Agilent G6854AA MassHunter Personal Pesticide Database Kit

Quick Start Guide

What is the MassHunter Personal Pesticide Database Kit ?

The MassHunter Personal Pesticide Database Kit lets you screen up to 1600 pesticides with accurate mass measurement, all in a single LC/MS analysis.

The MassHunter Personal Pesticide Database Kit helps minimize method development time for your Pesticides analysis. The database stores your retention times for compounds you target along with all entries in new databases that you name. You can add, remove and change the compounds in the database to meet the specific needs of your laboratory and your analyses.

The high mass accuracy of the Agilent time-of-flight (TOF) and tandem quadrupole time-of-flight (Q-TOF) LC/MS instruments provides the capability to screen and identify all compounds in the database that are detected by their exact mass and retention time (if known). Retention times can be

a search criterion specified as not required (non-targeted screen), as optional providing a targeted and non-targeted pesticide screen, or required (targeted screen only).

Kit Content

Agilent G6854AA MassHunter Personal Pesticide Database Kit Quick Start Guide (p/n 5990-4262EN) The Quick Start Guide provides an overview of the Database Kit, how to use it, and where to find further information. A copy of the Test Mix Report Example is also included in this document.

Agilent G6854AA MassHunter Personal Pesticide Database Quick Start Guide (p/n G6854-90003) The Quick Start Guide provides an overview of the MassHunter Personal Compound Database and Library program, how to use it with the Personal Pesticide Database, and where to find further information.

MassHunter Personal Pesticide Database Kit Support Disk (p/n G6854-90002)

The contents of the disk are:

- The TOF/Q-TOF LC/MS method **TestMix_pos.m** and **TestMix_neg.m** for running the test mix (positive & negative ion mode)
- A sample chromatogram and database screening report obtained with the test mix
- Example methods for acquisition and data analysis
- Technical note on accurate mass database
- Application notes that discuss screening with the MassHunter Personal Pesticide Database
- *Agilent G6854AA MassHunter Personal Pesticide Database Kit Quick Start Guide* (PDF)

MassHunter Personal Pesticide Database disk (p/n G6854-60005) Included in the kit is a disk that contains the MassHunter Personal Compound Database and Library program version B.03.01, the Personal Pesticide Database, the *Agilent G6854AA MassHunter Personal Pesticide Database Quick Start Guide* and related software license agreements. See "Installation" on page 4 for a list of software requirements.

ZORBAX LC Column (p/n 959764-902) Eclipse Plus C18, 2.1mm x 100, 1.8 µm.

LC/MS Pesticide Test Mix (p/n 5190-0469) Acidic and basic pesticides sample mixes (3 vials each) for your test runs.

QuEChERS SPE kit (p/n 5982-7005) AOAC method sample pack, 3 samples.

QuEChERS SPE kit (p/n 5982-7000) EN method sample pack, 3 samples.

Where to find more information

Application Notes and Publications You can find information about the MassHunter Personal Pesticide Database in the application notes and publications included on the support disk.

QuEChERS Extraction Procedures and Ready-to-use Kits The QuEChERS (Quick Easy, Cheap, Effective, Rugged and Safe) extraction procedure for pesticide residues in fruits and vegetables is being used by labs around the world. For a training video, references, and ready-to-use kits for doing QuEChERS extractions, go to http://www.chem.agilent.com/en-US/products/consumables/samplepreparation/sampliqspe/sampliqquechers

Alternatively, go to http://www.chem.agilent.com/ and type QuEChERS into the search field.

Before You Begin

Installation

1. Check that the Agilent 1200 Series LC is properly installed and verified.
2. On the Agilent 1200 Series Binary Pump SL, check that the mixer and damper are bypassed. See "To bypass mixer and damper" on page 23 for details.
3. Check that the Agilent 6200 Series Time-of-Flight LC/MS or Agilent 6500 Series Quadrupole Time-of-Flight instrument is properly installed and verified.
4. Check that the following programs are properly installed:
   - MassHunter Data Acquisition B.02.01 or higher
   - MassHunter Quantitative Analysis B.03.01 or higher
   - MassHunter Qualitative Analysis B.03.01 or higher
5. Install the MassHunter Personal Pesticide Database. Follow the installation instruction in the MassHunter Personal Pesticide Database *Quick Start Guide*.
6. Copy the methods on the support disk to the **D:\MassHunter\Methods** folder, or a folder under the **Methods** folder.

   The MassHunter Qualitative Analysis methods **TestMix_pos.m** and **TestMix_neg.m** contain both acquisition and data processing settings, and are to be used to run your test mixes.

   The methods **MFE_Pesticides.m** and **Find_by_formula_Pesticides.m** are data processing only methods.

Required Reagents and Parts

- LC/MS grade acetonitrile and water
- ZORBAX LC column, p/n 959764-902
- Glacial acetic acid 99.9% (highest purity)
- Formic acid (highest purity)
- Ammonium formate (highest purity)
- Ammonium acetate (highest purity)
- Ammonium hydroxide (highest purity)

Getting Started

The sample data files provided in the support disk were acquired with the test mixes on a system with the LC/MS system configured as described in "Installation" on page 4. Along with the sample data files are the methods with which these data files were acquired. If you review the acquisition method and sample data, you will get an idea of the data acquisition, data processing, and result interpretation from using the MassHunter Personal Pesticide Database Kit.

