

Workflow for Fast Lipid Tissue Screening using LESA-FT-ICR-MS

Jean R. N. Haler,^a Emma K. Sisley,^{b,c} Yarixa L. Cintron-Diaz,^a Sanjib N. Meitei,^d Helen J. Cooper,^b
Francisco Fernandez-Lima^{*a,c}

^a Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199

^b School of Biosciences, Edgbaston, University of Birmingham, Birmingham B15 2TT, UK

^c EPSRC Centre for Doctoral Training in Physical Sciences for Health, University of Birmingham, Birmingham, B15 2TT, UK

^d PREMIER Biosoft, Palo Alto, CA, US

^e Biomolecular Science Institute, Florida International University, Miami, Florida 33199

*Corresponding author e-mail: fernandf@fiu.edu

Supplementary Information

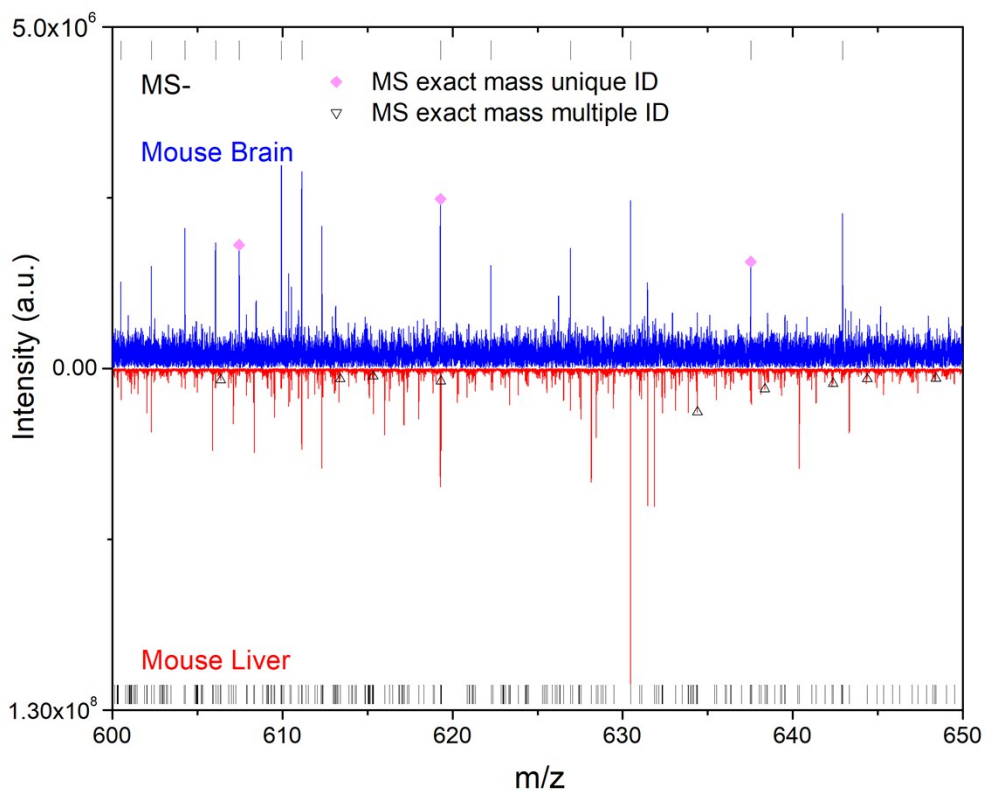


Figure S11: Extract from the negative ionization mode LESA-FT-ICR-MS spectra of mouse brain (top blue) and mouse liver (bottom red). The vertical lines on top of each spectrum represent the monoisotopic m/z peaks extracted for identification. The m/z peaks with unique and multiple lipid identifications are highlighted with pink and black markers.

