Investigation of Mainstream Tobacco Smoke Particulate Phase by HS-SPME-GC×GC-HRTOFMS

Radoslaw Lizak;[1] Liz Humston-Fulmer;[2] Joe Binkley;[2] Michal Brokl;[3] Christopher G. Wright;[3] Jean-François Focant.[1]

[1] Organic and Biological Analytical Chemistry Group, CART, University of Liège, Belgium
[2] LECO Separation Sciences, St. Joseph MI, USA
[3] Group Research and Development, British American Tobacco, Southampton, UK

Abstract

Recently, a method involving headspace solid-phase microextraction (HS-SPME) and comprehensive two-dimensional gas chromatography (GC×GC) coupled to time-of-flight mass spectrometry (TOFMS) was developed and applied to evaluate profiles of volatile compounds present in mainstream tobacco smoke particulate matter trapped on glass fiber filters.[1] Two cigarette types differing in a filter design were analyzed using optimized conditions. Principal component analysis (PCA) allowed a clear differentiation of the studied cigarette types. Fisher ratio analysis allowed identification of compounds responsible for the chemical differences between the cigarette samples.

In this study, in the quest of improving confidence in compound identification, we expended the procedure to high resolution TOFMS in order to add an extra dimension to the sets of data that are produced by means of accurate mass measurement. All details about sample preparation are available in the previous report.[1]For this study, we replicated the analyses of the 3R4F research reference cigarette over two different smoking regimes.

HS-SPME-GC×GC-HRTOFMS data files were acquired at 100Hz. Peak tables were run versus low resolution mass spectral libraries and accurate masse measurement permitted to further characterize analytes while preserving chromatogram integrity and keeping data file sizes below 0.5 Gb. Mass accuracies for middle range (100-200 uma) analytes were between 0.1 and 1ppm with good reproducibility between modulated slices. The added value of mass accuracies allows to further investigate unknown compounds that were highlighted as compounds of significance in our previous study.

References

1. M. Brokl, L. Bishop, C. G. Wright, C. Liu, K. McAdam, J.-F. Focant. Multivariate analysis of mainstream tobacco smoke particulate phase by headspace solid-phase micro extraction coupled with comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry. J. Chromatogr. A. 2014, 1370, 216-229.