

# ROMAN MANETSCH

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## EDUCATION / EMPLOYMENT HISTORY

### Education

- 6/1998 Diploma in Chemistry, University of Basel (Switzerland), Studies in Chemistry (main subject) and Biology (minor subject), Advisor: Professor Wolf-Dietrich Woggon  
Thesis: *Synthese potentieller Inhibitoren für die  $\beta$ -Carotin 15,15'-Dioxygenase (Synthesis of Potential Inhibitors of the Enzyme  $\beta$ -Carotene 15,15'-Dioxygenase)*
- 10/2002 Ph.D. in Chemistry, Institute of Organic Chemistry at the University of Basel (Switzerland); Advisor Professor Wolf-Dietrich Woggon and Co-Advisor Professor Jean-Louis Reymond (Department of Chemistry and Biochemistry at the University of Bern (Switzerland))  
Thesis: *Transition-State-Analoge für die Identifizierung des Enzyms Tocopherol-Cyclase und für die Herstellung katalytischer, monoklonale Antikörper (Transition State Analogues for the Identification of the Enzyme Tocopherol Cyclase and for the Preparation of Catalytic Monoclonal Antibodies)*

### Employment

- 11/2002 - 05/2005 Postdoctoral Fellow with K. Barry Sharpless, The Scripps Research Institute, La Jolla (CA)
- 08/2005 - 07/2011 Assistant Professor, Department of Chemistry, College of Arts and Science, University of South Florida, Tampa (FL)
- 08/2011 - 08/2014 Associate Professor, Department of Chemistry, College of Arts and Science, University of South Florida, Tampa (FL)
- 12/2012 - 10/2013 Sabbatical Researcher, Center for Proteomic Research, Novartis Pharma AG, Basel, Switzerland
- 09/2014 - present Associate Professor, Department of Chemistry and Chemical Biology, College of Science and Department of Pharmaceutical Sciences, Bouvé College of Health Sciences, Northeastern University, Boston (MA); Faculty Fellow, Center for Drug Discovery, Northeastern University, Boston (MA)

### Research Interests

The research interests of the Manetsch laboratory focus on organic, bioorganic, and click chemistry addressing fundamental aspects and diverse applications of medicinal chemistry of anti-infectives, as well as chemical probes for the study of specific proteins in complex biological matrices. Using synthetic chemistry in close conjunction with liquid chromatography with mass spectrometry detection (LC-MS and LC-MS/MS), the Manetsch laboratory developed kinetic Target-Guided Synthesis (TGS), a fragment-based lead discovery strategy, targeting protein-protein interactions associated with apoptosis. This LC-MS-based method is currently applied for the discovery of inhibitory agents or probe molecules to target malaria, leishmania, amoeba or bacterial infections. Furthermore, the Manetsch laboratory is interested in establishing reliable synthetic routes for the preparation of natural products or highly functionalized analogues with anti-infective activity. The synthetic capability enables the preparation of focused compound libraries required for detailed structure-activity and structure-property relationship studies (SAR and SPR). The Manetsch laboratory implemented LC-MS-based SPR assays and pharmacokinetics to routinely determine key physicochemical properties of small molecules. Using this hit-to-lead progression strategy, in vivo efficacious anti-malarial, anti-leishmanial, anti-amoeba and anti-bacterial (Gram-positive and/or Gram-negative) agents have been developed. For example, for approximately half a century, endochin, ICI56,780, WR243246, and 4(1*H*)-quinolone analogues thereof were known to be causal prophylactic and potent erythrocytic stage agents in avian but not in mammalian malaria models. In close collaboration with parasitology and pharmacology teams, our hit-to-lead optimization efforts

lead to 4(1*H*)-quinolones P4Q-391 and ELQ-300 with superb *in vivo* antimalarial activity (99% parasitemia suppression on day six post exposure at < 3 mg/kg doses) proving to be curative with all the mice surviving a *Plasmodium berghei* infection after 30 days. With the support of the non-profit organization Medicines for Malaria Venture, the frontrunner compound ELQ-300 entered preclinical development in 2013. As a third research field, the Manetsch laboratory developed chemical tools to identify and/or covalently label specific proteins in complex mixtures or entire proteomes. The Manetsch laboratory is currently studying and investigating various photoactivatable probes to study proteins related to energy metabolism and signal transduction. Furthermore, artemisinin-, primaquine- and chloroquine-based probes are currently under development to elucidate the mechanisms of antimalarial drug resistance in greater detail.

### Honors and Awards

- 2002 Ph.D. Summa Cum Laude
- 2003 Swiss National Science Foundation, Postdoctoral Fellowship
- 2003 Novartis Foundation (formerly the Ciba-Geigy Jubilee Foundation), Postdoctoral Fellowship
- 2004 Swiss National Science Foundation, Postdoctoral Fellowship
- 2012 Excellence in Innovation Award, University of South Florida

### RESEARCH ACTIVITIES

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#### Peer Reviewed Publications

(Corresponding author(s) is(are) indicated with asterisk(s)\*)

- 1) Parvatkar, P T; Smotkin, E S; **Manetsch, R\***. Total Synthesis of (±)-Decursivine *via* BINOL-Phosphoric Acid Catalyzed Tandem Oxidative Cyclization. *In preparation*.
- 2) Iyamu, I D; Roberts, B F; Cassandra, D; Wojtas, L; Kyle, D E; Chakrabarti, D; **Manetsch, R\***. Structure-Activity and Structure-Property Relationship Studies of Spirocyclic Chromane with Antimalarial Activity. *In preparation*.
- 3) Monastyrskiy, A; Brockmeyer, F; LaCrue, A N; Maignan, J R; Casandra, D; Mutka, T S; Sherwin Mashkouri, S; Kyle, D E; **Manetsch, R\***. Aminoalkoxycarbonyloxymethyl Ether Prodrugs with a pH-Triggered Release Mechanism: A Case Study Improving Solubility, Bioavailability, and Efficacy of Antimalarial 4(1*H*)-Quinolones with Single Dose Cures. *In preparation*.
- 4) Smith, K P; Dowgiallo, M D; Chiaraviglio, L; Parvatkar, P; Kim, C; **Manetsch, R**; Kirby, J E\*. A Whole-Cell Screen for Adjunctive and Direct Antimicrobials Active Against Carbapenem-Resistant *Enterobacteriaceae*. *Submitted*.
- 5) Donnelly, D P, Winters, J N; Conway, J B; Hossain, M A; Dowgiallo M D; Schmitt, N D; Rawlins C M; Salisbury, J P; Auclair, J R; **Manetsch, R**; Makowski L\*; Ondrechen M J\*; Agar, J N\*. Cyclic Thiosulfonates Stabilize Native Structure of Disease-Associated Variants of Cu/Zn-Superoxide Dismutase. *Submitted*.
- 6) Parvatkar, P T\*; **Manetsch R\***; Banik, B K\*. Metal-Free Cross-Dehydrogenative Coupling (CDC): Molecular Iodine as a Versatile Catalyst/Reagent for CDC Reaction. *Chemistry. Chem Asian J* 2019; 14, 6-30.
- 7) Donnelly, D P; Dowgiallo, M G; Salisbury, J P; Krishna, C; Iyengar, S; Chaudhari, M; Mathew, M; Miele, I; Auclair, J R; Lopez, S A, **Manetsch R**, Agar J N\*. Cyclic Thiosulfonates and Cyclic Disulfides Selectively Crosslink Thiols While Avoiding Modification of Lone Thiols. *J Am Chem Soc* 2018; 140, 7377–7380.
- 8) Neelarapu, R; Maignan, J R; Lichorowic, C L; Monastyrskiy, A; Mutka, T S; Lacrue, A N; Blake, L D; Casandra, D; Mashkouri, S; Burrows, J N; **Manetsch, R\*** Design and synthesis of orally bioavailable piperazine substituted 4(1*H*)-quinolones with potent antimalarial activity: structure-activity and structure-property relationship studies. *J Med Chem* 2018; 61, 1450–1473.
- 9) Kumar, A B; **Manetsch, R\***. Ammonia-free Synthesis of 3-Trifluoromethyl-3-Phenyldiaziridine. *Synth Commun* 2018; 48, 626–631.
- 10) Fleeman R, Van Horn K S, Barber M M, Burda W N, Flanigan D L, **Manetsch R\***, Shaw L N\*. Characterizing the Antimicrobial Activity of *N*<sup>2</sup>,*N*<sup>4</sup>-Disubstituted Quinazoline-2,4-Diamines Towards Multidrug Resistant *Acinetobacter baumannii*. *Antimicrob Agents Chemother* 2017; AAC.00059-17.

