Agilent SP1 7890-0568 3-in-1 GC/MSD DRS Analyzer

Installation and Checkout Guide

Agilent Technologies

Notices

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Contents

1 General Information for the 3-in-1 Analyzer

Objective

This document will guide you through the process of loading the semivolatiles (S-VOA) acquisition method, relocking the method, running the checkout sample, and analyzing the results using Deconvolution Reporting software (DRS). This process will be repeated for the volatiles (VOA) method. The pesticides method locking and DRS report are also discussed.

Read all sections in this chapter. You can then proceed to any section, depending upon which application will be run first.

- Chapter 2, “S-VOA Analyzer Specifics”
- Chapter 3, “VOA Analyzer Specifics”
- Chapter 4, “Pesticides Analyzer Specifics”

At the end of this document you will find Chapter 5, “Allowed 3-in-1 System Configurations” which shows allowed hardware options and Chapter 6, “Consumables and Supplies” which lists the replaceable parts and consumables used for these applications.

System Overview

The Agilent 3-in-1 GC/MSD DRS Analyzer, SP 7890-0568, is designed for the analyses of S-VOA, VOA, and pesticides compounds by GC/MSD, with Deconvolution Reporting software (DRS) for data reduction. The system includes an Agilent 7693A Autosampler, 7697A Headspace Sampler (HS), 7890A GC, and 5975C MSD.

A programmable temperature vaporizing multimode inlet (MMI) is used in hot splitless mode (HSL) for S-VOA and pesticide analyses. Cold splitless (CSL) and solvent vent modes (SV) are also available. A split-splitless (S/SL) inlet can be used in place of the MMI. A post column, 2-way purged splitter enables column backflushing of heavy matrix and column removal, without venting. A second inlet, S/SL, operates in hot split mode (HSP) for HS-VOA analyses.

The 2-way purged splitter operates as a column combiner. It combines the outlet flows from the S-VOA and VOA columns to a 1.1 m × 0.15 mm SilTek treated restrictor into the MSD transfer line. The 2-way purged splitter also provides makeup gas for good peak shapes and backflush flow.

The S-VOA DRS database-library (DBL) includes the single component analytes from USEPA methods 525 and 8270 plus others; 338 total. The Solvents-Plus DRS DBL includes the analytes from USEPA methods 524 and 8260 plus others; 369 total. The pesticides DRS DBL includes 927 pesticides and endocrine disruptors.

A top view schematic of the major components of the 3-in-1 Analyzer is shown in Figure 1 on page 8.

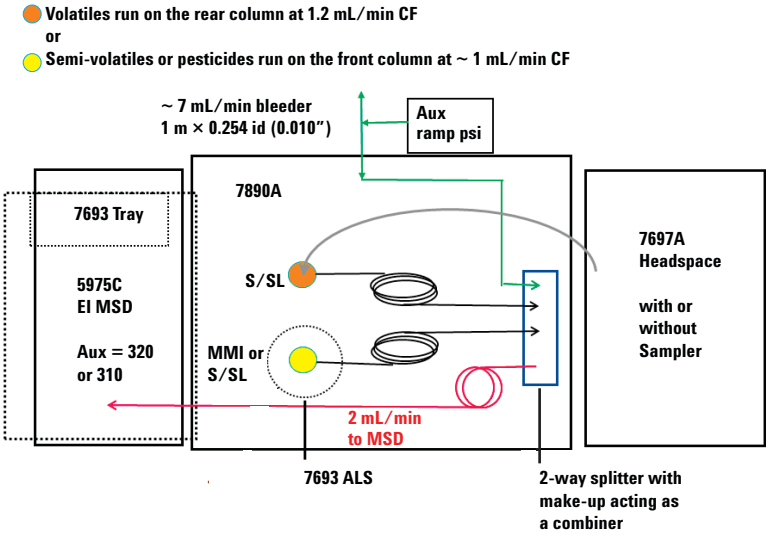

Figure 1 Top view of the 3-in-1 Analyzer

Before Getting Started

Agilent recommends that you watch the series of DRS training videos (p/n 5973-1731) before you follow these procedures. If you are not familiar with retention time (RT) locking, DRS, AMDIS Deconvolution software, or the QEdit function in the Agilent MSD ChemStation, these videos will be very helpful.

Installation Summary

1. Install the GC and MSD.
   - Connect all gases using required purifiers, and make sure supply pressures are high enough for the method (especially for backflushing at 60 psig).
   - Connect the AC power.
   - Start the GC gases flowing to purge the system.
2. Reconnect the CFT restrictor tube to the MSD from the plate located in oven.
3. Pump down the MSD with cool zones.
4. Check for leaks.
5. Load the following software:
   - MSD ChemStation
   - NIST 08 Library and AMDIS
   - DRS software
   - S-VOA DRS DBL, Solvents-Plus DRS DBL

   Copy files from the CD-ROM supplied by the Specials Group: (Detailed information is supplied in later sections).
   - Methods to Methods directory
   - Data files to Data directory
   - Macros to MSExe directory
   - AMDIS, MSSearch, and DRS config files to their respective directories
   - Tune file for MSD
6. Edit the **msdchem.ini** with the method desired for startup, such as **S-Voa_3in1_acq_BF.m**, to prevent Method Resolution.
7. Load and resolve methods. (Resolution may not be needed.)
8. Autotune the MSD.
9. Run a blank solvent.
10. Run the S-VOA checkout mix twice.
11. Relock the RT of the method on the second run.

12 Rerun the checkout sample with the relocked method, if needed.

13 In **DA**, run **Quant + DRS single** on the checkout sample data file.

14 Inspect the report to assure all peaks in the checkout mix are found with a match factor above the method default.

15 Run **Solvents+ checkout mix**, using headspace twice.

16 Relock the RT of method on the second run.

17 Rerun the checkout sample with the relocked method, if needed.

18 In **DA**, run **Quant + DRS single** on the checkout sample datafile.

19 Inspect the report to assure all peaks in the checkout mix are found with a match factor above the method default.

20 Archive:

- Stored method(s) with RTL calibration
- Autotune file
- Checkout sample data files
- DRS reports from checkout sample data files
- Any install notes for future service people (for example: AUX EPC supply pressure too low, so backflushing pressure reduced and time extended)

2-way Purged Splitter Plumbing and Operation Specifics

The 2-way purged splitter operates as a column effluent flow combiner. The splitter may be mounted on either side of the GC oven, as the restrictor is long enough to reach the MSD. The rear VOA column is connected with a SilTite ferrule to the first position closest to the makeup gas line from the Aux EPC module. This minimizes the chance of contamination from heavy matrix that may elute from the S-VOA column. The front S-VOA column is connected with a SilTite ferrule to the second (middle) position of the splitter. The restrictor is connected with a SilTite ferrule to the last position of the splitter, furthest from the makeup gas line.

The Aux EPC module is run in ramped pressure (RP) mode. This is done to maintain a constant 2 mL/min flow to the MSD as the oven temperature increases. It can not be run in constant pressure (CP) mode nor in constant flow (CF) mode. If run in CP mode, the flow to the MSD will be higher than 2 mL/min when the oven is cold. If run in CF mode, a true 2 mL/min will not be maintained due to the temperature differences between the oven and MSD transfer line.

Each of the three methods, S-VOA, VOA, and pesticides, has a different pressure ramp for the Aux EPC based on both the oven program and the transfer line temperature.

The restrictor (column 3) is a 1.1 m × 0.150 mm id piece of SilTek treated fused silica tubing (p/n 160-7625-5). It is connected to the splitter with a SilTite ferrule. The other end is connected to the MSD transfer line using either a SilTite or graphite/vespel ferrule with the appropriate nut.

