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Development and evaluation of portable NIR technology for the identification and quantification of Australian illicit drugs

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ABSTRACT

The efficient and accurate analysis of illicit drugs remains a constant challenge in Australia given the high volume of drugs trafficked into and around the country. Portable drug testing technologies facilitate the decentralisation of the forensic laboratory and enable analytical data to be acted upon more efficiently. Near-infrared (NIR) spectroscopy combined with chemometric modelling (machine learning algorithms) has been highlighted as a portable drug testing technology that is rapid and accurate. However, its effectiveness depends upon a database of chemically relevant specimens that are representative of the market. There are chemical differences between drugs in different countries that need to be incorporated into the database to ensure accurate chemometric model prediction. This study aimed to optimise and assess the implementation of NIR spectroscopy combined with machine learning models to rapidly identify and quantify illicit drugs within an Australian context. The MicroNIR (Viavi Solutions Inc.) was used to scan 608 illicit drug specimens seized by the Australian Federal Police comprising of mainly crystalline methamphetamine hydrochloride (HCl), cocaine HCl, and heroin HCl. A number of other traditional drugs, new psychoactive substances and adulterants were also scanned to assess selectivity. The 3673 NIR scans were compared to the identity and quantification values obtained from a reference laboratory in order to assess the proficiency of the chemometric models. The identification of crystalline methamphetamine HCl, cocaine HCl, and heroin HCl specimens was highly accurate, with accuracy rates of 98.4 %, 97.5 %, and 99.2 %, respectively. The sensitivity of these three drugs was more varied with heroin HCl identification being the least sensitive (methamphetamine = 96.6 %, cocaine = 93.5 % and heroin = 91.3 %). For these three drugs, the NIR technology provided accurate quantification, with 99 % of values falling within the relative uncertainty of ±15 %. The MicroNIR with NIRLAB infrastructure has demonstrated to provide accurate results in real-time with clear operational applications. There is potential to improve informed decision-making, safety, efficiency and effectiveness of frontline and proactive policing within Australia.

1. Introduction

The capacity for law enforcement to rapidly identify and quantify illicit drug seizures outside of forensic laboratories remains a constant challenge; particularly with the continuous rise in the amount of drugs seized [1]. Improving the current capabilities to obtain cost-effective and timely forensic information for investigative and intelligence activities is driving the decentralisation of the forensic laboratory [2]. Accordingly, there has been an influx in the establishment of in-field methods and techniques for illicit drug analysis. The preliminary identity of suspected drugs is commonly established through the use of colour tests [3]. However, a variety of analytical instrumentation exist and are used in different in-field contexts for identification (both for presumptive and confirmatory identification) based on different agencies and resources. These include ion mobility spectroscopy [4], Fourier-transform infrared (FTIR) spectroscopy [5], Raman spectroscopy [6], nuclear magnetic resonance (NMR) spectroscopy [7], electrochemical sensors [8] and various portable iterations of mass

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spectrometry techniques such as ambient ionisation techniques [9] or coupled to gas or liquid chromatography [3,10].

As has already been established elsewhere [3,10], these techniques have various limitations. Colour tests, sensors and spectroscopy techniques typically provide rapid results, but the former two have been criticised for their limitations in application and selectivity, and the latter often requires an increased level of expertise and experiences difficulty identifying more than one component at a time. Mass spectrometry techniques can require lengthy or intensive sample preparation methods (including harmful reagents), consist of long analysis times, complex interpretation and typically destroy the sample in the process [11].

Near-infrared (NIR) spectroscopy is an increasingly popular technique for in-field forensic drug identification and quantification [12]. Together with machine learning models via chemometric analysis, NIR spectroscopy can provide robust qualitative and quantitative information on suspected drug seizures [11]. NIR devices can be hand-held (readily miniaturised), fast, highly cost-effective (compared to other portable analytical techniques [13,14]) and accurate when combined with chemometric modelling [15]. Furthermore, it is easily integrated into current forensic workflows to ensure efficiency and validity to the sampling process; where drug identification and purity can have implications on subsequent forensic sampling processes [15]. NIR analysis is non-destructive, requires no sample preparation and can be done through a transparent material such as glass or plastic [13,14]. The preference for NIR as opposed to other spectroscopic techniques is its capacity to capture complex spectral data (in the form of combination bands and overtones) without any sample preparation by devices that are more readily miniaturisable and often cheaper compared to FTIR or Raman [14]. Issues in discerning polydrug mixtures by spectroscopic techniques can be overcome by the deconvolution of spectral data by chemometric modelling, which is readily compatible with NIR analysis [16].

The use of NIR spectroscopy in combination with chemometric modelling for identification and quantification of illicit drugs has been used in different countries, achieving highly selective and sensitive results [11,13,17,18]. Different chemometric models with different NIR spectrometers have been developed for cannabis, cocaine, heroin, methamphetamine, 3,4-methylenedioxymethamphetamine (MDMA) and other drugs to a lesser extent (such as ketamine or new psychoactive substances (NPS)) [12,13,19,20]. The MicroNIR (a NIR spectrometer) combined with chemometric models developed by the University of Lausanne (UNIL), have demonstrated high sensitivity and selectivity (achieving over 99 % in all instances) for cannabis, heroin base and cocaine hydrochloride (HCl). Furthermore, the quantification within certain purity ranges of heroin base (11.58 – 58.83 %) and cocaine HCl (21.23 – 98.53 %) were found to be within acceptable limits (95 % confidence interval) [11].