To review the Acquisition Method, use the MassHunter Data Acquisition program to open the method file **TestMix_pos.m**. The following data acquisition settings for the positive ion compounds are listed:

- Acquisition method information
- TOF/Q-TOF LC/MS settings
- Wellplate Sampler settings
- Binary Pump settings
- Thermostatted Column Compartment settings

The acquisition method parameters for the negative ion test mix are in the **TestMix_neg.m** acquisition method.

Note that both methods use two reference ions, which are dispensed from reference bottle A of the calibration delivery system. The two compounds used are from the API-TOF Reference Mass Solution (p/n G1969-85001) and are purine and HP-0921. Prepare the reference ion solution as recommended in the installation guide for your instrument. Do not use the trifluoracetic acid (TFA) found in the reference kit.

Make sure little residual or no signal from the TFA in the calibration mix comes from tuning or calibrating. Use the same reference solution for positive and negative ion analysis. If the purine does not give a usable signal in negative ion mode at m/z 119.06320, clean your ion source.

To run the test mix

Run the test mix (p/n 5190-0469) to get a better idea of how the MassHunter Personal Pesticide Database Kit will work for you.

1 Do a check tune to verify that the instrument operates properly.

Refer to the *Agilent 6200 Series TOF and 6500 Series Q-TOF LC/MS System Quick Start Guide* for instructions to tune the instrument.

2 Prepare the test mixes.

The concentration of the test mix stock solution is 100 ppm for both positive and negative mixes.

a Dilute 100 µL of the stock solution to 10.0 mL with acetonitrile to create the interim solution.

b Take 100 µL of the interim solution and dilute it to 10.0 mL with 10:90 acetonitrile:water.

c Transfer the final solution to a standard 2 mL sample vial for analysis.

The final solution is a 10 ppb working solution. Do this separately for the positive and negative test mixes.

3 Prepare mobile phases A and B.

- A= 5 mM acetic acid in water (300 µL glacial acetic acid in 1 L water)
- B= 100% acetonitrile

4 Run the test mix.

For the positive ion mix, load the method **TestMix_pos.m**. For the negative ion mix, load **TestMix_neg.m**. These methods use the system configuration as listed below. Systems that deviate from this configuration may not work with this method.

Column	2.1 x 100 ZORBAX Eclipse Plus C18 1.8 µm, p/n 959764-902
Wellplate Sampler	h-ALS-SL+, model# G1367D
Pump	Binary Pump – SL, Model 1312B configured with damper and mixer removed
Column Compartment	Column – SL, Model G1316B

5 Check that your method is set up to make a 5 µL injection.

6 Click **Run > Interactive Sample** to do a single sample run, or create a worklist to make multiple injections.

7 If you do not see all the peaks after you process your data:

a Extend your Stop time in the method to 15 minutes.

b Check that you detect reference ions between 10,000 and 100,000 counts, and that their *m/z* values are within a few millidaltons of the expected *m/z* values.

c Make sure your system is tuned and calibrated correctly.

d Run the test mix again.

This will not affect your results but will show if retention times are different on your system. (There are a number of reasons your retention times can change from those determined by Agilent, such as different instrument dead volume or configuration).

To process and interpret test mix data

In this topic, you process the data file that you created when you ran the test mix. The figures in this task are based on the example data file **Test_Mix_Pos.d** found on the support disk. Your results may differ slightly.

1 Open the MassHunter Qualitative Analysis program.

Click **Cancel** if you are asked to open a data file.

2 Process the data file for the positive ion test mix:

a Load the method **TestMix_pos.m**.

b Open the data file that you created when you ran the test mix.

You can also use example data file **Test_Mix_Pos.d** on the support disk. See Figure 1.

