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	
Fellowships and Awards		
2024	Best of Biophysical Journal 2023, article #5 entitled "Inner pore hydration free energy" selected for Best of Biophys. J. 2023 (link)	
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	
2022	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	

Publications

- 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
- 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
- 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

- 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,** The College of Idaho Natural Science Symposium, "Computer simulations of proteins help understand their function"
 - **Poster,** Biophysical Society Annual Meeting, "Computational mapping of allosteric modulators of the BK channel."
- 2023 **Poster,** Biophysical Society Annual Meeting, "A predictive model of voltage gating of BK channels via physical modeling and machine learning."
- Talk, University of Massachusetts Amherst ResearchFest (PH Terry award): "Predicting protein function with physics, experiments and machine learning."

 Poster, Biophysical Society Annual Meeting, "Free energy of hydrophobic dewetting in gating of BK channels"
- Talk, Northeastern Structural Symposium, "Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling"
 - **Poster,** University of Massachusetts Amherst ResearchFest (WE McEwen Award): "Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling"
- 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

Teaching

- 2022 **CIRTL Associate** achievement at the University of Massachusetts Amherst, for engaging in many trainings on evidence-based and inclusive teaching practices, including the preparation for the Teaching Fellowship to teach a First-year seminar.
- 2022 **Instructor of record** for First-year seminar, self-designed titled "Reconciling Atomic Chaos and Human Order" (info)
- 2020 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

promiscuity with physics-based modeling"

Mentoring Undergraduate research, Samantha Schultz (2020-2021), (publication #3); Callie Jillson (2019-2020)

Service

2024	Annual Cancer Research Retreat organization committee, University of Maryland, Baltimore
2019 –21	ResearchFest organization committee for Chemistry Dept., University of Massachusetts Amherst
2022, 2020	Alumni Networking Symposium organization committee , Chemistry-Biology Interface program, UMass Amherst
2021	Search committee , Grad Program Manager for Chemistry Dept. University of Massachusetts Amherst
	Journal Referee: Biophys. J., J. Chem. Theory Comput.

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, STEM outreach for middle-/high-schoolers in West Baltimore, CURE Program University of Maryland, 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

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2023- 24	Responsible Conduct of Research NIH training facilitator, University of Maryland, Baltimore	
2022	CITRL associate certification, University of Massachusetts Amherst, achieved through engaging in workshops and training on evidence-based and inclusive teaching practices (info)	
2021	Evidence-based Undergraduate STEM Teaching, online course (info) Inclusive STEM Teaching, online course (info)	