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A background image showing several laboratory glassware items, including test tubes and flasks, with a blurred, colorful background of red and blue. The glassware is arranged in a way that suggests a laboratory setting.

Cocaine and Heroin Content Determination with NIR

Confiscated street drug samples are mixtures with different drugs and cutting agents. Despite these different drug mixtures, exact NIR measurements are performed using the Buchi NIRFlex N-400 spectrometer. With Buchi NIRCal Chemometric Software only one calibration each for all heroin and all cocaine samples for a broad concentration range could be developed.

Cocaine and Heroin Content Determination with NIR

The identification and the estimation of the drug concentration of confiscated street drugs is one of the primary tasks of the scientific services of the municipal police of Zurich.

The scientific service of the municipal police Zurich has been using NIR technology as a standard method for street drug analyses for more than ten years. This analytical technique is primarily used to estimate the drug content in confiscated heroin and cocaine street drugs.

In 1991, the Federal Court of Switzerland decided to change the definition of severe cases of heroin and cocaine possession. Since that time the possession of more than 12 g of pure heroin and 18 g of pure cocaine are regarded as severe cases respectively. In such cases, the penalty is one year of imprisonment, in addition to up to a one million Swiss Frank fine. Because of this federal court decision, the number of court exhibits of street drugs has increased dramatically. In order to manage the high number of requested analyses, the municipal police of Zurich looked for a quick and reliable method for estimating drug concentrations.

The first tests with NIR spectroscopy were performed in 1991. Because of the promising results, a routine method was established for the InfraProver FT-NIR system from Bran+Luebbe in 1992. In 1993, the first instrument was bought followed by a second one in 1996.

Until today, the number of samples investigated has increased steadily. Furthermore, a change in consumer behaviour has occurred during the same period. After the disappearance of the „open drug scene“ heroin became the „loser drug“. The number of heroin samples investigated decreased while the number of cocaine samples increased drastically.

In 2004, more than 400 cocaine and more than 200 heroin analyses were performed. Generally the drug content of confiscations from „big deals“ were higher than those of the drugs sold on the streets (Fig. 1).

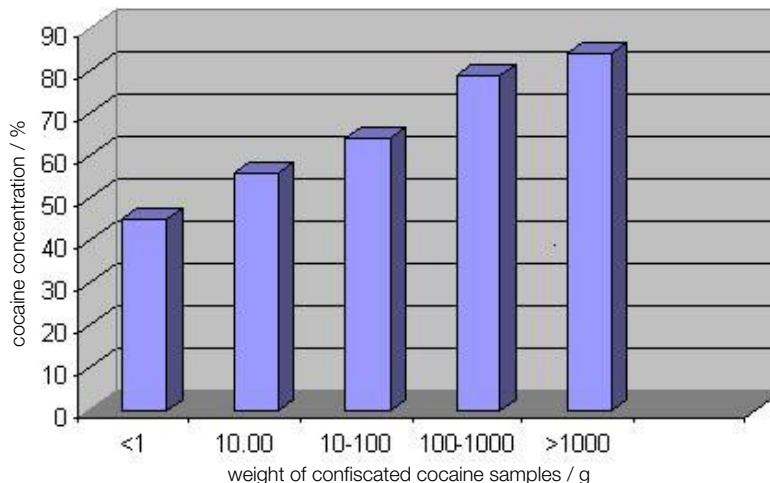


Fig. 1 Distribution of confiscated cocaine samples

For confiscated street drugs, the concentrations of heroin are normally considerably lower than those of cocaine.

The confiscated street drugs are mixtures of various active, excipient and cutting agents. For cocaine typical cutting agents are:

- Caffeine
- Lidocain
- Phenacetin
- various sugars (Lactose, Mannitol, Glucose, Dextrose etc..)

For heroin typical cutting agents are:

- Mixtures of Paracetamol, Caffeine and food colours

NIR Method

The first pre-investigation of the confiscated court exhibits is performed using color and immunological tests. Receiving positive results with the pre-investigations, the concentration of cocaine and heroin samples is estimated using NIR spectroscopy. Gas chromatography is used as a classical reference method which, however, takes much more time than NIR. For this reason, the predominant number of all confiscated samples are measured using NIR only. In order to get reliable results, the sample should be homogeneous. If that is not the case, it needs to be ground

in a mortar or mixed.

The NIR spectra of heroin and cocaine court exhibits show various characteristic absorption bands. Therefore, a distinct identification with NIR is possible (Fig. 2). However the principal interest was – of course – the quantification using NIR spectroscopy.

The first quantitative NIR calibration for **cocaine** was developed using court exhibits with drug concentrations between 31 and 89 %. The spectra were measured using the B+L InfraProver. The SEE (standard error of estimation) was 1.4 % and the SEP (standard error of prediction) was 3.4 % for the cocaine content using 130 spectra in the calibration and 14 spectra in the validation set.

The first NIR calibration for **heroin** was developed using spectra for concentrations in a range from 32 to 87 %. The SEE was 1.4 %, the SEP was 2.9 % using 129 spectra in the calibration and 15 spectra in the validation set.

In 2004, the B+L InfraProver spectra were transferred without any problems into the Buchi NIRCAl 4.21 software and new calibrations using the patented Calibration Wizard were calculated.

