



Mass Spectrometry Facility

Leadership



Sergey Pronin, PhD
Director, MS



Felix Grun, PhD
Manager

Mission

To support researchers with expertise and services in mass spectrometric analyses of proteins, oligonucleotides, metabolites and drugs.

- The MS Facility (Chemistry) provides both walk-up open access and staff services for a wide range of MS applications
- Staff provide weekly user/instrument training
- Additional MS services are available from the High-End Mass Spectrometry Facility (HMSF) and the Nutritional Metabolism & Disease Lab (NMDL)

Key Features

- Open Access:** Available 24/7
- 20 MS Instruments**
- User-run samples:** 300+ users/yr | 35,000+ samples/yr
- Low cost:** \$2 – \$30/sample
- Service requests:** via Agilent iLab or website
- Staff support:** Felix Grün, *Director*
Ben Katz, *Proteomics Specialist*
Chris Dickson, *GSR Fellow*

Capabilities

- Small molecule analysis – substrate/product monitoring
- Molecular formula (MF) validation ± 5 ppm
- Isotopic labelling analysis
- Polar/non-polar analyte detection/quantitation
- Air/temperature sensitive analytes
- Quantitation from biological/environmental matrices (targeted metabolomics)
- LC and UV/Vis complex mixture analysis (LC & GC) (global untargeted metabolomics)
- Polymer analysis (oligonucleotides, oligosaccharides)
- Peptide analyses (HRMS; in gel digestion, sequencing, aa modifications, PTMs)
- Intact protein analyses (up to 250 kDa)
- Ion mobility w/ MS (structural discrimination for isobaric species)
- Hydrogen-deuterium exchange (HDX) – protein-protein interactions
- Imaging mass spectrometry (IMS) –5–50 μm pixel res; 40 px/sec
- MS Software: MassLynx, PEAKS Studio 12, Progenesis Q1, BioPharmaLynx, MassHunter, Chromeleon 7, mzMine, Sirius, SciLS Lab Pro, ImageReveal. Remote login/access available

UCI Mass Spectrometry Facility
Department of Chemistry
<https://ucimsf.ps.uci.edu>

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Mass Spectrometry Facility Core Services
The Mass Spectrometry Facility (MSF) in the Department of Chemistry provides staff services and walk-up access to a variety of mass spectrometry instruments suitable for the analysis of small molecules, peptides/proteins and nucleic acids. The MSF provides services principally to faculty research groups in Chemistry and other UC departments/schools, but also accepts samples from outside academic/non-profit and commercial clients.

Instruments
ESI-LC-TOF
GC-MS
ESI-MS/MS
MALDI-TOF
IC
HPLC
ESI-LC-QDA
QQQ

Services
Open Access
User Training
Accurate Mass
Peptide Sequencing
Metabolomics
Custom
Rates
Calendars/Logbooks
Acknowledgments

MS News (Nature)
Latest news and research from Nature.com on the topic of Mass spectrometry

