



*Supplementary information*

# **Antibiotics in the Crab Ponds of Lake Guchenghu Basin, China: Occurrence, Temporal Variations and Ecological Risks**

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**Table S1** Details of antibiotics and their MRM parameters in RRLC-MS/MS

Class	Compound	Abbr <sup>a</sup>	CAS	Supplier	R.T. <sup>b</sup> (min)	MRM-transitions <sup>c</sup>	Fragmentor (V)	CE <sup>d</sup> (eV)
<b>ESI+</b>								
<b>Sulfonamides</b>		<b>SAs</b>						
	Sulfacetamide	SCT	144-80-9	Dr.Ehrenstorfer	0.79	<u>215→91.8</u>	40	28
						215→155.9	40	14
	Sulfachloryridazine	SCP	80-32-0	Dr.Ehrenstorfer	2.79	<u>284.8→155.8</u>	40	19
						284.8→107.9	40	32
	Sulfadiazine	SDZ	68-35-9	Dr.Ehrenstorfer	0.91	<u>250.9→155.7</u>	40	20
						250.9→92	40	32
	Sulfadoxine	SDO	2447-57-6	Dr.Ehrenstorfer	3.51	<u>310.9→155.9</u>	60	26
						310.9→107.9	60	33
	Sulfadimethoxine	SDM	122-11-2	Dr.Ehrenstorfer	5.86	<u>310.8→155.9</u>	100	27
						310.8→107.9	100	33
	Sulfamethazine	SMZ	57-68-1	Dr.Ehrenstorfer	1.83	<u>279→185.9</u>	75	23
						279→155.9	75	25
	Sulfathiazole	STZ	72-14-0	Dr.Ehrenstorfer	1.06	<u>256→155.8</u>	90	18
						256→91.8	90	30
	Sulfamethoxazole	SMX	723-46-6	Dr.Ehrenstorfer	3.42	<u>253.9→155.9</u>	90	22
						253.9→107.9	90	30
	Sulfamethoxazole-D <sub>4</sub> (IS) <sup>e</sup> SMX-D <sub>4</sub>		1020719-86-1	Dr.Ehrenstorfer	3.36	<u>258.1→159.9</u>	90	20
						258.1→111.9	90	32
	Sulfamerazine	SMR	127-79-7	Dr.Ehrenstorfer	1.31	<u>264.8→92.1</u>	70	34
						264.8→108.2	70	33
	Sulfamerazine-D <sub>4</sub> (IS)	SMR-D <sub>4</sub>		TRC	1.28	<u>269→159.9</u>	70	21
						269→109.8	70	27
	Sulfamonomethoxine	SMM	1220-83-3	Dr.Ehrenstorfer	2.7	<u>281.2→155.8</u>	110	24
						281.2→107.8	110	31
	Sulfapyridine	SPD	144-83-2	Dr.Ehrenstorfer	1.45	<u>249.9→155.9</u>	60	21
						249.9→92.1	60	33
	Sulfaquinoxaline	SQX	59-40-5	Dr.Ehrenstorfer	6.11	<u>300.9→91.8</u>	90	31
						301.3→107.9	90	32
	Sulfisoxazole	SX	127-69-5	Dr.Ehrenstorfer	4.15	<u>268→156.0</u>	90	17
						268→112.9	90	21
<b>diaminopyrimidines</b>	Trimethoprim	TMP	738-70-5	Dr.Ehrenstorfer	1.71	<u>291.1→122.9</u>	150	31
						291.2→230.1	150	31
	Trimethoprim-D <sub>3</sub> (IS)	TMP-D <sub>3</sub>		TRC	1.66	<u>294.4→123.1</u>	150	30
						294.4→230.0	150	47
<b>Tetracyclines</b>		<b>TCs</b>						
	Chlortetracycline	CTC	57-62-5	Dr.Ehrenstorfer	5.08	<u>479→444</u>	90	27
						479→462.1	90	23
	Doxycycline	DC	564-25-0	Dr.Ehrenstorfer	6.5	<u>445→428.1</u>	155	22
						445→410	155	32
	Thiabendazole-D <sub>4</sub> (IS)	TBD-D <sub>4</sub>	71535-97-2	TRC	1.09	<u>205.9→134.9</u>	180	45
						205.9→178.9	180	35
	Oxytetracycline	OTC	79-57-2	Dr.Ehrenstorfer	1.94	<u>461.1→426.1</u>	80	25
						461.1→443.1	80	17
	Tetracycline	TC	60-54-8	Dr.Ehrenstorfer	2.47	<u>445.1→410.0</u>	80	26
						445.1→426.8	80	17
	Tetracycline-D <sub>6</sub> (IS)	TC-D <sub>6</sub>		TRC	2.46	<u>451.3→416</u>	65	26
						451.3→114	65	16

