

## 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                                   |

### Fellowships and Awards

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| 2024     | <b>Best of Biophysical Journal 2023</b> , article #5 entitled “Inner pore hydration free energy...” selected for Best of Biophys. J. 2023 ( <a href="#">link</a> ) |
| 2023 –   | <b>T32 NIH Postdoctoral Fellowship (Cancer Biology)</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 NIH Graduate Fellowship (Chemistry-Biology Interface)</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   |

### Publications

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| 9. | <b>Nordquist E</b> , Jia Z, Chen J. Small molecule NS11021 promotes BK channel activation by increasing inner pore hydration. <b>J. Chem. Inf. Model.</b> 2024. bioRxiv DOI: <a href="https://doi.org/10.1101/2024.06.03.597166">10.1101/2024.06.03.597166</a>  |
| 8. | <b>Nordquist E<sup>#</sup></b> , Zhao M <sup>#</sup> , Kumar A, MacKerell A. Physics- and machine-learning based method to identify druggable binding sites using SILCS-Hotspots. <b>J. Comput. Aid. Mol. Des.</b> Submitted. 2024. chemRxiv DOI: <a href="https://doi.org/10.26434/chemrxiv-2024-hrqq9">10.26434/chemrxiv-2024-hrqq9</a>   |
| 7. | <b>Nordquist E<sup>#</sup></b> , 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. <b>PLOS Comput. Biol.</b> 2023 19(9): e1011460. DOI: <a href="https://doi.org/10.1371/journal.pcbi.1011460">10.1371/journal.pcbi.1011460</a> |
| 6. | Zhang L <sup>#</sup> , Barethiya S <sup>#</sup> , <b>Nordquist E</b> , Chen J. Machine Learning Generation of Dynamic Protein Conformational Ensembles. <b>Molecules</b> 2023, 28(10), 4047. DOI: <a href="https://doi.org/10.3390/molecules28104047">10.3390/molecules28104047</a>   |
| 5. | <b>Nordquist E</b> , Zhiguang J, Chen J. Inner pore hydration free energy controls activations of the big potassium channel and its mutants. <b>Biophys. J.</b> 2023, 122, 1158-1167. DOI: <a href="https://doi.org/10.1016/j.bpj.2023.02.005">10.1016/j.bpj.2023.02.005</a> (Selected part of Best of 2023 edition)  |
| 4. | <b>Nordquist E</b> , Clerico E, Chen J, Gierasch L. Computational Modeling of Hsp70-Client Interactions: Past, Present, and Future. <b>J. Phys. Chem. B</b> 2022, 126 (36), 6780–6791 DOI: <a href="https://doi.org/10.1021/acs.jpcc.2c03806">10.1021/acs.jpcc.2c03806</a>  |

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.jpcb.2c04157](https://doi.org/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](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)

## Presentations

2024	<b>Talk</b> , University of Maryland Baltimore Cancer Biology Research Retreat, “Physics- and machine-learning-based method for identifying druggable binding sites with SILCS-Hotspots” <b>Talk</b> , The College of Idaho Natural Science Symposium, “Computer simulations of proteins help understand their function” <b>Poster</b> , Biophysical Society Annual Meeting, “Computational mapping of allosteric modulators of the BK channel.”
2023	<b>Poster</b> , Biophysical Society Annual Meeting, “A predictive model of voltage gating of BK channels via physical modeling and machine learning.”
2022	<b>Talk</b> , University of Massachusetts Amherst ResearchFest (PH Terry award): “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 (WE McEwen Award): “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 First-year seminar, self-designed titled “Reconciling Atomic Chaos and Human Order” ( <a href="#">info</a> )
2020	<b>Guest lectures</b> , – Computer-aided Drug Design in Graduate Cancer Biology course; Discussion seminar moderator on AlphaFold2 at Amherst College Biophysics course; Lecture on molecular mechanics, additive force fields in UMass graduate Stat. Mech. course
2018	<b>TA</b> , General Chemistry I Lab  <b>Mentoring Undergraduate research</b> : Samantha Schultz (2020-2021), (publication #3); Callie Jillson (2019-2020)

## Service

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2024	<b>Annual Cancer Research Retreat organization committee</b> , University of Maryland, Baltimore
2019–21	<b>ResearchFest organization committee</b> for Chemistry Dept., University of Massachusetts Amherst
2022, 2020	<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:</b> Biophys. J., J. Chem. Theory Comput., J. Chem. Inf. Model.

## Outreach

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2024	<b>Guest presenter</b> , RAMP high-school scholars Lunch-and-Learn, University of Maryland, Baltimore ( <a href="#">info</a> ) <b>Poster judge</b> , Mount Royal Middle School Science Fair, Baltimore
2023	<b>Guest presenter and volunteer</b> , STEM outreach for middle-/high-schoolers in West Baltimore, CURE Program University of Maryland, Baltimore ( <a href="#">info</a> ) Interactive demos and STEM career discussions ( <a href="#">info</a> )
2020–23	<b>Reviewer for Journal of Emerging Investigators</b> , 25 articles by middle- / high-school students ( <a href="#">info</a> )
2022	<b>Lab workshop for girls summer science camp</b> , Eureka! at University of Massachusetts Amherst ( <a href="#">info</a> )

## Professional Development

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2023–24	<b>Responsible Conduct of Research NIH training facilitator</b> , University of Maryland, Baltimore
2022	<b>CITRL associate certification</b> , University of Massachusetts Amherst, achieved through engaging in workshops and training on evidence-based and inclusive teaching practices ( <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> )