APGC shown to boost food contaminant monitoring

By Joseph James Whitworth
21-Feb-2018 - Last updated on 21-Feb-2018 at 14:04 GMT

A technique for detection and quantification of contaminants in food samples of marine origin has been developed by IUPA researchers.

It uses a Waters Xevo TQ-S Triple Quadrupole Mass Spectrometer with atmospheric pressure gas chromatography (APGC).

Certain brominated flame retardants (BFRs), polyaromatic hydrocarbons (PAHs) and polychlorinated biphenyl (PCB) congeners have EU limits.

However, established presence in the food chain makes monitoring for them essential to ensure levels do not exceed the allowable concentration.

Dr Tania Portoles, of the Research Institute for Pesticides and Water (IUPA), University Jaume I in Spain, said BFRs reach the marine environment and are ingested by fish and shellfish.

"Since they are lipophilic substances, they cannot be excreted – they remain in the fats. Thus, we consume them when we eat a piece of tuna, for example. At high levels, they are toxic and can cause health problems including carcinogenesis, endocrine disruption and neurological problems."

Soft ionization

IUPA used a chemical ionization source, APGC, developed by Waters that results in a 'soft' ionization process. The organisation has 10 laboratories with 30 researchers.

Traditionally, determination of BFRs and other persistent organic pollutants used electron ionization (EI) as an ionization technique.

However, it can lead to fragmentation and the specific molecular ion is either not present or has a low intensity. This lack of specificity makes identification of compounds difficult and can reduce sensitivity.

IUPA found analysis of food samples by APGC improved selectivity when generating multiple reaction monitoring (MRM) transitions compared with the fragmentation experienced with EI source.

Soft ionization of APGC means reduced fragmentation for many compounds when compared with techniques such as EI. Reduced fragmentation can give higher sensitivity and specificity and simplify pre-cursor ion selection in MS/MS analyses.

Method development and validation

Dr Portolés used APGC to develop and test a method to increase the number of contaminants detected at lower concentrations in a variety of food samples.

With the Institute of Aquaculture Torre la Sal in Spain and the National Institute of Nutrition and Seafood Research (NIFES) in Norway, IUPA researchers used the Waters Xevo TQ-S with APGC for GC-MS/MS analysis of PAHs, PCBs and pesticides in 19 matrices – including fish tissues and feed ingredients.

The method used an Agilent gas chromatography system coupled to Waters' triple quadrupole tandem mass spectrometer with an atmospheric pressure chemical ionization source (GC-APCI-MS/MS).

It is based on a modification of the unbuffered QuEChERS method, using freezing as an additional clean-up step and applying a 20-fold dilution factor to the final extract.

Researchers found the ability to eliminate the matrix effect and remove time-consuming purification steps.

In addition to 24 PAHs, they tested for 15 pesticides and seven PCB congeners to widen method scope. The study was to determine trace levels (as low as 0.1 ng/L) of PAHs, PCBs, PBDEs and some emerging flame-retardants in 76 samples.

It allowed simultaneous quantification of 19 different matrices from aquaculture using solvent calibration.

The developed method was evaluated at 2, 5, and 50 ng g^-1 spiking levels. LOQs were 2 ng g^-1 for most analytes with LODs in the range of 0.5 to 2 ng g^-1.

Analysis of real-world samples revealed naphthalene, fluorene, phenanthrene, fluoranthene and pyrene at concentration levels ranging from 4.8 to 187 ng g^-1.

APGC alternative

Dr Portolés said APGC is an attractive alternative to EI (less fragmentation) and CI (more universal) and opens up new perspectives in quantitative analysis at trace levels and in universal wide-scope screening.

"With this interface, a soft and reproducible ionization is favored in GC, being the protonated molecule and/or the molecular ion the base peak of the spectrum in most cases. This notably facilitated the application of MS/MS methods (with triple quad or Q-Tof), and also the screening of contaminants with GC-MS focusing the search to the highly diagnostic molecular ion," she said.

"The versatility of the technique is high because you can have both GC and LC coupled to the same mass spectrometer. It is quite quick and easy to change from LC to GC and vice versa."

The APGC technique uses fewer solvents and materials compared to previously used methods and can determine compounds at a lower concentration.

This allows compliance with regulatory limits and the ability to inject less sample matrix, reducing effects of contamination on the GC-MS system and increasing uptime.

Source: Talanta Volume 172, 1 September 2017, Pages 109-119

"Multi-class determination of undesirables in aquaculture samples by gas chromatography/tandem mass spectrometry with atmospheric pressure chemical ionization: A novel approach for polycyclic aromatic hydrocarbons"

Authors: Portolés T, Garlito B, Nácher-Mestre J, Berntssen MHG, Pérez-Sánchez J.

RELATED TOPICS: WATERS, R&D, Meat, fish and poultry, Automation, Lab instruments and equipment