SNEHA RAY, Ph.D.

Research Scientist | Drug Discovery | Structural & Mechanistic Enzymology

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PROFESSIONAL SUMMARY

Research scientist with over a decade of experience in preclinical drug discovery for neglected tropical diseases, with a focus on structure-based drug design, protein biochemistry, and mechanistic enzymology. Internationally recognized for original contributions to covalent inhibitor design and antiparasitic drug development. Personally profiled by ACS Chemical Biology in their "Introducing Our Authors" feature. Co-first author of high-impact publications in Cell Chemical Biology, Chemical Science, ACS Chemical Biology, and Biochemistry. Established peer reviewer for seven international scientific journals. Track record of leading multi-national collaborative drug discovery programs; research contributions directly enabled securing over $1.5M in research funding and a collaborative agreement with industry. Mentored graduate and undergraduate researchers across multiple institutions.

EDUCATION

Ph.D., Chemistry — University at Buffalo, State University of New York, USA *2013 – 2019*

- CGPA: 3.98 / 4.0. Awarded competitive Teaching Assistantship and full out-of-state tuition scholarship based on academic merit.

M.Sc., Analytical Chemistry — St. Joseph's University (Bangalore University), India *2010 – 2012*

- CGPA: 8.7 / 10.0. University Gold Medalist (graduated with the top score across the University in M.Sc. Chemistry).

PROFESSIONAL EXPERIENCE

Instructor — University of Texas Southwestern Medical Center, Dallas, TX *2024 – Present*

- Spearheading a multi-group, multi-national antimalarial drug discovery effort, advancing novel lead compounds from target validation through lead optimization.
- Designing and executing experiments for structural and mechanistic elucidation of target–ligand interactions to drive structure–activity relationship (SAR) development.
- Coordinating cross-functional collaboration with medicinal chemists, structural biologists, and parasitologists across multiple institutions.

Content Editor — Bio-protocol LLC *2024 – Present*

- Selected and analyzed scientific content for journal publication; edited submissions to ensure accuracy, clarity, and adherence to scientific standards.
- Collaborated with editors and contributing authors across diverse subfields of biochemistry and molecular biology.

Postdoctoral Researcher — University of Texas Southwestern Medical Center, Dallas, TX *2019 – 2024*

Advisor: Prof. Margaret A. Phillips

Antimalarial drug discovery — Plasmodium falciparum

- Engineered a CRISPR-based protein production strategy in P. falciparum, enabling the first heterologous purification of a complex parasite drug target.
- Determined inhibitor binding mode in a unique hydrophobic pocket using cryo-EM, supporting rational lead optimization.

- Generated foundational data underpinning over $1M in collaborative grant funding, a patent, and an industry collaboration.

Antitrypanosomal drug discovery — Trypanosoma brucei

- Identified and validated a druggable enzyme target in T. brucei; developed high-throughput enzymatic and cell-based inhibition assays.
- Triaged screening data and assessed enzyme panels for broad-spectrum antiparasitic potential.
- Developed a metabolite extraction procedure for downstream metabolomic analysis.

Research Assistant (Ph.D. Candidate) — University at Buffalo, SUNY, NY *2013 – 2019*

Advisor: Prof. Andrew S. Murkin

- Discovered the mechanism by which 3-nitropropionate acts as a covalent inhibitor of Mycobacterium tuberculosis isocitrate lyase (MtICL) — the first demonstration of this mechanism for any enzyme (published in ACS Chemical Biology, 2018).
- Characterized the kinetics and biophysics of MtICL inhibition using kinetic isotope effects (KIE), NMR, ESI-MS, and X-ray crystallography.
- Identified active-site catalytic residues through site-directed mutagenesis and KIE analysis; synthesized 18O-, 3H-, and 14C-labeled probe compounds.
- Research contribution directly enabled securing a half-million-dollar NSF grant.

