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The analytical and chemometric procedures used to profile illicit drug seizures

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Abstract

Over the last 20 years there has been an increasing interest in the development of robust systems, both analytical and statistical, to enable the linkage of seizures of illicit drug to each other. Much of this work has concentrated on the analysis of synthetic drugs, such as amphetamine and its analogues. In recent years, the analysis of both organic and elemental impurities as well as isotope ratios has advanced the usefulness of the techniques available. The application of specific chemometric methods to the derived analytical data has begun to provide the possibility of robust methods by which the resultant information can be interrogated.

Keywords: Forensic analysis; Chemometrics; Drug analysis

1. Introduction

Conventional chemical profiling methods are based on determining and quantifying the illicit substance and identifying the organic impurities present. In the case of synthetic drugs, certain impurities may be route specific. Impurities are likely to be present in illicit seizures as a result of poor chemical handling during synthesis, side reactions of the intermediates formed, inadequate purification procedures and contamination, either in the reagents, the adulterants and diluents added in the reaction vessels or due to packaging and handling of the final tablets. Gas chromatography–mass spectroscopy (GC–MS) is routinely employed in organic profiling procedures, principally due to reliability, efficiency and definitive identification possible from the corresponding mass spectrum.

Organic impurity profiles can be used to assess variation within and between seizures, ultimately aiming to identify links between seizures which have originated from the same laboratory and possibly even from the same batch of illicit substance. Since illegally synthesised drugs may eventually be distributed in more than one country, the need for a universal method to establish links between seizures is apparent. Recent work has focused on the development of computer-based programs to improve the accumulation and appropriate accessibility of drug intelligence data. The potential of inorganic impurities to enhance current organic impurity profiling procedures is also under investigation.

Conventional physical and chemical profiling of illicit drugs aims to establish links among seizures, in order to:

1. identify dealer–user networks;
2. determine the geographical origin of the seizure;
3. monitor the length of time the clandestine laboratory has been in operation;
4. gather sufficient information to create national and international drug databases;
5. monitor the extent of international drug trafficking.

Early attempts to link illicitly produced tablets were based on physical descriptions. In 1976, Gomm et al. [1] compared amphetamine and LSD tablets based on the dimensions of the tablets and a microscopic examination of the surface. Today, conventional profiling of illicit drugs relies on a combination of physical, chemical and statistical techniques to establish links among seizures originating from a common source.

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2. Organic impurity profiling

In the case of synthetic drugs, links between seizures originating from a common batch of illicit substance may also be identified based on the presence or absence of specific organic impurities. The impurities may be present in the precursors or formed during the synthetic process. Impurities present in adulterants and diluents are also introduced during tablet preparation. Chromatographic techniques, such as HPLC [2], GC–FID [3] or GC–MS [4] are typically used to generate organic impurity profiles even though these (apart from HPLC) are destructive techniques and will result in loss of the sample. Extensive research into profiling amphetamine seizures is detailed in the literature, with the majority of studies concentrating on amphetamine synthesised by the Leuckart route, since this is the most commonly employed route in Europe [5]. A comprehensive review of mass spectral data for organic impurities in amphetamine and methamphetamine synthesised by the Leuckart route, among others, was published by Verweij [5].

The principle chemical precursors for the synthesis of 3,4-methylenedioxymethylamphetamine (3,4-MDMA) are isosafrole, safrole, piperonal and 3,4-MDP-2-P [6], all of which are controlled within the European Union. Despite this, there has been a significant increase in the production of 3,4-MDMA, which may be attributed to an increase in chemical and technical knowledge and the ease of obtaining synthetic recipes via the internet [6]. In initial studies, 3,4-MDMA was synthesised 'in-house' by researchers using various different synthetic routes, including the Leuckart [7,8], bromopropane [7] and reductive amination routes [4,7]. Although GC–FID [3], GC–MS [4,7] and HPLC [2,9] were the most common techniques employed in the analysis of the organic impurities, Renton et al. [8] also reported the use of ^{1}H and ^{13}C NMR spectrometries and UV and IR spectroscopies. Route specific organic impurities have been identified, for example, the imine, 1,2-(methylenedioxy)-4-(2-*N*-methyliminopropyl)benzene, in the reductive amination preparation [4] and 3,4-MDP-2-BP in the bromopropane method. However, it is often difficult to determine the route of synthesis based on the organic impurities present, since the same precursors, and hence the impurities associated, are common to a number of different routes.

