

Supporting Information

Analysis of 15 anti-obesity drugs in urine using thermal-assisted paper spray mass spectrometry

Shijia Jiang ^{a, b, †}, Junbo Zhao ^{a, †}, Hui Yan ^a, Ping Xiang ^a and Min Shen ^{a, *}

^a *Department of Forensic Toxicology, Shanghai Key Laboratory of Forensic Medicine, Shanghai Forensic Service Platform, Academy of Forensic Science, Shanghai, 200063, China*

^b *Criminal Justice College, East China University of Political Science and Law, Shanghai 200042, China*

^{*} *Corresponding author*

[†] *Equal contribution*

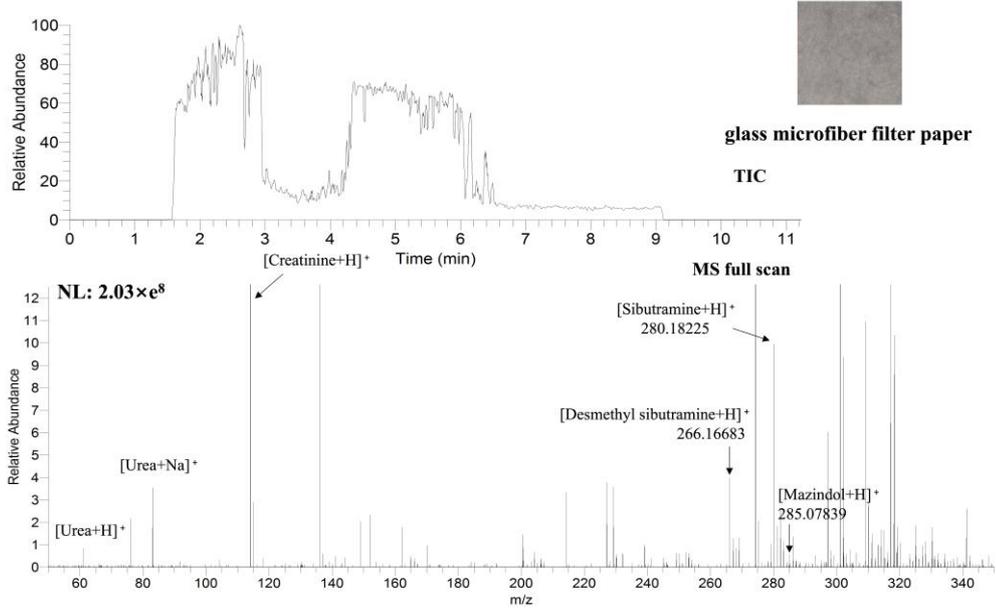
Table S1. Accurate mass identification for the major ionic species of anti-obesity drugs

Analyte	Ion Composition	Accurate mass		Error (ppm)
		Theoretical	Experimental	
Sibutramine	$C_{17}H_{27}ClN^+$	280.18265	280.18314	1.75
Cathinone	$C_9H_{12}NO^+$	150.09134	150.09103	-2.07
Desmethyl Sibutramine	$C_{16}H_{25}ClN^+$	266.16700	266.16730	1.13
Mazindol	$C_{16}H_{14}ClN_2O^+$	285.07892	285.07965	2.56
Amfepramone	$C_{13}H_{20}NO^+$	206.15394	206.15398	0.19
Didesmethyl Sibutramine	$C_{15}H_{23}ClN^+$	252.15135	252.15230	3.77
Fenfluramine	$C_{12}H_{17}F_3N^+$	232.13076	232.13101	1.08
Fluoxetine	$C_{17}H_{19}F_3NO^+$	310.14133	310.14206	2.35
Phendimetrazine	$C_{12}H_{18}NO^+$	192.13829	192.13834	0.26
Phenmetrazine	$C_{11}H_{16}NO^+$	178.12264	178.12276	0.67
Norfluoxetine	$C_{16}H_{17}F_3NO^+$	296.12568	296.12479	-3.01
Nordiazepam	$C_{15}H_{12}ClN_2O^+$	271.06327	271.06461	4.94
Phentermine	$C_{10}H_{16}N^+$	150.12773	150.12755	-1.20
Oxazepam	$C_{15}H_{12}ClN_2O_2^+$	287.05818	287.05948	4.53
Temazepam	$C_{16}H_{14}ClN_2O_2^+$	301.07383	301.07483	3.32

