IPSITA MOHANTY

+1 706-289-8326 ⋄ imm5615@psu.edu
Assistant Professor
Penn State, University Park, PA 16802

RESEARCH INTERESTS

Ipsita Mohanty, PhD, is an Assistant Professor of Pharmacology in the Departments of Veterinary and Biomedical Sciences and Nutrition. Her laboratory investigates the chemical language of host-microbiome communication by discovering and functionally characterizing previously unknown gut microbial metabolites that influence human health and disease. The Mohanty Lab integrates advanced untargeted LC-MS/MS metabolomics, proteomics, and integrated omics approaches with computational data science workflows to uncover novel microbial enzymes, decode metabolite transformation networks, and map how microbial chemistry shapes host physiology. A major focus is on microbially modified signaling molecules, including bile acids, indoles, carnitines, and acyl lipids, and to build large-scale computational metabolomics databases that link these molecules to diet, environment, aging, and human health and disease. Ultimately, the lab aims to generate an expansive spectral and mechanistic resource of microbial metabolites to enable new diagnostic, nutritional, and microbiome-based interventions that improve human health.

Key words: Untargeted LC-MS/MS metabolomics, data science, large-language models, structural elucidation, metagenomics, microbial metabolites, multi-omics, host signaling, aging, human diseases

POSITION

Assistant Professor of Pharmacology January 2026 - Present
Department of Veterinary and Biomedical Sciences
Department of Nutritional Sciences
Pennsylvania State University, Universitry Park, PA

Postdoctoral Researcher June 2022 - December 2025
Mentor: Dr. Pieter Dorrestein
University of California San Diego, San Diego, CA

EDUCATION

Doctor of Philosophy in Chemistry August 2017 - May 2022
PhD advisors: Dr. Vinayak Agarwal and Dr. Neha Garg
Georgia Institute of Technology, Atlanta, GA, CGPA: 3.42/4.00

Integrated Masters in Chemistry (B.Sc. and M.Sc.) August 2012 - May 2017
Drug Discovery (Micro Specialization)
Indian Institute of Technology, Kharagpur, India, CGPA: 8.77/10.00 (top of a class of 35)

GRANTS

NIH R21	Submitted my NIH R21 to the NIDDK in the February 2026 cycle. Pending Study Section Review
NIH K99/R00	Submitted my NIH K99/R00 to the National Institute of Aging (NIA) in the June 2024 cycle. Impact score: 28 (initial)/ 21 (resubmission). Pending Council Review

PUBLICATIONS

FIRST-AUTHOR

Mohanty, I., Xing, S., Castillo, V., Agongo, J., Patan, A., et al. (2026). MS/MS Mass Spectrometry Filtering Tree for Bile Acid Regio- and Stereoisomer Annotation. *ACS Analytical Chemistry*, 98(6), 4571-4584.

Mohanty, I., Mannochio-Russo, H., Abiead, Y. L., Schweer, J. V., Bittremieux, W., et al. (2024). The Underappreciated Diversity of Bile Acid Modifications. *Cell*, 187(7), 1801-1818.

Mohanty, I., Allaband, C., Mannochio-Russo, H., Abiead, Y. L., Hagey, L. R., Knight, R., Dorrestein, P. C. (2024). A Perspective: The changing metabolic landscape of bile acids, keys to metabolism and immune regulation. *Nature Reviews Gastroenterology and Hepatology*, 10.1038/s41575-024-00914-3.

Mohanty, I., Moore, S. G., Biggs, J. S., Freeman, C. J., Gaul, D. A., Garg, N., and Agarwal, V. (2021). Mass spectrometry-based stereochemical assignment and absolute abundance of non-proteinogenic amino acid homoarginine in marine sponges. *ACS Omega*, 48, 33200-33205.

Mohanty, I., Nguyen, N. A., Moore, S. G., Biggs, J. S., Gaul, D. A., Garg, N., and Agarwal, V. (2021). Enzymatic synthesis-assisted discovery of proline-rich macrocyclic peptides in marine sponges. *ChemBioChem*, 22, 1-6.

