Applications of Atmospheric Pressure Matrix-Assisted Laser Desorption/Ionization (AP/MALDI) with triple quadrupole mass analyzers

Nivedita Bhattacharya, Ph.D.

BARE FEET ANALYTICS

MassTech

Instrument port

Slot for inserting the target plate or slide

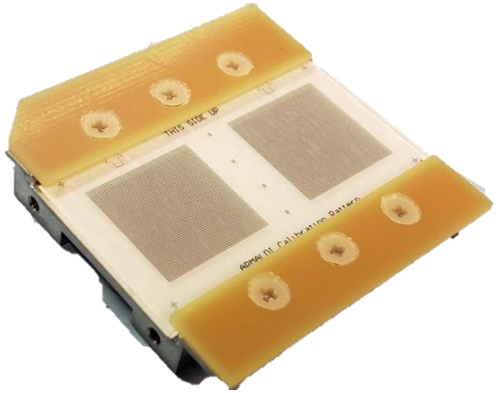
Power Supply

Laser **'ON'** indicator

LAN cable

External **control** port

High Throughput Analysis



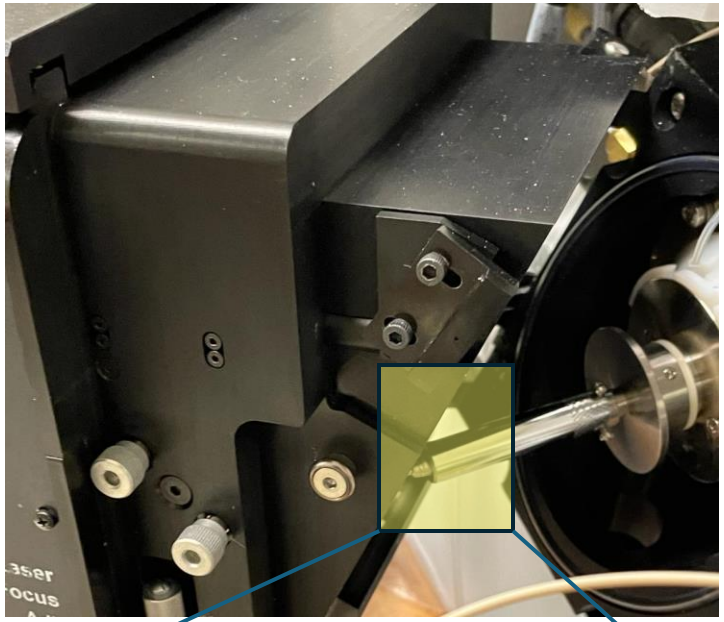
Mass Spectrometry Imaging

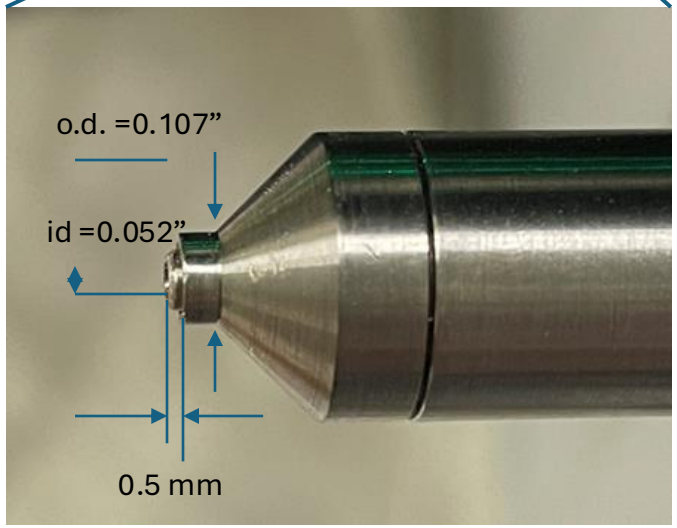
AP/MALDI(ng) specifications:

