

Supporting Information

Enantioseparation of Imazalil and Monitoring of Its Enantioselective Degradation in Apples and Soil using Ultra-high Performance Liquid Chromatography/Tandem Mass Spectrometry

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Sample Extraction and Purification

To minimize extraction interferences and to obtain better recoveries from the crude samples, six kinds of sorbents or sorbents mixtures (50 mg PSA, 50 mg C18, 50 mg Florisil, 50 mg PSA + 10 mg GCB, 50 mg C18 + 10 mg GCB, and 50 mg Florisil + 10 mg GCB) were tested at the spiking level of 200 µg/kg (*rac*-imazalil). PSA is applied to extract polar components such as fatty acids from non-polar samples whereas C18 is suitable for removing non-polar co-extractives from polar samples. Florisil is used for removing lipids and has a weak adsorption capacity for pigment. GCB is important for removal of visible pigments. The recoveries of imazalil enantiomers in apple and soil matrices were influenced by different sorbents, as showed in Figure S1. The 50 mg PSA showed the best purification and recoveries (range from 91.7% to 97.9%) for imazalil enantiomers in apples and soil. The recoveries for imazalil in apples were slightly reduced using GCB in sorbent mixtures since imazalil may be slightly retained by GCB.

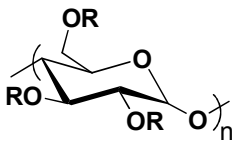
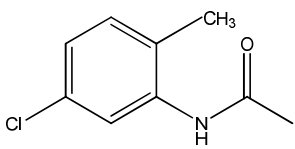
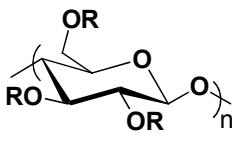
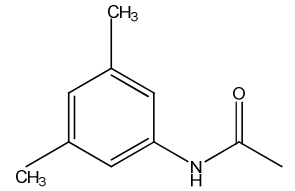
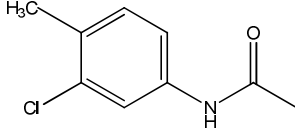
Table S1. Effect of ratios of ACN/water on chiral separation of imazalil enantiomers.

ACN/water (v/v) ^a	k ₁ ' ^b	k ₂ ' ^c	α	Rs
100:0	-	-	-	-
95:5	1.22	1.46	1.20	1.08
90:10	0.99	1.19	1.21	1.08
85:15	1.05	1.23	1.17	1.11
80:20	1.22	1.43	1.18	1.22
75:25	1.47	1.71	1.16	1.31
70:30	1.81	2.13	1.17	1.59
65:35	2.30	2.70	1.17	1.73
60:40	3.00	3.46	1.15	1.65

^a the mobile phase : ACN/water (v/v), flow rate : 0.5 mL/min, column temperature : 20°C.

^b k₁' was retention factor of first eluted -(S)-(+)-imazalil. ^c k₂' was retention factor of second eluted (R)-(-)-imazalil.

Table S2. Chemical structures of three polysaccharide based CSPs.

backbones	the name of the columns	side chains
 <p>Amylose-base column</p>	<p>LuxTM AMY lose-2 amylose <i>tris</i>-(5-chloro-2-methylphenylcarbamate)</p>	
 <p>Cellulose-based columns</p>	<p>Lux Cellulose-1 cellulose <i>tris</i>-(3,5-dimethylphenylcarbamate)</p> <p>Lux Cellulose-2 cellulose <i>tris</i>-(3-chloro-4-methylphenylcarbamate)</p>	 

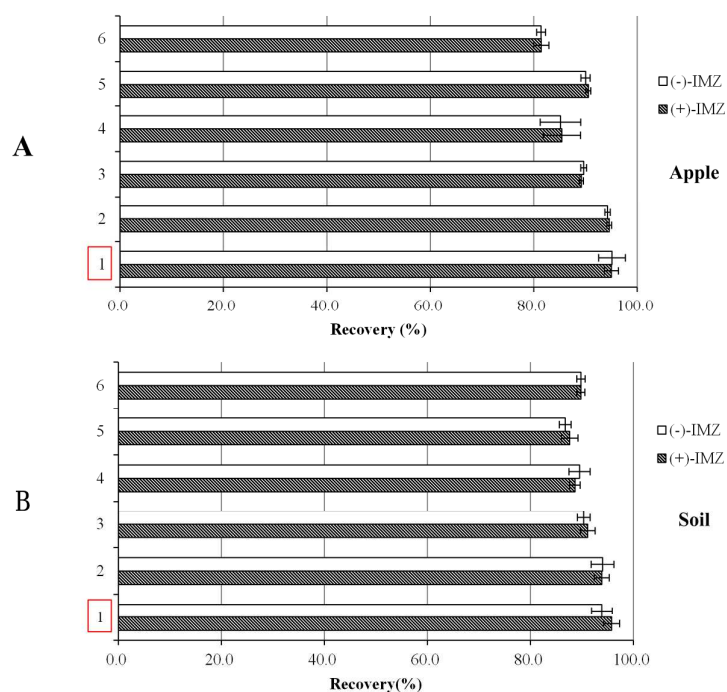


Figure S1. Effect of different sorbents (1: 50 mg PSA, 2: 50mgPSA+10 mg GCB, 3:50 mg C18, 4: 50 mg C18+10 mg GCB, 5: 50 mg Florisil, 6: 50 mg Florisil+10 mg GCB) on recoveries of imazalil enantiomers in different matrices (A: soil, B: apple) at 200 µg/kg.

