Supporting Information:

Generating fatty acid profiles in the gas-phase: fatty acid identification and relative quantitation using ion/ion charge inversion chemistry

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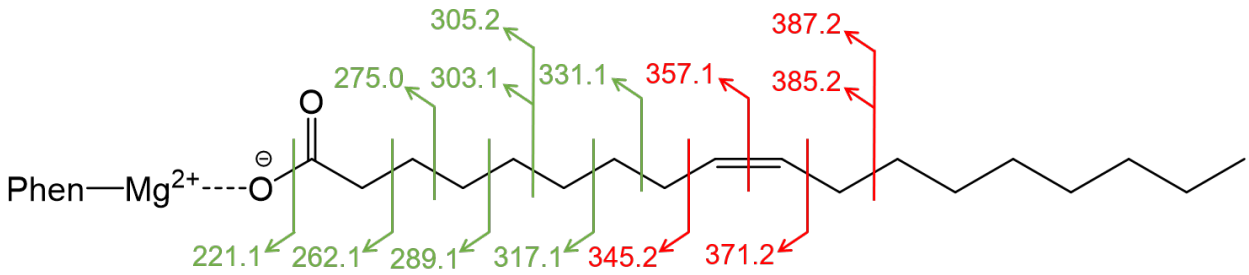

Figure S1. Structure and fragmentation pattern of [FA – H + MgPhen]$^+$ ion where FA = 18:1(9*Z*) (*i.e.* the *n*-9 isomer).

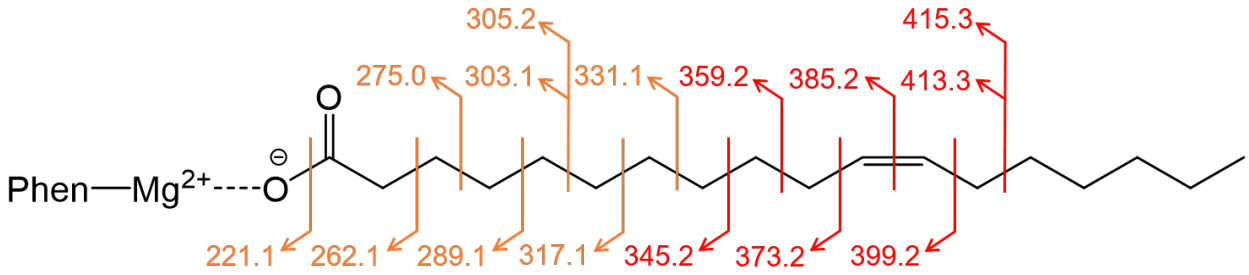

Figure S2. Structure and fragmentation pattern of [FA – H + MgPhen]$^+$ ion where FA = 18:1(11*Z*) (*i.e.* the *n*-7 isomer).

