Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

Rapid Characterization of Drugs in a Single Hair using Thermal Desorption Ionization Mass Spectrometry

Ran Kong[1, 2], Le Li[1, 2], Wanhui Liu[2], Ping Xiang[1]*, Junbo Zhao[1*]

1. Department of Forensic Toxicology, Shanghai Key Laboratory of Forensic Medicine, Shanghai Forensic Service Platform, Academy of Forensic Science, Shanghai, China
2. School of Pharmacy, Yantai University, Yantai, China

Table S1. Accurate mass identification for the major ionic species mentioned in the study

Compound	Elemental Composition	Experimental *m/z*	Theoretical *m/z*	Error (ppm)
MAMP	$C_{10}H_{16}N^+$	150.1281	150.1283	-1.33
AMP	$C_9H_{14}N^+$	136.1124	136.1126	-1.47
Tramadol	$C_{16}H_{26}NO_2^+$	264.1961	264.1964	-1.14
Methadone	$C_{21}H_{28}NO^+$	310.2169	310.2171	-0.64
Diazepam	$C_{16}H_{14}ClN_2O^+$	285.0788	285.0795	-2.46
Ocimene	$C_{10}H_{17}^+$	137.1324	137.1330	-4.38
Naphthalene	$C_{15}H_{25}^+$	205.1956	205.1956	0.00
CBN	$C_{21}H_{27}O_2^+$	311.2017	311.2011	1.93
THC/CBD	$C_{21}H_{31}O_2^+$	315.2329	315.2319	3.17
THCA	$C_{21}H_{29}O_4^+$	345.2068	345.2066	0.58
CBDA	$C_{22}H_{31}O_4^+$	359.2224	359.2222	0.56

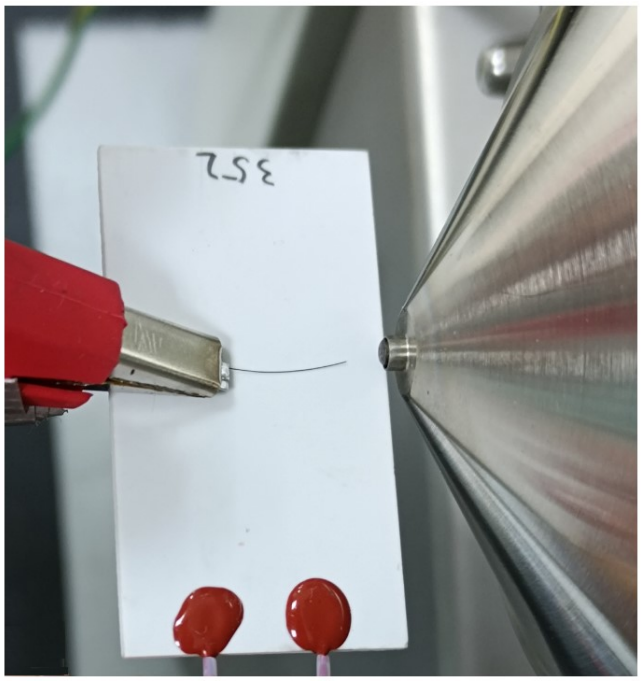

Figure S1. Graphical illustration of a TDI source coupled to an LTQ-Orbitrap mass spectrometer.

