

# Application Data Sheet

## No. 96

### GC-MS

Gas Chromatograph Mass Spectrometer

## An Investigation of Simultaneous Analysis Methods for 420 Residual Pesticide Compounds in Foods Using GC-MS/MS

Due to its excellent sensitivity and selectivity, GC-MS/MS is utilized for the analysis of residual pesticides in foods. The number of relevant pesticides grows yearly, and has reached 300 to 400 compounds. Due to limitations in MRM-related software functionality and detection sensitivity, analyzing so many pesticides requires the intended pesticides to be divided into multiple method files and then measured method by method. As a result, the number of analyses increases, and places a strain on laboratory productivity. Smart MRM<sup>®</sup>, the method creation function in GCMSsolution software, automatically creates the optimal methods for the simultaneous analysis of over 400 compounds, while ensuring sensitivity and accuracy are maintained. In addition, MRM analysis can be started without configuring troublesome transition settings by utilizing Smart Pesticides Database, which contains acquisition parameters for 479 compounds. Since this database contains retention indices, retention times can be corrected with a single n-alkane analysis (AART function). Using the corrected retention times allows the user to start creating MRM methods without purchasing or analyzing an analytical standard.

This data sheet reports batch analysis methods for 420 compounds (approximately 1,200 transitions) using Smart Pesticides Database and Smart MRM.

### Experiment

Commercially available spinach was pretreated with the QuEChERS method using Restek Q-sep<sup>™</sup>. Pesticides were added to the sample extract, with the concentration adjusted to 5 ng/mL. The prepared sample was then subjected to MRM analysis for 420 compounds under the analysis conditions registered in Smart Pesticides Database. Table 1 shows the analysis conditions. The retention times for the individual pesticides were corrected using the AART function based on an n-alkane analysis.

Table 1: Analysis Conditions

GC-MS:	GCMS-TQ8040		
Column:	SH-Rxi-5Sil MS (30 m long, 0.25 mm I.D., df = 0.25 μm) (Shimadzu, P/N: 221-75954-30)		
Glass Insert:	Sky Liner, Splitless Single Taper Gooseneck w/Wool (Restek, P/N: 567366)		
[GC]		[MS]	
Injection Unit Temp.:	250 °C	Interface Temp.:	250 °C
Column Oven Temp.:	50 °C (1 min) → (25 °C/min) → 125 °C (10 °C/min) → 300 °C (15 min)	Ion Source Temp.:	200 °C
Injection Mode:	Splitless	Solvent Elution Time:	1.5 min
High-Pressure Injection:	250 kPa (1.5 min)	Measurement Mode:	MRM
Carrier Gas Control:	Linear velocity (47.2 cm/sec)	Loop Time:	0.5 sec
Injection Volume:	2 μL		

### Analysis Results

Fig. 1 shows the mass chromatograms for malathion, trifloxystrobin, and fenbuconazole. Table 2 shows the area repeatability values for 240 of the 420 compounds (n = 5). By creating suitable MRM analysis methods utilizing Smart MRM, it is possible to analyze even 420 compounds simultaneously with favorable sensitivity and accuracy.

