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Providing illicit drugs results in five seconds using ultra-portable NIR technology: An opportunity for forensic laboratories to cope with the trend toward the decentralization of forensic capabilities

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ABSTRACT

The analysis of illicit drugs faces many challenges, mainly regarding the production of timely and reliable results and the production of added value from the generated data. It is essential to rethink the way this analysis is operationalised, in order to cope with the trend toward the decentralization of forensic applications. This paper describes the deployment of an ultra–portable near-infrared detector connected to a mobile application. This allows analysis and display of results to end users within 5 s. The development of prediction models and their validation, as well as strategies for deployment within law enforcement organizations and forensic laboratories are discussed.

1. Introduction

In the context of the analysis of illicit drugs, the time required to get an analytical response remains at the heart of the concerns of magistrates and police officers, who want to know rapidly if the seized product contains an illicit drug. In Switzerland, information about the purity of seized material is also required, as it allows categorization of the case as a minor crime (e.g., personal consumption) or a major one (e.g., trafficking). For example, if a person is arrested with less than 12 g of pure heroin or 18 g of pure cocaine, the prosecutor can dispose of the case by simply seizing the illicit drugs and imposing a fine. However, if these limits are exceeded, the case is classified as a trafficking offence and the prosecutor continues the inquiry. Such a legal system relies on the ability to obtain fast and reliable results from seized material, ideally at the street (as opposed to the laboratory) level. The gold standards for drug analysis are high-performance liquid chromatography (HPLC) or gas chromatography (GC) techniques, coupled with diode-array detection (DAD) [1], flame- ionization detection (FID) [2,3] or mass spectrometry (MS) [4,5]. The primary weak points of these analytical techniques are related to the sample preparation, the analysis time, and the destructive nature of the analysis. Additionally, these techniques quickly generate problematic workloads that prevent laboratories from meeting their customers' expectations. Finally, they are difficult to deploy at the street level. In this context, the search for a fast and portable analytical method is of great interest.

An elegant alternative, already intensively used in the pharmaceutical industry for quality control, is near-infrared (NIR) technology [6–8]. This technology has also been used for the analysis of falsified pharmaceuticals [9–12] and the identification and quantification of illicit drugs [13–18].

The development of portable analytical NIR capabilities offers the possibility of bringing the laboratory to the field. It also contributes to the trend toward decentralization and increasing need of rapid support and information for investigative and intelligence activities. As described by Casey et al. [19] in their study of the Kodak Syndrome, the decentralization and

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Fig. 1. Illustration of the MicroNIR Onsite W 1700 (Viavi Solutions Inc.).

commodification of forensic capabilities is an important challenge that all forensic laboratories have to face at some point.

In this paper, we propose the development and the validation of a methodology for the field deployment of a portable NIR analyser capable of rapid, non-destructive, and reliable identification and quantification of heroin, cocaine, and cannabis street samples. We will also describe how this technology can be implemented within forensic laboratories and law enforcement organizations through a dedicated mobile application. Finally, we will show how the information provided by the technology could be extracted in an intelligence-led perspective that allows laboratories to add value and benefit the legal system as a whole.

2. Material and methods

2.1. Portable NIR instrument

In this study, the MicroNIR Onsite W 1700 from Viavi Solutions Inc. was selected, due to its portability, ease of use, and Bluetooth connectivity (Fig. 1).

This system is ultra-compact, weighs only 250 g, and is powered by a Li-ion battery with a service life of more than 10 h. It is provided with Bluetooth connectivity and is distributed by Viavi Solutions Inc. (Santa Rosa, California, USA). The detector operates in the NIR spectral region (i.e., 950–1650 nm) and includes a linear variable filter (LVF) directly connected to a 128-pixel linear indium-gallium-arsenide (InGaAs) array detector. Two tungsten light bulbs act as the radiation source. The signal-to-noise ratio is 25.000, the integration time is 10 ms, and the system can perform 100 scans per analysis.

The NIR spectra obtain for heroin, cocaine and cannabis specimen are presented in Figs. 2–4, respectively.

2.2. Analytical workflow

The MicroNIR has been deployed in the field in conjunction with a dedicated mobile application (NIRLAB Mobile App), illustrated in Fig. 5. The main roles of the application are to send the recorded NIR spectrum to a database hosted in a secure cloud and to run the algorithms that have been developed for the identification and quantification of the illicit drugs present in the specimens investigated. The results of the calculations are then sent back to the mobile application, allowing a quasi-instantaneous (~5 s) consultation of the results by the user.

The type and purity of the illicit drugs, as well as the geolocation of the device at the time of the analysis, are stored in the database. The application makes it possible to visualize the data and perform subsequent analysis (e.g. spatial and temporal analysis, trend

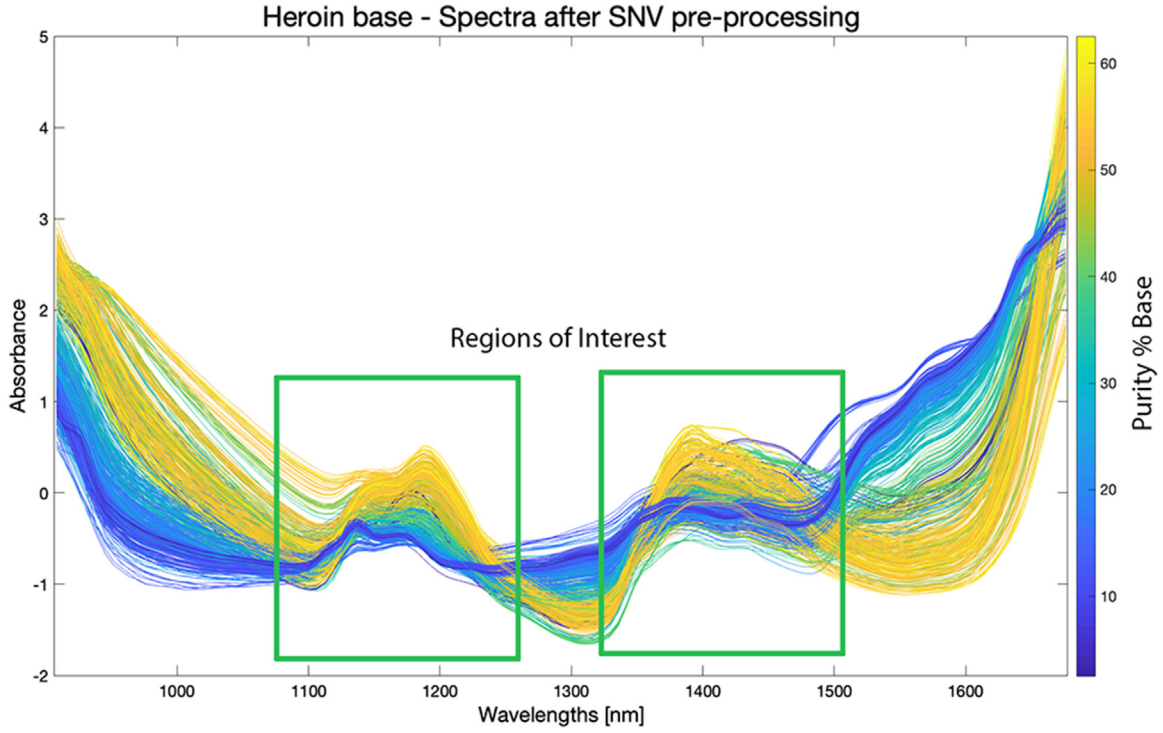

Fig. 2. Heroin base NIR spectra obtained using the MicroNIR Onsite W 1700 combined with a standard normal variate pre-processing.

