Man and wildlife are continuously exposed to relatively high amounts of toxic chemicals through nutrition, air, water, and even through the placenta during foetal life. The wide use of industrial and household chemicals has led to the increased public awareness on toxicity of these compounds. Moreover, several of them, notwithstanding their divergent chemical structure, have already been identified as endocrine disrupting chemicals (EDCs) [1].

During recent years several international studies were devoted to this topic, with a particular interest in estrogenic compounds in the environment. Research has shown that chronic exposure to these compounds may cause hormone related cancers, developmental abnormalities and a decreased sperm quality. Estrogenic compounds include natural substances like phytoestrogens and mycoestrogens and man-made chemicals like contraceptives, certain insecticides and herbicides, some PCBs, plasticisers and breakdown products of surfactants [2].

Besides environmental screening methods like immunoassays, an extensive amount of research is performed to develop new and improved methods for confirmation. To this end liquid chromatography coupled to mass spectrometry has been given a lot of attention. Liquid chromatography offers the advantages that a fairly simple sample preparation is sufficient and water-based samples can be easily handled. Mass spectrometry, on the other hand, is known for its selectivity and sensitivity. Although LC-triple quadrupole (QQQ) MS has been used in the majority of the applications, ion trap based mass analysers show great potential in routine analysis. Due to the ability to store and manipulate ions in time rather than space, they offer unique advantages over more traditional mass spectrometers in which ions pass through the instrument as a beam [3]. The biggest advantage is the capability to perform multi stage MS (MS^n), which is a powerful tool for structure elucidation and essential for selectivity in the analysis of complex environmental matrices. Furthermore, ion trap mass spectrometers show a full-scan sensitivity, clearly better than those of single quadrupoles. Finally, they are easy to use and to maintain.

This presentation examines the applicability of ion trap based mass spectrometers in environmental water analysis by means of a number of specific applications. The optimized analytical parameters, like eluent composition, flow, gradient programs, column types, and API interfaces will be discussed in detail for each method. Furthermore, appropriate sample preparation methods will be described. Finally, complete validation data for each analysis will be presented and examples of real-time water samples will be shown.

References

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