

*Developing a Model for Predicting the CID Mass Spectra of Ammoniated Triglycerides*

This project focuses on the development of an LC-MS-MS method for the positional analysis of complex mixtures of triglycerides (TAGs). Mass spectrometry is used to distinguish among positional isomers of TAGs. The intensities of diglycerol fragments resulting from the collisional-induced decomposition (CID) of ammoniated TAGs are dependent on fatty acid position. It is also evident from our most recent work that the intensities of the CID products of ammoniated TAGs are dependent on the degree of unsaturation and, to a lesser extent, on the chain length of the fatty acids. We have illustrated that calibration plots can be produced showing a linear dependence of fractional intensities of diglycerol fragments and fractional composition of positional isomers. We have designed a study that will be useful in quantifying the effects of fatty acid position, degree of unsaturation, and chain length on the CID spectra. This data will be used to estimate the fractional composition of any system of positional isomers. The accuracy and precision of this method will be explored, and the method will be applied to the analysis of complex mixtures, such as vegetable oils, animal fats, tissue, and blood. The development of this method will support a wide range of studies on metabolism, biosynthesis, and degradation of individual TAG species within biological systems.