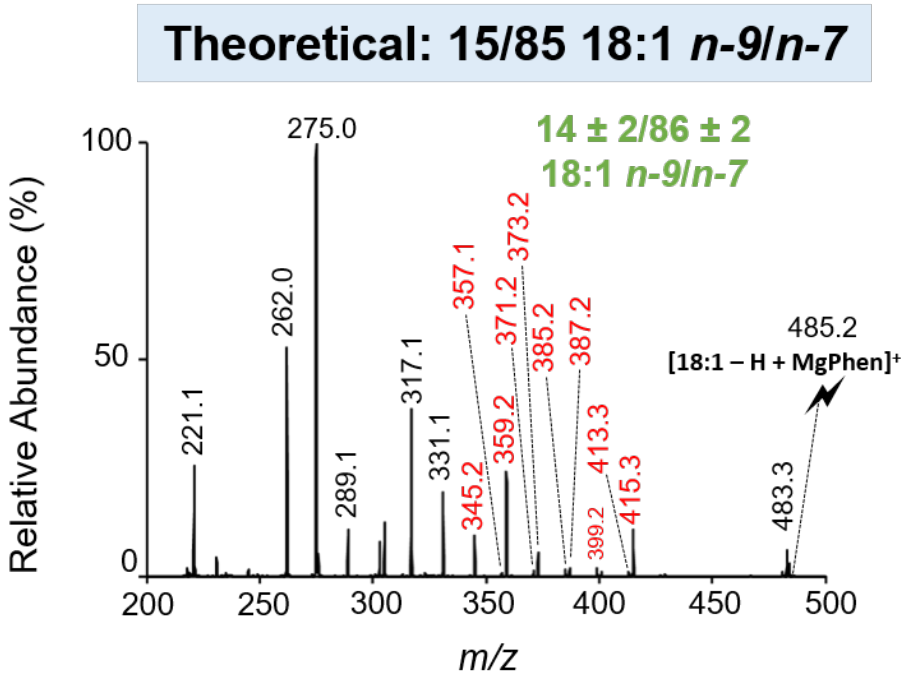

Figure S3. CID spectrum of [18:1 – H + MgPhen]$^+$ for the 15/85 *n*-9/*n*-7 18:1 FA mixture. Diagnostic product ions for relative quantitation are shown in red. The lightning bolt signifies the precursor ion collisionally activated. The calculated relative composition is shown in green.

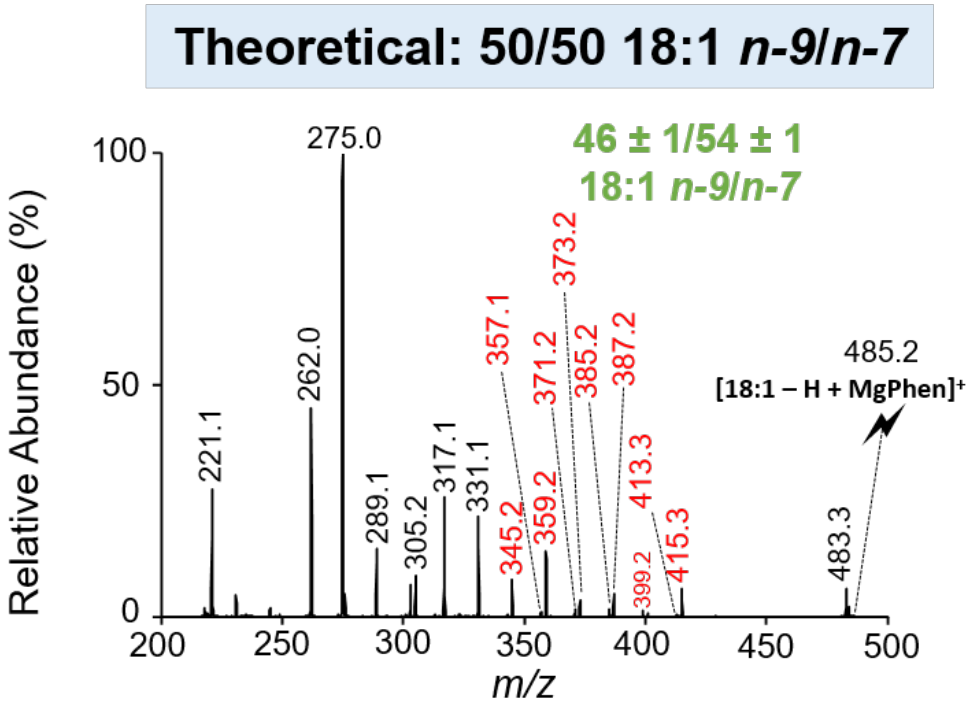

Figure S4. CID spectrum of [18:1 – H + MgPhen]$^+$ for the 50/50 *n*-9/*n*-7 18:1 FA mixture. Diagnostic product ions for relative quantitation are shown in red. The lightning bolt signifies the precursor ion collisionally activated. The calculated relative composition is shown in green.

