

Profiling the smell of death by TD-GCxGC-ToFMS

Stefanuto P.-H.¹, Stadler S.², Forbes S.², Focant J.-F.¹

¹ CART, Organic and Biological Analytical Chemistry, Department of Chemistry, University of Liège, Allée du 6 août B6c, 4000 Liège, Belgium. (phstefanuto@ulg.ac.be)

² Decomposition Chemistry Research Group University of Ontario Institute of Technology, 2000 Simcoe St. North, L1H 7K4 Oshawa Ontario, Canada.

The study of the 'smell of death' is an important part of thanatochemistry, the chemistry of death. Since 2004¹, an increasing number of studies are conducted to understand the body decomposition process by mean of the measurement of the Volatile Organic Compounds (VOCs) released by decaying bodies. However, the chemical profile of the decomposition odor is still far to be resolved. Indeed, the complexity of the VOC mixture makes it difficult to be carried out by classical GC-MS. Better understanding of the decomposition process could thus possibly be achieved using a multidimensional technique such as GCxGC-ToFMS.

In this study, we developed an analytical strategy based on direct sampling of cadaveric VOCs with a pumping device and sorbent tubes, followed by Thermal Desorption (TD) coupled to GCxGC-ToFMS.

Cadaveric specimen consisted of two domestic pigs (*Sus scrofa domesticus* L.) (25 kg) used to surrogate human models. Each pig had its own blank reference sample. They were let to decompose during 40 days. VOCs were collected at key dates of the decomposition process by trapping on Tenax-Carbopack® multisorbent tubes. All the tubes were desorbed in the GCxGC-ToFMS system by using the Markes Unity2® TD. This system allows split/trap cycles on other tubes for duplicate analysis (e.g. GC-MS and GCxGC-ToFMS analyses were compared).

The major challenge, for the analysis of such complex samples, is the optimization of the data processing. The first step was the data alignment and filtration to suppress the biota blank, possible column bleed, etc... based on t_{R_s} and mass spectral data. Multivariate analyses were used to extract potentially important biomarkers from the cleaned-up data set. The list of biomarkers included previously reported analytes but also new analytes that could potentially improve Post-Mortem Interval (PMI) determination². Additionally, these biomarkers were found to have time-dependent levels that could be paralleled to the various stages of the decomposition process. Moreover, VOC profiles of both pigs were compared to estimate the possible impact of corpse-to-corpse variability on the entire process.

¹ Vass, A. A. *et al.*, Decompositional odor analysis database. *Journal of forensic sciences* **49** (4), 760-9 (2004).

² Vass, A. A., The elusive universal post-mortem interval formula. *Forensic science international* **204** (1-3), 34-40 (2011).