Research Assistant — National Institute of Technology, Rourkela, India *2012 – 2013*

Advisor: Prof. Supratim Giri

- Synthesized amine-functionalized MCM-41 mesoporous silica nanoparticles for drug-delivery applications; studied release kinetics by UV/Vis and fluorescence spectroscopy.

AWARDS & HONORS

Competitive National & International Selections

- Selected to participate in RapiData 2025, Stanford Synchrotron Radiation Lightsource (SSRL), SLAC National Accelerator Laboratory — competitive international training program (2025).
- Recipient, Pacific Northwest Cryo-EM Center (PNCC) Grant — competitive national award supporting access to cryo-EM facilities (2023).
- Summer Research Fellowship, Indian Academy of Sciences — competitive national fellowship awarded to top science students across India (2011).

Institutional & Academic Honors

- Gold Medal in Chemistry, St. Joseph's College / Bangalore University — awarded to the top-scoring M.Sc. Chemistry graduate in the University (2012).
- UTSW Distinguished Postdoctoral Service Award, Nomination — Postdoctoral Association at UT Southwestern (2021).
- UTSW Postdoctoral Association Travel Award (Fall 2021).
- UTSW Certificate in Scientific Management (2023).
- Leadership Education Academy for Postdocs (LEAP) Training Certificate, UT Southwestern Graduate School of Biomedical Sciences (2021).
- Graduate Student Highlight selection, University at Buffalo — recognition for notable scholarly accomplishments (2018).
- GSEU Professional Development Award, University at Buffalo (2018).

- Mattern Tyler Award for Outstanding Teaching, Department of Chemistry, University at Buffalo (2016).
- GSEU Retention of Graduate Student Award for Academic Excellence, University at Buffalo (2015).
- Full Out-of-State Tuition Scholarship and Teaching Assistantship, University at Buffalo Department of Chemistry — awarded based on academic merit (2013).
- Undergraduate Merit Fellowship, St. Joseph's University (2007 – 2010).

ORIGINAL SCIENTIFIC CONTRIBUTIONS

- **First-ever demonstration of a novel covalent inhibition mechanism for an enzyme.** Discovered and characterized 3-nitropropionate as a masked-electrophile covalent inhibitor of Mycobacterium tuberculosis isocitrate lyase (MtICL) — establishing the nitro group as a novel masked electrophile, a mechanism not previously demonstrated for any enzyme. Published in ACS Chemical Biology (2018) and recognized as one of the top 20 most-downloaded articles in the journal.
- **Co-first-author discovery of species-selective, orally active proteasome inhibitors for malaria.** Co-led the identification and validation of piperidine carboxamides as reversible, orally active proteasome inhibitors with potent antimalarial activity. Published in Cell Chemical Biology (2024).
- **Novel framework for mechanism-based covalent inhibitor design.** Authored a Perspective in Biochemistry (2019) introducing new electrophiles and design strategies for targeted covalent inhibition — recognized by ACS Biochemistry as one of 2019's top-viewed papers.
- **Engineered protein-production strategy for a complex P. falciparum drug target.** Developed the first CRISPR-based heterologous expression and purification workflow for the target, enabling cryo-EM determination of inhibitor binding in a unique hydrophobic pocket — providing a foundation for next-generation antimalarial lead optimization.

