

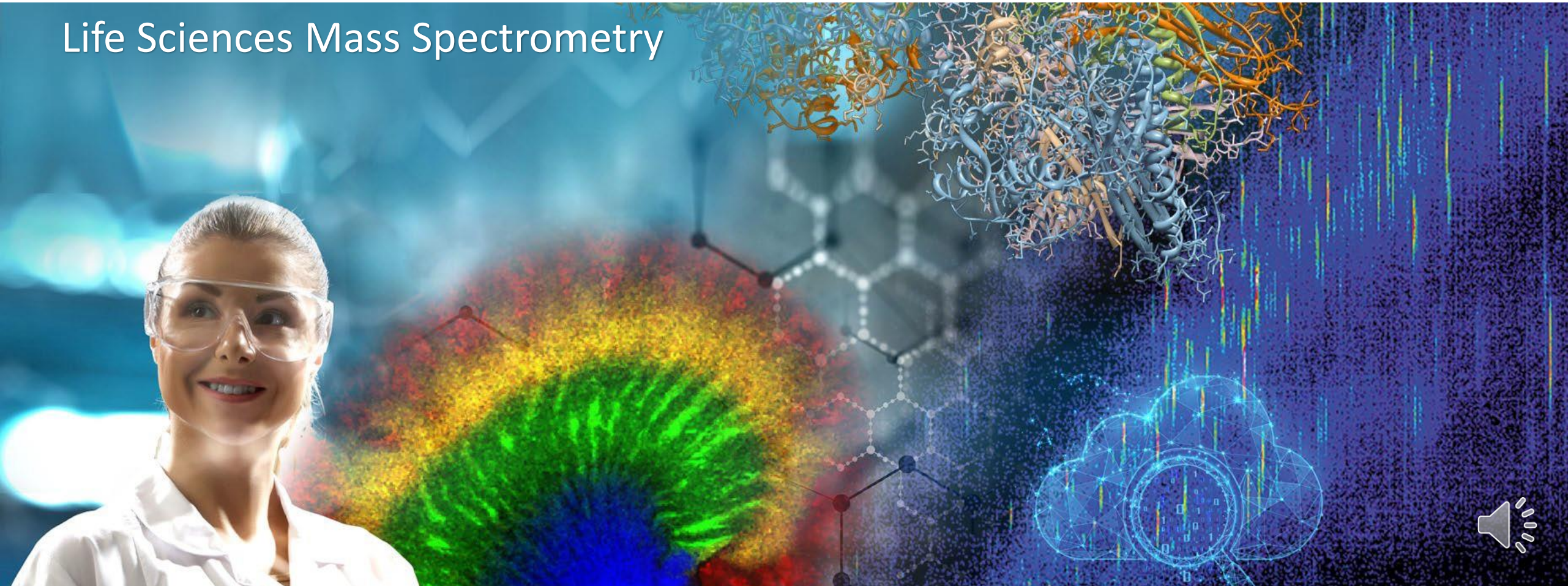
SpatialOMx[®] utilizing MALDI-2 technology adds tissue context to traditional Omics data for in-depth investigation of regional cellular processes



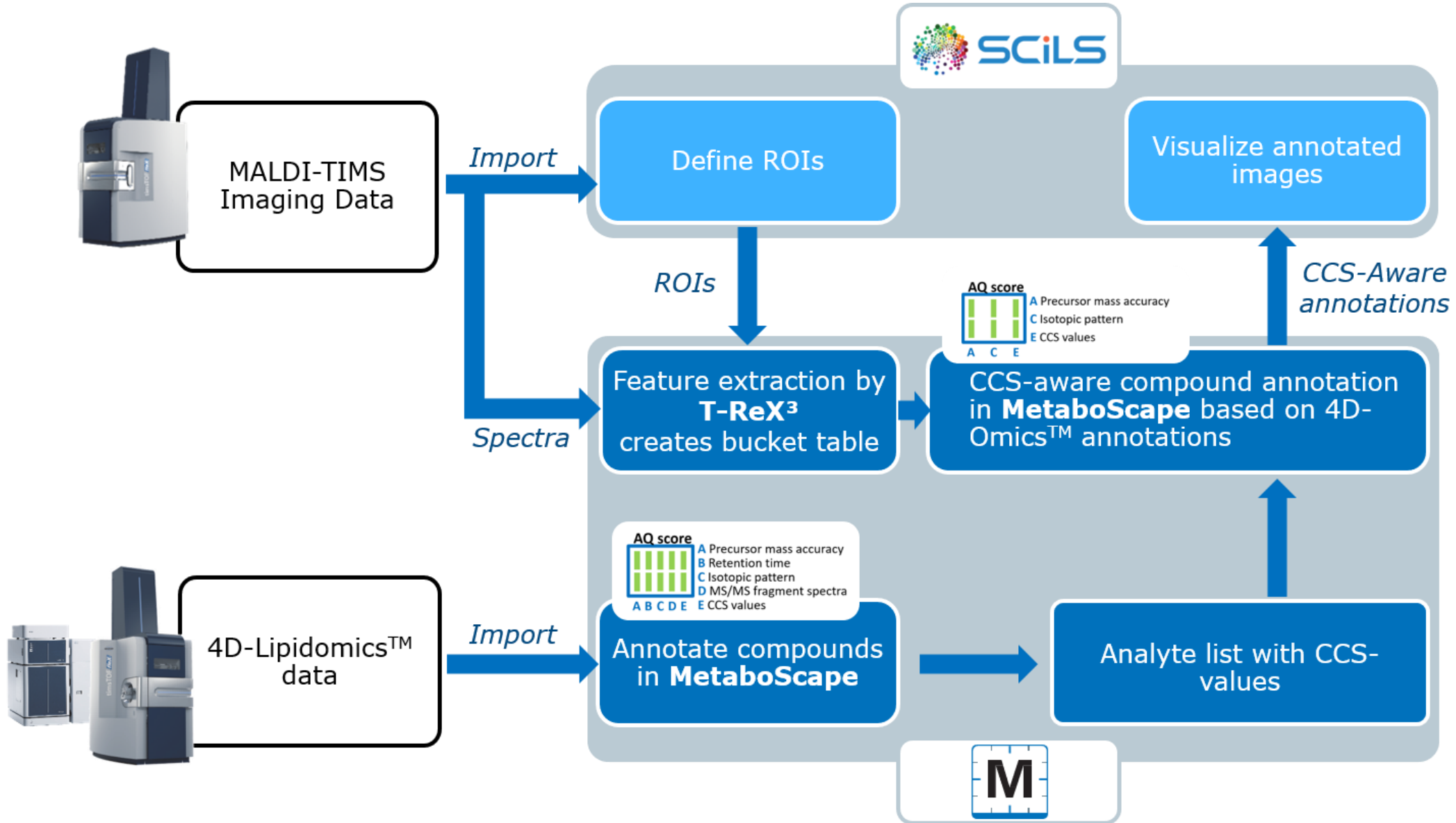
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Life Sciences Mass Spectrometry



