Supporting Information for:

Mapping the Distribution of Double Bond Location Isomers in Lipids across Mouse Tissues†

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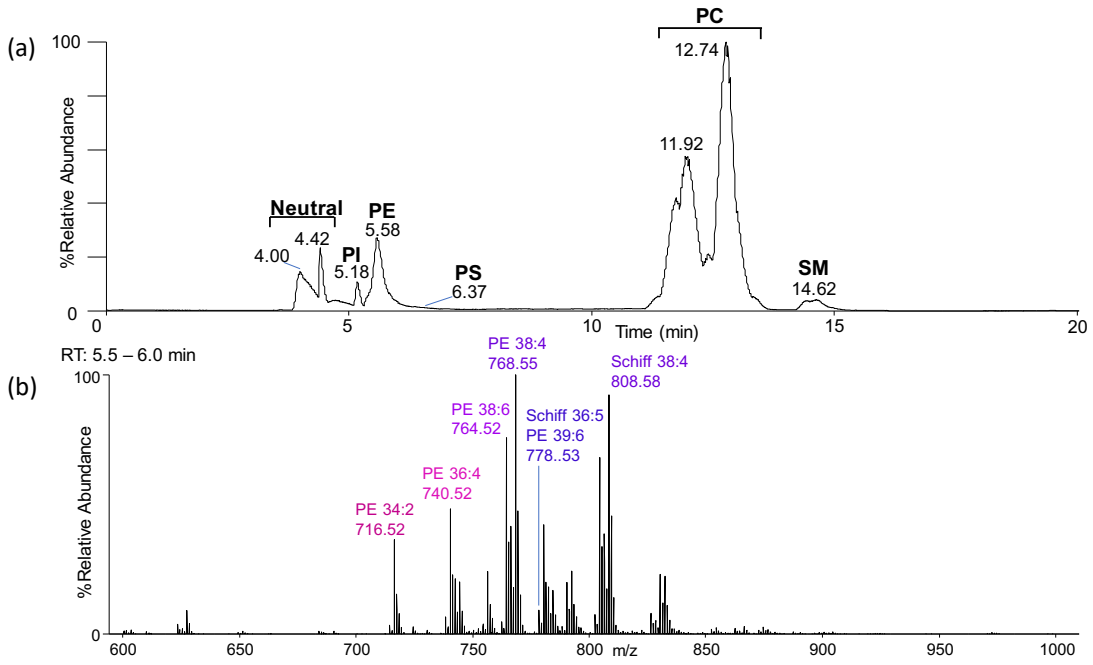


Fig. S1. (a) Base peak chromatogram of HILIC-MS of mouse liver extracts. (b) MS spectrum eluted between 5.5-6.0 min, the most abundant PE and corresponding Schiff Base products (noted as Schiff) are indicated.

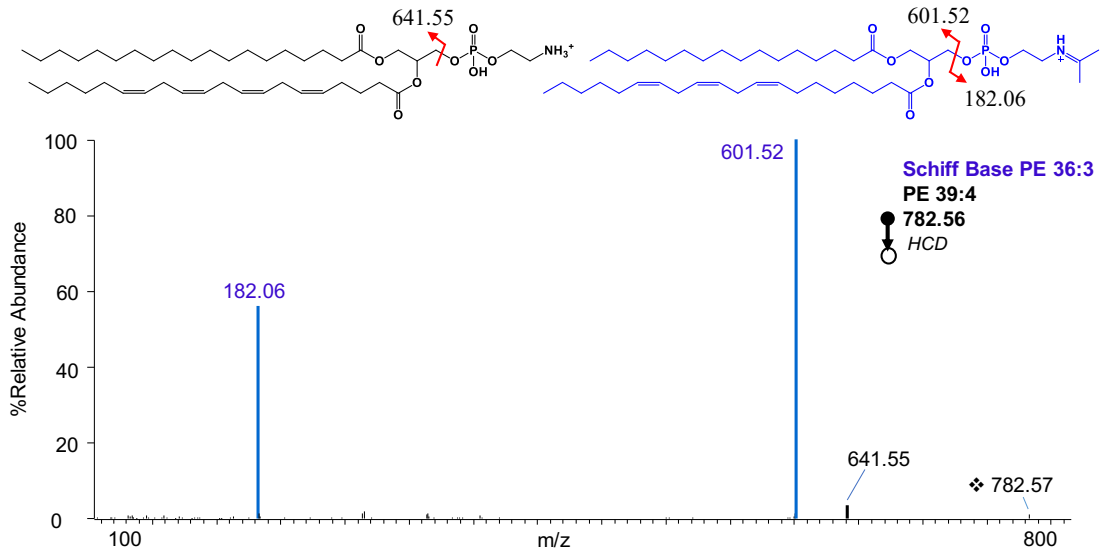


Fig. S2. MS^2 HCD spectrum of the isomeric PE 39:4 and the Schiff base product of PE 36:3 (*m/z* 782.56, RT 5-6 min) in mouse liver extracts. The structure of the two PE species is shown on top.

