

Alethiun LLC

Metabolomics, Liquid Chromatography, and Mass Spectrometry
Consulting and Algorithm Development

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Alethiun LLC provides software and research assistance for mass spectrometry based metabolomics researchers. The analysis of mass spectrometry datasets is a challenge lacking a comprehensive solution. This is especially true in the case of metabolomics.

It is easy to get metabolomic data but metabolomics is a hard science to do well.

I am Nathaniel Mahieu, the founder and primary consultant of Alethiun LLC. I look forward to chatting with you about your application and goals at no cost to you. Please feel free to contact me - I enjoy hearing about people's science. After our conversation, if I can suggest any existing approaches or solutions I will do so and additionally I will propose paths we could explore if we were to work together.

I have extensive experience in processing raw LC-MS data (1), have written from scratch an XCMS alternative including mass trace detection, mass and retention time alignment, chromatographic peak detection, mass relationship detection (2), consensus integration bound detection (3), and visualization. I have a deep understanding of biochemistry and can critically assess the value metabolomics can provide studies of biology. I additionally have directed the design of new mass spectrometry lab space and infrastructure, verifying that the plans we make on paper are what is delivered. My experience ranging from infrastructure to data analysis and biology gives me the breadth of understanding I need to advance your research goals.

How will Alethiun LLC provide value for your research program?

Researchers commonly attempt to implement their own data analysis algorithms in the absence of existing solutions. Processing mass spectrometry data (including liquid chromatography data) is a non-trivial task. Developing and automating custom data processing workflows is our primary skillset. If you have a labor intensive manual analysis we can work to automate the time consuming portions. More excitingly, we can create algorithmic approaches to extract information from your large datasets that would otherwise be impossible to extract manually. We can create workflows to process any data you collect and we can collaborate to extract the as much biologically relevant information from that data as possible. Finally, after exploring your research goals and related biology I will provide guidance and feasibility assessments as to whether your planned experiments and metabolomic approaches will provide the insight you desire.

Thank you, and I look forward to talking with you. - Nathaniel

- (1) Mahieu NG, 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](https://doi.org/10.1021/acs.analchem.7b02380)
- (2) Mahieu NG, 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.
- (3) Mahieu NG, J. L. Spalding, and G. J. Patti. **Wargroup: increased precision of metabolomic data processing by consensus integration bound analysis.** Bioinformatics, 2016; 32(2): pages 268-275
- (4) Mahieu NG, 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.