# Sudeshna Roy, Ph.D.

The University of Mississippi Department of BioMolecular Sciences School of Pharmacy

413 Faser Hall, University, MS 38677-1848

Email: <a href="mailto:roy@olemiss.edu">roy@olemiss.edu</a>
Phone: +1-662-915-2980

Website: <a href="http://roylaboratory.com/">http://roylaboratory.com/</a>

# **PROFESSIONAL APPOINTMENTS**

- NOT ESSIONAL AT TOMY MILENTS		
Assistant Professor of Medicinal Chemistry and Pharmacognosy Department of BioMolecular Sciences, The University of Mississippi		7/2017–current
Research Assistant Professor in the Research Institute of Pharmaceutical Sciences  7/2017–co School of Pharmacy, The University of Mississippi		
EDUCATION		
Postdoctoral Studies	University of North Carolina at Chapel Hill Division of Chemical Biology and Medicinal Chemistry, School of Pharmacy Advisor: Jeffrey Aubé, Ph.D.	2015–2017
Postdoctoral Studies	University of Kansas Department of Medicinal Chemistry, School of Pharmacy Advisor: Jeffrey Aubé, Ph.D.	2012–2015
Ph.D.	University of Missouri-St. Louis  Dissertation: Studies Toward Tetrahydrofuran-containing Natural Products: Total Synthesis of Amphidinolide C and Oxylipids Advisor: Christopher D. Spilling, Ph.D.	2007–2012

# M.S. University of Missouri-St. Louis

2007–2009

Specialization: Organic Chemistry

# M.Sc. University of Delhi, India

2005–2007

Specialization: Organic Chemistry

# B.Sc. St. Stephen's College, Delhi, India

2002-2005

Major: Chemistry

# **RESEARCH INTERESTS**

- 1. Target-based discovery of chemotherapeutics against *Mycobacterium tuberculosi*s and other antibiotic-resistant bacterial infections and targeted protein degradation.
- 2. Functionalization of fluoroalkenes.

HONORS AND AWARDS	
NIH Maximizing Investigators Research Award (MIRA) for Early Stage Investigators	2023
Sarah Isom Fellow, University of Mississippi	2023–2025
Rho Chi Pharmacy Honors Society	2020–Present
Awarded the Best Pharmacy Year1 Teaching Team of the Year (served as a co-instructor)	2020
Selected for NIGMS Mentoring Workshop for New Faculty in Organic and Biological Chemis	•
Travel Award, NSF Chemistry Early Career Investigator Workshop	2018
Selected for NSF Chemistry Early Career Investigator Workshop	2018
Elected member of the UNC-Chapel Hill chapter of Sigma Xi, The Scientific Research Honor	
Chancellor's Graduate Scholars Dissertation Fellowship, University of Missouri-St. Louis	2011–2012
Sigma Xi Award by the Graduate School, University of Missouri-St. Louis	2011
ACS Travel Award from the Division of Organic Chemistry for the 242nd National in Denver	
Graduate Research Fair Award, Ph.D. Natural Sciences Division	2009–2011
Outstanding Graduate Student Recognition from the Center of Teaching & Learning	2009–2010
RESEARCH SUPPORT (Ongoing & Completed)	
NIH R35GM150768 in NIGMS (Roy) Role: PI	09/01/2023-06/30/2028
Expanding the small molecule toolbox through novel applications of fluorinated alkenes	
NIH P20GM130460 in NIGMS GLYCORE (Sharp, Ross)	04/01/2023-03/31/2025
Role: Pilot Project PI (subaward)	0-70172023 0373172023
Chemical Programing of Bacterial Protease for Targeted Degradation of Peptidoglycan Bios	synthesis
Mississippi SMART Business Accelerator Program (Roy)	07/5/2023-07/04/2025
Role: PI	
Novel Chemotherapeutics for the Treatment of Tuberculosis	
Isom Fellowship (Roy)	05/10/2023-05/09/2025
Role: PI of the Fellowship	
Tuberculosis in Women and Children	
Nacuity Pharmaceuticals (Roy)	05/23/2022–12/31/2022
Role: PI Fluorinated analogs of N-acetyl cysteine amide	
	04 /05 /0000 04 /04 /0004
NIH P30GM122733 in NIGMS COBRE (Majumdar)	01/05/2023-01/04/2024
Role: PI of CORE Voucher	
Development of 1,2,4-triazoles for the treatment of tuberculous meningitis	
NIH R21AI142210 in NIAID (Roy)	7/1/2019-6/30/2022 (NCE)
Role: PI Target-based Chemotherapeutics Development Against Mycobacterium tuberculosis	
NSF XSEDE (Roy)	10/23/2019–04/22/2021
Role: PI	, , ,
Extended all-atom molecular dynamics simulations to understand the conformational change interesting with great molecular inhibitors.	ges of MraYMtb and its

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binding interactions with small molecule inhibitors

NIH P30GM122733 in NIGMS COBRE

5/31/2020-10/22/2021

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Role: PI of CORE Voucher

Search for natural product-inspired new chemical entities to treat pain, neuropsychiatric disorders, and addiction.