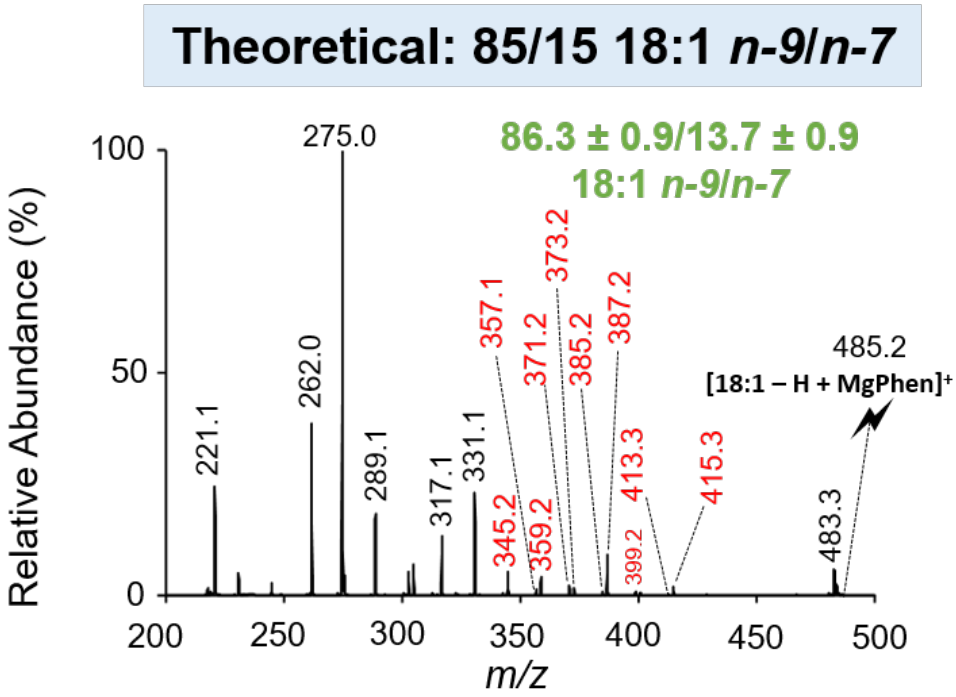

Figure S5. CID spectrum of [18:1 – H + MgPhen]$^+$ for the 85/15 *n*-9/*n*-7 18:1 FA mixture. Diagnostic product ions for relative quantitation are shown in red. The lightning bolt signifies the precursor ion collisionally activated. The calculated relative composition is shown in green.

Figure S6. Structure and fragmentation pattern of [FA – H + MgPhen]$^+$ ion where FA = 18:3(9*Z*,12*Z*,15*Z*) (*i.e.* the *n*-3 isomer).

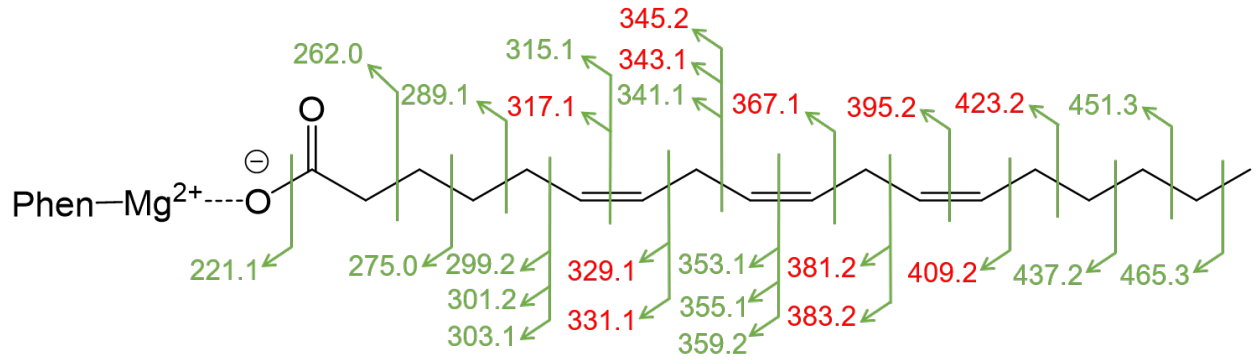

Figure S7. Structure and fragmentation pattern of [FA – H + MgPhen]$^+$ ion where FA = 18:3(6*Z*,9*Z*,12*Z*) (*i.e.* the *n*-6 isomer).

