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Dissipation and sorption-desorption of benziothiazolinone in agricultural soils and identification of its metabolites

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Tables

Table S1 Linear regression parameters of calibration curves and the matrix effect of benziothiazolinone in different matrices.

matrices	regression equation	R^2	ME (%)	LOD (mg/kg or mg/L)	LOQ (mg/kg or mg/L)
methanol	y = 1000000x + 238916	0.9977	—	—	—
water	y = 10 00000 x + 260705	0.9970	0	0.006	0.02
soil #1	y = 568966x + 87805	0.9988	-43.1	0.06	0.2
soil #2	y = 570007x + 104490	0.9972	-43.0	0.06	0.2
soil #3	y = 587573x + 86030	0.9988	-41.2	0.06	0.2
soil #4	y = 574896x + 65033	0.9989	-42.5	0.06	0.2
soil #5	y = 576898x + 88778	0.9987	-42.3	0.06	0.2

ME means matrix effect; LOD and LOQ represent the limits of detection and quantitation for the developed method, respectively.

Table S2 Recoveries and RSDs for benziothiazolinone in five soils.

matrices	spiked levels (mg/kg or mg/L)	recovery (%)					mean recovery (%)	RSD (%)
		1	2	3	4	5		
soil #1	0.2	88.14	80.79	80.23	78.53	85.31	82.60	4.82
	2	80.91	82.05	78.06	76.92	83.76	80.34	3.51
	10	75.54	73.78	74.19	74.05	74.46	74.40	0.92
soil #2	0.2	77.73	78.52	88.28	90.23	93.36	85.62	8.28
	2	97.48	89.94	94.97	97.48	99.37	95.84	3.81
	10	98.66	98.35	100.93	97.32	96.39	98.33	1.74
soil #3	0.2	100.65	97.17	93.68	94.12	99.78	97.08	3.27
	2	93.30	85.47	90.50	83.24	91.62	88.82	4.81
	10	101.44	98.56	101.24	96.80	101.24	99.85	2.09
soil #4	0.2	92.74	96.09	101.12	94.53	100.56	97.01	3.81
	2	98.22	102.96	101.78	106.51	108.88	103.67	4.01
	10	86.17	89.83	87.05	89.32	91.22	88.72	2.33
soil #5	0.2	96.56	103.09	98.63	102.41	104.12	100.96	3.19
	2	91.39	106.37	104.12	101.12	102.25	101.05	5.70
	10	95.37	101.68	103.71	99.85	100.56	100.23	3.08
water	0.02	101.93	101.40	106.98	103.00	100.31	102.72	2.50
	0.2	100.35	99.30	101.40	101.93	103.50	101.30	1.57
	2	105.28	104.15	98.49	100.75	103.58	102.45	2.71
	10	102.73	100.98	99.37	100.85	94.27	99.64	3.24

RSD means relative standard deviation.

Table S3 Sorption kinetics parameters of pseudo-first-order and pseudo-second-order models.

soils	$C_{s,exp}$ (mg/kg)	pseudo-first-order			pseudo-second-order		
		R^2	K_1 (min^{-1})	$C_{s,cal}$ (mg/kg)	R^2	K_2 (kg/(mg·min))	$C_{s,cal}$ (mg/kg)
#1	41.04	0.7752	8.06×10^{-3}	3.74	1	2.43×10^{-2}	41.15
#2	29.16	0.9449	3.22×10^{-3}	20.44	0.9865	3.10×10^{-2}	32.26
#3	25.83	0.9445	4.84×10^{-3}	19.36	0.6700	2.92×10^{-2}	34.25
#4	21.66	0.9609	8.52×10^{-3}	16.90	0.9039	4.01×10^{-2}	24.94
#5	19.92	0.8724	4.61×10^{-3}	10.94	0.1871	2.76×10^{-2}	36.23

$C_{s,exp}$ means the concentration (mg/kg) of BIT absorbed to the soils at the equilibrium state and is obtained from experiment; $C_{s,cal}$ is calculated using pseudo-first-order and pseudo-second-order models.

Table S4 Parameters of the intraparticle diffusion model.

