

***Supplementary Information for***

Occurrence, distribution and bioaccumulation of antibiotics in Liao River Basin in China

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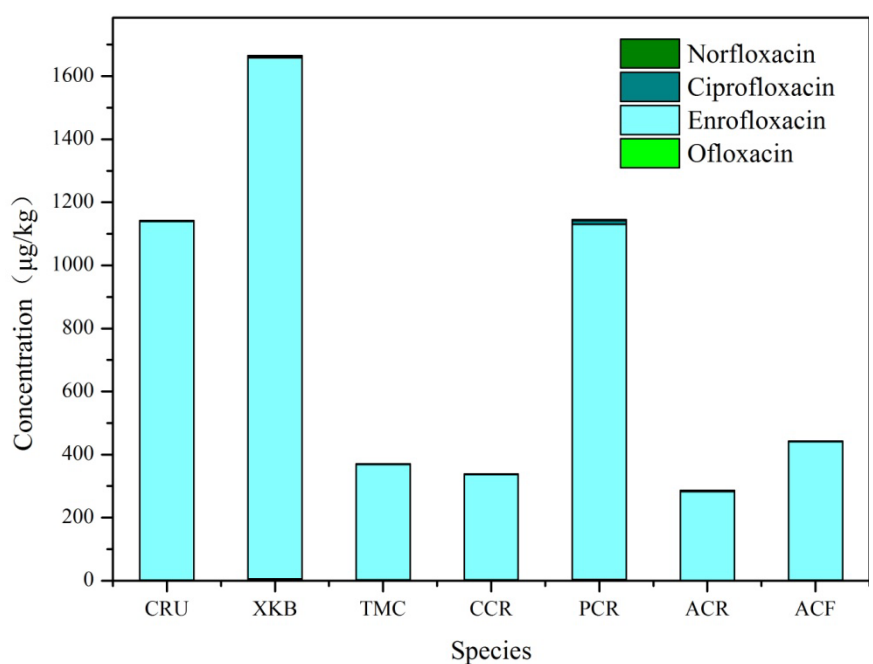


Figure S1. Concentrations of four quinolones in organism samples ( $\mu\text{g kg}^{-1}$ ).

Table S1 The biota samples collected from Liao River.

| Class      | Species                                                  | Abbreviation | n | Sampling site |
|------------|----------------------------------------------------------|--------------|---|---------------|
| Fish       | crucian<br>( <i>Carassius auratus</i> )                  | CRU          | 7 | L11           |
|            | Xingkai bitterling ( <i>Acheilognathus chankaensis</i> ) | XKB          | 5 | L11           |
|            | topmouth culter ( <i>Culter alburnus</i> )               | TMC          | 4 | L11           |
|            | Amur catfish ( <i>Slurus asotus</i> )                    | ACF          | 3 | L11           |
|            | Chinese mitten crab ( <i>Eriocheir sinensis</i> )        | CCR          | 4 | L47           |
| Crustacean | pea-crab ( <i>Pinnotheres sinensis</i> )                 | PCR          | 9 | L50           |
|            | Asian shore crab<br>( <i>Hemigraspus sanguineus</i> )    | ACR          | 7 | L49           |

