

ELIJAH KARVELIS

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Thorough and thoughtful computational structural biologist currently seeking a role where I can apply my expertise in physics-based and data-driven modeling to address critical problems in biomolecular engineering

EDUCATION

Massachusetts Institute of Technology — Cambridge, MA Doctorate in Biological Engineering Advisor: Bruce Tidor Thesis: <i>Computational Approaches for Understanding and Redesigning Enzyme Catalysis</i>	Expected April 2024 GPA: 5.0/5.0
University of Illinois — Urbana-Champaign, IL Bachelor of Science in Chemical Engineering	May 2018 GPA: 4.0/4.0

SKILLS

Methods	Molecular dynamics (MD), machine learning (ML), data science, protein design
Programming	Python, Unix/Linux, Bash, MATLAB
Software & packages	CHARMM, Gaussian, PyTorch, TensorFlow, Scikit-learn, Pandas, OSPREY

RELEVANT EXPERIENCE

Computational Modeling and Engineering of Enzyme Catalysis <i>Graduate Research Assistant (Tidor lab, CSAIL)</i>	MIT 2018 - present
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- Implemented [Transition Interface Sampling \(TIS\)](#) (using Python) to collect hundreds of thousands of hybrid QM/MM MD simulations (using CHARMM) of attempted enzyme-catalyzed reactions.
- Computed energies of activation using umbrella sampling with WHAM, collected simulations of thousands of turnover events, and used TIS to compute rate constants for 55 different enzyme variants.
- Trained ML models (using Scikit-learn and TensorFlow) to characterize key structural drivers of catalysis in a model enzyme, which were used to guide redesign trials for increased specific activity.
- Developed an approach combining ML models and simulations of turnover dynamics for enzyme redesign toward increased specific activity with an over 50% success rate (based on calculated results).
- Evaluated different deep learning models (using PyTorch) for mapping from turnover dynamics to overall activity, demonstrating that activity can be predicted from pre-reaction structural dynamics. [GitHub](#).
- Utilized and helped maintain the Tidor lab's private cluster, managing basic upkeep and troubleshooting tasks in a high-performance Unix-based computing environment.

In vitro Modeling of Glioblastoma Invasion <i>Undergraduate Research Assistant (Harley lab)</i>	UIUC 2016 - 2018
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- Developed a microfluidic platform for modeling glioblastoma in a vascularized brain-mimetic hydrogel with tunable properties, which was used to identify angiocrine signals affecting glioblastoma aggressiveness.

Teaching and Training

- TA'ed Principles of Molecular Bioengineering at MIT in Fall 2019, a graduate level course with 30+ students covering methods in biomolecular analysis and engineering. TA'ed hundreds of students across four different engineering courses at UIUC.
- Mentored and trained two undergraduate researchers and four rotating graduate students.
- Received the Kaufman Teaching Certificate and Graduate Research Mentorship Certificate from MIT.

PEER-REVIEWED PUBLICATIONS

Karvelis, E., Swanson, C., Tidor, B. Substrate turnover dynamics guide ketol-acid reductoisomerase redesign for increased specific activity. *Submitted*.

Karvelis, E., Tidor, B. Substrate-specific catalytic strategies uncovered across a panel of enzyme variants. *In preparation*.

Ngo, M. T., **Karvelis, E.**, Harley, B. A. C. Multidimensional hydrogel models reveal endothelial network angiocrine signals increase glioblastoma cell number, invasion, and temozolomide resistance. *Integrative Biology*, 12(6):139-149. 2020. <https://doi.org/10.1093/intbio/zya010>

SELECTED PRESENTATIONS

37th Annual Symposium of the Protein Society; Boston, MA: **Karvelis, E.**, Tidor, B. *Relating Turnover Dynamics to Catalytic Efficiency Identifies Enzyme Mutants with Increased Activity*. Poster. July 14, 2023.

ACS Spring 2023; Indianapolis, IN: **Karvelis, E.**, Tidor, B. *Turnover dynamics and machine learning guide redesigning KARI for increased catalytic activity*. Oral. March 29, 2023.

<https://acs.digitellinc.com/sessions/535607/view>

67th Biophysical Society Annual Meeting; San Diego, CA: **Karvelis, E.**, Tidor, B. *Using turnover dynamics to redesign KARI for improved catalytic activity*. Oral. Feb. 21, 2023.

<https://doi.org/10.1016/j.bpj.2022.11.1754>

Molecular Machine Learning Conference; Cambridge, MA: **Karvelis, E.** *Modeling substrate turnover dynamics to guide the redesign of a natural enzyme for increased activity*. Poster. Oct. 21, 2022.

Bioengineering and Toxicology Seminar; Cambridge, MA: **Karvelis, E.** *Understanding and Re-engineering Enzymes Using Molecular Dynamics*. Oral. February 12, 2021.

BMES National Conference; Phoenix, AZ: **Karvelis, E.** *Modeling Glioblastoma Invasion with Microfluidics*. Oral. Oct. 14, 2017.

Energy Biosciences Building Colloquium; Berkeley, CA: **Karvelis, E.** *High-throughput Identification of Genetic Interactions Using Barcoded Transposon Mutants*. Oral. Aug. 4, 2017.

BMES National Conference; Minneapolis, MN: **Karvelis, E.**, Ngo, M., Gilchrist, A., Kamm, R., Harley, B. *Utilizing Microfluidics to Recapitulate the Microenvironment of Glioblastoma*. Poster. Oct. 8, 2016.

SELECTED AWARDS

NSF GRFP Fellow: doctoral studies funding	2018 - 2021
MIT Viterbi Fellow: doctoral studies funding	2018
Stamps Leadership Scholar: generous award from UIUC	2014 - 2018
Amgen Scholar - UC Berkeley: research experience scholarship	2017
Goldwater Scholar: undergraduate award in STEM	2016
Phi Beta Kappa: honor society	2016
Bronze Tablet: UIUC graduation distinction	2018
Chancellor's Scholar: UIUC honors program	2014 - 2018
James Scholar: UIUC honors program	2014 - 2018

HOBBIES AND SERVICE

I enjoy playing guitar, basketball, and strength training. During my time at MIT, I served as the BE Social Chair, a member of CSAIL's Coffee Committee, tutored, and was an instructor for Momentum AI. In the past, I volunteered for several years at an exotic pet sanctuary, and I still enjoy learning about animals and wildlife.