However, the application and success of NIR chemometric analysis is highly dependent on building specific databases of relevant and known specimens. Chemometric models need to encompass a variety of sample characteristics, such as how a sample is scanned (direct contact or through a transparent medium such as plastic), chemical form (free base or salt form), colour of specimen and NIR device. The effectiveness of MicroNIR chemometric models, which have been built using European drug data, for drugs found in Australia remains unknown due to the absence of testing in Australian contexts. For example, within Australia, heroin is typically in the HCl salt form, and high purity crystalline methamphetamine is commonly seized [1], both of which are drug characteristics not currently optimised within the chemometric models developed with the MicroNIR. Hence, this study focused on the gap in MicroNIR implementation, specifically assessing its performance on chemically unique Australian drugs.

This study aimed to optimise and assess the implementation of NIR spectroscopy combined with machine learning models to rapidly identify and quantify illicit drugs within an Australian context. Specifically, this relates to developing crystalline methamphetamine HCl, cocaine HCl and heroin HCl qualitative and quantitative chemometric models.

2. Materials and methods

2.1. Specimen dataset

Existing chemometric models were optimised using NIR spectra collected from a convenience sample[1] of Australian illicit drug specimens (n=608). These specimens consisted of drugs previously seized and analysed by the Australian Federal Police (AFP) through standard crime scene processing (n=302) and state-based seizures via the AFP Enhanced National Intelligence Picture on Illicit Drugs (ENIPID) program (n=306) (process summarised in Fig. 1). The main drugs scanned consisted of crystalline methamphetamine HCl (n=314), cocaine HCl (n=184), heroin HCl (n=81). A variety of other substances (n=29) were also scanned in the interest of assessing the accuracy and selectivity of the chemometric models based on Australian drug seizures (see Supplementary materials for further details).

The true identity and quantification of these specimens was established by a combination of analytical techniques routinely conducted by the AFP and the National Measurement Institute (NMI). The following analytical techniques, validated and accredited according to ISO 17025, were used to accomplish this: FTIR, gas chromatography – mass spectrometry (GC-MS), liquid chromatography – mass spectrometry (LC-MS), and NMR. The recorded NIR spectra were pre-processed the same way as spectra already included in the UNIL database (see Section **2.4** Data pre-treatment, modelling and analysis for details), consisting of more than 45,000 NIR spectra of illicit drugs, medicines and common cutting agents. Newly scanned Australian drugs were collated with their true identities and quantification values provided by NMI and used to test existing chemometric models previously established by the NIRLAB database. Based on initial testing, the need for chemometric model development was evident. The results presented here are the product of the optimised chemometric models. The drug seizures sampled were diverse in terms of drug type, purity and adulteration to mimic drug seizures commonly seized by the AFP (see Fig. 2 for the composition of purity captured within this dataset based on the reference laboratory results). Herein, purity refers to the percentage of the main drug present within the specimen. The dataset was split into training (2/3) and validation (1/3) datasets for chemometric model optimisation.

The average, median, range and interquartile (IQR) range of purities for these drugs were: methamphetamine ($\bar{x}$ = 72.8 %, median = 80.0 %, 4.3–80.8 % and IQR = 77.6–80.3 %), cocaine ($\bar{x}$ = 65.9 %, median = 76.7 %, 6.1–87.5 % and IQR = 63.1–78.7 %) and heroin ($\bar{x}$ = 56.0 %, median = 70.2 %, 1.0–85.0 % and IQR = 30.8–77.8 %). These purities will be used to assess the accuracy of the machine learning model predictions.

2.2. NIR spectrometer

NIR spectra collection was accomplished by the MicroNIR Onsite W 1700 (Viavi Solutions Inc). The MicroNIR is ultracompact and lightweight; it uses two vacuum tungsten lamps for illumination, a linear variable filter as a dispersing element and the detector is a 128 pixel indium gallium arsenide (InGaAs) photodiode array. It operates within the 950 – 1650 nm NIR spectral range with a measurement time of 0.25 – 0.5 seconds, signal-to-noise ratio of 25,000:1, integration time of 10 ms and collects 125 data points.

[1] Convenience sampling within this work refers to accessing specimens that were available at the time of data collection. Specifically, they were historic illicit drug seizures that were held and accessible at AFP.

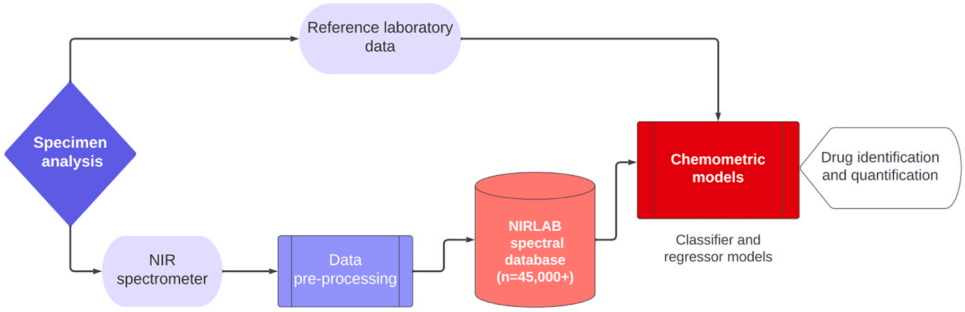

Fig. 1. Summary of the workflow for chemometric model output, involving the compilation of NIR spectra and reference laboratory data collected from diverse police seizures of illicit drugs.