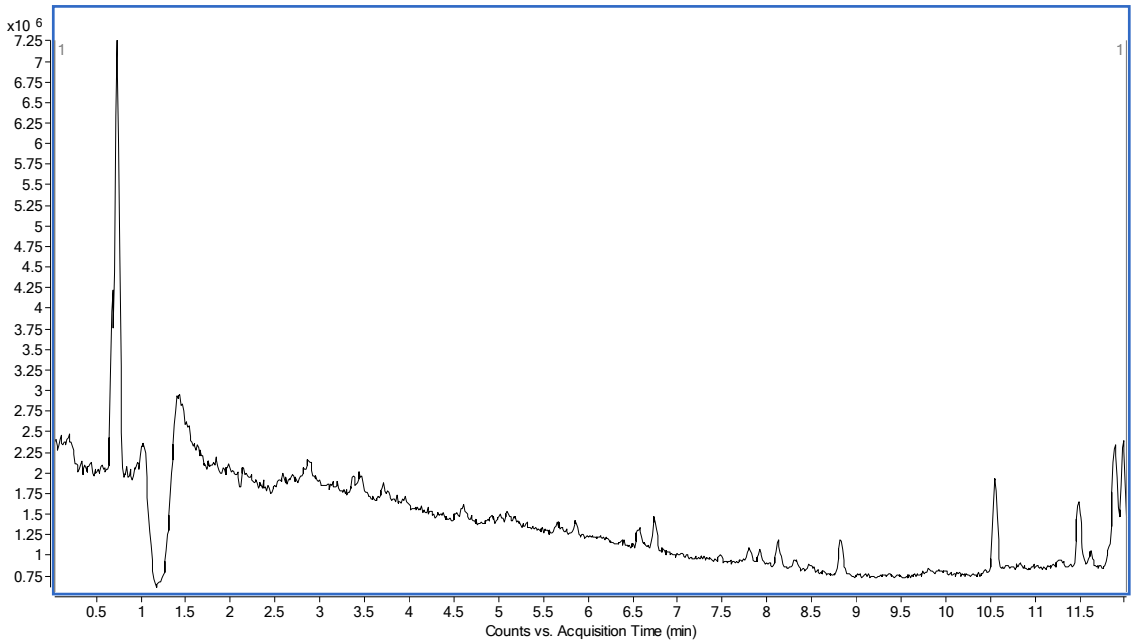


Figure 1 Example test mix chromatogram

c In the Method Explorer window, under **Chromatogram**, select **Define Chromatograms**. See Figure 2.

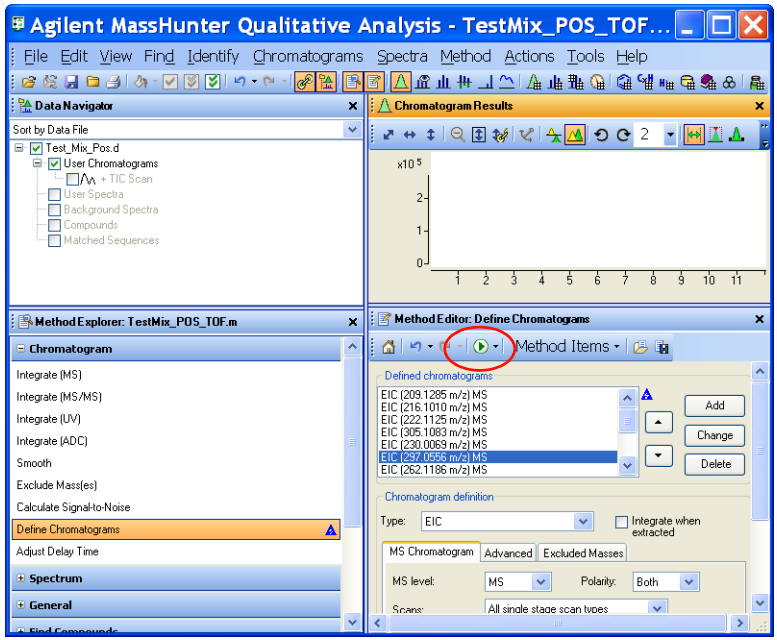


Figure 2 Define Chromatograms section selected. Click the green arrow (circled) to extract the ions.

A list of the exact *m/z* values of the compounds in the mixture is displayed in the Chromatograms > Define Chromatograms section.

3 Click the green arrow in the Chromatograms > Define Chromatograms section to extract the ions.

After the chromatograms are extracted, they are displayed in the Chromatogram Results window, as seen in Figure 3, if the view is in List Mode. In Figure 3, you can see the major peak in each EIC. The text mix data collected on your system will show a similar result.

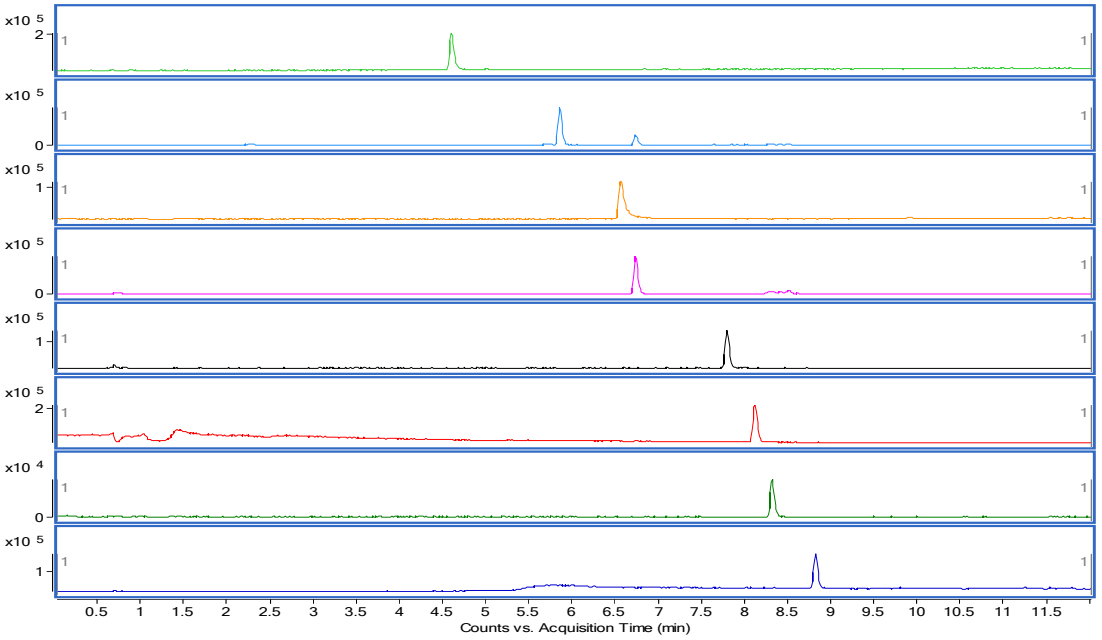


Figure 3 Extracted chromatograms

4 Repeat step 2 with the negative ion test mix. Use the data file that you collected from the negative ion test mix (or use **Test_Mix_Neg.d** file from the support disk), and load the **TestMix_neg.m** from the support disk.