- 11) Maignan J R, Lichorowic C L, Giarrusso J, Blake L D, Casandra D, Mutka T S, LaCrue A N, Burrows J N, Willis P A, Kyle D E, **Manetsch R\***. ICI 56,780 Optimization: Structure-Activity Relationship Studies of 7-(2-Phenoxyethoxy)-4(1*H*)-quinolones with Antimalarial Activity. *J Med Chem* 2016; 59, 6943-6960.
- 12) Roberts B F, Iyamu I D, Lee S, Lee E, Ayong L, Kyle D E, Yuan Y, **Manetsch R**, Chakrabarti D\*. Spirocyclic Chromanes Exhibit Antiplasmodial Activities and Inhibit All Intraerythrocytic Life Cycle Stages. *Int J Parasitol Drugs Drug Resist* 2016; 6, 85-92.
- 13) Kumar A B, Tipton J D, **Manetsch R\***. 3-Trifluoromethyl-3-aryldiazirine Photolabels with Enhanced Ambient Light Stability. *Chem Commun* 2016; 52, 2729-2732.
- 14) Van Horn K S, Zhu X, Pandharkar T, Yang S, Vesely B, Vanaerschot M, Dujardin J C, Rijal S, Kyle D E, Wang M Z, Werbovetz K A, **Manetsch R\***. Correction to Antileishmanial Activity of a Series of *N*(2),*N*(4)-Disubstituted Quinazoline-2,4-diamines. *J Med Chem* 2016; 59, 775.
- 15) Zhu X, Van Horn K S, Barber M M, Yang S, Wang M Z, **Manetsch R**, Werbovetz K A. SAR Refinement of Antileishmanial *N*<sup>2</sup>,*N*<sup>4</sup>-Disubstituted Quinazoline-2,4-diamines. *Bioorg Med Chem* 2015; 23, 5182-5189.
- 16) Mahajan S, **Manetsch R**, Merkler D J, Stevens S M Jr.\* Synthesis and Evaluation of a Novel Adenosine-ribose Probe for Global-scale Profiling of Nucleoside and Nucleotide-binding Proteins. *PLoS One*, 2015; 10, e0115644.
- 17) Monastyrskiy A, Namelikonda N K, **Manetsch R\***. Metal-Free Arylation of Ethyl Acetoacetate with Hypervalent Diaryliodonium Salts: an Immediate Access to Diverse 3-Aryl-4(1*H*)-Quinolones. *J Org Chem* 2014; 80, 2513-2502.
- 18) Cross R M, Flanigan D L, Monastyrskiy A, LaCrue A N, Saenz F E, Maignan J R, Mutka T S, White K L, Shackelford D M, Bathurst I, Fronczek F R, Wojtas L, Guida W C, Charman S A, Burrows J N, Kyle D E, **Manetsch R\***. Orally Bioavailable 6-Chloro-7-methoxy-4(1*H*)-quinolones Efficacious Against Multiple Stages of *Plasmodium*. *J Med Chem* 2014; 1693-1705.
- 19) Monastyrskiy A, Kyle D E, **Manetsch R\***. 4(1*H*)-Pyridone and 4(1*H*)-Quinolone Derivatives as Antimalarials with Erythrocytic, Exoerythrocytic, and Transmission Blocking Activities (Review). *Curr Top Med Chem* 2014; 1693-1705.
- 20) Campbell C O, Santiago D N, Guida W C, **Manetsch R**, Adams J H\*. In silico Characterization of an Atypical MAPK Phosphatase of *Plasmodium falciparum* as a Suitable Target for Drug Discovery. *Chem Biol Drug Des* 2014; 84, 158-168.
- 21) Van Horn K S, Zhu X, Pandharkar T, Yang S, Vesely B, Vanaerschot M, Dujardin J-C, Rijal S, Kyle D E, Wang M Z, Werbovetz Karl, **Manetsch R\***. Antileishmanial Activity of a Series of *N*<sup>2</sup>,*N*<sup>4</sup>-disubstituted quinazoline-2,4-diamines. *J Med Chem* 2014; 57, 5141-5156.
- 22) Kumar A B, **Manetsch R\***. Regioselective, Mild and Robust *O*2',*O*3'-Deacetylations of Peracetylated Ribonucleosides Using Tetra-*n*-butylammonium Fluoride. *Eur J Org Chem* 2014; 3551-3555.
- 23) Van Horn K S, Burda W N, Fleeman R, Shaw L N\*, **Manetsch R\***. Antibacterial Activity of a Series of *N*<sup>2</sup>,*N*<sup>4</sup>-Disubstituted Quinazoline-2,4-diamines. *J Med Chem* 2014; 57, 3075-3093.
- 24) Sáenz F E, LaCrue A N, Cross R M, Maignan J R, Udenze K O, **Manetsch R**, Kyle D K\*. 4-(1*H*)-Quinolones and 1,2,3,4-Tetrahydroacridin-9(10*H*)-ones Prevent the Transmission of *Plasmodium falciparum* to *Anopheles freeborni*. *Antimicrob Agents Chemother* 2013; 57, 61887-6195.
- 25) LaCrue A N, Sáenz F E, Cross R M, Udenze K O, Monastyrskiy A, Stein S, Mutka T S, **Manetsch R**, Kyle D E\*. 4(1*H*)-Quinolones with Liver Stage Activity Against *Plasmodium berghei*. *Antimicrob Agents Chemother* 2013; 57, 417-424.
- 26) Nilsen A, LaCrue A, White K. L , Forquer I P, Cross R M, Marfurt J, Mather M W, Delves M J, Shackelford D M, Sáenz F E, Morrisey J M, Steuten J, Mutka T, Li Y, Wirjanata G, Ryan E, Duffy S, Kelly J X, Sebayang B F, Zeeman A-M, Noviyanti R, Sinden R E, Kocken C H M, Price R N, Avery V M, Angulo-Barturen I, Jiménez-Díaz M B, Ferrer S, Herreros E, Sanz L M, Benito F J G, Bathurst I, Burrows J, Siegl P, Guy R K, Winter R W, Vaidya A B, Charman S A, Kyle D E, **Manetsch R\***, Riscoe M K\*. Quinolone-3-diarylethers: A New Class of Drugs for a New Era of Malaria Eradication. *Sci Transl Med* 2013; 5, 177ra37.
- 27) Kulkarni S S, Hu X, **Manetsch R\***. A Simple Base-mediated Amidation of Aldehydes with Azides. *Chem Commun* 2013; 49, 1193-1195.
- 28) Nacheva K P, Maza W A, Myers D Z, Fronczek F R, Larsen R W, **Manetsch R\***. Fluorescent Properties and Resonance Energy Transfer of 3,4-Bis(2,4-difluorophenyl)-maleimide. *Org Biomol Chem* 2012; 10, 7840-7846.

- 29) Kumar A B, Anderson J M, Melendez A L, **Manetsch R\***. Synthesis and Structure-Activity Relationship Studies of 1,3-Disubstituted 2-Propanols as BACE-1 Inhibitors. *Bioorg Med Chem Lett* 2012; 22, 4740-4744.
- 30) Namelikonda N K, **Manetsch R\***. Sulfo-Click Reaction *Via In Situ* Generated Thioacids and Its Application in Kinetic Target-Guided Synthesis. *Chem Commun* 2012; 48, 1526-1528.  
*Article has been published in the "Emerging Investigators 2012" issue.*
- 31) Cross R M, Namelikonda N K, Mutka T S, Luong L, Kyle D E, **Manetsch R\***. Synthesis, Antimalarial Activity, and Structure-Activity Relationship of 7-(2-Phenoxyethoxy)-4(1*H*)-quinolones. *J Med Chem* 2011; 54, 8321-8327.
- 32) Kumar A B, Anderson J M, **Manetsch, R\***. Design, Synthesis and Photoactivation Studies of Fluorous Photolabels. *Org Biomol Chem* 2011; 9, 6284-6292.
- 33) Cross M R, Maignan J R, Mutka T S, Luong L, Sargent J, Kyle D K, **Manetsch R\***. Optimization of 1,2,3,4-Tetrahydroacridin-9(10*H*)-ones as Antimalarials Utilizing Structure-Activity and Structure-Property Relationships. *J Med Chem* 2011; 54, 4399-4426.
- 34) Kulkarni S S, Hu X, Doi K, Wang H-G, **Manetsch R\***. Screening of Protein-Protein Interaction Modulators via Sulfo-Click Kinetic Target-Guided Synthesis. *ACS Chemical Biology* 2011; 6, 724-732.  
*Appeared in the list of 20 "most read" ACS Chemical Biology articles in the entire year of 2011.*
- 35) Cross R M, **Manetsch R\***. Divergent Route to Access Structurally Diverse 4-Quinolones via Mono or Sequential Cross-Couplings. *J Org Chem* 2010; 75, 8654-8657.
- 36) Cross M R, Monastyrskiy A, Mutka T S, Burrows J N, Kyle D K, **Manetsch R\***. Endochin Optimization: Structure-Activity and Structure-Property Relationship Studies of 3-Substituted 2-Methyl-3(1*H*)-quinolones with Antimalarial Activity. *J Med Chem* 2010; 53, 7076-7094.
- 37) Hu X, **Manetsch R\***, Kinetic Target-Guided Synthesis (Review). *Chem Soc Rev* 2010, 39, 1316-1324.
- 38) Hu X, Sun J, Wang H-G, **Manetsch R\***. Bcl-X<sub>L</sub>-Templated Assembly of Its Own Protein-Protein Interaction Modulator from Fragments Decorated with Thio Acids and Sulfonyl Azides. *J Am Chem Soc* 2008; 130, 13820-13821.
- 39) Radic Z, **Manetsch R**, Fournier D, Sharpless KB, Taylor P\*. Probing Gorge Dimensions of Cholinesterases by Freeze-Frame Click Chemistry. *Chem-Biol Interact* 2008; 175, 161-165.
- 40) Sharpless K B, **Manetsch R\***. In Situ Click Chemistry: A Powerful Means for Lead Discovery (Review). *Expert Opinion on Drug Discovery* 2006; 1, 525-538.
- 41) Radic Z, **Manetsch R**, Krasinski A, Raushel J, Yamauchi J, Garcia C, Kolb H C, Sharpless K B, Taylor P\*. Molecular basis of interactions of cholinesterases with tight binding inhibitors. *Chem-Biol Interact* 2005; 157, 133-141.
- 42) Krasinski A, Radic Z, **Manetsch R**, Raushel J, Taylor P, Sharpless K B, Kolb H C\*. Click Chemistry Screening *In Situ*: Target-Guided Optimization of Acetylcholinesterase Inhibitors. *J Am Chem Soc* 2005; 127, 6686-6692.
- 43) Zheng L, **Manetsch R**, Woggon W-D, Baumann U, Reymond J L\*. Mechanistic Study of Proton Transfer in Catalytic Antibody 16E7 by Site-Directed Mutagenesis and Homology Modeling. *Bioorg Med Chem* 2005; 13, 1021-1029.
- 44) **Manetsch R**, Krasinski A, Radic Z, Raushel J, Taylor P, Sharpless K B, Kolb H C\*. In Situ Click Chemistry: Enzyme Inhibitors Made to Their Own Specifications. *J Am Chem Soc* 2004; 126, 12809-12818.
- 45) **Manetsch R**, Zheng L, Reymond M T, Woggon W D, Reymond J-L\*. A Catalytic Antibody Against a Tocopherol Cyclase Inhibitor. *Chem Eur J* 2004; 10, 2487-2506.