Mohanty, I., Tapadar, S., Moore, S. G., Biggs, J. S., Freeman, C. J., Gaul, D. A., Garg, N., and Agarwal, V. (2021). Presence of bromotyrosine alkaloids in marine sponges is independent of metabolomic and microbiome architectures. *mSystems*, 6(2), e01387-20.

Mohanty, I., Moore, S. G., Yi, D., Biggs, J. S., Gaul, D. A., Garg, N., and Agarwal, V. (2020). Precursor-guided mining of marine sponge metabolomes lends insight into biosynthesis of pyrrole-imidazole alkaloids. *ACS Chem. Biol.*, 15(8), 2185–2194.

Mohanty, I., Podell, S., Biggs, J. S., Garg, N., Allen, E. E., and Agarwal, V. (2020). Multi-omic profiling of *Melophlus* sponges reveals diverse metabolomic and microbiome architectures that are non-overlapping with ecological neighbors. *Mar. Drugs*, 18(2), 124.

CO-AUTHOR

Pilley, S. E., ..., **Mohanty, I.**, (12th author), et al. (2026). A metabolic atlas of mouse aging. *Cell Metabolism*,38, 399-418.

Abiead, Y. L., **Mohanty, I.**, et al. (2025). A Perspective on Unintentional Fragments and Their Impact on the Dark Metabolome, Untargeted Profiling, Molecular Networking, Public Data, and Repository Scale Analysis. *JACS Au*, 12, 5828–5850.

Kvitne, K. E., Zuffa, S. Z., Charron-Lamoureux, V., **Mohanty, I.**, et al. (2025). Fecal microbial and metabolic signatures in children with very early onset inflammatory bowel disease. *NPJ Biofilms Microbiomes*, 12(1):33.

Kvitne, K. E., Allaband, C., ..., **Mohanty, I.**, (8th author), et al. (2025). Environmental and maternal imprints on infant gut metabolic development. *Cell Host Microbe*, 33(12), 2130-2147.

Brennan, C.,..., **Mohanty, I.**, (4th author), et al. (2025). Streamlined extraction of nucleic acids and metabolites from low- and high-biomass samples using isopropanol and matrix tubes. *Microbiology Spectrum*, 13:e01912-25.

Tronel, A., Roger-Margueritat, M., Plazy, C., Cunin, V., **Mohanty, I.**, et al. (2025). Untargeted and semi-targeted metabolomics approach for profiling small intestinal and fecal metabolome using high-resolution mass spectrometry. *Metabolomics*, 21(4), 84.

Ramos, S. F., Siguenza, N., Zhong, W., **Mohanty, I.**, Lingaraju, A., et al. (2025). Metatranscriptomics uncovers diurnal functional shifts in bacterial transgenes with profound metabolic effects. *Cell Host Microbe*, 33(7), 1057-1072.

Mannochio-Russo, H., Charron-Lamoureux, V.,....**Mohanty, I.**, (15th author)....., et al. (2025). The microbiome diversifies long-to short-chain fatty acid-derived N-acyl lipids. *Cell*, 188(15), 4154-4169.

Bae, H., Jung, S.,....**Mohanty, I.**, (13th author)....., et al. (2025). Cross-organ metabolite production and consumption in healthy and atherogenic conditions. *Cell*, 188(16), 4441-4455.

Abiead, Y. L., Strobel, M.,....**Mohanty, I.**, (13th author)....., et al. (2025). Enabling pan-repository reanalysis for big data science of public metabolomics data. *Nat. Comm.*, 16, 4838.

Abiead, Y. L., Rutz, A.,....**Mohanty, I.**, (13th author)....., et al. (2025). Discovery of metabolites prevails amid in-source fragmentation. *Nat. Metab.*, 7, 435-437.

