

## Supplemental Data

**Article Title:** Cocaine and metabolites concentrations in dried blood spots and venous blood after controlled intravenous cocaine administration

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**Supplemental Data Table 1.** Gas chromatography, mass spectrometry (MS), Deans switch, flame ionization (FID) and mass selective (MSD) detectors and back inlet (cold trap) method parameters for the detection and quantification of cocaine and benzoylecgonine (BE) in human venous blood.

Electron Ionization Parameters			
Deans switch		Back Inlet	
FID restrictor L.	212.7 cm	Initial T	250°C
FID restrictor i.d.	0.180 mm	Initial time	2.5 min
Aux 3 pressure	12.9 psi	Ramp #1	800°C/min
Front inlet		Final T; time	100°C; 5.3 min
Flow mode	Constant pressure	Ramp #2	800°C/min
Pressure	21.85 psi	Final T; time	250°C; 0 min
Total flow	55.3 mL/min	Oven	
Inlet T	250°C	Initial oven T	150°C
Injection mode	Splitless	Initial oven hold	0.5 min
Injection volume	2 µL	Ramp #1	30°C/min
Liner type	Single-taper glass wool	Final T; time	290°C; 0.5 min
FID and MSD		Ramp #2	75°C/min
FID T	250°C	Final T; time	180°C; 1.5 min
Hydrogen flow (OFF)	40 mL/min	Ramp #3	20°C/min
Air flow (OFF)	450 mL/min	Final T; time	280°C/min; 0 min
MSD reagent gas	Vacuum	Post Ramp	40°C/min
MSD transfer line T	280°C	Post T	320°C; 4 min
MS source T	230°C	Post time	4 min
MS quad T	150°C	Column 1 pressure	21.85 psi
EM offset (total)	506 (2612)	Column 2 pressure	12.9 psi

**Supplemental Data Table 2.** Demographic and self-reported cocaine histories for 13 cocaine users

Ppt	Race	Sex	Age (years)	Weight (lbs)	Days used in past 14 (SM or IV)	Mean use (SM or IV)	Age first use (SM or IV) (years)
A	AA	M	44.0	176	4 SM	2-3/week	38
B	AA	M	38.1	202	11 SM	5/week	32
C	More than 1	M	42.4	162	5 IV 0 SM	3/week 3-4/month	32 21
D	W	M	35.2	165	3 SM	1/week	25
E	AA	M	45.3	206	0 IV 5 SM	N/A 4/week	34 18
F	W	M	44.0	197	5 SM	Daily	18
G	W	M	42.5	180	6 IV 7 SM	3/week 2/week	28 31
H	AA	M	43.7	150	14 SM	Daily	21
I	AA	M	49.9	175	10 SM	4-5/week	25
J	AA	M	46.5	176	1 SM	3/week	15
K	W	M	39.2	175	0 IV 0 SM	N/A Daily	35 11
L	AA	M	48.8	153	10 SM	5-6/week	18
M	AA	F	36.6	140	0 SM	2/week	20

*Ppt* participant, *SM* smoked, *IV* intravenous, *AA* African-American, *W* White, *M* male

**Supplemental Data Table 3.** Potential exogenous interferences analyzed at 500 µg/L in dried blood spots (DBS) by liquid chromatography-high resolution mass spectrometry and in venous blood by two dimensional-gas chromatography mass spectrometry.

	Interferences
Group 1	morphine, normorphine, morphine-3-glucuronide, morphine-6-glucuronide, codeine, norcodeine, 6-monoacetyl-morphine, 6-acetyl codeine, hydrocodone, hydromorphone, oxycodone, noroxycodone, oxymorphone, noroxymorphone
Group 2	diazepam, lorazepam, alprazolam, imipramine, clomipramine, fluoxetine, norfluoxetine
Group 3	$\Delta^9$ -tetrahydrocannabinol, 11-hydroxy- $\Delta^9$ -tetrahydrocannabinol, 11-nor-9-carboxy- $\Delta^9$ -tetrahydrocannabinol, cannabidiol, cannabinol
Group 4	methamphetamine, amphetamine, <i>p</i> -hydroxymethamphetamine, <i>p</i> -hydroxyamphetamine, hydroxymethoxymethamphetamine, hydroxymethoxyamphetamine, methylenedioxyamphetamine, methylenedioxyamphetamine, methylenedioxyethylamphetamine, <i>p</i> -methoxyamphetamine, <i>p</i> -methoxymethamphetamine, ketamine, dextromethorphan, phentermine, ecgonine, norcocaine, cocaethylene, norcocaethylene
Group 5	(±)-ephedrine, (±)-pseudoephedrine, acetylsalicylic acid, ibuprofen, caffeine, acetaminophen
Group 6	cathinone, methcathinone, 4-fluoromethcathinone, methylone, ethylcathinone, $\alpha$ -pyrrolidinopentiophenone, buphedrone ephedrine, ethylone, 4-methoxymethcathinone, buphedrone, normephedrone, diethylcathinone, 3',4'-methylenedioxy- $\alpha$ -pyrrolidinopropiophenone, 4-methylephedrine, butylone, mephedrone, 4-methylethcathinone, 4-methyl-N-ethyl-norephedrine, 3',4'-methylenedioxy- $\alpha$ -pyrrolidinobutiophenone, Pentedrone, pentylone, 3',4'-dimethylmethcathinone, $\alpha$ -pyrrolidinopentiophenone, 4-methyl- $\alpha$ -pyrrolidinobutiophenone, 3',4'-methylenedioxyprovalerone, pyrovalerone, benzedrone, naphyrone

**Supplemental Data Figure 1a)** Liquid chromatography-high resolution mass spectrometry chromatogram of a dried blood spot (DBS) sample fortified at the limits of quantification (1  $\mu\text{g/L}$ ) for cocaine, benzoylecgonine (BE) and norcocaine and **b)** two dimensional-gas chromatography mass spectrometry chromatogram of a venous blood sample fortified at the LOQ (1  $\mu\text{g/L}$ ) for cocaine and BE.

