

ABSTRACT

Heroin profiling has been undertaken to derive forensic intelligence from the seized samples and make predictions as per the criminal activities. Six major tasks were performed to collect the relevant data from 311 heroin case samples submitted in 2010. Ten visual and physical characteristics were first collected from the case samples in Task 1. Subsequently in Task 2, five types of plastic films were successfully distinguished by attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) from the plastic packages used to contain the drug substances. This technique is rapid, robust and able to show repeatable (RSD < 2%) and reproducible (RSD < 3%) quantitative results when data normalization is used to minimize the variations arising from the poor optical contact and other uncontrolled factors. In Task 3, all the samples were analyzed by gas chromatography-mass spectrometry (GC-MS) and gas chromatography-flame ionization detection (GC-FID) to determine the levels of eight major compounds. Prior to analysis, the methods were also optimized and validated using chemical standards. The GC-FID method proved to be rapid (< 12 min), simple, precise (RSD < 5%), accurate (recoveries 99 – 102%) and robust for high throughput analysis. On the other hand, the GC-MS method is also found suitable for the profiling purpose. Furthermore, 8 links of simulated samples were analyzed following the procedures adopted by the case samples. This simulated dataset has successfully achieved eleven $\text{Normalization}_{\text{selected}} + \text{Standardization} (\text{N}_{\text{selected}} + \text{S})$ quotients for origin level sample classification where the clustering of case samples using principal component analysis (PCA) and hierarchical cluster analysis (HCA) operating with Ward-Manhattan is concerned. With the opium-based alkaloids, a novel tetrahedron model has also been developed to simplify the chemometric procedure involved in sample classification. Based on the purity level determined from the

previous task, the samples were analyzed using a sample weight equivalent to 15 mg heroin base or a 650 mg constant sample weight in Task 4 for impurity profiling. This was done after 12 impurity peaks were identified and a GC-FID method was optimized and validated. The method was also demonstrated to be rapid (< 35 min), precise (RSD $< 10\%$) and stable. Both of the sample weight approaches were statistically validated using samples of known relationships. Normalization + Standardization (N + S) was found to be the best pretreatment method and it performed particularly well in HCA operating with the Ward-Squared Euclidean and Ward-Squared Pearson. This technique was then applied to the case samples to evaluate the sample-to-sample relationships at the manufacturing level. Task 5 was carried out by quantifying trace elements. A method using inductively coupled plasma-mass spectrometry (ICP-MS) was validated using chemical standards and it proved stable for analysis. Highly variable ICP-MS data were often obtained but the intra-batch variation can be minimized via the Normalization + Fourth root (N + 4R) pretreatment method. This was verified by six batches of related samples using Ward-Squared Euclidean through HCA. Furthermore, various sources of metal contamination were also evaluated. The investigation showed that trace metals could only be used for street level sample classification. All the physical and chemical data were finally updated on a database in Task 6.