n means the total number of the organisms

Table S2 Optimized MS/MS parameters for the antibiotics analysis

| Analytes             | Parent ion (m/z) | Daughter ion<br>(m/z) | Fragmentor (V) | Collision Energy/<br>eV |
|----------------------|------------------|-----------------------|----------------|-------------------------|
| SCT                  | 215.0            | 156.0                 | 90             | 5                       |
|                      |                  | 108.0 <sup>a</sup>    |                | 18                      |
| STZ                  | 256.0            | 108.0                 | 110            | 20                      |
|                      |                  | 156.0 <sup>a</sup>    |                | 10                      |
| SPD                  | 250.1            | 108.0                 | 110            | 23                      |
|                      |                  | 156.0 <sup>a</sup>    |                | 12                      |
| SMA                  | 265.2            | 92.0                  | 110            | 25                      |
|                      |                  | 156.0 <sup>a</sup>    |                | 13                      |
| SMD                  | 279.2            | 156.0                 | 110            | 15                      |
|                      |                  | 186.1 <sup>a</sup>    |                | 12                      |
| SMP                  | 281.2            | 156.0 <sup>a</sup>    | 110            | 13                      |
|                      |                  | 215.1                 |                | 28                      |
| SCP                  | 285.2            | 156.0 <sup>a</sup>    | 100            | 10                      |
|                      |                  | 92.0                  |                | 25                      |
| SMX                  | 254.0            | 156.0 <sup>a</sup>    | 100            | 10                      |
|                      |                  | 92.0                  |                | 25                      |
| SCX                  | 301.1            | 156.0 <sup>a</sup>    | 125            | 10                      |
|                      |                  | 108.0                 |                | 30                      |
| SDX                  | 311.2            | 108.0                 | 100            | 35                      |
|                      |                  | 156.1 <sup>a</sup>    |                | 18                      |
| OFL                  | 362.2            | 261.2                 | 110            | 25                      |
|                      |                  | 318.2 <sup>a</sup>    |                | 15                      |
| ENR                  | 360.0            | 245.2                 | 130            | 15                      |
|                      |                  | 316.2 <sup>a</sup>    |                | 15                      |
| CIP                  | 332.2            | 231.1                 | 110            | 35                      |
|                      |                  | 314.3 <sup>a</sup>    |                | 20                      |
| NOR                  | 320.1            | 276.3                 | 90             | 18                      |
|                      |                  | 302.2 <sup>a</sup>    |                | 18                      |
| OTC                  | 461.2            | 442.8 <sup>a</sup>    | 120            | 5                       |
|                      |                  | 426.1                 |                | 15                      |
| TC                   | 445.0            | 427.0 <sup>a</sup>    | 120            | 10                      |
|                      |                  | 410.1                 |                | 15                      |
| CTC                  | 479.1            | 462.2 <sup>a</sup>    | 130            | 13                      |
|                      |                  | 444.1                 |                | 18                      |
| ERM-H <sub>2</sub> O | 716.5            | 558.0 <sup>a</sup>    | 150            | 25                      |
|                      |                  | 158.2                 |                | 25                      |
| ROM                  | 837.4            | 158.1 <sup>a</sup>    | 130            | 35                      |
|                      |                  | 679.4                 |                | 15                      |
| ERM                  | 734.5            | 158.2 <sup>a</sup>    | 90             | 35                      |
|                      |                  | 576.3                 |                | 15                      |
| CIP-D <sub>8</sub>   | 340.2            | 322.1                 | 120            | 18                      |

|                                   |       |                    |     |    |
|-----------------------------------|-------|--------------------|-----|----|
|                                   |       | 296.2 <sup>a</sup> |     | 18 |
| SAM- <sup>13</sup> C <sub>6</sub> | 277.0 | 162.0              | 100 | 10 |
| TRM- <sup>13</sup> C <sub>3</sub> | 198.1 | 140.1              | 120 | 15 |
| ERM- <sup>13</sup> C              | 720.6 | 162.2 <sup>a</sup> | 120 | 25 |
|                                   |       | 562.3              |     | 20 |

<sup>a</sup> quantitative ion

Table S3 Correlation coefficients ( $r^2$ ), linear range, recoveries (%) and limits of detection (LODs, S/N=3) of antibiotics

