

Nathaniel G. Mahieu

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Metabolomics Ph.D. with experience in biochemistry, mass spectrometry, liquid chromatography, software development, hardware, and bioinformatics. Leading expert in bioinformatic analysis of LC/MS-based untargeted metabolome data. Founding member of Alethiun LLC, specializing in mass spectrometry consulting and algorithm development.

EDUCATION

- 2011 – 2017 Doctor of Philosophy in Chemistry
Washington University in St. Louis, MO, USA
Thesis Research Advisor: Associate Professor Gary J. Patti
Dissertation Title: **Mapping Analyte-Signal Relations in LC-MS Based Untargeted Metabolomics**
My thesis work developed new experimental and bioinformatic solutions to address major challenges in mass spectrometry-based metabolomics. The addressed challenges include: 1. peak detection and integration bound selection (Mahieu 2016), 2. the prevalence of non-biological signals in datasets (Mahieu 2014) 3. annotation of complex relationships in spectral data (Mahieu 2016); and 4. annotation of the analyte content in untargeted datasets (Mahieu 2017).
- 2014 Johns Hopkins University, Online
Courses: Practical Machine Learning, Reproducible Research, and Exploratory Data Analysis
- 2007 – 2011 Bachelor of Science in Chemistry with honors and ACS certification
Bachelor of Science in Biochemistry with honors
University of Missouri in Columbia, MO, USA
Undergraduate Research Advisor: Professor Kent S. Gates
Undergraduate Thesis: **Synthesis of a 2-Nitroimidazole Derivative and Characterization of Tirapazamine (SR-4233) Analogues**

PROFESSIONAL COMPETENCIES

- Software Dev. Git, Linux, R, Ruby, Ruby on Rails, Apache, xHTML, CSS, JavaScript, MySQL, HTTP, Python, Autodesk Eagle, serial peripheral interface (SPI) hardware, basic circuit design
*Developed web applications starting in 2003 as a hobby. My knowledge developed in parallel with the maturation of modern web technologies giving me a deep understanding of these tools. I currently leverage these skills to accelerate my research, one such example is the *creDBle* metabolite database (Mahieu 2017, in preparation). Additionally, I have prototyped several hardware devices, fabricated PCB circuits, interfaced with that hardware, and written web interfaces for that hardware.*
- Bioinformatics Dynamic Time Warping (dtw), Graph Analysis (igraph), Plotting (ggplot2), Reproducible Research (knitr, sweave), Data Manipulation (data.table, plyr, reshape2, matrixStats), Parallel Processing (foreach, doRedis, doParallel), Mass Spectrometry Data Processing (custom algorithms, mzR, xcms, warpgroup, mz.unify, credential), Machine Learning (caret, ranger)

Projects accompanying my publications can be found at github.com/nathaniel-mahieu.

- Design Adobe Illustrator, InDesign, Acrobat
Took multiple ultimate jerseys (totaling approximately \$10,000 in orders) through the design and printing process using Adobe Illustrator. InDesign, Illustrator, and Acrobat are used to generate vector graphics and typeset posters and manuscripts.
- LC-MS Thermo Q-Exactive Plus, Agilent 6540 QTOF, Agilent 6530 QTOF, Agilent 6460 QqQ, AB Sciex 5600+ TripleTOF, Agilent 1260 Capillary LC, Agilent 1290 UPLC, Dionex RSLCnano, Dionex RSLC, chromatography at microflow (10 uL/min) to standard flow rates (0.4 mL/min), various reverse phase and HILIC column chemistries, Thermo Qual Browser, Agilent Qualitative Analysis, Thermo Compound Discoverer, Agilent MPP, Agilent Profinder, Thermo Xcalibur, Agilent Acquisition, Vista Flux.
Disassembled and reassembled the QTOFs and QqQ for preventative maintenance on four occasions. Performed the installation of a 6510 QTOF. As our lab's substitute for paying a service technician I became thoroughly acquainted with troubleshooting and repair of instruments. Developed and optimized targeted and untargeted methods for both chromatography and mass spectrometry. Beta tested several software packages including Agilent's Vista Flux and Thermo's Compound Discoverer. Consulted for Agilent developers on the design of the Vista Flux software in Santa Clara.

