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Challenges offered by hybrid high resolution mass spectrometry based metabolomics in food nutrition research

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Lipids are a large and diverse group of naturally-occurring compounds that store energy, give structure to cell membranes, and, as 'molecular messengers', they serve as signaling molecules. Considering foods nutritional value, lipids are one of the key components, they are e.g. a source of essential components such as polyunsaturated fatty acids (PUFA), they support absorption of fat soluble vitamins etc. For in-depth structural and quantitative characterization of various lipid classes and their distribution within food crops and/or products, instrumental platforms based on advanced chromatographic methods coupled with mass spectrometric detection represent currently the most challenging option. In our studies, we focused on application of these novel strategies for monitoring of lipids changes during storage and processing, i.e. under conditions when they may undergo various degradative processes such as oxidation. Worth to notice that compounds generated through oxidation reactions are related to undesirable sensory and biological effects. In addition to cytotoxic and genotoxic compounds, free radicals, products of lipids peroxidation also co-oxidize some vitamins, and thereby impair the nutritional quality of the foods. A high number of methodologies enabling determination of both primary and secondary oxidation products has been developed and implemented. However, some of these 'classic' approaches such as peroxide value illustrating early stages of lipids oxidation are highly empirical and their accuracy is rather questionable since the results vary with details of the analytical procedure. Also thiobarbituric acid (TBA) test often applied for measurement of the extent of lipids oxidation has been criticized as being non-specific and insensitive for the detection of low levels of malonaldehyde. Not surprising that introduction of modern instrumental techniques that enable rapid obtaining of more comprehensive and specific information is urgently needed. In addition to implementation of modern analytical methods for assessment of lipids qualitative parameters, we also were concerned with introduction of novel non-target screening strategies enabling lipids authentication. This presentation involves several case studies documenting challenges in lipids analysis: 1) Simple and fast sample preparation strategy based on partition in ternary solvent system enabling, in a single step, fractionation of fish lipid classes according their polarity. 2) Application of an ambient high resolution mass spectrometry (HRMS) employing direct Analysis in Real Time (DART) ion source for an assessment of lipids quality with regards to content of primary and secondary oxidation products 3) Authentication of food lipids using fingerprinting / profiling strategy based on DART-HRMS, lipidomics 4) Employing supercritical fluid chromatography (SFC) coupled with high definition mass spectrometry (HDMS) for analysis of frying oils and lipids isolated from human adipose tissue. Challenges offered by metabolomics in nutrition research are thoroughly discussed with a special focus on application of advanced multivariate statistical strategies enabling data interpretation.

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