Brennan, C., Belda-Ferre, P., Zuffa, S., Charron-Lamoureux, V., **Mohanty, I.**, Ackermann, G., Allaband, C., et al. (2024). Clearing the plate: A strategic approach to mitigate well-to-well contamination in large-scale microbiome studies. *mSystems*, 9:e00985-24.

Lee, M. H., Nuccio, S. P., **Mohanty, I.**, Hagey, L. R., Dorrestein, P. C., Chu, H., Raffatellu, M. (2024). How bile acids and the microbiota interact to shape host immunity. *Nature Reviews Immunology*, 10.1038/41577-024-01057-x.

Tang-Wing, C., **Mohanty, I.**, Bryant, M., Makowski, K., Melendez, D., et al. (2024). Impact of diet change on the gut microbiome of common marmosets (*Callithrix jacchus*). *mSystems*, 9:e00108-24.

Zhong, W., Olugbami, J. O., Rathakrishnan, P., **Mohanty, I.**, Moore, S. G., et al. (2024). Discovery and folding dynamics of a fused bicyclic cysteine knot undecapeptide from the marine sponge *Halichondria bowerbanki*. *The Journal of Organic Chemistry*, 89(17), 12748-12752.

Zhong, W., Deutsch, J. M., Yi, D., Abrahamse, N. H., **Mohanty, I.**, Moore, S. G., McShan, A. C., Garg, N., and Agarwal, V. (2023). Discovery and biosynthesis of ureidopeptide natural products macrocyclized via indole N-acylation in marine *Microbulbifer* spp. bacteria. *ChemBioChem*, e202300190.

Nguyen, N. A., Lin, Z., **Mohanty, I.**, Garg, N., Schmidt, E. W., and Agarwal, V. (2021). An obligate peptidyl brominase underlies the discovery of highly distributed biosynthetic gene clusters in marine sponge microbiomes. *J. Am. Chem. Soc.*, 143(27), 10221-10231.

PREPRINTS

Xing, S., ..., **Mohanty, I.**, (9th author), et al. (2026). Navigating the conjugated metabolome. *bioRxiv*; doi: 10.64898/2026.02.06.704496.

Patan, A., ..., **Mohanty, I.**, (9th author), et al. (2026). Navigating the conjugated metabolome. *bioRxiv*; doi: 10.1101/2025.11.18.689170.

Gouda, H., ..., **Mohanty, I.**, (12th author), et al. (2025). Learning molecular fingerprints of foods to decode dietary intake. *Research Square*; doi: 10.21203/rs.3.rs-7652253/v1.

Mannochio-Russo, H., ..., **Mohanty, I.**, (8th author), et al. (2025). Bridging Complexity and Accessibility in Metabolomics with MetaboApps. *ChemRxiv*; doi: 10.26434/chemrxiv-2025-3nq29.

CONTRIBUTIONS TO SCIENCE

Chemical profiling of marine sponges using mass spectrometry

Marine sponges are prolific producers of bioactive natural products, yet traditional discovery strategies have relied on large-scale "grind-and-find" isolation from kilograms of biomass. Regulatory changes and limited access to biomass have increasingly constrained these approaches. During my Ph.D. training, I developed and applied LC-MS/MS-based untargeted metabolomics to enable the discovery of sponge-derived natural products from sub-gram quantities of biomass, overcoming these limitations. Conventional natural product discovery is dominated by reverse-phase chromatographic methods that preferentially capture non-polar secondary metabolites, leading to systematic under-representation of polar biosynthetic intermediates. To address this gap, I implemented polar LC-MS/MS untargeted metabolomics workflows to identify previously inaccessible metabolites involved in natural product biosynthesis. Using this approach, I discovered and characterized L-homoarginine as a previously undescribed but essential intermediate in the biosynthesis of pyrrole-imidazole alkaloids (Mohanty, ACS Chem Biol, 2020). By designing experiments around appropriate positive and negative control sponge species and applying statistically robust metabolomics analyses, I linked these intermediates to specific biosynthetic pathways. This enabled the formulation of testable biosynthetic schemes, providing a foundation for subsequent genomic and transcriptomic mining of biosynthetic enzymes. Collectively, this work established a precursor-guided discovery strategy, in which biosynthetic intermediates-rather than final products alone-serve as entry points for natural product discovery. I extended this framework to other chemical classes in sponges and demonstrated how untargeted metabolomics can function as a discovery-first tool to reveal biosynthetic logic, broadly applicable to enzyme discovery and metabolite-driven pathway elucidation (Mohanty, mSystems, 2021; Mohanty, ChemBioChem, 2021).

