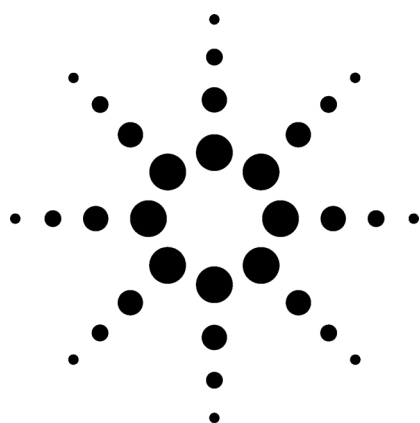


Semivolatiles Retention Time Locked (RTL) Deconvolution Databases for Agilent GC/MSD Systems



Application

Environmental

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Abstract

The G1677AA Semivolatiles Retention Time Locked database/library can provide rapid confirmation of environmental contaminants in complex matrices when used with Deconvolution Reporting Software. Separate methods and databases are included for wastewater and drinking water, with locked retention times. Compound lists are based on U.S. EPA Method 8270 (273 compounds) and Method 525 (119 compounds). Acquisition methods for both splitless and programmable temperature vaporizing inlets are provided. Full spectra are used for identification of deconvoluted analytes, not just a few extracted ions. When used with MSD ChemStation Rev E.02 or later, quantitation of the deconvoluted data from AMDIS is possible, in addition to the normal quantitation. The G1677AA Environmental Semivolatiles retention time locking database/library is an add-on product to the base deconvolution reporting software product G1716AA.

Introduction

Agilent Deconvolution Reporting Software (DRS) is a software package that combines the information from three separate processes into one easy-to-read report: 1) MSD ChemStation identification and quantitation, 2) industry standard AMDIS deconvolution with full spectrum identification 3) NIST full spectrum Search. The primary benefit of

DRS is significant time savings when interpreting results from complex matrix analyses.

Target compound identification and quantitation in environmental samples is often a tedious task and is therefore well suited to DRS. The list of target compounds varies widely, depending on geographic region, government requirements, and sample type. There is no universal list of analytes tied to specific methods that will satisfy all laboratories all of the time.

The United States Environmental Protection Agency (U.S. EPA) has published numerous GC/MSD methods for organic analytes in various matrices. U.S. EPA Method 525 is specified for drinking water and Method 8270 for wastewater, each having its own set of compounds. The compounds lists for these methods are extensive and form the basis for the deconvolution databases discussed in this note. Laboratories are not required to follow the U.S. EPA methods exactly to use the databases effectively. Compounds/spectra can easily be added by users to the databases for suitability in their own labs.

Databases/Libraries

Collections of mass spectral data are referred to as libraries or databases. DRS uses the combined general description of database/library (DBL). Retention time is a critical component of sample identification, and the compounds in these DBLs have been acquired using retention time locking (RTL).

The G1677AA Environmental Semivolatiles RTL DBL is a set of mass spectral libraries in the Agilent and NIST/AMDIS formats. There are three



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separate sets of files and methods. An 8270 set includes the mass spectra and locked retention times for 243 single-component semivolatiles compounds and internal standards specified by U.S. EPA Method 8270, plus 30 additional compounds of environmental interest – a total of 273 compounds. Two different 525 sets are included, one optimized for a split/splitless inlet and one optimized for a PTV inlet, designated as “long.” Each 525 set includes mass spectra and locked retention times for the same 119 single-component semivolatiles compounds and internal standards specified by U.S. EPA Method 525. A complete listing of the DBL compounds can be found in Appendix A.

Each DBL entry contains the following information:

- Mass spectrum acquired using Atune.u on a 5975 MSD
- Locked retention time determined on a 6890N/5975 or 7890A/5975 GC/MSD system. Compounds were injected at least once with phenanthrene-d10 locked to 9.500 ± 0.01 minutes. Phenanthrene-d10 was locked to 12.700 ± 0.01 minutes for the 525 PTV “long” method.
- Molecular formula
- Molecular weight (nominal mass)
- CAS number

Spectra were compared to those contained in the NIST05a Mass Spectral Library. Tests were performed on spiked samples containing hydrocarbon interferences and the results were compared to the list of spiked compounds.

Minimum system requirements for using the semi-VOAs DBLs

- G1716AA deconvolution reporting software, base product
- Agilent GC/MS system with E.02.00.xxx software preferred

Experimental

The instrument operating conditions used for acquiring the 8270 and 525 spectra and retention times are listed in Table 1. Splitless injection utilizing a split/splitless inlet with the column connected directly to the MSD was done. The thicker film 20-m column allows good separation of the early eluters from the solvent while providing a short run time of 17 min. An inlet temperature of 300 °C is optimum for later eluting PAHs but basic compounds, such as benzidine, have improved

response factors at lower inlet temperatures, 250 to 275 °C. Retention time locking to phenanthrene-d10 at 9.500 min was done in constant-flow mode, at 0.8 mL/min. The mass range of 35 to 500 is suitable for both lists of compounds. A 6-mm large-aperture drawout lens provides better high-end linearity at the expense of some sensitivity loss. The standard 3-mm lens could be used.

