Supporting Information

Coupling Headgroup and Alkene Specific Solution Modifications with Gas-Phase Ion/Ion Reactions for Sensitive Phospholipid Identification and Characterization

Elissia T. Franklin[a], Samuel W. J. Shields[b], Jeffrey C. Smith[b], Yu Xia[a,c], Scott A. McLuckey[a*]

a. *Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN, United States, 47907-2084, West Lafayette, IN, United States 47907-2084*
b. *Department of Chemistry and Institute of Biochemistry, Carleton University, 203 Steacie Building, 1125 Colonel By Drive, Ottawa, Ontario K1S 5B6, Canada*
c. *Department of Chemistry, Tsinghua University, Mengminwei Technical Building, Beijing, Haidian, China, 100084*

*Email: mcluckey@purdue.edu

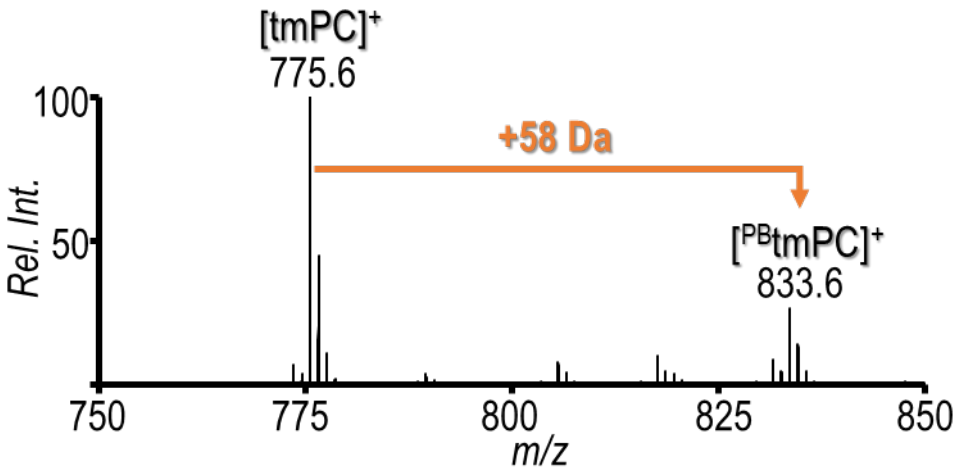

Figure S1: Positive ion mode mass spectrum of the PB reaction of [tmPC 16:0/18:1(9Z)]$^{+}$.

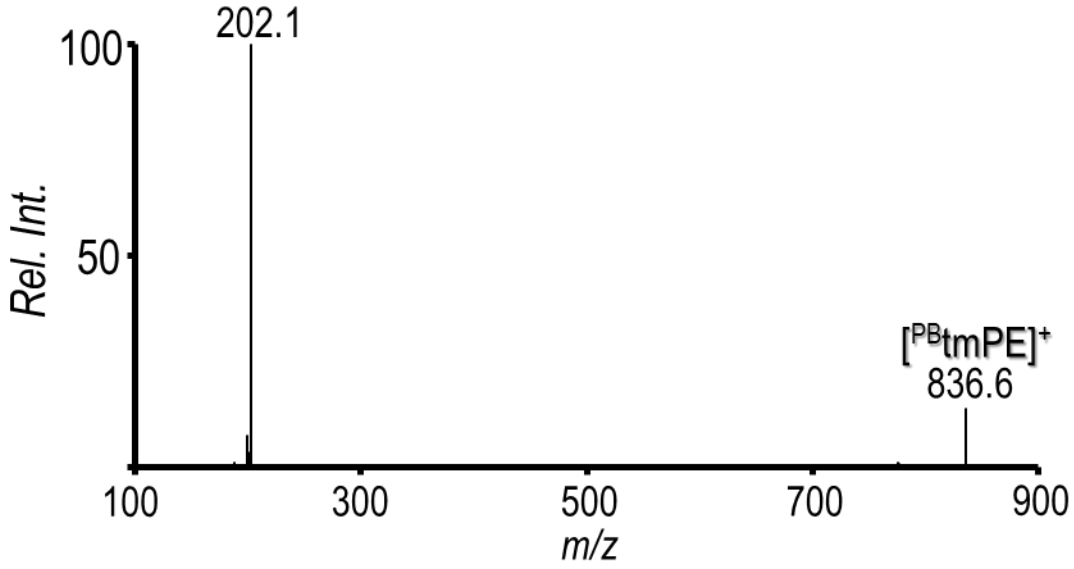

Figure S2: Positive ion mode CID spectrum of [^{PB}tmPE 16:0/18:1(9Z)]$^{+}$.