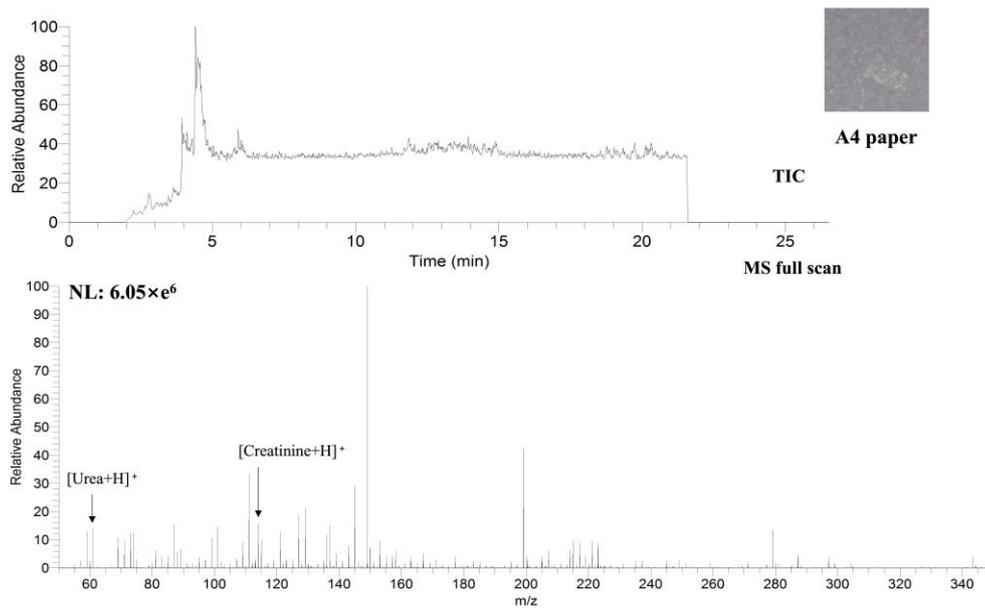
Table S2. Summary of optimal parameters

Parameter	Optimal value
the distance between paper tip and MS inlet	5 mm
paper substance	Whatman filter paper 1
voltage on paper substance	4.5 kV
spray solvent	MeOH: H ₂ O (90:10)

(a)



(b)



