

Screening for 926 Pesticides and Endocrine Disruptors by GC/MS with Deconvolution Reporting Software and a New Pesticide Library

Application Note

Food and Environmental

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Abstract

An updated and greatly expanded collection of mass spectral libraries has been introduced, replacing Agilent's RTL Pesticide Library and DRS pesticide solution. The new library contains 926 pesticides, endocrine disruptors, and related compounds – 359 more than the original library. Included are all compounds specified for GC/MS analysis in the new Japanese "Positive List" regulations. All compounds have locked retention times that can be accurately reproduced using an Agilent GC/MS system with the ChemStation's Retention Time Locking software. The new Database can be used as a standard GC/MS library for compound identification or with Agilent's Screener software for identifications based upon retention time and mass spectral matching. The greatest benefit accrues when these libraries are used with Agilent's new version of Deconvolution Reporting Software (part number G1716AA version A.03.00). This solution allows one to screen GC/MS files for all 926 pesticides and

endocrine disruptors in about two minutes per sample. Deconvolution helps identify pesticides that are buried in the chromatogram by co-extracted materials. The new database was compared to the smaller one for the DRS analysis of 17 surface water samples. With the new database, DRS found 99 pesticides, metabolites, fire retardants, and related contaminants that were not contained in the original RTL Pesticide and Endocrine Disruptor Library.

Introduction

Several years ago Agilent Technologies introduced Retention Time Locking (RTL) for gas chromatography (GC) and GC with mass spectral detection (GC/MS). RTL software makes it possible to reproduce retention times from run-to-run on any Agilent GC or GC/MS, in any laboratory in the world, so long as the same nominal method and GC column are used (1). Since any laboratory can reproduce retention times generated in another, it is possible to create mass spectral libraries that contain locked retention times. By locking their method to the published database, users can screen GC/MS files for all of the library's compounds. "Hits" are required to have the correct retention time as well as the correct spectrum, which eliminates many false positives and gives more confidence in compound identifications (2).



Agilent Technologies

More recently, Agilent introduced Deconvolution Reporting Software (DRS) that incorporates mass spectral deconvolution with conventional library searching and quantification. DRS results from a marriage of three different GC/MS software packages:

- 1) The Agilent GC/MS ChemStation,
- 2) The National Institute of Standards and Technology (NIST) Mass Spectral Search Program with the NIST '05 MS Library, and
- 3) The Automated Mass Spectral Deconvolution and Identification System (AMDIS) software, also from NIST.

The original DRS software was intended to be a comprehensive solution for pesticide analysis and, therefore, included the mass spectra (in AMDIS format) and locked retention times for 567 pesticides and suspected endocrine disruptors (3).

Recently, Agilent introduced an updated and greatly expanded Pesticide and Endocrine Disruptor Database (part number G1672AA) that now contains 926 entries. This represents the addition of 359 new compounds to the original library. At the same time, Agilent introduced a new version of the DRS software (part number G1716AA version A.03.00) that can be used with any Agilent-provided or user-developed DRS library.

Pesticide and Endocrine Disruptor Database Contents

The G1672AA Pesticide and Endocrine Disruptor Database contains virtually all GC-able pesticides, including those introduced very recently. In addition, the database includes numerous metabolites, more endocrine disruptors, important PCBs and PAHs, certain dyes (for example, Sudan Red), synthetic musk compounds, and several organophosphorus fire retardants.

This new database includes:

- A conventional mass spectral library for use with Agilent GC/MS ChemStations
- A screener database for use with Agilent's powerful screener software that is integrated into the GC/MS ChemStation
- Locked Retention Times for all 926 compounds that any Agilent 5975 or 5973 GC/MS user can reproduce in their laboratory
- Files for use with Agilent's G1716AA (A.03.00) Deconvolution Reporting Software
- An e-method that can be loaded into Agilent's G1701DA (version D.02.00 SP1 or higher) with instrument parameters for acquiring GC/MS files and analyzing the data with DRS. These parameters are listed in Table 1.
- Example files
- Application notes

On November 29, 2005, the Japanese Government published a "Positive List" system for the regulation of pesticides, feed additives, and veterinary drugs. Maximum Residue Limits (MRL) have been set for 758 chemicals while 65 others have been exempted from regulation. Fifteen substances must have no detectable residues. Other agricultural chemicals not mentioned have a uniform MRL of 0.01 ppm (4). This new regulation is scheduled to take effect on May 29, 2006.

Of the pesticides in the Japanese Positive List, 265 are to be analyzed by GC/MS. The new G1672AA Pesticide library contains mass spectra and locked retention times for all of these compounds. Thus, a laboratory could screen for all 265 "positive list" compounds and several hundred more pesticides in just 1–3 minutes after the GC/MS run.

Experimental

Table 1 lists the instrumentation, software, and analytical parameters used by Agilent for pesticide analysis. Depending upon the desired injection volume, a PTV inlet or split/splitless inlet can be used.

Table 1. Instrumentation and Conditions of Analysis

Gas Chromatograph	Agilent 6890N
Automatic Sampler	Agilent 7683 Injector and AutoSampler
Inlet	Agilent PTV operated in the solvent vent mode or Split/Splitless
Column	Agilent 30 m × 0.25 mm × 0.25 μm HP-5MSi (part number 19091S-433i)
Carrier gas	Helium in the constant pressure mode
Retention time locking	Chlorpyrifos-methyl locked to 16.596 min (nominal column head pressure = 17.1 psi)
Oven temperature program	70 °C (2 min), 25 °C/min to 150 °C (0 min), 3 °C /min to 200 °C (0 min), 8 °C /min to 280 °C (10–15 min)
PTV inlet parameters	Temp program: 40 °C (0.25 min), 1600 °C/min to 250 °C (2 min); Vent time: 0.2 min; Vent flow: 200 mL/min; Vent pressure: 0.0 psi; Purge flow: 60.0 mL/min; Purge time: 2.00 min
Injection volume	15 μL (using a 50-μL syringe)
Mass Selective Detector	Agilent 5975 inert
Tune file	Atune.u
Mode	Scan (or SIM with SIM DRS library)
Scan range	50–550 u
Source, quad, transfer line temperatures	230, 150, and 280 °C, respectively
Solvent delay	4.00 min
Multiplier voltage	Autotune voltage
Software	
GC/MSD ChemStation	Agilent part number G1701DA (version D02.00 sp1 or higher)
Deconvolution Reporting Software	Agilent part number G1716AA (version A.03.00) Deconvolution Reporting Software
Library searching software	NIST MS Search (version 2.0d or greater) (comes with NIST '05 mass spectral library – Agilent part number G1033A)
Deconvolution software	Automated Mass Spectral Deconvolution and Identification Software (AMDIS_32 version 2.62 or greater; comes with NIST '05 mass spectral library – Agilent part number G1033A)
MS Libraries	NIST '05 mass spectral library (Agilent part number G1033A) Agilent RTL Pesticide and Endocrine Disruptor Libraries in Agilent and NIST formats (part number G1672AA)

