

Supplementary Information

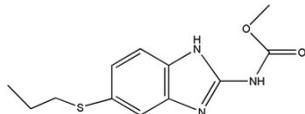
Occurrence, distribution and environmental risk of 19 anthelmintic drugs in river water and sediment from Jinjiang River, China

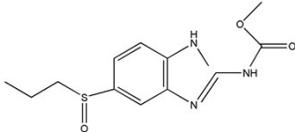
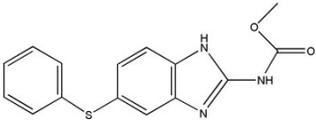
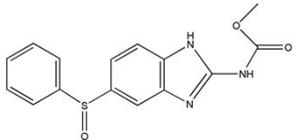
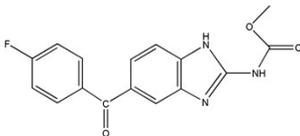
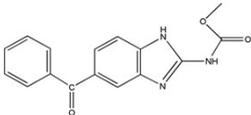
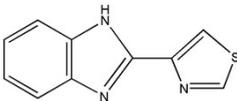
Sheng Yang¹, Mengxi Liao¹, Shijun Su¹, Sanglan Ding¹, Yiwen Li^{*1,2}, Zhiwei Gan^{*1}

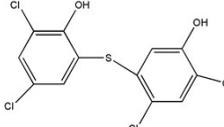
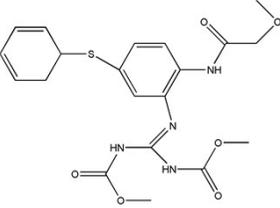
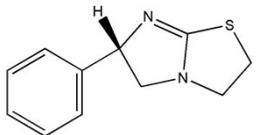
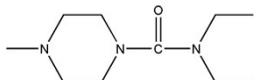
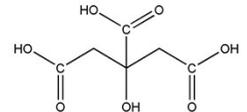
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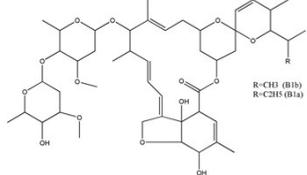
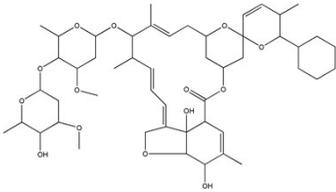
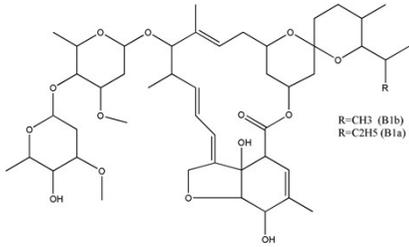
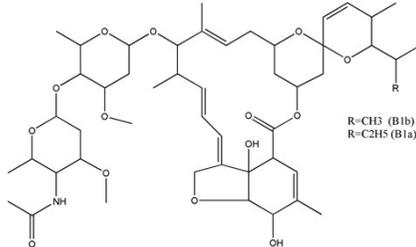
2. School of Chemical Engineering, Sichuan University, Chengdu 610065, China

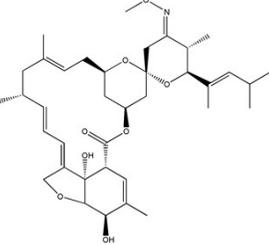
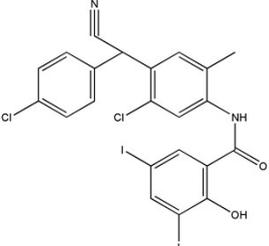
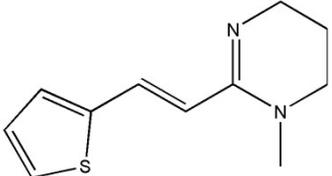
Table S1 The physicochemical data and structures of anthelmintic compounds

Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logK _{ow}	logK _{oc}	pK _a
Benzimidazoles	Albendazole	54965-21-8		10	3.07	2.94	3.37 ; 9.93

Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logKow	logKoc	pKa
	Ricobendazole	54029-12-8		62	1.2	\	3.5 ; 9.8 ; 7.8
	Fenbendazole	43210-67-9		0.01-0.04	1.95	3.37	\
	Oxfendazole	53716-50-0		407.2	1.63	\	\
	Flubendazole	31430-15-6		194.3	2.91	3.05	3.6 ; 9.6
	Mebendazole	31431-39-7		10	2.71	3	3.5
	Thiabendazole	148-79-8		\	2.47	2.69	4.7 ; 12

Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logKow	logKoc	pKa
	Bithionol	97-18-7		0.2	5.91	4.67	4.82 ; 10.5
Diphenylsulfides	Febantel	58306-30-2		76.9	1.53	1.45	4.8; 7.0; 7.4
Imidazothiazoles	Levamisole	14769-73-4		1116	2.87	1.88	7.0
Hexahydropyrazines	Diethylcarbamazine	1642-54-2	 	1*10 ⁶	\	\	7.7

Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logKow	logKoc	pKa
Macrocyclic lactones	Abamectin	71751-41-2		3.5*10 ⁻⁴	4	3.72-4.48	\
	Doramectin	117704-25-3		\	4.41	\	\
	Eprinomectin	70288-86-7		\	5.4	\	\
	Ivermectin	123997-26-2		\	3.22	\	\

Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logKow	logKoc	pKa
	Moxidectin	113507-06-5		4	4.77	3.9	\
Salicylanilides	Closantel	57808-65-8		1.5*10 ⁻⁵	8.11	5.72	4.18
Tetrahydropyrimidines	Morantel	15686-83-6		10	3.14	2.60	\

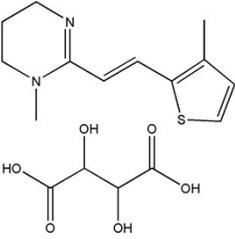
Anthelmintic Classes	Name	CAS number	Structural formula	solubility (mg/L)	logKow	logKoc	pKa
	Pyrantel	26155-31-7	 <chem>CN1CCN(CC1)C=N/C=C/C2=CC=C(S2)C(=O)C(O)C(O)C(=O)O</chem>	1.5*10 ⁵	\	\	\

Table S2 Geographical information and type of the sampling sites

Sampling sites	Description	Latitude	Longitude
S1	Suburban area	30°49'35"	103°58'16"
S2	Suburban area	30°49'3"	103°58'32"
S3	Upstream	Suburban area	103°59'19"
S4		Suburban area	104°0'36"
S5		Urban area	104°2'6"
S6		Urban area	104°3'26"
S7	Urban area	30°41'23"	104°3'28"
S8	Urban area	30°39'54"	104°05'28"
S9	Urban area	30°39'32"	104°2'5"
S10	Urban area	30°39'44"	104°2'3"
S11	Urban area	30°39'35"	104°2'13"
S12	Urban area	30°38'58"	104°3'43"
S13	Midstream	Urban area	104°4'58"
S14		Urban area	104°5'14"
S15	Urban area	30°35'31"	104°4'51"
S16	Urban area	30°33'38"	104°4'51"
S17	Urban area	30°31'47"	104°3'38"
S18	Urban area	30°30'26"	104°2'41"
S19	Suburban area	30°29'16"	104°3'7"
S20	Downstream	Suburban area	104°2'31"

S21	Suburban area	30°25'58"	104°1'22"
S22	Suburban area	30°24'49"	104°0'23"
S23	Suburban area	30°23'39"	103°59'3"
S24	Suburban area	30°21'39"	103°57'50"
S25	Suburban area	30°19'28"	103°58'18"
S26	Suburban area	30°18'14"	103°56'27"
S27	Suburban area	30°16'12"	103°55'60"
S28	Suburban area	30°13'32"	103°54'41"