Paired omics using metabolomics and 16S and whole-genome sequencing data

To move beyond single-omic descriptions of microbiomes, I integrated untargeted metabolomics with 16S rRNA gene and whole-genome sequencing data to establish functional links between microbial communities and metabolic outputs. Using paired omics analyses, I identified significant correlations between microbial taxa and metabolite features, demonstrating that microbial community composition plays a key role in shaping the overall metabolome,

even when global variation is modest (Mohanty, Mar. Drugs, 2020). These analyses were grounded in carefully designed positive and negative controls and supported by statistically robust correlation frameworks, enabling hypothesis generation around microbe-associated metabolic pathways. This paired-omics strategy emphasizes functional interpretation over taxonomic association alone and provides a generalizable framework for linking microbial ecology to biochemical phenotypes. Such approaches are now central to human microbiome research, where integrated microbiome-metabolome analyses have revealed disease-associated metabolic signatures and highlighted microbe-derived bile acids as key mediators of host-microbe interactions, particularly in inflammatory bowel disease. Recent studies combining microbiome profiling with metabolomics have shown that alterations in microbial community structure are associated with shifts in primary and secondary bile acid pools, linking dysbiosis to changes in host signaling, inflammation, and disease severity. Together, this work established a foundation for applying paired omics to uncover mechanistic microbe-metabolite relationships, with direct relevance to human disease and metabolism.

Discovery of novel bile acids by mining large-scale metabolomics data in public repositories

Bile acids are steroidal molecules regulating glucose metabolism and energy homeostasis, and are implicated in diseases including diabetes, obesity, and inflammatory bowel disease. Synthesized in the liver, bile acids are extensively modified by gut microbes, greatly expanding their chemical and functional diversity. Prior work using mass spectrometry identified over 150 microbially modified bile acids, establishing microbial bile acid metabolism as an underexplored axis of host-microbe communication. Building on this foundation, I applied MassQL (Mass Spectrometry Query Language), a computational framework for mining untargeted LC-MS/MS data for user-defined structural and fragmentation patterns, to expand bile acid chemical space. Using MassQL-based searches, I increased the bile acid modification pool from hundreds to thousands of candidate structures, revealing a broad diversity of microbial bile acid transformations. The MS/MS spectra of these candidate bile acids were curated into a publicly available spectral library, enabling reproducible detection (Mohanty, Cell, 2024; Mohanty, Nat. Rev. Gastroenterol. Hepatol., 2024; Mohanty, ACS Anal Chem, 2026). To provide biological context, I integrated curated metadata with standardized ontologies through ReDU (Reanalysis of Data User Interface) to associate subsets of candidate bile acids, including polyamine-amidated bile acids, with diet and disease states. In parallel, I used MASST (Mass Spectrometry Search Tool) to match candidate bile acid spectra against microbial reference datasets, supporting a microbial origin of specific bile acid modifications. My postdoctoral work established the first scalable, data-driven framework for bile acid discovery, integrating spectral mining, curated reference libraries, metadata harmonization, and repository-scale searching.

Leveraging public data with associated metadata for biological insights

Meta-analysis of large-scale public datasets enables powerful biological discovery beyond the scope of individual studies. While not yet routinely applied in metabolomics, we lead major efforts to develop tools, standards, and platforms that enable repository-scale re-analysis and cross-study integration. As a contributor and beta tester, I played an active role in shaping a pan-repository ecosystem that leverages standardized metadata and harmonized ontologies to uncover biologically meaningful patterns across thousands of datasets. This experience positioned me to apply meta-analysis as a discovery-driven approach, transforming fragmented public metabolomics data into interpretable biological insights.