Table 1. 8270 and 525 Methods – Gas Chromatograph and Mass Spectrometer Conditions

GC	Agilent Technologies 6890N or 7890A		
Inlet	EPC split/splitless – rear location		
Mode	Splitless, 0.5 µL injected		
Inlet temperature	300 °C		
Pressure	16.9 psi initial		
Purge flow	30.0 mL/min		
Purge time	0.75 min		
Gas saver	Off		
Gas type	Helium		
Liner	Agilent helix, single-taper, p/n 5188-5397		
Oven	240V		
Oven ramp	°C/min	Next °C	Hold min
Initial		40	1.00
Ramp 1	25	320	4.80
Total run time	17.0 min		
Equilibration time	0.5 min		
Oven max temp.	325 °C		
Column	Agilent Technologies DB-5.625, p/n 121-5622		
Length	20.0 m		
Diameter	0.18 mm		
Film thickness	0.36 µm		
Mode	Constant flow = 0.8 mL/min		
Pressure	16.7 psi initial		
Inlet	Rear		
Outlet	MSD		
Outlet pressure	Vacuum		
RTL	System retention time locked to phenanthrene-d10 at 9.500 min		
MSD	Agilent Technologies 5975, performance turbo		
Drawout lens	6-mm large-aperture drawout lens p/n G2589-20045		
Solvent delay	2.8 min		
Tune	Atune.u		
EM voltage	Tune voltage		
Mass range	35 to 500 amu		
Threshold	0		
Sampling	2		
Quad temperature	180 °C		
Source temperature	300 °C		
Transfer line temp.	280 °C		

The instrument operating conditions used for acquiring the 525 “long” retention times are listed in Table 2. A programmable temperature vaporizing inlet (PTV) was used with a 25-µL large volume injection (LVI). PTV-LVI is popular in labs requiring lower detection limits for drinking water. Active analytes have improved performance as they

vaporize at the lowest possible temperature compared to a hot splitless injection. Phenanthrene-d10 is used as the retention time locking compound at 12.700 min running in constant-flow mode at 1.5 mL/min. The PTV parameters are not directly transferrable to the 20-m column used in Table 1, without affecting retention times. The 30-m column provides better separation for SIM analysis, allowing more ions/compound or more SIM cycles/peak than a shorter run. Users can build their own SIM-based DBLs with a requirement of 4 ions/compound for best identification with deconvolution. Alternatively, SIM/scan data acquisition could be done with the SIM data used for quantitation and the scan data used for full-spectrum deconvolution. The 45 to 450 scan range is suitable for the 525 DBL. The sampling rate of two can be changed to one to maintain an equal number of scan cycles if SIM/scan is used.

Table 2. 525 Long Method – Gas Chromatograph and Mass Spectrometer Conditions

GC			
Agilent Technologies 6890N or 7890A			
Inlet	EPC PTV – front location		
Mode	Solvent vent – 25 uL injected		
Temp ramp	°C/min	Next °C	Hold min
Initial		20	0.60
Ramp 1	600	350	1.30
Ramp 2	10	250	0.00
Cryo	On		
Cryo use temperature	100 °C		
Cryo timeout	10.00 min (On)		
Cryo fault	On		
Pressure	11.77 psi (On)		
Vent time	0.60 min		
Vent flow	100.0 mL/min		
Vent pressure	0.0 psi		
Purge flow	50.0 mL/min		
Purge time	2.50 min		
Total flow	53.9 mL/min		
Gas saver	Off		
Gas type	Helium		
PTV Liner	Agilent multi-baffle liner, no packing, p/n 5183-2037		
Oven	120V		
Oven ramp	°C/min	Next °C	Hold min
Initial		40	2.50
Ramp 1	50	110	0.00
Ramp 2	10	320	1.10
Total run time	26 min		
Equilibration time	0.5 min		
Oven max temperature	325 °C		
Column	Agilent Technologies HP 5 MSi, p/n 19091S-433i		
Length	30.0 m		
Diameter	0.25 mm		
Film thickness	0.25 µm		
Mode	Constant flow – 1.5 mL/min		
Pressure	11.77 psi		

Inlet	Front
Outlet	MSD
Outlet pressure	Vacuum
RTL	System retention time locked to phenanthrene-d10 at 12.700 min