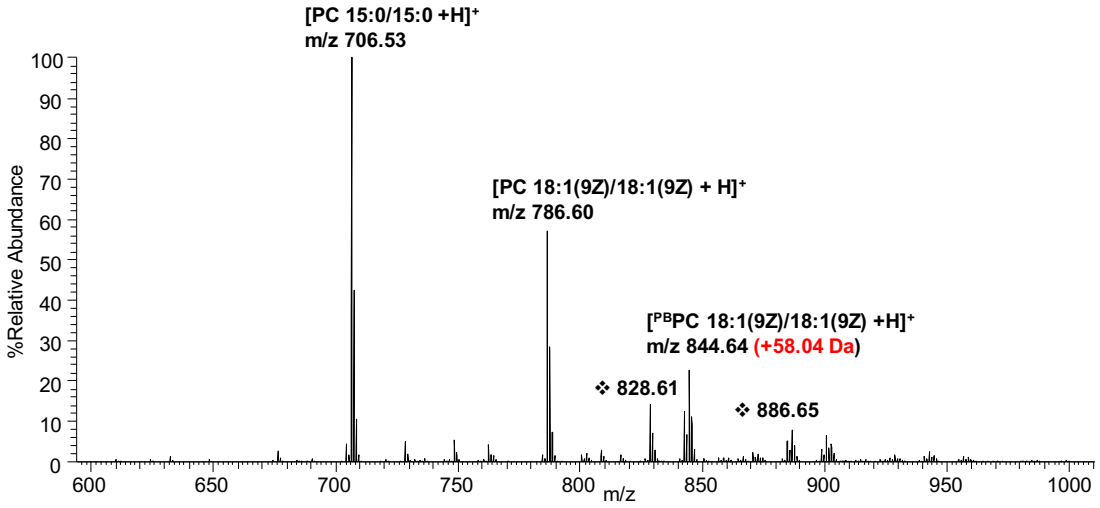


Fig. S3. MS spectrum of a mixture containing 5 µM PC 18:1(9Z)/18:1(9Z) and 5 µM PC 15:0/15:0 standards after 20 s PB reaction. The marked *m/z* 828.61 and *m/z* 886.65 represent Norrish Type II products of [PC 18:1(9Z)/18:1(9Z) $+NH_4]^+$ and [^{PB}PC 18:1(9Z)/18:1(9Z) $+NH_4]^+$ (+42 Da).

