Occurrence of pharmaceuticals and personal care products, and their associated environmental risks in Guanting Reservoir and its upstream rivers in north China

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| Classes                      | Compound      | acronym | CAS no.   | molecular formula | log\(k_w\)  | pKa\(^a\) | classification                                      |
|------------------------------|---------------|---------|-----------|-------------------|-------------|-----------|---------------------------------------------------|
| Acetaminophen                | ACE           | 103-90-2| \(C_8H_9NO_2\) | 0.46              | 9.38       |          | Analgesic, antipyretic                             |
| Caffeine                     | CAF          | 58-08-2 | \(C_8H_11NO_2\) | -0.07             | 10.40      |          | Central nervous system stimulant                   |
| Non-antibiotic pharmaceuticals (N-APs) | Diltiazem    | DTZ     | 42399-41-7 | \(C_{22}H_{26}N_2O_4S\) | 2.70        | 8.90     | Calcium channel blocker                            |
| Carbazepine                  | CBZ          | 298-46-4| \(C_{15}H_{12}N_2O_2\) | 2.47              | 7.00       |          | Anticonvulsant, antidepressant                     |
| Fluoxetine                   | FXT          | 54910-83-3 | \(C_{17}H_{18}F_3NO\) | 1.80              | -          |          | antidepressant                                    |
| Sulfadiazine                 | SDZ          | 68-35-9 | \(C_{10}H_{10}N_4O_2S\) | -0.34             | 2.0/6.48   |          | Sulfonamide antibiotic                            |
| Sulfamethoxazole             | SMX          | 723-46-6| \(C_{10}H_{12}N_2O_3S\) | 0.89              | 1.6/5.7    |          | Sulfonamide antibiotic                             |
| Sulfamethazine               | SMZ          | 57-68-1 | \(C_{10}H_{12}N_2O_3S\) | 0.14              | 2.65/7.65  |          | Sulfonamide antibiotic                             |
| Trimethoprim                 | TMP          | 738-70-5| \(C_{17}H_{11}N_2O_3\) | 0.91              | 7.12       |          | Antibacterial agent                                |
| Oxytetracycline              | OTC          | 79-57-2 | \(C_{18}H_{15}N_2O_8\) | 0.02              | 9.50       |          | Tetracycline antibiotic                            |
| Tetracycline                 | TC           | 60-54-8 | \(C_{20}H_{15}N_2O_8\) | -1.37             | 3.30       |          | Tetracycline antibiotic                            |
| Chlortetracycline            | CTC          | 57-62-5 | \(C_{22}H_{25}ClN_2O_8\) | -                 | 3.02/7.55/9.33 |          | Tetracycline antibiotic                            |
| Doxycycline                  | DOX          | 562-25-0| \(C_{20}H_{18}N_2O_8\) | 2.37              | 3.02/7.97/9.15 |          | Tetracycline antibiotic                            |
| Azithromycin                 | AZM          | 83905-01-5 | \(C_{20}H_{22}N_2O_2\) | 4.02              | 8.74       |          | Macrolide antibiotic                               |
| Erythromycin                 | ERY          | 114-07-8| \(C_{19}H_{22}NO_3\) | 3.06              | 8.90       |          | Macrolide antibiotic                               |
| Tylosin                      | TYL          | 1401-69-0 | \(C_{10}H_{17}NO_7\) | 1.05              | 7.10       |          | Macrolide antibiotic                               |
| Lincomycin                   | LIN          | 154-21-2| \(C_{23}H_{23}N_2O_8\) | 0.56              | 7.60       |          | Lincosomide antibiotic                             |
| Ofloxacin                    | OFL          | 82419-36-1 | \(C_{18}H_{20}F_3N_2O_4\) | -0.02             | -          |          | Quinolone antibiotic                               |

\(^a\): Stamatis and Konstantinou, 2013; Salgado et al., 2012; Chen et al., 2014; Yang et al., 2011; Marczak et al., 2015
Table S2. Sampling site information for samples of Guanting Reservoir

