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Exploring the added value of portable devices such as near infrared spectrometer in the field of illicit drugs analyses

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ABSTRACT

Facing the problem of backlogs in the forensic laboratories, the field of illicit drugs analyses has recently seen the development of different types of portable devices. Their main purpose is to be used directly by the police in order to reduce the number of specimens that are sent to the laboratories. Several portable devices have shown promising results. To avoid misuses, the added value of these devices should be explored, in order to establish "good practices" and keep the communication channels open between the police and the laboratories. Adapting sampling procedures around the use of portable devices allows for real-time qualitative and quantitative data. Forensic scientists can therefore rapidly assess whether every specimen in a seizure contain illicit drugs and if the seizure is composed of specimens showing different composition. Based on these information, forensic scientists can proceed to an intelligence-led sampling and prioritise specimens that would require further analyses. Additionally, the availability of more analysis data can strengthen the confidence in the reporting of the sampling process and the analyses results. Various scenarios have been tested in an operational context at the Geneva Cantonal Police Force using an ultraportable NIR device. The focus was oriented on sampling issues and the intelligence produced. Results indicate a great potential to detect the different classes within a seizure and therefore to ensure a representative sampling for further analyses.

1. Introduction

The increasing demand of forensic evidences in the judiciary procedures are leading to a saturation of the laboratory capabilities [1]. To limit further aggravation of this problem, several fields of forensic science are moving toward a trend of decentralisation. Instead of mandating an external laboratory to analyse traces, police forces and forensic services are equipping themselves with portable devices allowing in situ analyses. Among others, near infrared devices have shown promising results in the matter of decentralisation [2–5]. In order to maximise their potential and make the most of their use, it is important to study and develop the added value of portable devices for the police.

The most obvious advantage is the instantaneity of the information; by analysing their illicit drug seizures themselves, police forces get timely information, and avoid the administrative work and delay of an analysis' mandate to an external laboratory. Police may also easily analyse a higher amount of illicit drug specimens; thus having more data and taking intelligence-led decisions regarding the next steps of the investigation [6]. Specimens or samples can be selected for further analyses according to their additional information potential [7,8] or their representability of the different potential groups present within a seizure. These decisions being supported by scientific data, the results reported by forensic scientists are therefore strengthened.

Two specific applications will be presented in order to illustrate the added value of deploying such approach. The first one focus on sample preparation (unpacking) by providing approaches that drastically decrease the time needed for this step. The second one concern the sampling process, specifically the early detection and grouping of classes within a seizure.

1.1. Sample preparation

Several steps of sample preparation are required in order to perform analyses using laboratories equipment [9–11]. These steps can be time consuming, especially when working with large amount of small units that require their packaging to be removed and their content to be homogenised, as it is often the case in Switzerland with heroin bags and cocaine fingers [Fig. 1]. In the perspective to use portable NIR devices for intelligence and decision making

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Fig. 1. Top: 100 heroin bags coming from a single seizure, Bottom left: 161 cocaine fingers coming from a single seizure, Bottom right: Cocaine finger, unpacked cocaine finger, powdered and homogenised cocaine finger.

Fig. 2. Top: Measurements through the plastic of an heroin bag, Bottom left: Cutting a cocaine finger with an electric sheering prune, Bottom right: Measurements on the finger slices.

purposes, the possibility to skip these preparation steps must be considered. For instance, even though plastic do interfere with NIR spectra, it is still possible to analyse a drug sample through a plastic bag of reasonable thickness [Fig. 2 - Top]. As for cocaine fingers, the packaging is generally to thick and opaque to analyse it through its packaging. It is however possible to use an electric sheering prune to make a fast and clean cut of the finger, allowing measurements to be made on the slices [Fig. 2 - Bottom]. Using such approaches makes sample preparation less tedious and sampling gets faster. The forensic scientists can then quickly analyse a large part of the seizure and assess whether every specimen contain illicit drugs, if there are several classes within the seizure and choose which specimens are the most representative of the whole lot and/or might have the best intelligence potential.