PUBLICATIONS

- 2017 **N. G. Mahieu**, G.J. Patti
Systems-Level Annotation of a Metabolomics Data Set Reduces 25000 Features to Fewer than 1000 Unique Metabolites
Anal. Chem., acs.analchem.7b02380
- 2016 Y.J. Chen, **N. G. Mahieu**, X. Huang, M. Singh, P.A. Crawford, S.L. Johnson, R.W. Gross, J. Schaefer, G.J. Patti
Lactate metabolism is associated with mammalian mitochondria
Nat. Chem. Biol., vol. 12, pp. 937–943, 2016.
- 2016 **N. G. Mahieu**, J. L. Spalding, S. J. Gelman, and G. J. Patti
Defining and Detecting Complex Peak Relationships in Mass Spectral Data: The mz.unity Algorithm
Anal. Chem., vol. 88, no. 18, pp. 9037-9046, 2016.
- 2016 J. L. Spalding, K. Cho, **N. G. Mahieu**, I. Nikolskiy, E. M. Llufrío, S. L. Johnson, and G. J. Patti
Bar Coding MS2 Spectra for Metabolite Identification
Anal. Chem., vol. 88, no. 5, pp. 2538–2542, 2016.
- 2016 **N. G. Mahieu**, J. L. Genenbacher, and G. J. Patti
A roadmap for the XCMS family of software solutions in metabolomics
Curr. Opin. Chem. Biol., vol. 30, pp. 87–93, 2016.
- 2015 S. J. Gelman, **N. G. Mahieu**, K. Cho, E. M. Llufrío, T. A. Wenczewicz, and G. J. Patti
Evidence that 2-hydroxyglutarate is not readily metabolized in colorectal carcinoma cells
Cancer Metab., vol. 3, no. 1, p. 1, 2015.
- 2015 **N. G. Mahieu**, J. L. Spalding, and G. J. Patti
Warpgroup: increased precision of metabolomic data processing by consensus integration bound analysis
Bioinformatics, 2016; 32(2): pages 268-275
- 2014 Y.-J. Chen, X. Huang, **N. G. Mahieu**, K. Cho, J. Schaefer, and G. J. Patti
Differential incorporation of glucose into biomass during Warburg metabolism

Biochemistry, vol. 53, no. 29, pp. 4755–4757, 2014.

- 2014 H. P. Benton, J. Ivanisevic, **N. G. Mahieu**, M. E. Kurczyk, C. H. Johnson, L. Franco, D. Rinehart, E. Valentine, and others
Autonomous metabolomics for rapid metabolite identification in global profiling
Anal. Chem., vol. 87, no. 2, pp. 884–891, 2014.
- 2014 K. Cho, **N. G. Mahieu**, S. L. Johnson, and G. J. Patti
After the feature presentation: technologies bridging untargeted metabolomics and biology
Curr. Opin. Biotechnol., vol. 28, pp. 143–148, 2014.
- 2014 K. Cho, **N. Mahieu**, J. Ivanisevic, W. Uritboonthai, Y.-J. Chen, G. Siuzdak, and G. J. Patti
isoMETLIN: a database for isotope-based metabolomics
Anal. Chem., vol. 86, no. 19, pp. 9358–9361, 2014.
- 2014 **N. G. Mahieu**, X. Huang, Y.-J. Chen, and G. J. Patti
Credentialing features: a platform to benchmark and optimize untargeted metabolomic methods
Anal. Chem., vol. 86, no. 19, pp. 9583–9, Oct. 2014.
- 2013 J. D. Dougherty, S. E. Maloney, D. F. Wozniak, M. A. Rieger, L. Sonnenblick, G. Coppola, **N. G. Mahieu**, J. Zhang, J. Cai, G. J. Patti, and others
The disruption of Celf6, a gene identified by translational profiling of serotonergic neurons, results in autism-related behaviors
J. Neurosci., vol. 33, no. 7, pp. 2732–2753, 2013.
- 2013 I. Nikolskiy, **N. G. Mahieu**, Y.-J. Chen, R. Tautenhahn, and G. J. Patti
An untargeted metabolomic workflow to improve structural characterization of metabolites
Anal. Chem., vol. 85, no. 16, pp. 7713–7719, 2013.
- 2012 G. J. Patti, R. Tautenhahn, D. Rinehart, K. Cho, L. P. Shriver, M. Manchester, I. Nikolskiy, C. H. Johnson, **N. G. Mahieu**, and G. Siuzdak
A view from above: cloud plots to visualize global metabolomic data
Anal. Chem., vol. 85, no. 2, pp. 798–804, 2012.

