

## **SUPPLEMENTARY INFORMATION**

**Occurrence and preliminary environmental risk assessment of selected pharmaceuticals in the urban rivers, China**

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**Table S1. Range, and detection frequency (%) of pharmaceuticals in the three urban rivers during four sampling campaigns.**

Sampling campaign	Measurement	ATL	PRC	STZ	TMP	CAF	AZM	PNL	CBM	CLM	CLF	DCF	IBU
1 <sup>a</sup>	Range (ng/L)	0.6-91.1	12.4-728	0.4-8.2	3.8-25.6	85.4-2729.3	16.6-67.3	0.1-3.8	13.9-29.5	2.6-41.5	19.9-299.3	12.3-43.5	31-116.9
	FD <sup>e</sup> (%)	100	100	100	100	100	100	100	100	100	100	100	100
2 <sup>b</sup>	Range (ng/L)	2.4-7.9	2.3-1905.8	2-7.9	5.7-14.9	114.5-6868.8	n.d. <sup>f</sup> -8.3	n.d.-1.2	12.5-17.8	2-47.7	n.d.-11	15.1-54.4	n.d.-140.2
	FD (%)	100	100	100	100	100	94	72	100	100	61	100	94
3 <sup>c</sup>	Range (ng/L)	0.4-9.0	19.6-2744.7	n.d.-1.9	2.9-12.9	66.3-3888.0	n.d.-15.4	n.d.-8.8	8.6-16.1	0.8-39.8	1.2-5.1	5-32.1	7.3-58.6
	FD (%)	100	100	94	100	100	83	83	100	100	100	100	100
4 <sup>d</sup>	Range (ng/L)	0.9-3.7	1658.8-7023.7	10.3-56	5.3-16	3569.7-8662.4	n.d.-38.9	n.d.-2	0.6-8.9	n.d.-41	n.d.-3.8	1.8-63.8	43.4-194.6
	FD (%)	100	100	100	100	100	56	67	100	72	56	100	100

**Note:** <sup>a</sup> From May 28 to June 2, 2014, <sup>b</sup> September 12, 2014, <sup>c</sup> November 30, 2014, <sup>d</sup> January 29, 2015, <sup>e</sup> Frequency of detection (%), <sup>f</sup> Not detected (<LOQ).

**Table S2. Physicochemical properties of the target pharmaceuticals in this study.**

Compounds	Therapeutic groups	CAS No.	Molecular formula	Molecular Weight	Molecule structure	logKow	pKa
Azithromycin (AZM)	macrolides antibiotics	83905-01-5	C <sub>38</sub> H <sub>72</sub> N <sub>2</sub> O <sub>12</sub>	749.0		4.02 <sup>a</sup>	8.7 <sup>a</sup>
Clarithromycin (CLM)	macrolides antibiotics	81103-11-9	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	748.0		3.16 <sup>a</sup>	8.99 <sup>e</sup>
Sulfathiazole (STZ)	Antimicrobial sulfonamides	72-14-0	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	255.3		0.89 <sup>d</sup>	7.29 <sup>d</sup>
Trimethoprim (TMP)	Broad spectrum antibiotics	738-70-5	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>	290.3		0.91 <sup>d</sup>	7.12 <sup>d</sup>
Ibuprofen (IBU)	Anti-inflammatory/analgesic drugs	15687-27-1	C <sub>13</sub> H <sub>18</sub> O <sub>2</sub>	206.3		3.97 <sup>a</sup>	4.91 <sup>a</sup>
Diclofenac (DCF)	Non steroidal anti-inflammatory drugs (NSAID)	15307-79-6(Na) 15307-86-5	C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>	214.6		4.51 <sup>a</sup>	4.15 <sup>a</sup>

