PT16 Structural Characterisation of Triacylglycerols (TAGs) present in Very Low Density Lipoprotein by Ozone-Induced Dissociation (OzID)

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An advanced mass spectrometric approach was used for the near-complete structural characterisation of two abundant TAGs found in human VLDL.

Triacylglycerols (TAGs) are the most abundant lipids in nature and as a consequence more effort has been applied to the analysis of this lipid class than any other. Nevertheless, a complete structural analysis of TAGs requires numerous steps of derivatization and chromatography. In this study we have applied an advanced mass spectrometric approach for the examination of two abundant TAGs found in human very-low density lipoprotein (VLDL).
Complex mixtures of TAGs were isolated from VLDL obtained from 64-year-old females by HPLC.[1] A new online ozonolysis technique, ozone-induced dissociation (OzID) [2] was employed to unambiguously assign the double bond positions and provide near-complete structure elucidation for the intact TAGs. Multiple stages of MS were performed, utilizing different combinations of collision-induced dissociation (CID) and OzID to remove one or two of the three esterified fatty acids (FAs) and leave the remaining acyl chain/s for ozonolysis.
Two CID fragmentation mechanisms for the loss of FAs via either a five- or six-membered ring intermediate are proposed. The MS techniques used in this study have revealed that the “two” TAGs analysed are at least eleven distinct molecules with variation in the position of double bonds and FA attachment to the glycerol backbone. This study provides new insight into the diversity of TAG structure and how that was unattainable with traditional techniques.

1. Brohall, G., et al., *Prevalence of Diabetes and Impaired Glucose Tolerance in 64-Year-Old Swedish Women.* Diabetes care., 2006. 29(2): p. 363-367.
2. Thomas, M.C., et al., *Ozone-Induced Dissociation: Elucidation of Double Bond Position within Mass-Selected Lipid Ions.* Analytical Chemistry., 2008. 80(1): p. 303-311.