

Quick-DB for GCMS-TQ Series and GCMS-QP Series

GC/MS Residual Pesticides Database Ver. 2

Component No.	Sample No.	Type	Ret.	CE	Ref.	Type	Ret.	CE	Ref.	Quadratic	Quadratic	Quadratic	Linear	Linear
										Constant	1st	2nd	Constant	1st
1001	T	15.51021	8	100.00	Ref1	115.1483	8	100.00	154.06	0.00202698	0.00922177	-0.87286E-07	0.00428214	0.000764895
1002	T	16.01113	10	100.00	Ref1	145.0113	10	41.45	0.0094221	0.00916152	1.89586E-06	0.00187343	0.00852511	
1003	T	17.11483	4	100.00	Ref1	121.1477	8	48.09	0.0020823	0.00344821	7.30038E-07	0.000117927	0.00358754	
1004	T	18.1083	6	100.00	Ref1	105.1483	14	71.04	0.0054038	0.00764949	-2.80796E-06	0.0133218	0.0071263	
1005	T	19.01113	8	100.00	Ref1	155.0113	4	23.55	-0.00240438	0.000717643	4.26093E-07	-0.00364374	0.000799371	
1006	T	20.01113	6	100.00	Ref1	80.0113	20	8.73	0.00428732	0.000387048	-1.87214E-07	0.000963082	0.00034922	
1007	T	21.01113	14	100.00	Ref1	137.0113	20	37.81	0.0068932	0.0024216	-2.28744E-06	0.0118896	0.00198881	
1008	T	22.01113	8	100.00	Ref1	89.0113	20	6.86	0.00288972	0.0010384	-1.37427E-06	0.0028134	0.00076027	
1009	T	23.01113	8	100.00	Ref1	147.0113	12	33.87	0.0026114	0.00776134	-1.00079E-07	0.00021876	0.00774216	
1010	T	24.01113	14	100.00	Ref1	185.0113	14	29.42	0.0127189	0.017756	-2.11836E-07	0.0132826	0.0177154	
1011	T	25.01113	6	100.00	Ref1	142.0113	6	67.84	-0.00799668	0.00426789	5.00848E-06	-0.0014306	0.00523211	
1012	T	26.01113	24	100.00	Ref1	170.0113	14	101.96	0.000452064	0.00324207	1.40261E-06	-0.0018244	0.00352745	
1013	T	27.01113	4	100.00	Ref1	109.0113	12	25.42	0.0023824	0.0130605	6.29104E-06	0.020479	0.00622185	
1014	T	28.01113	12	100.00	Ref1	133.0113	12	130.03	-0.0049133	0.000252485	2.54937E-07	-0.014434	0.0142672	
1015	T	29.01113	14	100.00	Ref1	170.0113	14	71.03	0.0188323	0.0173207	-4.70214E-06	-0.00647349	0.000310373	
1016	T	30.01113	12	100.00	Ref1	109.0113	12	101.96	0.0140521	0.00664023	-2.22913E-06	0.0014058	0.0164288	

