**Supplementary material**

**Determining β-lactam antibiotics in aquatic products by modified QuECHERS combined with ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS)**

Lichun Li a,b,c, Yi Yin a,b,c\*,Guangming Zheng a,b,c, Shugui Liu a,b,c, Cheng Zhao a,b,c b, Lisha Ma a,b,c, Qi Shan a,b,c， Xiaoxin Dai a,b,c, Linting Wei a,b,c, Jiawei Lina,b,c ,Wenping Xie a,b,c,

a Ministry of Agriculture Laboratory of Quality & Safety Risky Assessment for Aquatic Product, Pearl River Fisheries Research Institute, Chinese Academic of Fishery Science, Guangzhou 510380, China

b Key Laboratory of Recreational Fisheries Research, Ministry of Agriculture, Pearl River Fisheries Research Institute, Chinese Academic of Fishery Science, Guangzhou 510380, China

c Key Laboratory of Aquatic Animal Immune Technology of Guangdong Province, Guangzhou 510380, China

\* Corresponding author at Pearl River Fisheries Research Institute, Chinese Academic of Fishery Science, Guangzhou 510380, China

Phone: +86 20 81616509

E-mail address: yin.yi@126.com

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**Fig.A1** Extracted ion chromatograms of nine β-lactam antibiotics at spiked concentration of 10 µg/kg in blank sample of *Ctenopharyngodon idella*

**Table.A1** Basic physico-chemical information and MRLs of nine β-lactam antibiotics

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compound** | **Structure** | **CAS** | **Molecular formula** | **Purity (%)** | **ADIa(µg/kg/day)** | **MRLb(µg/kg)** | **Foods** | **Country** |
| Penicillin G |  | 61-33-6 | C16H18N2O4S | 99.5 | 30 | 50[1] | fish | China |
| Amoxicillin |  | 26787-78-0 | C16H19N3O5S | 99.5 | 2.0 | 50[1] | fish | China |
| [Ampicillin](javascript:;) |  | 69-53-4 | C16H19N3O4S | 99.0 | 3.0 | 50[1] | fish | China |
| Cephalexin |  | 15686-71-2 | C16H17N3O4S | 98.3 | 54.4 | 200[1] | Cattle | China |
| Cefquinome |  | 84957-30-2 | C23H24N6O5S2 | 98.5 | 3.8 | 50[1] | Cattle | China |
| Ceftiofur |  | 80370-57-6 | C19H17N5O7S3 | 99.8 | 50 | 1000[1] | Cattle | China |
| Cefazolin |  | 25953-19-9 | C14H14N8O4S3 | 98.5 | - | 50[2] | Cattle | Japan |
| Cephapirin |  | 21593-23-7 | C17H17N3O6S2 | 99.4 | - | 30[2] | Cattle | Japan |
| Cefuroxime |  | 55268-75-2 | C16H16N4O8S | 99.1 | - | 20[2] | Cattle | Japan |
| Penicillin G-d7 |  | 352323-25-2 | C16H10D7KN2O4S | 98.0 | - | - | - | - |

a, ADI is allowable daily intake ;b, MRL is maximum residue limit.

**Table.A2 Chromatographic gradient conditions**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Time（ min） | Flow(mL·min-1) | Mobile phase A（%） | Mobile phase B（%） | curve |
| 0.00 | 0.4 | 90.0 | 10.0 | - |
| 1.00 | 0.4 | 90.0 | 10.0 | 6 |
| 3.00 | 0.4 | 70.0 | 30.0 | 6 |
| 5.00 | 0.4 | 60.0 | 40.0 | 6 |
| 5.01 | 0.4 | 90.0 | 10.0 | 6 |
| 8.00 | 0.4 | 90.0 | 10.0 | 6 |

**Table.A3 Concentration of β-lactam antibiotics residues found in real samples (n=3)**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Samples | Concentration of β-lactam antibiotics residues(µg/kg) | | | | | | | | |
| penicillin | amoxicillin | ampicillin | cephalexin | cefquinome | ceftiofur | cefazolin | cephapirin | cefuroxime |
| S1 | n.d.a | n.d. | n.d. | n.d. | n.d. | n.d. | 38.12±2.58 | n.d. | 25.31±2.61 |
| S2 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 11.51±1.03 |
| S3 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 16.42±0.99 | n.d. | n.d. |
| S4 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 17.65±0.45 | n.d. | n.d. |
| S5 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S6 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 75.15±3.61 |
| S7 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S8 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 27.81±3.79 |
| S9 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S10 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S11 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S12 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 24.52±1.99 | n.d. | n.d. |
| S13 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S14 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 27.55±1.22 | n.d. | 17.04±2.94 |
| S15 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 20.83±1.51 | n.d. | 33.98±3.32 |
| S16 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S17 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 18.43±1.45 | n.d. | n.d. |
| S18 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |
| S19 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | 15.21±2.54 | n.d. | n.d. |
| S20 | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. | n.d. |

a, n.d. is indicates that no detectable (<LOQ)

**References**

[1] China Food and Drug Administration, National Food Safety Standard-Maximum Residue Limits for Pesticides in Food, 2019.

[2] T.J.F.C. Foundation, Maximum Residue Limits (MRLs) List of Agricultural Chemicals in Foods, 2021. https://db.ffcr.or.jp/front/pesticide\_detail?id=38000