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

Application

Environmental

Author

Mike Szelewski
Agilent Technologies, Inc.
2850 Centerville Road
Wilmington, DE 19808
USA

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

separate sets of files and methods. An 8270 set includes the mass spectra and locked retention times for 243 single-component semivolatile 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 semivolatile 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 acqusition 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 semivolatile 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	525_Long_RTL_DRS.M
8270_RTL_DRS.M	525_RTL_DRS.M	525_Long.MSL
8270.MSL	525.MSL	525_Long.CID
8270.CID	525.CID	525_Long_cal_RT.CAL
8270_cal_RT.CAL	525_cal_RT.CAL	525_Long_cal_RT.CSL
8270_cal_RT.CSL	525_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

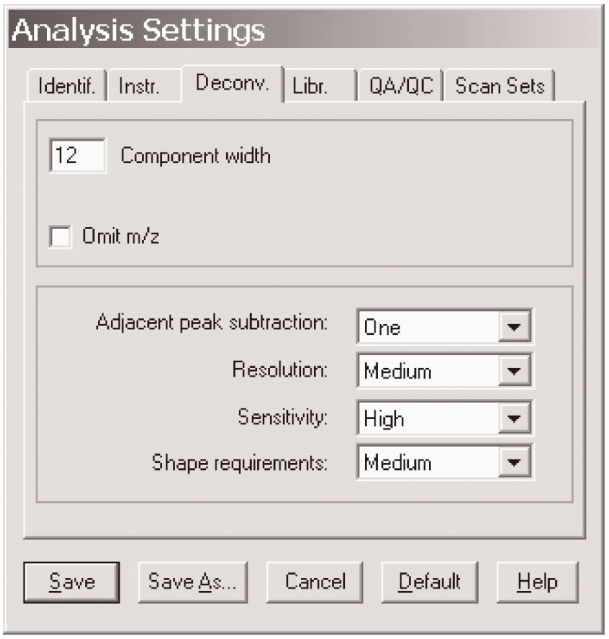
MSD ChemStation Library Files, *.L in **C:\Database**

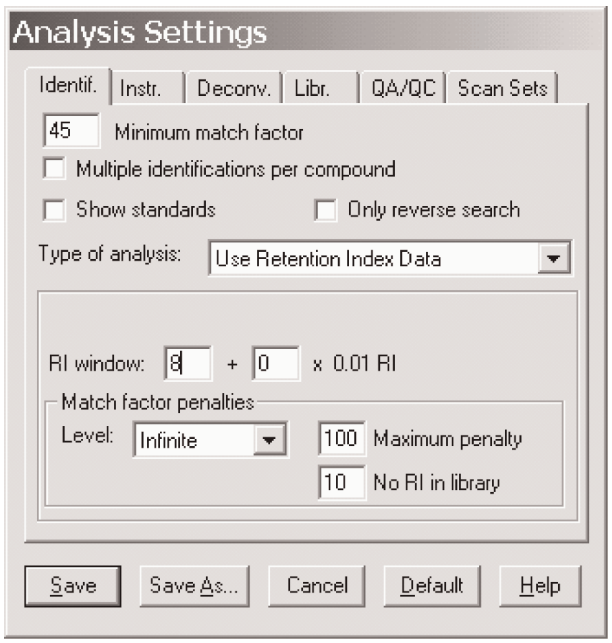
The MSD ChemStation methods contain a retention time locked quant database with single-point calibration. These methods can be used directly in data analysis, as described later. The methods also contain data acquisition parameters and retention time locking data. Users may have to resolve differences 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.



