Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Abnormal phospholipids distribution in the prefrontal cortex from a patient with schizophrenia revealed by matrix-assisted laser desorption/ionization imaging mass spectrometry

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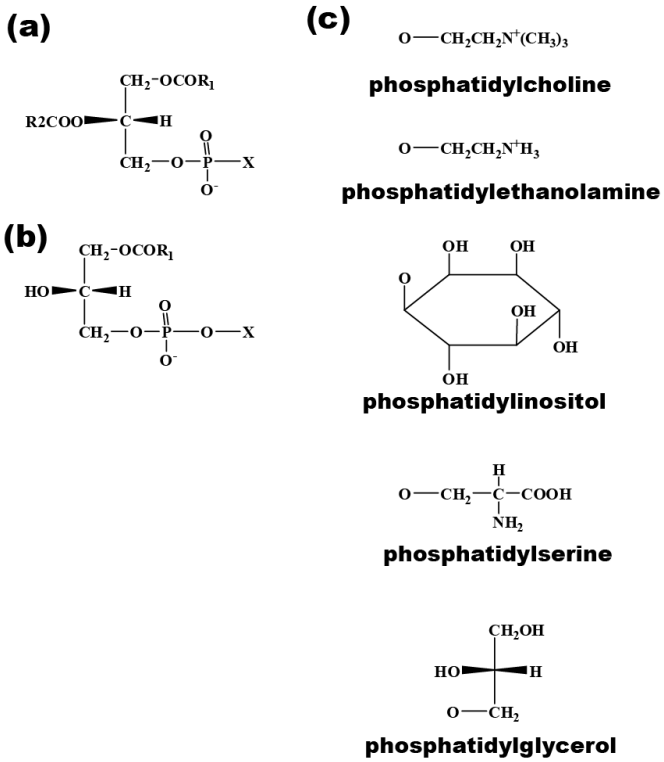

Figure S1. Structure of phospholipid classes.

Structures of the glycerol backbone of phospholipids (a) and lysophospholipids (b) are shown. They are subdivided into distinct classes (e.g., phosphatidylcholines, phosphatidylethanolamines, and phosphatidylinositols) based on the structure of the head group linked to the phosphate, attached at the *sn*-3 position of the glycerol backbone (c). They are further subdivided into numerous molecular species on the basis of the composition of fatty acyl residues linked to the *sn*-1 and *sn*-2 positions of the glycerol backbone.

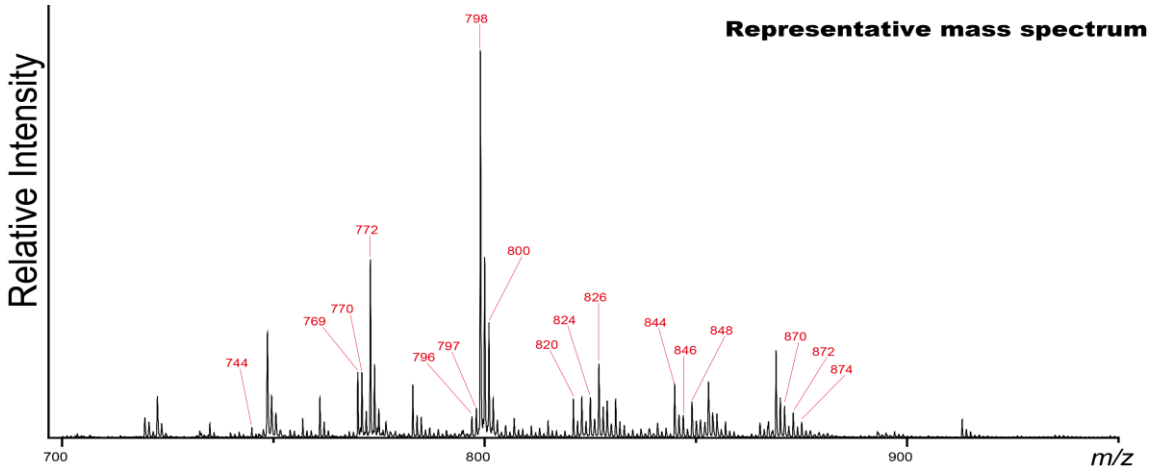

Figure S2. Overall mass spectrum obtained by MALDI-IMS of human postmortem brains, in positive ion detection mode.

