CCS-enabled SpatialOMx® for automatic annotation of lipids in MALDI Images based on 4D-Lipidomics™ data

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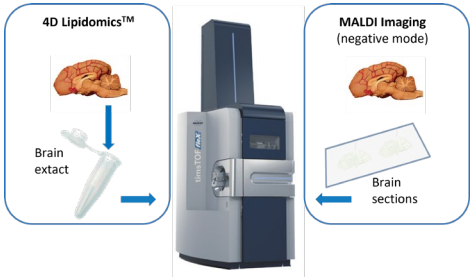
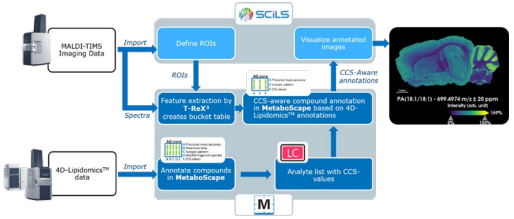
Introduction

The CCS-enabled SpatialOMx workflow opens new dimensions by combining the molecular and spatial information measured by MALDI-TIMS Imaging with highly confident 4D-Omics annotations. MetaboScape® 2021b and SCiLS™ Lab 2021b provide the interface to match data from both ionization techniques and enable automatic and CCS-enabled annotations of MALDI Imaging data. The CCS-value is a key component of this workflow.

Methods

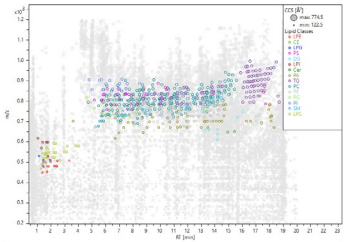


Mouse brain lipids were annotated after LC-ESI PASEF using a brain homogenate. Annotations were based on exact mass, retention time, MS/MS spectra and CCS-value. The resulting list was used to annotate lipids after MALDI Imaging of sections from the same brain sample. In addition to the exact mass, the mobility information (CCS-value) adds an additional confirmation criterion for reliable annotations.

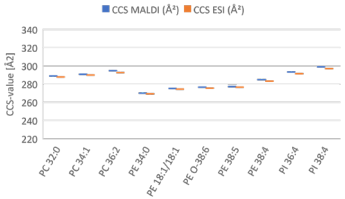


Computational pipeline using SCiLS™ Lab 2021b and MetaboScape® 2021b for CCS-enabled annotation of MALDI Imaging data.

Results



Annotated lipids from the 4D-Lipidomics™ (LC-ESI PASEF) experiment. 292 unique lipids were annotated in negative mode and 295 in positive mode using the rule-based lipid annotation tool of MetaboScape.

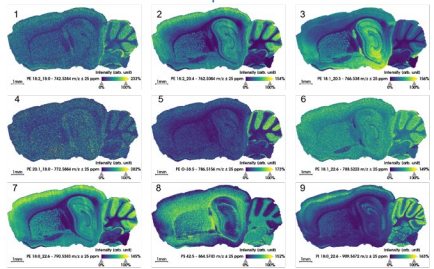


Reproducibility of CCS-values across ESI- and MALDI-ionization for different lipids.

Extract of feature table listing the selected lipids shown below*.

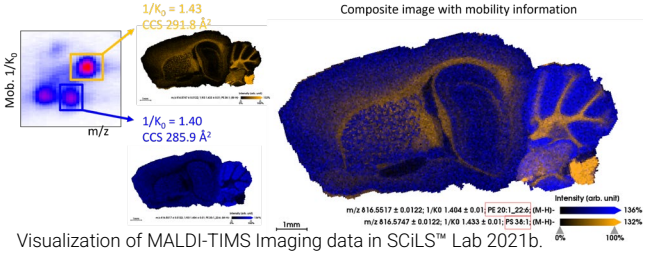
	m/z meas.	M meas.	Ions	Name	Δm/z [pp...	ΔCCS [%]	Molecular For...	Annotations	AQ
1	742.53843	743.54466		PE 18:2_18:0	-1.079	0.0	$C_{41}H_{79}NO_8P$		
2	762.50805	763.51533		PE 38:6	0.162		$C_{43}H_{71}NO_8P$		
3	766.53803	767.54380		PE 18:1_20:3	-1.559	0.2	$C_{43}H_{75}NO_8P$		
4	772.58837	773.59565		PE 20:1_18:0	2.842	0.2	$C_{43}H_{81}NO_8P$		
5	786.52735	787.53297		PS 18:1/18:1	-2.175		$C_{42}H_{78}NO_{10}P$		
6	788.52230	789.52957		PE 18:1_22:6	-1.626		$C_{45}H_{78}NO_8P$		
7	790.53831	791.54559		PE 18:0_22:6	-1.159	0.1	$C_{45}H_{80}NO_8P$		
8	864.57427	865.58155		PS 42:5	-2.010		$C_{48}H_{82}NO_{10}P$		
9	909.54725	910.55452		PI 18:0_22:6	-2.865	0.4	$C_{49}H_{83}O_{13}P$		

Visualization of annotated lipids in SCiLS™ Lab 2021b.



*Missing ΔCCS indicates that a different adduct was detected with ESI.

Feature table after automatic annotation (top) and spatial distribution (bottom) of nine representative lipids after annotation in MetaboScape 2021b. 82 lipids were detected in the negative mode MALDI Imaging data adding contextual information to the lipid annotation list after 4D-Lipidomics.



Visualization of MALDI-TIMS Imaging data in SCiLS™ Lab 2021b.

Conclusions

- Mobility enhanced MALDI-TIMS Imaging enables the separation of isobaric or even isomeric compounds and thereby delivers unprecedented imaging results, especially for spatial lipidomics.
- The novel CCS-enabled SpatialOMx® workflow increases the confidence in lipid annotations for MALDI images through the acquisition of CCS-tagged data.
- The CCS-enabled SpatialOMx® workflow is facilitated by a seamless communication between MetaboScape® 2021b and SCiLS™ Lab 2021b.

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