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

Research

Free energy calculations of hydrophobic dewetting in protein pores. Understanding the details of the gating mechanism of ion channels like the big potassium (BK) channel is a crucial for minimizing the effects of many diseases including cancer, stroke, asthma, and epilepsy. I have designed advanced protocols for sampling the free energy of desolvation in nanoscale pores. I used this method to explain the functional effects of experimentally-characterized mutations and to discover the mechanism of action of a known activator of BK.

Predictive modeling of protein function by integrating physics-based simulations and experiments using statistical learning. Predictive molecular models of protein function remain a grand challenge in biophysics, despite recent advances in structural biology and protein structure prediction. Currently there is a gap between structural and functional experimental data and atomistic, physics-based modeling. To bridge the gap, I have enriched available experimental functional data with physics-based modeling to describe the effects of mutations on protein function. Then, I used statistical learning methods to explain existing experimental data and to make novel predictions.

Publications

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.** (accepted) (bioRXiv)
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, DOI: 10.1016/j.bpj.2023.02.005
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
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

Fellowships and Awards

2023 –	**T32 Cancer Biology Postdoctoral Traineeship**, 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 Chemistry-Biology Interface Graduate Traineeship**, University of Masschusetts Amherst and National Institutes of Health (info)
2020	**William E. McEwen Poster Award**, Chemistry Dept., University of Massachusetts Amherst

Presentations

2022	**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”
2020	**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”
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”

Teaching

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; Amherst College Biophysics discussion seminar on AlphaFold2 (moderator); Graduate Statistical Mechanics, molecular mechanics, additive force fields
2018	**TA**, General Chemistry I Lab
	Mentoring Undergraduate research, Samantha Schultz (2020-2021), (publication #3); Callie Jillson (2019-2020)

Service

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. (1 article)

Outreach

2023	**Guest presenter and volunteer,** STEM outreach for middle-/high-schoolers in West Baltimore, CURE Program University of Maryland, Baltimore (info) Demo on Monte Carlo alogrithm to estimate pi (info)
2020–	**Reviewer for Journal of Emerging Investigators**, 23 articles by middle- / high-school students (info)
2022	**Girls summer science camp**, Eureka! at University of Massachusetts Amherst (info)

Professional Development

2022	**CITRL associate certification**, achieved through workshops and training for the (info)
2021	**Evidence-based Undergraduate STEM Teaching,** online course (info) **Inclusive STEM Teaching,** online course (info)