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No. AD-0103

Food Safety Analysis / LCMS-8050 & LCMS-IT-TOF

A Comparative Study of Targeted Screening Method by LC/MS/MS and Un-targeted Screening Method by LC-TOF in Residual Pesticides Analysis

ASMS 2015 WP 054

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Introduction

Advanced screening methods based on liquid chromatography-mass spectrometry (LC-MS) for detection of un-predicted residues of pesticides and veterinary drugs in agriculture products and food have been reported in recent years [1]. Without spectrum libraries like in GCMS, LC/MS/MS was initially not used in screening analysis. Whereas, high resolution LC-TOF was selected for screening analysis due to its accurate mass capability [1-2]. However, with rapid progress in data acquisition technique speed like UFMS (ultrafast MS) and high MRM capacity, new generation triple quadrupole LC/MS/MS has been used for targeted screening, e.g., of over a few hundred of pesticides in one analysis [3]. It is interesting to know the advantages and limitations of the two different screening approaches for pesticide residues in agriculture and food matrixes. We describe here a comparative study on targeted screening analysis based on MRM method on a UFMS-TQ system and un-targeted screening analysis based on high resolution MS full spectrum method on a LC-TOF system using same sample sets of mixed pesticides aiming at unveiling their capabilities and limitations in the challenging screening analysis.

Experimental

Mixed pesticide samples were obtained from a third party without information of compound number and names before completion of analysis. The unknown pesticide samples were analysed by two different screening methods on two LC-MS systems. A MRM-based targeted screening method was carried out on LCMS-8050, an ultrafast (UFMS) triple quadrupole system. Un-targeted screening ana-lysis of the same samples was carried out on LCMS-IT-TOF, a high resolution MS system. The two systems, analytical conditions and parameters are compiled into Table 1.

Table 1: Un-targeted screening analysis conditions of LCMS-IT-TOF

System & items		LCMS-8050*	LCMS-IT-TOF
LC conditions	Column	Shim-pack XR-ODS III (150 mmL. x 2mmi.D., 2.2µm)	Shim-pack XR-ODS III (150L x 2.0, 2.2µm)
	Flow Rate	0.4 mL/min	0.3 mL/min
	Mobile Phase	A : Water 5mM ammonium formate with 0.1% formic acid B : MeOHwith 5mM NH4 formate with 0.1% formic acid	A : Water 5 mmol/L NH4 formate, 0.1% formic acid B : MeOHwith 5 mmol/L NH4 formate, 0.1% FA
	Elution Mode	Gradient elution, 20 minute B: 5% (0 min) -> 100% (16min ~ 18min) -> 5% (18.1min ~20min)	Gradient elution, 35 min B: 15% (0min) -> 100% (25mins to 31min) -> 15% (31.1min to 35min)
	Oven Temp.	45 °C	50 °C
MS conditions	Interface	ESI heated	ESI (not heated)
	MS Mode	Schedule MRM, in positive and negative mode	Multi-event TIC, Positive and negative
	Interface Temp.	300 °C	RT
	Block Temp.	400 °C	250 °C
	DL Temp.	250 °C	200 °C
	Nebulizing Gas	Nitrogen, 2.0 L/min	Nitrogen, 1.5 L/min
	Heating Gas	Zero Air, 10 L/min	N.A.
	Drying Gas Flow	Nitrogen, 10 L/min	Nitrogen, 10 L/min
Inj Vol	Inj. Volume	1.0 µL	10 uL

* Refereed to method 1. The LC conditions of Method 2 and method 3 are different.

Results and Discussion

Description of targeted and un-targeted screening approaches

It has been accepted with unanimity that the MRM technique is one of best analytical methods in quantitative analysis of trace level organic compounds in complex matrix. Although MRM method has been used widely in quantitative analysis of thousands of compounds, it had not been used for screening analysis aiming at detection of concerned chemicals like pesticides in agriculture products until a recent time. The conventional method for screening analysis of pesticide residues is by GCMS with well-established spectrum library. However, GCMS with EI or CI ion source could not detect and quantify less and non-volatile pesticides effectively. In recent years, LC-MS with ESI interface has been increasingly used in analysis of pesticide residues using MRM method or high resolution TOF-MS method [1]. The so-called HRMS instruments like LC-TOF with its high mass-resolving power were first adopted in un-targeted screening analysis for pesticides and other chemical contaminants in agriculture products and food. A different methodology from GCMS isemployed, in which data analysis of the full spectra data is searched against a compound (molecular formula) database via accurate mass matching (+/-5ppm or better) to find candidates. The key advantages of this approach are: it does not need to restrict the retention time and the raw data can be re-analysed using different molecular formula database of any concerned compound or compounds group. On the hand, with rapid progress in instrumentation technology in recent years, new generation LC/MS/MS systems with ultrahigh data acquisition speed and extremely high capacity of MRM are invoked to use in screening analysis in food safety field. Targeted screening methods based on pre-loaded MRMs of hundred pesticides have been used increasingly as an alternative. This study is aimed at a comprehensive comparison between MRM-based targeted screening method and HRMS-based un-targeted screening method in detection and identification of pesticides in the unknown samples. Table 2 outlines the two methods used in this study, which were carried out on LCMS-8050, a latest model of LC/MS/MS with the highest performance specification of Shimadzu series, and LCMS-IT-TOF, a high resolution hydride MS system.