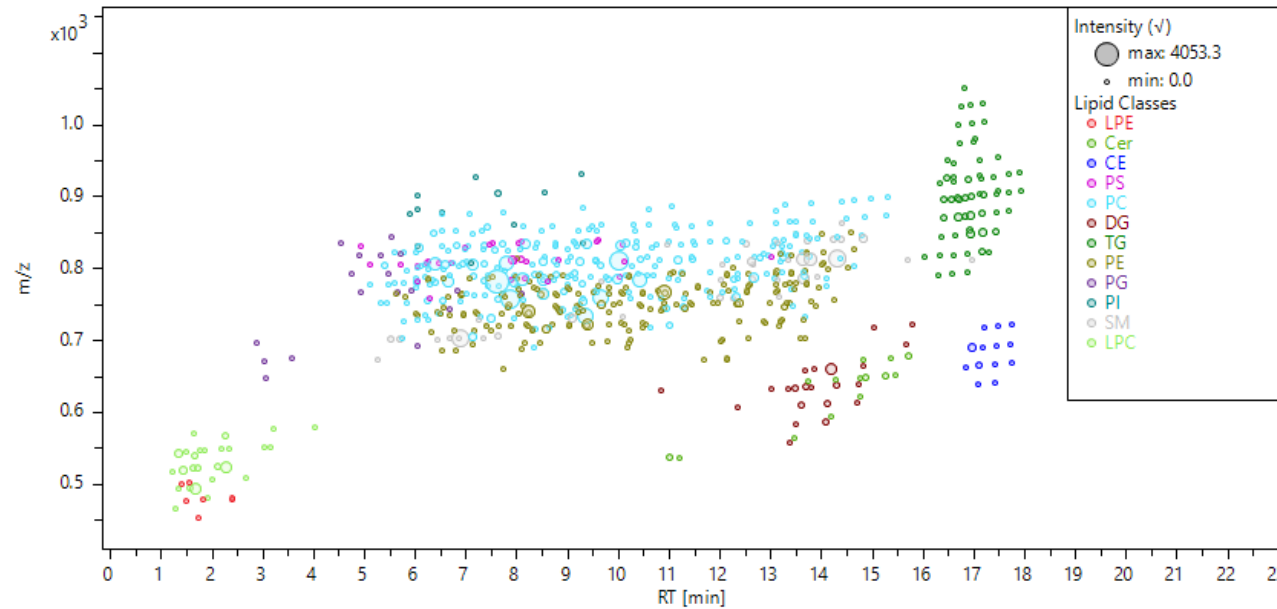
CCS-Aware SpatialOMx workflow with SCiLS™ and MetaboScape®



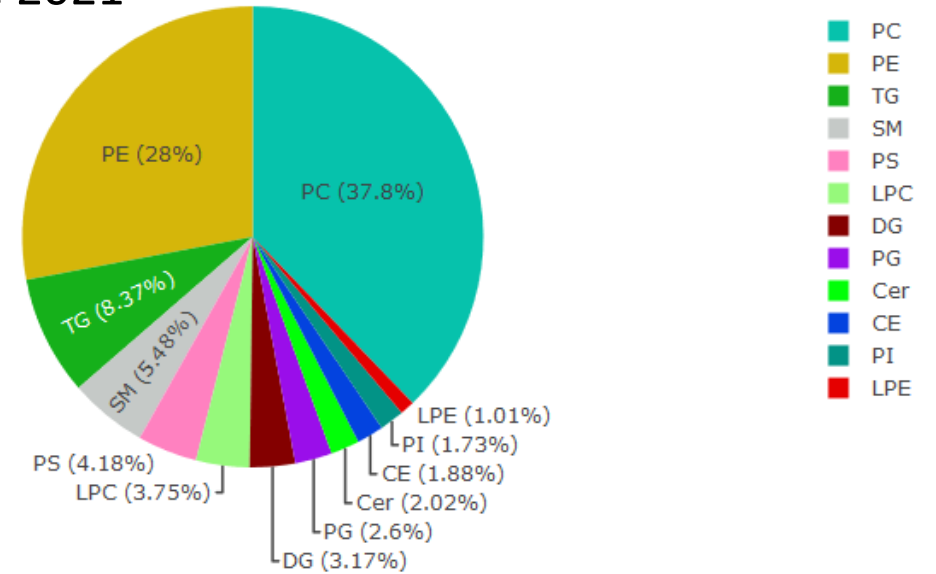
LC-ESI MS/MS lipid annotations from a rat kidney sample



