Method Development for the Characterization and Differentiation of Ky3R4F Cigarettes and Tobacco Heating Products Using TD-GC×GC-TOFMS/FID

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Tobacco smoke is generated at a wide range of temperatures, up to 900 °C, yielding a complex aerosol which contains thousands of compounds of different chemical classes and at very different concentrations [1]. The characterization of such a complex mixture has been widely documented in the literature but, generally, analyses have focused on some target compounds of toxicological interests which constituted only a small portion of the entire aerosol. Non-targeted approaches using comprehensive two-dimensional gas chromatography (GC×GC) have become a widely used analytical strategy to deal with the characterization of complex mixtures like tobacco smoke [1]. One of the limitations when collecting this type of sample is to obtain a representative fraction which preserves the integrity of the original test matrix and, hence, can be used for true quantification. In this study, the use of thermal desorption (TD) sorbent tubes for the sampling of aerosol from Ky3R4F reference cigarettes was optimized to avoid loss of chromatographic resolution and overloading of the signal due to highly concentrated compounds. In that sense, the possibility of directly coupling TD to GC×GC with dual detection based on Time-of-Flight Mass Spectrometry analyzer (TOFMS) and Flame Ionization Detector (FID) was investigated. Reliable characterization of mainstream smoke was achieved by simultaneous TOFMS identification and FID quantification. The developed method was also applied to a recently launched Tobacco Heating Product (THP), which heats the consumable instead of burning [2], and the obtained TD-GC×GC-TOFMS/FID data was used to highlight the statistically significant differences between the two types of products applying supervised and unsupervised data analysis.

[1] Brokl *et. al.* , J. Chromatogr. A, 1370 (2014) 216–229.
[2] Schaller *et. al.*, Regul. Toxicol. Pharmacol., 81 (2016) S27-S47.