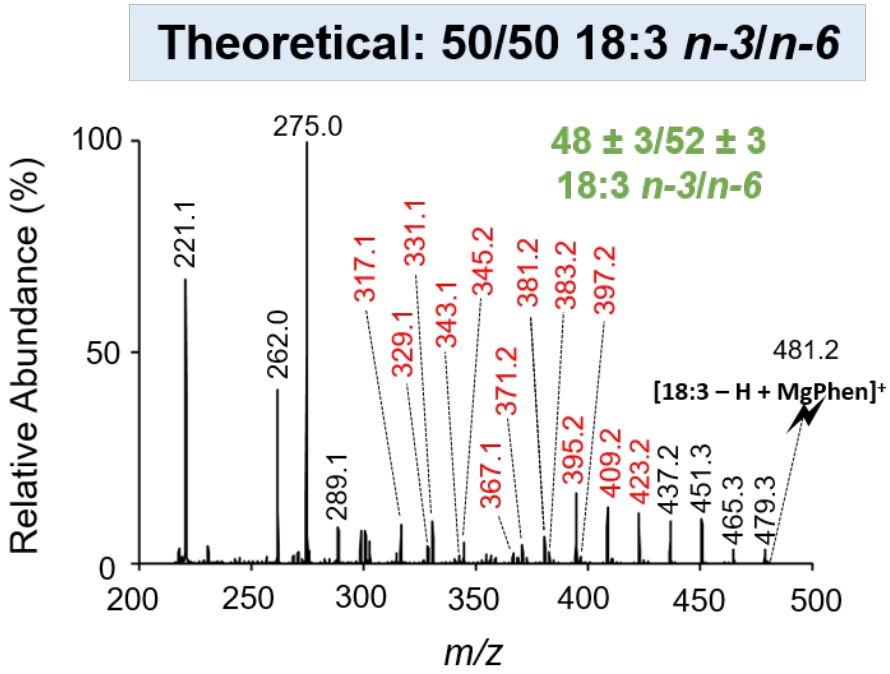

Figure S8. CID spectrum of [18:3 – H + MgPhen]$^+$ for the 50/50 *n*-3/*n*-6 18:3 FA mixture. Diagnostic product ions for relative quantitation are shown in red. The lightning bolt signifies the precursor ion collisionally activated. The calculated relative composition is shown in green.

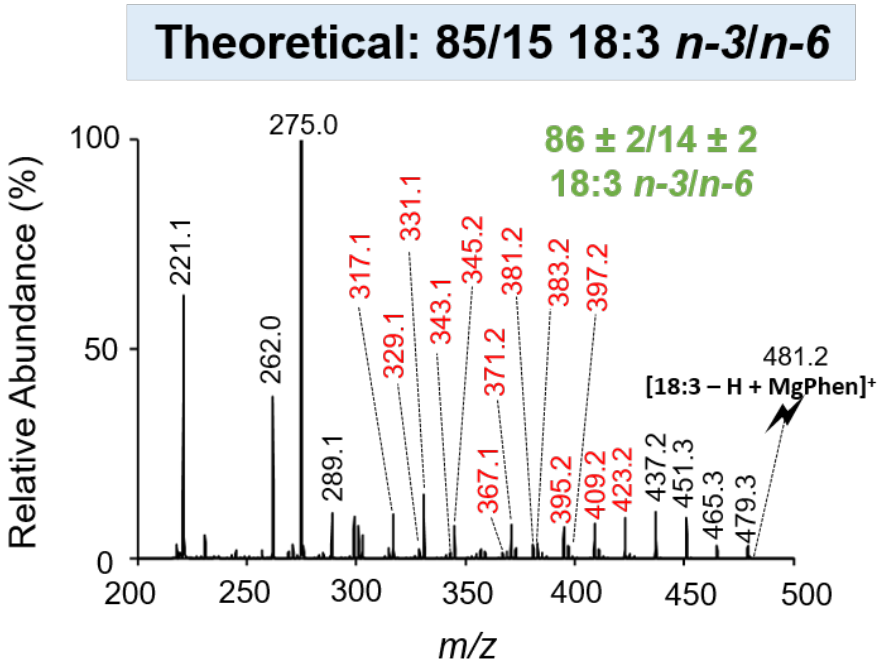

Figure S9. CID spectrum of [18:3 – H + MgPhen]$^+$ for the 85/15 *n*-3/*n*-6 18:3 FA mixture. Diagnostic product ions for relative quantitation are shown in red. The lightning bolt signifies the precursor ion collisionally activated. The calculated relative composition is shown in green.

