Agilent MassHunter Workstation– Unknowns Analysis

Familiarization Guide

Agilent Technologies

Notices

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In this Guide...

This guide presents step-by-step exercises to help you learn to use the Unknowns Analysis program. You can do these exercises with the demonstration analysis, method, and library files, shipped with the system installation disk, or with data you acquire.

Before you begin these exercises

Copy files from the installation disk to your hard disk

1. Insert the MassHunter Quantitative Analysis installation DVD into your computer.
2. Navigate to your DVD drive: **Data**,
3. If the folder is in a compressed format, extract the data files from their zip format.
4. Copy the **Data** folder from your installation disk in uncompressed format to any location on your hard disk.

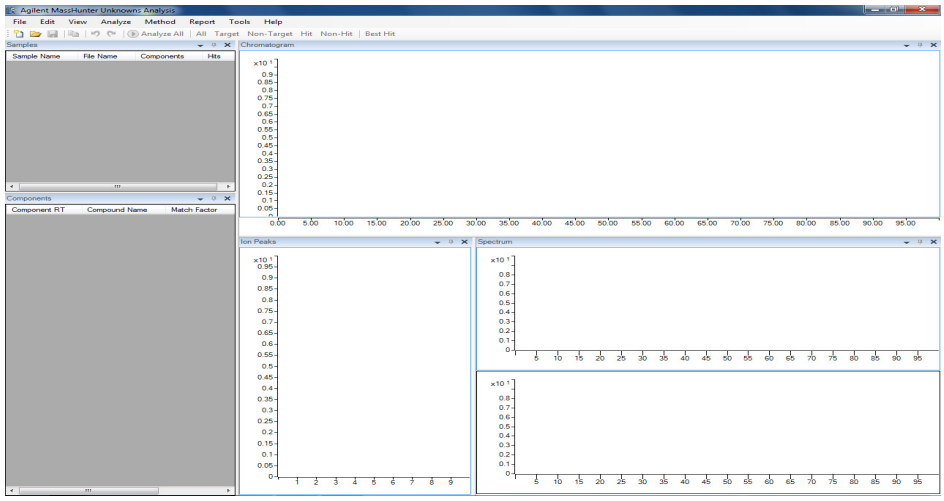
This folder contains all of the data, method, and library files needed for these exercises. Do not reuse the example data files on your system unless you know that they are identical to the originals on the disk. If the example data files already on the system do not match the original ones of the disk exactly, then the results obtained during these exercises will not match those shown in this guide.

Task 1: Identify Compounds with TIC Analysis

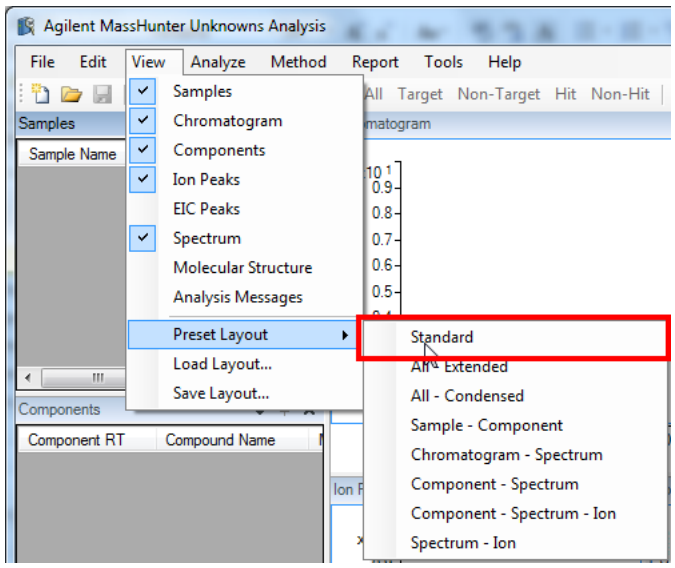
Create a new analysis

1. Start **Unknowns Analysis** by double-clicking the desktop icon.
   or
   Click **Start > Agilent > Quant Tools > Unknowns Analysis**.

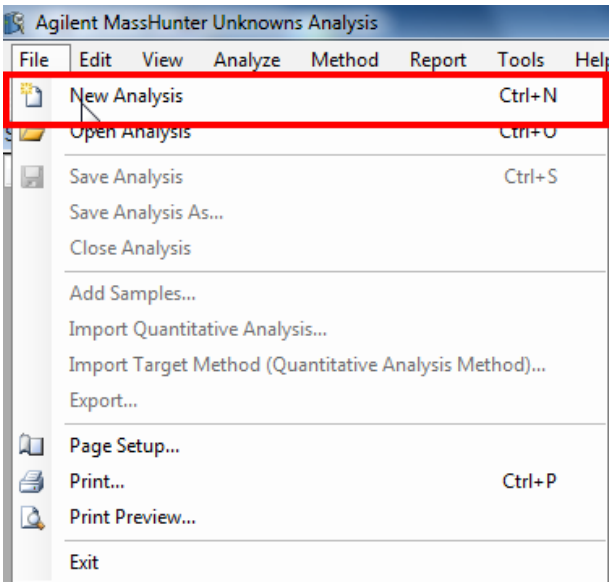
When you open the program, the default layout appears.



If the default layout is not present, click **View > Preset Layout > Standard** to restore the default layout before creating a new analysis.

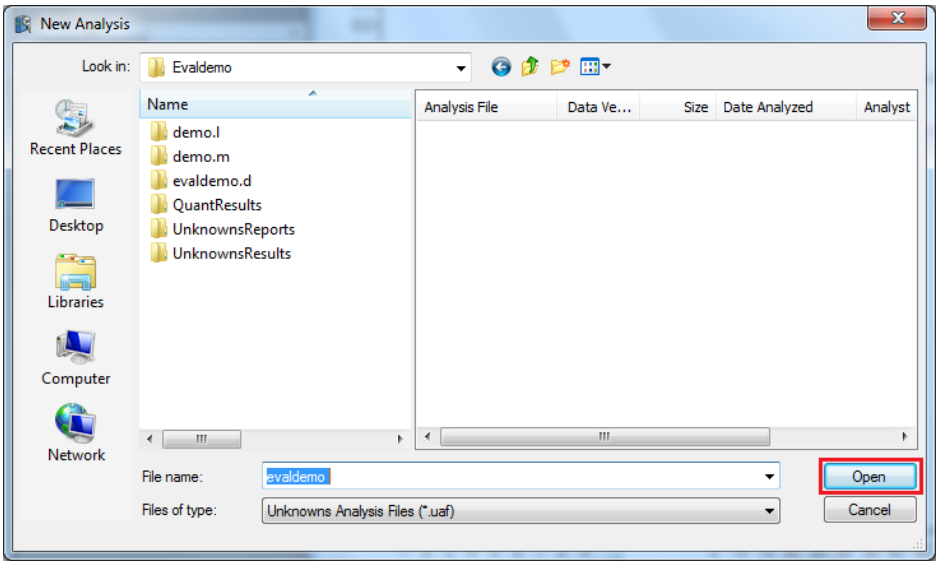


2. Select **File > New Analysis**.



3. Navigate to **MassHunter\Data\ Evaldemo**, or the folder where the data file to be analyzed is stored.

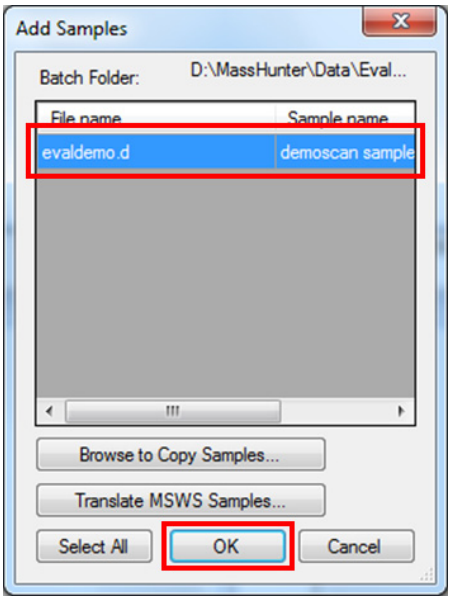
4. Type the analysis name **evaldemo** for the analysis, and click **Open**.



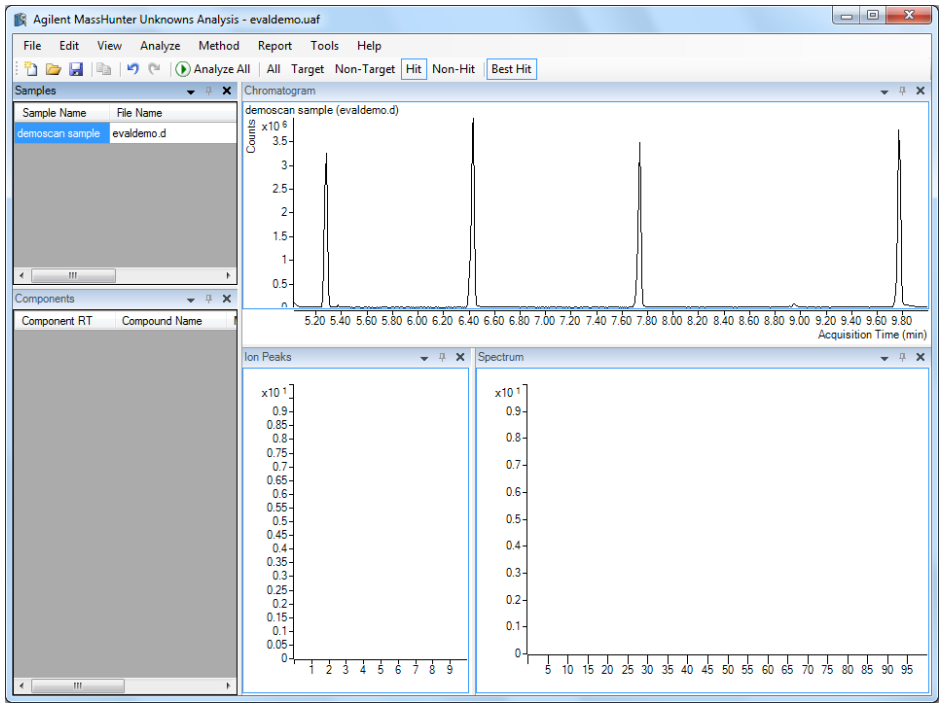
Add samples to the analysis

1. Select **File > Add Samples**.

2. Select the sample file(s) and click **OK** to add the sample to the batch.

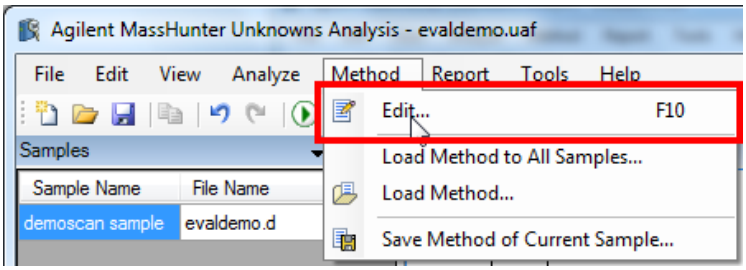


The Analysis table is no longer empty. It now contains the demo sample.

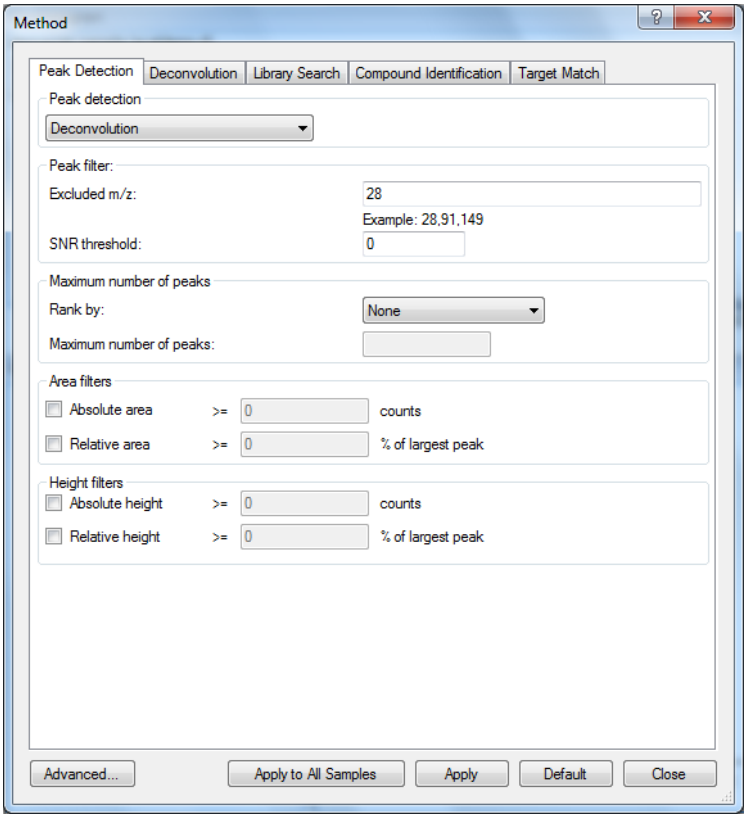


Set up the method for the analysis

Select **Method > Edit**.



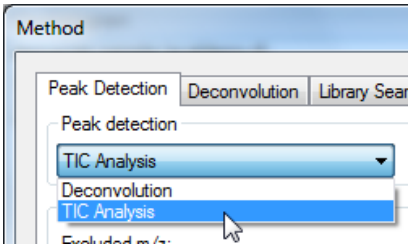
The Method dialog box standard view appears. For this task, we will use the **Standard** view.



Note that these are the default parameters for the method. You can click **Default** at the bottom of the Method dialog box to restore default parameters before creating a new method in the next step.

Set Peak Detection options

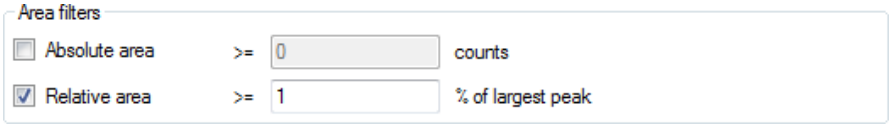
1. Select **TIC Analysis** from the **Peak detection** drop-down menu.



- **TIC Analysis**: Identifies the chromatographic peaks using integration instead of deconvolution.
- **Deconvolution:** Deconvolutes the components in the chromatogram and extracts the 'clean' spectra from background noise based on both retention time and peak shape.

