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Smart Pesticides Database™ Ver. 2

GC/MS Residual Pesticides Database

Supports the Simultaneous Analysis of 530 Residual Pesticides in Foods via GC-MS(/MS)

Smart Pesticides Database contains the retention indices and transitions for 530 pesticides. Ver. 2 additionally contains measurement ions for SIM mode, so it can be applied to both SIM and MRM analyses.
Thanks to the retention indices contained in the database and the AART function, retention times can be revised automatically without the use of pesticide standards.
Furthermore, the Smart MRM/SIM function allows automatic creation of the optimal measurement programs for multicomponent simultaneous analysis using MRM and SIM modes.
Lastly, the database can be customized to the GC conditions and the addition of new components.

Compound Name (E)	Ret. Index 1	Ret. Index 2	Ret. Index 3	Ion1				Ion2				Ion1			Ion2		
				Type	m/z	CE	Ratio	Type	m/z	CE	Ratio	Type	m/z	Ratio	Type	m/z	Ratio
Hymexazol	1201	1193	1191	T	99.0>71.0	8	100.00	Ref.1	99.0>54.0	26	6.13	T	99.0	100.00	Ref.1	71.0	18.40
Methamidophos	1240	1231	1229	T	141.0>95.0	8	100.00	Ref.1	141.0>79.0	22	31.28	T	141.0	100.00	Ref.1	94.0	337.84
Dichlorvos	1248	1244	1243	T	109.0>79.0	8	100.00	Ref.1	185.0>93.0	14	56.91	T	185.0	100.00	Ref.1	109.0	403.23
Nereistoxin	1285	1284	1274	T	149.1>71.1	8	100.00	Ref.1	149.1>102.1	6	67.94	T	70.0	100.00	Ref.1	149.0	51.20
Allidochlor	1290	1288	1283	T	132.1>56.0	8	100.00	Ref.1	138.1>96.0	6	26.15	T	138.0	100.00	Ref.1	173.0	6.98
Dichlobenil	1348	1345	1335	T	170.9>136.0	14	100.00	Ref.1	170.9>100.0	24	98.06	T	171.0	100.00	Ref.1	173.0	76.00
EPTC	1359	1358	1353	T	189.1>128.1	4	100.00	Ref.1	189.1>86.0	12	22.96	T	128.0	100.00	Ref.1	189.0	25.60
Biphenyl	1393	1391	1380	T	154.1>128.1	22	100.00	Ref.1	154.1>115.1	24	74.03	T	154.0	100.00	Ref.1	153.0	37.60
Propamocarb	1394	1393	1390	T	188.2>72.0	4	100.00	Ref.1	188.2>173.2	4	72.45	T	58.0	100.00	Ref.1	129.0	2.40
Mevinphos-1	1420	1420	1419	T	127.0>109.0	12	100.00	Ref.1	192.0>127.0	12	61.12	T	127.0	100.00	Ref.1	192.0	31.60

Enables Analysis Conditions Corresponding to a Variety of Needs

Supporting simultaneous multicomponent, high-speed analysis, the database can enable a choice of methods according to the usage.
In addition, the database contains retention indices for multiple columns with different polarities. As a result, even if peaks of target pesticides and contaminants overlap it can use a different column.
If the database is used in combination with the Twin Line MS system, analysis with different columns can be performed smoothly, without compromising the MS vacuum.

Provides Total Solution Including Certified Standard Substances, a Pretreatment Kit, and Consumables

If used in combination with the recommended certified standard substances, pretreatment kit, columns, and insert liners, the database enables high-accuracy pesticide analysis.
The recommended pretreatment kit and the recommended protocol can be applied even to high-matrix samples such as health foods and processed foods.

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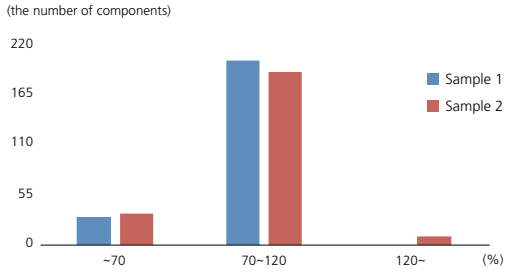
Verifying the Effectiveness of Recovery Tests of Health Foods

In conducting recovery tests in health foods for 220 pesticides, using the database, recommended pretreatment kit, pretreatment protocol, and certified standard substances, we succeeded in obtaining excellent ratios in over 80 percent of components.
Health foods contain many contaminants. Because it includes transitions for the separation of contaminants, the database minimizes their impact.
Additionally, the database can separate contaminants by allowing analysis with a different column, even if peaks of target pesticides and contaminants overlap.
If the database is used in combination with the Twin Line MS system, analysis with different columns can be performed smoothly, without compromising the MS vacuum.



Distribution of rates for two health food samples which were spiked with a pesticide standard sample so as to obtain a final concentration of 2.5 ng/mL each.

A printed handbook of the pretreatment protocol

A printed handbook of the recommended pretreatment protocol is provided (C146-E333), allowing customers to try the pretreatment process with ease.

Twin Line MS System

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 injection units.

Database Configuration

■ Product Contents

Database file and method files

■ Number of Pesticides Registered to the Database

530 compounds. Note: Commercially available standard mixtures are supported.

■ Applicable Instruments

GC-MS : GCMS-TQ™ Series
GCMS-QP2020 series, GCMS-QP2050
Excel® : Excel® 2021, 2019 (32/64-bit version)
Workstation : GCMSsolution™, LabSolutions™ DB GCMS, LabSolutions CS, LabSolutions GCMS

■ Recommended Consumables

Pretreatment Kit : Q-sep® QuEChERS Sample Prep Packets & Tubes (Restek)*
Certified Standard Substances
: GC Multiresidue Pesticide Kit (Restek)
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 221-75811-30
Column 3 : SH-I-5MS (30 m × 0.25 mm I.D., df = 0.25 mm), P/N 221-75940-30
Insert liner : Topaz® 3.5 mm I.D. Single Taper Inlet Liner w/ Wool (P/N 23336, Restek)

* For the recommended pretreatment protocol, contact Shimadzu.

Precautions

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 database 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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