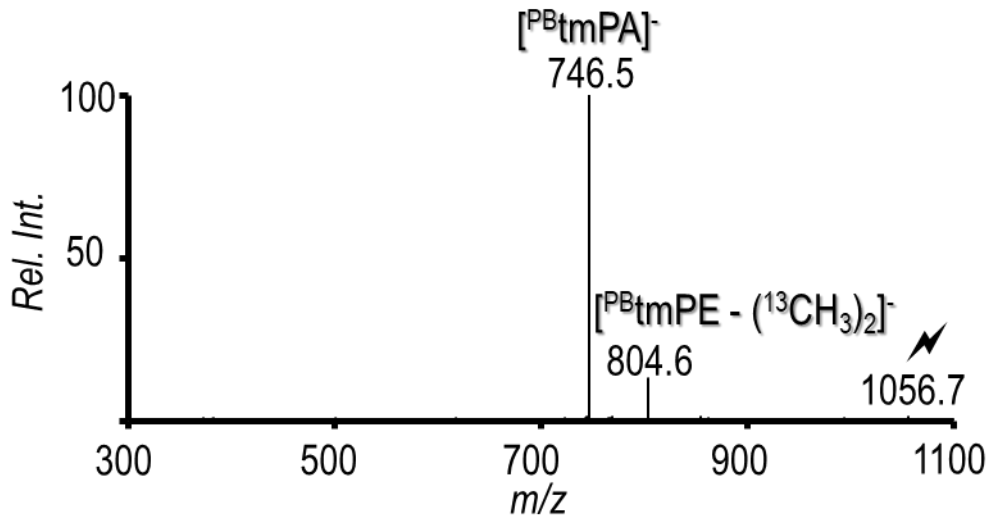

Figure S3: Isolation and sequential charge inversion of the PB product of positive ions at *m/z* 778 followed by CID of $[^{PB}tmPE + PDPA - 2H]^-$ at *m/z* 1056.7 from bovine liver polar lipid extract.

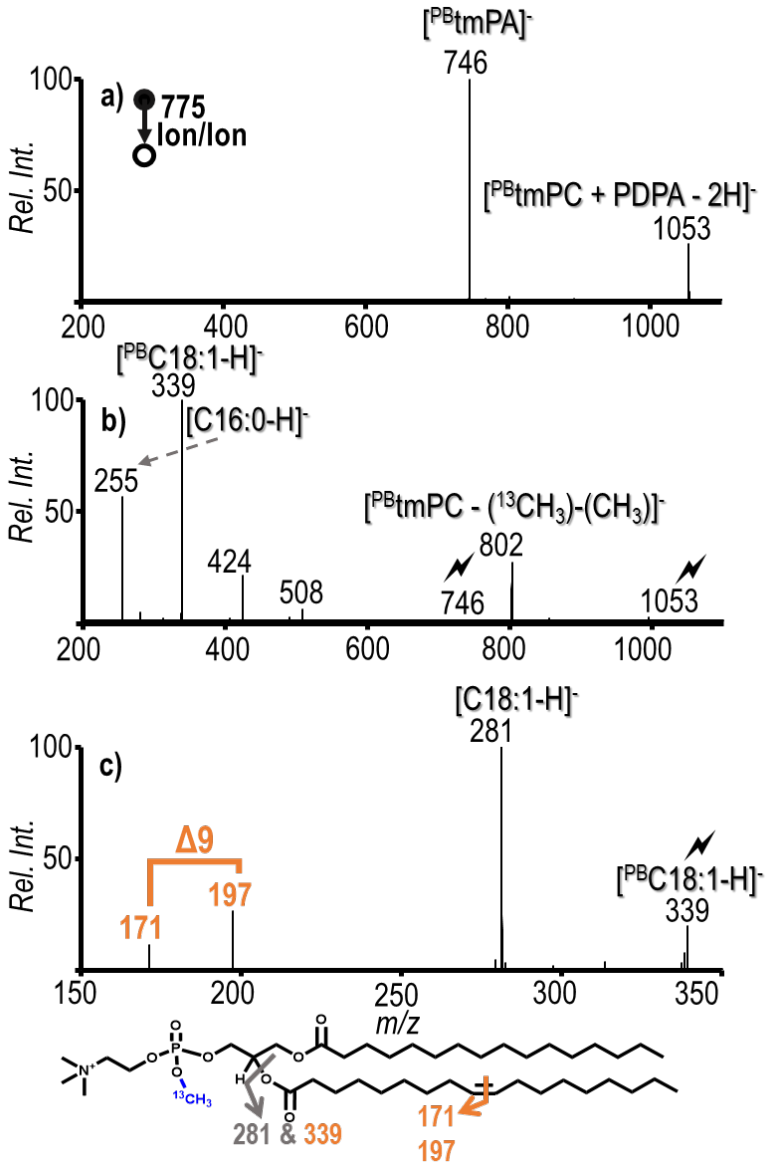

Figure S4: a) Post-ion/ion reaction between $[PDPA - 2H]^{2-}$ and $[^{PB}tmPC\ 16:0/18:1(9Z)]^{+}$; b) Ion trap CID of $[^{PB}tmPC + PDPA - 2H]^{-}$ followed by subsequent ion trap CID of $[^{PB}tmPA]^{-}$, c) Sequential steps of CID for the C=C localization.

