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Supplementary Material

2 Occurrence and risk assessment of current-use pesticides in 3 a tropical drinking water source reservoir in Hainan 4 Province, China

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19 **Text S1 Chemicals and reagents**

20 Oasis HLB SPE cartridges (Waters, 6 mL, 500 mg), were purchased from Waters (USA).
21 Chromatography grade solvents (n-Hexane (n-Hex), dichloromethane (DCM), acetone (ACE),
22 and ethyl acetate (EtAc)) were purchased from ANPEL Laboratory Technologies Inc.
23 (Shanghai, China).

24 **Text S2 Instrumental analysis.**

25 **UPLC-MS/MS**

26 Analysis of CUPs was performed using ultra-high-performance liquid chromatography-
27 triple quadrupole mass spectrometer (UPLC-MS/MS, Waters, TQ-S Micro) under positive
28 electrospray ionization (ESI+) in the multiple reaction monitoring (MRM) mode. A Waters
29 ACQUITY UPLC® T3 column (100 mm × 2.1 mm, 1.7 µm) was used to separate chemicals of
30 interest. The column temperature was 40 °C and the injection volume was 5 µL. The mobile
31 phases were (A) 0.05% acetic acid in MEOH and (B) 0.05% ammonium acetate and 0.05%
32 acetic acid in water with a flow rate of 0.4 mL/min. The gradient of separation was 15% A in 0–
33 1 min, 15–60% A in 1–6 min, 90% A in 6–13 min, 15% A in 13–15 min. Other MS conditions
34 were: Capillary voltage 4 kV, Drying gas temperature 350 °C and flow rate 10 mL/min,
35 Nebulizing gas pressure 50 psi, Sheath gas temperature 350 °C and flow rate 12 mL/min.

Table S1. General information for target chemicals.

Name	Abbreviations	CAS No.	molecular formulae	mass	Log Kow ^a
Dinotefuran	DNT	165252-70-0	C7 H14 N4 O3	202.21	-0.19
Acetamiprid	ACE	135410-20-7	C10 H11 CL1 N4	222.68	2.55
Nitenpyram	NTP	150824-47-8	C11 H15 CL1 N4 O2	270.72	0.4
Clothianidin	CLO	210880-92-5	C6 H8 CL1 N5 O2 S1	249.68	0.64
Thiacloprid	THA	111988-49-9	C10 H9 CL1 N4 S1	252.72	2.33
Thiamethoxam	THM	153719-23-4	C8 H10 CL1 N5 O3 S1	291.71	0.8
Imidacloprid	IMI	138261-41-3	C9 H10 CL1 N5 O2	255.67	0.56
Imidaclothiz	IMIT	105843-36-5	C7H8ClN5O2S	261.69	1.54
Flonicamid	FLO	158062-67-0	C9 H6 F3 N3 O1	229.16	0.5
Phoxim	PXM	14816-18-3	C12 H15 N2 O3 P1 S1	298.3	4.39
Dichlorvos	DCH	62-73-7	C4 H7 CL2 O4 P1	220.98	0.6
Malathion	MLT	121-75-5	C10 H19 O6 P1 S2	330.35	0.29
Dimethoate	DMT	60-51-5	C5 H12 N1 O3 P1 S2	229.25	0.72
Trichlorfon	TCF	52-68-6	C4 H8 CL3 O4 P1	257.44	0.42
Phorate	PHT	298-02-2	C7 H17 O2 P1 S3	260.37	3.62
Chlorpyrifos	CPF	2921-88-2	C9 H11 CL3 N1 O3 P1 S1	350.59	5.11
Atrazine	ATR	1912-24-9	C8 H14 CL1 N5	215.69	2.82
Butachlor	BTC	23184-66-9	C17 H26 CL1 N1 O2	311.86	4.84
Acetochlor	ATC	34256-82-1	C14 H20 CL1 N1 O2	269.77	3.37
Metalaxyl	MLX	57837-19-1	C15 H21 N1 O4	279.34	1.7
Carbendazim	CBZ	10605-21-7	C9 H9 N3 O2	191.19	1.55
Thiophanate-methyl	TPH	23564-05-8	C12 H14 N4 O4 S2	342.39	1.1
Pyraclostrobin	PCT	175013-18-0	C19 H18 CL1 N3 O4	387.83	5.45
Spirodiclofen	SPD	148477-71-8	C21 H24 CL2 O4	411.33	6.28
Indoxacarb	IDC	144171-61-9	C22 H17 CL1 F3 N3 O7	527.84	5.21
Emamectin benzoate	EMB	155569-91-8	C49 H77 NO13	888.13	/

37 a Data taken from the software EPI web 4.

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Table S2. Ions information for target chemicals.

