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Evaluation of the DART QDa System for Forensic Drug Screening

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GOAL

To assess the feasibility of using the DART™ QDa™ System for preliminary forensic drug screening.

BACKGROUND

Authorities worldwide are in a perpetual struggle to ensure public safety against the introduction of illicit drugs which include new psychoactive substances (NPS). Between 2009 and 2016, more than 700 NPS were reported to the United Nations Office on Drugs and Crime.[1]

The increase in both the number and diversity of the drugs involved presents a significant challenge for analytical laboratories. Within the E.U., more than 1 million seizures of illicit drugs are reported annually[2] which only adds to the workflow burden on these labs. Consequently, methods that can facilitate the rapid screening of drugs are of interest.

Previously, we have described a qualitative screening method for medicines based on the ACQUITY™ UPLC™ I-Class System in combination with the ACQUITY QDa™ Mass Detector.[3,4] This method involved a chromatographic separation (15 min) and generation of spectral data by the process of in-source collision-induced dissociation;[4-6] while performance was excellent, the relatively long chromatographic run time employed, in this case, may not be conducive to high numbers of samples. In contrast, the DART Source (IonSense Inc.) is an ambient ionization technology that requires minimal sample preparation and no chromatography.[7]

The DART QDa System can be used as an ultra-fast screening technique for seized material.

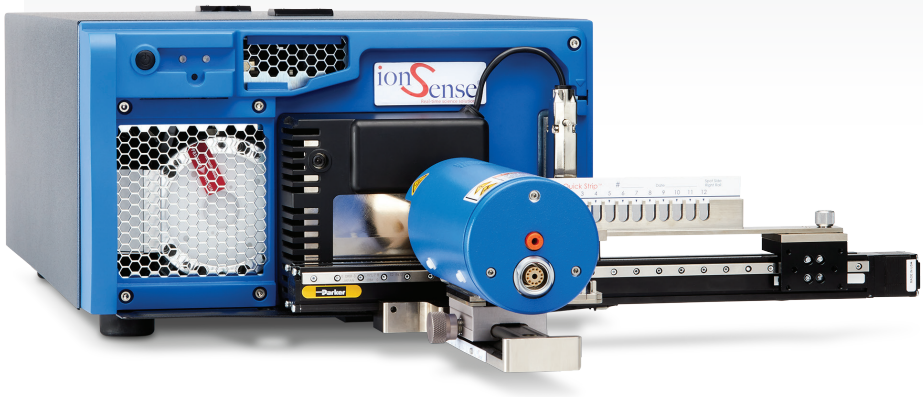

Figure 1. The DART QDa System with the QuickStrip holder.

This preliminary study was designed to evaluate the feasibility of using the DART Source in combination with the ACQUITY QDa (Figure 1) to perform a rapid qualitative screen of drugs. Reference standards were used for the initial evaluation. In addition, a series of unknown samples that had been confiscated at a UK music festival in 2017, by the Greater Manchester Police, UK, were analyzed. Music festivals present a unique opportunity to monitor drug trends and to better understand potential risk of these substances to public health.

THE SOLUTION

MATERIALS AND EXPERIMENTAL

Nine certified reference standards were purchased from Sigma-Aldrich (Poole, UK) at a concentration of 1 mg/mL in methanol. Prior to use, working solutions of the individual standards were prepared at 50 µg/mL by dilution with methanol; several mixtures, at various concentration ratios, were also prepared. The unknown samples were dissolved in methanol for analysis.

The DART QDa System used in these studies was equipped with a transmission module i.e., a railed system designed to automate sampling from a DART QuickStrip™ card; each card provides 12 sampling positions (Figure 1). Three microliter aliquots of each sample were spotted onto the card which was air dried for five minutes before being placed into the holder. Samples were passed in front of a flow of heated helium gas from the DART Source[5] which induced ionization.

Data were acquired in full scan at multiple cone voltages in positive mode using in-source collision-induced dissociation (Tables 1 and 2 list the ionization source conditions and the MS settings).

Data processing was achieved using Primary Ion Middle Ion Structural Analysis (PIMISA) software, from IonSense who also supplied a spectral library containing containing more than 800 substances.

DART conditions

Parameter	Settings
Polarity	Positive ion
DART gas and temp.	Helium at 300 °C
Rail speed (mm/sec)	1.0
QuickStrip card (no. of samples)	12

Table 1. DART ionization source conditions.

