## James C. Robertson

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### **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

#### **PUBLICATIONS**

- 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<sup>th</sup> 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
Research and Discovery in STEM for Women in Science and
Engineering, Stony Brook University

Fall 2018
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<sup>th</sup> 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

### TECHNICAL SKILLS & EXPERTISE

- Molecular dynamics simulations and data analysis primarily with AMBER software; additional experience with computational chemistry packages including OpenMM, NAMD, Gromacs, Gaussian, and the Schrödinger suite
- Utilizing High Performance Computing resources including Blue Waters at NCSA, and the following through XSEDE: Stampede, Maverick, Gordon, Comet, Keeneland, and Kraken
- Proficient in Linux, Python, bash, LaTex, and tel
- Familiarity with C++, R, html, perl, SQL, git, and methods in machine learning and data science
- Familiarity with instrumentation: NMR, GC-MS, FT-IR, ICP-OES, UV-Vis, capillary DNA

## sequencer, and thermal cyclers

# 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