Table S3 Mass spectrometer parameters for determination of target compound

Name	ESI mode	Retention time (min)	Precursor ion (m/z)	Daughter ions	DP ^a (volts)	EP ^b (volts)	CE ^c (volts)	CXP ^d (volts)	Corresponding internal standard
ALB	positive	4.18	266	234	100	10	29	12	ALB-D7
				190.9	100	10	44	12	
ALB-d7	positive	4.18	273.2	241.1	108	10	28	12	
				234	108	10	45	12	
RIC	positive	3.33	282	240	85	10	19	10	ALB-D7
				208	85	10	34	10	
FEN	positive	4.32	300	268	120	10	30	10	FEN-D3
				158.9	120	10	46	10	
FEN-d3	positive	4.32	303.2	268.1	120	10	30	10	
				159	120	10	46	10	
OXF	positive	3.55	316.3	159	110	10	45	11	FEN-D3
				191.1	110	10	28	11	
FLU	positive	3.97	314.2	282	120	10	33	13	FEN-D3
				122.9	120	10	48	13	
MEB	positive	3.89	296.1	263.9	120	10	30	8	FEN-D3
				105.1	120	10	43	8	
THI	positive	3.19	202.1	175	80	10	35	8	THI-D4
				130.9	80	10	45	8	
THI-d4	positive	3.19	206	179.1	80	10	31	10	
				135.2	80	10	46	10	
FEB	positive	4.35	447.1	383.1	95	6	27	5	FEB-D6
				415	95	6	19	5	
FEB-d6	positive	4.35	453.1	383.1	95	6	27	5	
				418.1	95	6	19	5	
LEV	positive	2.5	205.1	178	85	6	29	11	LEV-D5
				123	85	10	39	11	
LEV-d5	positive	2.5	210.1	183.1	95	10	30	10	
				128.1	95	10	38	11	
DIE	positive	2.28	200.2	100.2	60	10	20	10	DIE-D3
				127.1	60	10	20	10	
DIE-d3	positive	2.28	203	100.1	70	10	21	10	
				130.1	70	10	19	10	
ABA	positive	5.07	890.5	305.1	85	10	34	14	ROXI-D7
				567.4	85	10	21	14	
DOR	positive	5.25	916.5	331.2	80	10	35	13	ROXI-D7
				593.3	80	10	22	13	
IVE	positive	5.5	892.5	569.3	85	10	22	9	ROXI-D7

EPR	positive	4.97	914.5	307.1	85	10	35	9	ROXI-D7
				186.1	110	10	25	13	
				154	110	10	62	13	
MOX	positive	5.34	640.4	528.3	95	10	13	10	ROXI-D7
				687.6	120	10	31	9	
ROXI-D7	positive	4.39	845.6	158.2	120	10	41	9	
				498.3	95	10	18	10	
PYR	positive	2.54	207	150	85	10	38	10	LEV-D5
				136.1	85	10	41	10	
MOR	positive	3.02	221.1	122.9	90	10	44	10	LEV-D5
				164.2	90	10	36	10	
BIT	positive	4.91	352.9	160.8	-60	-10	-32	-10	FEB-D6
				191.9	-60	-11	-34	-10	
CLO	positive	4.87	660.7	126.9	-120	-12	-97	-8	CLO-C6
				344.8	-120	-13	-51	-8	
CLO-C6	positive	4.87	666.6	126.7	-120	-10	-90	-10	
				350.7	-120	-10	-50	-10	

a: declustering potential;

b: entrance potential;

c: collision energy;

d: collision outlet potential.