Results and Discussion

DRS, which has been described in preceding papers (3,5,6), can be summarized as follows:

Three separate, but complimentary, data analysis steps are combined into the DRS. First, the GC/MS ChemStation software performs a normal quantitative analysis for target pesticides using a target ion and up to three qualifiers. An amount is reported for all calibrated compounds that are detected. For other compounds in the database, an estimate of their concentration can be reported based upon an average pesticide response factor

that is supplied with the DRS software. The DRS then sends the data file to AMDIS, which deconvolutes the spectra and searches the Agilent RTL Pesticide Library using the deconvoluted full spectra. A filter can be set in AMDIS, which requires the analyte's retention time to fall within a user-specified time window. Because RTL is used to reproduce the RTL database retention times with high precision, this window can be quite small – typically 10–20 seconds. Finally, the deconvoluted spectra for all of the targets found by AMDIS are searched against the 147,000-compound NIST mass spectral library for confirmation; for this step, there is no retention time requirement.

This approach was rapidly adopted by many laboratories because of its ability to identify pesticides in complex chromatograms containing high levels of co-extracted interferences. Indeed, the solution proved to be so useful that users began to create their own DRS libraries (7). Therefore, the DRS was unbundled from the pesticide database so that it could be used with any agilent-provided or user-created database.

The original 567-compound RTL Pesticide Library (G1049A) included pesticides, a few metabolites, and most of the GC-amenable endocrine disruptors that were known at the time. The new version of the library includes many more pesticides, endocrine disruptors, and metabolites. This update also contains important compounds from other classes of contaminants that have been found in food and water supplies. Included are eighteen polychlorinated biphenyls (PCBs), four polybrominated biphenyls (PBBs), several polynuclear aromatic hydrocarbons (PAHs), several organophosphorus fire retardants, three important toxaphene congeners, and three Sudan dyes.

Advantages of Deconvolution

Figure 1 shows a screen from AMDIS that illustrates the power of this deconvolution software. The white trace in Figure 1A is the total ion chromatogram while the other three are extracted ions of a deconvoluted peak (a “component” in AMDIS terminology). Note that the TIC and extracted ions are not scaled to each other and this component is actually obscured by co-eluting compounds. Figure 1B juxtaposes the deconvoluted component spectrum (white) with the complete “undeconvoluted” spectrum (black). Clearly, this component is buried under co-eluting peaks that would ordinarily obscure the analyte. Figure 1C shows that the deconvoluted peak (white spectrum) is a good library match for norflurazon (black spectrum). The locked retention time for norflurazon in the RTL Pesticide Database is 26.933 min, which is just 2.3 seconds away from its observed RT in this chromatogram. Confidence in peak identifications is greatly enhanced by the combination of spectral deconvolution and locked retention time filtering.

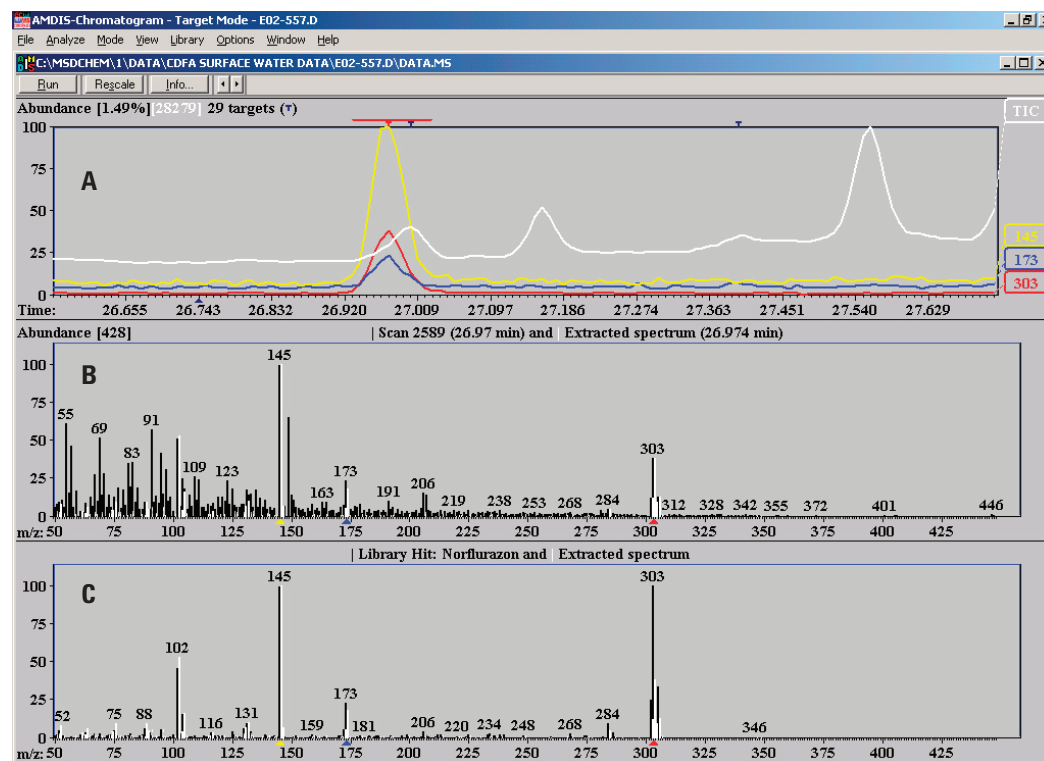


Figure 1. AMDIS screen showing the identification of norflurazon.

- A) The total ion and extracted ion chromatograms where norflurazon elutes.
- B) The deconvoluted component spectrum (white) juxtaposed with the spectrum at 26.972 min (black).
- C) The deconvoluted component matched to the library spectrum of norflurazon.

Surface Water Analysis - Revisiting an Earlier Study

In an earlier study, a comparison was made between Agilent's DRS and conventional pesticide analysis (3). The California Department of Food and Agriculture (CDFA) provided data files for 17 surface water extracts that had been analyzed in their laboratory. Since the GC/MS chromatograms were locked to the Agilent pesticide method, it was possible to analyze these data files using DRS without having to re-run the samples. The original DRS analysis was made using the 567-compound RTL Pesticide Database. For comparison, these same data files were re-analyzed using the new 926-compound RTL Pesticide Database. The chromatogram (Figure 2) and the DRS report (Figure 3) from one of these samples are shown below.

