

## 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; MIRTA, 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     | <b>371.1→242</b><br>371.1→111.9 | 40<br>30              | 28               | 3.3                  |
| ARI     | <b>448.1→285.2</b><br>448.1→176 | 40<br>40              | 46               | 5.7                  |
| CLM     | <b>315.1→85.9</b><br>315.1→57.8 | 32<br>30              | 46               | 5.5                  |
| NCLM    | <b>301.1→71.9</b><br>301.1→267  | 20<br>26              | 44               | 5.2                  |
| CLZ     | <b>327.1→270</b>                | 30                    | 46               | 5.0                  |
| NCLZ    | <b>313.1→270</b>                | 20                    | 34               | 4.4                  |
| ESC     | <b>325.2→108.8</b><br>325.2→262 | 34<br>26              | 44               | 4.5                  |

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|           |                            |          |    |     |
|-----------|----------------------------|----------|----|-----|
| FLUO      | 310.1→147.8                | 10       | 28 | 5.0 |
| DULO      | 298.1→153.8<br>298.1→187.9 | 10<br>10 | 16 | 4.9 |
| HALO      | 376.1→164.5<br>376.1→122.8 | 32<br>36 | 34 | 4.7 |
| MIRTA     | 286.1→195<br>286.1→71.9    | 36<br>30 | 46 | 4.5 |
| MPH       | 234.31→83.78               | 20       | 26 | 3.7 |
| OLAN      | 313.2→255.6<br>313.2→83.9  | 26<br>28 | 42 | 4.3 |
| QUE       | 384.1→252.9<br>384.1→220.9 | 30<br>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<br>278.1→57.9    | 16<br>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 |

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**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-desmethylvenlafaxine, 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) |     |     |     |     |     |      |      |     |      |
|----------|------------------------|-----|-----|-----|-----|-----|------|------|-----|------|
|          | C7                     | C6  | C5  | C4  | C3  | C2  | C1   | HQC  | MQC | LQC  |
| 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.