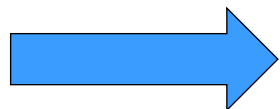
Rule-based Lipid Class annotation implemented in MetaboScape 2021



Overview of detected lipid classes



	RT [min]	CCS (Å ²)	m/z meas.	M meas.	Ions	MS/MS	Δm/z [ppm]	mSigma	MS/MS score	Name	Molecular For...	Annotations	AQ
692	16.70	323.0	896.77097	878.73748	± ■ ■		1.272	102.5	363.0	TG(22:6_16:0_1...	C ₅₇ H ₉₈ O ₆	LC	■ ■ ■
693	17.20	339.6	1004.86511	986.83082	± ■ ■		1.038	29.5	200.9	TG(62:8)	C ₆₅ H ₁₁₀ O ₆	LC	■ ■ ■

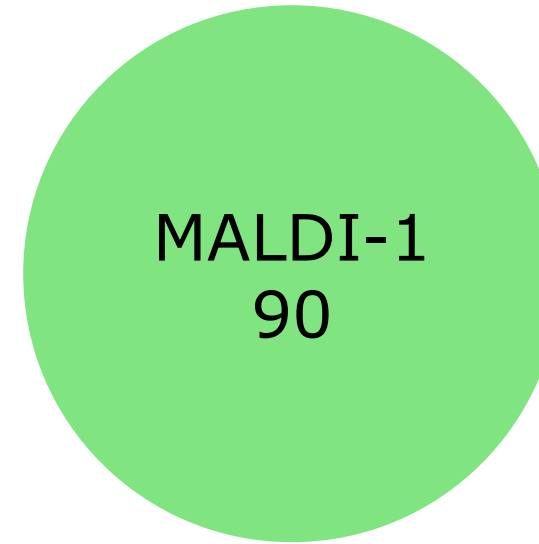
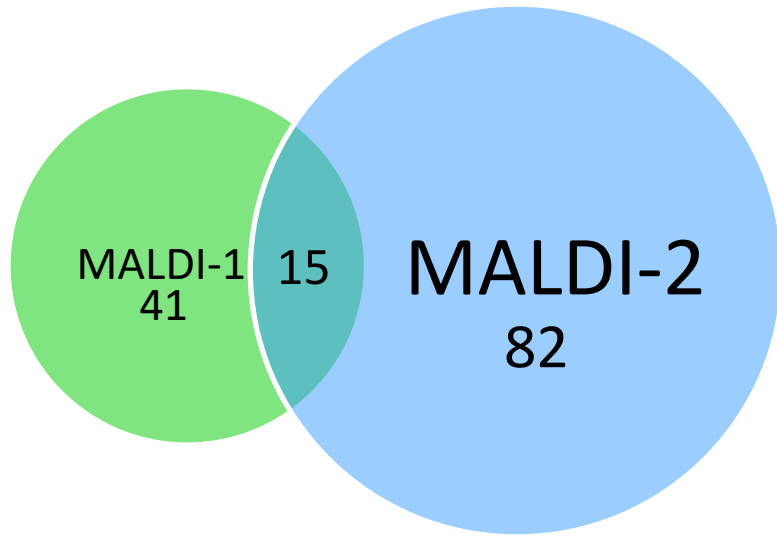


Overall, **693 lipids** were detected and annotated based characteristic fragments.