List of used lipid abbreviations

CAR: Acyl carnitines

Cer: Ceramides

CerP: Cer-1-phosphates

DG: Di(acyl/alkyl)glycerols

DGDG: Digalactosyldiacylglycerol

FA: Fatty acyls

HexCer: Hexosylceramides

HexSph: Hexosylsphingosines

LacCer: Lactosylceramides

LacSph: Lactosylsphingosine

LPA: Lysophosphatidic acid

LPC: Lysophosphatidylcholines

LPE: Lysophosphatidylethanolamines

LPG: Lysophosphatidylglycerol

LPI: Lysophosphatidylinositol

LPIP: Lysophosphatidylinositol monophosphate

LPS: Lysophosphatidylserine

MG: Mono(acyl/alkyl)glycerols

MGDG: Monogalactosyldiacylglycerols

MIPC: Mannosyl-PI-ceramides

NAE: N-acyl ethanolamines

NAT: N-acyl taurines

PA: Phosphatidic acids

PC: Phosphatidylcholines

PE: Phosphatidylethanolamines

PE-Cer: PE-ceramides

PG: Phosphatidylglycerols

PI: Phosphatidylinositols

PI-Cer: PI-ceramides

PIP: Phosphatidylinositol phosphates

PS: Phosphatidylserines

S1P: Sphingosine-1-phosphates

SHexCer: Sulfatides

SM: Sphingomyelin

SQDG: Sulfoquinovosyldiacylglycerols

TG: Tri(acyl/alkyl)glycerols

WE: Wax esters

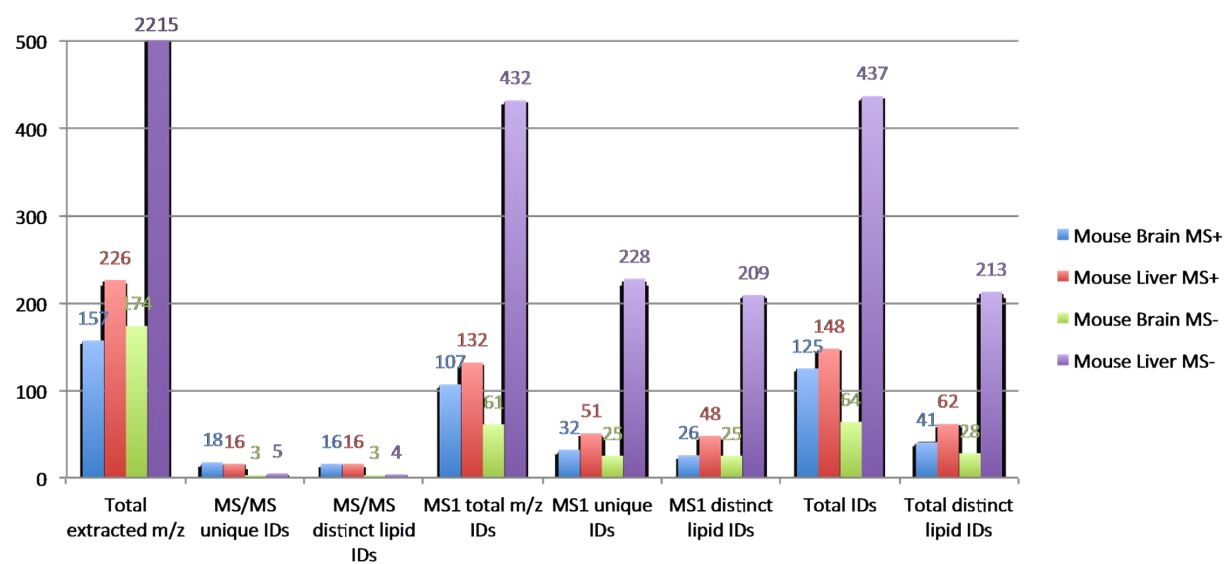


Figure SI2: Dataset descriptions of the positive and negative MB and ML FT-ICR-MS(MS) analyses.

Legends to the tables provided in the supplementary information file:

Table SI1: Summary of the mouse brain positive ionization LESA-FT-ICR MS1 exact mass assignments with multiple lipid identifications. The molecular ion species, chemical composition, lipid identifiers, theoretical mass, and mass error are provided.

Table SI2: Summary of the mouse liver positive ionization LESA-FT-ICR MS1 exact mass assignments with multiple lipid identifications. The molecular ion species, chemical composition, lipid identifiers, theoretical mass, and mass error are provided.

Table SI3: Summary of the mouse brain negative ionization mode LESA-FT-ICR-MS (MS1 and MS/MS). The molecular ion species, chemical composition, lipid class, theoretical mass, mass error, and identifiers are provided. HG denotes the head group and FA denotes fatty acids. MS1* designates exact mass lipid identifications where odd-chained lipids were discarded as biologically unlikely compared to the here reported even-chained lipid.

Table SI4: Summary of the mouse liver negative ionization mode LESA-FT-ICR-MS (MS1 and MS/MS). The molecular ion species, chemical composition, lipid class, theoretical mass, mass error, and identifiers are provided. HG denotes the head group and FA here denotes fatty acids. MS1* designates exact mass lipid identifications where odd-chained lipids were discarded as biologically unlikely compared to the here reported even-chained lipid.

Table SI5: Summary of the mouse brain negative ionization LESA-FT-ICR MS1 exact mass assignments with multiple lipid identifications. The molecular ion species, chemical composition, lipid identifiers, theoretical mass, and mass error are provided.

Table SI6: Summary of the mouse liver negative ionization LESA-FT-ICR MS1 exact mass assignments with multiple lipid identifications. The molecular ion species, chemical composition, lipid identifiers, theoretical mass, and mass error are provided.

Table SI7: Summary of the mouse brain and mouse liver lipid compositions, with the number of uniquely-identified lipids in each lipid class.