

Erik Nordquist

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Education

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

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

Work Experience

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

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

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

Fellowships and Awards

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

- **Nordquist E**, Zhao M, Yu W, MacKerell A. Computational Modeling of PROTAC Ternary Complexes as Ensembles Using SILCS-PROTAC. **J. Chem. Inf. Model.** (submitted) DOI: [10.26434/chemrxiv-2025-jk9sn](https://doi.org/10.26434/chemrxiv-2025-jk9sn)
- Patel R, **Nordquist E**, Polli J. Prediction of surfactant-mediated dissolution of poorly soluble drugs from drug particles. **Eur. J. Pharm. Sci.** 2025, 107052. DOI: [10.1016/j.ejps.2025.107052](https://doi.org/10.1016/j.ejps.2025.107052)
- **Nordquist E[#]**, Zhao M[#], Kumar A, MacKerell A. Physics- and Machine-Learning Based Method to Identify Druggable Binding Sites Using SILCS-Hotspots. **J. Chem. Inf. Model.** 2024, 64, 19, 7743-7757. DOI: [10.1021/acs.jcim.4c01189](https://doi.org/10.1021/acs.jcim.4c01189) ^{#Contributed equally.}
- **Nordquist E**, Jia Z, Chen J. Small Molecule NS11021 Promotes BK Channel Activation by Increasing Inner Pore Hydration. **J. Chem. Inf. Model.** 2024, 64, 19, 7616-7625. DOI: [10.1021/acs.jcim.4c01012](https://doi.org/10.1021/acs.jcim.4c01012)

- **Nordquist E[#]**, Zhang G[#], 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 19(9): e1011460. DOI: [10.1371/journal.pcbi.1011460](https://doi.org/10.1371/journal.pcbi.1011460) #Contributed equally.
- Zhang L, Barehiya S, **Nordquist E**, Chen J. Machine Learning Generation of Dynamic Protein Conformational Ensembles. **Molecules** 2023, 28(10), 4047. 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, 122, 1158-1167. DOI: [10.1016/j.bpj.2023.02.005](https://doi.org/10.1016/j.bpj.2023.02.005) Selected for Best of 2023 Edition.
- **Nordquist E[#]**, Schultz S[#], and Chen J. Using Metadynamics To Explore the Free Energy of Dewetting in Biologically Relevant Nanopores. **J. Phys. Chem. B** 2022, 126, 34, 6428-6437 DOI: [10.1021/acs.jpcb.2c04157](https://doi.org/10.1021/acs.jpcb.2c04157) #Contributed equally. **Note:** S. Schultz was an undergraduate I mentored during this project.
- **Nordquist E**, Clerico E, Chen J, Gerasch L. Computational Modeling of Hsp70-Client Interactions: Past, Present, and Future. **J. Phys. Chem. B** 2022, 126, 36, 6780–6791 DOI: [10.1021/acs.jpcb.2c03806](https://doi.org/10.1021/acs.jpcb.2c03806)
- **Nordquist E**, English C, Clerico E, Sherman W, Gerasch L, Chen J. Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. **PLOS Comput. Biol.** 2021, 17 (11): e1009567. 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 CL, 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, 41, 830–838. DOI: [10.1002/jcc.26133](https://doi.org/10.1002/jcc.26133)

Teaching and Mentoring

2025	Instructor of record , General Chemistry Lab, Stevenson University. Full teaching responsibility for one section of the lab class, including grading and office hours.
2022	Instructor of record , 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.” (link) Course goals: develop skills in scientific communication, and a perform 4-week mini research project. Assessments were primarily formative, with self-feedback to foster growth mindsets.
2020–24	Guest lectures: Computer-aided Drug Design in a graduate Cancer Biology course, UMB (2x); 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	Lab TA , 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	Talk , Frontiers at the Chemistry-Biology Interface Symposium, Johns Hopkins University, “Computational modeling of ternary complexes as ensembles using SILCS-PROTAC,” Baltimore, MD. Talk , Chemistry Department Seminar, George Washington University, “Computational design of PROTACs”, Washington D.C.
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2024	Talk , 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

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:

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

Outreach

2023–25	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)
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- Volunteer**, Halloween STEM outreach event at Community Engagement Center, University of Maryland, Baltimore
- 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

- 2025 **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

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