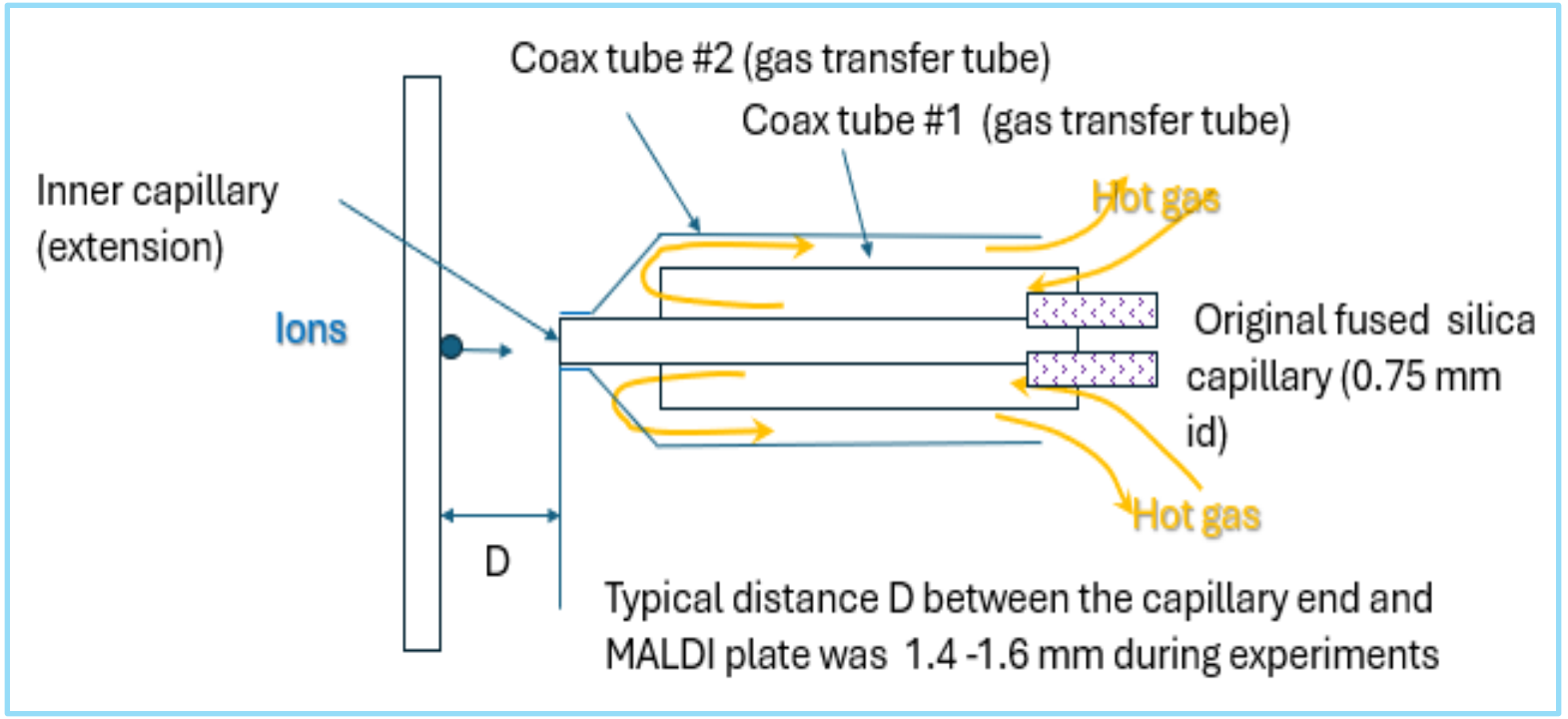
- Laser: 355 nm (Nd:YAG DPSS laser), 1-10 kHz
- MALDI spot size: 5-100 μm
- X-Y stage travel distance: 55 x 55 mm^2
- Sample monitoring: high resolution CCD camera

AP/MALDI QqQ MS

Double Coax Extender (2024)







Aflatoxin M1 analysis with AP/MALDI (single laboratory validation)

JOURNAL ARTICLE

Rapid and Quantitative Analysis of Aflatoxin M1 From Milk Using Atmospheric Pressure–Matrix Assisted Laser Desorption/Ionization (AP-MALDI)-Triple Quadrupole Selected Reaction Monitoring

Get access >

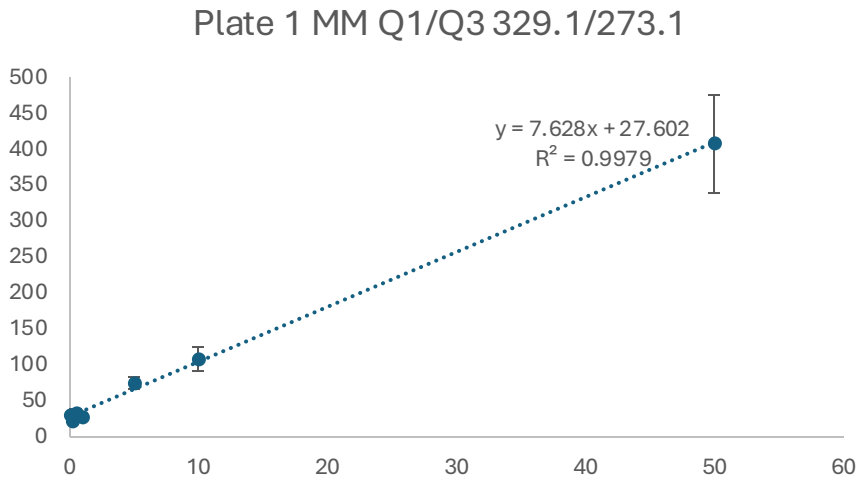
Vishal Mahale, Madhuri Gupta, Manisha Dhanshetty, Subodh Chawan, Eugene Moskovets, Kaushik Banerjee ✉, Nivedita Bhattacharya ✉, Venkateswarlu Panchagnula ✉

Journal of AOAC INTERNATIONAL, Volume 105, Issue 4, July-August 2022, Pages 1043–1050, https://doi.org/10.1093/jaoacint/qsac012