Gimeno et al. [6] presented a comprehensive study of mass spectral data of impurities present in samples containing 3,4-MDMA. The impurities were extracted from an alkaline solution into diethyl ether. Eight samples of 3,4-MDMA were analysed and mass spectra of all the impurities were obtained. The potential origin of various impurities was also discussed. For example, 1,3-benzodioxole and 3,4-methylenedioxytoluene were impurities identified in the samples, which are also present in safrole while 3,4-methylenedioxy-2-propanol in the samples was a product of the reduction of 3,4-MDP-2-P.

Research by Bohn et al. [10] isolated and identified twelve impurities in illicitly synthesised samples of 3,4-MDA and 3,4-MDMA. Impurities were isolated by preparative TLC and identified by ^{1}H NMR and mass spectrometries. Potential 'synthesis markers' were identified and it was concluded that the detection of such markers in illicit seizures could identify the synthetic route employed.

Chiarotti and Fucci [11] addressed the use of HPLC, GC, GC–MS and capillary electrophoresis (CE) for the analysis and comparison of heroin and cocaine seizures. An early study by Huizer [12] reported a method for the comparison of heroin samples using HPLC. Samples originating in the Middle East were characterised by relatively high levels of noscapine and papaverine, which were determined using UV detection. Further discrimination of the samples was possible based on the level of acetylthebaol present, which was determined by fluorimetric detection.

3. Isotopic analysis

The abundance of isotopes of elements, such as C and N, may differ due to environmental effects and has been exploited in classifying heroin [13,14] and cocaine [14,15] seizures according to geographical origin. Although 3,4-MDMA is a synthetic drug, safrole, which is used as a precursor, is a natural product. Variation in the $^{13}C/^{12}C$ and $^{15}N/^{14}N$ isotope ratios in seizures containing 3,4-MDMA may be expected due to the use of safrole either as a precursor in the bromopropane synthesis or as a pre-precursor for the synthesis of 3,4-MDP-2-P. In a study by Mas et al. [16], determination of the $^{13}C/^{12}C$ isotope ratio was used to identify common-batch members in seized samples of 3,4-MDMA. The carbon enrichment was calculated and expressed in the δ notation, following equation.

$$\delta^{13}C = \frac{10^{-3}[(^{13}C/^{12}C)_{SAMPLE} - (^{13}C/^{12}C)_{STANDARD}]}{(^{13}C/^{12}C)_{STANDARD}}$$

where $\delta^{13}C$ represents the carbon enrichment in permilles.

Six tablets were classified into four groups based on variation in the $\delta^{13}C$ values. The $\delta^{15}N$ values were also calculated following the above equation but replacing the $^{13}C/^{12}C$ isotope ratio with the $^{15}N/^{14}N$ isotope ratios. Further discrimination among seizures was possible, and it was concluded that tablets could still originate from different batches despite having comparable $\delta^{13}C$ values.

An intensive study by Carter et al. [17] applied GC–MS, GC–IRMS and elemental analysis–isotope ratio mass spectrometry (EA–IRMS) to characterise 50 illicit Ecstasy tablets. An 'isotopic fingerprint' of the illicit substance was generated for each tablet. Variation in the $\delta^{15}N$ value was used to link tablets to common batches and also to assess variation between seizures. Variation in the $\delta^{2}H$ and $\delta^{13}C$ values was less pronounced between tablets but provided further evidence to characterise the batches. Further work was reported to be in progress to investigate the route of synthesis for 3,4-MDMA based on the position of the ^{2}H substitution.

Desage et al. [18] applied GC–MS and GC with isotope ratio mass spectrometry (GC–IRMS) to classify heroin samples according to geographical origin. The samples, which originated from Turkey, Thailand, India, Pakistan and Nigeria, were differentiated based on the relative retention time and peak area of organic impurities and the corresponding mass spectral data. The mean ^{13}C enrichment, determined using GC–IRMS, was also found to vary according to geographical origin.