Table 2: Comparison of targeted & un-targeted screening methods

Item	Targeted Screening MRM method	Un-targeted screening HRMS method
No. of pesticides	fixed number (347, 167 & 121)*	not limited
Detection and identification method	Two pre-set MRM for each pesticide, intensity ratio	Accurate mass matching mass window (+/-) 5ppm
	Pre-determined RT with (+/-) 0.5 min window	Isotope pattern matching (scope > 50%)
Data analysis	Pre-set method, automated	allow re-process with specific database for data mining

* three method packages are used with different numbers of pesticides

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Results of targeted and untargeted screening of mixed pesticide samples

Figure 1 shows the MRM chromatograms of targeted screening analysis of the unknown mixed pesticide sample by three methods covering different numbers of compounds on LCMS-8050. The results of the screening by using three methods are shown in Figure 2. The total number of unique pesticides found in the unknown sample is 189.

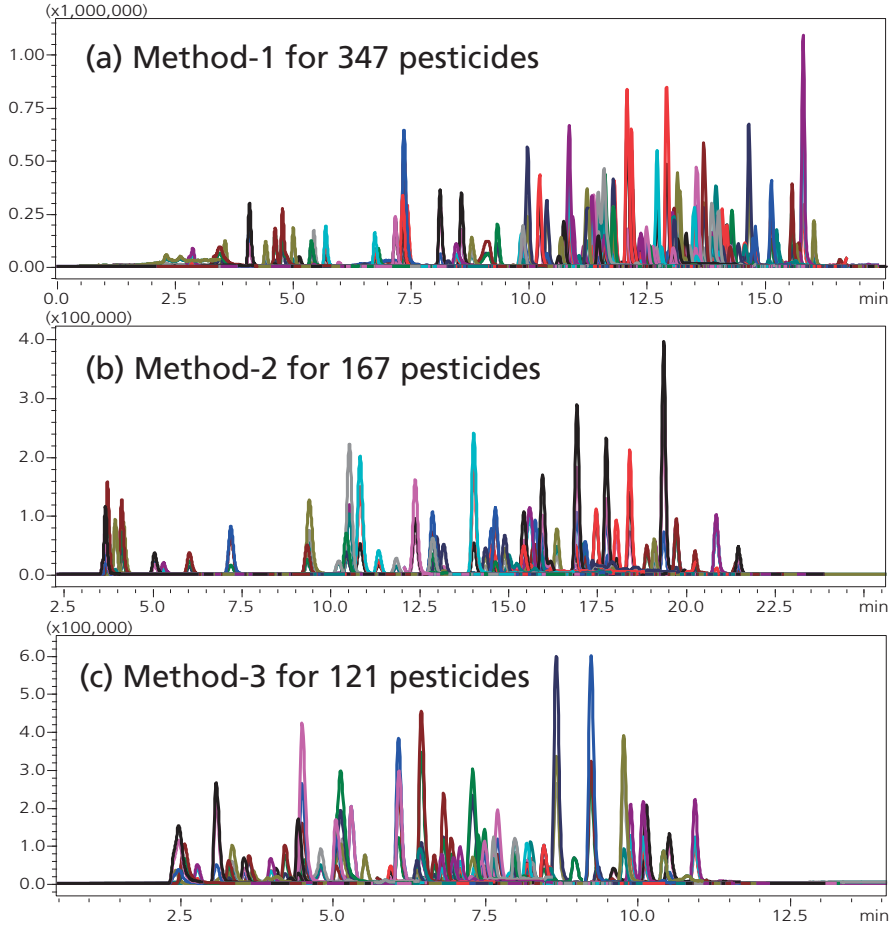

Figure 1: MRM chromatograms of targeted screening analysis of an unknown sample by three methods on LCMS-8050. The numbers of pesticides screened by the three methods are 347, 167 and 121, respectively.