## Book Chapters

- 1) Book chapter on "3',5'-Dimethoxybenzoin" by R. Matthew Cross and **Roman Manetsch**. *e-EROS Encycl. Reagents Org. Synth.* 2009.

## Patents

- 1) **Manetsch R**, Kyle D E, Monastyrskiy A, LcCrue A N, Maignan J R, Brockmeyer F M. Compounds and methods for their use in the treatment of malaria. US20190031613A1, 2019.

- 2) **Manetsch R**, Shaw L N, Van Horn K S, Burda W N. Compositions, methods of use, and methods of treatment. US10081607B2, 2018.
- 3) **Manetsch R**, Kumar A B, Tipton J. Photoactivatable probes and uses thereof. US10067136B1, 2018.
- 4) **Manetsch R**, Kyle D E, Raghupathi N, Maignan J R, Lichorowic C L, LaCrue A N. Quinolone-based compounds, formulations, and uses thereof. US10000452B1, 2018.
- 5) **Manetsch R**, Nacheva K P, Flanigan D L, Namelikonda N K, Iyamu I D, Kulkarni S S, Barber M M, Tipton J D, Wang HG, Doi K. Target Binding Molecules Identified by Kinetic Target-Guided Synthesis. US20160116482A1, 2016.
- 6) Riscoe M K, Kelly J X, Winter R W, Hinrichs D J, Smilkstein M J, Nilsen A, Burrows J N, Kyle D E, **Manetsch R**, Cross R M, Monastyrskyi A, Flanigan D L. Compounds Having Antiparasitic or Anti-Infectious Activity. US9206131B2, 2015.
- 7) **Manetsch R**, Shaw L N, Van Horn K S, Burda W N. Compositions, methods of use, and methods of treatment. US20150080409A1, 2015.
- 8) **Manetsch R**, Shaw L N, Van Horn K S, Burda W N. Compositions, methods of use, and methods of treatment. US8906918B1, 2014.
- 9) **Manetsch R**, Cross R M, Namelikonda N K, Kyle D E, Mutka T S, Lacrue A N, Maignan J R, Saenz F E. Preparation of 4(1*H*)-Quinolones Having Antimalarial Activity with Reduced Chemical Resistance. US8877752B2, 2014.
- 10) Riscoe M K, Kelly J X, Winter R W, Hinrichs D J, Smilkstein M J, Nilsen A, Burrows J N, Kyle D E, **Manetsch R**, Cross R M, Monastyrskyi A, Flanigan D L. Compounds Having Antiparasitic or Anti-Infectious Activity. US20140045888A1, 2014.
- 11) Riscoe M K, Kelly J X, Winter R W, Hinrichs D J, Smilkstein M J, Nilsen A, Burrows J N, Kyle D E, **Manetsch R**, Cross R M, Monastyrskyi A, Flanigan D L. Compounds Having Antiparasitic or Anti-Infectious Activity. US8598354B2, 2013.
- 12) Wang HG, **Manetsch R**, HuX, Kulkarni S S, Sun J. Acylsulfonamides and processes for producing the same. US8524947B2, 2013
- 13) Riscoe M K, Kelly J X, Winter R W, Hinrichs D J, Smilkstein M J, Nilsen A, Burrows J N, Kyle D E, **Manetsch R**, Cross R M, Monastyrskyi A, Flanigan D L. Compounds Having Antiparasitic or Anti-Infectious Activity. US20120115904A1, 2012.
- 14) **Manetsch R**, Kulkarni S S, Iyamu I D, Wang H-G, Doi K, Guida W C, Santiago D N, Duboulay C J. Target-Guided Synthesis of Acylsulfonamides that Target Bcl-2 Family Proteins with Potential Use in Treating Cancer. WO2012021486A2, 2012.
- 15) Adams J H, Balu B, Maher S P, Campbell C, **Manetsch R**. Methods for Treating and/or Preventing Malaria in Individuals that Use Plasmodium PF13\_0027 Gene and Dual-Specificity Protein Tyrosine Phosphatase as Targets. WO2010108177A2, 2010.
- 16) **Manetsch R**, Wang H-G, Hu X, Kulkarni S S, Sun J G. Target-Guided Synthesis of Triazoles in the Presence of a Bcl-2 Family Protein. WO2009105746A2, 2009.
- 17) **Manetsch R**, Wang H-G, Hu X, Kulkarni S S; Sun J G. Process for Preparation of Acylsulfonamides from Thioacids and Sulfonyl Azides in the Presence of a Bcl-2 Family Protein. WO2009105751A1, 2009.

### Invited Talks and Conferences

- 1) Kinetic Target-guided Synthesis: Mass Spectrometry-driven Medicinal Chemistry Targeting Protein-Protein Interactions; Roman Manetsch; 2018 Southeastern Chemical Biology Symposium, Athens, GA, United States, April 21, 2018.
- 2) Orally Bioavailable Antimalarial 4(1*H*)-Quinolone and 4(1*H*)-Quinolone Prodrugs with Single-Dose Cures; Roman Manetsch; International Pharma Conference and Expo, Rome, Italy, May 2-4, 2018.
- 3) Kinetic Target-guided Synthesis: a MS-based Fragment Evolution Platform; Roman Manetsch; International Pharma Conference and Expo, Rome, Italy, May 2-4, 2018.
- 4) Mass Spectrometry-guided Medicinal Chemistry Targeting Malaria and Cancer. Chemistry Department, University of Massachusetts Boston, September 27, 2017.
- 5) Mass Spectrometry-Driven Medicinal Chemistry Targeting Malaria and Cancer. Chemistry and Biochemistry Department, University of Massachusetts Dartmouth, September 27, 2017. February 11, 2016.

- 6) Kinetic Target-Guided Synthesis: A Fragment Evolution Strategy Based on Bioorthogonal Reactions. Fragment-based Lead Discovery Conference 2014, Basel, Switzerland, September 21 to 24, 2014.
- 7) Mass Spectrometry-Guided Approaches for Synthetic and Medicinal Chemistry. Pharmaceutical Sciences, University of Nebraska Medical Center, Omaha, NE, March 12, 2014.
- 8) Mass Spectrometry-Guided Approaches for Synthetic and Medicinal Chemistry. Department of Chemistry, Wayne State University, Detroit, MI, March 5, 2014.
- 9) Mass Spectrometry-Guided Approaches for Synthetic and Medicinal Chemistry. Department of Chemistry and Applied Biosciences, Swiss Federal Institute of Technology (ETH), Zürich, Switzerland, October 4, 2013.
- 10) Kinetic Target-guided Synthesis: A Mass Spectrometry-based Fragment Evolution Strategy for "Undruggable" Targets. 30<sup>th</sup> Winterschool on Proteinases and Their Inhibitors, Tiers am Rosengarten, February 27 to March 3, 2013.
- 11) Kinetic Target-Guided Synthesis: A Fragment-Based Discovery Strategy for "Undruggable" Targets Based on Bioorthogonal Reactions. Department of Chemistry, University of Basel, February 7, 2013.
- 12) Mass Spectrometry Guided Medicinal Chemistry of Antimalarial and Anticancer Agents. Department of Chemistry and Biochemistry, University of Bern, November 27, 2012.
- 13) Bringing 4(1*H*)-Quinolones and 3-Aryldiazirines Out of the "Dark" Ages. 6th International Conference, Chemistry of Nitrogen Containing Heterocycles, Kharkiv, Ukraine, November 12 to 16, 2012.
- 14) Kinetic Target-Guided Synthesis: A Fragment-Based Discovery Strategy for "Undruggable" Targets Based on Bioorthogonal Reactions. Drug Discovery Symposium, Novartis, Basel and Cambridge, October 22, 2012.
- 15) Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Glaxo Smith Kline, Research Triangle Park, NC, June 26, 2012.
- 16) Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Novartis, Basel, Switzerland, April 27, 2012.
- 17) Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Addex Pharmaceuticals, Geneva, Switzerland, April 23, 2012.
- 18) Mass Spectrometry Based Decisions Facilitating Synthetic and Medicinal Chemistry. Department of Chemistry, Clemson University, Clemson, SC, March 15, 2012.
- 19) Mass Spectrometry Based Decisions Facilitating Synthetic and Medicinal Chemistry. Department of Chemistry, Mississippi State University, MS, March 2, 2012.
- 20) Quinazolines with Anti-Leishmania Activity. Consortium for Parasitic Drug Development Meeting 2011. Clearwater, FL, November 1 to 3, 2011.
- 21) LC-MS-Guided Identification and Optimization of Anti-Cancer and Anti-Malarial Agents. Albert Einstein College of Medicine, Bronx, NY. June 21, 2011.
- 22) The Bioorthogonal Sulfo-click Reaction and its Use in Kinetic Target-Guided Synthesis Screening of Bcl-2 Proteins. Amgen, Thousand Oaks, CA, May 18, 2011.
- 23) LC-MS-Guided Identification and Optimization of Anti-Cancer and Anti-Malarial Agents. Department of Chemistry, Rice University, Houston, TX, April 27, 2011.
- 24) Bioorthogonality of the Sulfo-Click Reaction and its Use in Kinetic Target-Guided Synthesis. 241st ACS National Meeting and Exposition, Anaheim, CA, March 27 to 31, 2011.
- 25) Discovery and Optimization of Protein-Protein Interaction Modulators via Kinetic Target-Guided Synthesis. 18th International Molecular Medicine Tri-Conference, Mastering Medicinal Chemistry Summit. San Francisco, CA, February 23 to 25, 2011.
- 26) Targeting Protein-Protein Interactions via Kinetic Target-Guided Synthesis. The Fragment-Based Lead Discovery Conference 2010. Philadelphia, PA, October 10 to 13, 2010.
- 27) Two Case Studies of LC/MS-driven Drug Discovery: Targeting Bcl-2-Protein Interactions for Anti-Cancer and bc<sub>1</sub> for Anti-Malarial Agents. Department of Chemistry, University of Washington. Seattle, WA, October 20, 2010.
- 28) Targeting Protein-Protein Interactions and Malaria: Two Case Studies of LC/MS-driven Screening and Hit-to-Lead Optimization. The Scripps Florida Research Institute. Jupiter, FL, August 10, 2010.
- 29) Kinetic Target-Guided Synthesis Targeting Protein-Protein Interactions. "Short talk" and poster at the Gordon Research Conference on Chemistry and Biology of Peptides. Ventura, CA, February 28 to March 5, 2010.
- 30) LC/MS-based Drug Discovery Targeting Malaria and Cancer. Department of Chemistry, University of Tampa. Tampa, FL, November 17, 2009.