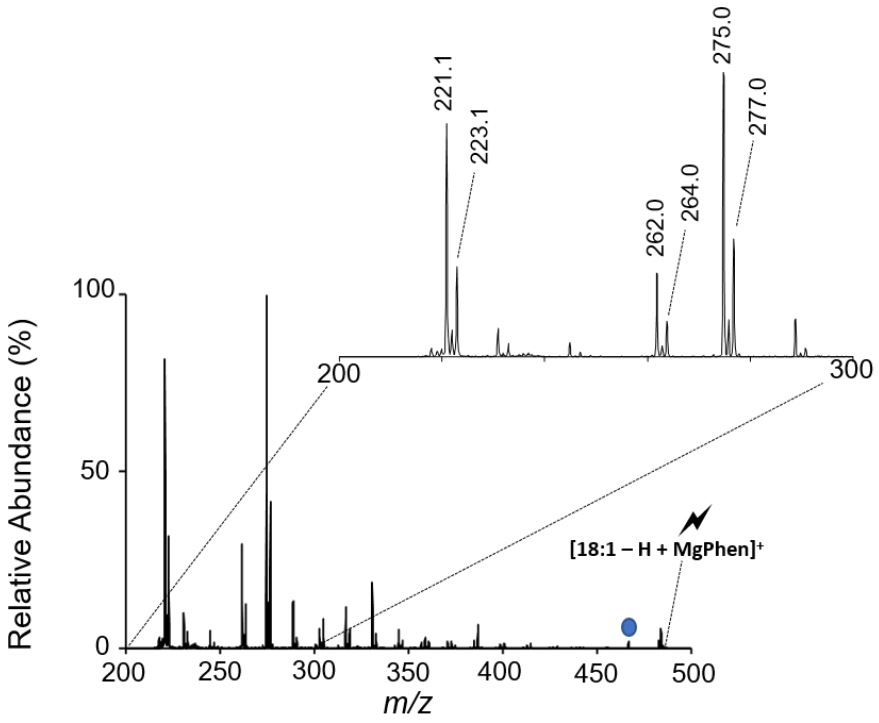

Figure S10. CID spectrum of [18:1 – H + MgPhen]$^+$ (*m/z* 485.2) derived from bovine liver extract. The blue circle represents a water loss from an ion isobaric to the charge-inverted 18:1 FA complex cation. There are notable +2 Da peaks observed at *m/z* 223.1, 264.0, and 277.0 due to the third isotope of the 18:2 FA in BLE.

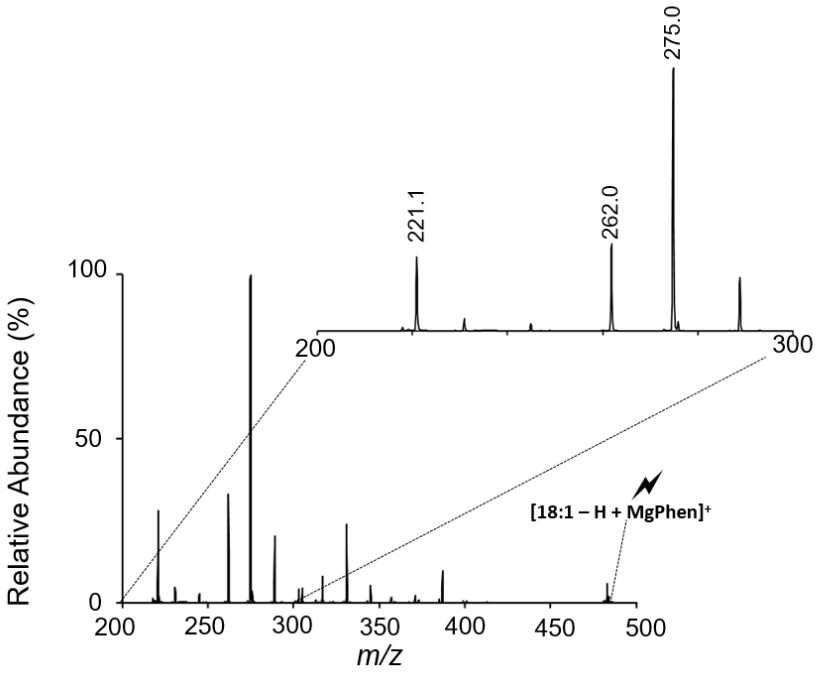

Figure S11. CID spectrum of $[18:1 - H + MgPhen]^+$ (*m/z* 485.2) derived from pure 18:1(9) standard. Note the absence of the notable +2 Da peaks at *m/z* 223.1, 264.0, and 277.0. Instead, only the product ions at *m/z* 221.1, 262.0, and 275.0 are observed.

