FINGERPRINTING / PROFILING: A NOVEL APPROACH FOR A HIGH THROUGHPUT AND COMPREHENSIVE ASSESSMENT OF QUALITY AND SAFETY OF FOOD LIPIDS

Jana Hajslova^{1*}, Tomas Cajka², Lukas Vaclavik³

^{1,2,3} Institute of Chemical Technology, Prague, Department of Food Chemistry and Analysis, Prague, Czech Republic

Lipids, the key component of many foodstuffs, are not only a source of essential components such as ω -3 and ω -6 fatty acids, but they are also accompanied by other important lipophilic components represented by vitamins, sterols etc. On the other hand, lipids may contain various toxic and /or antinutritive compounds generated from natural precursors as the result of (auto)oxidation processes or thermal processing. Chromatography, together with mass spectrometry, are essential analytical tools in this field. In addition to targeted compositional analysis, non-target fingerprinting / profiling techniques have recently emerged as the novel strategy for assessment of lipids quality and safety. In our study, ambient mass spectrometry employing DART (Direct Analysis in Real Time) and/or ASAP (Atmospheric Solids Analysis Probe) coupled with (ultra)high resolution mass spectrometry (MS) were used for characterization of various food lipids. In this way, not only intact triacyl glycerols but also their oxidation products such as hydroperoxides, epoxides etc., together with reactive polar breakdown products, can be detected. When using a simple sample preparation step, also occurrence of "emerging" processing contaminants 3-MCPD diesters could be documented. To obtain fingerprints of headspace volatiles, solid-phase microextraction-electron ionization high resolution mass spectrometry (HS-SPME-EI-HRMS) was employed. Advanced chemometric strategies represented by linear discrimination analysis (LDA) and neural networks (NN) were used for processing of generated data and quality markers identification.

Keywords: Lipidomics, fingerprinting, profiling

Acknowledgement: The financial support by the Ministry of Education, Youth and Sports of the Czech Republic (MSM 6046137305) is gratefully acknowledged.

^{*}Corresponding author - E-mail: jana.hajslova@vscht.cz , Phone: +420 2 2044 3185