Excluding phthalates, seven new compounds (shown with bold type in Figure 3) were identified using the 926-compound database: 4-chlorophenyl isocyanate (a phenylurea herbicide metabolite); 3,4-dichlorophenyl isocyanate (diuron metabolite); tris(2-chloroethyl) phosphate (a fire retardant); caffeine (a stimulant); Cyprodinil (a fungicide); desmethyl-norflurazon (a metabolite of norflurazon, an herbicide); and tris(2-butoxyethyl) phosphate (a fire retardant). Although caffeine is not generally considered to be dangerous, it is included in the database because it has been found frequently in sewage effluent and in numerous waterways together with a various pharmaceuticals and pesticides (8).

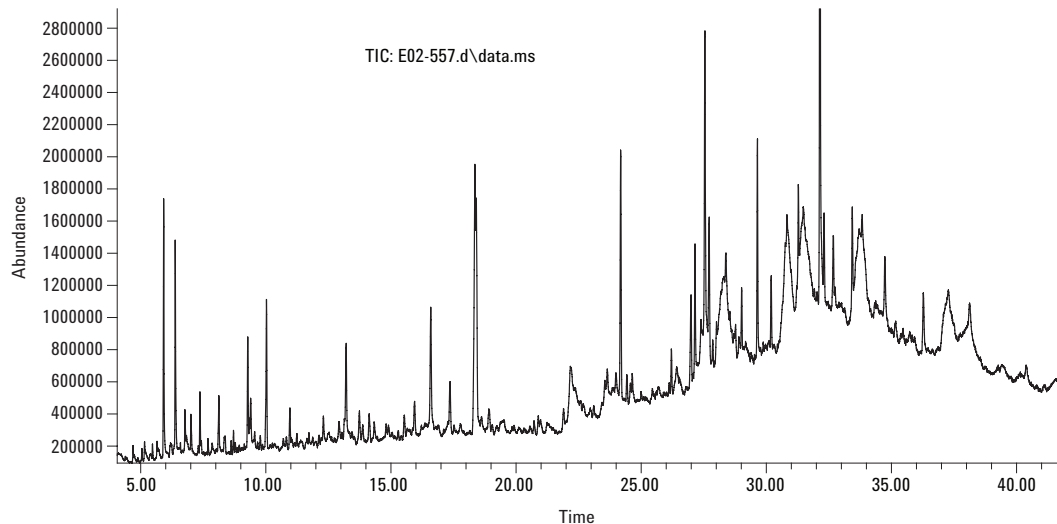


Figure 2. Chromatogram of a surface water extract that was analyzed by DRS using the new RTL Pesticide and Endocrine Disrupter Database. The results of this analysis are shown in Figure 3.

MSD Deconvolution Report

Sample Name: E02-557
Data File: C:\MSDCHEM\1\DATA\CDFA surface water data\E02-557.d
Date/Time: 11:24 AM Tuesday, Apr 4 2006

The NIST library was searched for the components that were found in the AMDIS target library.

RT	Cas #	Compound name	Agilent		RT Diff (sec.)	NIST	
			ChemStation amount (ng)	AMDIS match		reverse match	Hit number
4.4689	106445	4-Methylphenol		62	3.2		
4.4689	0000	3-Carbobenzyloxy-4-ketoproline				48	1
4.8840	104121	4-Chlorophenyl isocyanate		84	-1.8	86	2
6.3879	102363	Diuron Metabolite [3,4-Dichlorophenyl isocyanate]		99	3.1	95	1
6.8357	759944	EPTC		84	2.0	85	1
7.6988	95761	3,4-Dichloroaniline		93	2.1	89	2
7.9342	131113	Dimethylphthalate		67	1.7	84	2
8.1112	25013165	Butylated hydroxyanisole		63	-7.7		
8.1112	0000	7-Methoxy-2,2,4,8-tetramethyltricyclo [5.3.1.0(4,11)]undecane				62	1
8.941	29878317	Tolyltriazole [1H-Benzotriazole, 4-meth-]	1.29				
9.7903	134623	N,N-Diethyl-m-toluamide		85	2.2	84	2
10.0019	84662	Diethyl phthalate		98	2.6	92	1
10.7109	119619	Benzophenone		86	2.6	88	2
10.9684	126738	Tributyl phosphate		96	3.0	90	1
11.6491	1582098	Trifluralin		83	0.7	74	1
12.9326	122349	Simazine		88	1.4	86	2
13.4309	115968	Tris(2-chloroethyl) phosphate		79	1.0	78	1
13.7478	1517222	Phenanthrene-d10		95	1.3	83	1
15.4048	58082	Caffeine		80	1.6	74	1
15.9474	84695	Diisobutyl phthalate		90	3.2	88	4
16.5988	5598130	Chlorpyrifos Methyl		97	0.4	90	1
17.3653	7287196	Prometryn		90	1.5	84	1
18.4213	84742	Di-n-butylphthalate		99	0.4	94	1
18.9214	51218452	Metolachlor		90	0.7	87	1
20.5633	121552612	Cyprodinil		69	-0.1		
20.5633	76470252	9,9-Dimethoxy-9-sila-9, 10-dihydroanthracene				70	1
26.4247	23576241	Norflurazon, Desmethyl-		87	-4.5	69	2
26.9700	27314132	Norflurazon		87	1.5	79	1
26.9992	85687	Butyl benzyl phthalate		94	-0.5	94	1
27.3984	51235042	Hexazinone		89	0.8	83	1
28.0127	78513	Tris(2-butoxyethyl) phosphate		75	3.3	83	1
29.6537	117817	Bis(2-ethylhexyl)phthalate		98	0.3	90	3
33.9298	84764	Di-n-nonyl phthalate		65	-1.9		
33.9298	0000	Phthalic acid, 3,4-dichlorophenyl propyl ester				71	1
13.739		Phenanthrene-d10	10				

Figure 3. DRS report from the analysis of a surface water sample. The compounds shown in bold type were found by the new RTL Pesticide Database but not the original one because these compounds were not included.

For this sample, the ChemStation identified only tolyltriazole at 8.941 min, but AMDIS did not confirm this assignment, nor could it be confirmed manually. Butylated hydroxyanisole was tentatively identified by AMDIS with a low match value, but the retention time is off by -7.7 seconds which is considerably more than most other hits. This compound is not in the NIST library so it could not be confirmed. The ChemStation method used for this analysis required that all three qualifier ions fall within $\pm 20\%$ (relative) which is a rigorous requirement for such a complex sample. This explains why so few compounds were found by the ChemStation.