- 31) Kinetic Target-Guided Synthesis: A Fragment-Based Lead Discovery Method Targeting Protein-Protein Interactions. Department of Chemistry, Florida State University, Tallahassee, FL, November 20, 2008.
- 32) Target-Guided Synthesis: A New Approach for Drug Discovery. Florida Annual Meeting and Exposition 2008 (American Chemical Society Regional Meeting). Orlando, FL, May 8 to 10, 2008.
- 33) Target-Guided Synthesis: A New Approach for Drug Discovery. BioStat International / Molecular Medicine Seminar Series, College of Medicine, University of South Florida, Tampa, FL, March 31, 2006.

### Oral and Poster Presentations Manetsch Laboratory

(Oral presentations indicated by underlined author; first author is presenting author)

- 1) Matthew Dowgiallo, James E. Kirby, Roman Manetsch: Studies toward the total synthesis of streptolidine lactam and streptothricin F. Boston Symposium on Organic and Bioorganic Chemistry Boston MA, United States, October 2018
- 2) David Yingzhao Zhao, Roman Manetsch: Studies towards the total synthesis of anguidine. Boston Symposium on Organic and Bioorganic Chemistry Boston MA, United States, October 2018
- 3) Jackson G. Cacioppo, Brenda Winn, Chungsik Kim, Imran Elmaarouf, Meng Cui, Diomedes Logothetis, Roman Manetsch: Pyridyl- and pyrimidinyl-substituted diazirines as aromatic amino acid mimics and photoaffinity labels. Boston Symposium on Organic and Bioorganic Chemistry Boston MA, United States, October 2018
- 4) Mintesinot Kassu, Prakash Parvatkar, Roman Manetsch: Identification of potent protein-protein interaction modulators using kinetic target-guided synthesis. Boston Symposium on Organic and Bioorganic Chemistry Boston MA, United States, October 2018
- 5) Jennifer Winters, David McDonald, Elizabeth Taft, Jeffrey Agar, Roman Manetsch, Mary Jo Ondrechen: Cyclic disulfide compounds stabilize SOD1 dimers. 256th ACS National Meeting & Exposition, Boston, MA, United States, August 19 to 23, 2018 (2018), COMP-381.
- 6) David Yingzhao Zhao, Roman Manetsch: Studies towards the total synthesis of anguidine. 256th ACS National Meeting & Exposition, Boston, MA, United States, August 19 to 23, 2018 (2018), ORGN-644.
- 7) Matthew Dowgiallo, James Kirby, Roman Manetsch: Synthesis of a thiourea analogue of streptolidine lactam. 256th ACS National Meeting & Exposition, Boston, MA, United States, August 19-23, 2018 (2018), ORGN-643
- 8) Matthew Dowgiallo, James Kirby, Roman Manetsch: Studies Towards the Total Synthesis of Streptothricin F: Synthesis of Thiourea Analogue of Streptolidine Lactam. Natural Products and Bioactive Compounds Gordon Research Seminar, Andover NH, United States of America, July 2018
- 9) Jackson G. Cacioppo, Brenda Winn, Chungsik Kim, Imran Elmaarouf, Meng Cui, Diomedes Logothetis, Roman Manetsch: Pyridyl- and pyrimidinyl-substituted diazirines as aromatic amino acid mimics and photoaffinity labels. PharmSci Research Showcase, Boston, MA, United States, June 2018
- 10) Prakash T. Parvatkar, Eugene Smotkin, Roman Manetsch: BINOL-Phosphoric Acid Catalyzed Tandem Oxidative Cyclization: Synthesis, Antimalarial Activity Evaluation and SAR Studies of ( $\pm$ )-Decursivine. PharmSci Research Showcase, Boston, MA, United States, June 2018
- 11) Cynthia Lichorowic, Jordany R. Maignan, Raghupathi Neelarapu, Andrii Monastyrski, James V. Giarrusso, Tina S. Mutka, Lynn Blake, Debora Casandra, Alexis LaCruce, Dennis E. Kyle, Roman Manetsch: Optimization of 4(1*H*)-quinolone antimalarials for oral bioavailability and in vivo efficacy 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017. Pages MEDI-452.
- 12) Arun Babu Kumar, Jordan Anderson, Anthony Melendez and Roman Manetsch: Synthesis and SAR analysis of 1,3-disubstituted isopropanols as novel scaffold for  $\beta$ -secretase inhibition. 243rd American Chemical Society (ACS) National Meeting and Exposition, San Diego, CA, March 25 to 29, 2012.
- 13) Arun Babu Kumar: New series of 3-trifluoromethyl-3-aryldiazirine photo probes exhibiting enhanced stability to ambient light conditions. 243rd American Chemical Society (ACS) National Meeting and Exposition, San Diego, California, March 25 to 29, 2012.

*Awarded with an American Chemical Society Division of Medicinal Chemistry Student Travel Grant to attend the 243rd ACS National Meeting and Exposition in San Diego, CA.*