A bleed restrictor is attached to the makeup gas line with a T connector in between the Aux EPC and the splitter plate. This restrictor is 1 m × 0.010 mm id SS (p/n 0100-2354), and provides over pressure relief for pulsed injections and RT locking.

Backflushing Parameters

The S-VOA and pesticides methods include parameters for backflushing. The parameters are based on the MSD pump type. Agilent recommends that a turbo pump be used as they can handle higher flows and therefore shorter backflush times. **A diffusion pump can be used but the backflush time will be at least 10 minutes**. The Aux EPC pressure for backflushing with a diffusion pump can not exceed 25 psi, or excessive flow will go to the pump. Experiments have shown that the 10 minute backflush time is necessary to clean heavy hydrocarbons, often found in S-VOA samples, from the column. In all cases when backflushing the front S-VOA-pesticides column, set the rear VOA column inlet to a lower pressure (15 psi). This step is necessary to prevent the rear column from attempting to maintain a normal forward flow. However, the VOA method itself does not include backflushing due to the overall cleaner nature of the samples introduced. Listed in Table 1 are the pressures, flows, and times for backflushing for either the turbo or the diffusion pump. The void volumes for the pesticides method, not shown, are just slightly larger due to the oven temperature difference.

Table 1 Backflush parameters for the front column, using either the S-VOA or pesticides method

				Inlet pressure		Column flow		Front column
Method	**Pump**	**Aux EPC (psi)**	**Backflush (min)**	**Front (psi)**	**Rear (psi)**	**Front S-VOA (mL/min)**	**Rear VOA (mL/min)**	**Void volumes**
S-VOA	Turbo	60	5	1	15	–1.54	–3.3	8.6
	Diffusion	24	10	1	15	–0.36	–0.43	7.3

Software

All acquisition methods were built using the Agilent MSD Chemstation software E.02.01 or later. Data analysis methods were built using E.02.00. None of the methods are backward compatible. The NIST08 used was version 2.0 f, Oct 8, 2008. AMDIS version 2.66, create 121.82 was used to create all AMDIS files. Table 2 lists the methods and files that should be used for each of the 3-in-1 Analyzer modes of operation.

Table 2 Files for use with the 3 modes of the 3-in-1 Analyzer

	S-VOA	VOA	Pesticides
Acquisition	S-VOA_3in1_acq_BF.M	VOA_3in1_acq.M	Pest_3in1_acq_BF.M
Checkout DA	S-VOA_3in1_DA-checkout.M	VOA_3in1_DA-checkout.M	Pest_3in1_DA-checkout.M
Full DA	S-VOA_3in1_DA.m	VOA_3in1_DA.m	Pest_3in1_DA.m
Checkout msl	S-VOA_3in1_checkout.msl	VOA_3in1_checkout.msl	Pest_3in1_checkout.msl
Full msl	S-VOA_1.msl	CF_SOLV.MSL	RTLPest3.msl
*.cal	S-VOA_3in1.cal	VOA_3in1.cal	Pest_3in1.cal
*.csl	S-VOA_3in1.csl	VOA_3in1.csl	Pest_3in1.csl
Agilent.L	8270_DRS.L, 525_DRS.L	CF_SOLV.L	RTLPest3.L
Checkout.D	S-VOA_3in1_checkout.D	VOA_3in1_checkout.D	Pest_3in1_checkout.D
Onsite.ini	Onsite.ini	Onsite.ini	Onsite.ini
Default.ini	Default.ini	Default.ini	Default.ini
Nistms.ini	Nistms.ini	Nistms.ini	Nistms.ini
AmdisConfig.txt	AmdisConfig.txt	AmdisConfig.txt	AmdisConfig.txt

1 General Information for the 3-in-1 Analyzer

2
S-VOA Analyzer Specifics

The S-VOA portion of the 3-in-1 Analyzer is based on the SP1 7890-0459 S-VOA analyzer with modifications. The single-taper with glass wool liner, (p/n 5190-2293), introduced in early 2011, is UI deactivated and is used for HSL. CSL injections can be done using a 2 mm dimple liner (p/n 5190-2296) and conditions in *Application Note 5989-7875*. The 3-in-1 Analyzer uses a 20 m × 0.18 mm × 0.36 um DB-8270D column (p/n 121-9723) which is a more inert version of DB 5-MS. The system is RT locked to **Phenanthrene-d10 at 11.000 min**.

The S-VOA acquisition method, **S-voa_3-in-1_acq_bf.m**, contains both scan and SIM parameters. Scan only acquisitions can be run at a sampling rate of 2^2 or 2^1. The SIM parameters are those for the most common 100+ compounds from USEPA Method 525. If SIM/scan is run, the rate should be set to 2^1. With SIM/scan, the SIM signal can be used for quantitation of the most important analytes, and the scan signal can be used for deconvolution and identification of all 338 compounds.

The 338 compound quant database was taken from Agilent's G1677AA S-VOA DRS DBL, supplied with this analyzer. The RTs of the earliest and latest eluters have been slightly modified due to the Aux EPC pressure ramp. It is important to use the methods and files listed in Table 2 on page 13, for the best system performance.

The 338 compounds are listed in application note: *Semivolatiles Retention Time Locked (RTL) Deconvolution Databases for Agilent GC/MSD Systems*. Mike Szelewski, Agilent Technologies, Publication 5989-7875EN, www.agilent.com/chem. A copy of this application note is included on the G1677AA S-VOA DRS DBL CD that came with this analyzer.

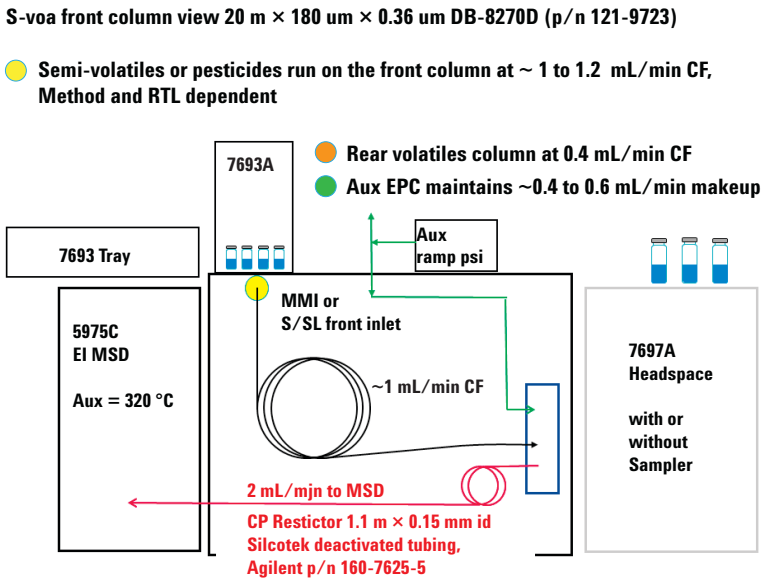

Figure 2 Front column view of the 3-in-1 Analyzer

Copying and Pasting S-VOA Files

Copy the S-VOA files from the CD supplied by the Specials Group and paste them into the location listed in Table 3. This CD is not one of the software installation CDs.

Table 3 Copying and pasting S-VOA files

File name	Location to paste the copied file
S-VOA_3in1_acq_BF.m S-VOA_3in1_DA-checkout.m S-VOA_3in1_DA.m	C:\MSDchem\1\Methods
S-VOA_3in1_checkout.D	C:\MSDchem\1\Data
S-VOA_3in1_checkout.msl S-VOA_3in1_checkout.cid S-VOA_3in1.cal S-VOA_3in1.csl	C:\NIST08\AMDIS32\Lib
Onsite.ini Default.ini	C:\NIST08\AMDIS32\Lib
Nistms.ini	C:\NIST08\Mssearch
AmdisConfig.txt	C:\Program Files\Agilent\MSD Deconvolution Reporting Software

Additional file information

Verify the following files in Table 4 were installed.

