Seized Drug Analysis using ASAP-MS and Multivariate Analysis Models

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INTRODUCTION

Illicit drug use and trafficking contribute to harm, instability, and violence. The analysis of seized drugs is essential for national and international efforts to control illegal substances. Drug control laboratories need analytical methods that deliver rapid, accurate results.

This study evaluated the RADIAN™ ASAP Mass Spectrometry (MS) device (Figure 1) as a rapid screening tool for detecting and differentiating drug substances in seized samples. Such data can provide insights into drug manufacturing, distribution, and the presence of harmful adulterants. The information can also be used to identify common or different manufacturing processes, cutting processes and packaging differences which can help identify the production location and its route to the location of seizure.

The use of multivariate analysis (MVA) software can take the "spectral fingerprint" of the samples and compare them to identify major component differences, or alternatively, subtle variations if the samples are very similar. A total of 172 suspect materials, in the form of MDMA tablets of 16 different shape and colour variants (Figure 3), confiscated at UK music events and night time venues, were provided by the police.

METHOD

Tablet samples were individually dissolved in methanol, diluted, and analysed using RADIAN ASAP MS with a four-function full scan acquisition (*m/z* 50–650) at 600°C.

The four functions were of increasing cone voltage to increase the production of fragment (product) ions to help improve spectral identification.

Data were acquired in triplicate using MassLynx™ Software.

A subset of samples was further analysed using AnalyzerPro™ XD Software with Multivariate Analysis (MVA) to assess similarities and differences between sample cohorts.

Figure 1. RADIAN ASAP MS

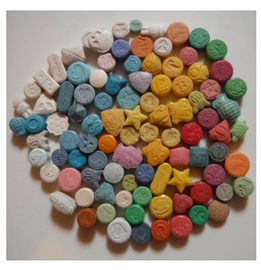

Figure 2. MDMA tablets

RESULTS AND DISCUSSION

Initial processing of the 172 tablets grouped into 16 cohorts based on shape and colour (Figure 3) were all identified as containing MDMA as the major component.

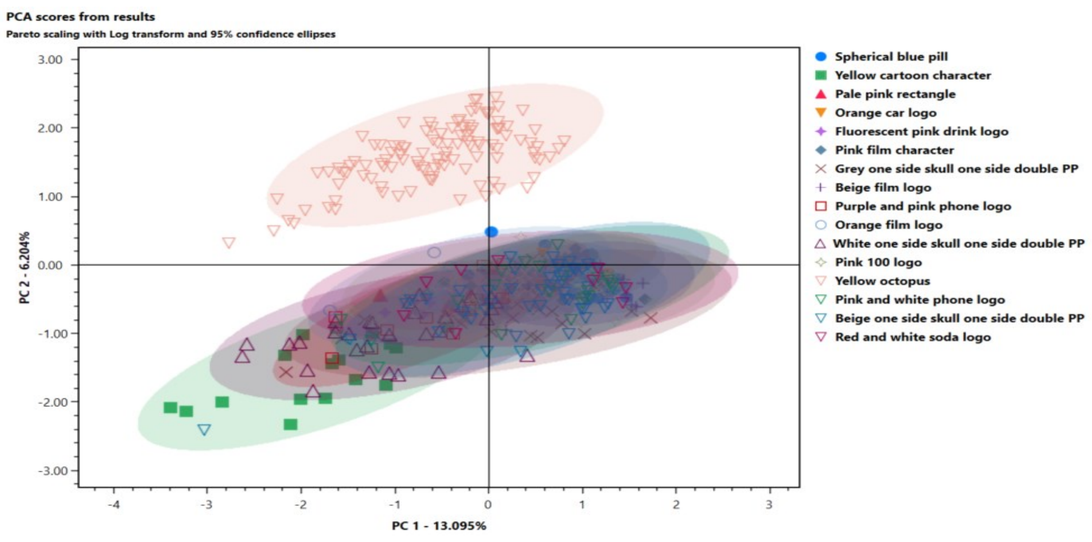

Figure 3. PCA of all categories

Principal Component Analysis (PCA) was performed using data from all four functions. One cohort, "Yellow Octopus," showed significant differences from the other sample types (Figure 3). This group contained both MDMA (*m/z* 194) and caffeine (*m/z* 195). The fragment ions (*m/z* 110 and 138) exhibited markedly different intensities in the higher energy functions compared to other tablet cohorts, suggesting a possible alternative cutting process.

A comparative analysis of the "Yellow Octopus" and "Orange Car Logo" cohorts revealed distinct masses unique to each group. In the Volcano Plot (Figure 4), green triangles indicate ions exclusive to "Yellow Octopus," while red triangles highlight those unique to "Orange Car Logo." The most prominent feature in "Yellow Octopus" is *m/z* 110, located at the top of the red rectangle. These cohort-specific masses may represent production markers, packaging residues, or by-products of differing cutting techniques.

