

Supporting Information

Chiral Pyrethroid Insecticide Fenpropathrin and its Metabolite: Enantiomeric Separation and Pharmacokinetic Degradation in Soils by Reverse-Phase High-Performance Liquid Chromatography

Ping Zhang^a, Qian Yu^a, Yuhan He^a, Wentao Zhu^b, Zhiqiang Zhou^b and Lin He ^{*a}

^a College of Plant Protection, Southwest University, Chongqing, China.

^b Beijing Advanced Innovation Center for Food Nutrition and Human Health, Department of Applied Chemistry, China Agricultural University, Beijing, China.

Page 2: Table S1 Enantiomeric separation results of fenpropathrin on three chiral columns used methanol/water or ACN/water as mobile phase

Page 3: Table S2 Effects of temperature on fenpropathrin separation with three types of chiral columns.

Page 4: Table S3 Experiment design and kinetic data for degradations of fenpropathrin and its metabolites 3-PBA in soils.

Page 5: Figure S1 Chromatograms for chiral resolutions on Lux Cellulose-1(methanol-water, A 95/5, B 90/10, C 85/15, D 80/20), Lux Cellulose-3(methanol-water, E 100/0, F 95/5, G 90/10, H 85/15) and Chiralpak IC(acetonitrile-water, I 65/35, J 60/40, K 55/45, L 50/50).

Table S1 Enantiomeric separation results of fenpropathrin on three chiral columns used methanol/water or ACN/water as mobile phase

Column	Mobile phase	Ratio (v/v)	k ₁	k ₂	α	R _s
Lux Cellulose-1	Methanol /H ₂ O	100/0	0.53	0.53	1.00	-
		95/5	1.24	1.33	1.07	0.61
		90/10	2.86	3.08	1.08	0.77
		85/15	6.93	7.50	1.08	0.87
		80/20	15.83	17.12	1.08	1.01
	ACN/H ₂ O	90/10	0.38	0.38	1.00	-
		80/20	1.36	1.36	1.00	-
		70/30	3.56	3.56	1.00	-
		60/40	10.09	10.09	1.00	-
Lux Cellulose-3	Methanol /H ₂ O	100/0	0.55	0.69	1.27	1.39
		95/5	1.34	1.68	1.26	1.72
		90/10	3.57	4.49	1.26	1.91
		85/15	7.61	9.52	1.25	2.30
	ACN/H ₂ O	75/25	1.05	1.10	1.05	0.62
		70/30	1.64	1.72	1.05	0.70
		65/35	2.66	2.80	1.05	0.78
		60/40	4.58	4.82	1.05	0.82
		55/45	8.21	8.65	1.05	0.87
		50/50	14.57	15.37	1.05	1.06
Chiralpak IC	Methanol /H ₂ O	100/0	0.26	0.26	1.00	-
		90/10	0.72	0.72	1.00	-
		80/20	3.27	3.27	1.00	-
		70/30	5.28	5.28	1.00	-
	ACN/H ₂ O	65/35	2.15	2.20	1.03	0.34
		60/40	3.65	3.76	1.03	0.47
		55/45	6.57	6.77	1.03	0.51
		50/50	11.74	12.13	1.03	0.64

Table S2 Effects of temperature on fenpropathrin separation with three types of chiral columns.

Column	Mobile phase (v/v)	Temperature (°C)	k ₁	k ₂	α	R _s
Lux Cellulose-1	Methanol/H ₂ O (85/15)	5	8.63	9.62	1.12	1.19
		10	7.44	8.18	1.10	1.14
		15	6.93	7.50	1.08	0.87
		20	5.95	6.38	1.07	0.82
		25	5.15	5.44	1.06	0.70
		30	4.56	4.77	1.05	0.59
		35	4.00	4.15	1.04	0.46
		40	3.49	3.58	1.03	0.36
Lux Cellulose-3	Methanol /H ₂ O (90/10)	5	6.16	7.70	1.25	1.53
		10	5.36	6.70	1.25	1.63
		15	4.51	5.66	1.25	1.76
		20	3.57	4.49	1.26	1.86
		25	3.22	4.05	1.26	1.91
		30	2.70	3.39	1.26	1.94
		35	2.29	2.87	1.26	2.17
		40	1.94	2.43	1.25	2.29
Lux Cellulose-3	ACN/H ₂ O (60/40)	5	4.09	4.37	1.07	0.92
		10	4.87	5.19	1.07	0.91
		15	4.82	5.11	1.06	0.86
		20	4.58	4.82	1.05	0.82
		25	4.45	4.65	1.05	0.70
		30	4.26	4.42	1.04	0.66
		35	4.04	4.16	1.03	0.62
		40	3.82	3.90	1.02	0.44
CHIRALPAK IC	ACN/H ₂ O (55/45)	10	5.88	6.08	1.03	0.57
		15	5.78	5.97	1.03	0.58
		20	5.45	5.61	1.03	0.57
		25	5.37	5.53	1.03	0.55
		30	5.22	5.37	1.03	0.53
		35	5.04	5.18	1.03	0.52
		40	4.84	4.96	1.03	0.49