MS News (Google)
Google News

Recent UCI MS Publications

Key Equipment & Technologies



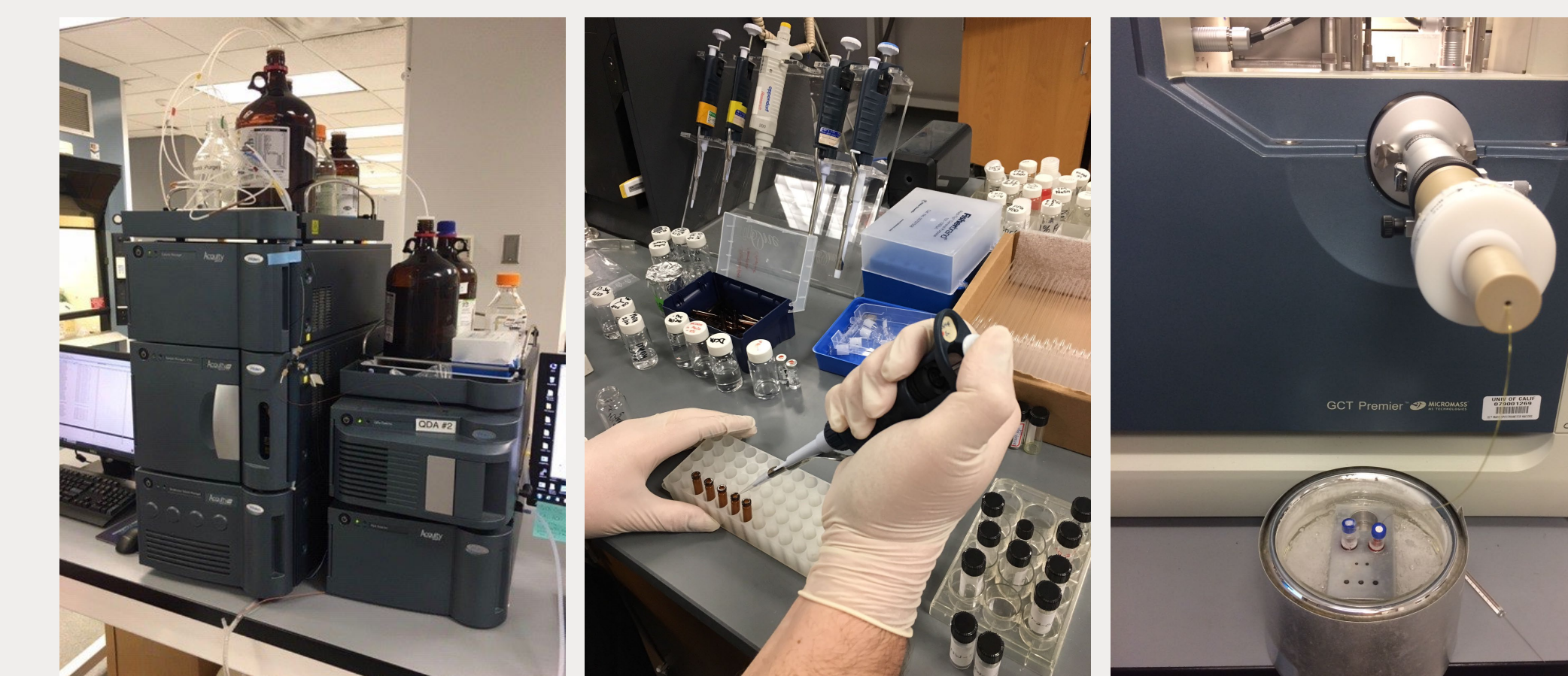
Waters Acquity Xevo G2-XS QTOF
LC-MS/MS; proteomics, metabolomics, sensitivity/quantitation; peptide sequencing, protein modifications

Agilent TD GC-MS/FID
Thermal desorption GC with MS and FID detectors for volatiles analysis; additional GC-MS instruments available



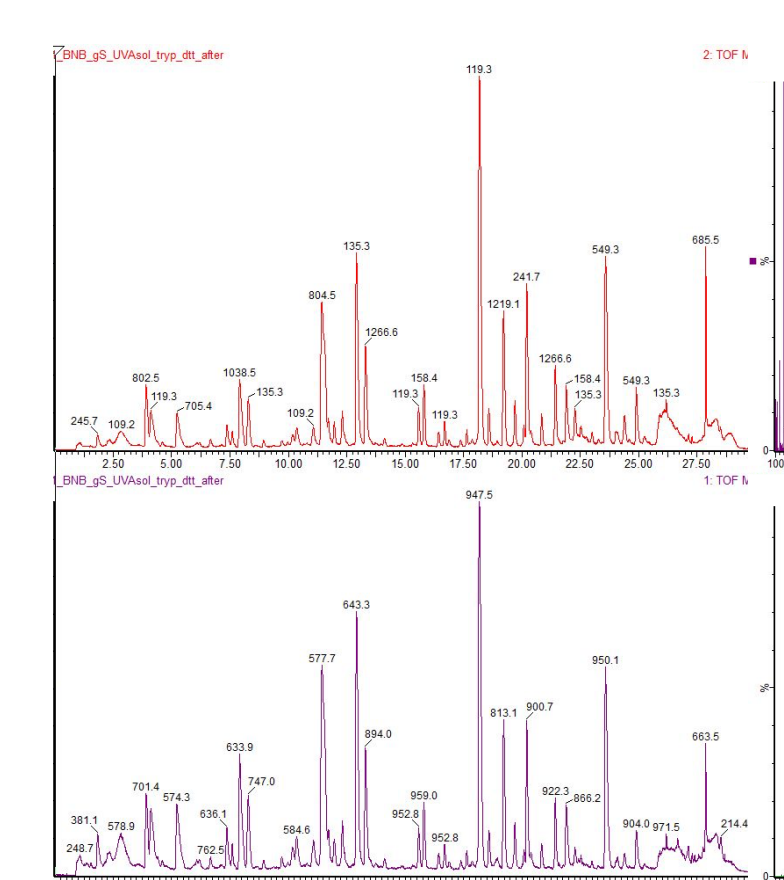
Waters Acquity TQ-Absolute Premier
UPLC triplequads for targeted quantitation of analytes from complex matrices