#### **RESEARCH SUPPORT** (Submitted & Pending)

NIH R01 (Stallings & Roy) in NIAID

10/15/2023-10/14/2028

Role: Multi-PI

Development of 1,2,4-Triazoles and their Derivatives as a New Treatment for Tuberculosis

Impact Score: 30; Percentile: 10

Status: Council Review Competed, requested and submitted JIT, waiting for the funding decision end of fiscal year

NIH R01 (Stallings & Roy) in NIAID

07/01/2024-06/30/2029

Role: Multi-PI

Development of 1,2,4-Triazoles and their Derivatives as a New Treatment for Tuberculosis

Status: Pending Council Review (This is an A1 submission of the above grant)

NIH R21 (Doering & Roy) in NIAID

12/01/2024-11/30/2026

Role: Multi-PI

Amino acid mimetics as anti-cryptococcal agents

Status: Pending Council Review

# **COLLABORATORS**

1. Christina Stallings, Ph.D., Washington University in St. Louis

- 2. Robert Doerksen, Ph.D., University of Mississippi
- 3. Christian Ducho, Ph.D., Saarland University, Germany
- 4. Tamara Doering, Ph.D., Washington University in St. Louis
- 5. Ryan Fortenberry, Ph.D., University of Mississippi
- 6. Michael Wall, Ph.D., Nacuity Pharmaceuticals
- 7. Soumyajit Majumdar, Ph.D., University of Mississippi
- 8. Mary Jackson, Ph.D., University of Colorado

#### **OTHER POSITIONS & SERVICE**

- Review Panel
  - 2019 American Chemical Society Petroleum Research Fund (ACS PRF) Doctoral New Investigator
  - 2020 NIGMS, Synthetic and Biological Chemistry B Study Section (SBCB) Review Panel
  - 2022 NIAID study section ZRG1 DCAI, Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)
  - 2023 NIAID DMID Omnibus BAA (HHS-NIH-NIAID-BAA2023-1), Research Area 002 Development of Therapeutic Candidates for Biodefense, Antimicrobial Resistant (AMR) Infections and Emerging Infectious Diseases (N01) contract proposals; Small Business: Anti-Infective Therapeutics DCAI (12)
    - NIAID study section ZRG1 DCAI, Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)
  - 2024 Small Business: Anti-Infective Therapeutics DCAI study section; Drug Discovery and Molecular Pharmacology A (DMPA) study section NIAID study section - ZRG1 DCAI, Small Business Innovation Research (SBIR) and Small Business

Technology Transfer (STTR)

- Discussion leader at conferences
  - 2021 Mid-South Glycoscience Meeting
  - 2022 Heterocycles Gordon Conference, Newport, RI
- Journal Referee

Nature Communications, MedChemComm, Journal of Natural Products, Israel Journal of Chemistry, Translational Research, Beilstein Journal of Organic Chemistry, Chemical Science, Organic and BioMolecular Chemistry, Chemical Toxicology, ACS Infectious Diseases, ACS Medicinal Chemistry Letters, European Journal of Organic Chemistry, Organic Letters

- Founder of the Chemistry Graduate Student Association, Treasurer at UMSL, 2009–2011
- Representative of Dept. of Chemistry & Biochemistry for Graduate Student Committee (Nominated), 2009–2011
- Participant in NIH Sponsored Fragment-based Drug Design Workshop, University of Kansas 2013
- NIH Sponsored Contemporary Medicinal Chemistry Workshop, University of Kansas 2012
   The Optimization of Drug Physicochemical Properties in Early Drug Discovery at KU Med Chem Fall Retreat 2012
- University of North Carolina at Chapel Hill's chapter of Sigma Xi, The Scientific Research Honor Society, 2016– Present
- American Chemical Society, 2008–Present
- American Association Pharmaceutical Sciences, 2017–Present

#### **PUBLICATIONS** (published n=24; submitted = 2)

- 1. Slone, S.; Anthony, S. R.; Green, L. C.; Nieman, M. L.; Alam, P.; Wu, X.; **Roy, S.**; Aubé, J.; Xu, L.; Lorenz, J. N.; Owens, A. P.; Kanisicak, O.; Tranter, M., HuR inhibition reduces post-ischemic cardiac remodeling by dampening acute inflammatory gene expression and the innate immune response. *Submitted to Journal of the American Heart Association* 
  - Non-peer-reviewed version of this article has been posted as a preprint: *bioRxiv*, **2023**. DOI: https://doi.org/10.1101/2023.01.17.524420
- 2. Berida, T.; Adekunle, Y. A.; Dada-Adegbola, H.; Kdimy, A.; **Roy, S.**; Sarkar, S. D., Plant Antibacterials: The Challenges and Opportunities. *Submitted to Fitoteria*.
- 3. Huang, T.-Y.; Djugovski, M.; Manning, D. L.; Adhikari, S.; **Roy, S.**, Morpholine-mediated defluorinative cycloaddition of *gem*-difluoroalkenes and organic azides. *Beilstein Journal of Organic Chemistry*, **2023**, *19*, 1545–1554. DOI: 10.3762/bjoc.19.111
  - Non-peer-reviewed version of this article has been posted as a preprint: *ChemRxiv*, **2023**. DOI: 10.26434/chemrxiv-2023-w2r84
- 4. Berida, T.; McKee, S. R.; Chatterjee, S.; Li, W.; Pandey, P.; Tripathi, S. D.; Doerksen, R. D.; Jackson, M.; Ducho, C.; Stallings, C. L.; Roy, S., Discovery, Synthesis, and Optimization of 1,2,4-Triazolyl Pyridines Targeting Mycobacterium tuberculosis. ACS Infectious Diseases 2023 9, 11, 2282–2298. DOI: 10.1021/acsinfecdis.3c00341 Non-peer-reviewed version of this article has been posted as a preprint: bioRxiv, 2023. DOI: 2022.11.14.516356
- Manning, D. L.; Huang, T.-Y.; Roy, S., The challenges and opportunities of developing small molecule inhibitors of MraY. Accepted in Annual Reports in Medicinal Chemistry, Special Volume on New Approaches Towards Novel Antibacterial Agents project. 2023. Invited Review. DOI: 10.1016/bs.armc.2023.09.005
- 6. Wu, X.; Ramesh, R.; Wang, J.; Zheng, Y.-G.; Armaly, A.; Wei, L.; Xing, M.; Roy, S.; Lan, L.; Gao, P.; Miao, Y.; Xu, L.; Aubé, J., Small molecules targeting the RNA-binding protein HuR inhibit tumor growth in xenografts. *Journal of Medicinal Chemistry* 2023, 66, 2032–2053. DOI: 10.1021/acs.jmedchem.2c01723
- 7. Green, L. C; Slone, S.; Anthony, S. R.; Guarnieri, A. Parkins, S.; Shearer, S. M.; Neiman, M. L.; **Roy, S.**; Aubé, J.; Wu, X.; Xu, L., Tranter, M., HuR-dependent expression of Wisp1 is necessary for TGF-induced cardiac myofibroblast activity. *Journal of Molecular and Cellular Cardiology* **2023**, 174, 38–46. DOI: 10.1016/j.yjmcc.2022.10.007