1.2. Sampling

Sampling might be considered as a trivial step of the analysis process of illicit drugs. It is, however, an important issue as it will influence the results reported by forensic scientists [9,12,13]. When it

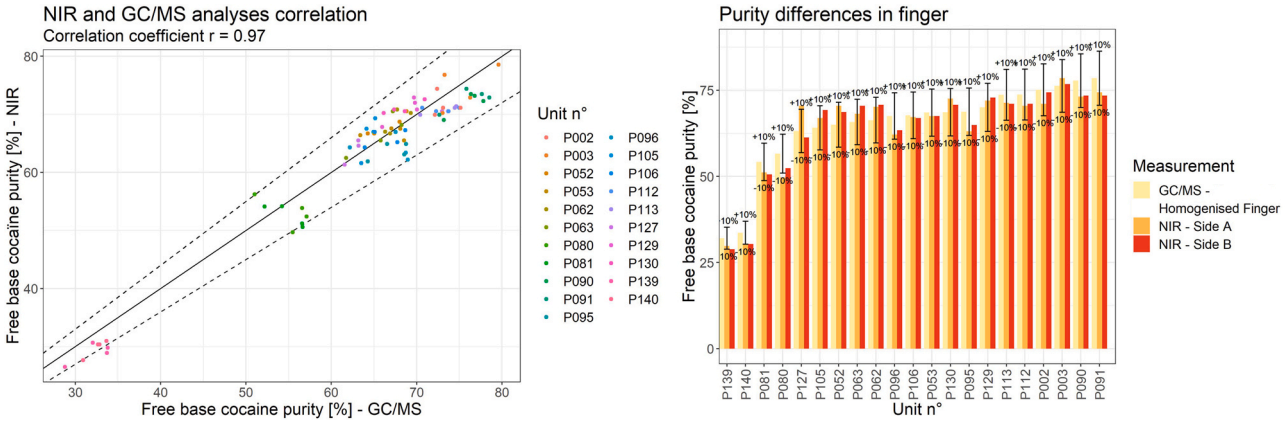

Fig. 3. Scenario 1 - Left: Correlation between NIR measurements and GC-MS analyses, Right: Purity variance within fingers.

comes to sampling an illicit drugs seizure, forensic scientists are faced with several aspects to consider. First, the purpose of the analyses must be determined. Qualitative, quantitative or profiling analyses require different sampling approaches [9]. Then, forensic and statistic considerations about the case will define how many samples should be analysed to be representative of the whole seizure.

However, beside the forensic and statistic aspects, cost and time of analysis also plays a role when it comes to sampling. Sampling guidelines usually require the analysis of a consequent amount of specimens for the sampled population to be considered as representative [14,15]. Unfortunately, forensic services cannot always afford to spend so much resources on every cases, as well as the Public Prosecutor Office who might wish to limit the cost for the analyses. Forensic scientists must therefore find a balance between the cost and time of analyses and the recommended amount of samples given the case's circumstances.

In that perspective, portable devices can offer excellent leads to this triage phase. The data they provide at an early stage of the investigation gives forensic scientists a better overview of the seized material. Intelligence-led decisions can therefore be taken to optimise the sampling.

2. Material and methods

In order to assess the feasibility of these approaches, three scenarios have been tested on real cases of the Geneva Cantonal Police Force, Switzerland. Four cases have been selected for additional analyses going beyond the scope of their court purposes. In these cases, analyses were carried out with both an ultraportable NIR device and GC-MS to confirm the results. Acquisition of data were made with a handheld MicroNIR™ OnSite-W using the parameters and algorithms developed by NIRLab [4]. Confirmatory analyses were done with a validated ISO 17021 GC-MS method as described by [4]. The main criteria for the GC-MS method are the following.

