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

Jean R. N. Haler, Emma K. Sisley, Yarixa L. Cintron-Diaz, Sanjib N. Meitei, Helen J. Cooper, Francisco Fernandez-Lima*

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 SI1: 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.