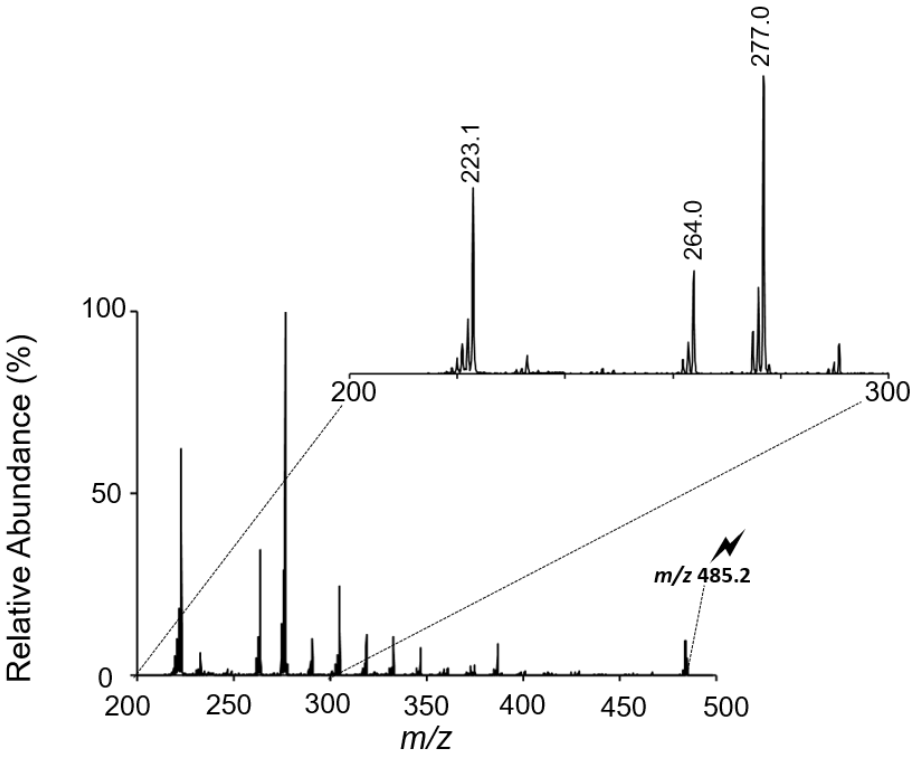

Figure S12. CID of the third isotope of [18:2 – H + MgPhen]$^+$ (*m/z* 485.2) derived from a pure 18:2 FA standard. Note the presence of the product ions *m/z* 223.1, 264.0, and 277.0 in the low mass region of the CID spectrum.