Class	Compound	Abbr	CAS	Supplier	R.T. (min)	MRM-transitions	Fragmentor (V)	CE <sup>d</sup> (eV)	
<b>Fluoroquinolones</b>		FQs				<u>331.9→314</u>	95	26	
	Ciprofloxacin	CFX	85721-33-1	Dr.Ehrenstorfer	2.14	331.9→288.1 <u>340.1→322</u>	95	24 30	
	Ciprofloxacin-D <sub>8</sub> (IS)	CFX-D <sub>8</sub>		Dr.Ehrenstorfer	2.12	340.1→296.1 <u>358→340.1</u>	95	26 31	
	Danofloxacin	DAN	112398-08-0	Dr.Ehrenstorfer	2.64	358→314 <u>400.2→356</u>	90	25 24	
	Difloxacin	DIF	98106-17-3	Dr.Ehrenstorfer	3.96	400.2→381.9 <u>360→316.2</u>	90	27 27	
	Enrofloxacin	EFX	93106-60-6	Dr.Ehrenstorfer	2.9	360→342 <u>365.1→321.1</u>	100	28 36	
	Enrofloxacin-D <sub>5</sub> (IS)	EFX- D <sub>5</sub>		Dr.Ehrenstorfer	2.87	365.1→347.1 <u>370.1→326</u>	70	30 25	
	Fleroxacin	FL	79660-72-3	Dr.Ehrenstorfer	1.91	370.1→268.9 <u>320→301.8</u>	115	36 26	
	Norfloxacin	NFX	70458-96-7	Dr.Ehrenstorfer	1.93	320→276 <u>351.8→265</u>	120	23 30	
	Lomefloxacin	LFX	98079-51-7	Dr.Ehrenstorfer	2.52	351.8→308 <u>363→72</u>	90	22 26	
	Marbofloxacin	MAR	115550-35-1	Dr.Ehrenstorfer	1.64	363→319.9 <u>362→261</u>	95	21 35	
	Ofloxacin	OFX	82419-36-1	Dr.Ehrenstorfer	1.97	362→318.1 <u>334→290</u>	124	26 26	
	Pefloxacin	PEF	70458-92-3	Dr.Ehrenstorfer	2.59	334→316 <u>386.1→368</u>	120	26 27	
	Sarafloxacin	SAR	98105-99-8	Dr.Ehrenstorfer	3.79	386.1→342.1 <u>263.3→129.0</u>	140	26 27	
	Carbadox	CAR	1791337	Dr.Ehrenstorfer	1.51	263.3→231.1	68	17	
	<b>Macrolides</b>		MLs						
		Azithromycin	ATM	830905-01-5	Dr.Ehrenstorfer	7.59	<u>749.5→158.2</u> 749.5→591.5	64	40 30
		Clarithromycin	CTM	81103-11-9	Dr.Ehrenstorfer	7.59	<u>748.9→158.2</u> 748.9→590.6	95	37 29
		Erythromycin-H <sub>2</sub> O	ETM-H <sub>2</sub> O	23893-13-2	TRC	7.44	<u>716.6→158.3</u> 716.6→558.5	85	42 21
		Erythromycin- <sup>13</sup> C-D <sub>3</sub> (IS)	ETM- <sup>13</sup> C-D <sub>3</sub>		TRC	7.44	<u>720.7→162.4</u> 720.7→562.5	97	42 22
Leucomycin		LCM	1392-21-8	Dr.Ehrenstorfer	7.46	<u>772.7→109.1</u> 772.7→174.2	132	63 44	
Oleandomycin		ODM	3922-90-5	Dr.Ehrenstorfer	7.67	<u>689→158.1</u> 689→544	100	42 28	
Roxithromycin		RTM	80214-83-1	Dr.Ehrenstorfer	7.63	<u>837.8→158.1</u> 837.8→679.8	102	47 29	
Tylosin		TYL	1401-69-0	Dr.Ehrenstorfer	7.26	<u>916.7→174.3</u> 916.7→772.4	141	55 41	