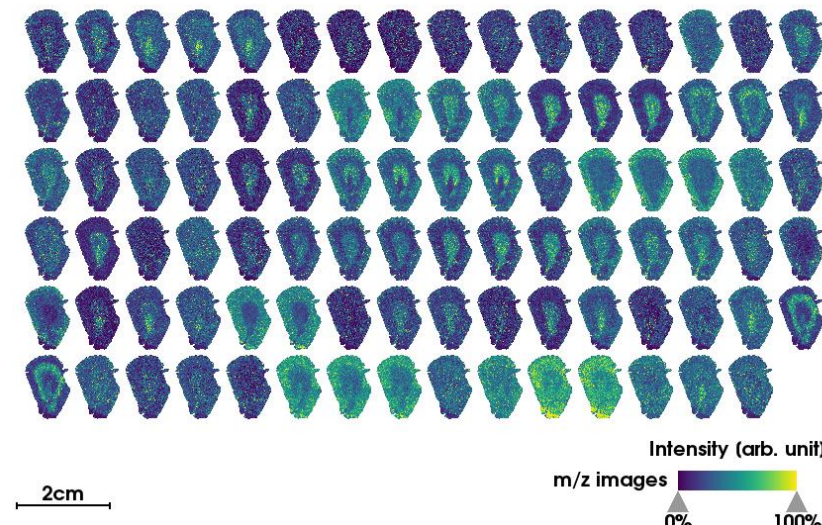
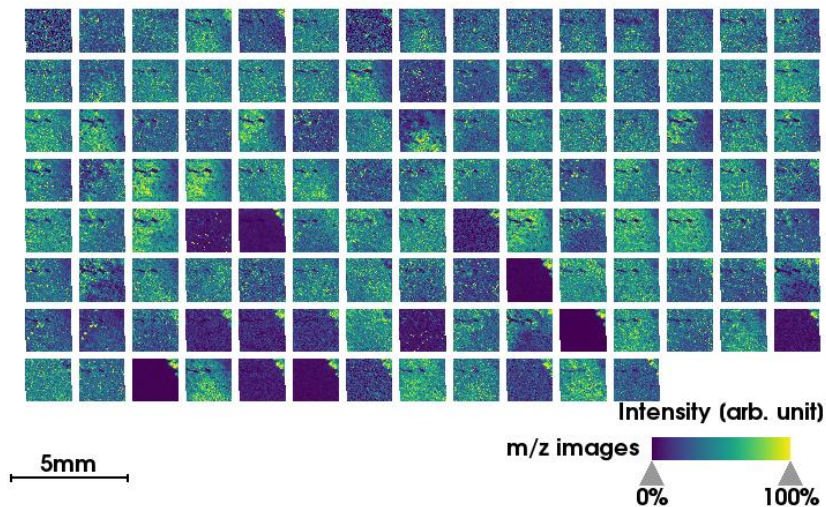
Automatic annotations of MALDI Imaging data

Positive mode lipid imaging

Negative mode lipid imaging

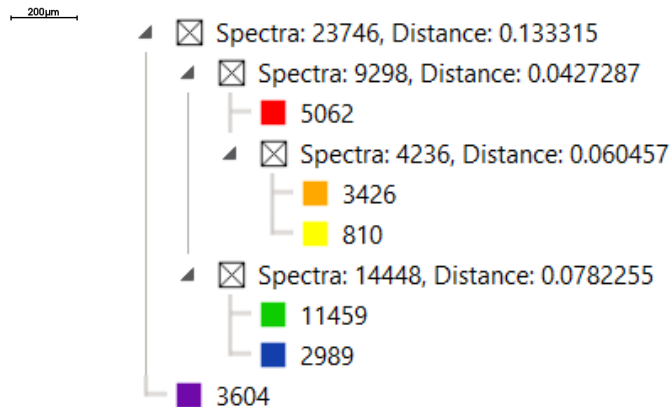
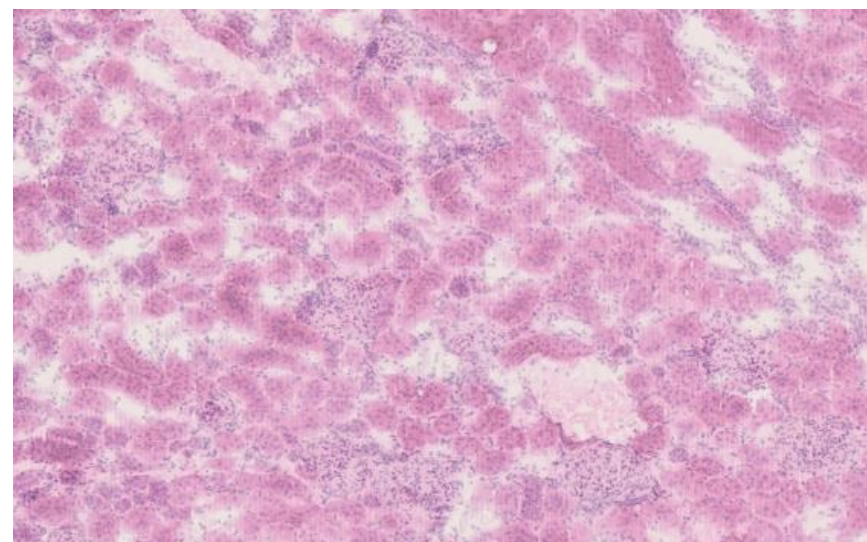
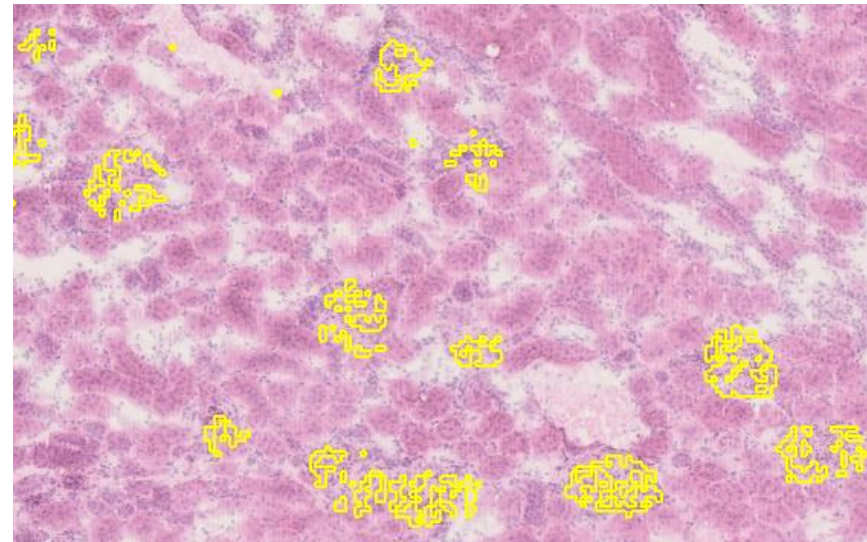
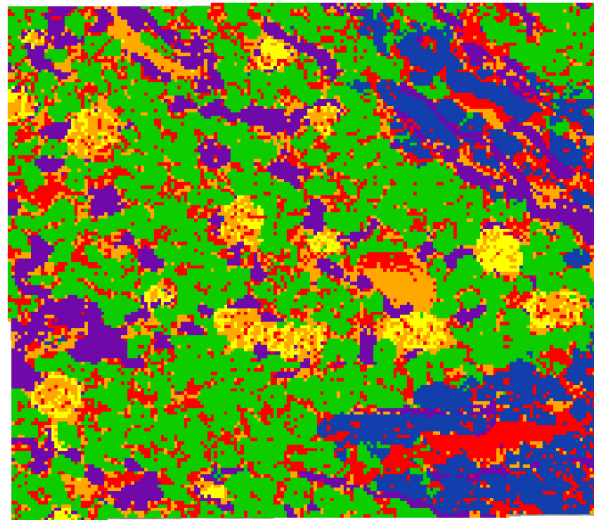


