

# Erik Nordquist

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## Education

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

## Appointments

2023– **Postdoctoral Fellowship**, University of Maryland, Baltimore, Department of Pharmaceutical Sciences. Advisor: Alexander D. MacKerell, Jr., Ph.D.

## Fellowships and Awards

2024 **Best of Biophysical Journal 2023**, publication titled “Inner pore hydration free energy...”  
**Talk award (3<sup>rd</sup>)**, Research Symposium, UM Greenebaum Comprehensive Cancer Center  
2023– **NIH T32 Postdoctoral Fellowship (Cancer Biology)**, University of Maryland, Baltimore  
2022 **Paul H. Terry Endowment Award**, Chemistry Dept., University of Massachusetts Amherst  
**CNS Teaching Fellowship**, College of Natural Sciences, University of Massachusetts Amherst ([link](#))  
2020–22 **NIH T32 Graduate Fellowship (Chemistry-Biology Interface)**, University of Massachusetts Amherst  
2020 **William E. McEwen Poster Award**, Chemistry Dept., University of Massachusetts Amherst

## Peer-Reviewed Publications

- **Nordquist E<sup>#</sup>**, Zhao M<sup>#</sup>, Kumar A, MacKerell A. Physics- and Machine-Learning Based Method to Identify Druggable Binding Sites Using SILCS-Hotspots. **J. Chem. Inf. Model.** 2024, 64, 19, 7743-7757. DOI: [10.1021/acs.jcim.4c01189](https://doi.org/10.1021/acs.jcim.4c01189) <sup>#</sup>Contributed equally.
- **Nordquist E**, Jia Z, Chen J. Small Molecule NS11021 Promotes BK Channel Activation by Increasing Inner Pore Hydration. **J. Chem. Inf. Model.** 2024, 64, 19, 7616-7625. DOI: [10.1021/acs.jcim.4c01012](https://doi.org/10.1021/acs.jcim.4c01012)
- **Nordquist E<sup>#</sup>**, 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. **PLOS Comput. Biol.** 2023 19(9): e1011460. DOI: [10.1371/journal.pcbi.1011460](https://doi.org/10.1371/journal.pcbi.1011460) <sup>#</sup>Contributed Equally.
- 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)
- **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](https://doi.org/10.1016/j.bpj.2023.02.005) Selected for Best of 2023 Edition.
- **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.jpcc.2c04157](https://doi.org/10.1021/acs.jpcc.2c04157) <sup>#</sup>Contributed equally.
- **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)

- **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)
- 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

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| 2024 | <p><b>Talk</b>, Institute for Bioscience and Biotechnology Research, University of Maryland Baltimore, Early-Career Research Symposium, “Computational design of PROTACs”, Rockville, MD.</p> <p><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.” (Talk award) Baltimore, MD.</p> <p><b>Talk</b>, The College of Idaho Natural Science Symposium, “Computer simulations of proteins help understand their function.” Caldwell, ID.</p> <p><b>Poster</b>, Biophysical Society Annual Meeting, “Computational mapping of allosteric modulators of the BK channel.” Philadelphia, PA.</p> |
| 2023 | <p><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.</p>  |
| 2022 | <p><b>Talk</b>, University of Massachusetts Amherst ResearchFest (PH Terry award): “Predicting protein function with physics, experiments and machine learning.” Amherst, MA.</p> <p><b>Poster</b>, Biophysical Society Annual Meeting, “Free energy of hydrophobic dewetting in gating of BK channels.” San Francisco, CA.</p>   |
| 2020 | <p><b>Talk</b>, Northeastern Structural Symposium, “Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling.” Virtual.</p> <p><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.</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.” Boston, MA.</p>  |

## Teaching and Mentoring

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| 2022    | <p><b>Instructor of record</b>, First-Year Seminar, self-designed, title: “Reconciling Atomic Chaos and Human Order”. Funded by UMass College of Natural Sciences Teaching Fellowship. (<a href="#">link</a>)</p>  |
| 2020–23 | <p><b>Guest lectures</b></p> <p>Computer-aided Drug Design in UMB Graduate Cancer Biology course (2x);</p> <p>Discussion seminar moderator on AlphaFold2 at Amherst College Biophysics course;</p> <p>Lecture on molecular mechanics, additive force fields in UMass Graduate Stat. Mech. Course</p> |
| 2018–19 | <p><b>Lab TA</b>, General Chemistry I Lab</p>  |

## Mentoring Experience with fellow trainees:

**Undergraduates (UMass):** Samantha Schultz (2020-2021); Callie Jillson (2019-2020)

**Graduate students (UMB):** Anthony O'Donnell (2024–); Zijin Xu (2024); Brandon Lowe (2023–)

## Service

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| 2023–24 | <p><b>Facilitator</b>, Responsible Conduct of Research NIH training, University of Maryland, Baltimore</p> |
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- 2024– **Organization committee, Annual Cancer Research Retreat**, University of Maryland, Baltimore
- 2020–20 **Organization committee, Alumni Networking Symposium**, Chemistry-Biology Interface program, University of Massachusetts Amherst (2x)
- 2020 **Search committee**, Grad. Program Manager, Chemistry Dept. University of Massachusetts Amherst
- 2019–21 **ResearchFest organization committee** for Chemistry Dept., University of Massachusetts Amherst

#### Journals Refereed for:

Comm. Chem., Biophys. J., J. Chem. Theory Comput., J. Chem. Inf. Model.

#### Outreach

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- 2024 **Guest presenter**, RAMP Program for STEM activity for high-schoolers in Baltimore, University of Maryland, Baltimore ([link](#)) (2x)  
**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 ([link](#)) (2x)
- 2020–23 **Reviewer for Journal of Emerging Investigators**, 25 articles by middle- / high-school students ([link](#))
- 2022 **Lab for girls' summer science camp**, Eureka! at University of Massachusetts Amherst ([link](#))

#### Professional Development

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- 2024 **Writing an Effective Teaching Philosophy Statement**, online CIRTl workshop  
**Teaching Biophysics at a PUI workshop**, Biophysical Society Annual Meeting
- 2024 **Safety preparedness trainings**, CPR/AED, Stop the Bleed, Civilian Active Shooter Events, and Fire Extinguishers, University of Maryland, Baltimore ([certificates](#))
- 2022 **CITRL associate certification**, University of Massachusetts Amherst, achieved through training on evidence-based and inclusive teaching practices ([link](#))
- 2021 **Evidence-based Undergraduate STEM Teaching**, online course ([link](#))  
**Inclusive STEM Teaching**, online course ([link](#))