Front Injector	
Sample washes	0
Sample pumps	2
Injection volume	25 microliters
Syringe size	50 microliters
PreInj. Solv A washes	0
PreInj. Solv B washes	1
PostInj. Solv A washes	2
PostInj. Solv B washes	2
Viscosity delay	1 second
Plunger speed	Variable
Injection speed	50 microliters/minute
Draw speed	600 microliters/minute
Dispense speed	6000 microliters/minute
PreInjection dwell	0 minutes
PostInjection dwell	0 minutes

MSD	
Agilent Technologies 5975C, performance turbo	
Drawout lens	6-mm large-aperture drawout lens p/n G2589-20045
Solvent delay	4 min
Low mass	45 amu
High mass	450 amu
Threshold	0
Sampling	2
Quad temperature	180 °C
Source temperature	300 °C
Transfer line temperature	280 °C
Tune type	Autotune
EM voltage	Tune voltage, 1247 V

Results and Discussion

Retention Time Locking – or Not

Maximum productivity from DRS is realized if the GC/MSD system is retention time locked. The DRS report displays RT differences of found targets from their expected RTs, which is important for differentiating compounds with similar spectra. AMDIS parameters can be set to exclude compounds found outside their expected RT windows, which eliminates false positives. Retention time locking also eliminates the need to change SIM acquisition times, a tedious task with multiple SIM groups. Therefore, it is strongly recommended that users run with an RTL system.

Although the majority of labs run RTL, some users may choose not to do so. Two different approaches can be used in this case, each with limited success.

Approach 1 – Updating the *.cal File

The *.cal file establishes the relationship between retention times found on any given day to those

expected in the AMDIS databases (*.msl and *.cid). For the semivolatiles DBL the *.cal files contain only ISTDs and surrogates. It is assumed that other analytes will track the retention time changes of these compounds. Whenever RTs change, the *.cal file RTs must be changed. This can be done by manually editing the RTs in the *.cal file using Notepad. Once all RTs have been updated, select Save, not Save As. A second choice is to have AMDIS rebuild the *.cal file. The procedure for this is in AMDIS Help.

Approach 2 – Updating the *.msl and *.cid Files

A menu item is provided in MSD data analysis, DRS > Update AMDIS Library RTs using quant database. This will update the RTs in both necessary AMDIS files using the current MSD quant database times and will save a copy of the original two AMDIS files.

Cautions: If the quant database contains an incorrect time, that time will be used. If the quant database does not contain a compound that is in the AMDIS files, AMDIS RTs will not be updated.

Using the Semivolatiles RTL DBL

The following files are installed:

8270_DRS_Demo.D	525_DRS_Demo.D	525_Long_DRS_Demo.D
8270_DRS.L	525_DRS.L	
8270_RTL_DRS.M	525_RTL_DRS.M	525_Long_RTL_DRS.M
8270.MSL	525.MSL	525_Long.MSL
8270.CID	525.CID	525_Long.CID
8270_cal_RT.CAL	525_cal_RT.CAL	525_Long_cal_RT.CAL
8270_cal_RT.CSL	525_cal_RT.CSL	525_Long_cal_RT.CSL

The typical locations into which the CD installer places the files are as follows:

Agilent MSD ChemStation datafiles *.D and Methods *.m in

C:\msdchem\MSDemo\Semivolatiles Example Data

C:\msdchem\MSDemo\Semivolatiles Example Methods

AMDIS files *.msl, *.cid, *.cal, and *.csl in

C:\NIST05\AMDIS32\LIB

MSD ChemStation Library Files, *.L in **C:\Database**

The MSD ChemStation methods contain a retention time locked quant database with single-point calibration. These methods can be used directly in data analysis, as described later. The methods also contain data acquisition parameters and retention time locking data. Users may have to resolve differences between their system and the method configuration upon loading the method in data acquisition. Additionally, new retention time locking data may have to be acquired. In most cases users will only have to relock their system if it is configured the same as the system in Table 1 or Table 2.

DRS in MSD Data Analysis

It is strongly recommended that an operator inexperienced in DRS first proceed to the General Help file section “Generating and Interpreting A Report Using DRS Manually/Interactively.” Complete all of the the Spinach A, B and C exercises for the best fundamental understanding of DRS. Then proceed as follows.