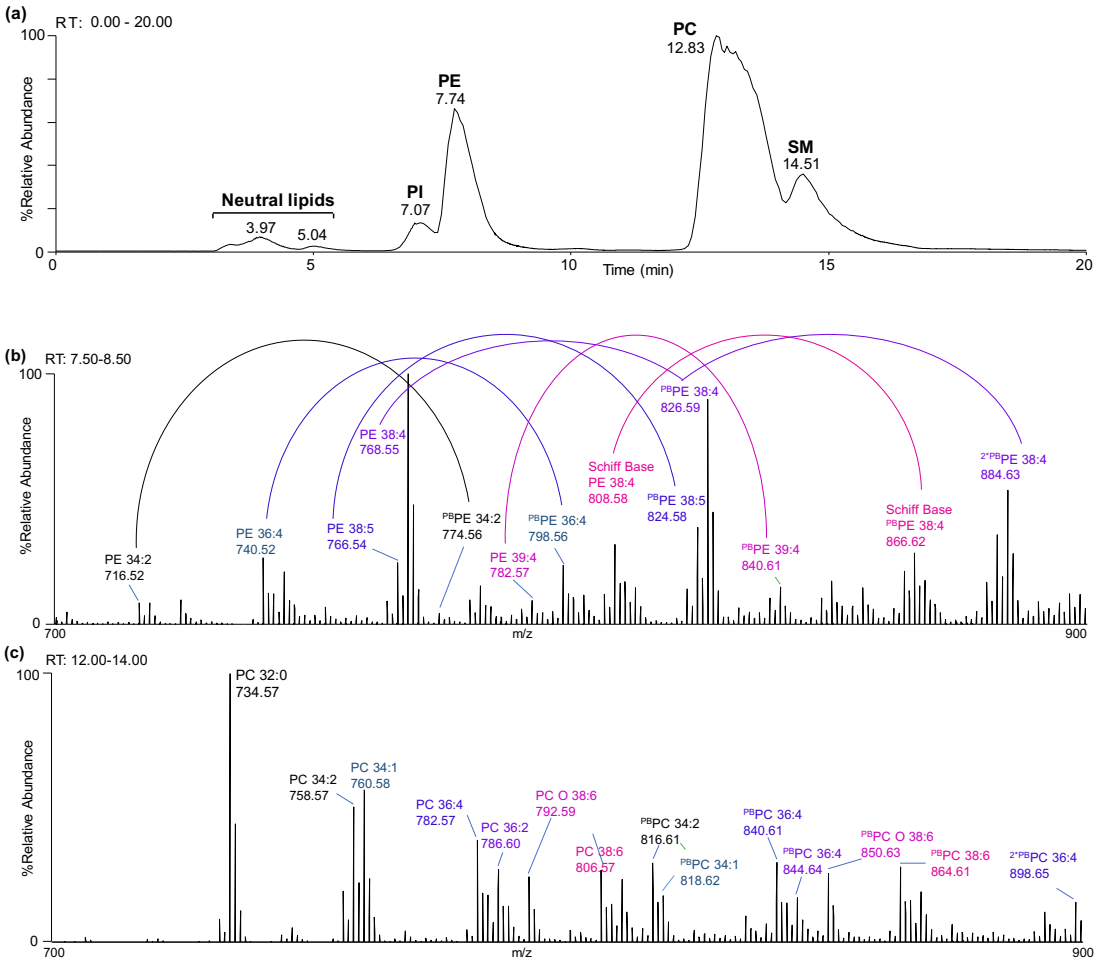


Fig. S4. (a) Base peak chromatography of LC-PB-MS of mouse kidney extracts with PB reaction. LC-PB-MS spectra of (b) PE (RT 7.5-8.5 min) and (c) PC (RT 12-14 min) from mouse kidney extracts. As an example, PE lipid species and their corresponding PB products are linked by lines. Over-reacted polyunsaturated species are labeled as ^{2*PB}PE and ^{2*PB}PC.

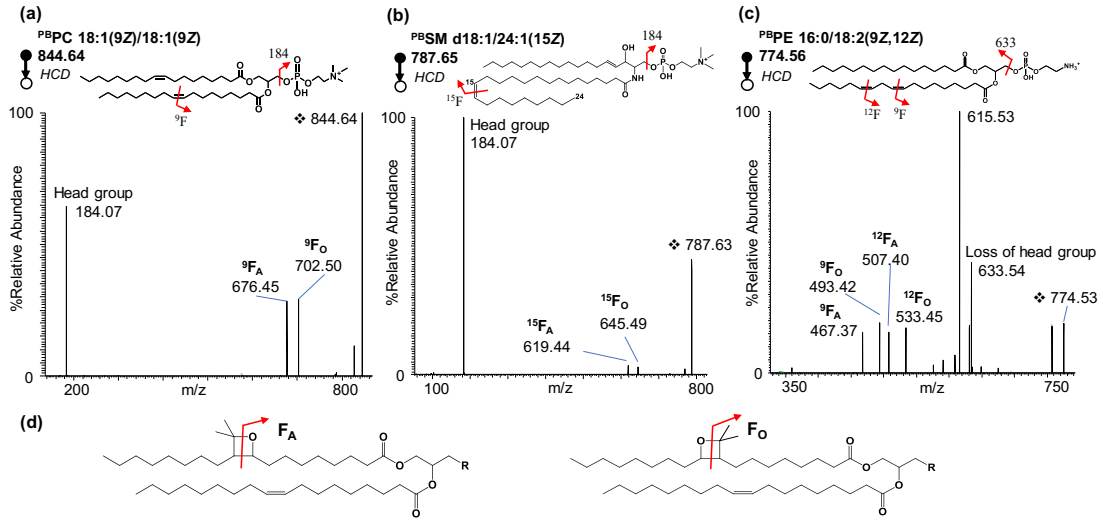


Fig. S5. MS^2 HCD spectra at NCE 15 of PB products of lipid standards: (a) ^{PB}PC 18:1(9Z)/18:1(9Z) *(m/z* 844.64), (b) ^{PB}SM 18:1;O2/24:1(15Z) (*m/z* 787.65), and (c) ^{PB}PE 16:0/18:2(9Z, 12Z) (*m/z* 774.56). (d) General structure of a pair of PB products, fragmented to diagnostic ions as F_A (aldehyde) and F_O (olefin), respectively.

