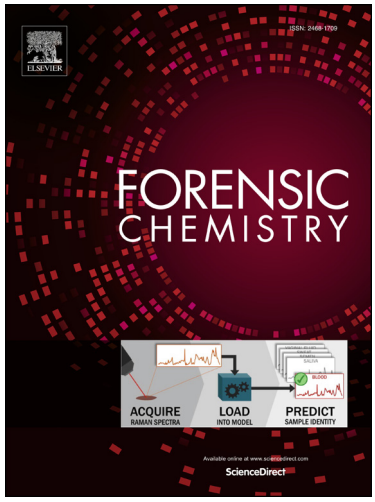


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# Application of *In silico* methods in forensic science: quantum chemistry and multivariate analysis applied to infrared spectra of new amphetamine- and cathinone-derived psychoactive substances.

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**ABSTRACT**

Identifying new psychoactive substances in a reliable manner is an exciting idea in forensic science. In this work, we apply in silico methods to recognize classes of drugs. We calculate the infrared spectra of 21 pairs of amphetamine and cathinone homologs by *in silico* techniques and compare the theoretical data with the experimental data. First, we submit each molecule to conformational analysis and use the minimum energy structure to determine the frequencies that generate the infrared spectra. We employ three different Density Functional Methods -B3LYP, B3LYP-D3 and M06-2X- and the 6-31G** basis set implemented on Gaussian 09 for this purpose. Application of supervised and unsupervised multivariate classification methods to the spectra helps us to evaluate the theoretical results. The *in silico* procedure adopted herein can predict the infrared values and provides valuable information about unknown substances. Therefore, this methodology could help to create an effective tool to identify unknown psychoactive substances.