Table S4 The method validation of target compounds

Analyte	External calibration R ²	IDLs ^a (ng/L)	IQLs ^b (ng/L)	River water		Sediment	
				MDLs ^c	MQLs ^d	MDLs	MQLs
				(ng/L)	(ng/L)	(ng/g)	(ng/g)
ALB	0.9992	1.8	6	0.03	0.09	0.02	0.07
RIC	0.9984	1.8	6	0.06	0.20	0.06	0.20
FLU	0.9995	6	20	0.09	0.30	0.20	0.61
FEN	0.9996	0.6	2	0.03	0.08	0.01	0.03
OXF	0.9994	1.8	6	0.05	0.14	0.03	0.11
MEB	0.9995	1.8	6	0.06	0.19	0.05	0.16
THI	0.9995	1.8	6	0.05	0.16	0.04	0.12
FEB	0.9991	0.6	2	0.03	0.09	0.02	0.06
LEV	0.9991	1.8	6	0.05	0.18	0.05	0.16
DIE	0.9997	6	20	0.08	0.25	0.15	0.46
ABA	0.9992	18	60	0.23	0.70	0.34	1.03
DOR	0.9983	6	20	0.22	0.65	0.33	1.01
IVE	0.9998	1.8	6	0.09	0.29	0.11	0.34
EPR	0.9992	18	60	0.24	0.75	0.38	1.14
MOX	0.9995	6	20	0.12	0.35	0.27	0.82
PYR	0.9995	18	60	0.35	1.07	0.75	2.26
MOR	0.9994	18	60	0.22	0.67	0.33	1.01
BIT	0.9991	6	20	0.09	0.26	0.11	0.35
CLO	0.9991	1.8	6	0.03	0.10	0.02	0.06

a: instrument detection limits;

b: instrument quantitation limits;

c: method detection limits;

d: method quantitation limits

Table S5 The results of absolute recoveries and matrix effect for target compound in the water and sediment samples (n=3, recovery (RSD) (%), matrix effect (RSD) (%))

Target compound	Matrix effect (RSD) (%)				Recovery (RSD) (%)					
	River water		Sediment		River water		Sediment			
Spiked concentration (ng/mL)	5	10	50	100	50 ng/g	5	10	50	100	50 ng/g
ALB	86±3.6	82±5.5	80±2.6	81±3.2	68±8.1	82±6.5	86±5.0	89±3.8	85±6.2	69±6.6
RIC	88±5.4	85±2.5	85±4.0	86±2.8	88±9.9	90±3.7	92±7.2	90±4.8	94±5.5	86±13.6
FEN	78±3.2	81±3.6	77±9.0	80±3.9	71±5.8	84±2.6	83±6.1	81±8.4	85±3.1	58±4.2
OXF	90±3.9	90±1.5	95±4.2	102±4.6	81±6.4	102±4.0	91±3.9	92±2.8	94±4.7	90±5.4
FLU	83±5.8	80±4.9	85±6.0	84±4.0	77±5.7	86±4.6	87±3.7	88±6.9	89±3.8	83±8.8
MEB	90±3.0	92±3.6	91±2.8	87±6.8	83±6.6	90±2.1	88±3.6	92±2.5	91±2.8	81±4.2
THI	83±2.2	84±6.8	81±6.0	83±3.0	75±9.4	88±3.2	87±5.6	89±4.9	90±2.1	78±7.3
FEB	75±11.5	80±8.9	81±6.3	79±3.3	69±6.9	82±4.5	80±3.2	79±6.8	80±5.2	69±8.1
LEV	91±3.3	90±2.3	93±7.7	89±6.4	86±6.8	90±3.9	88±2.5	87±4.0	87±4.4	80±5.6
DIE	89±3.1	88±5.7	87±3.6	90±3.8	90±7.7	84±2.4	82±4.6	84±3.5	80±3.7	62±7.6
ABA	83±4.5	84±12.4	84±3.8	86±8.2	81±6.9	49±4.5	47±5.2	50±6.2	53±4.6	58±3.9
DOR	85±8.8	86±4.5	84±4.7	89±3.4	73±7.8	41±6.4	43±3.8	45±2.5	45±7.1	48±5.3
IVE	91±6.0	89±4.9	88±3.9	92±5.6	83±6.1	43±3.1	44±5.0	42±2.3	46±4.7	45±8.8
EPR	89±4.0	84±2.3	85±4.5	82±5.6	76±5.5	46±2.9	45±2.3	42±6.3	47±4.7	59±4.3
MOX	80±4.4	80±3.8	84±4.4	81±5.7	80±5.2	43±4.7	37±11.2	39±6.0	40±4.6	42±3.8
PYR	89±5.4	87±8.2	86±6.6	90±8.4	82±8.9	82±3.9	83±5.5	85±6.9	86±4.5	79±6.7

MOR	78±4.8	77±7.1	80±6.5	78±3.7	83±10.5	76±2.8	74±6.5	78±4.1	81±5.3	81±7.1
BIT	76±1.7	75±5.8	73±1.7	76±2.7	53±14.7	53±9.7	51±9.2	49±11.0	54±8.1	31±3.1
CLO	57±4.6	59±8.6	56±6.8	57±9.5	48±5.5	26±2.4	34±6.7	26±4.1	25±3.4	10±1.7

Table S6 Toxicological data of target anthelmintics for aquatic ecosystems.