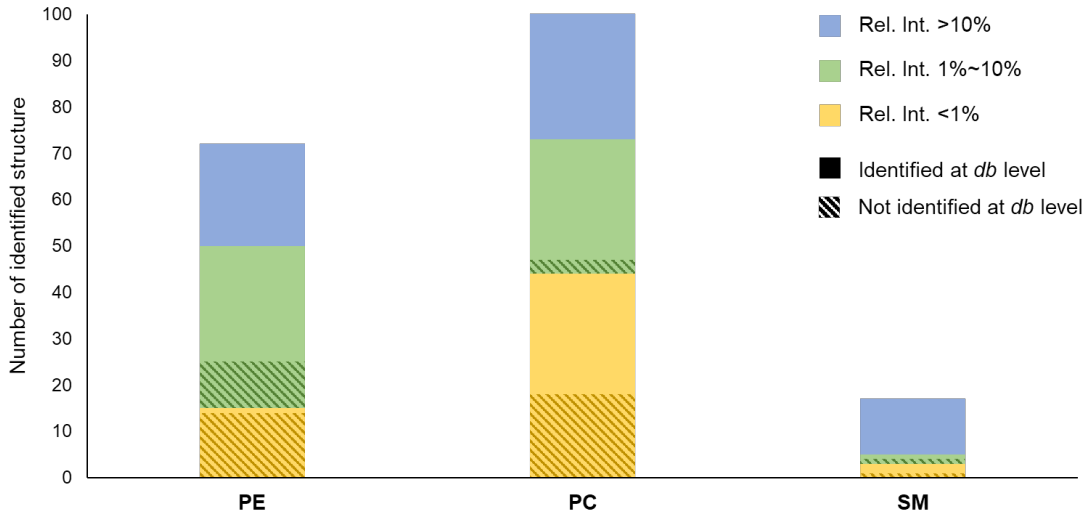