QDa conditions

Parameter	Settings
Acquisition software	MassLynx™
Analysis time (sec/sample)	5
Data acquisition	Full scan mass spectra
Cone voltage (V)	15, 30, 50, and 70
Acquisition range (*m/z*)	60–650
Sampling frequency (Hz)	5
Acquisition time (min)	3.5

Table 2. MS conditions.

RESULTS

Multi-cone voltage spectral data were acquired. Figure 2 shows the spectral data obtained at the various cone voltages for the drug amphetamine. With the PIMISA software, confidence in identification is achieved by matching the acquired data to the spectral library to obtain an average match score calculated across four cone voltages. The maximum score is 1 which can be considered to be equivalent to 100% match; for the purpose of this study, a minimum detection criteria of 0.7 (70% confidence) was applied to indicate a putative positive identification. Figure 3 shows an example of the spectral match of the acquired data of the individual standard of MDA to the supplied library. Successful identification was achieved for all of the individual standards analyzed (Table 3).

Mixtures of reference material prepared to contain both cocaine and clonazepam, at various concentration ratios, were also analyzed; both components were successfully identified with PIMISA with an average score confidence exceeding 90% (Table 4).

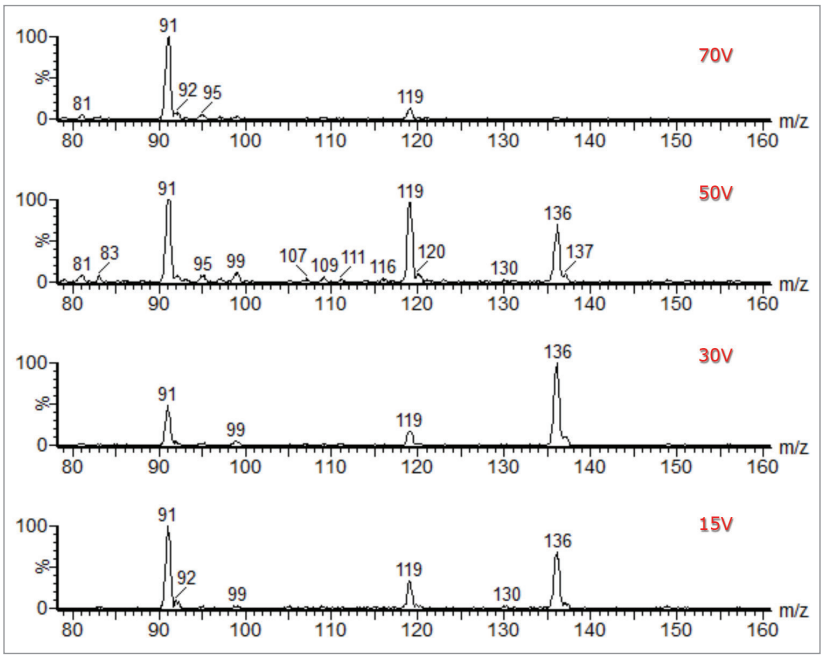

Figure 2. An example of smoothed MassLynx spectral data for amphetamine at multiple cone voltages.

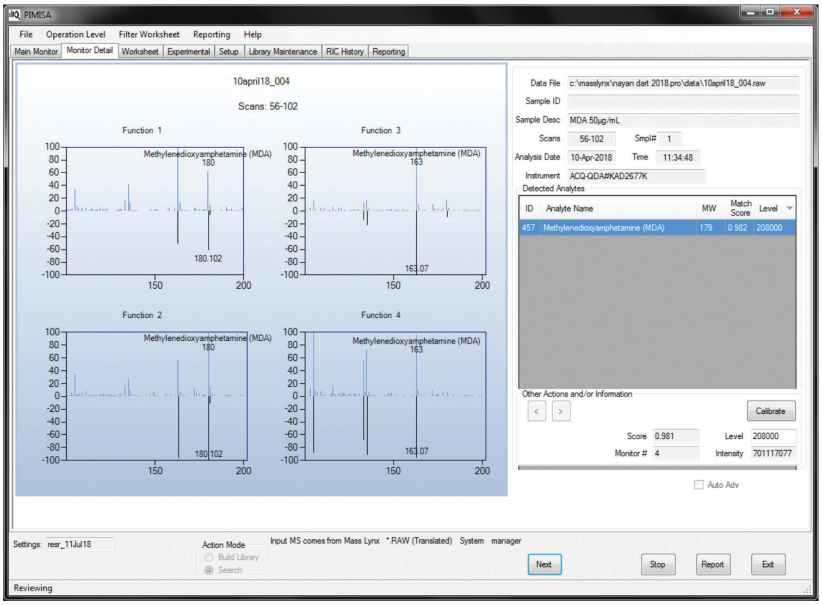

Figure 3. Spectral matching of 4 cone voltages (Functions 1–4) of the acquired data (upper trace) to the supplied library spectra (lower trace) for MDA.

