

## Erik Nordquist

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### Education

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| 2023 | <b>Ph.D. in Chemistry</b> , University of Massachusetts Amherst. Advisor: Jianhan Chen, Ph.D. |
| 2018 | <b>B.S. in Chemistry and Physics</b> , 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<sup>#</sup>**, Zhang G<sup>#</sup>, 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<sup>#</sup>, Barethiya S<sup>#</sup>, **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<sup>#</sup>**, Schultz S<sup>#</sup>, 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 –	<b>T32 Cancer Biology Postdoctoral Traineeship</b> , University of Maryland, Baltimore and National Institutes of Health ( <a href="#">info</a> )
2022	<b>Paul H. Terry Endowment Award</b> , Chemistry Dept., University of Massachusetts Amherst
2022	<b>Graduate Teaching Fellowship</b> , College of Natural Sciences, University of Massachusetts Amherst ( <a href="#">info</a> )
2020 –22	<b>T32 Chemistry-Biology Interface Graduate Traineeship</b> , University of Massachusetts Amherst and National Institutes of Health ( <a href="#">info</a> )
2020	<b>William E. McEwen Poster Award</b> , Chemistry Dept., University of Massachusetts Amherst

## Presentations

2022	<b>Talk</b> , University of Massachusetts Amherst ResearchFest; <a href="#">PH Terry Award</a> . “Predicting protein function with physics, experiments and machine learning.” <b>Poster</b> , Biophysical Society Annual Meeting; “Free energy of hydrophobic dewetting in gating of BK channels”
2020	<b>Talk</b> , Northeastern Structural Symposium, “Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling” <b>Poster</b> , University of Massachusetts Amherst ResearchFest; <a href="#">WE McEwen Award</a> ; “Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling”
2019	<b>Talk</b> , Biophysics at University of Massachusetts Amherst, “Understanding the origins of DnaK’s selective promiscuity with physics-based modeling” <b>Poster</b> , Molecular Biophysics in the Northeast, “Understanding the origins of DnaK’s selective promiscuity with physics-based modeling”

## Teaching

2022	<b>Instructor of record</b> for a self-designed first-year seminar ( <a href="#">info</a> )
2020	<b>Guest lectures</b> , Graduate Statistical Mechanics, molecular mechanics, additive force fields; Amherst College Biophysics discussion seminar of AlphaFold2 (moderator)
2018	<b>TA</b> , General Chemistry I Lab <b>Mentoring Undergraduate research</b> , Samantha Schultz (2020-2021), (publication #3); Callie Jillson (2019-2020)

## Service

2019 –21	<b>ResearchFest organization committee</b> for Chemistry Dept., University of Massachusetts
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	Amherst
2020, 2022	<b>Alumni Networking Symposium organization committee</b> , Chemistry-Biology Interface program, UMass Amherst
2021	<b>Search committee</b> , Grad Program Manager for Chemistry Dept. University of Massachusetts Amherst
	<b>Journal Referee, Biophys. J.</b> (1 article)

## Outreach

2020 –	<b>Reviewer for Journal of Emerging Investigators</b> , 22 articles by middle- / high-school students ( <a href="#">info</a> )
2022	<b>Girls summer science camp</b> , Eureka! at University of Massachusetts Amherst ( <a href="#">info</a> )

## Professional Development

2022	<b>CITRL associate certification</b> ( <a href="#">info</a> )
2021	<b>Evidence-based Undergraduate STEM Teaching</b> , online course ( <a href="#">info</a> ) <b>Inclusive STEM Teaching</b> , online course ( <a href="#">info</a> )