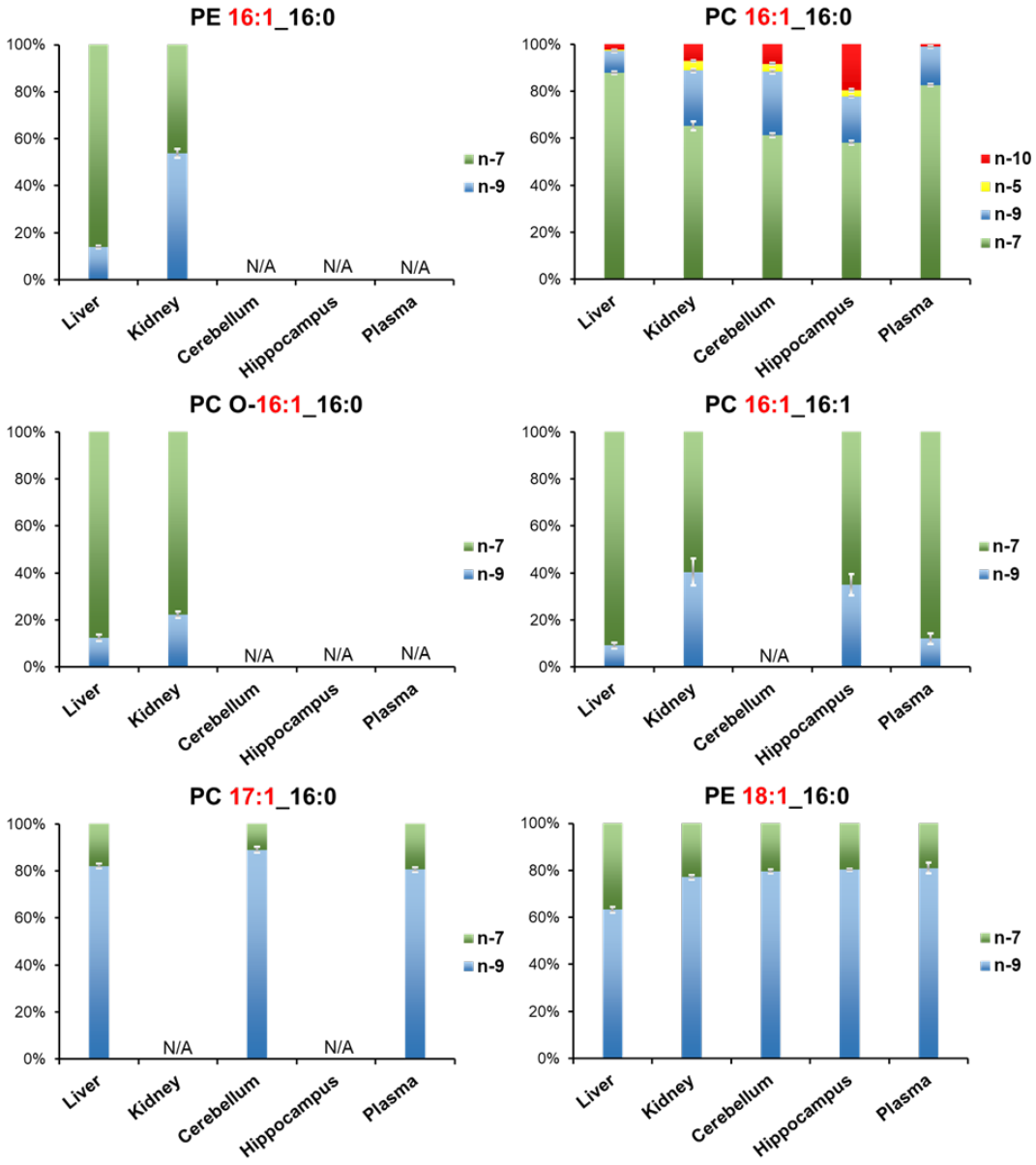
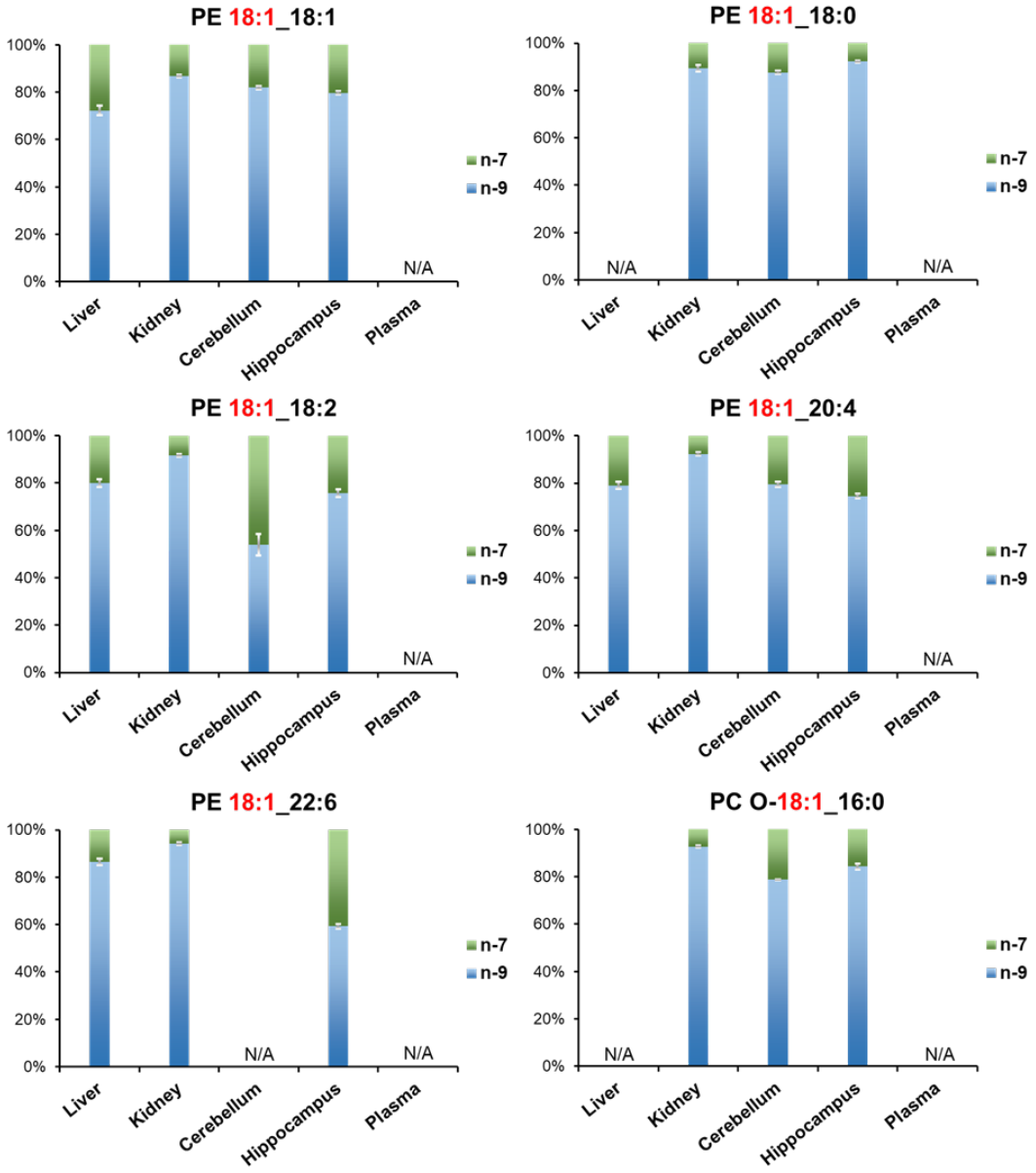
