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Application News

No. B81

MALDI-TOF Mass Spectrometry

Detection of Prescription Drugs and Cocaine in Urine using the MALDI-8020

Background

Clinical drug tests are used to analyse biological specimens, for example urine, hair, blood, breath, sweat, or saliva to determine the presence or absence of a specified drugs or related metabolites. Indications for drug testing include the following;

- Athletic drug testing.
- Pre-employment drug screening test or random drug testing to identify on-the-job drug abuse.
- Safety-related drug testing - where drug use could lead to safety issues (mental or physical impairment.)
- Post-accident drug testing - where drug use or misuse leads to an accident. This could include vehicular or work accidents and may result in casualties or property damage.

MALDI-TOF MS has the ability to quickly detect drug compounds in urine with minimal sample processing.

Michael Nairn

MALDI-8020

The MALDI-8020 developed by Shimadzu is a small footprint linear MALDI-TOF MS benchtop instrument and offers high performance featuring a 200 Hz solid state laser, sample loading times of less than 90 seconds and an automated source cleaning mode.

Table 1 Sample information

	Formula	$[M+H]^+$
Sample 1		
Mirtazapine	$C_{17}H_{19}N_3$	266.165
Promazine	$C_{17}H_{20}N_2S$	285.142
Trimipramine	$C_{20}H_{26}N_2$	295.217
Zolpidem	$C_{19}H_{21}N_3O$	308.176
Quetiapine	$C_{21}H_{25}N_3O_2S$	384.174
Sample 2		
Cocaine	$C_{17}H_{21}NO_4$	304.154
Cocaethylene	$C_{18}H_{23}NO_4$	318.170

Fig. 1 MALDI-8020 benchtop linear MALDI-TOF instrument

Samples and Methods

Prof. Franco Tagliaro from the University of Verona (Italy) kindly provided urine samples spiked with drug compounds and metabolites for analysis. These compounds were spiked at similar relative concentrations as would be produced by drug consumers. Sample 1 contained sedatives, antipsychotics and antidepressants. Sample 2 contained cocaine and metabolites of cocaine.

As urine contains a lot of salts, liquid-liquid extraction (LLE) was used to desalt, extract and enrich the samples prior to MALDI-TOF MS.

α-cyano-4-hydroxy-cinnamic acid (CHCA) was used as the MALDI matrix and was prepared at a concentration of 5 mg/mL in 1:1 ACN/0.1 % TFA mixture and mixed with cetyltrimethylammonium bromide (CTAB) in a molar ratio of 13250:1 CHCA:CTAB[*1]. CTAB was used as a quenching agent to reduce the intensity of the CHCA matrix peaks. The sample and matrix were spotted in a 1:1 ratio onto a Shimadzu FlexiMass-SR48 slide.

*1 Gottardo, R. (2012). Direct screening of herbal blends for new synthetic cannabinoids by MALDI-TOF MS https://doi.org/10.1002/jms.2036

Results

The MALDI-8020 was able to detect all the drug compounds present in samples 1 and 2 (Fig. 2, 3) with good mass accuracy. In addition, the data shows that the MALDI-8020 was able to distinguish Promazine which is 0.2Da smaller than the carbon-13 peak of CTAB.