HONORS/AWARDS

Elected Co-chair, Gordon Research Seminar(GRS) Metabolomics and Human Health March 2027

Best poster presentation, GRS Metabolomics and Human Health February 2025

Title: To separate or not to separate: MS/MS fragmentation-based uncoupling of bile acid isomers.

Early Career Rising Star Award, Metabolomics Association of North America October 2024

Invited talk title: MS2-fragmentation based filters reveal bile acid patterns in biology.

Invited speaker at Basic Science Emerging Topic Conference, Digestive Disease Week (DDW), Washington, D.C. May 2024

Title: Advancing Mass Spectrometry Insights in Metabolic Disorders and Liver Diseases

Invited speaker at American Gastroenterological Association session "Navigating the Microbial Landscape for Precision Nutrition", Digestive Disease Week (DDW), Washington, D.C. May 2024

Title: Impact of diet on microbial metabolites

Best oral presentation, Georgia Tech Chemistry graduate student retreat October 2021

Title: Querying the chemodiversity in marine sponges using mass spectrometry-based metabolomics

Outstanding student oral presentation, SIMB annual meeting August 2021

Title: Discovery of the non-proteinogenic amino acid homoarginine provides a key to unlock cryptic natural product biosynthetic pathways

Bagwell Undergraduate Research Mentor Fellowship August - December 2021

Department of Chemistry and Biochemistry, Georgia Tech

Best poster presentation, Georgia Tech Chemistry graduate student retreat November 2020

Title: Discovery of the non-proteinogenic amino acid homoarginine provides a key to unlock cryptic natural product biosynthetic pathways

Best oral presentation, 7th Annual Southeastern Biogeochemistry Symposium March 2020

Title: Multi-omic profiling of Melophlus sponges reveals diverse metabolomic and microbiome architectures that are non-overlapping with ecological neighbors

Best oral presentation, Georgia Tech Chemistry graduate student retreat October 2019

Title: Exploring the marine sponge-derived meroterpenoid chemistry using '-Omics' based approaches

William H. Emerson Fellowship August 2017 - May 2019

Department of Chemistry and Biochemistry, Georgia Tech

Institute silver medal May 2017

Department of Chemistry, IIT Kharagpur

Mitacs Globalink Fellowship May - July 2016

Mitacs Canada, Simon Fraser University Burnaby

Inspire SHE Scholarship August 2012 - May 2017

Department of Science and Technology, Government Of India

CONFERENCES

CHAIR

GRS Metabolomics and Human Health February 2025

Discussion leader at session: Assessing the Metabolome and Integration with other -Omics Technologies

MANA 6th Annual Conference October 2024

Chair at session: Single Cell Organisms and Microbiomes

ORAL PRESENTATIONS

MANA 6th Annual Conference October 2024

Oral talk title: Diving deeper into the bileome: MS2 fragmentation-based filtering identifies bile acid regio- and stereoisomers to reveal unique patterns in biology

Annual meeting Digestive Disease Week May 2024

Invited talk session 1: American Gastroenterological Association
Invited talk session 2: AASLD: Basic Science Emerging Topic Conference

MANA 5th Annual Conference October 2023

Oral talk title: Underappreciated diversity of bile acids: Hidden in plain sight

GRS Metabolomics and Human Health March 2023

Oral talk title: The underappreciated diversity and function of bile acid modifications

2021 SIMB annual meeting August 2021

Oral talk title: Discovery of the non-proteinogenic amino acid homoarginine provides a key to unlock cryptic natural product biosynthetic pathways

7th Annual Southeastern Biogeochemistry Symposium March 2020

Oral talk title: Multi-omic profiling of Melophlus sponges reveals diverse metabolomic and microbiome architectures that are non-overlapping with ecological neighbors

POSTER PRESENTATIONS

GRS and GRC Metabolomics and Human Health February 2025

Poster title: To separate or not to separate: MS/MS fragmentation-based uncoupling of bile acid isomers.