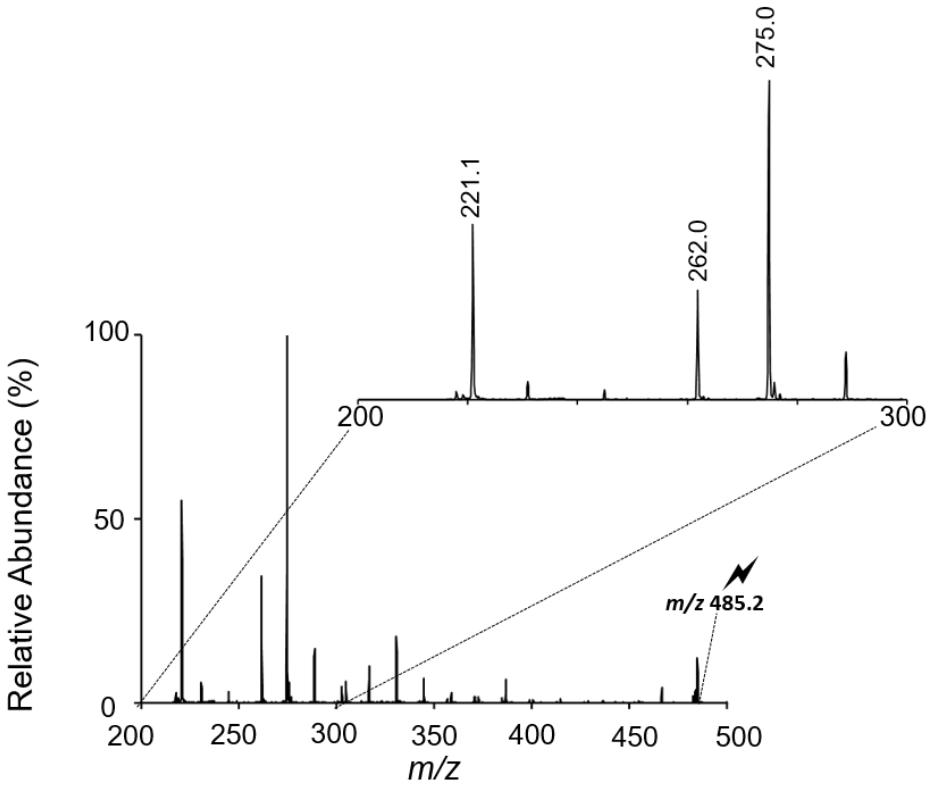

Figure S13. CID of the [18:2 – H + MgPhen]$^+$ (*m/z* 485.2) derived from bovine liver extract following monoisotopic isolation of the $[Mg(Phen)_3]^{2+}$ charge-inversion reagent prior to the ion/ion reaction. Note the absence of the product ions *m/z* 223.1, 264.0, and 277.0 in the low mass region of the CID spectrum.

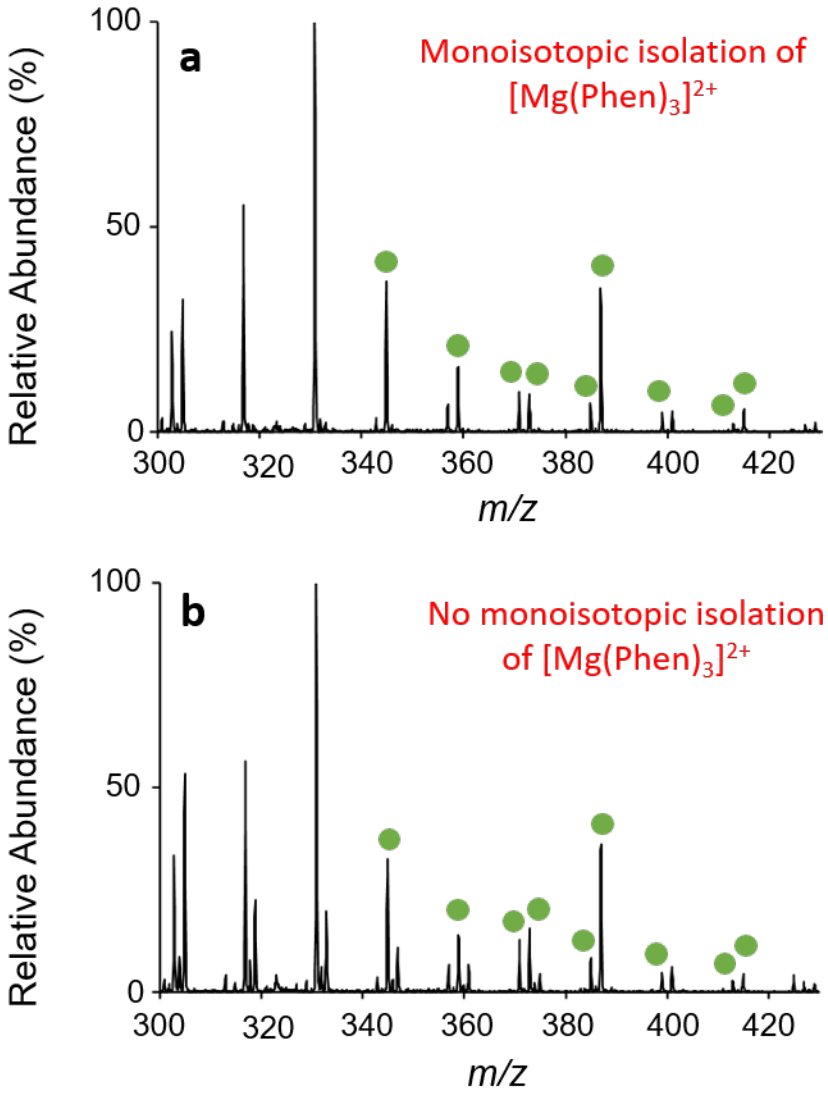

Figure S14. Enlargements of CID of the [18:1 – H + MgPhen]$^+$ (*m/z* 485.2) derived from bovine liver extract over the diagnostic product ion *m/z* region (a) with monoisotopic isolation of the $[Mg(Phen)_3]^{2+}$ charge-inversion reagent prior to the ion/ion reaction and (b) without monoisotopic isolation of the $[Mg(Phen)_3]^{2+}$ charge-inversion reagent prior to the ion/ion reaction. Diagnostic product ions used for the relative quantitation of 18:1 FA isomers are shown with green circles.