

Meagan C. Small

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EDUCATION

University of Maryland, Baltimore, Baltimore MD

Ph. D. in Pharmaceutical Sciences, June 2015 (anticipated)

Dissertation: "Computer-Aided Drug Design of Novel Macrolide Antibiotics to Address A2058-based Ribosomal Resistance"

Area of Specialization: Computer-aided drug design, molecular dynamics, force field development, docking

University of South Florida, Tampa FL

M.S. in Chemistry, August 2010

Thesis: "Time-resolved Thermodynamics of Heme Copper Oxidase Models"

Areas of Specialization: Spectroscopy, thermodynamics, and biophysics

University of South Florida, Tampa FL

B.S. in Chemistry, May 2007

Areas of Specialization: Physical chemistry

Honors: Graduated Cum Laude

University of South Florida, Tampa FL

B.S. in Biology, May 2007

Honors Thesis: "Microbial Diversity Using Phylogenetic Analysis of 16S rRNA from Jewfish Sink"

Areas of Specialization: Molecular biology and microbiology

Honors: Graduated Cum Laude

PUBLICATIONS

Peer-Reviewed Journal Articles

1. "Desmethyl Macrolides: Synthesis and Evaluation of 4-Desmethyl Telithromycin" Ian Glassford, Miseon Lee, Bharat Wagh, Venkata Velvadapu, Tapas Paul, Gary Sandelin, Charles DeBrosse, Dorota Klepacki, Meagan C. Small, Alexander D. MacKerell, Jr. and Rodrigo B. Andrade, **ACS Med Chem Let (2014, web)** ASAP: DOI 10.1021/ml5002097
2. "Desmethyl Macrolides: Synthesis and Evaluation of 4,8,10-Tridesmethyl Cethromycin" Bharat Wagh, Tapas Paul, Charles DeBrosse, Dorota Klepacki, Meagan C. Small, Alexander D. MacKerell, Jr. and Rodrigo B. Andrade, **ACS Med Chem Let (2013)**, 4(11): 1114-1118 DOI
3. "Impact of Ribosomal Modification on the Binding of Antibiotic Telithromycin Using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach" Meagan C. Small, Pedro Lopes, Rodrigo B. Andrade, Alexander D. MacKerell, Jr., **PLOS Computational Biology (2013)**, 9(6):e1003113
4. "Desmethyl Macrolides: Synthesis and Evaluation of 4,10-Didesmethyl Telithromycin" Venkata Velvadapu, Ian Glassford, Miseon Lee, Tapas Paul, Charles DeBrosse, Dorota Klepacki, Meagan C. Small, Alexander D. MacKerell, Jr. and Rodrigo B. Andrade, **ACS Med Chem Let (2012)**, 3(3):211-215

5. “Desmethyl Macrolides: Synthesis and Evaluation of 4,8-Didesmethyl Telithromycin”
Bharat Wagh, Tapas Paul, Ian Glassford, Charles DeBrosse, Dorota Klepacki, Meagan C. Small, Alexander D. MacKerell, Jr. and Rodrigo B. Andrade, **ACS Med Chem Let (2012)**, 3(12):1013-1018
6. “Scaled-Up Syntheses of Cuprilig for Removal of Nuisance Anions”
Dean F. Martin, Nicole Rubin, Meagan Small, **Florida Scientist (2010)**, 288:20
7. “Use of Model Compounds to Study Removal of Pharmaceuticals Using Octolig”
Wen-Shan Chang, Dean F. Martin, Meagan Small, **Technology and Innovation (2010)**, 12(1):71-77
8. “Removal of Selected Pharmaceuticals Using Octolig: A Supported Chelating Agent”
Wen-Shan Chang, Dean F. Martin, Meagan Small, **Technology and Innovation (2010)**, 12(2):143-152

Book Chapters

1. “Force field representation of biomolecular systems” Meagan C. Small and Alexander D. MacKerell, Jr., *In Silico Drug Discovery and Design: Theory, Methods, Challenges and Applications* (in press), CRC Press: Taylor & Francis Group, ISBN (978-1-4822-1783-4)