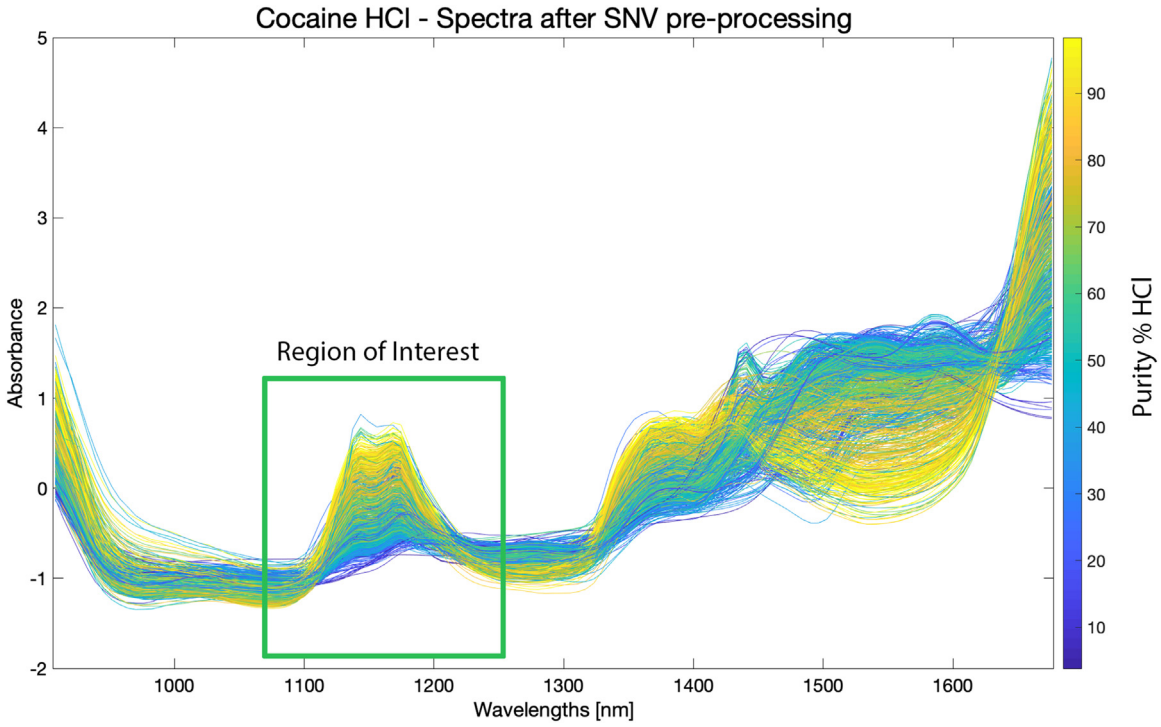

Fig. 3. Cocaine HCl NIR spectra obtained using the MicroNIR Onsite W 1700 combined with a standard normal variate pre-processing.

detection, illicit-drug monitoring). The fact that the NIRLAB architecture is accessible through the cloud means that the most recent updates (algorithms, library of substances) are immediately available to all users (see Fig. 6).

2.3. Chemometrics models

The chemometrics models were developed in Python, using the scikit-learn library version 0.21.3 [20]. Various combinations of algorithms and parameters were applied to the calibration dataset of cocaine and heroin street samples. The best results for cocaine and cannabis were obtained with a set of extremely randomized tree methods; for heroin, the best algorithms proved to be a group of gradient-boosting classifier and regressor methods. The difference observed in the type of algorithms yielding the best results is certainly due to the diversity of cutting agents in the calibration datasets, cocaine street samples being much more diversely cut than heroin street samples (see Figs. 7 and 8).

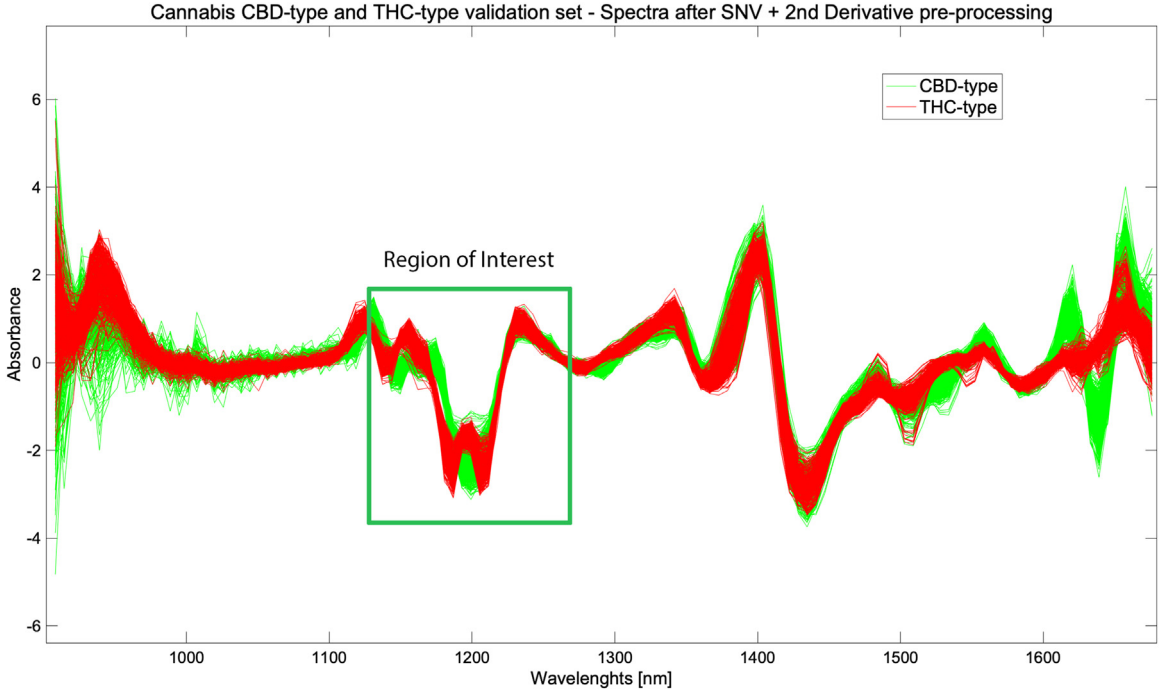

Fig. 4. Cannabis (THC and CBD types combined) NIR spectra after SNV + 2nd Derivative pre-processing.

