Rapid Detection of 25 Types of Narcotics by DART Coupled with Ultivo Triple Quadrupole MS (DART-MS/MS)

Jianzhong Li¹; Kerry SONG²; Xiaokun DUAN²; Charles LIU²; ¹ Agilent Technologies, Beijing, CHINA; ²ASPEC Technologies, Beijing, CHINA;

OVERVIEW

A rapid screening method for narcotics by DART-Ultivo MS/MS is described. DART-MS enables high-throughput in-situ analysis for forensic evidence detection which requires for speed and effectiveness. With multiple innovations, Agilent Ultivo mass spectrometer also provides high performance for rapid and mobile testing. This experiment uses DART- Ultivo system for rapid qualitative and quantitative analysis of 25 types of Narcotics samples.

INTRODUCTION

Narcotics have historically been used to refer to a number of mind-altering substances as well as to provide a broad legal designation for a range of illicit drugs; today, the Drug Enforcement Administration (DEA) more specifically defines narcotic drugs as those that relieve pain and dull the senses, and the use of the word is most commonly associated with opioid drugs. Some of the more widely-known narcotics and opioids drugs, e.g. heroin, codeine, oxycodone, morphine, fentanyl, et al. Opioid abuse, addiction, and overdose are considered serious public health concerns in the world.

Ultivo is a stackable Liquid Chromatography Triple Quadrupole (LC/TQ) mass spectrometer that eliminates the MS footprint by incorporating the MS into the LC stack, and represents a transformative approach to LC/TQ. Ultivo triple quadrupole LC/MS provides the performance found in larger comparable systems, but at a fraction of their size. Innovations such as the Vortex Collision Cell, Cyclone Ion Guide, and VacShield provide users the sensitivity, robustness, reliability, and performance required for the day-in, day-out challenges of high-throughput sample analysis.

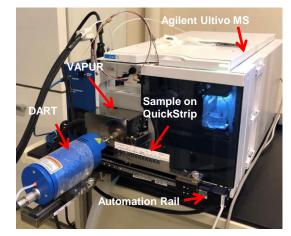
Increasing in cases involving narcotics of abuse leads to heavy burden for law enforcement agencies, exacerbating demand for rapid screening technique. This article introduced a fast qualitative and quantitative method which was combined DART with Agilent Ultivo system for testing 25 types of narcotics samples.

MATERIALS AND METHODS

The QuickStrip module (IonSense) was used for mixed standard of drugs and extract of authentic hair samples, with optimal linear rail speed at 0.5 mm/s and helium temperature at 350° C. Nitrogen gas was employed during method development phases for economics. All the standard solutions were prepared and dissolved to 1ng/mL, 2ng/mL, 5ng/mL, 10ng/mL, 20ng/mL, 50ng/mL, 100ng/mL by methanol. The DART source (IonSense) was coupled with a Ultivo triple quadrupole mass spectrometer (Agilent) in positive ion mode and scanned with scheduled MRM with optimized conditions. Data acquisition and processing were both accomplished with MassHunter software (Agilent).

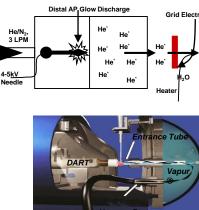
RESULTS

Fig 1. DART- Agilent Ultivo coupled with a VAPUR interface



DART[®] was connected to the Agilent Ultivo MS/MS through VAPUR interface. The distance between the DART[®] gun exit and VAPUR[®] inlet was 15 mm. The sampling glass rod was immersed for 1s into a 2 mL glass vial containing samples. The linear rail speed was 0.6 mm/s.

Fig 2. Schematic diagram and VAPUR® used in th



DART was operated at a flow rate of 2.5 L/min of He and a defaulted grid voltage of 30 V. The VAPUR ceramic tube was adjusted thus leaving a gap of 2mm between the VAPUR outlet and the inlet of MS. The vacuum pump (WELCH, USA) was maintained at a medium speed to help VAPUR efficiently collect and pull ions generated outside of the DART source and to separate ions from gas and other particle species.