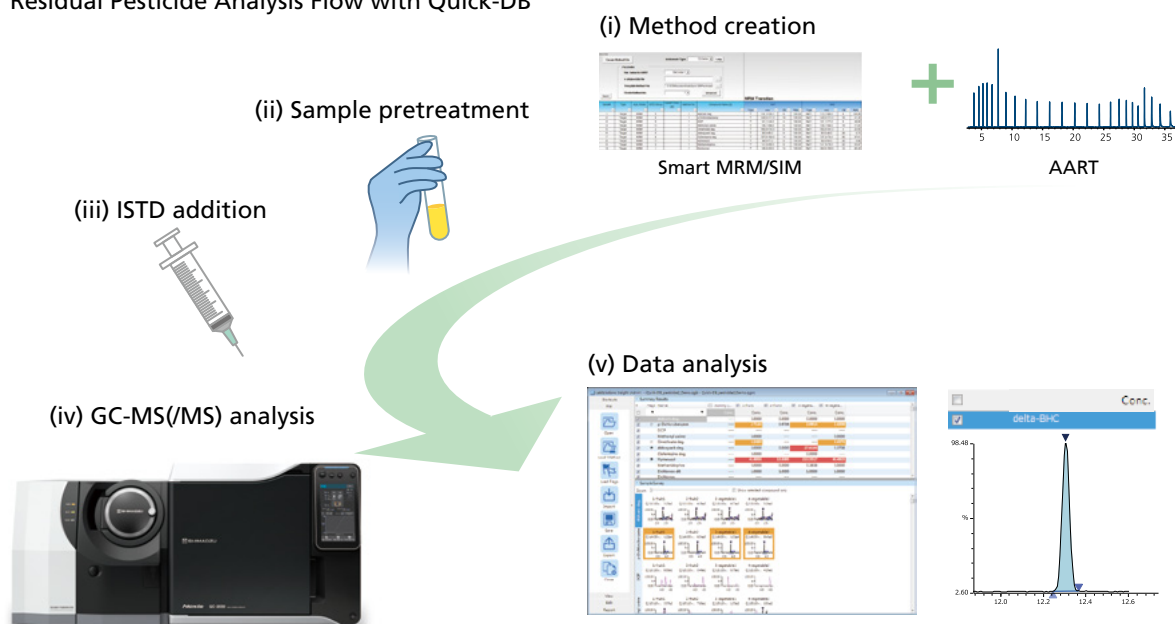
Simultaneous Screening of 491 Pesticides without Standard Samples

The increase in restricted pesticides caused by the introduction of the Positive List system for agricultural chemical residues in foods in Japan has resulted in an increasing number of samples to be analyzed. Increased purchasing costs and the control operations associated with these standard samples have become issues for the industry. This product is a GC-MS(/MS) analysis database pre-registered with calibration curves created using pesticide surrogates as internal standard substances. This allows for quick residual pesticide screening without the use of pesticide standard samples. In Ver. 2, the number of pesticides that can be analyzed in MRM mode is 491. Database customization has also been added.

1 Quantitation Analysis without Using Standard Samples

The database is registered with analytical conditions for 491 pesticides (retention indices, transitions, calibration curves, etc.). Retention indices can be used with the Automatic Adjustment of Retention Times (AART) function and automatic method creation function (Smart MRM™) to create quantitative analytical methods in SIM mode and MRM mode without using standard samples. The method files created are pre-registered with calibration curves created using pesticide surrogates as internal standard substances. This allows for the quantitative values to be calculated without using calibration curves obtained from standard samples.

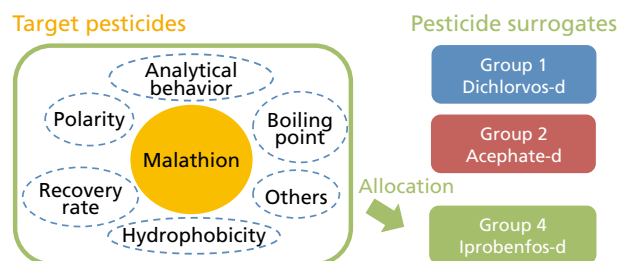
Residual Pesticide Analysis Flow with Quick-DB™



Quantitation Analysis Using Pesticide Surrogates as Internal Standard Substances

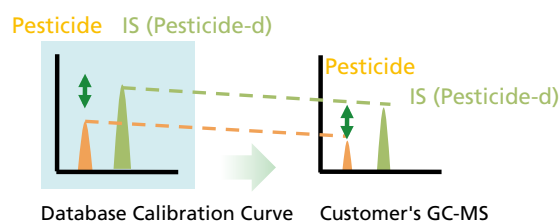
To increase quantitative analysis precision, quantitative values must be adjusted to compensate for pesticide losses during analysis and due to variations in GC-MS(/MS) sensitivity. The pesticide surrogates used are 19 pesticides labeled with stable isotope elements that behave almost identically to the target pesticides. The calibration curves contained in this product are created by grouping target pesticides based on similar behavioral and physical properties and allocating pesticide surrogates with similar physical properties to each group as internal standard substances. This allows for quantitative values to be calculated with high precision without using calibration curves created from standard samples.

