Inbuilt versus offline identification of novel psychoactive substances using handheld Raman spectroscopy

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Objective

The aim of this work is to compare the inbuilt and offline identification algorithms of NPS products using handheld Raman spectroscopy.

Introduction

Novel psychoactive substances (NPS) products represent a public health threat due to their unpredicted pharmacological effects/ side effects. Thus, these products often contain substance(s) that do not match their label claim. Handheld Raman spectroscopy offers a simple, rapid and no-destructive method for identification of NPS products.

Experimental

Materials

A total of seven NPS products were measured 'as received' using three handheld Raman spectrometers including: Thermo Truscan RM (now Antetech), Rigaku Xantus-1 and Rigaku FirstGuard instruments equipped with charged coupled device detectors and (785 nm or 1064 nm) laser excitation wavelengths.

Figure 1 Rigaku FirstGuard, Thermo TruscanRM Raman spectrometers and NPS products.

Method

- For inbuilt identification, libraries of substances commonly present in NPS products were created in the instruments. Then, test substances were compared against the libraries using probability algorithm.
- For offline identification, the spectra were exported to Matlab 7.0 where different algorithms were applied including: Correlation in wavelength space (CWS), distance based methods, principal component analysis (PCA) and fuzzy c-mean clustering (FCM).

Results and Discussion

The measurement time for the NPS products ranged between few seconds to few minutes depending on the Raman activity of the substances. Thus, pharmacologically active substances showed high Raman activity and good quality spectra. However, the Raman activity of pharmacologically inactive substances was often masked by fluorescence (Table 1).

Table 1 shows a list of substances present in legal high products and their corresponding Raman activity.

Substance	n	Maximum Peak position (cm^{-1})	Maximum Peak intensity	S/N ratio	Raman activity
Alginate sodium	9	1410	1701	10	Weak
Benzocaine	13	1278	34670	15.5	Medium
Caffeine	21	564	21790	61	Strong
Lactose	16	356	9997	15.3	Medium
Lidocaine hydrochloride	19	1449	8856	22.3	Medium
Maize starch	10	480	3783	12.2	Medium
Phenacetin	18	1612	13600	71	Strong
Procaine	18	1255	30040	18	Medium
Sucrose	10	539	2410	10.3	Weak

n: Number of samples, S/N: Signal to noise ratio

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In-built identification

The inbuilt algorithm was simple, rapid and easy to use (Figure 2). It could identify Raman active substances in pure and mixture samples provided there are signatures of these substances in the library. It was able to identify substances in six out of seven NPS products.

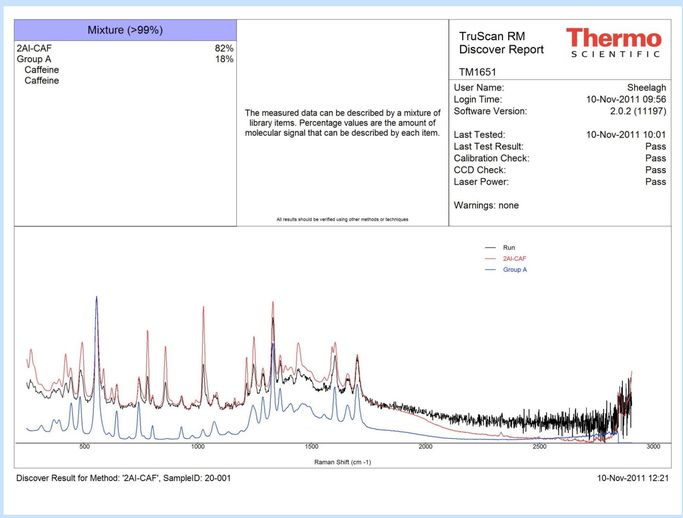

Figure 2 Raman spectrum of an NPS product (black) that matched the signature of 2-aminoindan and caffeine mixture (red) and caffeine (blue) .

Offline analysis

The offline spectral analysis offered more in-depth investigation of the content as well as the quality of the products. Thus, CWS was able to identify similarities between the products Raman spectra in relation to the individual impurities present in the products. On the other hand, distance based methods (Figure 3) and PCA methods offered more in-depth identification.

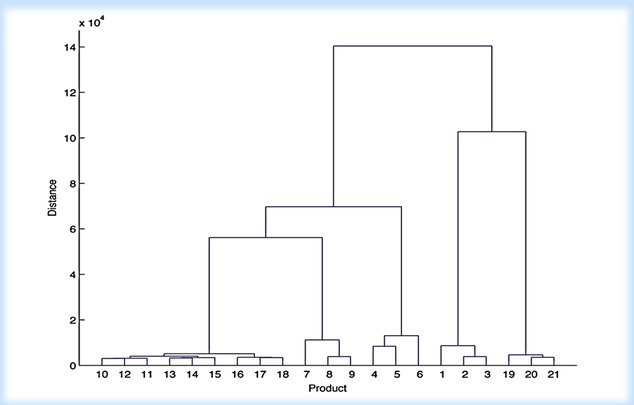

Figure 3 Dendrogram of Raman spectra of seven NPS products measured using the Rigaku FirstGuard Raman instrument. The clusters in the products explained the similarity in their constituents as follows: Cluster 1 (P1: 1- 3), cluster 2 (P2: 4 - 6), cluster 3 (P3: 7 - 9), cluster 4 (P4, P5 and P6: 10 - 18) and cluster 5 (19 - 21)

Multiple chemometric approach

PCA-FCM showed more accurate identification as each was able to cluster each product separately. Moreover, the combination of PCA and GMM was able to cluster products bought from the same website which could indicate their manufacturing site.

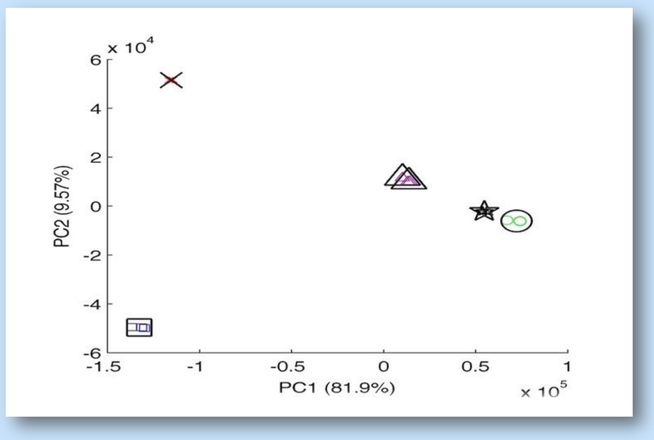

Figure 4 PCA-FCM applied to the seven NPS products showing cluster centres of the products.

Conclusion

Handheld Raman spectroscopy offered a powerful tool for identification of NPS products. Although the inbuilt algorithm offered a rapid and non-destructive method, offline analysis showed more accurate identification of NPS products.