Supporting Information

Quantitative Paper Spray Mass Spectrometry Analysis of Drugs of Abuse

Yuan Su [a], He Wang [a], Jiangjiang Liu [a], Pu Wei [b], R. Graham, Cooks [b,c], Ouyang Zheng*[a,c]

[a]*Weldon School of Biomedical Engineering, Purdue University, 206 South Martin Jischke Drive, West Lafayette, IN 47907, USA.*
[b]*Department of Chemistry and Center for Analytical Instrumentation Development, Purdue University, 560 Oval Drive, West Lafayette, IN 47907, USA.*
[c]*Center for Analytical Instrumentation Development, Purdue University, 560 Oval Drive, West Lafayette, IN 47907, USA.*
**Corresponding author. Email: ouyang@purdue.edu;*

Table S-1. Tandem mass spectrometric parameters for paper spray.

Drug	Precursor ion (*m/z*)	Product ion (*m/z*)	Collision energy (V)	Tube lens
Morphine $[C_{17}H_{19}NO_3+H]^+$	286.1	201.0 $-(C_4H_7NO)^1$	25	102
Morphine-d3	289.1	201.0 $-(C_4H_4D_3NO)$	25	102
Benzyolecgonine $[C_{16}H_{19}NO_4+H]^+$	290.0	168.0 $-(C_7H_6O_2)^2$	18	146
Benzyolecgonine-d3	293.0	171.0 $-(C_7H_6O_2)$	18	146
Cocaine $[C_{17}H_{21}NO_4+H]^+$	304.0	182.0 $-(C_7H_6O_2)^3$	20	78
Cocaine-d3	307.0	185.0 $-(C_7H_6O_2)$	20	78
6-acetylmorphine $[C_{19}H_{21}NO_4+H]^+$	328.3	164.9 $-(C_6H_{13}NO_4)^4$	26	117
6-acetylmorphine-d3	331.3	164.9 $-(C_6H_{10}D_3NO_4)$	26	117
Methamphetamine $[C_{10}H_{15}N+H]^+$	150.1	91.1 $-(C_3H_9N)^5$	24	69
Methamphetamine-d8	158.1	93.1 $-(C_3H_3D_6N)$	24	69
Oxycodone $[C_{18}H_{21}NO_4+H]^+$	316.1	298.0 $-(H_2O)^6$	20	80
		241.0 $-(C_3H_7O_2)$	26	80
Oxycodone-d6	322.1	304.8 $-(H_2O)$	20	80
		247.0 $-(C_3H_7O_2)$	26	80
Buprenorphine $[C_{29}H_{41}NO_4+H]^+$	468.2	396.1 $-(C_4H_8O)^7$	36	64
Buprenorphine-d4	472.2	400.1 $-(C_4H_8O)$	36	64

