Supplementary Information

Ion mobility spectrometry coupled with chemometrics for the rapid identification of six pesticide residues in rice samples

Pan Meng[a,b], Peng Li[c], Dairong Ding[a,b], Yuqi Gong[a,b], Xinyi Guo[a,b] and Min Sha[a,b]*

[a] School of Management Science and Engineering, Nanjing University of Finance and Economics, Nanjing 210023, China;

[b] Key Laboratory of Food Processing and Quality Control, Nanjing University of Finance and Economics, Nanjing 210023, China;

[c] School of Food Science and Engineering, Nanjing University of Finance and Economics, Nanjing 210023, China.

E-mail for the *corresponding author: minsha@nufe.edu.cn (M.S.)

Table S1. Numbers and corresponding concentrations of the solvent standard solutions for isoprothiolane (A) and propanil (B).

Solution Number for Isoprothiolane (A)	Solution Number for Propanil (B)	Concentration (mg/L)
M_1	M_2	0.0488
L_1	L_2	0.0977
K_1	K_2	0.1953
J_1	J_2	0.3906
I_1	I_2	0.7813
H_1	H_2	1.5625
G_1	G_2	3.125
F_1	F_2	6.25
E_1	E_2	12.5
D_1	D_2	25
C_1	C_2	50
B_1	B_2	100
A_1	A_2	1000

Table S2. Preparation details of the mixed spiked solutions of isoprothiolane (A) and propanil (B).

Set	No.	Minitab taguchi design level		Concentration level (mg/L)		Volume of each solution		
		A	B	A	B	Solvent standard solution for A	Solvent standard solution for B	Solvent
Training set	1	1	1	0.391	0.391	0.5 mL G_1	0.5 mL G_2	3 mL
	2	1	2	0.391	0.781	0.5 mL G_1	0.5 mL F_2	3 mL
	3	1	3	0.391	1.563	0.5 mL G_1	0.5 mL E_2	3 mL
	4	1	4	0.391	3.125	0.5 mL G_1	0.5 mL D_2	3 mL
	5	2	1	0.781	0.391	0.5 mL F_1	0.5 mL G_2	3 mL
	6	2	2	0.781	0.781	0.5 mL F_1	0.5 mL F_2	3 mL
	7	2	3	0.781	1.563	0.5 mL F_1	0.5 mL E_2	3 mL
	8	2	4	0.781	3.125	0.5 mL F_1	0.5 mL D_2	3 mL
	9	3	1	1.563	0.391	0.5 mL E_1	0.5 mL G_2	3 mL
	10	3	2	1.563	0.781	0.5 mL E_1	0.5 mL F_2	3 mL
	11	3	3	1.563	1.563	0.5 mL E_1	0.5 mL E_2	3 mL
	12	3	4	1.563	3.125	0.5 mL E_1	0.5 mL D_2	3 mL
	13	4	1	3.125	0.391	0.5 mL D_1	0.5 mL G_2	3 mL
	14	4	2	3.125	0.781	0.5 mL D_1	0.5 mL F_2	3 mL
	15	4	3	3.125	1.563	0.5 mL D_1	0.5 mL E_2	3 mL
	16	4	4	3.125	3.125	0.5 mL D_1	0.5 mL D_2	3 mL
Validation set	17	1	2	0.5	1	0.32 mL F_1	0.32 mL F_2	3.36 mL
	18	1	3	0.5	1.5	0.32 mL F_1	0.64 mL F_2	3.04 mL
	19	2	2	1	1	0.64 mL F_1	0.32 mL F_2	3.04 mL
	20	2	3	1	1.5	0.64 mL F_1	0.64 mL F_2	2.72 mL
	21	3	2	1.5	1	0.24 mL D_1	0.16 mL E_2	3.6 mL
	22	3	3	1.5	1.5	0.24 mL D_1	0.32 mL E_2	3.44 mL
	23	4	2	2	1	0.32 mL D_1	0.16 mL E_2	3.52 mL
	24	4	3	2	1.5	0.32 mL D_1	0.32 mL E_2	3.36 mL

Table S3. Peak intensity values corresponding to different concentrations of carbendazim standard solutions at 9.927 ms.