PRESENTATIONS

Computer-Aided Drug Design Symposium, Baltimore MD

Poster Presentation, June 2014

“Conformational Sampling of Desmethyl Telithromycin Using Hamiltonian Replica Exchange Molecular Dynamics”

University of Maryland School of Pharmacy Research Day, Baltimore MD

Poster Presentation, April 2014

“Conformational Sampling of Desmethyl Telithromycin Using Hamiltonian Replica Exchange Molecular Dynamics”

Second Nanomedicine Day, Baltimore MD

Poster Presentation, July 2013

“Impact of Ribosomal Modification on the Binding of Antibiotic Telithromycin using Empirical Force Field Simulations: Implications for Drug Design”

1st Annual Regional AAPS, West Virginia University, Morgantown WV

Poster Presentation, May 2013

“Impact of Ribosomal Modification on the Binding of Antibiotic Telithromycin using Computer Simulations”

University of Maryland School of Pharmacy Research Day, Baltimore MD

Poster Presentation, April 2013

“Impact of Ribosomal Modification on the Binding of Antibiotic Telithromycin using Empirical Force Field Simulations: Implications for Drug Design”

35th Annual Graduate Research Conference, Baltimore MD

Oral Presentation, April 2013

“Impact of Ribosomal Modification on the Binding of Antibiotic Telithromycin using Empirical Force Field Simulations: Implications for Drug Design”

244th American Chemical Society National Meeting and Exposition, Philadelphia PA

Poster Presentation, August 2012

“Investigations of the Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using Molecular Dynamics Simulations”

Mid-Atlantic Regional Meeting of ACS, Baltimore MD

Poster Presentation, May 2012

“Investigations of the Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using Molecular Dynamics Simulations”

34th Annual Graduate Research Conference, Baltimore MD

Poster Presentation, April 2012

“Investigations of the Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using Molecular Dynamics Simulations”

University of Maryland School of Pharmacy Research Day, Baltimore MD

Poster Presentation, March 2012

“Investigations of the Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using Molecular Dynamics Simulations”

4th Annual Frontiers at the Chemistry-Biology Interface Symposium, Newark DE

Poster Presentation, April 2011

“Conformational Sampling of Telithromycin/Cethromycin and Desmethyl Analogs”

33rd Annual Graduate Research Conference, Baltimore MD

Poster Presentation, April 2011

“Conformational Sampling of Telithromycin/Cethromycin and Desmethyl Analogs”

University of Maryland School of Pharmacy Research Day, Baltimore MD

Poster Presentation, March 2011

“Conformational Sampling of Telithromycin/Cethromycin and Desmethyl Analogs”

8th Annual Castle Conference, Tampa FL

Poster Presentation, April 2010

“Synthesis and Characterization of a Novel Calix[4]resorcinarene”

7th Annual Castle Conference, Tampa FL

Session Chair, April 2009

Presided over talks, mediated questions

53rd Annual Biophysical Society Meeting, Boston MA

Poster Presentation, February 2009

“Time-resolved Thermodynamics of CO Photolysis from an Engineered CuB Center in Sperm Whale Myoglobin”

60th Southeast Regional Meeting of ACS, New Orleans LA

Oral Presentation: Physical Chemistry Session, November 2008

“Time-resolved thermodynamics of CO Photolysis from an Engineered Copper Center in Sperm Whale Myoglobin”

AWARDS/HONORS

Department of Pharmaceutical Sciences Graduate Fellowship, University of Maryland, Baltimore, **2013**

Fred L & Helen M Tharp Endowed Scholarship, University of South Florida, **2009**

University of South Florida Presidential Scholarship, University of South Florida, **2007**

American Chemical Society Analytical Chemistry Award, University of South Florida, **2006**

Honors College Scholarship, University of South Florida, **2002-2007**

Florida Bright Futures Scholarship, University of South Florida, **2002-2007**