Table 4 Additional S-VOA file information

File name	Location to paste the copied file
8270_DRS.L, 525_DRS.L	These 2 libraries should have installed into C:\Database when the G1677AA S-VOA DRS database was installed.
Semivoas_1.msl Semivoas_1.cid	These 2 files should have installed into C:\NIST08\AMDIS32\Lib when the G1677AA S-VOA DRS database was installed.

Description of VOA Files

S-voa_3in1_acq_BF.m– the method that has been RT locked by the Specials Group using the installed column. This method will be relocked as part of the system installation and will be used for data acquisition of the checkout mix and customer samples in scan. The method includes SIM ions as discussed above.

S-Voa_3in1_DA-checkout.m–the data analysis method that contains 29 compounds in the quantitation database, that will be used for the DRS analysis of the checkout mix.

S-Voa_3in1_DA.m–the data analysis method that contains 338 compounds in the quantitation database that can be used for samples.

S-voa_3in1_Checkout.D–the datafile that was acquired by the Specials Group as final checkout. It can be used as a reference for the Checkout sample run as part of the system installation.

S-voa_3in1_checkout.msl, S-voa_3in1_checkout.cid, S-voa_3in1.cal, S-voa_3in1.csl–these are the AMDIS files designed for the S-VOA portion of the 3-in-1 Analyzer.

Semivoas_1.msl, Semivoas_1.cid–this is the 338 compound S-VOA DRS Database-Library and associated chemical information directory.

Onsite.ini, Default.ini, Nistms.ini, AmdisConfig.txt–these are configuration files specific to the analyzer and should over-write the exisiting files in the specified directories.

Loading and Relocking the S-VOA Method

The GC/MSD S-VOA checkout mix (p/n 5190-0473) is a solution of 29 compounds, each at 10 ppm (10 ng/µL), in dichloromethane (methylene chloride). The names and CAS numbers of the compounds in the mix are listed in Table 5 in RT order.

Table 5 S-VOA checkout mix compound list

Compound	RT	CAS number
N-Nitrosodimethylamine	3.770	62759
Aniline	6.190	62533
1,4-Dichlorobenzene-d4	6.538	3855821
Isophorone	7.299	78591
1,3-Dimethyl-2-nitrobenzene	7.707	81209
Naphthalene-d8	7.746	1146652
Hexachlorocyclopentadiene	8.614	77474
Mevinphos	9.016	7786347
Acenaphthene-d10	9.482	15067262
2,4-Dinitrophenol	9.542	51285
4-Nitrophenol	9.574	100027
2,4-Dinitrotoluene	9.671	121142
Fluorene	10.056	86737
4,6-Dinitro-2-methylphenol	10.078	534521
Trifluralin	10.190	1582098
Simazine	10.654	122349
Atrazine	10.680	1912249
Pentachlorophenol	10.796	87865
Terbufos	10.820	13071799

Table 5 S-VOA checkout mix compound list (continued)

Compound	RT	CAS number
Chlorothalonil	10.980	1897456
Phenanthrene-d10	11.000	1517222
Aldrin	11.816	309002
Heptachlor epoxide -isomer B	12.119	1024573
Endrin	12.833	72208
4,4'-DDT	13.158	50293
3,3'-Dichlorobenzidine	13.597	91941
Chrysene-d12	13.661	1719035
Benzo[b]fluoranthene	14.840	205992
Perylene-d12	15.363	1520963

Open one of the vials of the S-VOA checkout mix and transfer it to an autosampler vial. Place the autosampler vial in tray position 1. This will be used for relocking the previously locked method.

The S-VOA method is **RTLocked to Phenanthrene-d10 at 11.000 minutes.**

Loading the Acquisition Method

Open the ChemStation instrument control software and click **Method > Load Method** and choose the method called **S-voa_3in1_acq_BF.m**. This method should inject 1 µL, but verify the syringe size and injection volume after loading.

Making the Relocking Runs

NOTE

To save time, use the GC keyboard to set the current oven temperature to 250 °C while doing the next step. Do NOT save the method, as this is just temporary. This will preheat the oven and give better time matching in the relock step. As soon as the sequence starts, the oven temperature will return to 40 °C before the injection is made.

Relocking Sequence

1 Go to the **Sequence>Load Sequence** menu item in the ChemStation Instrument control software and load the file **Default.s**. Edit the sequence table to look like Figure 3.

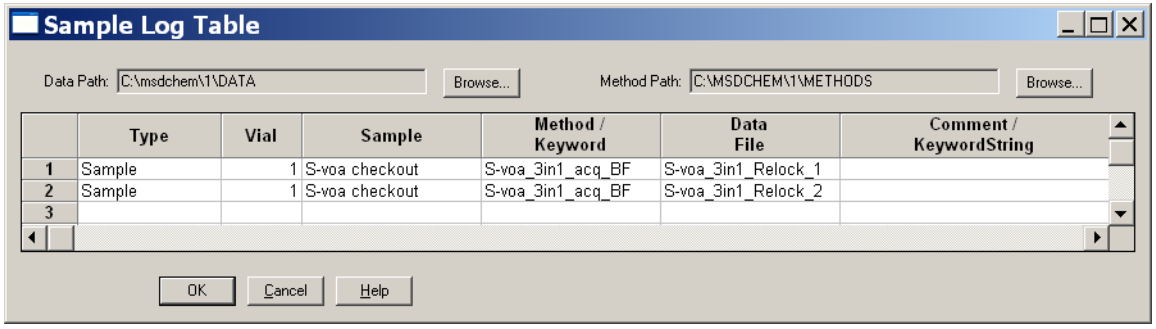

Figure 3 S-VOA sequence table for RTL relocking runs

2 Save the sequence as **Semivoas_Relock_Seq.s**. Make sure the vial of S-VOA checkout mix (p/n 5190-0473) is located in position 1 of the autosampler tray.

3 Go to the **Sequence>Run Sequence** menu item and run the sequence.

4 After the sequence is completed, start the **Instrument 1 Data Analysis** program.

5 Use the **Method>Load Method** menu item to load the same **S-voa_3in1_acq_BF.m** file that was run in the sequence.

6 Load the second run from the sequence (the first run was just to clean out the column) named **S-voa_3in1_Relock_2.D**.

7 Select the **View>RTLock Setup** menu item to open the **RTLock** screen. Proceed with relocking the acquisition method, **S-voa_3in1_acq_BF.m**, using datafile **S-voa_3in1_Relock_2.D**. The new inlet pressure has now been saved to the method.

NOTE The new pressure will not be applied to the method nor the GC until the method is reloaded or is run.

8 Select the **View>Return to Data Analysis** menu item to close the **RTLock Setup View.**

9 On the GC keyboard, press the **Front Inlet** key to view the pressure setpoints for the inlet the method is using.

10 In the **Data Acquisition** view, re-load your method **S-voa_3in1_acq_BF.m**.

You should see the new calculated locking pressure downloaded as the setpoint for the inlet.

Confirming the Lock

If the RT lock time of Phenanthrene-d10 was off by more than ± 0.010 minutes after relocking the method, an optional third run of the checkout mix can be made to verify the locking pressure and time.

The best way to do this is to add a line to the existing sequence, and then use the **Sequence > Position and Run** menu item.