The TIC for this data file is displayed when the file is opened.

5 Right-click on the TIC and click **Extract Defined Chromatogram**.

Again a plot of each extracted ion shows you that each compound is present. See Figure 4.

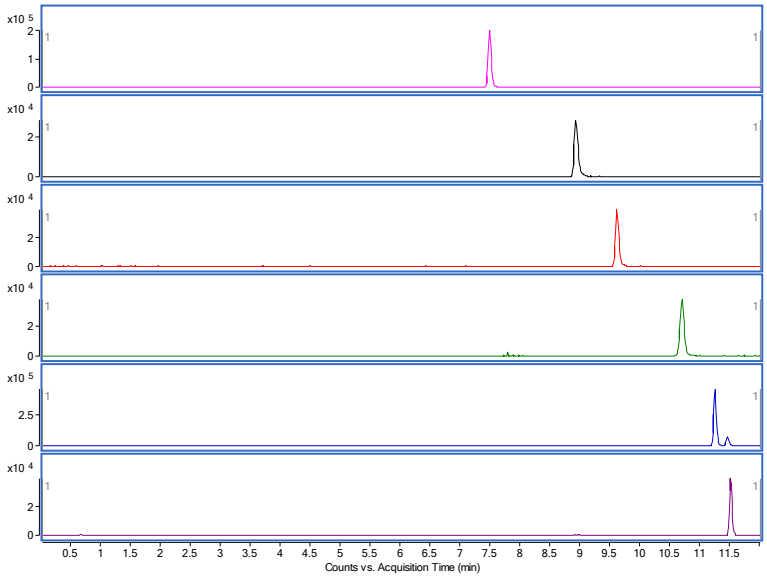


Figure 4 Extracted chromatograms

6 Load the **Find_by_formula_Pesticides.m** method from the support disk.

7 Locate the **Find Compounds by Formula** section in the Method Explorer. Review the settings in this method to become familiar with peak detection, mass tolerances and other settings. These settings may need to be adjusted for specific matrices.

8 Search for pesticide database compounds in the data file in a worklist with the **Find_by_formula_Pesticides.m** method:

a In the Method Explorer window, under **Worklist Automation**, click **Worklist Actions**.

b Make sure that these two actions are listed under **Actions to be run:**

Compound Automation without report
Generate Compound Report.

Make sure **Compound Automation with report** is *not* listed.

c Save the method.

d Click the green arrow () in the Method Editor toolbar.

The Qualitative Analysis program searches the data file for every compound in the pesticide database.

