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Analysis of complex mixtures by non-targeted approach using Fourier transform ion cyclotron resonance mass spectrometry

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Nowadays, the analysis of complex systems for different purposes is a great challenge. Two methodologies based on mass spectrometry may be used. The first one involves a targeted approach, which requires pretreatment steps including extraction, purification and separation (liquid or gas chromatography) before mass spectrometry measurement. This methodology is well suited for the quantization of targeted compounds but does not allow a global description of the sample to be achieved. Alternatively, the non-targeted methodology introduced few years ago may be used. Both approaches ensure to obtain complementary information. Non-targeted approach allows an exhaustive description of the complexity of the sample to be obtained, but it does not allow quantization. In contrast, non-targeted methodology ensures quantization but only on a restricted number of compounds. In contrast to the mass spectrometry targeted methods, the non-targeted approach systematically requires ultra-high resolution mass spectrometry, which allows the global composition of complex mixtures to be accurately detailed. More over, the ability of this instrument to be coupled with various ionization sources increases its capability to detect compounds with very different chemical properties and consequently to obtain an accurate description of the investigated sample. Considering the important analytical capacities of this approach, we will present two applications of this method. The first one in the field of environment chemistry for the analysis of particulate matter from different cigarette smokes which are some of the more important indoor pollutants and the second one in the field of the characterization of bio oils produced by pyrolysis of the biomass.

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Chemometric approach to optimize the operational parameters of ESI for the determination of contaminants of emerging concern in aqueous matrices by LC-IT-TOF-HRMSy

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Contaminants of emerging concern are organic compounds used in large quantities by the society for various purposes. They have shown biological activity at low concentrations and the difficulty to detect and quantify them in the environment stimulates the development of appropriate analytical methods. In this work, a chemometric approach to positive and negative ESI optimization for the simultaneous determination of contaminants of emerging concern in water samples by LC-IT-TOF-HRMS was applied. Three types of phase modifiers were used: formic acid, ammonium hydroxide and formic acid/ammonium formate. The effects of the operational parameters mobile phase modifier concentrations, mobile phase flow rate, heating block temperature and drying gas flow rate were evaluated by the 24−1 fractional factorial and Doehlert experimental designs. Factorial design indicated that ammonium hydroxide was more efficient compared to the other evaluated modifiers (higher ion intensities). Doehlert design allowed finding a region indicative of the optimum experimental conditions for most analytes. The best experimental condition observed was 3.5 mM ammonium hydroxide concentration; 0.0917 mL/min of mobile phase; 300 °C heating block temperature; and drying gas at 200 kPa. These optimized parameters resulted in decreased detection limits of the method. The optimized method was applied to the evaluation of water samples coming from the Rio Doce basin – Minas Gerais/Brazil utilizing principal component analysis and Kohonen neural network. In this way, the use of chemometric approaches showed to be a promising way to optimize the simultaneous determination of 21 contaminants of emerging concern in water by LC-IT-TOF-HRMS using ESI.

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