Rapid Structural Analysis of Triacylglycerols in Food using MALDI-TOF(/TOF) MS with monoisotopic precurcer selectivity

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Mass Spectrometry is widely accepted for lipid analysis coupled with liquid chromaotography or other separation techniques. Several types of mass spectrometer have MS/MS capability and use for structural analysis using low-energy collision-induced dissociation (CID) with atmospheric pressure chemical ionization (APCI) or electrospray ionization (ESI). However low-energy CID makes not enough information to decide positions of double bond in triacylglycerols (TAGs). High-energy CID is an especially attractive approach for TAGs analysis because charge-remote fragmentation provides much information about lipid structure including not only kinds of lipids but also position of doubule bonds. Monoisotopic precursor selectivity makes it possible to obtain product-ion mass spectra without interference from species that differed by a single double bond and also from isotope-ion. Complete structure determination of all TAGs, including structural isomers, was made possible by interpreting the charge-remote fragmentation resulting from high-energy CID of the sodiated TAGs.

However, large tandem magnetic sector mass spectrometers have fallen out of favor in recent years and high-energy CID appeared destined to become a “lost art” until the introduction of tandem time-of-flight (TOF/TOF) mass spectrometers by Cotter and Cornish in 1993. Recently, Pittenauer and Allmaier showed that TOF/TOF mass spectrometers have the potential to provide the same complete structural information as a tandem magnetic sector mass spectrometer. The principal limitation of this method was found to be the poor MS-I selectivity (4 to 6 Da window) of the TOF/TOF system, making it impractical to select precursor ions for TAGs with compositions that differ by two hydrogens.

We report that structural analysis of TAGs in foods using MALDI-TOF(/TOF) with new Spiral ion optics.