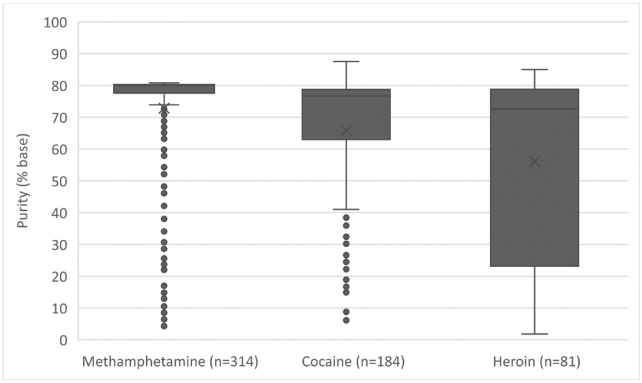

Fig. 2. Box and whisker plots representing the spread of purity (represented as free base form of drug) captured across methamphetamine, cocaine and heroin specimens as established by the reference laboratory (NMI). The purity was reported as 1.0 % when the purity was too low or too many adulterants were present to accurately quantify but the relevant drug was identified.

2.3. Sample collection

Specimens were scanned in triplicate (different spots/shaking between scans) by placing the NIR spectrometer on top of the specimen, pointing downwards. The same specimen was scanned by different types of contact between the NIR spectrometer and the specimen, and was scanned in different physical forms. This was to facilitate the most accurate optimisation of the chemometric models, that could be specific to specimen characteristics. There were two contact types: (1) direct contact between the MicroNIR and the drug specimen and (2) scanning the drug specimen through a low-density polyethylene sample bag. Low-density polyethylene sample bags produce a NIR signal that is interpretable; specific chemometric models were optimised by drug type that accounted for this signal in combination with the NIR signal produced by the drug being scanned (as opposed to subtraction of sample bag signal from the overall NIR spectrum). There were also two different physical forms scanned: non-homogenised and homogenised (homogenisation was achieved using a mortar and pestle).

Where possible all contact types and physical forms were scanned for one particular drug specimen. In some cases this was not possible. For example, where specimens were homogenised from standard operating procedures before scanning with the NIR device. Additionally, some plastic bag specimens were unable to be opened for direct contact scans due to restrictions relating to the chain of custody. Table 1 shows the breakdown of the type of spectra collected for each contact type and physical form.

2.4. Data pre-treatment, modelling and analysis

The raw spectral data collected from the MicroNIR was pre-processed for each drug type using a combination of standard normal variate (SNV) and/or Savitzky-Golay 2nd derivative (polynomial order = 2, window size = 3) [21]. This was done to reduce the influence of the instrument and transform the spectral data to a more appropriate format for the chemometric models [11]. Chemometric models were developed using the scikit-learn library (v.1.3.2) in Python [22]. The chemometric models first compared the scanned spectra against the database of illicit drug NIR spectra and assessed for similarity and outliers before being processed to produce an identification and a quantification (if possible). The entire NIR spectrum was analysed for this purpose, although regions of interest were specified, where diagnostic spectral details were examined for identification confirmation and quantitative analysis. Various algorithm combinations are employed across different drugs, including extremely randomised tree methods and gradient-boosting classifier and regressor methods. Identifications were typically reportable above 60 % confidence level and above the threshold of local outlier factor algorithm output, specific to each drug. Quantification values were only provided when the confidence level was 80 % or above (i.e. the number of scans identified as a drug does not equal the number of scans quantified). Within this work, sensitivity is defined as the percentage of true positive results predicted by the NIR technology, based on the total number of results that were actually positive (as identified by the reference laboratory). Accuracy is defined as the sum of the true positive and true negative predicted results as a percentage of the total number of results (i.e. the sum of true positive, true negative, false positive, false negative). Spectral and other data visualisations were made using a combination of Microsoft Excel (v.2305), Unscrambler (v.10.5.46461.632), Matlab PLS toolbox (v.9.2) and Tableau (v.2022.4.3)

Table 1
Composition of the NIR spectra collected within this study across different contact types and physical forms. This is inclusive of the three drugs targeted for chemometric model development (methamphetamine, cocaine, heroin) and all other drugs scanned for selectivity.

Physical form and contact type	Scans (n=3673)	Percentage (%)
Homogenised - plastic bag	1802	49.3
Homogenised - direct contact	883	24.0
Non-homogenised - plastic bag	369	10.3
Non-homogenised - direct contact	369	10.6
Other †	250	5.7

† Other physical forms scanned included: brick, bud, paper, pill and wet paste. Other contact types included: rigid plastic and glass.

2.5. Operational application

The methamphetamine specimens from the ENIPID specimens (n=188) were also compiled to assess the operational application of the MicroNIR with NIRLAB infrastructure. These specimens consisted of a broad range of purity and represented street-level specimens that are

typical of the drug distribution chain at the consumption level. This analysis consisted of a geographical examination to demonstrate the real-time investigative and intelligence capabilities of this technology from frontline implementation. Given that convenience sampling was employed to obtain drug specimens, only methamphetamine specimens are visualised here, to avoid a biased comparison with the other drugs captured. As with all specimens collected within this study, the drugs were obtained from previous seizures stored at AFP and scanned by the NIR spectrometer in the laboratory setting. Geographical information was then related based on case information via the postcode.

3. Results

The MicroNIR was successfully used to analyse 608 illicit drug specimens. The regions of interest for chemometric analysis were identified across the three drugs: crystalline methamphetamine HCl (1120 – 1200 nm, see Fig. 3 for example), cocaine HCl (1080 – 1250 nm) and heroin HCl (1100 – 1260 nm). The pre-processed spectra for crystalline methamphetamine HCl, cocaine HCl and heroin HCl for all specimens scanned within this study can be found within the Supplementary materials. There was a variable purity range across the methamphetamine, cocaine and heroin specimens sampled by the MicroNIR (Fig. 2). Methamphetamine purities were the highest and most closely clustered, and heroin the least within the specimens captured within this study.