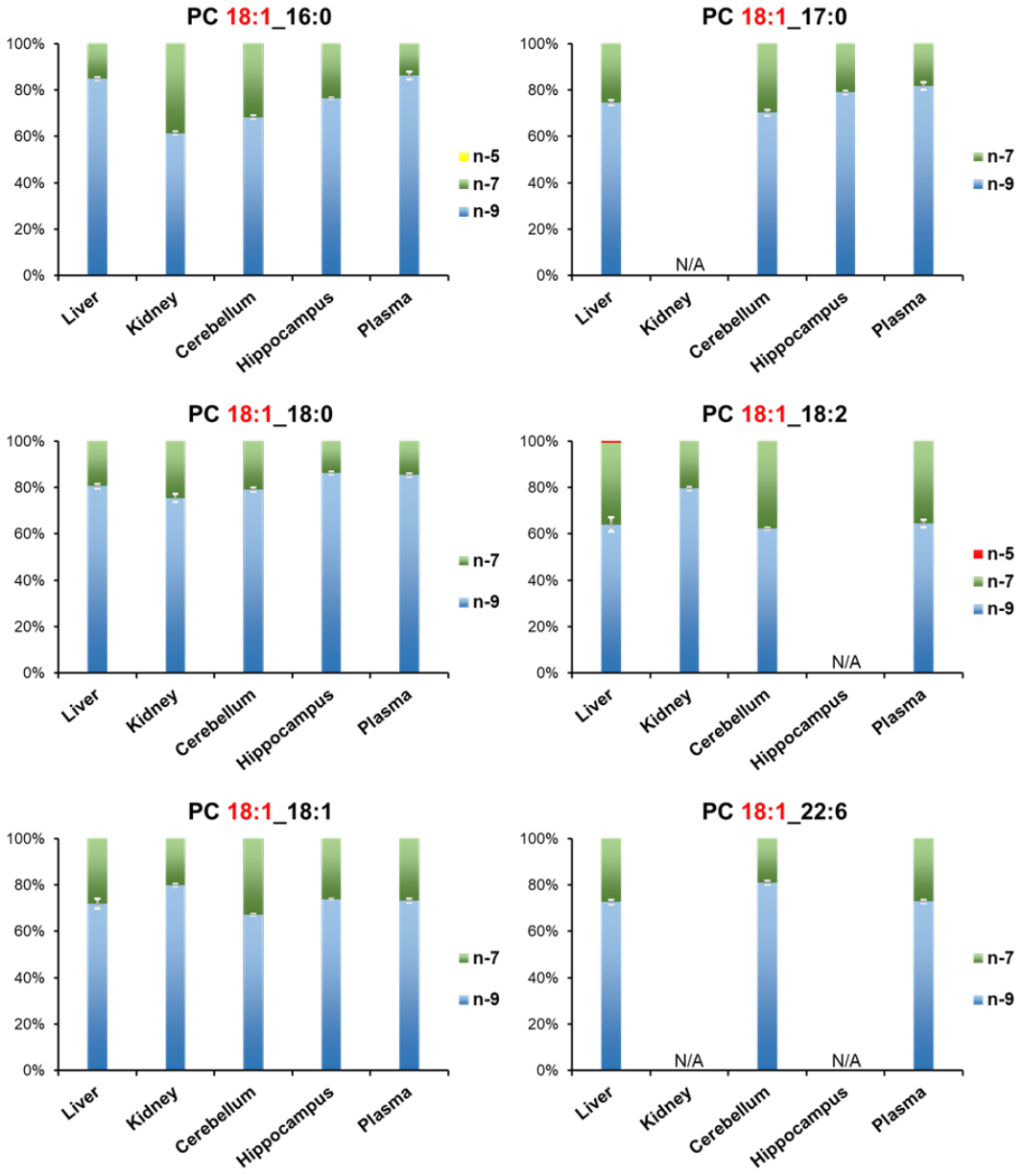
