

Discovery Metabolomics for Greater Biological Insight

Agilent 6546 LC/Q-TOF



Introduction

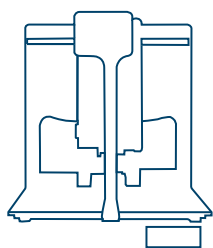
Endogenous metabolites reflect the functional state of a biological system. Profiling endogenous metabolites can be analytically challenging due to the complexity of biological systems. Agilent is a world leader in providing solutions for obtaining metabolomics data using high-resolution accurate mass LC/MS.

The power of discovery metabolomics lies in collecting quantitative and qualitative data with the greatest possible coverage of the metabolome. Agilent quadrupole time-of-flight (Q-TOF) technology provides fast data acquisition rates with a wide dynamic range. These features are a key requirement for the study of metabolites with a broad concentration range in biological systems. The Agilent 6546 LC/Q-TOF is the latest addition to the Agilent portfolio with many technological advancements.



The Agilent 6546 LC/Q-TOF is a mass spectrometer that provides a wide dynamic range, good mass accuracy, and outstanding isotope fidelity. All features are essential for high-performance discovery metabolomics analysis.

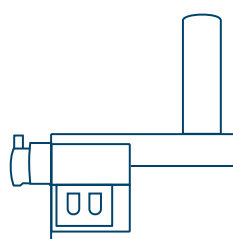
Workflow for discovery analysis of metabolomics samples



Sample preparation



Separation using
1290 Infinity II LC



Detection using
6546 LC/Q-TOF



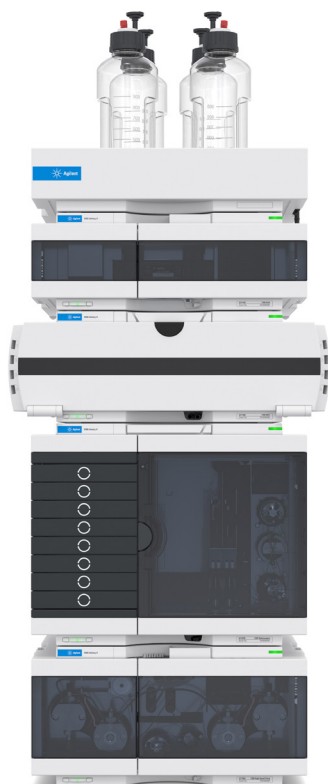
Data analysis using
MassHunter
software suite

Consumables and sample preparation

- Extensive range of LC columns and supplies for metabolites of different polarities, masses, and functional groups
- 96-well plate format of Solid Phase Extraction (SPE) for higher productivity
- Agilent Captiva EMR-Lipid for selective removal of major lipid classes from human specimens
- For more sample preparation techniques, [click here](#)



The Agilent Bravo Metabolomics Sample Prep Platform can be used with any LC/MS system. It incorporates room temperature quenching and Captiva EMR-Lipid removal technology.



