

# 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                                   |

## Appointments

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| 2023- | <b>Postdoctoral fellowship</b> , University of Maryland, Baltimore, Department of Pharmaceutical Sciences. Advisor: Alexander D. MacKerell, Jr., Ph.D. |
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## Fellowships and Awards

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| 2024    | <b>Best of Biophysical Journal 2023</b> , publication #4 entitled "Inner pore hydration free energy..." selected for Best of Biophysical Journal, 2023 ( <a href="#">link</a> )<br><b>Talk award (3<sup>rd</sup> place)</b> , University of Maryland Cancer Center Research Symposium |
| 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>CNS 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  |

## Peer-reviewed Publications

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| 7. | <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> Submitted, 2024. bioRxiv DOI: <a href="https://doi.org/10.1101/2024.06.03.597166">10.1101/2024.06.03.597166</a>   |
| 6. | <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> <sup>#</sup> Contributed equally.   |
| 5. | <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> <sup>#</sup> Contributed Equally. |
| 4. | <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)  |
| 3. | <b>Nordquist E<sup>#</sup></b> , Schultz S <sup>#</sup> , and Chen J. Using Metadynamics To Explore the Free Energy of Dewetting in Biologically Relevant Nanopores. <b>J. Phys. Chem. B</b> 2022, 126 (34), 6428-6437 DOI: <a href="https://doi.org/10.1021/acs.jpcb.2c04157">10.1021/acs.jpcb.2c04157</a> <sup>#</sup> Contributed equally.   |
| 2. | <b>Nordquist E</b> , English C, Clerico E, Sherman W, Gierasch L, Chen J. Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. <b>PLOS Comput. Biol.</b> 2021, 17 (11): e1009567. DOI: <a href="https://doi.org/10.1371/journal.pcbi.1009567">10.1371/journal.pcbi.1009567</a>  |

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)

## Review Articles and Book Chapters

2. 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)
1. **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)

## Presentations

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| 2024 | <b>Talk</b> , University of Maryland Greenbaum Comprehensive Cancer Center Research Symposium, “Physics- and machine-learning-based method for identifying druggable binding sites with SILCS-Hotspots.” (3 <sup>rd</sup> place) Baltimore, MD.<br><b>Talk</b> , The College of Idaho Natural Science Symposium, “Computer simulations of proteins help understand their function.” Caldwell, ID.<br><b>Poster</b> , Biophysical Society Annual Meeting, “Computational mapping of allosteric modulators of the BK channel.” Philadelphia, PA. |
| 2023 | <b>Poster</b> , Biophysical Society Annual Meeting, “A predictive model of voltage gating of BK channels via physical modeling and machine learning.” San Diego, CA.   |
| 2022 | <b>Talk</b> , University of Massachusetts Amherst ResearchFest (PH Terry award): “Predicting protein function with physics, experiments and machine learning.” Amherst, MA.<br><b>Poster</b> , Biophysical Society Annual Meeting, “Free energy of hydrophobic dewetting in gating of BK channels.” San Francisco, CA.   |
| 2020 | <b>Talk</b> , Northeastern Structural Symposium, “Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling.” Virtual.<br><b>Poster</b> , University of Massachusetts Amherst ResearchFest (WE McEwen Award): “Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling.” Amherst, MA.  |
| 2019 | <b>Talk</b> , Biophysics at University of Massachusetts Amherst, “Understanding the origins of DnaK’s selective promiscuity with physics-based modeling”<br><b>Poster</b> , Molecular Biophysics in the Northeast, “Understanding the origins of DnaK’s selective promiscuity with physics-based modeling.” Boston, MA.  |

## Teaching

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| 2022    | <b>Instructor of record</b> for First-year seminar, self-designed, title: “Reconciling Atomic Chaos and Human Order” ( <a href="#">info</a> )  |
| 2020-23 | <b>Guest lectures</b> ,<br>Computer-aided Drug Design in UMB Graduate Cancer Biology course;<br>Discussion seminar moderator on AlphaFold2 at Amherst College Biophysics course;<br>Lecture on molecular mechanics, additive force fields in UMass Graduate Stat. Mech. course |
| 2018-19 | <b>TA</b> , General Chemistry I Lab<br><br><b>Mentoring Undergraduate research:</b><br>Samantha Schultz (2020-2021, publication #3);<br>Callie Jillson (2019-2020)   |

## Service

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2023-24	<b>Facilitator, Responsible Conduct of Research NIH training</b> , University of Maryland, Baltimore
2024	<b>Annual Cancer Research Retreat organization committee</b> , University of Maryland, Baltimore
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
2020	<b>Alumni Networking Symposium organization committee</b> , Chemistry-Biology Interface program, University of Massachusetts Amherst
2019-21	<b>ResearchFest organization committee</b> for Chemistry Dept., University of Massachusetts Amherst
	<b>Journals Refereed for:</b> Biophys. J., J. Chem. Theory Comput., J. Chem. Inf. Model.

## Outreach

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2024	<b>Guest presenter</b> , RAMP Program for STEM activity for high-schoolers in Baltimore, 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> , CURE Program University of Maryland, Baltimore, STEM outreach for middle-/high-schoolers in 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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2022	<b>CITRL associate certification</b> , University of Massachusetts Amherst, achieved through 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> )