4D-Lipidomics™ based automated annotation of MALDI Imaging data using a dedicated bioinformatics pipeline

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ASMS reboot 2020, ID 302510, Code WP 262

Introduction
The complexity of lipid samples makes their analysis directly from tissue sections extremely challenging. Ion mobility helps in this respect by introducing an additional analytical dimension that can separate isomeric and isotopic molecules. Moreover, annotation of lipids from MALDI Imaging data is often hampered by the limited ability to perform large-scale MS/MS experiments directly from tissue. Here we demonstrate a workflow combining 4D-Lipidomics™ and MALDI Imaging data obtained from just one instrument, timsTOF fleX, in conjunction with a bioinformatics pipeline for automatic lipid annotation.

Methods
4D-Lipidomics™ workflow
MALDI Imaging (negative mode)

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Results

4D-Lipidomics results
Apply five quality criteria on PASEF empowered 4D-Lipidomics data for confident annotations. Merge positive and negative mode data to increase the number of hits.

MALDI Imaging results.
Region of interest (ROI) map of automatically generated molecular features.

4D-Molecular Imaging
Separate isobaric or isomeric compounds using trapped ion mobility spectrometry (TIMS). High resolving power. Molecular Imaging applying TIMS reveals distributions of isobaric compounds without having hundreds of thousands of resolving power.

Conclusions
• Highly confident annotations of PASEF empowered 4D-Lipidomics™ data were retrieved using five quality scoring criteria.
• SpatialOMx® workflow for automatic annotation of MALDI Imaging data using SCiLS Lab and MetaboScape presented.
• 4D-Molecular Imaging applying TIMS reveals distributions of isobaric compounds without having hundreds of thousands of resolving power.

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