212
annotated
images
with
MALDI-2



Lipids in renal glomeruli

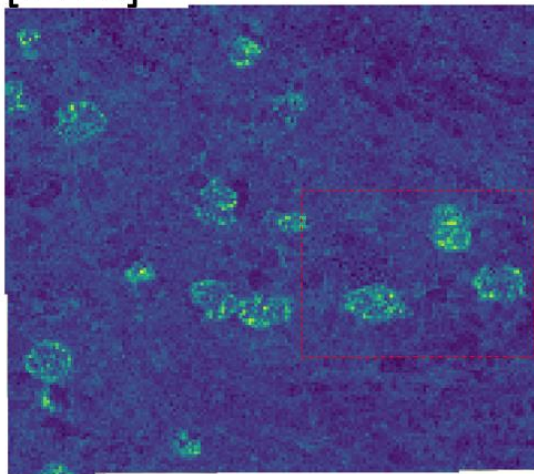
- Identify glomeruli regions in MALDI Imaging data by an unsupervised segmentation analysis



Lipids in renal glomeruli

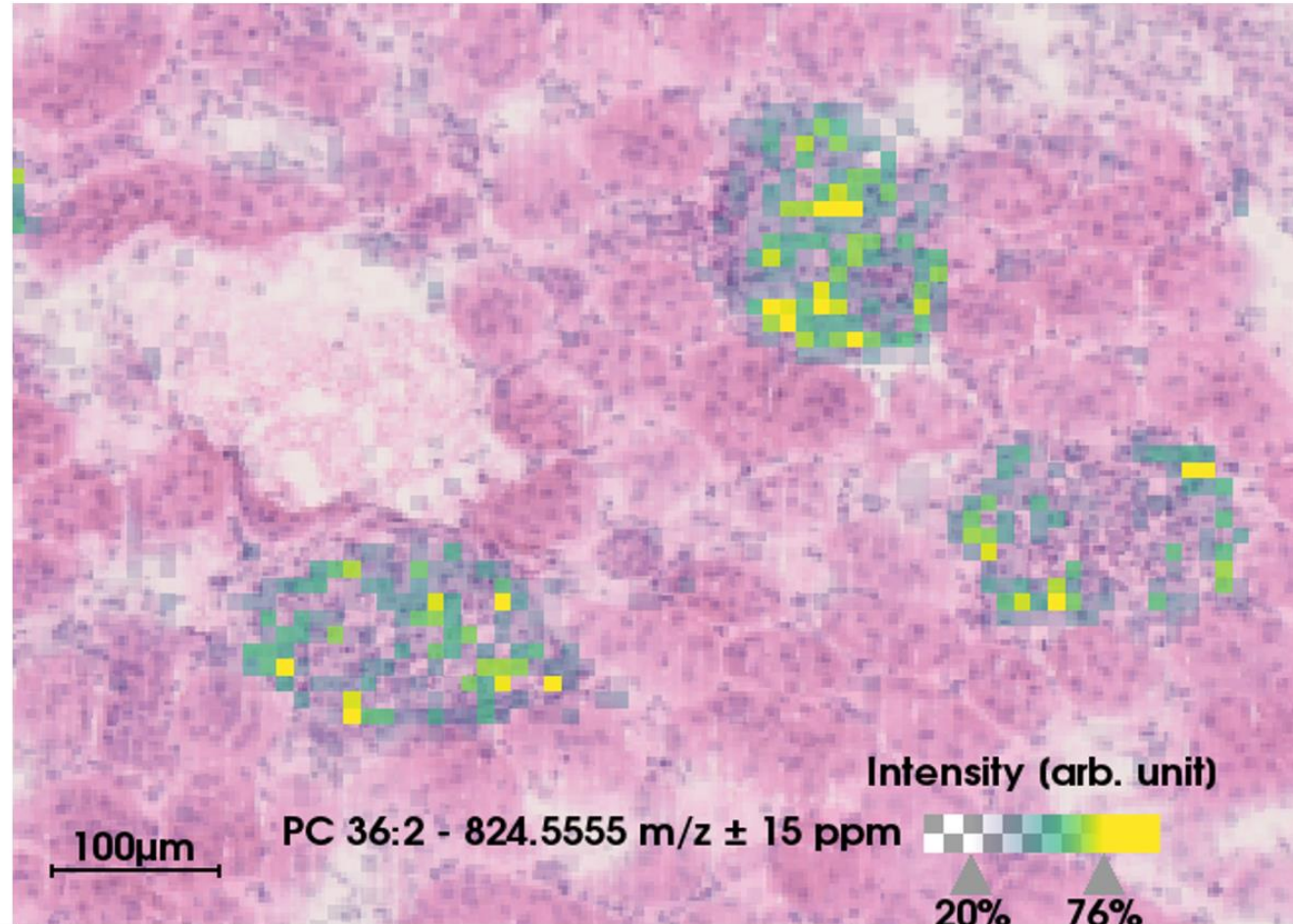
- Annotate lipids localized in glomeruli