The samples were prepared by weighing approximately 6 mg of the homogenised powder. The analysis is done in duplicate. The samples are then dissolved in a 500 µl solution of $CHCl_3$/pyridine 5:1 and 100 µl of MSTFA This solution is then heated at 80 °C in an air oven for 1 h. The analyses were separate on a HP-5MS column (12 m x 0.2 mm × 0.33 µm). The injection is made in a split mode with a general purpose split liner (vol. 870 µl, Agilent Technologies N°5183–4711 4 mm ID) packed with glass wool. 2 µl of the sample is injected at 270 °C with a total gas flow of 79.0 ml/mn and a split ratio of 80:1 (gas saver 15 ml/mn after 2 min). Helium is used as carrier gas with a constant flow mode (0.9 ml/mn). The temperature programme starts at 80 °C, then increases to 150 °C (100 °C/min), then increases to 250 °C (40 °C/min), then increases to 310 °C (60 °C/min) and holds for 1mn for a total run of 5.2 min. The mass spectrometer was operated with a solvent delay of 1.2 min. The scanning range was 10–550 amu, with a sampling rate of 5.2 scans/s. The temperature of the transfer line, the ion source and the quadrupole of the MS were set up at 280 °C, 230 °C and 150 °C respectively.

Pre-treatments on spectral data were performed using The Unscrambler® X software, and with Agilent ChemStation for GC-MS data. R software was then used on pre-treated data.

3. Results and discussion

3.1. Scenario 1

The first scenario tests the hypothesis that heterogeneity within cocaine fingers is low enough not to require homogenisation before NIR analysis. It also explores the possibility to separate and regroup classes based on their content. The scenario was tested with a box of cocaine seized in a car. The box contained 161 cocaine fingers distributed in 11 classes based on their aspect (i.e. powder colour and markings on the packaging).

Cocaine fingers were cut in three, as shown on Fig. 2 (Bottom), and measurements were made on both sides of each cut. The slices have then been scrapped and the powders obtained were analysed with GC-MS for comparison purpose with NIR results. The rest of the finger was then homogenised and analysed both with NIR and GC-MS. This methodology was followed in order to assess whether the content of the fingers was sufficiently homogeneous for measures taken on single points to approach the value of the homogenised sample.

The comparison between NIR measurements and GC-MS analyses present an excellent correlation and are mostly found within a 10% relative difference between the NIR and GC-MS purity [Fig. 3 - Left]. Most NIR analyses on the slices were also found within a 10% relative range of the GC-MS purity value for the homogenised fingers [Fig. 3 - Right], with an average NIR variance of 3.1 between side A and B. It has to be noted that the finger having the highest variance (P127) was also visually heterogeneous when cut (i.e. lump-like spots were visible). According to these observations, it appears that without clear signs of inhomogeneity, NIR analysis on non-homogenised fingers can still be a good estimator of their whole content.

Using the additional NIR data [Fig. 4], forensic scientists can decide if some classes could be regrouped and if subclasses should be separated. Indications on the similarities between the different fingers can be deduced from the NIR spectra, drug purity and cutting agents. Following the circumstances of the case, the analysis purposes and a pragmatic approach, these data can help to prioritise the samples requiring further analyses. The decision process for grouping different samples can then be clearly reported using explicative data.

