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ScienceDirect
Forensic Science International 178 (2008) 34–39
Forensic Science International
www.elsevier.com/locate/forsciint

Drug intelligence based on MDMA tablets data 2. Physical characteristics profiling

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Received 23 May 2007; received in revised form 17 January 2008; accepted 30 January 2008
Available online 19 March 2008

Abstract

One of the tasks of the European project entitled ''Collaborative Harmonisation of Methods for Profiling of Amphetamine Type Stimulants'' (CHAMP) funded by the sixth framework programme of the European Commission was to develop a harmonised methodology for MDMA profiling and the creation of a common database in a drug intelligence perspective. Part I was dedicated to the analysis of organic impurities formed during synthesis in order to investigate traffic tendencies and highlight potential links between samples, whereas this part focuses on physical characteristics of the MDMA tablets. Diameter, thickness, weight and score were demonstrated to be reliable and relevant features in this drug intelligence perspective. Distributions of samples coming from the same post-tabletting batch (post-TB) and samples coming from different post-TB were very well discriminated by using the squared Euclidean or the Manhattan distance on standardised data. Our findings demonstrated the possibility to discriminate between MDMA samples issued from different post-TB and to find out links between samples coming from a same post-TB. Furthermore, the hypothesis that most of the MDMA samples found on the international market come from the same countries was supported.

Keywords: Drug profiling; Intelligence; Statistics; MDMA; Ecstasy; Physical Characteristics

1. Introduction

The main objectives of the project entitled ''Collaborative Harmonisation of Methods for Profiling of Amphetamine Type Stimulants'' (CHAMP) funded by the sixth framework programme (contract no. 502126) of the European Commission included the development of harmonised profiling methods for amphetamine type stimulants (ATS) and a database with on-line access. A set of characteristics was measured on MDMA tablets and results were stored in the database: physical characteristics, chemical composition and organic impurities. Based on these features, a methodology was developed to highlight links between samples coming from different countries and to detect traffic tendencies. In the first part of this article, the potential of organic impurities was investigated for intelligence purposes. The present work focuses more particularly on physical characteristics, as they have been neglected in the literature regarding their use in a drug intelligence perspective. Physical characteristics are systematically recorded on Ecstasy tablets and moreover bring complementary information to organic impurities profiles since the two subsets of characteristics occur at different stages of the clandestine production of MDMA tablets: organic impurities are formed during the synthesis process, while physical characteristics are created during the tabletting process (see the first part of this article for more details [1]).

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0379-0738/$ – see front matter
doi:10.1016/j.forsciint.2008.01.014

The goal of this part of the project was to apply multivariate statistics on the physical characteristics of MDMA tablets in order to evaluate the possibility to differentiate different post-tabletting batches (post-TB) and the possibility of linking tablets from the same post-TB based on these features. The potential of these data for strategic intelligence purposes was also investigated. In a first step, pertinent variables (i.e. physical characteristics) were selected based on their reproducibility within and between partner laboratories and their discriminating power. The degree of similarity between samples coming from the same post-TB (i.e. linked) and, samples coming from different post-TB was evaluated to determine if the populations of linked and unlinked samples could be discriminated. Finally traffic tendencies between countries were investigated and potential links between street samples were searched for.

2. Materials and methods

2.1. Sampling

Two MDMA sample types were collected: test samples and street samples. The former were composed of 26 seizures made in Finland and Germany. Each of the seven partner laboratories received six tablets per test sample and carried out measurements on each tablet. Later each partner laboratory collected 80 street samples seized in their own country from 1996 to 2004, thus providing a total of 560 samples (Finland, The Netherlands, Czech Republic, France, Germany, Switzerland, USA). Street samples measurements were averaged from replicates made on five different tablets of a given seizure.

Replicate analyses on each given test sample were used to build a population of linked samples, while street samples mean measurements formed a population of unlinked samples. As mentioned in the first part, despite the fact that the samples origin was unknown, a seizure was considered to represent only one single post-TB, while different seizures were assumed to belong to different post-TB.

2.2. Physical features

The physical characteristics collected on each tablet were: physical form (such as powder, tablet, etc.), diameter, thickness, weight, shape top, shape side, edge profile, score (or breaking line), colour, colour variance, logo, category of logo.