These calibrations, including B+L InfraProver spectra only, were used for NIR

measurements with the Büchi NIRFlex N-400 between June and November 2004. For several samples, GC analyses were performed. These samples were used for new calibrations based on NIRFlex N-400 spectra.

The new NIRFlex calibrations clearly show an improved performance. For cocaine samples with a calibration range from 21 to 87%, the SEE is now only 1.5 % and the SEP is also 1.5 % using 107 samples with 536 spectra in the calibration and 34 samples with 171 spectra in the validation set.

In addition, the regression coefficient increased from 0.9674 for InfraProver to 0.9819 for NIRFlex N-400.

The new heroin calibration was calculated using samples in the concentration range between 4 and 78%. The SEE is 0.9 % and the SEP is also 0.9 % using 68 samples with 340 spectra in the calibration and 21 samples with 105 spectra in the validation set (Fig. 3); the regression coefficient is 0.9958.

It is obvious that the results could be improved considerably using the new calibrations developed with NIRFlex N-400 and NIRCal 4.21.

The considerable improvements in the quantitative NIR results using the Büchi NIRFlex N-400 and NIRCal 4.21 have different reasons:

Stable and satisfactorily working NIRFlex N-400:

- High-quality optical components for stable measurements
- Better cleaning possibilities of the reference plate at the Büchi NIRFlex N-400 resulting in more reliable spectra.

Efficient chemometric software NIRCal 4.21:

- Fast software – many calculations can be performed in a short time.
- Calibration Wizard for meaningful suggestions for pretreatments and number of calibration factors
- Easy visualization of calibration results
- Good software support

The acceptance of the NIR determination

NIR spectroscopy is regarded as

“extended pre-analysis” by the court. NIR results are rounded to the next 5 % level. If the amount of drug is in the range defined for “severe cases” (18 g pure cocaine or 12 g pure heroin) the result is verified by gas chromatography automatically. Without NIR spectroscopy the high number of confiscated heroin and cocaine drugs could not be measured with the existing personnel and laboratory status. In other words – despite the calibrations development NIR spectroscopy is a strong time and cost saving tool.

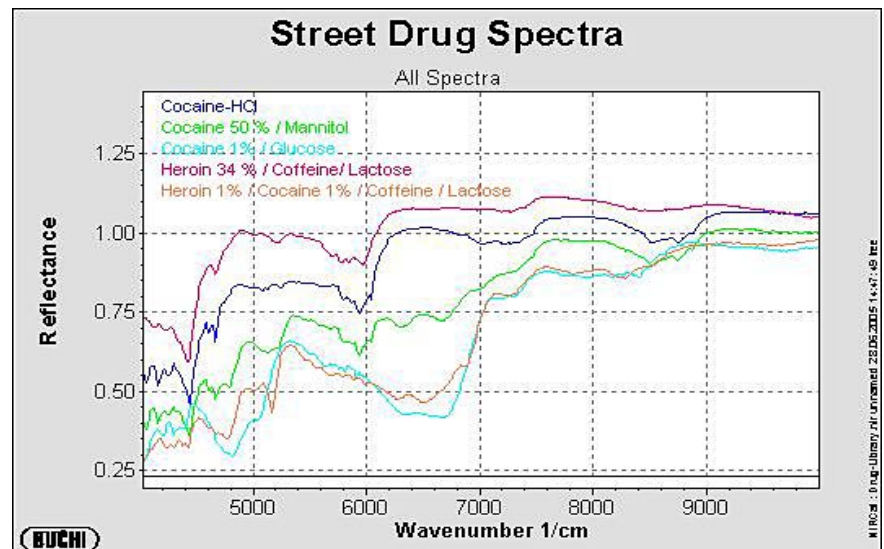


Fig.2: NIR spectra of some court exhibits

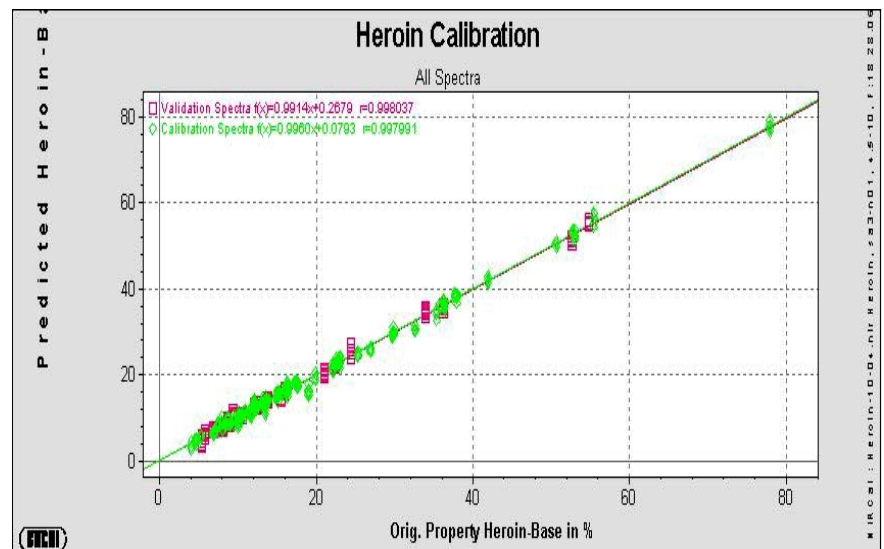


Fig.3: Quantitative ability for the determination of heroin content

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