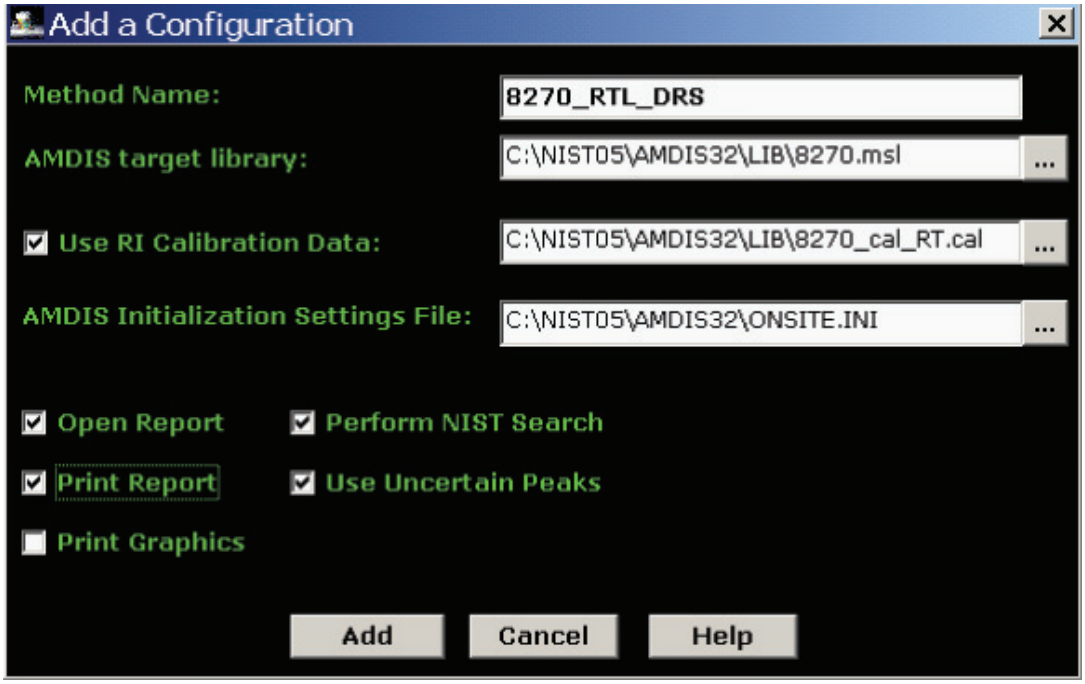


After AMDIS settings have been addressed, it will be necessary to configure a DRS method, depending on the analysis chosen. The relationship of the AMDIS and MSD ChemStation files are shown in the Table below.

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.

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

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

Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #
2-Fluorophenol	367124	7	
Heptachlor	76448	130	53
Heptachlor epoxide -isomer B	1024573	143	70
2,2',3,3',4,4',5-Heptachlorobiphenyl	35065306	203	
2,2',3,3',4,4',6-Heptachlorobiphenyl	52663715		104
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065293	195	
2,2',3,4,4',5',6-Heptachlorobiphenyl	52663691	187	
2,2',3,4',5,5',6-Heptachlorobiphenyl	52663680	184	
1,2,3,4,6,7,8-Heptachlorodibenzo-furan	67562394	215	
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	35822469	217	
Hexachlorobenzene	118741	106	30
2,2',3,4,4',5'-Hexachlorobiphenyl	35065282	180	
2,2',3,4,5,5'-Hexachlorobiphenyl	52712046	175	
2,2',3,5,5',6-Hexachlorobiphenyl	52663635	162	
2,2',4,4',5,5'-Hexachlorobiphenyl	35065271	170	
2,2',4,4',5,6'-Hexachlorobiphenyl	60145224		89
Hexachlorobutadiene	87683	47	
Hexachlorocyclopentadiene	77474	56	5
1,2,3,4,7,8-Hexachlorodibenzofuran	70648269	205	
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227286	209	
Hexachloroethane	67721	29	
Hexachlorophene	70304	214	
Hexachloropropene	1888717	46	
Hexamethylphosphoramid	680319	245	
Hexazinone	51235042		100
Hydroquinone	123319	244	
Indeno[1,2,3-cd]pyrene	193395	221	117
Isodrin	465736	140	
Isophorone	78591	34	2
Isosafrole	120581	61	
Kepone	143500	177	
Leptophos	21609905	201	
Malathion	121755	132	
Maleic anhydride	108316	243	
Merphos	150505		72
Mestranol	72333	242	
Methapyrilene	91805	138	
Methoxychlor	72435	188	106
3-Methylcholanthrene	56495	218	
4,4'-Methylenebis (2-chloroaniline)	101144	263	
4,4'-Methylenebis (N,N-dimethylaniline)	101611	262	
Methyl methanesulfonate	66273	6	
2-Methylnaphthalene	91576	53	
Methyl paraoxon	950356		46
Methyl parathion	298000	128	
2-Methylphenol	95487	20	
3-Methylphenol	108394	23	
4-Methylphenol	106445	22	
Metolachlor	51218452		62
Metribuzin	21087649		51
Mevinphos	7786347	63	9
Mexacarbate	315184	241	
MGK 264 - a	113484		67
MGK 264 - b	113484		69
Mirex	2385855	204	
Molinate	2212671		20
Monocrotophos	6923224	98	
Naphthalene	91203	43	
Naphthalene-d8	1146652	30	
1,4-Naphthoquinone	130154	65	
1-Naphthylamine	134327	80	
2-Naphthylamine	91598	78	
Napropamide	15299997		83
Nicotine	54115	58	
5-Nitroacenaphthene	602879	255	
2-Nitroaniline	88744	64	
3-Nitroaniline	99092	70	
4-Nitroaniline	100016	87	
5-Nitro-o-anisidine	99592	254	
Nitrobenzene	98953	32	
Nitrobenzene-d5	4165600	31	
4-Nitrobiphenyl	92933	258	
Nitrofen	1836755	165	
2-Nitrophenol	88755	35	
4-Nitrophenol	100027	74	
4-Nitroquinoline-1-oxide	56575	136	
5-Nitro-o-toluidine	99558	85	
N-Nitrosodiethylamine	55185	8	
N-Nitrosodimethylamine	62759	2	
N-Nitrosodi-n-butylamine	924163	49	
N-Nitrosodi-n-propylamine	621647	25	
N-Nitrosodiphenylamine	86306	90	
N-Nitrosomethylethylamine	10595956	4	
N-Nitrosomorpholine	59892	27	
N-Nitrosopiperidine	100754	33	
N-Nitrosopyrrolidine	930552	24	
trans-Nonachlor	39765805		81
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