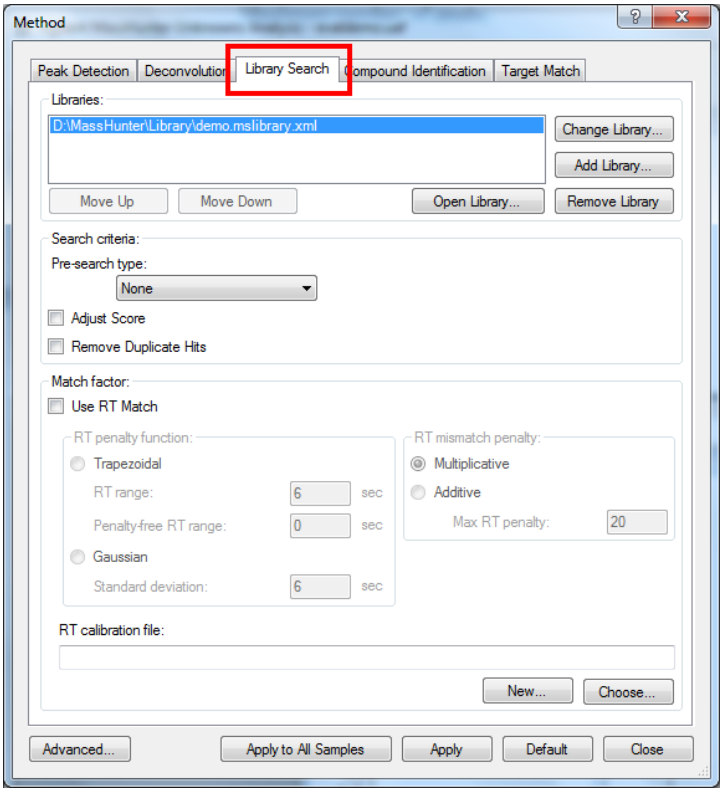
2. In the **Maximum number of peaks** section, select **Area** from the **Rank by** drop-down menu, and enter **5** for the **Maximum number of peaks**.

3. In the **Area filters** section, select **Relative area** and enter **1** for the **% of largest peak**.

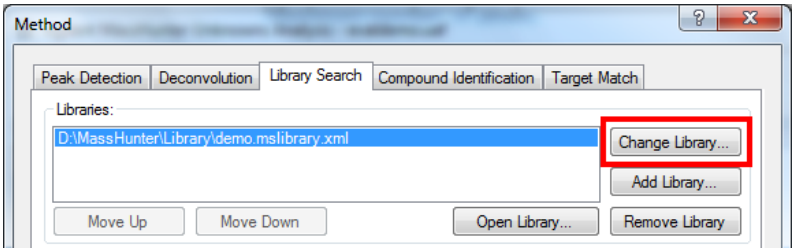


Set Library Search options

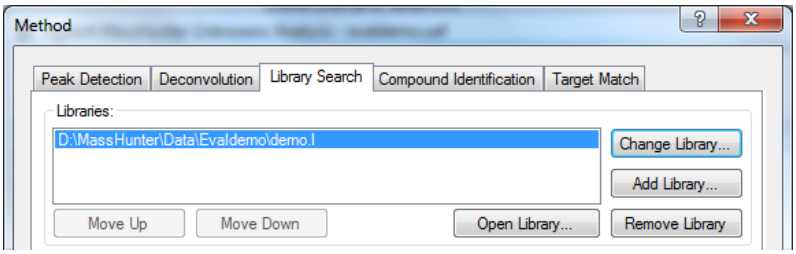
1. Click **Library Search**.



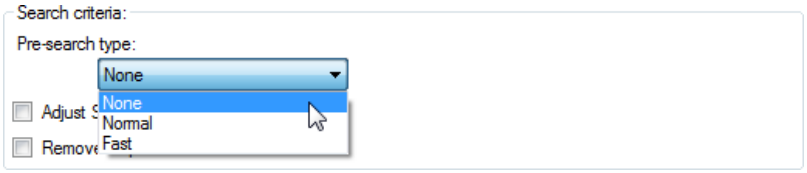
2. Click **Change Library**.



3. Navigate to **MassHunter\Data\Evaldemo**, or the relevant folder, select **demo.L**, and click **Open**.



4. In the **Search criteria** section, select **None** from the **Pre-search** drop-down menu.

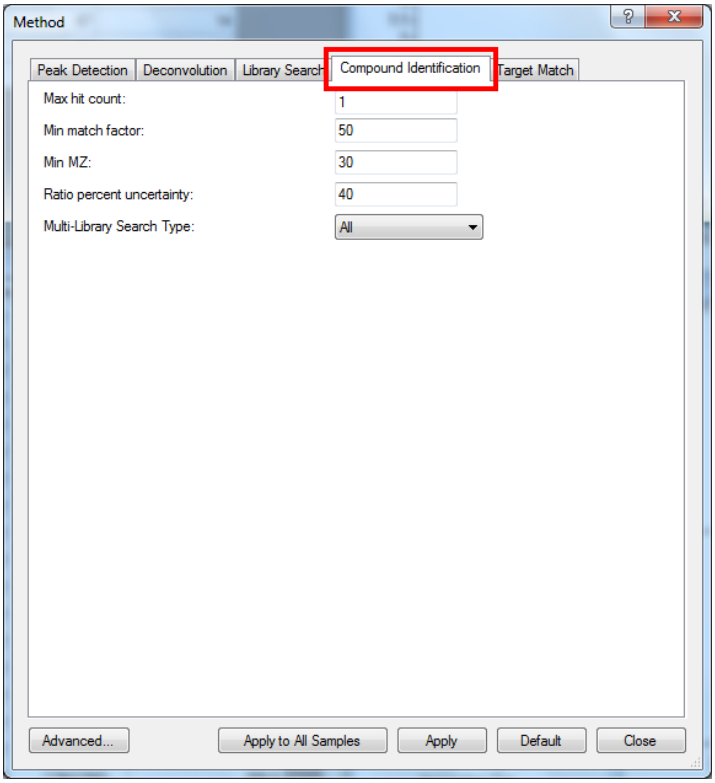


There are 3 Pre-search types: **None**, **Normal**, and **Fast**. By default, Unknowns Analysis uses **Normal**.

- **None**: The library search is not subjected to a preliminary screening process.
- **Normal**: The screening algorithm uses the entire library as the list of candidates if the indexing scheme does not produce enough candidates. It is 50-100 times faster than no pre-search, with essentially zero false negatives rate for high-scoring hits (match score > 80).
- **Fast**: The screening algorithm uses whatever list of candidates it gets from the index and avoids the entire library-search even if there are not enough candidates found. The speed is 100-1000 times faster than no pre-search, with ≥1% false negatives rate for high-scoring hits.

Set Compound Identification options

1. Click **Compound Identification**.



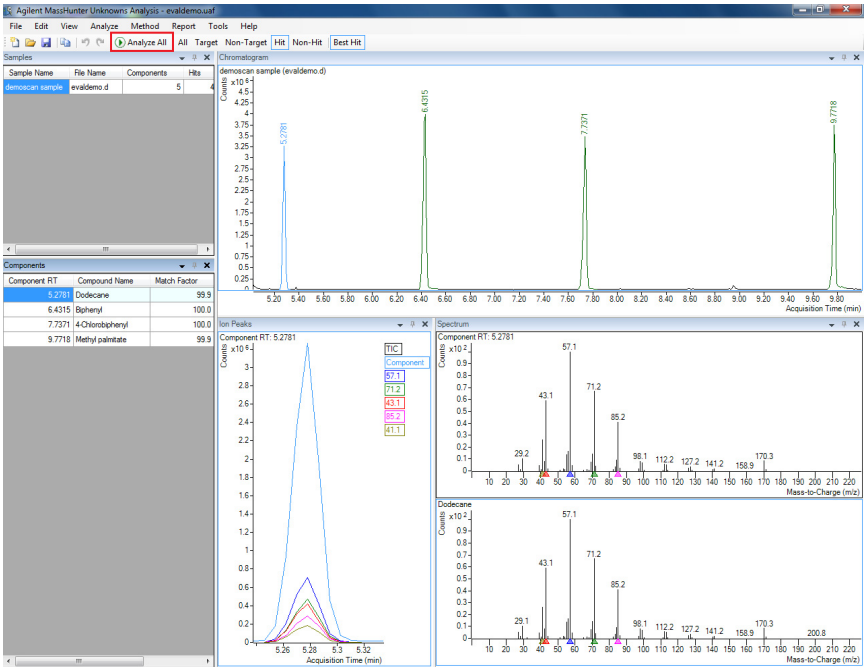
For this task, we will use the default Compound Identification parameters.

2. Click **Apply to All Samples**, and then click **Close**.

Analyze and review results

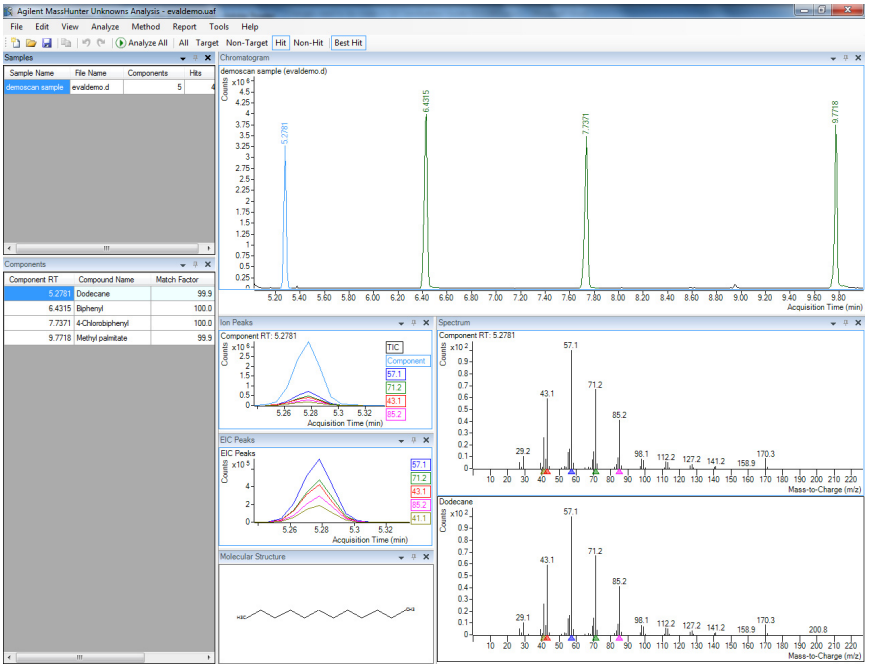
1. Click **Analyze All**.

After the analysis is complete, the main view that appears should look like the example below. This is the default layout and contains the default column settings. If you see a different layout than the one in the example below, select **View > Preset Layout > Standard** to reset the standard layout.



2. Select **View > Preset Layout > All-condensed**.

The system displays the All-condensed view.



3. Select the **demoscan sample** from the **Sample** table.

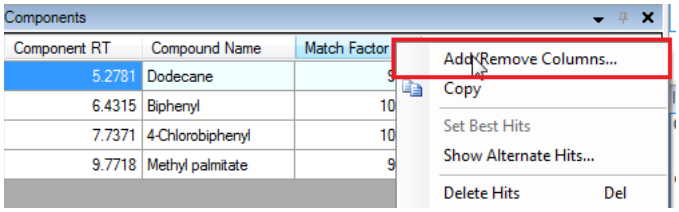
4. Right-click any column header in the **Components** window, and select **Add/Remove Columns**.

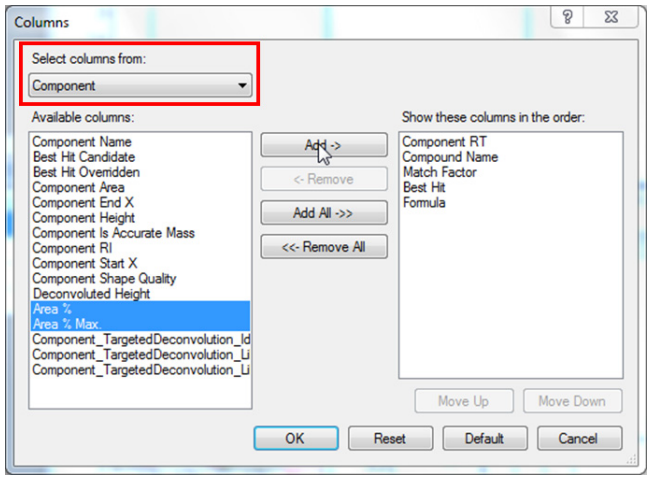
5. Select **Component** from the **Select columns from** drop-down menu.

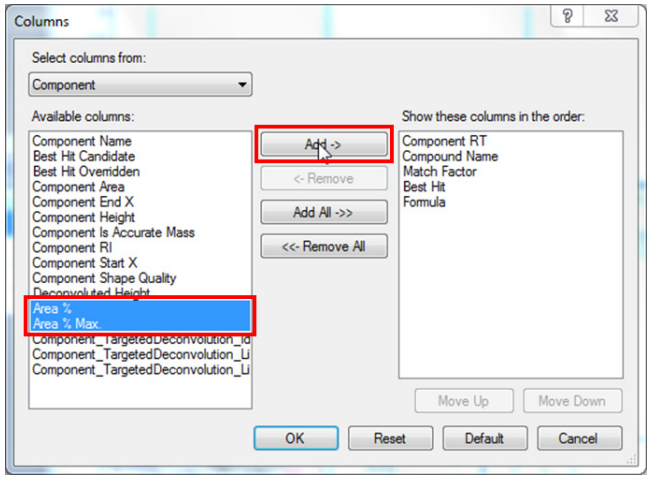
6. Select **Area %** and **Area % Max** from the **Available columns** list, and click **Add**.

Click one of the following toolbar buttons to view the changes in the **Components** window:

- **All**: View all the peaks.
- **Hit**: View the peaks that are found in the library search.
- **Non-Hit**: View the peaks that are not found in the library search.