Cyprodinil (20.563 min) was identified by AMDIS but the NIST library search failed to confirm its presence. The next line shows that the best NIST library match is an anthracene derivative that is nothing like cyprodinil. This result was obtained when AMDIS was configured to “use uncertain peaks” as shown in Figure 4. When this feature is

turned off in DRS Compound Identification Configuration, the best NIST library hit for this spectrum is, indeed, cyprodinil. When a compound's identity is ambiguous, as with cyprodinil, it may be useful to perform the DRS search both ways and compare the results.

In the comparison described earlier (3), DRS was able to identify all 37 pesticides found by the CDFA chemist. However, DRS completed the task for all 17 samples in about 20 minutes compared to ~8 hours for the manual procedure (Table 2). Moreover, DRS identified one false positive in the CDFA report and found 34 additional pesticides and related compounds.

Using the new 926-compound Database, it took 32 minutes to analyze all of the samples and DRS was able to find an additional 99 pesticides, metabolites, fire retardants, and related compounds (Table 2).

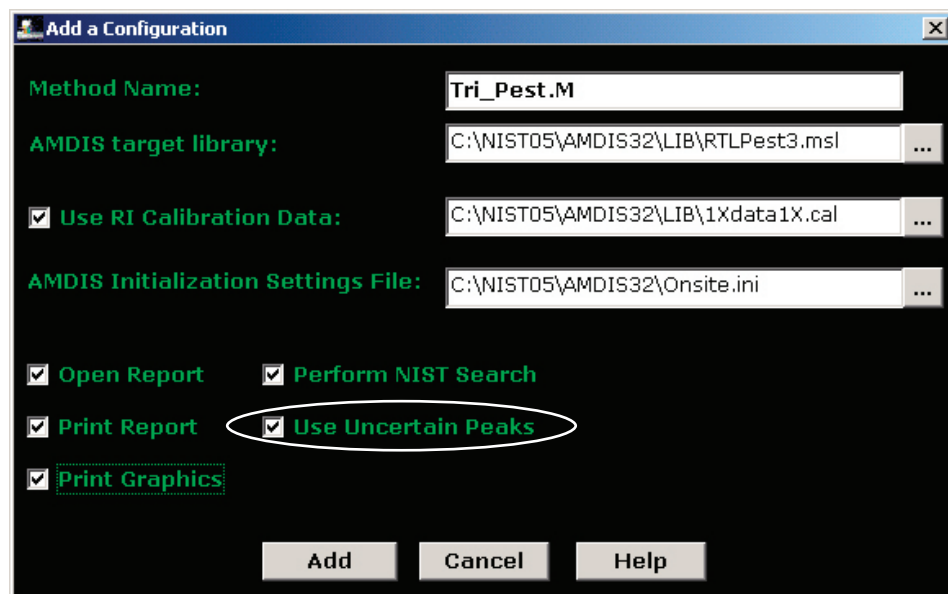


Figure 4. DRS configuration screen for the method called **Tri_Pest**. When the box labeled “Use Uncertain Peaks” is checked, AMDIS will use uncertain peaks for library searches. When unchecked, AMDIS ignores uncertain mass spectral peaks. Sometimes, this can affect the quality of a library match.

Table 2. Comparison of the Results Obtained by Screening 17 Surface Water Extracts Using Traditional Methods (CDFA) and Using DRS With Two Different Databases – the G1049A With 567 Compounds and the G1672AA With 926 Entries

	CDFA	Agilent DRS (Original G1049A database)	Agilent DRS (G1672 AA database)
Targets found (not counting ISTD)	37	Same 37 +34 more	Same 37 +99 more
False positives	1	0	0
Processing time	~8 hrs (ChemStation only)	20 minutes	32 min

Handling Stereoisomers

Many pesticides have multiple stereoisomers with virtually identical mass spectra. For example, cyfluthrin has four diastereomers arising from its three chiral centers. It is very difficult and sometimes impossible to determine the elution order of these isomers and most analysts report them as a sum of the isomer amounts. Agilent's G1049A RTL Pesticide database arbitrarily assigned each isomer a Roman numeral with I for the earliest eluting isomer, II for the next, and so on. The same Chemical Abstracts Service number (CAS #) was assigned to all of the isomers. Generally, it was a CAS # for the compound with "unstated stereochemistry." This caused some incompatibility with AMDIS as explained below.

AMDIS software differentiates among compounds using a "chemical identification number." The easiest and most consistent approach is to use each compound's CAS #. The default setting for AMDIS is to allow each CAS # to be used only once when analyzing a GC/MS data file. While this seems logical, it requires that each database entry have a different CAS #. It is possible to allow multiple hits per compound by checking the box in AMDIS found in the drop down menu under Analyze/Settings/Identif. However, this allows multiple peaks to be assigned the same compound name.

In the new RTL Pesticide Database (G1672AA), the Roman numeral designations remain and the first isomer in the series is given its genuine CAS #. Subsequent isomers in the series are given unique, but fictitious "CAS #s" generated by Agilent. The compound's real CAS # appears in braces after the compound name. For example, the cyfluthrin isomers are entered into the database as shown in Table 3.

Table 3. Method for Listing Compounds with Multiple Stereoisomers in the New G1672AA RTL Pesticide Database

RT	Compound name*	CAS #**
32.218	Cyfluthrin I	68359-37-5
32.359	Cyfluthrin II {CAS # 68359-37-5}	999028-03-4
32.477	Cyfluthrin III {CAS # 68359-37-5}	999029-03-7
32.536	Cyfluthrin IV {CAS # 68359-37-5}	999030-03-4

* In a series, the earliest eluting isomer is identified with "I" and is assigned its legitimate CAS #. Subsequent isomers are assigned unique, but fictitious CAS #s (see footnote **). Their actual CAS # is put in braces behind the compound name.

** Cyfluthrin I has been given its genuine CAS #. Cyfluthrin II-IV have been given unique numbers that can be distinguished from actual CAS numbers because they all have six digits before the first hyphen (9 total) and all begin with the series 999.

Figure 5 shows how permethrin was identified in a spinach sample using both databases with AMDIS configured to allow one hit per compound. Using the older 567-compound database (G1049A) only one permethrin isomer was identified because its CAS # could be used only once. With the new format used in the 926-compound RTL Pesticide Database (G1672AA), both isomers of permethrin were identified. Not surprisingly, the NIST library search found no hits with the same fictitious CAS # assigned to permethrin II. So, the software printed the best match on the following line. This compound, a cyclopropanecarboxylic acid derivative, is a permethrin isomer.