3.1. Qualitative result summary

3.1.1. Drug identity performance

Across the drugs examined by the NIR technology, no false positives were detected; all specimens that were not cocaine HCl, crystalline methamphetamine HCl and heroin HCl were identified as such (true negative rate = 100 %). Overall, the accuracy was high for all three drugs (see Fig. 4): crystalline methamphetamine HCl (98.4 %), cocaine HCl (97.5 %) and heroin HCl identification (99.2 %). However, differences were observed when the sensitivity of the three drugs were examined. The best performance was observed by crystalline methamphetamine; 96.6 % of the 1735 NIR scans of crystalline methamphetamine HCl were correctly identified and 3.4 % were false negatives. Cocaine HCl identification also performed well, which is related to the high number and diversity of cocaine HCl specimens that have already been captured within the UNIL database of NIR spectra. Of the 1406 NIR scans of cocaine HCl specimens, 93.5 % were correctly identified as cocaine HCl and the remaining 6.5 % of cocaine HCl scans were false negatives. The least successful identification occurred with heroin; out of the 345 scans of heroin HCl specimens, 91.3 % were correctly identified, while 8.7 % resulted in false negatives. For all three drugs, the false negative results were either reported as an unknown result or the major adulterant present was identified (i.e. the most abundant compound in that specimen). Considering the 100 % true negative rate, henceforth only the true positive and false negative rates will be compared for simplicity. For the drugs scanned other than methamphetamine, cocaine or heroin, there was never a false positive.

3.1.2. Comparison of contact types and physical forms

In order to obtain the most accurate results, the chemometric models were optimised to specific contact types and physical forms (see Fig. 5). The ability to input the contact type and physical form of the drug specimen and utilise algorithms that are specific to those parameters enables the most successful predictions. Hence there was a focus within this study to scan the same drug seizure by direct contact and through plastic bags, as well as in both homogenised and non-homogenised forms of the drugs wherever possible. For the drugs scanned by different contact types, direct contact produced the highest sensitivity (98.4 % true positive) with only a small number of false negatives (1.6 %). Drug specimens scanned through plastic bags observed a larger percentage of false negatives (7.4 %) but were still highly sensitive (92.6 % true positive). For the comparison of physical forms, specimens that were non-homogenised had a lower percentage of false negatives than specimens that were homogenised (0.7 % compared to 6.6 %, respectively). Overall, the sensitivity was high across non-homogenised and homogenised specimens (99.3 % and 93.4 % true positives, respectively).

3.2. Quantitative result summary

The final optimised quantification chemometric models for cocaine HCl, crystalline methamphetamine HCl and heroin HCl demonstrated accurate purity predictions (see Fig. 6). For each of the three drugs examined within this study, 99 % of results were quantified within the relative uncertainty ±15 % base purity (within respective drug types). Furthermore, there was good correlation between the reference laboratory purity value (i.e. the true value) and the purity predicted by the chemometric models utilising NIR data. The R^2 values were highest for methamphetamine (0.981), followed by cocaine (0.940) and heroin (0.834). There was no notable separation in quantification between contact types across the three drugs. Some separation was observed for cocaine; direct contact scans slightly overestimated purity and plastic

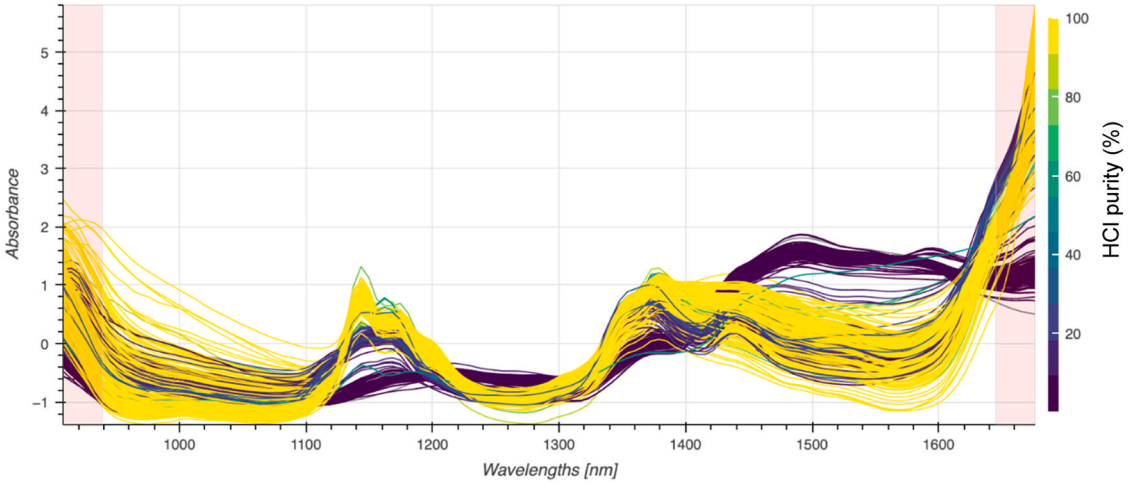

Fig. 3. Overlaid NIR spectra of crystalline methamphetamine HCl specimens (direct contact only) visualised by HCl salt purity. Raw NIR data was pre-processed by SNV.