| Sites | Coordinates        | Date           | Location         |
|-------|--------------------|----------------|------------------|
| L01   | 115°46'36.84"E 40°22'16.752"N | August, 01 2017 | Guanting Reservoir |
| L02   | 115°45'43.56"E 40°21'43.344"N | August, 01 2017 | Guanting Reservoir |
| L03   | 115°45'48.24"E 40°21'38.592"N | August, 01 2017 | Guanting Reservoir |
| L04   | 115°45'54.72"E 40°21'27.072"N | August, 01 2017 | Guanting Reservoir |
| L05   | 115°44'30.12"E 40°20'52.26"N | August, 01 2017 | Guanting Reservoir |
| L06   | 115°44'13.56"E 40°21'5.04"N  | August, 01 2017 | Guanting Reservoir |
| L07   | 115°43'54.48"E 40°21'13.32"N | August, 01 2017 | Guanting Reservoir |
| L08   | 115°43'11.99"E 40°20'55.788"N | August, 01 2017 | Guanting Reservoir |
| L09   | 115°41'25.08"E 40°20'20.04"N | August, 01 2017 | Guanting Reservoir |
| L10   | 115°37'35.40"E 40°18'25.668"N | August, 01 2017 | Guanting Reservoir |
| L11   | 115°37'9.12"E 40°17'29.076"N | August, 01 2017 | Guanting Reservoir |
| L12   | 115°36'59.04"E 40°16'56.279"N | August, 01 2017 | Guanting Reservoir |
| L13   | 115°36'26.48"E 40°16'18.336"N | August, 01 2017 | Guanting Reservoir |
| L14   | 115°36'9.72"E 40°14'7.799"N  | August, 01 2017 | Guanting Reservoir |
| R01   | 115°52'28.20"E 40°26'47.868"N | August, 04 2017 | Guishui River   |
| R02   | 114°30'20.52"E 40°37'1.235"N | August, 02 2017 | Yongding River  |
| R03   | 115°28'1.20"E 40°21'25.128"N | August, 02 2017 | Yongding River  |
| R04   | 115°21'18.72"E 40°21'15.696"N | August, 02 2017 | Sanggan River   |
| R05   | 115°12'40.32"E 40°21'30.96"N | August, 02 2017 | Sanggan River   |
| R06   | 115°18'20.88"E 40°24'52.344"N | August, 02 2017 | Yanghe River    |
| R07   | 115°7'9.84"E 40°31'4.295"N  | August, 02 2017 | Yanghe River    |
| R08   | 114°58'19.91"E 40°37'10.488"N | August, 02 2017 | Yanghe River    |
| Analytes | Parent ion (m/z) | Daughter ion (m/z) | Fragmentor/ Collision energy/ | |
|----------|-----------------|-------------------|-----------------------------|---|
| ACE      | 152             | 110               | 90                          | 15 |
|          |                 | 65                | 90                          | 35 |
| CAF      | 195             | 138               | 110                         | 15 |
|          |                 | 110               | 110                         | 25 |
| DTZ      | 415             | 178               | 130                         | 25 |
|          |                 | 150               | 130                         | 25 |
|          |                 | 194               | 110                         | 15 |
| CBZ      | 237             | 156               | 110                         | 15 |
|          |                 | 92                | 110                         | 25 |
|          |                 | 156               | 110                         | 15 |
| SMX      | 254             | 92                | 110                         | 25 |
|          |                 | 156               | 90                          | 25 |
| SMZ      | 279             | 186               | 90                          | 25 |
|          |                 | 156               | 90                          | 25 |
| TMP      | 291             | 261               | 110                         | 25 |
|          |                 | 230               | 110                         | 25 |
|          |                 | 444               | 130                         | 13 |
| OTC      | 461             | 426               | 130                         | 17 |
|          |                 | 427               | 110                         | 5  |
| TC       | 445.2           | 410               | 110                         | 15 |
|          |                 | 426               | 110                         | 15 |
|          |                 | 427               | 110                         | 5  |
| CTC      | 479             | 462               | 110                         | 15 |
|          |                 | 197               | 110                         | 35 |
| DOX      | 445.2           | 428               | 110                         | 15 |
|          |                 | 154               | 110                         | 35 |
|          |                 | 591.2             | 130                         | 30 |
| AZM      | 749.5           | 158               | 130                         | 35 |
|          |                 | 576               | 90                          | 15 |
| ERY      | 734.5           | 158               | 90                          | 35 |
|          |                 | 772               | 110                         | 35 |
| TYL      | 916.3           | 174               | 110                         | 35 |
Table S4. Water quality parameters in surface water samples collected from Guanting Reservoir and its upstream rivers