- 8. Pandey, P.; Chatterjee, S.; Berida, T.; Doerksen, R. J.; **Roy, S.**, Identification of Potential Non-nucleoside MraY Inhibitors for Tuberculosis Chemotherapy from Structure-Based Virtual Screening. *Journal of Biomolecular Structure & Dynamics* **2022**, 40, 4832–4849. DOI: 10.1080/07391102.2020.1862705
- 9. Stoddard, S. V.; Stoddard, S. D; Oelkers, B. K.; Fitts, K.; Whalum, K.; Hemphill, A. D.; Manikonda, J.; Martinez, L. M.; Riley, E. G.; Roof, C. M.; Sarwar, N.; Thomas, D. M.; Ulmer, E.; Wallace, F. E.; Pandey, P.; Roy, S., Optimization Rules for SARS-CoV-2 Mpro Antivirals: Ensemble Docking and Exploration of the Coronavirus Protease Active Site. *Viruses* 2020, *12*, 942. DOI: 10.3390/v12090942
- 10. Wu, X.; Gardashova, G.; Lan, L.; Han, S.; Zhong, C.; Marquez, R.; Wei, L.; Wood, S.; Roy, S.; Gowthaman, R.; Karanicolas, J.; Gao, P.; Dixon, D.; Welch, D.; Li, L.; Ji, M.; Aubé, J.; Xu, L., Targeting the interaction between RNA-binding protein HuR and FOXQ1 suppresses breast cancer invasion and metastasis. *Communications Biology* 2020, *3*, 193. DOI: 10.1038/s42003-020-0933-1
- 11. Jana, S.; Adhikari, S.; Cox, M. R.; **Roy, S.**, Regioselective synthesis of 4-fluoro-1,5-disubstituted-1,2,3-triazoles from synthetic surrogates of α-fluoroalkynes. *Chemical Communications* **2020**, *56*, 1871–1874. DOI: 10.1039/C9CC09216A
- 12. Andrade, D.; Mehta, M.; Griffith, J.; Oh, S.; Corbin, J.; Babu, A.; De, S.; Chen, A.; Zhao, Y. D.; Husain, S.; Roy, S.; Xu, L.; Aube, J.; Janknecht, R.; Gorospe, M.; Herman, T.; Ramesh, R.; Munshi, A., HuR Reduces Radiation-Induced DNA Damage by Enhancing Expression of ARID1A. *Cancers* 2019, 11, 2014. DOI:10.3390/cancers11122014
- 13. Allegri, L.; Baldan, F.; **Roy, S.**; Aubé, J.; Russo, D.; Filetti, S.; Damante, G., The HuR CMLD-2 Inhibitor Exhibits Antitumor Effects via MAD2 Downregulation in Thyroid Cancer Cells. *Scientific Reports* **2019**, Article number: 7374. DOI: 10.1038/s41598-019-43894-0
- 14. Green, L.G.; Anthony, S. R.; Slone, S.; Lanzillotta, L.; Nieman, M. L.; Wu, X.; Robbins, N.; Jones, S. M.; Roy, S.; Owens, A. P.; Aubé, J.; Xu, L.; Lorenz, J. N.; Blaxall, B. C.; Rubinstein, J.; Benoit, J. B.; Tranter, M., Human Antigen R as a Therapeutic Target in Pathological Cardiac Hypertrophy. *JCI Insight* 2019; 4(4):e121541. DOI: 10.1172/jci.insight.121541
- 15. Spicer, T. P.; Gardiner, D. L.; Schoenen, F. J.; Roy, S.; Griffin, P. R.; Chase, P.; Scampavia, L.; Hodder, P.; Trenholme, K. R., Identification of Antimalarial Inhibitors Using Late-Stage Gametocytes in a Phenotypic Live/Dead Assay. *SLAS DISCOVERY: Advancing Life Sciences R&D* **2019**, *24*, 38–46. DOI: 10.1177/2472555218796410
- 16. **Roy, S.**; Motiwala, H. M.; Koshlap, K. M.; Aubé, J., Hexafluoroisopropanol and Acetyl Chloride Promoted Catalytic Hydroarylation with Phenols. *European Journal of Organic Chemistry* **2018**, 306–315. DOI: 10.1002/ejoc.201701256
- 17. Muralidharan, R.; Mehta, M.; Ahmed, R.; **Roy, S.**; Xu, L.; Aubé, J.; Chen, A.; Zhao, Y.; Herman, T.; Ramesh, R.\*; Munshi, A., HuR-targeted small molecule inhibitor exhibits cytotoxicity towards human lung cancer cells. *Scientific Reports* **2017**, *7*, Article number: 9694. DOI: 10.1038/s41598-017-07787-4
- 18. **Roy, S.\***; Sileikyte, J.; Neuenswander, B.; Hedrick, M. P.; Chung, T. D. Y.; Aubé, J.; Schoenen, F. J.\*; Forte M. A.\*; Bernardi, P.\*, *N*-Phenylbenzamides as Potent Inhibitors of the Mitochondrial Permeability Transition Pore. *ChemMedChem* **2016**, *11*, 283–288. DOI: 10.1002/cmdc.201500545 \*co-corresponding author
- 19. **Roy, S.**; Sileikyte, J.; Schiavone, M.; Neuenswander, B.; Argenton, F.; Aubé, J.; Hedrick, M. P.; Chung, T. D. Y.; Forte M. A.; Bernardi, P.; Schoenen, F. J., Discovery, Synthesis, and Optimization of Diarylisoxazole-3-carboxamides as Potent Inhibitors of the Mitochondrial Permeability Transition Pore. *ChemMedChem* **2015**, *10*, 1655–1671. DOI: 10.1002/cmdc.201500284 {Designated as *Very Important Paper (VIP)*}