Compound name	CAS #	8270_DRS.L entry #	525_DRS.L entry #
Octachlorodibenzofuran	39001020	220	
Octachlorodibenzo-p-dioxin	3268879	219	
Octamethyl pyrophosphoramide	152169	239	
4,4'-Oxydianiline	101804	261	
Parathion (ethyl)	56382	134	
Pebulate	1114712		14
Pentachlorobenzene	608935	75	
2,2',3,4,5'-Pentachlorobiphenyl	38380028	156	
2,2',3',4,6'-Pentachlorobiphenyl	60233252		71
2,2',4,5,5'-Pentachlorobiphenyl	37680732	148	
2,3,3',4',6-Pentachlorobiphenyl	38380039	158	
1,2,3,7,8-Pentachlorodibenzofuran	57117416	198	
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	40321764	202	
Pentachloroethane	76017	14	
Pentachloronitrobenzene	82688	113	
Pentachlorophenol	87865	112	37
cis-Permethrin	54774457		110
trans-Permethrin	51877748		111
Perylene-d12	1520963	206	115
Phenacetin	62442	101	
Phenanthrene	85018	122	42
Phenanthrene-d10	1517222	88	32
Phenobarbital	50066	236	
Phenol	108952	11	
Phenol-d5	4165622	10	
p-Phenylenediamine	106503	50	
Phorate	298022	102	
Phosalone	2310170	200	
Phosmet	732116	196	
Phosphamidon I	13171216	118	
Phthalic anhydride	85449	235	
2-Picoline (2-Methylpyridine)	109068	5	
Piperonyl sulfoxide	120627	234	
Prometon	1610180		34
Prometryn	7287196		56
Propyzamide (Pronamide)	23950585	114	41
Propachlor	1918167		23
Propazine	139402		36
Propylthiouracil	51525	233	
Pyrene	129000	147	76
Pyrene-d10-ss	1718521		74
Pyridine	110861	3	
Resorcinol	108463	232	
Safrole	94597	52	
Simazine	122349		33
Simetryn	1014706		52
Stirofos (Tetrachlorvinphos)	22248799		77
Strychnine	57249	231	
Sulfallate	95067	230	
Sulfotepp	3689245	95	
Tebuthiuron	34014181		18
Terbacil	5902512		48
Terbufos	13071799	121	40
Terbutryne	886500		57
Terphenyl-d14	1718510	157	
1,2,4,5-Tetrachlorobenzene	95943	54	
2,2',3,5'-Tetrachlorobiphenyl	41464395	135	
2,2',4,4'-Tetrachlorobiphenyl	2437798		60
2,2',5,5'-Tetrachlorobiphenyl	35693993	133	
2,3',4,4'-Tetrachlorobiphenyl	32598100	144	
2,3,7,8-Tetrachlorodibenzofuran	51207319	178	
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746016	183	
2,3,4,6-Tetrachlorophenol	58902	79	
Tetrachlorvinphos	961115	151	
Tetraethylpyrophosphate (TEPP)	107493	81	
Thiophenol (Benzenethiol)	108985	229	
Thionazin	297972	83	
Toluene diisocyanate	584849	228	
o-Toluidine	95534	28	
Toxaphene	58002190	227	
Triadimefon	43121433		65
2,4,6-Tribromophenol	118796	96	
1,2,4-Trichlorobenzene	120821	42	
2,2',5-Trichlorobiphenyl	37680652	117	
2,4,5-Trichlorobiphenyl	15862074		50
2,4',5-Trichlorobiphenyl	16606023	127	
2,4,5-Trichlorophenol	95954	59	
2,4,6-Trichlorophenol	88062	57	
Tricyclazole	41814782		84
O,O,O-Triethyl phosphorothioate	126681	38	
Trifluralin	1582098	92	27
2,4,5-Trimethylaniline	137177	269	
Trimethyl phosphate	512561	226	
1,3,5-Trinitrobenzene	99354	99	
Triphenylphosphate-ss	115866		102
Tris(2,3-dibromopropyl) phosphate	126727	224	
Tri-p-tolylphosphate	78320	225	
Vernolate	1929777		10

www.agilent.com/chem

Printed in the USA
February 8, 2008
5989-7875EN

Agilent Technologies