| Sites | DOC (mg L\(^{-1}\)) | TN (mg L\(^{-1}\)) | TP (mg L\(^{-1}\)) | NH3-N (mg L\(^{-1}\)) |
|-------|----------------------|---------------------|---------------------|----------------------|
| L01   | 13.17                | 0.326               | 0.013               | 0.27                 |
| L02   | 10.11                | 0.280               | 0.022               | 0.16                 |
| L03   | 10.75                | 0.234               | 0.026               | 0.14                 |
| L04   | 11.52                | 0.222               | 0.023               | 0.16                 |
| L05   | 11.65                | 0.230               | 0.016               | 0.30                 |
| L06   | 11.47                | 0.329               | 0.016               | 0.11                 |
| L07   | 12.52                | 0.322               | 0.020               | 0.11                 |
| L08   | 10.58                | 0.249               | 0.025               | 0.10                 |
| L09   | 11.24                | 0.276               | 0.012               | 0.25                 |
| L10   | 10.48                | 0.234               | 0.030               | 0.16                 |
| L11   | 7.98                 | 0.257               | 0.027               | 0.18                 |
| L12   | 9.58                 | 0.268               | 0.023               | 0.12                 |
| L13   | 10.89                | 0.130               | 0.026               | 0.19                 |
| L14   | 7.83                 | 0.283               | 0.039               | 0.22                 |
| R01   | 14.65                | 1.261               | 0.140               | 0.26                 |
| R02   | 6.33                 | 2.024               | 0.325               | 0.16                 |
| R03   | 8.74                 | 0.188               | 0.075               | 0.12                 |
| R04   | 17.19                | 0.479               | 0.037               | 0.59                 |
| R05   | 3.20                 | 1.775               | 0.025               | 0.23                 |
| R06   | 4.64                 | 1.073               | 0.104               | 0.16                 |
| R07   | 11.67                | 2.116               | 0.467               | 0.77                 |
| R08   | 21.98                | 1.100               | 1.639               | 0.87                 |
| R09   | 14.47                | 0.855               | 0.143               | 19.70                |
| R10   | 13.55                | 1.146               | 0.206               | 1.02                 |
| R11   | 6.45                 | 0.164               | 0.083               | 0.45                 |
| R12   | 2.33                 | 0.617               | 0.089               | 0.04                 |
| R13   | 0.61                 | 0.398               | 0.080               | 0.06                 |
| R14   | 1.91                 | 0.797               | 0.007               | 0.07                 |
Table S5. Environmental risk assessment for selected PPCPs in GTR and its upstream rivers

| Analytes | EC50 (mg/L) | PNEC (μg·L⁻¹) | Maxium MEC (ng·L⁻¹) | RQ       |
|----------|-------------|----------------|----------------------|----------|
|          |             |                | GTR                  | Upstream rivers | GTR     | Upstream rivers |
| ACE      | 9.2         | 9.2⁷           | 506.47               | 901.73    | 5.51E-02 | 9.80E-02       |
| CAF      | 69         | 69⁸            | 620.39               | 707.51    | 0.009    | 0.010          |
| DTZ      | 8.2        | 8.2⁹           | 17.37                | 8.64      | 2.12E-03 | 1.05E-03       |
| CBZ      | 31.6       | 31.6³          | 5.90                 | 11.47     | 0.000    | 0.000          |
| FXT      | 41         | 41²            | 3.40                 | 4.45      | 8.29E-05 | 1.09E-04       |
| SDZ      | 10         | 10⁶            | 23.51                | 20.58     | 0.002    | 2.06E-03       |
| SMX      | 20         | 20⁴            | 44.39                | 42.59     | 0.002    | 0.002          |
| SMZ      | 15.6       | 15.6³          | 25.68                | 14.11     | 0.002    | 9.03E-04       |
| TMP      | 1.0        | 1³             | 15.26                | 20.23     | 0.015    | 0.020          |
| OTC      | 2.0        | 2⁸             | 30.45                | 36.26     | 0.015    | 0.018          |
| TC       | 3400       | 3400⁸          | 14.86                | 18.86     | 4.37E-06 | 5.55E-06       |
| CTC      | 5.0        | 5³             | 15.38                | 19.68     | 0.003    | 3.94E-03       |
| DOX      | 430        | 430⁴           | 10.11                | 12.76     | 2.35E-05 | 2.97E-05       |
| AZM      | 0.45       | 0.45²³         | 16.72                | 25.71     | 0.037    | 0.057          |
| ERY      | 0.04       | 0.04³          | 27.56                | 63.69     | 0.689    | 1.592          |
| TYL      | 0.34       | 0.34³          | 1.49                 | 0.00      | 0.004    | 0.000          |
| LIN      | 14.0       | 13.98³         | 10.53                | 59.19     | 0.001    | 0.004          |
| OFL      | 100        | 100²           | 26.37                | 36.73     | 2.64E-04 | 3.67E-04       |

⁷ Lin et al., 2008; ⁸ Muñoz et al., 2008; ⁹ Kim et al., 2007; ³ Schwab et al., 2005; ⁴ Bu et al., 2013; ⁵ Ji et al., 2012; ⁶ Verlicchi et al., 2014; ⁷ Isidori et al., 2005
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