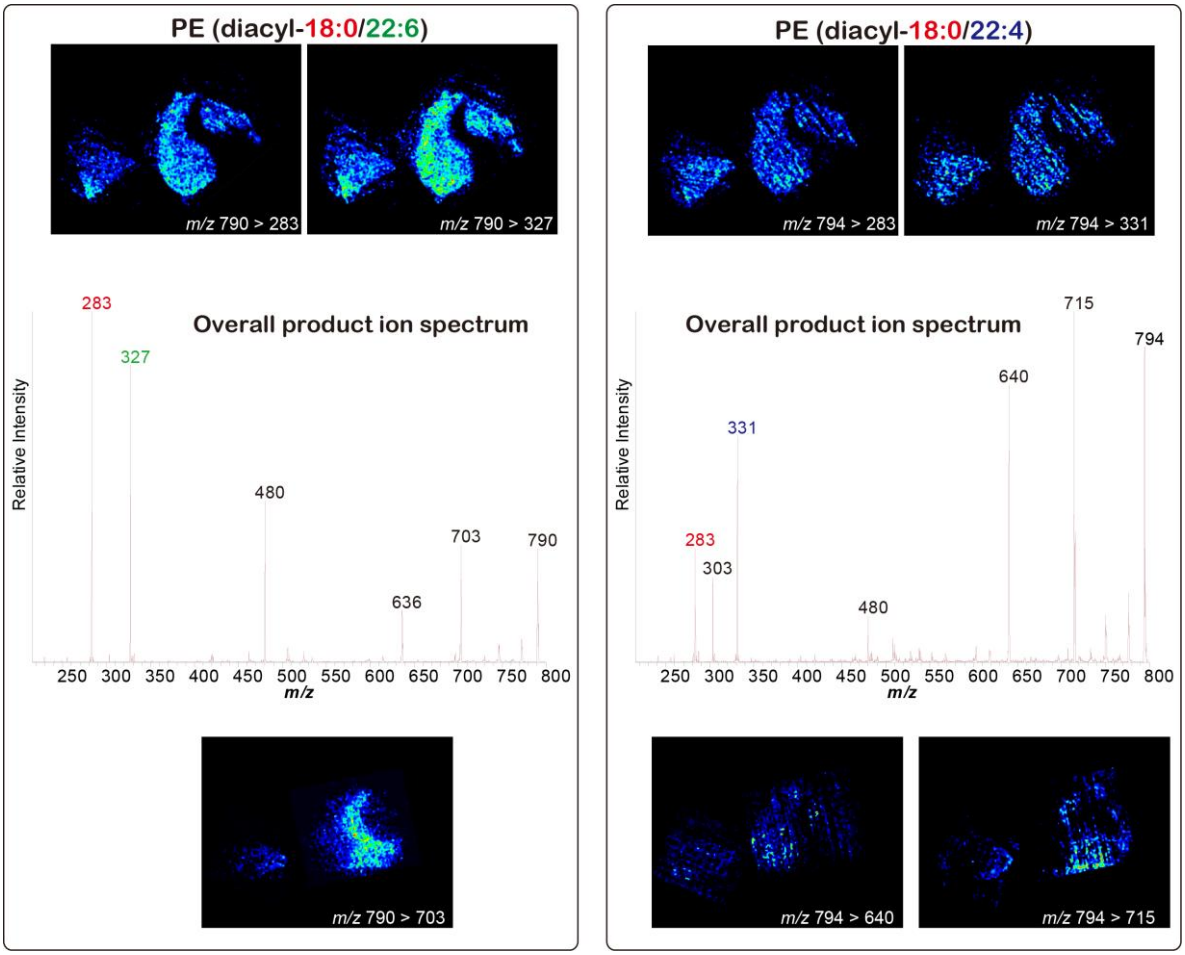

Figure S3. Results of MS/MS imaging of PE species in negative ion detection mode.

