

ROMAN MANETSCH - CV

Professor, Department of Chemistry and Chemical Biology and Department of Pharmaceutical Sciences, and Faculty Fellow, Center for Drug Discovery and Barnett Institute for Chemical and Biological Analysis; Northeastern University, 102 Hurlig Hall, 360 Huntington Avenue, Boston, MA 02115 (USA);
ORCID: 0000-0001-7038-6867; Email: r.manetsch@northeastern.edu; webpage: www.manetschlab.com

EDUCATION, EMPLOYMENT HISTORY, AND RESEARCH INTERESTS

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 β -Carotin 15,15'-Dioxygenase (Synthesis of Potential Inhibitors of the Enzyme β -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 (Research on catalytic antibodies was conducted in collaboration with the laboratory of Professor Jean-Louis Reymond, Department of Chemistry and Biochemistry at the University of Bern, Switzerland). Thesis: *Transition-State-Analogue 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 (USF), Tampa (FL)
- 08/2011 - 08/2014 Associate Professor, Department of Chemistry, College of Arts and Science, University of South Florida (USF), Tampa (FL)
- 12/2012 - 10/2013 Sabbatical Researcher, Center for Proteomic Research, Novartis Pharma AG, Basel, Switzerland
- 09/2014 – 06/2023 Associate Professor, Department of Chemistry and Chemical Biology, College of Science, and Department of Pharmaceutical Sciences, Bouvé College of Health Sciences, Northeastern University (NEU), Boston (MA)
- 07/2023 – present Professor, Department of Chemistry and Chemical Biology, College of Science, and Department of Pharmaceutical Sciences, Bouvé College of Health Sciences; Faculty Fellow, Center for Drug Discovery, and Faculty Fellow, Barnett Institute for Chemical and Biological Analysis, Northeastern University (NEU), Boston (MA)

Overarching Research Interests

The Manetsch group focuses on conducting medicinal chemistry research aimed at addressing unmet health needs (anti-malarials, anti-biotics, drug resistance, others). The laboratory leverages expertise in organic, analytical, and medicinal chemistry for impactful collaborative research. Research endeavors serve as valuable training opportunities for students interested in pursuing a career in organic and pharmaceutical chemistry.

Research Summary

The research interests of the Manetsch laboratory center on organic, bioorganic, and click chemistry addressing both fundamental principles and diverse applications within the field of medicinal chemistry, with a specific emphasis on anti-infectives. Additionally, the laboratory explores the development of chemical probes tailored for studying specific proteins in complex biological matrices.

The Manetsch laboratory developed kinetic target-guided synthesis (KTGS), a fragment-based lead discovery strategy, using synthetic chemistry in close conjunction with liquid chromatography and mass spectrometry detection (LC-MS and LC-MS/MS), to target protein-protein interactions associated with apoptosis. KTGS involves the biological target participating in the irreversible assembly of its own inhibitory bidentate ligand from a pool of complementary reactive fragment series. This LC-MS-based approach is currently applied for the discovery of inhibitors or probe molecules to treat or detect malaria, amoebic, or bacterial infections.

The Manetsch laboratory is also interested in synthetic chemistry for the preparation of anti-infective natural products. The anti-biotic streptothricin scaffold has been overlooked by the synthetic chemistry community until now. The Manetsch laboratory developed a convergent, diversity-enabling total synthesis of the natural product streptothricin F, which opens up new avenues for medicinal chemistry exploration. Key transformations of the synthetic approach include a Burgess reagent-mediated 1,2-anti-diamine installation, a diastereoselective azidation of a lactam enolate, and a Lewis acid-mediated desulfurization-guanidination. The recently disclosed synthesis represents the second total synthesis of streptothricin F, and the first through a diversity-enabling convergent route (35 total steps, with the longest linear sequence of 19 steps, and 0.40% overall yield for streptothricin F). With this synthetic approach, the Manetsch laboratory has converted the natural product streptothricin F into a promising antibiotic scaffold, poised for further optimization. Accordingly, the Manetsch laboratory is pursuing medicinal chemistry-guided analog generation of streptothricin F to explore streptothricin analogs for potential therapeutic uses and for structural biology investigations using cryogenic electron microscopy (cryo-EM).

Synthetic routes also enable the preparation of compound libraries for detailed structure-activity and structure-property relationship studies (SAR and SPR, respectively). The Manetsch laboratory implemented LC-MS-based physicochemical property profiling and pharmacokinetics to determine and optimize the bioavailability of small molecules. Using this hit-to-lead progression strategy, *in vivo* efficacious anti-malarial and anti-bacterial (Gram-positive and/or Gram-negative) agents have been developed. For example, for nearly half a century, 4(1*H*)-quinolones endochin, ICI56,780, and WR243246 were recognized for their causal prophylactic and potent erythrocytic stage activity in avian models, yet their efficacy in mammalian models remained unestablished. In close collaboration with parasitology and pharmacology colleagues, our hit-to-lead optimization efforts led to 4(1*H*)-quinolones P4Q-391 and ELQ-300 displaying exceptional *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.

Finally, the Manetsch laboratory developed photoactivatable probes as well as cyclic thiosulfonates to covalently label specific proteins in complex mixtures or entire proteomes. We are currently investigating whether the efficacy, low toxicity, and pharmacodynamics of crosslinker-mediated SOD1 stabilization make cyclic thiosulfonates a promising therapeutic approach for SOD1-related familial amyotrophic lateral sclerosis (fALS).

Honors and Awards

- 2002 Ph.D. Summa Cum Laude, University of Basel
- 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

PUBLICATIONS, BOOK CHAPTERS, AND PATENTS

Peer Reviewed Publications

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

- 67) Kassu, M; Zulauf, K E; Ross, J N; Kirby, J E; Manetsch, R*. Development of CGS-15943 Adjunctives for the Disruption of Plasmid Maintenance in Multidrug Resistant *E. coli*. *ACS Infect Dis* **2025**; 11, 80-87.
- 66) Huang, L; Kim, T; Armendarez, O J; Deravi, L F; Parvatkar, P T*; Manetsch, R*. Efficient Biomimetic Total Synthesis, Characterization, and Antioxidant Activity of Ommatins. *JACS Au* **2024**; 4, 4307-4316.
- 65) Van Horn, K S; Zhao Y; Parvatkar PT; Maier J; Mutka T; Lacrue, A N; Brockmeier F; Ebert, D; Wu, W; Casandra, D R; Namelikonda, N; Yacoub, J; Sigal, M; Knapp, S; Floyd, D; Waterson, D; Burrows, J N; Duffy, J; DeRisi, J L; Kyle, D E; Guy, R K; Manetsch, R*. Optimization of Asymmetric Dihydropyridines as Antimalarials. Manuscript Optimization of diastereomeric dihydropyridines as antimalarials. *Eur J Med Chem* **2024**; 275, 116599.

- 64) Parvatkar, P T; Diagne, K; Zhao, Y; Manetsch, R*. Indoloquinoline Alkaloids as Antimalarials: Advances, Challenges, and Opportunities. *ChemMedChem* **2024**; 19(18):e202400254.
- 63) Huang, L; Parvatkar, P T; Wagner, A; Kulkarni, S S; Manetsch, R*. Chemoselective seleno-click amidation in kinetic target-guided synthesis. *Chem Commun* **2024**; 60, 12722-12725.
- 62) Hossain, M A; Sarin, R; Donnelly, D P; Miller, B C; Weiss, A; McAlary, L; Antonyuk, S V; Salisbury, J P; Amin, J; Conway, J B; Watson, S S; Winters, J N; Xu, Y; Alam, N; Brahme, R R; Shahbazian, H; Sivasankar, D; Padmakumar, S; Sattarova, A; Ponmudiyan, A C; Gawde, T; Verrill, D E; Yang, W; Kannapadi, S; Plant, L D; Auclair, J R; Makowski, L; Petsko, G A; Ringe, D; Agar, N Y R; Greenblatt, D J; Ondrechen, M J; Chen, Y; Yerbury J J; Manetsch, R; Hasnain, S S; Brown, R H Jr; Agar, J N*. Evaluating protein cross-linking as a therapeutic strategy to stabilize SOD1 variants in a mouse model of familial ALS. *PLoS Biol.* **2024**; 22(1):e3002462.
- 61) Parvatkar, P T; Manetsch, R; The emergence of sulfo-click amidation in kinetic target-guided synthesis. *Med Chem Res* **2024**; 33, 1307–1314.
- 60) Parvatkar, P T; Maher, S P; Zhao, Y; Cooper, C A; de Castro, S T; Péneau, J; Vantaux, A; Witkowski, B; Kyle, D E; Manetsch, R*. *In vitro* Antimalarial Activity of Trichothecenes Against Liver and Blood Stages of *Plasmodium* Species. *J Nat Prod* **2024**; 87, 315-321.
- 59) Kassu, M; Parvatkar, P; Milanes, J; Monaghan, N P; Kim, C; Dowgiallo, M; Zhao, Y; Asakawa, A; Huang, L; Wagner, A; Miller, B; Carter, K; Barrett K F; Tillery L M; Barrett L K; Phan I Q; Subramanian S; Myler, P J; Van Voorhis, W C; Leahy, J W; Rice, C A; Kyle, D E; James Morris, J; Manetsch, R*. Shotgun Kinetic Target-Guided Synthesis Approach Enables the Discovery of Small Molecule Inhibitors against Pathogenic Free-Living Amoeba Glucokinases. *ACS Infect Dis* **2023**; 11, 2190-2201.
- 58) Parvatkar, P*; Wagner, A; Manetsch, R*: Biocompatible Reactions: Advances in Kinetic Target-Guided Synthesis (Review). *Trends Chem* **2023**; 9, 657-671.
- 57) Di Marco, C N*; Terrell, L; Sanchez, R; Rueda, L; Shuster, L; Nartey, E N; McHugh, C; Mack, J F; Shu, A; Tian, X; Medina, J R; Rivero, R; Manetsch, R; Heerding, D; Mangatt, B. Design and synthesis of aminopyridine containing biaryls reducing c-MYC protein levels in cells. *Bioorg Med Chem Lett* **2023**; 92, 129385.
- 56) Morgan, C E; Kang, Y S; Green, A B; Smith, K P; Dowgiallo, M G; Miller, B C; Chiaraviglio, L; Truelson, K A; Zulauf, K E; Rodriguez, S; Kang, A D; Manetsch, R; Yu, E W; Kirby, J E*. Streptothricin F is a bactericidal antibiotic effective against highly drug-resistant gram-negative bacteria that interacts with the 30S subunit of the 70S ribosome. *PLoS Biol* **2023**; 21(5): e3002091.
- 55) Nacheva, K; Kulkarni, S S; Kassu, M; Flanigan, D; Monastyrskiy, A; Iyamu, I D; Doi, K; Barber, M; Namelikonda, N; Tipton, J D; Parvatkar, P; Wang, H G; Manetsch, R*. Going beyond Binary: Rapid Identification of Protein-Protein Interaction Modulators Using a Multifragment Kinetic Target-Guided Synthesis Approach. *J Med Chem* **2023**; 66, 5196-5207.
- 54) Dowgiallo, M; Miller, B; Kassu, M; Smith, KP; Fetigan, A; Guo, J; Kirby, J; Manetsch, R*. The convergent total synthesis of streptothricin F. *Chem Sci* **2022**; 13, 3447-3453.
- 53) Iyamu, I D; Zhao Y; Parvatkar P T; Roberts B F; Casandra D R; Wojtas L; Kyle D E; Chakrabarti D; Manetsch R*. Structure-activity and structure-property relationship studies of spirocyclic chromanes with antimalarial activity. *Bioorg Med Chem* **2022**; 57, 116629.
- 52) Maher S P; Vantaux A; Cooper C A; Chasen N M; Cheng W T; Joyner C J; Manetsch R; Witkowski B; Kyle D*. A phenotypic screen for the liver stages of *Plasmodium vivax*. *Bio Protoc* **2021**; 11, e4253.
- 51) Parvatkar, P T; Smotkin, E S; Manetsch, R*. Total Synthesis of (±)-Decursivine via BINOL-Phosphoric Acid Catalyzed Tandem Oxidative Cyclization. *Sci Rep* **2021**; 11, 19915.
- 50) Kim, C; Kassu, M; Smith, KP; Kirby, JE; Manetsch, R*. Pyrazole-Thiazole Core-Containing Analogs Exhibit Adjunctive Activity with Meropenem against Carbapenem-Resistant Enterobacteriaceae (CRE). *ChemMedChem* **2021**; 16, 2775–2780.
- 49) 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(1H)-Quinolones with Single Dose Cures. *J Med Chem* **2021**; 64, 6581–6595.
- 48) Lichorowic, C L; Zhao, Y; Maher, S P; Padín-Irizarry, V; Mendiola, V C; de Castro, S T; Worden, J A; Casandra D; Kyle, D E; Manetsch R*. Synthesis of Mono- and Bis-peroxide-bridged Artemisinin Dimers to Elucidate the Contribution of Dimerization to Antimalarial Activity. *ACS Infect Dis* **2021**; 7, 2013–2024.