72nd ASMS Conference on Mass Spectrometry and Allied Topics June 2024

Poster title: To separate or not to separate: MS/MS fragmentation-based uncoupling of bile acid regio- and stereoisomers.

GRC Metabolomics and Human Health March 2023

Poster title: The underappreciated diversity of bile acid modifications

4th International Conference on Natural Product Discovery and Development in the Genomic Era, SIMB February 2023

Poster title: Integrated analysis of public untargeted metabolomics data reveals underappreciated diversity of bile acids

69th ASMS Conference on Mass Spectrometry and Allied Topics November 2021

Poster title: Querying the chemodiversity in marine sponges using mass spectrometry-based metabolomics

Atlanta Athens Mass Spectrometry Discussion Group Symposium September 2019

Poster title: Exploring the marine sponge-derived meroterpenoid natural product chemistry using '-Omics' based approaches

Emory Microbiome Research Centre Symposium August 2019

Poster title: Exploring the marine sponge-derived meroterpenoid natural product chemistry using '-Omics' based approaches

TEACHING/WORKSHOPS

WORKSHOPS

Presented on MassQL at the MANA interest group Software and Data Exchange (SODA) workshop conducted on zoom — July 2024

Presented and conducted a workshop on GNPS workflows at the MANA 5th Annual Conference. — October 2024

Presented on GNPS dashboard and MassQL at the 2023 SIMB conference. — February 2023

UNIVERSITY TEACHING

Instructor, Research Practice in VBSC (VBSC 415), Penn State — January 12, 2026 - present

Guest Lecture, Childhood Obesity (Nutrition 532), Penn State — February 2, 2026

Special Lecture, Bioinformatics for Immunologists (BGGN 239), UCSD — June 2, 2025

Teaching assistant for Biochemistry lab II, Georgia Tech — January - April 2020

Teaching assistant for organic synthesis laboratory, Georgia Tech — May - December 2019

MENTORING

Mentor, Womxn in Metabolomics (WomiX) 2025 Mentorship Program — March 2025 - present

Mentor to more than 10 undergraduate students, University of California San Diego — August 2023 - May 2024

Mentor to 5 undergraduate students, Georgia Tech — August 2020 - May 2022

Student mentor, IIT Kharagpur — August 2016 - May 2017

LEADERSHIP/COMMUNITY ENGAGEMENT

Interest groups, Metabolomics Association of North America (MANA) — January 2024 - January 2025
Council member in the Early Career Member Council. Organized the largest Early Career Members networking event at the 6th Annual MANA conference with more than 80 participants. Led a recruiter roundtable event for early-career researchers with 38 attendees. I am also a member of the Womxn in Metabolomics group. Part of the special interest group aimed at fostering communication between women researchers in metabolomics.

Executive board, Postdoctoral Association, UCSD — August 2023 - August 2025
As co-vice chair of community engagement, I organize career fairs and networking events for postdocs at UCSD. Along with the team, I organized an industry networking event with 200 postdocs in attendance in March 2024.

Postdoctoral Association, UCSD — June 2023, December 2022
Volunteered for a science outreach program in a San Diego junior school

Junior STEM, Georgia Tech — January - April 2020
Volunteered for Junior STEM's "STEP INTO STEM" science outreach program

Centre for Chemical Evaluation (CCE), Georgia Tech — October 2020
Volunteered at CCE's Buzz on Biotech initiative and demonstrated science experiments to middle school students

Asha for Education, Georgia Tech — October 2020
Served as President of the Atlanta chapter and volunteered in fundraising events and Georgia Tech game day concessions. Volunteered at the At-Promise youth and community center, supported by the Atlanta Police Foundation.