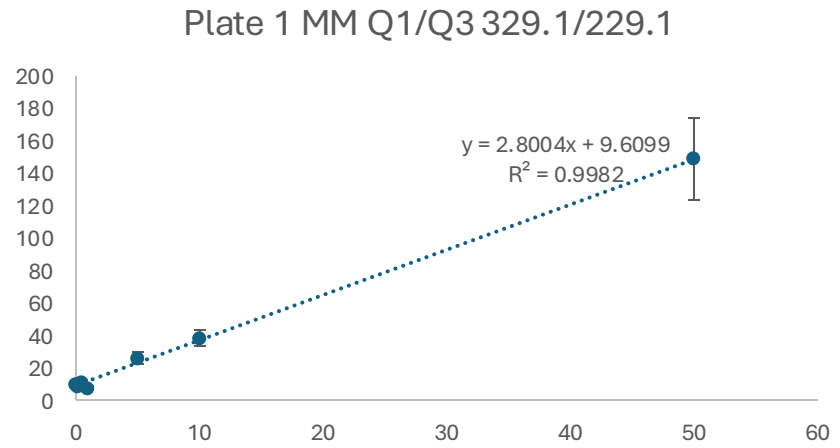
Published: 02 February 2022 **Article history** ▾

- ✓ Developed AP/MALDI QqQ method
- ✓ Method validated with UHPLC FLR
- ✓ Test the "fitness-of-purpose" for the developed method based on established guidelines

Limit of Quantitation (LOQ) of AFM1 with AP/MALDI



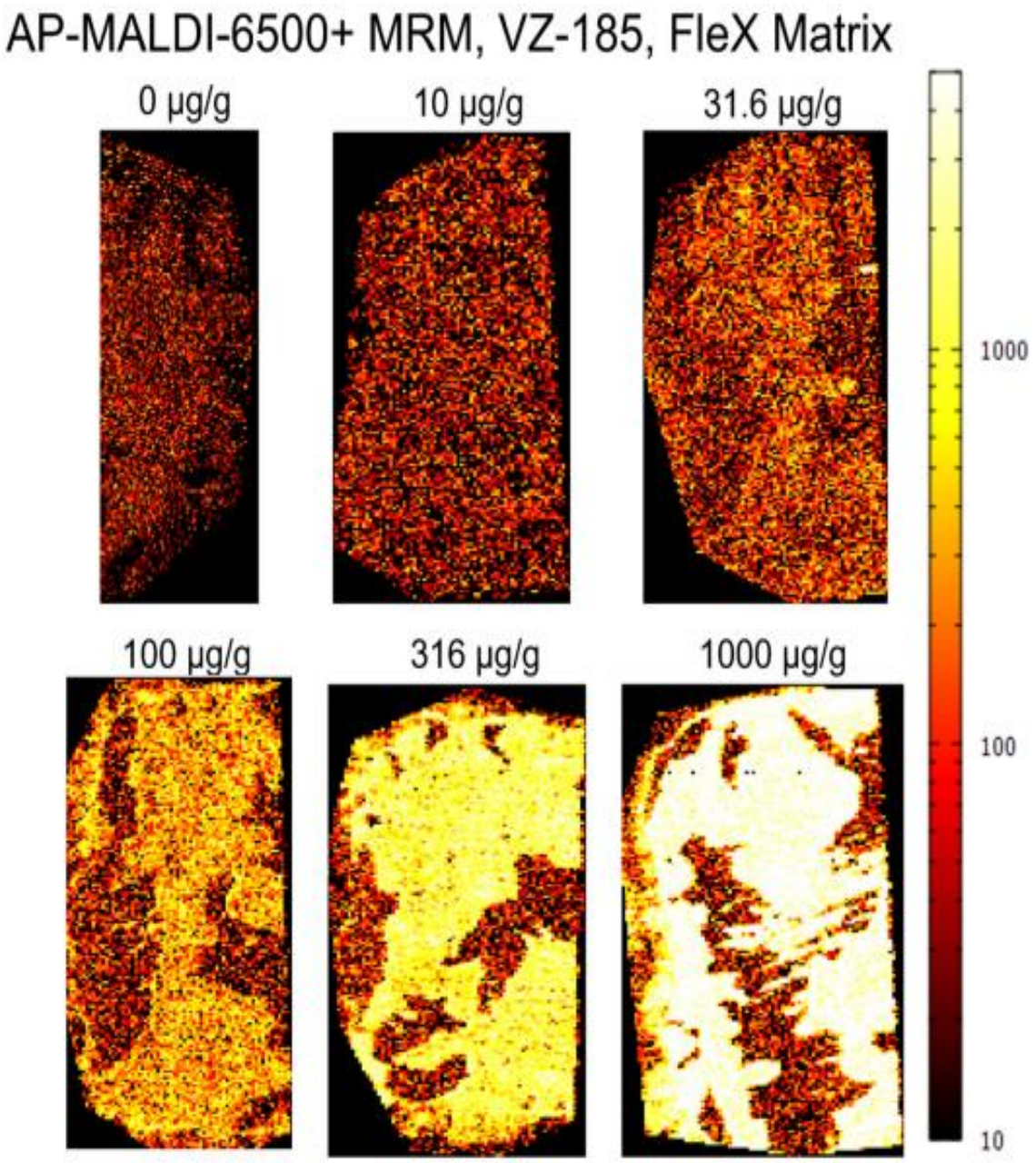
Concentration (in ppb)	Ion intensity Q1/Q3 (329/273) ± SD (n=4)	Ion intensity Q1/Q3 (329/229) ± SD (n=4)
0.2	29.4 ± 3.8	14.0 ± 2.2
0.4	29.2 ± 5.6	12.0 ± 2.0
2	50.0 ± 10.5	17.5 ± 2.6
4	69.3 ± 8.0	28.5 ± 3.8
10	100.2 ± 9.8	39.4 ± 6.7
20	184.7 ± 19.7	69.0 ± 8.9
50	195.7 ± 33.6	73.8 ± 11.6
100	753.8 ± 136.1	322.7 ± 58.7
1000	8021.8 ± 1089.9	3140.7 ± 540.6