INVITED ORAL PRESENTATIONS

- 2017 Podium Presentation, American Society for Mass Spectrometry Annual Meeting (ASMS)
“Annotation of Challenging Signals in Untargeted Metabolomics”
- 2015 Metabolomics Short Course Lecture, Mass Spectrometry: Applications to the Clinical Lab (MSACL)
“Credentialing Metabolomic Features”
- 2015 Metabolomics Short Course Lecture, MSACL
“Metabolomic Extractions”
- 2014 Metabolomics Short Course Lecture, ASMS
“Metabolomic Extractions”
- 2013 Podium Presentation and Young Investigator Award, MSACL
“Untargeted Profiling of Metabolite Classes by Mass Spectrometry”

AWARDS

2016	Steve Berger Award, <i>Agilent</i>
2014	Graduate Student Award, <i>American Society for Mass Spectrometry</i>
2014	Young Investigator Award, <i>Mass Spectrometry: Applications to the Clinical Lab</i>
2012	Graduate Assistance in Areas of National Need Fellowship
2011	Best Undergraduate Senior Thesis, <i>Biochemistry</i>
2011	Dean's List recognition all eight semesters of undergraduate study
2010	Life Sciences Undergraduate Research Opportunities Program
2010	Undergraduate Research Mentorship Program
2007	Missouri Bright Flight Scholarship and Mizzou Excellence Scholarship
2006	Missouri Boys State
2005	Missouri Scholars Academy

POSTER PRESENTATIONS

2016	"Analyte or Amalgamation? Exploring Relationships and Redundancy in Metabolomic Datasets", MSACL
2016	"Metabolomic Analyte or Amalgamation? Exploring Relationships and Redundancy in Mass Spectrometry Datasets", ASMS
2015	"Comprehensive Annotation of an Untargeted Metabolomic Dataset: <i>Escherichia coli</i> ", MSACL
2015	"Warpgroup: Advances in LC/MS Based Omics Processing, Quantitation, and Coverage", ASMS
2014	"Optimizing and Benchmarking Untargeted Metabolomics - Quantitative Evaluation of Instrumentation and Methodology to Allow Cross-Lab Comparisons", ASMS
2014	"Optimizing and Benchmarking Untargeted Metabolomics", NIH Metabolomics Resource Cores Spring Symposium

EXPERIENCE

2017 – Present	Mass Spectrometry Consulting and Algorithm Development Alethiun LLC
2016 – 2017	Reviewer, BMC Bioinformatics
2015	Laboratory Infrastructure Design <i>Served as chief consultant in designing two mass spectrometry-based research laboratories housing 16 instruments. Design required coordination with architects (Feeler Architects), engineers (Ross & Baruzzini, Jacobs Engineering), and construction contractors (Lawlor Corporation) to establish requirements for power quality, mechanical controls, compressed air generation, nitrogen purification, and system redundancy in addition to reviewing laboratory drawings and elevations. 150 hours</i>
2010 – 2011	Undergraduate Researcher University of Missouri
2008 – 2010	Quality Control Analyst Teva Pharmaceuticals

- 2009 – 2010 Tutor, Total Person Program
University of Missouri Athletics
- 2008 – 2009 Director, Missouri Loves Company
University of Missouri Men's Ultimate
- Organized and managed an event for 1500 players with a revenue of \$20,000. Identified an opportunity to relocate and improve the event resulting in an increase from 40 teams to 56 teams the following year. Established MLC as one of the premier fall tournaments and a preview of spring nationals with 5 of 16 nationals qualifying teams in attendance.*

TEACHING EXPERIENCE

- 2016 – Present Graduate Student Mentor, Fuad Nasser
- 2016 Center for the Integration of Research, Teaching, and Learning, Associate
- 2016 Teaching Citation
- Teaching Philosophy Statement available upon request*
- 2015 Undergraduate Research Mentor, David Lee, 70 hours
- 2014 Undergraduate Research Mentor, Lauren Becker, 100 hours
- 2013 – 2014 Teaching Assistant, Biochemistry II
- 2011 – 2012 Teaching Assistant, Organic Chemistry Lab I and II