- **Area %**: Percentage of the peak area sum
- **Area % Max**: Percentage of the largest peak area

7. Verify that the selected columns are moved to the **Show these columns in the order** list, and click **OK**.

8. From the **Components** table, select a component in the **Component RT** column.

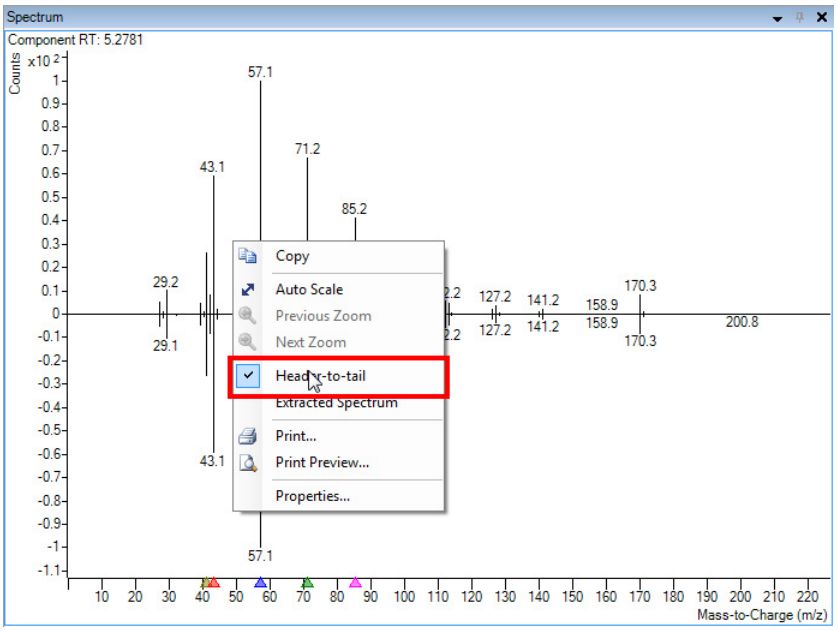
Components

Component RT	Compound Name	Match Factor	Best Hit	Formula	Area %	Area % Max.
5.2781	Dodecane	99.9	☑	C12H26	19.158	63.44
6.4315	Biphenyl	100.0	☑	C12H10	30.196	100.00
7.7371	4-Chlorobiphenyl	100.0	☑	C12H9Cl	25.572	84.69
9.7718	Methyl palmitate	99.9	☑	C17H34O2	23.731	78.59

View the **Chromatogram**, **Spectrum**, **Ion Peaks**, **EIC Peaks**, and **Molecular Structure** for the selected component.

In the **Spectrum** window, the top spectrum is from the component, and the bottom spectrum is from the library. The **Match Factor** in the **Components** table reflects how closely the two spectrum match.

To change to the Header-to-tail view, right-click inside the **Spectrum** window and select **Header-to-tail**.



The **Ion Peaks** and **EIC Peaks** windows show the extracted chromatograms of the selected ions. The EIC traces and their numeric identifiers to the right of the display are color-coded.

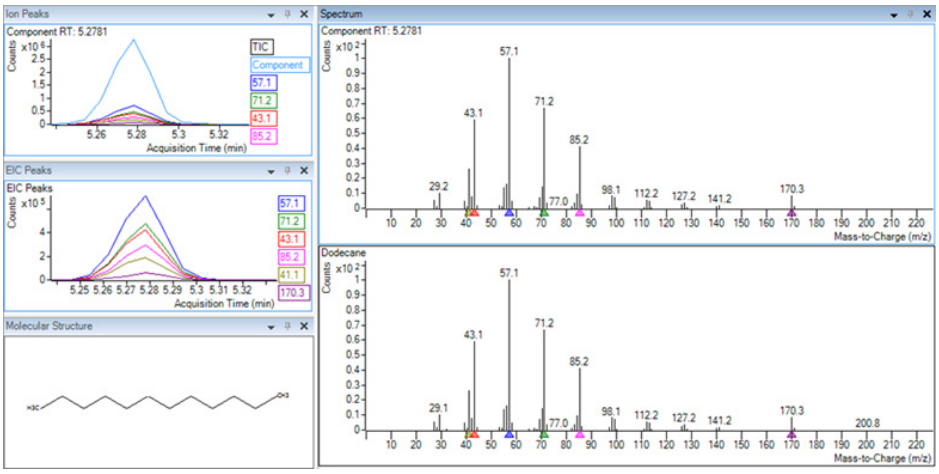
To interactively add the ion chromatogram traces in the **Ion Peaks** and **EIC Peaks** window to the display, click in any **Mass Spectral Display** area of the **Spectrum** window. If the selected *m/z* chromatogram is not already displayed, it will be added to the **Ion Peaks** and **EIC Peaks** window and a ▲ symbol of the same color will be at the appropriate *m/z* position below the x-axis in the **Spectrum** window.

9. To save the analysis, select **File > Save Analysis**.

10. Click **File > Exit**.

To remove an ion chromatogram trace (and its numeric identifier) from the **Ion Peaks** and **EIC Peaks** window, click on its numeric identifier or on the corresponding *m/z* value position in the **Spectrum** window.

The **Molecular Structure** is from the library. If the searched library does not contain the structures for the entries, nothing will be displayed in the **Molecular Structure** window.

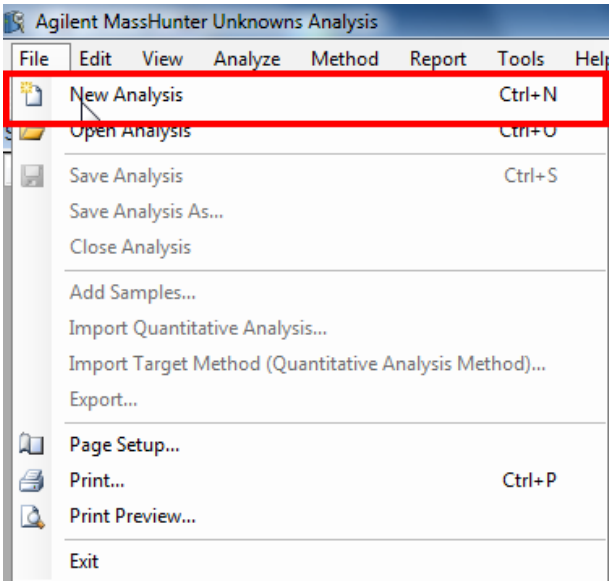


Task 2: Identify Compounds with Deconvolution

Create a new analysis

1. Start **Unknowns Analysis** by double-clicking the desktop icon.
   or
   Click **Start > Agilent > Quant Tools > Unknowns Analysis**.

2. Select **File > New Analysis**.



3. Navigate to \ ***Your Directory***\ **RI-PEST-MATRIX**\.

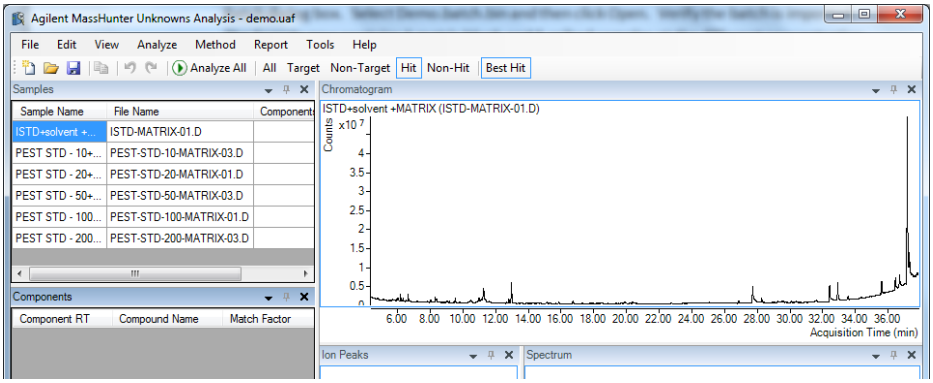
4. Type the analysis name **demo**, and click **Open**.

Add samples to the analysis

1. Select **File > Import Quantitative Analysis**.

2. Select **Demo.batch.bin**, and click **Open**.

Verify the batch is imported. The **Sample** window now contains one matrix blank and five spiked samples at the different concentration levels. The **Chromatogram** shows the TIC of the sample selected in the **Sample** window.

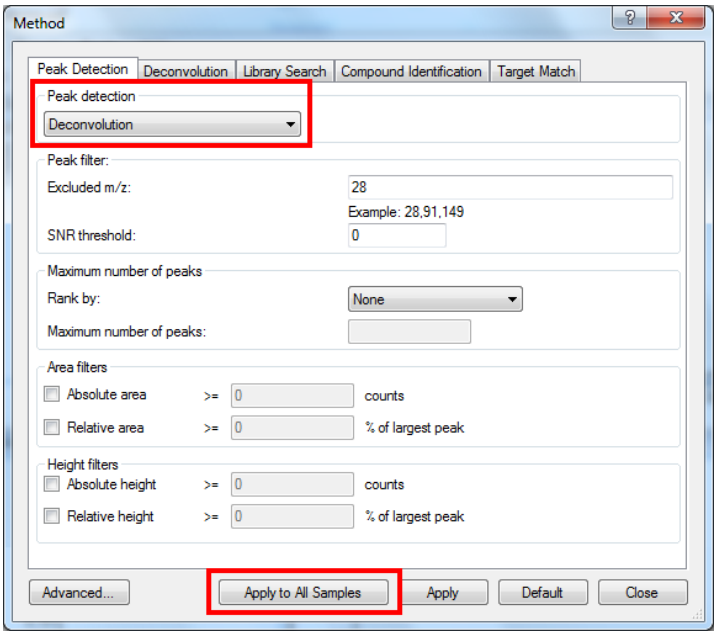


Set up the method for the analysis

Press **F10** or select **Method > Edit**.

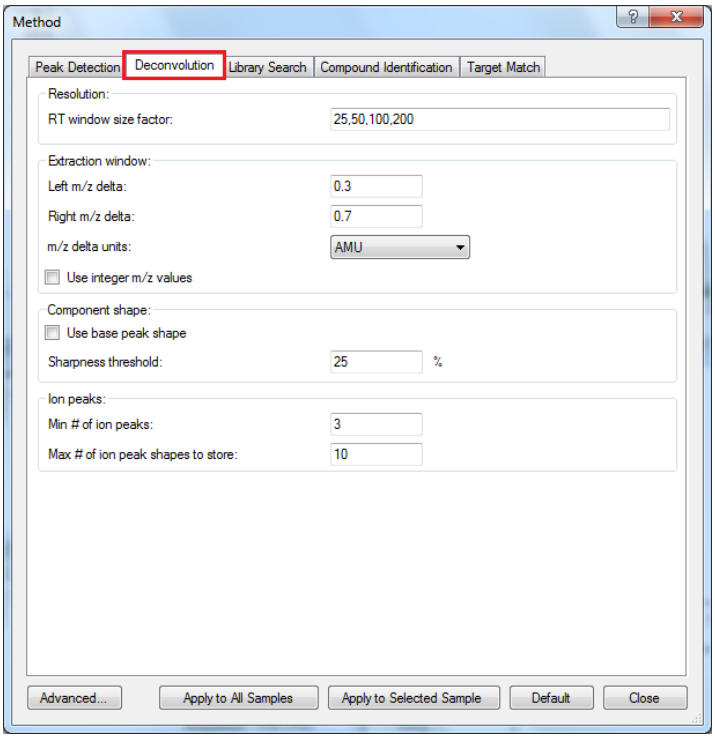
Set Peak Detection options

Select **Deconvolution** from the **Peak detection** drop-down menu, and click **Apply to All Samples**.

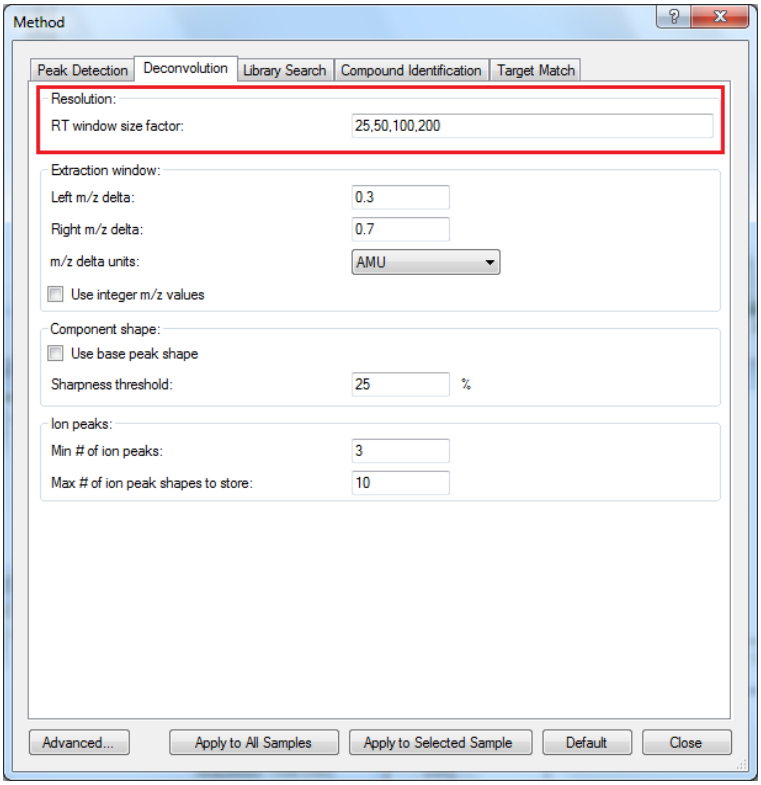


Set Deconvolution options

1. Click **Deconvolution**.

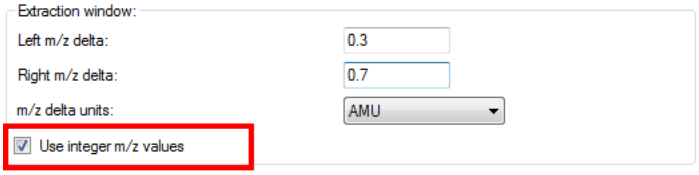


The default parameters for deconvolution display. By default, there are four values (25, 50, 100, 200) for the **RT window size factor**. Select any set of Window Size Factor (WSF) values in a comma-separated format.



The WSF represents a dimensionless scale of the correlation window for grouping ion peaks into components, equivalent to Resolution and AMDIS. A smaller value (higher resolution) separates closely spaced peaks, finds more components, and runs longer. A larger value is used for wider peaks. Using multiple values covers all kinds of peaks without manual optimization.