Target ADs	Species group	Species	Endpoint test	Exposure time (h)	Critical effects	Toxicological data (ng/L)	Reference	AF	PNEC _{Ecotox} (ng/L)
ALB	Fish	zebrafish	Growth inhibition	144	NOEC	2.2×10^4	(Carlsson. et al., 2013)	100	220
	Fish	zebrafish	Growth inhibition	144	EC ₅₀	42×10^3	(Carlsson. et al., 2013)	1000	42
	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	42.8×10^3	(Oh. et al., 2006)	1000	42.8
RIC	/								
FEN	Fish	zebrafish	Growth inhibition	144	EC ₅₀	2.4×10^4	(Carlsson. et al., 2013)	1000	24
	Fish	zebrafish	Growth inhibition	144	NOEC	2.0×10^4	(Carlsson. et al., 2013)	100	200
	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	9.8×10^3	(Oh. et al., 2006)	1000	9.8
	Fish	zebrafish	Growth inhibition	144	EC ₅₀	6.8×10^6	(Carlsson. et al., 2013)	1000	6.8×10^3

	Fish	zebrafish	Growth inhibition	144	NOEC	4.6×10^6	(Carlsson. et al., 2013)	100	4.6×10^4
	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	5.4×10^5	(Oh. et al., 2006)	1000	540
FLU	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	54.8×10^3	(Oh. et al., 2006)	1000	54.8
MEB	organisms	<i>Hybrid Snakehead</i>	Growth inhibition	48	EC ₅₀	2.1×10^6	(Lin. et al., 2010)	1000	2.1×10^3
THI	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	3.1×10^5	(Oh. et al., 2006)	1000	308.8
BIT	organisms	<i>Oryzias latipes</i>	Growth inhibition	96	EC ₅₀	2.4×10^5	(Yoshimura et al., 2005)	1000	240
	Fish	zebrafish	Growth inhibition	144	NOEC	2.0×10^5	(Carlsson. et al., 2013)	100	2×10^3
FEB	Fish	zebrafish	Growth inhibition	144	EC ₅₀	3.4×10^5	(Carlsson. et al., 2013)	1000	340
	Daphnia magna	<i>D. magna</i>	Growth inhibition	96	EC ₅₀	2.03×10^4	(Oh. et al., 2006)	1000	20.3

LEV	organisms	Oryzias latipes	Growth inhibition	96	EC ₅₀	37.3 × 10 ⁶	(Yoshimura et al., 2005)	1000	37.3 × 10 ³
DIE	/								
	algae	S. subspicatus	Growth inhibition	72	EC ₅₀	4.4 × 10 ⁶	(Tişler. et al., 2006)	1000	4400
ABA	organisms	zebrafish	Growth inhibition	96	EC ₅₀	5.04 × 10 ⁴	(Tişler. et al., 2006)	1000	50.4
	organisms	zebrafish	Growth inhibition	48	EC ₅₀	3.3 × 10 ⁴	(Novelli, Vieira et al. 2012)	1000	33
	organisms	zebrafish	Growth inhibition	144	EC ₅₀	5.8 × 10 ⁵	(Carlsson. et al., 2013)	1000	580
DOR	organisms	zebrafish	Growth inhibition	144	NOEC	4.6 × 10 ⁵	(Carlsson. et al., 2013)	100	4.6 × 10 ³
	Daphnia magna	<i>D. magna</i>	Growth inhibition	48	EC ₅₀	25	(Boxal. et al., 2003)	1000	0.025
IVE	organisms	zebrafish embryo	Growth inhibition	144	EC ₅₀	4.4 × 10 ⁵	(Carlsson. et al., 2013)	1000	440
	organisms	zebrafish embryo	Growth inhibition	144	NOEC	2.2 × 10 ⁵	(Carlsson. et al., 2013)	100	2.2 × 10 ³