- ✓ LOQ of the method is lower than mandated regulated limits of the FDA
- ✓ Calibration curves across 3 days exhibited excellent $R^2 = 0.99$
- ✓ RSDs of qualifier (Q1/Q3 – 329.1/273.1) to quantifier (Q1/Q3 329.1/229.1) ion ratios for matrix-matched calibrants and QC samples

For more details, please visit poster ThP 637 (Thursday)

AP/MALDI QqQ for Tissue Imaging



pharmaceuticals

MDPI

Article

Evaluation of Quantitative Platforms for Single Target Mass Spectrometry Imaging

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TP 292

Instrumentation: General

Multivendor and Multiplatform Comparison of Linearity and Sensitivity in Mass Spectrometry Imaging

by Andrew Bowman, AbbVie, Inc., North Chicago, IL

Bowman A. *et. al., Pharmaceuticals*, **2022**, 15, 1180

Application Note

Biotherapeutics and Biosimilars

Agilent

Trusted Answers

Imaging Lipids in a Brain Injury Model with AP-MALDI on the Agilent 6495 Triple Quadrupole and 6560 Ion Mobility Mass Spectrometers

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Abstract

This application note demonstrates the interface of an atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI) source to an Agilent 6495 triple quadrupole (TQ) mass spectrometer and an Agilent 6560 ion mobility Q-TOF mass spectrometer. The ability to image endogenous lipids across mouse brain tissue using selective precursor to product ion transitions on the TQ mass spectrometer is demonstrated. It is further demonstrated that the same AP-MALDI source can be used to generate mass spectrometry images of endogenous lipids using an ion mobility-enabled Q-TOF mass spectrometer. As a result, these data highlight the compatibility of using AP-MALDI on Agilent mass spectrometers to selectively detect and image endogenous mouse brain lipids.

