Factors Affecting Incurred Pesticide Extraction in Cereals

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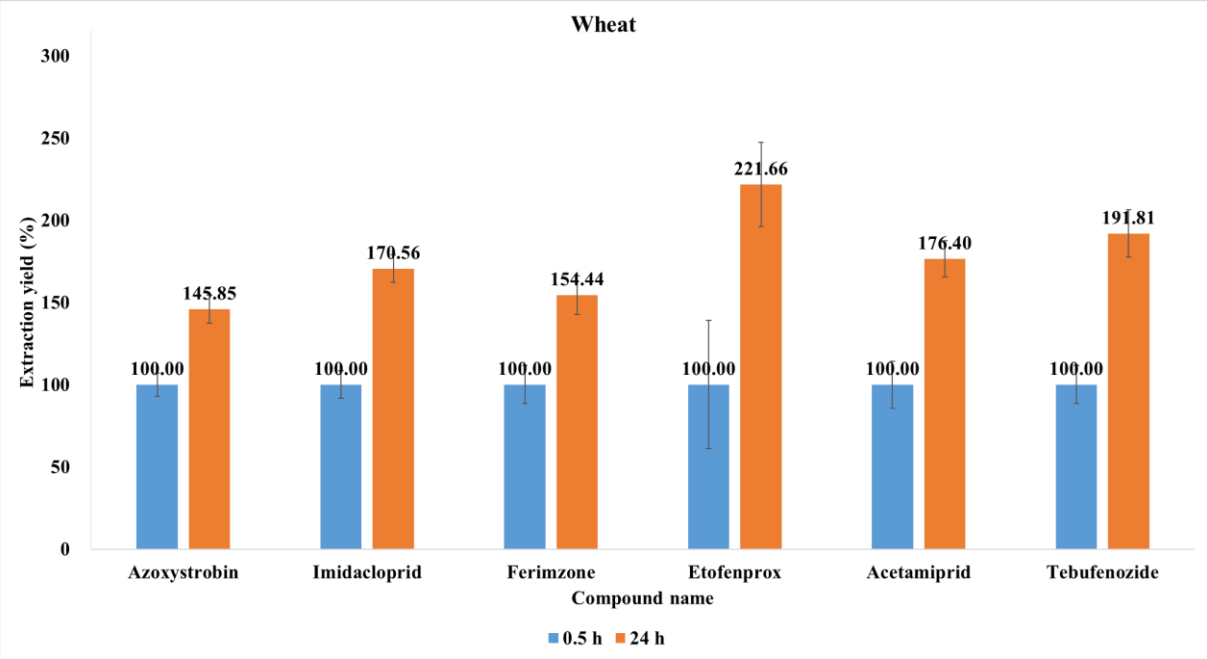

Figure S1. Immersion time optimization. The average extracted pesticide residues concentration at 0.5 h was set as the 100% extraction yield.