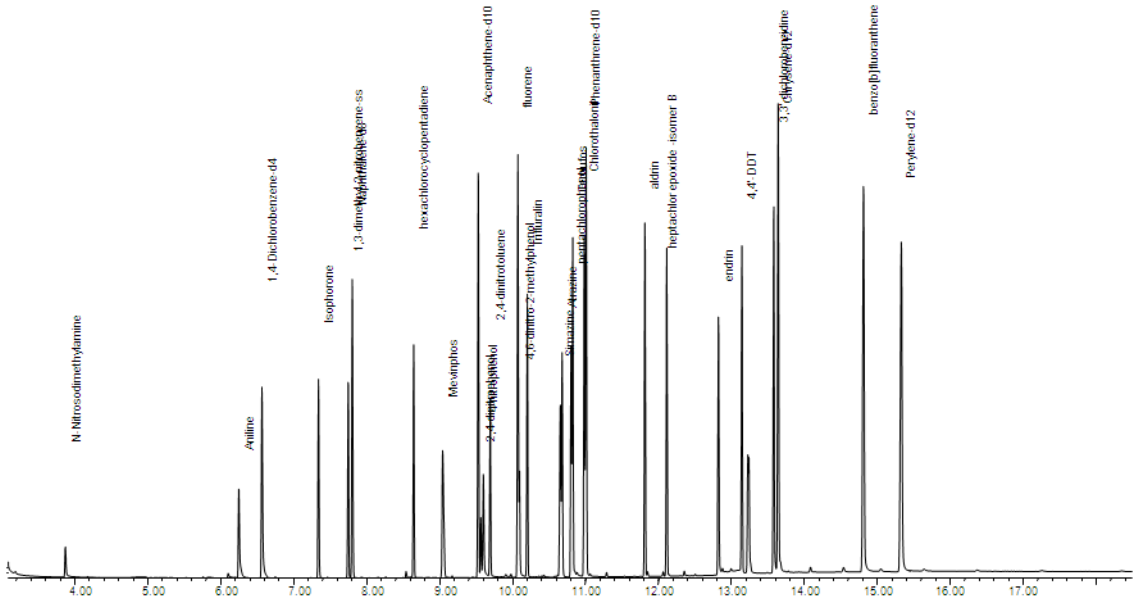

Figure 4 S-VOA checkout mix total ion chromatogram

DRS Analysis of the S-VOA Checkout Mix

This step is to confirm that the RTs across the entire elution range of the chromatogram match those in the method closely enough to have all peaks fall in their recognition windows.

1 In **Data Analysis**, using the **Method > Load Method...** menu item, load the **method S-Voa_3in1_DA-checkout.m**.

2 Using the **File > Load Data File...** menu item, load the last **checkout mix relocking** run that was made. Select the menu item **DRS > Quant + DRS single file**. After a moment, you will see activity on the computer as DRS performs a quantitative analysis, deconvolutes the mass spectra, and searches the **S-voa_3in1_checkout.msl AMDIS** database, then searches the **NIST08 library**. Depending upon the deconvolution settings chosen, the DRS process will typically take 2–4 minutes. At this point, DRS will generate a report that looks similar to (but not necessarily identical to) Figure 5 on page 25.

3 Inspect the report and compare it to the list of compounds in the sample.

Also note that the **ChemStation Amount** column gives only estimated amounts for the compounds that it identified. These amounts are based on a single point response factor that is supplied with your method. You must calibrate any compounds that you wish to quantify as you do with any other GC/MS method.

The **AMDIS** amount column is completed after the QEdit process.

The **AMDIS** column of the DRS report should find all the analytes in the test mix, typically with match factors > 90 and with **RT** differences of < 10 seconds.

MSD Deconvolution Report
Sample Name: S-VOA checkout
Data File: C:\msdchem\1\DATA\S-voa_3in1_checkout.D
Date/Time: 8:52:43 AM Wednesday, May 25, 2011

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	
RT	Cas number	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec	Revers Match	Hit Num.
3.7997	62759	N-Nitrosodimethylamine	6.77		96	2.0	84	1
6.1762	62533	Aniline	10		99	4.7	96	1
6.4935	3855821	1,4-Dichlorobenzene-d4	10		99	6.1	91	1
7.2780	78591	Isophorone	10		96	4.4	95	1
7.6890	81209	1,3-dimethyl-2-nitrobenzene (ss)	10		96	3.7	95	1
7.7469	1146652	Naphthalene-d8	10		100	2.3	90	1
8.5964	77474	Hexachlorocyclopentadiene	10		98	1.2	91	1
9.0028	7786347	Mevinphos	10		95	0.6	90	2
9.4978	15067262	Acenaphthene-d10	10		98	–0.1	81	1
9.5359	51285	2,4-Dinitrophenol	10		91	0.1	91	1
9.5676	100027	4-Nitrophenol	9.48		95	0.3	93	1
9.6660	121142	2,4-dinitrotoluene	10		96	0.1	92	1
10.0484	86737	Fluorene	10		98	0.0	93	1
10.0698	534521	4,6-Dinitro-2-methylphenol	10		96	–0.0	93	1
10.1747	1582098	Trifluralin	10		95	–0.1	93	1
10.6410	122349	Simazine	10		93	0.7	84	2
10.6642	1912249	Atrazine	10.97		96	0.3	91	1
10.7841	87865	Pentachlorophenol	10		97	–0.0	92	1
10.8089	13071799	Terbufos	10		95	0.0	91	1
10.9678	1897456	Chlorothalonil	10		100	0.2	95	1
10.9973	1517222	Phenanthrene-d10	10		96	0.0	86	2
11.8117	309002	Aldrin	10		98	–0.8	92	1
12.1149	1024573	Heptachlor epoxide -isomer B	10		97	–1.1	93	1
12.8343	72208	Endrin	10		98	–1.7	94	1
13.1563	50293	4,4'-DDT	10		93	–2.0	90	1
13.5999	91941	3,3'-Dichlorobenzidine	10		96	–2.2	97	1
13.6598	1719035	Chrysene-d12	10		98	–2.2	91	1
14.8425	205992	Benzo[b]fluoranthene	10		100	–3.8	95	2
15.3696	1520963	Perylene-d12	10		98	–4.6	85	1

Figure 5 Example of S-VOA checkout mix DRS report

3
VOA Analyzer Specifics

The VOA portion of the 3-in-1 Analyzer is based on the SP1 7890-0567 HS VOA Analyzer.

The straight bore no taper liner, (p/n 8004-0157), has a 1.2 mm id and gives good peak shapes and sensitivity at a 20:1 split. The liner is inserted upside-down, that is with the counterbore, if present, at the top. This is not the normal position but it helps guide the megabore transfer line into the liner. The column is a 30 m × 0.25 mm × 1.0 um DB-5 MS UI column (p/n 121-5533UI). The column length above the inlet ferrule should be ~20 mm.

The rear inlet top weldment is replaced with the accessory 7890A S/SL MMI Weldment for Headspace, (p/n G3521A). This eliminates splicing the transfer line into the carrier line. The septum purge line exists but the carrier is fed directly from the inlet EPC module to the headspace sampler. The original weldment is included if needed.

The 7697A Headspace sampler is interfaced to the 7890 rear inlet using a length of 530 um SilTek deactivated fused silica tubing through the transfer line. At the GC inlet, the tubing is

punctured through the septum and trimmed to a length of ~30 mm. The tubing is inserted into the liner, using the counterbore in the liner as a lead-in. The standard green septum nut and septum complete the seal.

The system is RT locked to Toluene-d8 at 7.790 minutes.

The VOA acquisition method, **VOA_3-in-1_acq.m**, contains both scan and SIM parameters. Scan only acquisition, run at a sampling rate of 2^2, is used for RT locking and checkout. The SIM parameters are those for the 63 most commonly measured compounds from USEPA Method 524. If SIM/scan is run, the rate should be set to 2^1. With SIM/scan, the SIM signal can be used for quantitation of the most important analytes and the scan signal can be used for deconvolution and identification of all 369 compounds.

The 369 compound quant database was taken from Agilent's G1678AA Solvents-Plus DRS DBL, supplied with this analyzer. The retention times from the CF methodology with a CP post column splitter were used as a starting point. The retention times of the earliest and latest eluters have been slightly modified due to the Aux EPC pressure ramp. It is important to use the methods and files listed in Table 2 on page 13, for best system performance.