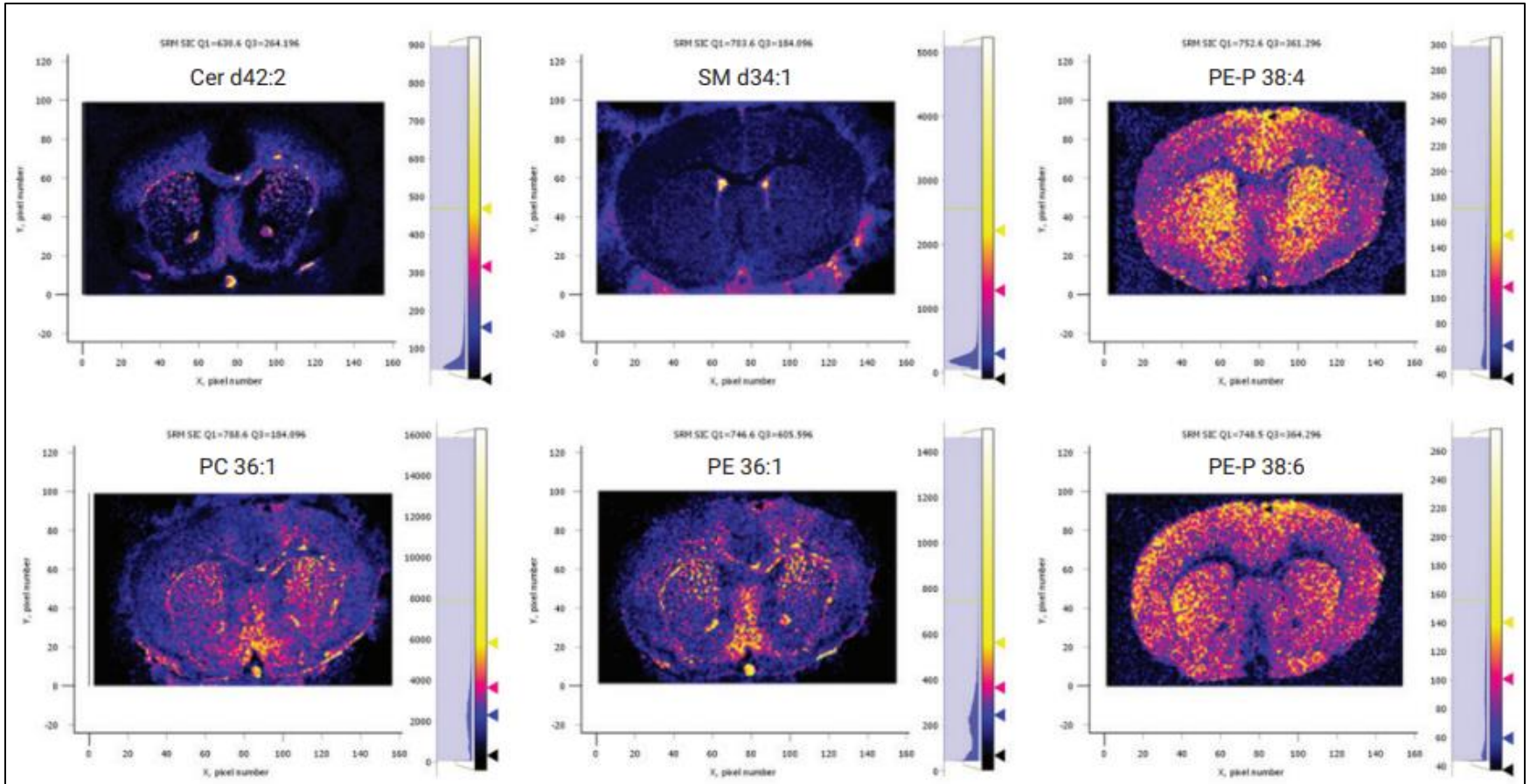


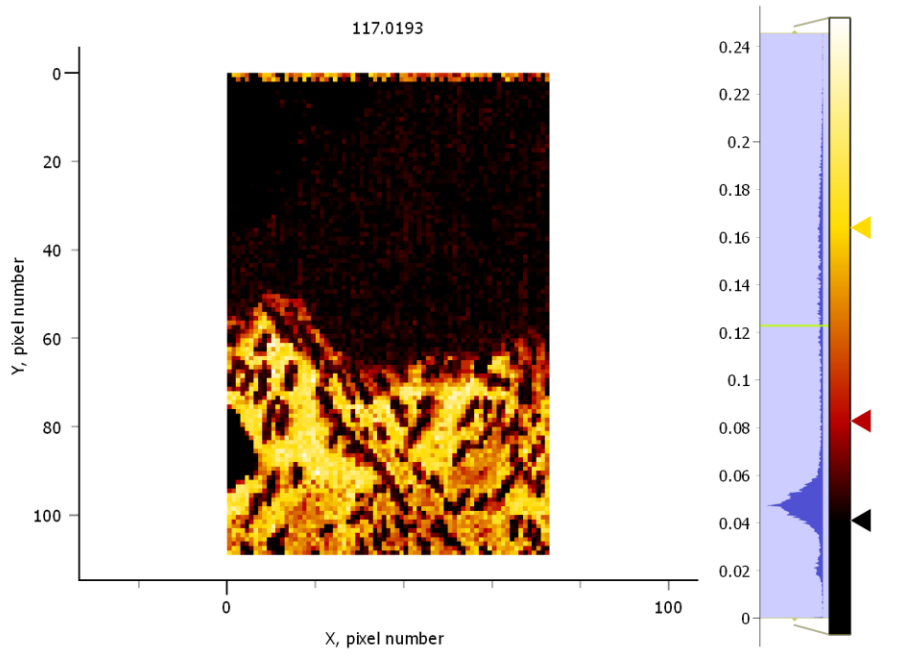
Figure 3. AP-MALDI triple quadrupole images of selected lipids.

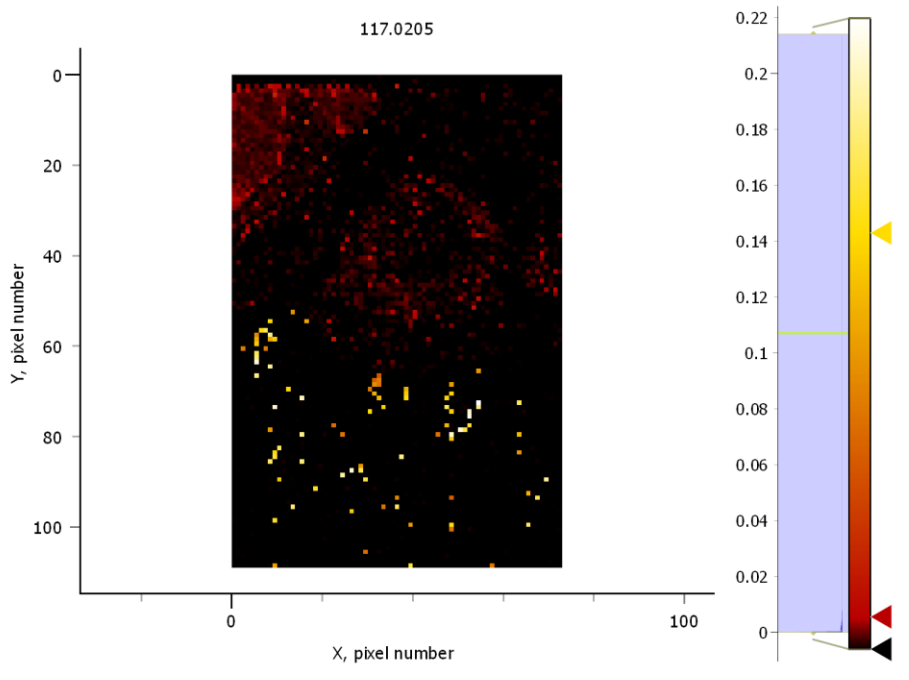
Targeted lipid MRM transitions.

