ON-SPOT IDENTIFICATION OF NOVEL PSYCHOACTIVE SUBSTANCES USING HANDHELD RAMAN SPECTROSCOPY

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Objective

The aim of this work was to identify novel psychoactive substances (NPS) products using handheld Raman spectroscopy.

Introduction

NPS products represent a major health threat due to their unpredicted effects/adverse effects. This is mainly attributed to the the fact that these products often contain pharmacological active/ inactive substances that do not match their label claim. NPS products could be encountered anywhere including parties, nightclubs and users homes. This stimulates the need to develop rapid and non-destructive methods for their analysis. Handheld Raman spectroscopy offers this advantage.

Experimental

Materials

A total of 318 NPS products were used in this work. The products had diverse formulation (powders, tablets, liquids and gels), colours and shapes.

Instrumentation

Products were measured as received using the Rigaku FirstGuard handheld Raman instrument equipped with 1064 nm laser power and a charged coupled device detector.

Method

❑Spectral measurement was made at 490 mW laser power and 2 sec exposure time. Each spectrum was the sum of three scans and required less than a minute.

❑Spectra were compared instantly against the instrumental in-built algorithm. The latter algorithm utilised Hit Quality Index (HQI) to compare the test spectrum against the library spectra. HQI was displayed as a percentage match and was based on correlation coefficient values.

❑As the Raman signal was often masked by noise (photon shot-, sample-, detector- and spectral- generated), an HQI > 50% was considered a similar item and > 95% as identical.

Results and Discussion

Raman spectroscopy

Raman spectroscopy offered an advantage in identifying the purity of NPS products. This was because pharmacologically active substances (such as caffeine) are Raman active and vice versa. Thus, pharmacologically inactive substances often fluoresce upon interaction with laser which often decreases/masks the Raman activity of the measured product. Moreover, Raman spectroscopy required no sample preparation and could measure the sample regardless of its physical state (solid, liquid and gels).

More specifically, handheld Raman spectroscopy offers many advantages:

- ❑ It is of portable, mobile and of light weight so can be used easily in any field.
- ❑ It operates under wide temperature range (-25°C – 40°C).
- ❑ It is equipped with a long life time battery and in-built computer.
- ❑ Its straightforward interface allows it to be used by non-experts.

NPS products identification

The in-built algorithm was able to identify 170 (54%) NPS products. The largest number of products matched the following substances: p-hydroxy codeine, ketamine, MDMA, lactose, caffeine, polystyrene, acacia and cocaine hydrochloride (Table 1). In addition, less matches were obtained for the following substances: Cyclodextrin, benzene, paracetamol, sucrose, amfetamine sulfate, dextrin, propylene glycol, quinine sulfate, titanium dioxide and urea.

Table 1 The number of products (N) and mean HQI values matching each of the listed substances.

Substance	N	Mean values
p-hydroxy cocaine	36	69.5 (60.2 - 64)
Ketamine	35	76.9 (53.6 - 82)
MDMA	19	63.3 (54.7 - 100)
Lactose	18	67 (50.5 - 100)
Caffeine	13	74.2 (55.7 - 100)
Polystyrene	11	65.5 (50.6 - 74)
Acacia	7	55.5 (50.4 - 62)
Cocaine hydrochloride	4	83.5 (65.7 - 100)

Of the remaining products, 34 were not Raman active and 114 could not be identified because they had no library reference spectra. The Raman intensity and number of peaks indicated to a degree the percentage match and purity of the product. For instance, a product that had an HQI = 80% against caffeine showed the same spectral features of caffeine but with less intensity (Figure 1).

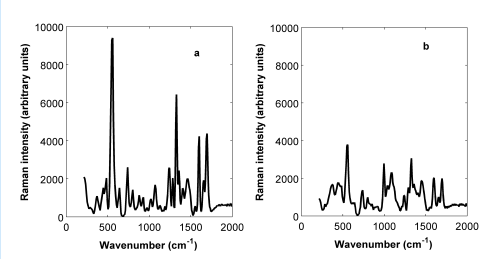

Figure 1 The Raman spectra of (a) caffeine and b) a product that contained caffeine (HQI = 80%) measured using the Rigaku First Guard Raman instrument.

In this respect, the purity of the products varied between the individual substances. This was demonstrate by the variation in the match values obtained for the individual products (Figure 2).

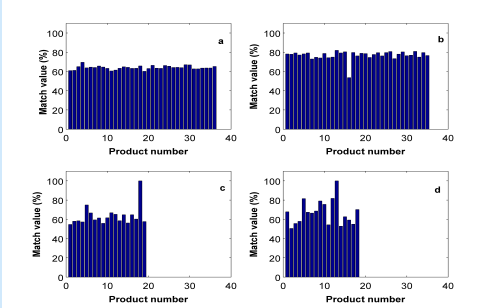

Figure 2 Match values (HQI, %) of the individual products against (a) p-hydroxy cocaine, (b) ketamine, (c) MDMA and lactose.

Conclusion

Handheld Raman spectroscopy offered a rapid and non-destructive method for the identification of NPS products. The instrumental in-built algorithm could identify 54% of the NPS products measured.

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