

# Erik Nordquist

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## Education

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| –    | <b>Ph.D. in Chemistry</b> , University of Massachusetts Amherst |
| 2018 | <b>B.S. in Chemistry and Physics</b> , The College of Idaho     |

## Research

**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.

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

## Publications

7. **Nordquist E**, Guohui Z, Jiamin C, Chen J. Functional effects of novel mutations of big potassium channel predicted via physics-based and statistical modeling. (forthcoming, April 2022)
6. **Nordquist E**, Zhiguang J, Chen J. Big potassium channel activator modulates dewetting of the inner pore. (forthcoming, March 2022)
5. **Nordquist E**, Zhiguang J, Chen J. Inner pore hydration free energy controls activations of the big potassium channel and its mutants. Biophys. J. (submitted)
4. **Nordquist E**, Clerico E, Chen J, Gierasch L. Computationally-aided modeling of Hsp70-client interactions: past, present, and future. J. Phys. Chem. B 2022. [DOI](#)
3. **Nordquist E**<sup>#</sup>, Schultz S<sup>#</sup>, Chen J. Using metadynamics to explore the free energy of dewetting in biologically-relevant nanopores. J. Phys. Chem. B 2022. [DOI](#)
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 Comp Bio (2021). [DOI](#)
1. Gong X, Chiricotto M, Liu X, **Nordquist E**, Feig M, Brooks C, Chen J. Accelerating the GBMV/SA implicit solvent model using GPUs. J Comput Chem (2020). [DOI](#)

## Fellowships and Awards

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| 2022 | <b>Dr. Paul H. Terry Endowment Award</b> , University of Massachusetts Amherst Chemistry                                      |
| 2022 | <b>Graduate Teaching Fellowship</b> , Coll. of Natural Sciences, University of Massachusetts Amherst ( <a href="#">info</a> ) |

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| 2020<br>– 22 | <b>Chemistry-Biology Interface Traineeship</b> , National Institutes of Health and University of Massachusetts Amherst ( <a href="#">info</a> ) |
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## Presentations

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

## Teaching

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| 2022 | <b>Instructor of record</b> for a self-designed first-year seminar ( <a href="#">info</a> )  |
| 2020 | <b>Guest lecture</b> , Graduate Statistical Mechanics, molecular mechanics and empirical force fields                                      |
| 2018 | <p><b>TA</b>, General Chemistry I Lab</p> <p><b>Mentoring Undergraduates</b>, Samantha Schultz (2020-2021); Callie Jillson (2019-2020)</p> |

## Service

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

## Outreach

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| 2020<br>– | <b>Reviewer for Journal of Emerging Investigators</b> , 15 articles authored by middle- and 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

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