GCXGC-TOFMS FOR VOC ANALYSES: FORENSIC AND MEDICAL APPLICATIONS

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Introduction

Amongst the various fields of application of GCxGC-TOFMS, the analysis of biological samples for target or screening purposes represents quite a growing area of interest. Both signal and peak capacity enhancement properties of the technique are challenged through strategies ranging from, for example, low pg target analyses of selected persistent organic pollutants (POPs) in human matrices to characterization of variations in complex metabolite fingerprint as a result of the progression of a disease. The analysis of volatile organic compounds (VOCs) released from various biological sources is also a challenging area of research. A few examples include the study of VOC mixtures released from decaying bodies, human breath, etc... For each of those, the idea is obviously to gather more information from what can usually be expected using classical GC-MS analyses. Although GCxGC-TOFMS can easily produce better resolved chromatograms and complementary deconvoluted mass spectral signals, the complexity of the generated data sets makes its proper use relatively complex.

Results and Discussion

First, the gain in 'what you can see' is potentially challenged by the fact that 'what you now see' is potentially originating from levels where the surrounding environment of the target samples plays an important role in the composition of the mixture. Generally, taking the 'blank' contribution into account is thus the first step to go over and renders peak alignments and mass spectral comparison extremely important, even before real sample-to-sample comparison. Statistical consideration of the individual-to-individual variation is also a major challenge that precedes dedicated data mining and proper peak assignment in target samples. Ultimately, from this exhaustive data processing exercise, you can potentially contribute to better characterize specific product markers, improve post mortem interval (PMI) estimation, correlate the presence of certain VOCs with various diseases, etc… (Figure 1) but such comprehensive VOC analyses remain analytically challenging.

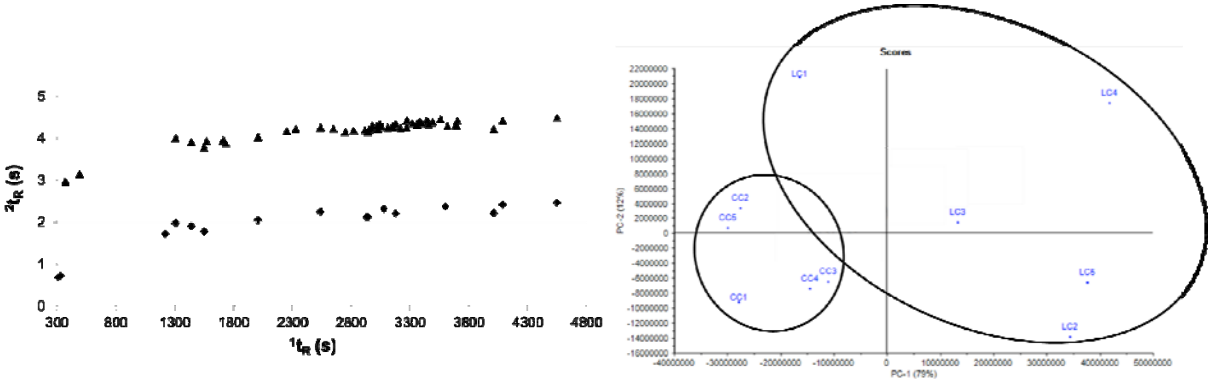

Fig. 1: Left: Searching for graves: Apex plot for gravesoil (triangles, n = 47 hits) and control soils (diamonds, n = 16 hits) after running an alkane-specific VB script for discrimination. Gravesoil ^2t_R have been shifted of 2 s for clarity. (C Brasseur *et al.*, J Chromatogr A, doi:10.1016/j.chroma.2012.03.048)
Right: Diagnostic potential: PCA plot showing the difference between breath VOC mixtures of lung cancer patient versus controls. (PH Stefanuto, F Schleich, R Louis, JF Focant, under progress investigation)