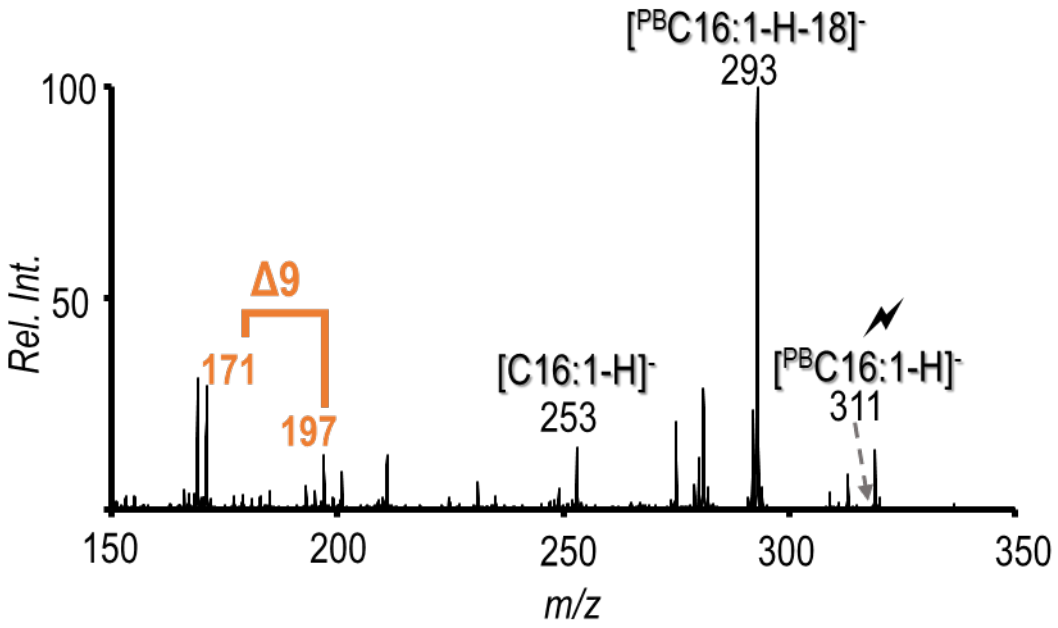

Figure S5: Charge inversion of positive ion mode m/z 836 (PB product of m/z 778) followed by multiple steps of ion trap CID and sequential CID spectrum of m/z 311.

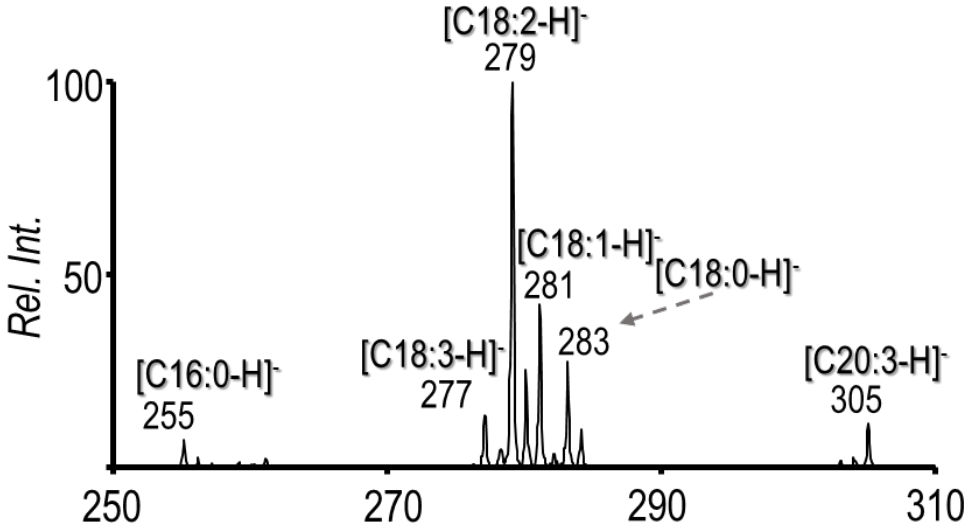

Figure S6: Charge inversion via ion/ion reaction with PDPA of ions at *m/z* 802 followed by sequential steps of CID for fatty chain determination.