Supplemental figures for: Imaging Regiospecific Lipid Turnover in Mouse Brain with Desorption Electrospray Ionization Mass Spectrometry

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Supplemental Figure S1: Urine and blood deuterium enrichments for the mice used in this study were combined to measure an average body water turnover for these mice. There was an initial bolus to 2.1 molar percent excess (MPE), followed by an increase to 5.3 MPE. Body water turnover rate was 0.27 per day, resulting in a body water half-life of 2.5 days in these mice. This body water turnover rate was used to define a curve of deuterium enrichment for calculating turnover of the individual lipids.



Supplemental Figure S2: Stable carbon hydrogen bonds which could incorporate deuterium during metabolic labeling are indicated with asterisks. The biologically predicted number of deuterium sites are close to the theoretical expectations based on the biosynthesis of AA and DHA. Because of the isobaric diversity that is likely present for the PS and PI lipids, it is not possible to specify the deuterium incorporation sites for these lipids in the hydrophobic tails.

Supplemental Figure S3 Overall Figure Legend

Supplemental Figure S3, A-D: Lipid fragmentation from brain samples

compared to standards. Fragmentation spectra for lipids at 303.3, 327.3, 834.6, and 885.6 m/z at 40 eV collision energy (top spectra, each panel) matched with fragmentation spectra for the corresponding commercial lipid standards (bottom spectra, each panel, inverted) under identical DESI conditions.

303.25 m/z



Supplemental Figure S3A: Fragmentation of 303.25 m/z peak and arachidonic acid standard. Despite not being able to identify structures to accompany all fragments, good agreement between sample and standard spectra allow us to confidently identify the lipid at 303.25 m/z as arachidonic acid.

327.3 m/z



Supplemental Figure S3B: Fragmentation of 327.3 m/z peak and docosahexaenoic acid standard. Despite not being able to identify structures to accompany all fragments, good agreement between sample and standard spectra allow us to confidently identify the lipid at 327.3 m/z as docosahexaenoic acid.

834.6 m/z



Supplemental Figure S3C: Fragmentation of 834.6 m/z peak and phosphatidylserine standard. Although the PS standard was not an exact match for the target in the brain samples (parent ion m/z of 788.5, see Methods), the lipid standard enabled us to confirm that the species at 834.6 m/z is a phosphatidylserine.

885.6 m/z



Supplemental Figure S3D: Fragmentation of 885.6 m/z peak from brain sample and phosphatidylinositol standard. Despite not being able to identify structures to accompany all fragments, good agreement between sample and standard spectra allow us to confidently classify the lipid at 885.6 m/z as a phosphatidylinositol.

Supplemental Figure S4 Overall Figure Legend

Supplemental Figure S4, A-C: Concentration as the relative ion intensity (right hand column), and isotope ratio images scaled either within the timepoint (right column) or across all the timepoints (middle column) for arachidonic acid (AA, S4A), docosahexaenoic acid (DHA, S4B), and phosphotidyl inositol (PI, S4C). A representative stained tissue slice is shown (top left), with the areas of the cortex and caudoputamen (CA) highlighted in the cartoon (top right).



Supplemental Figure S4A: Concentration/ Isotope maps for AA



Supplemental Figure S4B : Concentration/ Isotope maps for DHA



Supplemental Figure S4C : Concentration/ Isotope maps for PI



Supplemental Figure S5: Signal purity tested by spatial distribution of neutromers. The isotope pattern of the phosphotidyl inositol (PI) overlays a second unidentified species at 888.7. The MO-M2 neutromers of PI (885.6, 886.6, 887.6) have the same distribution (left image). Moving from the left hand side to the right hand side of the 888 peak produces a very different intensity distribution.