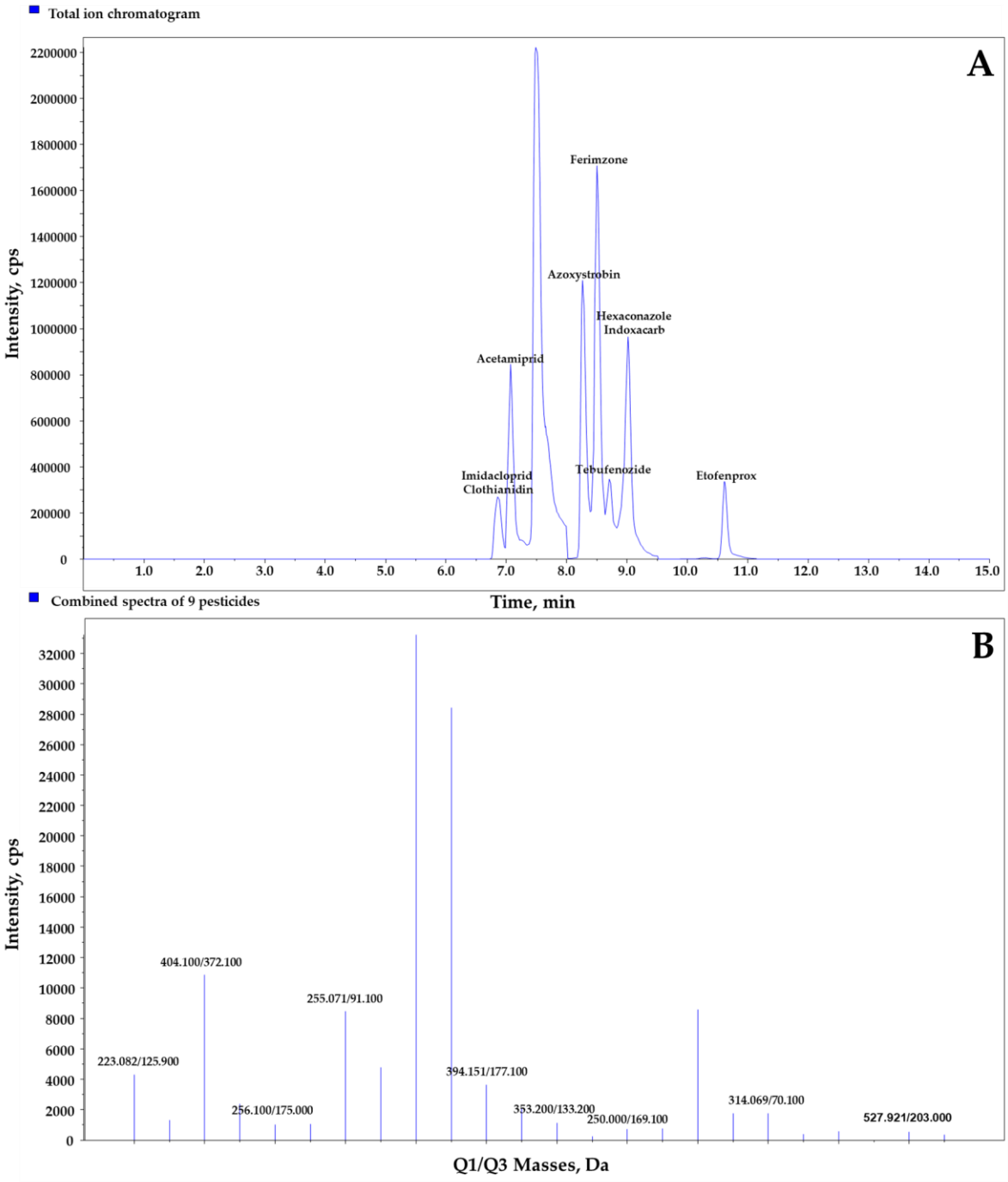

Figure S2. Total ion chromatogram (A) and combined spectra of 9 pesticides (B) at 50 ppb in rice.