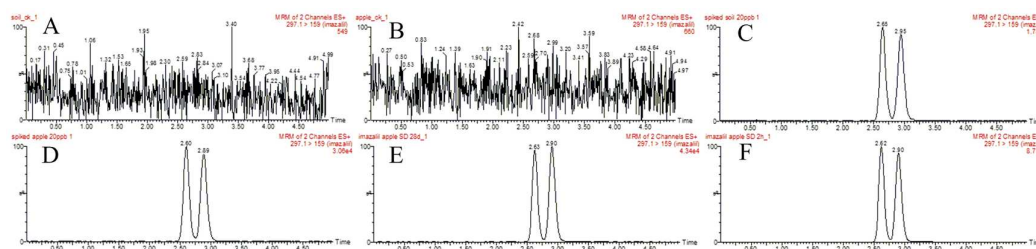


Figure S2. Typical UPLC-MS/MS (MRM) chromatograms of imazalil enantiomers (A: bank soil sample, B: blank apple sample, C: spiked soil sample-20 µg/kg, D: spiked apple sample-20 µg/kg, E: apple sample in Shandong-28 d after treatment, F: apple sample in Shandong-2 h after treatment.

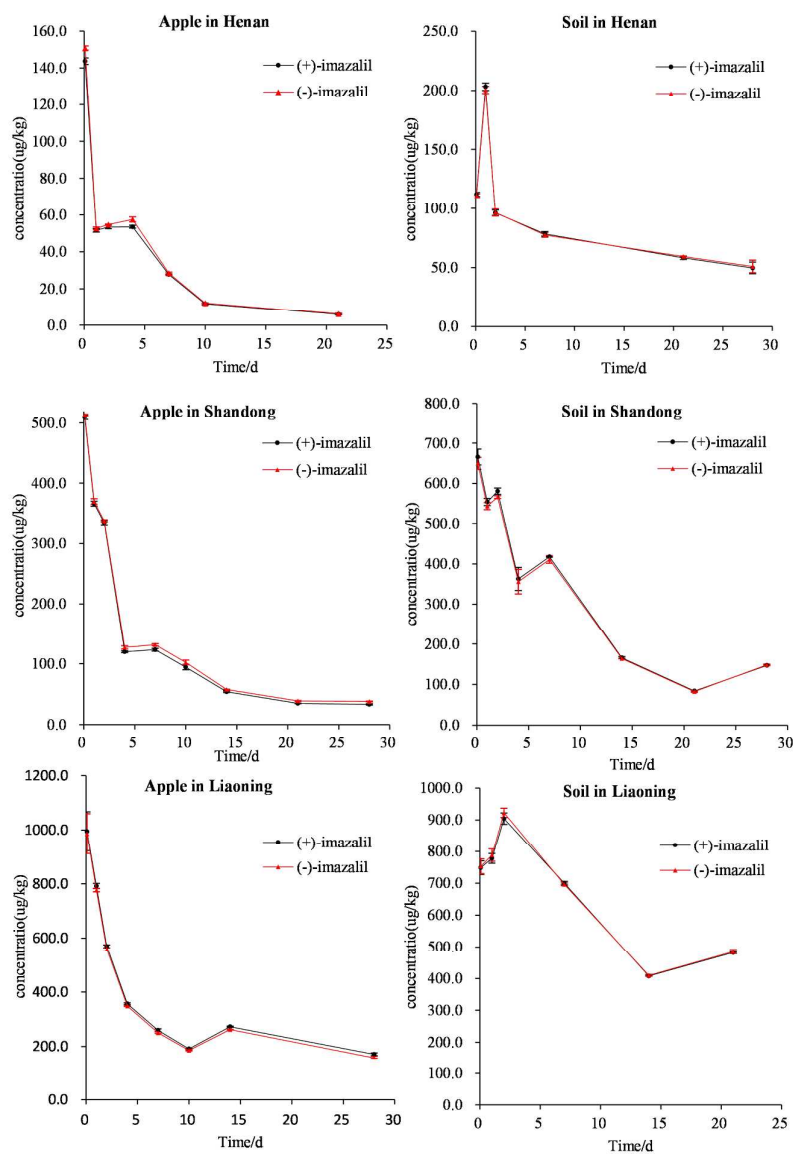


Figure S3. Concentration versus time plots of imazalil enantiomers in apple and soil in three provinces.