2. In the **Extraction Window** section, select **Use integer m/z values**.

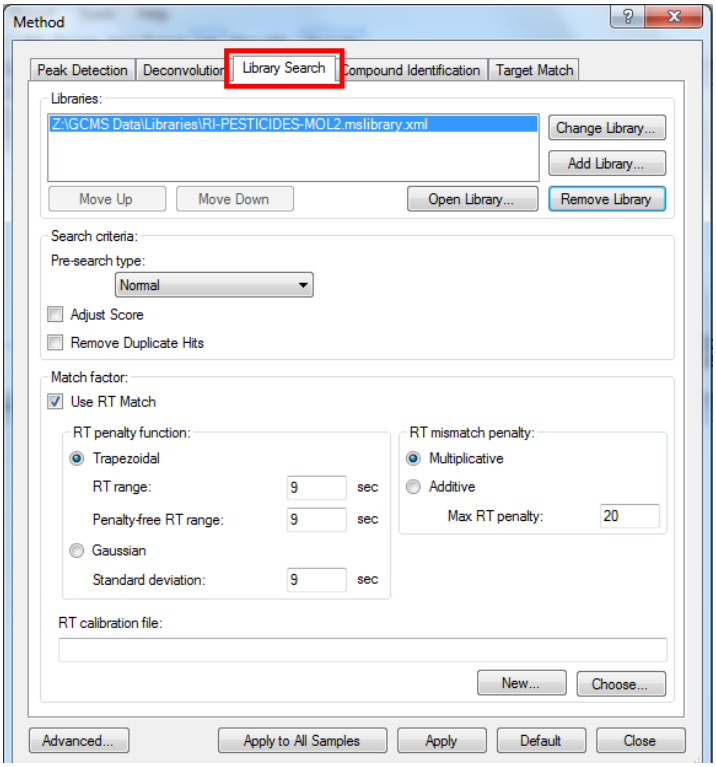


Use integer m/z values runs the deconvolution with both integer and filtered *m/z*, and provides the best results.

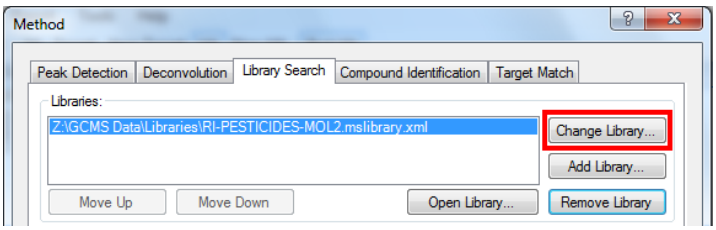
3. Click **Apply to All Samples**.

Set Library Search options

1. Click **Library Search**.

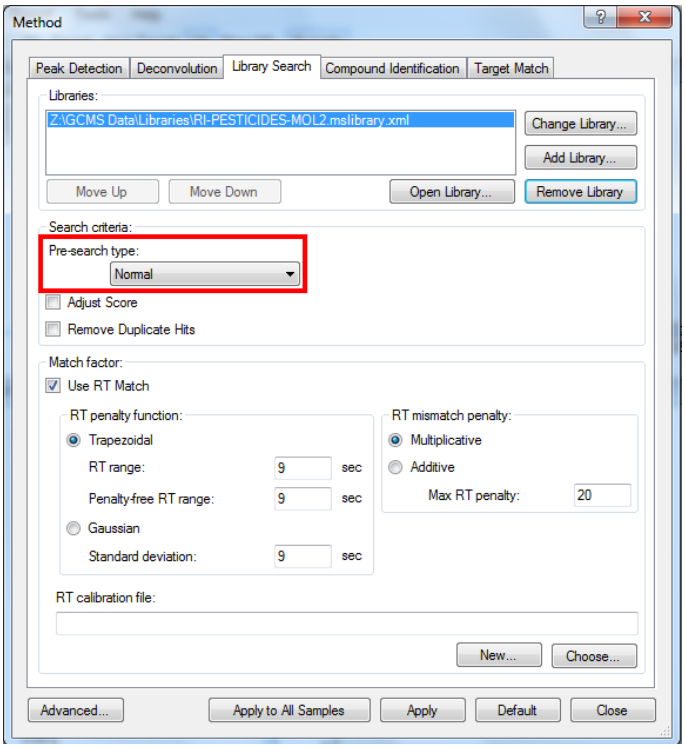


2. Click **Change Library**.



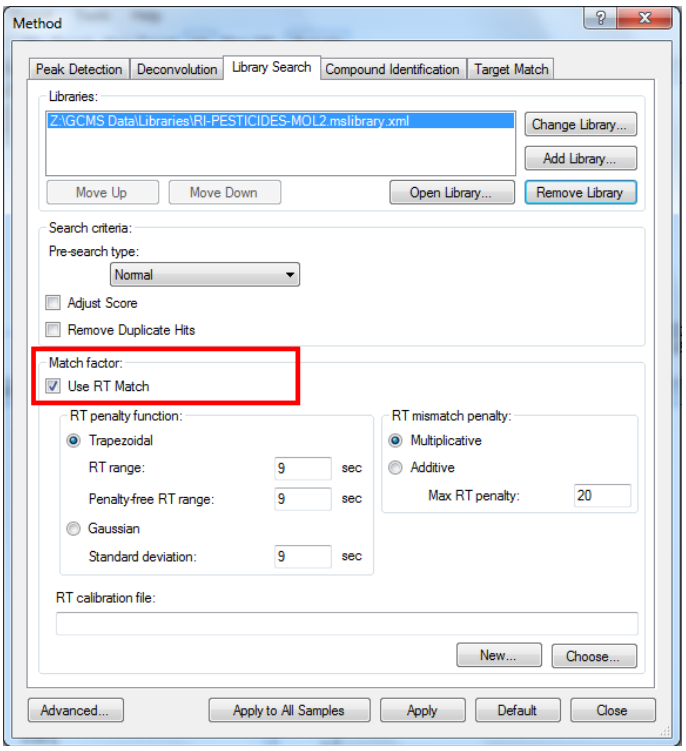
3. Navigate to the relevant folder, select **RI-PESTICIDES-MOL2.mslibrary.xml**, and click **Open**.

4. In the **Search criteria** section, select **Normal** from the **Pre-search type** drop-down menu.

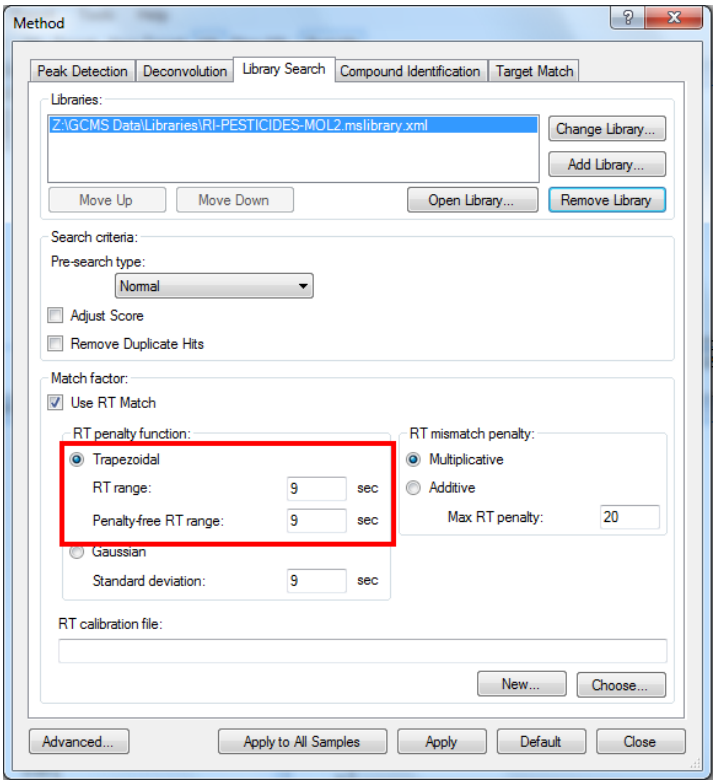


- Select **Adjust Score** to give the closest library match scores to NIST.
- Select **Remove Duplicate Hits** to remove duplicate hits that appear in the hit list for a given target spectrum. This deals with duplicate and highly similar library entries such as seen in NIST, and only returns the single library entry with the highest fit score.

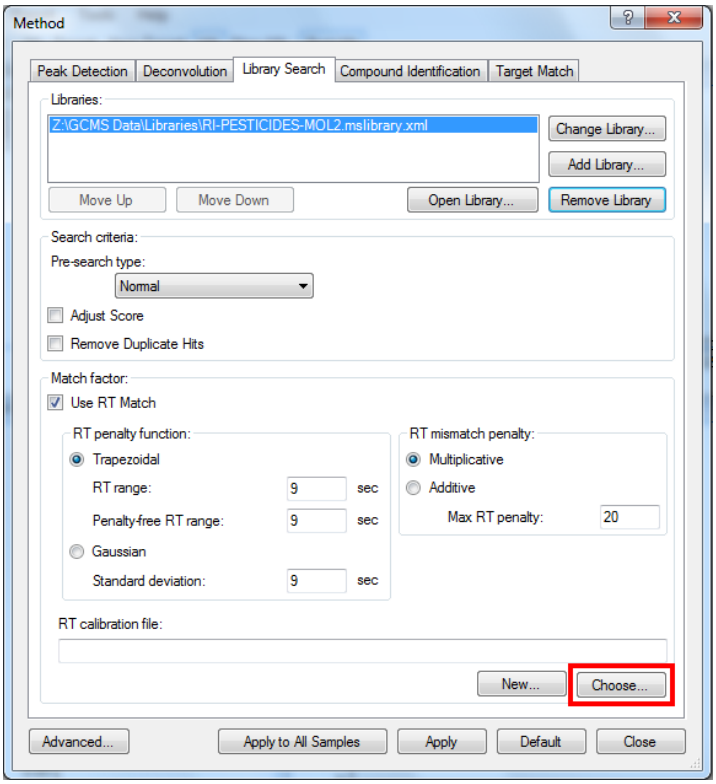
5. In the **Match factor** section, select **Use RT Match**.



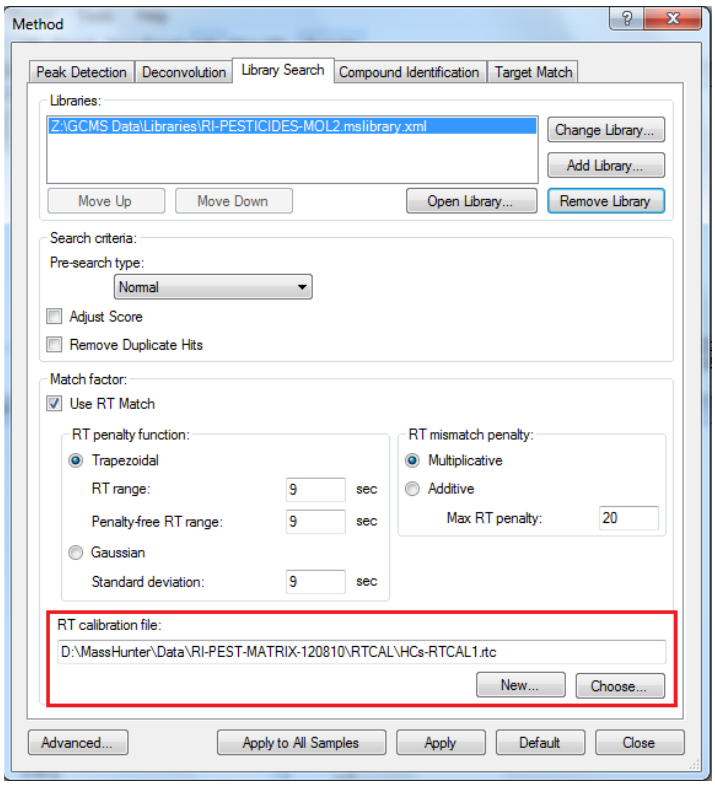
6. In the **RT penalty function** section, select **Trapezoidal** and enter the following:
   RT range: 9
   Penalty-free RT range: 9



7. In the RT calibration file section, click **Choose**.

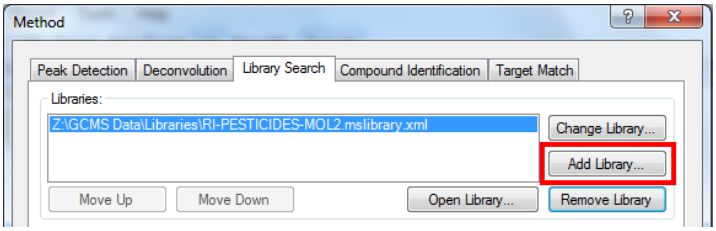


8. Navigate to the relevant folder, and select **HCs-RTCAL1.rtc**.



RT/RI calculation is used with library matching to lower the false positive rate. The window is set to ±9 seconds to qualify the hits from the Library Search.

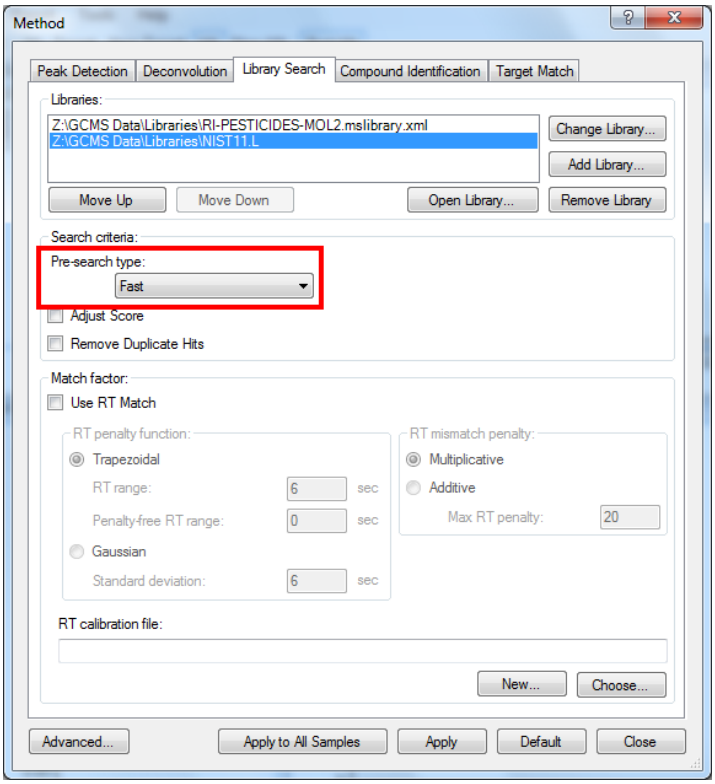
9. In the **Libraries** section, click **Add Library**.



10. Navigate to the relevant folder, and select **NIST11.L**.

Multiple libraries can be used in Library Search. For this example, the target MS library contains 900+ pesticides with Retention Indexes (RI) information. NIST11.L can be used for the additional confirmation.

