# Sanjay Iyer

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## RESEARCH

Developed Artificially Intelligent (AI) workflows that leverage Large Language Models (LLMs) to guide users and streamline chemical analyses, integrating Python scripts for process automation alongside evolutionary and Bayesian optimization algorithms for efficiently exploring complex experimental search spaces.

## RESEARCH EXPERIENCE

**Graduate Research Assistant, Purdue University** **08/2020 – Present**

- Pioneered the first LLM-powered AI Agent end-to-end workflow with real-time quality control for chip-based nanoESI-MS/MS
- Implemented an AI-driven evolutionary algorithm approach to optimize HPLC/$MS^2$ parameters for complex mixture separation
- Spearheaded the development of CLAW (Comprehensive Lipidomic Automation Workflow) for large scale lipidome profiling using mass spectrometry with multiple reaction monitoring (MRM)
- Engineered an automated analysis script and algorithm for online liquid chromatography ozone electrospray ionization (LC–OzESI)-MRM to identify double bond locations in both mono- and polyunsaturated fatty acids
- Architected AI agents within CLAW to guide users through both traditional MRM and OzESI analyses, facilitating species-level profiling and double bond localization
- Constructed Docker-based microservices for a closed-loop optimization workflow powered by blockchain infrastructure
- Automated the optimization of experimental parameters in pulsed neutral reagent introduction for tandem mass spectrometry, leveraging diagnostic gas-phase ion-molecule reactions
- Implemented multi-objective optimization in a continuous flow reaction using Bayesian Optimization to simultaneously balance multiple performance metrics

## WORK EXPERIENCE

**Purdue University, West Lafayette, IN** **08/2020 – Present**
**Teaching Assistant**

- Assisted in designing Python-based lessons for advanced physical chemistry lab courses (CHM 37301 and 37401), utilizing libraries such as NumPy, Pandas, and Matplotlib.

**Kaleido Biosciences Lexington, MA** **01/2019 – 07/2020**
**Research Associate II**

- Developed and validated advanced GCMS methods for analyzing microbiome metabolic therapies (MMTs) and authored supporting SOPs and Certificates of Analysis.
- Characterized MMTs for patent applications and managed batch closures for ten production campaigns.
- Processed over 1,000 samples and ensured operational efficiency of GCMS and LC systems.

**Vertex Pharmaceutical, Boston, MA** **08/2018 – 01/2019**
**Research Associate I**

- Conducted analysis and method development on drug substance ensuring compliance with cGMP standards and quality control.
- Maintained and troubleshot GC-MS systems to deliver accurate and reliable analytical results.

**Cabot Corporation, Billerica, MA** **12/2017 – 07/2018**
**Research Associate I**

- Conducted GC-MS analysis of over 300 carbon black samples across seven global production sites

**PUBLICATIONS**

1. Iyer, S.; Beveridge, C.; Randolph, C. E.; Muhoberac, M.; Manchanda, P.; Walker, K. A.; Tichy, S.; Chopra, G. CLAW-MRM: Comprehensive Lipidomics Automation Workflow for Multiple Reaction Monitoring Using Large Language Models. *Analytical Chemistry* 2025, 97 DOI: 10.1021/acs.analchem.4c05039.
2. **Iyer, S.;** Beck, A. G.; Fine, J.; Chopra, G. *Paddy: An Evolutionary Optimization Algorithm for Chemical Systems and Spaces*. Digital Discovery 2025, 4 (5), 1352–1371. https://doi.org/10.1039/D4DD00226A**.**
3. Beveridge, C.; Muhoberac, M.; **Iyer, S**.; Randolph, C.; Tichy, S.; Chopra, G. *Automating Lipidomics Experiments and Analysis using Large Language Models*. (In preparation)
4. Randolph, C. E.; Manchanda, P.; Beveridge, C.; **Iyer, S**.; Sharma, K.; Poad, B. L. J.; Blanksby, S. J.; Tichy, S.; Chopra, G.* *Brain Region-specific Deep Profiling of Lipid Droplets Reveal Compositional Differences in Alzheimer's Disease and Aging*. (In preparation)
5. Anyaeche, R. O.; Beck, A.; Wijewardhane, P.; **Iyer, S**.; Fu, Y.; Liu, J. K.-Y.; Zhang, J.; Alzarieni, K. Z.; Feng, E.; Hilger, R. T.; Welch, C.; Kenttämaa, H. I.; Chopra, G. *Machine Learning-Guided Automated HPLC/MS2 Platform Based on Diagnostic Gas-phase Ion-molecule Reactions for Structural Characterization of Unknown Compounds in Mixtures*. (In preparation)
6. Randolph, C. E.; Manchanda, P.; Arora, H.; **Iyer, S**.; Saklani, P.; Beveridge, C.; Chopra, G. *Mass Spectrometry-Based Single-Cell Lipidomics: Advancements, Challenges, and the Path Forward*. TrAC, Trends Anal. Chem. 2023.
7. Dunlap, J. H.; Ethier, J. G.; Putnam-Neeb, A. A.; **Iyer, S**.; Luo, S.-X. L.; Feng, H.; Torres, J. A. G.; Doyle, A. G.; Swager, T. M.; Vaia, R. A.; Mirau, P.; Crouse, C. A.; Baldwin, L. A. *Continuous Flow Synthesis of Pyridinium Salts Accelerated by Multi-Objective Bayesian Optimization with Active Learning*. Chem. Sci. 2023. (Pick of the week)
8. Randolph, C. E.; Beveridge, C. H.; **Iyer, S**.; Blanksby, S. J.; McLuckey, S. A.; Chopra, G. *Identification of Monomethyl Branched-Chain Lipids by a Combination of Liquid Chromatography Tandem Mass Spectrometry and Charge-Switching Chemistries*. J. Am. Soc. Mass Spectrometry. 2022.

