

SUPPLEMENTARY DATA

Table S1. Multiple reaction monitoring (MRM), transitions, collision energies, cone voltages, and retention times for the 18 analytes and six internal standards in plasma (MRM transitions used for quantification are shown in bold). 9-OH-RISP, 9-hydroxy-risperidone; AMI, amisulpride; AMI-d5, amisulpride-d5; ARI, aripiprazole; CLM, clomipramine; CLZ, clozapine; CLZ-d8, clozapine-d8 ; DULO, duloxetine; ESC, escitalopram; FLUO, fluoxetine; FLUO-d5, fluoxetine-d5; HALO, haloperidol; HALO-d4, haloperidol-d4; MIRT, mirtazapine; MPH, methylphenidate; NCLM, norclomipramine; NCLZ, norclozapine; ODV, O-desmethyl-venlafaxine; OLAN, olanzapine; QUE, quetiapine; QUE-d8, quetiapine-d8; RISP, risperidone; VNLF, venlafaxine; VNFL-d6, venlafaxine-d6.

Analyte	MRM transitions (m/z)	Collision energy (eV)	Cone voltage (V)	Retention time (min)
AMI	371.1→242	40	28	3.3
	371.1→111.9	30		
ARI	448.1→285.2	40	46	5.7
	448.1→176	40		
CLM	315.1→85.9	32	46	5.5
	315.1→57.8	30		
NCLM	301.1→71.9	20	44	5.2
	301.1→267	26		
CLZ	327.1→270	30	46	5.0
NCLZ	313.1→270	20	34	4.4
ESC	325.2→108.8	34	44	4.5
	325.2→262	26		

FLUO	310.1→147.8	10	28	5.0
DULO	298.1→153.8 298.1→187.9	10 10	16	4.9
HALO	376.1→164.5 376.1→122.8	32 36	34	4.7
MIRTA	286.1→195 286.1→71.9	36 30	46	4.5
MPH	234.31→83.78	20	26	3.7
OLAN	313.2→255.6 313.2→83.9	26 28	42	4.3
QUE	384.1→252.9 384.1→220.9	30 36	36	4.9
RISP	411.2→190.9	36	30	4.2
9-OH-RISP	427.61→207.09	36	30	3.9
VNLF	278.1→260 278.1→57.9	16 36	36	4.0
ODV	264.36→57.84	20	26	3.3
AMI-d5	375.2→242	30	38	3.2
CLZ-d8	338.2→275	30	46	4.9
FLUO-d5	315.1→152.8	10	28	5.0
HALO-d4	384.1→252.9	30	36	4.7
QUE-d8	392.1→257.9	34	36	4.9
VLNF-d6	284.3→266.2	16	28	4.0

Table S2. Calibration curve spiking solutions prepared by serial dilutions in methanol from first working solutions at the concentrations of 50 µg/ml for 10 molecules (amisulpride, aripiprazole, clomipramine, clozapine fluoxetine, norclozapine, norclomipramine, O-desmethyl-venlafaxine, quetiapine, venlafaxine), 5.0 µg/ml for 6 molecules (9-hydroxy-risperidone, duloxetine, escitalopram, mirtazapine, olanzapine, risperidone) and for methylphenidate, and 0.5 µg/ml for haloperidol. 10M: amisulpride, aripiprazole, clomipramine, clozapine fluoxetine, norclozapine, norclomipramine, O-desmethylvenlafaxine, quetiapine, venlafaxine; 6M: 9-OH-risperidone, duloxetine, escitalopram, mirtazapine, olanzapine, risperidone; MPH, methylphenidate; HALO, haloperidol.

Analytes	Concentrations (µg/mL)									
	C7	C6	C5	C4	C3	C2	C1	HQC	MQC	LQC
10M	10	8	5	4	2	1	0.5	9.0	3.0	1.5
6M	1.5	1.2	0.75	0.6	0.3	0.15	0.075	1.35	0.45	0.225
MPH	0.15	0.12	0.075	0.06	0.03	0.0115	0.0075	0.45	0.15	0.075
HALO	0.5	0.4	0.25	0.20	0.10	0.05	0.025	0.135	0.045	0.0225

Table S3. Calibration standard concentrations obtained by spiking blank plasma with appropriate amount of secondary working solution. 10M: amisulpride, aripiprazole, clomipramine, clozapine fluoxetine, norclozapine, norclomipramine, O-desmethyl-venlafaxine, quetiapine, venlafaxine; 6M: 9-hydroxy-risperidone, duloxetine, escitalopram, mirtazapine, olanzapine, risperidone; MPH, methylphenidate; HALO, haloperidol.

Analytes	Concentrations (ng/mL)							HQC	MQC	LQC
	C7	C6	C5	C4	C3	C2	C1			
10M	1000	800	500	400	200	100	50	900	300	150
6M	150	120	75	60	30	15	7.5	135	15	22.5
MPH	15	12	7.5	6	3	1.5	0.75	45	15	7.5
HALO	50	40	25	20	10	5	2.5	13.5	4.5	2.25

Supplementary Data S4. Detailed formula used to calculate the Relative Infant Dosage (RID).

$$RID = \frac{D(infant)}{D(mother)} \times 100$$

with:

- $D(infant)$, in mg/kg: daily dose ingested by the infant, adjusted by weight.

$$D(infant) = \frac{C(milk) \times V(milk)}{W(infant)}$$

- $C(milk)$, mg/mL: measured concentration of the drug in breast milk.
- $V(milk)$, in mL: volume of breast milk ingested daily by the infant. If not known, $V(milk)$ is estimated at 150 mg/kg/day (Larsen et al., 2015). For the mixed diet, $V(milk)$ was calculated as follows:

$$V(milk) = V(feed) \times n(feeds)$$

with:

- $V(feed)$, where (mL: volume of the feed. If unknown, $V(feed)$ was estimated by dividing 150 mg/kg/day by the total food intake per day.
- $n(feeds)$: number of feeds per day.
- $W(infant)$, kg: weight of the infant at the time of breast milk sampling.
- $D(mother)$, in mg/kg: daily intake of the mother adjusted by weight at the time of breast milk sampling.