Full name	Abbreviation	CAS	Precursor (m/z)	Quantitative ion (m/z)	Cone (V)	Collision (V)
Current-Use Pesticides (CUPs)						
Dinotefuran	DNT	165252-70-0	203	113/129	15	10
Acetamiprid	ACE	135410-20-7	223	56/126	30	15/20
Nitenpyram	NTP	150824-47-8	271.1	125.9/224.9	15	45229
Clothianidin	CLO	210880-92-5	250	132/169	25	45214
Thiacloprid	THA	111988-49-9	253	90.1/126	40	35/20
Thiamethoxam	THM	153719-23-4	292	132/211.2	25	45219
Imidacloprid	IMI	138261-41-3	256.1	175.1/209.1	25	20/15
Imidaclothiz	IMIT	105843-36-5	262.08	95/122.24/180.98	22	42/26/14
Flonicamid	FLO	158062-67-0	230.1	148.05/203.07	35	25/15
Phoxim	PXM	14816-18-3	299	129/153	12	45120
Dichlorvos	DCH	62-73-7	221	79/109	23	34/22
Malathion	MLT	121-75-5	331	99/127	12	45286
Dimethoate	DMT	60-51-5	230.1	125/199	5	45219
Trichlorfon	TCF	52-68-6	257	79/109	35	30/15
Phorate	PHT	298-02-2	261	75.1/97.05	15	45285
Chlorpyrifos	CPF	2921-88-2	349.9	97/198	27	30/20
Atrazine	ATR	1912-24-9	216.1	96.1/174.2	39	23/18
Butachlor	BTC	23184-66-9	312.2	57.3/238.2	26	45282

Acetochlor	ATC	34256-82-1	270	148/224	20	45275
Metalaxyll	MLX	57837-19-1	280.1	192.1/220.1	10	20/15
Carbendazim	CBZ	10605-21-7	192.1	132.1/160.1	10	30/15
Thiophanate-methyl	TPH	23564-05-8	343	93/151	25	30/20
Pyraclostrobin	PCT	175013-18-0	388.1	163/193.9	5	45285
Spirodiclofen	SPD	148477-71-8	411.4	71.16/313.1	35	45214
Indoxacarb	IDC	144171-61-9	528	150/203	5	25/30
Emamectin benzoate	EMB	155569-91-8	886.6	126/158	20	30/35
Carbendazim-d3	CBZ-d3	/	195.1	64.99/132.08/160.08	6	40/30/14
Acetamiprid-d3	ACE-d3	/	226.15	59.07/90.08/125.97	16	14/32/18
Clothianidin-d3	CLO-d3	/	253.09	113.06/131.94/171.99	18	22/14/10
imidacloprid-d3	IMD-d3	/	260.14	87.07/179.1/213.14	24	14/16/12

Table S3. Recovery and MQL for each target chemical.

No.	Compounds	Recovery (%)	MQL (ng/L)
1	DNT	98.3	1.00
2	ACE	79.7	0.208
3	NTP	65.8	0.417
4	CLO	90.4	1.67
5	THA	87.3	0.060
6	THM	82.1	0.357
7	IMI	101	0.833
8	IMIT	104	0.909
9	FLO	62.9	0.526
10	PXM	60.0	0.250
11	DCH	59.0	1.67
12	MLT	82.0	0.132
13	DMT	75.1	0.625
14	TCF	61.1	1.000
15	PHT	57.2	1.43
16	CPF	53.8	0.833
17	ATR	90.7	0.294
18	BTC	78.8	1.25
19	ATC	56.2	0.192
20	MLX	81.0	0.167
21	CBZ	59.1	0.238
22	TPH	68.0	0.109
23	PCT	85.1	0.109
24	SPD	111	0.185
25	IDC	91.5	0.962
26	EMB	53.0	0.833

45 **Table S4.** Aquatic life benchmarks and lowest PNEC for CUPs detected in reservoirs.

No.	Pesticides	Abbreviation	Aquatic Life Benchmarks ^a (µg/L)	Lowest PNEC ^b (µg/L)
1	Acetamiprid	ACE	2.1	0.024
2	Clothianidin	CLO	0.05	2.23
3	Thiamethoxam	THM	0.74	0.042
4	Imidacloprid	IMI	0.01	0.0013
5	Flonicamid	FLO	3000	62
6	Dichlorvos	DCH	0.0058	0.0006
7	Atrazine	ATR	5	0.6
8	Metalaxyl	MLX	1200	100
9	Carbendazim	CBZ	0.99	0.44
10	Spirodiclofen	SPD	1.95	0.2

46 a: the Aquatic Life Benchmarks for freshwater chronic invertebrates came from the United States

47 Environmental Protection Agency (USEPA) (Aquatic Life Benchmarks and Ecological Risk

48 Assessments for Registered Pesticides | USEPA)

49 b: The lowest PNECs can be found online at NORMAN Ecotoxicology Database (norman-

50 network.com)

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Table S5. Relative chronic reference dose (cRfD) of six NNIs and Relative potency factor (RPF) of six NNIs normalized to IMI.

	CRfD(mg/kg bw/d) ^a	RPF ^b
IMI	0.057	1
THM	0.006	9.5
ACE	0.071	0.803
CLO	0.0098	5.816
DNT	0.02	2.85

^a U.S.EPA has enacted chronic reference dose (cRfD) for some individual NNIs based on the no-observed-adverse-effect level (NOAEL)¹.