**PRESENTATIONS**

**Poster, ASMS Spring, Baltimore, MD** **2025**

- Large Language Model-Driven AI Agents for Automated Workflows on a Chip-based nanoESI-MS/MS Platform with Real-Time Quality Control

**Poster, ASMS Spring, Anaheim, CA** **2024**

- Artificially Intelligent Copilot for Automating LC-OzESI-MRM Lipidomics Experiments and Analysis using Large Language Models

**Oral, ACS Spring, New Orleans, LA** **2024**

- CLAW: Comprehensive Lipidomic Automation Workflow using a Large Language Models User **Interface**

**Poster, ASMS Spring, Houston, TX** **2023**

- Automated Multiple Reaction Monitoring(MRM)-profiling and ozone electrospray ionization (OzESI)-MRM Informatics Platform for High-throughput Lipidomics

**Oral, ASMS Spring, Minneapolis, MN** **2022**

- Machine Learning-Guided Automated HPLC/MS/MS Platform Based on Diagnostic Ion-Molecule Reactions for Structural Elucidation of Unknown Compounds

**Poster, Center for Biological Metrology (CBM) Fall, Virtual Event** **2021**

- Fully Autonomous Platform for Tandem Mass Spectrometry Experiments Based on Diagnostic Gas-phase Ion-molecule Reactions

**Oral, ACS Fall, Atlanta GA** **2021**

- Automating the Optimization of Experimental Parameters for the Pulsed Introduction of Neutral Reagents in Tandem Mass Spectrometry Experiments Based on Diagnostic Gas-phase Ion-molecule Reactions

**Oral, University of Tennessee Knoxville REU, Knoxville TN** **2017**

- Synthesis of pH-Responsive Binary Heterografted Bottlebrushes with Well-Defined V-Shaped Side Chain Architecture

## EDUCATION

**Purdue University, West Lafayette, IN** **08/2020 - Present**
*PhD in Chemistry*
Advisor: Gaurav Chopra

**Salem State University, Salem, MA** **01/2015 – 12/2017**
*B.S. Chemistry Magna Cum Laude*

## SELECTED AWARDS AND HONORS

- Purdue College of Science Graduate Travel Award **2025**
- Purdue Graduate Student Government Travel Award **2025**
- Charles J. Cleary Scientific Achievement Award **2024**
- Chemical Sciences Pick of the Week **2023**
- ACS Division of Organic Chemistry Award **2017**
- Deans List **2015-2017**

## PROFESSIONAL CERTIFICATIONS

- Complex Carbohydrate Research Center Polysaccharide Course, Athens GA, Techniques for Characterization of Carbohydrate Structure of Plant and Microbial Polysaccharides **2019**
- Agilent GC Workshop, Cambridge MA, Eliminate the Fear Factor **2019**

## SKILLS & INTERESTS

- AI Agents, Large Language Models, Machine Learning
- Python, Linux, R