Erik Nordquist

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Education

2023	**Ph.D. in Chemistry**, University of Massachusetts Amherst. Advisor: Jianhan Chen, Ph.D.
2018	**B.S. in 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,** article #5 entitled "Inner pore hydration free energy…" selected for Best of Biophysical Journal, 2023 (link) **Talk award (3rd place),** University of Maryland Cancer Center Research Symposium
2023-	**T32 NIH Postdoctoral Fellowship (Cancer Biology)**, University of Maryland, Baltimore and National Institutes of Health (info)
2022	**Paul H. Terry Endowment Award**, Chemistry Dept., University of Massachusetts Amherst **Graduate Teaching Fellowship**, College of Natural Sciences, University of Massachusetts Amherst (info)
2020-22	**T32 NIH Graduate Fellowship (Chemistry-Biology Interface)**, University of Massachusetts Amherst and National Institutes of Health (info)
2020	**William E. McEwen Poster Award**, Chemistry Dept., University of Massachusetts Amherst

Peer-reviewed publications

9. **Nordquist E**, Jia Z, Chen J. Small molecule NS11021 promotes BK channel activation by increasing inner pore hydration. **J. Chem. Inf. Model.** Submitted, 2024. bioRxiv DOI: 10.1101/2024.06.03.597166
8. **Nordquist E**#, Zhao M#, Kumar A, MacKerell A. Physics- and machine-learning based method to identify druggable binding sites using SILCS-Hotspots. **J. Comput. Aid. Mol. Des.** Submitted, 2024. chemRxiv DOI: 10.26434/chemrxiv-2024-hrqq9 #Equal Contributions
7. **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 #Equal Contributions
6. 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
5. **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 part of Best of 2023 edition)

4. **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
3. **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 [#]Equal Contributions
2. **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
1. 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

2024	**Talk,** University of Maryland Greenbaum Comprehensive Cancer Center Research Symposium, "Physics- and machine-learning-based method for identifying druggable binding sites with SILCS-Hotspots." (3rd place) 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

2022	**Instructor of record** for First-year seminar, self-designed titled "Reconciling Atomic Chaos and Human Order" (info)
2020 -23	**Guest lectures**, Computer-aided Drug Design in Graduate Cancer Biology course;

	Discussion seminar moderator on AlphaFold2 at Amherst College Biophysics course; Lecture on molecular mechanics, additive force fields in UMass graduate Stat. Mech. course
2018	**TA**, General Chemistry I Lab
	Mentoring Undergraduate research: Samantha Schultz (2020-2021, publication #3); Callie Jillson (2019-2020)

Service

2023-24	**Facilitator, Responsible Conduct of Research NIH training,** University of Maryland, Baltimore
2024	**Annual Cancer Research Retreat organization committee,** University of Maryland, Baltimore
2022	**Alumni Networking Symposium organization committee,** Chemistry-Biology Interface program, University of Massachusetts Amherst
2021	**Search committee,** Grad Program Manager for Chemistry Dept. University of Massachusetts Amherst
2020	**Alumni Networking Symposium organization committee,** Chemistry-Biology Interface program, University of Massachusetts Amherst
2019-21	**ResearchFest organization committee** for Chemistry Dept., University of Massachusetts Amherst
	Journals Refereed for: Biophys. J., J. Chem. Theory Comput., J. Chem. Inf. Model.

Outreach

2024	**Guest presenter,** RAMP high-school scholars Lunch-and-Learn, University of Maryland, Baltimore (info) **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 West Baltimore (info) Interactive demos and STEM career discussions (info)
2020-23	**Reviewer for Journal of Emerging Investigators**, 25 articles by middle- / high-school students (info)
2022	**Lab workshop for girls' summer science camp**, Eureka! at University of Massachusetts Amherst (info)

Professional Development

2022	**CITRL associate certification**, University of Massachusetts Amherst, achieved through training on evidence-based and inclusive teaching practices (info)
2021	**Evidence-based Undergraduate STEM Teaching,** online course (info) **Inclusive STEM Teaching,** online course (info)