Exhaustive and Reliable Data Analysis for Untargeted Metabolomics

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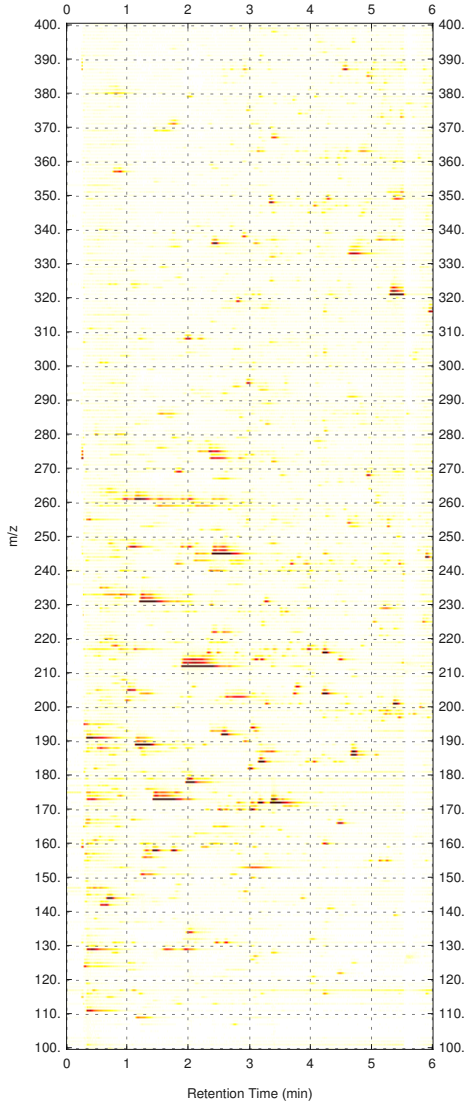
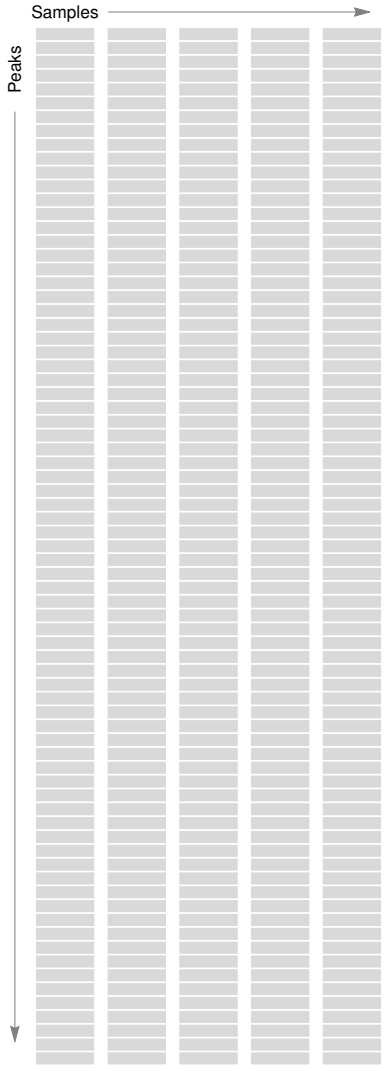
From Raw Data to Compound List

Use high quality expert curated data for your downstream statistical analysis!