^b RPF: Relative potency factor was calculated based on cRfD of each NNI normalized by cRfD of IMI.

57 RPFk=cRfD imidacloprid / cRfDk, where k means NNIs.

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Table S6. The daily water ingestion rate (DIR) for estimation of human exposure.

Group	Age	DIR ($L \cdot kg^{-1} bw \cdot d^{-1}$)
Infants	<1 year	0.089
Toddlers	1-3 years	0.031
Children	4-11 years	0.029
Teenagers	11-21 year	0.016
Adults	≥ 21 year	0.02

60 Data source: USEPA exposure factors handbook, based on “Consumer-Only Estimates of Direct and
61 Indirect Water Ingestion^{2,3}.

Table S7. Concentrations (ng/L) of CUPs in surface water in the study area.

Chemicals	Range	Median	Mean	Sd	DF (%)
DNT	n.d.– 2.07	n.d.	0.07	0.39	3.45
ACE	n.d.– 95	0.53	6.92	17.9	72.4
NTP	n.d.– 0.492	n.d.	0.034	0.13	6.9
CLO	n.d.– 210	11.9	36.5	51.7	89.7
THA	n.d.– 0.39	n.d.	0.013	0.072	3.45
THM	n.d.– 539	25.1	103	153	75.9
IMI	n.d.– 210	6.94	23.5	44.1	65.5
IMIT	n.d.– 1.4	n.d.	0.048	0.26	3.45
FLO	n.d.– 2.04	n.d.	0.24	0.48	27.6
Σ NNI	n.d.– 755	71	170	208	96.6
PXM	n.d.– n.d.	n.d.	n.d.	n.d.	0
DCH	n.d.– 286	3.41	21.5	63.9	75.9
MLT	n.d.– 16.3	n.d.	1.32	3.61	37.9
DMT	n.d.– n.d.	n.d.	n.d.	n.d.	0
TCF	n.d.– 46.9	n.d.	2.24	8.72	20.7
PHT	n.d.– n.d.	n.d.	n.d.	n.d.	0
CPF	n.d.– 32	n.d.	2.01	6.2	24.1
Σ OPPs	n.d.– 297	3.91	27.1	67.8	79.3
ATR	n.d.– 1.39	n.d.	0.15	0.37	17.2
BTC	n.d.– n.d.	n.d.	n.d.	n.d.	0
ATC	n.d.– 55.4	n.d.	3.26	11.4	10.3
MLX	n.d.– 69.9	11.4	16.5	16.6	93.1
CBZ	n.d.– 322	5.71	26.5	64.7	86.2
TPH	n.d.– 6.14	n.d.	0.50	1.57	10.3
PCT	n.d.– 63.7	0.18	3.62	11.9	51.7
SPD	n.d.– 245	n.d.	23.1	59.9	48.3
IDC	n.d.– 6.84	n.d.	0.24	1.27	3.45
EMB	n.d.– 5.88	n.d.	0.20	1.09	3.45
Σ Others	n.d.– 439	28.3	74.1	103	93.1
Σ CUPs	n.d.– 821	119	244	241	96.6

Table S8. IMI-equivalent estimated daily intake (IMIeq EDI) of NNIs (pg/kg bw/d) from Hailan Province, China.

	Median					95 th percentile				
	Infants	Toddlers	Children	Teenagers	Adults	Infants	Toddlers	Children	Teenagers	Adults
Water ingestion rate a (L/kg bw/day)	0.089	0.031	0.029	0.016	0.02	0.089	0.031	0.029	0.016	0.02
Six NNIs										
ACE	27.1	9.45	8.84	4.88	6.09	39	13.6	12.7	7.02	8.77
CLO	4590	1600	1500	826	1030	8070	2810	2630	1450	1810
THM	9110	3170	2970	1640	2050	43600	15200	14200	7830	9790
IMI	0	0	0	0	0	602	210	196	108	135
Total NNIs										
IMIeq EDI	13700	4780	4470	2470	3090	52300	18200	17000	9400	11800

65 a : Parameters used for EDI of NNIs according to USEPA exposure factors handbook (page 3e43), based on “Consumer-Only Estimates of Direct and Indirect Water Ingestion

66 (L/kg bw/d)”. IMI-equivalent EDI of each NNI was calculated by multiplying EDI of each NNI and corresponding relative potency factor (RPF); \sum IMIeq EDI: Summing up IMIeq

67 EDI of each NNI¹.

68

Table S9. The concentrations of NNIs (ng/L) in surface water at each sampling site within the study area.