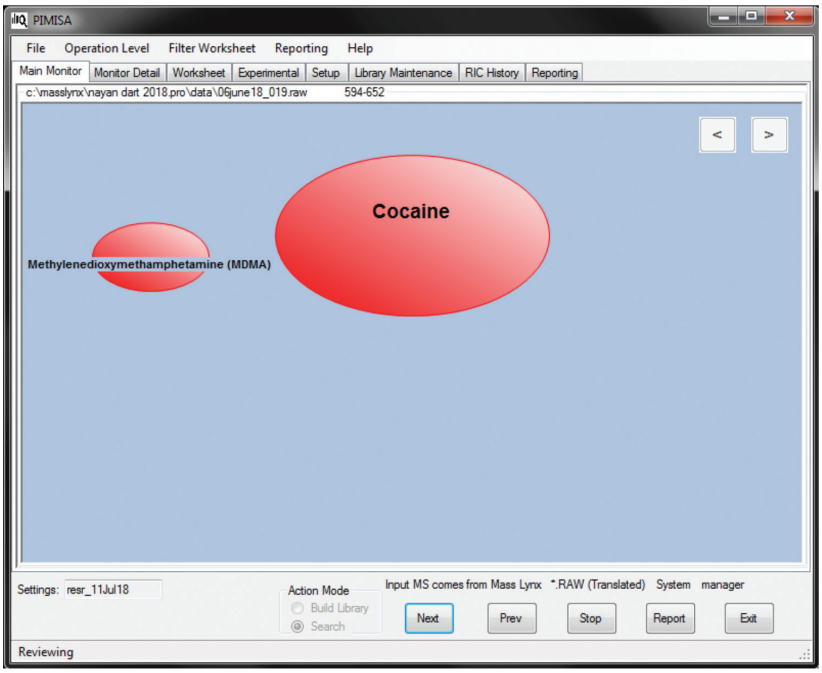

Figure 4. An example of a processed dataset illustrating the successful identification and relative peak area abundance of cocaine and MDMA (ecstasy) within a drug seizure tablet.

Individual Reference Standards	Average Match (%)
Amphetamine	97
Clonazepam	100
Cocaine	92
Ketamine	98
MDA	90
Morphine	99
Naproxen*	89
Sertraline*	91
THC	99

Table 3. Average PIMISA match scores for the individual standards.
**Supplied library modified by adding new data for these two analytes.*

Mixtures	Average Match (%)
Clonazepam:Cocaine (50 µg/mL: 50 µg/mL)	Clonazepam = 91 Cocaine = 95
Clonazepam:Cocaine (50 µg/mL: 10 µg/mL)	Clonazepam = 99 Cocaine = 94
Clonazepam:Cocaine (10 µg/mL: 50 µg/mL)	Clonazepam = 90 Cocaine = 95

Table 4. Average PIMISA match scores for mixtures.

The seized drug samples were also analyzed using the DART QDa System. PIMISA provided putative positive identification of drug substances found either as an individual component or in combination with other drugs. Figure 4 shows an example of the results from one of the seized samples. Analysis of the other confiscated samples revealed a high abundance of the following drug substances: ketamine, MDMA, cocaine, either alone or in the presence of other substances, as well as sildenafil and paracetamol. All DART QDa System results were independently confirmed by an alternative methodology based on an ACQUITY UPLC I-Class/Xevo™ G2-XS QTof.

SUMMARY

This study has shown the potential of the DART QDa System as an initial ultra-fast screening technique for seized material. The acquired data demonstrated excellent agreement with the supplied spectral library, resulting in high match factors and putative positive identification for known drug standards and for the unknown drug seizures. The results obtained with the DART QDa System were confirmed using an alternative method based on UPLC-QTof technology.

References

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