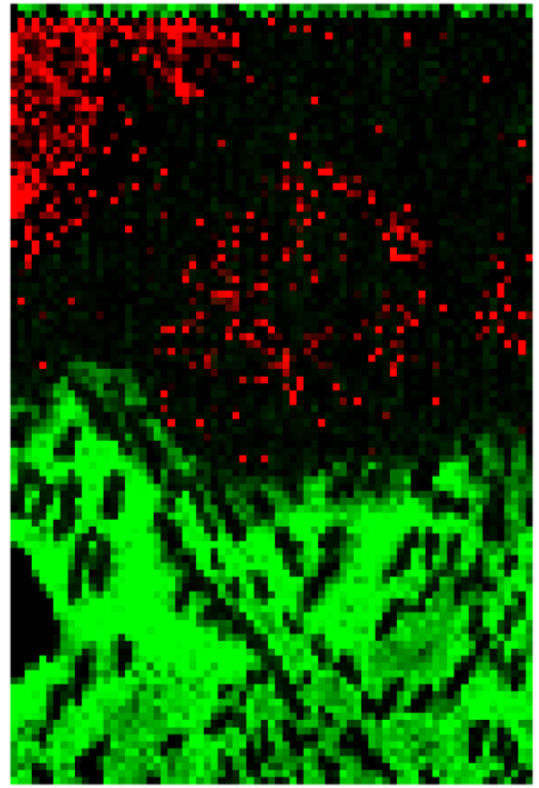
Targeted Lipid Transitions			
Lipid	Ion	Precursor	Product Ion
Cer d42:2	$[M+H-H_2O]+$	630.6	264.2
SM(d34:1)	[M+H]+	703.6	184.1
HexCer(d42:2)	$[M+H-H_2O]+$	792.7	264.2
LPE 18:0	[M+H]+	482.3	341.3
LPC 16:0	[M+H]+	496.3	184.1
LPC 18:0	[M+H]+	524.4	184.1
PC 32:0	[M+H]+	734.6	184.1
PC 34:1	[M+H]+	760.6	184.1
PC 36:1	[M+H]+	788.6	184.1
PC 38:4	[M+H]+	810.6	184.1
PE 36:1	[M+H]+	746.6	605.6
PE 38:2	[M+H]+	772.6	631.6
PE 40:6	[M+H]+	792.6	651.6
PE P-38:6	[M+H]+	748.5	364.3
PE P-38:4	[M+H]+	752.6	361.3
PE P-40:6	[M+H]+	776.6	385.3

AP/MALDI MSI of liver tumor – Exploris 240

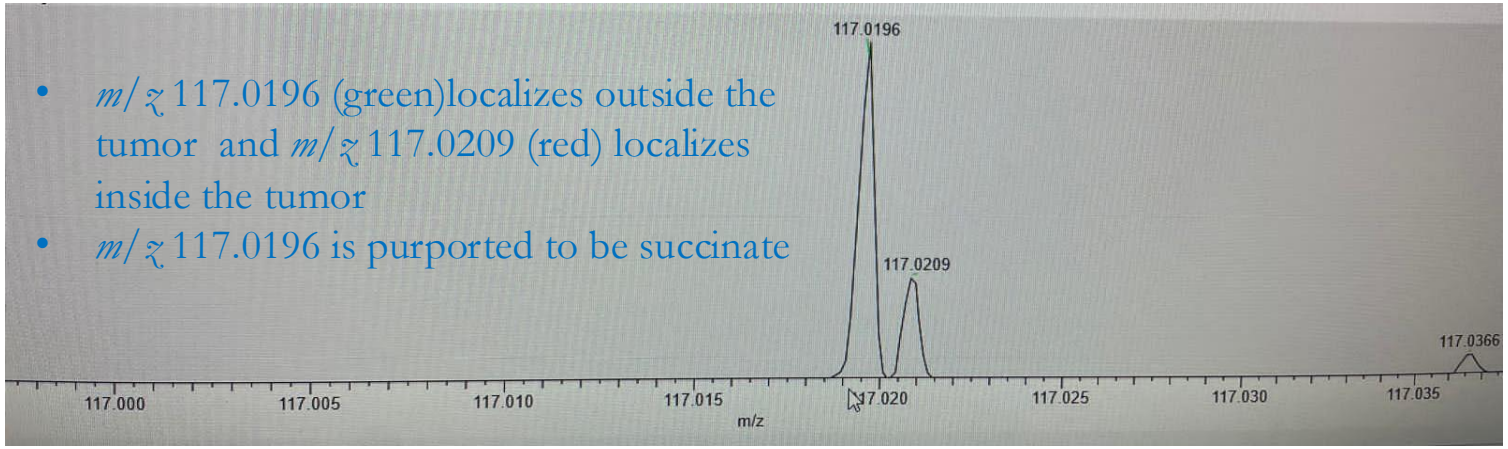
Prof. Gary Patti, Dr. Vika Anokhina, Washington University St. Louis