Based on the results of LC/ESI-MS/MS, the most and second-most abundant PE species were subjected to MS/MS imaging in the negative ion detection mode, using 9-aminoacidine as a matrix. For both PE (diacyl-18:0/22:6) and PE (diacyl-18:0/22:4), fatty acid ions were detected at each data point; they produced specific imaging results for each PE molecular species (upper panels). However, other intense product ions showed distinct distribution images from the PEs, thus indicating a common, identical nominal mass with the precursor PE ion and other one.

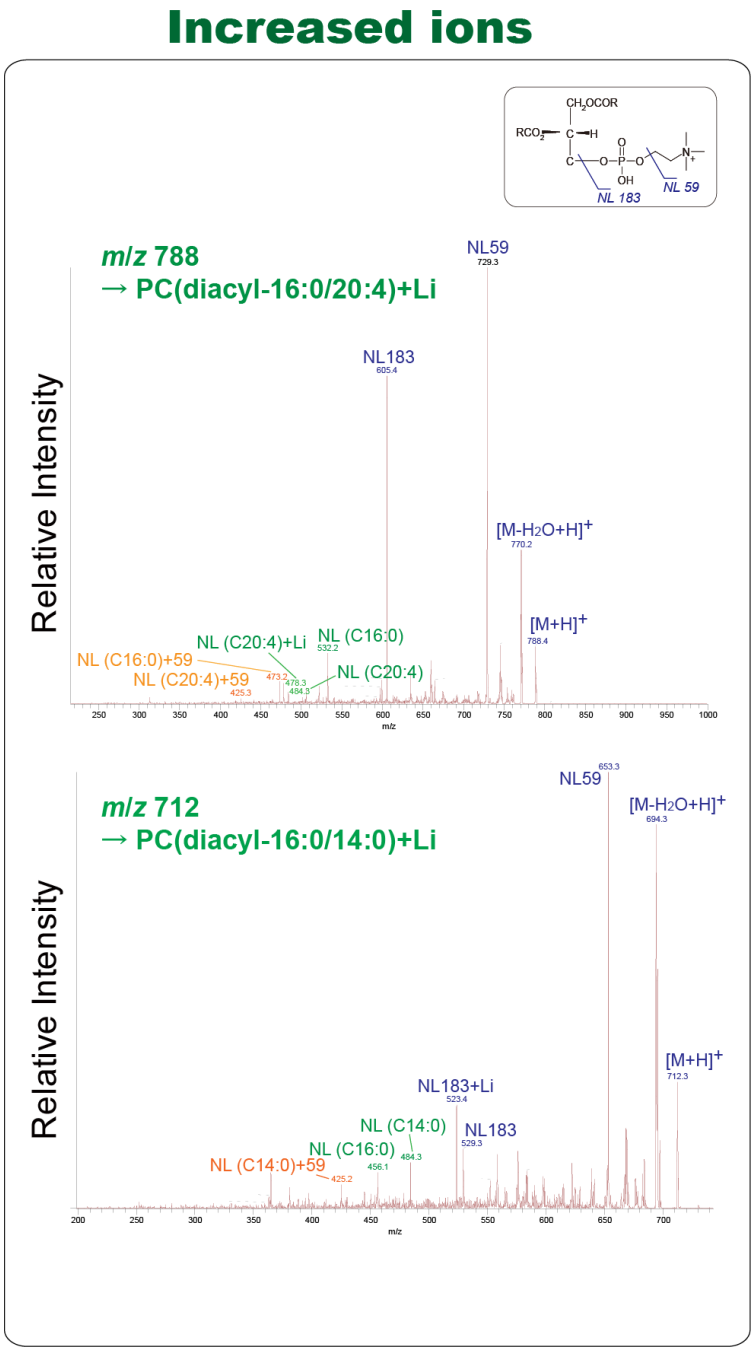

Figure S4. On tissue MS/MS of molecules showing considerably changed ratios (for increased ions).