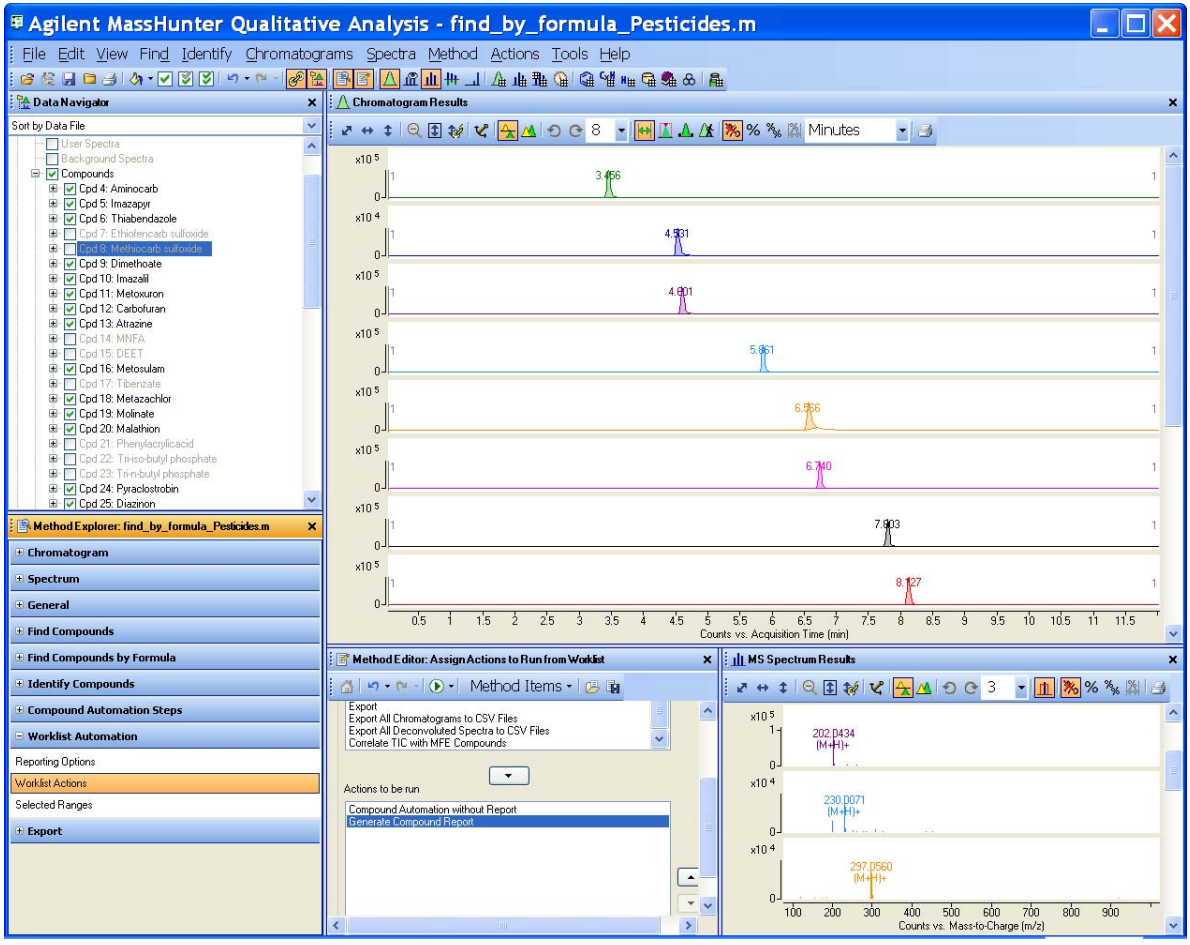


Figure 5

Note that all the isomers of dinoseb are listed in the compounds found in the database.

9 Load the method file **MFE_Pesticides.m**.

10 In the Method Explorer, locate the Find Compounds > Find by Molecular Formula section and review the settings in all tabs.

11 Review all settings in the Extractor tab.

12 Search for pesticide database compounds in the data file:

a In the Method Explorer window, under **Worklist Automation**, click **Worklist Actions**.

b Click the green arrow in the Method Editor toolbar.

The Find by Molecular Feature algorithm is much faster than the Find by Formula algorithm, but it may not be as thorough. The compound report generated from this method using Worklist automation is shown below:

Data File	TestMix_pos_13.d	**Sample Name**	test_Mix_pos_1
Sample Type	Sample	**Position**	P1-F2
Instrument Name	CAS6530_1	**User Name**	
Acq Method	CO_pos_ultra.m	**Acquired Time**	6/1/2009 3:28:51 PM
IRM Calibration Status	Success	**DA Method**	MFE_Pesticides.m
Comment			

Compound Table

Compound Label	RT	Mass	Name	DB Formula	DB Diff (ppm)
Cpd 19: Aminocarb	3.472	208.1213	Aminocarb	C11 H16 N2 O2	-0.44
Cpd 40: Imazapyr	4.543	261.1113	Imazapyr	C13 H15 N3 O3	-0.03
Cpd 41: Thiabendazole	4.612	201.036	Thiabendazole	C10 H7 N3 S	0.2
Cpd 52: Ethiofencarb sulfoxide	5.176	241.0777	Ethiofencarb sulfoxide	C11 H15 N O3 S	-1.91
Cpd 62: Dimethoate	5.866	228.9998	Dimethoate	C5 H12 N O3 P S2	-0.75
Cpd 65: Imazalil	6.549	296.0488	Imazalil	C14 H14 Cl2 N2 O	-1.58
Cpd 66: Imazalil	6.579	296.0485	Imazalil	C14 H14 Cl2 N2 O	-0.65
Cpd 68: Metoxuron	6.746	228.0666	Metoxuron	C10 H13 Cl N2 O2	-0.09
Cpd 85: Carbofuran	7.805	221.1054	Carbofuran	C12 H15 N O3	-1.05
Cpd 88: Atrazine	8.138	215.094	Atrazine	C8 H14 Cl N5	-0.92
Cpd 89: DEET	8.2	191.1309	DEET	C12 H17 N O	0.53
Cpd 90: Tibenzate	8.323	228.0607	Tibenzate	C14 H12 O S	1
Cpd 91: Metosulam	8.33	417.0069	Metosulam	C14 H13 Cl2 N5 O4 S	-0.98

Cpd 92: Fluoroglycofen	8.33	419.0033	Fluoroglycofen	C16 H9 Cl F3 N O7	-3.28
Cpd 93: Tibenzate	8.433	228.0608	Tibenzate	C14 H12 O S	0.39
Cpd 97: Tibenzate	8.527	228.0609	Tibenzate	C14 H12 O S	-0.12
Cpd 99: Metazachlor	8.837	277.0983	Metazachlor	C14 H16 Cl N3 O	-0.53
Cpd 107: Molinate	9.927	187.1027	Molinate	C9 H17 N O S	2.02
Cpd 111: Malathion	10.448	330.036	Malathion	C10 H19 O6 P S2	0.2
Cpd 113: Phenylacrylicacid	10.558	148.0522	Phenylacrylicacid	C9 H8 O2	1.59
Cpd 121: Tri-n-butyl phosphate	11.177	266.1645	Tri-n-butyl phosphate	C12 H27 O4 P	0.58
Cpd 123: Tri-n-butyl phosphate	11.272	266.1646	Tri-n-butyl phosphate	C12 H27 O4 P	0.32
Cpd 125: Pyraclostrobin	11.477	387.0989	Pyraclostrobin	C19 H18 Cl N3 O4	-0.9
Cpd 127: Diazinon	11.497	304.1012	Diazinon	C12 H21 N2 O3 P S	-0.56