Study Area	Site	DNT	ACE	NTP	CLO	THA	THM	IMI	IMIT	FLO
Reservoirs	R-1	n.d.	0.558	n.d.	13.4	n.d.	34.1	6.5	n.d.	n.d.
	R-2	n.d.	0.486	n.d.	2.7	n.d.	10.5	n.d.	n.d.	n.d.
	R-3	n.d.	0.38	n.d.	14.6	n.d.	38.3	5.74	n.d.	n.d.
	R-4	n.d.	0.528	n.d.	16.2	n.d.	60.3	6.94	n.d.	n.d.
	R-5	n.d.	0.362	n.d.	9.18	n.d.	25.1	n.d.	n.d.	n.d.
	R-6	n.d.	n.d.	n.d.	3.95	n.d.	10.7	n.d.	n.d.	n.d.
	R-7	n.d.	n.d.	n.d.	3.9	n.d.	6.39	n.d.	n.d.	0.704
	R-8	n.d.	0.525	n.d.	8.88	n.d.	10.8	n.d.	n.d.	0.527
	R-9	n.d.	n.d.	n.d.	3.38	n.d.	n.d.	n.d.	n.d.	n.d.
Upstream River Basin	R-10	n.d.	n.d.	n.d.	4.98	n.d.	6.84	n.d.	n.d.	0.702
	U-1	n.d.	5.49	n.d.	95	n.d.	465	96	n.d.	0.528
	U-2	n.d.	13.7	n.d.	69.9	n.d.	65	11.7	n.d.	n.d.
	U-3	n.d.	4.87	0.492	102	n.d.	198	40.5	n.d.	0.932
	U-4	n.d.	n.d.							
Agricultural Sources	A-01	n.d.	0.784	n.d.	5.76	n.d.	9.08	15.9	n.d.	n.d.
	A-02	n.d.	5.4	n.d.	n.d.	n.d.	293	8.86	n.d.	2.04
	A-03	n.d.	n.d.	n.d.	210	n.d.	539	5.93	n.d.	n.d.
	A-04	n.d.	95	0.49	123	n.d.	n.d.	n.d.	n.d.	n.d.
	A-05	n.d.	17.1	n.d.	15.4	n.d.	21.3	38.7	n.d.	n.d.
Domestic Sources	A-06	2.07	13.9	n.d.	126	n.d.	n.d.	210	n.d.	1.11
	D-1	n.d.	21.9	n.d.	91.2	n.d.	216	25.7	n.d.	n.d.
	D-2	n.d.	4.74	n.d.	8.98	0.388	45.1	11.8	n.d.	n.d.
	D-3	n.d.	0.515	n.d.	29.3	n.d.	313	92.9	n.d.	n.d.
	D-4	n.d.	2.46	n.d.	8.91	n.d.	n.d.	8.16	n.d.	n.d.

	D-5	n.d.	2.62	n.d.	57.3	n.d.	333	54.6	n.d.	0.536
	D-6	n.d.	0.374	n.d.	11.9	n.d.	234	17.8	n.d.	n.d.
	D-7	n.d.	8.96	n.d.	18	n.d.	42.9	18	1.4	n.d.
	D-8	n.d.	n.d.	n.d.	3.83	n.d.	n.d.	n.d.	n.d.	n.d.
	D-9	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	4.42	n.d.	n.d.

70 n.d.: not detected.

71

72 **Table S10** The concentrations of OPPs (ng/L) in surface water at each sampling site within the study area.

Study Area	Site	PXM	DCH	MLT	DMT	TCF	PHT	CPF
Reservoirs	R-1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	R-2	n.d.	6.05	n.d.	n.d.	n.d.	n.d.	n.d.
	R-3	n.d.	2.32	n.d.	n.d.	n.d.	n.d.	n.d.
	R-4	n.d.	3.3	n.d.	n.d.	n.d.	n.d.	n.d.
	R-5	n.d.	2.51	n.d.	n.d.	n.d.	n.d.	n.d.
	R-6	n.d.	4.18	n.d.	n.d.	n.d.	n.d.	n.d.
	R-7	n.d.	1.88	n.d.	n.d.	n.d.	n.d.	n.d.
	R-8	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	R-9	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	R-10	n.d.	3.91	n.d.	n.d.	n.d.	n.d.	n.d.
Upstream River Basin	U-1	n.d.	6.05	0.553	n.d.	4.15	n.d.	3.61
	U-2	n.d.	2.95	n.d.	n.d.	n.d.	n.d.	n.d.
	U-3	n.d.	3.6	n.d.	n.d.	3.24	n.d.	1.76
	U-4	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Agricultural Sources	A-01	n.d.	3.69	0.396	n.d.	n.d.	n.d.	n.d.
	A-02	n.d.	2.4	n.d.	n.d.	n.d.	n.d.	n.d.
	A-03	n.d.	n.d.	0.134	n.d.	n.d.	n.d.	1.96

