

Supplementary Information

Illicit Drugs, Metabolites and Adulterants in Wastewater: Monitoring Community Drug Abuse in the Brazilian Federal District during the 2014 Soccer World Cup

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Table S1. Retention time, MS/MS parameters and multiple reaction monitoring (MRM) conditions

Analyte	Retention time / min	DP ^a / V	EP ^b / V	CEP ^c / V	Reaction transitions / Da	CE ^d / eV	CXP ^e / V
COC	0.36	41	3.5	20	304.2→182.2	23	4
					304.2→105.2	43	4
					304.2→119.0	39	4
AEME	0.46	81	3	10	182.2→108.2	21	4
					182.2→119.1	23	4
					182.2→122.1	25	4
BE	0.94	46	5.5	16	290.2→168.2	27	4
					290.2→77.2	79	4
					290.2→105.1	45	4
Nor-BE	1.12	56	7	12	276.2→154.1	19	4
					276.2→136.1	29	4
					276.2→105.1	39	4
Nor-COC	1.59	61	6.5	18	290.2→168.2	19	4
					290.2→136.2	31	4
					290.2→77.2	67	4
EME	1.75	36	6	12	200.2→182.2	19	4
					200.2→82.1	37	4
					200.2→94.1	49	4

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Table S1. Retention time, MS/MS parameters and multiple reaction monitoring (MRM) conditions (cont.)

Analyte	Retention time / min	DP ^a / V	EP ^b / V	CEP ^c / V	Reaction transitions / Da	CE ^d / eV	CXP ^e / V
AE	1.88	56	9.5	10	168.2→136.2	13	4
					168.2→91.1	29	4
					168.2→108.1	23	4
ECG	2.16	36	5.5	8	186.2→168.2	19	4
					186.2→136.1	29	4
					186.2→68.1	39	4
LEV	2.17	61	9	12	205.2→91.2	45	4
					205.2→178.1	27	4
					205.2→123.1	39	4
PHE	2.28	51	9.5	10	180.2→110.2	27	4
					180.2→138.1	21	4
					180.2→65.1	47	4
AMP	2.29	16	4	12	136.2→119.1	13	4
					136.2→90.9	23	4
MAMP	3.06	26	6	10	150.2→91.1	27	4
					150.2→119.0	13	6
MDA	3.07	21	5	10	180.2→163.2	13	4
					180.2→105.1	29	4
					180.2→77.1	49	4
MDMA	3.07	26	5	10	194.2→163.2	15	4
					194.2→105.1	33	4
					194.2→77.1	57	4
MDEA	3.18	36	7	12	208.3→163.2	17	6
					208.3→105.2	31	4
					208.3→77.2	57	4
MBDB	3.96	36	6	12	208.3→135.1	27	4
					208.3→77.2	55	4
					208.3→177.2	13	4

^aDP: declustering potential; ^bEP: entrance potential; ^cCEP: collision cell entrance potential; ^dCE: collision energy; ^eCXP: collision cell exit potential. COC: cocaine; AEME: anhydroecgonine methyl ester; BE: benzoylecgonine; Nor-BE: nor-benzoylecgonine; Nor-COC: norcocaine hydrochloride; EME: ecgonine methyl ester; AE: anhydroecgonine hydrochloride; ECG: ecgonine hydrochloride; LEV: levamisole; PHE: phenacetin; AMP: (±)-amphetamine; MAMP: (±)-methylamphetamine hydrochloride; MDA: (±)-3,4-methylenedioxyamphetamine; MDMA: (±)-3,4-methylenedioxymethamphetamine; MDEA: (±)-3,4-methylenedioxyethylamphetamine; MBDB: (±)-3,4-methylenedioxy-*N*-methyl-butanphenamine.

Table S2. Analytical parameters of the method

Analyte	LOD ^a / ($\mu\text{g L}^{-1}$)	LOQ ^a / ($\mu\text{g L}^{-1}$)	Linear range ^b / ($\mu\text{g L}^{-1}$)	R ²	Recovery ^c / %
COC	0.14	0.34	1.0-20	0.993	107 \pm 4
AEME	1.3	4.2	12.5-50	0.996	96 \pm 4
BE	0.32	1.1	2.5-100	0.997	95 \pm 5
Nor-BE	0.26	0.86	2.5-25	0.991	97 \pm 4
Nor-COC	0.19	0.62	1.0-50	0.999	61 \pm 10
EME	0.51	1.7	2.5-150	0.999	NR ^d
AE	0.37	1.2	5.0-100	0.998	100 \pm 6
ECG	0.26	0.85	2.5-250	0.999	NR
LEV	0.21	0.71	5.0-50	0.994	106 \pm 7
PHE	0.10	0.34	2.0-100	0.997	90 \pm 4
AMP	0.73	2.4	8.0-150	0.994	56 \pm 3
MAMP	0.72	2.4	12.5-200	0.999	59 \pm 9
MDA	1.0	3.3	10-200	0.990	91 \pm 7
MDMA	0.34	1.1	1.0-150	0.999	82 \pm 3
MDEA	0.34	1.1	1.0-150	0.999	72 \pm 4
MBDB	0.29	0.96	6.0-150	0.999	72 \pm 7