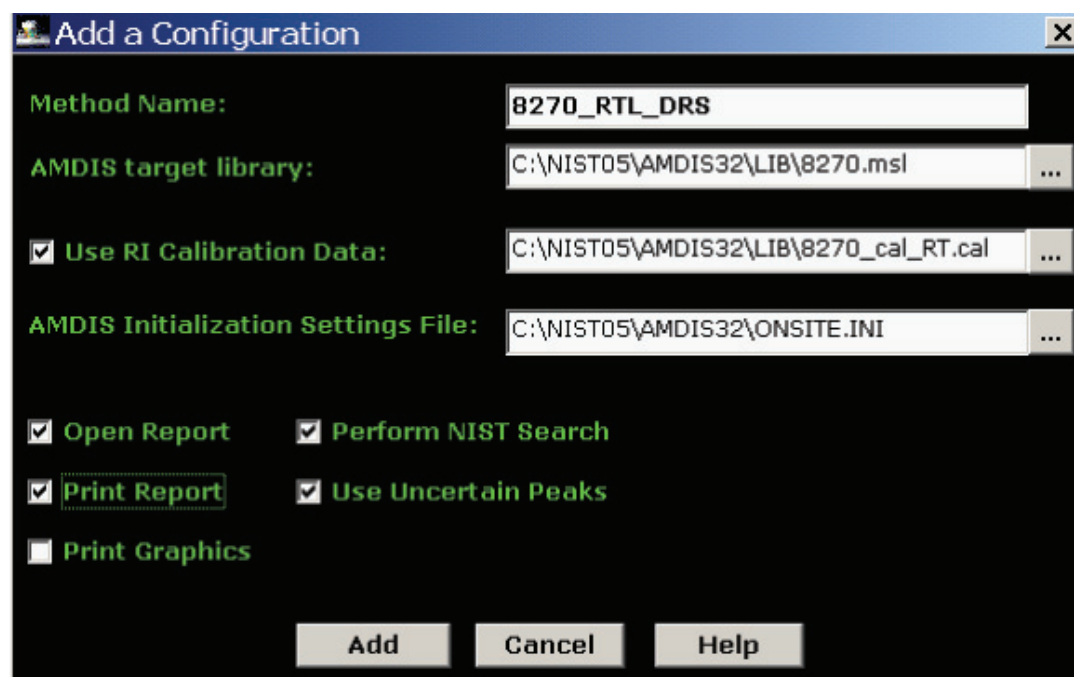
Open AMDIS as a standalone application and then select Analyze > Settings. Verify that the settings are as shown below, then select Save. If prompted to reanalyze, select No, then exit AMDIS. The settings will be permanently saved in the AMDIS initialization file onsite.ini.

After AMDIS settings have been addressed, it will be necessary to configure a DRS method, depending on the analysis chosen. The relationship of the AMDIS and MSD ChemStation files are shown in the Table below.

MSD ChemStation method	MSD ChemStation select library	DRS configurator method	DRS configurator AMDIS target library	DRS configurator RI calibration file	DRS configurator AMDIS .ini file
8270_RTL_DRS.m	8270_DRS.L	8270_RTL_DRS	8270.msl	8270_cal_RT.cal	Onsite.ini
525_RTL_DRS.m	525_DRS.L	525_RTL_DRS	525.msl	525_cal_RT.cal	Onsite.ini
525_long_DRS.m	525_DRS.L	525_long_DRS	525_long.msl	525_long_cal_RT.cal	Onsite.ini

A DRS method must be configured for each of the applications that will be used. Let's look at one example of using the semivolatiles DBL, in this case the 8270 set.

1. Configure a NEW DRS Method using the Method Configurator as shown below.



2. Select Add then Exit > Exit and Save.
3. In the MSD ChemStation, Data Analysis View, Load Method 8270_RTL_DRS.m.
4. Load datafile 8270_DRS_Demo.D.
5. From the Data Analysis View DRS menu, select Quant + DRS Single File.

At the end of the DRS process a report similar to the one shown should be generated.

