Advanced approaches for imaging and characterization of complex samples using the advantages of selected spectroscopic, chromatographic and chemometric methods

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In PhD thesis, I have proposed and described several approaches to solving complex analytical problems by combining inexpensive, fast, and non-destructive analytical methods with modern machine learning approaches. Machine learning techniques, despite their great potential, are not popular enough in analytical laboratories and research groups. My research is concerned with the development of new non-invasive methods for the characterization of heterogeneous samples that are complex mixtures of diverse chemical compounds. I have used hyperspectral imaging techniques (NIR-HSI), selected spectroscopic techniques (NIR), and chromatographic method (TLC). Using the synergy of these techniques, as well as designing new chemometric strategies for the interpretation of instrumental data, I have developed novel approaches to facilitate the examination of chemically complex samples.

Research material considered in my experiments included meat samples, polymer wastes, and polymer feedstock material samples, as well as fountain pen ink samples. Such a wide range of diverse samples with different origin and characteristics allowed me to confirm not only the effectiveness but also the versatility of the proposed analytical strategies. Similar samples are regularly delivered to laboratories worldwide where they are subject to detailed analyses or quality control aimed at detecting batches of products not conforming to the manufacturer's or consumer's expectations.

My research work had two main objectives. The first one was to develop approaches for more efficient characterization of complex samples. The increase in efficiency includes a reduction of both the cost and time of measurement and analysis, as well as an expansion of the possibilities offered by widely available laboratory equipment when supported by the here-proposed modern methods of data processing and interpretation. The second objective was to address some of the drawbacks of the selected analytical methods and processes. Sample processing itself (e.g., dilution, purification, homogenization, sample exposure to analytical chemical reagents) is often a major source of laboratory error. Simplifying or eliminating the sample preparation step can increase efficiency increase of many laboratory methods. At the same time, sample processing itself supports the partial removal of information that can be crucial for material identification and analytical problem-solving. The proposed solutions reduce these problems and enable analytical chemists to make use of some of the instrumental data usually neglected during the analytical process, allowing for a more detailed characterization of laboratory samples.