IPSITA MOHANTY

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RESEARCH INTERESTS

I take a multi-pronged approach that combines **LC-MS/MS-based untargeted metabolomics, big data mining from public repositories, and structural elucidation using fragmentation spectra** to decode how microbial metabolites influence host signaling pathways. During my doctoral research, I mapped the diverse microbial communities of marine sponges and uncovered structurally unique molecules produced by the sponge-microbe holobiont. As a postdoctoral researcher in the Dorrestein lab, I use mass spectrometry-based computational tools to discover novel microbial metabolites from large-scale public repositories of untargeted LC-MS/MS data. In my own research group, I aim to identify previously unknown microbial metabolites, such as bile acids and other steroids, that play critical roles in aging and its associated diseases. Through extensive collaborations, I will integrate mechanistic studies in animal models to elucidate how these microbial metabolites function as communication signals between microbes and their hosts.

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

EDUCATION

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

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)

SKILLS

Grantsmanship	Submitted my NIH K99/R00 to the National Institute of Aging (NIA) in the June 2024 cycle. Impact score: 28 (initial)/ 21 (resubmission).
Computational skills	Big data mining, MS/MS data acquisition and analysis, Structure elucidation using computational tools, Spectral database generation, Linux, R scripting
Wet lab skills	DNA extraction, Polymerase Chain Reaction (PCR), Gel electrophoresis, Restriction enzyme digestion, Cloning, Protein purification using FPLC, sample preparation for mass spectrometry analysis, organic synthesis
Software	Bruker data analysis, Thermo Xcalibur, GNPS, Qiita, QIIME2, Illustrator, Origin
Soft skills	Peer-reviewed 10 manuscripts, Teamwork, Leadership, Interpersonal skills, Effective scientific communication

PUBLICATIONS

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.

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.

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.

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.

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.

PREPRINTS

Mohanty, I., Xing, S., Castillo, V., Agongo, J., Patan, A., et al. (2025). MS/MS mass spectrometry filtering tree for bile acid isomer annotation. *bioRxiv*; doi: 10.1101/2025.03.04.641505.

Zuffa, S. Z., ..., **Mohanty, I.**, (6th author), ..., Dorrestein, P. C. (2025). Empirically establishing drug exposure records directly from untargeted metabolomics data. *bioRxiv*; doi: 10.1101/2025.04.28.651123.

Kvitne, K. E., Zuffa, S. Z., Charron-Lamoureux, V., **Mohanty, I.**,..., Dorrestein, P. C. (2025). Fecal Microbial and Metabolic Signatures in VEO-IBD: Implications for Unique Pathophysiology. *bioRxiv*; doi: 10.1101/2025.04.26.650779.

Zhao, H. N., ..., **Mohanty, I.**, (31st author), ..., Dorrestein, P. C. (2024). Empirically establishing drug exposure records directly from untargeted metabolomics data. *bioRxiv*; doi: 10.1101/2024.10.07.617109.

PROJECTS

Exploring the diversity of bile acids using mass spectrometry-based tools June 2022 - Present
Postdoctoral project; Dr. Pieter C. Dorrestein
Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego

- Using data patterns in the MS/MS fragmentation spectra selective to bile acids, 5576 putative bile acids were discovered from public untargeted LC-MS/MS fragmentation data available in the GNPS/MassIVE repository. The bile acid-specific MS/MS spectra extracted from the repository were added to a spectral resource available for researchers to accelerate the discovery of novel bile acids and their potential biological functions.
- I developed a workflow that utilizes the ratios of relative intensities of diagnostic MS/MS fragment ions to design filters capable of distinguishing between regio- and stereoisomers of bile acids. This method is compatible with MS/MS fragmentation spectra from any LC-MS/MS dataset, including previously acquired data, significantly reducing the need for synthesizing multiple bile acid isomers for validation studies. Serving as a proof of concept, this approach can be expanded to distinguish other metabolite isomers.

Chemical profiling of marine sponges with multi-omics based approaches August 2017 - May 2022
Doctoral thesis project; Dr. Vinayak Agarwal and Dr. Neha Garg
Department of Chemistry and Biochemistry, Georgia Tech

I employed LC-MS/MS metabolomics and 16S sequencing-based tools to explore the chemical and biological diversity of small organic molecules (natural products) found in marine sponges and their bacterial symbionts. My research examined the chemical diversity of under-studied sponges and discovered many novel analogs. I have also pursued the isolation, structural characterization and biochemical reconstitution of the biosynthetic pathway for novel natural products.

Characterization of the polar character of azaenediynes August 2016 - May 2017
Master thesis project; Dr. Amit Basak
Department of Chemistry, IIT Kharagpur

I studied the regioselectivity in addition of nucleophiles to the p-benzyne intermediates derived from unsymmetrical aza-substituted enediynes via Bergman cyclization using experimental and computational analyses. I specifically synthesized the azaenediynes intermediates in the Bergman cyclization reaction using multi-step total synthesis.

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

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 - TBD

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 - present
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 - present
Serving as the co-vice-chair of community engagement, I organize career fairs and networking events for postdocs at UCSD. Along with the team I organized a indutry networking event with 200 postdocs in attendance in March 2024.

Postdoctoral Association, UCSD June 2023, December 2022
Volunteered for science outreach program in 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 fund-raising events and Georgia Tech game day concessions. Volunteered at the At-Promise youth and community center supported by Atlanta Police foundation.