Additional information on using a headspace with the Solvents-Plus DRS DBL can be found in the following application note: *Headspace Volatiles using a Headspace-GC/MSD Analyzer*. Mike Szelewski, Agilent Technologies, Publication 5990-7907EN, www.agilent.com/chem. A copy of this application note is included on the CD that came with this analyzer.

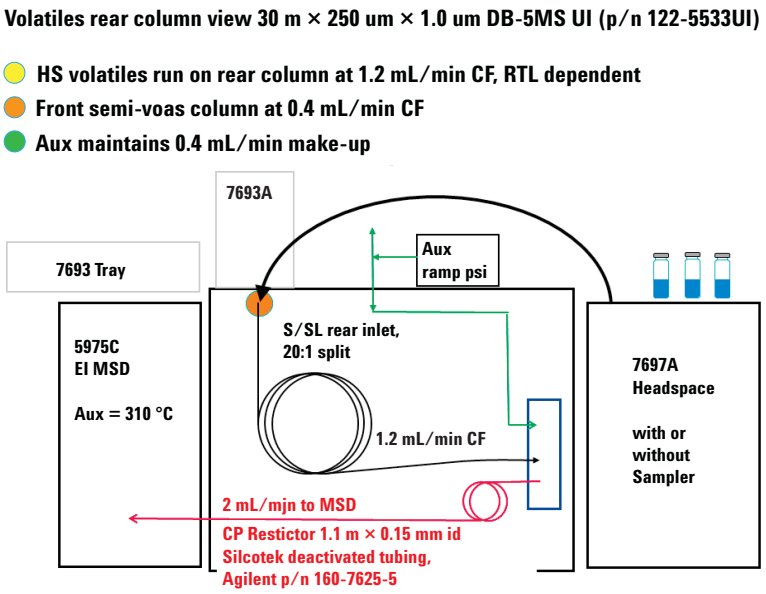

Figure 6 Rear column view of the 3-in-1 Analyzer

Copying and Pasting VOA Files

Copy the VOA files from the CD supplied by the Specials Group and paste them into the location listed in Table 6. This CD is not one of the software installation CDs.

Table 6 Copying and pasting VOA files

File name	Location to paste the copied file
VOA_3in1_acq.m VOA_3in1_DA-checkout.m VOA_3in1_DA.m	C:\MSDchem\1\Methods
VOA_3in1_checkout.D	C:\MSDchem\1\Data
VOA_3in1_checkout.msl VOA_3in1_checkout.cid VOA_3in1.cal VOA_3in1.csl	C:\NIST08\AMDIS32\Lib
Onsite.ini Default.ini	C:\NIST08\AMDIS32\Lib
Nistms.ini	C:\NIST08\Mssearch
AmdisConfig.txt	C:\Program Files\Agilent\MSD Deconvolution Reporting Software

Additional file information

Verify the following files in Table 7 were installed.

Table 7 Additional VOA file information

File name	Location to paste the copied file
CF_SOLV.L, CP_SOLV.L	These 2 libraries should have installed into C:\ Database when the G1678AA Solvents-Plus DRS database was installed.
CF_SOLV.msl CF_SOLV.cid	These 2 files should have installed into C:\ NIST08\AMDIS32\Lib when the G1678AA Solvents-Plus DRS database was installed.

Description of VOA Files

VOA_3in1_acq.m–the method that has been RT locked by the Specials Group using the installed column. This method will be relocked as part of the system installation and will be used for data acquisition of the checkout mix and customer samples in scan. This method includes the SIM ions discussed above.

VOA_3in1_DA-checkout.m–the data analysis method that contains 20 compounds in the quantitation database, that will be used for the DRS analysis of the checkout mix.

VOA_3in1_DA.m–the data analysis method that contains 369 compounds in the quantitation database that can be used for samples.

VOA_3in1_Checkout.D–the datafile that was acquired by the Specials Group as final checkout. It can be used as a reference for the checkout sample run as part of the system installation.

VOA_3in1_checkout.msl, VOA_3in1_checkout.cid, VOA_3in1.cal, VOA_3in1.csl–these are the AMDIS files designed for the VOA portion of the 3-in-1 Analyzer.

CF_SOLV.msl, CF_SOLV.cid–this is the 369 compound Solvents-Plus DRS Database-Library and associated chemical information directory file.

Onsite.ini, Default.ini, Nistms.ini, AmdisConfig.txt–these are configuration files specific to the analyzer and should overwrite the exisiting files in the specified directories.

Loading and Relocking the Headspace VOA Method

The GC/MSD Solvents-Plus checkout mix (p/n G3440-85012) is a solution of 20 compounds, each at 500 ppm (500 ng/µL), in n-propanol. If the checkout mix is unavailable, an alternate mix containing toluene-d8 can be used for relocking, such as Ultra Scientific (p/n STS-310). The names and CAS numbers of the compounds in the G3440-85012 mix are listed in Table 8 on page 33 in RT order.

Table 8 Solvents-Plus checkout mix compound list

Compound	RT	CAS number
Pentane	3.284	109660
Allyl chloride	3.718	107051
Allyl ether	6.275	557404
Propyl acetate	6.613	109604
Propylene glycol	7.045	57556
Toluene-d8	7.790	2037265
n-Octane	8.371	111659
2-Methylbutyl acetate	9.857	624419
Diethyl disulfide	11.004	110816
Phenol	11.698	108952
o-Ethyltoluene	12.054	611143
p-Isopropyltoluene (p-Cymene)	12.864	99876
Indene	13.398	95136
Nitrobenzene	14.108	98953
1-Nonanol	15.077	143088
Decanal	15.702	112312
n-Nitroso-di-n-butylamine	16.670	924163
1,8-Octanediol	17.745	629414
2,6-Di-tert-butyl-4-methylphenol (BHT)	20.111	128370
n-Hexadecane	21.091	544763

The VOA method should be RT locked to toluene-d8 at 7.790 minutes. If a toluene-d8 standard is not available, the system RT lock can be checked with chlorinated tap water. Chloroform should elute at ~ 5.08 min, bromodichloromethane

at ~ 6.80 min, and dibromochloromethane at ~ 8.63 min. These three compounds are commonly found in chlorinated drinking water in the 1–50 ppb range.

Standards Preparation for Relocking the VOA Column

Partially fill two 20 mL headspace vials with 10 mL water. Spike 2 uL of the Solvents-Plus checkout mix into each of the headspace vials. The resulting concentration is 100 ppb in the water. Place the vials in the first two tray positions. These will be used for relocking the previously locked method.

Loading the VOA Acquisition Method

Open the ChemStation instrument control software and click **Method > Load Method** and choose the method called **VOA_3in1_acq.m.**

Relocking Sequence

The process here is similar to that used for relocking the S-VOA method.

1. Set up a two line sequence using the method **VOA_3in1_acq.m**. Name the datafiles **VOA_3in1_Relock_1** and **VOA_3in1_Relock_2.**
2. Save the sequence as **VOA_Relock_Seq.s** and run the sequence.
3. After the sequence is completed, start the **Instrument 1 Data Analysis** program.
4. Use the **Method > Load Method** menu item to load the same **VOA_3in1_acq.m** file that was run in the sequence.
5. Load the second run from the sequence (the first run was just to clean out the column) named **VOA_3in1_Relock_2.D.**

6 Select the **View > RTLock Setup** menu item to open the **RTLock** screen. Proceed with relocking the acquisition method, **VOA_3in1_acq.m**, using datafile **VOA_3in1_Relock_2.D**. The new inlet pressure has now been saved to the method.

NOTE The new pressure will not be applied to the method or to the GC until the method is reloaded or is run.