- 20. **Roy, S.**; Sutivisedsak, N.; Hamper, B. C.; Lyss, A. M.; Spilling, C. D., A Practical and Scalable Synthesis of (*S*)- and (*R*)-1- (Dimethoxyphosphoryl)allyl Methyl Carbonates. *Synthesis* **2015**, *47*, 3669–3672. DOI: 10.1055/s-0035-1560487
- 21. Schroeder, C. E.; Yao, Y.; Sotsky, J.; Smith, R. A.; **Roy, S.**; Chu, Y-K, Guo, H.; Tower, N. A.; Noah, J. W.; McKellip, S.; Sosa, M.; Ramussen, L.; Smith, L. H.; White. E. L.; Aubé, J.; Jonsson, C. B.; Chung, D.; Golden, J. E., Development of (*E*)-2-((1,4-dimethylpiperazin-2-ylidene)amino)-5-nitro-*N*-phenylbenzamide, ML336: Novel 2 Amidinophenylbenzamides as Potent Inhibitors of Venezuelan Equine Encephalitis Virus. *Journal of Medicinal Chemistry* **2014**, *57*, 8608–8621. DOI: 10.1021/jm501203v
- 22. Sileikyte, J.; Roy, S.; Porubsky, P.; Neuenswander, B.; Wang, J.; Hedrick, M.; Pinkerton, A. B.; Salaniwal, S.; Kung, P.; Mangravita-Novo, A.; Smith, L. H.; Bourdette, D. N.; Jackson, M. R.; Aubé, J; Chung, T. D. Y.; Schoenen, F. J.; Forte M. A.; Bernardi, P., Small Molecules Targeting the Mitochondrial Permeability Transition. Probe Reports from the NIH Molecular Libraries Program. Submitted in April 2014; Peer-reviewed in July 2014. <a href="http://www.ncbi.nlm.nih.gov/books/NBK280049/">http://www.ncbi.nlm.nih.gov/books/NBK280049/</a>
- 23. Chung, D.; Schroeder, C. E.; Sotsky, J.; Yao, T.; **Roy, S.**; Smith, R. A.; Tower, N. A.; Noah, J. A.; McKellip, S.; Sosa, M.; Rasmussen, L.; White, E. L.; Aubé, J.; Golden, J. E., ML336: Development of Quinazolinone-Based Inhibitors Against Venezuelan Equine Encephalitis Virus (VEEV). Probe Reports from the NIH Molecular Libraries Program. Submitted in December 2012; Peer-reviewed in February 2013. http://www.ncbi.nlm.nih.gov/books/NBK179829/
- 24. **Roy, S.**; Spilling, C. D.\* "An Expeditious Total Synthesis of Both Diastereomeric Lipid Dihydroxytetrahydrofurans from *Notheia Anomala*" *Organic Letters* **2012**, *14*, 2230–2233. DOI: 10.1021/ol300597u
- 25. **Roy, S.**; Spilling, C. D., Synthesis of the C(18)-C(34) Fragment of Amphidinolide C and the C(18)-C(29) Fragment of Amphidinolide F. *Organic Letters* **2010**, *12*, 5326–5329. DOI: 10.1021/ol102345v
- 26. Ranu, B. C.; Banerjee, S.; **Roy, S.**, A Task Specific Basic Ionic Liquid, [BmIm]OH-promoted Efficient green and One-pot Synthesis of Tetrahydrobenzo[b]pyran Derivatives. *Indian Journal of Chemistry* **2008**, *47B*, 1108–1112. DOI: 10.1002/chin.200846133

# **PATENTS**

- 1. **Roy, S.**; Djugovski, M.; Huang, T.-Y., UM-51201-8220 Compounds for the Treatment of Retinitis Pigmentosa and Methods of Making and Using the Same. 63/510,709, provisional patent application filed on 6/28/2023.
- 2. **Roy, S.**; Berida, T.; Stallings, C. L.; Manning, D.L.; McKee, S., UM9470 Cysteine-based Peptidomimetics with Antimycobacterial and Antifungal Properties. 63/490,049, provisional patent filed on 3/14/2023.
- 3. **Roy, S.**, Berida, T.; Doerksen, R. J.; Stallings, C. L., and McKee, S.; Ducho, C. D., UM9470 Selective Agents Targeting Mycobacterium Tuberculosis. 63/267,357, patent filed on 1/31/2023.
- 4. Aubé, J.; **Roy, S.**; Xu, L.; Wu, X.; Lan, L., Inhibitors of RNA-Binding Proteins, Compositions Thereof, and Therapeutic Uses Thereof. 62/841,600, patent filed on 05/01/19.
- 5. **Roy, S.**; Bernardi, P.; Forte, M. A.; Schoenen, F. J.; Sileikyte, J., Small Molecule Inhibitors of the Mitochondrial Permeability Transition Pore (mtPTP). PCT Int. Appl. (2016), WO 2016073633 A1 20160512.