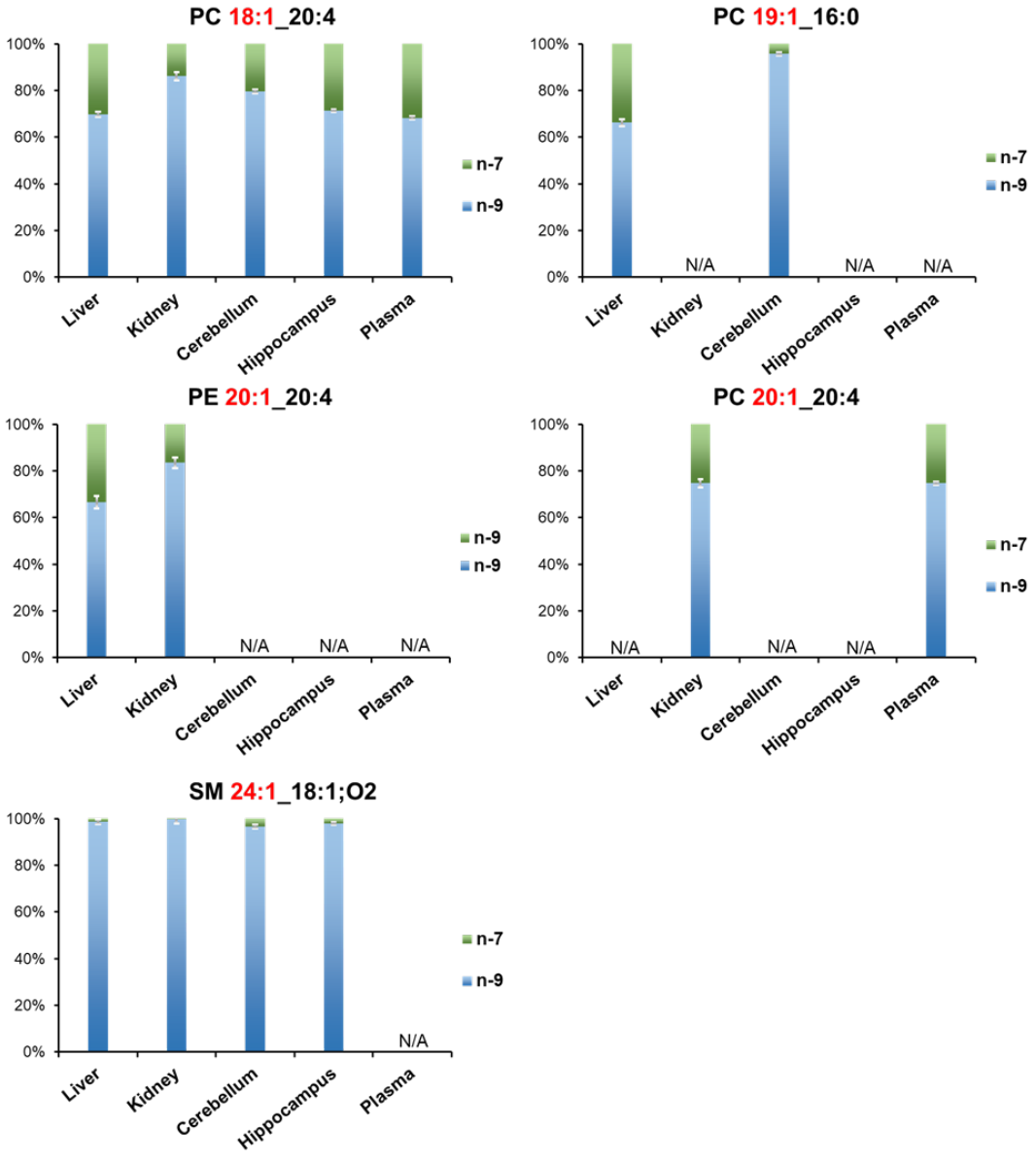