[M+K]⁺

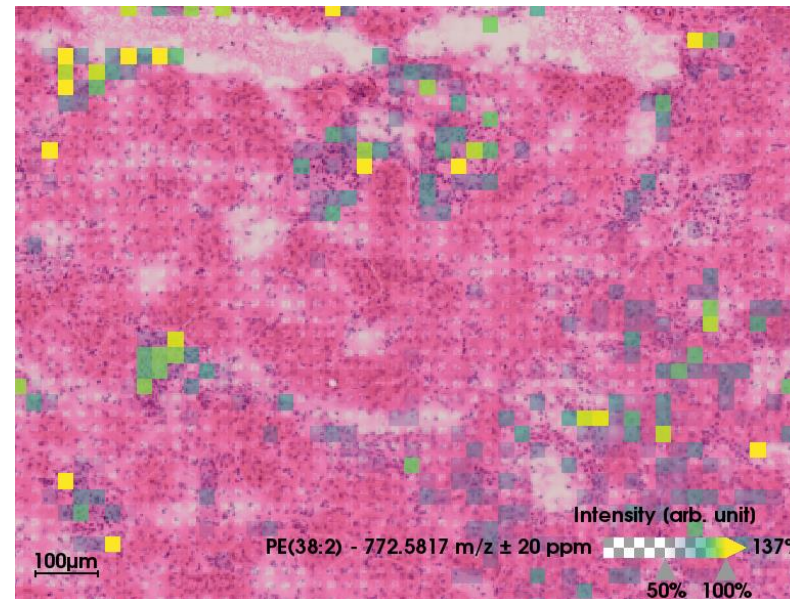
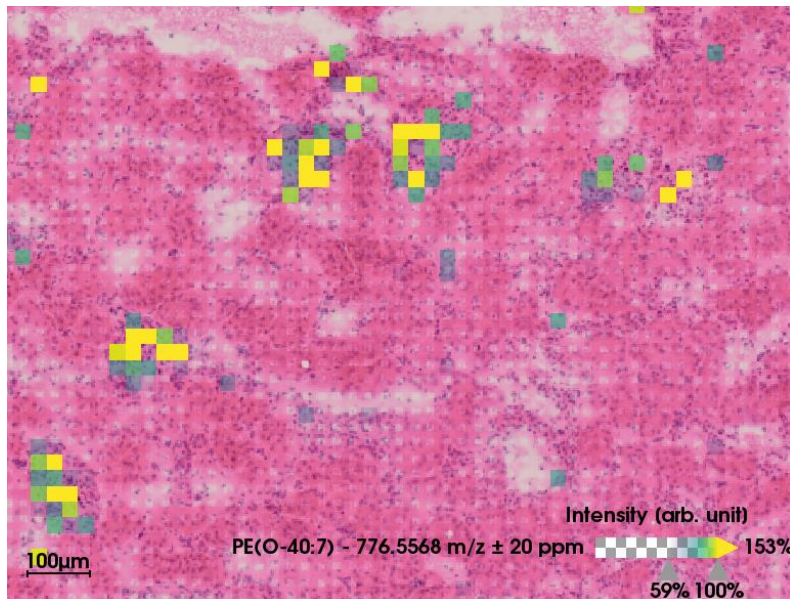
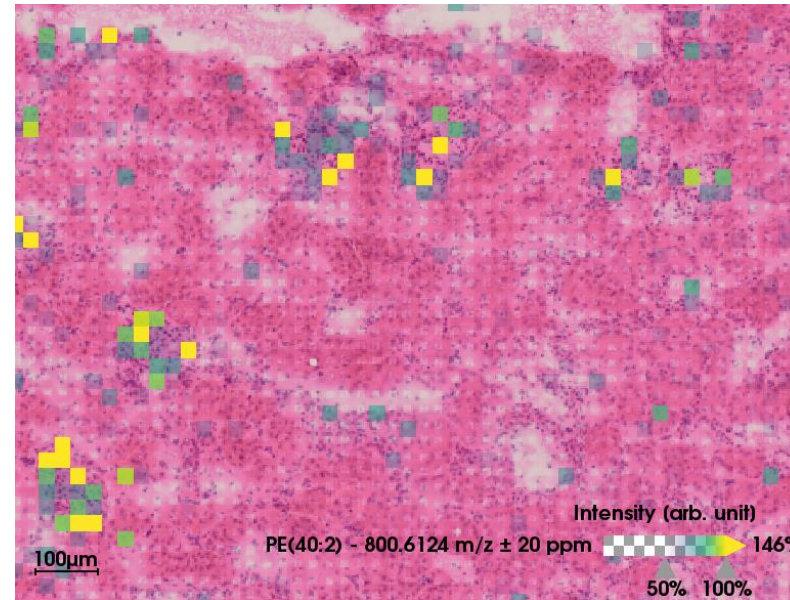
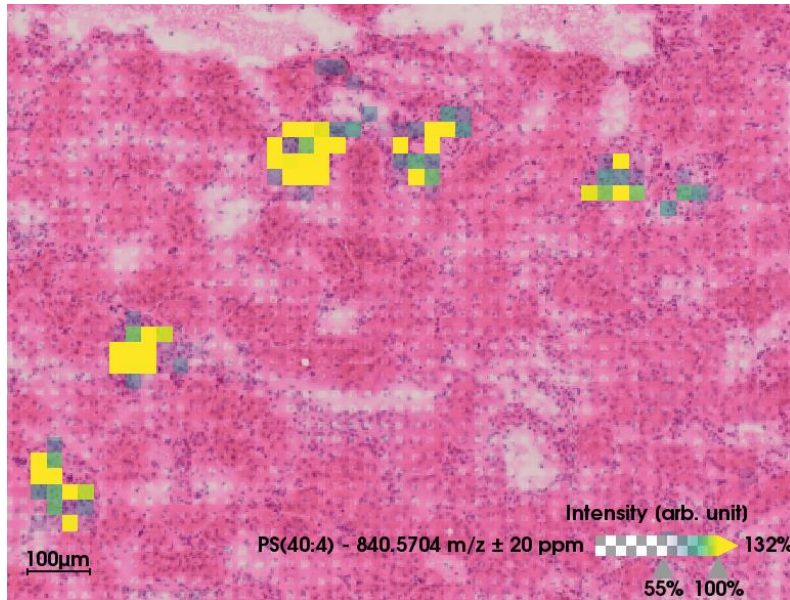


