

Supporting Information

**Quantitative Paper Spray Mass Spectrometry
Analysis of Drugs of Abuse**

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

Drug	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	Collision energy (V)	Tube lens
Morphine [C ₁₇ H ₁₉ NO ₃ +H] ⁺	286.1	201.0 -(C ₄ H ₇ NO) ¹	25	102
Morphine-d3	289.1	201.0 -(C ₄ H ₄ D ₃ NO)	25	102
Benzoyllecgonine [C ₁₆ H ₁₉ NO ₄ +H] ⁺	290.0	168.0 -(C ₇ H ₆ O ₂) ²	18	146
Benzoyllecgonine-d3	293.0	171.0 -(C ₇ H ₆ O ₂)	18	146
Cocaine [C ₁₇ H ₂₁ NO ₄ +H] ⁺	304.0	182.0 -(C ₇ H ₆ O ₂) ³	20	78
Cocaine-d3	307.0	185.0 -(C ₇ H ₆ O ₂)	20	78
6-acetylmorphine [C ₁₉ H ₂₁ NO ₄ +H] ⁺	328.3	164.9 -(C ₆ H ₁₃ NO ₄) ⁴	26	117
6-acetylmorphine-d3	331.3	164.9 -(C ₆ H ₁₀ D ₃ NO ₄)	26	117
Methamphetamine [C ₁₀ H ₁₅ N+H] ⁺	150.1	91.1 -(C ₃ H ₉ N) ⁵	24	69
Methamphetamine-d8	158.1	93.1 -(C ₃ H ₃ D ₆ N)	24	69
Oxycodone [C ₁₈ H ₂₁ NO ₄ +H] ⁺	316.1	298.0 -(H ₂ O) ⁶	20	80
		241.0 -(C ₃ H ₇ O ₂)	26	80
Oxycodone-d6	322.1	304.8 -(H ₂ O)	20	80
		247.0 -(C ₃ H ₇ O ₂)	26	80
Buprenorphine [C ₂₉ H ₄₁ NO ₄ +H] ⁺	468.2	396.1 -(C ₄ H ₈ O) ⁷	36	64
Buprenorphine-d4	472.2	400.1 -(C ₄ H ₈ O)	36	64