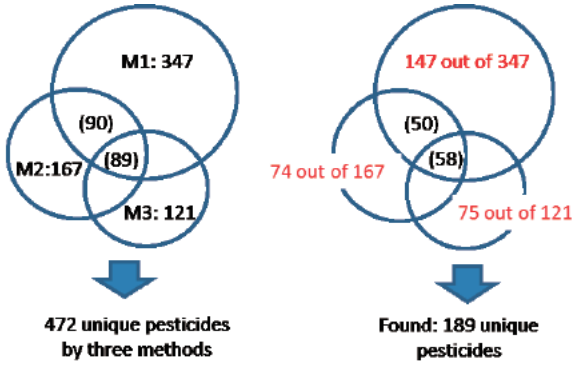

Figure 2: Numbers of pesticides of three MRM method packages covered are Method-1: 347, Method-2: 167 and Method 3: 121 (left). A total of 189 pesticides were found in the unknown mixed pesticide sample by the three methods (right).

Figure 3 shows multi-event TICs of un-targeted screening analysis of the unknown mixed pesticide sample on LCMS-IT-TOF. The so-called multi-event method was described elsewhere [4]. Instead of a single event of full mass range (m/z100~900), the data acquisition was performed in ten separate events, each covering a narrow mass range. This method was proven to be more sensitive than a single event method due to a lower baseline [4]. A total of 83 pesticides was detected and confirmed from this un-targeted screening analysis using a compound database of 450 pesticides (see Table 3). Fifty-three out of the eighty-three (70%) found pesticides were also found in targeted screening by LCMS-8050. In addition, 37 candidates were suspected present in the sample. Nine out of 37 suspected candidates (24%) were also found in the targeted screening analysis by LCMS-8050.

Comparison of targeted and untargeted screening

As shown in Figure 4, nine pesticides found in the unknown sample by both targeted and untargeted screening methods are selected randomly to compare the detection results individually. A general impression is that for those firmly detected pesticides, the detection results by both HRMS method on LC-TOF and MRM method on LC/MS/MS are qualified as screening candidates. The absolute detection sensitivity of MRM-based targeted screening are obviously higher than that of HRMS-based un-targeted screening. There are instrumentation factors and methodology factors. The LCMS-8050 is a latest model of triple quadrupole system with extremely high sensitivity, which contributes at least partially to the results of more pesticides found. However, this study is focused on the methodology factors. One of the key ideas of un-targeted screening by HRMS is that the method should avoid discrimination of any mass in data acquisition step. This means that all ions of a sample including matrix and solvent clusters are detected equally. As a result, some peaks of interesting compounds may be interfered to become shoulder or tailing peaks or submerged peaks due to high baseline. These can make peak detection more difficult in the subsequent data analysis step due to inappropriate integration parameters being applied. This was proven by reversed searching of those pesticides that were not found by un-targeted screening but found by MRM method in the LC-TOF raw data. By entering the exact masses of these pesticides to extract the corresponding EIC, additional 69 pesticides were found from the LC-TOF raw data. Figure 5 shows a few examples of the EICs obtained by this method. It can be that all these peaks in TICs are severely disturbed or merged by the baseline.

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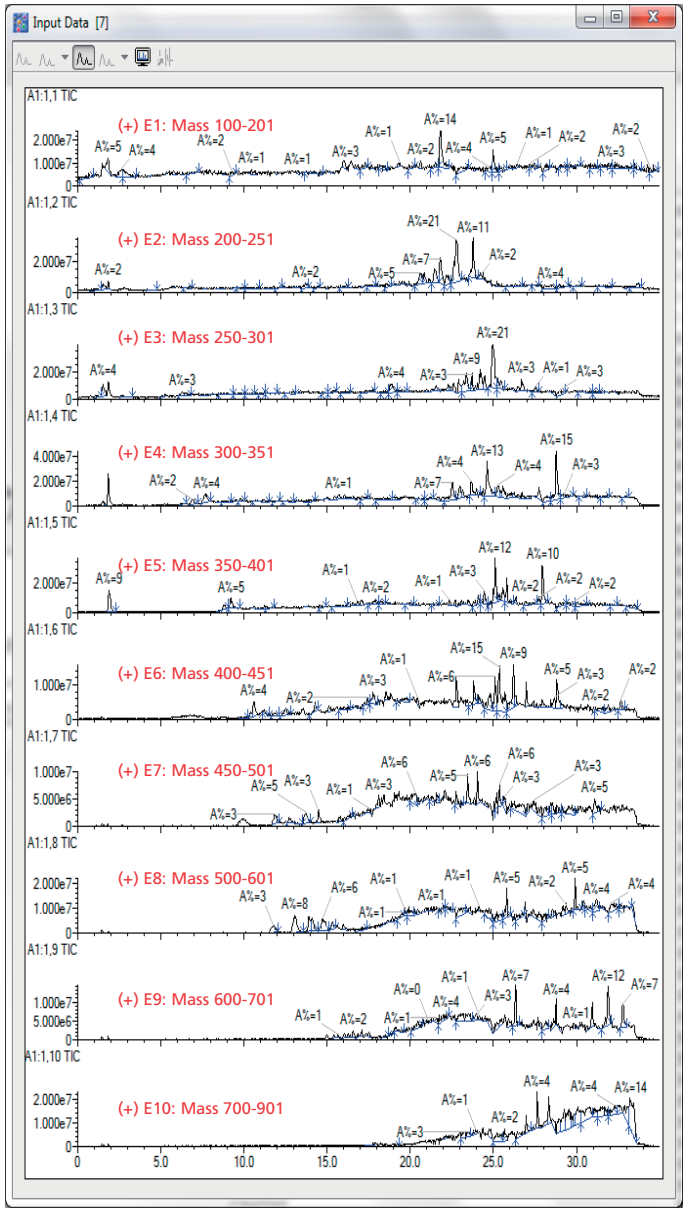