Soil	First linear region			Second linear region			Third linear region		
	K_{p1}	C_1	R^2	K_{p2}	C_2	R^2	K_{p3}	C_3	R^2
#1	2.29	20.45	1	0.36	35.27	0.985	0.01	40.81	0.5973
#2	5.10	-24.59	1	0.69	9.54	0.9545	0.21	21.16	0.9940
#3	3.20	-14.99	0.9291	0.26	16.01	0.9751	0.10	22.16	0.8722
#4	5.76	-30.12	1	0.55	10.56	0.9817	0.03	20.58	0.4233
#5	6.08	-32.94	1	0.24	12.92	0.7788	0.09	16.81	0.7491

Figures

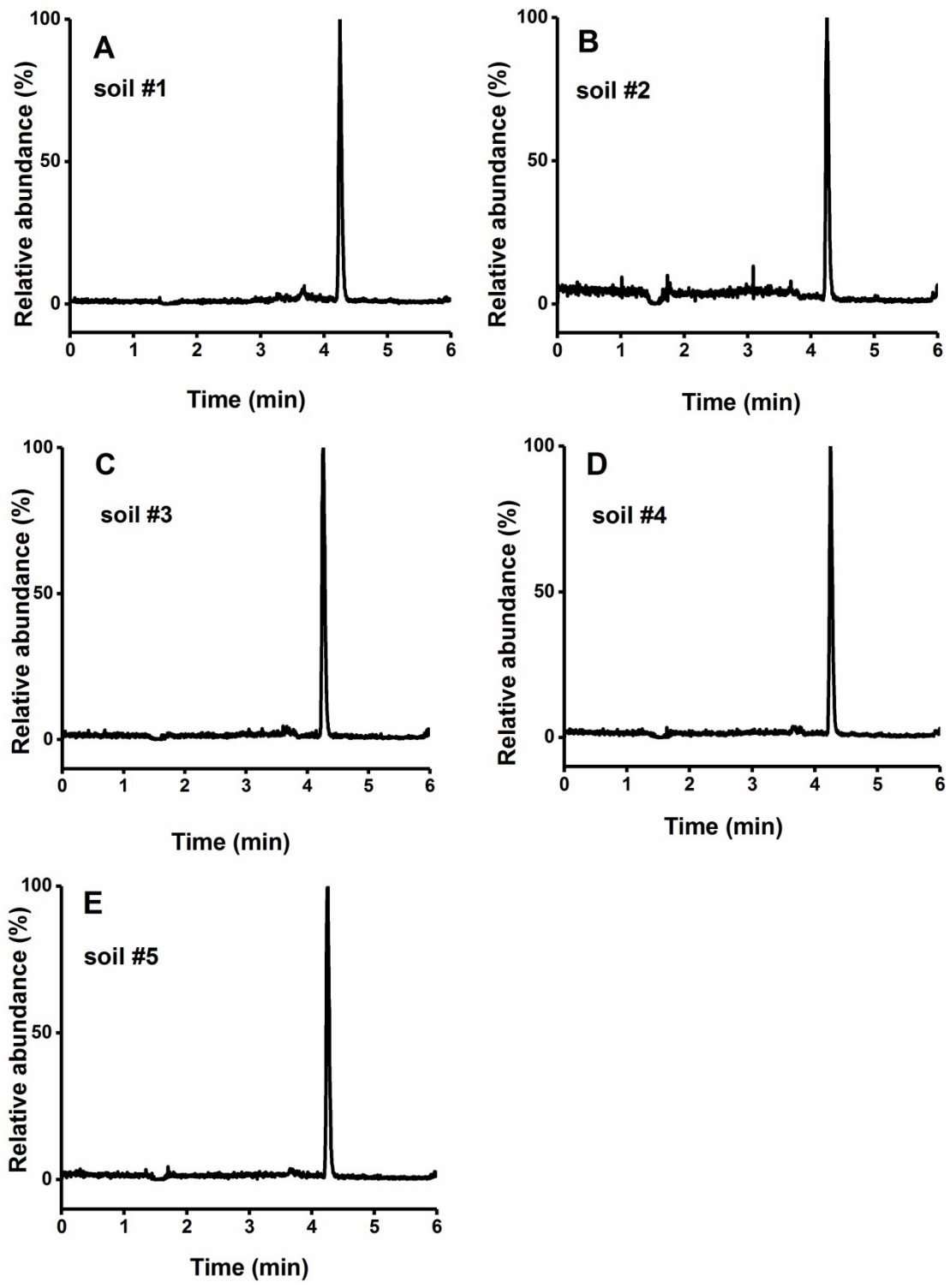

Fig. S1 Representative chromatogram of benziothiazolinone in five soils: matrix-matched standard solution (2 mg/kg) for (A) soil #1, (B) soil #2, (C) soil #3, (D) soil #4, (E) soil #5.

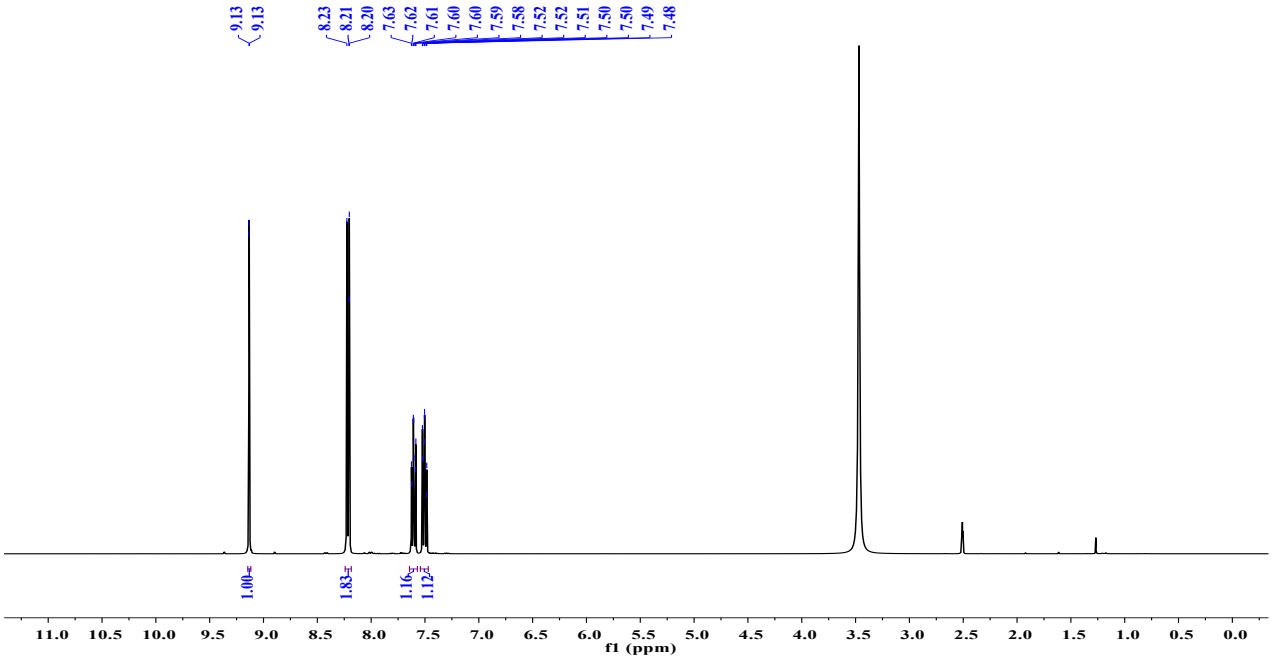

Fig. S2 The ^{1}H NMR spectrum of TP 2 in DMSO-*d6* at 400 MHz.