- 47) Aluri, K C; Hossain, M A; Kanetkar, N; Miller, B C; Dowgiallo, M G; Sivasankar, D; Sullivan, M R; Manetsch, R; Konry, T; Ekenseair, A; Agar*, J N. Cyclic thiosulfonates as a novel class of disulfide cleavable cross-linkers for rapid hydrogel synthesis. *Bioconjugate Chemistry* **2021**; 32, 584–594.
- 46) Tillery, L; Barrett, K; Goldstein, J; Lassner, J W; Osterhout, B; Tran, N L; Xu, L; Young, R M; Craig, J; Chung, I; Dranow, D M; Abendroth, J; Delker, S L; Davies, D R; Mayclin, S J; Clahoun, B; Bolejack, M J; Staker, B; Subramanian, S; Phan, I; Lorimer, D D; Myler, P J; Edwards, T E; Kyle, D E; Rice, C A; Morris, J C; Leahy, J W; Manetsch R; Barett; L K, Smith, C L; Van Voorhis, W C*. Naegleria fowleri: protein structures to facilitate drug discovery for the deadly, pathogenic free-living amoeba. *PLoS One* **2021**; 16(3): e0241738.
- 45) Krohn-Brennan, T; Manetsch, R; O'Doherty, G A; Kirby J E*. New Strategies and Structural Considerations in Development of Therapeutics for Carbapenem-Resistant Enterobacteriaceae: New Therapies for CRE. *Transl Res* **2020**; 220, 14–32.
- 44) 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. *SLAS Discov* **2019**; 24, 842–853.
- 43) Parvatkar, P T*; Manetsch R*; Banik, B K*. Metal-Free Cross-Dehydrogenative Coupling (CDC): Molecular Iodine as a Versatile Catalyst/Reagent for CDC Reaction (Review). *Chemistry. Chem Asian J* **2019**; 14, 6–30.
- 42) 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.
- 41) Neelapapu, R; Maignan, J R; Lichorowic, C L; Monastyrskyi, 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(1H)-quinolones with potent antimalarial activity: structure–activity and structure–property relationship studies. *J Med Chem* **2018**; 61, 1450–1473.
- 40) Kumar, A B; Manetsch, R*. Ammonia-free Synthesis of 3-Trifluoromethyl-3-Phenyl-diaziridine. *Synth Commun* **2018**; 48, 626–631.
- 39) McQueen, A; Blake, L D; Azhari, A; Kemp, M T; McGaha, T W Jr; Namelikonda, N; Larsen, R W; Manetsch, R; Kyle, D E*. Synthesis, Characterization, and Cellular Localization of a Fluorescent Probe of the Antimalarial 8-Aminoquinoline Primaquine. *Bioorg Med Chem* **2017**; 27, 4597–4600.
- 38) Namelikonda, N K; Monastyrskyi, A; Manetsch, R*. Scalable Multigram Syntheses of Antimalarial 4(1H)-Quinolones ELQ-300 and P4Q-391. *Eur J Org Chem* **2017**; 23, 3328–3334.
- 37) Blake, L D; Johnson, M E; Siegel, S V; McQueen, A; Iyamu, I D; Shaikh, A K; Shultis, M W; Manetsch, R; Kyle, D E*. Menoctone Resistance in Malaria Parasites is Conferred by M133I Mutations in Cytochrome b that are Transmissible Through Mosquitoes. *Antimicrob Agents Chemother* **2017**; 61, AAC.00059-17. E00689-17/13.
- 36) Brockmeyer, F; Manetsch, R*. Progress in the Optimization of 4(1H)-Quinolone Derivatives as Antimalarials Targeting the Erythrocytic, the Exoerythrocytic and the Transmitting Stages of the Parasite (Review). *Chimia* **2017**; 71, 213–219.
- 35) Fleeman R, Van Horn K S, Barber M M, Burda W N, Flanagan D L, Manetsch R*, Shaw L N*. Characterizing the Antimicrobial Activity of N²,N⁴-Disubstituted Quinazoline-2,4-Diamines Towards Multidrug Resistant *Acinetobacter baumannii*. *Antimicrob Agents Chemother* **2017**; AAC.00059-17.
- 34) 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(1H)-quinolones with Antimalarial Activity. *J Med Chem* **2016**; 59, 6943–6960.
- 33) 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.
- 32) Kumar A B, Tipton J D, Manetsch R*. 3-Trifluoromethyl-3-aryldiazirine Photolabels with Enhanced Ambient Light Stability. *Chem Commun* **2016**; 52, 2729–2732.
- 31) Zhu X, Van Horn K S, Barber M M, Yang S, Wang M Z, Manetsch R, Werbovetz K A*. SAR Refinement of Antileishmanial N²,N⁴-Disubstituted Quinazoline-2,4-diamines. *Bioorg Med Chem* **2015**; 23, 5182–5189.
- 30) 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.

- 29) 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* **2015**; 80, 2513–25020
- 28) Cross R M, Flanigan D L, Monastyrskiy A, LaCrue A N, Saenz F E, Maignan J R, Mutka T S, White K L, Shackleford 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.
- 27) 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.
- 26) 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 Dis* **2014**; 84, 158–168.
- 25) 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*²,*N*⁴-disubstituted quinazoline-2,4-diamines. *J Med Chem* **2014**; 57, 5141–5156; [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].
- 24) 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*²,*N*⁴-Disubstituted Quinazoline-2,4-diamines. *J Med Chem* **2014**; 57, 3075–3093.
- 22) 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, 6187–6195.
- 21) 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.
- 20) Nilsen A, LaCrue A, White K. L , Forquer I P, Cross R M, Marfurt J, Mather M W, Delves M J, Shackleford D M, Sáenz F E, Morrissey 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.
- 19) Kulkarni S S, Hu X, Manetsch R*. A Simple Base-mediated Amidation of Aldehydes with Azides. *Chem Commun* **2013**; 49, 1193–1195.
- 18) 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.
- 17) 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.
- 16) 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.
- 15) 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.
- 14) Kumar A B, Anderson J M, Manetsch, R*. Design, Synthesis and Photoactivation Studies of Fluorous Photolabels. *Org Biomol Chem* **2011**; 9, 6284–6292.
- 13) 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.

- 12) 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.
- 11) Cross R M, Manetsch R*. Divergent Route to Access Structurally Diverse 4(1*H*)-Quinolones via Mono or Sequential Cross-Couplings. *J Org Chem* **2010**; 75, 8654–8657.
- 10) Cross M R, Monastyrskyi 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.
- 9) Hu X, Manetsch R*, Kinetic Target-Guided Synthesis (Review). *Chem Soc Rev* **2010**, 39, 1316–1324.
- 8) Hu X, Sun J, Wang H-G, Manetsch R*. Bcl-X_L-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.
- 7) 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.
- 6) 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.
-----Publications Prior Independent Career at the University of South Florida-----
- 5) 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.
- 4) 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.
- 3) 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.
- 2) 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.
- 1) 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 "A Comprehensive Review of 4(1*H*)-Quinolones and 4(1*H*)-Pyridines for the Development of an Effective Antimalarial" in *Plasmodium* Species and Drug Resistance by Ami H. Asakawa and Roman Manetsch, IntechOpen, **2021**.
- 2) Book chapter on "3',5'-Dimethoxybenzoic acid" in *e-EROS Encycl. Reagents Org. Synth.* by R. Matthew Cross and Roman Manetsch, Wiley, **2009**.

