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ACCEPTED MANUSCRIPT

COCAINE AND ADULTERANTS ANALYSIS IN SEIZED DRUG SAMPLES BY INFRARED SPECTROSCOPY AND MCR-ALS

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Highlights:

- Direct FTIR analysis of seized cocaine samples;
- Cocaine and adulterants determination;
- Validation with a significative number of seized samples (n>700);
- Qualitative and quantitative analysis by MCR-ALS;

ABSTRACT

Cocaine use has been reported for more than 2500 years, but along this period of time its damage to society in general became evident. Nowadays, cocaine is classified as an illicit drug and studies which give support to drug enforcement institutions, particularly in the area of police intelligence, are very relevant. Often, trafficked cocaine is not traded in its pure form, but mixed with adulterants and diluents. In the analysis of seized samples, the reference method is based on gas chromatography, however the interest in the use of vibrational spectroscopy has increased. This work aims at developing a method for determination of the concentrations of cocaine, adulterants and diluents in cocaine samples employing Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) associated with Multivariate Curve Resolution with Alternating Least-Squares (MCR-ALS). A total of 6 adulterants, 3 diluents, 2 forms of cocaine (base and hydrochloride) were determined and the method developed based on 55 synthetic mixtures prepared according to a mixture design and 20 seized samples. For validation purposes 708 seized samples and 9 synthetic mixtures were analyzed. The results proved to be satisfactory, showing that the proposed method has a great

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