| Groups        | Analytes             | Surrogates                        | $r^2$  | Linear range<br>( $\mu\text{g L}^{-1}$ ) | Recovery (%) |           |           | LOD                             |                                    |                                    | LOQ                             |                                    |                                    |
|---------------|----------------------|-----------------------------------|--------|------------------------------------------|--------------|-----------|-----------|---------------------------------|------------------------------------|------------------------------------|---------------------------------|------------------------------------|------------------------------------|
|               |                      |                                   |        |                                          | Water        | Sediment  | Organism  | Water<br>( $\text{ng L}^{-1}$ ) | Sediment<br>( $\text{ng g}^{-1}$ ) | Organism<br>( $\text{ng g}^{-1}$ ) | Water<br>( $\text{ng L}^{-1}$ ) | Sediment<br>( $\text{ng g}^{-1}$ ) | Organism<br>( $\text{ng g}^{-1}$ ) |
| Quinolones    | NOR                  | CFX-D <sub>8</sub>                | 0.9974 | 0.5-500                                  | 87.5±7.4     | 87.6±4.6  | 81.8±3.8  | 0.9                             | 0.8                                | 2.1                                | 2.9                             | 2.3                                | 6.5                                |
|               | CIP                  | CFX-D <sub>8</sub>                | 0.9987 | 0.5-500                                  | 82.7±11.4    | 75.8±7.6  | 72.5±9.2  | 1.1                             | 1.2                                | 0.8                                | 3.6                             | 3.9                                | 2.7                                |
|               | ENR                  | CFX-D <sub>8</sub>                | 0.9990 | 0.5-500                                  | 97.4±8.9     | 71.5±13.7 | 85.2±7.0  | 0.4                             | 0.6                                | 2.3                                | 1.2                             | 1.7                                | 7.0                                |
|               | OFL                  | CFX-D <sub>8</sub>                | 0.9988 | 0.5-500                                  | 104.0±8.5    | 113.7±1.9 | 87.8±3.6  | 0.3                             | 0.3                                | 1.1                                | 0.9                             | 1.0                                | 3.5                                |
|               | SCT                  | SAM- <sup>13</sup> C              | 0.9987 | 0.1-500                                  | 88.0±0.8     | 63.0±4.1  | 72±4.8    | 0.05                            | 0.1                                | 0.2                                | 0.1                             | 0.3                                | 0.8                                |
|               | STZ                  | SAM- <sup>13</sup> C              | 0.9974 | 0.1-500                                  | 84.2±5.9     | 123.5±5.0 | 93.6±7.1  | 0.2                             | 0.3                                | 0.6                                | 0.8                             | 0.8                                | 1.7                                |
|               | SMX                  | SAM- <sup>13</sup> C              | 0.9991 | 0.1-500                                  | 101.0±4.3    | 102.1±1.3 | 90.7±9.9  | 0.2                             | 0.4                                | 0.3                                | 0.7                             | 1.1                                | 1.0                                |
| Sulfonamides  | SDX                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9987 | 0.2-500                                  | 88.3±2.7     | 106.9±5.2 | 82.6±6.7  | 0.1                             | 0.2                                | 0.9                                | 0.4                             | 0.6                                | 2.5                                |
|               | SPD                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9985 | 0.2-500                                  | 98.0±5.3     | 108.6±4.6 | 90.2±3.3  | 0.1                             | 0.2                                | 0.6                                | 0.4                             | 0.7                                | 1.8                                |
|               | SMD                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9996 | 0.1-500                                  | 121.0±5.6    | 119.8±2.2 | 100.5±14  | 0.08                            | 0.1                                | 0.6                                | 0.2                             | 0.3                                | 1.6                                |
|               | SMA                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9993 | 0.1-500                                  | 102.0±3.7    | 99.1±2.5  | 97.2±1.2  | 0.15                            | 0.3                                | 0.2                                | 0.5                             | 1.2                                | 0.7                                |
|               | SMP                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9986 | 0.1-500                                  | 101.0±3.5    | 132.3±1.6 | 96.8±4.2  | 0.05                            | 0.1                                | 0.2                                | 0.2                             | 0.4                                | 0.8                                |
|               | SCX                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9977 | 0.2-500                                  | 107.0±7.1    | 117.0±8.5 | 96.7±9.1  | 0.04                            | 0.1                                | 0.6                                | 0.1                             | 0.3                                | 1.9                                |
|               | SCP                  | SAM- <sup>13</sup> C <sub>6</sub> | 0.9985 | 0.2-500                                  | 112.0±7.3    | 96.8±3.4  | 114.4±4.6 | 0.07                            | 0.2                                | 0.6                                | 0.2                             | 0.7                                | 1.5                                |
| Tetracyclines | TC                   | TRM- <sup>13</sup> C <sub>3</sub> | 0.9934 | 1-500                                    | 84.4±5.6     | 67.1±5.1  | 111.4±3.2 | 0.9                             | 0.5                                | 2.3                                | 3.0                             | 1.5                                | 6.2                                |
|               | OTC                  | TRM- <sup>13</sup> C <sub>3</sub> | 0.9934 | 1-500                                    | 90.0±7.1     | 63.4±10.3 | 109.2±8.2 | 0.7                             | 0.7                                | 1.1                                | 2.1                             | 2.4                                | 3.4                                |
|               | CTC                  | TRM- <sup>13</sup> C <sub>3</sub> | 0.9905 | 1-500                                    | 101.0±6.1    | 77.2±8.6  | 103.0±1.6 | 0.9                             | 1.0                                | 1.0                                | 2.9                             | 3.4                                | 2.9                                |
| Macrolides    | ROM                  | ERM- <sup>13</sup> C              | 0.9934 | 0.5-500                                  | 71.5±13.7    | 82.4±2.6  | 74.8±7.0  | 0.2                             | 0.4                                | 0.9                                | 0.7                             | 1.3                                | 2.8                                |
|               | ERM-H <sub>2</sub> O | ERM- <sup>13</sup> C              | 0.9992 | 0.1-500                                  | 113.7±1.9    | 103.1±1.0 | 96.8±4.4  | 0.3                             | 0.5                                | 1.5                                | 1.1                             | 1.8                                | 4.2                                |

Table S4 Concentrations of antibiotics in water and sediment in each site.