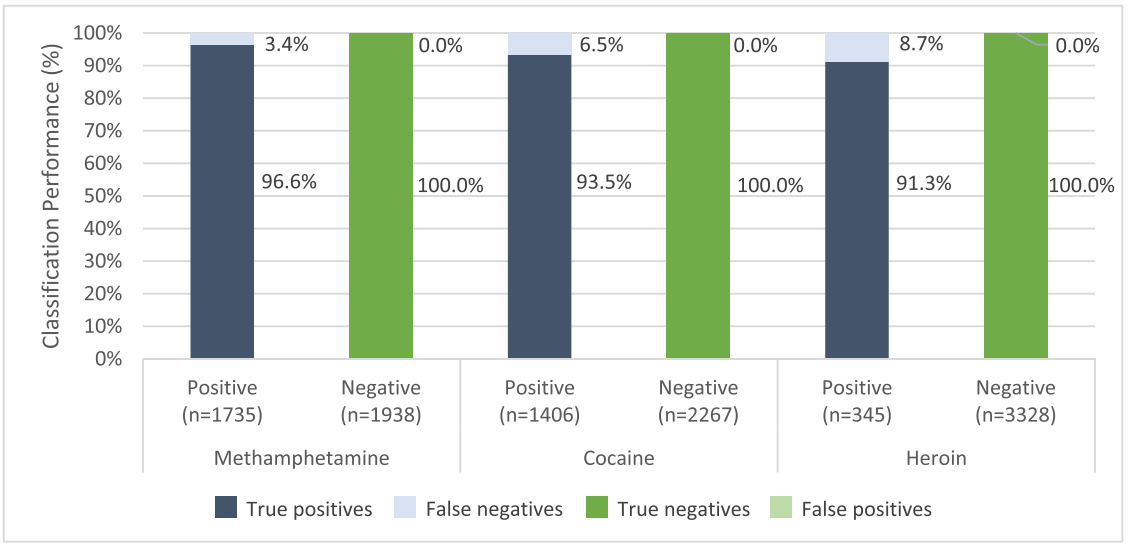

Fig. 4. Visualisation of confusion matrix demonstrating the classification performance for crystalline methamphetamine HCl, cocaine HCl and heroin HCl. Positive and negative columns are based upon reference laboratory identification with series within the columns representing whether the predicted identity by the NIR technology was true or false.

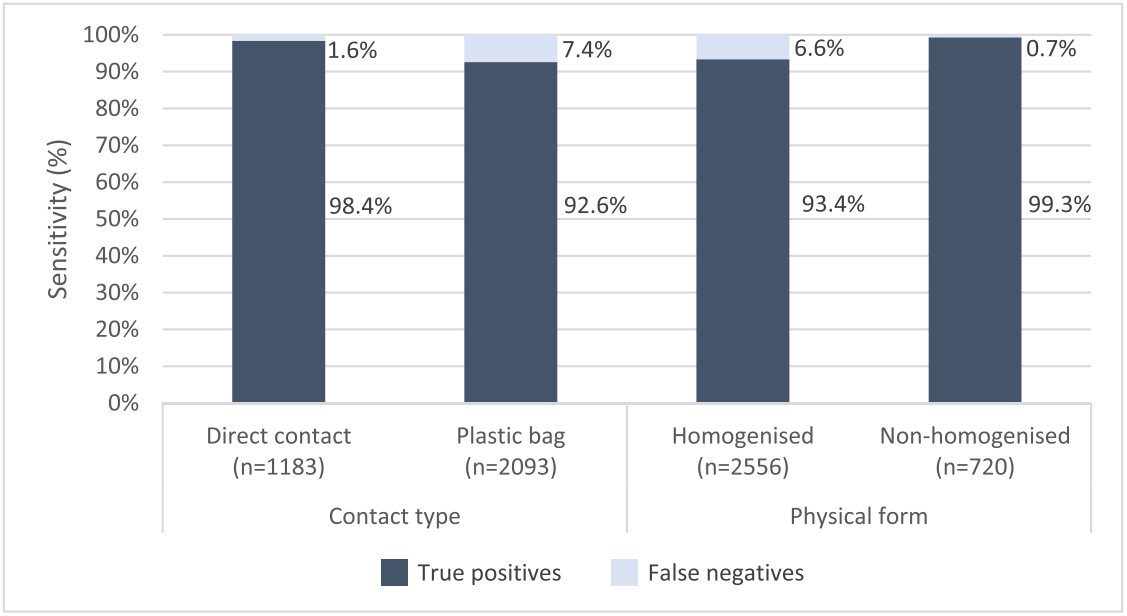

Fig. 5. Comparison of sensitivity of identification across different physical forms and contact types for crystalline methamphetamine HCl, cocaine HCl and heroin HCl specimens (other drugs scanned as well as different specimen forms/contact methods are removed).

bags underestimated purity. However, this was still largely within the relative uncertainty limits.

3.3. Operational application

A geographical analysis of the methamphetamine specimens by the NIR technology was accomplished (see Fig. 7). The average purity of methamphetamine specimens captured was high (77.3 % base purity) and does not appear to vary much across the region examined. When examining the number of methamphetamine seizures it was unsurprising to find the frequencies concentrated in the centre of the city examined here. However, a number of hotspots are highlighted; the largest number of seizures within a postcode captured in this sample occurred on the north-western corner of the city examined. Other points of interest include seizures where the average purity across the postcode is low which highlights more distinctive behaviour among the actors within the drug distribution chain. While this information can be obtained by traditional analytical methods (i.e., mass spectrometry), this example application demonstrates the capacity of NIR technology to accomplish this proactively and in real-time. The collection of geolocation data in the field and the automated workflow make this information instantly accessible to decision-makers, eliminating the wait for transport, laboratory processing times, and manual data collation and summarising tasks. The application of NIR technology in this way facilitates real-time decision-making.