Database Search Results

Compound	Hits
Aminocarb	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Aminocarb	TRUE	C11 H16 N2 O2	208.1213	208.1212	-0.44	3.472

Database Search Results

Compound	Hits
Imazapyr	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Imazapyr	TRUE	C13 H15 N3 O3	261.1113	261.1113	-0.03	4.543

Database Search Results

Compound	Hits
Thiabendazole	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Thiabendazole	TRUE	C10 H7 N3 S	201.036	201.0361	0.2	4.612

Database Search Results

Compound	Hits
Ethiofencarb sulfoxide	2

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Ethiofencarb sulfoxide	TRUE	C11 H15 N O3 S	241.0777	241.0773	-1.91	5.176
Methiocarb sulfoxide		C11 H15 N O3 S	241.0777	241.0773	-1.91	5.176

Database Search Results

Compound	Hits
Dimethoate	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Dimethoate	TRUE	C5 H12 N O3 P S2	228.9998	228.9996	-0.75	5.866

Database Search Results

Compound	Hits
Imazalil	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Imazalil	TRUE	C14 H14 Cl2 N2 O	296.0488	296.0483	-1.58	6.549

Database Search Results

Compound	Hits
Imazalil	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Imazalil	TRUE	C14 H14 Cl2 N2 O	296.0485	296.0483	-0.65	6.579

Database Search Results

Compound	Hits
Metoxuron	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Metoxuron	TRUE	C10 H13 Cl N2 O2	228.0666	228.0666	-0.09	6.746

Database Search Results

Compound	Hits
Carbofuran	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Carbofuran	TRUE	C12 H15 N O3	221.1054	221.1052	-1.05	7.805

Database Search Results

Compound	Hits
Atrazine	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Atrazine	TRUE	C8 H14 Cl N5	215.094	215.0938	-0.92	8.138

Database Search Results

Compound	Hits
DEET	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
DEET	TRUE	C12 H17 N O	191.1309	191.131	0.53	8.2

Database Search Results

Compound	Hits
Tibenzate	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Tibenzate	TRUE	C14 H12 O S	228.0607	228.0609	1	8.323

Database Search Results

Compound	Hits
Metosulam	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Metosulam	TRUE	C14 H13 Cl2 N5 O4 S	417.0069	417.0065	-0.98	8.33

Database Search Results

Compound	Hits
Fluoroglycofen	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Fluoroglycofen	TRUE	C16 H9 Cl F3 N O7	419.0033	419.002	-3.28	8.33

Database Search Results

Compound	Hits
Tibenzate	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Tibenzate	TRUE	C14 H12 O S	228.0608	228.0609	0.39	8.433

Database Search Results

Compound	Hits
Tibenzate	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Tibenzate	TRUE	C14 H12 O S	228.0609	228.0609	-0.12	8.527

Database Search Results

Compound	Hits
Metazachlor	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Metazachlor	TRUE	C14 H16 Cl N3 O	277.0983	277.0982	-0.53	8.837

Database Search Results

Compound	Hits
Molinate	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Molinate	TRUE	C9 H17 N O S	187.1027	187.1031	2.02	9.927

Database Search Results

Compound	Hits
Malathion	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Malathion	TRUE	C10 H19 O6 P S2	330.036	330.0361	0.2	10.448

Database Search Results

Compound	Hits
Phenylacrylicacid	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Phenylacrylicacid	TRUE	C9 H8 O2	148.0522	148.0524	1.59	10.558

Database Search Results

Compound	Hits
Tri-n-butyl phosphate	2

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Tri-n-butyl phosphate	TRUE	C12 H27 O4 P	266.1645	266.1647	0.58	11.177
Tri-iso-butyl phosphate		C12 H27 O4 P	266.1645	266.1647	0.58	11.177

Database Search Results

Compound	Hits
Tri-n-butyl phosphate	2

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Tri-n-butyl phosphate	TRUE	C12 H27 O4 P	266.1646	266.1647	0.32	11.272
Tri-iso-butyl phosphate		C12 H27 O4 P	266.1646	266.1647	0.32	11.272

Database Search Results

Compound	Hits
Pyraclostrobin	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Pyraclostrobin	TRUE	C19 H18 Cl N3 O4	387.0989	387.0986	-0.9	11.477

Database Search Results

Compound	Hits
Diazinon	1

Compound	Best	Formula	Mass	Tgt Mass	Diff (ppm)	RT
Diazinon	TRUE	C12 H21 N2 O3 P S	304.1012	304.1011	-0.56	11.497

--- End Of Report ---

You can run **MFE_Pesticides.m** or **Find_by_formula_Pesticides.m** in one of two ways:

- As part of a worklist, if the method has the worklist actions as specified in step 8. To do so, save the method to the same name as your acquisition method.
- As a separate data analysis method. To do so, add the column **Override DAmethod** into the worklist in the Data Acquisition program (see Figure 6).