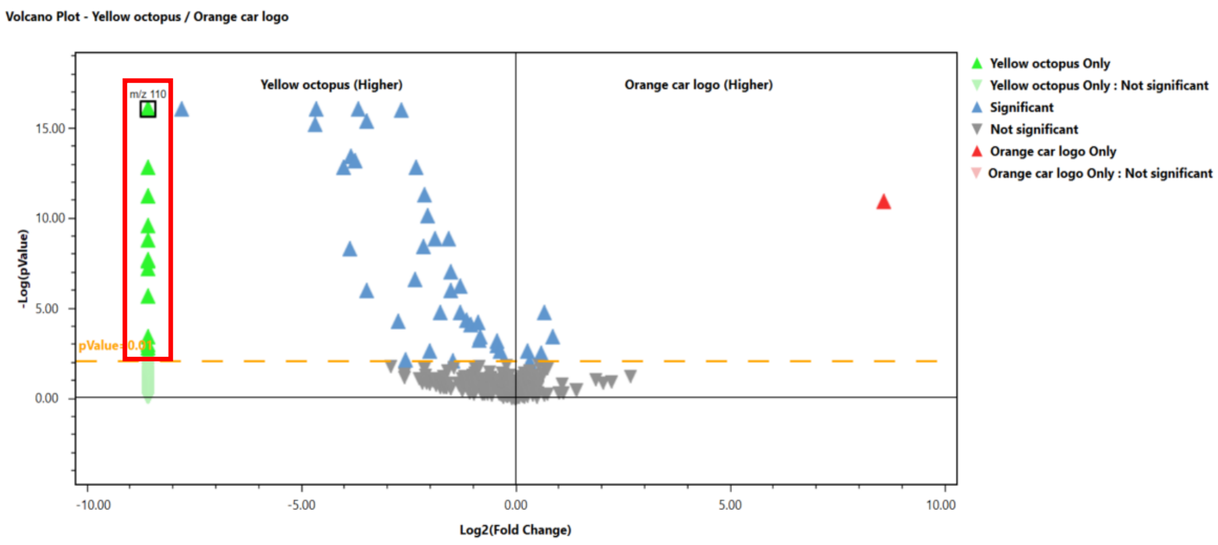

Figure 4. Volcano Plot Function Four

Further statistical interrogation was performed across all 16 cohorts using only the first (low-energy) acquisition function, isolating the molecular (precursor) ions that analysts can most readily recognize. By systematically comparing every cohort combination, we identified masses that were uniquely present in specific tablet cohorts over the full acquisition mass range. Figure 5 illustrates these cohort-specific ions using a feature map. A more in-depth analysis can also be undertaken where multiple feature maps can be created so that additional fragmentation information can be obtained.

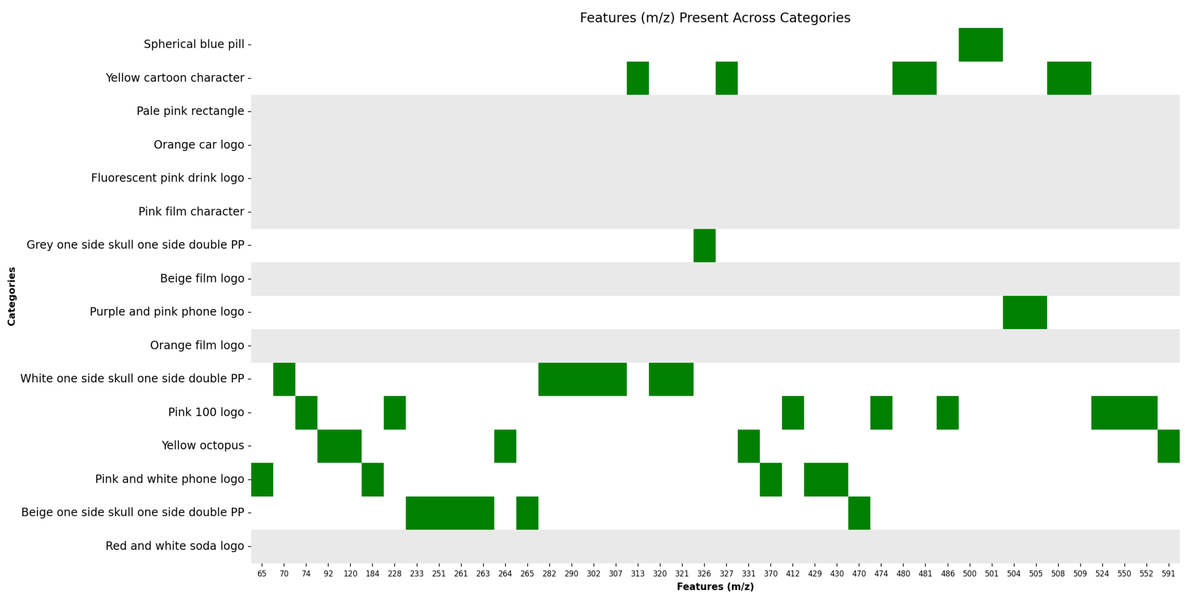

Figure 5. Comparison of unique features per categories

The grey lines within the feature map, show tablets that have no mass differences within the first energy function, suggesting these have been processed and manufactured in a similar way.

The green squares are unique masses which could be investigated to identify if these are produced through the manufacture or processing of the material.

CONCLUSIONS

The RADIAN ASAP MS, combined with Multivaariate Analysis, effectively screes seized samples and differentiates MDMA tablet cohorts.

Caffeine concentration was identified as a main differentiator between one cohort (yellow octopus) compared to the other cohorts showing a potential different cutting process from manufacture to seizure.

The detection of caffeine in a specific group highlights the method's ability to identify unique chemical markers, offering valuable insights for forensic investigations into drug production and adulteration.

Unique components were identified in several tablets which could be investigated to identify if they are unique production/processing markers.