

FT-ICR MS: the solution to the coincidence mass of the ions in soybean oil

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Soybean oil is a complex mixture containing a wide range of compounds, i.e. triacylglycerols, mono and diacylglycerols, free fatty acids, oxidized products, and others. Typical soybean oil fingerprint MS shows ions in the form of sodium (Na^+) and potassium (K^+) adducts. Therefore, may arise a question if a particular ion is in the form of K^+ adduct or it is an oxidized compound in the form of Na^+ adduct. Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) is a technique that allows a detailed characterization of organic compounds due to its high resolution and mass accurate. This technique permits differentiate molecules by their exact mass to the fourth decimal place. Thus, the aim of this work was to use FT-ICR MS to resolve the question about the coincidence of mass between Na^+ and K^+ ions in soybean oil. 1 μL soybean oil and 1 μL oxidized soybean oil (submitted to 110° C and 10L h^{-1} of air during 5 hours) was diluted in 100 μL toluene:methanol (1:1). These solutions were directly analyzed by a FT-ICR MS (LTQ FT Ultra Mass Spectrometer, ThermoScientific, Germany) with an electrospray (ESI) source (Advion BioSciences, United States) in the positive ion mode. The mass spectra were recorded in the mass/charge (m/z) range of 500-1100. Significant differences were observed in the ESI (+) FT-ICR MS spectra of soybean oil and oxidized soybean oil. For soybean oil, the predominant ions were triacylglycerols (TAG) in the $[\text{TAG} + \text{Na}^+]$ form of m/z 877 (PLL), 899 (LLL_n), 901 (LLL), 903 (LLO), and 905 (LOO). In this conditions almost not observed the presence of $[\text{TAG} + \text{K}^+]$. The oxidized soybean oil spectra demonstrated a decrease in TAG ions and an increase of ions corresponding to oxidation compounds as TAG + Ox (m/z 917 – LLL + Ox), TAG + 2Ox (m/z 933 – LLL + 2Ox) TAG + 3Ox (m/z 949 – LLL + 3Ox), and TAG + 4Ox (m/z 965 – LLL + 4Ox). Oxidation compounds were observed mainly in the form of Na^+ adducts. From this FT-ICR MS data is possible to note that the increase of 16 units in m/z of TAG ions in soybean oil during oxidation process do not correspond a $[\text{TAG} + \text{K}^+]$ but an oxidation compound containing one more oxygen molecule (TAG + Ox + Na^+).