MALDI Mass Spectrometric Imaging of Cardiac Tissue Following Myocardial Infarction in a Rat Coronary Artery Ligation Model

Prepared for Resubmission to Analytical Chemistry (12/11/1 Revision)

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Figure S-5. MS² spectrum using CID of m/z 546 (**a**) and MS³ spectrum using CID of m/z 546 \rightarrow 487 (**b**) from infarcted cardiac tissue. The structure of LPC 18:0 and an MS² image of m/z 546 \rightarrow 487 from cardiac tissue following LAD coronary artery ligation is shown as an inset in (**a**).

Figure S-6. MS² spectrum of m/z 848 using PQD from infarcted cardiac tissue. The structure of PC (18:0/20:4) and an MS² image of m/z 848 \rightarrow 789 from cardiac tissue following LAD ligation are shown as an inset.



Figure S-1. MS image of m/z 132 intensity divided by the TIC from control cardiac tissue.



Figure S-2. MS spectra of 100 ppm LPC 17:0 synthetic standard spotted with 40 mg/mL DHB in 70:30 MeOH:H₂O (v/v) with 10 mM NaOAc (a) or 10 mM KOAc (b).



Figure S-3. MS² spectra of the $[M+H]^+$ at m/z 510 (a) and the $[M+Na]^+$ at m/z 532 (b) and MS³ spectrum of $m/z 532 \rightarrow 473$ (c). All spectra were acquired from a 100 ppm standard of LPC 17:0 spotted with 40 mg/mL DHB in 70:30 MeOH:H₂O (v/v) with 10 mM NaOAc.



Figure S-4. MS² spectra of the $[M+K]^+$ at m/z 548 (a) and MS³ spectrum of m/z 548 \rightarrow 489 (b). All spectra were acquired from a 100 ppm standard of LPC 17:0 spotted with 40 mg/mL DHB in 70:30 MeOH:H₂O (v/v) with 10 mM KOAc.



Figure S-5. MS^2 spectrum using CID of m/z 546 (**a**) and MS^3 spectrum using CID of m/z 546 \rightarrow 487 (**b**) from infarcted cardiac tissue. The major fragment in (**a**) is a NL of 59, indicating an alkali metal adduct of a PC. Furthermore, in (**b**), the 22 Da difference between m/z 363 and 341 indicate a sodiated PC. Also, the fragment ion at m/z 147 is indicative of sodiated cyclophosphane, a characteristic ion of sodiated PCs. The ion was identified as the [M+Na]⁺ of LPC 18:0. The structure and an MS² image of m/z 546 \rightarrow 487 from cardiac tissue following LAD coronary artery ligation is shown as an inset in (**a**).



Figure S-6. MS^2 spectrum of m/z 848 using PQD from infarcted cardiac tissue. A NL of 59 indicates an alkali metal adduct of a PC. The 38 Da difference between m/z 655 and 627 and the fragment ion at m/z 163 (potassiated cyclophosphane) indicate a potassiated PC. MS^3 demonstrated a minor NL of 284, indicating a stearic fatty acid tail in the *sn*-1 position of the glycerol backbone (data not shown). Therefore, the ion was identified as the $[M+K]^+$ of PC (18:0/20:4). The structure and an MS^2 image of m/z 848 \rightarrow 789 from cardiac tissue following LAD ligation are shown as an inset. Unlike CID, PQD is not hindered by a LMCO, providing the potential for a larger number of characteristic ions within one MS^2 experiment. For example, when isolating the ion at m/z 848, the typical LMCO for CID on a linear ion trap is m/z 230, excluding the characteristic potassiated cyclophosphane ion (m/z 163).