# **OUTREACH**

- 1. Hosted the following high school students for 4 weeks that participated in the ARISE@UM, A Research Immersive STEM Experience at the University of Mississippi, program
  - Participated in a zoom seminar, Summer 2020 & 2021 (in person activities canceled due to COVID-19)
  - Claire Cizdziel, Oxford High School, Summer 2019
  - Abigail Moeller, Excelsior Classical, Summer 2019
  - Lithika Polepalli, Mississippi School of Math and Science, Summer 2018
  - Sarena Patel, Mississippi School of Math and Science, Summer 2018
- 2. Participated in the UM Science Technology Engineering Math Summer Research Experience of Undergraduate Program (STEMS REU) as a sponsoring faculty and hosted the following students
- Matthew Saucier, University of Mississippi, Summer 2019
- Matthew Saucier, University of Mississippi, Summer 2018
- Peggy McCluggage, University of Mississippi, Summer 2018
- 3. Participated in the UM pharmacy SRFP, Summer Research Fellowship Program, as a sponsoring faculty and hosted the following students
- J.D. Olivet, University of Mississippi, Summer 2019

# **MEDIA**

# ChemComm Milestones – Sudeshna Roy, 03 Nov 2020

To celebrate the publication of Dr. Roy's first article in ChemComm (also her first independent research article), Harriet Kent interviewed about the research focus, the journey toward becoming a PI and setting up the lab, and what the future holds for the independent research into combating deadly bacterial infections.

# **Isom Center Fellowship Supports Innovative Research, 15 AUG 2023**

Announcement of recipients of 2023 Isom Center Fellowships. Dr. Roy's research into how tuberculosis and HIV treatment affect women and children is specifically called out as an interesting research opportunity opened by the new cross-disciplinary approach taken by the Isom Center.

#### **TEACHING EXPERIENCE**

University of Mississippi

1. PHCY 401: Foundations of BioMolecular Sciences I, 3 Credit Hours

Fall 2018, 107 Pharmacy Year I students. Instructor for 4 weeks

Fall 2019, 109 Pharmacy Year I students. Instructor for 4 weeks

Fall 2020, 98 Pharmacy Year I students. Instructor for 4 weeks

Fall 2021, 106 Pharmacy Year I students. Instructor for 4 weeks

Fall 2022, 77 Pharmacy Year I students. Instructor for 4 weeks

Fall 2023, 64 Pharmacy Year I students. Instructor for 2 weeks

2. PHCY 401 (Remediation): Foundations of BioMolecular Sciences I, 3 Credit Hours

Wint 2023, 1 Pharmacy Year I student. Instructor of record for 2weeks

3. MEDC 416: Medicinal Chemistry of Therapeutic Agents I, 3 Credit Hours

Fall 2018, 120 Pharmacy Year II students. Instructor for 2 weeks

4. MEDC 501: Advanced Medicinal Chemistry I, 3 Credit Hours

Fall 2018, 1 BioMolecular Sciences graduate student. Instructor for 4 weeks

Fall 2019, 5 BioMolecular Sciences graduate students. Instructor for 4 weeks

Fall 2020, 7 BioMolecular Sciences graduate students. Instructor for 4 weeks

Fall 2021, 5 BioMolecular Sciences graduate students. Instructor for 4 weeks

Fall 2022, 2 BioMolecular Sciences graduate students. Instructor for 4 weeks

Fall 2023, 3 BioMolecular Sciences graduate students. Instructor for 2 weeks

5. MEDC 714: Chemotherapeutic Agents, 3 Credit Hours

Spring 2019, 6 BioMolecular Sciences graduate students. Instructor of Record

# 6. MEDC 507: Organic Chemistry of Drug Synthesis, 3 Credit Hours

Spring 2020, 9 BioMolecular Sciences graduate students. Instructor of Record Spring 2022, 9 BioMolecular Sciences graduate students. Instructor of Record Spring 2024, 6 BioMolecular Sciences graduate students. Instructor of Record

# 7. PHCY 603: Professional studies in Integrated Systems – Genitourinary and Reproductive Health, 3 Credit Hours

Fall 2020, Pharmacy Year 3 students. Total contact time 4+ hours as an instructor

Fall 2021, Pharmacy Year 3 students. Total contact time 3+ hours as an instructor

Fall 2022, Pharmacy Year 3 students. Total contact time 3+ hours as an instructor

Fall 2023, Pharmacy Year 3 students. Total contact time 3+ hours as an instructor

# 8. BMS 610: Carbohydrates and Glycoconjugates, 3 Credit Hours

Spring 2023, Graduate course. Total contact time 3+ hours as an instructor

# University of Missouri-St. Louis, as a graduate student

1. Instructor of Organic Chemistry Laboratory Course

Summer 2012

2. Laboratory & Workshop Teaching Assistant for General Chemistry

Spring 2011, Fall 2007

3. Laboratory Teaching Assistant for Organic Chemistry

Summer-Fall 2010, Spring 2011

4. Laboratory & Workshop Teaching Assistant for General Chemistry

Spring 2008

# **CURRENT RESEARCH GROUP**

# **Graduate Research Assistants (duration, department)**

- 1. Mario Djugovski (Aug 2020–current, Medicinal Chemistry div in BioMolecular Sciences). Expected graduation May 2025.
- 2. Destinee Manning (Jul 2021–current, Medicinal Chemistry div in BioMolecular Sciences). Expected graduation May 2025.
- 3. Tzu-Yu Huang (Sept 2021–current, Medicinal Chemistry div in BioMolecular Sciences). Expected graduation May 2025.