2.3. Statistical analysis

The numerical data obtained were treated statistically using the SPSS® 12.0 software (SPSS Inc.). For each test sample, the relative standard deviation (RSD) was calculated within each laboratory (six single measurements) and between laboratories (seven mean measurements). Then the variables distributions within the street samples population were determined to obtain an estimation of their discriminating power.

A discriminant analysis was performed in order to investigate the possibility to distinguish the 26 test samples (assumed to be different) on the basis of the reliable and relevant external characteristics of MDMA tablets. Each test sample was characterized by seven mean observations, one per partner laboratory. For each observation, the result of this multivariate analysis was represented on a two-dimensional scatter-plot defined by the first and second discriminant axes [2]. The correlation of each variable with each discriminant axis was calculated.

Distances were measured between linked and unlinked samples in order to check if a separation between the distributions of these two sets of distances was possible [3,4]. The aim was to demonstrate the possibility to highlight links between samples based on the distance value separating them. The linked samples (same post-TB) were the measurements made on a same MDMA test sample by different laboratories, whereas the unlinked samples referred to the measurements taken on different MDMA street samples (different seizures, different post-TB). Pre-treatment methods had to be applied because the calculation of distances can be sensitive to differences in scale between variables [4]. Three methods were selected: standardisation (i.e. subtract the mean value and divide by the standard deviation), fourth square root and ranking 0–1 (i.e. subtract the minimal value and divide by the interval: max.–min.). Two distance metrics were then used: squared Euclidean distance and Manhattan distance.

Area under the receiver operating characteristic (ROC) curve was used to evaluate the efficiency of the combination of a pre-treatment and distance metric described above in order to discriminate the populations of linked and unlinked samples. ROC curve is constructed by plotting the true positive rate (sensitivity) in function of the false positive rate (1-specificity) for different decision thresholds (distance values). The area under the ROC curve theoretically ranges from 0.5 (distributions completely overlapped) to 1 (distributions perfectly separated) [5].

Boxplots and stacked bar plots were drawn in order to represent and to compare data distributions of MDMA street samples between laboratories.

A principal component analysis (PCA), performed by using The Unscrambler® 9.2 (Camo Process AS), was carried out on the continuous physical variables of street samples of all partner laboratories in order to detect patterns between countries.

3. Results and discussion

3.1. Selection of variables

The following variables were not reproducible between laboratories and were therefore not selected: shape side, edge profile, colour, colour variance and logo. These characteristics were not reliable because they are highly operator dependent and the different possible outputs are difficult to clearly define. Physical form and shape top were identical for all the samples, which indeed were all tablets and round. Hence these variables were not relevant. Only the following physical features were selected: diameter (RSD $< 1\%$), thickness (RSD $< 5\%$), weight (RSD $< 5\%$) and score (binary variable: which takes value 1 if a score is present, 0 if not). These were found reliable (low RSD values).

The selected physical features also proved to be relevant, as their values were widely distributed (Figs. 1–3). A score was presented by 56.5% of street samples tablets. The diameter distribution in street samples tablets (Fig. 1) highlighted three main classes of diameter: 7, 8 and 9 mm. This observation and the low RSD values obtained might be explained by the fact that the diameter is a fixed variable for a given tabletting machine.

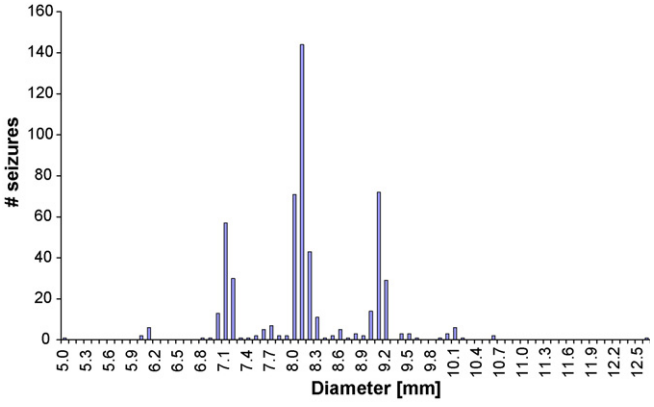

Fig. 1. Distribution of diameter values of MDMA street samples of the seven partner countries. Three frequent classes of values were found: 7, 8 and 9 mm.

