Abstract

Methods of analytical chemistry are widely used in lipidomics. Separation techniques coupled to mass spectrometry or nuclear magnetic resonance are used very often. They make it possible to identify lipids present in the matrix in very small quantities.

This work summarizes the application of modern analytical methods and instrumentation for identifying and characterizing lipids in vernix caseosa. It is shown how I contributed during the Ph.D. studies to the elucidation of the structure and characterization of unknown lipid classes followed by more detailed description of those lipid classes already identified in vernix caseosa.

An integral part of my work was the application of the method enabling the localization of double bonds developed by our laboratory in triacylglycerols and 1,2-diol diesters in vernix caseosa. This analytical method is based on the formation of an acetonitrile adduct in an ionization source of a mass spectrometer enabling atmospheric pressure ionization. The complexity of the triacylglycerol class did not allow a complete characterization of the double bonds. However, the fragmentation mostly showed that double bonds up to *n*-12 position are present, but small peaks in some spectra also indicated double bonds at more distant positions from the chain termini. I have also collaborated on the characterization of chain branching and the position of double bonds of triacylglycerols. The analyzes showed branching in *iso*-, *anteiso*- and other positions and double bonds even in unusual positions. In collaboration on the characterization of 1,2-diol diesters, we were able to localize the double bonds in the *n*-7, *n*-9 and *n*-5 positions.

Another part of this work was the hydrolysis of whole vernix lipidome and analysis of methyl esters of fatty acids. The results showed 167 mostly saturated molecular species containing a large number of branching sites in their chains. These results were part of a study focused on the difference in lipid composition in the cohort of 20 newborn subjects.

1-*O*-acylceramides are a new lipid subclass that I identified and characterized in the investigated matrix. The results showed more than 2,000 molecular species with mainly saturated fatty acid chains. Another newly characterized lipid class that we identified was cholesterol esters of ω- (-(*O*-acyl)-hydroxy fatty acids.

The results of my work confirm the complexity of the lipid composition of vernix caseosa and contribute to understanding the importance of this unique biofilm.