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Rapid qualitative and quantitative analysis of methamphetamine, ketamine, heroin, and cocaine by near-infrared spectroscopy

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Highlights:

- NIR methods for qualitative and quantitative analysis of drugs have been established.
- 1118 samples were used for the model building and validation purposes.
- The RMSEC, RMSECV, and RMSEP for all models were less than 1.6%, 2.9%, and 3.6%, respectively.

ABATRACT

Rapid and nondestructive near infrared spectroscopy (NIR) methods have been developed for simultaneous qualitative and quantitative analysis of methamphetamine, ketamine, heroin, and cocaine in seized samples. This is the first systematic report regarding a qualitative and quantitative procedure of applying NIR for drug analysis. A total of 282 calibration samples and 836 prediction samples were used for the building and validating of qualitative and quantitative models. Two qualitative analysis modeling methods for soft independent modeling by class analogy (SIMCA) and supporting vector machine (SVM) were compared. From its excellent performance in rejecting false positive results, SIMCA was chosen. The drug concentrations in the calibration and validation sample sets were analyzed using high-performance liquid chromatography. Based on the use of first-order derivative spectral data after standard normal variate (SNV) transformation correction, in the wavelength range from 10000 to 4000 cm^{-1}, four partial least squares quantitative-analysis models were built. The coefficients of determination for all calibration models were >99.3, and the RMSEC, RMSECV, and RMSEP were all less than 1.6, 2.9, and 3.6%, respectively. The results obtained here indicated that NIR with chemometric methods was accurate for qualitative and quantitative analysis of drug samples. This methodology provided a potentially useful alternative to time-consuming gas chromatography-mass spectroscopy and high-performance liquid chromatography methods.

Keywords: Near infrared spectroscopy, Qualitative and quantitative analysis, Methamphetamine, Ketamine, Heroin, Cocaine, SIMCA, Partial least squares

1. Introduction

Methamphetamine, ketamine, heroin, and cocaine are the four most common drugs in China,