7 Select the **View > Return to Data Analysis** menu item to close the **RTLock Setup View**.

8 On the GC keyboard, press the **Back Inlet** key to view the pressure setpoints for the inlet the method is using. In the **Data Acquisition** view, re-load your method **VOA_3in1_acq.m.**

You should see the new calculated locking pressure downloaded as the setpoint for the inlet.

Confirming the Lock

After relocking the method, a third run (optional) of the checkout mix can be made to verify the locking pressure and time, if the RT lock time of toleune-d8 was off by more than ± 0.010 minutes.

The best way to do this is to add a line to the existing sequence and then use the **Sequence > Position and Run** menu item.

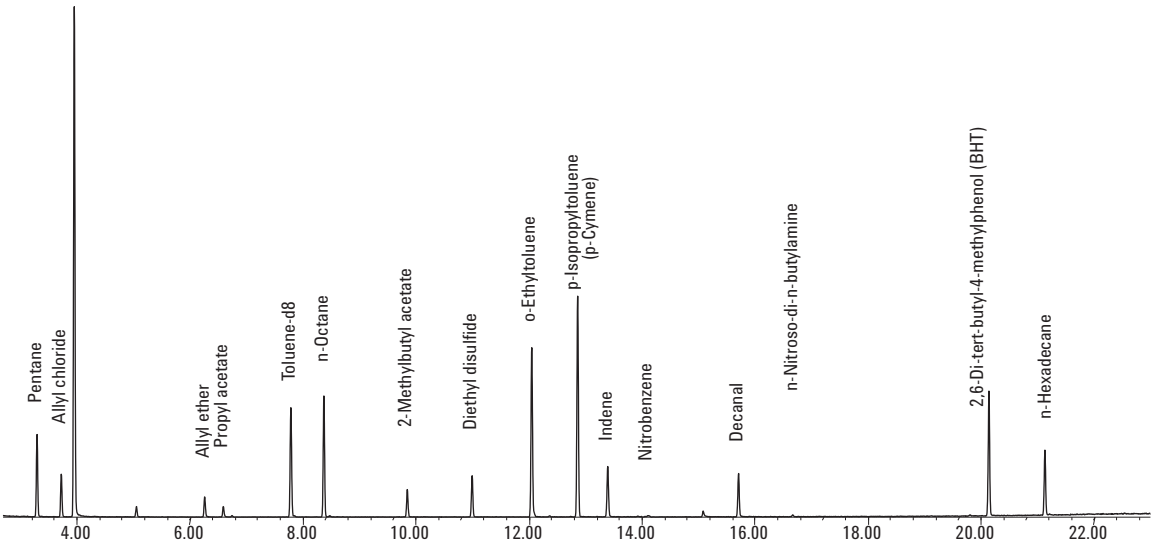

Figure 7 Solvents-Plus checkout mix total ion chromatogram

When run using headspace, some compounds may have a much lower response, such as propylene glycol, phenol, or 1,8-octanediol, due to their solubility in water.

DRS Analysis of the Solvents-Plus Checkout Mix

This step is to confirm that the retention times across the entire elution range of the chromatogram match those in the method closely enough to have all peaks fall in their recognition windows.

1 In Data Analysis using the **Method > Load Method...** menu item, load the method **VOA_3in1_DA-checkout.m.**

2 Using the **File > Load Data File...** menu item, load the last checkout mix relocking run that was made. Select the menu item **DRS > Quant + DRS single file**. After a moment, you will see activity on the computer as DRS performs a quantitative analysis, deconvolutes the mass spectra and searches the **VOA_3in1_checkout.msl** AMDIS database. Depending upon the deconvolution settings chosen, the DRS process will typically take 2 to 4 minutes. At this point, DRS will generate a report that looks similar to (but not necessarily identical to) Figure 7 on page 36.

3 Inspect the report and compare it to the list of compounds in the sample.

Also note that the **ChemStation Amount** column gives only estimated amounts for the compounds that it identified. These amounts are based on a single point response factor that is supplied with your method. You must calibrate any compounds that you wish to quantify as you do with any other GC/MS method.

The **AMDIS** amount column is completed after the QEdit process.

The **AMDIS** column of the DRS report should find all the analytes in the test mix, typically with match factors > 80 and with RT differences of < 10 seconds.

MSD Deconvolution Report

Sample Name: 2 uL 500ppm VOA COM

Data File: C:\msdchem\1\DATA\VOA_3in1_Relock_2.D

Date/Time: 2:31:01 PM Thursday, May 26, 2011

Adjacent Peak Subtraction = 1

Resolution = Medium

Sensitivity = High

Shape Requirements = Medium

The NIST library was not searched for the components that were found in the AMDIS target library.

			Amount (ppb)		AMDIS		NIST	
RT	Cas number	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec	Reverse Match	Hit Num.
3.2976	109660	Pentane	10		100	–0.0		
3.7269	107051	Allyl chloride	9.97		100	–0.0		
6.2628	557404	Allyl ether	10		98	0.0		
6.5954	109604	Propyl acetate	10		98	0.1		
7.7893	2037265	Toluene-d8	10		100	–0.0		
8.375	111659	n-Octane	10		84	0.0		
9.8501	624419	2-Methylbutyl acetate	10		99	0.0		
10.9992	110816	Diethyl disulfide	10.01		100	–0.0		
12.0524	611143	o-Ethyltoluene	10		100	0.0		
12.8663	99876	p-Isopropyltoluene (p-Cymene)	10		100	–0.0		
13.3979	95136	Indene	10		100	–0.0		
14.1014	98953	Nitrobenzene	9.46		76	–0.5		
15.079	143088	1-Nonanol	10.17		83	0.1		
15.7087	112312	Decanal	10		97	–0.0		
16.670	924163	n-Nitroso-di-n-butylamine	10					
20.1332	128370	2,6-Di-tert-butyl-4-methylphenol (BHT)	10		99	0.0		
21.1227	544763	n-Hexadecane	10		97	–0.2		

Figure 8 Example of Solvents-Plus checkout mix DRS report

4
Pesticides Analyzer Specifics

The pesticide portion of the 3-in-1 Analyzer uses the S-VOA hardware and column with method modifications, see Figure 2 on page 16. The pesticides method is not RT locked by the Specials Group, and should be done on site by the user after the S-VOA Analyzer section is completed.

The single-taper with glass wool liner, (p/n 5190-2293), introduced in early 2011, is UI deactivated and is used for HSL. CSL injections can be done using a 2 mm dimple liner (p/n 5190-2296) and conditions in *Application Note 5989-7875*. The 3-in-1 Analyzer uses a 20 m × 0.18 mm × 0.36 um DB-8270D column (p/n 121-9723) which is a more inert version of DB 5-MS. The Pesticide Analyzer should be RT locked to lindane at 9.100 minutes.

The pesticides acquisition method, **Pest_3in1_acq_bf.m**, is scan only and can be run at a sampling rate of 2^2 or 2^1. Users may want to run SIM for some compounds, and if SIM/scan is run, the rate should be set to 2^1. With SIM/scan, the SIM signal can be used for quantitation of the most important analytes and the scan signal can be used for deconvolution and identification of the remaining pesticides.

The 927 compound quant database was taken from Agilent's G1672AA pesticides DRS DBL, but has been modified. The original pesticides DRS DBL was built using a 30 m × 250 um × 0.25 um column running in constant pressure mode. The 3-in-1 Analyzer pesticides column is a 20 m × 180 um × 0.36 um column running in constant flow mode. The original 927 pesticides DBL was mapped to the 3-in-1 Analyzer column running in CF mode. More than 50 index peaks were used with a 6th order curve fit to translate the RTs. All of the 927 pesticides were not rerun on the 3-in-1 Analyzer column. The translated RTs should be ± 0.10 minutes from actual, with some outliers, as shown in Figure 9 on page 47. Because all of the RTs are not precise, this modified pesticides database will be provided at no charge, only as part of the 3-in-1 Environmental Analyzer.