Patents

- 20) Manetsch R.; Parvatkar, P. T.; Huang, L.; Chiaraviglio, L.; Kirby, J. E.; Maher, S. P.; Kyle, D. E.; Hussain, A.; Deravi, L.; Kim, T.; Armendarez, O. Scalable Total Synthesis of Ommatins and their Application in Photocatalysis and Photodynamic Therapies. Provisional Patent Application Number: 63/684,151. **2024**.
- 19) Wagner, A. N., Trombley, R., Podgurski, M. E., Smith, J. R., Cui, M., Marin, A. A., Ruberto, A., Maher, S. P., Kyle, D. E., Manetsch, R. Plasmodium *falciparum* Formate-Nitrite Transporter (PfFNT) Inhibitors. Provisional Patent Application Number: 63/507,757. **2023**.
- 18) Kyle, D E; Maher, S; Asakawa, A H; Diagne, K D; Manetsch, R; Marin, A A; Marasciullo, A; Consoli, C E; De Castro, S T; McWhorter, O I; Cui, M. Tetrahydroacridinone Analogues for Treatment and Prevention of Malaria. Provisional Patent Application Number: 63/507,750. **2023**.
- 17) Manetsch R, Ferreira G C, Stojanovski B M, Nacjewa K P. 5-aminolevulinate synthase inhibitors and methods of use thereof. US11,479,532, **2022**.
- 16) 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. US10,551,389B2, **2020**.
- 15) Manetsch R, Van Horn K S, Burda W N, Shaw L N, Fleeman R, Barber M, Flanigan D L. N²,N⁴-Disubstituted quinazoline-2,4-diamines and uses thereof. US10,323,007B1, **2019**.

- 14) Manetsch R, Shaw L N, Van Horn K S, Burda W N. Compositions, methods of use, and methods of treatment. US10,081,607B2, **2018**.
- 13) Manetsch R, Kumar A B, Tipton J. Photoactivatable probes and uses thereof. US10,067,136B1, **2018**.
- 12) Manetsch R, Kyle D E, Raghupathi N, Maignan J R, Lichorowic C L, LaCrue A N. Quinolone-based compounds, formulations, and uses thereof. US10,000,452B1, **2018**.
- 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. US9206131B2, **2015**.
- 10) Manetsch R, Shaw L N, Van Horn K S, Burda W N. Compositions, methods of use, and methods of treatment. US8,906,918B1, **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. US8,877,752B2, **2014**.
- 8) 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. US20140045,888A1, **2014**.
- 7) 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. US8,598,354B2, **2013**.
- 6) Wang HG, Manetsch R, HuX, Kulkarni S S, Sun J. Acylsulfonamides and processes for producing the same. US8,524,947B2, **2013**.
- 5) 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. US20,120,115,904A1, **2012**.
- 4) 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**.
- 3) 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**.
- 2) 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**.
- 1) 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**.

SELECTED RESEARCH ACTIVITIES

Selected Talks and Conferences

- Discovery and Synthesis of Anti-bacterials and Anti-malarials. Department Of Chemistry, University of New Haven, October 27, 2023.
- The Antimicrobial Activity of Streptothricins and the Convergent Synthesis of Streptothricin F. Boston Area Antimicrobial Resistance Network Meeting. December 2, 2022.
- Transforming Bricklike 4(1*H*)-Quinolones into Orally Bioavailable Antimalarials Targeting Liver, Blood, and Transmitting Stages of the Parasite. Global Conference on Pharmacy and Pharmaceutical Sciences. Virtual, November 15, 2021.
- Unconventional Selection and Optimization Approaches to Find the Right One. Department Of Chemistry, Georgia State University. Atlanta, GA, United States. September 24, 2021.
- Transforming Bricklike 4(1*H*)-Quinolones into Orally Bioavailable Antimalarials Targeting Liver, Blood, and Transmitting Stages of the Parasite. Pharmaceutical Research and Drug Development. Virtual, September 20 - 22, 2021.
- A Divergent Total Synthesis of Streptothricin F. 3rd International Conference on PharmaScience Research and Development. Virtual, February 22 - 24, 2021.
- Mass Spectrometry-Guided Synthesis for the Discovery and Development of Anti-Malarial Agents. Institut for Kemi, Danmarks Tekniske Universitet. Lyngby, Denmark, October 30, 2019.

- Kinetic target-guided synthesis to discover new Leads for *N. fowleri*. Amoeba Science Meeting. Orlando, FL, United States, September 14, 2019.
- Mass Spectrometry-Guided Discovery and Development of Anti-Malarial Agents. Departamento de Química en Ciencias Farmacéuticas, Universidad Complutense de Madrid. Madrid, Spain, July 9, 2019.
- Kinetic Target-guided Synthesis: Mass Spectrometry-driven Medicinal Chemistry Targeting Protein-Protein Interactions. 2018 Southeastern Chemical Biology Symposium. Athens, GA, United States, April 21, 2018.
- Orally Bioavailable Antimalarial 4(1*H*)-Quinolone and 4(1*H*)-Quinolone Prodrugs with Single-Dose Cures. International Pharma Conference and Expo. Rome, Italy, May 2-4, 2018.
- Kinetic Target-guided Synthesis: a MS-based Fragment Evolution Platform. International Pharma Conference and Expo. Rome, Italy, May 2 - 4, 2018.
- Mass Spectrometry-guided Medicinal Chemistry Targeting Malaria and Cancer. Chemistry Department, University of Massachusetts Boston. Boston, MA, United States, September 27, 2017.
- Mass Spectrometry-Driven Medicinal Chemistry Targeting Malaria and Cancer. Chemistry and Biochemistry Department, University of Massachusetts Dartmouth. Dartmouth, MA, United States, February 11, 2016.
- Kinetic Target-Guided Synthesis: A Fragment Evolution Strategy Based on Bioorthogonal Reactions. Fragment-based Lead Discovery Conference 2014. Basel, Switzerland, September 21-24, 2014.
- Mass Spectrometry-Guided Approaches for Synthetic and Medicinal Chemistry. Pharmaceutical Sciences, University of Nebraska Medical Center. Omaha, NE, United States, March 12, 2014.
- Mass Spectrometry-Guided Approaches for Synthetic and Medicinal Chemistry. Department of Chemistry, Wayne State University. Detroit, MI, United States, March 5, 2014.
- 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.
- Kinetic Target-guided Synthesis: A Mass Spectrometry-based Fragment Evolution Strategy for "Undruggable" Targets. 30th Winterschool on Proteinases and Their Inhibitors. Tiers am Rosengarten, Italy, February 27 - March 3, 2013.
- Kinetic Target-Guided Synthesis: A Fragment-Based Discovery Strategy for "Undruggable" Targets Based on Bioorthogonal Reactions. Department of Chemistry, University of Basel. Basel, Switzerland, February 7, 2013.
- Mass Spectrometry Guided Medicinal Chemistry of Antimalarial and Anticancer Agents. Department of Chemistry and Biochemistry, University of Bern. Bern, Switzerland, November 27, 2012.
- Bringing 4(1*H*)-Quinolones and 3-Aryldiazirines Out of the "Dark" Ages. 6th International Conference, Chemistry of Nitrogen Containing Heterocycles. Kharkiv, Ukraine, November 12-16, 2012.
- Kinetic Target-Guided Synthesis: A Fragment-Based Discovery Strategy for "Undruggable" Targets Based on Bioorthogonal Reactions. Drug Discovery Symposium, Novartis. Basel, Switzerland and Cambridge, MA, United States, October 22, 2012.
- Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Glaxo Smith Kline. Research Triangle Park, NC, United States, June 26, 2012.
- Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Novartis. Basel, Switzerland, April 27, 2012.
- Kinetic Target-Guided Synthesis: Fragment-Based Discovery Strategies Based on Bioorthogonal Reactions. Addex Pharmaceuticals. Geneva, Switzerland, April 23, 2012.
- Mass Spectrometry Based Decisions Facilitating Synthetic and Medicinal Chemistry. Department of Chemistry, Clemson University. Clemson, SC, United States, March 15, 2012.
- Mass Spectrometry Based Decisions Facilitating Synthetic and Medicinal Chemistry. Department of Chemistry, Mississippi State University. Mississippi State, MS, United States, March 2, 2012.
- Quinazolines with Anti-Leishmania Activity. Consortium for Parasitic Drug Development Meeting 2011. Clearwater, FL, United States, November 1 - 3, 2011.
- LC-MS-Guided Identification and Optimization of Anti-Cancer and Anti-Malarial Agents. Albert Einstein College of Medicine. Bronx, NY, United States, June 21, 2011.
- The Bioorthogonal Sulfo-click Reaction and its Use in Kinetic Target-Guided Synthesis Screening of Bcl-2 Proteins. Amgen. Thousand Oaks, CA, United States, May 18, 2011.
- LC-MS-Guided Identification and Optimization of Anti-Cancer and Anti-Malarial Agents. Department of Chemistry, Rice University. Houston, TX, United States, April 27, 2011.
- Bioorthogonality of the Sulfo-Click Reaction and its Use in Kinetic Target-Guided Synthesis. 241st ACS National Meeting and Exposition. Anaheim, CA, United States, March 27 to 31, 2011.