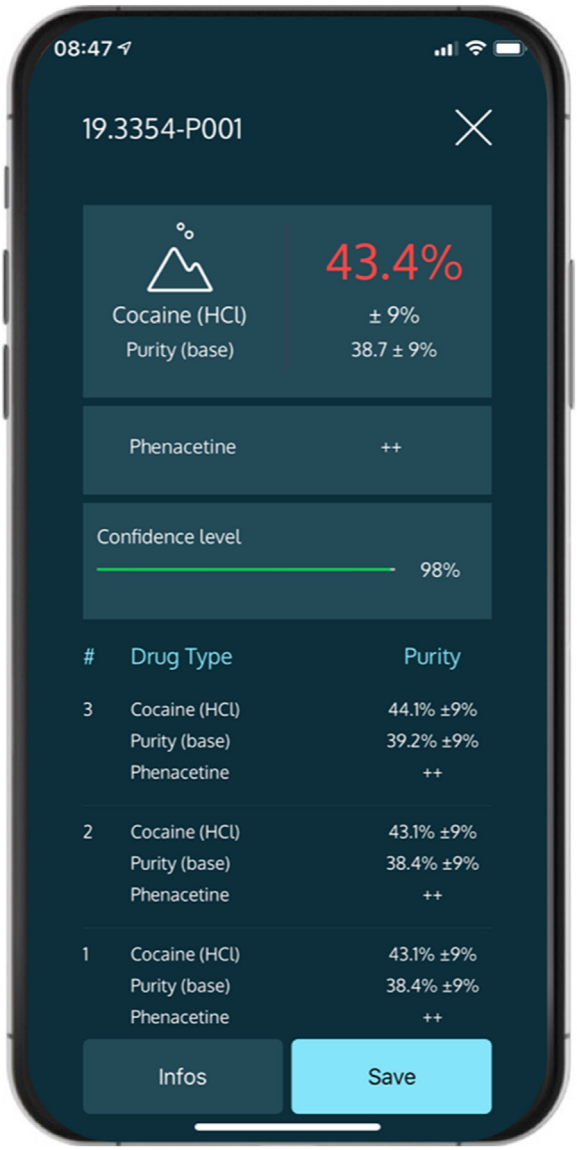

Fig. 5. Screenshot of the mobile application developed to communicate with the MicroNIR device.

To avoid prediction over-fitting, grouped k-fold cross-validation was used (number of splits equal to 5). This method ensures that the replicate measurements (3 per sample) are grouped together during the cross-validation and therefore not split between the calibration and validation datasets.

2.4. Calibration and validation datasets

To evaluate the performance of the MicroNIR chemometric models, a two-step approach was deployed, focusing on qualitative and quantitative performance assessment following an ISO 17025 scheme.

The models were trained on a large collection of unique specimens of cocaine, heroin, and cannabis street samples, as well as cutting agents and other non-illicit substances, seized by the police in the French-speaking part of Switzerland from 2016 to 2020. This allowed collection of as many specimens as possible and, most importantly, maximized the representativity of the illicit-market specimens, in terms of composition and purity.

Because the NIR-based technique is non-destructive, all the specimens were first analysed using the MicroNIR device (three NIR spectra per specimen, obtained from random spots). The composition and purity of the specimens were then determined using our routine, validated, GC–MS method. The results of these analyses constituted the reference dataset. The specimens were further split into two datasets (see Table 1): a calibration and a validation dataset, using the Kennard-Stone selection method [21] in order to maximize the variability of the specimens in each dataset.

2.4.1. Step 1 – qualitative performance assessment

Because it is important to ensure that no alarm is triggered when cocaine, heroin, or cannabis are absent, a qualitative evaluation of the selectivity of the cocaine and heroin detection models was performed. The samples for this evaluation consisted of a set of 182 mixtures of pharmaceuticals and typical cutting agents of various types and concentrations. The sensitivity and selectivity of the cocaine and heroin models were also tested on an external validation set, through the prediction of an additional 610 specimens actually containing cocaine and 184 specimens actually containing heroin that were not used to calibrate and validate the model.

To evaluate the cannabis sensitivity, the 221 cannabis specimens from the validation set were used (see Table 1).

2.4.2. Step 2 – quantitative performance assessment

The quantitative approach is challenging, as the composition of heroin and especially cocaine is complex and changes over time. For cocaine samples, it is not rare to encounter mixtures of four to five different cutting agents [22]. This is a challenge for the NIR technology, primarily because unlike GC and HPLC, no separation step is undertaken. The greater variability of the mixtures encountered must therefore be taken into account when developing the chemometrics models.

To evaluate the performance of the NIR models, the qualitative and quantitative results were compared to those of the reference dataset, which were obtained using the routine, validated, GC–MS method used in our laboratory.

Figs. 7 and 8 illustrate the variety of cutting-agent combinations in cocaine and heroin street samples, respectively, that have been identified using GC–MS. For cocaine specimens, there are no fewer than 321 combinations. This high variability is a challenge for a non-separative method like NIR spectroscopy.

3. Results

3.1. Qualitative evaluation

The confusion matrices illustrated in Tables 2 and 3 present the results obtained for the qualitative assessment of the cocaine and heroin prediction models, respectively.

Of the 2047 specimens containing cocaine only 12 were not predicted containing cocaine by the developed model. The sensitivity for the cocaine model is therefore equal to 0.994, which is excellent considering the number of specimens and their complex and variable matrix.

To measure the sensitivity of the heroin model, out of 600 specimens only 1 was not predicted containing heroin, resulting in a sensitivity of the model equal to 0.998, which is also excellent.

In addition to the sensitivity, it was important to evaluate the true negative rate (selectivity) of both models. Therefore, the 182 mixtures not containing heroin nor cocaine were processed using each model. None of them was predicted containing heroin or cocaine, leading to a general selectivity of the method of 1.00.

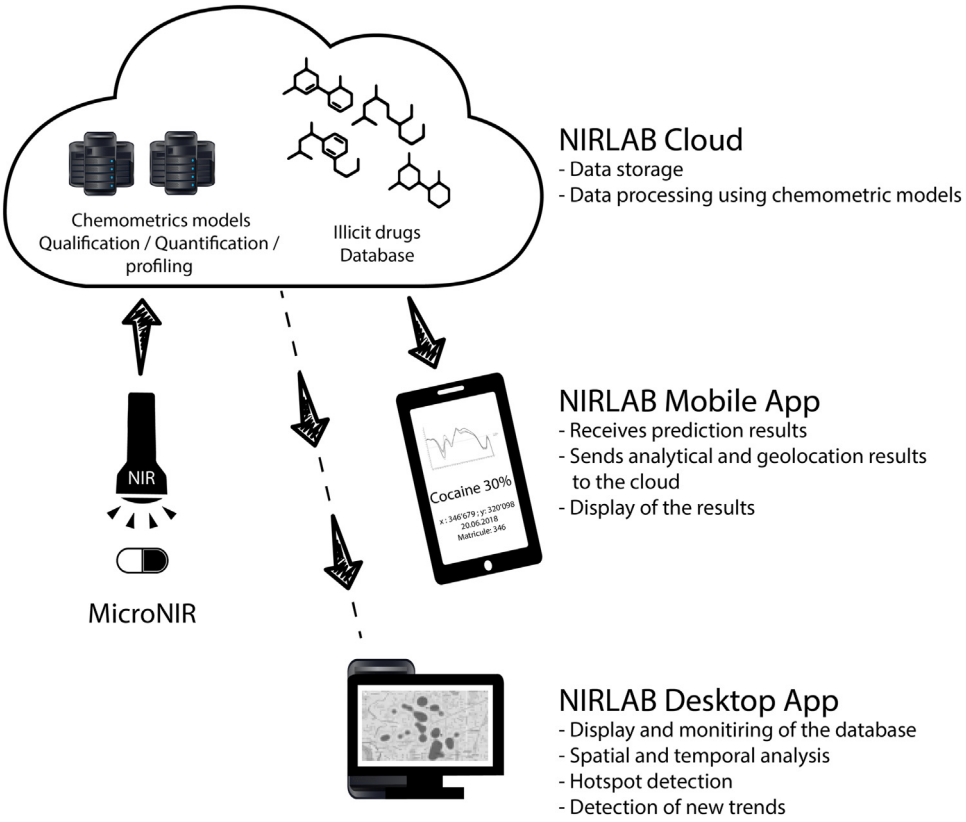

Fig. 6. Illustration of the architecture of the NIRLAB application.