MSD Deconvolution Report

Sample Name: 5ppm 8270sm + 50GKD

Data File: C:\msdchem\1\DATA\8270_D~1.D

Date/Time: 05:00 PM Monday, Dec 17 2007

Adjacent Peak Subtraction = 1

Resolution = Medium

Sensitivity = High

Shape Requirements = Medium

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

R.T.	Cas #	Compound Name	Amount (ng)		AMDIS		NIST	
			Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
2.8499	62759	N-Nitrosodimethylamine	5.56		93	-0.5	96	1
4.7302	62533	Aniline			98	4.2	96	1
5.0358	3855821	1,4-Dichlorobenzene-d4	40		99	-0.2	93	1
5.2143	106445	4-Methylphenol			66	-7.7	89	1
5.3059	98862	Acetophenone			49	-4.6		
5.3059	105055	Benzene, 1,4-diethyl-					89	1
6.2476	1146652	Naphthalene-d8	40		99	-0.1	86	1
6.2679	91203	Naphthalene	3.77		58	-0.1		
6.2679	5405798	3-Hexanone, 2,2-dimethyl-					81	1
6.787	680319	Hexamethylphosphoramid	0.28					
6.9442	91576	2-Methylnaphthalene			97	0.1	91	1
7.761	95830	4-Chloro-1,2-phenylenediamine	0.69					
7.845	5131602	4-Chloro-1,3-phenylenediamine	0.1					
7.9945	15067262	Acenaphthene-d10	40		98	-0.1	82	1
8.0256	51285	2,4-Dinitrophenol			58	0.0	68	1
8.0572	100027	4-Nitrophenol	2.44		81	-0.1	92	1
8.195	132649	Dibenzofuran	0.11					
8.3833	84662	Diethyl phthalate	0.23		78	-0.2	75	1
8.530	99558	5-nitro-o-toluidine	0.11					
8.5420	86737	Fluorene			56	0.0	80	58
8.5644	534521	4,6-Dinitro-2-methylphenol			89	-0.1	88	1
8.6164	86306	N-Nitrosodiphenylamine			45	-0.8		
8.6164	3892000	Pentadecane, 2,6,10-trimethyl-					84	1
9.2806	92671	4-Aminobiphenyl	6.1		94	-0.1	89	2
9.2829	87865	Pentachlorophenol	4.22		91	-0.1	66	11
9.4964	1517222	Phenanthrene-d10	40		97	-0.1	86	1
9.5139	120127	Anthracene			52	-3.4	70	15
9.5175	85018	Phenanthrene			68	-0.2	80	1
10.0286	84742	di-n-Butyl phthalate			74	-0.1	84	9
10.8285	92875	Benzidine	5.67		97	0.8	91	1
12.1025	91941	3,3'-Dichlorobenzidine	5.3		95	-0.4	97	1
12.1665	1719035	Chrysene-d12	40		93	-0.3	92	1
12.168	56553	Benz[a]anthracene	0.06					
12.168	218019	Chrysene	0.08					
12.168	732116	Phosmet	0.27					
13.3443	207089	Benzo[k]fluoranthene			93	-2.4	94	2
13.3443	205992	Benzo[b]fluoranthene	5.75		95	-0.2	90	2
13.381	207089	Benzo[k]fluoranthene	5.89					
13.8809	1520963	Perylene-d12	40		99	-0.6	77	1

This report is based on DRS revision A.04. Previous DRS revisions do not have AMDIS settings in the header, nor do they have a column for the amount calculated from AMDIS. The AMDIS calculated amount will be available after using QEdit in MSD ChemStation, Rev E.02 and later. Please consult the DRS A.04 Help section “Using QEdit with DRS Quantitative Data” for details.

The user can also configure DRS methods for either of the 525 sets of files, similar to that shown above for the 8270 set. Methods and demo datafiles are provided.

Conclusions

The Semivolatiles RTL DBL can provide rapid confirmation of environmental contaminants in complex matrices when used with DRS. Separate databases are provided for wastewater and drinking water, with locked retention times. Full spectra are used for identification of deconvoluted analytes. When used with MSD ChemStation Rev E.02 or later, quantitation on the deconvoluted data from AMDIS is possible, in addition to the normal quantitation. The G1677AA Environmental Semivolatiles RTL DBL is an add-on product to the base DRS product G1716AA.

For More Information

For more information on our products and services, visit our Web site at www.agilent.com/chem.

Appendix A

Lists of Compounds

Combined alphabetical listing of compounds from both the 8270_DRS.L and the 525_DRS.L, including CAS number and library entry number. Italics indicate the additional 30 compounds in the 8270 DBL. Retention time information can be found in the method quant databases, the Agilent libraries, or the AMDIS databases.

Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #	Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #
Acenaphthene	83329	71		gamma-BHC (lindane)	58899	115	39
Acenaphthene-d10	15067262	55	1	Bis(2-chloroethoxy)methane	111911	39	
Acenaphthylene	208968	69	12	Bis(2-chloroethyl) ether	111444	13	
Acetophenone	98862	26		Bis(2-chloroisopropyl) ether	108601	21	
2-Acetylaminofluorene	53963	185		Bis(2-ethylhexyl)phthalate	117817	191	108
1-Acetyl-2-thiourea	591082	271		Bromacil	314409		58
Alachlor	15972608		54	4-Bromophenyl phenyl ether	101553	103	
Aldrin	309002	137	61	Bromoxynil	1689845	97	
Ametryn	834128		55	Butachlor	23184669		79
2-Aminoanthraquinone	117793	267		Butifos	78488		85
Aminoazobenzene	60093	253		Butyl benzyl phthalate	85687	173	95
4-Aminobiphenyl	92671	111		Butylate	2008415		8
3-Amino-9-ethylcarbazole	132321	264		Captafol	2425061	186	
Anilazine	101053	141		Captan	133062	142	
Aniline	62533	12		Carbaryl	63252	129	
o-Anisidine	90040	240		Carbazole	86748	126	
Anthracene	120127	124	43	Carbofuran	1563662	110	
Aramite	140578	155		Carbophenothion	786196	176	
Atraton	1610179		31	Carboxin	5234684		88
Atrazine	1912249		35	Chlordane (NOS)	57749	252	
Azinphos-methyl	86500	199		alpha-Chlordane	5103719		80
Azobenzene (conv: 1,2-diphenylhydrazine)	103333	93		gamma-Chlordane	5103742		73
Barban	101279	160		Chlorfenvinphos	470906	145	
Benz[a]anthracene	56553	193	103	4-Chloroaniline	106478	44	
Benzidine	92875	149		Chlorobenzilate	510156	164	91
Benzo[a]pyrene	50328	216	114	<i>2-Chlorobiphenyl</i>	2051607	73	16
Benzo[b]fluoranthene	205992	212	112	5-Chloro-2-methylaniline	95794	256	
Benzo[ghi]perylene	191242	223	119	4-Chloro-3-methylphenol	59507	51	
Benzo[k]fluoranthene	207089	213	113	3-(Chloromethyl)pyridine	3099318	276	
Benzoic acid	65850	37		1-Chloronaphthalene	90131	270	
p-Benzoquinone	106514	238		2-Chloronaphthalene	91587	62	
Benzyl alcohol	100516	18		Chloroneb	2675776		17
alpha-BHC (alpha-HCH)	319846	104	28	2-Chlorophenol	95578	15	
beta-BHC (beta-HCH)	319857	109	38	4-Chloro-1,2-phenylenediamine	95830	260	
delta-BHC (delta-HCH)	319868	123	47	4-Chloro-1,3-phenylenediamine	5131602	259	
				4-Chlorophenyl phenyl ether	7005723	84	

Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #	Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #
Chlorothalonil	1897456		49	3,3'-Dimethylbenzidine	119937	174	
Chlorpropham	101213		26	a,a-Dimethylphenethylamine	122098	40	
Chlorpyrifos	2921882		63	1,3-Dimethyl-2-nitrobenzene-ss	81209		3
Chrysene	218019	194	105	2,4-Dimethylphenol	105679	36	
Chrysene-d12	1719035	153	99	Dimethyl phthalate	131113	66	11
Coumaphos	56724	208		Di-n-butyl phthalate	84742	131	59
p-Cresidine	120718	237		1,2-Dinitrobenzene	528290	274	
Crotoxyphos	7700176	146		1,3-Dinitrobenzene	99650	67	
Cyanazine	21725462		64	1,4-Dinitrobenzene	100254	273	
Cycloate	1134232		25	4,6-Dinitro-2-methylphenol	534521	89	
2-Cyclohexyl-4,6-dinitro-phenol	131895	266		2,4-Dinitrophenol	51285	72	
Dacthal (DCPA)	1861321		66	2,4-Dinitrotoluene	121142	76	19
4,4'-DDD	72548	167	93	2,6-Dinitrotoluene	606202	68	15
4,4'-DDE	72559	154	86	Dinocap I	39300453	190	
4,4'-DDT	50293	179	98	Di-n-octyl phthalate	117840	207	
Demeton-O	298033	251		Dinoseb	88857	119	
Demeton-S	126750	107		Diphenamid	957517	239	68
Diallate	2303164	100		Diphenylamine	122394	91	
2,4-Diaminotoluene	95807	268		5,5-Diphenylhydantoin	57410	257	
Diazinon	333415		44	1,2-Diphenylhydrazine	122667	272	
Dibenz[a,h]anthracene	53703	222	118	Disulfoton	298044	120	45
Dibenz(a,i)acridine	224420	250		Disulfoton sulfone	2497065		75
Dibenzofuran	132649	77		Disulfoton sulfoxide	2497076		6
Dibenzo(a,e)pyrene	192654	249		Endosulfan I	959988	150	78
Dibrom (naled)	300765	94		Endosulfan II	33213659	169	92
1,2-Dibromo-3-chloropropane	96128	275		Endosulfan sulfate	1031078	182	96
Dichlone	117806	116		Endrin	72208	166	90
1,2-Dichlorobenzene	95501	19		Endrin aldehyde	7421934	172	94
1,3-Dichlorobenzene	541731	16		Endrin ketone	53494705	189	
1,4-Dichlorobenzene	106467	17		EPN	2104645	197	
1,4-Dichlorobenzene-d4	3855821	1		EPTC	759944		7
3,3'-Dichlorobenzidine	91941	192		Ethion	563122	168	
2,3-Dichlorobiphenyl	16605917	105	29	Ethoprophos	13194484		24
2,4-Dichlorophenol	120832	41		Ethyl carbamate	51796	246	
2,6-Dichlorophenol	87650	45		Ethyl methanesulfonate	62500	9	
Dichlorvos	62737	48	4	Etridiazole	2593159		13
Dicrotophos	141662	248		Famphur	52857	171	
Dieldrin	60571	161	87	Fenamiphos	22224926		82
Di(2-ethylhexyl)adipate	103231		101	Fenarimol	60168889		109
Diethyl phthalate	84662	82	22	Fensulfotion	115902	159	
Diethylstilbestrol	56531	181		Fenthion	55389	139	
Diethyl sulfate	64675	247		Fluchloralin	33245395	125	
Dimethoate	60515	108		Fluoranthene	206440	152	
3,3'-Dimethoxybenzidine	119904	265		2-Fluorobiphenyl	321608	60	
p-(Dimethylamino)azobenzene	60117	163		Fluorene	86737	86	21
7,12-Dimethylbenz[a]anthracene	57976	211		Fluridone	59756604		116