Concentration (mg/L)	Peak Intensity Value
0.04883	1.195797
0.09766	1.786731
0.19531	2.659581
0.39063	4.976288
0.78125	7.53898
1.5625	10.41300244
3.125	10.81165471
6.25	10.81190267

Table S4. Peak intensity values corresponding to different concentrations of flutolanil standard solutions at 14.079 ms.

Concentration (mg/L)	Peak Intensity Value
0.1953125	1.62915394
0.390625	1.73781459
0.78125	1.98169018
1.5625	2.51557757
3.125	5.30126309
6.25	10.41300244
12.5	10.81165471
25	10.81190267

Table S5. Peak intensity values corresponding to different concentrations of pirimiphos-methyl standard solutions at 12.836 ms.

Concentration (mg/L)	Peak Intensity Value
0.0488	1.54457961
0.0977	1.79743223
0.1953	2.04262666
0.390625	3.02739687
0.78125	3.88944724
1.5625	5.05762937
3.125	7.33010082
6.25	9.0291605
12.5	9.80669851

Table S6. Peak intensity values corresponding to different concentrations of carbendazim matrix standard solutions at 9.914 ms.

Concentration (mg/L)	Peak Intensity Value
0.0488	0.4016378
0.09766	0.49517052
0.1953125	0.65965523
0.390625	0.90353857
0.78125	1.41689547
1.5625	2.59273858
3.125	3.32604957
6.25	4.62136822
12.5	6.66956139
25	9.95048676

Table S7. Peak intensity values corresponding to different concentrations of flutolanil matrix standard solutions at 14.079 ms.

Concentration (mg/L)	Peak Intensity Value
0.1953	1.21132021
0.3906	1.44815384
0.78125	1.22270755
1.5625	1.30998145
3.125	1.60265458
6.25	2.43126898
12.5	3.33163866
25	4.38325307
50	5.35753183

Table S8. Peak intensity values corresponding to different concentrations of pirimiphos-methyl matrix standard solutions at 12.836 ms.

Concentration (mg/L)	Peak Intensity Value
0.1953	1.04895086
0.3906	1.04986304
0.78125	1.24496818
1.5625	1.49466177
3.125	2.02364126
6.25	2.89871514
12.5	3.83053813
25	5.98262897
50	8.05755048

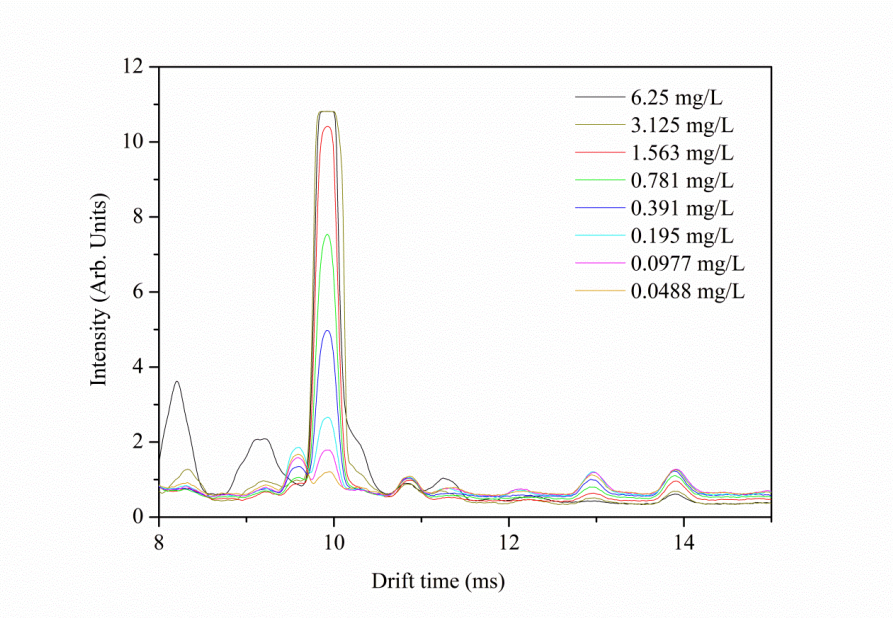

Fig. S1. Ion mobility spectra of carbendazim standard solutions at different concentrations.