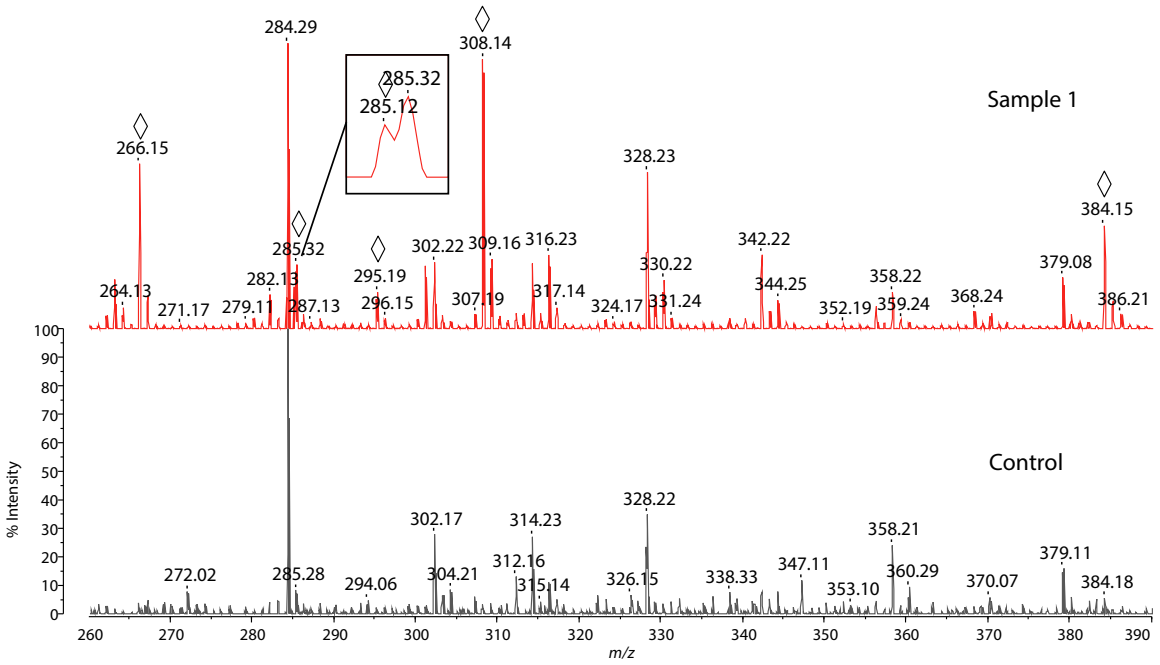

Fig. 2 Peaks consistent with spiked drug molecules are marked with a diamond shape.
The MALDI-8020 is able to distinguish Promazine that is 0.2Da smaller than the secondary isotope of cetyltrimethylammonium bromide

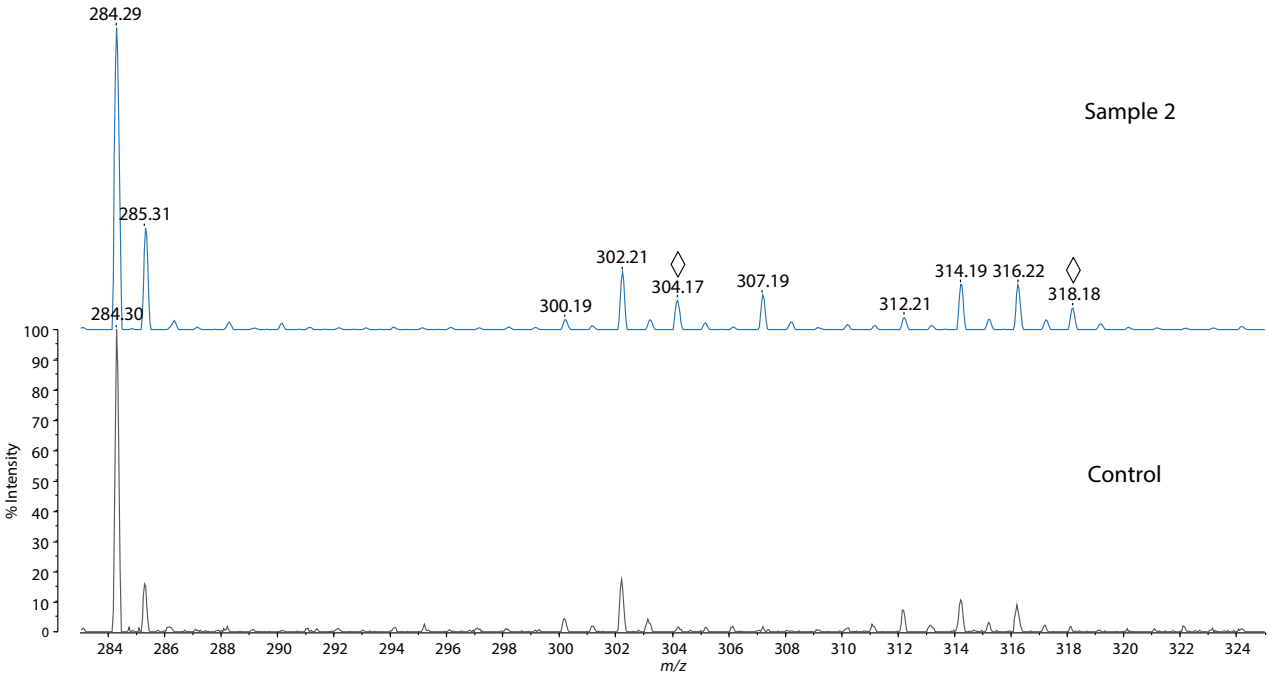

Fig. 3 Peaks consistent with spiked drug molecules are marked with a diamond shape.
The MALDI-8020 was able to detect Cocaine $[M+H]^+$ and its metabolites.

First Edition: May 2018

Shimadzu Corporation
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