

Supplementary material

Table S1. MS/MS standards optimization parameters. The table lists, for each standard, the recording mode (polarity), precursor ion (m/z), fragmentor, fragment ions (m/z), collision energy (CE), retention time (t_R), slope (a) and section on the x-axis (b), R^2 , linearity range (linearity), detection limit (LOD), and quantification limit (LOQ).

Standard	Polarity	Precursor (m/z)	Fragmentor (V)	Product ions (m/z)	CE (V)	t_R (min)	Y=ax + b		R^2	Linearity range ($\mu\text{g/mL}$)	LOD ($\mu\text{g/mL}$)	LOQ ($\mu\text{g/mL}$)
							Slope (a)	Intercept (b)				
Dopamin	+	153.9	60	118.6	10	1.0	37355.512266	-49.952304	0.9947	0.01-1	0.00441	0.01337
				<u>90.9</u>	20							
Octopamin	+	153.9	60	136.9	4	0.5	109396.977405	10.295928	0.9992	0.0001-1	0.000311	0.000941
				<u>90.8</u>	24							
				<u>120.9</u>	4							
Tyramin	+	137.9	60	90.9	22	1.5	167336.717374	79.131000	0.9975	0.001-1	0.001561	0.004729
				<u>77.0</u>	30							

*Quantifier ions are underlined.

Table S2. MS/MS parameters for components semiquantified without standards: acetylcholine (ACh), gamma-aminobutyric acid (GABA) and glutamate, N-acetyl dopamine, N-acetyl tyramine, cocaine (COC) and methamphetamine (METH). The table list the recording mode (polarity), precursor ion (m/z), fragmentor, fragment ions (m/z), collision energy (CE), and retention time (t_R).

Compound	Polarity	Precursor (m/z)	Fragmentor (V)	Product ions (m/z)	CE (V)	t_R (min)
ACh	+	147.0	135	<u>88.0</u>	25	0.6
				87.0	25	
GABA	+	103.9	135	69.0	5	0.6
				<u>45.0</u>	25	
				43.0	25	
Glutamate	+	147.9	135	129.0	25	0.7
				101.0	25	
				<u>84.0</u>	25	
N-acetyl dopamine	+	196.0	135	154.0	15	4.6
				137.0	15	
				119.0	30	
				91.0	30	
METH	+	150.5	135	<u>91.2</u>	20	5.2
N-acetyl tyramine	+	180.0	135	138.0	30	5.3
				121.0	30	
				91.0	40	
				<u>77.0</u>	40	

COC	+	304.1	100	<u>182.1</u>	30	7.2
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*Quantifier ions are underlined.