Erik Nordquist

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Education

–	**Ph.D. in Chemistry**, University of Massachusetts Amherst
2018	**B.S. in Chemistry and Physics**, 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**[#], Schultz S[#], 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

2022	**Dr. Paul H. Terry Endowment Award**, University of Massachusetts Amherst Chemistry
2022	**Graduate Teaching Fellowship**, Coll. of Natural Sciences, University of Massachusetts Amherst (info)

2020 – 22	**Chemistry-Biology Interface Traineeship**, National Institutes of Health and University of Masschusetts Amherst (info)

Presentations

2022	**Talk,** University of Massachusetts Amherst ResearchFest; P.H. 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; W.E. McEwen Poster 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 a self-designed first-year seminar (info)
2020	**Guest lecture**, Graduate Statistical Mechanics, molecular mechanics and empirical force fields
2018	**TA**, General Chemistry I Lab
	Mentoring Undergraduates, Samantha Schultz (2020-2021); Callie Jillson (2019-2020)

Service

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

Outreach

2020 –	**Reviewer for Journal of Emerging Investigators**, 15 articles authored by middle- and high-school students (info)
2022	**Girls summer science camp**, Eureka! at University of Massachusetts Amherst (**info**)

Professional Development

2022	**CITRL associate certification** (info)

2021 **Evidence-based Undergraduate STEM Teaching,** online course (info)

Inclusive STEM Teaching, online course (info)