

GONÇALO JORGE GOUVEIA

phone: (706) 308-7500

e-mail: gjgouveia@googlemail.com

Research Interests: Chemical structure elucidation of unknown metabolites and confident spectral annotation of metabolomics data is challenging and requires the integration of multiple data streams. Yet, robust computational capabilities are still lacking. My research interests lie in developing holistic strategies that take advantage of classical biochemistry experiments, novel experimental designs, analytical platforms, biological materials, and computational methods to facilitate the discovery and identification of metabolites. This is critical for the successful translation of metabolomics outcomes and advancement of biological discovery. In addition, I am a trained Drugs and Toxicology Forensic Scientist. Prior to my graduate education, I specialized in analytical chemistry method development and the implementation of quality control and assurance practices in targeted high-throughput analysis. Similarly, these much-needed practices play a critical role in metabolomics research, ensuring reproducibility and public confidence in metabolomics outputs.

Education

2018 - 2022: University of Georgia, Complex Carbohydrate Research Centre, USA

PhD. graduate from the Biochemistry and Molecular Biology Department: *The role of model organisms, biochemistry, and separation science to improve metabolomics outcomes: a path to integration.* Mentored by Prof. Arthur Edison.

2019: Birmingham Metabolomics Training Centre, University of Birmingham

Metabolomics Data Processing and Data Analysis: Course aimed at implementing tools and approaches to analyse metabolomics data.

2015: Arizona State University, USA

Robert F. Borkenstein course: Pharmacology of drugs and their effects on psychomotor performance and driving. Advanced professional course for toxicologists and law enforcement professionals.

2005-2006: London South Bank University, UK.

MSc. in Forensic Science: Thesis: "Applications of ^1H NMR to Bio-samples in order to determine the Estimated Time since Death".

2000-2005: University of South Wales, School of Applied Sciences, UK.

BSc. (Hons.) in Forensic Science.

Publications

Erik R. Andersson, Amanda L. Bayless, [...], **Gouveia, G.J.**, [...], Robert Powers, Valérie Copié, and Teklab Gebregiorgis
Securing the Future of NMR Metabolomics Reproducibility: A Call for Standardized Reporting. *Analytical Chemistry* 2025
97 (38), 20655-20666, 10.1021/acs.analchem.5c03274

Gouveia, G.J., Head, T., Cheng, L.L. *et al.* Perspective: use and reuse of NMR-based metabolomics data: what works and what remains challenging. *Metabolomics* 20, 41 (2024). 10.1007/s11306-024-02090-6

Powers, R., Andersson, E., [...], **Gouveia, G.J.**, [...], Wishart, D., 2024, Best Practices in NMR Metabolomics: Current State, *TrAC*, 10.1016/j.trac.2023.117478.

Broeckling, C.D., [...], **Gouveia, G.J.**, [...], Mosley, J.D, 2023, Current practices in LC-MS untargeted metabolomics: a scoping review on the use of pooled QC samples. (*Submitted to ACS Analytical Chemistry*).

Asef, K.C., [...], **Gouveia, G.J.**, [...], Fernández, F.M., 2023, Unknown Metabolite Identification Using Machine Learning Collision Cross-Section Prediction and Tandem Mass Spectrometry, *ACS Analytical Chemistry* 2023 95 (2), 1047-1056, 10.1021/acs.analchem.2c03749

Wishart, D.S., [...], **Gouveia, G.J.**, [...], Uchimiya, M., 2022, NMR and Metabolomics—A Roadmap for the Future, *Metabolites*, 12, 678, 10.3390/metabo12080678

Shaver, A. O., Garcia, B. M., **Gouveia, G.J.***, et. al., 2022, An anchored experimental design and meta-analysis approach to address batch effects in large-scale metabolomics, *Frontiers in Molecular Biosciences*, 10.3389/fmolb.2022.930204