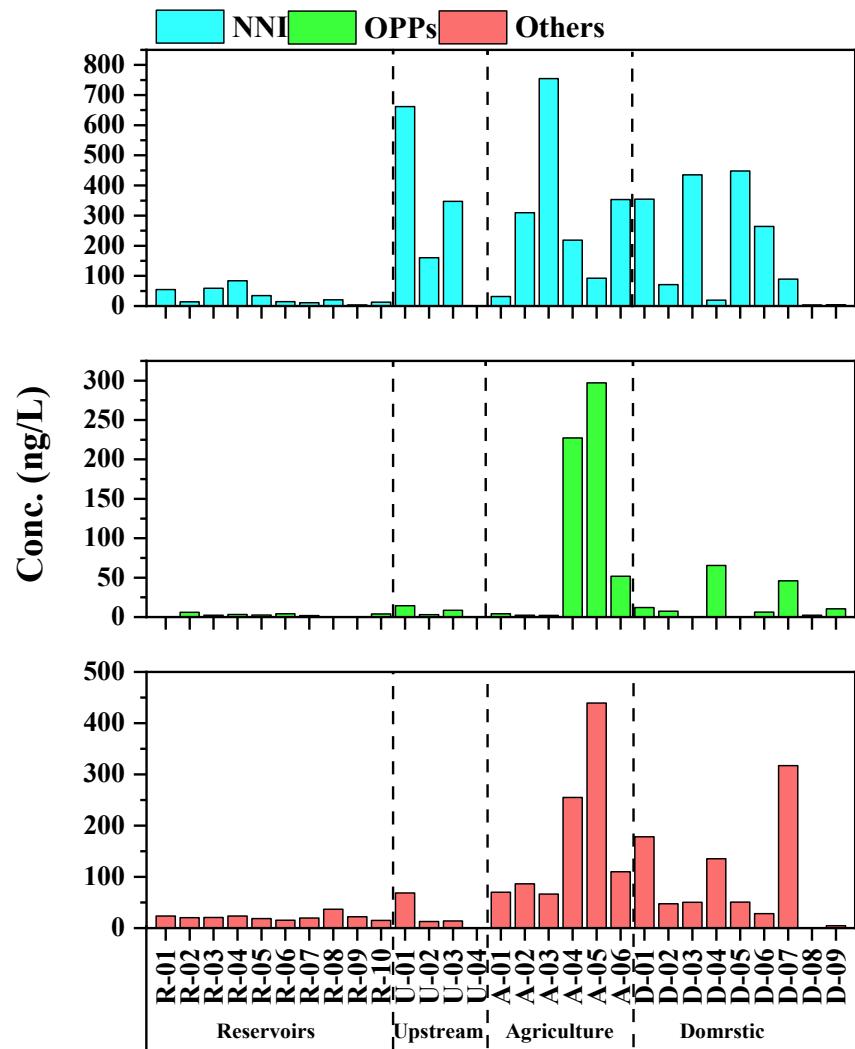
	A-04	n.d.	207	16.3	n.d.	1.56	n.d.	1.82
	A-05	n.d.	286	8.21	n.d.	2.6	n.d.	n.d.
	A-06	n.d.	4.66	0.166	n.d.	46.9	n.d.	n.d.
	D-1	n.d.	3.41	0.155	n.d.	n.d.	n.d.	8.51
	D-2	n.d.	4.96	2.51	n.d.	n.d.	n.d.	n.d.
	D-3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Domestic Sources	D-4	n.d.	48.1	8.64	n.d.	n.d.	n.d.	8.68
	D-5	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	D-6	n.d.	6.05	0.172	n.d.	n.d.	n.d.	n.d.
	D-7	n.d.	13	1.06	n.d.	n.d.	n.d.	32
	D-8	n.d.	2.31	n.d.	n.d.	n.d.	n.d.	n.d.
	D-9	n.d.	4.08	n.d.	n.d.	6.48	n.d.	n.d.

73 n.d.: not detected.

Table S11. The concentrations of OthPs (ng/L) in surface water at each sampling site within the study area.

Study Area	Site	ATR	BTC	ATC	MLX	CBZ	TPH	PCT	SPD	IDC
Reservoirs	R-1	0.34	n.d.	n.d.	14.2	6.51	n.d.	n.d.	2.72	n.d.
	R-2	n.d.	n.d.	n.d.	13.7	6.64	n.d.	n.d.	n.d.	n.d.
	R-3	1.39	n.d.	n.d.	13	3.96	n.d.	n.d.	2.18	n.d.
	R-4	n.d.	n.d.	n.d.	18.1	5.53	n.d.	n.d.	n.d.	n.d.
	R-5	n.d.	n.d.	n.d.	12.8	5.71	n.d.	n.d.	n.d.	n.d.
	R-6	n.d.	n.d.	n.d.	10.2	5.12	n.d.	n.d.	n.d.	n.d.
	R-7	n.d.	n.d.	n.d.	11.2	5.39	n.d.	n.d.	2.9	n.d.
	R-8	0.57	n.d.	n.d.	21.1	12.6	n.d.	n.d.	2.5	n.d.
	R-9	n.d.	n.d.	n.d.	12.4	7.39	n.d.	n.d.	2.52	n.d.
	R-10	n.d.	n.d.	n.d.	11.4	3.53	n.d.	n.d.	n.d.	n.d.
Upstream River Basin	U-1	n.d.	n.d.	11.8	42.5	6.79	n.d.	7.65	n.d.	n.d.
	U-2	n.d.	n.d.	n.d.	4.22	5.66	n.d.	0.29	2.8	n.d.
	U-3	n.d.	n.d.	n.d.	4.47	4.75	n.d.	2.49	2.28	n.d.
	U-4	n.d.								
Agricultural Sources	A-01	n.d.	n.d.	n.d.	55.4	n.d.	n.d.	0.177	14.5	n.d.
	A-02	n.d.	n.d.	n.d.	34	40.2	n.d.	1.82	10.3	n.d.
	A-03	n.d.	n.d.	55.4	3.1	7.26	n.d.	0.626	n.d.	n.d.
	A-04	1.3	n.d.	n.d.	4.11	3.15	n.d.	1.74	245	n.d.
	A-05	n.d.	n.d.	n.d.	11	322	n.d.	63.7	42.3	n.d.