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2-Fluorophenol	367124	7		Methyl parathion	298000	128	
Heptachlor	76448	130	53	2-Methylphenol	95487	20	
Heptachlor epoxide -isomer B	1024573	143	70	3-Methylphenol	108394	23	
2,2',3,3',4,4',5-Heptachlorobiphenyl	35065306	203		4-Methylphenol	106445	22	
2,2',3,3',4,4',6-Heptachlorobiphenyl	52663715		104	Metolachlor	51218452		62
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065293	195		Metribuzin	21087649		51
2,2',3,4,4',5',6-Heptachlorobiphenyl	52663691	187		Mevinphos	7786347	63	9
2,2',3,4',5,5',6-Heptachlorobiphenyl	52663680	184		Mexacarbate	315184	241	
1,2,3,4,6,7,8-Heptachlorodibenzo- furan	67562394	215		MGK 264 - a	113484		67
1,2,3,4,6,7,8-Heptachlorodibenzo- p-dioxin	35822469	217		MGK 264 - b	113484		69
Hexachlorobenzene	118741	106	30	Mirex	2385855	204	
2,2',3,4,4',5'-Hexachlorobiphenyl	35065282	180		Molinatate	2212671		20
2,2',3,4,5,5'-Hexachlorobiphenyl	52712046	175		Monocrotophos	6923224	98	
2,2',3,5,5',6-Hexachlorobiphenyl	52663635	162		Naphthalene	91203	43	
2,2',4,4',5,5'-Hexachlorobiphenyl	35065271	170		Naphthalene-d8	1146652	30	
2,2',4,4',5,6'-Hexachlorobiphenyl	60145224		89	1,4-Naphthoquinone	130154	65	
Hexachlorobutadiene	87683	47		1-Naphthylamine	134327	80	
Hexachlorocyclopentadiene	77474	56	5	2-Naphthylamine	91598	78	
1,2,3,4,7,8-Hexachlorodibenzofuran	70648269	205		Napropamide	15299997		83
1,2,3,4,7,8-Hexachlorodibenzo- p-dioxin	39227286	209		Nicotine	54115	58	
Hexachloroethane	67721	29		5-Nitroacenaphthene	602879	255	
Hexachlorophene	70304	214		2-Nitroaniline	88744	64	
Hexachloropropene	1888717	46		3-Nitroaniline	99092	70	
Hexamethylphosphoramid	680319	245		4-Nitroaniline	100016	87	
Hexazinone	51235042		100	5-Nitro-o-anisidine	99592	254	
Hydroquinone	123319	244		Nitrobenzene	98953	32	
Indeno[1,2,3-cd]pyrene	193395	221	117	Nitrobenzene-d5	4165600	31	
Isodrin	465736	140		4-Nitrobiphenyl	92933	258	
Isophorone	78591	34	2	Nitrofen	1836755	165	
Isosafrole	120581	61		2-Nitrophenol	88755	35	
Kepone	143500	177		4-Nitrophenol	100027	74	
Leptophos	21609905	201		4-Nitroquinoline-1-oxide	56575	136	
Malathion	121755	132		5-Nitro-o-toluidine	99558	85	
Maleic anhydride	108316	243		N-Nitrosodiethylamine	55185	8	
Merphos	150505		72	N-Nitrosodimethylamine	62759	2	
Mestranol	72333	242		N-Nitrosodi-n-butylamine	924163	49	
Methapyrilene	91805	138		N-Nitrosodi-n-propylamine	621647	25	
Methoxychlor	72435	188	106	N-Nitrosodiphenylamine	86306	90	
3-Methylcholanthrene	56495	218		N-Nitrosomethylethylamine	10595956	4	
4,4'-Methylenebis (2-chloroaniline)	101144	263		N-Nitrosomorpholine	59892	27	
4,4'-Methylenebis (N,N-dimethylaniline)	101611	262		N-Nitrosopiperidine	100754	33	
Methyl methanesulfonate	66273	6		N-Nitrosopyrrolidine	930552	24	
2-Methylnaphthalene	91576	53		trans-Nonachlor	39765805		81
Methyl paraoxon	950356		46	Norflurazon	27314132		97
				2,2',3,3',4,4',5,5',6-Nonachlorobi- phenyl	40186729	210	
				2,2',3,3',4,5',6,6'-Octachlorobi- phenyl	40186718		107