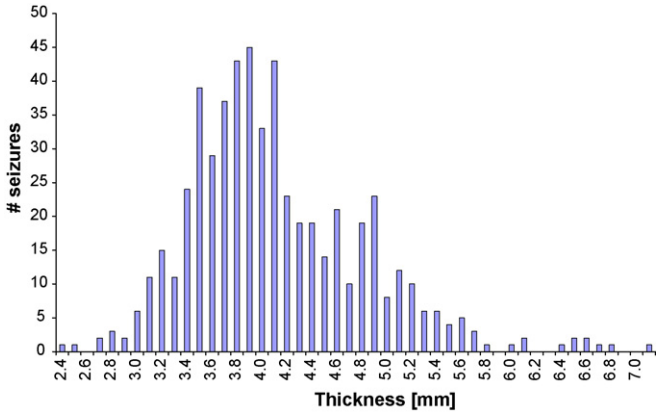

Fig. 2. Distribution of thickness values of MDMA street samples of the seven partner countries. A broad variation was found, with a mean value of 4.1 mm.

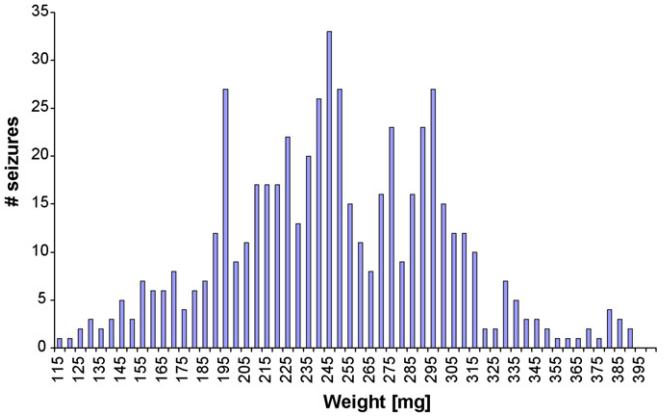

Fig. 3. Distribution of weight values of MDMA street samples of the seven partner countries. A broad variation was found, with a mean value of 251 mg.

Within seizure variability of weight and thickness are slightly larger mainly due to inhomogeneous fabrication process and friability of tablets. In fact thickness and weight depend on the quantity of powder per tablet and the set pressure of the punches for a given post-TB [6]. Their RSD values were effectively slightly higher than for diameter and their distribution were broad and clearly continuous (Figs. 2 and 3). In order to handle this variability, average values made on at least five different tablets of a given seizure were introduced in the database. This insured RSD values under 5% within and between countries.

Discrimination was possible between the 26 test samples on the basis of the selected features (Fig. 4). Correct classification rate reached 94.5%. The first discriminant function accounted for 72.3% of the total variance, while the second one explained 20.3% of it. The first discriminant function was mainly correlated to diameter and weight, and the second function was mainly correlated to thickness and weight (Table 1). The selected features proved thus to be discriminant between samples.

3.2. Separation of linked and unlinked samples distributions

Given the promising results provided by the discriminant analysis, the selected physical characteristics were further used

