

Erik Nordquist

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20 Penn St, Baltimore, MD 21201

Education

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| 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](https://doi.org/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](https://doi.org/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.jpcc.2c03806](https://doi.org/10.1021/acs.jpcc.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.jpcc.2c04157](https://doi.org/10.1021/acs.jpcc.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](https://doi.org/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](https://doi.org/10.1002/jcc.26133)

Fellowships and Awards

2023 –	T32 Cancer Biology Postdoctoral Fellowship , 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 Fellowship , University of Massachusetts 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 algorithm to estimate pi ([info](#))
- 2020 – **Reviewer for Journal of Emerging Investigators**, 24 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](#))