11. Select **Fast** from the **Pre-search type** drop-down menu.

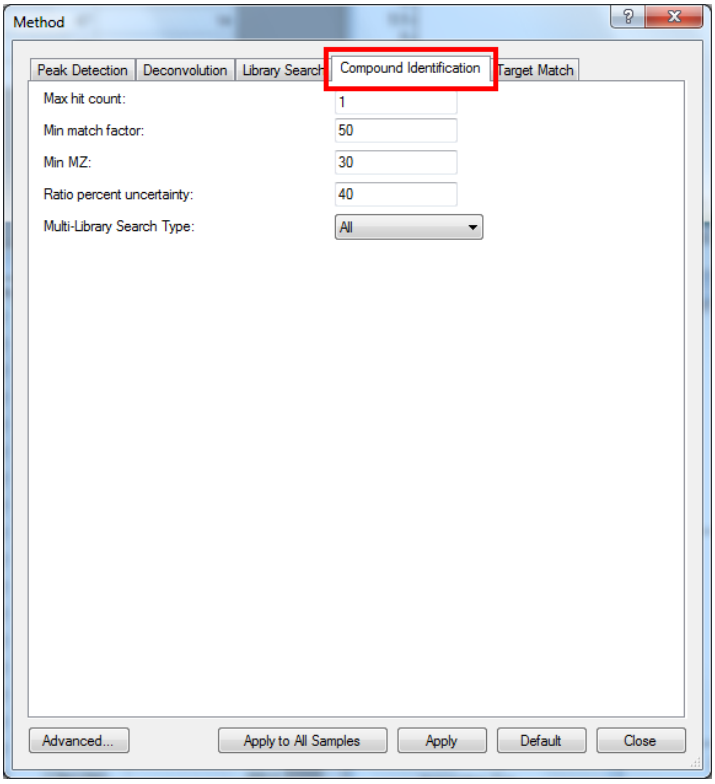


12. Click **Apply to All Samples**.

You are able to set different Library Search parameters for different libraries.

Set Compound Identification options

Click **Compound Identification**.

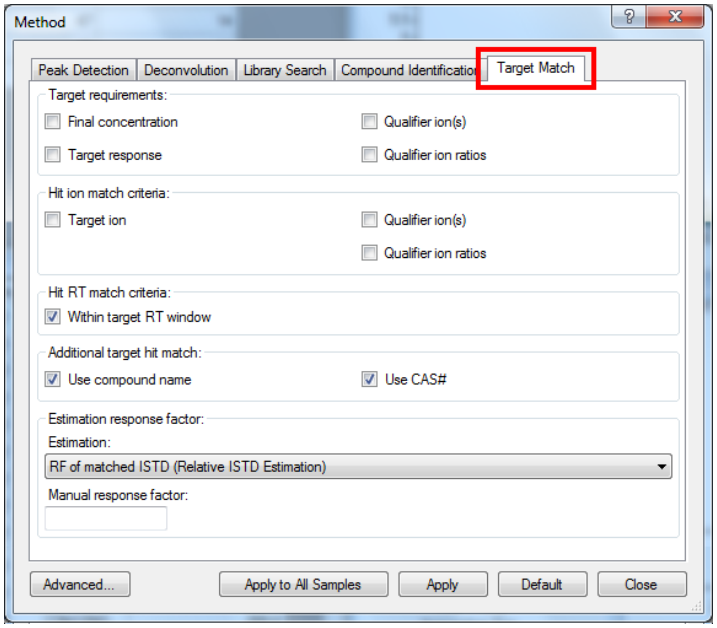


For this example, the **Min match factor** is set to 50 for the compound identification from the Library Search.

- **Max hit count**: The maximum number of Library Search hits to report per component.
- **Min MZ**: The lower *m/z* limit for library match score calculation.
- **Ratio percent uncertainty**: Only applicable when **Pre-search type** is selected in Library Search. The larger the value, the more Library Search candidates are generated, and the longer the library search process.
- **All**: Search all libraries (default)
- **Multi-Library Search Type**: If multiple libraries were used, two search modes are available:
  - **All**: Search all libraries (default)
  - **StopWhenFound**: Stop searching the library when enough candidates are found

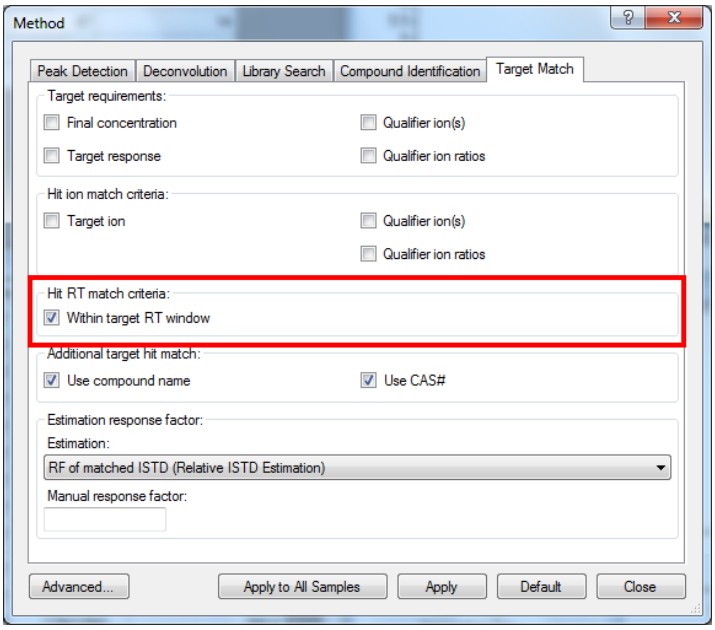
Set Target Match options

1. Click **Target Match**.

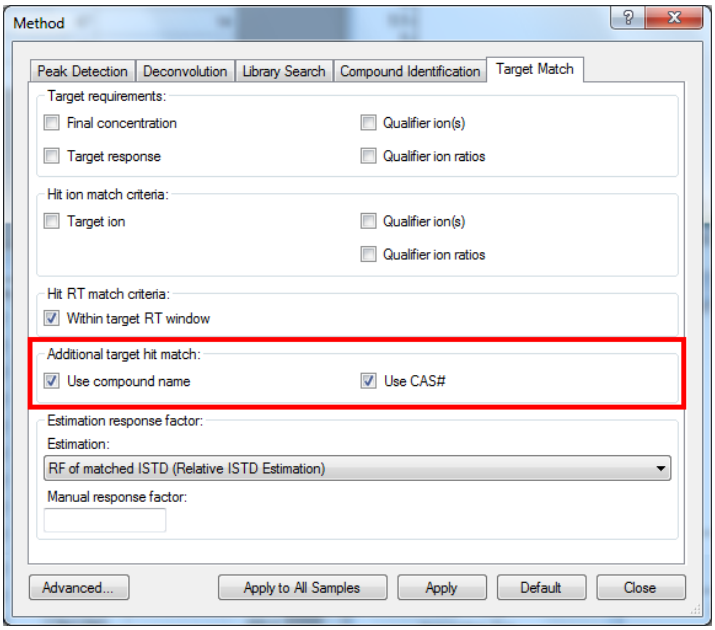


Target Match identifies quantitation targets using the quantitation method. The goal of identifying non-target compounds is simplified by filtering out the target matches. RT window, compound name, and CAS# can be applied for **Target Match**.

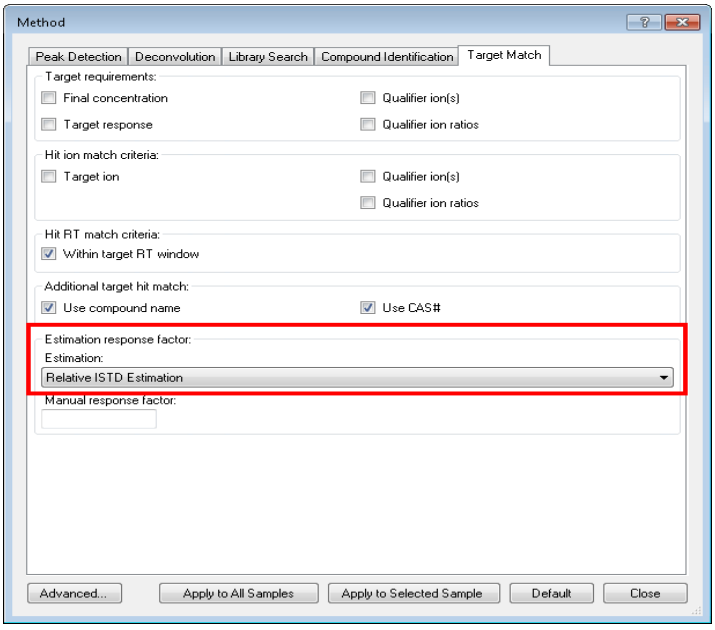
2. In the **Hit RT match criteria** section, select **Within target RT window**.



3. In the **Additional target hit match** section, select **Use compound name** and **Use CAS#**.



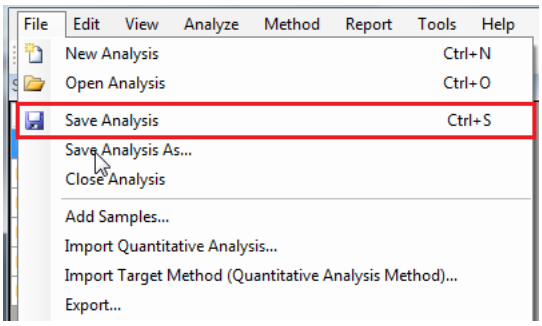
4. In the **Estimation response factor** section, select **RF of matched ISTD** from the **Estimation** drop-down menu.



Concentration estimation leverages the Quant target **Response Factors** (RF), which are applied to Non-Target hits as well. Estimation of response factors is flexible, and can be adjusted to suit the particular analytical requirements.

5. Click **Apply to All Samples**, and then click **Close**.

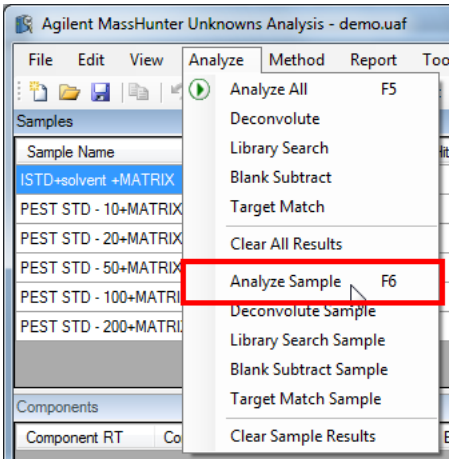
6. To save the analysis, select **File > Save Analysis**.



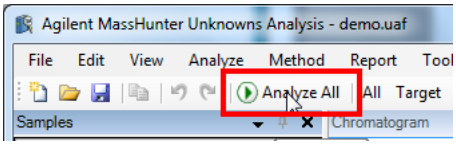
Analyze and review results

1. In the **Sample** window, select the sample **ISTD+solvent+MATRIX**.

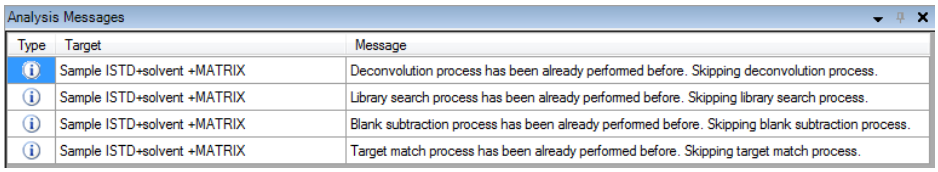
2. Select **Analyze > Analyze Sample**.



To analyze the rest of the sample, click **Analyze All**. The analysis starts from where it left off and skips the sample(s) previously analyzed if no parameter in the method has been changed.



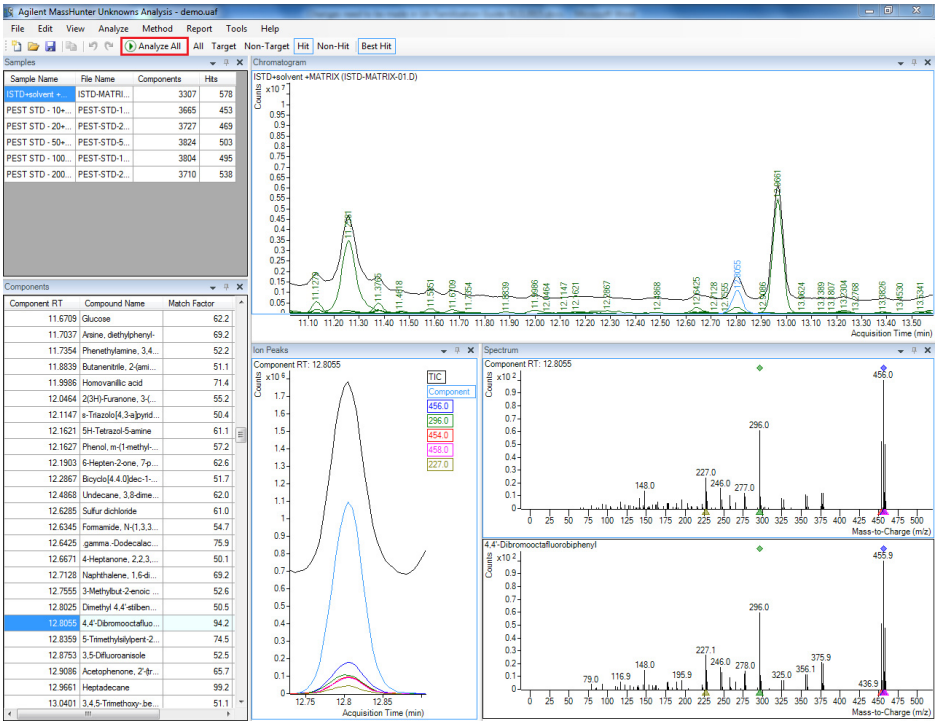
View validation information in the Analysis Messages.



Analysis Messages

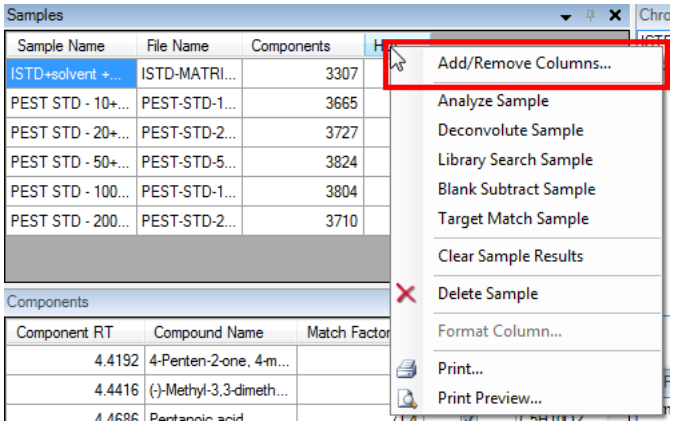
Type	Target	Message
ⓘ	Sample ISTD+solvent +MATRIX	Deconvolution process has been already performed before. Skipping deconvolution process.
ⓘ	Sample ISTD+solvent +MATRIX	Library search process has been already performed before. Skipping library search process.
ⓘ	Sample ISTD+solvent +MATRIX	Blank subtraction process has been already performed before. Skipping blank subtraction process.
ⓘ	Sample ISTD+solvent +MATRIX	Target match process has been already performed before. Skipping target match process.