We identified detailed fatty acid constituents of each PCs by replacing adducted alkali metal from potassium to lithium, by adding 20 mM of lithium acetate in the matrix solution. In each mass spectrum, the presence of a choline containing head group ([NL] of 59 u) and phosphate ([NL] of 183 u) was confirmed. MS/MS subjecting lithium adducted molecules provides increased acyl-chain loosed fragment ions, therefore, we could precisely identify the fatty acid moiety ([NL] of acyl-chain).

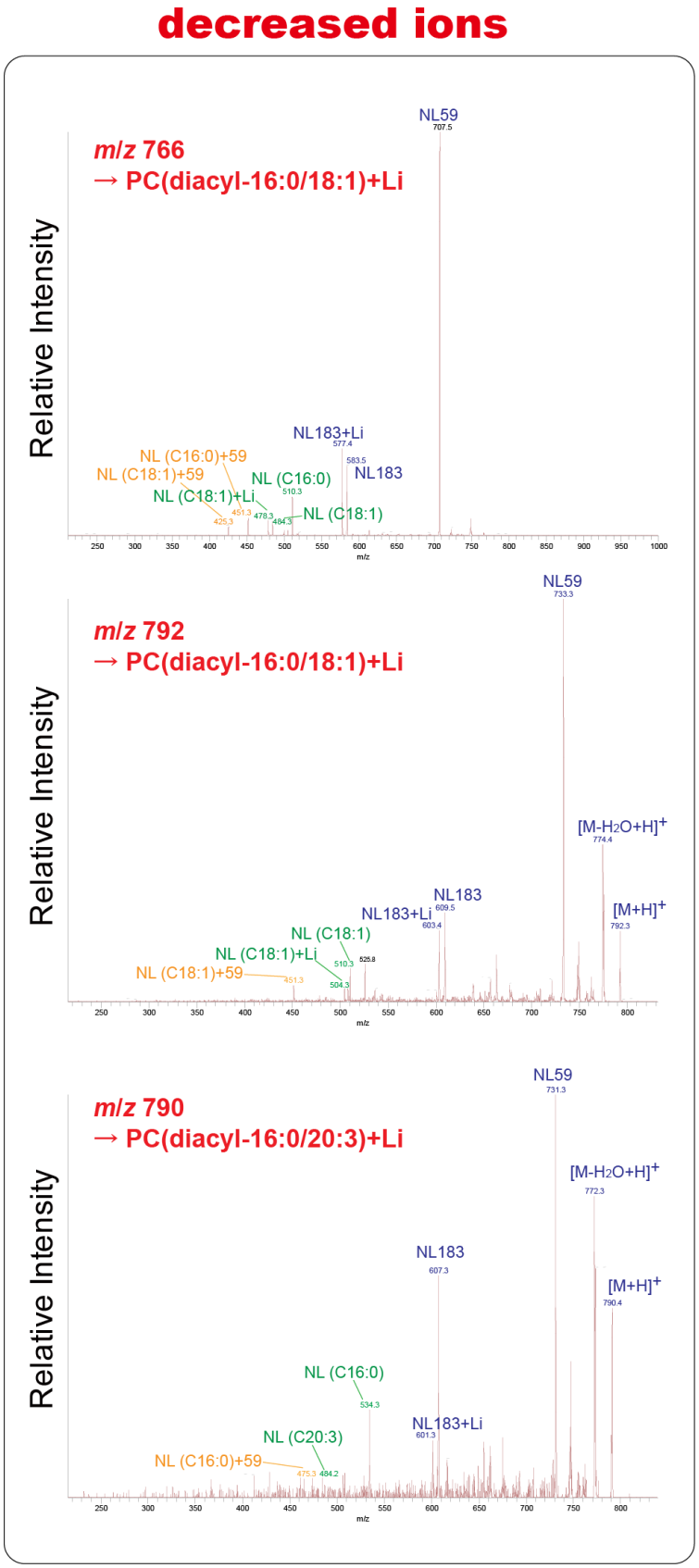

Figure S5. On tissue MS/MS of molecules showing considerably changed ratios (for deased ions).