Supplementary information for:

**Hippocampal lipid differences in Alzheimer’s disease: A human brain study using Matrix-Assisted Laser Desorption/Ionization-Imaging Mass Spectrometry**

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Figure S1: MS/MS spectra of selected m/z lipid species. Figure showing MS/MS spectra, acquired using MALDI-TOF-TOF and/or LC-MS/MS (as indicated), and analyzed using the LIPID MAPS database (Fahy et al., 2007) or LipidSearch software (Thermo Scientific, USA), respectively. (A) m/z 600.5, (B) m/z 647.5, (C) m/z 774.6, (D) m/z 228.6, and (E) m/z 779.6. The matched output from the LIPID MAPS database for the MALDI-TOF-TOF MS/MS data is shown in Table S1.
Figure S1 (continued): MS/MS spectra of selected m/z lipid species. MS/MS spectra, acquired using MALDI-TOF-TOF and/or LC-MS/MS (as indicated), and analyzed using the LIPID MAPS database (Fahy et al., 2007) or LipidSearch software (Thermo Scientific, USA), respectively. (F) m/z 786.6, (G) m/z 794.6, (H) m/z 795.7, and (I) 796.6. The matched output from the LIPID MAPS database for the MALDI-TOF-TOF MS/MS data is shown in Table S1.
Figure S1 (continued): MS/MS spectra of selected m/z lipid species. MS/MS spectra, acquired using MALDI-TOF-TOF and/or LC-MS/MS (as indicated), and analyzed using the LIPID MAPS database (Fahy et al., 2007) or LipidSearch software (Thermo Scientific, USA), respectively. (J) m/z 797.7, (K) m/z 810.6, (L) m/z 885.6, and (M) m/z 718.6 (detected in positive ion mode). The matched output from the LIPID MAPS database for the MALDI-TOF-TOF MS/MS data is shown in Table S1.
Table S1: A summary of the matched output from LIPID MAPS (Fahy et al., 2007) for the product ions generated using MALDI-TOF/TOF-MS/MS, for the m/z species shown in Figure S1.

| Lipid Species | MS/MS Product ions | LIPID MAPS database output |
|---------------|--------------------|----------------------------|
| m/z 647.5 PA 32:0-H\(^-\) (Figure S1B) | m/z 78 PO\(_3\)-ion | |
| | m/z 96 H\(_2\)PO\(_4\)-ion | |
| | m/z 153 Glycerol-3-phosphate ion with loss of H\(_2\)O | |
| | m/z 255 sn1 RCOO-ion | |
| | sn2 RCOO- ion | |
| | m/z 391 Neutral loss of sn1 RCOOH group from [M-H]\(^-\) | |
| | Neutral loss of sn2 RCOOH group from [M-H]\(^-\) | |
| | m/z 409 Loss of sn1 acyl chain as RCOOH group from [M-H]\(^-\) | |
| | Loss of sn2 acyl chain as RCOOH group from [M-H]\(^-\) | |
| m/z 774.6 PE 39:7-H\(^-\) (Figure S1C) | m/z 283 Loss of CO\(_2\) from sn2 RCOO \(^-\) ion (PUFA) | |
| | m/z 327 sn2 RCOO- ion | |
| | m/z 446 Neutral loss of sn2 RCOOH group from [M-H]\(^-\) | |
| | m/z 464 Loss of sn2 acyl chain as ketene (RCH=C=O) from [M-H]\(^-\) | |
| m/z 778.6 PE 39:5-H\(^-\) (Figure S1D) | m/z 331 sn1 RCOO- ion | |
| | m/z 446 Neutral loss of sn1 RCOOH group from [M-H]\(^-\) | |
| | m/z 464 Loss of sn1 acyl chain as ketene (RCH=C=O) from [M-H]\(^-\) | |
| m/z 779.6 PG 37:6-H\(^-\) 17:2/20:4 OR 22:6/15:0 (Figure S1E) | m/z 303 sn1/2 RCOO- ion | |
| | m/z 419 Loss of sn1/2 acyl chain as ketene (RCH=C=O) and glycerol from [M-H]\(^-\) | |
| | m/z 327 sn1 RCOO- ion | |
| m/z 786.6 PS 36:2-H\(^-\) (Figure S1F) | m/z 417 Neutral loss of sn1/2 RCOOH group and serine from [M-H]\(^-\) | |
| | m/z 435 Loss off sn1/2 acyl chain as ketene (RCH=C=O) and serine from [M-H]\(^-\) | |
| | m/z 699 Loss of serine from precursor ion | |
| m/z 794.6 PE 40:4-H\(^-\) (Figure S1G) | m/z 283 sn2 RCOO- ion | |
| | m/z 331 sn1 RCOO- ion | |
| | m/z 480 Loss of sn1 acyl chain as ketene (RCH=C=O) from [M-H]\(^-\) | |
Table S1 (continued): A summary of the matched output from LIPID MAPS (Fahy et al., 2007) for the product ions generated using MALDI-TOF/TOF-MS/MS, for the m/z species shown in Figure S1.

| Lipid Species | MS/MS Product ions | LIPID MAPS database output |
|---------------|-------------------|-----------------------------|
| m/z 795.7 PG 38:5-H⁻ (Figure S1H) | m/z 153 | Glycerol-3-phosphate ion with loss of H₂O |
|               | m/z 283 | sn1 RCOO⁻ ion |
|               | m/z 419 | Neutral loss of sn1/2 RCOOH group and glycerol from [M-H]⁻ |
|               | m/z 437 | Neutral loss of sn1/2 RCOOH group and glycerol from [M-H]⁻ |
|               | m/z 153 | Loss of sn1/2 acyl chain and glycerol from [M-H]⁻ |
|               | m/z 283 | Glycerol-3-phosphate ion with loss of H₂O |
|               | m/z 331 | Loss of CO₂ from sn1 RCOO⁻ ion (PUFA) |
|               | m/z 327 | sn2 RCOO⁻ ion |
|               | m/z 283 | sn1 RCOO⁻ ion |
| m/z 810.6 PS 38:4-H⁻ (Figure S1K) | m/z 283 | sn1 RCOO⁻ ion |
|               | m/z 303 | sn1 RCOO⁻ ion |
|               | m/z 419 | Neutral loss of sn1 RCOOH group and glycerol from [M-H]⁻ |
| m/z 885.6 PI 38:4-H⁻ (Figure S1L) | m/z 283 | sn1 RCOO⁻ ion |
|               | m/z 303 | sn2 RCOO⁻ ion |
|               | m/z 315 | Glycerophosphoinositol-2H₂O |
|               | m/z 419 | Neutral loss of sn2 RCOOH group and inositol from [M-H]⁻ |
|               | m/z 439 | Neutral loss of sn1 RCOOH group and inositol from [M-H]⁻ |
|               | m/z 581 | Neutral loss of sn2 RCOOH group from [M-H]⁻ |
|               | m/z 599 | Loss of sn2 acyl chain as ketene (RCH=C=O) from [M-H]⁻ |
|               | m/z 601 | Neutral loss of sn1 RCOOH group from [M-H]⁻ |

Reference:
Fahy E, Sud M, Cotter D, Subramaniam S (2007) LIPID MAPS online tools for lipid research. Nucleic Acids Research 35:W606-W612.