	Sample Name	Sample Position	Method	Override DA Method	Data File
✓	reagent blank 1	P1-A1	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	reagent blank
✓	2ppb neat in 20:80 ACN	P1-A2	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	2ppb neat stc
✓	reagent blank 2	P1-A1	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	reagent blank
✓	Spinach AOAC zero	P1-A3	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	Spinach AOA
✓	Spinach AOAC 10ppb	P1-A4	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	Spinach AOA
✓	reagent blank 3	P1-A1	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	reagent blank
✓	Spinach EN zero	P1-A5	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	Spinach EN z
✓	Spinach EN 10ppb (2p	P1-A6	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	Spinach EN 1
✓	reagent blank 4	P1-A1	D:\MassHunter\damethods\find	D:\MassHunter\damethods\MFE_	reagent blank

Figure 6

Using these features of the MassHunter Data Acquisition program for TOF and Q-TOF, and the Qualitative Analysis program, in combination with the Personal Pesticide Database, samples can be screened for targeted pesticides and a large number of non-targeted pesticides with the benefit of automated screening and reporting.

If you need only to screen for compounds in a non-targeted analysis, you need not customize the database and can use it directly for the screen. Remember, however, that compounds in the database that are not detected can still be present. Some compounds in the database simply will not ionize by common techniques used for LC/MS, such as electrospray or APCI.

To develop a targeted analysis

The use of the database to screen samples can be a powerful tool to detect and identify pesticides that you have no reason to believe are present. If you need to confirm whether a list of targeted compounds is either present or not present in the sample, then those compounds must be analyzed, retention times recorded, and detection limits determined.

1 Run standards of targeted compounds and create custom databases from the MassHunter Personal Pesticide Database.

   The Technical Note on the MassHunter Personal Pesticide Database (p/n 5990-3976EN) on the support disk describes how to create a custom database, and to add retention times for your compounds and chromatographic conditions to that database.

   An example of the addition of retention times to a custom database for the negative ion test mix is given in the application note p/n 5990-4251EN. In that application note the example of the negative ion mix where retention times have been added, dinoseb is the only reported isomer because its entry matches the retention time in the custom database.

   The MassHunter Personal Compound and Database and Library (PCDL) program, supplied with the MassHunter Personal Pesticide Database Kit, is an updated version of the MassHunter Personal Compound Database program described in the technical note. The PCDL program contains additional fields such as IUPAC names and ChemSpider links (and the ability to add spectra to a spectral library), but the functionality is the

same as described in the technical note. For a description of PCDL, see *An Application Kit for the Screening of Samples for Analytes of Forensic and Toxicological Interest using TOF or Q-TOF LC/MS with a Personal Forensics/Toxicology Database* (p/n 5990-4257EN).

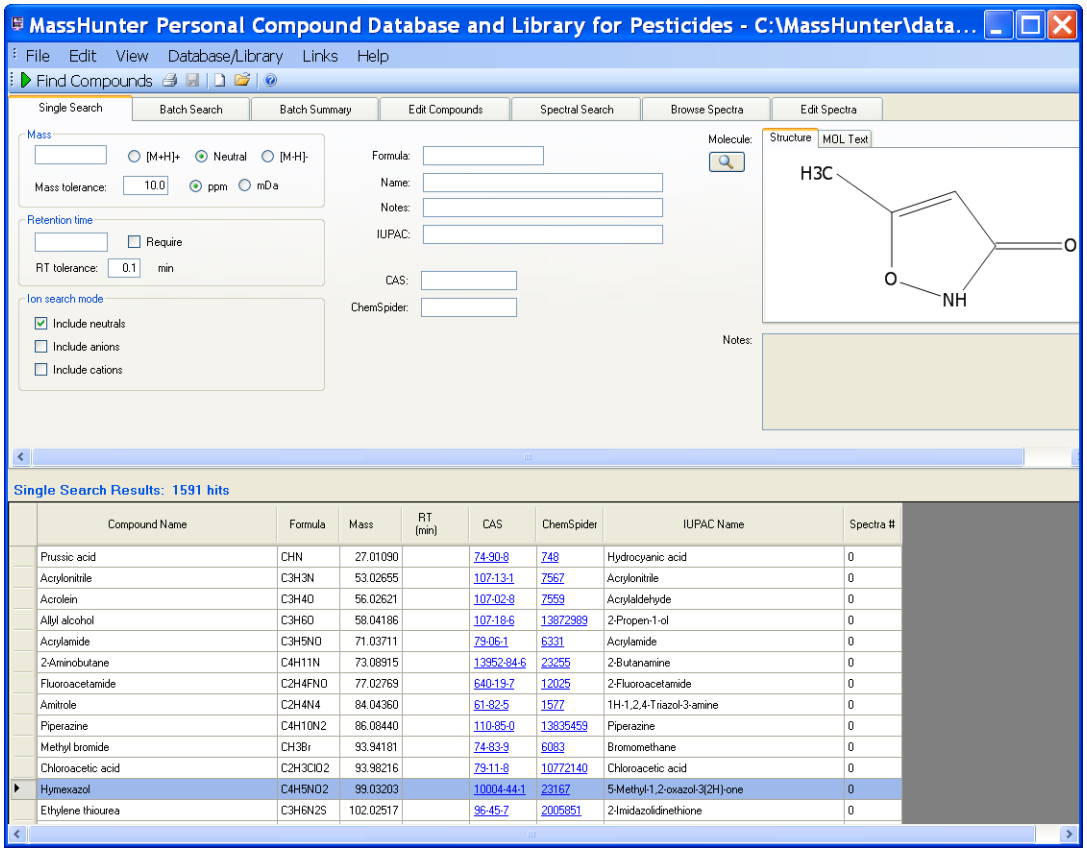


Figure 7 The MassHunter Personal Compound Database and Library program displaying the Pesticides database. Please note the additional columns in the PCDL database now available (Chemspider numbers with link and the IUPAC names).