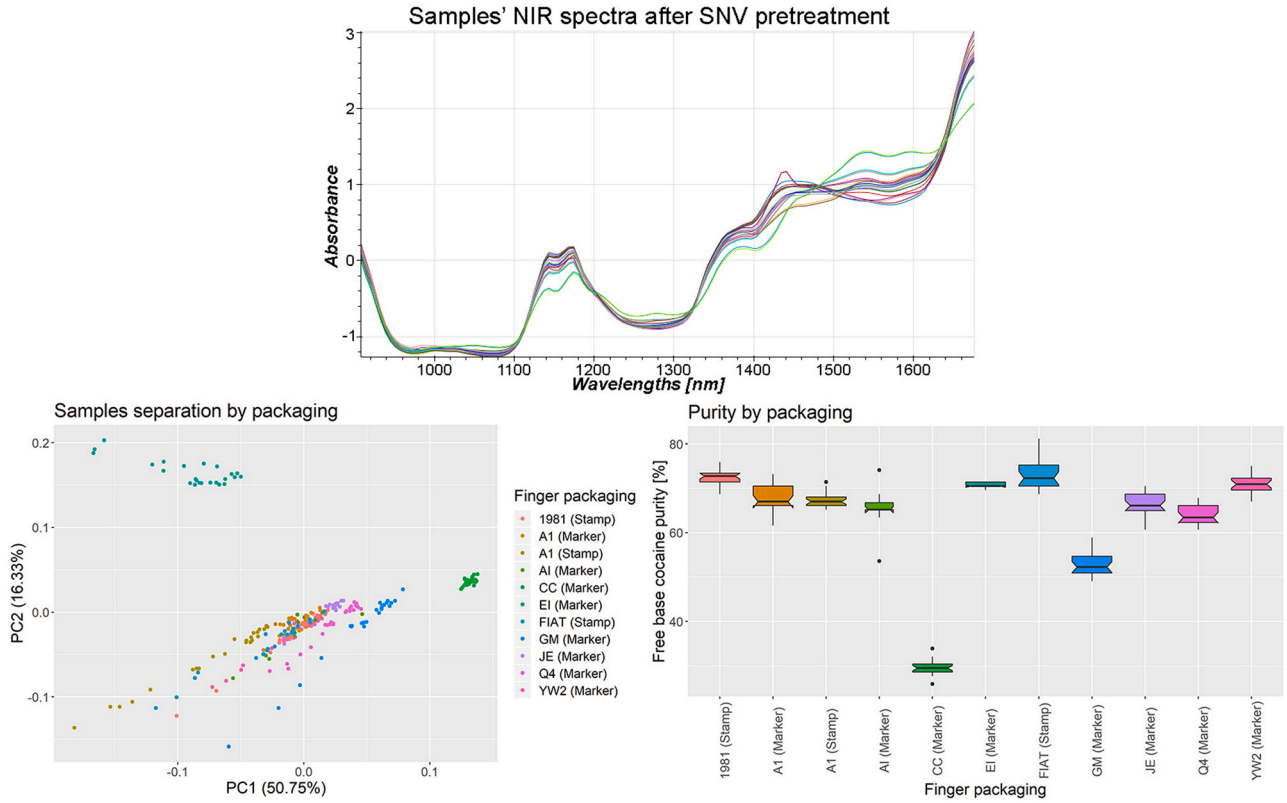

Fig. 4. Scenario 1 - Top: NIR spectra after Standard Normal Variate (SNV) pretreatment, Bottom left: Principal Component Analysis (PCA) by packaging logo, Bottom right: Cocaine purity by packaging logo.

3.2. Scenario 2

The second scenario focus on the hypothesis that early data from NIR analysis allow to separate subclasses and provide a more representative sampling. Here, a seizure of 100 cocaine fingers that were ingested by a body packer was used to test this hypothesis. The fingers couldn't be differentiated on their visual aspect. Therefore, a single class was made with this seizure. The ENFSI Bayesian sampling plan [14] was used to define a sample size of 26 units (parameters: N = 100, k = 0.9, r = 0, CL = 0.95, a = 3, b = 1) that have been analysed both with NIR spectrometer and GC-MS. The remaining 74 fingers were only analysed with NIR. As it appeared in Scenario 1 that sample preparation was not necessarily required when using a NIR device, the fingers were only cut and not homogenised for the NIR analysis. The GC-MS confirmatory analyses were performed on samples from the fingers after homogenisation.

As it can be seen in the Fig. 5, the Standard Normal Variate (SNV) plot of the 9th specimen differentiate itself from the 25 other plots. A slight difference appears in the wavelengths range from 1100 nm to 1200 nm, resulting from a difference in cocaine purity. However, the main difference doesn't reside in the cocaine region of interest but in the wavelength influenced by the cutting agents, ranging from 1300 nm to 1700 nm (cf. [4]).

In an intelligence perspective, it is especially relevant to proceed with further analyses for the 9th specimen and any of the 25 other samples. The GC-MS analysis confirmed a difference both in purity and in cutting agents.

