Performance of quadrupole-ion-trap mass spectrometry for the analysis of furan

Scholl G.[a], Scippo M.L.[b], Maghuin-Rogister G.[b], De Pauw E.[a], Eppe G.[a]
[a]CART, Mass Spectrometry Laboratory, Faculty of Sciences, University of Liège
[b]CART, Laboratory of food analysis, Faculty of Veterinary Medicine, University of Liège

The furan is a small organic molecule (MW=68) that can be found in food and feed, and classified as possibly carcinogenic to humans by the IARC (group 2B). Furan has been identified in a number of foods that undergo heat treatment such as canned and jarred foods. The pathways of formation are not yet well known and includes several mechanisms such as Maillard reaction, carbohydrate thermal decomposition, amine decarboxylation-reduction, …

Based on the literature currently available, gas chromatography connected to mass spectrometry is the method that fits with the necessary sensitivity and specificity (ppb level in food). According to physical properties of the furan, it allows an easy transfer in the gas phase. So gas phase extraction techniques like headspace or solid phase microextraction (SPME) are used. These extraction techniques can be hyphenated with GC/MS in an integrated analysis method using isotopic dilution technique for the quantitative aspect.

In the mass spectra of the furan, there's two ions of interest : the molecular ion (m/z = 68) and the main fragment ion ($C_3H_3^+$; m/z = 39). The chromatogram constructed with the signal of the molecular ion is use for quantification. And the one constructed with the signal of the main fragment ion is use to check the presence of interferences through the ion ratio measure.

To obtain the required sensitivity and specificity, quadrupole mass spectrometer in Selected Ion Monitoring scan mode (SIM) is used, but ion-trap can also achieve these requirements. For the analysis of so low masses ion-trap is commonly used in full-scan mode, but the high chemical noise and the number of interfering compounds limits the analytical performances. So, as we need better one, we turn to SIM mode that provides good results. But, in a way to achieve the maximum performance with an ion-trap, we develop a two step scanning mode : time resolute isolation-detection scan. In the first step, we isolate the ions of interest in the trap (like as MRM isolation step in an ion-trap) and in the second one, we eject and detect only these ions.

The obtained results, in term of chemical noise and peak intensity, with this scanning mode are better than with SIM. So it provides enough sensitivity and specificity to analyze furan.

As we develop an integrated analytical procedure for the analysis of furan, we optimize the SPME and headspace extraction conditions, with the developed detection mode, using a Central Composite Design experiment plan and compare their analytical performances.