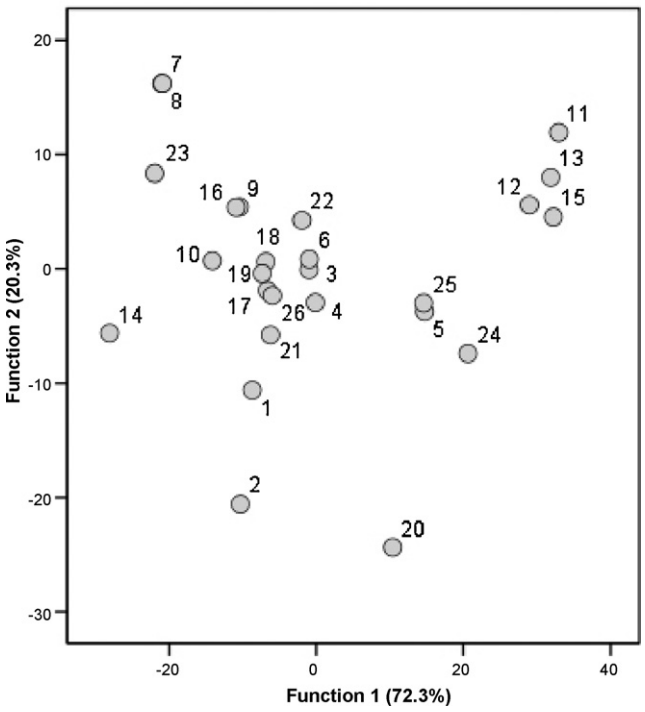

Fig. 4. Results of the discriminant analysis performed on the four selected external characteristics (diameter, thickness, weight and score) of the 26 MDMA test samples: representation of the centroids of the seven measurements (one by laboratory) of each test sample on the first two discriminant functions.

to estimate the power of the separation between distributions of linked and unlinked samples. The results of area under the ROC curve, used to quantify the efficiency of each combination of pre-treatment and distance metric in order to discriminate these populations, are given in Table 2. Whatever the pre-treatment method and the distance metric, separation between populations of linked and unlinked samples proved to be excellent. An example of ROC curve is given in Fig. 5. These findings demonstrate the possibility to discriminate between samples issued from different post-TB.

The distributions of distances calculated between linked and unlinked samples were visualized by histogram plots. The example shown in Fig. 6 illustrates the small overlapping area between the two populations of interest. Histogram plots of distances calculated on data pre-treated by fourth square root or ranking 0–1 show a clear separation between two groups of distances between unlinked samples (Fig. 7), due to the dichotomy of values taken by the score. The pre-treatments by ranking 0–1 and fourth square root attributed too much importance to the score variable in the calculation of distances,

Table 1
Discriminant analysis of the four selected external characteristics: correlation coefficients of diameter, thickness, weight and score with the first and the second discriminant function

	Function 1	Function 2
Diameter	0.861	−0.276
Weight	0.591	0.572
Thickness	0.165	0.890
Score	−0.030	−0.236

Table 2
Values of area under the ROC curves, when linked samples are measurements made on a same test sample by different laboratories, and unlinked samples are measurements made on different street samples by a same laboratory (the data of all the laboratories are however considered)

	Standardisation	Ranking 0–1	4th square root
Squared Euclidean	0.983	0.959	0.984
Manhattan	0.982	0.955	0.984

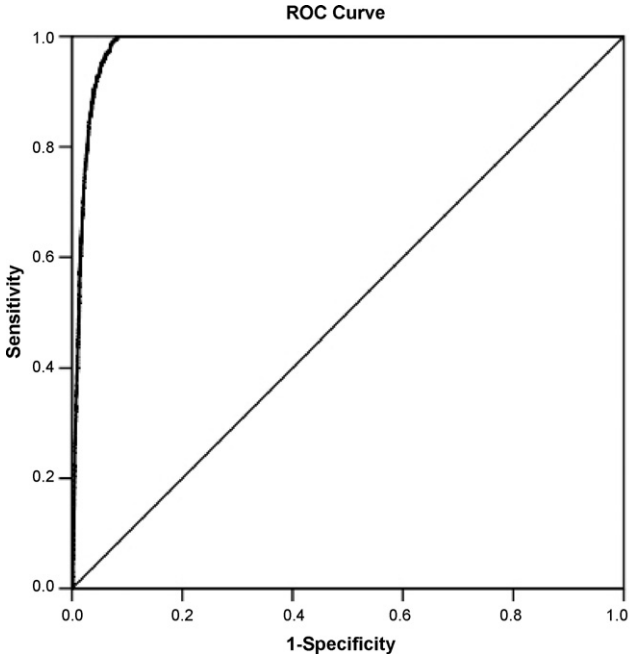

Fig. 5. Example of ROC curve of the combination standardisation and Manhattan distance: linked samples are measurements made on a same test sample by different laboratories, and unlinked samples are measurements made on different street samples by a same laboratory (the data of all the laboratories are however considered).