- Garcia, B.M., **Gouveia, G.J.**, Shaver, A.O., Amster, I.J., Edison, A.S., and Leach III, F.E., 2022, Taguchi Design of Experiments for Untargeted Metabolomics Sample Preparation. Chemrxiv, 10.26434/chemrxiv-2022-znvj7
- Lippa, K.A. , [...], **Gouveia, G.J.**, [...], Wilson, I., Ubhi, B.K., 2021, *Reference Materials for MS-based Untargeted Metabolomics and Lipidomics: A Review by the Metabolomics Quality Assurance and Quality Control Consortium (mQACC)*, Metabolomics, 10.1007/s11306-021-01848-6 (Voted best Review Article in Metabolomics 2023)
- Gouveia, G.J.**, Shaver, A.O., Garcia, B.M., Morse, A.M., Andersen, E.C., Edison, A.S., McIntyre, L.M., 2021, *Long-Term Metabolomics Reference Material*, Anal. Chem., 10.1021/acs.analchem.1c01294
- Edison, A.S., Colonna, M., **Gouveia, G.J.**, Holderman, N.R., Judge, M.T., Shen, X. and Zhang, S., 2021, *NMR: Unique Strengths That Enhance Modern Metabolomics Research*, Anal. Chem., 93, 1, 478–499
- Borchert, A.J.*, **Gouveia, G.J.***, Edison A.S. and Downs, D.M., 2020, *¹H NMR metabolomics corroborates serine hydroxymethyltransferase as the primary target of 2-aminoacrylate in a ridA mutant of Salmonella enterica*. mSystems Mar 2020, 5 (2) e00843-19; DOI: 10.1128/mSystems.00843-19
- *Co-first authors**
- Shaver, A.O., **Gouveia, G.J.***, Kirby, P.S., Andersen, E.C., Edison, A.S., 2020, Culture and Assay of Large-Scale Mixed-Stage Caenorhabditis elegans Populations. J. Vis. Exp., e61453, doi:10.3791/61453.
- Nothaft, H., [...], **Gouveia, G.J.**, [...], Szymanski, C., et al., 2017, *Co-administration of the Campylobacter jejuni N-glycan based vaccine with probiotics improves vaccine performance in broiler chickens*. Applied and Environmental Microbiology Nov 2017, 83 (23) e01523-17; DOI: 10.1128/AEM.01523-17
- Rooney, B.*, **Gouveia, G.J.***, et al. 2017 *A study of blood alcohol and drug concentrations in UK motorists prior to the introduction of fixed DUID limits*. Journal of Analytical Toxicology, Volume 41, Issue 2, March 2017, Pages 140–145, DOI: 10.1093/jat/bkw109

***Co-first authors**

Nearing submission:

Gouveia, G.J. *, Qu, D. *, Bills, B., Li, G., Wang, X., Kline, J., Ferber, A., Acikalin, U., Gomes, C. P., Schroeder, F. C.; *Omics-scale Molecular Formula Inference from Isotopic Fine Structure with DeepIFSReasoner*.
***Co-first authors in alphabetical order**

Acikalin, U. *, Ferber, A. *, Feng, D. *, **Gouveia, G.J. ***, Qu, D. *, [...], Gomes, C. P., Schroeder, F. C.; *In-Silico Mass-Spectrometry Mapping of the Small-Molecule Universe*.
***Co-first authors in alphabetical order**

Employment

2024 - Present: Cornell University, Boyce Thompson Institute, hosted by Prof. Frank Schroeder

Senior Research Associate: Working in collaboration with the Schroeder and Gomes lab to bridge Analytical Chemistry and Computer Science developing a revolutionary approach to identify and annotate known and unknown compounds from LC-MS spectra. This is one of the biggest bottlenecks in current modern biology which will pave the way for novel applications from agriculture to precision medicine.

2022 – 2024: Institute of Bioscience and Biotechnology Research, NIST (National Institute of Standards and Technology) and University of Maryland, hosted by Dr. Frank Delaglio

Post-Doctoral Research Scientist: Working with NIST scientists for direct knowledge transfer to industry and clinical applications. Developed methods to improve production and quality of CAR-T cells defining QA/QC attributes that inform CAR-T therapy success. Using the newly developed NISTCHO cells as a model system using inline, Low-Field Benchtop NMR, continuous metabolite measurements to better define attributes that predict desired physiological properties and outcomes. In addition to this project, I developed novel strategies to integrate LC-MS and NMR data to define the commercially released Research Grade Reference Material generating a comprehensive list of highly confident metabolite annotations.

2016 – 2017: University of Georgia, hosted by Prof. Arthur Edison

Laboratory Manager and Research Professional: QA/QC implementation as well as design and development of high-throughput protocols for the Edison Lab. Analysis of metabolomics samples and data for the University of Florida Southeast Centre for Integrated Metabolomics Core Facility.

2014 – 2016: LGC Forensics, Drugs & Toxicology Departments, United Kingdom

Toxicology Reporting Scientist: analyse, report and peer-review Alcohol and Drugs analysis (HS-GC, GC-MS, LC-MS) in biological samples. I have testified in over 1000 cases providing scientific advice as an expert witness. Analytical chemistry method development and validation (to ISO standards).

Complex Case Scientist: consisted in the examination of illicit laboratories and illicit cannabis cultivations as well as analytical chemistry method development.

Drugs Reporting Scientist: analysis of drugs of abuse by GC-MS, FTIR, and HPLC seized by law enforcement and the subsequent reporting in a court of law.