Table S1. Method validation for rice, wheat, barley, and oat

Matrix	Compound	LOQ_{method} (ng/g)	R^2	Linear range (µg/kg)	10 ng/g		50 ng/g		Matrix effect (%)
					Recovery (%)	RSD (%)	Recovery (%)	RSD (%)	
Rice	Acetamiprid	10	0.997	1–50	97.31	0.41	115.93	0.53	-17.4
	Azoxystrobin		0.999		114.24	0.75	117.88	1.08	-20.4
	Imidacloprid		0.998		103.17	3.75	115.79	0.53	-16.6
	Ferimzone		0.993		88.46	3.14	117.44	2.21	-38.3
	Etofenprox		0.994		86.63	4.85	92.58	6.01	-35.5
	Tebufenozide		0.999		94.86	12.87	105.31	5.22	-20.5
	Clothianidin		0.998		103.58	1.05	117.14	0.20	-26.1
	Hexaconazole		0.998		99.55	4.53	116.98	0.29	-27.1
	Indoxacarb		0.992		90.33	3.01	107.96	0.81	-17.4
Wheat	Acetamiprid	10	0.999	1–50	98.63	0.87	112.59	4.68	-9.8
	Azoxystrobin		0.998		91.27	1.78	115.35	4.12	-13.6
	Imidacloprid		0.999		111.46	1.86	111.57	4.36	-8.0
	Ferimzone		0.999		81.28	3.75	117.66	3.22	-30.4
	Etofenprox		0.999		105.86	1.81	104.50	3.91	-25.2
	Tebufenozide		0.997		103.65	9.87	114.15	6.00	-12.1
	Clothianidin		0.999		102.77	0.44	108.60	3.04	-13.7
	Hexaconazole		0.999		95.27	11.20	106.96	5.21	-10.9
	Indoxacarb		0.999		102.92	1.06	115.39	3.31	-9.8
Barley	Acetamiprid	10	0.999	1–50	88.30	1.37	107.65	1.54	-1.1
	Azoxystrobin		0.997		82.10	2.18	116.18	1.77	-6.6
	Imidacloprid		0.999		92.11	4.32	105.45	3.44	-1.4
	Ferimzone		0.993		96.84	1.56	116.10	2.09	-31.2
	Etofenprox		0.999		116.82	2.12	104.54	4.61	-25.0
	Tebufenozide		0.997		84.06	0.90	117.73	4.50	-5.4
	Clothianidin		0.999		93.55	0.75	105.95	2.63	-19.7
	Hexaconazole		0.999		96.08	2.88	101.45	1.45	-7.1
	Indoxacarb		0.999		94.22	1.09	101.31	2.41	-1.1
Oat	Acetamiprid	10	0.999	1–50	97.10	0.86	106.90	1.11	-7.2
	Azoxystrobin		0.998		89.61	2.01	112.64	1.21	-6.8
	Imidacloprid		0.999		110.34	3.54	103.37	1.69	-0.8
	Ferimzone		0.993		101.09	0.41	114.27	1.06	-51.4
	Etofenprox		0.998		72.01	1.17	83.64	5.59	-30.2
	Tebufenozide		0.999		104.02	1.67	97.63	4.49	-9.6
	Clothianidin		0.999		101.64	2.83	100.54	1.66	-14.7
	Hexaconazole		0.999		106.53	3.52	94.27	2.39	-11.0
	Indoxacarb		0.999		110.39	1.29	111.82	1.00	-7.2

RSD: Relative Standard Deviation

Table S2. MRM conditions

Compound	Q1 Mass (Da)	Q3 Mass (Da)	Time (min)	DP (V)	EP (V)	CE (V)	CXP (V)
Acetamiprid	223.082	125.900	7.00	96	10	29	10
		90.100				43	8
Azoxystrobin	404.100	372.100	8.25	74	10	19	4
		344.100				27	4
Imidacloprid	256.100	175.000	6.80	89	10	25	4
		209.000				23	4
Ferimzone	255.071	91.100	8.50	121	10	45	8
		65.100				73	6
Etofenprox	394.151	177.100	10.64	61	10	21	18
		107.000				61	12
Tebufenozide	353.200	133.200	8.70	81	10	23	4
		296.900				15	4
Clothianidin	250.000	169.100	6.80	94	10	21	4
		132.000		71		35	4
Hexaconazole	314.069	70.100	8.90	106	10	25	6
		159.000				43	12
Indoxacarb	527.920	203.000	8.86	166	10	57	22
		149.900				33	18