4. Raman spectroscopy

Bell et al. [19] concentrated on the analysis of Ecstasy and related β-phenethylamines, including 3,4 methylenedioxyamphetamine (3,4-MDA); 3,4 methylenedioxyethylamphetamine (3,4-MDEA); *N*-methyl-1-(1,3-benzodioxol-5-yl)-2-butylamine (MBDB) and amphetamine sulphate, using Raman spectroscopy with far-red excitation (783 nm). It was possible to differentiate the spectra of the illicit substances based on differences in the position of vibrational bands, even in the presence of adulterants and diluents. Semi-quantitative analysis was possible based on the relative intensity of the band. In addition, the spectra could distinguish different hydrated forms of the illicit substance, which could be used to link seizures to a common batch. In a later study, Bell et al. [20] applied Raman spectroscopy to profile the composition of illicit Ecstasy tablets. A sample population of 400 tablets was selected from a seizure, which contained more than 50,000 tablets in eight different bags. Despite significant variation within each bag, the contents of each were classified based on the diluent present. It was possible to differentiate samples, which contained the same diluent according to the degree of hydration of the illicit substance and the ratio of illicit substance to diluent. The study concluded that a physical description of seizures and quantification of the illicit substance were not sufficient for definitive characterisation due to significant variation observed within each sample population. The detailed Raman spectra obtained conveyed this variation and the rapid analysis time coupled with non-destructive sampling was an obvious advantage in large samples where high throughput is desirable.

5. Other spectroscopic techniques

Conventional analytical techniques used for chemical profiling purposes destroy at least a portion of the sample. Sondermann and Kovar [21] synthesised 3,4-MDMA and 3,4-MDEA and simulated illicit preparations by mixing the illicit substance with a variety of diluents, including magnesium stearate, lactose, sorbitol and starch. Near infrared (NIR) spectroscopy was employed to analyse the preparations and it was possible to identify the illicit substance in each preparation. The analysis was rapid and simple, with the advantage of being non-destructive.

6. Elemental analysis

Recent inorganic impurity profiling studies in illicit drug seizures have employed electrothermal atomic absorption spectrometry (ET–AAS), which is sufficiently sensitive although is mainly limited to single element determination. Infante et al. [22] identified Cd, Ca, Cu, Fe, Mn and Zn in 198 illicit heroin seizures and investigated correlation between these elements. The presence of calcium in 93% of the seizures was attributed to adulterants, such as calcium bicarbonate, while Fe was a component in the metal containers used to extract morphine from the opium poppy. Of the elements studied, Cd, Zn, Cu and Fe were identified as metals, which could increase the toxicity of the illicit substance.

Barmejo-Barrera et al. [23] optimised methods for the determination of Pb in heroin and cocaine samples. In the presence of $Pd(NO_3)_2$ as a chemical modifier, the analyte was stable at pyrolysis temperatures up to 1000 °C. The limit of detection was 31.4 μg Pb kg^{-1} and the characteristic mass of Pb was 24.4 pg kg^{-1}. Analytical recoveries were between 98 and 105% in the concentration range 2.5–40 μg Pb L^{-1}.

In a separate study, the same authors reported an optimised method for the detection of trace levels of Cr in cocaine and heroin samples [24]. The sensitivity, precision, accuracy and detection limits afforded by two different chemical modifiers, $Mg(NO_3)_2$ and HNO_3, were compared and the advantage of including a cooling step prior to atomisation was again considered. The method was also applied for the determination of Ag and Mn in heroin and cocaine seizures in a later study [25].

Flame atomic absorption spectrometry (FAAS), flame atomic emission spectrometry (FAES) and ET–AAS, were applied for the quantification of 15 metals in 46 cocaine seizures [26]. Due to the range in concentration of each metal determined in the seizures, the metal concentrations were normalised. In this procedure, the mean of the variable in all samples is subtracted from the variable in each sample and divided by the standard deviation of the variable in all samples. It was possible to classify the seizures according to geographical origin using principle component analysis (PCA), cluster analysis (CA) and linear discriminant analysis (LDA).