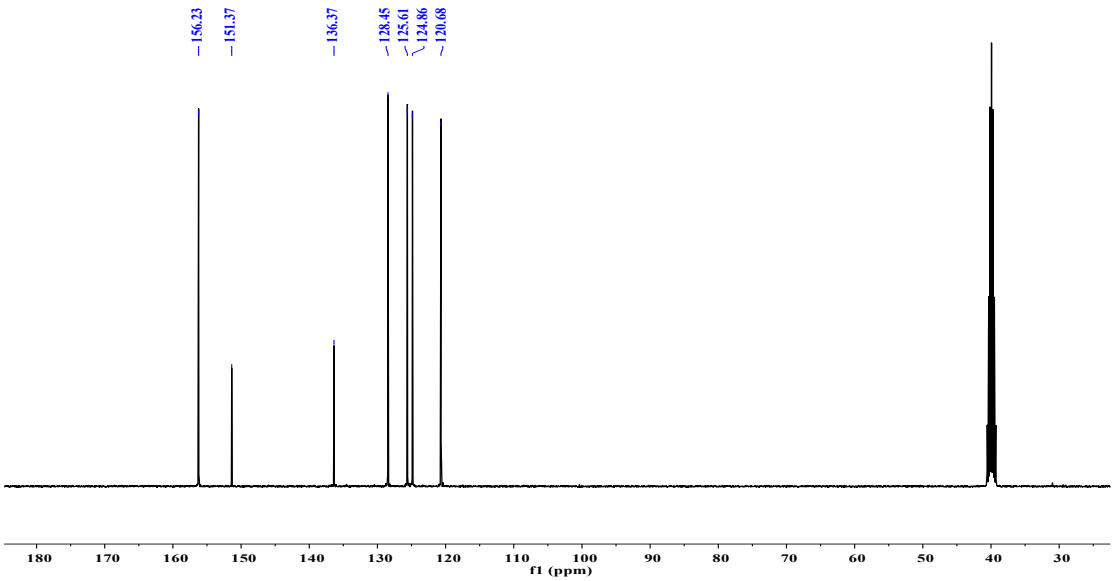

Fig. S3 The ^{13}C NMR spectrum of TP 2 in DMSO-*d6* at 101 MHz.

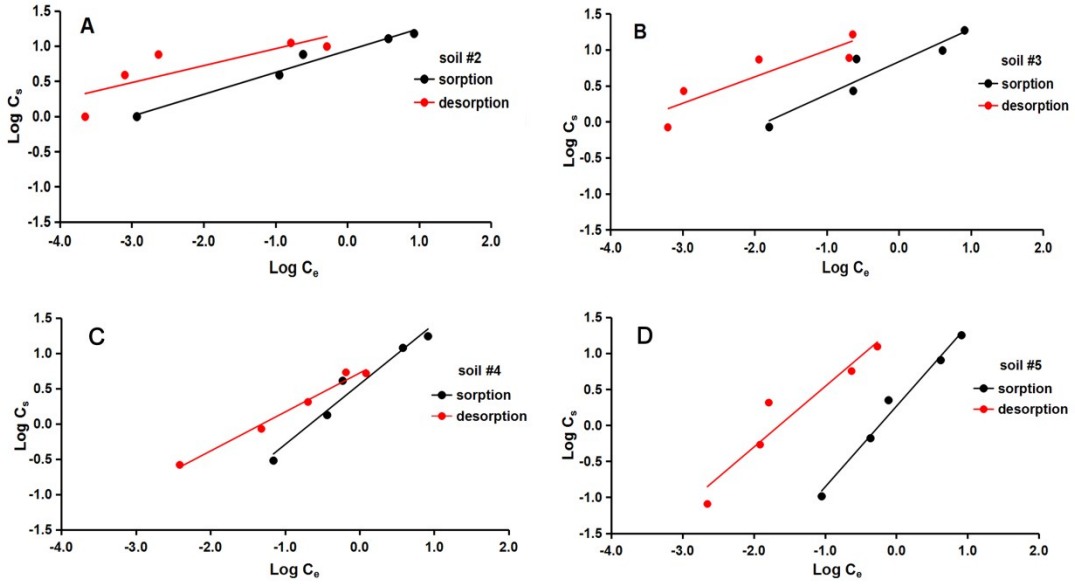

Fig. S4 Freundlich sorption-desorption isotherms of benziothiazolinone: (A) in soil #2, (B) in soil #3, (C) in soil #4, (D) in soil #5.