A dedicated statistical model was also developed for the differential identification of THC-type cannabis and CBD-type cannabis. As indicated in Table 1, 244 specimens of THC-type cannabis and 195 specimens of CBD-type cannabis were used to develop the chemometrics model. The selectivity and sensitivity of the model were perfect: all cannabis specimens were identified as cannabis-positive and no false positive were detected. Furthermore, as illustrated in Fig. 9, a perfect separation of the two cannabis populations was achieved with the validation set. Therefore, this functionality was implemented in the MicroNIR, allowing police officers to quickly and reliably test cannabis seizures.

3.2. Quantitative models

When plotting the MicroNIR purity values predicted by the cocaine and heroin models with the reference ones obtained by GC–MS, both values are shown to be in agreement (see Figs. 10 and 11, respectively), illustrating the efficiency of prediction models based on NIR analysis.

The R^2 values corresponding to the heroin and cocaine models are equal to 0.984 and 0.964, respectively. However, as discussed by Bland and Altman [23], the R^2 is not necessary the criterion of choice for assessing agreement between two methods. We have opted to look at the dispersion of the relative error between the NIR prediction model and the reference method (GC–MS). It is apparent that approximately 95% of the results are in the range of ±15%, both for cocaine (Fig. 10) and heroin specimens (Fig. 11). These results are comparable to the relative expended uncertainty obtained during the accreditation of the method (see the part dedicated to the Quantitative Validation under ISO 17025 norm).

3.3. Quantitative validation as requested by ISO 17025 norm

Once the models have been developed and their performance validated, the methodology has been validated using the e-noval (version ENOV-4.1c software) from Pharmalex [24] that tests several widely-recognized validation criteria like: trueness, precision (repeatability and intermediate precision), accuracy, uncertainty of measurements, linearity, limits of quantitation (LOQ) and the purity range.

To provide an overview of the quantification quality, we decided to present the experimental design used as well as the uncertainty that has been measured for the MicroNIR validation. This uncertainty has also been compared with the reference values obtained by the validated GC–MS method.

The design used for this validation was the following: five different levels of purity have been chosen for cocaine (i.e., 20%, 40%, 60%, 80%,100%) and six for heroin (i.e., 5%, 10%, 15%, 20%, 40%, 60%). For each of these levels, four different specimens were selected to best represent the matrix variability present in the heroin and cocaine populations. Tables S1 and S2 in supplementary data list all specimens used in the experimental design. It should be noted that the reference values are those obtained by the validated GC–MS method used in the laboratory. We introduced the inter-user and inter-device variability aspects by providing four different users a microNIR device each (hence four different devices in total) to carry out the analyses. For each analyzed specimen, three replicates were performed, and the average values were introduced in the experimental design. Thus, for cocaine 240 analyses were performed, of which 80 average values were calculated and introduced in the e-noval validation software; for heroin, 288 measurements were made and 96 average values were obtained.

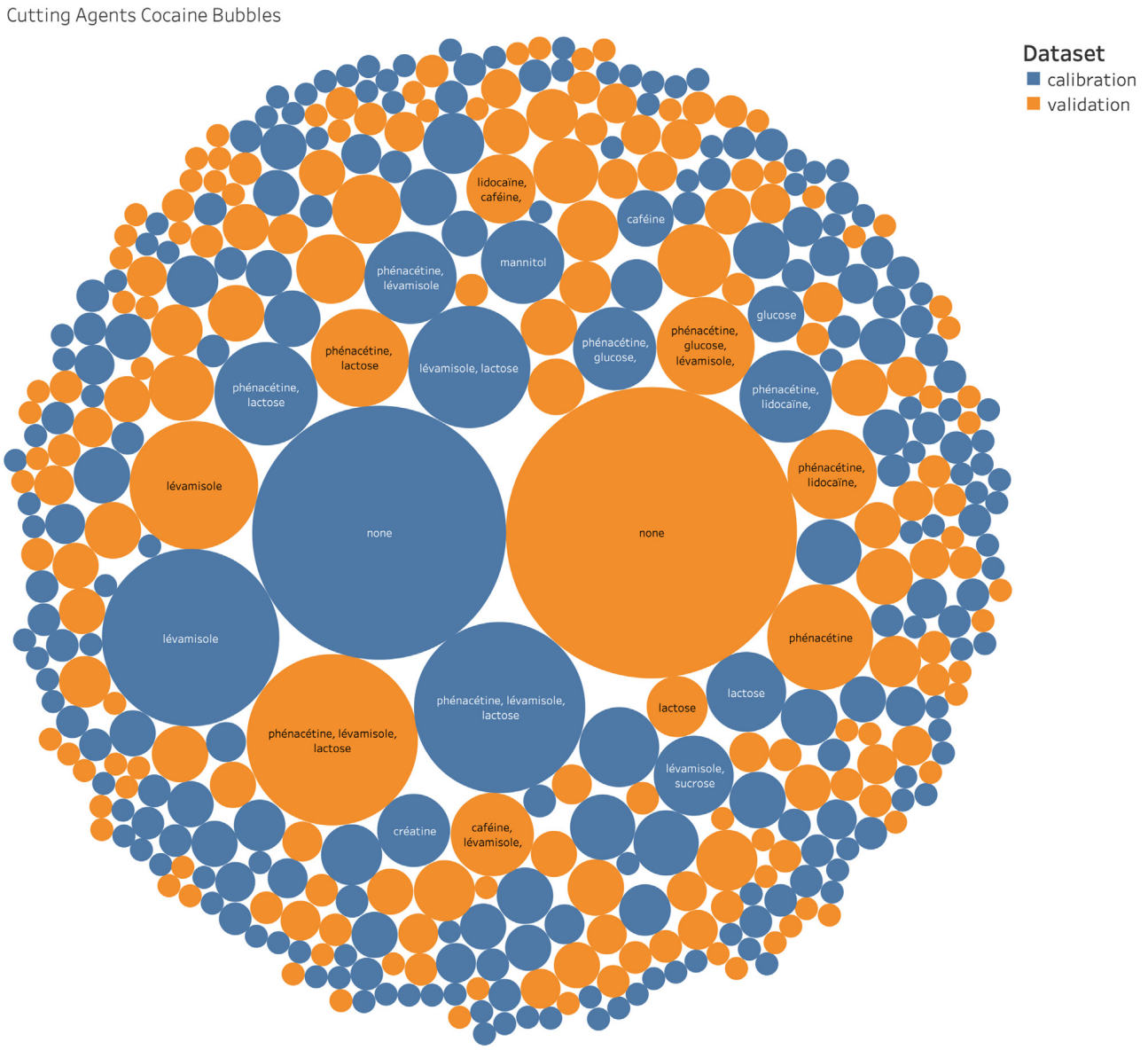

Fig. 7. Schematic illustration of the numerous cutting-agent combinations that were identified by GC–MS analysis of cocaine street specimens. Each bubble represents a specific combination of cutting agents observed in the validation (orange) and calibration (blue) datasets. The bigger the bubble the more prevalent the cutting agent combination. The two largest bubbles represent uncut cocaine specimens. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

The acceptance limits were set at +/− 30% total error for cocaine and +/− 40% total error for heroin. The β-expectation tolerance intervals were computed with a risk of 5%.