Few reports of trace metal profiling in other drug seizures are available in the literature. Methamphetamine is a major drug of abuse in Japan and is mainly synthesised by an ephedrine reduction reaction. Relatively few organic impurities are produced in this synthesis, creating difficulties for conventional organic impurity profiling methods. Suzuki et al. [27] applied inductively coupled plasma–mass spectrometry (ICP–MS) and ion chromatography (IC) to identify and quantify metals present in methamphetamine samples synthesised by this route. Solutions of methamphetamine crystals were analysed and Na, Pd, Ba, I and Br were identified as the major elements. Samples were taken from different positions of the same crystal and higher concentrations of each element were determined on the surface of the crystal

compared to within the crystal. Bromine and chlorine anions were detected at significant concentrations in all samples using IC. No statistical analysis of the experimental data was reported. A recent review [28] of the analytical techniques used for comparative studies of heroin and cocaine seizures stated that the application of AAS for the determination of trace metals in the seizures was limited due to problems in evaluating the results.

Marumo et al. [29] identified inorganic impurities present in methamphetamine samples using a combination of ICP–MS, FAAS and ET–AAS. Seventeen of the seized samples were classified into five groups based on the concentrations of Na and Ba present. Wells et al. [30] analysed 96 separate heroin seizures for 35 elements by ICP–MS. The results were statistically treated to illustrate similarities and differences among the seizures. There was similar correlation in the elements present in seizures known to originate from the same geographical region. More robust statistical analysis was applied in a study by Myors et al. [31] to classify heroin samples of known origin. A total of 73 elements were quantified using ICP–MS and hierarchical cluster analysis, K-means cluster analysis and PCA were used for classification. The study required the analysis of more samples of known origin in order to impart more significance to the classification obtained. In both studies, ICP–MS was shown to be a reliable and sensitive method for the determination of trace elements in illicit heroin seizures. Rapid and simultaneous multi-element analysis was possible although the technique is limited by expensive instrumentation and high maintenance costs.

Comment et al. [32] analysed two different Ecstasy seizures by ICP–MS and ICP–atomic emission spectrometry (ICP–AES). They reported that heating solutions of the tablets in nitric acid in a microwave oven was a more effective method of sample preparation than vortexing and sonicating the solutions. ICP–MS was shown to be more sensitive than ICP–AES for all the elements studied and was used to generate inorganic impurity profiles for a number of Ecstasy seizures. Elements, such as Si, K and Fe, were determined in both the seizures and also in samples, which contained no illicit substance. These elements are abundant in the environment and will prove of little use in profiling illicit seizures. It was possible to establish preliminary links among case samples, based on the inorganic impurity profile although further information, such as a physical description of the seizures and the organic impurity profiles, was essential to confirm the linkage.

7. Chemometric methods for the classification of synthetic drug seizures

Illegally synthesised drug are likely to be distributed in more than one country, and thus the need for a universal method to establish links between seizures originating from a common source is apparent. Computer methods [33–36] for the comparison of impurity profiles have improved visual classifications of seizures and are a significant step towards creating an international database [32,37] of reference data, which could ultimately be used to monitor the extent of drug trafficking. The method and types of statistical and chemometric techniques commonly applied to drug profiling include specifically the use of PCA, HCA, LDA and more recently artificial neural networks (ANN). PCA and HCA are generally viewed as exploratory methods of data analysis [38] from which natural clusters in the data set can be identified. Both procedures are examples of unsupervised pattern recognition methods [37], where no knowledge concerning the origin of the samples is necessary. HCA gives no indication of the variables, which contribute most to the classification of objects in the data set unlike PCA where the loadings indicate the variation contained within each variable. There may be a loss of information in the dendrogram generated by HCA, especially if clusters are not well resolved. However, HCA does present all the variation in the data set, in contrast to PCA where only a percentage of the variation is typically presented.