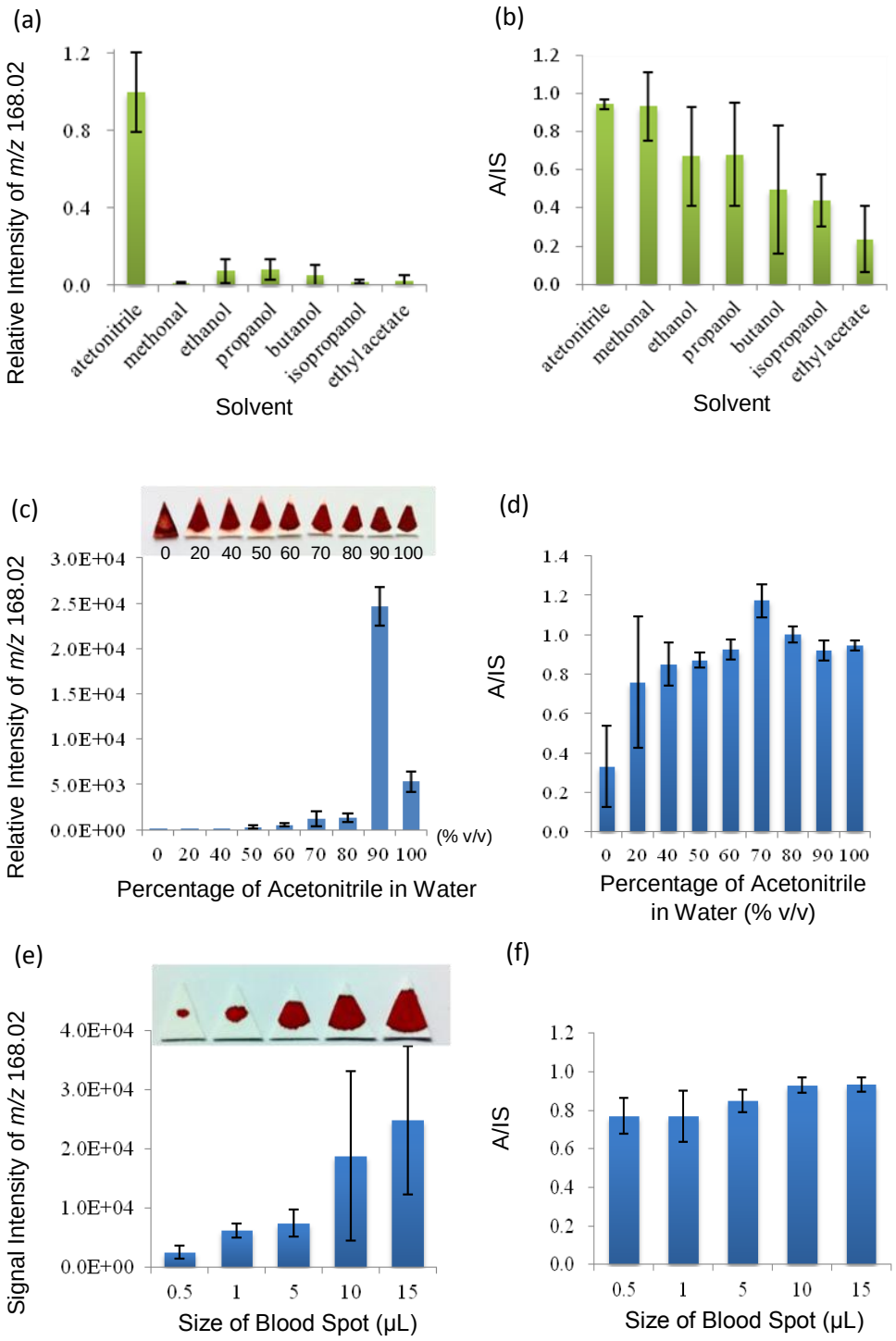

Fig. S1. Optimization of experimental conditions for quantitative paper spray mass spectrometry. Effect of spray solvent on (a) the signal intensity and (b) the ratio of analyte to internal standard (A/IS) of benzyolecgonine [$(M+H)^+$, *m/z* 290.0, product ion, *m/z* 168.0]. Effect of acetonitrile percentage in water on (c) the signal intensity and (d) the ratio of analyte to internal standard (A/IS) of benzyolecgonine. Effect of blood size on (e) the signal intensity and (f) the ratio of analyte to internal standard (A/IS) of benzyolecgonine.