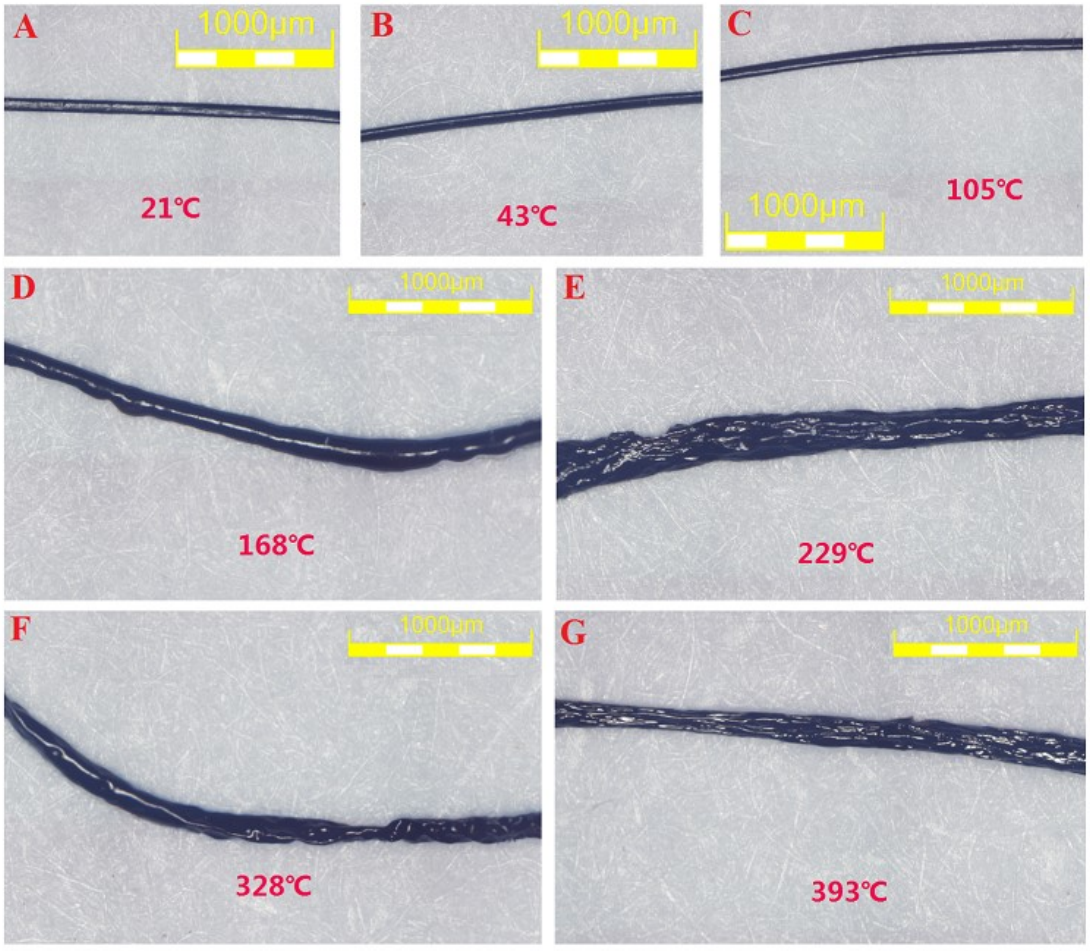

Figure S2. Electron microscope images of a single hair at different MCH temperatures**.**

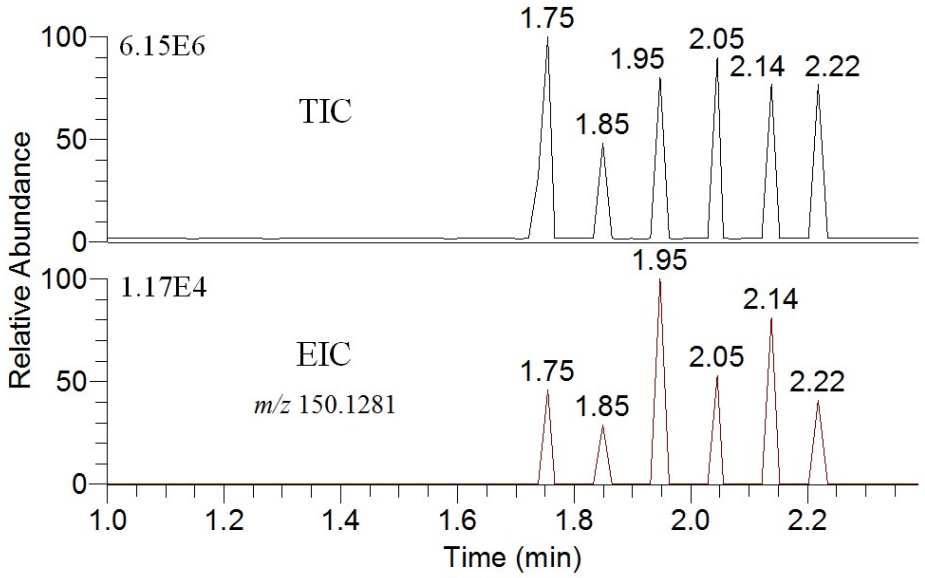

Figure S3. Total ion chromatogram (TIC) and extracted ion chromatogram (EIC) were obtained by added the solvent six times for analysis of methamphetamine (*m/z* 150.1281) in hair sample by TDI-MS.