Separation with Agilent 1290 Infinity II LC

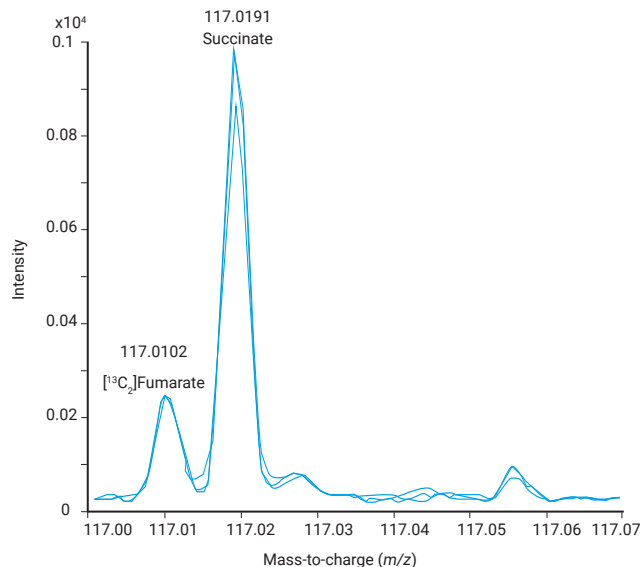
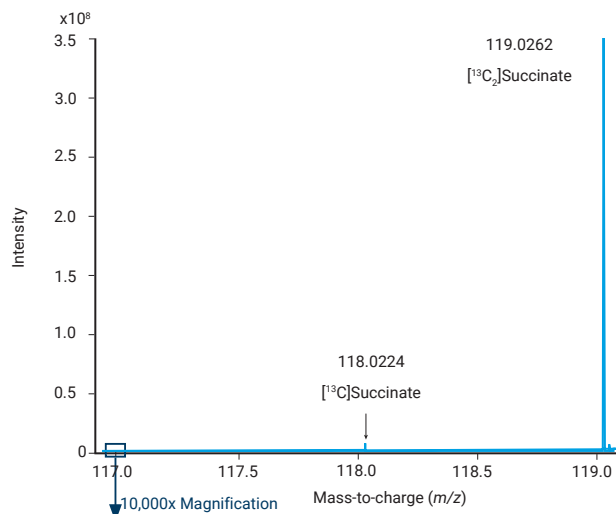
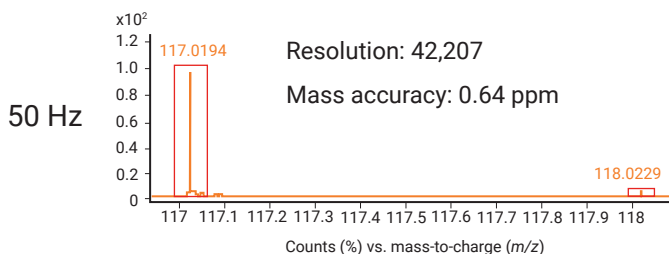
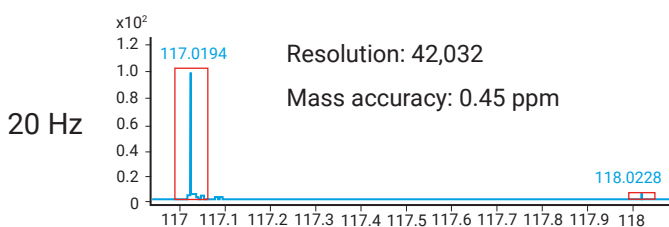
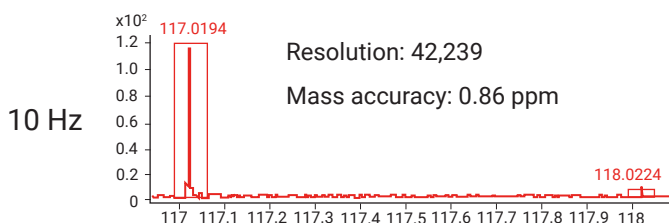
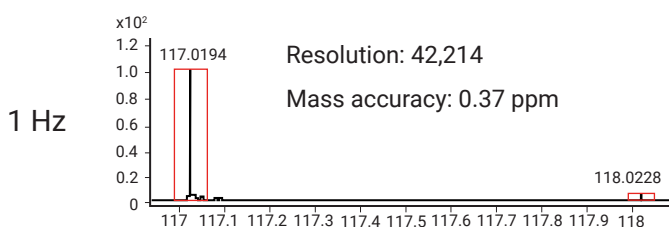
- More chromatographic resolution and lowest system dispersion with specially designed components in the sample flow path
- Less than 10 ppm carryover
- Greater flexibility and capacity to run microplates and vials in the multi sampler
- For additional information on HPLC systems, [click here](#)

The Agilent 1290 Infinity II LC is designed for higher sample throughput. It gives robust, excellent performance and can be seamlessly integrated into existing laboratory environments.

Detection With 6546 LC/Q-TOF



- Higher sensitivity, resolution, dynamic range, and isotopic fidelity for advanced metabolomics research
- Metabolite identification using accurate mass MS/MS analysis
- For more Q-TOF LC/MS instrument options, [click here](#)