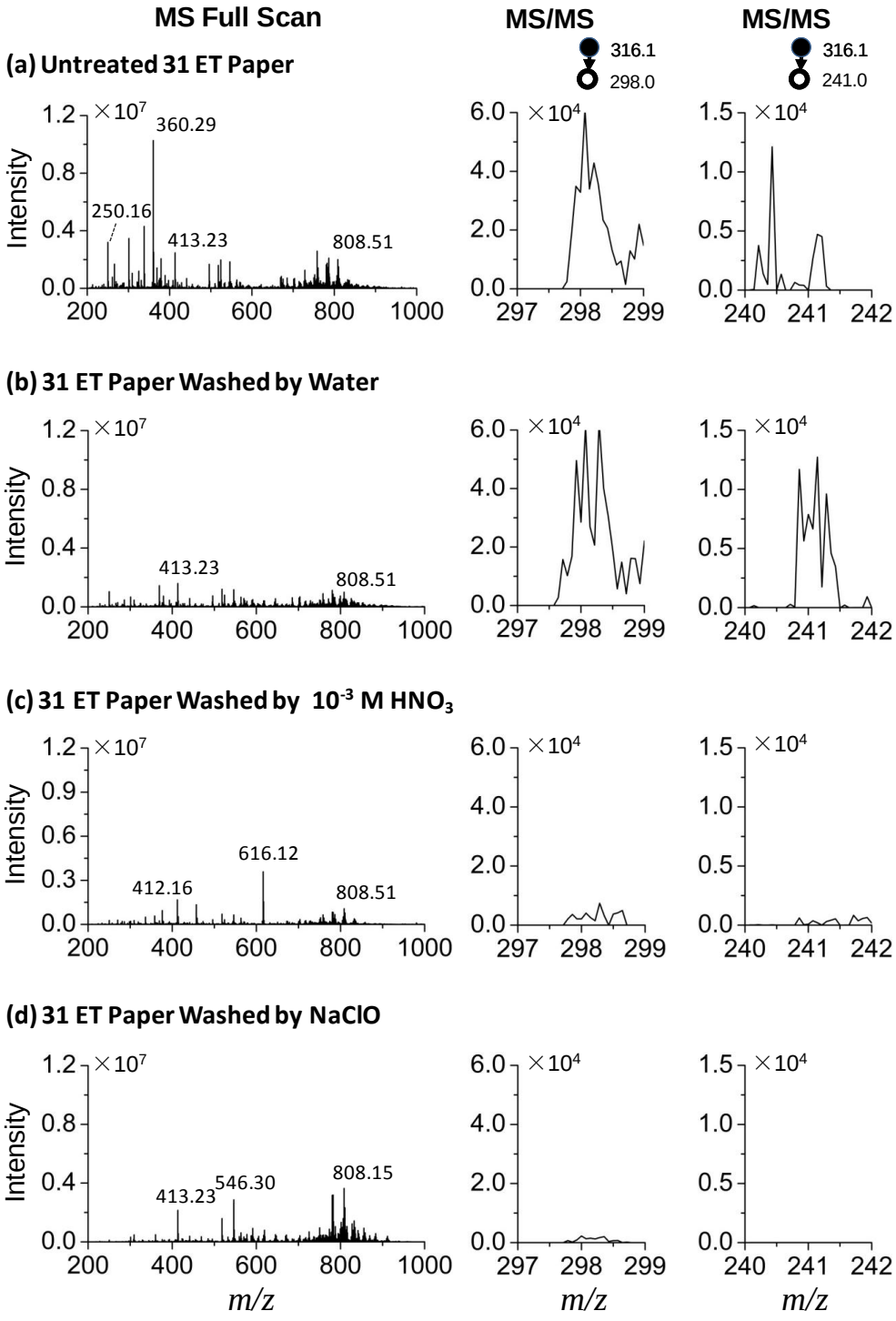

Fig. S2. MS spectra (mass range: *m/z* 200-1000) by Orbitrap and MS/MS spectra (parent ion: *m/z* 316.1, mass range: 297.0-299.0 and 240.0-242.0) by TSQ for blank dried blood spot with different treatment of paper: (a) untreated 31 ET paper, (b) 31 ET paper washed by water, (c) 31 ET paper washed by 10^{-3} M HNO3 aqueous solution and (d) ET paper washed by NaClO aqueous solution (Cl% = 1.5 g/L, pH=12). Paper spray solvent: 90% acetonitrile: 10% water solution; solvent volume: 25 μL; Voltage: 3.5 kV.

References

[1] C. Poeaknapo, U. Fisinger, M. H. Zenk and J. Schmidt, *Phytochemistry,* 2004, **65,** 1413–1420.

[2] W. F. Smyth, *Electrophoresis*, 2005, **26,** 1334–1357.

[3] O. Curcuruto, F. Guidugli and P. Traldi, *Rapid Commun. Mass Spectrom.* 1992, **6,** 436-437.

[4] K. Raith and R. Neubert, J. Am. Soc. Mass Spectrom., 2003, **14,** 1262–1269.

[5] W. E. Steiner, B. H. Clowers, K. Fuhrer, M. Gonin, L. M. Matz, W. F. Siems, A. J. Schultz and H. H. Hill, *Rapid Commun. Mass Spectrom.* 2001, **15,** 2221-2226.

[6] K. Pennanen, T. Kotiaho, K. Huikko and R. Kostiainen, *J. Mass Spectrom.,* 2001, **36,** 791–797.

[7] D. Favretto, G. Frison, S. Vogliardi and S. D. Ferrara, *Rapid Commun. Mass Spectrom.* 2006, **20,** 1257-1265.