So long as the NIST library search is turned on in DRS, it will always print another line after reporting a compound with a fictitious CAS #. Note that these fictitious CAS #s always contain 9 digits and begin with 999.

A)

RT	Cas #	Compound name	Agilent			NIST	
			ChemStation amount (ng)	AMDIS match	RT Diff (sec.)	reverse match	Hit number
31.6158	52645531	Permethrin II		88	3.9	91	3

B)

RT	Cas #	Compound name	Agilent			NIST	
			ChemStation amount (ng)	AMDIS match	RT Diff (sec.)	reverse match	Hit number
31.4127	52645531	Permethrin I		78	2.6	81	3
31.6088	999046036	Permethrin II {CAS # 52645-53-1}		65	3.5		
31.6088	51877748	Cyclopropanecarboxylic acid, 3-(2,2-dichlorovinyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester, (1R-trans)-				95	1

Figure 5. A) A single isomer of permethrin was identified by DRS using the G1049A 567-compound database when AMDIS was not allowed to use multiple hits per compound. B) Two permethrin isomers are identified by DRS with the G1672AA 926-compound database under the same circumstances.

Conclusions

The new G1672AA RTL Pesticide and Endocrine Disruptor library contains substantially more target analytes than its predecessor. With the addition of 359 new compounds, it is the most comprehensive library of its type available today. Many new pesticides, metabolites, and endocrine disruptors were added along with important PCBs, PBBs, PAHs, synthetic musk compounds, Sudan dyes, and organophosphorus fire retardants. The database contains all of the analytes specified for GC/MS analysis in the new Japanese “Positive List” regulations.

When combined with the complete DRS solution, one can screen GC/MS data files for all 926 compounds in about two minutes per sample. This is the fastest, most comprehensive, most accurate, and least tedious method for screening food and environmental samples for these compounds.

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Appendix A

Lists of Compounds in Databases

1,2,4-Trichlorobenzene	2,6-Dimethylaniline	Acetochlor
1,2-Dibromo-3-chloropropane	2-[3-Chlorophenoxy]propionamide	Acifluorfen methyl ester
1,3,5-Tribromobenzene	2-Chlorophenol	Aclonifen
1,3-Dichlorobenzene	2-Ethyl-1,3-hexanediol	Acrinathrin
17 α -Ethinylestradiol	2-ethyl-6-methylaniline	Alachlor
1-naphthalenol	2-Hydroxyestradiol	Aldrin
2-(1-naphthyl)acetamide	2-Methyl-4,6-dinitrophenol	Allidochlor
2-(2-Butoxyethoxy)ethyl thiocyanate	2-Methylphenol	Ametryn
2-(Octylthio)ethanol	2-Nitrophenol	Amidithion
2,3,4,5-Tetrachloronitrobenzene	2-Phenoxypropionic acid	Aminocarb
2,3,4,5-Tetrachlorophenol	3,4,5-Trimethacarb	Amitraz
2,3,4,6-Tetrachlorophenol	3,4-Dichloroaniline	Amitraz metabolite [Methanimidamide, N-(2,4-dimethylphenyl)-N'-methyl-]
2,3,5,6-Tetrachlorophenol	3,5-Dichloroaniline	Ancymidol
2,3,5,6-Tetrachloro-p-terphenyl	3-Aminophenol	Anilazine
2,3,5-Trichlorophenol	3-Chloro-4-fluoroaniline	Aniline
2,3,5-Trimethacarb	3-Chloro-4-methoxyaniline	Anilofos
2,3,6-Trichloroanisole	3-Chloroaniline	Anthracene
2,3,7,8-Tetrachlorodibenzofuran	3-Hydroxycarbofuran	Aramite I
2,3,7,8-Tetrachlorodibenzo-p-dioxin	3-Indolylacetoneitrile	Aramite II {CAS # 140-57-8}
2,4,5,6-Tetrachloro-m-xylene	3-Trifluormethylaniline	Atraton
2,4,5-T methyl ester	4,4'-Dichlorobenzophenone	Atrazine
2,4,5-Trichloroaniline	4,4'-Oxydianiline	Atrazine-desethyl
2,4,5-Trichlorophenol	4,6-Dinitro-o-cresol (DNOC)	Azaconazole
2,4,5-Trichloro-p-terphenyl	4-Aminodiphenyl	Azamethiphos
2,4,5-Trimethylaniline	4-Bromoaniline	Azibenzolar-S-methyl
2,4,6-Tribromoanisole	4-Chloro-2-methylaniline	Azinphos-ethyl
2,4,6-Tribromophenol	4-Chloro-3-methylphenol	Azinphos-methyl
2,4,6-Trichloroanisole	4-Chloroaniline	Aziprotryn metabolite [2-Amino-4-isopropylamino-6-methylthio-1,3,5-triazine]
2,4,6-Trichlorophenol	4-Chlorophenyl isocyanate	Aziprotryne
2,4-D methyl ester	4-Isopropylaniline	Azobenzene
2,4-D sec-butyl ester	4-Methylphenol	Azoxybenzene
2,4-DB methyl ester	4-Nitrophenol	Azoxystrobin
2,4'-Dichlorobenzophenone (2,4'-Dicofol decomposition product)	4-Nonylphenol	Barban
2,4-Dichlorophenol	5,7-Dihydroxy-4'-methoxyisoflavone	Beflubutamid
2,4-Dichlorophenyl benzenesulfonate	9,10-Anthraquinone	Benalaxyl
2,4-Dimethylaniline	Acenaphthene	Benazolin-ethyl
2,4-Dimethylphenol	Acenaphthylene	Bendiocarb
2,6-Dichlorobenzamide	Acephate	Benfluralin
2,6-Dichlorobenzonitrile	Acequinocyl	
	acetamiprid	