Class	Compound	Abbr	CAS	Supplier	R.T. (min)	MRM-transitions	Fragmentor (V)	CE <sup>d</sup> (eV)
<b>ionophores</b>		IPs						
	Salinomycin	SAL	53003-10-4	Dr.Ehrenstorfer	9.99	<u>773.6→431.4</u>	160	68
						773.6→265.2	160	70
	Narasin	NAR	55134-13-9	TRC	10.2	<u>787.7→431.6</u>	175	69
						787.7→531.5	175	62
	Monensin	MON	17090-79-8	Dr.Ehrenstorfer	10	<u>693.5→675.7</u>	170	52
						693.5→479.4	170	70
<b>aminocoumarins</b>	Novobiocin	NOV	303-81-1	Dr.Ehrenstorfer	17.3	<u>613.6→189.1</u>	145	24
						613.6→133		72
<b>lincosamides</b>	Lincomycin	LIN	154-21-2	Dr.Ehrenstorfer	1.23	<u>407.5→126.1</u>	80	32
						407.5→359.1	80	26
	Lincomycin-D <sub>3</sub> (IS)	LIN-D <sub>3</sub>		TRC	1.23	<u>410.6→129.1</u>	80	30
						410.6→362.2	90	25
<b>ESI-</b>								
<b>chloramphenicol derivatives</b>								
	Florfenicol	FF	73231-34-2	Dr.Ehrenstorfer	2.92	<u>355.7→335.8</u>	60	12
						355.7→184.5	60	25
	Chloramphenicol	CAP	154-75-2	Dr.Ehrenstorfer	3.63	<u>320.8→152</u>	40	21
						320.8→256.8	40	15
	Chloramphenicol-D <sub>5</sub> (IS)	CAP-D <sub>5</sub>		Dr.Ehrenstorfer	3.61	<u>325.7→156.8</u>	55	23
						325.7→261.8	55	16

<sup>a</sup> Abbreviation. <sup>b</sup> Retention time. <sup>c</sup> The selected ions for the antibiotic compounds were  $[M+H]^+$ , except ionophore compounds ( $[M+Na]^+$ ), florfenicol and chloramphenicol ( $[M-H]$ ). The underlined MRM transitions were used for quantification. <sup>d</sup> Collision energy. <sup>e</sup> Internal standard.



**Table S2.** Concentrations of antibiotics in ponds around Lake Guchenghu (ng/L).

Analytes	Fre. <sup>a</sup> (%)			Max <sup>b</sup>			Min <sup>c</sup>			Med <sup>d</sup>			Mean		
	spring	summer	autumn	spring	summer	autumn	spring	summer	autumn	spring	summer	autumn	spring	summer	autumn
SAs	80	100	100	79.9	672	431	ND <sup>e</sup>	21.7	11.5	42.0	117	169	39.6	198	175
SMX	40	20	20	17.5	21.7	6.40	ND	ND	ND	ND	ND	ND	6.00	4.34	1.28
SDZ	40	80	80	63.2	654	430	ND	ND	ND	ND	115.2	169	24.5	187	169
TMP	60	60	40	24.5	17.1	15.8	ND	ND	ND	4.40	3.20	ND	9.12	6.82	4.18
MLs	100	100	100	405	2530	313	2.10	1.30	1.90	9.70	417	201	89.2	691	166
RTM	0	0	40	ND	ND	0.20	ND	ND	ND	ND	ND	ND	ND	ND	0.05
LCM	20	0	0	8.00	ND	ND	ND	ND	ND	ND	ND	ND	1.60	ND	ND
CTM	0	60	20	ND	76.2	0.05	ND	ND	ND	ND	3.20	ND	ND	17.1	0.01
ETM-H <sub>2</sub> O	100	100	100	405	2450	312	1.10	1.30	1.90	2.10	411	201	82.8	674	165
ATM	20	0	20	24.2	ND	5.60	ND	ND	ND	ND	ND	ND	4.84	ND	1.12
CFX	40	0	0	46.5	ND	ND	ND	ND	ND	ND	ND	ND	16.8	ND	ND
MON	80	80	60	326	328	2.45	ND	ND	ND	3.60	6.6	0.4	102	82.5	0.72
FF	60	100	60	161	248	261	ND	21.0	ND	84.0	141	56.0	78.0	138	81.2
LIN	80	80	80	4.40	2.80	2.30	ND	ND	ND	1.40	1.90	0.80	2.02	1.58	0.94
ALL	100	100	100	558	3520	1000	148	190	14.5	365	686	429	328	1110	423

a Frequency of detection of each antibiotic in all surface water samples

b Maximum concentration

c Minimum concentration

d Median concentration

e Not detected



Table S3. Canonical correspondence analysis of the antibiotic concentrations and environmental parameters in crab ponds

Axes	1	2	3	4	Total variance
Eigenvalues :	0.195	0.104	0.072	0.013	1.000
Species-environment correlations :	0.666	0.674	0.765	0.443	
Cumulative percentage variance					
of species data :	19.5	29.9	37.2	38.5	
of species-environment relation :	50.8	77.8	96.5	100.0	
Sum of all eigenvalues					1.000
Sum of all canonical eigenvalues					0.385



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