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Abstract:

The development of suitable analytical methods to obtain metrologically traceable results in the determination of toxicants in food matrices is an important issue, as food represents the main way of assumption of many contaminants, among which the Polycyclic Aromatic Hydrocarbons (PAHs). The present work deals with the set up and internal validation of an analytical method carried out at INRiM for the quantification by gascromatography coupled with mass spectrometry (GC-MS) of some priority PAHs in green tea (*Camellia sinensis*) and yerba mate (*Ilex Paraguaiensis*), in order to obtain metrologically traceable results. Two approaches for the quantification were applied: an external calibration, for determining the GC-MS calibration curves by means of standard reference solutions and an internal calibration by using perdeuterated standards. For the external calibration, Weighted (WLS) and Weighted Total (WTLS) Least Squares fitting procedures were applied. The measurement uncertainty evaluation was carried out by applying the Law of Propagation of Uncertainty.

Keywords: metrological traceability, measurement uncertainty, polycyclic aromatic hydrocarbons, food, green tea, yerba mate

1. Introduction

1.1. Polycyclic Aromatic Hydrocarbons (PAHs)

Polycyclic Aromatic Hydrocarbons (PAHs) are organic micropollutants having an aromatic planar structure. They are present in all the environmental compartments and in food. PAHs are formed from incomplete combustion of organic substances, generated by anthropogenic sources (vehicular and industrial emissions, domestic heating, power plants, food cooking, tobacco) or natural sources to a less extent (bushfires, agricultural combustion, volcanic eruptions) [1] The formation mechanism of PAHs has not been completely clarified but the more accredited hypothesis is based on three formation steps: pyrolisis, pyrosynthesis and, finally, polymerisation.

PAHs are characterised by high stability and low reactivity, and for this reason they can be detected even at great distance from the emission sources. Their vapour pressure is generally low and reduces with increasing molecular weight. This trend influences the different percentages of PAHs distributed in the gaseous phase in atmosphere and adsorbed on soils, particulate matter and vegetation. PAHs having from 2 to 4 aromatic rings tend to stay in the gaseous form and have short half-life. PAHs with 5 or more benzene rings, which are the compounds with greater toxicological interest, do not persist for long periods in the atmosphere as gaseous molecules [2].

There is great concern for PAHs, due to their fallouts on human health. Scientific evidence showed that some PAHs may have carcinogenic effects. The most harmful of them is benzo[a]pyrene (BaP), which was classified as carcinogenic agent to humans (Group 1) by the International Agency for Research on Cancer (IARC) [3] and assumed as the marker molecule for the carcinogenic risk of the entire PAH class. Other PAHs are classified as non carcinogenic (group 3), possible carcinogenic (group 2B) or probable carcinogenic (group 2A).

The mutagenic and carcinogenic actions are due to the formation of PAHs derivatives by means of metabolic reactions occurring in the living organisms, meant to facilitate the expulsion of these compounds. The PAHs toxicity will depend on the balance between the metabolite formation rate and the rate of its removal. These metabolites, generally diol epoxides, can bind to the DNA chains, damaging their structures and thus leading to mutations and eventually to carcinogenesis [4].

The more validated hypothesis relates the PAHs reactivity to the number and relative position of the condensed rings. Experimental observations proved that a necessary condition for the PAH carcinogenic action to occur, is the presence in the structure of more than 4 benzene condensed rings. Indeed, the condensation reduces the aromatic properties facilitating the metabolic reactions and the consequent formation of carcinogenic metabolites. The presence of the so called “bay region”,