- 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, United States, February 23 - 25, 2011.
- Targeting Protein-Protein Interactions via Kinetic Target-Guided Synthesis. The Fragment-Based Lead Discovery Conference 2010. Philadelphia, PA, United States, October 10 - 13, 2010.
- Two Case Studies of LC/MS-driven Drug Discovery: Targeting Bcl-2-Protein Interactions for Anti-Cancer and bc₁ for Anti-Malarial Agents. Department of Chemistry, University of Washington. Seattle, WA, United States, October 20, 2010.
- 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, United States, August 10, 2010.
- 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, United States, February 28 - March 5, 2010.
- LC/MS-based Drug Discovery Targeting Malaria and Cancer. Department of Chemistry, University of Tampa. Tampa, FL, United States, November 17, 2009.
- Kinetic Target-Guided Synthesis: A Fragment-Based Lead Discovery Method Targeting Protein-Protein Interactions. Department of Chemistry, Florida State University. Tallahassee, FL, United States, November 20, 2008.
- Target-Guided Synthesis: A New Approach for Drug Discovery. Florida Annual Meeting and Exposition 2008 (American Chemical Society Regional Meeting). Orlando, FL, United States, May 8 - 10, 2008.
- Target-Guided Synthesis: A New Approach for Drug Discovery. BioStat International / Molecular Medicine Seminar Series, College of Medicine, University of South Florida. Tampa, FL, United States, March 31, 2006.

Selected Oral and Poster Presentations by Graduate Students and Postdocs

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

- 154) Khaly Diagne, Ami Asakawa, Anthony Marasciullo, Caroline Consoli, Logan Helms, Adriana A. Marin, Steven Maher, Dennis E. Kyle, and Roman Manetsch. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 153) Brandon C. Miller, Matthew G. Dowgiallo, Mintesinot Kassu, Kenneth P. Smith, Christopher E. Morgan, Yuliya A. Marusyk, Hanna R. Warinner, Andrew Fetigan, Yoon-Suk Kang, Alex B. Green, Lucius Chiaraviglio, Katherine A. Truelson, Katelyn E. Zulauf, Shade Rodriguez, Anthony D. Kang, Jason J. Guo, Edward W. Yu, James E. Kirby, Roman Manetsch. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 152) Lili Huang, Prakash Parvatkar, Lucius Chiaraviglio, James E. Kirby, Roman Manetsch. Scalable Total Synthesis of Ommatins and their Antioxidant Activity. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 151) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification and structural optimization of a core-independent carboxamide chemotype as novel *P. falciparum* inhibitors. Division of Medicinal Chemistry Award Session, ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 150) Roger Trombley, Alicia Wagner, Jacqueline Smith, Maris Podgurski, Benjamin Liebson, Mai Shaalan, Meng Cui, Steven P. Maher, Anthony Ruberto, Dennis E. Kyle, Roman Manetsch. Optimization of an in-house discovered pyrazine carboxamide scaffold as a potent, fast-acting antimalarial. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 149) Yuliya A. Marusyk, Brandon C. Miller, Matthew G. Dowgiallo, Mintesinot Kassu, Kenneth P. Smith, Christopher E. Morgan, Edward W. Yu, James E. Kirby, Roman Manetsch. Systematic improvements to the diversity-enabling, convergent synthesis of streptothricin F analogs. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 148) Prakash T. Parvatkar, Steven P. Maher, Yingzhao Zhao, Caitlin A. Cooper, Sagan T. de Castro, Julie Péneau, Amélie Vantaux, Benoît Witkowski, Dennis E. Kyle, Roman Manetsch. Antimalarial Activity of Trichothecenes against Liver and Blood Stages of Plasmodium Species. ACS National Meeting. Denver, CO, United States. August 18 - 22, 2024.
- 147) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification and structural optimization of a core-independent carboxamide chemotype as novel *P. falciparum* inhibitors. Northeast Student Chemistry

Research Conference. Boston, MA, United States. April 20, 2024. (*Most Promising Female Scientist Award*)

- 146) Roger Trombley, Alicia Wagner, Jacqueline Smith, Maris Podgurski, Benjamin Liebson, Mai Shaalan, Meng Cui, Steven P. Maher, Anthony Ruberto, Dennis E. Kyle, Roman Manetsch. Optimization of an in-house discovered pyrazine carboxamide scaffold as a potent, fast-acting antimalarial. Northeast Student Chemistry Research Conference. Boston, MA, United States. April 20, 2024.
- 145) Yuliya A. Marusyk, Brandon C. Miller, Matthew G. Dowgiallo, Mintesinot Kassu, Kenneth P. Smith, Christopher E. Morgan, Edward W. Yu, James E. Kirby, Roman Manetsch. Systematic improvements to the diversity-enabling, convergent synthesis of streptothricin F analogs. Northeast Student Chemistry Research Conference. Boston, MA, United States. April 20, 2024.
- 144) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification and structural optimization of a core-independent carboxamide chemotype as novel *P. falciparum* inhibitors. Frühjahrssymposium (Spring Symposium) 2024 of the JungChemikerForum (JCF) of the German Chemical Society (GDCh). Ulm, Germany. March 13 – 16, 2024.
- 143) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification and structural optimization of a core-independent carboxamide chemotype as novel *P. falciparum* inhibitors. Molecular Approaches to Malaria 2024. Lorne, Australia. February 18 – 22, 2024
- 142) Brandon C. Miller, Matthew G. Dowgiallo, Mintesinot Kassu, Kenneth P. Smith, Christopher E. Morgan, Yuliya A. Marusyk, Hanna R. Warinner, Andrew Fetigan, Yoon-Suk Kang, Alex B. Green, Lucius Chiaraviglio, Katherine A. Truelson, Katelyn E. Zulauf, Shade Rodriguez, Anthony D. Kang, Jason J. Guo, Edward W. Yu, James E. Kirby, Roman Manetsch. Antimicrobial and Structural Characterization of Streptothricin F, and the Convergent Synthesis of Streptothricin Analogs. Boston Area Antimicrobial Resistance Network Meeting. Boston, MA, United States, December 8, 2023.
- 141) Brandon C. Miller, Matthew G. Dowgiallo, Mintesinot Kassu, Kenneth P. Smith, Christopher E. Morgan, Yuliya A. Marusyk, Hanna R. Warinner, Andrew Fetigan, Yoon-Suk Kang, Alex B. Green, Lucius Chiaraviglio, Katherine A. Truelson, Katelyn E. Zulauf, Shade Rodriguez, Anthony D. Kang, Jason J. Guo, Edward W. Yu, James E. Kirby, Roman Manetsch. Antimicrobial and Structural Characterization of Streptothricin F, and the Convergent Synthesis of Streptothricin Analogs. Boston Symposium on Organic and Bioorganic Chemistry. Boston, MA, United States. Oct. 5, 2023.
- 140) Ami Asakawa, Khaly Diagne, Anthony Marasciullo, Caroline Consoli, Logan Helms, Adriana A. Marin, Meng Cui, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacridones (THAs). Boston Symposium on Organic and Bioorganic Chemistry. Boston, MA, United States. Oct. 5, 2023.
- 139) Lili Huang, Mintesinot Kassu, Prakash Parvatkar, Roman Manetsch. Expanding the Scope of the Sulfo-Click Reaction and Kinetic Target-Guided Synthesis. Merck, BSOBC. Boston, MA, United States. October 5, 2023.
- 138) Ami Asakawa, Khaly Diagne, Anthony Marasciullo, Caroline Consoli, Logan Helms, Adriana A. Marin, Meng Cui, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacridones (THAs). Gordon Research Seminar: Medicinal Chemistry Strategies and Case Studies in Drug Discovery. New London, NH, United States. Aug 5 - 6, 2023.
- 137) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. 3 Chemotypes and 2 SARs from 1 Virtual Hit: the Identification and Optimization of Antimalarial Inhibitors. Pfizer, Chemistry Spotlight. Cambridge, MA, United States. August 23, 2023.
- 136) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. 3 Chemotypes and 2 SARs from 1 Virtual Hit: the Identification and Optimization of Antimalarial Inhibitors. ACS National Meeting. San Francisco, CA, United States. August 12 – 18, 2023.
- 135) Jacqueline Smith, Alicia Wagner, Roger Trombley, Maris Podgurski, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Synthesis of Nicotinamide-Based Anti-Malarial Therapeutics. ACS National Meeting. San Francisco, CA, United States. August 12 – 18, 2023.
- 134) Maris Podgurski, Alicia Wagner, Roger Trombley, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Structure-activity and structure-property