Fig. S6. Total number of identified structures of PE, PC, and SM in mouse liver. 58 PE, 100 PC, and 17 SM species are identified with relative intensity ranging from 0.05% to 100% relative to the most abundant species in each subclass. Open color graph bars indicate structures identified at the DBL level, while diagonally striped graph bars only at subclass or chain composition level.


PE 16:1_16:0
PC 16:1_16:0
PC O-16:1_16:0
PC 16:1_16:1
PC 17:1_16:0
PE 18:1_16:0
100%
80%
60%
40%
20%
0%
N/A
Liver
Kidney
Cerebellum
Hippocampus
Plasma
n-10
n-5
n-9
n-7


PE 18:1_18:1
PE 18:1_18:0
PE 18:1_18:2
PE 18:1_20:4
PE 18:1_22:6
PC O-18:1_16:0
100%
80%
60%
40%
20%
0%
n-7
n-9
N/A
Liver
Kidney
Cerebellum
Hippocampus
Plasma


PC 18:1_16:0
PC 18:1_17:0
PC 18:1_18:0
PC 18:1_18:2
PC 18:1_18:1
PC 18:1_22:6
100%
80%
60%
40%
20%
0%
Liver
Kidney
Cerebellum
Hippocampus
Plasma
n-5
n-7
n-9
N/A


PC 18:1_20:4
PC 19:1_16:0
PE 20:1_20:4
PC 20:1_20:4
SM 24:1_18:1;O2
100%
80%
60%
40%
20%
0%
Liver
Kidney
Cerebellum
Hippocampus
Plasma
n-7
n-9
N/A

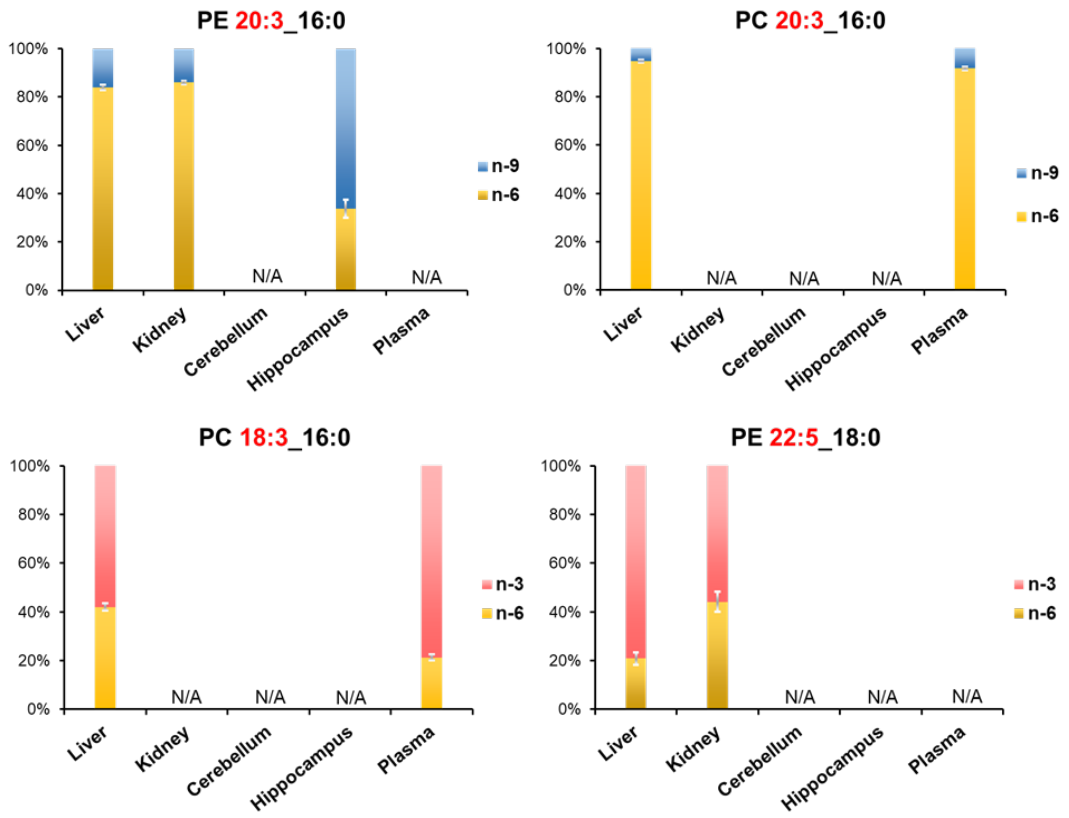


Fig. S7. %Relative composition of DBL isomers of lipids across tissues. The analyzed fatty acyl chains are labeled in red in each lipid name. Non-identified or non-quantified samples are marked as N/A. Standard deviations are shown on each segment of the graph bars.