Figure 3: Multi-event TICs of un-targeted screening of an unknown mixed pesticide sample on LC-MS-IT-TOF.

Table 2 Result of un-targeted screening of pesticides of unknown mixed pesticide sample on LCMS-IT-TOF

S. No	RT	Area	Meas. m/z	Pred. m/z	Pesticide name	Formula (M)	Ion	Diff (mDa)	Isotope	by MRM
1	1.8	2,099,891	189.1612	189.1598	Propamocarb	C9 H20 N2 O2	[M+H]+	1.4	yes	yes
2	1.8	2,133,120	142.0085	142.0086	Methamidophos	C2 H8 N O2 P S	[M+H]+	-0.1	yes	yes
3	23.2	4,220,339	270.1511	270.1489	mepronil	C17 H19 N O2	[M+H]+	2.2	yes	yes
4	9.2	21,961,421	355.1584	355.1628	Isoxaben	C18 H24 N2 O4	[M+Na]+	-4.4	Yes	no
5	11.8	4,164,019	238.0824	238.0830	atrazine	C8 H14 N5 Cl	[M+Na]+	-0.6	Yes	yes
6	13.3	4,476,595	192.0762	192.0768	Carbendazim	C9 H9 N3 O2	[M+H]+	-0.6	yes	yes
7	13.3	3,212,352	230.0036	230.0069	dimethoate	C5 H12 N O3 P S2	[M+H]+	-3.3	yes	yes
8	13.8	16,673,818	223.0756	223.0745	acetamiprid	C10 H11 N4 Cl	[M+H]+	1.1	yes	no
9	13.8	16,673,818	223.0756	223.0747	Aldoxycarb (Aldicarbsulfone)	C7 H14 N2 O4 S	[M+H]+	0.9	yes	yes
10	15.4	17,341,491	253.0290	253.0253	Asulam	C8 H10 N2 O4 S	[M+Na]+	3.7	yes	no
11	15.4	17,341,491	253.0290	253.0309	Thiacloprid	C10 H9 N4 S Cl	[M+H]+	-1.9	yes	yes
12	16.3	14,762,458	190.0435	190.0433	tricyclazole	C9 H7 N3 S	[M+H]+	0.2	yes	no
13	18.5	4,308,480	201.0353	201.0313	Cloprop	C9 H9 O3 Cl	[M+H]+	4.0	yes	no
14	19.2	4,696,806	224.0916	224.0917	Bendiocarb	C11 H13 N O4	[M+H]+	-0.1	yes	yes
15	19.3	17,418,650	222.1104	222.1125	carbofuran	C12 H15 N O3	[M+H]+	-2.1	yes	yes
16	19.6	23,308,032	229.1110	229.1118	tebuthiuron	C9 H16 N4 O S	[M+H]+	-0.8	yes	yes
17	19.9	14,864,960	236.0717	236.0740	carboxin	C12 H13 N O2 S	[M+H]+	-2.3	yes	yes
18	20.3	4,718,208	215.0560	215.0582	monolinuron	C9 H11 N2 O2 Cl	[M+H]+	-2.2	yes	yes
19	20.4	4,432,947	226.0888	226.0896	Methiocarb	C11 H15 N O2 S	[M+H]+	-0.8	yes	yes
20	20.5	20,994,829	233.0877	233.0896	Flumeturon	C10 H11 N2 O F3	[M+H]+	-1.9	yes	yes
21	20.7	4,856,192	213.0816	213.0789	Chlortoluron	C10 H13 N2 O Cl	[M+H]+	2.7	yes	yes
22	20.8	28,004,557	239.148	239.1503	Pirimicarb	C11 H18 N4 O2	[M+H]+	-2.3	yes	yes
23	20.9	12,987,392	210.1584	210.1601	Dimethirimol	C11 H19 N3 O	[M+H]+	-1.7	yes	yes
24	21.0	4,668,646	246.0432	246.044	forchlorfenuron	C12 H10 N3 O Cl	[M-H]-	-0.8	yes	yes
25	21.1	18,761,882	214.1102	214.1121	simetryne	C8 H15 N5 S	[M+H]+	-1.9	yes	no
26	21.2	6,553,958	194.1170	194.1176	isoprocarb (MIPC)	C11 H15 N O2	[M+H]+	-0.6	yes	yes