- relationship studies of *Plasmodium falciparum* formate nitrite transporter (*PfFNT*) inhibitors. ACS National Meeting. San Francisco, CA, United States. August 12 – 18, 2023.
- 133) Khaly Diagne, Ami Asakawa, Raghupathi Neelarapu, Jordany R. Maignan, Alexis N. LaCrue, Debora Casandra, Jeremy N. Burrows, Dennis E. Kyle, and Roman Manetsch. Synthesis of novel 4(1*H*)-Quinolone inhibitors of cytochrome *bc*₁ complex in *Plasmodium falciparum*. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 132) Yuliya Marusyk, Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Hanna Warinner, Andrew Fetigan, Edward Yu, James Kirby, Roman Manetsch. The convergent total synthesis of antibacterial natural product streptothricin F and derivatives. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 131) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. 3 Chemotypes and 2 SARs from 1 Virtual Hit: the Identification and Optimization of Antimalarial Inhibitors. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 130) Maris Podgurski, Alicia Wagner, Roger Trombley, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Structure-activity and structure-property relationship studies of *Plasmodium falciparum* formate nitrite transporter (*PfFNT*) inhibitors. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 129) Jacqueline Smith, Alicia Wagner, Roger Trombley, Maris Podgurski, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Synthesis of Nicotinamide-Based Anti-Malarial Therapeutics. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 128) Roger Trombley, Alicia Wagner, Jacqueline Smith, Maris Podgurski, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Discovery and optimization of the scaffold core of a novel *Plasmodium falciparum* formate nitrite transporter (*PfFNT*) inhibitor. ACS Northeast Regional Meeting. Boston, MA, United States. June 14 – 19, 2023.
 - 127) Maris Podgurski, Alicia Wagner, Roger Trombley, Jacqueline Smith, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Structure-activity and structure-property relationship studies of *Plasmodium falciparum* formate nitrite transporter (*PfFNT*) inhibitors. Northeast Student Chemistry Research Conference. Boston, MA, United States. April 22, 2023.
 - 126) Jacqueline Smith, Alicia Wagner, Roger Trombley, Maris Podgurski, Meng Cui, Adriana A. Marin, Edward Yu, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Synthesis of Nicotinamide-Based Anti-Malarial Therapeutics. Northeast Student Chemistry Research Conference. Boston, MA, United States. April 22, 2023.
 - 125) Anna Meglan, Alicia Wagner, Adriana A. Marin, Kimberly Stieglitz, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Autophagy-related Protein 8 (*PfAtg8*) Inhibitors via KTGS. American Society of Biochemistry and Molecular Biology Annual Meeting. Seattle, WA, United States, March 25 – 28, 2023.
 - 124) Ami Asakawa, Khaly Diagne, Anthony Marasciullo, Caroline Consoli, Logan Helms, Adriana A. Marin, Meng Cui, Steven P. Maher, Dennis E. Kyle Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacrin-9(10*H*)-ones (THAs). Northeast Regional Meeting. Boston, MA, United States. June 14 – 17, 2023.
 - 123) Yuliya Marusyk, Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Hanna Warinner, Andrew Fetigan, Edward Yu, James Kirby, Roman Manetsch. Antimicrobial and Structural Characterization of Streptothricin F, and the Convergent Synthesis of Streptothricin Analogs. Boston Area Antimicrobial Resistance Network Meeting 2022. Boston, MA, United States, December 2, 2022.
 - 122) Alicia Wagner, Roger Trombley, Maris Podgurski, Jacqueline Smith, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Formate Nitrite Transporter (*PfFNT*) Inhibitors via Virtual Screen. ACS Northeast Regional Meeting 2022. Rochester NY, United States, October 2 – 5, 2022.
 - 121) Anna Meglan, Alicia Wagner, Yisakor Assefa, Sagan Thomas De Castro, Olivia Isabelle Mcwhorter, Adriana A. Marin, Kimberly Stieglitz, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Autophagy-related Protein 8 (*PfAtg8*) Inhibitors via Two Screening Methods. ACS Northeast Regional Meeting 2022. Rochester NY, United States, October 2 – 5, 2022.

- 120) Ling Cheng, Lili Huang, Wei Wang, Rick L. Tarleton, Roman Manetsch. Design and Development of *Trypanosoma cruzi* Benzoxaborole Prodrug. ACS Northeast Regional Meeting 2022. Rochester NY, United States, October 2 – 5, 2022.
- 119) Lili Huang, Alona Botnar, Chungsik Kim, Dennis E. Kyle, Roman Manetsch. Clickable Gibberellic Acid Derivatives and Early Recrudescence Phenotype from Artemisinin-Induced Dormancy. ACS Northeast Regional Meeting 2022. Rochester NY, United States, October 2 – 5, 2022.
- 118) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Yuliya Marusyk, Hanna Warinner, Andrew Fetigan, Edward Yu, James Kirby, Roman Manetsch. Antimicrobial and Structural Characterization of Streptothricin F, and the Convergent Synthesis of Streptothricin Analogs. ACS Northeast Regional Meeting 2022. Rochester NY, United States, October 2 – 5, 2022.
- 117) Ami Asakawa, Anthony Marasciullo, Caroline Consoli, Bruno Quiroga, Sagan Thomas De Castro, Olivia Isabelle Mcwhorter, Adrianna A. Marin, Meng Cui, Steven Maher, Dennis E. Kyle, Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacrin-9(10*H*)-ones (THAs) and the Development of Quantitative Structure-Activity Relationship (QSAR) Models. Northeast Regional Meeting. Rochester, NY, United States. Oct 02 - 05, 2022.
- 116) Ami Asakawa, Anthony Marasciullo, Caroline Consoli, Bruno Quiroga, Sagan Thomas De Castro, Olivia Isabelle Mcwhorter, Adrianna A. Marin, Meng Cui, Steven Maher, Dennis E. Kyle, Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacrin-9(10*H*)-ones (THAs) and the Development of Quantitative Structure-Activity Relationship (QSAR) Models. Empowering Women in Organic Chemistry. Cambridge, MA, United States. June 23 – 24, 2022.
- 115) Lili Huang, Alona Botnar, Chungsik Kim, Dennis E. Kyle, Roman Manetsch. Clickable Gibberellic Acid Derivatives and Early Recrudescence Phenotype from Artemisinin-Induced Dormancy. Empowering Women in Organic Chemistry. Hybrid conference. Cambridge, MA, United States, June 23 – 24, 2022
- 114) Ling Cheng, Lili Huang, Wei Wang, Rick L. Tarleton, Roman Manetsch. Design and Development of *Trypanosoma cruzi* Benzoxaborole Prodrug. Empowering Women in Organic Chemistry. Hybrid conference. Cambridge, MA, United States, June 23 – 24, 2022.
- 113) Alicia Wagner, Roger Trombley, Maris Podgurski, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Formate Nitrite Transporter (PfFNT) Inhibitors via Virtual Screen. Empowering Women in Organic Chemistry. Hybrid conference. Cambridge, MA, United States, June 23 – 24, 2022.
- 112) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Yuliya Marusyk, Hanna Warinner, Andrew Fetigan, Edward Yu, James Kirby, Roman Manetsch. Antimicrobial and Structural Characterization of Streptothricin F, and the Convergent Synthesis of Streptothricin Analogs. New England Glyco-Chemistry Meeting. Waltham, MA, United States, June 11, 2022.
- 111) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Andrew Fetigan, Hanna Warinner, Jason Guo, Edward Yu, James Kirby, Roman Manetsch. Studies Towards the Convergent Total Synthesis of Streptothricin Analogs. Northeast Student Chemistry Research Conference. Virtual conference. Boston, MA, United States, April 23, 2022.
- 110) Alicia Wagner, Roger Trombley, Maris Podgurski, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Formate Nitrite Transporter (PfFNT) Inhibitors via Virtual Screen. Northeast Student Chemistry Research Conference. Virtual conference. Boston, MA, United States, April 23, 2022.
- 109) Lili Huang, Alona Botnar, Chungsik Kim, Dennis E. Kyle, Roman Manetsch. Clickable Gibberellic Acid Derivatives and Early Recrudescence Phenotype from Artemisinin-Induced Dormancy. Northeast Student Chemistry Research Conference. Virtual conference. Boston, MA, United States, April 23, 2022.
- 108) Alicia Wagner, Mintesinot Kassu, Tsedey Ayele, Anna Meglan, Yisakor Assefa, Adriana A. Marin, Meng Cui, Kimberly Stieglitz, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Autophagy-related Protein 8 (Atg8) Inhibitors via Two *In Silico* Screening Methods. Malaria: Confronting Challenges From Drug Discovery to Treatment. Breckenridge, CO, United States. April 10 – 13, 2022.
- 107) Mintesinot Kassu, Prakash Parvatkar, Jillian Milanes, Chungsik Kim, Matthew Dowgiallo, Yingzhao Zhao, Lili Huang, Ami Asakawa, Alicia Wagner, Brandon Miller, Karissa Carter, James Morris, Roman Manetsch. Discovery of *Plasmodium vivax* Hexokinase Inhibitors using High-Throughput Kinetic Target-Guided Synthesis Approach. Malaria: Confronting Challenges From Drug Discovery to Treatment. Breckenridge, CO, United States. April 10 – 13, 2022.

- 106) Lili Huang, Alona Botnar, Chungsik Kim, Dennis E. Kyle, Roman Manetsch. Clickable Gibberellic Acid Derivatives and Early Recrudescence Phenotype from Artemisinin-Induced Dormancy. Malaria: Confronting Challenges From Drug Discovery to Treatment. Breckenridge, CO, United States, April 10 – 13, 2022.
- 105) Ami Asakawa, Anthony Marasciullo, Caroline Consoli, Bruno Quiroga, Sagan Thomas De Castro, Olivia Isabelle Mcwhorter, Adrianna A. Marin, Meng Cui, Steven Maher, Dennis E. Kyle, Roman Manetsch. Design and Development of Antimalarial 1,2,3,4-Tetrahydroacrin-9(10*H*)-ones (THAs) and the Development of Quantitative Structure-Activity Relationship (QSAR) Models. Malaria: Confronting Challenges From Drug Discovery to Treatment. Breckenridge, CO, United States. April 10 – 13, 2022.
- 104) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Andrew Fetigan, Hanna Warinner, Jason Guo, Edward Yu, James Kirby, Roman Manetsch. Studies Towards the Convergent Total Synthesis of Streptothricin Analogs. Frühjahrssymposium (Spring Symposium) 2022 of the JungChemikerForum (JCF) of the German Chemical Society (GDCh). Leibniz Universität Hannover. Hannover, Germany, March 23, 2022.
- 103) Mintesinot Kassu, Prakash Parvatkar, Jillian Milanes, Christopher Rice, Chungsik Kim, Matthew Dowgiallo, Yingzhao Zhao, Lili Huang, Ami Asakawa, Alicia Wagner, Brandon Miller, Karissa Carter, Bart Staker, Isabelle Phan, Peter Myler, Wesley Van Voorhis, James Morris, Dennis Kyle, Roman Manetsch. Shotgun Kinetic Target-Guided Synthesis Approach Enables the Discovery of Small Molecule Inhibitors against Pathogenic Amoeba Glucokinases. Boston Symposium on Organic and Bioorganic Chemistry. Virtual conference. Boston, MA, United States, November 4, 2021.
- 102) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Andrew Fetigan, Jason Guo, Edward Yu, James Kirby, Roman Manetsch. Studies Towards the Convergent Total Synthesis of Streptothricin Analogs. Boston Symposium on Organic and Bioorganic Chemistry. Virtual conference. Boston, MA, United States, November 4, 2021.
- 101) Alicia Wagner, Maris Podgurski, Meng Cui, Adriana A. Marin, Steven P. Maher, Dennis E. Kyle, Roman Manetsch. Identification of *Plasmodium falciparum* Formate Nitrite Transporter (PfFNT) Inhibitors via Virtual Screen. Boston Symposium on Organic and Bioorganic Chemistry. Virtual conference. Boston, MA, United States, November 4, 2021.
- 100) Mintesinot Kassu, Prakash Parvatkar, Jillian Milanes, Christopher Rice, Chungsik Kim, Matthew Dowgiallo, Yingzhao Zhao, Lili Huang, Ami Asakawa, Alicia Wagner, Brandon Miller, Karissa Carter, Bart Staker, Isabelle Phan, Peter Myler, Wesley Van Voorhis, James Morris, Dennis Kyle, Roman Manetsch. Shotgun Kinetic Target-Guided Synthesis Approach Enables the Discovery of Small Molecule Inhibitors against Pathogenic Amoeba Glucokinases. 262nd American Chemical Society National Meeting and Exposition. Hybrid conference. August 22 – 26, 2021.
- 99) Ami Asakawa, Anthony Marasciullo, Sagan Thomas De Castro, Isabelle Mcwhorter, Meng Cui, Steven Maher, Dennis E. Kyle, Roman Manetsch. Development of quantitative activity relationship (QSAR) models to assist in the design and development of antimalarial 1,2,3,4-tetrahydroacrin-9(10*H*)-ones (THAs). 262nd American Chemical Society National Meeting and Exposition. Hybrid conference. August 22 – 26, 2021.
- 98) Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Kenneth Smith, Christopher Morgan, Andrew Fetigan, Jason Guo, Edward Yu, James Kirby, Roman Manetsch. Studies Towards the Convergent Total Synthesis of Streptothricin Analogs. New England Glyco-Chemistry Meeting. Virtual conference. Boston, MA, United States, May 2021.
- 97) Hanna Warinner, Brandon Miller, Matthew Dowgiallo, Mintesinot Kassu, Andrew D. Fetigan, Roman Manetsch. New England Glyco-Chemistry Meeting. Virtual conference. Synthesis of the Gulosamine Moiety of Streptothricin F. Boston, MA, United States, May 2021.