Allocation of Pesticide Surrogates Based on Physical Properties of Target Pesticides



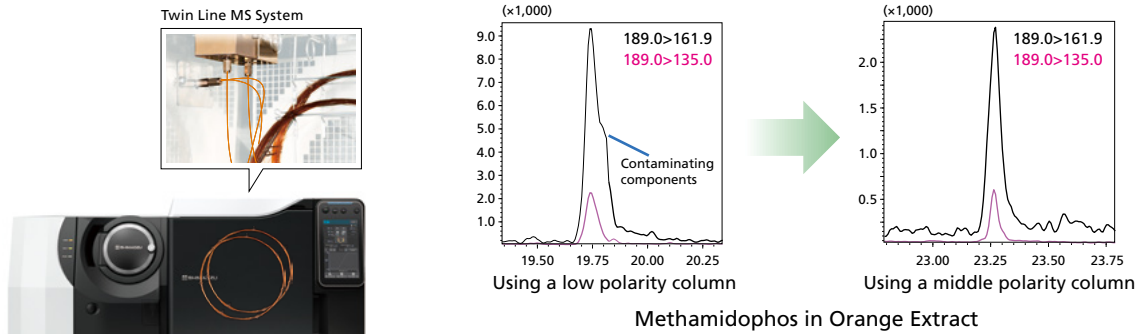
Sensitivity Variation Adjustments Using Pesticide Surrogates

Pesticide surrogates can also be used to adjust differences in target pesticide responses observed in calibration curves and a customer's instrument due to variations in GC-MS(/MS) sensitivity.



2 Reliable Target Pesticide Detection of High Matrix Samples

When analyzing high matrix samples such as those that have undergone simple pretreatment by a QuEChERS method, detection and quantitation may not be achieved in either SIM mode or MRM mode due to the influence of contaminants on the target pesticides. Using two columns of different polarity allows for peak separation between the target pesticide and contaminants. This product is compatible with the Twin Line MS system, and can be used to reliably detect pesticides in high matrix samples.

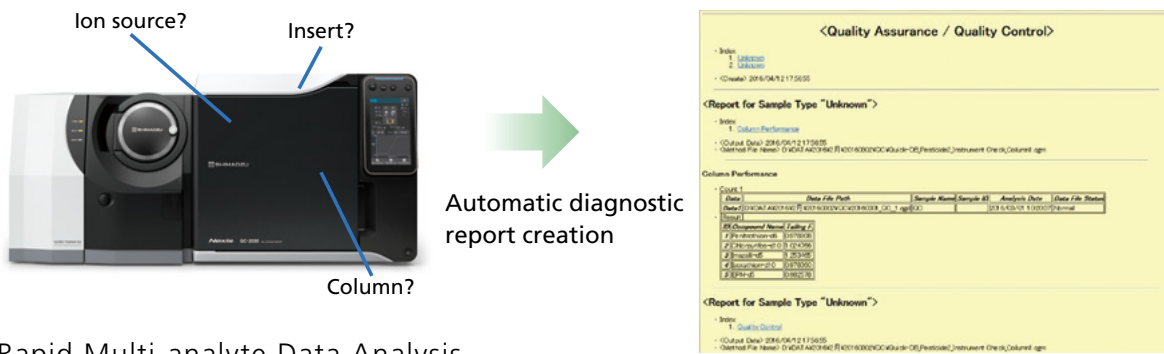


Analysis can be performed smoothly on different columns without interrupting the MS vacuum by simultaneously attaching the mass spectrometer to the outlets of two different columns installed in two separate vaporizing chambers.