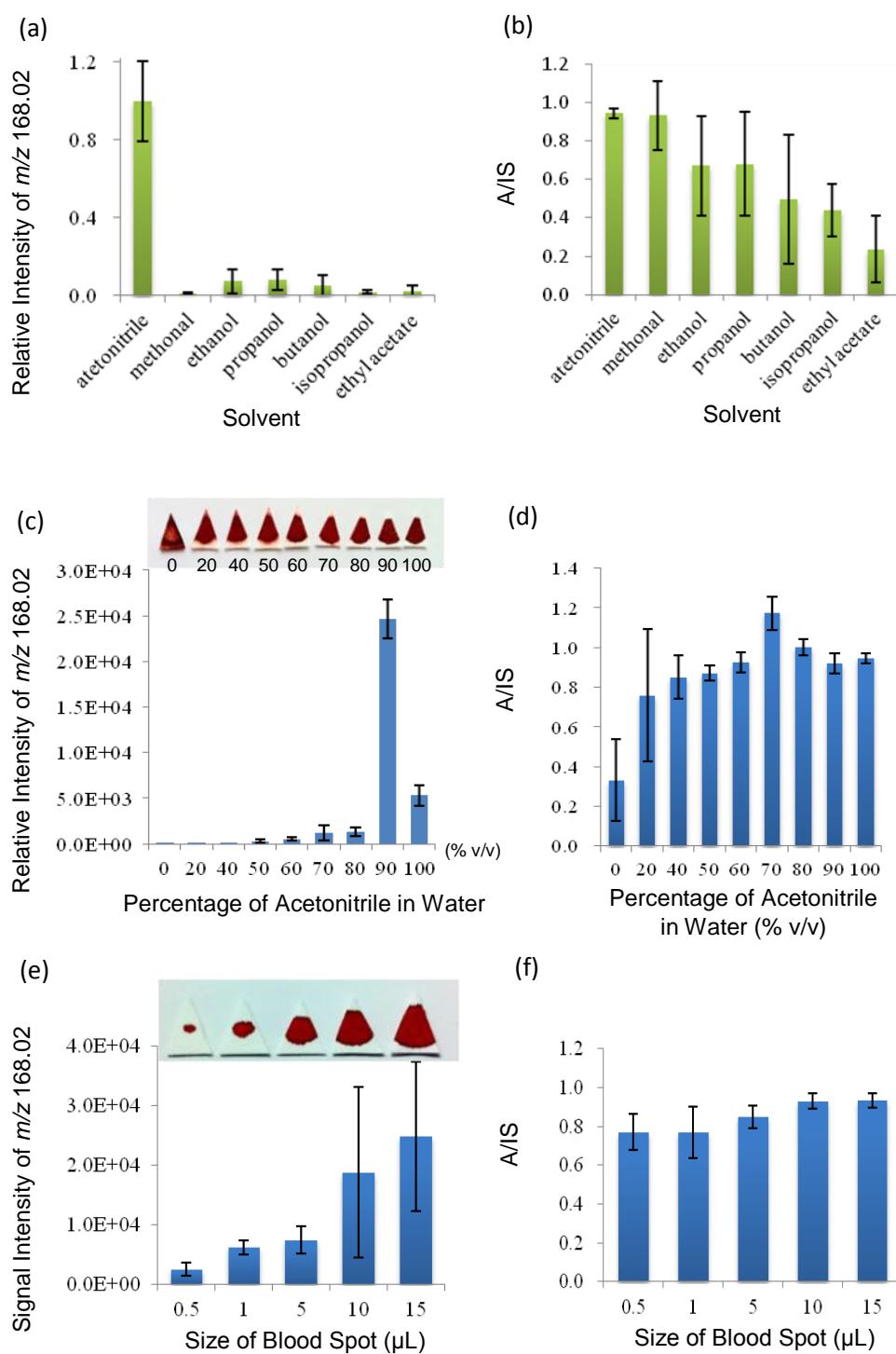


Fig. S1. Optimization of experimental conditions for quantitative paper spray mass spectrometry. Effect of spray solvent on (a) the signal intensity and (b) the ratio of analyte to internal standard (A/IS) of benzyloecgonine $[(\text{M}+\text{H})^+, m/z 290.0]$, product ion, $m/z 168.0$. Effect of acetonitrile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

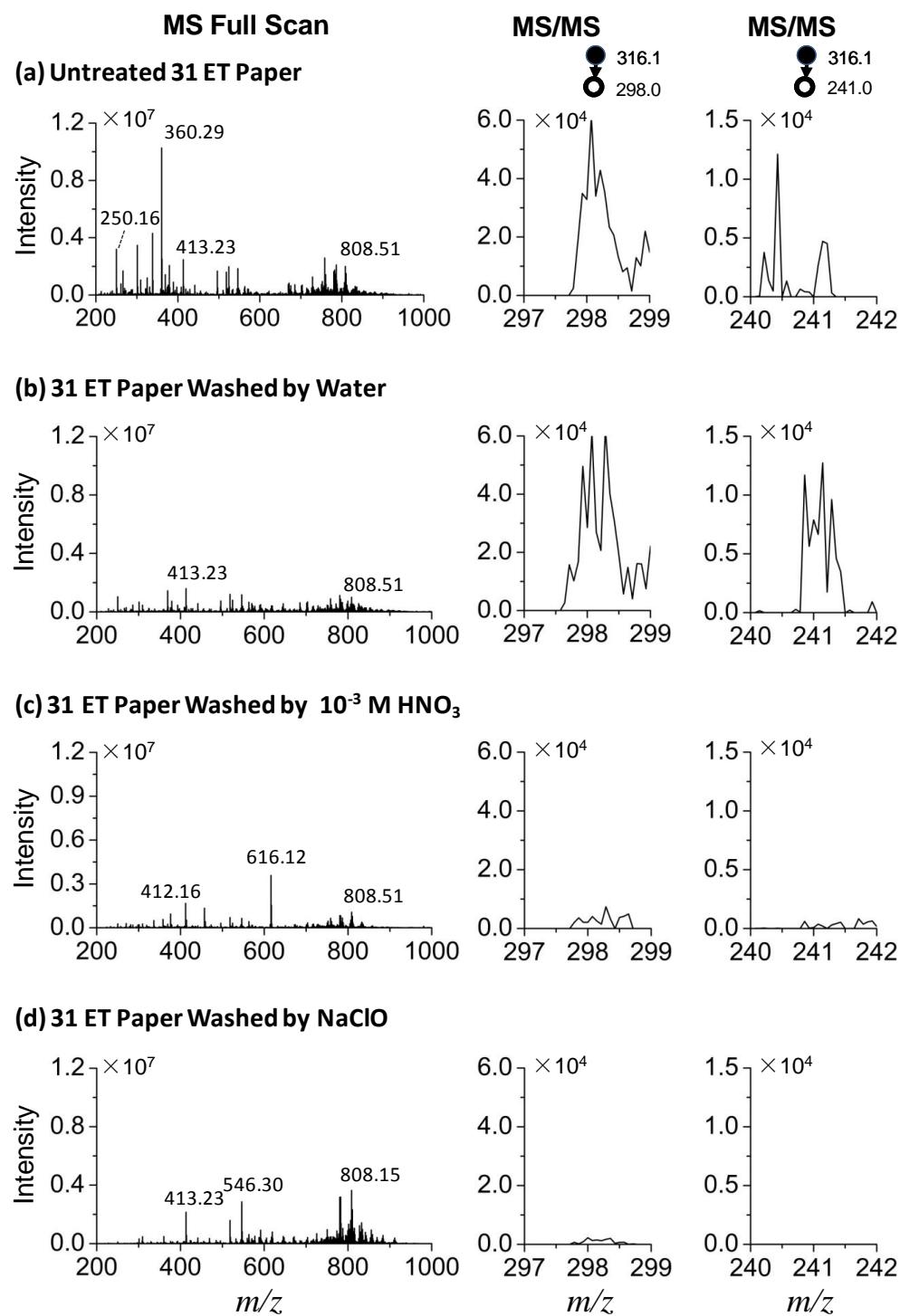


Fig. S2. MS spectra (mass range: m/z 200-1000) by Orbitrap and MS/MS spectra (parent ion: m/z 316.1, mass range: 297.0-299.0 and 240.0-242.0) by TSQ for blank dried blood spot with different treatment of paper: (a) untreated 31 ET paper, (b) 31 ET paper washed by water, (c) 31 ET paper washed by 10^{-3} 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 μ L; Voltage: 3.5 kV.

References

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