Heroin Profiling Unit Manager: I oversaw this unit implementation, management of staff and training. This included method development, validation, and creation of standard operating procedures and successful ISO17025 accreditation.

Internal Auditor: perform internal audits and define correction actions against international standards (ISO17025/9001) in addition to the roles of Drugs and Toxicology Reporting Scientist.

Intelligence Representative at LGC: processing and analysing data collected at a national scale by all the forensic service providers for The London Metropolitan Police and National Crime Agency.

Trainer: Evidential Drug Identification Testing (EDIT) – Training and certification of police officers to carry out field drug testing approved by the United Kingdom Home Office.

2009 – 2010: Forensic Science Services, Drugs Department, London, UK

Drug Profiling Unit: Responsible for development, revision, and implementation of quality control systems, ensuring ISO17025 quality standards, troubleshooting and maintenance of analytical instruments (GC-MS and GC-FID).

Forensic analyst: carried out analysis of drugs of abuse by GC-MS, FTIR, HPLC and NMR.

2006 – 2009: London South Bank University

Industry funded research internship: title “¹H NMR analysis of GRINrx Dentifrice formulations and their interactions with salivary Biomolecules” presented at the International Association for Dental Research conference in New Orleans, USA, 2007.

Awards & Service

2024: Recipient of the Best Poster award at the Metabolomics Association of North America (MANA) Conference

2021: Recipient of the Karl-Erik L. Eriksson Scholarship

Referee for: ACS Analytical Chemistry, PeerJ, Analytical Science Advances, Metabolites, EMBO Press and Journal of Chromatography B.

2025-2026: Member of the Scientific Organizing Committee for the Annual MANA Conference.

2023-present: Chair of the MANA Early Career Member network.

Chair of the International Metabolomics Quality Assurance and Quality Control Consortium (mQACC) outreach working group.

2024-2025: Member of the Organizing Committee of the Annual MANA Conference.

Presentations

Oral presentations

2026: Invited for 2026 Division of Systems Biology at Imperial College London – date TBD – Prof. Ian Wilson

2025: Invited speaker to the Montreal Mass Spectrometry Discussion group – Nov 2025 – Prof. Chaurand

2025: Invited speaker to the Concordia University Departmental Seminar – Nov 2025 – Prof. Vuckovic

2025: Oral presenter at the annual 2025 Metabolomics Association of North America conference:

Molecular formulas from isotopic fine structures of ultra-high-resolution LC-MS

2024: Workshop panellist to the 2023 Metabolomics Society Annual Conference:

NMR metabolomics workshop: Building a metabolomics fraction library

Invited speaker and panellist to the FDA Chemometrics for governmental agencies workshop:
NMR Metabolomics from Design to Metabolite ID

2022: Invited speaker to the NIH Workshop on Measurement Needs for Medical Products:
Long-Term Metabolomics Reference Material.

Invited speaker to the Biomolecular Structure and Function Group at NIST:
Long-Term Metabolomics Reference Material.

2021: Invited speaker to the 1st Brazilian Metabolomics Network Meeting:
Long-Term Metabolomics Reference Material.

Metabolomics Association of North America Conference.

Building a metabolomics fraction library.

Invited speaker to the Metabolomics Consortium Collaborative Series:

*Dissecting 2-aminoacrylate global stress outcomes in *S. enterica* using ¹H NMR Metabolomics.*

Invited speaker to the Eriksson Lecture Series, UGA:

*¹H NMR Metabolomics Corroborates Serine Hydroxymethyltransferase as the Primary Target of 2-Aminoacrylate in a *ridA* Mutant of *Salmonella enterica*.*

2020: Invited speaker at the Metabolomics QA and QC Consortium (mQACC):
Long-Term Metabolomics Reference Material.

2019: SouthEast Magnetic Resonance Conference:
C. elegans reference material development for metabolite ID.

Poster presentations

2024: Metabolomics Society and Metabolomics Association of North America

2021: NIH Common Fund Metabolomics Consortium Meeting

2020: Metabolomic Association of North America
NIH Common Fund Metabolomics Consortium Meeting

2019: Metabolomics Society
American Society of Mass Spectrometry
NIH Common Fund Metabolomics Consortium Meeting

2018: Metabolomics Society

2017: Metabolomics Society

2016: The Allied Genetics Conference
SouthEast Magnetic Resonance Conference

Professional Memberships

2020-Present: American Society of Pharmacognosy

2018-Present: Metabolomics Association of North America
International Metabolomics Society

2016-2020: American Society for Mass Spectrometry

2012-2023: Royal Society of Chemistry

2014-2017: United Kingdom and Ireland Association of Forensic Toxicologists