Sam DeLuca

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EDUCATION

Ph.D Chemical and Physical Biology — Vanderbilt University, Nashville, TN, 2008-March 2014 (expected)

B.S. Bioinformatics and Molecular Biology — Rensselaer Polytechnic Institute, Troy, NY, 2004-2008

RESEARCH EXPERIENCE

Vanderbilt University — **Advisor: Dr. Jens Meiler** **2008-present**

Development of a novel virtual High Throughput Screening (vHTS) software tool

- Designed and implemented RosettaHTS, a vHTS tool integrating structure-based small molecule docking with Artificial Neural Network techniques to predict ligand binding affinity.
- Wrote approximately 35,000 lines of C++ to develop RosettaHTS, a virtual screening tool integrated with the Rosetta software suite. Rosetta is a 2 million-line C++ application developed by a consortium of 24 research groups in 8 countries around the world.
- Curated a high quality protein-ligand interaction dataset to train and optimize RosettaHTS.
- Collaborated extensively with scientists at Vanderbilt and other universities during the software development process.
- Collaborated with a group of scientists to design and implement a MySQL based system for managing and analyzing large protein structure datasets.

Development of a knowledge-based energy potential for improving protein design predictions

- Implemented an energy potential to design proteins by analyzing the chemical environment of experimentally determined protein structures.
- Optimized the parameters of the energy potential using particle swarm optimization.
- Benchmarked the optimized parameters to demonstrate efficacy of the new energy function.

Led the migration of the Rosetta project from SVN version control software to Git

- Wrote Python tools to partially automate the migration process.
- Developed a new version control workflow in collaboration with the Rosetta developer community.
- Coordinated the migration process with the Rosetta developer community to minimize disruption of development activity.
- Wrote documentation and support information for the new version control workflow.

Rensselaer Polytechnic Institute — **Advisor: Dr. Chris Bystroff** **2004-2006 (Undergraduate Research)**

Development of ECOME, an interactive ecosystem simulation

- ECOME was designed to explore the effect of the introduction of civilization on an established ecosystem.
- Wrote a networked Java GUI which allowed the simulation to be modified interactively.
- Results were presented as a poster in 2005 at the IEEE Computational Systems Bioinformatics Conference.

Harvard Children's Hospital — **Advisor: Dr. Michael Freeman** **2006-2008 (Undergraduate Research)**

Identification of prostate cancer related genes

- Employed Perl scripts and the Ingenuity Pathway Analysis toolkit to analyze data from RNA expression microarrays to identify potential genes related to prostate cancer.
- Performed PCR experiments to validate the microarray data.
- Used siRNA to study the effect of previously identified genes on prostate cancer cell proliferation *in vitro*.

TEACHING, MENTORING AND OUTREACH EXPERIENCE

Instructor — Aspirnaut, Vanderbilt University **2012-2013**

Taught science classes to 3-6th grade students via video conferencing

- The Aspirnaut program is run by Vanderbilt University to provide high quality science instruction to students in rural school districts
- Taught 2-4 lab-based classes per month in a wide range of science topics using video conferencing technology

Instructor — Rosetta Workshop, Vanderbilt University **2011-2013**

Organized and team-led workshops to train scientists to use the Rosetta modeling suite

- Three workshops were conducted in March 2011, November 2012, and April 2013.
- Workshops limited to 15 attendees to maximize interaction between attendees and instructors.
- Created and presented hands-on tutorials to immerse participants in using the Rosetta modeling software suite.
- Consulted and discussed the individual scientific problems of the attendees and provided advice and guidance for successfully applying Rosetta modeling techniques.

Instructor — Rosetta Bootcamp, UNC Chapel Hill **2013**

Team-taught workshop in Rosetta development for new programmers in the rosetta community

- The first Rosetta "bootcamp" was held in 2012 to provide 25 new programmers with the basic knowledge necessary to be an effective Rosetta developer.
- Composed and taught 3 lectures describing introductory C++ and version control skills.
- Covered other material, including the Rosetta software architecture and techniques for numeric computing.

General Chemistry Lab, Vanderbilt University — Graduate Teaching Assistant **2010**

Taught and graded a freshman chemistry lab section

- Provided theoretical and practical instruction in basic chemistry lab procedures.
- Graded papers, homework assignments and lectures.

Intro to Cell Biology, Rensselaer Polytechnic Institute — Undergraduate Teaching Assistant **2008**

Taught a freshman chemistry lab section

- Managed lab stock solutions and materials.
- Instructed students in basic cell culture techniques.

AWARDS AND FELLOWSHIPS

- 2013 — Vanderbilt Graduate Student Travel Award
- 2013 — Rosetta award for service to the community
- 2011 — PhRMA Foundation Pre-doctoral Fellowship in Informatics
- 2011 — Rosetta award for service to the community
- 2010 — Vanderbilt Graduate Student Travel Award
- 2009 — Vanderbilt Graduate Student Travel Award
- 2007 — Tri-Beta Biological Honors society, Officer
- 2004 — Rensselaer Medal

POSTERS AND PRESENTATIONS

2013

- Poster — Vanderbilt Chemical and Physical Biology Retreat
- Poster — Gordon Conference – Computer Aided Drug Design
- Talk — Vanderbilt Molecular Biophysics Training Program Seminar
- Poster — RosettaCon

2012

- Poster — From Computational Biophysics to Systems Biology (CBSB)
- Poster — Vanderbilt Chemical and Physical Biology Retreat
- Talk — Vanderbilt Molecular Biophysics Training Program Seminar
- Talk — RosettaCon

2011

- Poster — Biophysical Society Meeting
- Poster — RosettaCon
- Talk — Vanderbilt Chemical and Physical Biology Retreat

2010

- Poster — RosettaCon
- Poster — Vanderbilt Chemical and Physical Biology Retreat

2009

- Poster — eCheminfo Conference
- Talk — RosettaCon

PUBLICATIONS