Intensity (arb. unit)
0% 100%
PC 36:2 - 824.5555 m/z ± 15 ppm

- PC (36:2)
- PC (38:2)
- SM (36:1)
- SM (40:1)



Annotated lipids in renal glomeruli: MALDI-2



- PC (36:2)
- SM (36:1)
- SM (40:1)

Unique in MALDI-2:

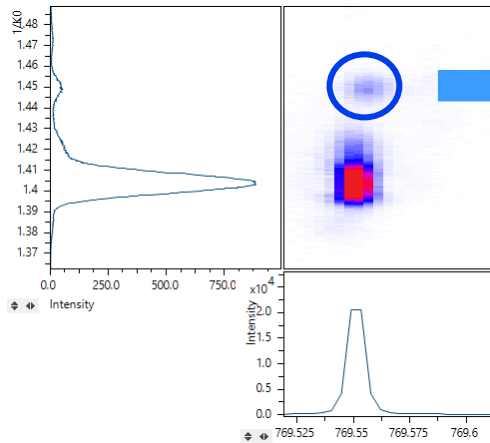
- PS (40:4)
- PE (40:2)
- PE(O-40:7)
- PE (38:2)

The TIMS advantage of the timsTOF fleX

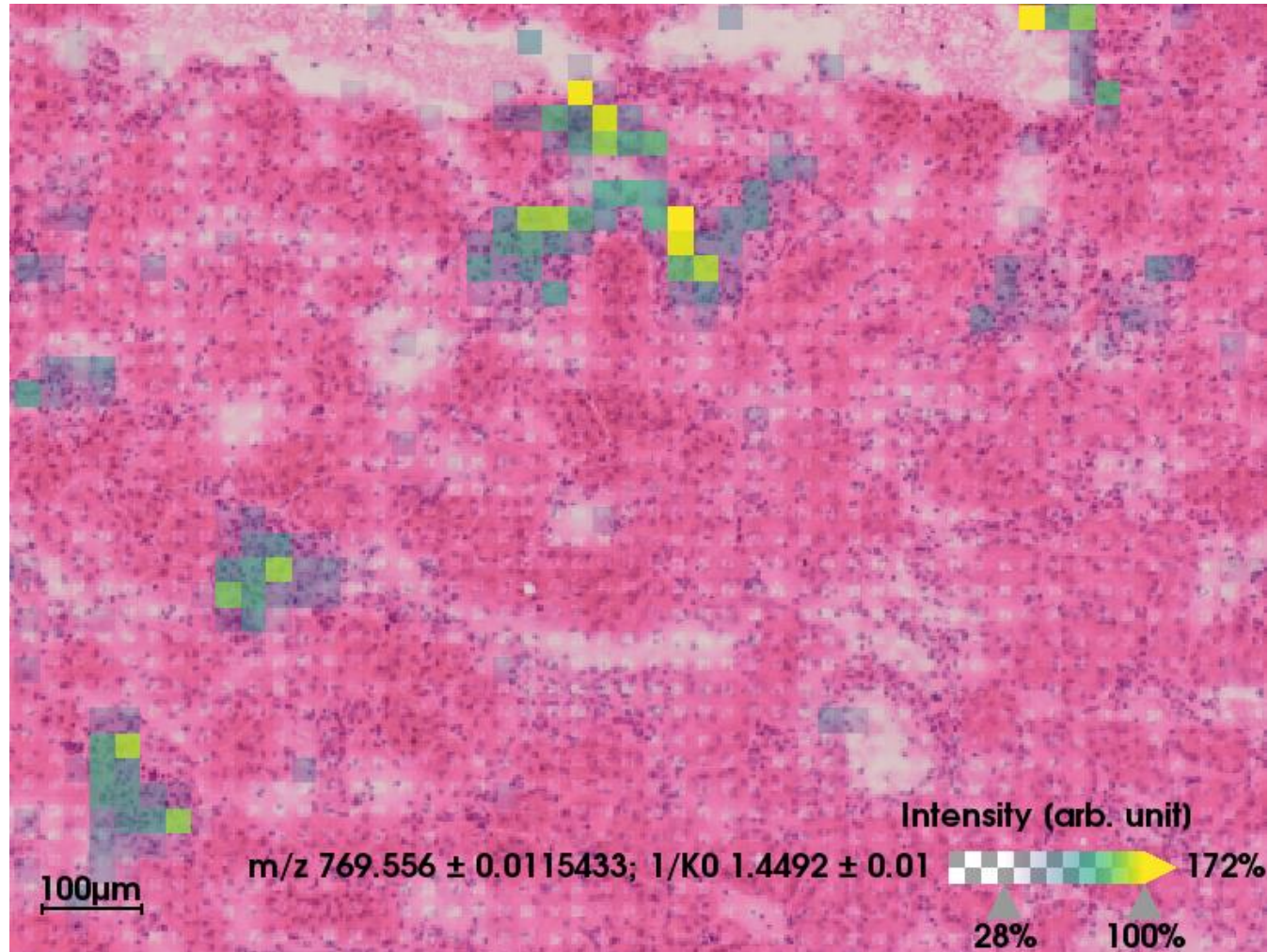
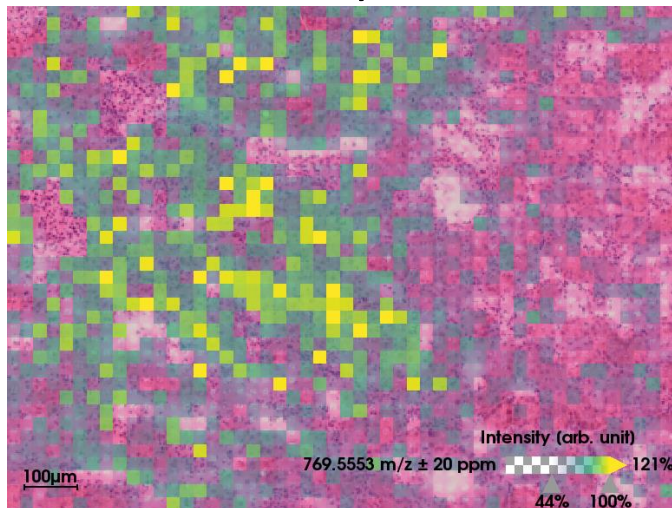
TIMS benefit is especially valuable for MALDI-2 data



SM (36:1); with mobility information

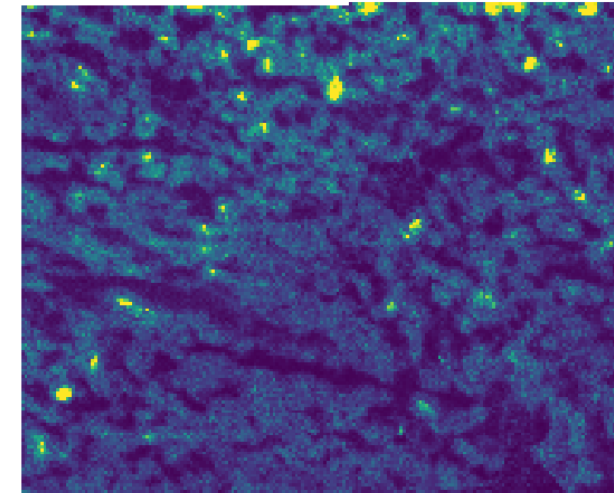


Without mobility information

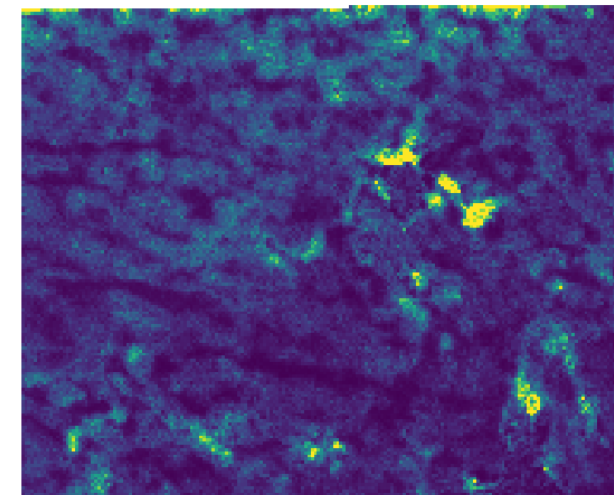


Conclusions

- SpatialOMx is a workflow for automatic annotation of compounds in MALDI images based on confident 4D-Omics data.
- The CCS-value adds an additional confidence criterion for matching of ESI and MALDI data.
- Lipids specifically localized in small tissue regions such as glomeruli were annotated.
- MALDI-2 extends the analytical range to compounds that are not detectable with MALDI-1.
- MALDI-TIMS imaging is especially helpful to separate isobaric compounds in complex MALDI-2 data.



Intensity (arb. unit)
400µm Cholesterol - 369.351 m/z ± 15 ppm 866%



Intensity (arb. unit)
400µm Vitamine E - 430.3781 m/z ± 15 ppm 274%