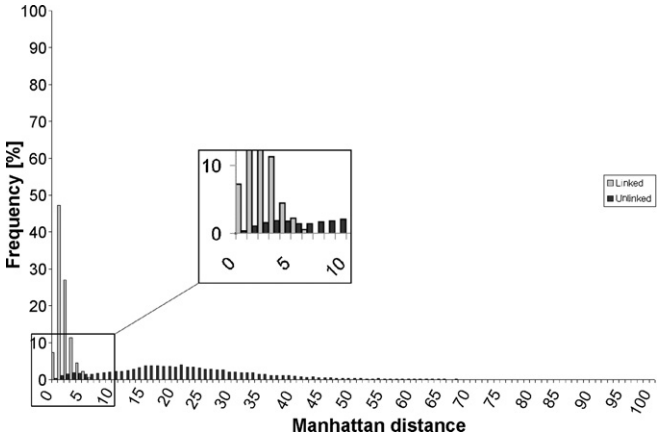

Fig. 6. Histogram of distributions of Manhattan distances calculated between linked and unlinked samples, where data were normalised by standardisation.

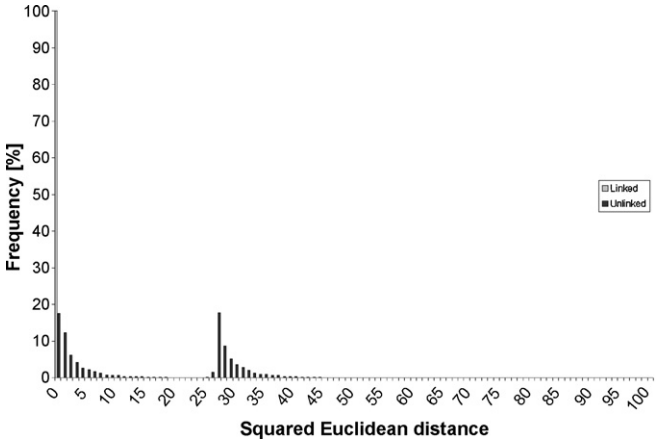

Fig. 7. Histogram of distributions of squared Euclidean distances calculated between linked and unlinked samples, where data were normalised by fourth square root.

generating large distances between samples presenting a different value of score. The best pre-treatment method proved thus to be standardisation.

3.3. Drug intelligence

3.3.1. Strategic intelligence

Boxplots were drawn for each continuous variable (diameter, thickness, weight) in order to represent and to compare data distributions of MDMA street samples between partner laboratories. Stacked bars were plotted to visualise the distributions of the score variable (Fig. 8). Whereas no general trend could be extracted from the boxplots of diameter and thickness because their values were not that much different between countries, diameter values of the tablets analyzed in the USA were definitely less variable than in other countries, and all grouped around 8 mm. This could be explained by the use of an 8 mm tabletting machine type or a specific source of importation in the USA. In addition, although the medians of diameter values were located at 8 mm for each laboratory, diameters values were on average smaller in Germany, Czech Republic and the Netherlands that in the other countries. Finally, in the USA, a far greater proportion of tablets without score were observed.

A principal component analysis was carried out on the continuous physical variables of all partner laboratories to try to highlight patterns between countries. No groups of countries could be extracted (Fig. 9), but the set of observations appeared grouped in three diagonals. It was found that this pattern was not due to differences in physical properties between countries, but to the fact that most of diameter values were grouped in three classes: 7, 8 and 9 mm. The lack of differences in physical properties of tablets between the countries supports the hypothesis that most of the street samples found on the international market comes from the same countries [7].

These findings must be taken with care, because the samples of this study were not collected at the same period in all the countries. Hence these tendencies should be further confirmed.