RECOGNITION OF SCHOLARLY WORK

- **Featured Author Profile, "Introducing Our Authors," ACS Chemical Biology (2018)** — selected by the editors as one of six profiled authors of the journal's June 2018 issue. ACS Chem. Biol. 13, 1409–1411 (2018), DOI: 10.1021/acschembio.8b00523.
- **Top 20 Most-Downloaded Article, ACS Chemical Biology (May–June 2018)** — for "The Nitro Group as a Masked Electrophile in Covalent Enzyme Inhibition" (DOI: 10.1021/acschembio.8b00225). Recognition issued by Editor-in-Chief Prof. Laura L. Kiessling, July 2018.
- **One of 2019's Top-Viewed Papers, ACS Biochemistry** — for "New Electrophiles and Strategies for Mechanism-Based and Targeted Covalent Inhibitor Design," featured by the journal's official social media channel as a highlighted Perspective from the Mechanistic Enzymology Special Issue.
- **Independent acknowledgment for medicinal chemistry expertise** in Ullah et al., Journal of Antimicrobial Chemotherapy (2020), an antimalarial rate-of-kill study from Keele University, Liverpool School of Tropical Medicine, and UT Southwestern — credited by name for medicinal chemistry advice on a study of MMV Malaria Box compounds.
- **Graduate poster selected for SciMix, ACS Spring National Meeting (2018)** — competitive selection for the flagship multidisciplinary poster session of the American Chemical Society.
- **Graduate Student Highlight, University at Buffalo (2018)** — featured by the University at Buffalo Department of Chemistry for notable scholarly accomplishments.

PEER REVIEW SERVICE (JUDGING THE WORK OF OTHERS)

Invited expert reviewer for seven international peer-reviewed scientific journals across chemistry, biochemistry, infectious diseases, and biomedical research. Selected by editors based on demonstrated subject-matter expertise.

Total: 17 reviews for 7 publications.

- Springer Nature
- Scientific Reports (Springer Nature)
- Bio-Protocol
- Frontiers in Chemistry
- PLoS Neglected Tropical Diseases
- Canadian Journal of Infectious Disease
- Disease Markers

PEER-REVIEWED PUBLICATIONS

- Gahalawat, S., **Ray, S.**, … Phillips, M. A., Ready, J. M. "Optimization of Species-Selective Reversible Proteasome Inhibitors for the Treatment of Malaria." *J. Med. Chem.* 68, 21, 23485–23520 (2025).
- Banerjee, A., Brisco, T., **Ray, S.**, … Phillips, M. A., Smith, M. W. "Synthesis of the 5/5-Spiroindimicin Alkaloids: Development of a General Synthetic Approach and Biological Investigations." *Organic & Biomolecular Chemistry* 22, 9413–9425 (2024).
- Lawong, A.*, Gahalawat, S.*, **Ray, S.***, … Phillips, M. A. "Identification of Potent and Reversible Piperidine Carboxamides That Are Species-Selective Orally Active Proteasome Inhibitors to Treat Malaria." *Cell Chemical Biology* 31, 1–15 (2024). *Co-first authors.
- Zhang, Z., **Ray, S.**, … Phillips, M. A., Smith, M. W. "Total Synthesis of (+)-Spiroindimicin A and Congeners Unveils Their Antiparasitic Activity." *Chemical Science* 12, 10388–10394 (2021).
- **Ray, S.**, Murkin, A. S. "New Electrophiles and Strategies for Mechanism-Based and Targeted Covalent Inhibitor Design." *Biochemistry* 58 (52), 5234–5244 (2019). *Recognized as one of 2019's top-viewed papers by ACS Biochemistry.*
- **Ray, S.**, Kreitler, D. F., Gulick, A. M., Murkin, A. S. "The Nitro Group as a Masked Electrophile in Covalent Enzyme Inhibition." *ACS Chemical Biology* 13 (6), 1470–1473 (2018). DOI: 10.1021/acschembio.8b00225. *Top 20 most-downloaded ACS Chemical Biology article, May–June 2018.*

INVITED TALKS & CONFERENCE PRESENTATIONS

Invited & Selected Talks

- Structural Biology Work in Progress Meeting, Dallas, TX (2024, 2025)
- Structural Biology Interface Meeting, Dallas, TX (2025)
- Parasitology Work in Progress Meeting, Dallas, TX (2024)
- Molecular Parasitology Meeting, Woods Hole, MA (2021, 2024)
- Buffalo Protein Club, Hauptman-Woodward Institute, Buffalo, NY (2017)
- Organic Chemistry and Chemical Biology Seminar, University at Buffalo (2017)
- Ontario–Quebec Physical Organic Mini-Symposium, St. Catharines, ON, Canada (2016) — international audience

