Differential mobility spectrometry resolves chlorine- and acetate-adducts of phosphatidylcholine (PC)

SelexION® Technology

The resolution of isobaric lipid species—specifically the ability to distinguish lipid adducts, such as the chlorine- and acetate adducts of PC, is critical for molecular species identification and accurate quantitation in lipidomics analysis.

The challenge:

A typical solvent for lipid analysis contains volatile salts such as ammonium acetate to improve ionization. In biological samples, Cl- ions are present, and they compete with the solvent anions to form lipid adducts, which increases the number of isobars in the sample. HPLC may not be sufficient to resolve these isobars; as a result, both may be co-isolated during precursor ion selection during MS/MS. Characterization of PC in the negative ion mode can be particularly challenging, because it exists as a mixture of anionic adducts/ions, depending on the solvent composition in which they are dissolved. Product ion analysis (MS/MS) of this mixture is key to determine composition, however mixtures of adducts can generate confounding results, which can lead to mis-identification and incorrect quantification.

The solution:

Differential ion mobility separation (DMS) as provided by the SelexION Technology isolates molecules based on their electrostatic properties (i.e., dipole moment), and consequently these isobars can be separated using an adduct-specific compensation voltage (CoV) during analysis via infusion or HPLC. SelexION Technology isolates the lipid adducts prior to MS/MS analysis and therefore generates spectra that are adduct-specific and clear of isobaric interference from other adducts. This enables clear identification and accurate quantification of the target lipid molecule.

SelexION Technology can isolate the different adducts of PC, which enables correct identification and accurate quantitation of individual PC molecular species.

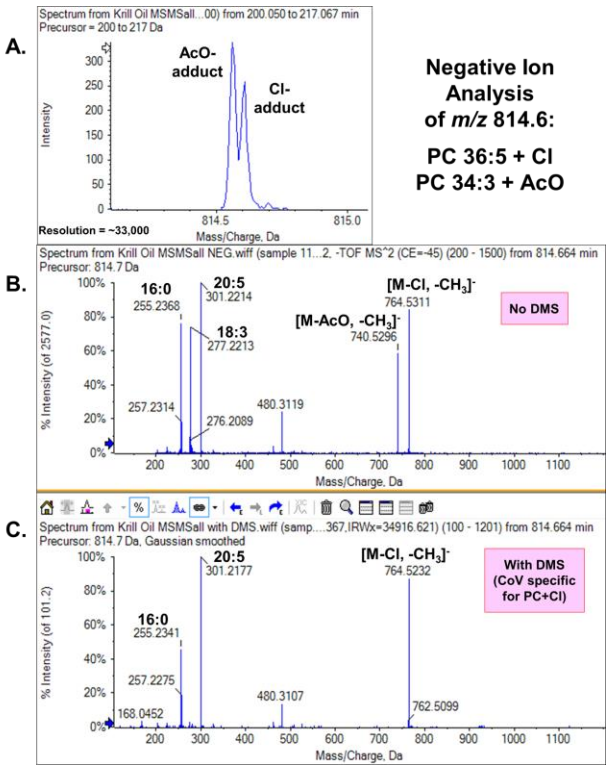

Figure 1. Resolution of PC-adducts by SelexION Technology. Krill oil was diluted in a mixture of methanol and dicholoromethane (1:1, v/v) containing 10 mM ammonium acetate and infused into a TripleTOF® 5600+ System equipped with a SelexION Device. **A**) A TOF MS scan of m/z 814-815 shows acetate- and chlorine-adducts of the PC molecular species. This 1 Da range is the typical isolation window of precursor ions during MS/MS analysis on most unit- and high-resolution instruments. **B)** MS/MS analysis of m/z 814.6 shows a convolved spectrum of the chlorine and acetate adducts. Note, fragment 255 (palmitic acid; 16:0) is common to both precursors. **C**) With the DMS device set to resolve chlorine adducts, the MS/MS spectrum reflects a single molecular species that is identifiable and quantifiable, PC (16:0/20:5) + Cl.

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