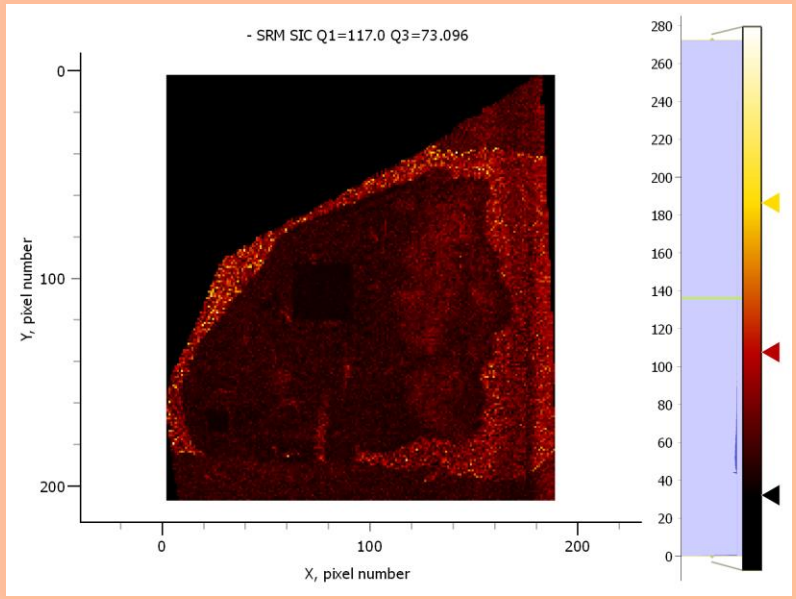


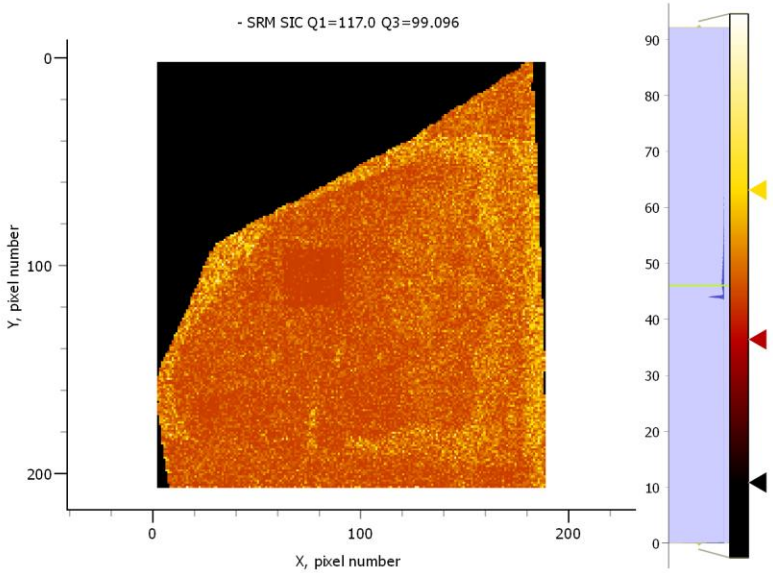


- *m/z* 117.0196 (green)localizes outside the tumor and *m/z* 117.0209 (red) localizes inside the tumor
- *m/z* 117.0196 is purported to be succinate