| Site | Water (ng L <sup>-1</sup> ) |        |       |         |         | Sediment (µg kg <sup>-1</sup> , dw) |       |       |       |        |
|------|-----------------------------|--------|-------|---------|---------|-------------------------------------|-------|-------|-------|--------|
|      | Σ SAs                       | Σ QNs  | Σ TCs | Σ MCs   | Total   | Σ SAs                               | Σ QNs | Σ TCs | Σ MCs | Total  |
| L1   | 72.23                       | 29.50  | 23.98 | 21.24   | 146.95  | 0.00                                | 0.00  | 0.00  | 0.00  | 0.00   |
| L2   | 193.62                      | 216.81 | 0.00  | 111.38  | 521.81  | 0.00                                | 3.15  | 0.00  | 0.60  | 3.76   |
| L3   | 76.64                       | 83.32  | 0.00  | 39.40   | 199.36  | 0.00                                | 21.85 | 0.00  | 0.00  | 21.85  |
| L4   | 65.76                       | 50.06  | 0.00  | 151.35  | 267.17  | 0.00                                | 0.00  | 0.00  | 0.00  | 0.00   |
| L5   | 59.22                       | 132.29 | 8.95  | 21.66   | 222.12  | 0.00                                | 0.00  | 0.00  | 0.00  | 0.00   |
| L6   | 64.17                       | 0.00   | 0.00  | 25.78   | 89.96   | 1.54                                | 9.26  | 0.00  | 8.51  | 19.31  |
| L7   | 50.55                       | 128.15 | 9.64  | 36.86   | 225.20  | 0.00                                | 12.21 | 16.25 | 0.00  | 28.46  |
| L8   | 59.54                       | 28.66  | 7.41  | 17.82   | 113.43  | 0.00                                | 1.24  | 7.03  | 1.82  | 10.09  |
| L9   | 140.79                      | 251.84 | 66.48 | 263.78  | 722.89  | 0.00                                | 15.72 | 21.17 | 31.82 | 68.71  |
| L10  | 70.73                       | 28.02  | 0.00  | 24.09   | 122.84  | 0.00                                | 0.00  | 4.85  | 1.27  | 6.13   |
| L11  | 90.26                       | 36.41  | 0.00  | 43.54   | 170.20  | 0.00                                | 0.00  | 3.75  | 1.37  | 5.11   |
| L12  | 59.97                       | 28.65  | 13.18 | 11.65   | 113.46  | 0.00                                | 0.92  | 0.00  | 0.00  | 0.92   |
| L13  | 46.98                       | 143.07 | 0.00  | 16.31   | 206.35  | 0.00                                | 0.00  | 0.00  | 0.00  | 0.00   |
| L14  | 103.86                      | 70.36  | 0.00  | 83.63   | 257.85  | 0.00                                | 7.84  | 0.00  | 0.00  | 7.84   |
| L15  | 100.92                      | 38.09  | 0.00  | 40.45   | 179.46  | 0.00                                | 16.39 | 2.50  | 0.00  | 18.89  |
| L16  | 45.06                       | 190.47 | 0.00  | 27.93   | 263.46  | 0.00                                | 60.81 | 31.52 | 83.27 | 175.60 |
| L17  | 84.12                       | 388.34 | 24.85 | 3162.22 | 3659.53 | 0.00                                | 11.10 | 2.94  | 0.00  | 14.04  |
| L18  | 98.43                       | 0.00   | 0.00  | 21.22   | 119.65  | 0.00                                | 12.48 | 7.10  | 14.07 | 33.65  |
| L19  | 66.52                       | 27.88  | 0.00  | 18.59   | 112.99  | 0.00                                | 14.23 | 4.66  | 19.10 | 37.99  |
| L20  | 145.67                      | 30.92  | 0.00  | 20.04   | 196.63  | 0.00                                | 8.90  | 2.44  | 0.00  | 11.34  |
| L21  | 71.98                       | 23.52  | 19.03 | 230.03  | 344.56  | 0.00                                | 12.29 | 2.66  | 0.00  | 14.95  |
| L22  | 1484.62                     | 187.75 | 0.00  | 410.15  | 2082.52 | 0.00                                | 54.16 | 3.73  | 7.74  | 65.63  |
| L23  | 52.79                       | 23.48  | 0.00  | 178.89  | 255.16  | 0.00                                | 19.72 | 2.58  | 0.00  | 22.29  |

