James Jeffryes



Education

Doctor of Philosophy June 2017 Northwestern University Evanston, IL

Chemical Engineering, Advised by Keith Tyo & Christopher Henry

Thesis: Enumerating the Potential Metabolome through Simulation of Enzyme-catalyzed and

Spontaneous Reactions

Bachelor of Science May 2012 Rose-Hulman Institute of Technology Terre Haute, IN

Chemical Engineering & Biochemistry and Molecular Biology, Magna Cum Laude

Experience

Since July 2017 Postdoctoral Researcher at Argonne National Laboratory

Mathematics and Computer Science Division, Lemont, IL

 Integrating bioinformatics tools into Department of Energy Biological Knowledge Base as a member of an Agile development team

Aug 2016 Nov 2016 Data Science & Computational Biology Intern at Intrexon Corporation

Industrial Products Division, South San Fransisco, CA

- Developed a pipeline for aggregation, annotation and prioritization of enzymes with novel biosynthetic potential.
- Cleaned, parsed and utilized substrate and reaction data from external databases.
- Built and deployed a containerized Flask microservice, bringing analysis results directly to wet-lab scientists.
- · Constructed visualizations for complex, hierarchical, and heterogeneous biological data.

Jun 2017 Mar 2013 Graduate Research Assistant at Argonne National Laboratory

Mathematics and Computer Science Division, Lemont, IL

- Collaborated in a cross-functional team including plant biologists and analytical chemists to uncover novel enzyme functions and the resulting metabolic products.
- Generated computational predictions of enzymatic and spontaneous chemical activities to build
 a searchable databases of putative metabolites.
- Implemented a API in Python to enable database integration into Department of Energy Biological Knowledge Base and 3rd party workflows.
- Co-developed and maintained an AngularJS web application at minedatabase.mcs.anl.gov to facilitate broad use of the metabolite database.

Summer 2011

Summer Research Student at Colorado St. University

Colorado Center for Biofuels and Biorefining, Fort Collins, CO

- Constructed a partial astaxanthin synthesis pathway in *E. coli* with cloning techniques and performed homologous recombination in *Synechocystis*.
- Adapted a carotenoid extraction protocol for Synechocystis to enable quantitative HPLC analysis.

Technical Skills

Data Science	Python, Machine learning with scikit-learn & dask, Cluster computing, MongoDB, Redis, SQL
Bioinformatics	BLAST & Multiple sequence alignment, Ancestral sequence reconstruction, Homology modeling
Cheminformatics	QSAR modeling, Compound & reaction database design, ChemAxon suite, OpenBabel, RDKit
Web Development	APIs and microservices with Flask & Docker, JavaScript, Angular.js, Node.js, Protractor testing

Selected Awards

2016	Data Smackdown Champion	2014 - 2015	Fellowship in Leadership
	Enova International		Northwestern University
2015	NIH Travel Grant	2013	Outstanding Teaching Assistant Finalist
	Metabolomics Society		Northwestern University

Research Communication

Publications

- 1. O. Frelin, L. Huang, G. Hasnain, **J. Jeffryes**... A. Hanson "A novel directed-overflow and damage-control N-glycosidase in riboflavin biosynthesis" *Biochem. J.* **466**, 137-145 (2015)
- 2. **J. Jeffryes**, R. Colestani, M. El-Badawi, T. Kind... C. Henry "MINEs: Open access databases of computationally predicted enzyme promiscuity products for untargeted metabolomics" *J. Cheminformatics* 7:44 (2015)
- 3. C. Lerma-Ortiz*, **J. Jeffryes***, A. Cooper... C. Henry & A. Hanson "Nothing of chemistry disappears in biology": The Top 30 damage-prone metabolites *Biochem. Soc. Trans.* **44**, 961-71 (2016) *these authors contributed equally to this work
- 4. D. Pertusi, M. Moura, **J. Jeffryes** & K. Tyo "Elucidating substrate-level enzymatic promiscuity using cheminformatic methods" *Metabolic Engineering* In Review
- 5. **J. Jeffryes** C. Lerma-Ortiz A. Golubev... K. Tyo & C. Henry "CD-MINE: a database of curated and predicted spontaneous metabolic reactions" *ACS Synthetic Biology* In Preparation

Select Conference Presentations

- 1. **J. Jeffryes**, C. Lerma-Ortiz, T. Niehaus... C. Henry *Mining metabolism for unannotated enzymatic functions and serendipitous metabolic pathways* Poster Presentation at **Metabolic Engineering 11** June 27, 2016
- J. Jeffryes, C. Lerma-Ortiz, A.J. Cooper... C. Henry Detection of novel metabolites and enzyme functions through in silico expansion of metabolic models Oral Presentation at 251st American Chemical Society National Meeting & Exposition March 13, 2016
- 3. J. Jeffryes, R. Colestani, M. El-Badawi, T. Kind... C. Henry MINEs: Open access databases of computationally predicted enzyme promiscuity products for untargeted metabolomics Oral Presentation at 11th International Conference of the Metabolomics Society July 2, 2015

Teaching Experience

Leadership Coach	Worked with undergraduate students to identify and overcome leadership challenges in their organizations though one-on-one mentoring organized by Northwestern University's Center for Leadership.
Workshop Instructor	Developed and taught a 2-day workshop on cheminformatics and MINE databases for graduate students, postdoctoral fellows, and faculty from University of Florida and University of California-Davis
Research Mentor	Advised Tom Aunins, a Chemical Engineering undergraduate student, in writing a successful Undergraduate Research Grant application and conducting summer research.
Teaching Assistant	Kinetics, Energetics & Bioreactor Design, 3 quarters. Paradigms & Strategies of Leadership, 1 quarter Computational Biology, 1 quarter