EPR	Daphnia magna	<i>D. magna</i>	Growth inhibition	48	EC ₅₀	4.5 × 10 ²	(Boxal. et al., 2003)	1000	0.45
MOX	/								
CLO	/								
PYR	/								
MOR	/								

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Mean	7.94	1.31	0.70	0.82	15.88	1.83	2.40	0.25	0.73	0.88	1.85	2.13	nq	nq	nq	nq	nq	nq	nq
Med. ^c	2.91	0.37	0.22	0.47	0.69	0.39	0.32	0.10	nq	0.18	0.31	nq	nd	nd	nd	nd	nd	nq	nd
Feq. ^d	24/25	25/25	24/25	25/25	24/25	22/25	22/25	18/25	25/25	16/25	23/25	22/25	4/25	7/25	9/25	8/25	4/25	11/25	11/25

Table S8 The K_{d,s} value of 19 anthelmintics

Compound	ALB	RIC	FEN	OXF	FLU	MEB	THI	FEB	BIT	LEV	CLO	DIE	ABA	DOR	IVE	EPR	MOX	PYR	MOR
K _{d,s} Summer	24921	112	1246	71	3960	2050	174	389	-	1476	730	1953	-	-	-	-	-	428	-
Winter	218	24	61	203	964	534	296	130	-	194	1270	2000	-	-	459	-	-	-	-

Table S9 Correlation analysis among different anthelmintics in the Jinjiang River in summer

	ALB	RIC	FEN	OXF	FLU	MEB	THI	FEB	BIT	LEV	CLO	DIE	ABA	DOR	IVE	EPR	MOX	PYR	MOR
ALB	1																		
RIC	0.122	1																	
FEN	.715**	.438*	1																
OXF	0.084	.618**	.433*	1															
FLU	0.347	.522**	.708**	.843**	1														
MEB	.416*	.617**	.768**	.876**	.916**	1													
THI	0.334	.602**	.672**	.875**	.850**	.916**	1												
FEB	-0.426	0.14	-0.135	-0.253	-0.274	-0.303	-0.248	1											
BIT	-0.092	.426*	0.323	.561**	.550**	.509**	.420*	-0.022	1										
LEV	.666**	.496**	.841**	.405*	.583**	.699**	.697**	0.016	0.031	1									
CLO	0.316	.412*	.644**	.456*	.611**	.625**	.488**	-0.085	.501**	.444*	1								
DIE	.563**	0.375	.792**	0.375	.577**	.638**	.652**	0.172	0.024	.934**	.499**	1							
ABA	0.124	0.396	.487*	0.257	.424*	.403*	0.306	.592**	.454*	0.367	.718**	.486*	1						
DOR	0.069	0.392	.448*	0.245	.403*	0.374	0.269	.632**	.444*	0.32	.660**	.450*	.974**	1					
IVE	.578**	.421*	.675**	.502*	.660**	.701**	.548**	-0.411	.438*	.468*	.826**	.463*	.503*	.495*	1				
EPR	0.17	-0.284	0.176	-0.176	0.069	-0.109	-0.137	0.361	0.159	-0.05	0.197	0.088	.517**	.544**	0.135	1			
MOX	0.047	0.323	.417*	0.206	0.371	0.366	0.267	.714**	0.398	0.381	.468*	.464*	.828**	.806**	0.176	.410*	1		
PYR	0.14	.789**	0.227	0.182	0.113	0.243	0.185	0.236	0.155	0.335	0.174	0.19	0.261	0.218	0.138	-0.283	0.377	1	
MOR	.789**	0.202	.794**	0.315	.534**	.583**	.598**	-0.175	-0.017	.836**	0.263	.820**	0.187	0.199	.490*	0.232	0.207	0.049	1