2 If targeted analysis is needed, run standards in groups of no more than 50 compounds each. Use the chromatographic method of choice.

3 On each data set, find compounds by molecular feature to get the needed mass list, then either:

- From the MassHunter Qualitative Analysis program, copy and paste the compounds into the **Mass List** table on the Batch Search tab of the Personal Compound Database and Library (PCDL) program *or*
- From the MassHunter Qualitative Analysis program, export the mass list to a **.csv** file and then import the compounds into the **Mass List** table on the Batch Search tab.

The ability to create custom databases with your own retention time gives the MassHunter Personal Pesticide Database Kit its power and flexibility.

To bypass mixer and damper

The Binary Pump SL is delivered in standard configuration (damper and mixer connected). This step shows how to bypass the damper and mixer and convert the pump to low delay volume mode.

Configurations where only the damper or the mixer is disconnected while the other part is still in line are not supported by Agilent Technologies.

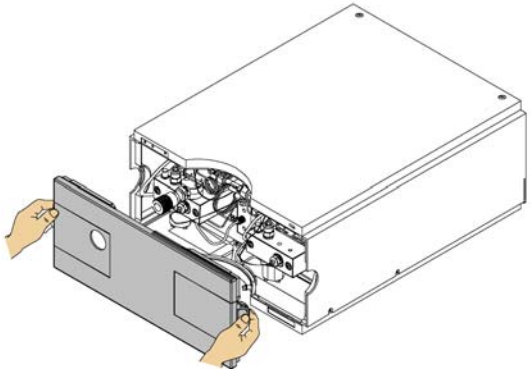
Tools required

- Wrench, 1/4-inch x 5/16-inch (p/n 8710-0510)
- Wrench, open end, 14-mm (p/n 8710-1924)
- Hex Driver, 1/4-inch, slitted (p/n 5023-0240)

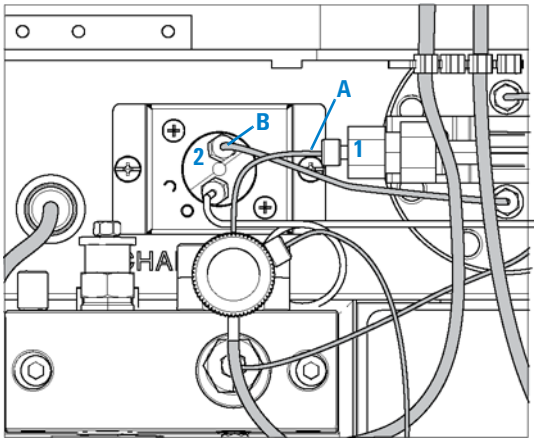
Preparations for this procedure

- Flush the system (water if buffers were used, otherwise IPA).
- Turn the flow off.

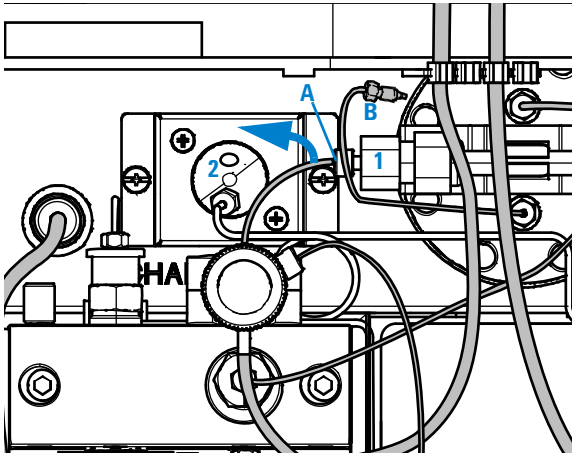
1 Remove the front cover by pressing the clip fastener on both sides of the cover.



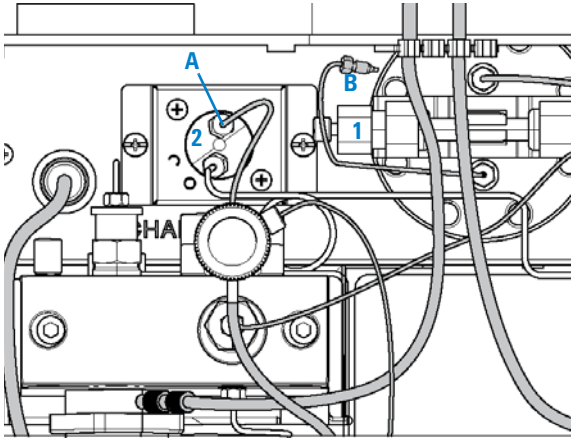
2 Use the 1/4 inch hex driver to remove fitting **B** from port *2* of the pressure sensor.



3 Fold capillary end **B** away. It remains unconnected. Disconnect fitting **A** from outlet **1** of the mixer.



4 Connect fitting **A** to port **2** of the pressure sensor. Seal port **1** of the mixer with a plastic blank nut.



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In This Guide

This Quick Start Guide describes how to use the MassHunter Personal Pesticide Database Kit.

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