Supervised pattern recognition methods require prior knowledge of the sample origin to develop models, which are subsequently used to assign unknown samples to a parent group. Discriminant analysis techniques such as LDA are examples of parametric supervised techniques and are applied in cases where the data set is known to be normally distributed. For data sets in which this assumption cannot be made, non-parametric methods such as ANN algorithms can be applied to discriminate samples of different origin. Artificial neural network algorithms have the potential to provide complete solutions in the identification of patterns in data in even the most complex applications [37].

Johnston and King [39] developed one of the first chemometric models to be applied to illicit drug samples, using linear discriminant analysis to predict the origin of heroin samples based on the concentration of selected alkaloids and adulterants present. Profiles of each sample were obtained using HPLC and GC–FID and the LDA model correctly predicted the origin of the samples in 83% of cases. Currently, the majority of studies have concentrated on the application of computerised profiling methods for amphetamine and methamphetamine seizures.

Jonson and Strömberg [33] developed a computerised method for the comparison of impurity profiles from samples of amphetamine, which were generated by GC–MS. The quotients of selected impurities were calculated based on the peak area and impurity profiles with similar quotients were matched. The method is easily set up in laboratories in different countries, enabling similar comparison techniques to be employed at an international level.

The same authors [24] presented a method for the classification of amphetamine synthesised by the Leuckart route. Amphetamine was synthesised in the laboratory and analysed by GC–FID. Similar organic impurity profiles were obtained for amphetamine synthesised by the same route

while amphetamine samples synthesised by different routes showed quite different impurity profiles, enabling classification on two levels. The computerised quotient method [22] was applied to detect 'batch relations' among seizures, which may indicate the distribution of the batch within or between countries. Second level classification required the detection of 'source relations' between different batches produced by the same synthetic route. Further development of the computerised classification method could eliminate the inevitable subjectivity associated with visual assessment of impurity profiles. In addition, computerised comparisons are accessible to drug intelligence units and are ideal when large sample numbers are considered.

Jonson [34] reported improvements in the earlier computer-aided comparisons previously reported. A total of 136 amphetamine samples were analysed by GC–FID and the impurity profiles were assessed visually and using the computer classification method. There was good agreement between the computer-generated classification of seizures and those proposed on a visual basis. In addition, tentative classification of the seizures was achieved by principle component analysis.

Perkal et al. [37] generated organic impurity profiles for 224 samples of methamphetamine hydrochloride using capillary GC–FID. Canonical variate analysis was applied to classify the samples according to three different synthetic routes. Samples originating from a common batch were identified using a quotient method based on the number of peaks matched in the profiles compared. Based on an analysis of the impurities present, 60 samples were likely to have been synthesised by the reduction of ephedrine or pseudoephedrine and 14 samples from the Leuckart synthesis. It was not possible to identify the synthetic route in the remaining 150 samples. Of the 224 impurity profiles generated, 161 common batches were identified. The study also reported the development of an Australian National Drugs Intelligence database, based on a chemical characterisation of the seizure and common drug logos. The ultimate aim was to provide a computerised database, which was accessible to drug investigators throughout Australia, in an attempt to uncover national distribution networks of illicit drugs.

Statistical analysis and chemometric procedures were applied by Krawczyk and Parczewski [40] in the classification of 1000 amphetamine samples, based on 15 chromatographic peaks. Organic impurity profiles were considered similar where the Euclidean distance between them was less than 1. The method was successfully applied by the Polish police force to identify drug-trafficking networks and seize clandestine laboratories. The authors indicated that research would continue to improve the efficiency of the method.

8. Conclusions

The use of drug profiling and its potential to link seized illicit synthetic and semi synthetic drugs is not a new development in Forensic drug chemistry. However, with the use and development of robust validated analytical techniques, the surety of links between samples can be made with greater confidence. There are interesting and emerging developments in the usage of chemometric data analysis techniques, particularly the use of artificial neural networks to combine organic and elemental profiles, which will provide great assistance to analysts in interpreting the complex impurity patterns derived from analysis.

The application of advanced chemometric techniques should be encouraged in interpreting the results of forensic analysis particularly in areas where pattern recognition is involved, such as drug profiling or interpretation of fire debris analysis. Here is an area where experienced analytical chemists who use these techniques can help in the interpretation of such data.

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