- 14) K. Van Horn, X. Zhu, T. Pandharkar, B. Vesely, M. Z. Wang, D. Kyle, K. Werbovetz, R. Manetsch: 2,4-diaminoquinazolines as anti-leishmanials. 243rd American Chemical Society National Meeting and Exposition. San Diego, CA, March 25 to 29, 2012.
- 15) Kurt S. Van Horn, Whitney Burda, Lindsey Shaw, Roman Manetsch: 2,4-diaminoquinazolines as anti-bacterials. 243rd American Chemical Society National Meeting and Exposition. San Diego, CA, March 25 to 29, 2012.
- 16) Shikha Mahajan, David Merkler, Roman Manetsch: Proteomic profiling of adenine nucleotides and nucleoside analogs binding proteins using activity-based protein profiling probes. 242nd ACS National Meeting and Exposition, Denver, CO, United States, August 28 to September 1, 2011.
- 17) R. Matthew Cross: Identification of an Early Lead and Optimization Strategies for the Development of an Orally Bioavailable Late Lead 4(1*H*)-Quinolone with Antimalarial Activity. Florida Annual Meeting and Exposition 2011 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2011.
- 18) Shikha Mahajan: Synthesis of biotinylated-azido-adenine ribose derivative analogues: Potential activity-based protein profiling probes. Florida Annual Meeting and Exposition 2011 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 12 to 14, 2011.
- 19) Katya Nacheva: 3,4-Bis(2,4-Difluorophenyl)-Maleimide as Fluorescence Probe and its Incorporation in a Fluorescent Resonance Energy Transfer Substrate of  $\beta$ -Secretase. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2011.
- 20) Andrii Monastyrskiy: Synthesis and Evaluation of 4(1*H*)-quinolones Prodrugs Targeting Multi-drug Resistant *P. falciparum* Malaria. 2011 USF Raymond Castle Student Research Conference, Tampa, April 9th, 2011.
- 21) Katya Nacheva: Fluorescence and Resonance Energy Transfer of 3,4-bis(2,4-difluorophenyl)-maleimide. Raymond Castle conference, University of South Florida, Tampa, FL, April 9, 2011.
- 22) Shikha Mahajan, David Merkler, Roman Manetsch: Protein Profiling of Adenine Nucleotides and Nucleoside Analogues Binding Proteins using Novel Activity Based Protein Profiling Probes. Sanibel Conference, American Society of Mass Spectrometry, St. Pete Beach, FL, United States, January 21 to 24, 2011.
- 23) Andrii Monastyrskiy, Roman Manetsch, Tina S Mutka, Alexis Lacrue, Fabian Saenz, Dennis E. Kyle: Synthesis and Evaluation of 4(1*H*)-quinolones Prodrugs Targeting Multi-drug Resistant *P. falciparum* Malaria. Florida Annual Meeting and Exposition 2011 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 12 to 14, 2011.  
*Awarded with the 1<sup>st</sup> prize in graduate poster competition.*
- 24) R. Matthew Cross, Andrii Monastyrskiy, Jordany Maignan, Tina Mutka, Dennis E. Kyle, Roman Manetsch: Design of novel 4-(1*H*)-quinolones targeting multi-drug resistant *P. falciparum* malaria. Gordon Research Conference, Bryant University, Smithfield, RI, July 18 to 23, 2010.
- 25) R. Matthew Cross: Synthesis and Structure-Activity Relationship Studies of 4(1*H*)-Quinolones Targeting Multi-drug Resistant *P. falciparum* Malaria. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 15, 2010.
- 26) Niranjana Namelikonda, Sameer Kulkarni, Kenichiro Doi, Hong-Gang Wang, Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2010.
- 27) Katya Nacheva, William A. Maza, Randy W. Larsen, Roman Manetsch: 3,4-Bis(2,4-Difluorophenyl)-Maleimide as Fluorescence Probe and its Incorporation in a Fluorescent Resonance Energy Transfer Substrate of  $\beta$ -Secretase. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2010.
- 28) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated-azido-adenine ribose derivative analogues: Potential activity-based protein profiling probes. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2010.
- 29) Jordany R. Maignan, Andrii Monastyrskiy, Matthew R. Cross, Tina Mutka, Dennis E. Kyle, Roman Manetsch: The Use of an HPLC-based Assay to Determine Aqueous Solubility of Compounds with Biological Activity. Florida Annual Meeting and Exposition 2010 (American Chemical Society Regional Meeting). Palm Harbor, FL, May 13 to 14, 2010.
- 30) Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. 2010 CHI's Fragment-Based Drug Discovery Conference, San Diego, CA, April 27 to 29, 2010.



- 31) Andrii Monastyrskiy, David, Flanigan, R. Matthew Cross, Tina Mutka, Dennis Kyle, Roman Manetsch: Design of Novel 4(1*H*)-quinolones Targeting Multi-Drug Resistant *P. falciparum* Malaria. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 32) Sameer Kulkarni: Kinetic Target-Guided Synthesis for the Identification of Bcl-X<sub>L</sub>-Protein Interaction Modulators. 2010 USF Raymond Castle Student Research Conference, Tampa, April 17, 2010.  
*Awarded second place in the Bioorganic, Natural and Organic Chemistry Division.*
- 33) Kurt Van Horn, Anuradha Srivastava, Dennis Kyle, Roman Manetsch: Anti-leishmanial Activity of a new series of Quinazolines. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 34) Lisa Luong, R. Matthew Cross, Justin Sargent, Jordany Maignan, Tina Mutka, Dennis Kyle, Roman Manetsch: 1,2,3,4-Tetrahydroacridones as Potential Inhibitors of Atovaquone-Resistant and Atovaquone-Susceptible *P. falciparum* isolates TM90-C2B and W2. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 35) Jordan Anderson, Arun Babu Kumar, Roman Manetsch: Design of a Small Molecule Inhibitor of  $\beta$ -Secretase. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 36) Jordany Maignan, Andrii Monastyrskiy, Lisa Luong, R. Matthew Cross, Roman Manetsch: The Development and Use of an HPLC-based Assay to Determine Aqueous Solubility of Compounds with Biological Activity. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 37) Anthony Melendez, Arun Babu Kumar, Jordan Anderson, Hong-Gang, Roman Manetsch: Synthesis of 1,3-Disubstituted Isopropanols as Potential Small Molecule Inhibitors for BACE-1 and Protein-Protein Interaction. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 38) Sameer Kulkarni, Niranjana Namelikonda, Kenichiro Doi, Hong-Gang Wang, Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. 2010 USF Raymond Castle Student Research Conference, Tampa, FL, April 17, 2010.
- 39) R. Matthew Cross, David L. Flanigan, Andrii Monastyrskiy, Tina Mutka, Dennis E. Kyle, Roman Manetsch: Design of novel 4-(1*H*)-quinolones targeting multi-drug resistant *P. falciparum* malaria. American Chemical Society National Meeting and Exposition, San Francisco, CA, March 21 to 25, 2010.
- 40) R. Matthew Cross: Synthesis and structure-activity relationship studies of 4(1*H*)-quinolones targeting multi-drug resistant *P. falciparum* malaria. American Chemical Society National Meeting and Exposition, San Francisco, CA, March 21 to 25, 2010.
- 41) Katya Nacheva, David Mayer, Roman Manetsch: In Situ Click Chemistry Reaction Templated by bCAII. Symposium on Drug Design, Discovery and Delivery 2009. Blase Alfano Center, University of South Florida, Tampa, FL, October 14 to 16, 2009.
- 42) Arun Babu Kumar, Jordan Anderson, Roman Manetsch: Development of a Labeling Probe for the Discovery and Identification of Saccharide-Binding Proteins. Symposium on Drug Design, Discovery and Delivery 2009 (FCoE-BITT), Tampa, FL, October 14-16, 2009
- 43) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated-azido-adenine ribose derivative analogues: Potential activity-based protein profiling probes. Symposium on Drug Design, Discovery and Delivery (Florida Centre of Excellence for Biomolecular Identification and Targeted Therapeutics). University of South Florida, Tampa, FL, October 14 to 16, 2009.
- 44) Sameer Kulkarni, Xiangdong Hu, Kenichiro Doi, Hong-Gang Wang, Roman Manetsch, Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. 2009 Symposium on Drug Design, Discovery and Deliver, Florida Center of Excellence for Biomolecular Identification and Targeted Therapeutics, University of South Florida, Tampa, FL, October 14 to 16, 2009.
- 45) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated azido adenineribose derivative analogues: Potential activity based protein profiling probes. VIII European Symposium of the Protein Society, Zurich, Switzerland, June 14 to June 18, 2009
- 46) Roman Manetsch, Sameer Kulkarni, Xiangdong Hu, Hong-Gang Wang: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. Gordon Research Conference, Proctor Academy, Andover, NH, June 14 to 19, 2009.
- 47) Petoria Gayle, Sameer Kulkarni, Xiangdong Hu, Hong-Gang Wang, Roman Manetsch: Protein-Protein Interaction Modulators and Role of Kinetic Target Guided Synthesis. 2009 USF Raymond Castle Student Research Conference, Tampa, FL, April 18, 2009.

- 48) Kurt Van Horn, Roman Manetsch: Templated Assembly of DNA Fragments via Complimentary Reactive Functionalities. 2009 USF Raymond Castle Student Research Conference, Tampa, FL, April 18, 2009.
- 49) Mario Martinez, Xiangdong Hu, Hong-Gang Wang, Roman Manetsch: Development of a SAR-by-MS Screening Platform Targeting Bcl-2 Proteins. 2009 USF Raymond Castle Student Research Conference, Tampa, FL, April 18, 2009.
- 50) Mario Martinez, Xiangdong Hu, Hong-Gang Wang, Roman Manetsch: Development of SAR-by-MS for proteins of the Bcl-2 family. USF's Undergraduate Research Symposium and Celebration, Tampa, FL, April 4, 2009.

*Awarded with the 1<sup>st</sup> prize for best oral presentation by an undergraduate student*