Prior to 2021, 96 presentations by co-workers.

RESEARCH FUNDING

Funding Summary

- Active Awards, December 2023: Total funding (Northeastern University and collaborating institutions), direct and indirect costs \$11,578,964; Funding Manetsch Laboratory, direct and indirect costs \$4,448,501; Funding Manetsch Laboratory, direct costs \$2,840,248.

- Completed Awards at Northeastern University: Funding Manetsch laboratory, direct and indirect costs \$1,735,730; Funding Manetsch Laboratory, direct costs \$1,348,254.
- Completed Awards at University of South Florida: Funding Manetsch laboratory, direct and indirect costs \$3,322,928; Funding Manetsch Laboratory, direct costs \$2,062,934.

Current/Active Awards – External

(unless specified, total budget comprises of direct and indirect costs)

- 5) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R21AI171727): The Activation of Benzoxaborole Prodrug AN15368, a Clinical Candidate for Chagas Disease. Total budget \$422,035 (\$31,400 Manetsch total budget; \$20,000 Manetsch direct costs) 04/01/2023 - 03/31/2025. Contact PI Rick L. Tarleton (University of Georgia, Athens) and CIs Michael Zhuo Wang (University of Kansas), and Roman Manetsch.
- 4) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R01AI157208): Use of De Novo Synthesis Approaches and Structure-guided Design to Optimize Therapeutic Properties of Streptothricin Class Antimicrobials. Total budget \$3,977,758 (\$1,413,000 Manetsch total budget; \$900,000 Manetsch direct costs) 09/01/2020 - 08/31/2025. Contact PI James E. Kirby (Beth Israel Deaconess Medical Center) and PIs Edward Yu (Case Western Reserve University), and Roman Manetsch; CI George O'Doherty (Northeastern University).
- 3) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R01AI153290): Lead Optimization and Target Identification of Drugs Targeting Hypnozoites. Total budget \$3,506,812 (\$1,166,812 Manetsch total budget; \$750,000 Manetsch direct costs) 08/01/2020 - 07/31/2025. Contact PI Dennis E. Kyle (University of Georgia, Athens) and PIs Benoit Witowski (Institute Pasteur in Cambodia), and Roman Manetsch.
- 2) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R01AI144464): Orally Bioavailable 4(1H)-Quinolones with Multi-Stage Antimalarial Activity. Total budget \$3,672,359 (\$1,837,289 Manetsch total budget; \$1,170,248 Manetsch direct costs) 04/11/2019 - 04/10/2025 (NCE). Contact PI Roman Manetsch and PI Dennis E. Kyle (University of Georgia, Athens).
- 1) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R01AI 154860): De Novo Synthesis, and Functional and Structural Characterization of Novel Aminoglycoside Analogues to Bypass Resistance Mechanisms and Optimize Selectivity. Total budget \$3,261,596 (\$1,233,200 NEU total budget; \$4,424 Manetsch direct costs) 08/01/2020 - 07/31/2025 (NCE). Contact PI James E. Kirby (Beth Israel Deaconess Medical Center) and PIs Edward Yu (Case Western Reserve University), and George O'Doherty (Northeastern University); CI Roman Manetsch.

Completed Awards - External

(unless specified, total budget comprises of direct and indirect costs)

- 15) National Institutes of Health, National Institute on Deafness and Other Communication Disorders (R21DC020136): Molecular Mechanism of the Bitter Taste of HIV/AIDS Drugs and its Inhibition. Total budget \$431,750 (\$20,844 Manetsch direct costs) 07/01/2022 - 06/30/2024. PI Meng Cui (Northeastern University); CI Diomedes Logothetis (Northeastern University) and Roman Manetsch.
- 14) National Institutes of Health, National Institute of Allergy and Infectious Diseases (R21AI140212): 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 - 02/28/2023 (NCE). Contact PI Roman Manetsch and PI James E. Kirby (Beth Israel Deaconess Medical Center).
- 13) Medicines for Malaria Venture (RD-17-0036): Antimalarial Compounds Targeting Liver Stages of *Plasmodium vivax*. \$475,079 Manetsch direct costs 01/01/2018 - 12/31/2022 (award is renewed annually). Contact PI Dennis E. Kyle, and PI Roman Manetsch. Note: Medicines for Malaria Venture provided additional resources for evaluating compounds in academic and industrial laboratories partnering with Medicines for Malaria Venture. Furthermore, in 2020-2022, synthetic chemists (2.0 FTEs) at TCG Lifesciences (Kolkata, India) dedicated to this project were funded by Medicines for Malaria Venture. The scope of this work focused on the development of a compound series displaying anti-hypnozoite activity.
- 12) National Institutes of Health, National Institute of Allergy and Infectious Diseases (5R33-AI119114): Plasmid Eviction to Restore Susceptibility in Carbapenem-Resistant Enterobacteriaceae. Total budget \$1,679,792 (\$91,020 Manetsch total budget; \$57,975 Manetsch direct costs) 07/01/2018 - 06/30/2022 (NCE). PI James E. Kirby (Beth Israel Deaconess Medical Center) and CI Roman Manetsch.

- 11) Amyotrophic Lateral Sclerosis Association (18-IIA-420): Tethering SOD1 Cysteine Pairs with Cyclic Disulfides: a New Method for Protein Stabilization. Total budget \$300,000 (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.
- 10) 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 provided additional resources for evaluating our prodrug compound in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies have been charged directly to Medicines for Malaria Venture. The scope of this work focused on evaluating whether our prodrug approach has potential for clinical development.
- 9) 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).
- 8) 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.
- 7) 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 Werbovetz (The Ohio State University, Department of Medicinal Chemistry); CIs Roman Manetsch and Zhuo (Michael) Wang (University of Kansas, Pharmaceutical Chemistry).
- 6) 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 provided additional resources for evaluating our compound in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies have been charged directly to Medicines for Malaria Venture.
- 5) 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 provided additional resources for evaluating our compounds in academic and industrial laboratories partnering with Medicines for Malaria Venture. The costs associated to these studies have been charged directly to Medicines for Malaria Venture.
- 4) 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)
- 3) James and Esther King Biomedical Research Program, Florida Department of Health (07KN-08): Bcl-X_L-Templated Assembly of Compounds Modulating Bcl-X_L-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).
- 2) 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).

- 1) 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.

Completed Awards - Internal

(unless specified, total budget comprises of direct and indirect costs)

- 8) NEU 2023 Tier 1 Seed Grant: Strategy for Broad Spectrum Corona Virus Treatment. \$50,000 direct costs (no indirect costs allowed); (\$25,000 Manetsch direct costs) 07/01/2022 - 09/30/2023. PI Jeffrey N. Agar (Northeastern University); CI Roman Manetsch.
- 7) 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.
- 6) 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.
- 5) 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.
- 4) 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).
- 3) 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-Aminolevulinate Synthase. \$40,000, 09/01/2007 - 08/31/2009. PI Roman Manetsch.
- 2) 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).
- 1) 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).