27	21.2	10,335,846	222.0673	222.0696	Methabenzhiazuron	C10 H11 N3 O S	[M+H]+	-2.3	yes	yes
28	21.2	3,616,870	302.1092	302.1099	flutriafol	C16 H13 N3 O F2	[M+H]+	-0.7	yes	yes
29	21.4	3,713,178	248.0554	248.0585	forchlorfenuron	C12 H10 N3 O Cl	[M+H]+	-3.1	yes	yes
30	21.4	7,629,670	207.1465	207.1492	Isoproturon	C12 H18 N2 O	[M+H]+	-2.7	yes	yes
31	21.5	29,246,131	233.0233	233.0243	diuron(DCMU)	C9 H10 N2 O Cl2	[M+H]+	-1.0	yes	yes
32	21.5	21,697,280	280.1526	280.1543	metalaxyl	C15 H21 N O4	[M+H]+	-1.7	yes	yes
33	21.6	8,570,214	298.2717	298.2741	spiroxamine	C18 H35 N O2	[M+H]+	-2.4	yes	yes
34	21.8	9,574,400	199.1806	199.1805	Cycluron	C11 H22 N2 O	[M+H]+	0.1	yes	yes
35	22.3	13,953,843	297.0537	297.0556	Imazalil	C14 H14 N2 O Cl2	[M+H]+	-1.9	yes	yes
36	22.3	7,779,904	299.0559	299.0614	quinalphos	C12 H15 N2 O3 P S	[M+H]+	-5.5	yes	no
37	22.3	27,524,147	247.0318	247.0325	Fludioxonil	C12 H6 N2 O2 F2	[M-H]-	-0.7	yes	yes
38	22.4	6,889,062	404.1225	404.1241	Azoxystrobin	C22 H17 N3 O5	[M+H]+	-1.6	yes	yes
39	22.5	35,051,597	331.1150	331.1208	Halofenozide	C18 H19 N2 O2 Cl	[M+H]+	-5.8	Yes	yes
40	22.5	7,491,968	332.1186	332.1080	isofenphos-methyl	C14 H22 N O4 P S	[M+H]+	10.6	Yes	no
41	22.5	4,282,573	302.1380	302.1387	Fenoxycarb	C17 H19 N O4	[M+H]+	-0.7	yes	yes
42	22.6	15,515,878	233.1619	233.1648	Siduron	C14 H20 N2 O	[M+H]+	-2.9	yes	no
43	22.6	22,200,499	228.1263	228.1277	Ametryn	C9 H17 N5 S	[M+H]+	-1.4	yes	yes
44	22.9	45,391,386	277.1418	277.1424	Ferimzone (Z or F)	C15 H18 N4	[M+Na]+	-0.6	yes	no
45	23.0	9,554,406	324.1196	324.1206	flutolanil	C17 H16 N O2 F3	[M+H]+	-1.0	yes	no
46	23.0	13,692,800	327.0066	327.0185	diclofop	C15 H12 O4 Cl2	[M+H]+	-11.9	Yes	no
47	23.0	14,694,170	329.0032	329.0075	disulfoton sulfone	C8 H19 O4 P S3	[M+Na]+	-4.3	no	no
48	23.1	8,170,342	388.1302	388.1310	dimetomorph	C21 H22 N O4 Cl	[M+H]+	-0.8	yes	yes
49	23.3	10,796,544	299.0851	299.0849	mefenacet	C16 H14 N2 O2 S	[M+H]+	0.2	yes	no
50	23.3	10,632,934	291.0898	291.0895	Chloroxuron	C15 H15 N2 O2 Cl	[M+H]+	0.3	yes	yes
51	23.5	8,188,646	374.1951	374.1962	Spirotetramat	C21 H27 N O5	[M+H]+	-1.1	yes	yes
52	23.5	3,252,198	321.2117	321.2173	Iprovalicarb	C18 H28 N2 O3	[M+H]+	-5.6	Yes	yes
53	23.5	4,293,837	372.0280	372.0288	tetraconazole	C13 H11 N3 O F4 Cl2	[M+H]+	-0.8	yes	yes
54	23.6	22,224,717	224.1164	224.1182	Mepanipyrim	C14 H13 N3	[M+H]+	-1.8	yes	yes