Out of the validation results, it can be concluded that the NIR method can advantageously replace the GC/MS for on-site analysis of cocaine and heroin samples. Indeed, the tolerance intervals of samples containing cocaine−HCl between 21.23–98.53% and heroin-base between 11.58–58.83% are comprised in the acceptance limits meaning that 95% of future measurements will have an accuracy (total error) below these limits (see values in Tables 4 and 5). Below these concentrations, the error of prediction is too high and no more acceptable.

Another interesting output is that the majority of the variability of the method comes from the intra-series (repeatability) part of the random error. This suggests that the majority of the random error comes from the sample itself and the way it is presented to the MicroNIR system. The inter-user and inter-equipment errors seem to be very small which is positive for the further deployment of this strategy.

The relative expanded uncertainty (REU) values measured for both heroin and cocaine and heroin specimens have been confronted with those obtained by the ISO 17025 validated GC–MS method used in routine in the laboratory (see Table 6).

3.4. The case of Cannabis Typing

Since 2016, the Swiss legislation regarding cannabis products has evolved: samples characterized by a THC level lower than 1% are considered legal. As a consequence, hundreds of stores are now selling cannabis-based products containing less than 1% THC and various amounts of CBD, a legal active compound [25] used mainly for medical (relaxation, sleep aid) and cosmetic purposes. Resulting from this change of legislation, police forces faced a new issue: “How to quickly determine whether a sample claimed

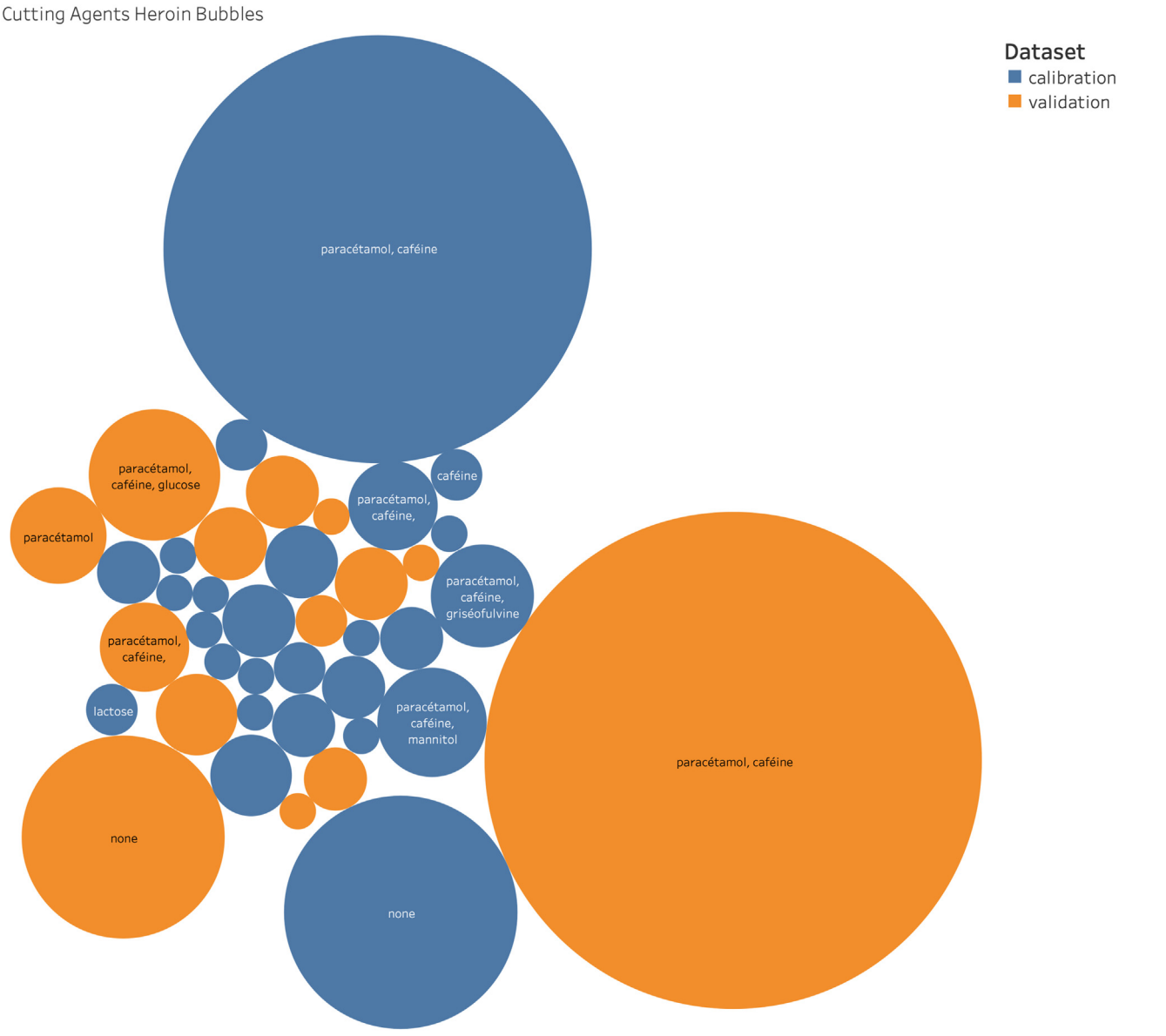

Fig. 8. Schematic illustration of the numerous cutting-agent combinations that were identified by GC–MS analysis of heroin street specimens. Each bubble represents a different combination of cutting agents observed in the validation (orange) and calibration (blue) datasets. The bigger the bubble the more prevalent the cutting agent combination. The two largest bubbles represent heroin cut with paracetamol and caffeine. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

Table 1
Total number of cocaine, heroin, and cannabis street samples seized by the police, as well as their distribution in the calibration and validation datasets, and the purity ranges (obtained by GC–MS).

Substance	Total	Calibration	Validation	Purity Range
Cocaine	1437	966	471	5% - 100%
Heroin	416	246	170	3% - 67%

Substance	Total	Calibration	Validation
Cannabis CBD	293	195	98
Cannabis THC	367	244	123
Total	660	439	221

Table 2
Confusion matrix of cocaine predictions for 2047 specimens (calibration, validation and external validation) of cocaine. P = Positive, N = Negative, TP = True Positive, FP = False Positive, TN = True negative, FN = False negative.

Cocaine (2047 samples)		microNIR		
Non-cocaine (182 samples)		P = 2035	N = 194	
GC–MS	P = 2047	TP = 2035	FN = 12	Sensitivity = 0.994 (TP/P)
	N = 182	FP = 0	TN = 182	Selectivity = 1 (TN/N)

Table 3
Confusion matrix of heroin predictions for 674 specimens (calibration, validation and external validation) of heroin. P = Positive, N = Negative, TP = True Positive, FP = False Positive, TN = True negative, FN = False negative.

Heroin (600 samples)		microNIR		
Non-heroin (182 samples)		P = 599	N = 183	
GC–MS	P = 600	TP = 599	FN = 1	Sensitivity = 0.998 (TP/P)
	N = 182	FP = 0	TN = 182	Selectivity = 1 (TN/N)

to be legal by its owner actually contains less than 1% THC?". Some indicative tests do exist, but the results are difficult to assess, and the procedure is destructive for the questioned sample. Therefore, police officers prefer to send the samples to the forensic laboratory for further analysis. If the specimen is determined to be illicit (i.e., more than 1% THC), the offender is responsible for the analysis costs. On the contrary, the analysis of licit samples is paid for by the State. This situation is not satisfying for both the consumers and the police officers. In this specific scenario, the use of a MicroNIR device combined with a dedicated prediction model could represent a unique and extremely valuable alternative in terms of ease of use, quickness of response and limited cost.