Paracetamol (PRC)	Antipyretic analgesics	103-90-2	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>	151.2	0.46 <sup>a</sup>	9.38 <sup>a</sup>
Atenolol (ATL)	Cardioselective beta blockers	29122-68-7	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	266.3	0.16 <sup>a</sup>	9.6 <sup>e</sup>
Propranolol (PNL)	Beta-blockers	525-66-6	C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>	259.4	3.48 <sup>a</sup>	9.1 <sup>b</sup>
Clofibrilic acid (CLF)	Lipid regulators	882-09-7	C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>	214.6	2.57 <sup>b</sup>	3.2 <sup>b</sup>
Carbamazepine (CBZ)	Psychiatric- antiepileptics	298-46-4	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O	236.3	2.45 <sup>d</sup>	7.0 <sup>d</sup>
Caffeine (CAF)	Psychomotor stimulants	58-08-2	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	194.2	-0.07 <sup>a</sup>	10.4 <sup>a</sup>

Note: <sup>a</sup> Data from Kosma et al.<sup>1</sup>; <sup>b</sup> Data from Camacho- Muñoz et al.<sup>2</sup>; <sup>c</sup> Data from Zhang et al.<sup>3</sup>; <sup>d</sup> Data from Kim et al.<sup>4</sup>; <sup>e</sup> Data from the manufacturers.

**Table S3. Details of sampling along Qiujiang (QJ) River, Dongzoumatang (DZM) River and Yangshupugang (YSP) River in Shanghai, China.**

<b>River</b>	<b>Flow rate (m<sup>3</sup>/s)</b>	<b>Length (km)</b>	<b>Width (m)</b>	<b>Depth (m)</b>	<b>Sampling section</b>	<b>Sampling campaign</b>
<b>QJ</b>	5.4-24.0	7.0	30-40	0.8-1.8 <sup>a</sup> 3.9-4.0 <sup>b</sup>	Q1-Q6	May 28 to June 2, 2014 September 12, 2014 November 30, 2014 January 29, 2015
<b>DZM</b>	4.8-20.5	5.0	20-30	2.2-2.4 <sup>a</sup> 3.8-4.0 <sup>b</sup>	D1-D6	
<b>YSP</b>	14.2-28.3	4.5	~27	~3.5	Y1-Y6	

Note: <sup>a</sup> Depth during the normal low water level; <sup>b</sup> Depth during the normal high water level.

**Table S4. Retention times and their optimal MS/MS parameters using hot electrospray ionization of target pharmaceuticals.**

Compound	Mw (Da)	Precursor ion (m/z)	Product ion (m/z)	Collision energy (eV)	S-Lens RF (v)	Ionization mode	Retention time (min)
<b>PNL</b>	259.4	260.2	116.1 *	17	85	HESI+	5.93
			183.1	17	85		
<b>AZM</b>	749.0	749.5	591.5 *	24	163	HESI+	5.32
			158.1	37	79		
<b>CBZ</b>	236.3	237.1	194.1 *	19	77	HESI+	6.61
			193.1	33	77		
<b>CLM</b>	748.0	748.4	158.1 *	26	129	HESI+	7.14
			590.5	14	129		
<b>STZ</b>	255.3	256.0	156.0 *	14	71	HESI+	2.72
			108.1	23	71		
<b>TMP</b>	290.3	291.1	230.1 *	23	109	HESI+	3.74
			261.1	24	109		
<b>ATL</b>	266.3	267.1	145.1 *	25	86	HESI+	1.80
			190.1	17	86		
<b>PRC</b>	151.2	152.0	110.1 *	15	66	HESI+	2.44
			65	29	66		
<b>CAF</b>	194.2	195.1	138.1 *	19	79	HESI+	3.98
			110.1	33	79		
<b>IBU</b>	206.3	205.0	161.0 *	7	42	HESI-	7.32
<b>CLF</b>	214.6	213.0	127.0 *	20	53	HESI-	5.98
<b>DCF</b>	296.2	294.0	250.1 *	14	59	HESI-	7.15
			214.1	21	59		
<b>PRC-d<sub>3</sub></b>	154.2	155.1	111.1*	15	74	HESI+	2.43
			93.1	21	74		
			107.1*	19	57	HESI-	2.38
			118.1	34	57		
<b>STZ-d<sub>4</sub></b>	259.3	260.0	160.0*	14	84	HESI+	2.68
			96.1	25	84		
			160.0*	19	58		
258.0	20	58					

Note: \* product ion for quantification.

## References

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