3.3. Scenario 3

Scenario 3 tests the hypothesis that plastic interferences on NIR spectra are low enough to allow the use of NIR analysis through plastic bags for sampling purposes. Two different cases have been

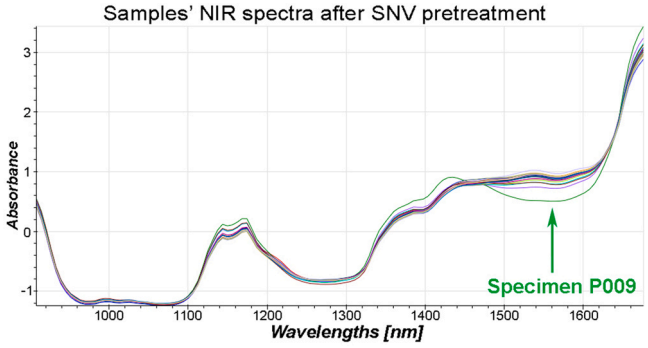

Fig. 5. Scenario 2 - NIR spectra after SNV pretreatment.

used to illustrate the influence of the plastic bags on the results of heroin analyses. Case A was a seizure of two packs of 100 heroin bags in the backpack of a dealer. This case was focused on the comparison between analyses through the packaging and in direct contact of the drug and fourteen specimens were selected for this purpose. Case B was a seizure of 61 heroin bags confiscated on a second dealer, out of which 30 units were selected for the direct contact and through plastic analyses comparison.

As shown in [Fig. 6], the plastic bags' interferences in the spectra are different in case A and case B due to difference inherent of the packaging itself. The algorithms were able to recognise heroin through the packaging used for case A. As for case B, several spectra were labelled as being close to heroin spectrum rather than to be formally recognised as such.

Even when the algorithms do not recognise the illicit drugs, the information coming from the spectra can still give an insight on the content of the seizure. The similarities – and differences – between measures of different specimens can be a good estimator of the

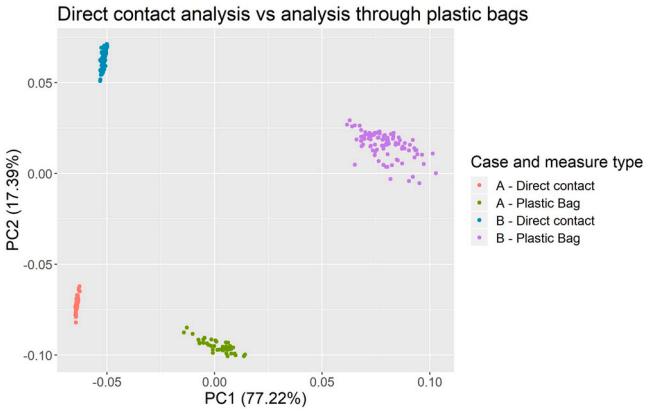

Fig. 6. Case 3 - PCA by measurement type.

homogeneity of the units within a seizure. This information helps the selection of samples for direct contact or even GC-MS analysis and an appropriate extrapolation of data. This can help forensic scientists to communicate their findings in a transparent manner and thus strengthening the confidence in their report. Additionally, the early detection of heterogeneity within a seizure serves intelligence purpose, as distinct specimens can be sent to the laboratory for further analyses. The forensic laboratory can then make the most of their chemical profile, produce high value intelligence and give inputs to direct the investigation.

4. Conclusion

The possibility to analyse illicit drugs without requiring sample preparation allows the forensic scientists to easily gather analytical data from more specimens than it is feasible when using laboratory equipment, and thus gaining more insight on the seizure. Even when algorithms are unable to clearly qualify and quantify a substance, the spectral data allow for an intelligence-led selection of samples that should require further analyses. Forensic scientists are then able to prioritise the samples according to the resources available for a given case and can quickly and wisely make decisions on what happens next in the investigation. These choices being based on analytical data, the forensic scientists' conclusions regarding the seizure can be strengthened.

Moreover, a prioritisation between samples for further analyses reduces the laboratories' analysis workload, and shift it to data treatment. Therefore, laboratories have more resources to optimise the use of chemical profiling and adding more value to the intelligence generated out of the case and analysis data.

CRediT authorship contribution statement

Marc Wermelinger: Writing – review & editing, Software, Conceptualization, Methodology, Investigation. **Florentin Coppey**: Review & editing, Methodology. **Laëtitia Gasté**: Review & editing, Methodology. **Pierre Esseiva**: Writing – review & editing, Conceptualization, Methodology, Supervision.

Conflict of interest

The authors have no conflict of interest related to this work.

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