|     |        |         |        |         |         |      |        |        |        |        |
|-----|--------|---------|--------|---------|---------|------|--------|--------|--------|--------|
| L24 | 69.60  | 114.10  | 0.00   | 29.70   | 213.40  | 0.00 | 3.73   | 9.42   | 0.00   | 13.15  |
| L25 | 75.24  | 30.50   | 14.64  | 36.63   | 157.01  | 0.91 | 2.38   | 30.84  | 14.06  | 48.18  |
| L26 | 90.21  | 135.47  | 17.55  | 30.46   | 273.69  | 2.63 | 53.27  | 42.83  | 21.06  | 119.78 |
| L27 | 67.19  | 83.39   | 43.26  | 78.31   | 272.15  | 0.00 | 24.24  | 2.46   | 0.00   | 26.70  |
| L28 | 80.86  | 83.64   | 0.00   | 116.06  | 280.56  | 0.00 | 8.32   | 28.64  | 21.28  | 58.25  |
| L29 | 69.46  | 283.64  | 51.96  | 196.69  | 601.74  | 0.00 | 116.99 | 30.34  | 42.63  | 189.96 |
| L30 | 676.25 | 113.97  | 27.75  | 260.21  | 1078.19 | 1.61 | 63.00  | 369.46 | 308.56 | 742.62 |
| L31 | 74.45  | 124.43  | 0.00   | 241.60  | 440.49  | 0.58 | 5.94   | 10.13  | 96.15  | 112.81 |
| L32 | 97.11  | 288.12  | 13.96  | 339.07  | 738.27  | 0.00 | 6.11   | 25.85  | 117.91 | 149.87 |
| L33 | 140.73 | 217.54  | 0.00   | 301.50  | 659.77  | 0.00 | 1.98   | 23.63  | 38.22  | 63.83  |
| L34 | 63.88  | 23.35   | 0.00   | 8.13    | 95.37   | 0.00 | 35.37  | 2.59   | 0.00   | 37.96  |
| L35 | 72.91  | 83.28   | 14.96  | 29.67   | 200.83  | 0.00 | 21.64  | 167.67 | 2.39   | 191.70 |
| L36 | 90.32  | 22.92   | 0.00   | 26.53   | 139.78  | 0.00 | 14.25  | 192.63 | 30.83  | 237.71 |
| L37 | 81.99  | 88.36   | 44.46  | 45.60   | 260.41  | 0.00 | 39.48  | 64.52  | 375.13 | 479.14 |
| L38 | 2.15   | 22.98   | 0.00   | 0.00    | 25.13   | 1.22 | 13.49  | 0.00   | 4.69   | 19.41  |
| L39 | 1.79   | 24.64   | 0.00   | 5.00    | 31.42   | 2.57 | 9.95   | 0.00   | 0.00   | 12.52  |
| L40 | 48.72  | 80.06   | 0.00   | 103.30  | 232.08  | 0.00 | 49.21  | 14.54  | 20.21  | 83.96  |
| L41 | 44.17  | 55.00   | 0.00   | 156.55  | 255.71  | 0.00 | 24.64  | 3.05   | 12.44  | 40.13  |
| L42 | 58.55  | 23.98   | 25.05  | 158.49  | 266.06  | 0.80 | 31.97  | 2.56   | 0.00   | 35.32  |
| L43 | 50.78  | 319.46  | 0.00   | 16.42   | 386.65  | 1.24 | 24.52  | 2.29   | 20.03  | 48.08  |
| L44 | 94.10  | 1068.52 | 770.50 | 2040.51 | 3973.63 | 0.00 | 5.18   | 404.82 | 20.66  | 430.66 |
| L45 | 73.30  | 190.84  | 0.00   | 140.35  | 404.49  | 0.00 | 23.93  | 3.51   | 15.50  | 42.94  |
| L46 | 58.00  | 187.79  | 6.52   | 120.96  | 373.27  | 0.00 | 10.70  | 15.51  | 24.17  | 50.37  |
| L47 | 59.61  | 289.22  | 0.00   | 208.44  | 557.27  | 0.45 | 72.44  | 25.14  | 177.14 | 275.17 |
| L48 | 55.02  | 45.59   | 0.00   | 121.96  | 222.56  | 0.30 | 32.02  | 5.67   | 44.86  | 82.85  |
| L49 | 50.44  | 42.66   | 0.00   | 205.99  | 299.09  | 0.00 | 40.96  | 10.29  | 47.92  | 99.17  |

|     |       |       |       |       |        |      |       |      |       |       |
|-----|-------|-------|-------|-------|--------|------|-------|------|-------|-------|
| L50 | 45.49 | 32.63 | 14.25 | 97.81 | 190.19 | 0.00 | 27.36 | 3.68 | 12.92 | 43.96 |
|-----|-------|-------|-------|-------|--------|------|-------|------|-------|-------|