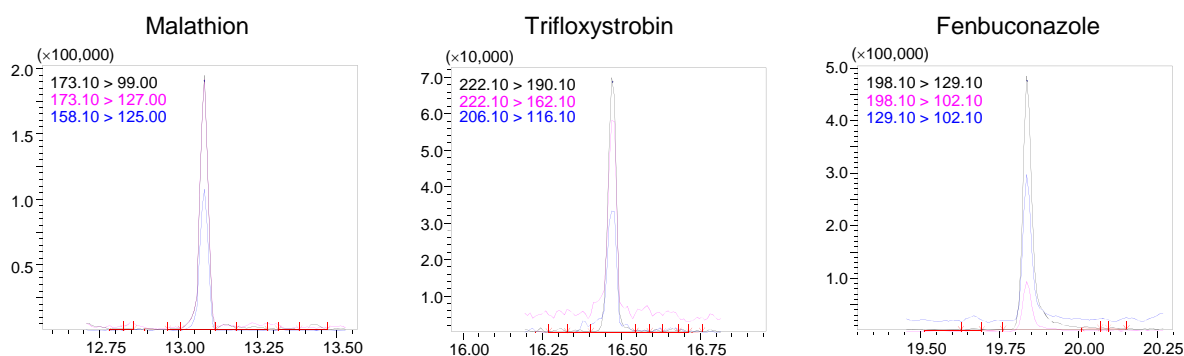


Fig. 2: Mass Chromatograms for the Pesticides

\*Supported by GCMSsolution ver. 4.20 and later.

Table 2: Area Repeatability for 240 Compounds (n = 5)