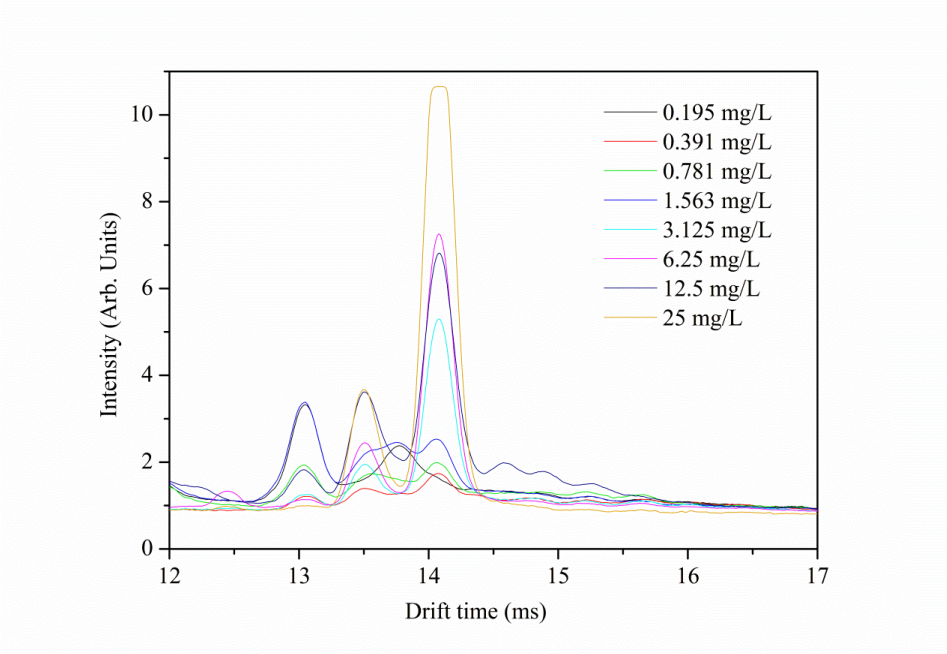

Fig. S2. Ion mobility spectra of flutolanil standard solutions at different concentrations.

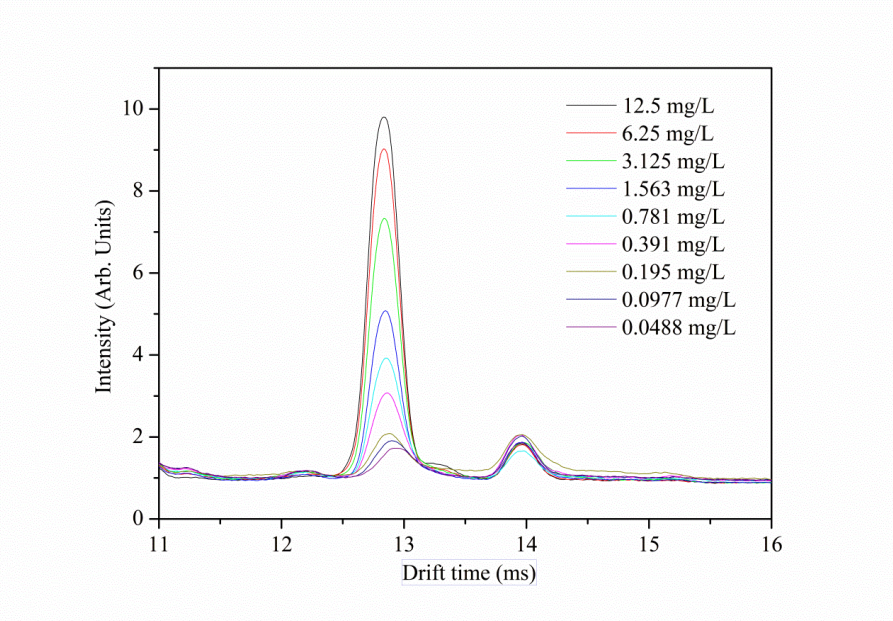

Fig. S3. Ion mobility spectra of pirimiphos-methyl standard solutions at different concentrations.