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Octachlorodibenzofuran	39001020	220		Simazine	122349		33
Octachlorodibenzo-p-dioxin	3268879	219		Simetryn	1014706		52
Octamethyl pyrophosphoramidate	152169	239		Stirofos (Tetrachlorvinphos)	22248799		77
4,4'-Oxydianiline	101804	261		Strychnine	57249	231	
Parathion (ethyl)	56382	134		Sulfallate	95067	230	
Pebulate	1114712		14	Sulfotepp	3689245	95	
Pentachlorobenzene	608935	75		Tebuthiuron	34014181		18
2,2',3,4,5'-Pentachlorobiphenyl	38380028	156		Terbacil	5902512		48
2,2',3',4,6'-Pentachlorobiphenyl	60233252		71	Terbufos	13071799	121	40
2,2',4,5,5'-Pentachlorobiphenyl	37680732	148		Terbutryne	886500		57
2,3,3',4',6'-Pentachlorobiphenyl	38380039	158		Terphenyl-d14	1718510	157	
1,2,3,7,8-Pentachlorodibenzofuran	57117416	198		1,2,4,5-Tetrachlorobenzene	95943	54	
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	40321764	202		2,2',3,5'-Tetrachlorobiphenyl	41464395	135	
Pentachloroethane	76017	14		2,2',4,4'-Tetrachlorobiphenyl	2437798		60
Pentachloronitrobenzene	82688	113		2,2',5,5'-Tetrachlorobiphenyl	35693993	133	
Pentachlorophenol	87865	112	37	2,3',4,4'-Tetrachlorobiphenyl	32598100	144	
cis-Permethrin	54774457		110	2,3,7,8-Tetrachlorodibenzofuran	51207319	178	
trans-Permethrin	51877748		111	2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746016	183	
Perylene-d12	1520963	206	115	2,3,4,6-Tetrachlorophenol	58902	79	
Phenacetin	62442	101		Tetrachlorvinphos	961115	151	
Phenanthrene	85018	122	42	Tetraethylpyrophosphate (TEPP)	107493	81	
Phenanthrene-d10	1517222	88	32	Thiophenol (Benzenethiol)	108985	229	
Phenobarbital	50066	236		Thionazin	297972	83	
Phenol	108952	11		Toluene diisocyanate	584849	228	
Phenol-d5	4165622	10		o-Toluidine	95534	28	
p-Phenylenediamine	106503	50		Toxaphene	58002190	227	
Phorate	298022	102		Triadimefon	43121433		65
Phosalone	2310170	200		2,4,6-Tribromophenol	118796	96	
Phosmet	732116	196		1,2,4-Trichlorobenzene	120821	42	
Phosphamidon I	13171216	118		2,2',5-Trichlorobiphenyl	37680652	117	
Phthalic anhydride	85449	235		2,4,5-Trichlorobiphenyl	15862074		50
2-Picoline (2-Methylpyridine)	109068	5		2,4',5-Trichlorobiphenyl	16606023	127	
Piperonyl sulfoxide	120627	234		2,4,5-Trichlorophenol	95954	59	
Prometon	1610180		34	2,4,6-Trichlorophenol	88062	57	
Prometryn	7287196		56	Tricyclazole	41814782		84
Propyzamide (Pronamide)	23950585	114	41	0,0,0-Triethyl phosphorothioate	126681	38	
Propachlor	1918167		23	Trifluralin	1582098	92	27
Propazine	139402		36	2,4,5-Trimethylaniline	137177	269	
Propylthiouracil	51525	233		Trimethyl phosphate	512561	226	
Pyrene	129000	147	76	1,3,5-Trinitrobenzene	99354	99	
Pyrene-d10-ss	1718521		74	Triphenylphosphate-ss	115866		102
Pyridine	110861	3		Tris(2,3-dibromopropyl) phosphate	126727	224	
Resorcinol	108463	232		Tri-p-tolylphosphate	78320	225	
Safrole	94597	52		Vernolate	1929777		10

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