ABSciex 5500 & Bruker ultraflexxtreme
MALDI instruments for protein analysis and imaging mass spectrometry (IMS)

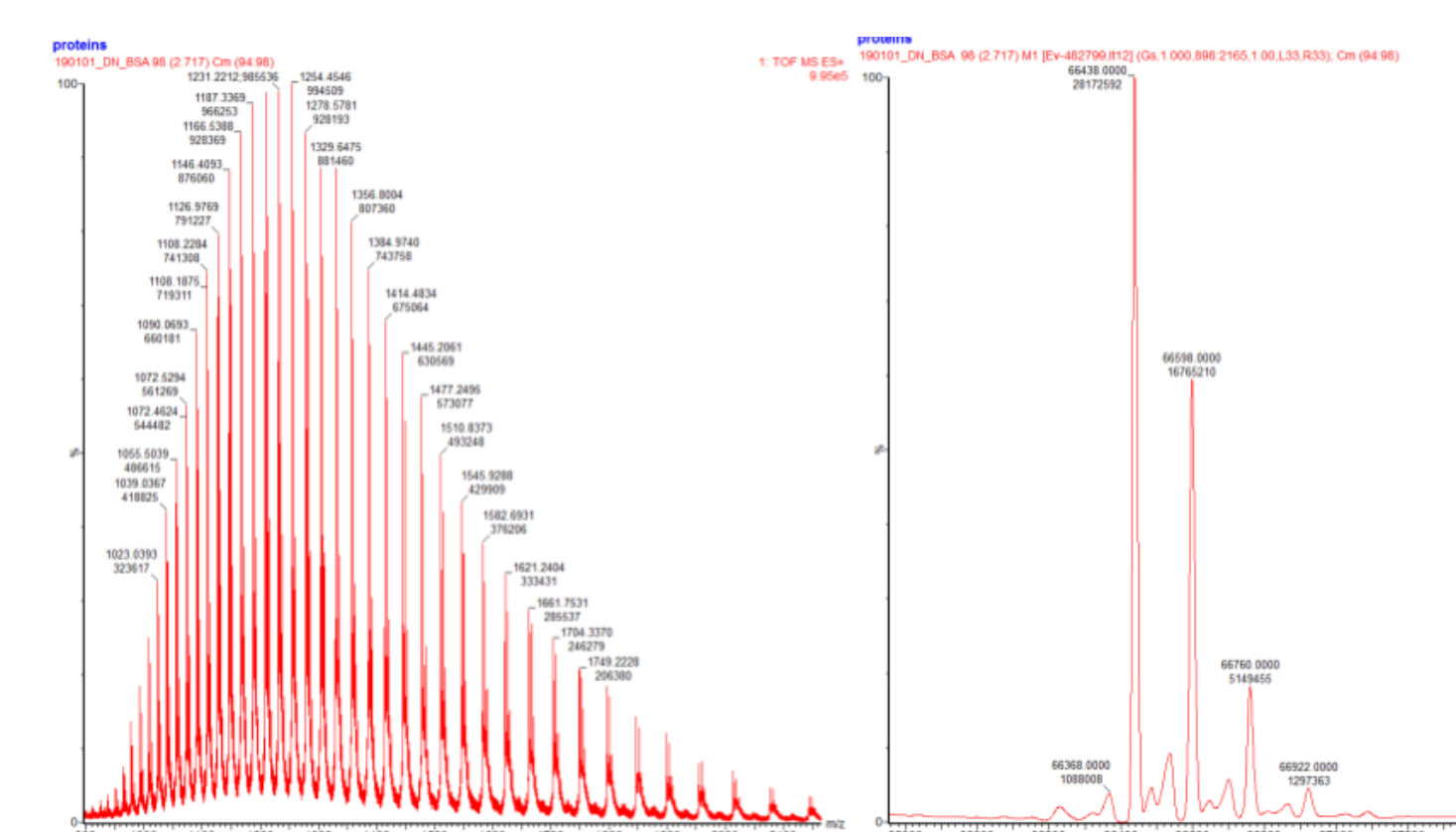


Waters Acquity QDAs
