THE POWER OF KNOWING NOW: RAPID DRUG SCREENING USING ASAP-MS

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** TAKE HOME **

Small-footprint ASAP-MS device

Super-easy, rapid identification of drug substances

- **Replicate results obtained within 2 min**
- **Very good qualitative agreement with HRMS screening**

SCAN ME

Forensic use only

AIM

To evaluate the performance of a new compact device based on Atmospheric Solids Analysis Probe-Mass Spectrometry (ASAP-MS) for rapid drug screening and to compare data with an established screening method based on high-resolution mass spectrometry (HRMS).

CURRENT ANALYTICAL CHALLENGES

High number of seized samples requiring analysis, puts laboratories under pressure to produce results quickly

Ever-increasing diversity of substances received including traditional drugs and novel psychoactive substances (NPS)

Lengthy analysis times associated with some traditional screens such as TLC or GC-MS. Large seizures require multiple analysis (random sampling)

Performance of some traditional screens can be insufficient *e.g.*, colorimetric tests are not available for all drugs or can suffer from false positives

EXPERIMENTAL

ASAP-MS

The science bit:

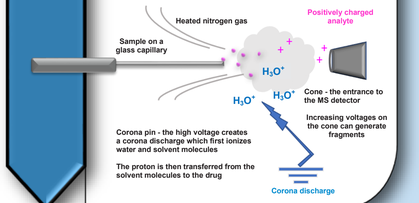
Atmospheric Solids Analysis Probe (ASAP) in conjunction with Mass Spectrometry (MS)

ASAP
Permits direct MS analysis without complex sample preparation or chromatography

= Easy, rapid sample introduction

MS
- MS system collects the *m/z* information relating to the intact drug molecule as well as the fragmented molecule
- Application of increasing cone voltages can generate specific fragment ions *i.e.,* a molecular fingerprint (**Figure 1**)

= More information, more specificity, more confidence in identification



- Certified reference materials (CRM) were prepared at 50 µg/mL in methanol
- Pharmaceuticals and seized pill/tablets/powders were initially dissolved in 10 mL of methanol:water (50/50, v/v) then diluted further (1:20) in methanol
- All samples were analysed by the **Dip & Detect Workflow** and the parameters detailed in **Table 1**
- Data was processed in near real-time by LiveID 2.0 library matching software which enables real-time matching of acquired data to the reference library
- LiveID calculates an average match factor (maximum is 1000) using a reverse-fit model
  - For these studies a match factor of 850 was used as the reporting cut-off, match factors ≥900 were considered as high confidence detections

Parameter	Setting
Ionization mode	ASAP+
Corona pin	3 µA
Desolvation gas	Nitrogen at 600 °C
Cone	15, 25, 35, 50 V
Acquisition mode	Full scan MS (continuum mode) *m/z* 50-600
Scan speed	5 Hz

Table 1. RADIAN-ASAP parameters, the same parameters were used for creation of the reference library and subsequent routine analysis.

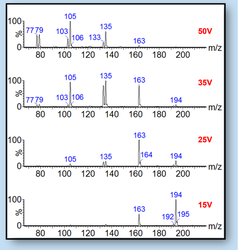
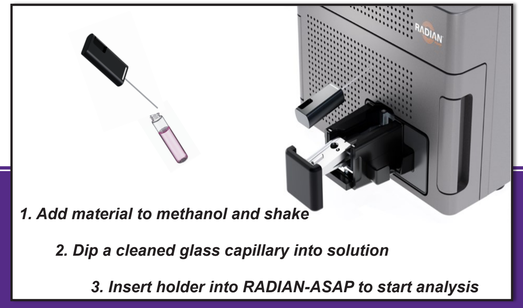


Figure 1. Analysis of MDMA CRM. Collection of MS data at 4 cone voltages results in collision–induced dissociation and generation of a highly-specific spectral fingerprint comprising the precursor ion at m/z 194 and fragment ions.

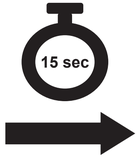
WORKFLOW: Dip & Detect

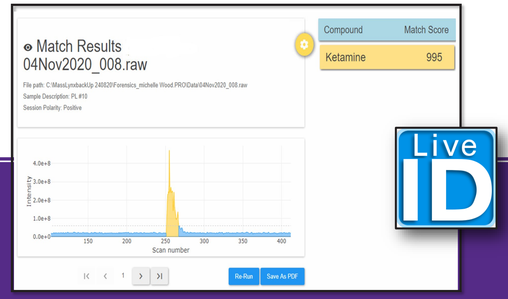


1. Add material to methanol and shake

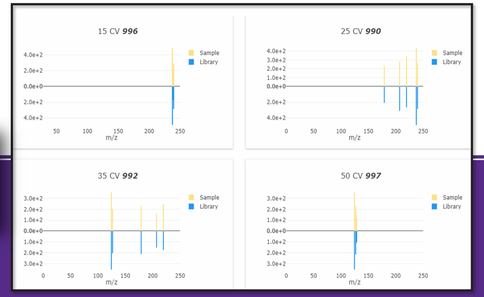
2. Dip a cleaned glass capillary into solution

3. Insert holder into RADIAN-ASAP to start analysis





Live ID



RESULTS & DISCUSSION

- Insertion of the capillary holder initiates data collection at 4 cone voltages and generates a spectral fingerprint, for each analyte, that confers high specificity for drug identification (**Figure 1**)
- LiveID compares the spectral data acquired for samples against a prepared reference library; this matching can be performed in near real-time with a result provided in seconds
- The **Workflow** shows an example of the output obtained following analysis of ketamine CRM and demonstrated a high confidence identification
- CRM for 40 common illicit drugs were analysed. 97.5% resulted in match factors ≥ 877 and in the majority of cases (90%) only one drug was proposed
- More than 60 samples seized by the Police were analysed using RADIAN-ASAP
  - These data were compared with an established high-resolution mass spectrometry (HRMS) screening method (UNIFI™ Forensic Toxicology Screening Solution, Waters Corp)
- Analysis of the confiscated samples revealed a high proportion of ketamine (40%), MDMA (30%), cocaine (20%). Drug mixtures were also identified.
- **Figure 2** shows duplicate analysis for a seized blue 'Punisher' pill. **Figure 3** shows the data for duplicate analysis of a confiscated 'Xanax' pill
- Confirmatory analysis by HRMS showed excellent agreement (> 95%) with the major components identified by ASAP-MS

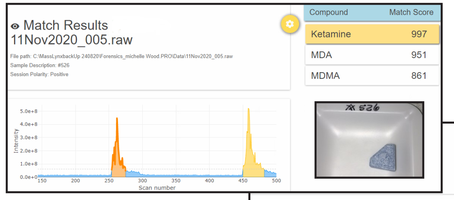


Figure 2. Duplicate 'Dip and Detect' analysis. The results were independently confirmed by the 15 min HRMS screening technique.

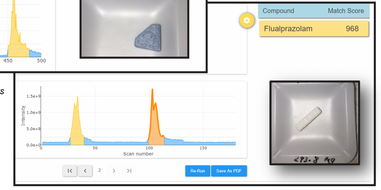


Figure 3. Duplicate analysis of a 'Xanax' sample. Instead of alprazolam, flualprazolam - a 'designer' benzodiazepine, was identified with high confidence.