Tab 1. Conditions for mass spectrometry

Compound name	Precursor (m/z)	Product (m/z)	Fragmentor (V)
Codeine	300.2	165.1 / 215.1	160
Papaverine	340.2	202.0 / 171.0	160
Acetylcodeine	342.3	225.1 / 282.1	165
Heroin	370.3	268.3 / 328.2	170
Cocaine	304.2	182.1 / 150.1	125
Meperidine	248.2	220.1 / 174.1	140
CBD	315.3	193.1 / 259.3	125
Caffeine	195.1	138.1 / 110.1	120
Morphine	286.2	165.0 / 201.0	155
Amphetamine	136.1	119.1 / 91.1	70
Fentanyl	337.3	188.1 / 105.2	130
THC	315.2	193.1 / 259.1	135

s of DART®	
nis study	





CE (V)
55 / 30
30 / 45
30 / 25
30 / 30
20/30
25 / 20
25 / 20
20 /25
50 / 30
8 / 20
25 / 45
25 / 20

Compound name	Precursor (m/z)	Product (m/z)	Fragmentor (V)	CE (V)
Triazolam	343.1	315.1 / 308.1	180	30 / 30
JWH073	328.3	155.0 / 127.0	150	25 / 55
JWH-122	356.2	214.2 / 169.1	170	25 / 30
JWH-210	370.3	183.1 / 214.2	180	30 / 30
JWH-203	340.2	125.1 / 214.1	150	35 / 30
Midazolam	326.2	291.2 / 209.0	170	30 / 40
Paracetamol	152.1	110.1 / 65.1	110	15 / 35
Ketamine	238.0	125.0 / 179.0	100	35 / 20
Thebaine	312.2	58.2 / 266.1	100	15 / 16
Methadone	310.3	265.2 / 105.1	110	15 / 30
Nitrazepam	282.1	236.0 / 180.1	140	30 / 45
Promethazine	285.2	86.1 / 198.0	100	20 / 30
Methcathinone	164.1	146.1 / 131.1	90	10 / 20
MDMA	194.1	163.1 / 105.0	90	10 / 30
Chlordiazepoxide	300.1	282.1 / 227.0	145	25 / 25
Cathinone	150.1	132.1 / 117.0	80	10 / 25
Methaqualone	251.1	132.0 / 91.0	145	30 / 50

Fig 3. Cali. curves of : (a) Methagualone; (b) Ketamine ; (c) Nitrazepam ; (d) Cocaine

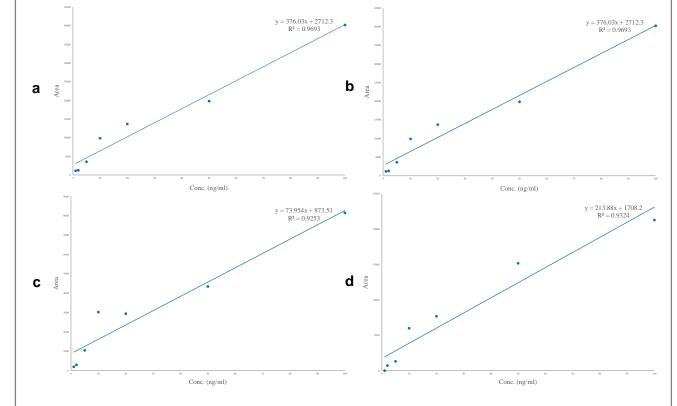
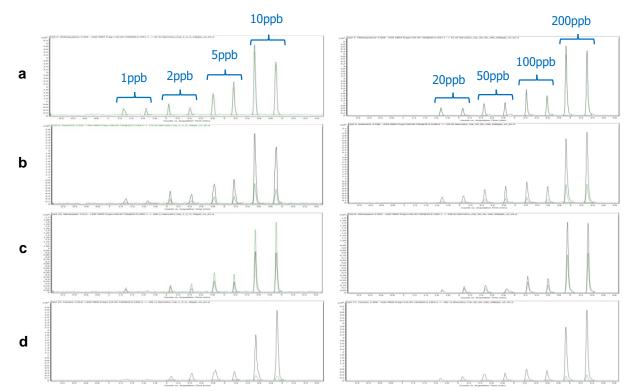


Fig 4. Detection of four Drugs by DART-Ultivo (a) Methaqualone; (b) Ketamine ; (c) Nitrazepam ; (d) Cocaine



CONCLUSIONS

A DART-Ultivo MS/MS method was established to rapidly gualitative and guantitative of 25 types of narcotics samples. The results were encouraging. All 25 types of drugs in different types showed positive results at concentrations of 1ng/mL, and good linearity over the evaluated range (1 – 100 ng/mL). Take Methagualone, Ketamine, Nitrazepam and Cocaine for examples. The linearity is between 92.53-96.93% from 1 to 100ng/mL in 6 orders of magnitude. The signal-to-noise ratio (S/N) were \geq 3 at concentration of 1ng/ml, which meets the requirement of quantitation limit S/N>10. Similarly, codeine, papaverine, fentanyl, midazolam cathinone and other 20 drugs were also analyzed by DART-Ultivo.

This method could successfully be used to analyze narcotics of abuse rapidly and confidently with minimal sample preparation (no derivatization steps and radiation-free). The advantage of this method includes fast response and ease of operation. The highthroughput potential for the analysis of various compounds makes this approach a promising alternative for the forensic science laboratory.





