Shotgun Approach for Quantitative Imaging of Phospholipids Using Nanospray Desorption Electrospray Ionization Mass Spectrometry

Ingela Lanekoff[1,*], Mathew Thomas[2], Julia Laskin[1,*]

1) Physical Sciences Division, Pacific Northwest National Laboratory, Richland, USA

2) Computational Science and Mathematics Division, Pacific Northwest National Laboratory, Richland, USA

Supporting Information

Table S1. Carbon factors used for quantification by accounting for the number of carbons in the acyl chain and adduct (Na or K).

#C	CF $[M+Na]^+$	CF $[M+K]^+$
25	1.00	1.00
30	1.11	1.18
32	1.15	1.25
34	1.20	1.33
36	1.24	1.40
38	1.28	1.47
40	1.33	1.54
42	1.37	1.62
43	1.39	1.65
44	1.42	1.69
46	1.46	1.76

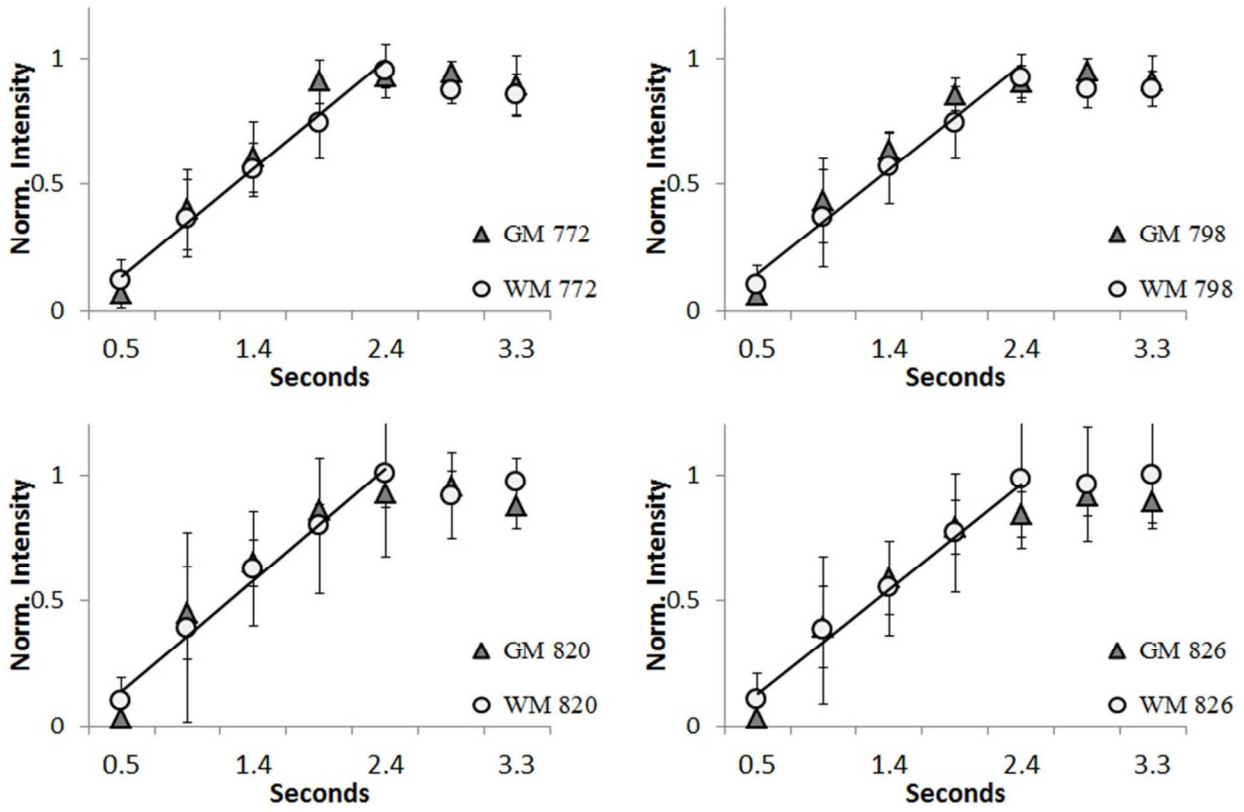

Figure S1. Localized extraction of four different PC as $[M+K]^+$: PC 32:0 (772), PC 34:1 (798), PC 36:4 (820), and PC 36:1 (826) in the white matter (WM), shown as white circles, and gray matter (GM), shown as gray triangles. The error bars show the standard deviation of the normalized intensity over five spots per region. The average time between acquired spectra was 0.47 seconds.