4. Discussion

The MicroNIR with NIRLAB infrastructure examined here showcased the potential to increase efficiency and effectiveness of frontline policing

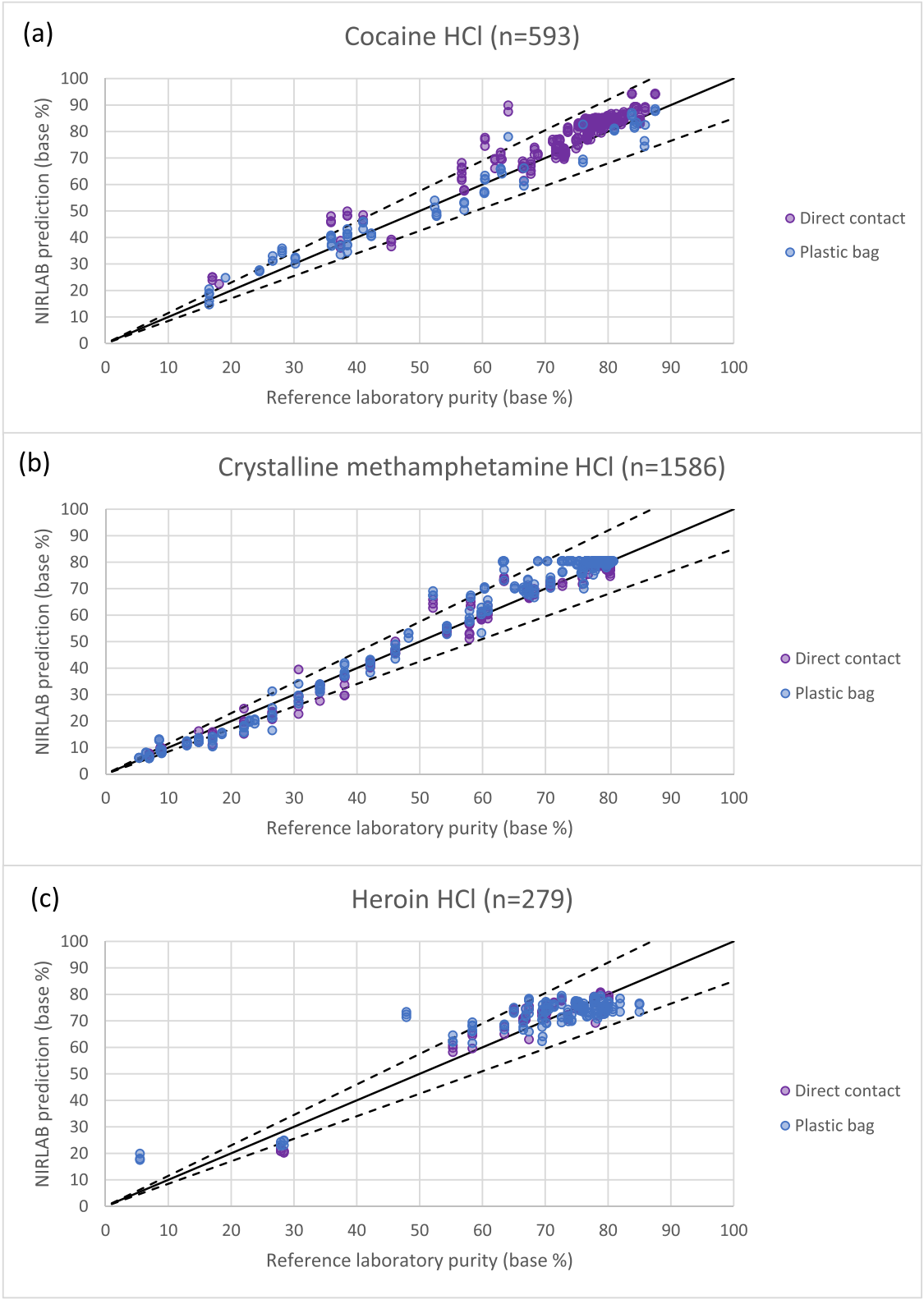

Fig. 6. Correlation of NIRLAB predicted purity value and the reference laboratory purity determination for (a) cocaine, (b) methamphetamine and (c) heroin. Purity is represented in the percentage of the free base form of the drug. The relative uncertainty of the purity estimate is represented as dashed lines which are ±15 % purity.

through its capacity to rapidly and accurately identify and quantify illicit drug seizures. The classification results of crystalline methamphetamine HCl, cocaine HCl and heroin HCl demonstrated a high accuracy and sensitivity for the identification ability of the MicroNIR. Moreover, the absence of any false positives in this study underscores the efficacy of this technology in law enforcement. It can help prevent operational inefficiencies arising from the unnecessary charging of individuals for drug possession when no drugs are actually present. The