Benfuracarb	Bromophos-ethyl	Chlordimeform
Benfuresate	Bromopropylate	Chlorethoxyfos
Benodanil	Bromoxynil	Chlorfenapyr
Benoxacor	Bromoxynil octanoic acid ester	Chlorfenethol
Bentazone	Bromuconazole I	Chlorfenprop-methyl
Bentazone methyl derivative	Bromuconazole II {CAS # 116255-48-2}	Chlorfenson
Benthiocarb	Bufencarb	Chlorfenvinphos
Benzene, 1,3-bis(bromomethyl)-	Bupirimate	Chlorfenvinphos, <i>cis</i> -
Benzenesulfonamide	Buprofezin	Chlorfenvinphos, <i>trans</i> -
Benzidine	Butachlor	Chlorflurecol-methyl ester
Benzo(a)anthracene	Butafenacil	Chlormefos
Benzo(a)pyrene	Butamifos	Chlornitrofen
Benzo[b]fluoranthene	Butoxycarboxim	Chlorobenzilate
Benzo[g,h,i]perylene	Butralin	Chloroneb
Benzo[k]fluoranthene	Butyl benzyl phthalate	Chloropropylate
Benzophenone	Butylate	Chlorothalonil
Benzoximate metabolite	Butylated hydroxyanisole	Chlorotoluron
Benzoylprop ethyl	Cadusafos	Chlorpropham
Benzyl benzoate	Cafenstrole	Chlorpyrifos
b-Estradiol	Caffeine	Chlorpyrifos Methyl
BHC alpha isomer	Captafol	Chlorthal-dimethyl
BHC beta isomer	Captan	Chlorthiamid
BHC delta isomer	Carbaryl	Chlorthion
BHC epsilon isomer	Carbetamide	Chlorthiophos
Bifenazate metabolite (5-Phenyl-o-anisidine)	Carbofuran	Chlorthiophos sulfone
Bifenox	Carbofuran-3-keto	Chlorthiophos sulfoxide
Bifenthrin	Carbofuran-7-phenol	Chlozolate
Binapacryl	Carbophenothion	Chrysene
Bioallethrin	Carbosulfan	Cinerin I
Bioallethrin S-cyclopentenyl isomer	Carboxin	Cinerin II
Bioresmethrin	Carfentrazone-ethyl	Cinidon-ethyl
Biphenyl	Carpropamid	cis-Chlordane
Bis(2,3,3,3-tetrachloropropyl) ether	Carvone	Clodinafop-propargyl
Bis(2-butoxyethyl) phthalate	Cashmeran	Clomazone
Bis(2-ethylhexyl)phthalate	Cekafix	Cloquintocet-mexyl
Bisphenol A	Celestolide	Coumaphos
Bitertanol I	Chinomethionat	Crimidine
Bitertanol II {CAS # 55179-31-2}	Chloramben methyl ester	Crotoxyphos
Boscalid (Nicobifen)	Chloranocryl	Crufomate
Bromacil	Chlorbenside	Cyanazine
Bromfenvinphos-(E)	Chlorbenside sulfone	Cyanofenphos
Bromfenvinphos-(Z)	Chlorbicyclen	Cyanophos
Bromobutide	Chlorbromuron	Cyclafuramid
Bromocyclen	Chlorbufam	Cycloate
Bromophos	Chlordecone	Cyclopentadecanone
	Chlordene, <i>trans</i> -	Cycluron

Cyflufenamid	Dichlofluanid metabolite (DMSA)	Dinocap I
Cyfluthrin I	Dichlone	Dinocap II {CAS # 39300-45-3}
Cyfluthrin II {CAS # 68359-37-5}	Dichlormid	Dinocap III {CAS # 39300-45-3}
Cyfluthrin III {CAS # 68359-37-5}	Dichlorophen	Dinocap IV {CAS # 39300-45-3}
Cyfluthrin IV {CAS # 68359-37-5}	Dichlorprop	Di-n-octyl phthalate
Cyhalofop-butyl	Dichlorprop methyl ester	Dinoseb
Cyhalothrin I (lambda)	Dichlorvos	Dinoseb acetate
Cyhalothrin (Gamma)	Diclobutrazol	Dinoseb methyl ether
Cymiazole	Diclocymet I	Dinoterb
Cymoxanil	Diclocymet II {CAS # 139920-32-4}	Dinoterb acetate
Cypermethrin I	Diclofop methyl	Di-n-propyl phthalate
Cypermethrin II {CAS # 52315-07-8}	Dicloran	Diofenolan I
Cypermethrin III {CAS # 52315-07-8}	Dicrotophos	Diofenolan II {CAS # 63837-33-2}
Cypermethrin IV {CAS # 52315-07-8}	Dicyclohexyl phthalate	Dioxabenzofos
Cyphenothrin <i>cis</i> -	Dicyclopentadiene	Dioxacarb
Cyphenothrin <i>trans</i> - {CAS # 39515-40-7}	Dieldrin	Dioxathion
Cyprazine	Diethyl ethyl	Diphacinone
Cyproconazole	Diethofencarb	Diphenamid
Cyprodinil	Diethyl dithiobis(thionoformate) (EXD)	Diphenyl phthalate
Cyprofuram	Diethyl phthalate	Diphenylamine
Cyromazine	Diethylene glycol	Dipropetryn
d-(<i>cis-trans</i>)-Phenothrin-I	Diethylstilbestrol	Dipropyl isocinchomeronate
d-(<i>cis-trans</i>)-Phenothrin-II {CAS # 260002-80-2}	Difenoconazol I	Disulfoton
Dazomet	Difenoconazol II {CAS # 119446-68-3}	Disulfoton sulfone
DDMU [1-Chloro-2,2-bis(4'-chlorophenyl)]	Difenoxuron	Ditalimfos
Decachlorobiphenyl	Diflufenican	Dithiopyr
Deltamethrin	Diisobutyl phthalate	Diuron
Demephion	Dimefox	Diuron Metabolite [3,4-Dichlorophenyl isocyanate]
Demeton-S	Dimepiperate	Dodemorph I
Demeton-S-methylsulfon	Dimethachlor	Dodemorph II {CAS # 1593-77-7}
Desbromo-bromobutide	Dimethametryn	Drazoxolon
Desmedipham	Dimethenamid	Edifenphos
Desmetryn	Dimethipin	Empenthrin I
Dialifos	Dimethoate	Empenthrin II {CAS # 54406-48-3}
Di-allate I	Dimethomorph-(E)	Empenthrin III {CAS # 54406-48-3}
Di-allate II {CAS # 2303-16-4}	Dimethomorph-(Z) {CAS # 110488-70-5}	Empenthrin IV {CAS # 54406-48-3}
Diamyl phthalate	Dimethylphthalate	Empenthrin V {CAS # 54406-48-3}
Diazinon	Dimethylvinphos(z)	Endosulfan (alpha isomer)
Diazinon-oxon	Dimetilan	Endosulfan (beta isomer)
Dibenz[a,h]anthracene	Dimoxystrobin	Endosulfan ether
Dicamba	Di-n-butylphthalate	Endosulfan lactone
Dicamba methyl ester	Di-n-hexyl phthalate	Endosulfan sulfate
Dicapthon	Diniconazole	Endrin
Dichlofenthion	Dinitramine	Endrin aldehyde
Dichlofluanid	Di-n-nonyl phthalate	Endrin ketone
	Dinobuton	

