# ELIJAH KARVELIS

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Thorough and thoughtful computational biophysicist with a passion for combining physics-based and data-driven approaches to address critical problems in biomolecular engineering; currently seeking a role in this area

## EDUCATION

**Massachusetts Institute of Technology, Cambridge** *2018 - Present*
Doctorate, Biological Engineering (Advisor: Bruce Tidor) GPA: 5.0/5.0

**University of Illinois, Urbana-Champaign** *2014 - 2018*
Bachelor of Science, Chemical Engineering GPA: 4.0/4.0

## TECHNICAL SKILLS AND EXPERIENCE

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|---|---|
| **Methods** | Molecular dynamics, machine learning, data science, protein design |
| **Programming** | Python, Unix/Linux and familiarity with Bash and MATLAB |
| **Software & packages** | CHARMM, Gaussian, PyTorch, TensorFlow, Scikit-learn, Pandas, OSPREY |

## RELEVANT RESEARCH EXPERIENCE

**Computational Modeling and Engineering of Enzyme Catalysis** MIT 2019 - present
*Graduate Research Assistant*

- Implemented Transition Interface Sampling to collect and process hundreds of thousands of hybrid QM/MM molecular dynamics simulations of attempted enzyme-catalyzed reactions. Used this platform to (i) compute energies of activation, (ii) collect simulations of thousands of turnover events, and (iii) calculate rate constants using kinetic data for 55 different enzyme variants.
- Trained machine learning models to characterize key structural drivers of catalysis in a model enzyme.
- Developed an approach, combining machine learning models and simulations of turnover dynamics, for rational enzyme redesign toward increased activity with an over 50% success rate (based on calculated results) for a natural enzyme-substrate system.
- Identified three unique mechanisms by which designed mutants achieved increased specific activity.
- Evaluated different deep learning models 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** UIUC 2016 - 2018
*Undergraduate Research Assistant*

- Developed a microfluidic platform for modeling glioblastoma invasion in the context of a vascularized brain-mimetic hydrogel with tunable biochemical and biophysical properties.

**Teaching and Training**
*Teaching Assistant and Graduate Research Assistant*

- TA'ed Principles of Molecular Bioengineering (20.420) at MIT in Fall 2019, a graduate level course covering methods in biomolecular analysis and engineering. TA'ed for four different engineering courses at UIUC.
- Mentored and trained two undergraduate researchers and four rotating graduate students.
- Kaufman Teaching Certificate (in progress) and Graduate Research Mentorship Certificate from MIT

## SELECTED AWARDS

**NSF GRFP Fellow**: doctoral studies funding *2018 - 2021*
**MIT Viterbi Fellow**: doctoral studies funding *2018*
**Stamps Leadership Scholar**: UIUC's most generous and selective award *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 Recipient**: designates top 3% of UIUC graduates *2018*
**Chancellor's Scholar**: UIUC's highest honors program (125/7000 students) *2014 - 2018*
**James Scholar**: UIUC honors program (top 20% of students) *2014 - 2018*

## PEER-REVIEWED PUBLICATIONS

Karvelis, E., Swanson, C., Tidor, B. Substrate turnover dynamics guide ketol-acid reductoisomerase redesign for increased specific activity. *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/zyaa010

## 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.

## 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.