^aMethod limit of detection (LOD) and limit of quantification (LOQ) considering a pre-concentration factor of 10; ^blinear range for instrumental analytical curves; ^cgeometric mean considering a group of eight authentic sewage samples spiked with 100 or 1000 $\mu\text{g L}^{-1}$ of each analyte; ^dNR: not recovered. COC: cocaine; AEME: anhydroecgonine methyl ester; BE: benzoylecgonine; Nor-BE: nor-benzoylecgonine; Nor-COC: norcocaine hydrochloride; EME: ecgonine methyl ester; AE: anhydroecgonine hydrochloride; ECG: ecgonine hydrochloride; LEV: levamisole; PHE: phenacetin; AMP: (\pm)-amphetamine; MAMP: (\pm)-methamphetamine hydrochloride; MDA: (\pm)-3,4-methylenedioxyamphetamine; MDMA: (\pm)-3,4-methylenedioxymethamphetamine; MDEA: (\pm)-3,4-methylenedioxyethylamphetamine; MBDB: (\pm)-3,4-methylenedioxy-*N*-methyl-butanphenamine.

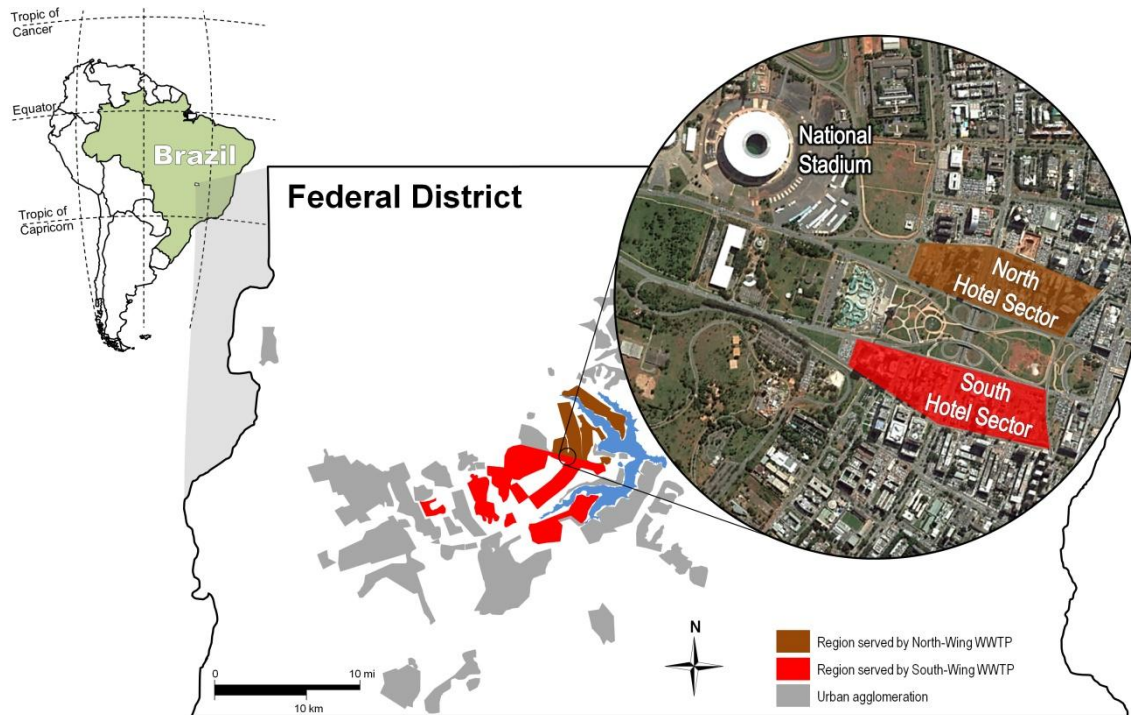


Figure S1. Map of Brasília, in Brazil, showing the Pilot Plan, the regions covered by the North-Wing WWTP (dark orange) and by the South-Wing WWTP (red). In detail, the localization of both Hotel Sectors as well as the National Stadium.