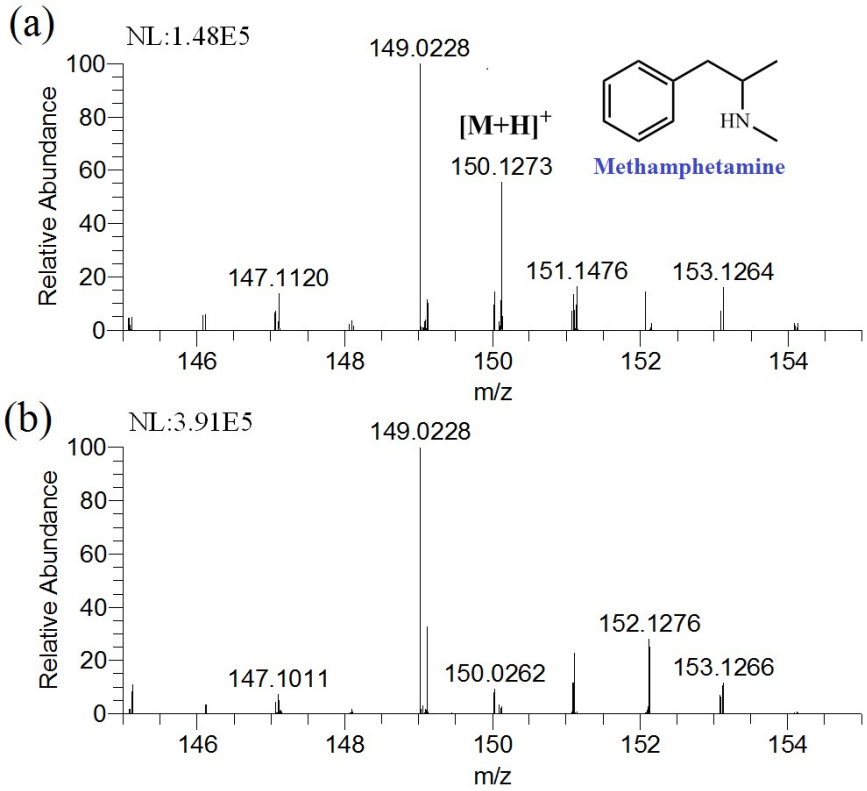

Figure S4. DART direct analysis of hairs from the methamphetamine users: (a) A wisp hair (about 30 hairs), (b) a single hair. The MAMP ion could only be observed in a wisp hair. The helium temperature was set to 250 °C.