- 51) Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. 2009 CHI's Fragment-Based Drug Discovery Conference, San Diego, CA, April 6 to 8, 2009.
- 52) Arun Babu Kumar, Jordan Anderson, Roman Manetsch: Development of a labeling probe for the discovery and identification of saccharide-binding proteins. American Chemical Society National Meeting and Exposition, Salt Lake City, UT, March 22 to 26, 2009.
- 53) Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interaction Modulators. 2009 Molecular Medicine Tri-Conference, San Francisco, CA, February 3 to 5, 2009.
- 54) Jordany Maignan, R. Matt Cross, Tina Mutka, Dennis Kyle, Roman Manetsch: SAR Study of 1,2,3,4-Tetrahydroacridones for the Development of Chemotypes Targeting Atovaquone Resistant Malaria Parasites. 2008 Poster Symposium & Competition "Global Challenges for the 21<sup>st</sup> Century" Tampa, FL, November 6, 2008
- 55) Sameer Kulkarni, Jiazhi Sun, Hong-Gang Wang, Roman Manetsch: Targeting protein-protein interactions via in situ click chemistry. American Chemical Society National Meeting and Exposition, Philadelphia, PA, August 17 to 21, 2008.
- 56) Xiangdong Hu, Jiazhi Sun, Hong-Gang Wang, Roman Manetsch: Bcl-templated assembly of its own protein-protein interaction modulators. American Chemical Society National Meeting and Exposition, Philadelphia, PA, August 17 to 21, 2008.
- 57) Sameer Kulkarni, Xiangdong Hu, Hong-Gang Wang, Roman Manetsch: Application of Target Guided Synthesis (TGS) approach: Targeting protein-protein interactions, Florida Annual Meeting and Exposition 2008 (American Chemical Society Regional Meeting). Orlando, FL, May 8 to 10, 2008.
- 58) Arun Babu Kumar, Jordan Anderson, Roman Manetsch: Development of a Labeling Probe for the Discovery and Identification of Saccharide-Binding Proteins. Florida Annual Meeting and Exposition 2008 (American Chemical Society Regional Meeting), Orlando, FL, May 8 to 10, 2008.
- 59) Arun Babu Kumar, Roman Manetsch. 2008 USF Raymond Castle Student Research Conference. Development and synthesis of photoaffinity labeling probe for target selective proteomics. Tampa, FL, April 19, 2008.
- 60) Sameer Kulkarni, Jiazhi Sun, Hong-Gang Wang, Roman Manetsch: Kinetic Target-Guided Synthesis for the Identification of Bcl-xL-Protein Interactions Modulators. 2008 USF Raymond Castle Student Research Conference, Tampa, FL, April 19, 2008.
- 61) Christi Young, Roman Manetsch, Edwin Rivera, Alberto van Olphen, Alfredo E. Cardenas: Molecular dynamics of the RNA-binding domain of Influenza A NS1. American Chemical Society National Meeting and Exposition, New Orleans, LA, April 6 to April 10, 2008.
- 62) Richard M. Cross, Gregory A. Hunter, Gloria C. Ferreira, Roman Manetsch: Screening of libraries for inhibitors or activators of the enzyme 5-aminolevulinic synthase. American Chemical Society National Meeting and Exposition, New Orleans, LA, April 6 to April 10, 2008.
- 63) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated azido adenineribose derivative analogues: Potential activity based protein profiling probes. American Chemical Society National Meeting and Exposition, New Orleans, LA, April 6 to April 10, 2008.
- 64) Mario Martinez, Shikha Mahajan, Roman Manetsch: Development of a Photoaffinity Labeling Probe. USF's Undergraduate Research Symposium and Celebration, Tampa, FL, April 2, 2008.

*Awarded with the 1<sup>st</sup> prize for best oral presentation by an undergraduate student*

- 65) Richard M. Cross, Tina Mutka, Dennis E. Kyle, Roman Manetsch: Quinolones as Novel Chemotypes Targeting Atovaquone Resistant Malaria Parasites. 18<sup>th</sup> Annual 2008 USF Health Research Day, Tampa, FL, February 22, 2008.

- 66) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated-azido-adenine-ribose derivatives analogues: Potential activity based protein profiling (ABPP) probes. 18<sup>th</sup> Annual 2008 USF Health Research Day, Tampa, FL, February 22, 2008.
- 67) Xiangdong Hu, Sameer S. Kulkarni, Lisa Malmgren, Jiazhi G. Sun, Hong-Gang Wang, Roman Manetsch: Bcl-X<sub>L</sub>-templated assembly of its own protein-protein interaction modulators. 18<sup>th</sup> Annual 2008 USF Health Research Day, Tampa, FL, February 22, 2008.
- 68) Arun B. Kumar, Roman Manetsch: Development of a Labeling Probe for the Discovery and Identification of Saccharide-Binding Proteins. 18<sup>th</sup> Annual 2008 USF Health Research Day, Tampa, FL, February 22, 2008.
- 69) Shikha Mahajan, David Merkler, Roman Manetsch: Synthesis of biotinylated-azido-adenine ribose derivative analogues: Potential activity based protein profiling probes. Symposium on Drug Design, Discovery and Delivery (Florida Centre of Excellence for Biomolecular Identification and Targeted Therapeutics). University of South Florida, Tampa, Florida, FL, October 25 to 26, 2007.
- 70) Richard Matthew Cross, Zoran Radic, Palmer Taylor, Roman Manetsch: Synthesis of IBTZ6PA2: A potential acetylcholinesterase inhibitor displaying improved species specificity. Florida Annual Meeting and Expedition 2007 (American Chemical Society Regional Meeting). Orlando, FL, April 12, 2007.

## RESEARCH FUNDING

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### Pending Awards

(unless specified, funding amounts comprise of direct and indirect costs)

- 1) National Institutes of Health, National Institute of Allergy and Infectious Diseases (RO1AI144464): Orally Bioavailable 4(1*H*)-Quinolones with Multi-Stage Antimalarial Activity. Total budget \$3,672,359 (\$1,837,289 Manetsch total budget; \$1,170,248 Manetsch direct costs) 04/01/2019 - 03/31/2024. Contact PI **Roman Manetsch** and PI Dennis E. Kyle (University of George, Athens). Impact score 32, percentile 14; NIAID 2019 RO1 payline percentile 14; JIT submitted on January 18, 2019; animal protocol approval requested by NIH; approval expected on March 21, 2019.
- 2) National Institutes of Health, National Institute of Allergy and Infectious Diseases (RO1AI148901): Structure-based Development of Drugs to Treat Primary Amoebic Meningoencephalitis. Total budget \$3,912,640 (\$762,174 Manetsch total budget; \$485,461 Manetsch direct costs) 09/01/2019 - 08/31/2024. Contact PI Dennis E. Kyle (University of George, Athens), PI Jim Leahy (University of South Florida), PI James Morris (Clemson University), PI Wesley Van Voorhis (University of Washington) and PI **Roman Manetsch**.
- 3) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R01GM135731-01): MS-Enabled Cyclic Thiosulfinate Crosslinkers. Total budget \$3,142,032 (\$1,472,903 Manetsch total budget; \$938,155 Manetsch direct costs) 09/01/2019 - 08/31/2024. Contact PI Jeffrey N. Agar (Northeastern University), PI **Roman Manetsch**, and CI Mary Jo Ondrechen.

### Current Awards

(unless specified, funding amounts comprise of direct and indirect costs)

- 1) National Institutes of Health, National Institute of Allergy and Infectious Diseases (1R21AI140212): Development of Streptothricin Class Antimicrobials as Novel Therapeutics. Total budget \$467,498 (\$215,185 Manetsch total budget; \$137,061 Manetsch direct costs) 03/01/2019 - 02/28/2021. Contact PI **Roman Manetsch** and PI James E. Kirby (Beth Israel Deaconess Medical Center).
- 2) Medicines for Malaria Venture (RD-17-0036): Antimalarial Compounds Targeting Liver Stages of *Plasmodium vivax*. \$435,079 direct costs (no indirect costs allowed); (\$251,493 Manetsch direct costs) 01/01/2018 - 12/31/2018 (award is renewed annually). Contact PI Dennis E. Kyle, and PI **Roman Manetsch**. Note: Medicines for Malaria Venture provides additional resources for evaluating our prodrug compound in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies will be charged directly to Medicines for Malaria Venture. The scope of this work focuses on the development of a compound series displaying anti-hyponozoite activity.

- 3) National Institutes of Health, National Institute of Allergy and Infectious Diseases (5R33-AI119114): Plasmid Eviction to Restore Susceptibility in Carbapenem-Resistant Enterobacteriaceae. Total budget unknown (\$91,020 Manetsch total budget; \$57,975 Manetsch direct costs) 07/01/2018 - 06/30/2020. PI James E. Kirby (Beth Israel Deaconess Medical Center) and CI **Roman Manetsch**.
- 4) Amyotrophic Lateral Sclerosis Association (18-IIA-420): Tethering SOD1 Cysteine Pairs with Cyclic Disulfides: a New Method for Protein Stabilization. Total budget \$300,00 (10% indirect costs allowed); (\$92,937 Manetsch total budget; \$84,488 Manetsch direct costs), 10/01/2017 - 09/31/2020. PI Jeffrey N. Agar (Northeastern University), CI Mary Jo Ondrechen (Northeastern University), and CI **Roman Manetsch**.

### Grants Expired

(unless specified, funding amounts comprise of direct and indirect costs)

