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, Ion channels

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

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. Med. Chem.** (submitted) DOI: 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
- **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 [#]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

- **Nordquist E[#],** Zhang G[#], Barethiya 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 [#]Contributed equally.
- Zhang L, Barethiya S, **Nordquist E**, Chen J. Machine Learning Generation of Dynamic Protein Conformational Ensembles. **Molecules** 2023, 28(10), 4047. DOI: 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 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 [#]Contributed equally. **Note:** S. Schultz was an undergraduate I mentored during this project.
- **Nordquist E**, Clerico E, Chen J, Gierasch 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
- **Nordquist E**, English C, Clerico E, Sherman W, Gierasch 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
- 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

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.

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)

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 **CITRL 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.