3.5. Routine implementation

Routine implementation of the handheld NIR within a law enforcement unit requires close collaboration with the forensic laboratory. Indeed, it is essential to guarantee the models performance, particularly through the monitoring of the accuracy levels [26]. The continuous performance of the method is assessed by monitoring predictions of control specimens (samples analysed with the reference GC–MS method and resulting in a consensus purity) for each device and by picking random specimens (e.g. 10%) to be analysed by the forensic laboratory with the GC–MS method. The control specimens are analysed periodically and have shown highly stable purity over time.

For both accuracy and calibration monitoring, acceptance criteria have been established, and control charts displaying the bias (the difference between the NIR-predicted value and the expected value) have been produced. For the error during the validation step, a conservative decision limit equal to 15% was chosen.

Specimens that result in a negative prediction by the MicroNIR device will also be sent to the forensic laboratory to determine if they constitute false negatives or if they contain a product that is not yet in the database. In the case of a false negative, the results will be added to the calibration set and the algorithm retrained. For unknown samples, the relevance of adding the product in the models will be assessed. If it is concluded that the product should be added, the algorithms will be tuned in order to recognize it.

3.6. Geo-referencing

As the system is connected to a mobile phone application, it is possible to associate the MicroNIR analysis with the GPS coordinates of the site at which the sample was obtained as well as the timestamp of the analysis. This offers an opportunity to geo-reference the analyses and to report them on a map for forensic-intelligence purposes. Spatiotemporal visualization can indeed provide a way to monitor the appearance of new products on the market or to detect the presence of high-purity samples in a specific area.

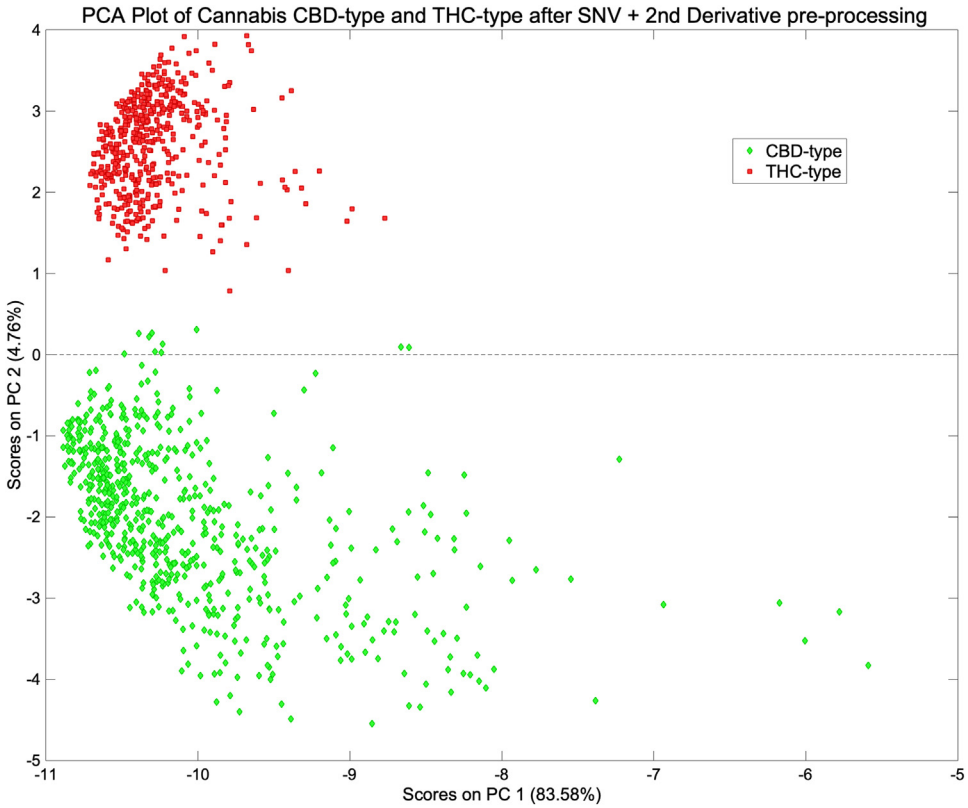

Fig. 9. Separation of the two populations of cannabis, THC (red) and CBD (green), using the scores of the two main principal components obtained by principal components analysis (PCA). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

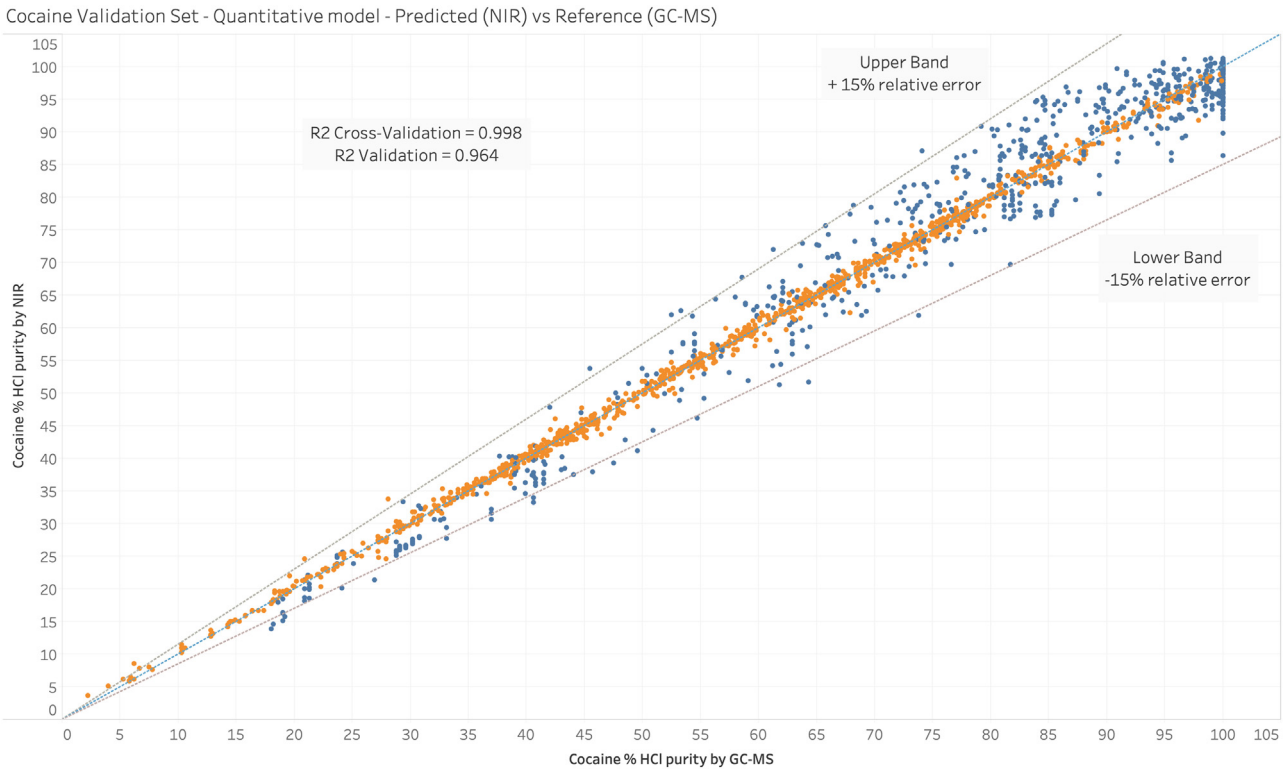

Fig. 10. Correlation of GC–MS quantification and NIR prediction of cocaine purity for the calibration (N = 966, orange) and validation (N = 471, blue) datasets. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