- 1) Medicines for Malaria Venture (16/00421): Prodrugs of Antimalarial 4(1*H*)-Quinolones. \$24,218.41 direct costs (no indirect costs allowed); (\$24,218.41 Manetsch direct costs) 06/01/2016 - 05/31/2017. PI **Roman Manetsch**. Note: Medicines for Malaria Venture provides additional resources for evaluating our prodrug compound in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies will be charged directly to Medicines for Malaria Venture. The scope of this work focuses on evaluating whether our prodrug approach has potential for clinical development.
- 2) National Institutes of Health, National Institute of General Medical Sciences (1R01GM097118): Drugs Targeting Erythrocytic and Exoerythrocytic Stages of Malaria. Total budget \$1,361,229 (\$952,861 Manetsch total budget; \$657,146 Manetsch direct costs) 09/15/2011 - 05/31/2017. PI **Roman Manetsch**; CI Dennis Kyle (University of South Florida, Department of Global Health).
- 3) National Institutes of Health, National Institute of Allergy and Infectious Diseases Partnerships with Product Development Public-Private Partnerships (1R01AI090662): Drug Validation of New Antimalarial Leads. Total budget \$5,721,270 (\$1,111,636 Manetsch total budget; \$766,646 Manetsch direct costs), 06/01/2011 - 07/31/2017. Lead PI Jeremy Burrows (Medicines for Malaria Venture) and PIs Kip Guy (St. Jude Children's Research Hospital, Chemical Biology and Therapeutics), Dennis Kyle (University of South Florida, Department of Global Health), David Floyd (Rutgers, Department of Chemistry), and **Roman Manetsch**.
- 4) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R21): Antileishmanial Lead Optimization of Quinazolines. Total budget \$432,963 (\$115,274 Manetsch budget; \$78,418 Manetsch direct costs), 07/01/2012 - 06/30/2014. PI Karl Werbovets (The Ohio State University, Department of Medicinal Chemistry); CIs **Roman Manetsch** and Zhuo (Michael) Wang (University of Kansas, Pharmaceutical Chemistry).
- 5) Medicines for Malaria Venture (11/0022): Quinolones for Single Exposure Radical Cure, \$182,108 direct costs (no indirect costs allowed); (\$83,724 Manetsch direct costs), 03/01/2012 – 12/31/2012 (continuation upon meeting milestones). PI Dennis Kyle (University of South Florida, Department of Global Health); CI **Roman Manetsch**. Note: Medicines for Malaria Venture provides additional resources for evaluating our prodrug compound in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies will be charged directly to Medicines for Malaria Venture.
- 6) Medicines for Malaria Venture (08/0068): Quinolone and 1,2,3,4-Tetrahydroacridone Chemotypes for Malaria Drug Discovery. \$859,086 direct costs (no indirect costs allowed); (\$449,127 Manetsch budget; direct costs), 11/01/2008 – 12/31/2012 (annually renewed; notified on 05/22/2012 that project will be terminated due to successful delivery of a preclinical candidate, which has been taken forward by MMV's translational team). PI **Roman Manetsch**; CI Dennis Kyle (University of South Florida, Department of Global Health). Note: Medicines for Malaria Venture provides additional resources for evaluating our compounds in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies will be charged directly to Medicines for Malaria Venture.
- 7) Bankhead-Coley Biomedical Research Program, Florida Department of Health (08BN-04): Chemical Tools for Proteomic Profiling. Total budget \$375,000 (10% indirect costs allowed); (\$173,610 Manetsch total budget; \$157,827 Manetsch direct costs), 07/01/2008 – 12/31/2011. PI **Roman Manetsch**; CI David Merkler (University of South Florida, Department of Chemistry), Mentor Mark McLaughlin (University of South Florida, Department of Chemistry)

- 8) Florida Center of Excellence - BITT Seed Grant: Evaluation of a Phosphotyrosin Phosphatase as an Antimalarial Drug Target. \$75,000 direct costs (no indirect costs allowed); (\$33,000 Manetsch direct costs), 07/01/09 – 12/31/11. PI John Adams (University of South Florida, Department of Global Health); CI **Roman Manetsch**.
- 9) Florida Center of Excellence - BITT Seed Grant: Characterization of Candida Cytochrome b5 Reductase as Pharmacological Target, \$75,000 direct costs (no indirect costs allowed); (\$33,000 Manetsch direct costs), 07/01/09 – 12/31/11. PI Andreas Seyfang (University of South Florida, Molecular Medicine); CI **Roman Manetsch**.
- 10) James and Esther King Biomedical Research Program, Florida Department of Health (07KN-08): Bcl-X<sub>L</sub>-Templated Assembly of Compounds Modulating Bcl-X<sub>L</sub>-Protein Interactions. Total budget \$375,000 (10% indirect costs allowed); (\$337,612 Manetsch total budget; \$306,920 Manetsch direct costs), 07/01/2007 – 12/31/2010. PI **Roman Manetsch**; Mentor Wayne Guida (University of South Florida, Department of Chemistry).
- 11) Johnnie B. Byrd, Sr. Alzheimer's Center and Research Institute, Seed Grant: Adenylomics and Caffeinylics. Total budget \$40,793 (10% indirect costs allowed); (\$21,443 Manetsch total budget; \$19,494 Manetsch direct costs), 09/01/2008 – 08/31/2009. PI **Roman Manetsch**; CI David Merkler (University of South Florida, Department of Chemistry).
- 12) Florida Center of Excellence - BITT Seed Grant, GALS007: Adenylomics. \$75,000 direct costs (no indirect costs allowed); (\$37,000 Manetsch direct costs), 05/01/2008 – 04/30/2009. PI David Merkler (University of South Florida, Department of Chemistry); CI **Roman Manetsch**.
- 13) Florida Center of Excellence - BITT Seed Grant, GALS008: SAR Study of Quinolones and 1,2,3,4-Tetrahydroacridones for the Development of Novel Chemotypes Targeting Atovaquone Resistant Malaria Parasites. \$75,000 direct costs (no indirect costs allowed); (\$38,000 Manetsch direct costs), 05/01/2008 – 04/30/2009. PI **Roman Manetsch**; CI Dennis Kyle (University of South Florida, Department of Global Health).
- 14) Florida Center of Excellence - BITT Thrust Graduate Scholar, Ph.D. scholarship for graduate student Richard M. Cross: Discovery of Lead Compounds Targeting the Enzyme 5-Aminolevulinic Synthase. \$40,000, 09/01/2007 – 08/31/2009. PI **Roman Manetsch**.
- 15) University of South Florida, Interdisciplinary Research Development Grant: Development of Novel Antiviral Compounds Targeting Non-structural Protein 1. \$49,872 direct costs (no indirect costs allowed); (\$16,624 Manetsch direct costs), 03/01/2006 – 02/29/2008. PI **Roman Manetsch**; CIs Alberto van Olphen (University of South Florida, Center for Biological Defense) and Edwin Rivera (University of South Florida, Department of Chemistry).
- 16) University of South Florida, Interdisciplinary Research Development Grant: Development of Novel Antiviral Compounds Against Influenza. \$19,994 direct costs (no indirect costs allowed); (\$6,372 Manetsch direct costs), 02/01/2006 – 01/31/2007. PI Alberto van Olphen (University of South Florida, Center for Biological Defense); CIs **Roman Manetsch** and Edwin Rivera (University of South Florida, Department of Chemistry).
- 17) American Cancer Society Institutional Grant Program, Cycle 20, Fall 2005: Bcl-xL-Templated Assembly of Compounds Modulating Bcl-xL. \$20,000 direct costs (no indirect costs allowed), 04/01/2006 – 03/31/2007. PI **Roman Manetsch**.

## TEACHING AND TRAINING ACTIVITIES

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### Courses (NEU)

- 1) *CHM2315 Organic Chemistry 1: Chemistry Majors*: Fall 2015
- 2) *CHM5626 Organic Synthesis*: Fall 2016, Fall 2017, Fall 2018.
- 3) *PHSC5400 Principles of Drug Design*: Fall 2016, Fall 2017, Fall 2018.
- 4) *CHEM5676 Bioorganic Chemistry (1 lecture)*: Spring 2016, Spring 2017, Spring 2018, Spring 2019.
- 5) *PHSC5360 Anti-Infectives* (course coordination): Summer 2018, Summer 2019

### Courses (USF)

- 1) CHM2210 *Organic Chemistry I*: Spring 2007, Spring 2008, Fall 2008, Spring 2009, Fall 2009, Spring 2010, Spring 2011, Spring 2014 (undergraduate level course).
- 2) CHM2211 *Organic Chemistry II*: Spring 2012 (undergraduate level course).
- 3) CHM6250/5225 *Advanced Organic Chemistry I*: Fall 2005, Fall 2006, Fall 2007, Fall 2013 (dual listed graduate and undergraduate level course).
- 4) CHM6935 *Graduate Seminar*: Fall 2006, Spring 2007, Fall 2007, Spring 2008, Fall 2008, Spring 2009, Fall 2009, Spring 2010, Fall 2010, Spring 2011, Fall 2011, Spring 2012 (coordinating CHM6935 Graduate Seminar program).
- 5) CHM6938/4932 *Spectroscopy*: Fall 2010, Fall 2011 (dual listed graduate and undergraduate level course).
- 6) CHM6938/PHC7931 *Drug Discovery for Tropical Diseases*: Spring 2010, Spring 2012, Spring 2014 (graduate level course).

### Postdoctoral Associates

- 1) Dr. Chungsik Kim (09/2016 – present)
- 2) Dr. Prakash Parvatkar (09/2016 – 08/2018)
- 3) Dr. Abdul Shaikh (09/2015 – 08/2017)
- 4) Dr. Fabian Brockmeyer (06/2015 – 05/2017)
- 5) Dr. Yana Sakhno, 06/2012 - 08/2013
- 6) Dr. Raghupathi Neelarapu, 05/2012 - 07/2014
- 7) Dr. Nirranjan Namelikonda, 05/2009 - 09/2014
- 8) Dr. David Flanigan, 04/2009 - 10/2014
- 9) Dr. Yijun Yiang, 09/2009 - 12/2010
- 10) Dr. Xiangdong Hu, 09/2006 - 04/2009