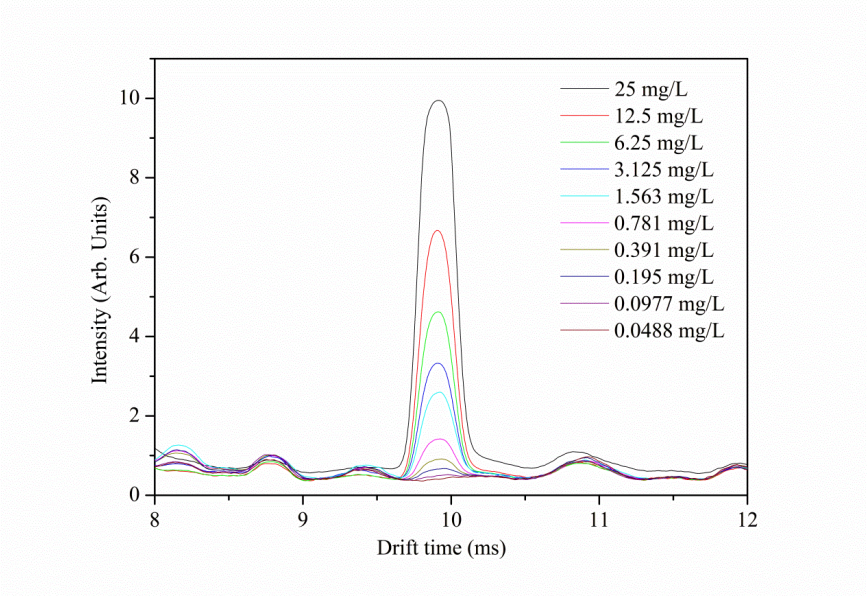

Fig. S4. Ion mobility spectra of carbendazim matrix standard solutions at different concentrations.

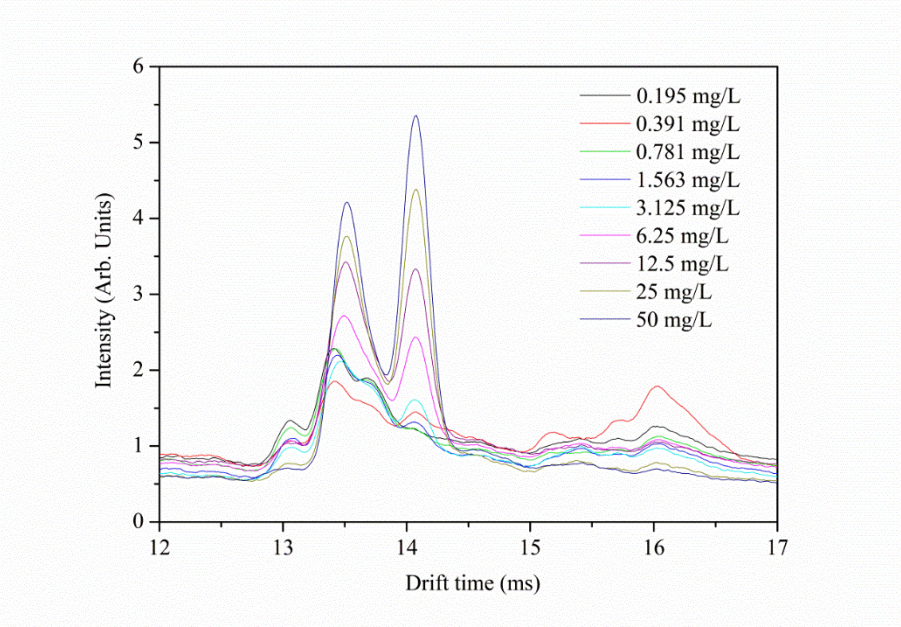

Fig. S5. Ion mobility spectra of flutolanil matrix standard solutions at different concentrations.

