Steve J Bertolani

Phone 916 996 8734
Email: sjbertolani@ucdavis.edu
LinkedIn: steve-j-bertolani
Github: sjbertolani

Education

Ph.D. - Physical Chemistry, UC Davis 2012-2018
Ph.D. Advisor - Justin Siegel
-Thesis Topic - Improving enzyme active site models with chemical reaction information. By mining data from solved protein structures in the enzyme subclass, we are able to add extra information into the creation of in silico computer models of enzymes as reactions occur. This yields increased accuracy in select cases.

-Designed and implemented a computation pipeline (GEO mining) that allows modeling, docking and design of O(1k-100k+) enzymes in parallel, versus traditional methods which design O(1-10). Used for multiple systems and projects. Allows diverse searching of protein sequence space and rapidly identifies good candidates for new enzyme specificities. Combines bioinformatics, structural informatics, state-of-the-art protein homology modeling and molecular docking and design.

B.S. in Chemistry, CSU-Sacramento 2012
Research Advisor - Ben Gherman
-Research Topic - DFT calculations on peptide deformylase biomimetic. Using the Gaussian quantum chemistry package to calculate minimized energy structures and transition state structures to estimate the cooperativity of hydrogen bond donors and acceptors in the peptide deformylase reaction.

Peer-Reviewed Publications

Mak, WS, **Bertolani, SJ**, Wang, XK, Arenas, R, Tang, WQ, Tagkopoulos, I, Wilson, DK, Siegel, JB, " Discovery, Design, and Structural Characterization of Alkane-Producing Enzymes across the Ferritin-like Superfamily", *Biochemistry*, 2020, 59, 40, 3834-3843, https://doi.org/10.1021/acs.biochem.0c00665

Le K, Adolf-Bryfogle J, Klima J,Lyskov S,Labonte J, **Bertolani S**, Roy Burman A, Leaver-Fay A, Weitzner B, Maguire J, Rangan R, Adrianowycz M, Alford R, Adal A, Nance M, Das R, Dunbrack R, Schief W, Kuhlman B, Siegel J, Gray J. "PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design**",** *Preprints*, 2020, 2020020097 (doi: 10.20944/preprints202002.0097.v1

Contreras, SC, **Bertolani, SJ**, Siegel, JB, “A benchmark for homomeric enzyme active site structure prediction highlights the importance of accurate modeling of protein symmetry”, *ACS Omega* 2019**,** https://doi.org/10.1021/acsomega.9b02636

Bertolani, SJ, Siegel, JB, “Integration of geometric constraints inferred from enzyme reaction chemistry can increase enzyme active site modeling accuracy”*, PLOS One 2019, 14(4): e0214126*

Nuñez, NN, Khuu, C, Babu, CS, **Bertolani, SJ**, Rajavel, AN, Spear, JE, Armas, JA, Wright, JD , Siegel, JB, Lim, C, David, SS, “The Zinc Linchpin Motif in the DNA Repair Glycosylase MUTYH: Identifying the Zn 2+ Ligands and Roles in Damage Recognition and Repair”, *JACS 2018 140(41), 13260-13271*

O’Brien, TE, **Bertolani, SJ,** Zhang, Y, Siegel, J, Tantillo, DJ, “Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases-Bornyl Diphosphate Synthase as a Representative Case”, *ACS Catalysis* 8(4), 3322-3330, 2018

Woo J, Seo E, **Bertolani SJ**, Siegel JB, Park E, Dinesh-Kumar S, “Comparative analyses of ubiquitin-like ATG8 and cysteine protease ATG4 autophagy genes in the plant lineage and cross-kingdom processing of ATG8 by ATG4 “, *Autophagy 12(11)*, 2054-2068, 2016

O’Brien, TE, **Bertolani, SJ**, Tantillo, DJ, Siegel, JB, “Mechanistically informed predictions of binding modes for carbocation intermediates of a sesquiterpene synthase reaction”, *Chemical Science,* 2016, 7(7), 4009-4015

Mak WS, Tran S, Marcheschi R, **Bertolani SJ**, Thompson J, Baker D, Liao JC, Siegel JB, “Integrative genomic mining for enzyme function to enable engineering of a non-natural biosynthetic pathway”, *Nature communications* 2015, 6,10005

Carlin DA, **Bertolani SJ**, Siegel JB, “Biocatalytic conversion of ethylene to ethylene oxide using an engineered toluene monooxygenase”, *Chemical communications* 2015 , 51(12), 2283-2285

Other Publications

Bertolani SJ, Carlin DA, Siegel JB, “Computational Introduction of Catalytic Activity into Proteins”, *Methods Mol Biol, 1414*, 213-31, 2016

Grants/Awards/Training

Biopharma Partnering Coordinator Internship, Office of Technology Management 2017-2018
PyRosetta 2.0 Manual (Rosetta Commons - $50k, joint w/ Johns Hopkins) 2017

(To expand project on https://github.com/sjbertolani/pyrosettabook; declined due to time constraints)

Superfund Research Program GSR Traineeship (Summer), UC Davis 2016
Peter A. Rock Graduate Fellowship in Chemistry, UC Davis 2016
UC Davis & Humanities Graduate Research Award, UC Davis 2015
Chemistry Graduate Program Fellowship, UC Davis 2014
Edmund & Wilma Fink Memorial Award in Physical Chemistry, UC Davis 2013
ACS Western Regional Meeting- Undergraduate Poster Presentation Award 2011
SURE Grant - computational chemistry under Dr. Ben Gherman 2011
Hyperchem Award 2011

Patents

Discovery of enzymes from the alpha-keto acid decarboxylase family US Patent 10,829,756

Presentations & Posters

Bertolani SJ, "Modeling enzyme active sites", RosettaCon, Leavenworth, WA. July 2017 (Presentation)

Bertolani SJ, "Enzyme Design with PyRosetta", Winter RosettaCon, San Diego, CA. Feb 2017 (Presentation)

Bertolani SJ, "Modeling enzyme active sites with chemical constraints", Winter RosettaCon, San Diego, CA. Feb 2017 (Presentation)

Bertolani SJ, "Homology models of enzymatic active sites", Winter RosettaCon, Burlington, Vermont. March 2016 (Presentation)

Mak WS, Tran S, Marcheschi R, **Bertolani SJ***, Thompson J, Baker D, Liao JC, Siegel JB "Integrative Genomic Mining for Enzyme Function to Enable Engineering of a Non-Natural Biosynthetic Pathway", SIMB 2015, Philadelphia PA, USA *presented joint work

Bertolani SJ, Zamora AE, Gherman BF, "Computational Study of Hydrogen Bonding Residues and Thiolate Coordination in the Active Site of Eubacterial Peptide Deformylase" (poster) 43rd Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011

Mentoring/Teaching Experience

TA for CHE 130B (Computational Drug Discovery & Design) 2015-17
TA for CHE 110A (Introductory Quantum Chemistry) 2013
TA for CHE2 series (General Chemistry & Laboratory) 2012-14

REU Mentor for NSF program #1659649
(Maya, Currently a Ph.D. student at George Washington) 2015
REU Mentor for NSF program #1659649 (Tommy) 2017

Undergraduate Mentor to Morgan Nance
(Currently a Ph.D. student at John Hopkins) 2014-16