** . Correlation is significant at the 0.01 level (2-tailed)

* . Correlation is significant at the 0.05 level (2-tailed)

Table S10 Correlation analysis among different anthelmintics in the Jinjiang River in winter

	ALB	RIC	FEN	OXF	FLU	MEB	THI	FEB	BIT	LEV	CLO	DIE	ABA	DOR	IVE	EPR	MOX	PYR	MOR
ALB	1																		
RIC	.644**	1																	
FEN	.907**	.499**	1																
OXF	.810**	.732**	.847**	1															
FLU	.820**	.655**	.788**	.747**	1														
MEB	.927**	.721**	.901**	.946**	.788**	1													
THI	.875**	.606**	.913**	.827**	.864**	.868**	1												
FEB	0.195	0.057	0.107	0.162	-0.052	0.238	-0.049	1											
BIT	-0.028	0.151	0.039	0.113	0.03	0.111	0.126	-0.176	1										
LEV	.886**	.620**	.934**	.854**	.829**	.898**	.954**	-0.049	0.112	1									
CLO	.554**	.477*	.543**	.577**	.392*	.662**	.522**	0.305	0.128	.513**	1								
DIE	.509**	0.094	.650**	.557**	0.313	.508**	.505**	0.215	0.025	.525**	0.135	1							
ABA	.384*	-0.059	.427*	0.199	0.296	0.234	0.33	0.004	-0.314	0.291	-0.097	.398*	1						
DOR	0.355	-0.159	.439*	0.177	0.23	0.214	0.334	-0.016	-0.263	0.288	-0.047	.448*	.925**	1					
IVE	0.323	-0.254	.418*	0.141	0.317	0.178	0.228	0.072	-0.376	0.214	-0.213	.404*	.879**	.851**	1				
EPR	0.31	-0.287	.436*	0.162	0.264	0.206	0.241	0.028	-0.25	0.254	-0.179	.404*	.879**	.817**	.942**	1			
MOX	0.311	0.113	.449*	0.29	0.347	0.242	.387*	-0.046	-0.116	0.357	-0.173	.539**	.709**	.709**	.640**	.526**	1		
PYR	.636**	.978**	.484*	.689**	.651**	.700**	.610**	-0.056	0.176	.630**	.458*	0.038	-0.111	-0.204	-0.321	-0.346	0.079	1	
MOR	.570**	0.144	.631**	.482*	.529**	.480*	.567**	-0.102	-0.045	.618**	-0.09	.644**	.476*	.419*	.456*	.503**	.495*	0.181	1

** . Correlation is significant at the 0.01 level (2-tailed)

* . Correlation is significant at the 0.05 level (2-tailed)

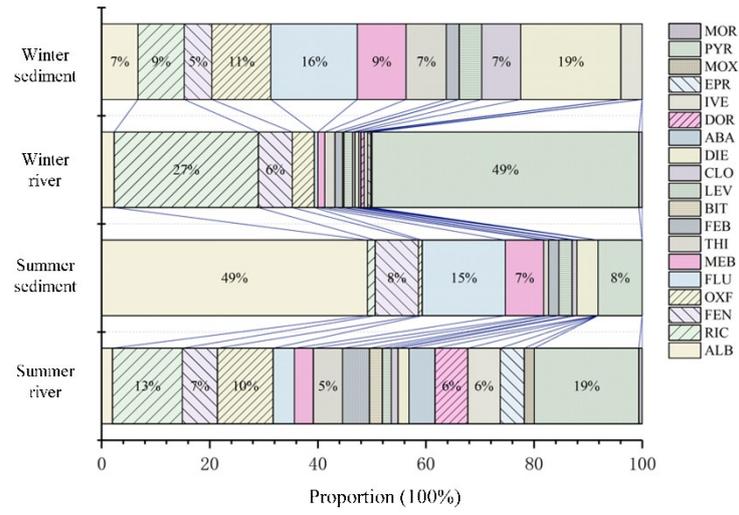


Fig. S1 Percentage compositions of 19 anthelmintics in the river and sediment samples in Chengdu, China