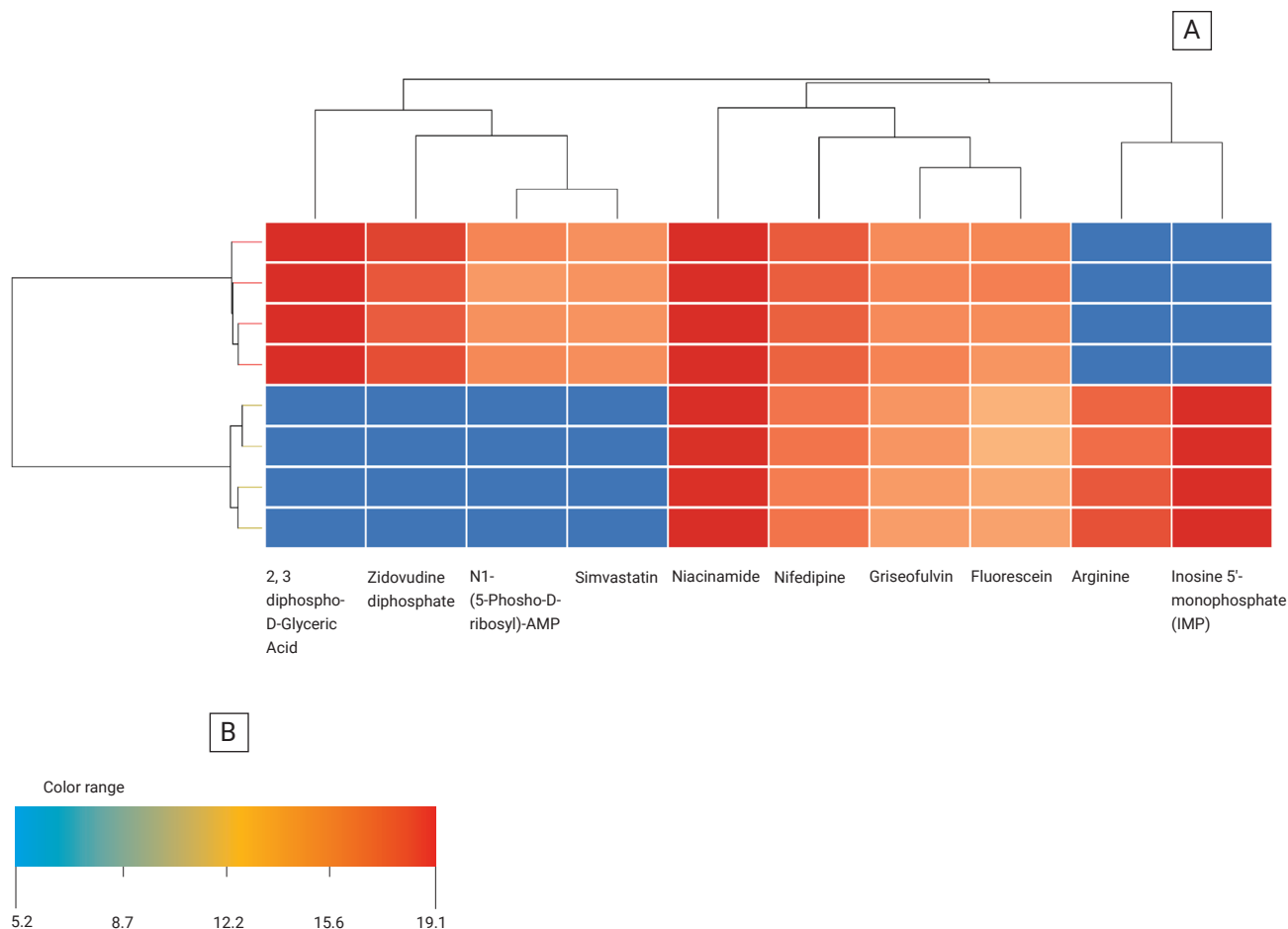


Resolution is independent of the acquisition rate for succinic acid with the Agilent 6546 LC/Q-TOF.

Intrascan dynamic range of the Agilent 6546 LC/Q-TOF. A 1X ¹³C-enriched *E. coli* extract was spiked with ¹³C₂-succinate. Three technical replicates are superimposed. Despite the vast difference in intensities (10⁴ to 10⁸ counts), accuracy and resolution is preserved, allowing precise determination of both high- and low-abundance peaks within the same spectrum.

Q-TOF data processing and analysis with Agilent MassHunter software suite

- MassHunter Profinder for batch feature extraction of raw data with powerful editing and visualization capabilities
- Mass Profiler Professional (MPP) for statistical analysis and intuitive visualization tools including univariate and multivariate analysis, principal component analysis (PCA), clustering, and class prediction analysis
- Highly curated Agilent METLIN Metabolomics Database and Library for metabolite identification
- Additional fit-for-purpose software for even deeper insights: MassHunter VistaFlux for qualitative flux analysis, MassHunter Classifier software for easy classification of unknown samples, and MassHunter Lipid Annotator software to enable lipid annotation of large datasets and downstream lipid profiling workflows



Hierarchical clustering in MPP connects compounds and/or samples in a tree structure using their abundance profiles. Figure A shows a dendrogram of ten compounds found in two groups of samples. It shows the relationship between compounds in one dimension and between samples in the other dimension. Figure B shows a legend for the heatmap.

Conclusion

Metabolomics solutions from Agilent enable a streamlined end-to-end workflow. The portfolio of products and software solutions turns large sample sets into meaningful information. Agilent instruments, columns, and software solutions can help to effectively address metabolomics challenges.

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