55	23.6	2,692,378	331.0377	331.0376	fensulfothion oxon sulfone	C11 H17 O6 P S	[M+Na]+	0.1	yes	no
56	23.6	1,709,030	364.0728	364.0737	flufenacet	C14 H13 N3 O2 F4 S	[M+H]+	-0.9	yes	yes
57	23.6	24,522,573	242.1420	242.1434	terbutryn	C10 H19 N5 S	[M+H]+	-1.4	yes	no
58	23.7	3,835,955	325.0499	325.0521	Cyazofamid	C13 H13 N4 O2 S Cl	[M+H]+	-2.2	yes	yes
59	23.7	5,997,939	434.9291	434.9314	fipronil	C12 H4 N4 O F6 S Cl2	[M-H]-	-2.3	yes	yes
60	23.7	4,849,434	337.1188	337.1215	fenbuconazole	C19 H17 N4 Cl	[M+H]+	-2.7	yes	yes
61	23.8	4,287,360	351.2091	351.2078	tebufenozide	C22 H28 N2 O2	[M-H]-	1.3	yes	yes
62	23.8	2,937,792	373.1276	373.1305	cafenstrole	C16 H22 N4 O3 S	[M+Na]+	-2.9	yes	no
63	23.9	1,753,805	273.0575	273.0535	MCPB	C11 H13 O3 Cl	[M+HCOO]-	4.0	Yes	no
64	23.9	1,035,021	705.0070	705.0125	Flubendiamide	C23 H22 N2 O4 F7 S I	[M+Na]+	-5.5	yes	no
65	24.0	20,307,021	495.1966	495.1978	Hydramethylnon	C25 H24 N4 F6	[M+H]+	-1.2	yes	yes
66	24.0	6,955,098	275.0699	275.0712	Neburon	C12 H16 N2 O Cl2	[M+H]+	-1.3	yes	yes
67	24.1	6,011,315	327.1729	327.1703	Dimoxystrobin	C19 H22 N2 O3	[M+H]+	2.6	yes	yes
68	24.2	4,694,272	284.0676	284.0716	penconazole	C13 H15 N3 Cl2	[M+H]+	-4.0	yes	yes
69	24.2	2,102,426	308.1516	308.1524	tebuconazole	C16 H22 N3 O Cl	[M+H]+	-0.8	Yes	yes
70	24.3	1,700,864	342.0218	342.0240	Prothioconazole	C14 H15 N3 O S Cl2	[M-H]-	-2.2	yes	no
71	24.4	5,576,806	732.4687	732.4681	Spinosyn A	C41 H65 N O10	[M+H]+	0.6	yes	yes
72	24.4	5,144,832	342.0771	342.0771	propiconazole	C15 H17 N3 O2 Cl2	[M+H]+	0.0	yes	yes
73	24.7	2,588,186	326.0808	326.0821	Diniconazole	C15 H17 N3 O Cl2	[M+H]+	-1.3	yes	no
74	24.8	5,358,285	748.4970	748.4994	Spinetoram	C42 H69 N O10	[M+H]+	-2.4	yes	yes
75	24.9	1,791,821	346.0915	346.0929	Triflumizole	C15 H15 N3 O F3 Cl	[M+H]+	-1.4	yes	yes
76	25.1	4,002,662	383.1694	383.1635	Furathiocarb	C18 H26 N2 O5 S	[M+H]+	5.9	yes	yes
77	25.2	9,050,906	505.1075	505.1105	Metaflumizone	C24 H16 N4 O2 F6	[M-H]-	-3.0	yes	yes
78	25.5	12,471,642	360.1752	360.1770	etoxazole	C21 H23 N O2 F2	[M+H]+	-1.8	yes	yes
79	25.7	2,695,757	422.2068	422.2074	Fenpyroximate (E or F)	C24 H27 N3 O4	[M+H]+	-0.6	yes	yes
80	25.8	2,013,440	374.0978	374.0934	Pyrazophos	C14 H20 N3 O5 P S	[M+H]+	4.4	yes	no
81	25.8	7,307,520	373.0971	373.0950	Quizalofop-Ethyl	C19 H17 N2 O4 Cl	[M+H]+	2.1	yes	no
82	26.2	8,095,296	447.1116	447.1057	orthosulfamuron	C16 H20 N6 O6 S	[M+Na]+	5.9	Yes	no