#### **PAST MEMBERS**

#### Postdoctoral Research Associates (duration)

- 1. Sampad Jana (Mar 2018–Sept 2019)
- 2. Shamba Chatterjee (Apr 2018–May 2021)

#### **Graduate Students (time in lab, graduation date)**

- 1. Sweta Adhikari, M.S. (Jul 2017–Dec 2019) in Pharmaceutical Sciences with emphasis on Medicinal Chemistry *Thesis: A Study to Regioselectively Access Fluorinated Triazoles and Isoxazoles*
- 2. Hamdan Alferaei, M.S. (Jan 2020–Dec 2021) in Pharmaceutical Sciences with emphasis on Medicinal Chemistry *Thesis: Applications of Fluoronitroalkenes in 1,3-Dipoplar Cycloaddition and 1,4-Conjugate Addition*
- 3. Tomayo Berida, Ph. D. (Jul 2018–May 2023), in Pharmaceutical Sciences with emphasis on Pharmacognosy Dissertation: Development of Narrow-spectrum Agents & MraY Inhibitors Targeting Multidrug-resistant Mycobacterium tuberculosis
- 4. Benjamin Sawyer (Aug 2019–May 2024, Medicinal Chemistry div in BioMolecular Sciences). Expected graduation May 2024. \*Transfer student from Dr. Hoang Le's lab, who is now employed at NIH NIDA.

#### Associate R&D Staff

1. Sweta Adhikari (Jan 2020–Jun 2020)

- 2. Matt Saucier (Aug 2020-June 2021)
- 3. Peggy McCluggage (Aug 2020–June 2021)

#### Undergraduate Students (time in the lab, degree program, graduation date)

- 1. Hannah Chasteen (Aug-Dec 2017, B.S. in Forensic Chemistry, transferred)
- 2. Lilly Nguyen (Aug 2017–May 2018, B.S. in Biology, May 2020)
- 3. Galina Ostrovsky\* (Jan 2018–Nov 2018, B.A. in Biochemistry and Spanish, May 2019)
- 4. Jay D. Olivet\* (Jan 2018–May 2019, B.S. in Pharmaceutical Sciences, May 2020, transferred to Samford University)
- 5. Matthew Saucier\* (Jan 2018–May 2020, B.A. in Biochemistry, May 2020)
- 6. Peggy McCluggage\* (Jan 2018–May 2020, B.A. in Biochemistry, May 2020)
- 7. Micah Stewart\* (Jan 2019–May 2020, B.A. in Biochemistry, May 2020)
- 8. Emmanuel Hodges (Fall 2019, B.S. in Pharmaceutical Sciences, May 2021)
- 9. Micaela Shields\* (Aug 2020–Dec 2020, B.A. in Biochemistry, May 2023)
- 10. Lindsey Hohlt (Aug 2020-May 2021, B.S. in Pharmaceutical Sciences, May 2022)

#### **RESEARCH COMMITTEE MEMBER**

Type: Dissertation (duration, degree, department)

- 1. Amna Adam (Fall 2015–May 2020, Ph.D., Medicinal Chemistry div in BioMolecular Sciences)
- 2. Mohammed Hawwal (Fall 2016–May 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences)
- 3. Shukria Akbar (Fall 2016– May 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences)
- 4. Barbara I. Adaikpoh (Fall 2016–May 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences)
- 5. AyoOluwa O. Aderibigbe (Fall 2016–July 2021, Ph.D., Medicinal Chemistry div in BioMolecular Sciences).
- 6. Anthony Devdass (Fall 2017–May 2022, Ph.D., Inorganic div in Chemistry and Biochemistry)
- 7. Vijayan Sajith (Fall 2017 May 2022, Ph.D., Organic div in Chemistry and Biochemistry)
- 8. Nicholas Akins (Fall 2017–May 2021, Ph.D., Medicinal Chemistry div in BioMolecular Sciences)
- 9. Kayleigh Barlow (Spring 2018-current, Ph.D., Physical Chemistry div in Chemistry and Biochemistry)
- 10. Md Imdadul Khan (Fall 2018–November 2022, Ph.D., Medicinal Chemistry div in BioMolecular Sciences)
- 11. Christine Curiac (Fall 2018–November 2022, Ph.D., Organic div in Chemistry and Biochemistry)
- 12. Morgan Perkins (Fall 2018–November 2022, Ph.D., Physical Chemistry div in Chemistry and Biochemistry)
- 13. Megan Davis (Spring 2019–February 2023, Ph.D., Physical Chemistry div in Chemistry and Biochemistry)
- 14. Ravinder Kaur (Fall 2019–current, Ph.D., Organic div in Chemistry and Biochemistry)
- 15. Ashly Antony (Fall 2022-current, Ph.D., Inorganic div in Chemistry and Biochemistry)

Type: Thesis/Dissertation (duration, degree, department, graduation date)

