Modelling of nonselective analytical signals in course of quality monitoring

Quality of products depends on many parameters including their unique chemical composition. By definition, the global approach for the quality evaluation is necessary. It often requires more than controlling one or two parameters at once. Thus, the evaluated product is described by possibly reach in chemical information instrumental signal(s) (containing the inputs of several chemical components included in the product). The nonselective signals (e.g. chromatograms or spectra) are frequently used. They are considered as chemical fingerprints since the information they contain is unique. Nevertheless, the complex chemical composition of products leads to overlaps of particular signals relevant to different components. Isolation of significant information from such complex data facilitates the application of chemometric approaches. Considering their advantages the chemical fingerprints are used to evaluate quality of food products, in process analytical technology, and to monitor the environment.

The aim of the research was to extract the relevant information form the nonselective signals to develop novel analytical approaches for the quality evaluation. Approaches to evaluate the quality of sugar (in course of its color and ash content), diesel oil (in course of the level of the imposed excise duty) and food products as coffee, pepper mint, oregano, basil, tomato paste, and rooibos tea (in course of their total antioxidant capacity and total polyphenol content) are developed. The nonselective signals like excitation-emission fluorescence matrices, high performance liquid chromatograms detected by diode array detector (HPLC-DAD) and infrared spectra were registered for the products. They were efficiently modelled using selected chemometric methods. New chemical approaches have been developed and validated according to their chemometric and analytical parameters.

The application of nonselective signals in the developed approaches significantly reduces or fully eliminates the use of classic, laborious, time and money consuming, analytical methods. All of performed experiments were designed following the green chemistry approach i.e. to limit the amount of harmful chemical wastes. Thus, the nonselective signals were collected for raw samples (without any laboratory preparation) or using the distilled water as the only solvent.

Considering their high efficiency the developed approaches can be recommended for the routine laboratory or on-line quality evaluation. It should be emphasized, the presented results refer to the preliminary studies and the application should be preceded by the additional experiments (taking into account the various changes of chemical composition of samples).