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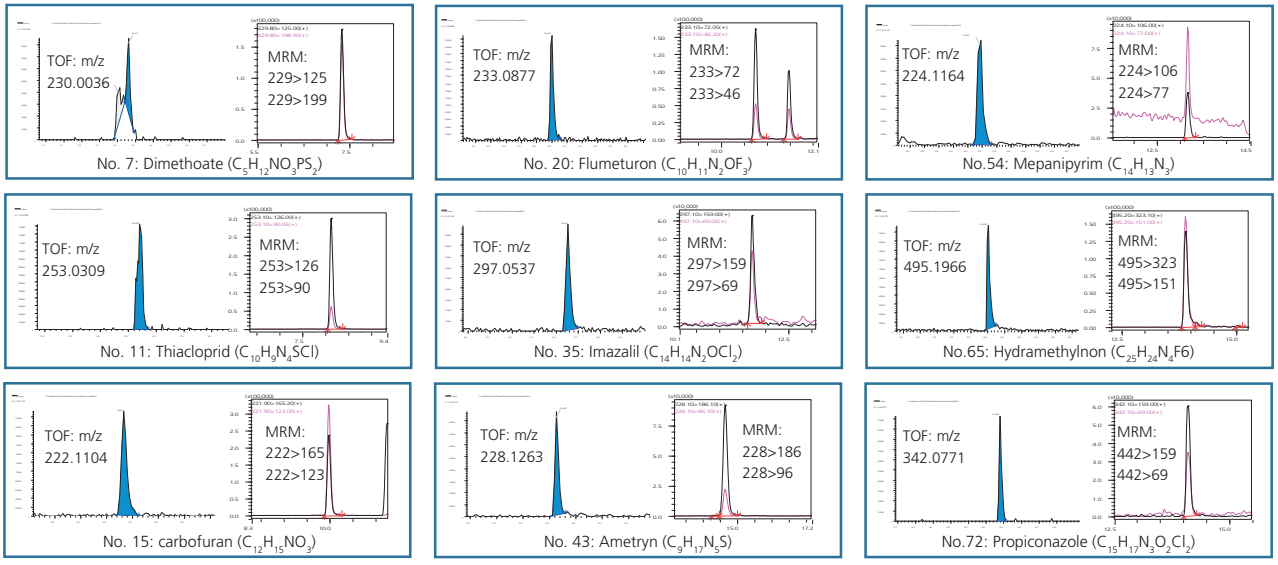

