Transfer of heroin profiling method from conventional GC-MS to Fast-GC-MS and UHPLC-MS/MS.

Benjamin Debrus (1), Julian Broséus (2), Davy Guillarme (3), Philippe Hubert (1), Jean-Luc Veuthey (3), Pierre Esseiva (2), Serge Rudaz (3)

1) Laboratory of Analytical Chemistry, University of Liège, Belgium.
2) Institut de Police Scientifique, School of Criminal Sciences, University of Lausanne, Switzerland.
3) School of Pharmaceutical Sciences, University of Genève, Switzerland.

Introduction: Classical databases used to profile heroin samples are actually feeded with GC-MS data. Despite its ability to obtain suitable results for the classification of heroin samples and the establishment of chemical similarity [1], this chromatographic technique could be time-consuming and not available in all laboratories.

Aim: The aims of the study were, firstly, to optimize the separation and detection of the relevant components for classification of heroin samples. Secondly, to shorten the GC-MS analysis time thanks to geometrical transfer (Fast-GC). Thirdly, to use alternative fast chromatographic techniques, such as UHPLC, for the analysis of heroin samples after optimisation with dedicated modelisation software. In this work, a particular attention was paid to the development of generic chemometric strategies to convert data afforded by any other analytical technique to compare with the results obtained with the classical GC-MS.

Method: The selected variables are the normalized area of specific fragments of six alkaloids co-extracted from opium with heroin. These alkaloids are meconin, acetylcodeine, acetylthebaol, 6-monoacetylmorphine, papaverin and noscapin. Linear and non-linear transformation methods were evaluated for comparison purpose.

Results: Using geometrical transfer rules and chemometric strategies, the original GC-MS method of 30 min was shortened to less than 5 min in fast-GC-MS. While correlation between the variables coming from Fast-GC and GC was around 98%, a conversion factor was mandatory to implement the original database with Fast-GC-MS values. Concerning UHPLC, electrospray ionisation was found to be adapted for the detection of the above mentioned compounds in less than 4 min. and can also be provide results which can be added to the original database after data correction.

Conclusions: Using those strategies, analysis times were reduced down to 5 min and the time devoted to derivatization (mandatory for GC-MS and Fast-GC) could be avoided with the help of liquid based separation techniques. The time needed to establish the chemical similarity between heroin samples is now shorter and give the opportunity to the forensic scientist to play a deeper role with the investigators.

References:
[1] Guéniat O. and Esseiva P., Heroin and cocain profiling, 1st Edition, 2005, Lausanne.