After the analysis is complete, the main view that appears should look like the example below. This is the default layout and contains the default column settings.

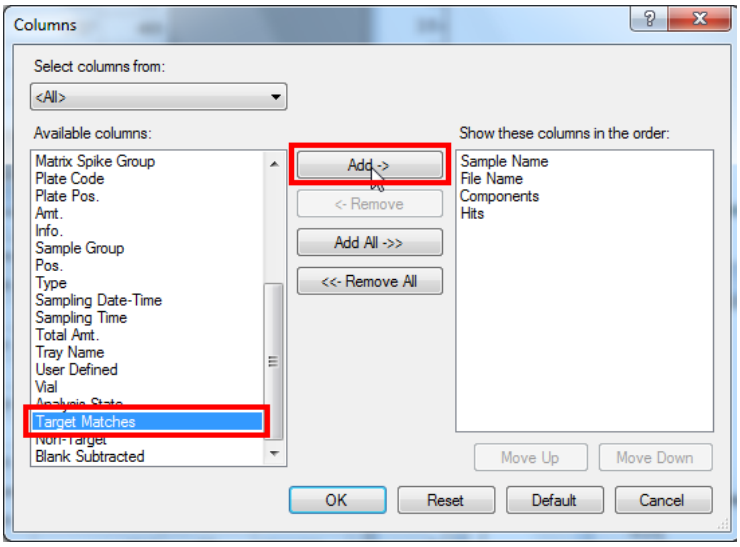


Review best hit results

1. Right-click any column header in the **Samples** window, and select **Add/Remove Columns**.

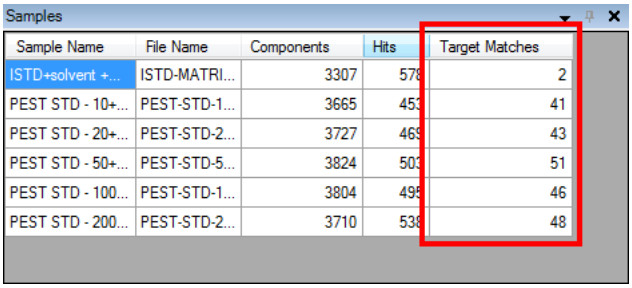


2. Select **Target Matches** from the **Available columns** list and click **Add**.



3. Verify that the selected column is moved to the **Show these columns in the order** list, and click **OK**.

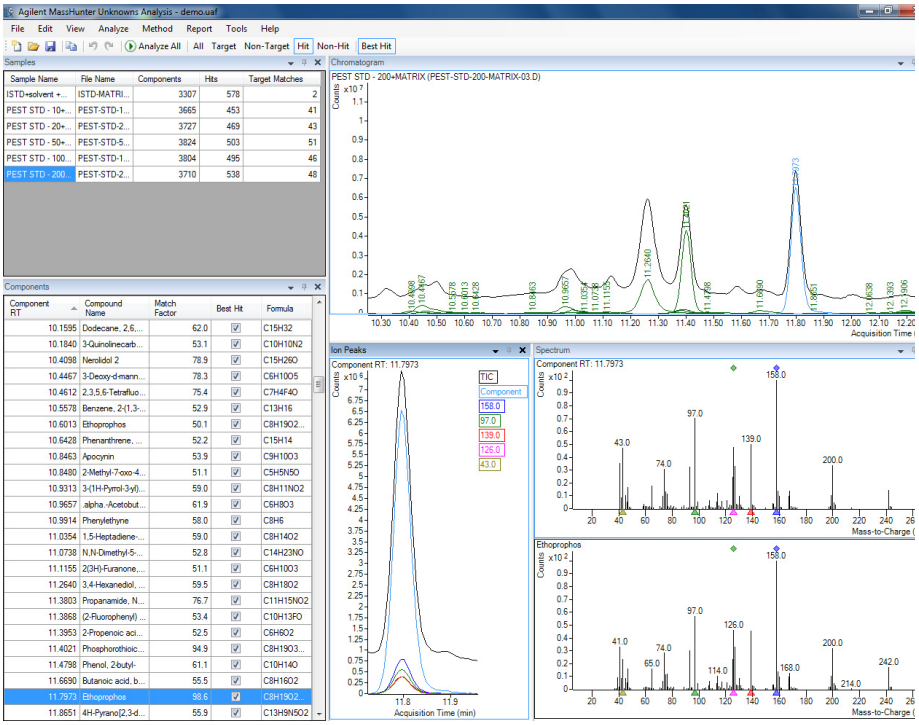
The **Target Matches** column is added to the **Samples** window.



4. Select the last sample in the **Samples** window.

Click one of the following toolbar buttons to view the changes in the **Components**, **Chromatogram**, **Ion Peaks**, and **Spectrum** windows:

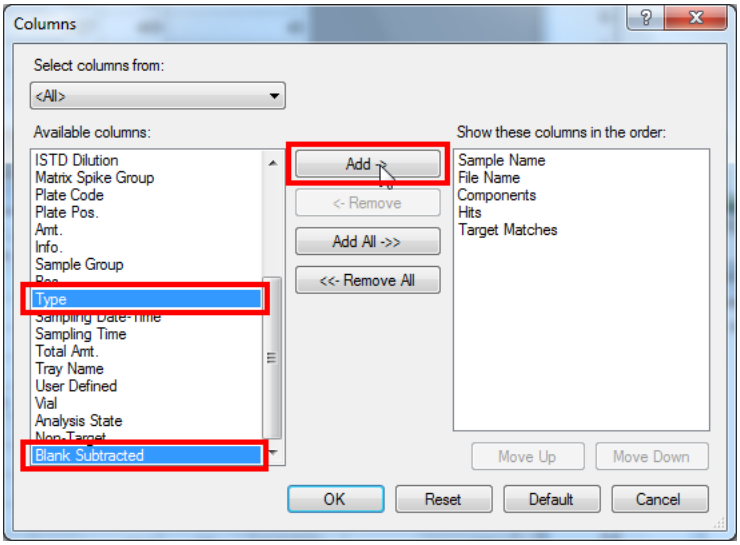
- **All**: View all the peaks.
- **Target**: View the peaks that are also in the quantitation method.
- **Non-Target**: View the peaks that are not in the quantitation method.
- **Hit**: View the peaks that are found in the library search.
- **Non-Hit**: View the peaks that are not found in the library search.
- **Best Hit**: View the component with the highest library match score among the multiple hits of the same compound from different resolutions.



Review blank hit subtraction results

1. Right-click any column header in the **Samples** window, and select **Add/Remove Columns**.

2. Select **Type** and **Blank Subtracted** from the **Available columns** list, and click **Add**.



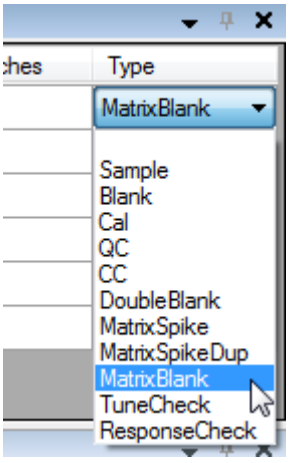
3. Verify that the selected columns are moved to the **Show these columns in the order** list, and click **OK**.

The **Type** and **Blank Subtracted** columns are added to the **Samples** window.

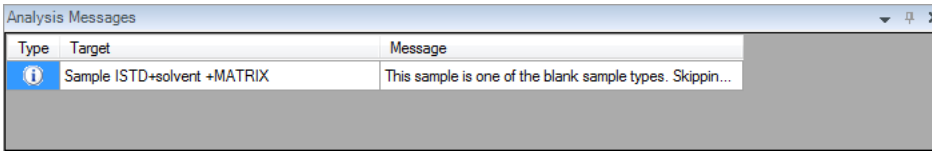
Samples

Sample Name	File Name	Components	Hits	Target Matches	Type	Blank Subtracted
ISTD+solvent +MATRIX	ISTD-MATRI...	3307	578	2	MatrixBlank	0
PEST STD - 10+MATRIX	PEST-STD-1...	3665	453	41	Cal	183
PEST STD - 20+MATRIX	PEST-STD-2...	3727	469	43	Cal	167
PEST STD - 50+MATRIX	PEST-STD-5...	3824	503	51	Cal	153
PEST STD - 100+MATRIX	PEST-STD-1...	3804	495	46	Cal	160
PEST STD - 200+MATRIX	PEST-STD-2...	3710	538	48	Cal	149

4. Note the list of available samples in the **Type** drop-down menu.



The values shown in the **Blank Subtracted** column in the **Samples** window represent the number of hits that were blank subtracted from the samples. Verify that the message "This sample is one of the blank sample types. Skipping blank subtraction process." for the **ISTD+solvent+MATRIX** sample appears in the **Analysis Messages** window.



Close the **Analysis Messages** window.

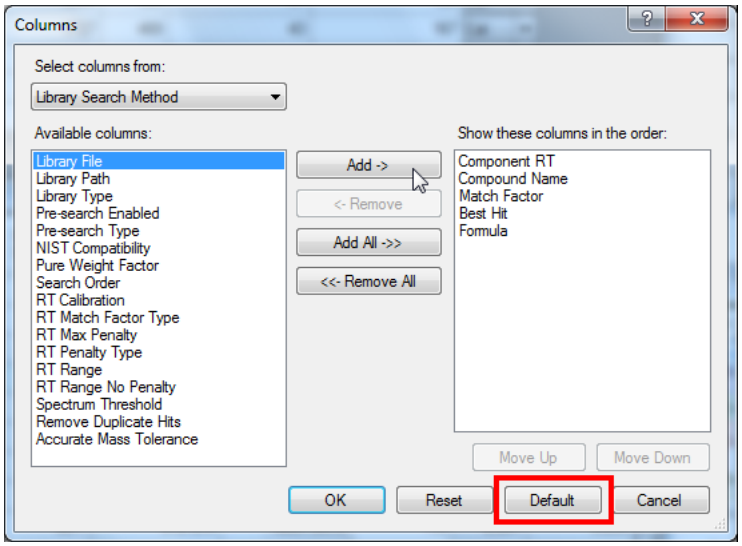
Hits in a sample are marked as **Blank Subtracted Hits** when the same hit is found in the blank with RT±5FWHM. FWHM of a typical GC-MS peak is 1-2s. If we use 2s on this estimation, 5FWHM = 10s = 0.17min. You can see the **Blank Subtracted** hits only when you click **All** in the toolbar.

Blank Hit Subtraction is performed against the "blank" sample(s). The hit(s) in any sample(s) with **Sample Type** classified as **Blank**, **DoubleBlank**, or **MatrixBlank** will automatically get subtracted from all the standard samples during the process. You can designate the "blank" sample for blank subtraction purposes by changing the **Sample Type** in the **Sample**. No **Blank Subtraction** happens if there is no "blank" sample(s). Change the sample type to turn off **Blank Subtraction**.

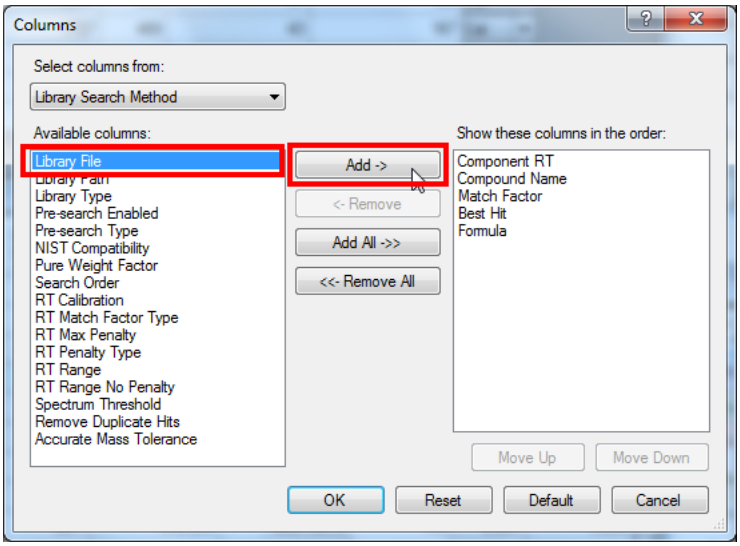
Use Show Alternate Hits to evaluate results

1. Right-click any column header in the **Components** window, and select **Add/Remove Columns**.

2. Click **Default**.

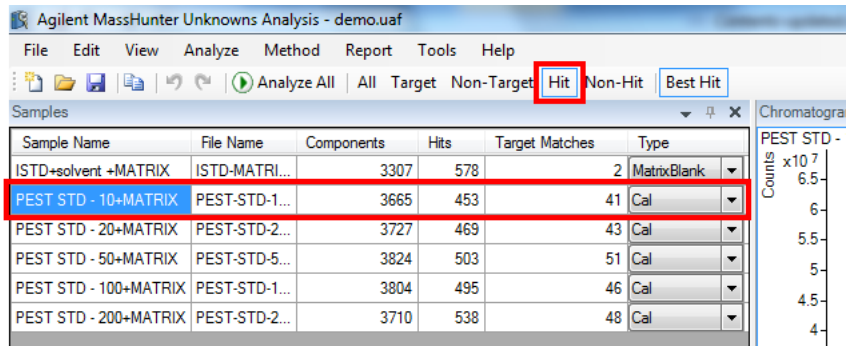


3. Select **Library File** from the **Available columns** list, and click **Add**.

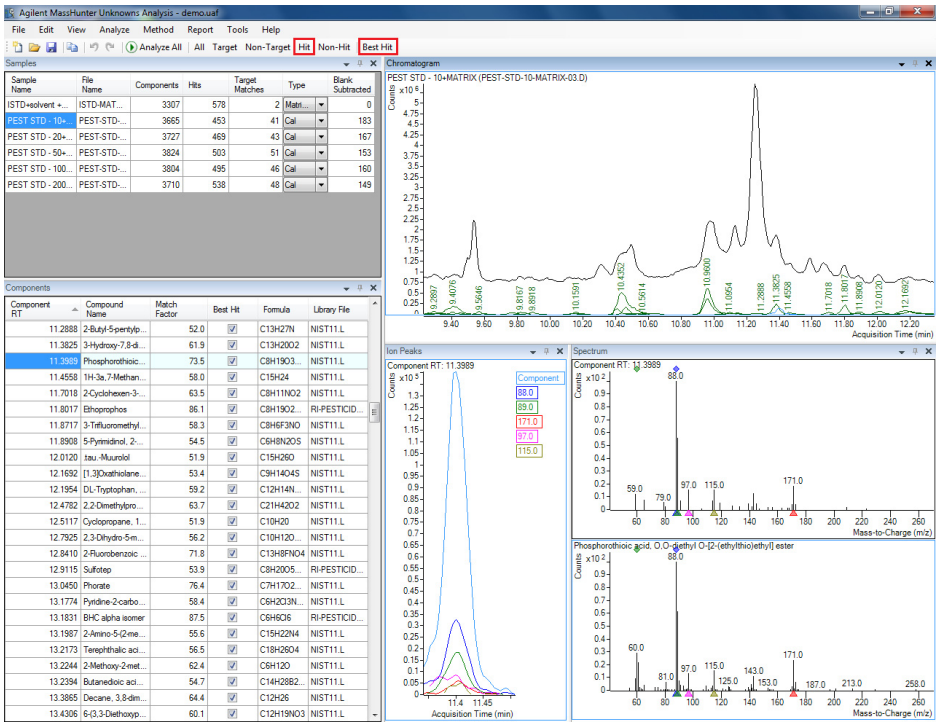


4. Verify that the selected columns are moved to the **Show these columns in the order** list, and click **OK**.

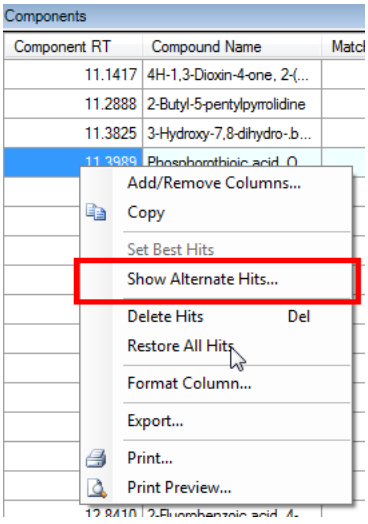
5. Select the **PEST STD-10+MATRIX** sample in the **Samples** window and click **Hit** in the toolbar to view the changes in the **Components** window.