For best system performance, it is important to use the methods and files listed in Table 2 on page 13.

Copying and Pasting Pesticides Files

Copy the pestidides files from the CD supplied by the Specials Group and paste them into the location listed in Table 9. This CD is not one of the software installation CDs.

Table 9 Copying-pasting pesticides files

File name	Location to paste the copied file
Pest_3in1_acq_BF.m Pest_3in1_DA-checkout.m Pest_3in1_DA.m	C:\MSDchem\1\Methods
Pest_3in1_checkout.D	C:\MSDchem\1\Data
Pest_3in1_checkout.msl Pest_3in1_checkout.cid Pest_3in1.cal Pest_3in1.csl RTLPest3.msl RTLpest3.cid	C:\NIST08\AMDIS32\Lib
Onsite.ini Default.ini	C:\NIST08\AMDIS32\Lib
Nistms.ini	C:\NIST08\Mssearch
AmdisConfig.txt	C:\Program Files\Agilent\MSD Deconvolution Reporting Software
RTLPest3.L	C:\Database

Description of Pesticides Files

Pest_3in1_acq_BF.m–the method has not been RT locked by the Specials Group. This method should be RT locked by the user for data acquisition of the checkout mix and samples. On loading the method, Method Resolution will be required.

Pest_3in1_DA-checkout.m–the data analysis method that contains 20 compounds in the quantitation database, and will be used for the DRS analysis of the checkout mix.

Pest_3in1_DA.m–the data analysis method that contains 927 compounds in the quantitation database that can be used for samples. The RTs have been translated as described earlier and can be updated by users, if needed, after running standards.

Pest_3in1_Checkout.D–an example datafile that can be used as a reference for the checkout sample run.

Pest_3in1_checkout.msl, Pest_3in1_checkout.cid, Pest_3in1.cal, Pest_3in1.csl–these are the AMDIS files designed for the pesticides portion of the 3-in-1 Analyzer.

RTLPest.msl, RTLPest3.cid–this is the 927 compound pesticides DRS Database-Library and associated directory file, provided at no charge. The G1672AA pesticides DBL product should not be purchased nor installed.

Nistms.ini, AmdisConfig.txt, Default.ini–these are configuration files specific to the Analyzer and should overwrite the exisiting files in the specified directories.

Onsite.ini–this is an **AMDIS** configuration file specific to the Analyzer and should overwrite the exisiting file in the specified directory. When running **Pesticides**, the **RI Window** in **AMDIS** should be changed to 45. This can be found under the **Analyze > Settings... Identification** tab in **AMDIS**.

Loading and Relocking the Pesticides Method

The GC/MSD pesticides checkout mix (p/n 5190-0468) is a solution of 20 compounds, each at 10 ppm (10 ng/µL), in acetone. The names and CAS numbers of the compounds in the mix are listed in Table 10 in RT order.

Table 10 Pesticides checkout mix compound list

Compounds	RT	CAS number
Dichlorvos	4.892	62737
Mevinphos	6.006	7786347
Ethalfluralin	7.750	55283686
Trifluralin	7.862	1582098
Atrazine	8.786	1912249
Lindane	9.100	58899
Chlorpyrifos methyl	10.055	5598130
Heptachlor	10.448	76448
Malathion	10.706	121755
Chlorpyrifos	10.890	2921882
p,p'-DDE	12.838	72559
Dieldrin	13.059	60571
Hexazinone	14.406	51235042
Propargite	14.564	2312358
Leptophos	15.896	21609905
Fenarimol	16.444	60168889
Mirex	16.483	2385855
Coumaphos	17.107	56724
Ethofenprox	18.146	80844071
Deltamethrin	19.793	52918635

Open one of the vials of the pesticides checkout mix and transfer it to an autosampler vial. Place the autosampler vial in tray position one. This will be used for RT locking the method.

The method, **PEST_3in1_acq_BF.m**, should be **RTLocked to Lindane at 9.100** minutes.

RT Locking the Method

The method, **PEST_3in1_acq_BF.m**, should be RT locked in **Data Acquisition**. The procedure for this is found in the MSD Chemstation Help, by Searching **rtlocking** and then select **To lock an MS method**. An outline of the steps is as follows:

1. Load the acqusition method, **PEST_3in1_acq_BF.m**, in the **Data Acqusition View** and **Resolve** if necessary.
2. Place a vial of the pesticides checkout mix in position one of the autosampler.
3. Acquire the initial 5 RT locking runs.
4. A new Data Analysis session will start after completion of the 5 runs.
5. Select the peak for locking. Lindane should elute close to 9 minutes.
6. Complete the remaining dialogue box inputs.
7. Reload the method in **Data Acquisition.**

Relocking Sequence

The process here is similar to that used for relocking the S-VOA method.

1. Set up a two-line sequence using the method **PEST_3in1_acq_BF.m**. Name the datafiles **PEST_3in1_Relock_1** and **PEST_3in1_Relock_2**.
2. Save the sequence as **PEST_Relock_Seq.s** and run the sequence.
3. After the sequence is completed, start the **Instrument 1 Data Analysis** program.
4. Use the **Method > Load Method** menu item to load the same **PEST_3in1_acq_BF.m** file that was run in the sequence.
5. Load the second run from the sequence (the first run was just to clean out the column) named **PEST_3in1_Relock_2.D**.

6 Select the **View > RTLock Setup** menu item to open the **RTLock** screen.

7 Proceed with relocking the acquisition method, **PEST_3in1_acq_BF.m**, using datafile **PEST_3in1_Relock_2.D.** The new inlet pressure has now been saved to the method.

NOTE The new pressure will not be applied to the method until the method is reloaded or is run.

8 Select the **View > Return to Data Analysis** menu item to close the **RTLock Setup View**.

9 On the GC keyboard, press the **Front Inlet** key to view the pressure setpoints for the inlet the method is using.

10 In the **Data Acquisition** view, re-load your method **PEST_3in1_acq_BF.m**.

You should see the new calculated locking pressure downloaded as the setpoint for the inlet.

Confirming the Lock

After relocking the method, a third run (optional) of the checkout mix can be made to verify the locking pressure and time, if the RT lock time of lindane was off by more than ± 0.010 minutes from the expected 9.100 minutes.

The best way to do this is to add a line to the existing sequence and then use the **Sequence > Position** and **Run** menu item.

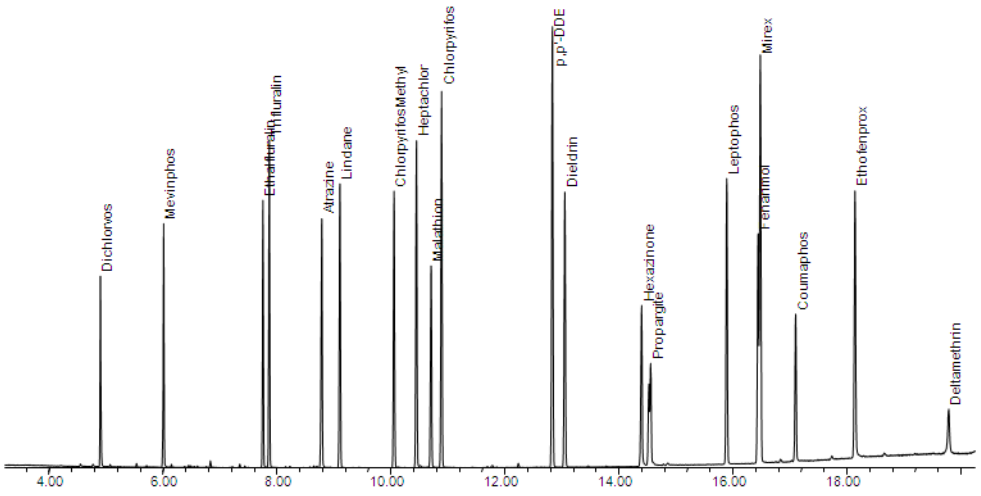

Figure 9 Pesticides checkout mix total ion chromatogram

DRS Analysis of the Pesticides Checkout Mix

This step is to confirm that the retention times across the entire elution range of the chromatogram match those in the method closely enough to have all peaks fall in their recognition windows.