Selected Poster Presentations

- ACS Spring National Meeting (SciMix selection), New Orleans, LA (2018)

- Midwest Enzyme Chemistry Conference, Chicago, IL (2017)
- Enzyme Mechanisms Conference, St. Pete Beach, FL (2017)
- UTSW Biochemistry Symposium, Pegasus Park, Dallas, TX (2022, 2023)
- UTSW Biochemistry Retreat, Pottsboro, TX (2024)
- UB Graduate Student Symposium, Buffalo, NY (2015)

LEADERSHIP & PROFESSIONAL SERVICE

Chair, National Postdoctoral Appreciation Week (NPAW), UT Southwestern PDA *2021*

- Lead organizer of the National Postdoc Appreciation Week Symposium (Sept. 20–24, 2021), coordinating a week-long program of national-scope events and speakers.
- Managed correspondence and records for the PDA Executive Board.

Acting Vice-President, Postdoctoral Association at UT Southwestern *2021 – 2022*

- Organized multiple events promoting visibility of biomedical scientists in the local community.
- Contributed to institutional initiatives supporting postdoctoral career development.

Lab Safety Program Lead, Murkin Group, University at Buffalo *2015 – 2018*

- Planned and implemented lab-safety programs in compliance with Environmental, Health, and Safety (EHS) regulations.

MENTORSHIP & TEACHING

Mentor, Department of Biochemistry, UT Southwestern Medical Center *2021 – Present*

- Trained and supervised graduate students and research assistants in parasitic cell handling, enzyme purification, and assay development — from concept design through troubleshooting and data presentation.

Mentor, Research Foundation, University at Buffalo *2015 – 2018*

- Mentored graduate and undergraduate researchers in organic synthesis, enzyme purification, and assay development.

Teaching Assistant, Department of Chemistry, University at Buffalo *2013 – 2015*

- Supervised four undergraduate and graduate-level courses (10–50 students each) in advanced organic chemistry, reaction kinetics, and enzyme kinetics.
- Developed laboratory experiments, lectures, exams, and homework materials.

CERTIFICATIONS & PROFESSIONAL DEVELOPMENT

Research Compliance Training

- Human Subject Protection (HSP) Course (Researchers), CITI Program — University of Texas Southwestern Medical Center. Completed July 2024 (valid through July 2027).
- Research HIPAA, CITI Program — University of Texas Southwestern Medical Center. Completed July 2024.

Continuing Education

- Introduction to Python Nanocourse — Lyda Hill Department of Bioinformatics, UT Southwestern Medical Center (October 21–22, 2025).

TECHNICAL SKILLS

Biochemistry: Protein expression (bacterial, insect, parasite cells); chromatography (FPLC/HPLC); cryo-EM; X-ray crystallization; SDS-PAGE; enzyme kinetics; enzyme- and cell-based assay development; chemical library screening; kinetic and binding isotope effect (KIE/BIE) analysis.

Molecular Biology: CRISPR-based protein production; cloning; site-directed mutagenesis; DNA prep and electrophoresis; transformation; bacterial, insect, and parasite cell culture and harvesting.

Organic & Medicinal Chemistry: Synthesis of bioactive natural products; mechanism-based covalent inhibitor design; isotope-labeled probe synthesis; nanoparticle synthesis.

Analytical & Biophysical: 1D/2D NMR (1H, 13C); UV/Vis; fluorescence; FTIR; ESI-MS; ICP-MS; GE ÄKTA purification; stopped-flow kinetics; SEM; XRD; analytical ultracentrifugation; automated liquid handlers (Tecan, BioTek MultiFlo FX); automated Western blot; proteomics.

Computational & Programming: Python (scientific computing — UTSW Bioinformatics nanocourse, 2025); data handling and visualization; basic statistical analysis.

Professional: Multi-stakeholder project leadership; scientific writing; grant writing; international collaboration; mentorship; public speaking to international audiences.

References available on request.