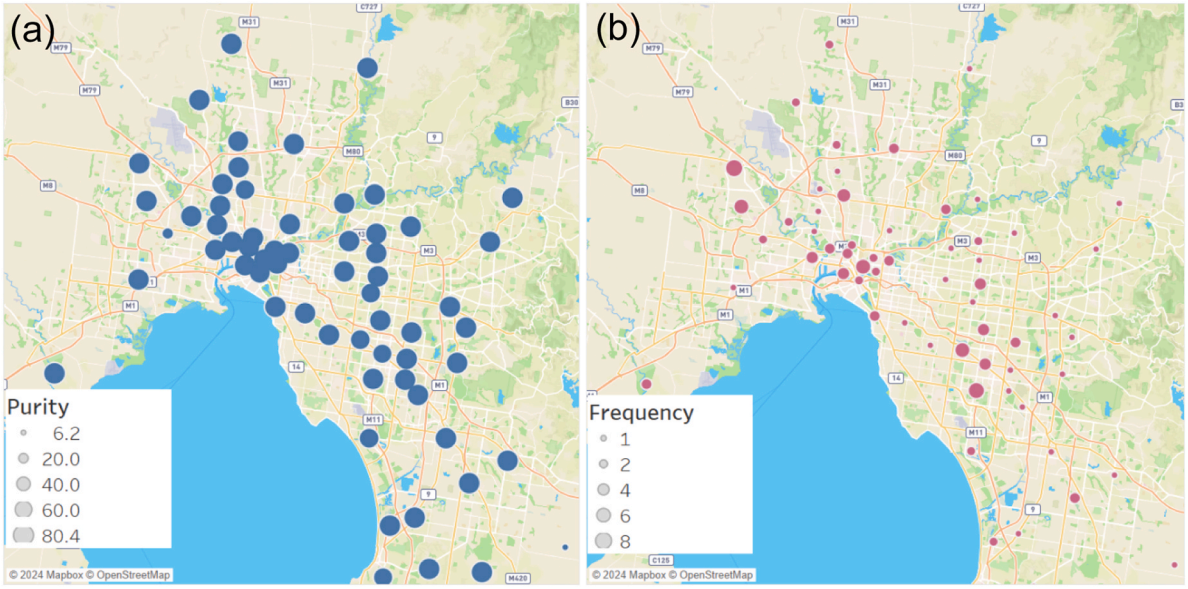

Fig. 7. Geographical visualisation depicting origin of methamphetamine drug seizures identified and quantified by MicroNIR and NIRLAB. Seizures are visualised in two different formats: (a) average purity across the same postcode and (b) frequency of seizures detected within the same postcode.

high sensitivity for the three drugs examined was comparable to other implementations of NIR spectroscopy for illicit drugs, typically reporting a sensitivity (i.e. true positive rate) above 90 % for a variety of different drugs including cannabis, methamphetamine, MDMA, ketamine, heroin, cocaine and some NPS [11,12,19,20,23,24]. Furthermore, the classification results were comparable (and in some cases superior) to the accuracies and sensitivities of other portable drug testing technologies such as colour tests [25], FTIR spectroscopy [23], Raman spectroscopy [26,27], portable mass spectrometry [28] and ion mobility spectrometry [29]. Whilst performing comparably to other drug testing technologies, the strength of this technology stems from a combination of factors: almost instantaneous results, cost-effective, non-destructive, accessible results by non-chemists and increased safety (scanning through transparent materials such as glass or plastic). Furthermore, the ability to provide information on the purity of the main drug and the presence of other major cutting agents. These combination of strengths are not seen by any other portable drug testing technology.

Heroin HCl classification was the least successful in terms of its sensitivity. One explanation for the classification performance of heroin is related to the difference between Australian heroin specimens to previously scanned heroin specimens used to build chemometric models. There are chemical differences between the heroin HCl scanned within this study in Australia and the heroin base scanned within Switzerland that was initially used to build the relevant chemometric models [11]. Furthermore, commonly Australian heroin is white [1] whereas Switzerland heroin is often brown, related to the former being in the HCl salt form and the latter in the free base form [30,31]. The colour of heroin and MDMA has been previously shown to significantly change the NIR spectrum but can be accounted for with the appropriate chemometric model optimisation [19].

More broadly, the false negatives that did occur were caused by two main factors: when there was only a small percentage of the drug was present and homogenised scans of drugs within plastic bags. A small percentage of drug present meant that other components (i.e. the cutting agents) made up the majority of the signal of the NIR spectrum, which limited the machine learning algorithms ability to link to a known/similar specimen that had been previously collected and stored within the database. This typically resulted in the major cutting agent being identified as the main component (or otherwise provided an unknown substance result). This information is still useful for flagging specimens of concern that might require further testing; for example, a substance that was only identified as lidocaine is potentially related to low purity cocaine, which was recently identified as an emerging health concern within New South Wales [32].

The other variable that had the largest number of false negative results were homogenised specimens scanned through plastic bags. It is interesting to note it is specifically the combination of these two variables that performed poorly; homogenised specimens scanned by direct contact and non-homogenised specimens scanned by either contact type all had less than 3 % false negatives within their respective categories. Similarly, the specimens that fell outside the relative uncertainty range when quantified were all homogenised, and mostly scanned through plastic bags. A small number of cocaine specimens that were scanned by direct contact were also outside the uncertainty range, but this was due to their physical colour (brown instead of white) or being low purity/heavily adulterated. This issue in identification and quantification of homogenised plastic bags specimens was likely related to the robustness of the chemometric models employed here. The classification algorithms were able to account for small differences in new NIR scans to the known scans within the database (such as only the homogenisation process or scanned through a plastic bag) but the combination of these variables presents a NIR spectrum that is too unfamiliar to provide an identification. It is likely that homogenisation process increases the influence of small impurities specific to the Australian drug landscape, making them more representative within the scan and thus increasing their likelihood of interfering with identification. Another hypothesis for why the combination of homogenisation and scanning through plastic bags caused lower sensitivity is related to the space between individual drug molecules within a specimen. The homogenisation process decreased the space between molecules causing more diffusion of the NIR light meaning that spectral features related to the plastic bag were better represented in the NIR spectrum. Conversely, for example with crystalline methamphetamine there is more space between the methamphetamine molecules due to the space between crystals meaning that there might be less diffusion and the NIR light is able to bounce back like from a mirror, thus not capturing NIR spectral features from the plastic bag (see NIR peak at approximately 1200 nm present only within homogenised specimens scanned through plastic bags in Figure A5 in Supplementary materials).

The distinctive nature of NIR measurement of illicit drugs through plastic bags has already been established for the MicroNIR employed here. A previous study has found that the performance of the

identification of heroin specimens can be different on a case-by-case basis and the success is influenced by the heterogeneity of the specimen [15]. Another study observed issues with identification in plastic bags for complex mixtures which resulted in false positives (other substances detected as cocaine and methamphetamine) [13]. It is important to note that a different NIR instrument and machine learning workflow was employed for this study. However, it is evident that plastic bags have an influence on NIR spectra (see Supplementary materials for overlaid NIR spectrum of a sample of plastic bags used in this study). Since NIR radiation is being absorbed by the plastic bag, it leaves less energy to be absorbed by the components of the drug specimen [33]. This interference from the plastic bag in the NIR spectrum when combined with other factors such as heterogeneity or presence of other compounds, inhibits the success of the predicted values such as was observed within this study.