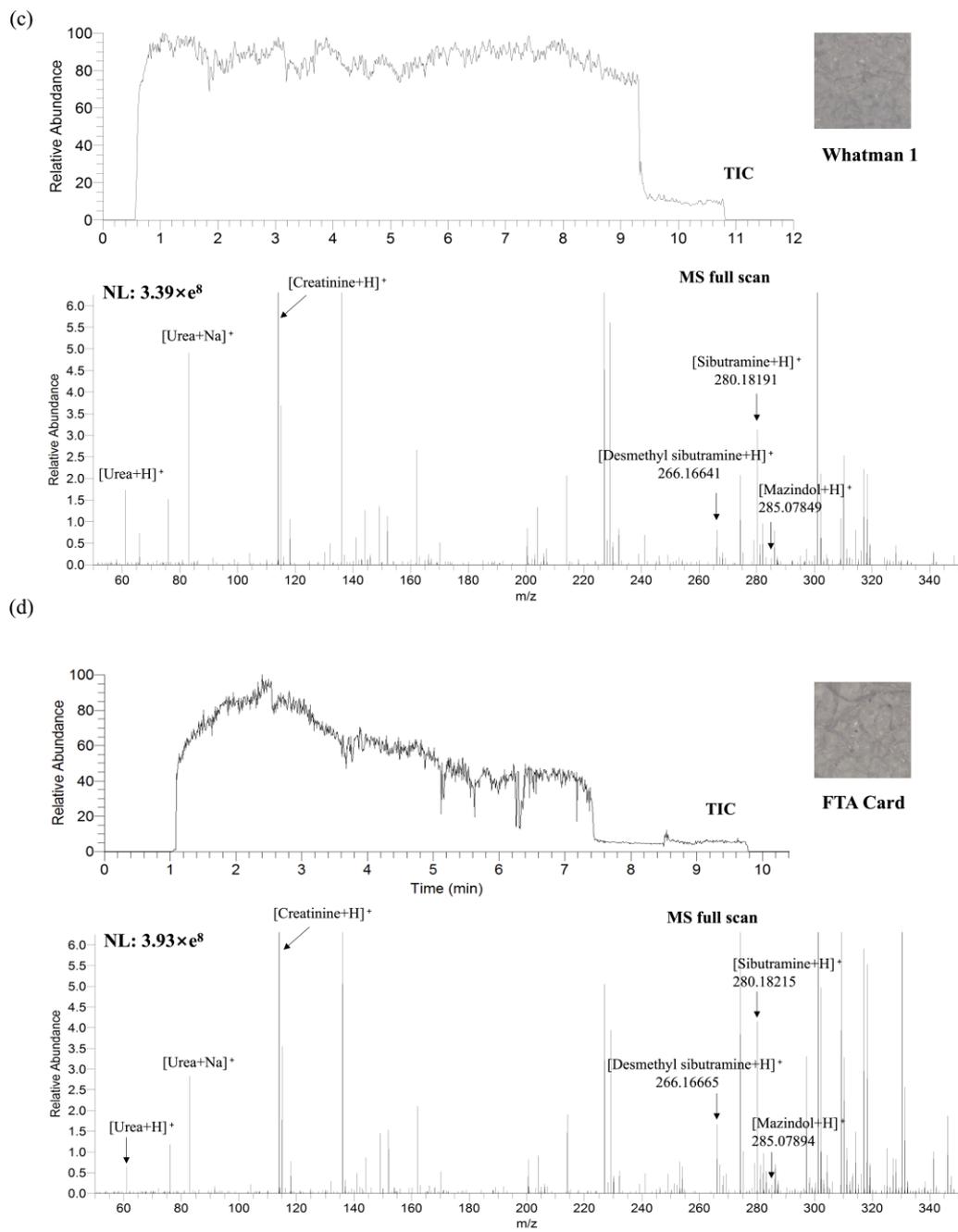


Fig. S1 The detected intensity, TIC and microstructure of (a) glass microfiber filter paper (47mm in diameter), (b) A4 paper, (c) Whatman1 and (d) FTATM card.

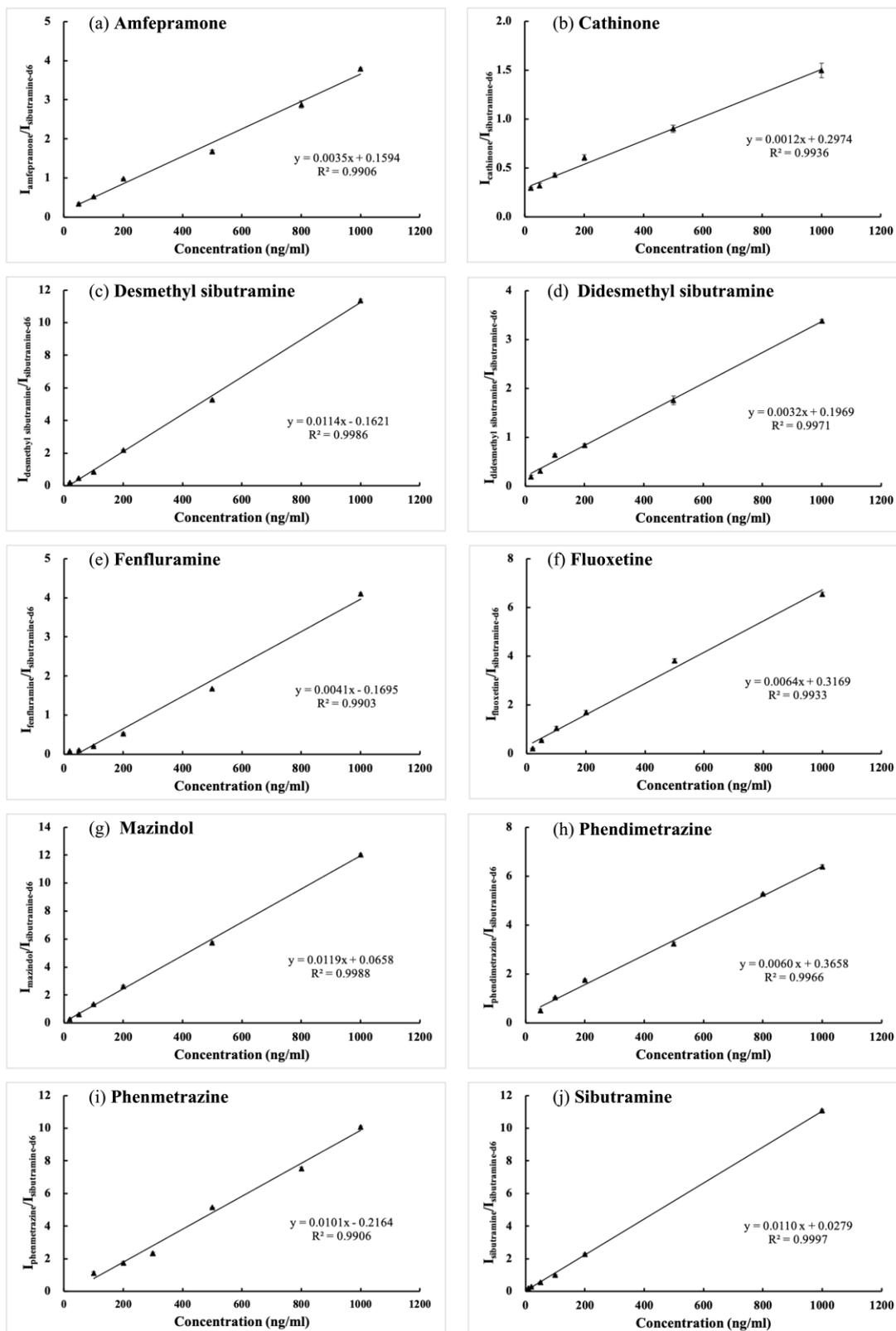


Fig. S2 Linearity between the concentrations of drugs and the intensity ratios of drugs to sibutramine- d_6 . The error bar represents the standard deviation of samples analyzed in triplicate.