Table S3 Experiment design and kinetic data for degradations of fenpropathrin and its metabolites 3-PBA in soils.

Experiment	Spiked compound	Soil type	Detected compound	$k \times 100$ (day ⁻¹)	$t_{1/2}$ (day)	R^2
E1	Rac- fenpropathrin	Non-sterilized soil	S-fenpropathrin	3.9	17.8	0.867
			R-fenpropathrin	5.5	12.6	0.917
E2	Rac- fenpropathrin	Sterilized soil	S-fenpropathrin	/	/	/
			R-fenpropathrin	/	/	/
E3	Rac- fenpropathrin	Artificial soil	S-fenpropathrin	/	/	/
			R-fenpropathrin	/	/	/
E4	3-PBA	Non-sterilized soil	3-PBA	17.2	4.0	0.924
E5	3-PBA	Sterilized soil	3-PBA	/	/	/
E6	3-PBA	Artificial soil	3-PBA	/	/	/

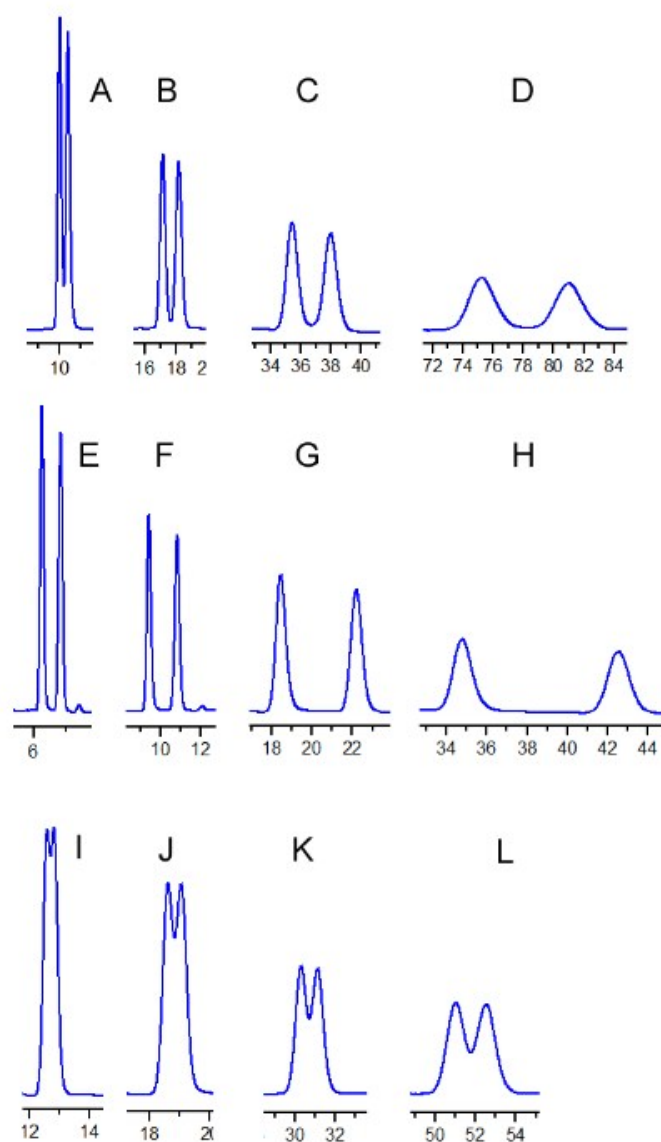


Figure S1 Chromatograms for chiral resolutions on Lux Cellulose-1(methanol-water, A 95/5, B 90/10, C 85/15, D 80/20), Lux Cellulose-3(methanol-water, E 100/0, F 95/5, G 90/10, H 85/15) and Chiralpak IC(acetonitrile-water, I 65/35, J 60/40, K 55/45, L 50/50).