TEACHING AND TRAINING ACTIVITIES

Courses at NEU

Student's evaluations are given in parenthesis (instructor effectiveness; # of responded evaluations/# of enrolled students)

- 8) *CHEM2315 Organic Chemistry 1* (undergraduate level course): Fall 2015 (3.3/5.0; 31/49).
- 7) *PHSC2650 Intro to Health Science Research* (1 lecture/course; undergraduate level course): Spring 2022 (4.7/5.0; 18/23), Spring 2023 (5.0/5.0; 5/10).
- 6) *CHEM5626 Organic Synthesis* (graduate level course): Fall 2016 (5.0/5.0; 6/9), Fall 2017 (4.9/5.0; 14/15), Fall 2018 (4.9/5.0; 17/19), Fall 2019 (4.8/5.0; 14/15), Fall 2020 (4.8/5.0; 5/8), Fall 2021 (4.9/5.0; 16/20), Fall 2022 (4.8/5.0; 17/24); Fall 2023 (4.9/5.0; 13/21); Fall 2024 (4.9/5.0; 15/31).
- 5) *CHEM5676 Bioorganic Chemistry* (1 lecture/course, graduate level course): Spring 2016 (not evaluated), Spring 2017 (4.8/5.0; 9/11), Spring 2018 (4.8/5.0; 12/13), Spring 2019 (not evaluated), Spring 2020 (not evaluated), Spring 2022 (not evaluated); Spring 2023 (4.8/5; 20/21).
- 4) *PHSC5360 Anti-Infectives* (unless specified, 5 lectures/course and course coordination; graduate level course): Summer 2018 (4.1/5.0; 138/144), Summer 2019 (4.1/5.0; 109/114); Summer 2020 (4.1/5; 135/140);

- Summer 2021 (4.2/5; 85/88); Summer 2022 (3.7/5; 95/95); Summer 2023 (4.1/5; 91/94); Summer 2024 (1 lecture/course; not evaluated).
- 3) *PHSC5400 Principles of Drug Design* (graduate level course): Fall 2016 (4.6/5.0; 10/12), Fall 2017 (4.9/5.0; 9/9), Fall 2018 (4.9/5.0; 8/9), Fall 2019 (4.9/5.0; 10/12), Fall 2020 (5.0/5.0; 5/6), Fall 2021 (5.0/5.0; 5/6), Fall 2022 (4.9/5.0; 5/6).
 - 2) *PHSC5450 Contemporary Approaches to Drug Design* (1 lecture/course, graduate level course): Spring 2023 (not evaluated); Spring 2024 (4.9/5.0; 8/10).
 - 1) *PHSC6314 Special Topics Pharm Science* (1 lecture/course, graduate level course): Summer 2020 (not evaluated).

Courses at USF

- 6) *CHM2210 Organic Chemistry I* (undergraduate level course, 160-320 enrolled students): Spring 2007, Spring 2008, Fall 2008, Spring 2009, Fall 2009, Spring 2010, Spring 2011, Spring 2014.
- 5) *CHM2211 Organic Chemistry II* (undergraduate level course): Spring 2012 (undergraduate level course, 160-320 enrolled students).
- 4) *CHM6250/5225 Advanced Organic Chemistry I* (dual listed graduate and undergraduate level course, 15-30 enrolled students): Fall 2005, Fall 2006, Fall 2007, Fall 2013.
- 3) *CHM6935 Graduate Seminar* (course coordination, graduate level course, 70-100 enrolled students): Fall 2006, Spring 2007, Fall 2007, Spring 2008, Fall 2008, Spring 2009, Fall 2009, Spring 2010, Fall 2010, Spring 2011, Fall 2011, Spring 2012.
- 2) *CHM6938/4932 Spectroscopy* (dual listed graduate and undergraduate level course, 15-30 enrolled students): Fall 2010, Fall 2011.
- 1) *CHM6938/PHC7931 Drug Discovery for Tropical Diseases* (graduate level course, 25-40 enrolled students): Spring 2010, Spring 2012, Spring 2014.

Senior Research Scientist

- 1) Dr. Prakash Parvatkar, September 2022 – present

Postdoctoral Associates

- 10) Dr. Chungsik Kim, September 2016 – August 2020
- 9) Dr. Prakash Parvatkar, September 2016 – August 2018
- 8) Dr. Abdul Shaikh, September 2015 – August 2017
- 7) Dr. Fabian Brockmeyer, June 2015 – May 2017
- 6) Dr. Yana Sakhno, June 2012 – August 2013
- 5) Dr. Raghupathi Neelapapu, May 2012 – July 2014
- 4) Dr. Niranjana Namelikonda, May 2009 – September 2014
- 3) Dr. David Flanigan, April 2009 – October 2014
- 2) Dr. Yijun Yang, September 2009 – December 2010
- 1) Dr. Xiangdong Hu, September 2006 – April 2009

Thesis and Dissertation Research Supervision

- 28) Arif Hussain (Chemistry and Chemical Biology), 2023 – present, Ph.D. student
- 27) Benjamin Liebson (Chemistry and Chemical Biology), 2023 – present, Ph.D. student
- 26) Mai Shaalan (Chemistry and Chemical Biology), 2023 – present, Ph.D. student
- 25) Ling Cheng (Pharmaceutical Sciences), 2021 – 2023, *Optimization of Antiparasitic Small Molecule Inhibitors and Fluorescent Probes*, M.S. from NEU
- 24) Khaly Diagne (Chemistry and Chemical Biology), 2021 – present, Ph.D. candidate
- 23) Yuliya Marusyk (Chemistry and Chemical Biology), 2021 – present, Ph.D. candidate
- 22) Roger Trombley (Chemistry and Chemical Biology), 2021 – present, Ph.D. candidate
- 21) Alicia Wagner (Chemistry and Chemical Biology), 2020 – present, Ph.D. candidate
- 20) Ami Asakawa (Pharmaceutical Sciences), 2019 – 2024. *Lead optimization of 1,2,3,4-Tetrahydroacridin-9(10H)-ones and development of QSAR models for antimalarial drug discovery*. Ph.D. from NEU
- 19) Christina Di Marco (GlaxoSmithKline; co-advisor Dr. Brandon Turunen), 2019 – 2023. *Innovative Cancer Treatments via Small Molecules and Cytotoxicity Targeting Chimeras (CyTaCs)*, industrial Ph.D. from NEU
- 18) Lili Huang (Chemistry and Chemical Biology), 2019 – 2024. *Total synthesis of ommatins, hit-to-lead optimizations of antimalarials, and development of chalcogen click chemistry towards kinetic target-guided*

- synthesis. Ph.D. from NEU
- 17) Brandon Miller (Chemistry and Chemical Biology), 2019 – 2024. *Explorations of synthetic methodologies for two therapeutic frameworks: synthesis optimizations of first-generation streptothricin F intermediates, a second-generation formal synthesis of streptothricin F, and the synthesis and molecular probe development of cyclic thiosulfonates*. Ph.D. from NEU
 - 16) Mintesinot Kassu (Chemistry and Chemical Biology), 2018 – 2024. *Alternative drug discovery platforms for the identification of anti-infective agents*. Ph.D. from NEU
 - 15) Jackson Cacioppo (Chemistry and Chemical Biology), 2017 – 2019. *Synthesis of 3-Trifluoro-methyl-3-Pyrimidinyl Diazirines as Photoreactive Amino Acid Analogs*. M.S. from NEU
 - 14) Matthew Dowgiallo (Chemistry and Chemical Biology), 2015 – 2020. *Combating the Rise of Antimicrobial Resistance: Permeation and Efflux Multiparameter Optimization and A Divergent Total Synthesis of Streptothricin F*. Ph.D. from NEU
 - 13) Yingzhao (David) Zhao (Chemistry and Chemical Biology), 2015 – 2020. *Studies towards the Total Synthesis of Anguidine and Anguidine-like Scaffolds*. Ph.D. from NEU
 - 12) Megan Barber, 2012 – 2015, *2,4-Disubstituted Quinazolines with Antileishmanial or Antibacterial Activity*. M.S. from USF
 - 11) 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
 - 10) 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
 - 9) 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
 - 8) Andrii Monastyrskyi, 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
 - 7) 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
 - 6) Kurt Van Horn, 2007 – 2013. *Anti-Parasitic and Anti-Bacterial Agents: Studies on 1,4-Dihydropyridines and 2,4-Diaminoquinazolines*. Ph.D. from USF
 - 5) 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
 - 4) 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
 - 3) Shikha Mahajan, 2006 – 2012. *Protein Profiling of Adenine Nucleoside and Nucleotide Analogs Binding Proteins Using N⁶-Biotinylated-8-azidoadenosine Analogs as Affinity Based Protein Profiling Probes*. Ph.D. from USF (primary advisor David Merkler, Co-advisor Roman Manetsch)
 - 2) 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
 - 1) Lisa M. 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

- 41) Sriram Kompella, July 2024 – present
- 40) Caroline Lynch, January 2024 – present
- 39) Allyson Kleinmann, January 2024 – present
- 38) Mya Gaddy (REU student from Lafayette College), May 2023 – August 2023
- 37) Kaia Ellis (REU student from Kennesaw State University), May 2022 – August 2022
- 36) Jacqueline Smith, June 2022 – June 2024
- 35) Nathan Tang, January 2022 – May 2023
- 34) Portia Aning, January 2022 – present
- 33) Maris Podgurski, September 2021 – June 2024
- 32) Victor Velazquez (student from Roxbury Community College), September 2021 – January 2022
- 31) Caroline Consoli, September 2021 – May 2022
- 30) Bruno Quiroga, August 2021 – May 2022
- 29) Yisakor Assefa (student from Roxbury Community College), June 2021 – August 2021
- 28) Anthony Marasciullo, January 2021 – May 2022

- 27) Hanna Warinner (student from University of Bath (UK)), November 2020 – August 2021
- 26) Anna Meglan, April 2020 – May 2023
- 25) Tsedey Ayele (student from Roxbury Community College), May 2020 – December 2020
- 24) Karissa Carter (REU student from Norfolk State University), May 2019 – August 2019
- 23) Loren Po, January 2018 – December 2019
- 22) Grace Kiser, February 2018 – December 2018
- 21) Andrew Fetigan, January 2016 – April 2019
- 20) Liu Li, January 2016 – August 2016
- 19) Imran Sharif Elmaarouf, February 2016 – April 2019
- 18) Daniel Assad Saad September 2017 – December 2018
- 17) Michael Shultis, February 2015 – December 2016
- 16) Jackson Goodman Cacioppo, July 2016 – December 2016
- 15) Susan Anne Roberts, August 2016 – December 2016
- 14) Tanner C Jenkins, October 2016 – December 2016
- 13) Madeline L MacDonnell, January 2016 – March 2016
- 12) Jake Ganley, January 2016 – June 2017
- 11) Lisa Barton, January 2015 – April 2016
- 10) Lauren Bertino, January 2016 – March 2016
- 9) Danielle Lefebvre, February 2016 – April 2016
- 8) Clarissa Santori, August 2016 – December 2017
- 7) Fabiola Caban (REU student from the Universidad Ana G. Méndez, San Juan, Puerto Rico), May 2016 – August 2016
- 6) James Giarrusso, 2011 – 2013
- 5) Niles Gunsalus, 2010 – 2012
- 4) Anthony Melendez, 2010 – 2012
- 3) Lisa Luong, 2009 – 2011
- 2) Jordan Anderson, 2008 – 2011
- 1) Mario Martinez, 2007 – 2009

Honors Undergraduate Thesis

- 4) Alexandra Griffin, 2010 – 2011
- 3) Lisa Luong, 2010 – 2011
- 2) Jordan Anderson, 2010 – 2011
- 1) Mario Martinez, 2008 – 2009

Doctoral Committee Service, NEU (students that are not members of the Manetsch laboratory).