Basic LC-MS/PDA systems for small molecule analyses

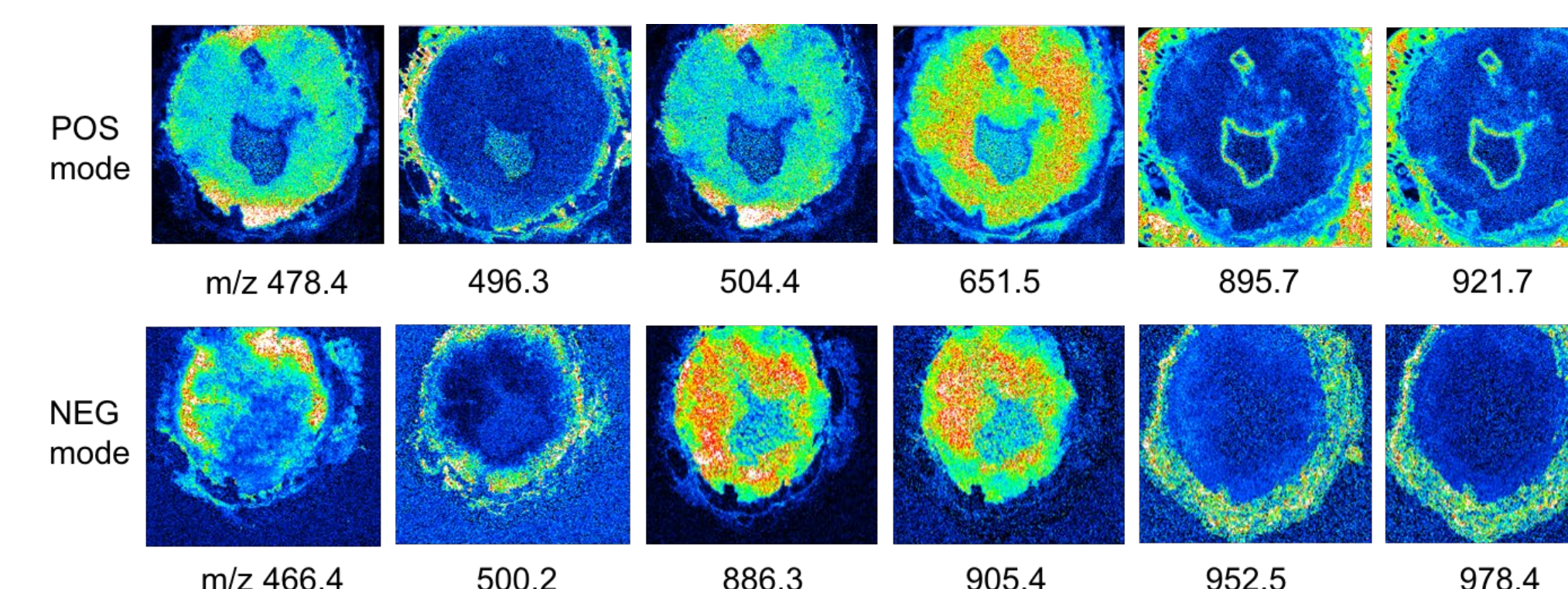
Sample prep:
HRMS sample prep for flow-ESI, MALDI targets and LIFDI (e.g. organometallic at -65 °C under inert atmosphere)