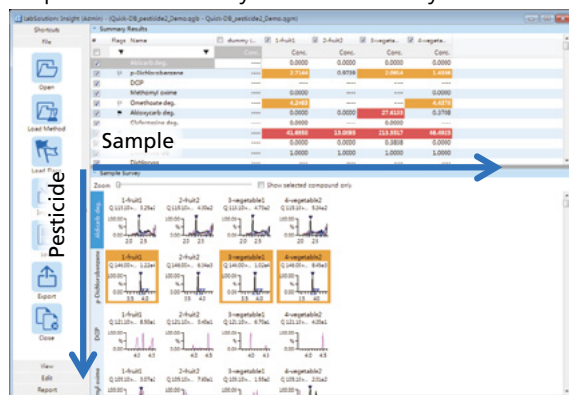
3 Accelerating All Operations, from Precision Control to Data Analysis

Rapid Precision Control with QA/QC Functions Designed Especially for Pesticide Analysis

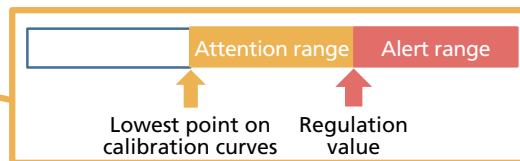
Periodic precision control of instruments is needed to maintain the reliability of data during daily analyses. This product comes with QA/QC methods created especially for pesticide analysis. These methods allow for quick confirmation of instrument status by simply analyzing pesticide surrogates before analyzing the target sample.



Rapid Multi-analyte Data Analysis



This product comes with the LabSolutions Insight™ file registered with the lowest point on calibration curves for target pesticides. Whether a pesticide has been detected or not can be determined instantaneously based on flagging (color coding of the chromatogram graphs), which allows for rapid data analysis.



4 Possibility of Customizing Database

This product is the world's only customizable database for residual pesticide screening. Additional analytical conditions (including calibration curve information) can be added to the database. Also, the target pesticides being measured can be changed for each sample, allowing the customer to analyze particular target pesticides.

Serial#	Type	Acq. Mode	ISTD Group	Level1 Conc (IS)	Method No.	Compound Name (E)	Ret. Index 1	tea	apple	tomato
1	Target	MFM	5		1	Aldicarb deg.	881	x		x
2	Target	MFM	9		1	p-Dichlorobenzene	1023	x	x	x
3	Target	MFM	9		1	DCIP	1057	x	x	
4	Target	MFM	11		1	Methomyl oxime	1064	x	x	x
5	Target	MFM	2		1	Omethoate deg.	1099	x		x
4E2	Target	MFM	1		1	new 1	2000	x		x
4E3	Target	MFM	2		1	new 2	2500	x	x	x
4E4	Target	MFM	3		1	new 3	3000		x	x

Additional pesticides can be registered

When target pesticides differ for each test sample (food), target pesticides for each food can be recorded in the database so methods are created that analyze only these recorded compounds.

Product Specifications

Product Contents

Database file, method files, LabSolutions Insight damp file, report format files

Number of Pesticides Registered to the Database

For GC-MS (Scan/SIM modes): 474 compounds (317 for Scan mode, 157 for SIM mode)

For GC-MS/MS (MRM mode): 491 compounds

Applicable Instruments

GC/MS: GCMS-TQ™ series, GCMS-QP2020 series, GCMS-QP2010 Ultra

GC/MS Workstation: GCMSsolution™ + LabSolutions Insight

LabSolutions™ DB GCMS/LabSolutions CS + LabSolutions Insight DB/CS

Consumables

Column 1: SH-I-5Sil MS 30 m×0.25 mm I.D., df=0.25 mm (P/N 221-75954-30)

Column 2: SH-200MS 30 m×0.25 mm I.D., df=0.25 mm (P/N 221-75954-30)

Insert liner: Topaz Liner Splitless Single Taper Gooseneck w/Wool, P/N 23336 (Restek)

Internal standard: PL Pesticide Surrogate standards Mix I, II (P/N 99056136, 99056191) (Hayashi Pure Chemical Ind., Ltd.)

This product was created based on results obtained by the Aichi Science and Technology Foundation "Knowledge Hub" Priority Research Project and Food Safety & Security Technology Development Project.

1. The accuracy of the information contained in the database and the usefulness of information obtained as a result of the use of this information is not guaranteed.
2. Be sure to test the qualitative and quantitative information obtained with this system using a standard sample for confirmation.
3. To reliably identify substances registered with this database, perform measurement using the system requirements of the method file included with the product.

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