Compound Name	%RSD	Compound Name	%RSD	Compound Name	%RSD	Compound Name	%RSD
Dichlorvos	6.37	Propanil	1.78	Fenothiocarb	2.83	Pyridaphenthion	3.17
Dichlobenil	2.87	Acetochlor	3.83	alpha-Endosulfan	13.10	Iprodione	8.59
EPTC	2.28	Bromobutide	4.15	Butamifos	4.96	Acetamiprid	7.64
Butylate	2.55	Chlorpyrifos-methyl	2.91	Flutriafol	5.72	Phosmet	10.86
Etridiazole	8.94	Vinclozolin	3.91	Fenamiphos	6.49	Bifenthrin	6.12
Methacrifos	3.84	Parathion-methyl	6.53	Napropamide	8.75	EPN	7.46
Clothianidin	9.96	Tolclofos-methyl	2.70	Flutolanil	6.05	Bromopropylate	3.29
Chloroneb	3.36	Simeconazole	4.94	Hexaconazole	8.09	Picolinafen	3.06
Crimidine	3.31	Alachlor	4.17	Prothiofos	3.47	Fenoxycarb	5.28
2-Phenylphenol	2.74	Simetryn	3.24	Fludioxonil	2.39	Bifenazate	3.52
Isoprocarb	4.68	Metalaxyl	2.51	Isoprothiolane	4.10	Etoxazole	7.00
Tecnazene	3.66	Fenchlorphos	2.94	Pretilachlor	3.01	Fenpropathrin	6.37
Omethoate	6.96	Prometryn	4.12	Profenofos	2.96	Fenamidone	2.31
Propoxur	9.13	Pirimiphos-methyl	3.14	Tricyclazole	5.31	Tribufos	6.29
Propachlor	2.73	Fenitrothion	4.47	Uniconazole	3.63	Bifenox	7.37
Ethofophos	2.55	Ethofumesate	4.15	Oxadiazon	2.86	Furametpyr	4.71
Ethalfuralin	3.83	(E)-Dimethylvinphos	4.82	Thifluzamide	5.38	Tetradifon	7.80
Chlorpropham	3.21	Bromacil	7.35	Tribufos	2.04	Pentoxazone	5.03
Trifluralin	5.56	Esprocarb	3.06	Myclobutanil	2.62	Phosalone	8.42
Dicrotophos	5.78	Malathion	7.44	Flusilazole	6.76	Leptophos	4.31
Benfluralin	5.09	Quinoclamine	6.49	Oxyfluorfen	12.31	Azinphos-methyl	4.17
Salithion	2.10	Metolachlor	1.79	Bupirimate	3.78	Cyhalothrin-1	9.01
Sulfotep	3.61	Chlorpyrifos	3.63	Buprofezin	5.30	Cyhalothrin-2	8.68
Monocrotophos	5.44	Thiobencarb	7.20	Kresoxim-methyl	2.86	Cyhalofop-butyl	1.48
Cadusafos	3.25	(Z)-Dimethylvinphos	2.82	Carboxin	3.94	Mefenacet	4.52
Phorate	1.99	Diothofencarb	2.10	Diclobutrazol	4.21	Pyrazophos	5.85
alpha-BHC	4.14	Fenthion	6.45	(Z)-Metominostrobin	6.00	Fenarimol	4.05
Thiometon	3.57	Chlorthal-dimethyl	3.06	Azaconazole	2.75	Azinphos-ethyl	3.58
Dicloran	6.15	Fenpropimorph	4.62	Cyflufenamid	9.37	Pyraclufos	7.94
Dimethoate	5.51	Parathion	8.92	Chlorfenapyr	7.41	Fenoxaprop-ethyl	9.11
Furilazole	2.52	Triadimefon	3.61	Isoxathion	9.27	Fluquinconazole	11.11
Carbofuran	8.29	Tetraconazole	6.35	(Z)-Pyrinobac-methyl	2.59	Pyridaben	5.75
Simazine	4.30	Isocarbophos	8.27	Chlorobenzilate	1.33	Butafenacil	4.30
Atrazine	1.34	Nitrothal-isopropyl	6.41	Fensulfthion	6.20	Etobenzanid	2.99
Dimethipin	8.14	Phthalide	5.64	beta-Endosulfan	7.09	Fenbuconazole	2.93
Swep	3.23	Bromophos	3.73	Diniconazole	3.46	Cypermethrin-1	14.35
beta-BHC	1.62	Fosthiazate-1	5.22	Oxadixyl	4.14	Cypermethrin-2	9.04
Chlorbufam	7.21	Fosthiazate-2	8.17	Ethion	3.10	Cypermethrin-3	9.50
Clomazone	3.10	Pendimethalin	6.83	Fluacrypyrim	3.59	Cypermethrin-4	9.03
Quintozene	2.85	(E)-Chlorfenvinphos	3.27	Mepronil	1.35	Halfenprox	4.03
Propazine	6.04	Cyprodinil	4.35	Triazophos	6.34	Flucythrinate-1	7.57
gamma-BHC	4.52	Fipronil	6.31	Chlornitrofen	5.56	Flucythrinate-2	7.78
Terbufos	2.88	Dimethametryn	2.44	Carbophenothion	3.72	Quizalofop-ethyl	5.45
Cyanophos	4.00	Penconazole	4.01	Cyanofenphos	4.13	Etofenprox	4.39
Fonofos	5.74	Chlozolinate	10.85	Trifloxystrobin	2.52	Silafluofen	1.71
Propyzamide	1.97	Tolyfluanid	5.13	Edifenphos	7.31	Fluridone	2.51
Pyroquilon	4.53	Isofenphos	2.82	Norflurazon	4.58	Pyrimidifen	4.83
Diazinon	3.33	Phenthoate	3.43	Propiconazole-1	7.77	Flumioxazin	13.53
Pyrimethanil	3.55	Quinalphos	7.29	Propiconazole-2	7.45	Fenvalerate-1	7.70
Isazofos	3.89	Thiabendazole	3.55	Quinoxifen	2.34	Fenvalerate-2	5.06
Tefluthrin	2.58	Dimepiperate	2.29	(E)-Pyrinobac-methyl	0.69	Pyraclostrobin	3.40
Terbacil	6.73	Procymidone	1.15	Endosulfan sulfate	12.96	Difenoconazole-1	9.02
Etrimfos	3.20	Bromophos-ethyl	1.78	Lenacil	2.35	Difenoconazole-2	3.94
delta-BHC	7.35	Methodathion	2.84	Chloridazon	7.76	Indoxacarb	13.62
Tri-allate	4.62	Chlorbenside	3.44	Tebuconazole	5.87	Azoxystrobin	8.90
Tebupirimfos	3.79	Propaphos	7.33	Piperonyl butoxide	3.48	Dimethomorph-1	6.48
Iprobenfos	2.12	Tetrachlorvinphos	6.45	Epoxiconazole	0.42	Dimethomorph-2	7.81
Benoxacor	9.77	Trichlamide	13.53	Zoxamide	7.71	Tolfenpyrad	5.71
Dichlofenthion	2.62	Paclbutrazol	3.63	Pyributicarb	5.85	Imibenconazole	7.03
Dimethenamid	2.55	Butachlor	4.03	Chlormethoxyfen	4.34	Cinidon-ethyl	10.40

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