

Erik Nordquist

✉ enordquist@rx.umaryland.edu

🌐 eriknordquist.com

20 Penn St, Baltimore, MD 21201

Education

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| 2023 | Ph.D. in Chemistry , University of Massachusetts Amherst. Advisor: Jianhan Chen, Ph.D. |
| 2018 | B.S. in Chemistry and Physics , The College of Idaho |

Appointments

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| 2023- | Postdoctoral fellowship , 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 | Best of Biophysical Journal 2023 , publication #4 entitled "Inner pore hydration free energy..." selected for Best of Biophysical Journal, 2023 (link)
Talk award (3rd place) , University of Maryland Cancer Center Research Symposium |
| 2023- | T32 NIH Postdoctoral Fellowship (Cancer Biology) , University of Maryland, Baltimore and National Institutes of Health (info) |
| 2022 | Paul H. Terry Endowment Award , Chemistry Dept., University of Massachusetts Amherst |
| 2022 | CNS Teaching Fellowship , College of Natural Sciences, University of Massachusetts Amherst (info) |
| 2020-22 | T32 NIH Graduate Fellowship (Chemistry-Biology Interface) , University of Massachusetts Amherst and National Institutes of Health (info) |
| 2020 | William E. McEwen Poster Award , Chemistry Dept., University of Massachusetts Amherst |

Peer-reviewed Publications

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| 7. | Nordquist E[#] , Zhao M [#] , Kumar A, MacKerell A. Physics- and machine-learning based method to identify druggable binding sites using SILCS-Hotspots. J. Chem. Inf. Model. Submitted, 2024. chemRxiv DOI: 10.26434/chemrxiv-2024-hrqq9 [#] Contributed equally. |
| 6. | Nordquist E , Jia Z, Chen J. Small molecule NS11021 promotes BK channel activation by increasing inner pore hydration. J. Chem. Inf. Model. Submitted, 2024. bioRxiv DOI: 10.1101/2024.06.03.597166 |
| 5. | Nordquist E[#] , Zhang G [#] , 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. 2023 19(9): e1011460. DOI: 10.1371/journal.pcbi.1011460 [#] Contributed Equally. |
| 4. | Nordquist E , Zhiguang J, Chen J. Inner pore hydration free energy controls activations of the big potassium channel and its mutants. Biophys. J. 2023, 122, 1158-1167. DOI: 10.1016/j.bpj.2023.02.005 (Selected part of Best of 2023 edition) |
| 3. | Nordquist E[#] , Schultz S [#] , 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 [#] Contributed equally. |
| 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 |

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

Teaching

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| 2022 | Instructor of record for First-year seminar, self-designed, title: “Reconciling Atomic Chaos and Human Order” (info) |
| 2020-23 | Guest lectures ,
Computer-aided Drug Design in UMB 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 |
| 2018-19 | TA , General Chemistry I Lab

Mentoring Undergraduate research:
Samantha Schultz (2020-2021, publication #3);
Callie Jillson (2019-2020) |

Service

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

Outreach

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

Professional Development

2022	CITRL associate certification , University of Massachusetts Amherst, achieved through training on evidence-based and inclusive teaching practices (info)
2021	Evidence-based Undergraduate STEM Teaching , online course (info) Inclusive STEM Teaching , online course (info)