1. Raw Data →

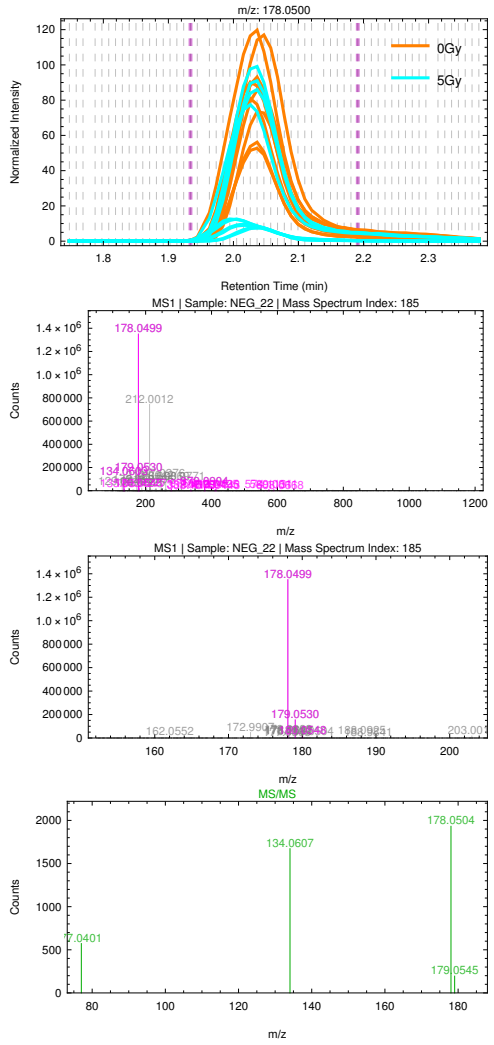


2. Curated Peak List →

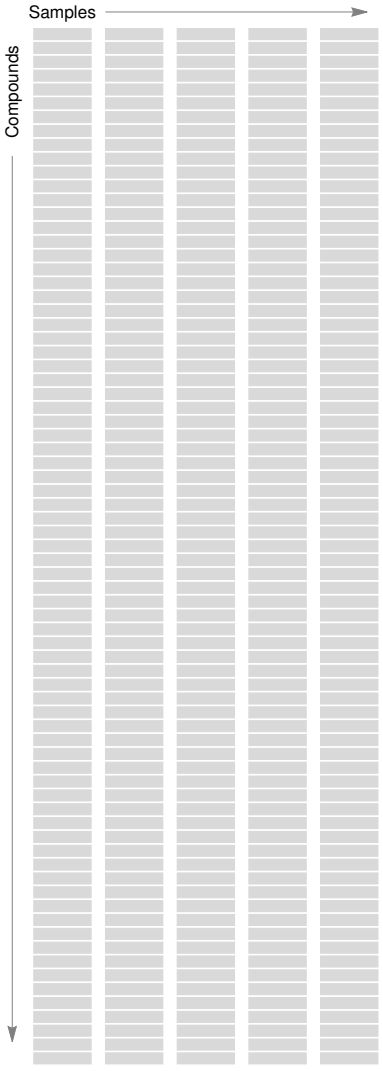


3. Interpretation →

Putative Chemical Formula: C9H9NO3
Putative Identity: Hippuric acid



4. Compound List



Example Analysis

- The Association of Biomolecular Resource Facilities (ABRF) Metabolomics Research Group (MRG) 2016 Study

  https://abrf.org/research-group/metabolomics-research-group-mrg

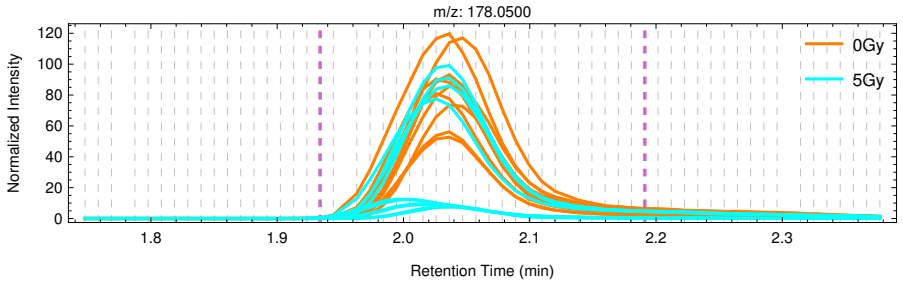
  https://abrf.org/sites/default/files/2016_mrg_study_outline_060716.pdf

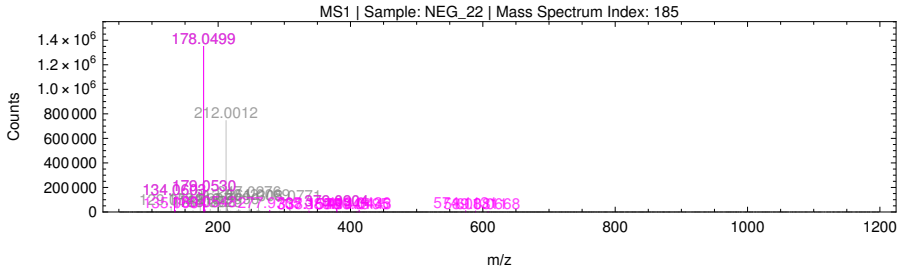
- Urine samples from mice exposed to 5 Gray of external X-ray (n = 5) and those exposed to sham irradiation - control group (n = 5)
- Each sample analyzed twice in both positive and negative polarity modes (UPLC-Q-TOF)
- Pooled sample analyzed in MS^E mode in both positive and negative polarity
- Authors provided raw data as well as peak lists from automated analysis
- The assignment: "*...report on the top 50 features that show statistically significant differences in relative abundances between the two study groups...*"