- 1. Maali Alshammari (Spring 2017–May 2019, M.S. in Pharmaceutical Sciences, Medicinal Chemistry div in BioMolecular Sciences, May 2019)
  - Title: Synthesis of Fluoroflavones as Potential Neuroprotective Agents.
- 2. Ibrahim Almarabi (Spring 2017–May 2019, M.S. in Pharmaceutical Sciences, Pharmacognosy div in BioMolecular Sciences, May 2019)
  - Thesis Title: Phytochemical Investigations and Drug Interaction Potential of Cyanotis vaga (Luor.) Schult. & Schult. f.
- 3. Kyra Dodson (Fall 2016–Jul 2019, M.S. in Chemistry, Organic div Chemistry and Biochemistry, Dec 2019) *Title: Design Strategies for Histone Deacetylase Inhibitors.*
- 4. Sweta Adhikari (Fall 2017–Fall 2019, M.S. in Pharmaceutical Sciences, Medicinal Chemistry div in BioMolecular Sciences, Dec 2019)

<sup>\*</sup>Indicates Honors Program

- 5. Amna Adam (Fall 2015–April 2020, Ph.D. in Pharmaceutical Sciences, Medicinal Chemistry div in BioMolecular Sciences, April 2020)
  - Title: Application of Fluorinated Reagents in Synthesis and Drug Discovery.
- 6. Nicholas Akins (Fall 2017–May 2021, Ph.D., Medicinal Chemistry div in BioMolecular Sciences, April 2021) Dissertation Title: Design and Synthesis of Salvanorin-Based Compounds for the Opioid Receptors.
- 7. Shukria Akbar (Fall 2016–May 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences, April 2021) Dissertation Title: Responses of Predatory Myxobacteria to Preys Signalling Molecules & Features of a Pseudomonas Prey Avoiding Predation.
- 8. Barbara I. Adaikpoh (Fall 2016–May 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences, April 2021) Dissertation Title: Responses of Myxobacteria to Plant-Related Chemosignals Suggest Their Roles in the Rhizobiome.
- 9. Mohammed Hawwal (Fall 2016–Jul 2021, Ph.D., Pharmacognosy div in BioMolecular Sciences, April 2021) Dissertation Title: Isolation of Marker Compounds From Copaiba Essential Oil and Mimosa Pigra for Quality Evaluation of Dietary Supplements.
- 10. AyoOluwa O. Aderibigbe (Fall 2016–Jul 2021, Ph.D., Medicinal Chemistry div in BioMolecular Sciences, Jul 2021) Dissertation Title: Computational Studies of Non-Active Functional States of the Cannabinoid Receptor 1 and its Ligands.
- 11. Hamdan Alferaei (Spring 2020–Fall 2021, M.S. in Pharmaceutical Sciences, Medicinal Chemistry div in BioMolecular Sciences, Dec 2021)
- 12. Anthony Devdass (Fall 2017–May 2022, Ph.D., Inorganic div in Chemistry and Biochemistry, April 2022)

  Dissertation Title: Molecular Design of Transition Metal Complexes for Photocatalytic CO₂ reduction and Redox Mediation in Dye-Sensitized Solar Cells.
- 13. Vijayan Sajith (Fall 2017–May 2022, Ph.D., Organic div in Chemistry and Biochemistry, April 2022) Dissertation Title: Effect of Heterocycles on Biologically relevant Molecules.
- 14. Md Imdadul Khan (Fall 2018–December 2022, Ph.D., Medicinal Chemistry div in BioMolecular Sciences, November 2022)
  - Dissertation Title: Progress in Natural Product-Inspired Drug Discovery.
- 15. Christine Curiac (Fall 2018 December 2022, Ph.D., Organic div in Chemistry and Biochemistry, November 2022) Dissertation Title: Controlling Rate of Interfacial Electron Transfers via Synthetic Modulation of Organic Chromophores.
- 16. Morgan Perkins (Fall 2018–December 2022, Ph.D., Physical Chemistry div in Chemistry and Biochemistry, October 2022)
  - Dissertation Title: : Exploring Non-Covalent Interactions with Quantum Chemical Tools.
- 17. Tomayo Berida, Ph. D. (Jul 2018–May 2023), in Pharmaceutical Sciences with emphasis on Pharmacognosy Dissertation: Development of Narrow-spectrum Agents & MraY Inhibitors Targeting Multidrug-resistant Mycobacterium tuberculosis

Type: Honors College Thesis (degree program, graduation date)

- 1. Cassidy Baldwin (B.S. in Biology, May 2018)
  - Title: Techniques for the synthesis of difluorinated organic molecules using magnesium bases.
- 2. Matt Saucier (B.A. in Biochemistry with Minor in Biology, May 2020)
  - Title: Synthesis of Fluorinated Pyrazoles via Intra- and Intermolecular Cyclization Reactions.
- 3. Peggy McCluggage (B.A. in Biochemistry with Minor in Biology, May 2020) *Title: Design and Synthesis of Novel Analogs as Potential Antitubercular Agents.*
- 4. Micah Stewart (B.A. in Biochemistry with Minor in Biology, May 2020)
  - Title: Silver-Catalyzed Synthesis of Disubstituted Fluorinated Isoxazoles.
- 5. Eli Bettiga (B.A. in Biology with Minor in Biochemistry, May 2021)

  Title: Synthesis of Novel Long Chain Unsaturated Fatty Acids Analogs of Capsaicin.

