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## Cocaine profiling: implementation of a predictive model by ATR-FTIR coupled with chemometrics in forensic chemistry

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### Abstract

In this study, a strategy based on Infrared Spectroscopy with Fourier Transformed and Attenuated Total Reflectance associated with chemometrics (ATR-FTIR) is proposed to identify the chemical “fingerprint” of cocaine samples. To this end, standard mixtures of cocaine and cuttings at different ratios were investigated in order to develop a multivariate classification model to simultaneously predict the composition of the samples and to obtain a profile of adulteration of cocaine seizures. In addition, the application of a Partial Least Squares (PLS) and Principal Component Regression (PCR) calibration approaches were found to be a useful tool to predict the content of cocaine, caffeine, procaine, lidocaine and phenacetin in drug seizures. The achieved results on real confiscated samples, in cooperation with the Italian Scientific Investigation Department (Carabinieri-RIS) of Rome, allow to consider ATR-FTIR followed by chemometrics as a promising forensic tool in such situations involving profile comparisons and supporting forensic investigations.

**Keywords:** ATR-FTIR spectroscopy, Cocaine, Profiling, Chemometrics, Forensic chemistry

### 1. Introduction

Cocaine is the most widely used illicit drug, and its “origin” is always the focus of intense investigation aimed at identifying the trafficking routes. The classification of cocaine seizures according to its form (composition, cutting agents) provides useful information to enhance the existence of cocaine illicit networks and supply the police intelligence [1-6].

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