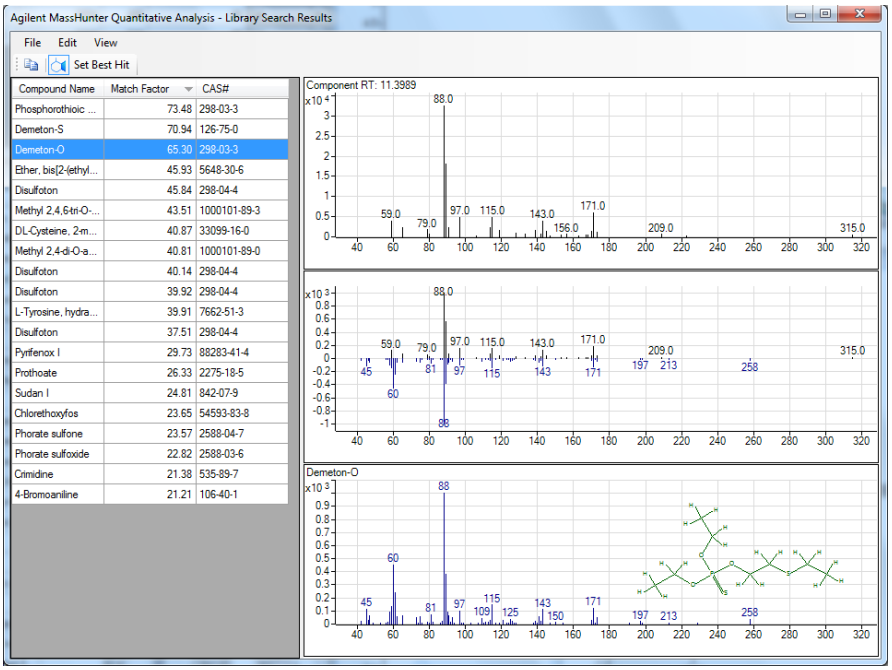
Verify that the Best Hits are from different libraries.



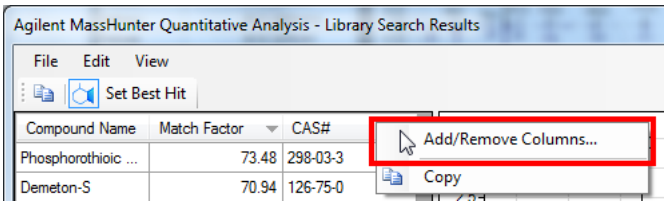
6. Right-click **Phosphorothioic acid** in the **Components** window and select **Show Alternate Hits**.



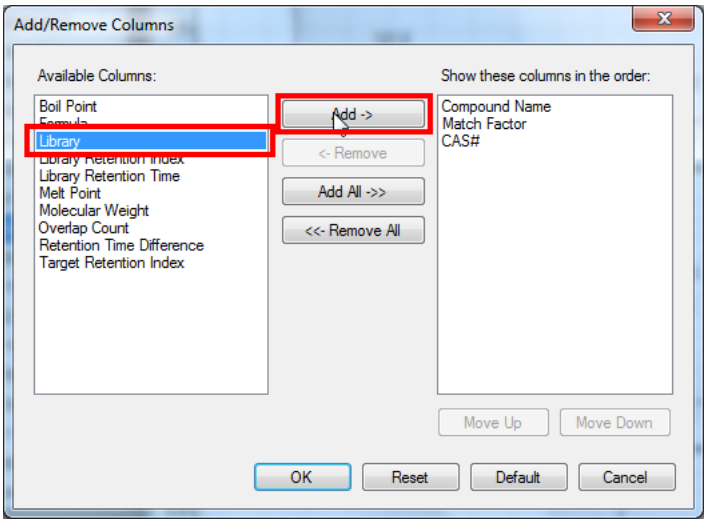
The **Library Search Results** are displayed.



7. Right-click any column header in the **Library Search Results** window, and select **Add/Remove Columns**.

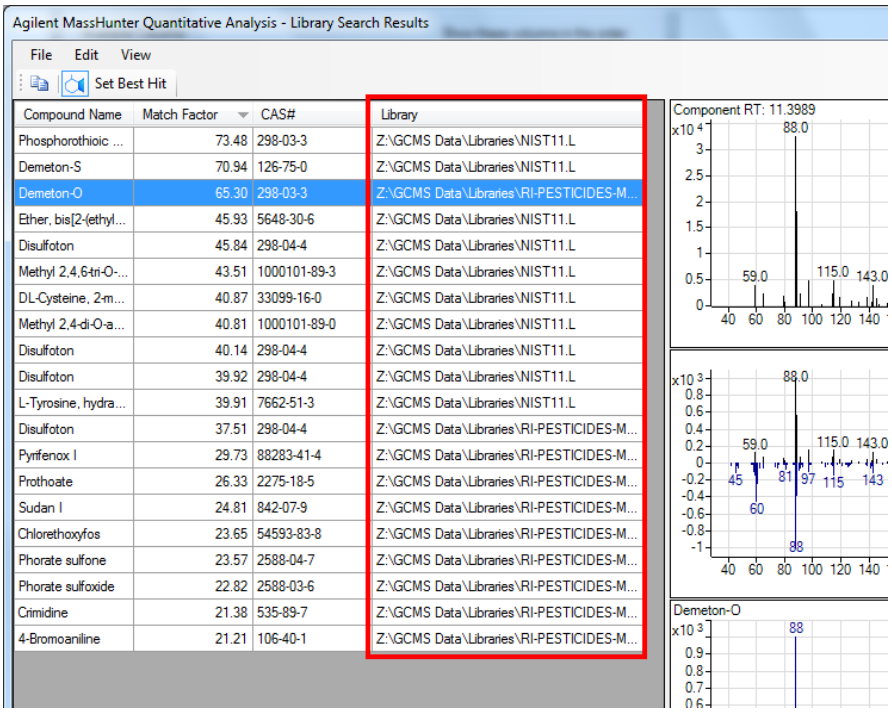


8. Select **Library** from the **Available Columns** list, and click **Add**.

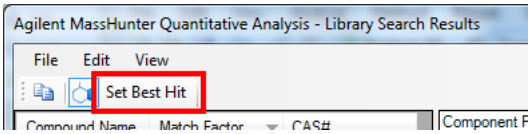


9. Verify that the selected columns are moved to the **Show these columns in the order** list, and click **OK**.

The **Library** column is added to the table.



10. Select **Demeton-S** and click **Set Best Hit**.



Verify that the selected compound replaced the previous compound as the current **Best Hit** in the **Component** table.

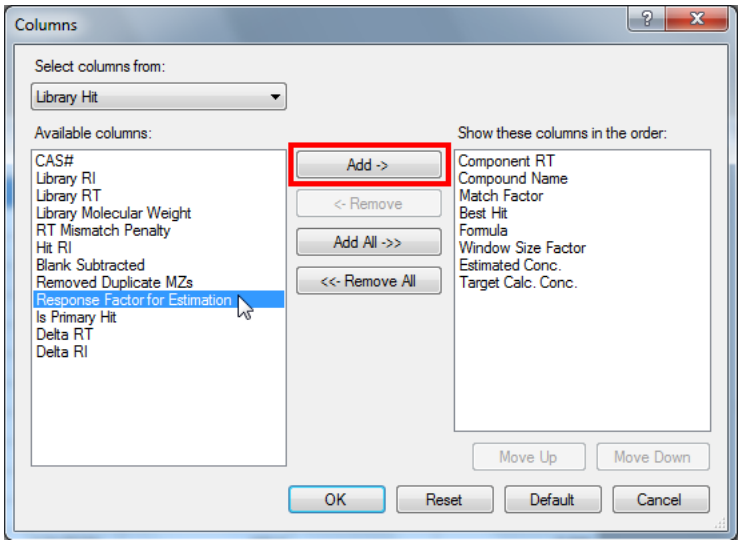
Components

Component RT	Compound Name	Match Factor	Best Hit	Formula	Library File
11,1417	4H-1,3-Dioxin-4-one,...	50,4	☑	C9H14O3	NIST11.L
11,2888	2-Butyl-5-pentylpyrrol...	52,0	☑	C13H27N	NIST11.L
11,3825	3-Hydroxy-7,8-dihydr...	61,9	☑	C13H20O2	NIST11.L
11,3989	Demeton-S	70,9	☑	C8H19O3...	NIST11.L
11,4558	1H-3a,7-Methanoaz...	58,0	☑	C15H24	NIST11.L
11,7018	2-Cyclohexen-3-ol-1-...	63,5	☑	C8H11NO2	NIST11.L
11,8017	Ethoprophos	86,1	☑	C8H19O2...	RI-PESTICIDES-MOL2....
11,8717	3-Trifluoromethylben...	58,3	☑	C8H6F3NO	NIST11.L
11,8908	5-Pyrimidinol, 2-meth...	54,5	☑	C6H8N2OS	NIST11.L
12,0120	.tau.-Muurolol	51,9	☑	C15H26O	NIST11.L
12,1692	[1,3]Oxathiolane-4-a...	53,4	☑	C9H14O4S	NIST11.L
12,1954	DL-Tryptophan, N-m...	59,2	☑	C12H14N...	NIST11.L
12,4782	2,2-Dimethylpropano...	63,7	☑	C21H42O2	NIST11.L
12,5117	Cyclopropane, 1,1,2...	51,9	☑	C10H20	NIST11.L
12,7925	2,3-Dihydro-5-methyl...	56,2	☑	C10H12O...	NIST11.L
12,8410	2-Fluorobenzoic aci...	71,8	☑	C13H8FNO4	NIST11.L

Review concentration estimation results

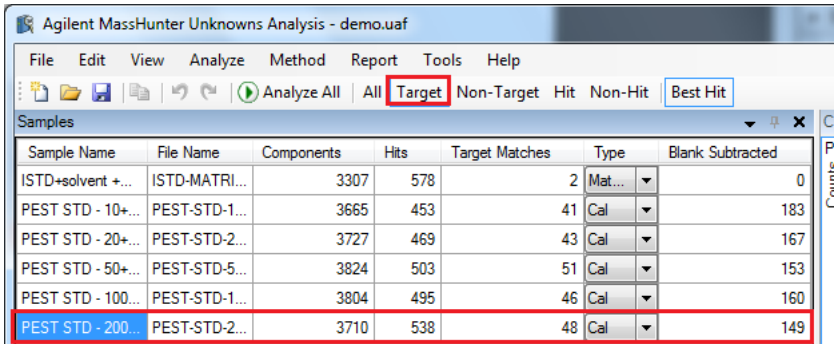
1. Right-click any column header in the **Components** window, and select **Add/Remove Columns**.

2. Select **Base Peak Deconvoluted Area**, **Response Factor for Estimation**, **Target Multiplier**, **Estimated Conc.**, and **Target Calc. Conc.** from the **Available columns** list, and click **Add**.



3. Verify that the selected columns are moved to the **Show these columns in the order** list, and click **OK**.

4. Select the **PEST STD-200+MATRIX** sample in the **Samples** window, and click **Target** in the toolbar to view the changes in the **Components** window.



The estimated concentration results are listed in the **Estimated Conc.** column. For target compounds, you are able to compare with the Quant calculated concentrations.