	A-06	n.d.	n.d.	n.d.	69.9	26.9	n.d.	13	n.d.	n.d.
	D-1	n.d.	n.d.	27.5	4.75	139	5.43	1.6	n.d.	n.d.
	D-2	n.d.	n.d.	n.d.	20.1	19.5	6.14	1.85	n.d.	n.d.
	D-3	n.d.	n.d.	n.d.	11.4	10.5	n.d.	n.d.	28.5	n.d.
	D-4	n.d.	n.d.	n.d.	4.95	4.84	n.d.	2.91	110	6.84
Domestic Sources	D-5	0.612	n.d.	n.d.	36.8	8.93	n.d.	4.23	n.d.	n.d.
	D-6	n.d.	n.d.	n.d.	22.9	3.05	n.d.	2.41	n.d.	n.d.
	D-7	n.d.	n.d.	n.d.	6.99	104	2.97	0.526	202	n.d.
	D-8	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	D-9	n.d.	n.d.	n.d.	4.55	n.d.	n.d.	n.d.	n.d.	n.d.

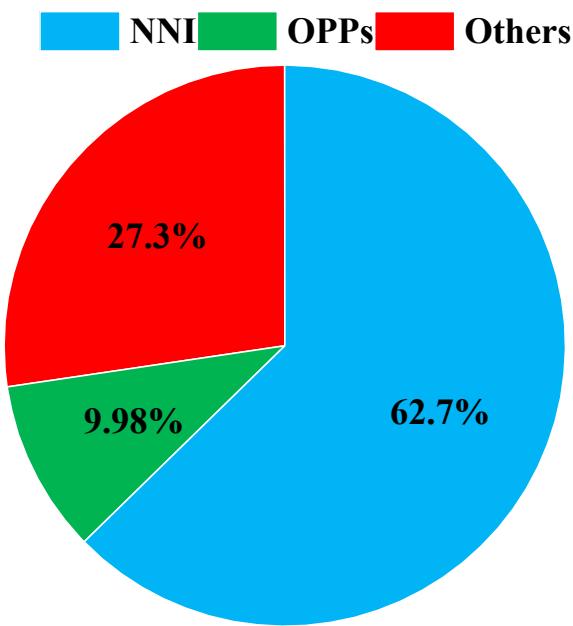


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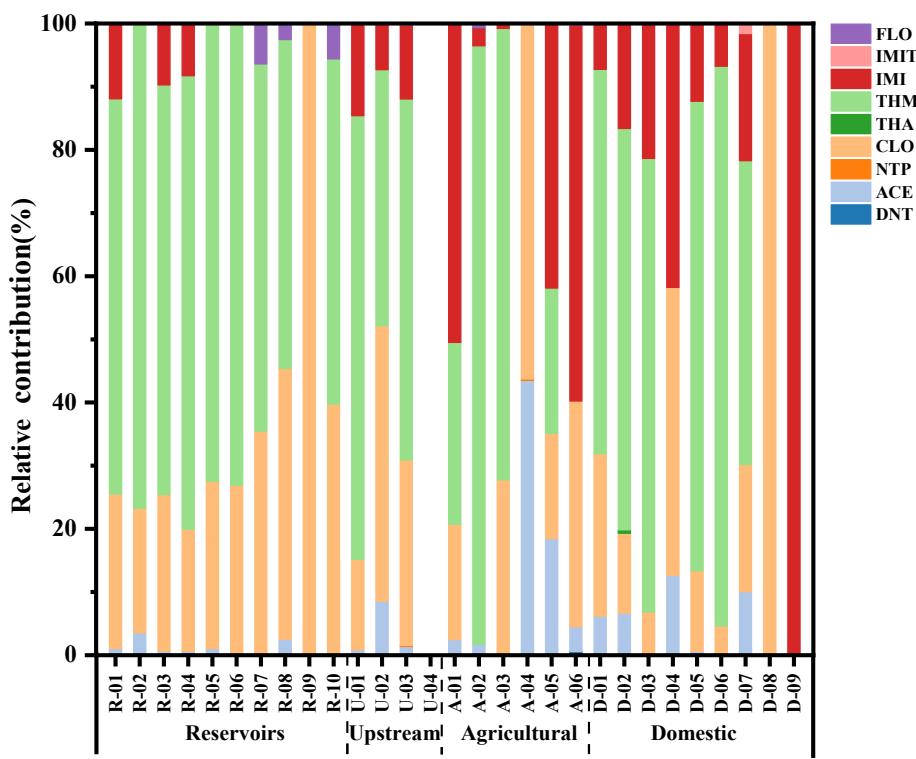
Figure S1. Concentrations of NNI, OPPs, and other pesticides in water at various sites

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81 **Figure S2.** Pie chart of the percentage of NNI, OPPs, and other pesticides in the study area.