The operational compatibility of the MicroNIR with NIRLAB infrastructure has been highlighted through this study. In relation to frontline policing, this technology has demonstrated its capacity to be user-friendly, cost-effective, fast, accurate and increase safety by minimising exposure to potential high risk drugs by the ability to scan through plastic bags. It could facilitate more informed decision-making by frontline police based upon robust analytical information. This would help avoid wasting resources in the instance of false positives that might have occurred from a lack of information or less specific testing (such as colour tests). At a tactical/strategic level, this technology shows great potential for proactive policing through real-time intelligence and investigative activities based on in-field analytical data. This was highlighted in the geographical mapping capabilities from the example of the ENIPID seizures that is not delayed by lengthy lead times from forensic laboratory analysis. This illustration demonstrated the capacity to solve security-related problems by providing investigative leads based upon hotspot detection or aberrations in criminal behaviour that can lead to more meaningful impacts on the criminality associated with illicit drugs. More broadly, the streamlined nature of this data source enables a more efficient distillation of trends in the illicit drug market, enabling a better understanding of the illicit drug problem under a forensic intelligence paradigm [34]. The beneficial applications of the portable NIR technology, optimised within this study, extend beyond law enforcement contexts. Implementations in frontline healthcare settings could enhance clinical management and offer valuable insights into street-level drug consumption. Obtaining information about the identity and purity of drugs at the consumption level enables both police and health organisations to allocate resources and tailor messaging. This enhanced understanding can have broader implications in terms of harm minimisation and public health efforts, addressing the illicit drug problem more comprehensively [35].

Further research into decentralising the forensic laboratory is paramount to improving casework efficiency and effectiveness in an increasingly complex transnational serious and organised crime environment [2]. The development and implementation of portable technologies does not aim to replace conventional laboratory-based techniques but to support them by reducing the time spent on straight forward analyses (i.e. pure/traditional drugs) to enable reprioritisation on more complicated specimens (i.e. complex mixtures or NPS). Moreover, this technology serves a role in forensic laboratories as a screening tool, ensuring consistent sampling from seizures and preventing inefficiencies caused by the necessity to resample due to disparate samples. This is essential when drug-related crime is only increasing [36] whilst resourcing in terms of equipment or analysts cannot keep up; illuminating the need to find solutions that work more efficiently with fewer resources. NIR spectroscopy combined with chemometric modelling here has demonstrated an ultra-portable technology that is fast, accurate and user-friendly; highlighting its compatibility with decentralisation.

There are a number of limitations to discuss within this work. Only low-density polyethylene plastic bags were used in the development of the chemometric models. As has already been highlighted, different low-density plastic bags have slight differences in the NIR spectrum, which can influence the accuracy of the model prediction. However, this remains fit for purpose for use within AFP but further expansion should explore this. Within this study, given the logistical and legality issues of handling illicit drugs, convenience sampling was employed. Hence, the authors have refrained from holistic summaries on drug trends based upon the data collected within this study, instead focusing on the strengths of the NIR technology and providing examples of how it can be used operationally. A large number of the specimens scanned were of higher purity, which is related to the level of the drug distribution chain that AFP captures in seizures. This is further evident by the lower purity specimens having more issues with identification and quantification. Whilst this illustrates a gap in the chemometric models, it does not negate their usefulness. It in fact highlights that the current implementation is fit for purpose for AFP given the accuracy for the type of samples they often capture (i.e. high purity trafficking specimens opposed to low purity consumption specimens). Furthermore, this gap could be easily addressed by targeting the types of specimens not captured within the current dataset and optimise the chemometric models accordingly.

5. Conclusions

The optimisation and assessment of hand-held NIR spectroscopy (MicroNIR) combined with machine learning models (NIRLAB) for rapid identification and quantification of crystalline methamphetamine HCl, cocaine HCl and heroin HCl was accomplished within this study. The identification of crystalline methamphetamine HCl, cocaine HCl and heroin HCl specimens was accurate (98.4 %, 97.5 % and 99.2 %, respectively) and sensitive (96.6 %, 93.5 % and 91.3 %, respectively). There was never a single false positive detected across the scans collected across the three targeted drugs. The quantification of all three drugs was accurate within the uncertainty limits of ±15 % for 99 % of specimens. Issues in identification and quantification typically arose due to low purity specimens or from the combination of scanning through plastic and the homogenisation process. However, the MicroNIR with chemometric modelling provided by NIRLAB has demonstrated to be an accurate portable drug testing technology that is compatible to operational implementation within Australia. Furthermore, it provides great potential for intelligence and investigative activities in order to better understand the illicit drug problem in real time and affect more meaningful change more efficiently based upon analytical data. Expansion of this technology within Australia could facilitate the optimisation of chemometric models for drugs other than the three prioritised here, and upscaling implementation will provide further insight into the suitability of this NIR technology for portable drug testing in relevant policing and health-related contexts.

CRediT authorship contribution statement

Natasha Stojanovska: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Pierre Esseiva:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Claude Roux:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization. **Scott Chadwick:** Writing – review & editing, Supervision, Project administration, Methodology, Conceptualization. **Florentin Coppey:** Writing – review & editing, Visualization, Validation, Methodology, Formal analysis, Data curation. **Harrison Fursman**: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Marie Morelato:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of Competing Interest

None

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.forsciint.2024.112179.

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