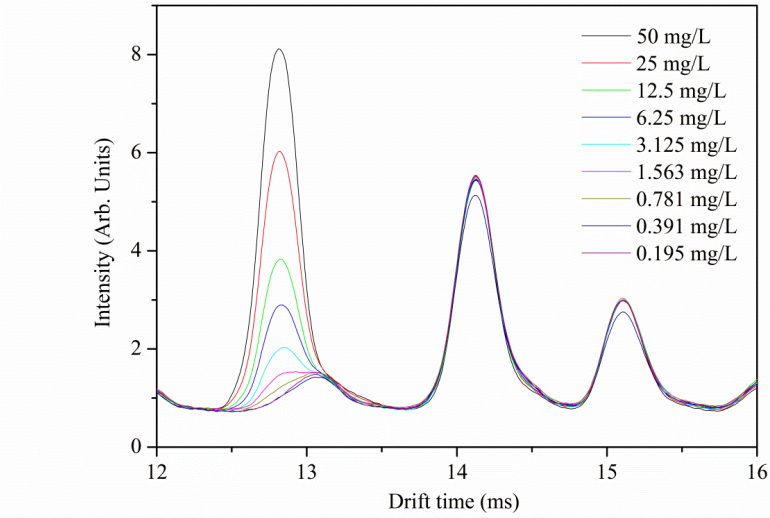

Fig. S6. Ion mobility spectra of pirimiphos-methyl matrix standard solutions at different concentrations.

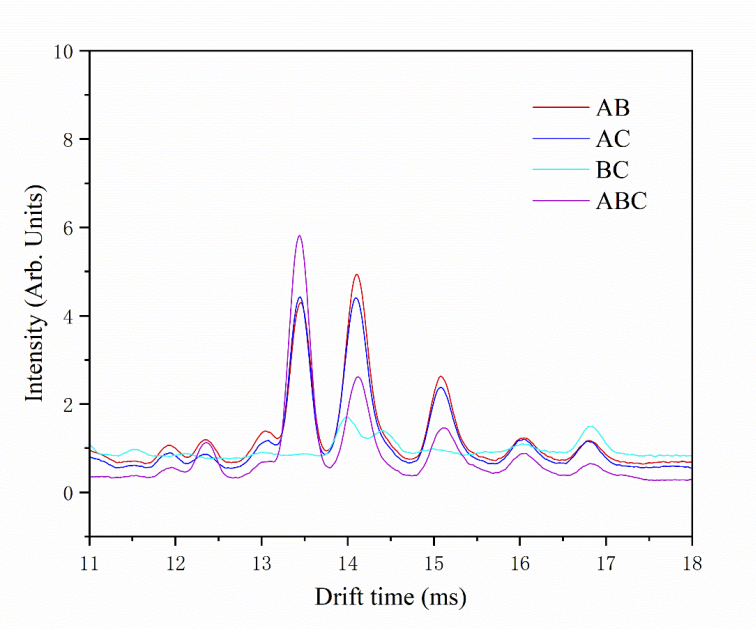

Fig. S7. Ion mobility spectra of the matrix standard solutions of mixed pesticide samples spiked at a concentration of 3.125 mg/L in positive ionization mode.

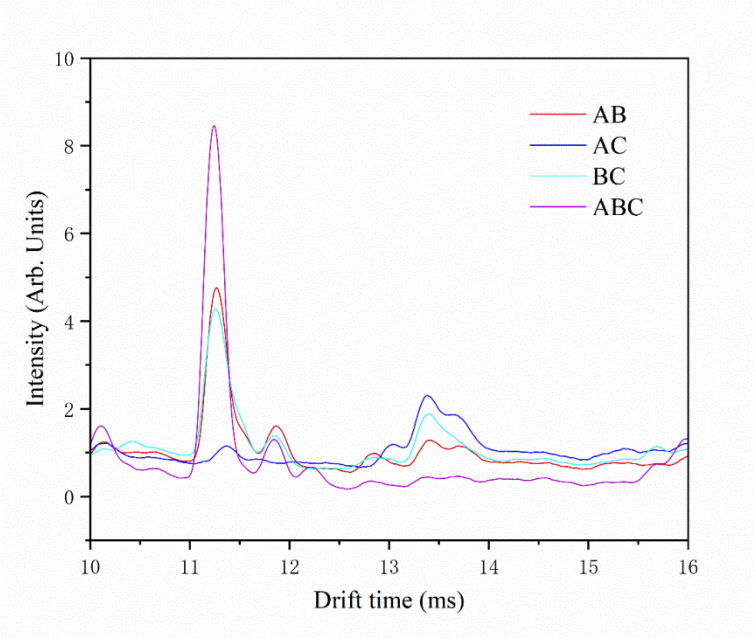

Fig. S8. Ion mobility spectra of the matrix standard solutions of mixed pesticide samples spiked at a concentration of 3.125 mg/L in negative ionization mode.