DanVanatta

Computational Biochemist

contact

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programming

Python(numpy, matplotlib)
Bash, C++, Ruby
R, Matlab, SQL, VMD
Gromacs & MSMBuilder

databases

Uniprot/Swissprot
PharmGKB
Entrez

interests

Rock Climbing,
Basketball, Guitar,
Mountain Biking

education

2009–2014 **Ph.D.,** Chemistry — **Stanford University**
Dissertation: *Simulations of Antibiotic Resistance in Bacteria*

2005–2009 **B.S. Honors,** Chemistry — **University of California, Berkeley**

research

2009– **Graduate Researcher** — **Stanford University**
Advisor: Vijay Pande

- Generated and analyzed large scale datasets with molecular dynamics and Markov Models on distributed computing network Folding@Home.
- Developed novel algorithms and work flows to interpret computational models based on experimental data.
- Statistically evaluated the activation pathways of conformational change in key bacterial signaling protein (NtrC) to discover stabilizing molecular interactions.
- Recapitulated experimental binding trend for vancomycin with cell wall precursor and applied statistical analysis to calculate error bars.
- Tested and improved in-house analysis pipelines (MSMBuilder and Folding@Home)

2008–2009 **Undergraduate Researcher** — **UC Berkeley**
Advisor: Phillip Geissler

Created C++ program to model self-assembly of nano rods for use in solar panels

2007-2008 **Undergraduate Researcher** — **UC Berkeley**
Advisor: Richard Andersen

Synthesized and analyzed bonding of air-sensitive transition metal - ligands

publications

2014 **Dan Vanatta**, Vijay Pande. Origin of Molecular Resistance to Vancomycin. *Submitted to JCTC.*

2014 **Dan Vanatta**, Diwakar Shukla, Morgan Lawrenz, Vijay Pande. A Network of "Molecular-Switches" Control the Activation of Key Bacterial Signaling Protein. *In review at Nat. Comm.*

2014 Diwakar Shukla, **Dan Vanatta**, Vijay Pande. Activation of Kinases by Phosphorylation. *In preparation*

teaching

2009–2010	**Teaching Assistant** Organic Chemistry Lecture & Lab	**Stanford University**
2007-2008	**Undergraduate Student Instructor** ChemScholars & General Chemistry	**UC Berkeley**
2007-2009	**Willard Youth Support Program** Volunteer Math Tutor & Mentor	**Willard Middle School, Berkeley, CA**

academic projects

2013 Researched pharmacogenomic potential of the interaction between metoprolol and Cytochrome P450.

2012 Wrote Python code to:

- Perform global ends-free and local alignment using Needleman-Wunsch dynamic programming algorithm with affine gap penalty
- Classify gene expression microarray experiments using K-nearest neighbor supervised machine learning algorithm.
- Cluster genes with similar expression profiles using K-means unsupervised machine learning algorithm.
- Build a network of protein connections using a cheminformatic approach to compare proteins by examining the similarity of ligands they bind.

invited presentations

2013	Molecular-Switches Control the Activation of NtrC	**CMAD Seminar, Stanford, CA**
2012	Predicting Conformational Change in NtrC	**Student Seminar, Stanford, CA**
2010	New Directions in Predictions of Protein Allostery	**A.S.P. retreat, Las Vegas, NV**

posters

2013	Molecular-Switches Control the Activation of NtrC	**BPS 2014, SF, CA**
2012	Understanding Protein Conformational Change	**CUP XII, Santa Fe, NM**

awards

2014-	**Simbios Fellowship**	**Stanford University**
2010-2014	**Stanford Center for Molecular Analysis and Design Fellowship**	**Stanford University**
2012-2013	**Hong Kong Graduate Fellowship**	**Stanford University**
2007	**Bruce Howard Memorial Scholarship**	**UC Berkeley**