1. In **Data Analysis,** using the **Method > Load Method...** menu item, load the method **Pest_3in1_DA-checkout.m.**
2. Using the **File > Load Data File...** menu item, load the last checkout mix relocking run that was made. Select the menu item **DRS > Quant + DRS single file**. After a moment, you will see activity on the computer as DRS performs a quantitative analysis, deconvolutes the mass spectra and searches the **Pest_3in1_checkout.msl AMDIS** database, then searches the NIST08 library. Depending upon the deconvolution settings chosen, the DRS process will typically take 2–4 minutes. At this point, DRS will generate a report that looks similar to (but not necessarily identical to) Figure 10 on page 49.
3. The DRS Report for the pesticides checkout mix shows two compounds, dieldrin and mirex, with RT differences of > 30 sec with respect to the **AMDIS** database **RTLPest3.msl**. Differences such as these can be expected for a subset of the database due to the translation that was described earlier. The GC/MSD Chemstation quantitation database (qdb.mth) time were translated using the index compounds. The expected RTs in the **RTLPest3.msl** were not changed from the original values. Instead a modified RT calibration file, **Pest_3in1.cal** is used to translate the retention times.

   Also note that the **ChemStation Amount** column gives only estimated amounts for the compounds that it identified. These amounts are based on a single point response factor that is supplied with your method. You must calibrate any compounds that you wish to quantify as you do with any other GC/MS method.

   The **AMDIS Amount** column is completed after the QEdit process.

MSD Deconvolution Report

Sample Name: Pesticides Checkout

Data File: C:\msdchem\1\DATA\Pest_3in1_checkout.D

Date/Time: 9:31:29 AM Tuesday, June 07, 2011

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 (ppm)		AMDIS		NIST	
RT	Cas number	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
4.8939	62737	Dichlorvos	10		99	0.0	94	1
6.0058	7786347	Mevinphos	10		100	–0.0	91	2
7.752	55283686	Ethalfluralin	10		99	0.1	95	1
7.8602	1582098	Trifluralin	10		98	–0.0	93	1
8.7850	1912249	Atrazine	10		98	–0.0	93	1
9.1017	58899	Lindane	10		99	–0.0	94	1
10.0547	5598130	Chlorpyrifos Methyl	10		99	–0.0	90	1
10.4477	76448	Heptachlor	10		100	0.0	95	1
10.7060	121755	Malathion	10		99	0.0	93	1
10.8886	2921882	Chlorpyrifos	10		100	–0.1	93	1
12.8357	72559	p,p'-DDE	10		100	–0.0	96	1
13.058	60571	Dieldrin	10		99	37.7	96	2
14.407	51235042	Hexazinone	10		99	0.3	88	1
14.532	2312358	Propargite	10		84	0.0	86	1
15.8956	21609905	Leptophos	10		100	–0.0	78	1
16.447	60168889	Fenarimol	10		90	0.4	88	1
16.486	2385855	Mirex	10		98	38.9	94	1
17.1035	56724	Coumaphos	10		99	–0.1	94	1
18.1467	80844071	Ethofenprox	10		95	–0.0	93	1
19.7897	52918635	Deltamethrin	10		86	0.5	92	1

Figure 10 Example of pesticides checkout mix DRS report

5 Allowed 3-in-1 System Configurations

GC	7890A
Oven	120V or 240V
Front inlet	S/SL or MMI for S-VOA–checkout is hot splitless
Rear inlet	S/SL for VOAs
Splitter	Purged 2-way acting as a column effluent combiner
Aux EPC	3 channel
Aux Temp	MSD aux heater option
Autosampler	7693 with tray is recommended, but an Injector only is allowed
Inlet weldment	Rear inlet top weldment replaced with G3521A for interfacing the headspace sampler
MSD	5975C
Pump type	Either a turbo or a diffusion pump is allowed, however, Agilent strongly recommends the turbo pump
Headspace	7697A with 111 sample capacity is recommended, but the 12 position headspace is allowed
Software	GC/MSD Chemstation NIST08 DRS base product G1716AA S-VOA DRS DBL G1677AA Solvents-Plus DRS DBL G1678AA

Pesticides DRS DBL included on the Specials CD at no charge. Do not order.

6 Consumables and Supplies

Below is a list of consumables and parts that are used with the Agilent 3-in-1 Analyzer.

Table 11 Agilent 3-in-1 Analyzer consumables and parts

3-in-1 Columns and column accessories	Part number
S-VOA-Pesticide Column, Agilent J&W DB-8270D GC Column, 20 m × 0.18 mm × 0.36 um	121-9723
VOA Column, Agilent J&W DB-5 MSUI GC Column, 30 m × 0.25 mm × 1.0 um	121-5533UI
Restrictor tubing, 0.15 mm SilTek deactivated, 5 m 1.1 m × 0.15 mm used in oven from 2-way splitter to MSD transfer line	160-7625-5
Column ferrule, MMI, graphite (10/pk), for inlets	5080-8853
Column nut, GC capillary (2/pkg), for inlets	5181-8830
MSD Transfer line ferrule, 0.4 mm graphite/vespel, long 10pk	5062-3508
Column nut for MSD tranfer line when using p/n 5062-3508	05988-20066
Restrictor tubing, 0.53 mm SilTek deactivated, 5 m for headspace	Restek p/n 10028

Table 11 Agilent 3-in-1 Analyzer consumables and parts (continued)

GC inlet and instrument supplies	Part number
S-VOA Inlet liner, MMI or S/SL, 4 mm id with UI deactivated wool	5190-2293
S-VOA Inlet liner, MMI, cold splitless only, 2 mm id	5190-2296
VOA inlet liner, 1.2 mm straight for interfacing headspace 5pk	8004-0157
Septum, advanced green (50/pkg)	5183-4759
O-ring, inlet liner non-stick (10/pkg)	5188-5365
ALS syringe, 10 µL tapered fixed needle, PTFE-tipped plunger, 6pk	G4513-80208
ALS syringe, 10 µL tapered fixed needle, PTFE-tipped plunger	G4513-80200
Capillary flow parts	
Internal nut for capillary flow devices	G2855-20530
SilTite ferrule for 0.25 mm and smaller columns (10/pkg)	5188-5361
2-Way purged splitter, plate only	G3180-61500
Bleed line, 0.0625 in OD × 0.010 in id × 100 cm, 316SS tubing	0100-2354
1/16 in Brass Swagelok tee	0100-0680
Bleed tee ferrule, 1/16 in Vespel (10/pkg)	0100-1329
Useful tools	
MSD column installation tool	G1099-20030
Ferrule pre-swage tool for capillary flow devices	G2855-60200
Chemical standards	
S-VOA Locking-Checkout Standard, 3 ampoules, 1 mL	5190-0473
Pesticides Locking-Checkout Standard, 3 ampoules, 1 mL	5190-0468
VOA (Solvent+) Locking-Checkout Standard	G3440-85012

Table 11 Agilent 3-in-1 Analyzer consumables and parts (continued)

CDs	
DRS video CD "DRS Familiarization Videos"	5973-1731
CD disk (Installation guide, Methods, Autotune file, AMDIS settings, configured DRS methods, checkout datafiles and DRS report)	not a replaceable part

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