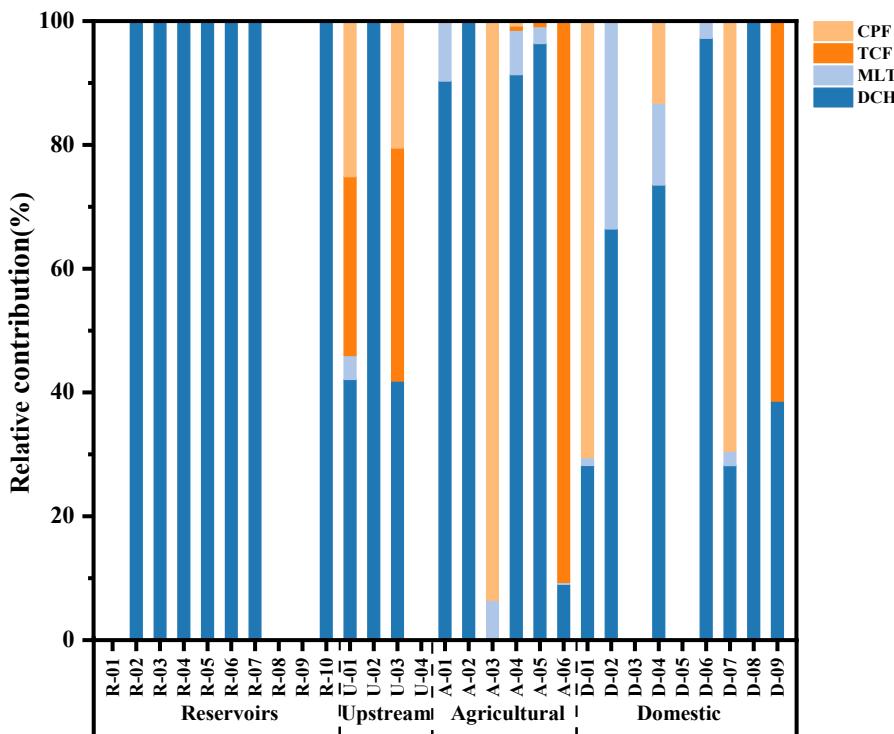


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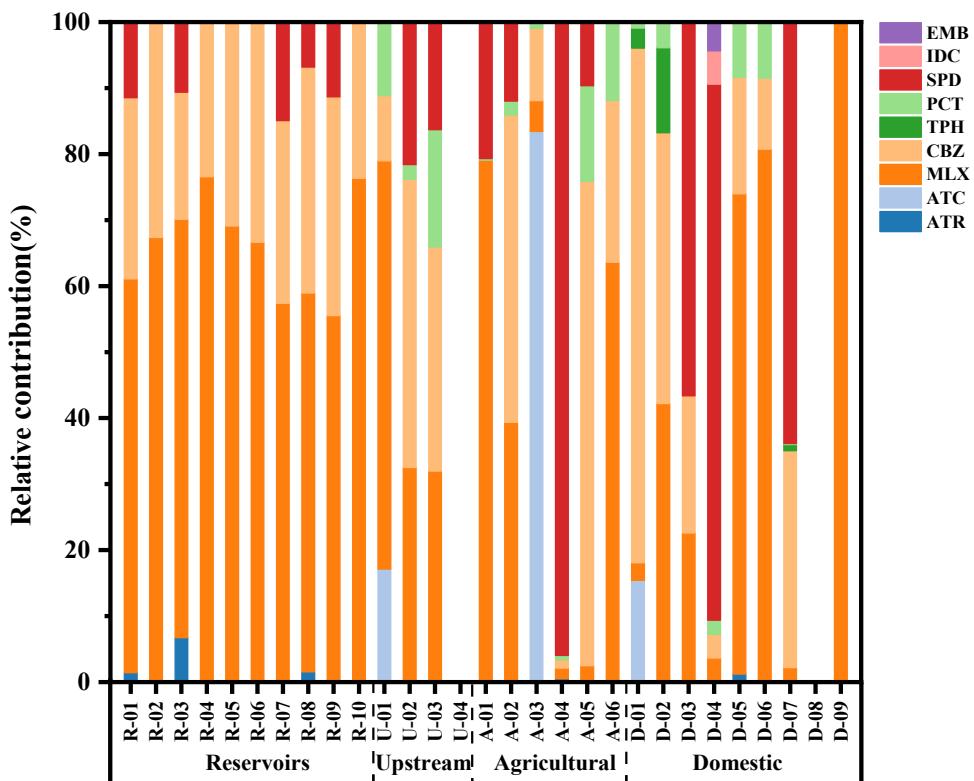
Figure S3. The relative contribution of NNIs at each sampling site.