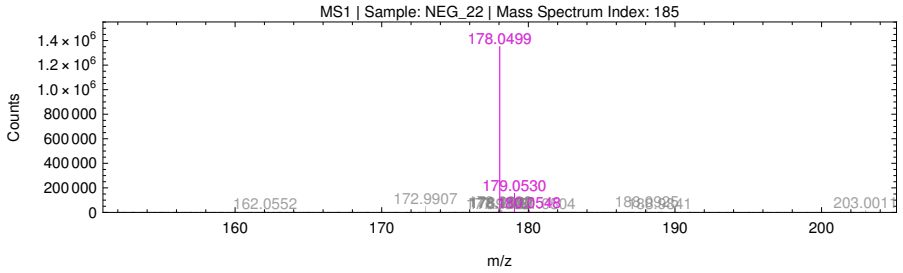
Compound Interpretation

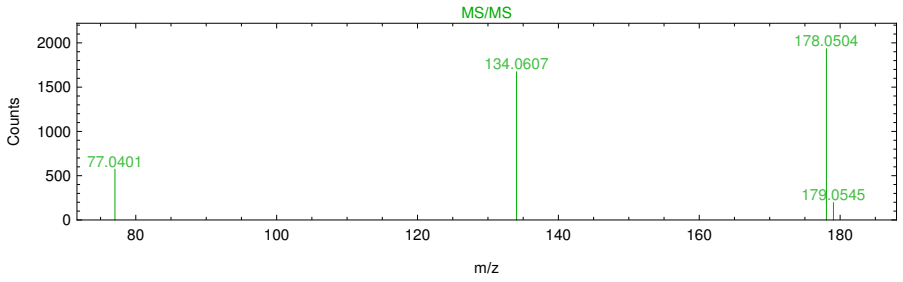
Putative Chemical Formula: C9H9NO3 **Putative Identity:** Hippuric acid **Note:** MassBank: KO001092

Negative Mode:

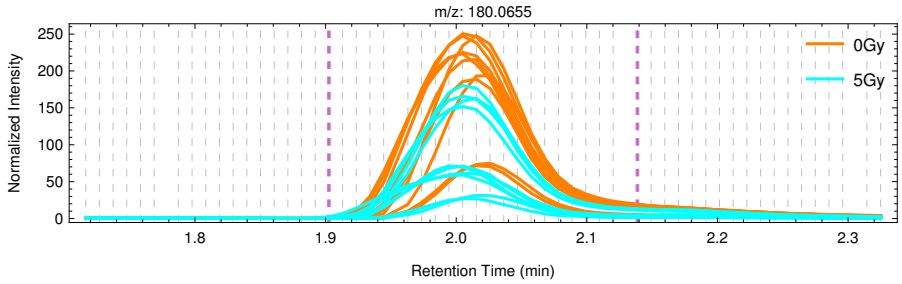


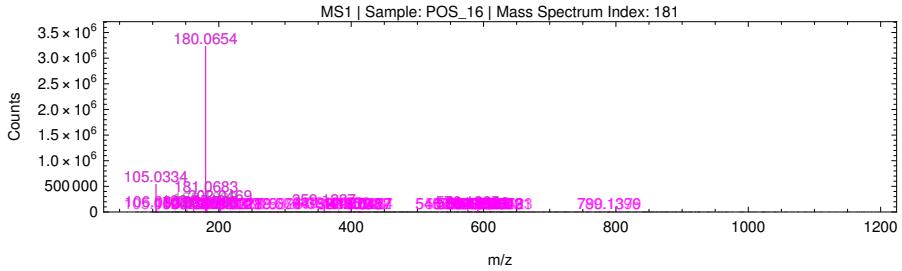


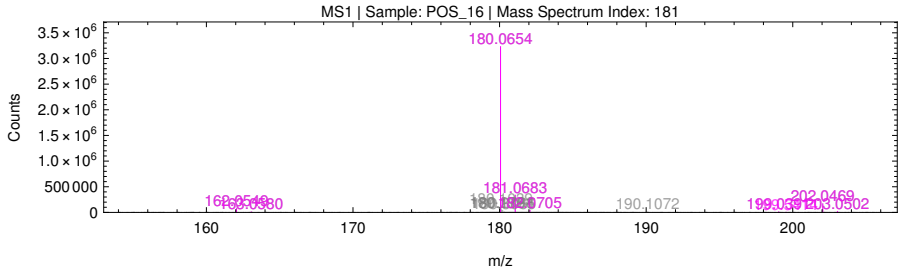


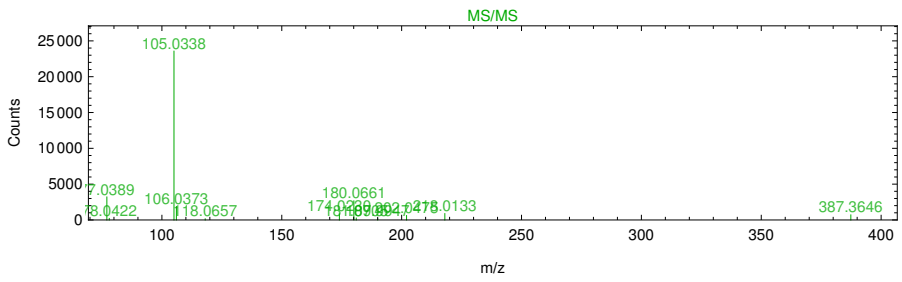


Positive Mode:



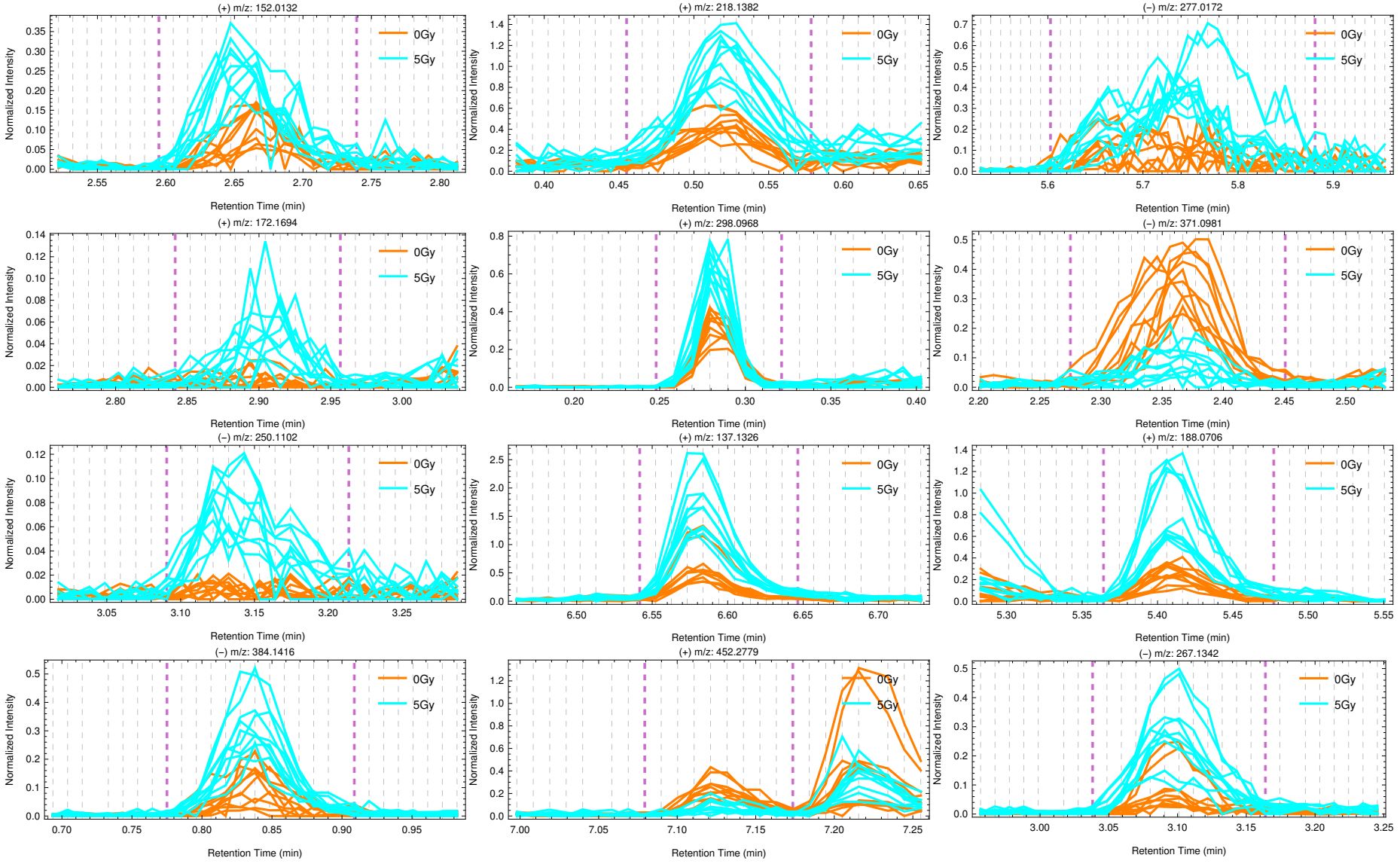






Compounds with Significant Differences

None of the peaks below were found in peak lists provided by the authors of the study.



Thank You!

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Additional References

- Untargeted Metabolomics Suffers from Incomplete Data Analysis
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- Unexpected Metabolites
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  http://www.mdpi.com/1660-3397/11/10/3617/htm
- Unexpected Metabolic Capabilities
  http://dx.doi.org/10.1039/c1mb05196b
- Metabolic Interactions
  http://www.nature.com/articles/ncomms9289
- Interpretation of Mass Spectra
  http://pubs.acs.org/doi/abs/10.1021/ac402180c
- Metabolite Turnover
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- Enzyme Discovery
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