Erik Nordquist

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Education

2023 **Ph.D.** Chemistry, University of Massachusetts Amherst. Advisor: Jianhan Chen, Ph.D.
2018 **B.S.** Chemistry and Physics, The College of Idaho

Appointments

2023– **Postdoctoral Fellowship**, University of Maryland, Baltimore, Department of Pharmaceutical Sciences. Advisor: Alexander D. MacKerell, Jr., Ph.D.

Fellowships and Awards

2024 **Best of Biophysical Journal 2023,** publication titled "Inner pore hydration free energy…"
Talk award (3rd), Research Symposium, UM Greenebaum Comprehensive Cancer Center
2023– **NIH T32 Postdoctoral Fellowship (Cancer Biology)**, University of Maryland, Baltimore
2022 **Paul H. Terry Endowment Award**, Chemistry Dept., University of Massachusetts Amherst
CNS Teaching Fellowship, College of Natural Sciences, University of Massachusetts Amherst (link)
2020–22 **NIH T32 Graduate Fellowship (Chemistry-Biology Interface)**, University of Massachusetts Amherst
2020 **William E. McEwen Poster Award**, Chemistry Dept., University of Massachusetts Amherst

Peer-Reviewed Publications

- Patel R, **Nordquist E**, Polli J. Prediction of surfactant-mediated dissolution of poorly soluble drugs from drug particles. Eur. J. Pharm. Sci. (under revision)
- **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.
- **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

Presentations

2025 **Talk**, Chemistry Department Seminar, George Washington University, "Computational design of PROTACs", Georgetown, MD.

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.

Teaching and Mentoring

2022 **Instructor of record,** First-Year Seminar, self-designed, title: "Reconciling Atomic Chaos and Human Order". Funded by UMass College of Natural Sciences Teaching Fellowship. (link)

2020–23 **Guest lectures**

Computer-aided Drug Design in UMB Graduate Cancer Biology course (2x);
Discussion seminar moderator on AlphaFold2 at Amherst College Biophysics course;
Lecture on molecular mechanics, additive force fields in UMass Graduate Stat. Mech. Course

2018–19 **Lab TA**, General Chemistry I Lab

Mentoring Experience with fellow trainees:

Undergraduates (UMass): Samantha Schultz (2020-2021); Callie Jillson (2019-2020)
Graduate students (UMB): Anthony O'Donnell (2024–); Zijin Xu (2024); Brandon Lowe (2023–)

Service

2023–24 **Facilitator**, Responsible Conduct of Research NIH training, University of Maryland, Baltimore
2024– **Organization committee, Annual Cancer Research Retreat**, University of Maryland, Baltimore
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 organization committee** for Chemistry Dept., University of Massachusetts Amherst

Journals Refereed for:
Comm. Chem., Biophys. J., J. Chem. Theory Comput., J. Chem. Inf. Model.

Outreach

2024 **Guest presenter,** RAMP Program for STEM activity for high-schoolers in Baltimore, University of Maryland, Baltimore (link) (2x)
Poster judge, Mount Royal Middle School Science Fair, Baltimore
2023 Guest presenter and volunteer, CURE Program University of Maryland, Baltimore, STEM outreach for middle-/high-schoolers in Baltimore (link) (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

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, and Fire Extinguishers, University of Maryland, Baltimoire (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.