From Sample to Biology, One Streamlined Workflow for Lipidomics

Key benefits

- Supports multiple data acquisitions including iterative MS/MS, auto MS/MS, and IM All Ions MS/MS
- Brand new theoretical lipid annotation tool Agilent MassHunter Lipid Annotator, with a modified LipidBlast database underlying the MS/MS workflow
- Complements existing MS workflows with Agilent MassHunter Profinder and Mass Profiler Professional (MPP)
- Unique data visualization methods such as mass defect plots, retention time (RT) versus mass plots, and lipid matrices help decipher trends in large lipid datasets

Agilent MassHunter Lipid Annotator software is built on an algorithm that uses probability theory and least squares fit to annotate lipids based on an updated *in silico* MS/MS database for Q-TOF CID fragmentation modeled from lipid standards for each lipid class. The Lipid Annotator software uses iterative MS/MS data to make rapid and accurate lipid annotations, and automatically generate PCDL spectral libraries with RT information. The lipidomics workflow additionally includes MassHunter Profinder and Mass Profiler Professional (MPP), and personal compound database, and library (PCDL) manager.

The Lipid analysis workflow in MPP includes lipid class normalization based on internal standards and additional visualization features including lipid matrices, Kendrick mass defect plot, and a scatterplot that is colored based on lipid class.

There are complementary data visualizations between Lipid Annotator and MPP. A color-coded pie chart from Lipid Annotator gives an overview of lipid classes identified (Figure 1). This is accompanied by a matching color-coded scatterplot showing the mass and RT for the lipids identified. This allows the user to gain insight into the important lipid classes in each sample. More detailed visualizations in the form of matrix plot are provided in MPP, providing the user with the ability to evaluate statistical changes in lipids across sample sets (Figure 2).

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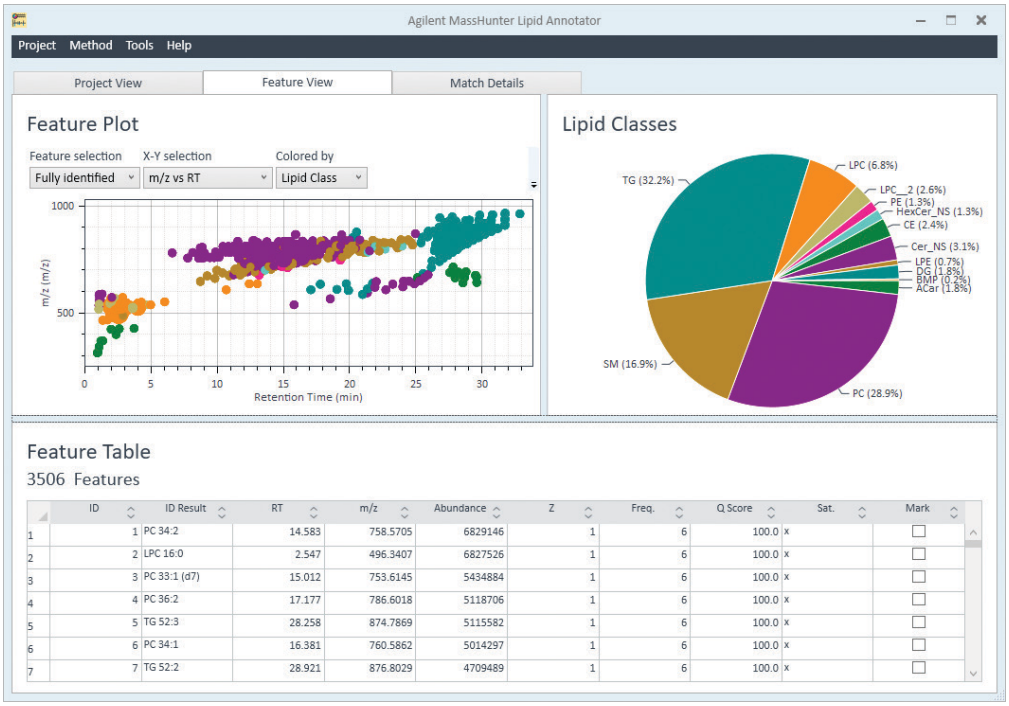
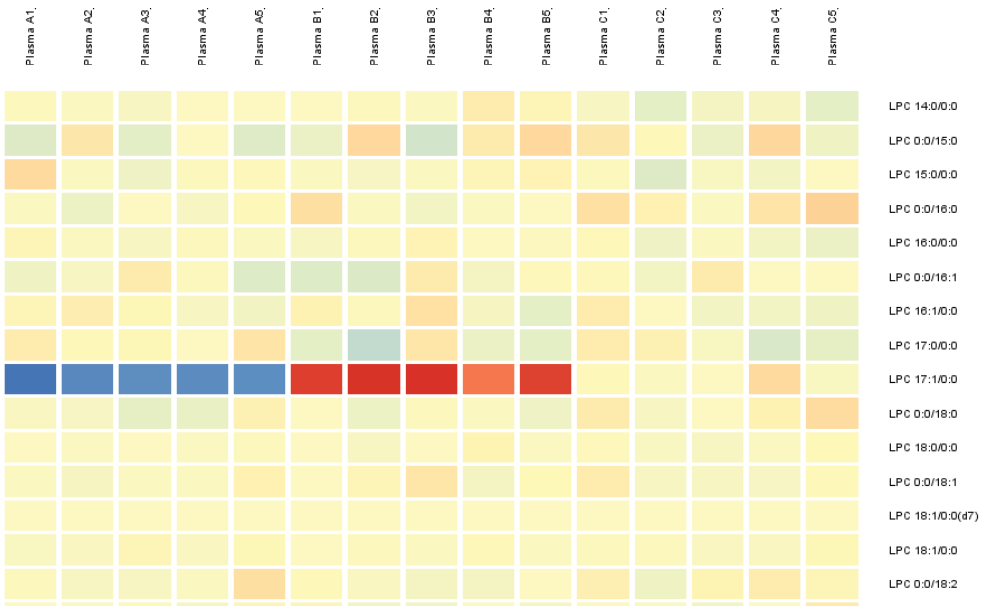


	ID	ID Result	RT	m/z	Abundance	Z	Freq.	Q Score	Sat.	Mark
1	1	PC 34:2	14.583	758.5705	6829146	1	6	100.0	x	
2	2	LPC 16:0	2.547	496.3407	6827526	1	6	100.0	x	
3	3	PC 33:1 (d7)	15.012	753.6145	5434884	1	6	100.0	x	
4	4	PC 36:2	17.177	786.6018	5118706	1	6	100.0	x	
5	5	TG 52:3	28.258	874.7869	5115582	1	6	100.0	x	
6	6	PC 34:1	16.381	760.5862	5014297	1	6	100.0	x	
7	7	TG 52:2	28.921	876.8029	4709489	1	6	100.0	x	

Figure 1. Lipid Annotator software identified 461 lipids from six pooled plasma Iterative MS/MS files. Sum composition lipid names, and where possible, more specific constituent lipid-level names, were exported to PCDL format in an automated fashion.



... + 16 more LPCs

Figure 2. Lipid matrix plot showing relative abundance differences between sample groups for the LPC lipid class. The spiked-in standard of LPC 17:1 shows the expected up (red) and down (blue) regulated pattern.

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