DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

Comparative research of ionic liquid and standard matrices used in MALDI ionization mass spectrometry

Matrix-assisted laser desorption/ionization time of flight mass spectrometry (MALDI-TOF-MS) has previously been used to identify large biomolecules such as proteins, polymers, nucleic acids and peptides. Normally, standard matrices such as derivatives of benzoic, cinnamic acid or sinapic acids were used to research these compounds. Unfortunately, due to their crystallization on the plate, qualitative and quantitative analysis of low molecular weight compounds, especially pharmaceuticals, has been so far unreliable. The main reason was the large number of signals coming from the matrix ionization, what prevented the identification of test substances. The problem was also the uneven distribution of the compound on the surface of the crystals, which limited the repeatability of the measurements and prolonged time of analysis. Research published in 2001, which concerned the second generation of ionic liquids, also named ionic liquid matrices, has been revolutionary in this field.

Ionic Liquid Matrices (ILMs) are organic salts formed by a simple neutralization reaction. The substrates of this reaction are the crystalline standard MALDI matrix (e.g. α -cyano-4-hydroxy cinnamic acid) and organic base (e.g. diisopropylethylamine), which are taken in equimolar amounts during the synthesis. In 2001 ionic liquid matrixes have been used in the MALDI-MS technique for the first time, but despite of many benefits, they are not commonly used in the low molecular weight compounds analysis. This is mainly due to the lack of knowledge concerning their nature and potential possibilities of application.

Therefore, the **main scientific objective of the presented project is to compare the ionic liquid and standard matrices used in MALDI spectrometry**, which will consist of evaluating the application potential for quantitative and qualitative analysis of various groups of low molecular weight compounds. The main research hypothesis, assumes that **ionic liquid matrices, thanks to liquid character, ionic structure and superior to conventional materials homogeneity are characterized by a competitive ionic potential of low molecular weight analytes and does not generate a high background on MS spectra during MALDI-TOF analysis**. To prove this, the basic research is planned. It should be noted that preliminary studies have already been carried out and the positive results are the motivation for the further study of the nature of ionic liquid matrices and the development of their application potential in MALDI spectrometry.

The scheme of the research which has been planned under this project should lead to the selection of the most effective among the selected matrix for quantitative analysis of chosen groups of low molecular weight compounds. In addition, the analytical procedure of this research, assumes also the risk of discarding matrices which will not fulfil the criteria. The first step will be to investigate the ionic nature of liquid matrices by determining the relationship between viscosity and conductivity (Walden's plot). In the second step, the homogeneity of the obtained spot (matrix/analyte mixture) and the repeatability of the measurements will be checked. The third step is determining the ionization potential of selected group of low molecular compounds using the five ILMs chosen after preliminary research. In the next step, quantitative analysis using external and internal calibration (isotopically labelled internal standard by ²H or ¹³C atoms) will be performed by MALDI-MS, which will enable the comparison of the quality of the analysis using ILMs and standard matrices. The project will end the validation of final analysis of selected analytes. The method with the best results will allow the analysis of real samples (e.g. analysis of pharmaceuticals residues in the environment).

The successful completion of the project will allow to develop cheap, easy and what more competitive to commonly used chromatographic methods the analytical tool, which is MALDI-MS spectrometric technique. It is worth to mention that the use of this technique is part of the green chemistry and environmentally friendly because of low solvent consumption and low waste. The implementation of the project will make an important contribution to the development of science, in particular analytical and physical chemistry.