SUPPORTING INFORMATION

for

Structural characterization of glycerophospholipids by combinations of ozone- and collision-induced dissociation mass spectrometry: The next step towards “top-down” lipidomics

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**Scheme S-1:** The substitution mechanism with a five-membered ring intermediate driven by the
sn-2 fatty acyl chain during CID/OzID fragmentation of [TG 16:0/18:1/16:0 + Na]⁺.
Scheme S-2: Proposed structures of major product ions forming in CID/OzID from [PC 16:0/18:2 + Na]+.
Scheme S-3: A mechanism proposed for the formation and (CID/OzID)$^2$ fragmentation of the m/z 614/615 ion resulting from the PC 16:0/18:1(9Z) standard.
**Figure S-1:** (a) CID spectrum of [TG 16:0/18:1/16:0 + Na]$^+$ precursor ion at m/z 855, (b) CID/OzID spectrum of m/z 599 fragment ion [TG 16:0/18:1/16:0 + Na - 16:0]$^+$ formed in (a).

**Figure S-2:** ESI-MS mass spectra obtained in positive ion mode for lipids extracts from (a) cow brain and (b) cow kidney. The ions observed represent the [M + Na]$^+$ adducts of a wide range of phospholipids present in the samples.
Figure S-3: Duplicate measurement of CID/OzID spectra generated by initially mass-selecting [M + Na]^+ adduct ions at m/z 782 from (a), (b) and (c) bovine brain and (d), (e), (f) bovine kidney extracts.
Figure S-4: Duplicate measurement of CID/OzID² spectra generated by initially mass-selecting [M + Na]⁺ adduct ions at m/z 782 from (a), (b) and (c) bovine brain and (d), (e), (f) bovine kidney extracts. The magnifying factor of 20 times is the same for all spectra.
**Figure S-5:** Duplicate measurement of (CID/OzID)² spectra generated by initially mass-selecting [M + Na]⁺ adduct ions at m/z 782 from (a), (b) and (c) bovine brain and (d), (e), (f) bovine kidney extracts. The magnifying factor of 5 times is the same for all spectra.