- 30) Novera Alam, Chemistry and Chemical Biology
- 29) Wei-Ting Chang, Chemistry and Chemical Biology
- 28) Arezou Dilmaghanimarand, Chemistry and Chemical Biology
- 27) Yang Fang, Chemistry and Chemical Biology
- 26) Ian Hicks, Chemistry and Chemical Biology
- 25) Wensheng Yang, Chemistry and Chemical Biology
- 24) Bohui Li, Chemistry and Chemical Biology
- 23) Yaning Li, Chemistry and Chemical Biology
- 22) Caroline Millard, Chemistry and Chemical Biology
- 21) Hayden Motter, Chemistry and Chemical Biology
- 20) Vijaymahantesh Pattanashettr, Chemistry and Chemical Biology
- 19) Jess Pennington, Chemistry and Chemical Biology
- 18) Debarpita Ray, Chemistry and Chemical Biology
- 17) Mengqi Ren, Chemistry and Chemical Biology
- 16) Vinou Val, Chemistry and Chemical Biology
- 15) Yuhan Wang, Chemistry and Chemical Biology
- 14) Chenyang Xue, Chemistry and Chemical Biology
- 13) Olusegun Abolarin, Pharmaceutical Sciences
- 12) Harvens Beauzile, Pharmaceutical Sciences
- 11) Brittany Brems, Pharmaceutical Sciences

- 10) Krista Brown, Pharmaceutical Sciences
- 9) Wilder Felix, Pharmaceutical Sciences
- 8) Markos Georgiadis, Pharmaceutical Sciences
- 7) Maria Gerasi, Pharmaceutical Sciences
- 6) Otto Holbrook, Pharmaceutical Sciences
- 5) Sahil Seth, Pharmaceutical Sciences
- 4) Arslan Sheikh, Pharmaceutical Sciences
- 3) Michael Speziale, Pharmaceutical Sciences
- 2) Negar Shahsavari, Biology
- 1) Sean A. Chin Chan, The H. Lee Moffitt Cancer Center and Research Institute, Florida

External Ph.D. Thesis Examiner

- 3) Sean Chin Chan, Drug Discovery, the H. Lee Moffitt Cancer Center, Tampa (FL), USA (2021)
- 2) Peter Mubanga Cheuka, Department of Chemistry, University of Cape Town, South Africa (2018)
- 1) Leon Jacobs, Stellenbosch University, South Africa (2018)

External M.S. Thesis Examiner

- 1) Pieter Cilliers, Department of Pharmacy, North-West University, South Africa (2018)

SERVICE (2014-present)

Service to the Department of Chemistry and Chemical Biology, College of Science

- 7) Merit Review Committee Department of Chemistry and Chemical Biology (2023)
- 6) Safety Officer of the Department of Chemistry and Chemical Biology (2016 – 2023)
- 5) Chair of Antimicrobials and Disease Strategy faculty search (joint search with the Biology, Chemical Engineering, and Pharmaceutical Sciences departments). Faculty search ended successfully with the hire of Dr. Thiago dos Santos (2022 – 2023)
- 4) Executive Committee of the Department of Chemistry and Chemical Biology (2016 – 2023)
- 3) Student Recruiting/Admissions Committee of Chemistry and Chemical Biology (2015, and 2017 – 2022)
- 2) Committee for (Bio)Analytical Chemistry faculty search. Faculty search ended successfully with the hire of Dr. Leila Deravi (2015 – 2016)
- 1) Committee CCB laboratory design in new building of Northeastern University, EXP Research Center (2019 – 2020)

Service to the Department of Pharmaceutical Sciences, Bouvé College of Health Sciences

- 6) Committee for faculty search in Drug Discovery and Development with a focus on mental health and addiction (joint search with the Center for Drug Discovery) (2023 – 2024)
- 5) Associate Chair for Research (2021 – 2023)
- 4) Chair of Drug Discovery and Artificial Intelligence faculty search (joint search with the Bioengineering Department) (2021– 2022)
- 3) Student Recruiting/Admissions Committee of Pharmaceutical Sciences (2016 – 2020)
- 2) Instrumentation Committee of Pharmaceutical Sciences (2016 – 2017)
- 1) Committee for Natural Product Chemistry faculty search (joint search with Chemistry and Chemical Biology) (2015 – 2016)

Service to the College of Science and Bouvé College of Health Sciences

- 4) Committee for Anti-microbial Discovery faculty search in the Department of Biology. Faculty search ended successfully with the hire of Dr. Nick Takacs (2021-2022)
- 3) Department Search Representative,* search for Analytical and/or Environmental Chemistry Faculty Position (2021)
- 2) Department Search Representative,* search for Sustainable Energy and Materials Faculty Position (2021)
- 1) Pharmacy's Academic and Professional Standing Committee** (2020 – 2021)

[*Department Search Representative to assist with sorting through the long list of faculty candidates and to justify why each woman or racial minority candidate is not included on the short list of the invited/interviewed candidates. The Department Search Representative is not a member of the search committee. The Representative is given access to search folders and work in a two-

day turnaround so as not to delay the search process. There are up to ~10 candidates to sort through. The service of the Department Search Representative is counted as CoS and Department service; **Pharmacy's Academic and Professional Standing Committee at its core is tasked with ensuring student academic and professional success, and reviewing students who may experience academic and/or professional concerns within the School of Pharmacy e.g. course deficiencies, failures, dismissals. The committee meets at the beginning of the semester for 4-7 hours to process student's requests from the previous semester.]

Service to the University

- 4) Faculty Director for the Nuclear Magnetic Resonance Core Facility (2021 – present)
- 3) Chair of NEU's Laboratory Safety Hygiene Committee (2020 – 2023)
- 2) NEU's Laboratory Safety Hygiene Committee (2016 – 2023)
- 1) Committee member focusing on the design of research resumption tracking software called Service Now SNOW*** (2020 – 2021)

[***The committee comprises of staff and administrators from various Colleges and Departments. The committee meets weekly for approximately 60 minutes. As the only faculty member in the committee, I am responsible that software design meets the needs of faculty members.]

Service to the Discipline

- 11) 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.
- 10) Reviewer National Institutes of Health:
 - NIH/ZRG1 IDM-T(82), R21s, and R03s (March 2015)
 - NIH/DDR, R01s (June 2015)
 - NIH/ZAI1 LC-M-J, Special Emphasis Panel International Centers of Excellence for Malaria Research U19 (September 2016)
 - 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 (October 2018)
 - NIH/ZRG1 IDM-S(83) A R03s and R15s (July 2019)
 - NIH/ZRG1 IDM-Y(82), R03s, and R21s (March 2020)
 - NIH/Emergency COVID-19 and SARS/CoV-2 Grants Review, R01s and R21s (July 2020)
 - NIH/Emergency COVID-19 and SARS/CoV-2 Grants Review, R01s and R21s (September 2020)
 - NIH/Emergency COVID-19 and SARS/CoV-2 Grants Review, R01s and R21s (January 2021)
 - NIH Special Emphasis Panel, Drug Discovery and Mechanisms of Resistance in Eukaryotic Pathogenic Organisms, R01s and R21s (December 2021)
 - NIH/ZRG1, AIDC-B(83), Special Emphasis Panel on Eukaryotic Pathogen Drug Discovery and Resistance R01s and R21s (July 2022)
 - NIH/SBCB, R01s, R15s, R21s, and R03s (October 2022)
 - NIH/ARIT, Anti-Infective Resistance and Targets, R01s, R15s, R21s, and R03s (March 2024)
 - NIH/BQQ, Development of Medical Countermeasures for Biodefense and Emerging Infectious Diseases (June 2024)
- 9) Reviewer Department of Defense:
 - Peer Review Medical Research Program (PRMRP) Preapplications – Malaria (July 2014)
 - PRMRP Applications – Malaria (November 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)
 - PRMRP Preapplications – Malaria (June 2021)

- PRMRP Applications – Malaria (November 2021)
 - PRMRP Applications – Malaria (August 2022)
- 8) Reviewer grant applications for Deutsche Forschungsgemeinschaft (German Research Foundation) (2023)
 - 7) Reviewer grant applications for Dana-Farber Cancer Institute/Northeastern University, Joint Program in Cancer Drug Development (2015).
 - 6) 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).
 - 4) Conference Session Chair: Boston Symposium on Organic Chemistry and Bioorganic Chemistry, Boston, USA (October 2015); International Pharma Conference and Expo, Rome, Italy, (May 2018); Amoeba Summit, Orlando, USA (September 2019); 3rd International Conference on PharmaScience Research and Development, virtual (February 2021); Boston Symposium on Organic Chemistry and Bioorganic Chemistry, Boston, USA (October 2024).
 - 3) Active Member of Science Department Advisory Board, Roxbury Community College, Massachusetts (2019 – present); research advising with Professor Kimberly Stieglitz of undergraduate student Tsedey Ayele (June-December 2020) and Yisakor Assefa (June-September 2021); projects conducted in my laboratory
 - 2) Advisor of research tool development project by Computer Science undergraduate students of Northeastern University Sandbox Computer Science Club (September 2019 – December 2020)
 - 1) 1-day organic chemistry program for high school students showcasing the use of analytical instrumentation to characterize small molecules (August 2024 – present)