



**Gas Chromatography-Atmospheric Pressure Chemical
Ionization-Tandem Mass Spectrometry Methods
for the Determination of Environmental Contaminants**

av

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Abstract

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The recent developments and improvements of instrumental methods for the analyses of the environmental contaminants, especially the persistent organic pollutants (POPs), have made it possible to detect and quantify these at very low concentrations in environmental and biotic matrices.

The main objective of this thesis is to demonstrate the capability of the atmospheric pressure chemical ionization technique (APCI), using gas chromatography coupled to tandem mass spectrometry for the determination of a wide range of environmental contaminants, including the POPs regulated by Stockholm Convention, such as polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs), but also the derivatives of PBDEs and novel brominated flame retardants (NBFRs).

The APCI was operated in charge transfer condition, preferably producing molecular ions. Multiple reaction monitoring (MRM) experiments were optimized by adjusting cone voltage, collision energy and dwell time. Optimization of source parameters, such as gas flows and temperatures was also performed. Low concentration standards were analyzed, achieving a visible chromatographic peak for 2 fg 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) demonstrating the excellent sensitivity of the system. Adequate linearity and repeatability were observed for all the studied compounds. The performance of APCI methods was validated against the conventional methods using gas chromatography coupled to high resolution mass spectrometry for chlorinated compounds in a wide range of matrices including environmental, air, human and food matrices.

The GC-APCI-MS/MS method was successfully applied to a set of 75 human serum samples to study the circulating levels of POPs in epidemiologic studies. Moreover the method was utilized to establish temporal trends of POPs in osprey eggs samples collected during the past five decades.

Keywords: PCDD/Fs, PCBs, OCPs, PBDEs, NBFRs, APCI, MS/MS, HRMS, human serum, osprey egg.

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