

TD-GC×GC-LRTOFMS/FID AND TD-GC×GC-HRTOFMS FOR THE ANALYSIS OF VAPOUR PHASE OF CIGARETTE SMOKE AND TOBACCO HEATING PRODUCT AEROSOL

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There is an ongoing interest in the development of novel tobacco products for the purpose of tobacco harm reduction. Recently, new generations of tobacco heating (heat-not-burn) products (THPs) were introduced [1]. Such products can vary significantly from tobacco cigarettes and a full characterization of its total aerosol chemical composition is needed for toxicological assessment. In this context, we have developed an analytical method based on thermal desorption and comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry and flame ionisation detection (TD-GC×GC-TOFMS/FID). The splitting of the flow between the detectors was achieved using a controlled flow splitter (CFT) with different lengths and diameters of capillary column to reach a 1:1 split ratio between FID and TOFMS. A simple sample collection, extraction and introduction method was developed based on thermal desorption. The TD-GC×GC approach was further transferred to high-resolution time-of-flight mass spectrometry (HRTOFMS) to enhance the identification of compounds of interest. In this work we will discuss the benefits and challenges associated with sample introduction, optimisation of TD-GC×GC-LRTOFMS/FID and its alignment with TD-GC×GC-HRTOFMS instrument. The enhanced confidence in peak assignment using linear retention indices, mass spectral matches against library (from LRTOFMS and HRTOFMS) and accurate mass values will be highlighted. Finally, the qualitative and semi-quantitative comparison of vapour fraction of selected THP aerosol vs 3R4F reference cigarette smoke, based on their chemical classes, will be discussed. The results confirm the superior capability of the developed methods in analysing complex aerosol mixtures generated from the different tobacco products and highlight the relative simplicity of the THP aerosols in comparison to mainstream cigarette smoke.

[1] M.R. Smith, et.al., *Regulatory Toxicol. and Pharmacol.*, **81** (2016) S17-S26.