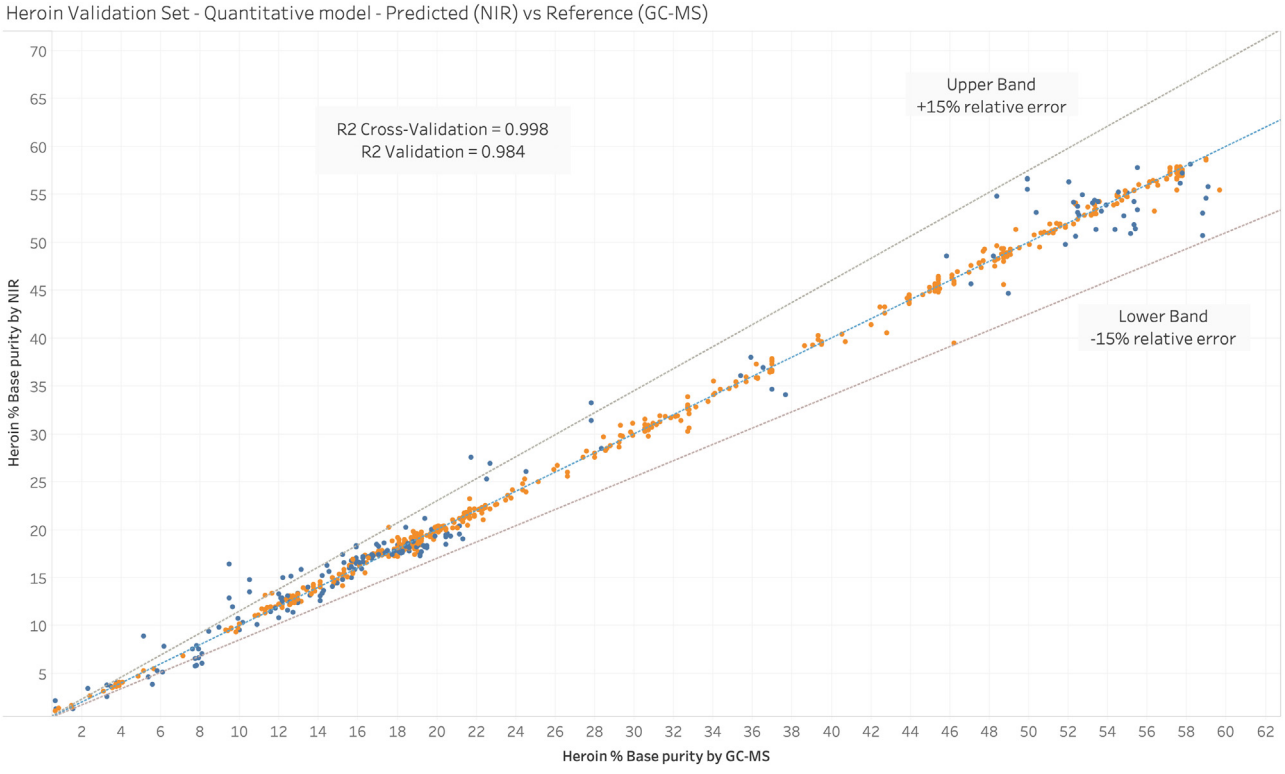

Fig. 11. Correlation of GC–MS quantification and NIR prediction of heroin purity for the calibration (N = 246, orange) and validation (N = 170, blue) datasets. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

Table 4
Validation criteria for the assay of heroin-base.

	Concentration level (%)	Heroin-base
Trueness		
Relative bias (%)	5	39.21
	10	9.03
	15	5.31
	20	−4.46
	40	0.08
	60	−6.94
Intra-assay precision		
Repeatability (RSD%)	5	63.95
	10	15.32
	15	4.04
	20	2.52
	40	4.83
	60	3.85
Between-assay precision		
Intermediate precision (RSD%)	5	63.95
	10	15.32
	15	4.98
	20	2.68
	40	4.83
	60	3.85
Relative expanded uncertainty		
(%)	5	131.8
	10	31.59
	15	10.56
	20	5.59
	40	9.97
	60	7.94
Accuracy		
Relative β -expectation tolerance limits (%)	5	[−101.5, 179.9]
	10	[−24.68, 42.74]
	15	[−6.55, 17.17]
	20	[−10.47, 1.56]
	40	[−10.56, 10.71]
	60	[−15.41, 1.53]

Table 5
Validation criteria for the assay of cocaine−HCl.

	Concentration level (%)	Cocaine-HCl
Trueness		
Relative bias (%)	20	10.87
	40	−3.23
	60	3.22
	80	−0.77
	100	−4.92
Intra-assay precision		
Repeatability (RSD%)	20	7.27
	40	6.04
	60	6.05
	80	3.73
	100	3.34
Between-assay precision		
Intermediate precision (RSD%)	20	7.49
	40	6.04
	60	6.05
	80	3.73
	100	3.34
Relative expanded uncertainty		
(%)	20	15.52
	40	12.45
	60	12.48
	80	7.69
	100	6.88
Accuracy		
Relative β -expectation tolerance limits (%)	20	[−5.76, 27.49]
	40	[−16.51, 10.06]
	60	[−10.10, 16.53]
	80	[−8.99, 7.44]
	100	[−12.26, 2.42]

4. Discussion

The handheld NIR analytical approach proposed in this study brings the laboratory to the field [27,28] and provides users with real-time information about the type and the purity of the product investigated. It has been very useful in helping law enforcement organizations decide whether to proceed with investigations. One illustration of its application is the quick determination of cannabis type (i.e., illegal or legal regarding the Swiss legislation) in the field, an efficient and cost-effective answer to a challenge that has arisen in Switzerland since the legalisation of cannabis with THC content lower than 1% in 2016. Rapid, on-site NIR predictions coupled with a mobile phone application provide a clear and reliable answer that quickly provides law enforcement officers with information about the follow-up associated to a questioned specimen, while avoiding systematic analysis by the forensic laboratory. Among the advantages offered by such a system, in comparison to other approaches (e.g. colorimetric testing), are the non-destructive character of the analysis (no substance is destroyed during testing) and the ability to provide more than just a colorimetric answer, thanks to the combination of qualitative data, quantitative data, and geolocation information. Considering that one analysis takes only a few seconds, and that the answer is reported as quickly to the police officer, portable NIR spectroscopy is a promising approach to on-site drug analysis.

This technological improvement will also deeply transform the role of the traditional laboratory. We do not foresee the disappearance of laboratories, but rather laboratories taking on new roles consisting of more challenging and less routine activities. Indeed, one reason for the long response time of laboratories is the high workload generated by the need to perform “routine” qualitative and quantitative analyses; for example, the vast majority of illicit drug samples seized by Swiss police are cocaine and heroin. These “routine” analyses highly affect the time that forensic experts can spend on more interesting cases (e.g. identification of new psychoactive substances, extraction of illicit drugs impregnated in clothes). An approach combining routine field analyses with laboratory analysis of special samples only offers the experts an opportunity to focus on more challenging forensic cases that allow them to fully deploy their expertise.