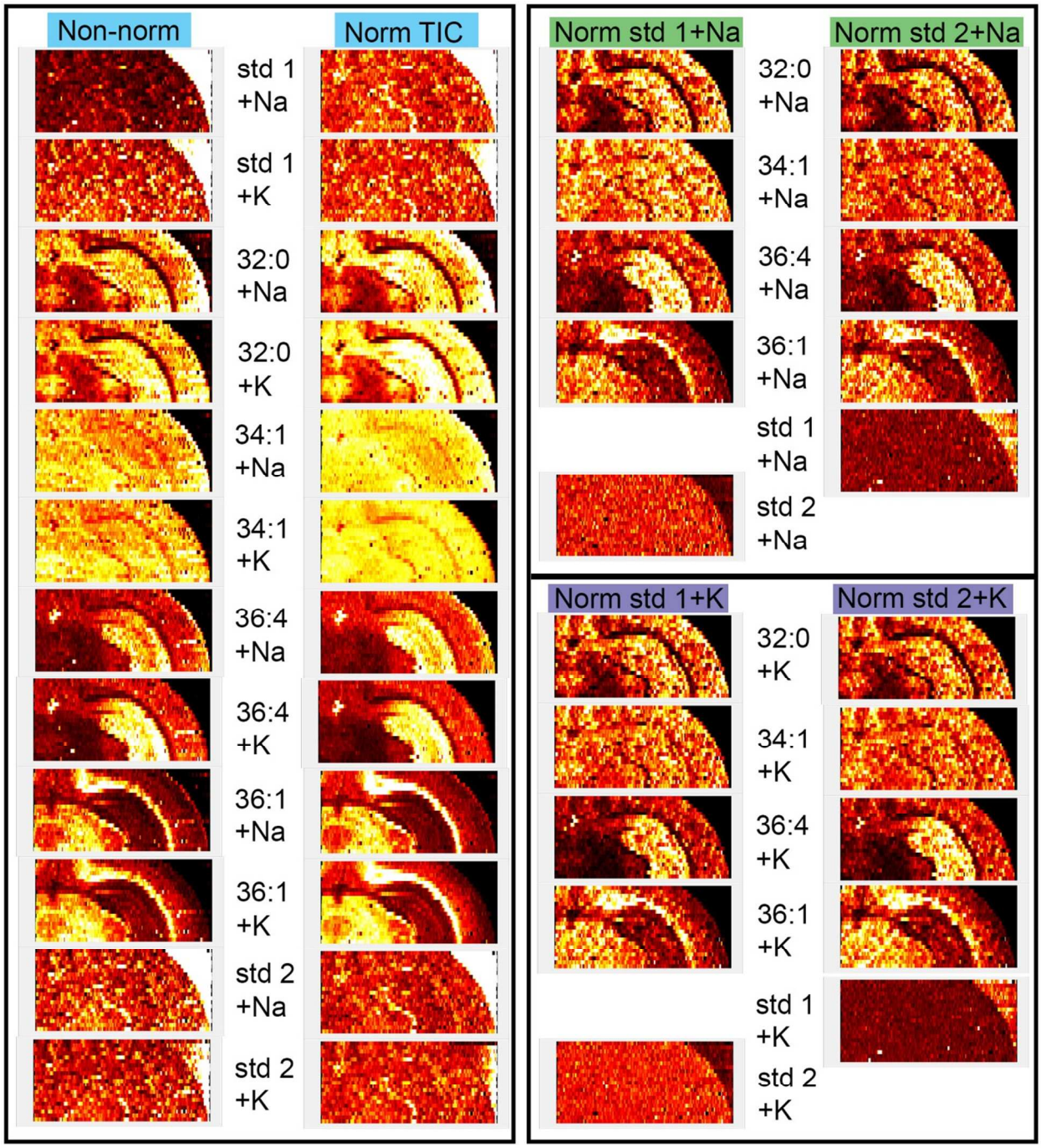

Figure S2. Ion images of endogenous PC 32:0, PC 34:1, PC 36:4, and PC 36:1 ($[M+Na]^+$ and $[M+K]^+$) and PC standards PC 25:0 (std 1) and PC 43:6 (std 2) ($[M+Na]^+$ and $[M+K]^+$), shown as non-normalized, normalized to TIC and normalized to the standards std 1 ($[M+Na]^+$ and $[M+K]^+$) and std 2 ($[M+Na]^+$ and $[M+K]^+$).

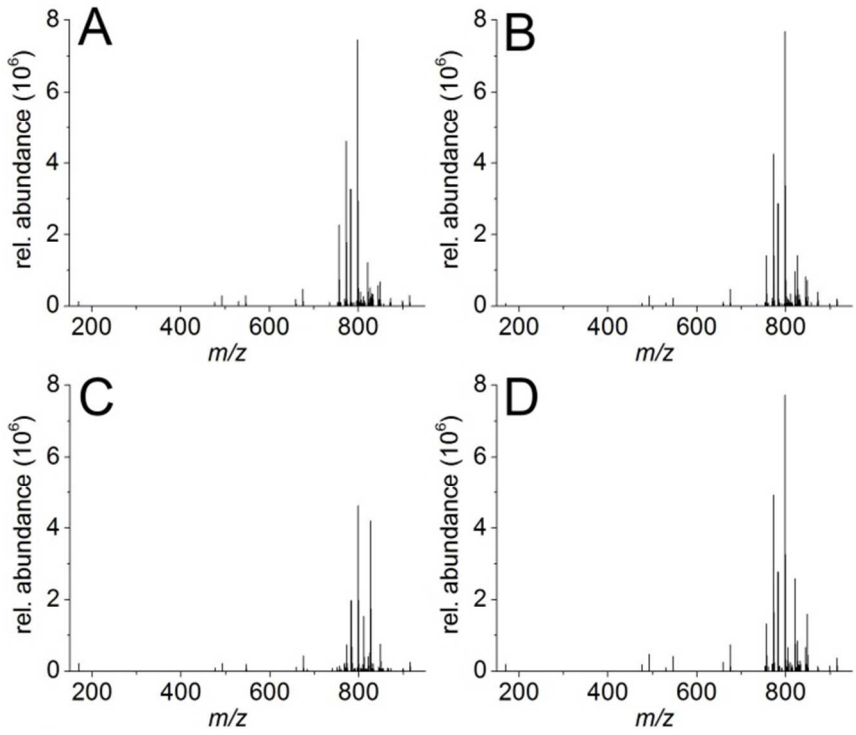

Figure S3. Single representative spectra from four different brain regions, 100-1000 Da. A) Neocortical layers I-IV, B) neocortical layers V-VI, C) white matter, and D) hippocampus. No normalization for the y-axis is performed.

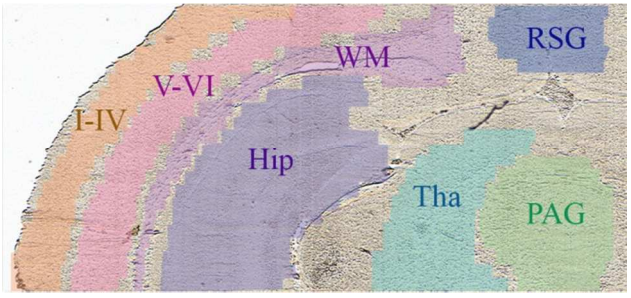

Figure S4. Seven regions of interest used for shotgun-like quantification of PC species in brain regions (Table 1 and Figure 5). I-IV = neocortical layers I-IV; V-VI = neocortical layers V and VI; RSG= retrosplenial granular Cx, b, and c; Hip = hippocampus; WM = white matter (corpus callosum); Tha = thalamus; and PAG = Periaqueductal gray (lateral and dorsomed).