3.3.2. Operational intelligence

A final aim of this work was to investigate the potential of the method to point out links between samples. The same procedure as for organic impurities profiles comparison was

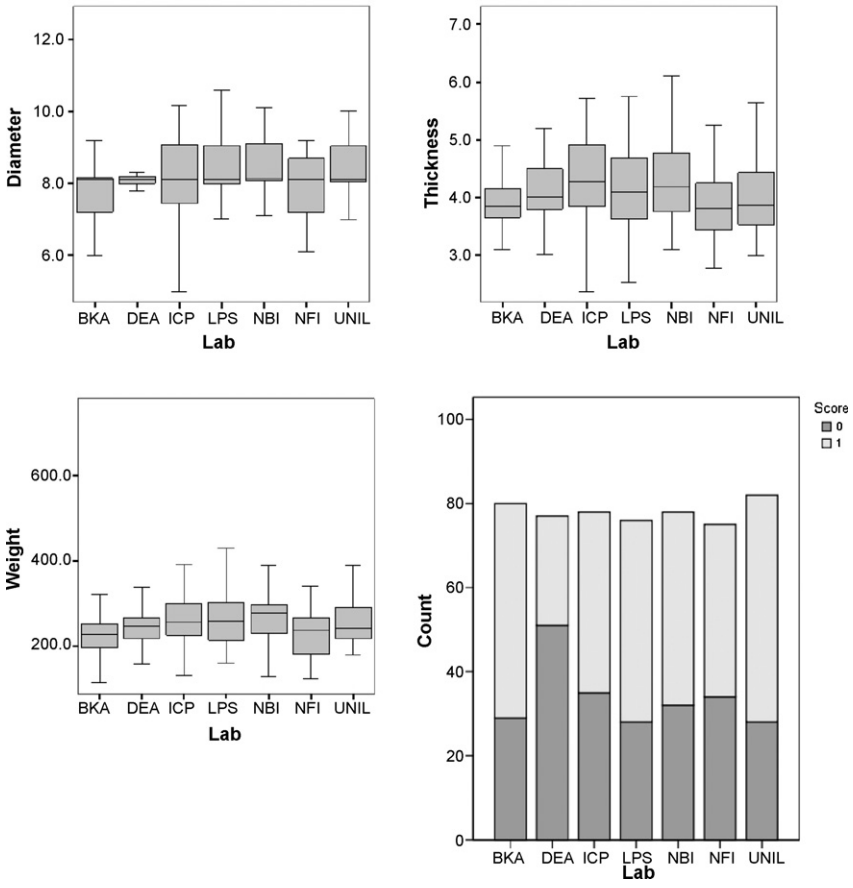

Fig. 8. Boxplots and stacked bars of physical properties (diameter, thickness, weight and score) of MDMA street samples within each one of the seven partner laboratories.

used. A distance value was fixed as a threshold from which deciding whether two samples are linked or not. The threshold was chosen to tolerate a false positive rate of 2% (on the basis of the distances between street samples) [8]. A systematic search was carried out on street samples to highlight links based on organic impurities between countries. Several links were highlighted within and between countries. For example, a link was highlighted between two samples seized in the Netherlands (NL 60) and in Switzerland (CH2), because the squared Euclidean value between the samples was under the given threshold (<0.04). Tablets from these seizures showed corresponding physical characteristics, except from the logo (Fig. 10). The different logos can be explained by the use of several punches on a tabletting machine. Two types of links may be revealed between samples: organic impurities corresponding profiles support the hypothesis that the seized tablets came from the same pre-tabletting batch (pre-TB) batch, while corresponding physical characteristics support the hypothesis that the seized tablets came from the same post-TB. The chemical composition and organic impurities profiles did also correspond between samples NL 60 and CH2 (Table 3).

The tablets were seized in the Netherlands in July 2004 and in Switzerland in October 2004. Later, in January 2007, a

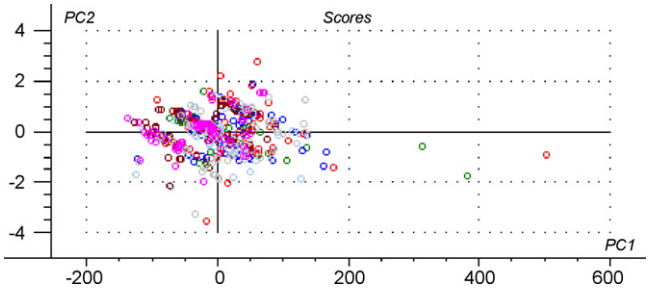

Fig. 9. Results of the principal component analysis on continuous physical variables (diameter, thickness and weight) of street samples of all partner laboratories.