Timely analyses allow the laboratory to respond to urgent requests from people in the field and become a key player in the system. Because the laboratory in this decentralized environment is responsible for the quality of the results, it is its duty to monitor the handheld device analytical response and continuously train the chemometrics models when new psychoactive substances or cutting agents appear on the market. We believe that this approach will reinforce the ties between law enforcement organizations and the forensic laboratory, which is essential if the laboratory is to take into account the needs and preoccupations of police officers and prosecutors. Furthermore, this approach also promotes the experts’ skills and

Table 6
Comparison of Relative Expanded Uncertainty (%) for MicroNIR quantification versus reference GC–MS quantification method.

Cocaine MicroNIR method		Cocaine ISO 17025 validated GC–MS method	
Concentration (%)	Relative Expanded Uncertainty (%)	Concentration (%)	Relative Expanded Uncertainty (%)
$21.2 \leq C < 40.5$	15.5	$1.15 \leq C < 5.5$	17.0
$40.5 \leq C < 81.6$	12.5	$5.5 \leq C < 69.8$	10.0
$81.6 \leq C \leq 98.5$	7.7	$69.8 \leq C < 87.3$	13.0
Heroin MicroNIR method		**Heroin ISO 17025 validated GC–MS method**	
Concentration (%)	Relative Expanded Uncertainty (%)	Concentration (%)	Relative Expanded Uncertainty (%)
$10 \leq C < 15$	31.0	$1.2 \leq C < 4.5$	24.0
$15 \leq C < 58.8$	10.0	$3.9 \leq C < 7.7$	11.0
		$7.7 \leq C \leq 63.8$	6.0

contribution and, by removing routine cases from their workload, frees up time for them to propose new development in the field. This portable solution paves the way for new opportunities in drug enforcement, by virtue of its ability to associate geolocation data with analytical results in real time, and to identify hot spots and the introduction of unusual products. Moreover, the implementation of this rapid and simple analytical technique makes it possible to collect information on all seized specimens. Using an ultra-portable system connected to smartphone breaks the barriers of cost associated with the illicit drugs analysis and offers a full vision of the totality of the samples seized. It is thus possible to better monitor the illicit market and rapidly detect new trends or modifications of the market structure (e.g. change in the purity of an illicit drug or emergence of a new illicit drug in a specific area).

The qualitative assessments of the MicroNIR performance demonstrates its efficiency to identify illicit drugs. It is important to mention that these assessments were performed by considering a large dataset of street samples. This was especially true for the qualitative assessment for which a total of 2047 specimens of cocaine, 600 specimens of heroin and 660 specimens of cannabis were used. Even if the selectivity and sensitivity are high, it has to be mentioned that the system recognizes only the substances that have been used to train the algorithms.

Therefore, if a new, unknown, product (like new psychoactive substances (NPS)) is analysed by the system, it will not be recognized by it. This is also true regarding the amount of an illicit substance present in the analysed matrix. If, for example, traces of cocaine are present in a questioned specimen (i.e. 1–2% of cocaine mixed with a cutting agent), it is highly unlikely that the models will be able to recognize the specimen as containing cocaine. The situation is similar with traces of fentanyl mixed with sugar. If the proportion of the substance of interest is too small (approximately below 3%), the system will not be able to detect it. Despite these limitations, this approach can recognize the majority of the "classic" illicit drugs present on the street. Consequently, it frees up precious time for the forensic laboratory, which can hence focus on the analysis of unusual specimens. Once a new compound or mixture is identified, it can be added to the chemometric models and enrich the analytical potential of the handheld tool. This is particularly valuable given that the algorithms and the databases are remotely hosted (i.e.in t he cloud). This is an essential feature, as the illicit-drug market changes rapidly (e.g. emergence of new products, changes in the purity of a specific illicit drug) and it is consequently expected that the model will require regular updates. However, thanks to the centralization of the database and to cloud processing, users will always be using the latest version of the models.

For the quantitative assessment of the methodology, the results also illustrate the ability of the prediction models to accurately predict the purity of questioned specimens, with uncertainties close to these obtained with the validated GC–MS method, considered as a reference. Such results are not trivial to achieve, as street-drug seizures are highly variable in terms of purity and composition. As mentioned above, the prediction models must be periodically updated to reflect the current street market profile. Such an update has to be performed in close collaboration with a forensic laboratory that has the analytical capabilities to identify NPS or new cutting agents. This illustrates how collaboration between field-users and the laboratory could take place.

Another application that could be developed by exploiting the MicroNIR results concerns its potential to highlight similarities between specimens that could be used in a profiling perspective [3]. Again, the idea is not to replace the profiling approach based on large databases but to provide rapid information about the similarity between two samples and promote the use of profiling information in a law-enforcement context. Currently, it must be admitted that the use of profiling information faces problems related to the response time as well as police priorities. When a link between two seizures is highlighted but the results take two months to obtain or are not a priority for the police, the information will simply be filed without further investigation. On the other hand, the MicroNIR approach allows automatic comparison of the NIR spectra from two specimens. If the analysis indicates that the spectra are indistinguishable, there is a high probability that the specimens are similar. This could motivate a police officer to submit the specimens to the laboratory for confirmatory analysis and the production of an analytical report. This constitutes a shift from the current approach, which focuses on the construction of a huge database of illicit-drug profiles, to a more pragmatic vision centred on case-to-case analysis. At the moment, the situation is unsatisfactory, and the great majority of links is not investigated, either because they do not fit the priorities of the criminal investigation or because the information is reported after the case has already been closed. At the moment, the potential of MicroNIR for profiling purposes has still to be demonstrated and evaluated, but it could be an important and valuable development for the methodology.

Finally, as described above, the use of this handheld technology creates new opportunities for illicit-drug analysis. The results are reliable, rapid, and directly available through a mobile application. Moreover, given the current digital revolution, it is also important for forensic laboratories to move in this direction and provide applications that not only fit the information requirements of users, but also promote closer collaboration with law enforcement organizations and other stakeholders on the adoption of problem-oriented and intelligence-led strategies [19]. This paves the way for laboratories fully exploiting the possibilities of their data and bringing real value-added knowledge to their customers.

5. Conclusion

The democratization of portable and handheld analytical technologies that can deliver rapid and accurate information to law enforcement officers during their investigations opens the door to a new type of activity for the forensic laboratory. It also stimulates reflection within forensic laboratories regarding their role and the best way to enhance their results and adopt a more relevant and central role. Furthermore, it is an excellent opportunity for the laboratory to reconnect with police investigations and intelligence, something that has been neglected for many years [19]. In this study, we demonstrated how an approach based on a portable NIR device can be applied to cocaine, heroin, and cannabis street samples. By providing qualitative and quantitative information, as well as by helping answer the question of the legality of a seized sample, this approach clearly presents advantages over conventional protocols and helps filling the gap between police forces on the street and the forensic laboratory.

We believe it is essential to initiate this change to the way forensic laboratories consider their tasks and their roles. By failing to undertake these transformations, it is likely that forensic laboratories will experience difficult times.

CRediT authorship contribution statement

Florentin Coppey: Writing - review & editing, Software, Conceptualization, Methodology, Investigation. **Andy Bécue:** Writing - review & editing, Supervision. **Pierre-Yves Sacré:** Conceptualization, Methodology, Investigation. **Eric M. Ziemons:** Conceptualization, Methodology, Writing - review & editing. **Philippe Hubert:** Conceptualization, Methodology, Investigation. **Pierre Esseiva:** Writing - review & editing, Supervision, Methodology, Conceptualization.

Declaration of Competing Interest

The authors report no declarations of interest.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at https://doi.org/10.1016/j.forsciint.2020.110498.

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