James C. Robertson
Philadelphia Area, PA USA jcrobertsonphd.com
jamescampbellrobertson@gmail.com (541) 227-9540

EXPERIENCE

Research Scientist in Computational Chemistry **2019 - current**
Janssen Research and Discovery, Spring House, PA

NIH IRACDA NY-CAPS Postdoctoral Scholar **2016 - 2019**
Protein Folding Simulations
Laufer Center for Physical and Quantitative Biology, Stony Brook University
Advisor: Ken A. Dill

EDUCATION

Ph.D. Medicinal Chemistry **May 2016**
Molecular Dynamics Simulations of DNA: Force Field Evaluation and Backbone Substate Dynamics In Free and Protein-Bound DNA
University of Utah College of Pharmacy
Advisor: Thomas E. Cheatham, III

B.S. Chemistry with ACS Certificate in Biochemistry **June 2011**
Southern Oregon University, Ashland, OR
Graduated Cum Laude

TECHNICAL SKILLS & EXPERTISE

- Computational chemistry software and tools for structure-based and ligand-based drug design: Schrödinger including LiveDesign, OpenEye, RDKit, CCG MOE, and Pipeline Pilot
- Molecular dynamics simulations and data analysis with AMBER, Desmond, OpenMM, NAMD, and Gromacs
- Scientific computing: scripting workflows and implementing new algorithms; expertise with UNIX/Linux; extensive use of High Performance Computing CPU/GPU resources
- Machine learning and data science primarily with Python and Jupyter notebooks; familiarity with R

PUBLICATIONS

- Robertson JC*, Nassar R*, Liu C, Brini E, Dill KA, Perez A. NMR-assisted protein structure prediction with MELDxMD. **2019,** *Proteins: Structure, Function, and Bioinformatics,* 87 (12), 1333-1340. (***co-first authors**)
- Robertson JC, Perez A, Dill KA. MELD x MD Folds Nonthreadables, Giving Native Structures and Populations. **2018,** *J. Chem. Theory Comput.*, DOI: 10.1021/acs.jctc.8b00886
- Galindo-Murillo R*, Robertson JC*, Zgarbová M, Šponer J, Otyepka M, Jurečka P, Cheatham III, TE. Assessing the Current State of AMBER Force Field Modifications for DNA. **2016,** *J. Chem. Theory Comput.,* 12 (8), 4114-4127. (***co-first authors**)
- Robertson JC, Cheatham III, TE. DNA Backbone BI/BII Distribution and Dynamics in E2 Protein-Bound Environment Determined by Molecular Dynamics Simulations, **2015,** *J. Phys. Chem. B,* 119, 14111-14119.

- Robertson JC, Hurley N, Tortorici M, Ciossani G, Borrello MT, Vellore NA, Ganesan A, Mattevi A, Baron R. Expanding the Druggable Space of the LSD1/CoREST Epigenetic Target: New Potential Binding Regions for Drug-Like Molecules, Peptides, Protein Partners, and Chromatin, **2013,** *PLoS Comp. Biol.,* 9(7):e1003158. doi:10.1371/journal.pcbi.1003158
- Dixon AS, Miller GD, Bruno BJ, Constance JE, Woessner DW, Fidler TP, Robertson JC, Cheatham III TE, Lim CS. Improved Coiled-Coil Design Enhances Interaction with Bcr-Abl and Induces Apoptosis, **2012,** *Mol. Pharm.,* 9, 187-195.

NATIONAL PRESENTATIONS & POSTERS

Presentations:

- "Landing a Tenure Track Faculty Position" **Stony Brook University Center for Inclusive Education Faculty Career Month** Stony Brook, NY *April 2019*
- "Bringing Better Physics to Protein Structure Prediction with MELD-accelerated Molecular Dynamics" **American Physical Society March Meeting** Boston, MA *March 2019*
- "BI/BII Backbone Sub State Dynamics in Protein-bound DNA" **American Chemical Society Spring Meeting** San Diego, CA *Spring 2016*
- "Using Configurational Ensembles to Expand LSD1/CoREST Druggability" 94^{th} **Annual AAAS Pacific Division Meeting** Las Vegas, NV *June 2013*
- "Ensemble-Based Virtual Screening of LSD1/CoREST" **SC12 Early Research Showcase, SC12** Salt Lake City, UT *Nov 2012*

Posters:

- "Protein Structures and Populations with MELD x MD" **CASP13** Riviera Maya, MX *December 2018*
- "MELD Folds Nonthreadable Proteins" **IRACDA** Atlanta, GA *July 2018*
- "MELD Folds Nonthreadable Proteins" **Blue Waters Symposium** Sunriver, OR *June 2018*
- "MELD Threads the Needle: Physics-Based Simulations Fold Nonthreadable Proteins" **IRACDA** Birmingham, AL *June 2017*
- "Assessing the Current State of AMBER Force Field Modifications for DNA" **American Chemical Society Spring Meeting** San Diego, CA *Spring 2016*
- "Human Low Molecular Weight Protein Tyrosine Phosphatases: Molecular Dynamics of A and B Isoforms" **International Society of Quantum Biology and Pharmacology President's Meeting** Telluride, CO *June 2014*
- "Molecular Dynamics Generated Ensemble for Structure-Based Drug Design" **Biophysical Society 58th Annual Meeting** San Francisco, CA *Feb 2014*
- "Ensemble-Based Virtual Screening of LSD1/CoREST" **SC12 Early Research Showcase, SC12** Salt Lake City, UT *Nov 2012*
- "Ensemble-Based Virtual Screening of LSD1/CoREST" **Utah Bioscience Symposium** Salt Lake City, UT *Sep 2012*
- "Primer-Directed Biocement and Kinase Searches from *Phragmatopoma lapidosa* and *Pectinaria gouldii* cDNA" **American Chemical Society Spring Meeting** Anaheim, CA *Spring 2011*

TEACHING EXPERIENCE

Instructor **Fall 2018**

Research and Discovery in STEM for Women in Science and Engineering, Stony Brook University — Stony Brook, NY

Adjunct Assistant Professor — **Spring 2018**
Principles of Chemistry II, SUNY Old Westbury — Old Westbury, NY

Curriculum Committee — **Spring 2018**
College Chemistry I and II, Suffolk County Community College — Selden, NY

Teaching Assistant — **Fall 2016**
Physical and Quantitative Biology, Stony Brook University — Stony Brook, NY

Teaching Assistant — **Spring 2014**
Physiological Chemistry II, University of Utah College of Pharmacy — Salt Lake City, UT

Guest Lecturer — **Fall 2014**
Organic Medicinal Chemistry, University of Utah College of Pharmacy — Salt Lake City, UT

Peer Led Team Learning — **2009-2010**
Organic Chemistry, Southern Oregon University — Ashland, OR

Pedagogy Workshops and Courses Completed — **2014-present**

- Scientists Teaching Science: A Short Course in Best Practices in Science Education • Alan Alda Center for Communicating Science Boot Camp: Improvisation for Scientists & Distilling Your Message • Flipping the Classroom • Building a Fool-Proof Syllabus • Evidence-based Instructional Practices: Process Oriented Guided Inquiry Learning • Evidence-based Instruction: Active Learning/Effective Questioning/Clickers • Overview of Scientific Teaching • Establishing Rapport: Secret Ingredient for Successful Teaching • Active Learning • Classroom Civility • Multimedia in Canvas • Spicing Up Your Lecture

LEADERSHIP, SERVICE, OUTREACH & AWARDS

- $100 3rd Place: Postdoc Spotlight *Stony Brook University* Fall 2018
- $5000 Wolf Prize: Excellence in teaching, research, and service *University of Utah* May 2016
- Instructor: Academic Writing Workshops *Stony Brook University* June 2017
- Member and Chair: Student Advisory Committee for Retention, Promotion, and Tenure *University of Utah College of Pharmacy* 2014-2016
- President: Chemistry Club *Southern Oregon University* 2010-2011 (Member 2009-2011)
- National Science Foundation Research Experience for Undergraduates *Coe College* 2010
- AAAS Pacific Division Student Travel Grant 94^{th} *Annual AAAS Pacific Division Meeting Las Vegas, NV* June 2013
- Coyner Graf Memorial Scholarship (1 year of tuition) *Southern Oregon University* 2010-2011
- National Science Foundation Research Experience for Undergraduates Chemistry Leadership Group Travel Award *ACS Spring Meeting* 2011
- Department of Chemistry Outstanding Service Award *Southern Oregon University* 2010-2011
- Department of Chemistry Award in Inorganic Chemistry *Southern Oregon University* 2010-

2011

MEMBERSHIPS & AFFILIATIONS

- American Chemical Society
- American Chemical Society Computers in Chemistry Division
- American Physical Society
- Biophysical Society
- American Association for the Advancement of Science
- New York Academy of Sciences