EPN	Fenoprop methyl ester	Fluoxastrobin <i>cis</i> -
Epoxiconazole	Fenothiocarb	Fluquinconazole
EPTC	Fenoxanil	Flurenol-butyl ester
Erbon	Fenoxaprop-ethyl	Flurenol-methylester
Esfenvalerate	Fenoxycarb	Fluridone
Esprocarb	Fenpiclonil	Flurochloridone I
Etaconazole	Fenpropathrin	Flurochloridone II {CAS # 61213-25-0}
Ethalfuralin	Fenpropidin	Flurochloridone, deschloro-
Ethidimuron	Fenson	Fluroxyppy-1-methylheptyl ester
Ethiofencarb	Fensulfothion	Flurprimidol
Ethiolate	Fensulfothion-oxon	Flurtamone
Ethion	Fensulfothion-oxon -sulfone	Flusilazole
Ethofenprox	fensulfothion-sulfone	Fluthiacet-methyl
Ethofumesate	Fenthion	Flutolanil
Ethofumesate, 2-Keto	Fenthion sulfoxide	Flutriafol
Ethoprophos	Fenthion-sulfone	Fluvalinate-tau-I
Ethoxyfen-ethyl	Fenuron	Fluvalinate-tau-II {CAS # 102851-06-9}
Ethoxyquin	Fenvalerate I	Folpet
Ethylenethiourea	Fenvalerate II {CAS # 51630-58-1}	Fonofos
Etoxazole	Fepropimorph	Formothion
Etridiazole	Fipronil	Fosthiazate I
Etridiazole, deschloro- (5-ethoxy-3-dichloromethyl-1,2,4-thiadiazole)	Fipronil, desulfinyl-	Fosthiazate II {CAS # 98886-44-3}
Etrimfos	Fipronil-sulfide	Fuberidazole
Eugenol	Fipronil-sulfone	Furalaxyl
Exaltolide [15-Pentadecanolide]	Flamprop-isopropyl	Furathiocarb
Famoxadon	Flamprop-methyl	Furilazole
Famphur	Fluacrypyrim	Furmecyclox
Fenamidone	Fluazifop-p-butyl	Halfenprox
Fenamiphos sulfoxide	Fluazinam	Haloxifop-methyl
Fenamiphos-sulfone	Fluazolate	Heptachlor
Fenarimol	Flubenzimine	Heptachlor epoxide isomer A
Fenazaflor	Fluchloralin	Heptachlor exo-epoxide isomer B
Fenazaflor metabolite	Flucythrinate I	Heptenophos
Fenazaquin	Flucythrinate II {CAS # 70124-77-5}	Hexabromobenzene
Fenbuconazole	Fludioxonil	Hexachlorobenzene
Fenchlorazole-ethyl	Flufenacet	Hexachlorophene
Fenchlorphos	Flumetralin	Hexaconazole
Fenchlorphos-oxon	Flumiclorac-pentyl	Hexazinone
Fenclorim	Flumioxazin	Hexestrol
Fenfuram	Fluometuron	Hydroprene
Fenhexamid	Fluoranthene	Imazalil
Fenitrothion	Fluorene	Imazamethabenz-methyl I
Fenitrothion-oxon	Fluorodifen	Imazamethabenz-methyl II {CAS # 81405-85-8}
Fenobucarb	Fluoroglycofen-ethyl	Imibenconazole
Fenoprop	Fluoroimide	Imibenconazole-desbenzyl
	Fluotrimazole	

Indeno[1,2,3-cd]pyrene	Mecoprop methyl ester	Monocrotophos
Indoxacarb and Dioxacarb decomposition product [Phenol, 2-(1,3-dioxolan-2-yl)-]	Mefenacet	Monolinuron
Ioxynil	Mefenpyr-diethyl	Musk amberette
Ioxynil octanoate	Mefluidide	Musk Ketone
Ipconazole	Menazon	Musk Moskene
Iprobenfos	Mepanipirim	Musk Tibetene (Moschustibeten)
Iprodione	Mephosfolan	Musk xylene
Iprovalicarb I	Mepronil	Myclobutanil
Iprovalicarb II {CAS # 140923-25-7}	Metalaxyl	N,N-Diethyl-m-toluamide
Irgarol	Metamitron	N-1-Naphthylacetamide
Isazophos	Metasystox thiol	Naled
Isobenzan	Metazachlor	Naphthalene
Isobornyl thiocynoacetate	Metconazole I	Naphthalic anhydride
Isocarbamide	Metconazole II {CAS # 125116-23-6}	Naproanilide
Isocarbophos	Methabenzthiazuron [decomposition product]	Napropamide
Isodrin	Methacrifos	Nicotine
Isufenphos	Methamidophos	Nitralin
Isufenphos-oxon	Methfuroxam	Nitrapyrin
Isomethiozin	Methidathion	Nitrofen
Isoprocarb	Methiocarb	Nitrothal-isopropyl
Isopropalin	Methiocarb sulfone	N-Methyl-N-1-naphthyl acetamide
Isoprothiolane	Methiocarb sulfoxide	Nonachlor, <i>cis</i> -
Isoproturon	Methomyl	Nonachlor, <i>trans</i> -
Isoxaben	Methoprene I	Norflurazon
Isoxadifen-ethyl	Methoprene II {CAS # 40596-69-8}	Norflurazon, desmethyl-
Isoxaflutole	Methoprotryne	Nuarimol
Isoxathion	Methoxychlor	o,p'-DDD
Jasmolin I	Methoxychlor olefin	o,p'-DDE
Jasmolin II	Methyl (2-naphthoxy)acetate	o,p'-DDT
Jodfenphos	Methyl paraoxon	Octachlorostyrene
Kinoprene	Methyl parathion	o-Dianisidine
Kresoxim-methyl	Methyl-1-naphthalene acetate	o-Dichlorobenzene
Lactofen	Methyldymron	Ofurace
Lenacil	Metobromuron	Omethoate
Leptophos	Metolachlor	o-Phenylphenol
Leptophos oxon	Metolcarb	Orbencarb
Lindane	Metominostrobin (E)	<i>ortho</i> -Aminoazotoluene
Linuron	Metominostrobin (Z) {CAS # 133408-50-1}	Oryzalin
Malathion	Metrafenone	Oxabetrinil
Malathion-o-analog	Metribuzin	Oxadiazon
MCPA methyl ester	Mevinphos	Oxadixyl
MCPA-butoxyethyl ester	Mirex	Oxamyl
MCPB methyl ester	Molinate	Oxycarboxin
m-Cresol	Monalide	Oxychloridane
Mecarbam		Oxydemeton-methyl
		Oxyfluorfen