# **SELECTED PROFESSIONAL PRESENTATIONS**

# 2024

• Roy, S. "Unlocking the Potential of 1,2,4-Triazolyl Derivatives as a New Treatment for Tuberculosis" Gordon Research Conference New Antibacterial Discovery and Development, Ventura, CA, Mar 2024 (Poster)

#### 2023

• Roy, S. "Crafting Small Molecules to Probe Biology and Treat Human Diseases" University of Nebraska at Omaha, Feb 2023 (*Invited Talk*)

#### 2022

- Roy, S. "Search for Narrow-spectrum Antibacterials & Ways to Access Fluorinated Molecules" 71st Southwest Regional Meeting (SWRM) of the American Chemical Society (SERMACS), Baton Rouge, LA, Nov 2022 (*Invited Talk*)
- Roy, S. "New Classes of Antimycobacterial Chemotherapeutics" Gordon Research Conference New Antibacterial Discovery and Development, Lucca, Italy, Jul 2022 (*Poster*)
- Roy, S. "Polarity Reversal and Functionalization of fluorinated alkenes" Gordon Research Conference Heterocycles, Newport, RI, Jun 2022 (*Poster*)
- Roy, S. "Crafting Small Molecules to Probe Biology and Treat Human Diseases" Saarland University, Germany, Jul 2022 (Invited Talk)
- Roy, S. "Crafting Small Molecules to Probe Biology and Treat Human Diseases" IQUIR-CONICET, Argentina, Apr 2022 (Invited Talk)
- Roy, S. "Crafting Small Molecules to Probe Biology and Treat Human Diseases" University of Illinois, Chicago, Jan 2022 (*Invited Talk*)

#### 2019

- Roy, S.; Jana, S.; Adhikari, S.; Cox, M. R. "Use of  $\alpha$ -Fluoronitroalkenes as a Synthetic Equivalent for Unstable Fluoroalkynes to Access 4-Fluoro-1,5-disubstituted-1,2,3-triazoles" Gordon Research Conference Heterocycles, Newport, RI, Jun 2019 (*Poster*)
- Roy, S.; Pandey, P.; Chatterjee, S.; Stallings, L. C.; Doerksen, R. J. "Structure-based Virtual Screening Approach to Identify Novel MraY Inhibitors for Tuberculosis Chemotherapy" Keystone Symposia on Tuberculosis: Mechanisms, Pathogenesis and Treatment (A3), Banff, Canada, Jan 2019 (*Poster*)

#### 2018

- Roy, S. "Small Molecule Tools in Chemistry and Biology" Invited Lecture, Department of Chemistry and Biochemistry, University of Mississippi, Apr 26, 2018 (*Talk*)
- Roy, S. "Small Molecule Tools in Chemistry and Biology" Invited Lecture, Chemistry Department, Jackson State University, Nov 16, 2018 (Talk)
- Roy, S. "Small Molecule Tools to Investigate Chemical and Biological Processes" Invited Lecture, Jan 2018 (Talk)
  - -Indian Association of Cultivation of Sciences, India
  - -Indian Institutes of Science Education and Research, India
  - -Jadavpur University, India
  - -National Institute of Pharmaceutical Education and Research, India

#### 2017

• Roy, S. "Small Molecule Tools to Investigate Chemical and Biological Processes" *Invited Lecture*, The University of Mississippi, Department of BioMolecular Sciences, Oxford, Mississippi, Mar 2017 (*Talk*).

#### 2015

• **Roy, S.** "Discovery and Optimization of Novel Inhibitors of the Mitochondrial Permeability Transition Pore" 25<sup>th</sup> International Society of Heterocyclic Chemistry Congress, Santa Barbara, Aug 2015 (*Talk*).

#### 2011

- **Roy, S**; Spilling, C. D. "Synthesis of the C(10)-C(17) Unit of Amphidinolides C, C2, & F, Potent Cytotoxic Macrolides" *Joint 46th Midwest and 39<sup>th</sup> Great Lakes Regional Meeting of the ACS*, St. Louis, Oct 2011 (*Poster*).
- **Roy, S.**; Spilling, C. D. "Stereoselective Synthesis of Tetrahydrofuran Rings: An Expeditious Entry to Epoxy Lipids from Australian Brown Alga" Abstracts of Papers, *242*<sup>nd</sup> ACS National Meeting, Denver, Aug 2011 (*Talk*).
- Roy, S.; Spilling, C. D. "Stereoselective Synthesis of Tetrahydrofuran Ring-Containing Biologically Active Natural Products" Graduate School Research Fair, UMSL, St. Louis, MO, (*Received an Award* in Ph.D. Natural Sciences Division) Apr 2011 (*Poster*).
- Roy, S.; Spilling, C. D. "Synthetic Studies toward Amphidinolide C & Amphidinolide F: Potent Cytotoxic Macrolides" *Invited Lecture*, University of Kalyani, West Bengal, India, Jan 2011 (*Talk*).

#### 2010

Roy, S.; Spilling, C. D. "Synthetic Studies toward Amphidinolide C & Amphidinolide F: Potent Cytotoxic Macrolides"
 Abstracts of Papers, 23<sup>rd</sup> Annual Organic Chemistry Day, Columbia, MO; Graduate School Research Fair, UMSL, St. Louis, MO, Apr 2010 (Poster).

#### 2009

- Roy, S.; Spilling, C. D. "Synthesis of the C(18)-C(34) Fragment of Amphidinolide C & the C(18)-C(29) Fragment of Amphidinolide F, Potent Cytotoxic Macrolides" 2009 Graduate School Research Fair, UMSL, St. Louis, MO, (Received the Sigma Xi Award as well as the First Place in Ph.D. Chemistry Division (Poster).
- Roy, S.; Spilling, C. D. "Synthesis of the C(18)-C (34) Fragment of Amphidinolide C & the C(18)-C(29) Fragment of Amphidinolide F, Potent Cytotoxic Macrolides" Abstracts of Papers, 238<sup>th</sup> ACS National Meeting, Washington DC, Aug 2009 (Talk).