Mass Spectrometry Imaging of Lipids: Generation of Untargeted Consensus Spectra
Reveals Spatial Distributions in Niemann-Pick Disease, Type C1

Supplemental Information

Authors and Affiliations

Fernando Tobias¹, Matthew T. Olson², and Stephanie M. Cologna¹,³

1. Department of Chemistry, University of Illinois at Chicago, Chicago, IL 60607, USA
2. Department of Laboratory Medicine and Pathology, Mayo Clinic, Jacksonville, FL 32224, USA
3. Laboratory for Integrative Neuroscience, University of Illinois at Chicago, Chicago, IL 60607, USA
Supplemental Figure S1. Averaged mass spectra of the cerebellum in positive ion mode (m/z 600 – 1000) from two biological replicate sections of *Npc1*+/+ (panels A and C) and *Npc1*−/− (panels B and D). Arrows indicate 1,5-DAN matrix cluster ions which indicate consistent coating due to their similar relative abundance.
Supplemental Figure S2: LC-ESI-MS/MS of gangliosides (A) GM3(d36:1), (B) GM3(d38:1), (C) GM2(d36:1), (D) GM2(d38:1) and (E) GM1(d36:1), (F) GM1(d38:1) detected from MALDI-MSI from whole cerebellar lipid extracts, n = 3 with replicate injections, p-value < 0.0001, ***. Significance was calculated using an unpaired t-test. Each analysis has been normalized to the protein concentration.
Supplemental Figure S3. On tissue MS/MS collected for m/z 1382.9 assigned to GM2(d36:1). The two major fragment ions observed are noted in red on the provided structure and labeled in red.

Supplemental Figure S4. On tissue MS/MS of m/z 1410.8 assigned to GM2(d18:1/20:0). The two signature fragment ions indicating the head group assignment are labeled on the structure in red.
Supplemental Figure S5. On tissue MS/MS of m/z 1544.8 assigned to GM1(d18:1/18:0). The two notable fragment ions of the lipid head group observed are provided in red and labeled on the proposed structure.

Supplemental Figure S6. On tissue MS/MS of m/z 1572.8 assigned to GM1(d18:1/20:0). Only one discernable fragment ion was assigned at 290.5Da indicating cleavage of the sugar head group. The putative structure is included for reference.
Supplemental Figure S7. On tissue MS/MS of parent ion assigned to GM3(d18:1/18:0) observed at m/z 1179.8. Two prominent fragment ions were observed and labeled on the structure provided.

Supplemental Figure S8. On tissue MS/MS of ganglioside GM3(d18:1/20:0) observed at m/z 1207.8. The two indicative fragment ions are noted in red on the structure provided.