Figure 4: Individual comparisons of detection of nine pesticides (out of 83) in an unknown sample by targeted and un-targeted screening methods.

But, they could be detected if their EICs were extracted successfully. This results indicate that HRMS based un-targeted screening is highly depending on the data analysis method. The current peak picking algorithm could not find effectively the distorted and submerged peaks. More sensitive peak picking programs (different algorithm) are required for effective detection of distorted and submerged peaks in LC-TOF data.

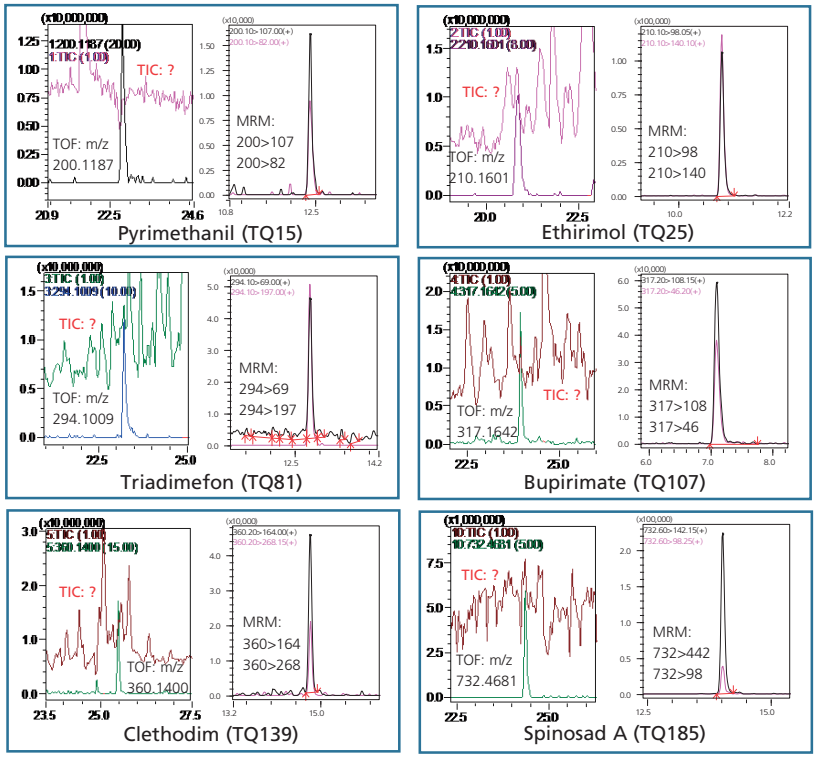

Figure 4 Sixty-nine additional pesticides were confirmed exist in the unknown sample by re-exploring the LC-TOF raw data through extracting the exact masses of pesticides found by MRM method (displaying 6 only).

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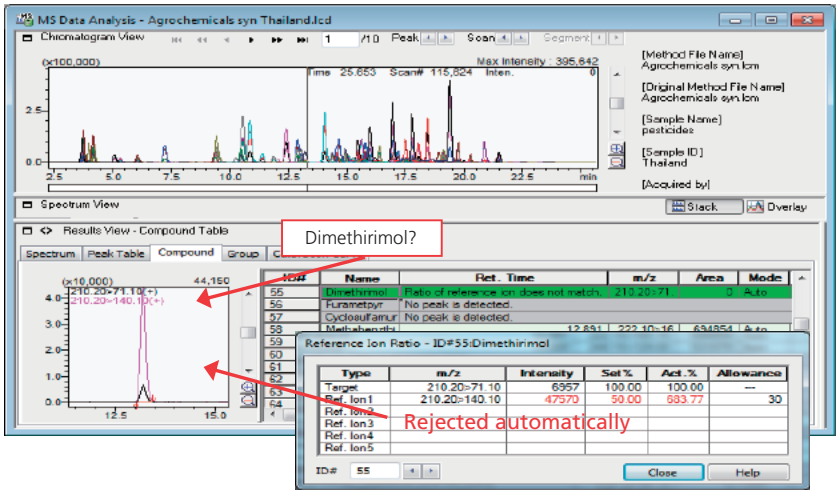

Figure 5: The Identification of a peak for dimethirimol was rejected automatically by the method due to un-matching of intensity ratio of MRMs.

In contrast, the MRM targeted screening method does not affected by data analysis. While, matrix effect is the only factor that may cause false positive and false negative detection. The screening reliability of MRM method is considerably high due to the excellent mass selectivity and specific RT of every compounds. In addition, the confirmation MRM (reference ion) and its intensity ratio with the main MRM (quantifier ion) provides additional selectivity and confirmation, which could reduce further false positive results. Figure 6 shows one example, a peak corresponding to dimethirimol appeared at the expected RT with two MRMs. However, the data analysis program rejected it as a found pesticide due to the intensity ratio of the MRM pair was out of the defined range. This result may have two possibilities: it is another compound or there is a co-elute peak which MRM is same as the confirmation MRM (210>140) of dimethirimol. The MRM-based targeted screening methods have been increasingly adopted in analysis of pesticides and other chemical contaminants in food safety analysis due to several facts. First, the number of pesticides that can be covered (screened) in a single run has increased drastically due to the improvements in triple quadrupole instrumentation and software technologies. Second, MRM database of most pesticides become available for various LC/MS/MS systems from vendors or research institutes. Third, MRM targeted screening approach can be fully automated from data acquisition to data analysis and reporting, which is favorited in routine inspection analysis in food safety labs.

Conclusions

This is a preliminary comparative study of MRM-based targeted screening method and HRMS based un-targeted screening method for detection of pesticides. HRMS method on LC-TOF is an ideal approach for screening of un-limited pesticides in samples. This approach requires advanced data acquisition method and high sensitivity in full spectrum mode to detect all ions without discrimination. However, data analysis may be very challenging in peak picking of distorted and submerged peaks due to matrix interference of actual food samples. On the other hand, the MRM-based targeted screening approach has been increasingly adopted in food safety analysis because of its operation easiness and high reliability in detection and identification of targeted pesticides. Further studies with more quantitative comparison of the two screening approaches and their performances for different samples are needed.

A Comparative Study of Targeted Screening Method by LC/MS/MS and Un-targeted Screening Method by LC-TOF in Residual Pesticides Analysis

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First Edition: May, 2015

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