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Figure S4. The relative contribution of OPPs at each sampling site.



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Figure S5. The relative contribution of Other Pesticides at each sampling site.

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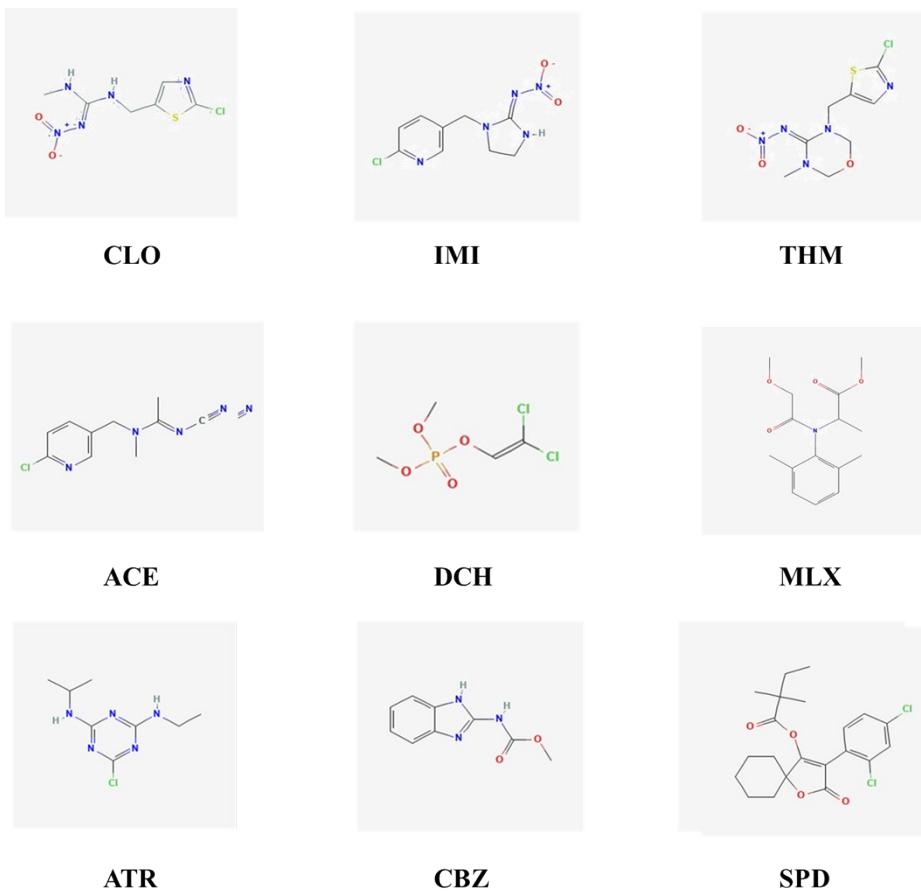
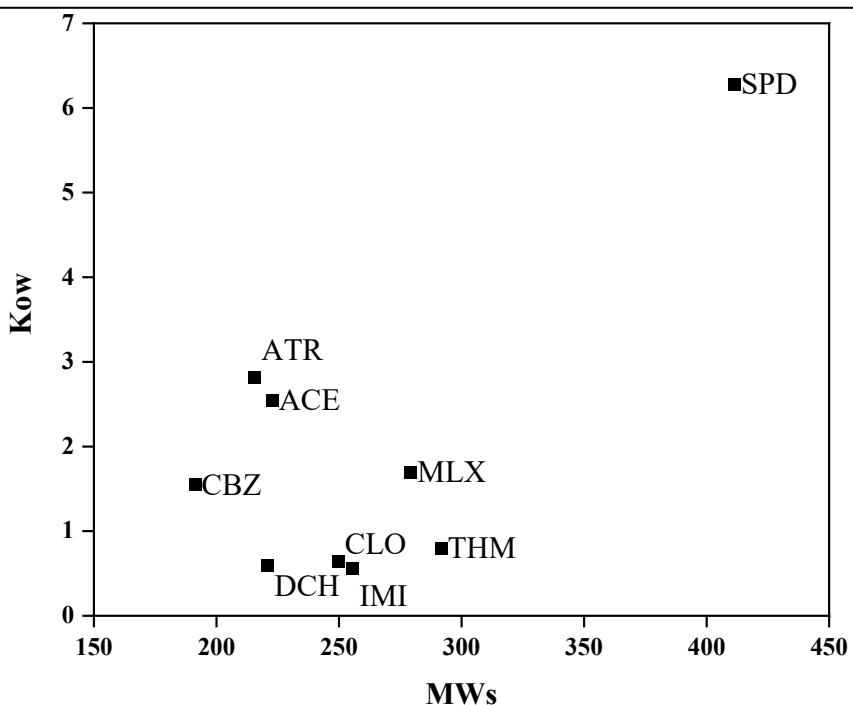


Fig.S6 Chemical Structure Depiction of the main detected pesticides in the study area.



93 **Fig.S7** Scatter plot of molecular weight (MWs) vs. Octanol-Water Partition Coefficient (K_{OW}).

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