DP: Declustering Potential

EP: Entrance Potential

CE: Collision Energy

CXP: Cell Exit Potential

Table S3. Average extracted pesticide residue concentrations by particle size

Crop	Pesticide	Extracted pesticide residue by cereal particle size (mg/kg, n = 3)				
		<10-mesh	10–20-mesh	20–40-mesh	40–60-mesh	> 60-mesh
Rice	Acetamiprid	14.0 e	29.6 d	50.6 c	89.9 b	131.8 a
	Azoxystrobin	14.1 d	16.6 d	45.6 c	133.3 b	246.9 a
	Imidacloprid	21.4 e	44.6 d	73.4 c	125.6 b	183.5 a
	Ferimzone	18.3 d	28.0 d	74.9 c	197.2 b	326.0 a
	Etofenprox	5.9 c	5.2 c	8.0 c	22.1 b	42.8 a
	Tebufenozide	5.6 c	6.2 c	18.6 c	61.8 b	138.8 a
	Clothianidin	1.6 e	2.3 d	3.6 c	5.1 b	7.1 a
	Hexaconazole	20.1 d	29.1 d	71.3 c	183.9 b	328.4 a
	Indoxacarb	10.5 d	11.1 d	38.7 c	153.9 b	318.6 a
Wheat	Acetamiprid	38.1 d	67.9 c	87.8 a	86.8 a	77.4 b
	Azoxystrobin	24.1 d	40.3 c	70.6 b	83.0 a	74.5 b
	Imidacloprid	44.1 d	77.3 c	100.6 a	99.0 a	89.8 b
	Ferimzone	47.2 c	88.1 b	106.5 a	109.8 a	86.4 b
	Etofenprox	19.6 d	22.3 d	42.5.c	61.6a	56.7 b
	Tebufenozide	35.2 e	45.8 d	69.6 c	101.6 a	81.3 b
	Clothianidin	7.4 c	12.9 b	14.7 b	18.2 a	14.2 b
	Hexaconazole	31.4 d	56.6 c	72.8 ab	76.3 a	61.5 bc
	Indoxacarb	47.8 e	60.7 d	92.9 c	131.4 a	117.2 b
Barley	Acetamiprid	41.4 e	56.6 d	99.6 c	116.5 b	116.5 a
	Azoxystrobin	24.6 e	32.6 d	109.7 c	175.3 b	192.8 a
	Imidacloprid	43.0 e	56.0 d	101.4 c	117.4 b	118.7 a
	Ferimzone	29.2 e	43.8 d	124.1 c	162.4 b	167.4 a
	Etofenprox	31.0 e	34.2 d	104.2 c	206.1 b	232.3 a
	Tebufenozide	45.8 e	48.8 d	154.0 c	289.7 b	309.2 a
	Clothianidin	5.4 e	7.4 d	13.1 c	14.3 b	14.4 a
	Hexaconazole	20.8 e	26.7 d	73.9 c	97.0 b	104.6 a
	Indoxacarb	43.2 e	49.9 d	181.3 c	346.3 b	394.1 a
Oat	Acetamiprid	22.9 c	59.6 a	62.7 a	58.3 ab	51.4 b
	Azoxystrobin	18.4 d	39.9 c	49.7 b	59.6 a	57.9 a
	Imidacloprid	28.6 c	69.5 a	73.5 a	69.4 a	59.6 b
	Ferimzone	19.0 c	68.6 ab	79.9 a	76.1 ab	66.5 b
	Etofenprox	16.6 c	20.9 bc	26.4 b	36.9 a	37.4 a
	Tebufenozide	17.6 d	24.3 cd	27.6 c	44.1 b	53.2 a
	Clothianidin	3.1 c	7.5 a	8.1 ab	7.4 ab	6.5 b
	Hexaconazole	12.1 d	37.8 c	48.2 a	46.6 ab	41.3 bc
	Indoxacarb	38.3 c	46.9 c	66.1 b	89.7 a	93.8 a

Notes: Same lowercase letters across a row indicate no significant differences among residue concentrations of same pesticide ($p < 0.05$). Extraction efficiency: a > b > c > d > e