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Untargeted Metabolomics

Untargeted analysis covers a detection of metabolites without prior selection. This approach provides a more comprehensive view of a sample and enables a discovery of unknown compounds which might turn out to be a significant. Identification of compounds is based on comparison to an own library of analytical reference standards and various external libraries. Compounds are identified on different levels of certainty or remain unidentified.

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workflow - untargeted metabolomics

- Design experiment
- Sample collection
- Sample preparation
- LC-HRMS analysis
  (chromatography, mass spectrometry, data acquisition)
- Data processing
  (integration, normalization, identification)
- Analysis and preliminary interpretation

Vanquish™ Flex UHPLC system
Orbitrap Exploris 120 (Thermo Scientific)
Compound Discoverer Software (Thermo Scientific)

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LC-HRMS analysis

chromatography: stationary phase

RP (reverse-phase)

HILIC

high resolution mass spectrometry: ionisation mode

positive

negative

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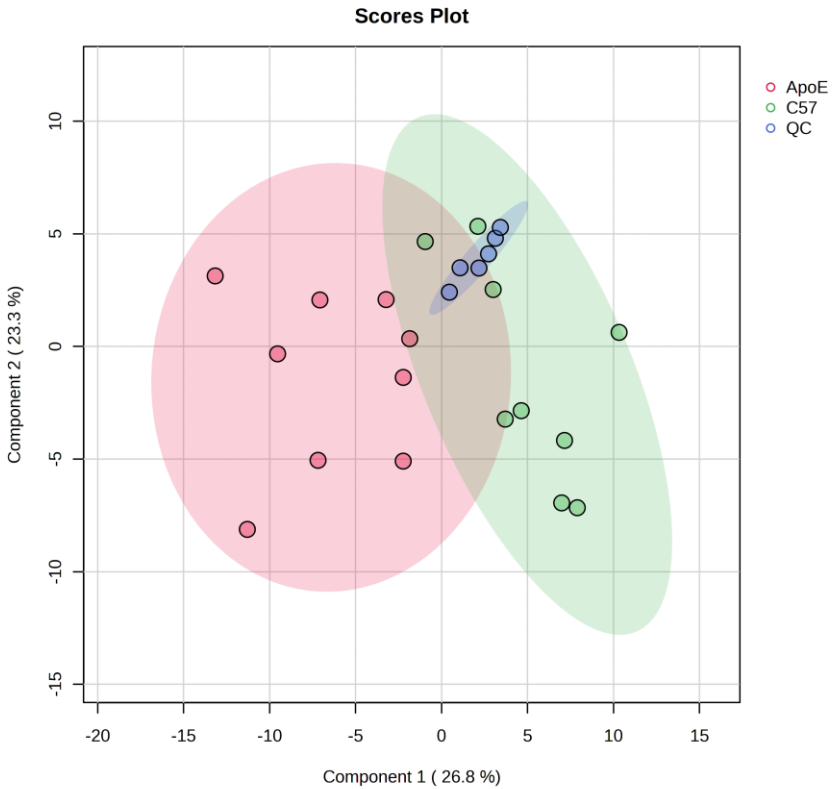
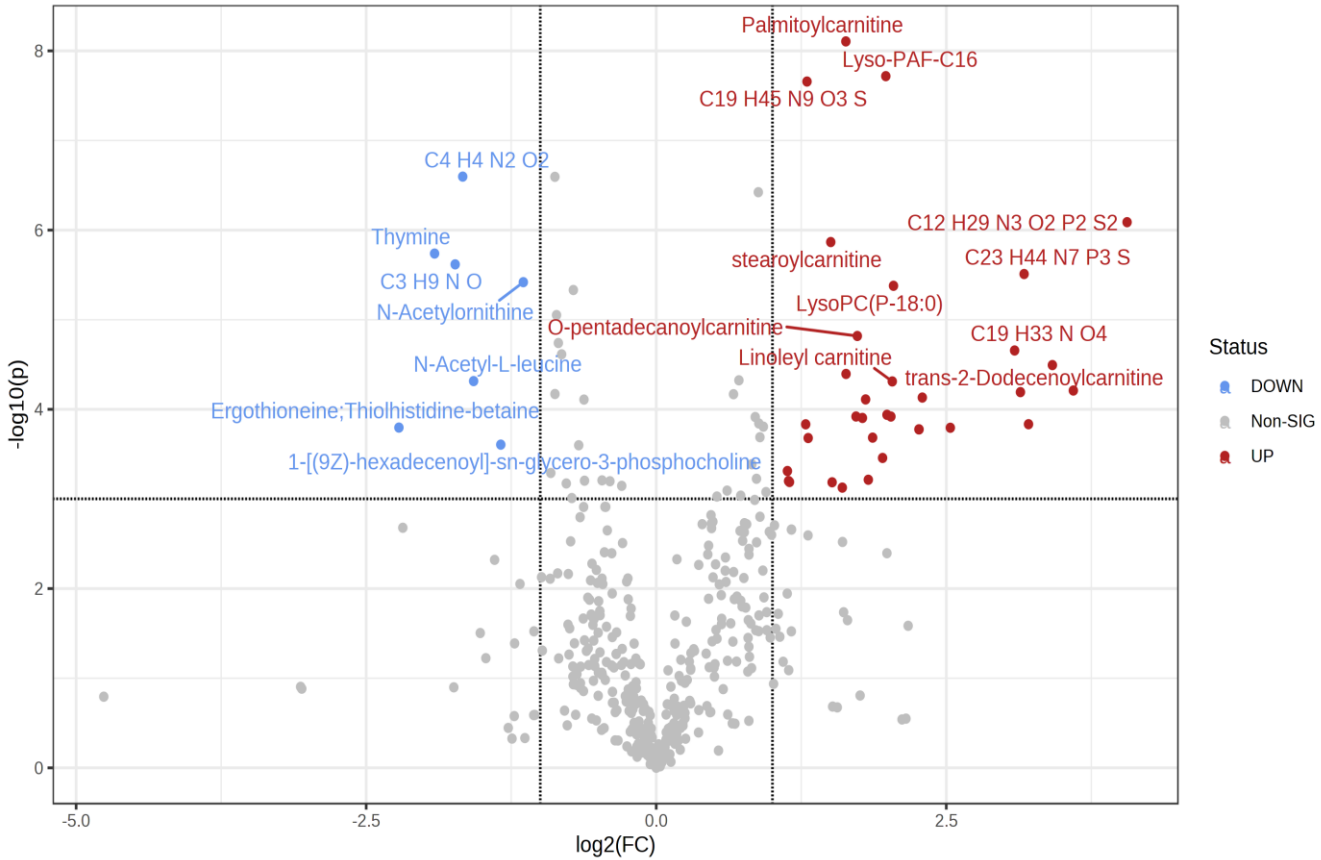
Plasma metabolites profile in ApoE/LDLR-/- and C57BL/6J female mice.

LC-HRMS analysis (RP, positive mode)



Partial Least Squares Discriminant Analysis (PLS-DA)
Metabo Analyst 5.0



Differential metabolite identification for the experimental dataset using Volcano Plot (Metabo Analyst 5.0)

JCET unpublished data

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