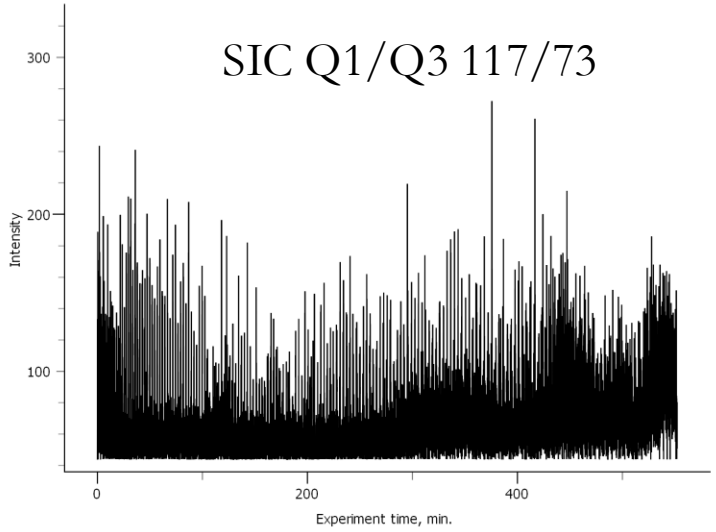


AP/MALDI QqQ MSI of liver tumor

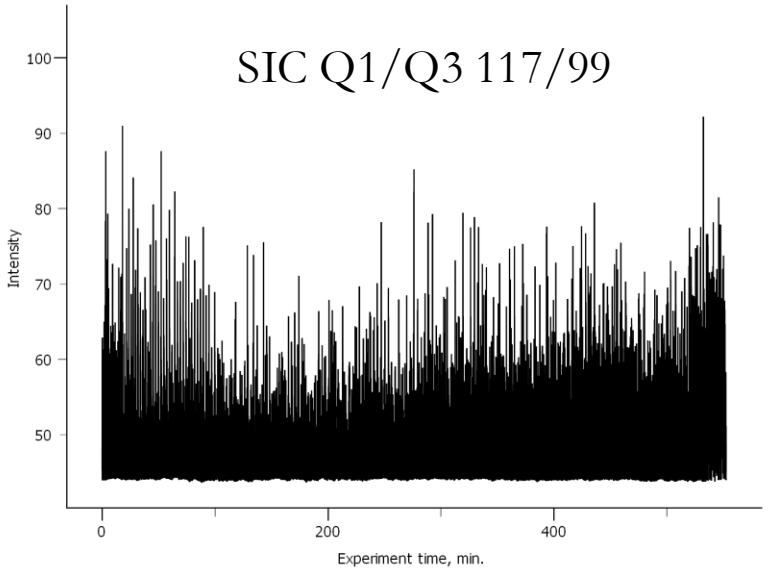




SIC Q1/Q3 117/73



SIC Q1/Q3 117/99



Thank You

Barefeet Analytics Private Limited

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Akshay Vasekar

MassTech Inc.

Venkat Panchagnula
Eugene Moskovets
Konstantin Novoselov

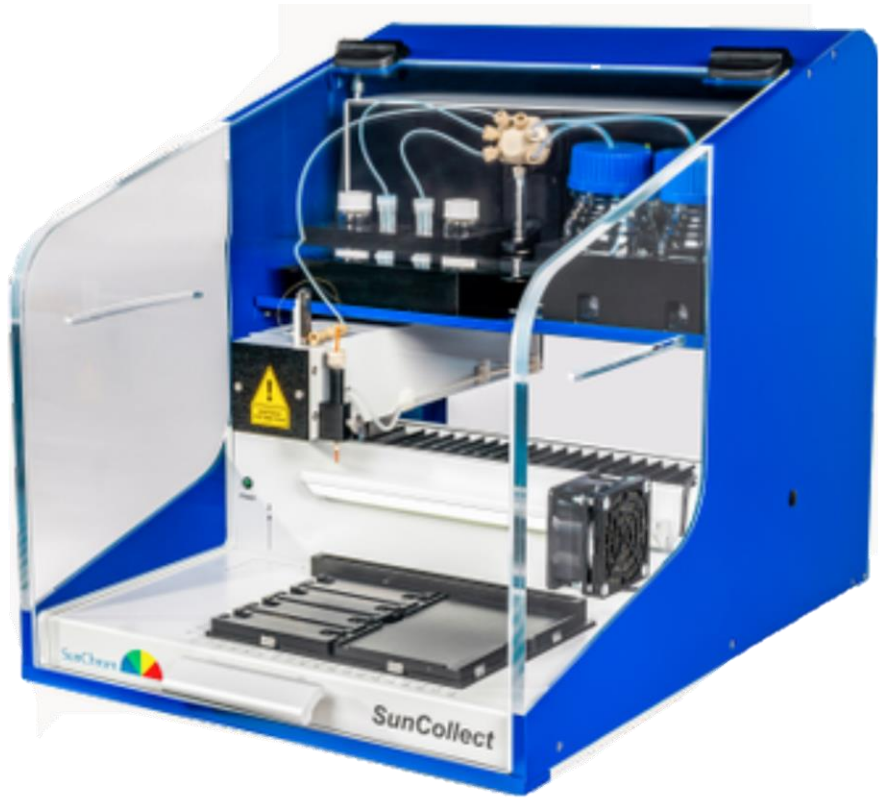
Backup Slides

Analytical method variables

De Sante Guidelines is followed by food industry for validation of chromatography and MS methods

ANALYTICAL QUALITY CONTROL AND METHOD VALIDATION PROCEDURES FOR PESTICIDE RESIDUES ANALYSIS IN FOOD AND FEED SANTE 11312/2021

MS detector/Characteristics		Acquisition	Requirements for identification	
Resolution	Typical systems (examples)		minimum number of ions	additionally
Unit mass resolution	Single MS quadrupole, ion trap, TOF	full scan, limited *m/z* range, SIM	3 ions	S/N ≥ 3[d] Analyte peaks from both product ions in the extracted ion chromatograms must fully overlap.
	MS/MS triple quadrupole, ion trap, Q-trap, Q-TOF, Q-Orbitrap	selected or multiple reaction monitoring (SRM, MRM), mass resolution for precursor-ion isolation equal to or better than unit mass resolution	2 product ions	Ion ratio from sample extracts should be within **±30% (relative)** of average of calibration standards from same sequence
Accurate mass measurement	High resolution MS: (Q-)TOF (Q-)Orbitrap	full scan, limited *m/z* range, SIM, fragmentation with or without precursor-ion selection, or combinations thereof	2 ions with mass accuracy ≤ 5 ppm[a, b, c]	S/N ≥ 3[d] Analyte peaks from precursor and/or product ion(s) in the extracted ion chromatograms must fully overlap. Ion ratio: see D12


SunCollect