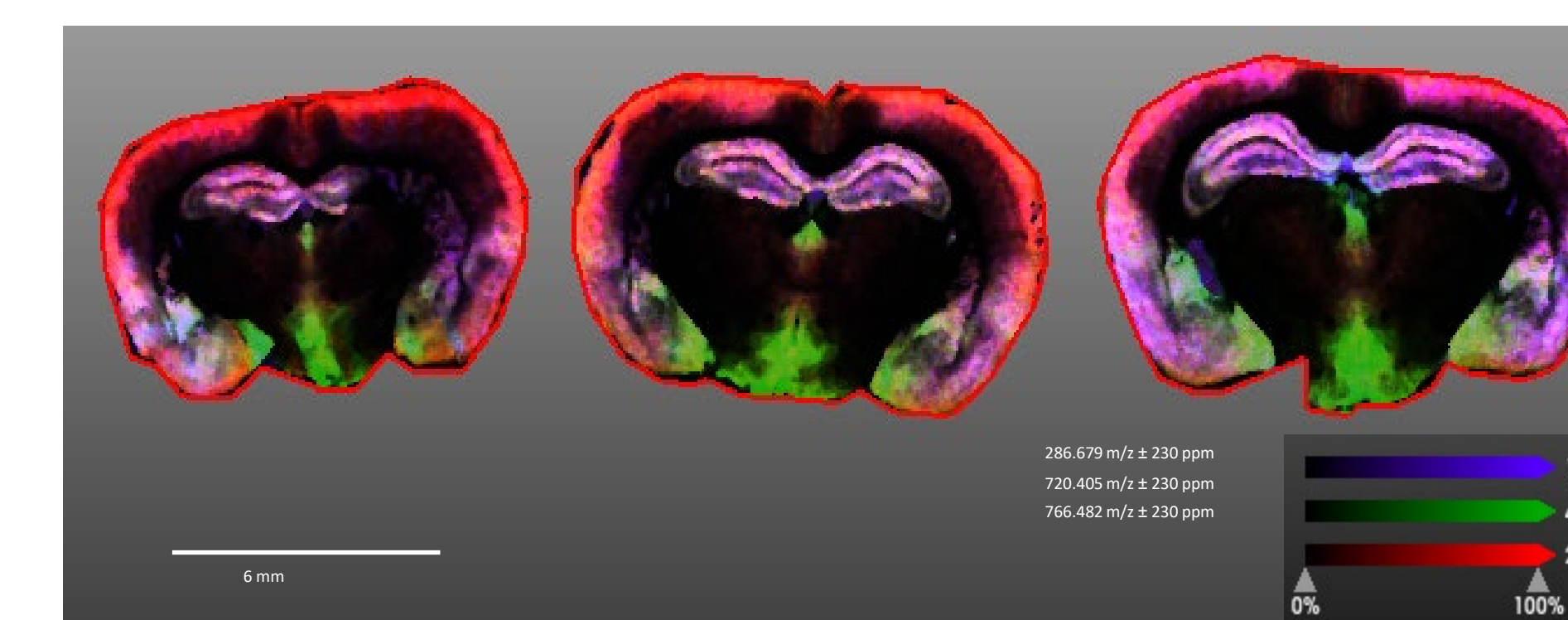
Peptide sequencing
Protein digestion, LC and nanoLC peptide separation, MS and MSMS data acquisition & analysis



Protein HRMS analysis
Multiple charge state ladder deconvolution of BSA ($m/z = 66438$); 5 min high-throughput analysis up to 250 kDa, w/ buffer



SW480 Tumor Xenograft Metabolic Heterogeneity Revealed by MALDI IMS
SW480 xenografts sectioned fresh frozen at 12 μm onto ITO slides, vacuum dried and matrix applied by sublimation: positive mode DHB (1.5 μm), negative mode 9AA (0.9 μm). Component features show complementary (m/z 478.4 v. 496.3) or strongly correlated (m/z 895.7/921.7 and 952.5/978.4) distribution patterns defining distinct zones of metabolite/lipid distributions within the tumor.



Metabolite/Lipid Imaging of 5xfAD v Control Mouse Brains
C57BL6 (control) or 5xfAD mice (7 months) were fresh frozen at 20 μm onto ITO slides. 9-AA matrix was applied by sublimation/recrystallization. Sections were imaged in reflector negative mode (RN) at 50 μm pixel resolution. False color composite image for three metabolite/lipid m/z markers is shown.

Untargeted metabolomics
Cloud mirror plot of *Anopheles stephensi* v *Aedes Chetumal*. Circles represent “ m/z_{rt} ” features with p -values < 0.0001 , fold change > 1.5 . Green (upper panel) up-regulated in *Aedes*; red (lower half) up-regulated in *Anopheles*. Candidate metabolite IDs were derived by searching METLIN, HMDB and MetaScope databases with exact $m/z \pm 20$ ppm.



Shimadzu iMScope
AP-MALDI QTOF for high-throughput and high resolution IMS

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