

**XV REUNIÓN CIENTÍFICA  
SOCIEDAD ESPAÑOLA DE CROMATOGRAFÍA  
Y TÉCNICAS AFINES · SECyTA 2015**

*XV SCIENTIFIC MEETING  
OF THE SPANISH SOCIETY OF CHROMATOGRAPHY  
AND RELATED TECHNIQUES · SECyTA2015*

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**POTENTIAL OF ATMOSPHERIC PRESSURE CHEMICAL IONIZATION SOURCE FOR THE QUANTIFICATION OF A WIDE RANGE OF HALOGENATED PERSISTENT POLLUTANTS IN COMPLEX SAMPLES**

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Gas chromatographs coupled to mass spectrometers (GC-MS) have been extensively applied for the determination of volatile and semi-volatile, non-polar, compounds in fields like food safety, environmental or toxicological studies. Most methods reported in the literature use electron ionization (EI) [1], which may result in extensive fragmentation of analytes compromising both, selectivity and sensitivity. This makes also difficult the application of tandem MS due to lack of specific/abundant precursor ions [2].

The analysis of persistent organic pollutants, including brominated flame retardants (BFRs), polychlorinated dibenzodioxins, polychlorinated dibenzofurans and dioxin-like polychlorinated biphenyls (dl-PCBs), relies on the use of methods based on GC-MS operating in EI or negative chemical ionization (NCI) modes using quadrupole, triple quadrupole, ion trap or magnetic sector analyzers [3]. These halogenated contaminants are examples of compounds for which a softer, reproducible and robust ionization technique might be favorable since they show high fragmentation in EI and low specificity in NCI [4]. In this work the potential of atmospheric pressure chemical ionization (APCI) combined with GC and triple quadrupole mass analyzer has been investigated, using BFRs, PCDD/PCDF and dl-PCBs as model compounds for their determination in different complex samples, including marine samples, milk, feed and animal fat and interlaboratory studies samples.

Ionization and fragmentation behavior of 14 PBDEs and 3 novel BFRs as well as 10 PCDD/PCDF and 7 dl-PCB congeners by APCI has been studied. The formation of highly abundant (quasi) molecular ions has been the main goal because of the expected improvement in specificity obtained when using it as precursor ion in tandem MS. The convenience of using modifiers for the ionization step has been studied and discussed for each family of compounds with the aim of obtaining the maximum sensitivity in combination of acceptable reproducibility and optimum specificity/selectivity. The improved detectability (LODs between 1 and 20 fg) achieved when using APCI compared to EI has been demonstrated. The application to different complex samples has shown the feasibility of the methods at trace levels for unambiguous identification and determination of the compounds investigated. These results highlight the potential of APCI as the reference for quantification of halogenated pollutants in the next years.

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