### Thesis and Dissertation Research Supervision

- 1) Lili Huang (Chemistry and Chemical Biology), 2019 - present, Ph.D. candidate
- 2) Ami Asakawa (Pharmaceutical Sciences), 2019 - present, Ph.D. candidate
- 3) Brandon Miller (Chemistry and Chemical Biology), 2019 - present, Ph.D. candidate
- 4) Mintesinot Kassu (Chemistry and Chemical Biology), 2018 - present, Ph.D. candidate
- 5) Jackson Cacioppo (Chemistry and Chemical Biology), 2017 - present, M.S. candidate, graduation expected Spring 2019
- 6) Matthew Dowgiallo (Chemistry and Chemical Biology), 2016 - present, Ph.D. candidate, graduation expected Fall 2019
- 7) Yingzhao (David) Zhao (Chemistry and Chemical Biology), 2015 - present, Ph.D. candidate, graduation expected Spring 2020
- 8) Iredia D. Iyamu (Chemistry and Chemical Biology), 2010 - 2016, *Design, Synthesis and Evaluation of Spirocyclic Chromanes, Dihydropyridines, and Naphtoquinones as Antimalarial Agents*, Ph.D. from NEU
- 9) Cynthia Lichorowic (Chemistry and Chemical Biology), 2010 - 2016, *Studies on Antimalarial Activity, Physicochemical Properties and Mechanism of Action of 4(1H)-quinolones and Artemisinin*, Ph.D. from NEU
- 10) Megan Barber, 2012 - 2015. *2,4-Disubstituted Quinazolines with Antileishmanial or Antibacterial Activity*, M.S. from USF
- 11) Jordany R. Maignan, 2009 – 2015, *Development of Orally Bioavailable 4(1H)-Quinolones and 1,2,3,4-Tetrahydroacridin-9(10H)-ones with Potent Antimalarial Activity*, Ph.D. from USF
- 12) Andrii Monastyrskiy, 2008 - 2014, *Synthesis and Evaluation of 3-Aryl-4(1H)-Quinolones as Orally Active Antimalarials: Overcoming Challenges in Solubility, Metabolism, and Bioavailability*, Ph.D. from USF
- 13) Kurt Van Horn, 2007 - 2013, *Anti-Parasitic and Anti-Bacterial Agents: Studies on 1,4-Dihydropyridines and 2,4-Diaminoquinazolines*, Ph.D. from USF
- 14) Katya Nacheva, 2007 - 2012, *Design and Synthesis of a Molecular Fluorescent Probe and its Role of Kinetic Target-Guided Synthesis to Identify Inhibitors of Enzymatic and Protein-Protein Interaction Targets*, Ph.D. from USF
- 15) Sameer S. Kulkarni, 2006 - 2012, *Development and Optimization of Kinetic Target-Guided Synthesis Approaches Targeting Protein-Protein Interactions of the Bcl-2 Family*, Ph.D. from USF
- 16) Arun B. Kumar, 2006 - 2012, *Design, Synthesis and Evaluation of Novel Diazirine Photolabels with Improved*

*Ambient Light Stability and Fluorous-Based Enrichment Capacity*, Ph.D. from USF

- 17) Shikha Mahajan, 2006 - 2012, *Protein Profiling of Adenine Nucleoside and Nucleotide Analogs Binding Proteins Using N<sup>6</sup>-Biotinylated-8-azidoadenosine Analogs as Affinity Based Protein Profiling Probes*, Ph.D. from USF (primary advisor David Merkler, Co-advisor Roman Manetsch)
- 18) R. Matthew Cross, 2005 - 2011, *Lead Discovery and Optimization Strategies Towards the Development of 4(1H)-Quinolone and 1,2,3,4-Tetrahydroacridone Analogs with Antimalarial Activity*, Ph.D. from USF
- 19) Lisa Malmgren, 2005 - 2007, *Using in Situ Click Chemistry to Modulate Protein-Protein Interactions: Bcl-xL as a Case Study*, M.S. from USF

### **Undergraduate Research**

- 1) Loren Po, January 2019 – present
- 2) Andrew Fetigan, January 2016 - present
- 3) Liu Li, January 2016 - August 2016
- 4) Imran Sharif Elmaarouf, February 2016 - present
- 5) Grace Kiser, February 2018 - December 2018
- 6) Daniel Assad Saad September 2017-December 2018
- 7) Michael Shultis, February 2015 - December 2016
- 8) Jackson Goodman Cacioppo, July 2016 - December 2016
- 9) Susan Anne Roberts, August 2016 - December 2016
- 10) Tanner C Jenkins, October 2016 - December 2016
- 11) Madeline L MacDonnell, January 18, 2016 - March 2016
- 12) Jake Ganley, January 2016 - June 2017
- 13) Lisa Barton, January 2015 - April 2016
- 14) Lauren Bertino, January 2016 - March 2016
- 15) Danielle Lefebvre, February 2016 - April 2016
- 16) Clarissa Santori, August 2016 - December 2017
- 17) Fabiola Caban (REU student), summer 2016
- 18) James Giarrusso, 2011 - 2013, BS in Chemistry in 2012
- 19) Niles Gunsalus, 2010 - 2012, BS in Chemistry in 2012
- 20) Lisa Luong, 2009 - 2011, BS in Biomedical Sciences in 2011
- 21) Jordan Anderson, 2008 - 2011, BS in Chemistry in 2011
- 22) Mario Martinez, 2007 - 2009, BS in Chemistry in 2009

### **Honors Undergraduate Thesis**

- 1) Alexandra Griffin, 2010 - 2011, BS in Biomedical Sciences in 2011
- 2) Lisa Luong, 2010 - 2011, BS in Biomedical Sciences in 2011
- 3) Jordan Anderson, 2010 - 2011, BS in Chemistry in 2011
- 4) Mario Martinez, 2008 - 2009, BS in Chemistry in 2009

### **Doctoral Committee Service** (students that are not members of the Manetsch laboratory).

- 1) Dana Klug, Chemistry and Chemical Biology
- 2) Andrew Spaulding, Chemistry and Chemical Biology
- 3) Debarpita Ray, Chemistry and Chemical Biology
- 4) John de la Parra, Chemistry and Chemical Biology
- 5) Daniel Donnelly, Chemistry and Chemical Biology
- 6) Westley Tear, Chemistry and Chemical Biology
- 7) Kelly Bachovchin, Chemistry and Chemical Biology
- 8) Othman Benchama, Pharmaceutical Sciences
- 9) Peter Schaffer, Pharmaceutical Sciences
- 10) Lucas Cantwell, Pharmaceutical Sciences
- 11) Austen Casey, Pharmaceutical Sciences
- 12) Dimitris Gazgalis, Pharmaceutical Sciences
- 13) Brenda Winn, Pharmaceutical Sciences

### **External examiner**

- 1) External examiner of Ph.D. theses: Peter Mubanga Cheuka, Department of Chemistry, University of Cape Town, South Africa (2018); Leon Jacobs, Stellenbosch University, South Africa (2018).
- 2) External examiner of M.S. thesis: Pieter Cilliers, Department of Pharmacy, North-West University, South Africa (2018).

### **SERVICE**

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#### **Service to the Department of Chemistry and Chemical Biology, Northeastern University**

- 1) Safety Officer of the Department of Chemistry and Chemical Biology (2016 – present)
- 2) Executive Committee of the Department of Chemistry and Chemical Biology (2016 – present)
- 3) Student Recruiting/Admissions Committee of Chemistry and Chemical Biology (2015, and 2017 – present)
- 4) Committee for (Bio)Analytical Chemistry faculty search. Faculty search ended successfully with the hire of Dr. Leila Deravi (2015)

#### **Service to the Department of Pharmaceutical Sciences, Northeastern University**

- 1) Student Recruiting/Admissions Committee of Pharmaceutical Sciences (2016 – present)
- 2) Instrumentation Committee of Pharmaceutical Sciences (2016-2017)
- 3) Committee for Natural Product Chemistry faculty search (joint search with Chemistry and Chemical Biology) (2015 and 2016)

#### **Service to Northeastern University**

- 1) NEU's Laboratory Safety Hygiene Committee (2016 – present)

#### **Service to the Discipline**

- 1) Reviewer of scientific manuscripts: ACS Chemical Biology, ACS Infectious Diseases, ACS Medicinal Chemistry Letters, Angewandte Chemie International Edition, Antimicrobial Agents and Chemotherapy, Bioorganic and Medicinal Chemistry, Bioorganic and Medicinal Chemistry Letters, ChemBioChem, Chemical Biology and Drug Design, Chemical Science, Chemical Reviews, Chemistry – An Asian Journal, Chemistry – A European Journal, ChemMedChem, Drug Discovery Today, European Journal of Medicinal Chemistry, European Journal of Organic Chemistry, Helvetica Chimica Acta, Heterocyclic Communications, Journal of the American Chemical Society, Journal of Computer-Aided Molecular Design, Journal of Natural Products, Journal of Organic Chemistry, Journal of Medicinal Chemistry, Medicinal Research Reviews, Nature Chemistry, Organic and Biomolecular Chemistry, Organic Letters, Proceedings of the National Academy of Sciences, RSC Advances.
- 2) Reviewer National Institutes of Health: NIH/ZRG1 IDM-T (82) R21s and R03s (October 2014); NIH/ZRG1 IDM-T (82) R21s and R03s (March 2015); NIH/DDR RO1s (June 2015); NIH/SBCA R01s, R03s, R15s, and R21s (June 2017); NIH/ZAI1 LG-M (J2) Special Emphasis Panel RFA AI-17-042, Centers of Excellence for Translational Research (U19).
- 3) Reviewer Department of Defense: Peer Review Medical Research Program (PRMRP) Preapplications – Malaria (July 2014); PRMRP Applications – Malaria (December 2014); PRMRP Preapplications – Malaria (June 2015); PRMRP Preapplications – Malaria (July 2016); Military Infectious Diseases Research Program (MIDRP) panel on antiparasitic drugs (February 2017); PRMRP Preapplications – Malaria (July 2018); MIDRP panel on antiparasitic drugs (February 2019).
- 4) Reviewer grant applications for the Dutch Product Development Partnership III Fund (2015).
- 5) Reviewer grant applications for King Abdulaziz City for Science and Technology (KACST); review organized by the American Association for the Advancement of Science (AAAS) (2018).
- 6) Reviewer grant applications for Dana-Farber Cancer Institute/Northeastern University, Joint Program in Cancer Drug Development (2015).