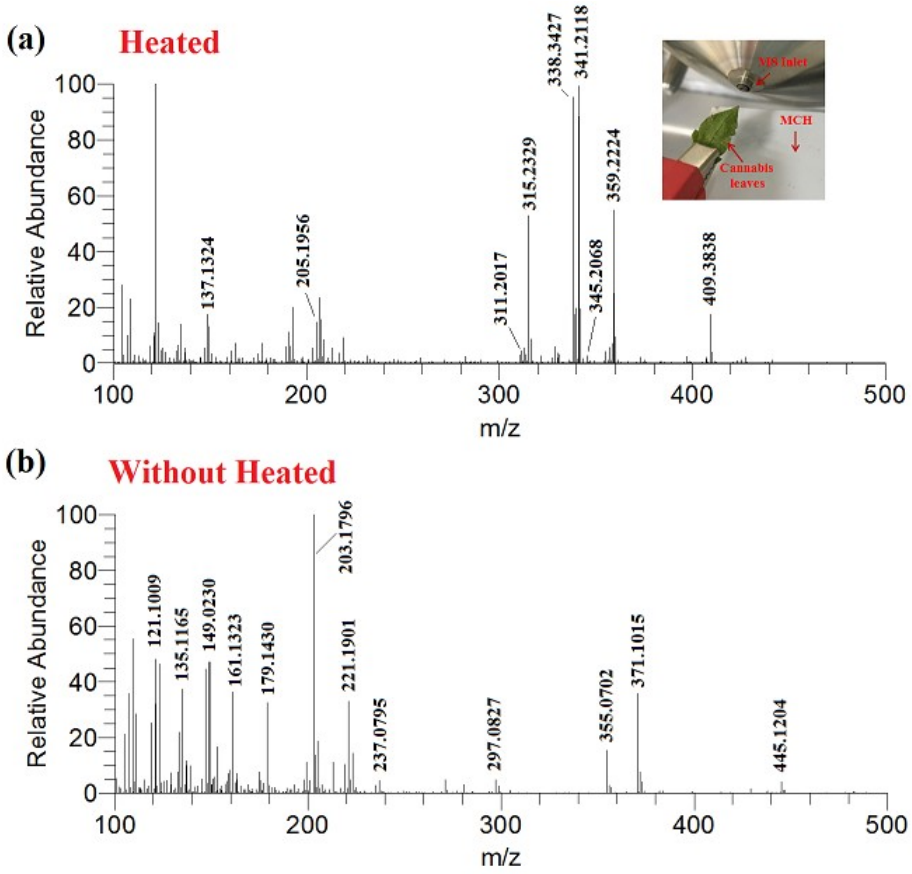

Figure S5. The fresh cannabis leaves were analyzed by TDI-MS. (a) The mass spectrum of cannabis leaf was obtained with heated by the MCH. (b) The mass spectrum of cannabis leaf was obtained without heated by the MCH. The mainly detected active components in cannabis leaves were cannabinoids, such as cannabidiol/Δ^9-tetrahydrocannabinol (CBD/THC, 315.2329), Δ^9-tetrahydrocannabinolic acid (THCA, 345.2068), cannabinol (CBN, 311.2017), and cannabidiolic acid (CBDA, 359.2224).

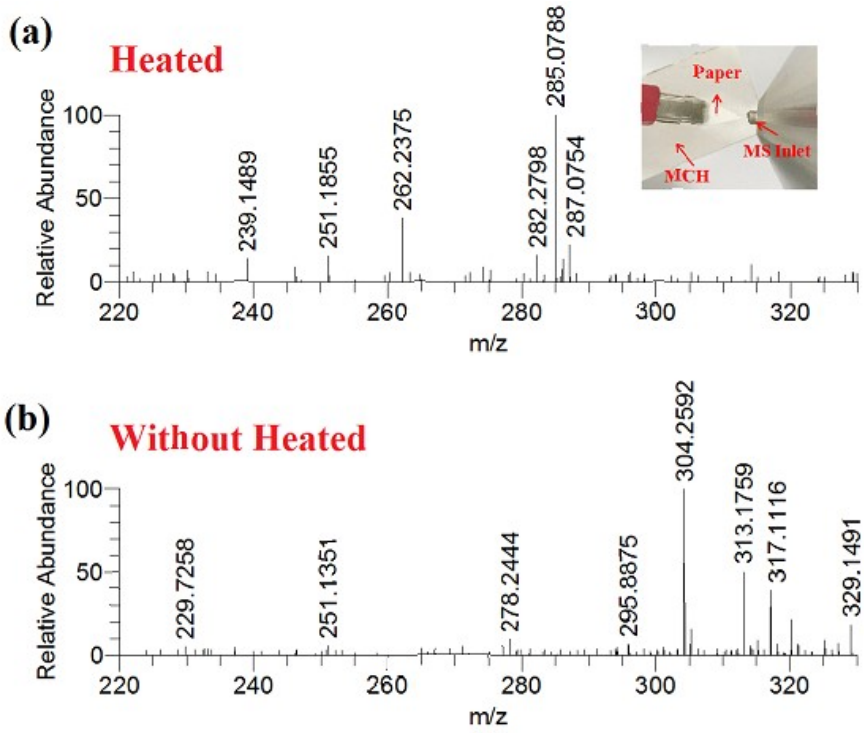

Figure S6. The mass spectra were obtained by paper spray direct ionization of the urine sample which was containing the drug of the diazepam. (a) The urine sample was analyzed by paper spray with heated. (b) The urine sample was analyzed by paper spray without heated.