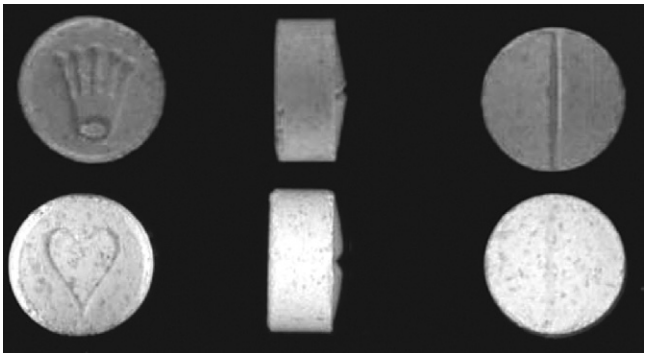

Fig. 10. Photography of the tablets from street samples CH2 (above) and NL 60 (below). Light source was not standardised. Tablets from both seizures showed corresponding physical characteristics, except from the logo.

Table 3
Link between MDMA samples from the Netherlands (NL) and Switzerland (CH) based on the external characteristics (diameter, thickness, weight and score)

Sample	Logo	Colour	Score	Diameter (mm)	Thickness (mm)	Weight (mg)	Purity (%)	Adulterants	Lactose	Organic impurities
NL 60	Heart	Beige	Yes	8.1	3.8	247	27	Caffeine	Yes	Corresponding
CH2	Rolex	Beige	Yes	8.1	4.1	242	28	Caffeine	Yes	Corresponding

The organic impurities profile did also corresponding.

clandestine laboratory that was not active anymore was found in the Netherlands. This laboratory produced MDMA by the H_2/Pt reductive amination synthesis route and also had seven tabletting machines, some identicals, producing tablets in the same range of physical characteristics as the two seizures NL 60 and CH2. Several types of punches, including rolex and heart logos, were found. These observations supported the hypothesis that the seized tablets came from the same pre-TB and the same post-TB.

4. Conclusion

This study focused on multivariate statistical analysis of physical characteristics of MDMA tablets to demonstrate their potential in a drug intelligence perspective. It was demonstrated that diameter, weight, thickness and score were adequate features in order to discriminate between samples coming from different post-TB (or seizures). First, it must be emphasized that, for each continuous physical property (diameter, thickness and weight), the mean values of at least six measurements made on different tablets of any seizure should be introduced in the database to handle the within seizure variability. Distances metrics were then calculated between all possible pairs of linked (coming from a same seizure) and unlinked (coming from different seizures) samples. Overlapping of these two distributions was quantified by the area under the ROC curve. It appeared that Manhattan and squared Euclidean distances applied to standardised data were very efficient methods to discriminate between the two distributions of linked and unlinked samples.

Trends of external characteristics between countries or groups of countries were then searched for. It appeared that weight and thickness values were very similar between all the countries, and that diameter values were slightly lower in Germany, Czech Republic and the Netherlands than in the other countries. Furthermore, a greater proportion of tablets without score were observed in MDMA tablets seized in USA than in other involved European countries. Whatever the country, most of the diameter values were grouped in three classes: 7, 8 and 9 mm, except in the USA where all values were around 8 mm. It must however be kept in mind that these tendencies would need to be confirmed since samples were not collected at the same period in all the countries.

The results of this study demonstrate that physical properties can be used in drug intelligence purposes, and that the selected statistical methods can be applied to highlight links between samples with similar physical properties and to discriminate samples with different external characteristics, i.e. coming from different post-TB. A link between samples based on physical characteristics does not mean that the same press was used. It may be another press with the same settings in respect to diameter, thickness, weight and score. A link found between samples should therefore be confronted to other information on the samples (such as contextual information or other characteristics) in order to allow a more precise understanding of the traffic.

Acknowledgements

The CHAMP project was supported by a research grant of the sixth framework programme of the European Commission (EC) (contract no. 502126) and the Federal Office of Education and Science in Switzerland (contract no. 04.0005).

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