p,p'-DDD	Phenanthrene	Promecarb
p,p'-DDE	Phenanthrene-d10	Promecarb artifact [5-isopropyl-3-methylphenol]
p,p'-DDM [<i>bis</i> (4-chlorophenyl)methane]	Phenakapton	Prometon
p,p'-DDT	Phenol	Prometryn
p,p'-Dibromobenzophenone	Phenothiazine	Propachlor
p,p'-Dicofol	Phenothrin I	Propamocarb
Paclobutrazol	Phenothrin II	Propanil
Paraoxon	Phenoxyacetic acid	Propaphos
Parathion	Phenthoate	Propargite
PBB 52 Tetrabrombiphenyl	Phorate	Propargite metabolite [Cyclohexanol, 2-(4-tert-butylphenoxy)]
PBB 101	Phorate sulfone	Propazine
PBB 15	Phorate sulfoxide	Propetamphos
PBB 169 Hexabrombiphenyl	Phorate-oxon	Propham
PCB 101	Phosalone	Propiconazole-I
PCB 105	Phosfolan	Propiconazole-II {CAS # 60207-90-1}
PCB 110	Phosmet	Propisochlor
PCB 118	Phosphamidon I	Propoxur
PCB 126	Phosphamidon II {CAS # 13171-21-6}	Propyzamide
PCB 127	Phthalide	Prosulfocarb
PCB 131	Phthalimide	Prothioconazole-desthio
PCB 136	Picloram methyl ester	Prothiofos
PCB 138	Picolinafen	Prothoate
PCB 153	Picoxystrobin	Pyracarbolid
PCB 169	Pindone	Pyraclufos
PCB 170	Piperalin	Pyraflufen-ethyl
PCB 180	Piperonyl butoxide	Pyrazon
PCB 30	Piperophos	Pyrazophos
PCB 31	Pirimicarb	Pyrazoxyfen
PCB 49	Pirimiphos-ethyl	Pyrene
PCB 77	Pirimiphos-methyl	Pyrethrin I
PCB 81	Plifenat	Pyrethrin II
p-Dichlorobenzene	p-Nitrotoluene	Pyributicarb
Pebulate	Potasan	Pyridaben
Penconazole	Prallethrin, <i>cis</i> -	Pyridaphenthion
Pendimethalin	Prallethrin, <i>trans</i> - {CAS # 23031-36-9}	Pyridate
Pentachloroaniline	Pretilachlor	Pyridinitril
Pentachloroanisole	Probenazole	Pyrifenox I
Pentachlorobenzene	Prochloraz	Pyrifenox II {CAS # 88283-41-4}
Pentachloronitrobenzene	Procymidone	Pyriftalid
Pentachlorophenol	Prodiamine	Pyrimethanil
Pentanochlor	Profenofos	Pyrimidifen
Permethrin I	Profenofos metabolite (4-Bromo-2-chlorophenol)	Pyriminobac-methyl (E)
Permethrin II {CAS # 52645-53-1}	Profluralin	Pyriminobac-methyl (Z) {CAS # 136191-64-5}
Perthane	Prohydrojasmon I	
Phantolide	Prohydrojasmon II {CAS # 158474-72-7}	
Phenamiphos		

Pyriproxyfen	Tecnazene	Triadimenol
Pyroquilon	Tefluthrin, <i>cis</i> -	Tri-allate
Quinalphos	Temephos	Triamiphos
Quinoclamine	Terbacil	Triapenthenol
Quinoxifen	Terbucarb	Triazamate
Quintozene metabolite (pentachlorophenyl methyl sulfide)	Terbufos	Triazophos
Quizalofop-ethyl	Terbufos-oxon-sulfone	Tributyl phosphate
Rabenzazole	Terbufos-sulfone	Tributyl phosphorotrithioite
Resmethrin	Terbumeton	Trichlamide
Resmethrine I	Terbuthylazine	Trichlorfon
Resmethrine II {CAS # 10453-86-8}	Terbuthylazine-desethyl	Trichloronate
Rotenone	Terbutryne	Triclopyr methyl ester
S,S,S-Tributylphosphorotrithioate	Tetrachlorvinphos	Triclosan
Schradan	Tetraconazole	Triclosan-methyl
Sebuthylazine	Tetradifon	Tricresylphosphate, <i>meta</i> -
Sebuthylazine-desethyl	Tetraethylpyrophosphate (TEPP)	Tricresylphosphate, <i>ortho</i> -
Secbumeton	Tetrahydrophthalimide, <i>cis</i> -1,2,3,6-	Tricresylphosphate, <i>para</i>
Silafluofen	Tetramethrin I	Tricyclazole
Silthiopham	Tetramethrin II {CAS # 7696-12-0}	Tridemorph, 4-tridecyl-
Simazine	Tetrapropyl thiodiphosphate	Tridiphane
Simeconazole	Tetrasul	Trietazine
Simetryn	Thenylchlor	Triethylphosphate
Spirodiclofen	Theobromine	Trifenmorph
Spiromesifen	Thiabendazole	Trifloxystrobin
Spiroxamine I	Thiazopyr	Triflumizole
Spiroxamine II {CAS # 118134-30-8}	Thifluzamide	Trifluralin
Spiroxamine metabolite (4-tert-butylcyclohexanone)	Thiofanox	Triphenyl phosphate
Sudan I	Thiometon	Tris(2-butoxyethyl) phosphate
Sudan II	Thionazin	Tris(2-chloroethyl) phosphate
Sudan Red	Thymol	Tris(2-ethylhexyl) phosphate
Sulfallate	Tiocarbazil I	Triticonazole
Sulfanilamide	Tiocarbazil II {CAS # 36756-79-3}	Tryclopyrbutoxyethyl
Sulfentrazone	Tolclofos-methyl	Tycor (SMY 1500)
Sulfotep	Tolfenpyrad	Uniconazole-P
Sulfur (S8)	Tolyfluanid	Vamidothion
Sulprofos	Tolyfluanid metabolite (DMST)	Vernolate
Swep	Tolyltriazole [1H-Benzotriazole, 4-methyl-]	Vinclozolin
Tamoxifen	Tolyltriazole [1H-Benzotriazole, 5-methyl-]	XMC (3,4-Dimethylphenyl N-methylcarbama
TCMTB	Tonalide	XMC (3,5-Dimethylphenyl N-methylcarbama
Tebuconazole	Toxaphene Parlar 26	Zoxamide
Tebufenpyrad	Toxaphene Parlar 50	Zoxamide decomposition product
Tebupirimifos	Toxaphene Parlar 62	
Tebutam	<i>trans</i> -Chlordane	
Tebuthiuron	Transfluthrin	
	Traseolide	
	Triadimefon	

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