

Supplementary Materials

Distribution of Heavy Metals and Organic Compounds: Contamination and Associated Risk Assessment in the Han River Watershed, South Korea

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Table S1. ICP-MS conditions

	Instrument parameters	Setting range for normal sensitivity	Setting range for CRI mode
Gas flow	Plasma flow(L/min)	18.0	18.0
	Auxiliary flow(L/min)	1.50	1.50
	Sheath gas flow(L/min)	0.16	0.16
	Nebulizer flow(L/min)	0.92	0.92
Sample introduction	RF power(kW)	1.40	1.40
	Sampling depth(mm)	6.5	6.5
	Pump rate (rpm)	5	5
	First extraction lens(volts)	-20	-20
Ion optics	Second extraction lens	-185	-185
	Third extraction lens	-220	-220
	Conner lens	-220	-220
	Mirror lens right	37	37
	Mirror lens left	40	40
	Mirror lens bottom	33	33
	Entrance lens	-3	-3
	Entrance plate	-30	-30
CRI gas	Fringe bias	-3.8	-3.8
	Pole bias	0.0	0.0
	Skimmer gas source	-	H ₂
	Skimmer gas flow	-	60

Table S2. Liquid chromatograph condition

Column	Hypersil GOLD C18(50mm)		
	Time	A%	B%
Pump 1	0.00	98	2
	1.00	98	2
	3.00	2	98
	7.00	2	98
	7.01	98	2
	10.00	98	2
	A:0.1% formic acid water B : acetonitrile		
Column	Hypersil GOLD aQ(20mm)		
	Time	A%	B%
Pump 2	0.00	98	2
	1.01	98	2
	1.20	98	2
	8.00	98	2
	10.00	98	2
	A:0.1% formic acid water B : acetonitrile		

* Column temperature: ambient; injection volume:1000 μL

Table S3. Method detection limit (MDL) for target compounds

Compounds	Spiked Conc. (ng/L)	Measured Conc. (ng/L)	Mean (ng/L) ± SD	Recovery (%)	MDL (μg/L)
Cr*	0.1	0.0095, 0.0990, 0.1003, 0.1059, 0.0987, 0.1047, 0.1161	0.1028±0.007	102.8	0.022
As*	0.3	0.2897, 0.2908, 0.3093, 0.3067, 0.3013, 0.2990, 0.2955	0.2989±0.007	99.6	0.024
Hg	0.5	0.3362, 0.3880, 0.4553, 0.4180, 0.3859, 0.4147, 0.4046	0.4004±0.037	80.1	0.115
Aldicab	10	10.3, 11.1, 9.1, 11.5, 9.1, 10.5, 9.6	10.18±0.96	101.8	0.0030
Methomyl	5	4.7, 3.9, 4.6, 4.5, 3.9, 5.2, 5.4	4.61±0.57	92.2	0.0018
Molinate	5	6.2, 5.2, 5.7, 5.4, 6.3, 6.0, 5.3	5.73±0.46	114.7	0.0015
MCPA	5	4.5, 3.7, 4.5, 4.7, 4.3, 4.4, 4.7	4.38±0.36	87.7	0.0011
Carbaryl	10	11.3, 12.2, 9.4, 11.2, 10.9, 11.1, 10.7	10.97±0.84	109.7	0.0027
2,4-D	5	5.6, 4.3, 5.6, 5.7, 5.1, 5.1, 5.8	5.32±0.53	106.4	0.0017
Carbofuran	5	5.7, 4.6, 5.7, 5.5, 5.6, 5.2, 5.7	5.44±0.39	108.9	0.0012
Bisphenol A	5	5.9, 4.6, 5.4, 4.8, 5.6, 5.1, 5.7	5.28±0.47	105.6	0.0015
Quinoline	10	9.1, 8.0, 9.2, 9.3, 9.8, 9.2, 10.2	9.26±0.69	92.6	0.0022

* Cr and As: μg/L

Table S4. Linearity of calibration and equation of target compounds

Compounds	Equation	Linearity(r^2)
Cr	$Y = 30378x + 47018$	0.9999
As	$Y = 3954.9x + 70.756$	1.0000
Hg	$Y = 1870.3x + 1309.2$	0.9990
Aldicab	$Y = 0.00202299x - 0.00983077$	0.9981
Methomyl	$Y = 0.0627686x - 0.120973$	0.9965
Molinate	$Y = 0.0748761x - 0.080387$	0.9986
MCPA	$Y = 0.0504372x - 0.00639455$	0.9995
Carbaryl	$Y = 0.00190959x - 0.00641905$	0.9989
2,4-D	$Y = 0.0351863x - 0.00134848$	0.9995
Carbofuran	$Y = 0.0606644x + 0.00748371$	0.9979
Bisphenol A	$Y = 0.0850283x + 0.681573$	0.9995
Quinoline	$Y = 0.0176491x + 0.0887547$	0.9979

Table S5. Aquatic toxicity data and PNEC values of target compounds on aquatic organisms

Compounds	Species	Test duration/endpoint	Parameter	Concentration ($\mu\text{g}/\text{L}$)	Reference	AF	PNEC ($\mu\text{g}/\text{L}$)
Cr	<i>O. mossambicus</i>	7 d/ abnormality	NOEC	400	Poongothai et al., 1996	10	40
As	<i>D. rerio</i>	24 h/ oxygen consumption	NOEC	500	Babich et al., 2020	50	10
Hg	<i>S. acutus var. acutus</i>	23 d/ biomass	NOEC	200	Butler et al., 2012	100	2
Molinate	<i>M. australiensis</i>	8d/ mortality	NOEC	110	Julli and Krassoi., 1995	10	11
Carbofuran	<i>P. promelas.</i>	33 d/ survival	NOEC	67.6	Call and Geiger, 2015	10	6.8
Bisphenol A	<i>P. promelas.</i>	164 h/ survival	NOEC	130	Mihaich et al., 2012	100	1.3
Quinoline	<i>C. riparius</i>	4d/ mortality	LC50	4896.7	Bleeker et al., 1998	1000	4.9