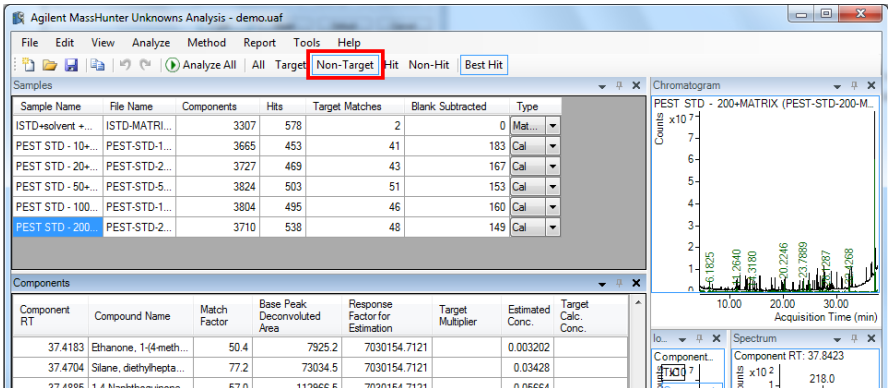
Estimated Concentration is calculated using the following formula:

$$EstimatedConcentration = \frac{BasePeakDeconvolutedArea}{RFforEstimation} \times Multiplier$$

Components

Component RT	Compound Name	Match Factor	Base Peak Deconvoluted Area	Response Factor for Estimation	Target Multiplier	Estimated Conc.	Target Calc. Conc.
11.4021	Phosphorothioic aci...	94.9	2721304.4	14882.6150	1.0	182.9	144.4
11.7973	Ethoprophos	98.6	2129122.9	23030.7854	1.0	92.45	80.33
12.9031	Sulfotep	97.3	1015154.5	14085.4273	1.0	72.07	60.25
13.0452	Phorate	97.5	3420580.5	36958.8482	1.0	92.55	69.61
13.1816	BHC alpha isomer	98.8	1624103.4	30149.9823	1.0	53.87	50.11
13.7016	Pentachloroanisole	98.8	1731347.2	31680.1152	1.0	49.84	50.17
13.7651	Dimethoate	96.0	2679103.0	27597.5245	1.0	97.08	79.42
14.3218	BHC beta isomer	98.5	1014024.0	16466.2678	1.0	59.17	49.7
14.5841	Lindane	98.0	1123973.2	20441.2941	1.0	54.99	50.04
15.0133	Fonofos	97.4	2705421.8	35661.4284	1.0	75.86	60.31
15.5881	Diazinon	98.2	2028613.6	19208.4327	1.0	98.63	79.78
15.6787	Disulfoton	85.7	1203625.2	14752.9912	1.0	81.59	61.33
15.6842	BHC delta isomer	96.2	1201797.5	22136.8200	1.0	54.29	50.04
17.7267	Methyl parathion	86.9	1539303.6	7893.1866	1.0	108	71.86
17.7336	Chloropyriphos-methyl	91.9	2612062.4	25588.5789	1.0	102.1	81.29
17.9452	Heptachlor	95.7	598014.1	9867.5025	1.0	60.6	50.24

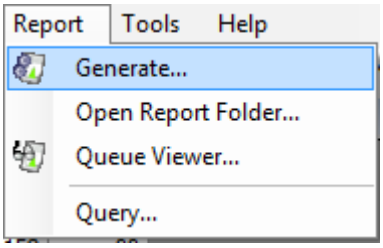
5. Click **Non-Target** in the toolbar to view the estimated concentrations for Non-Targets.



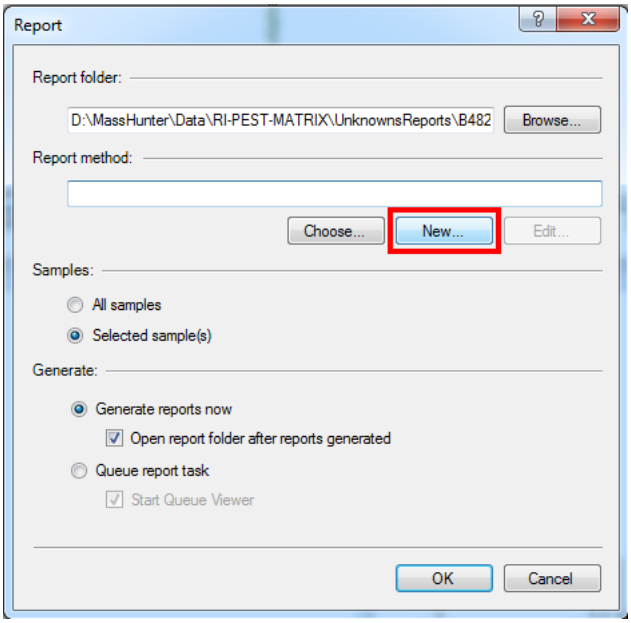
6. To save the analysis, select **File > Save Analysis**.

Task 3: Generate the Report

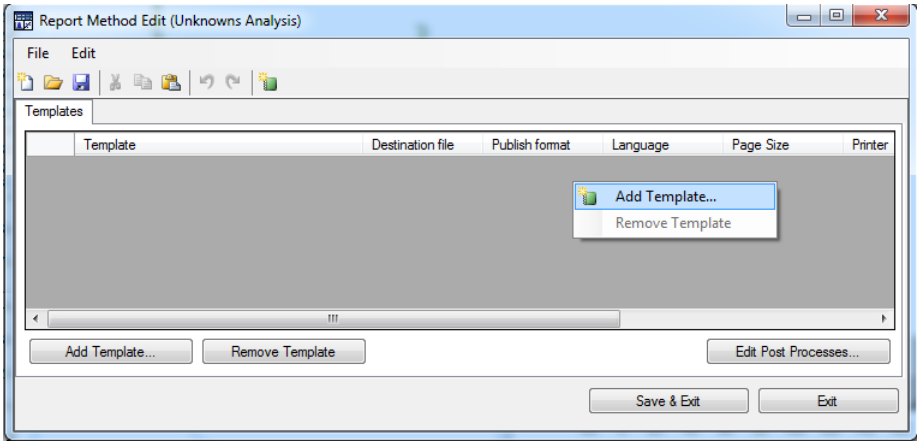
1. Select **Report > Generate**.



2. Under **Report method**, click **New**.

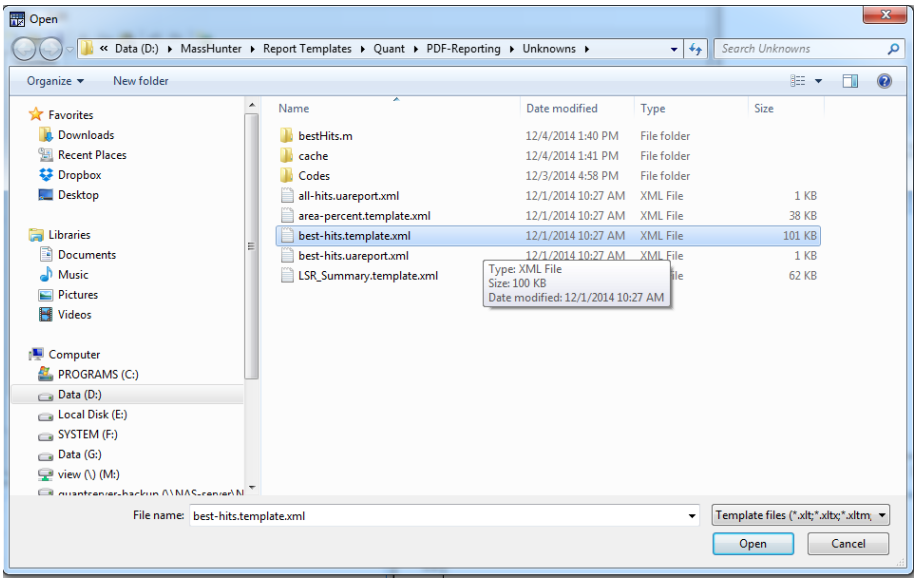


3. Right-click in the window and select **Add Template**.

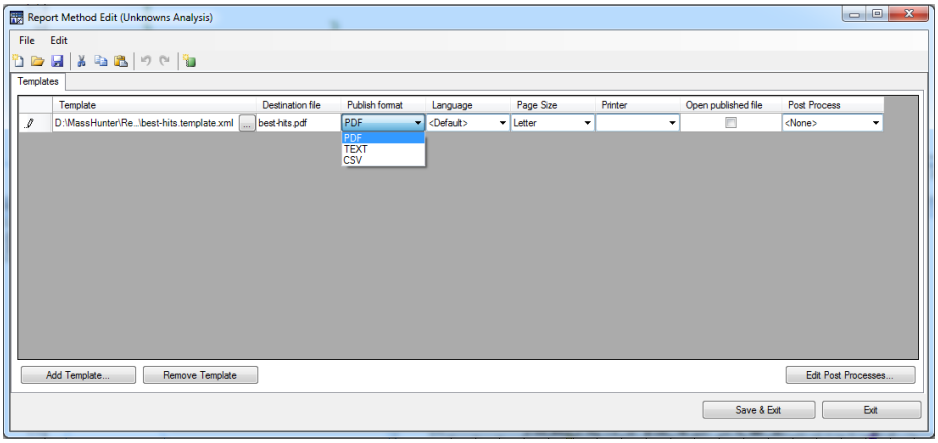


Task 3: Generate the Report

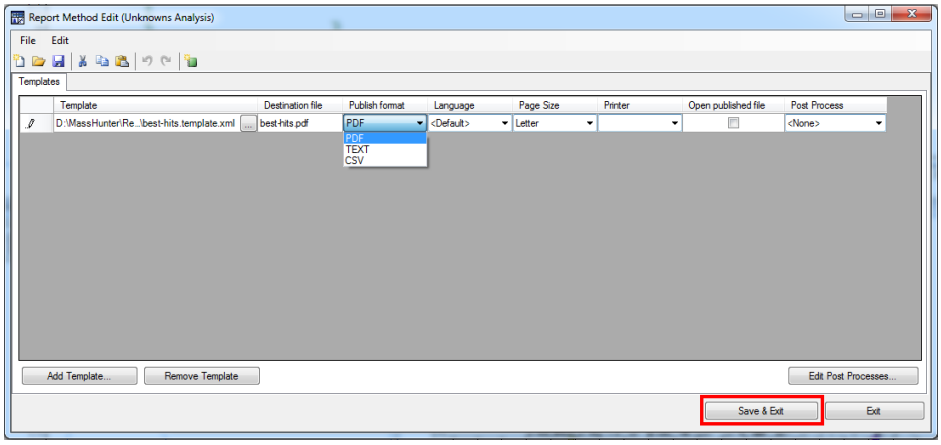
4. Navigate to **D:\MassHunter\Report Templates\Quant\PDF-Reporting\Unknowns**, select **best-hits.template.xml**, and click **Open**.



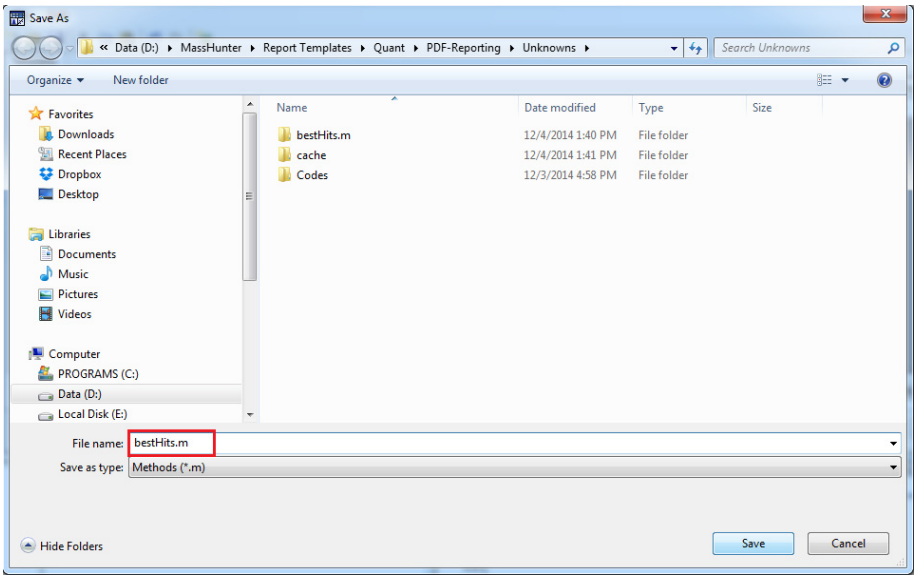
Once the template(s) is selected, you can configure the **Report Publish Format** with *PDF, TEXT, and CSV,* **Language** with *English, Chinese, Japanese, and Russian,* **Page Size, Printer** with *A4 and Letter*, and whether or not to **Open published file** after generating the report. The **Post Process** is also available to process the report further after finishing the report task.



5. Click **Save & Exit** to save the Report Method in a desired location.



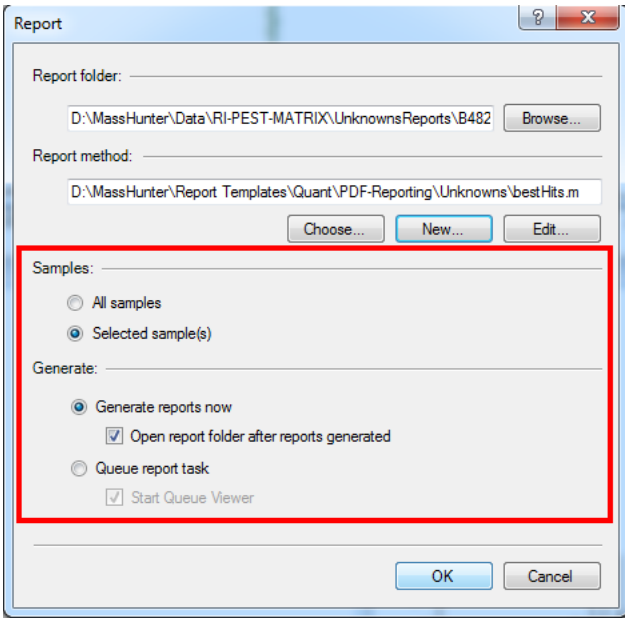
Report Methods have a **.m** extention.



Task 3: Generate the Report

6. For samples, you can generate a report for **All samples** or the **selected Sample(s).**

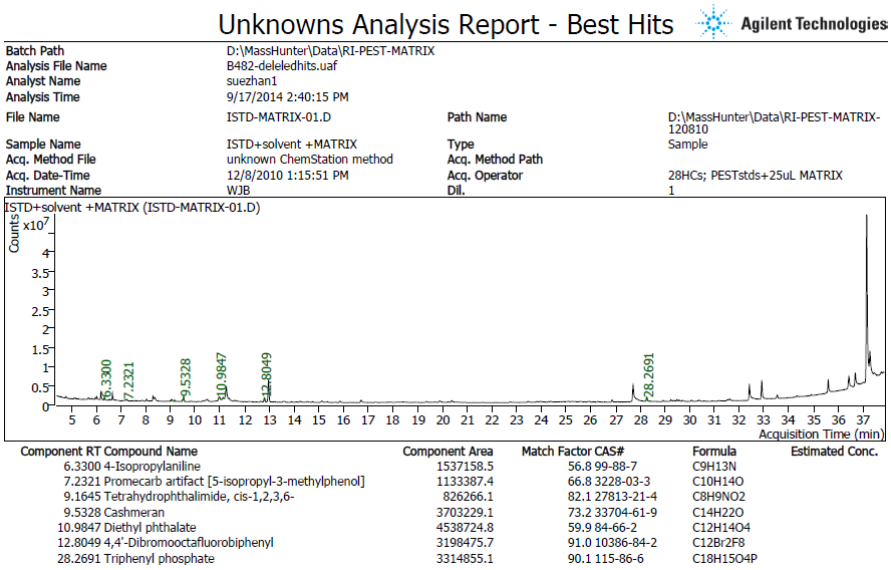
   For Report Generating modes, you can select **Generate reports now** or **Queue report task**.



7. Click **OK** to begin generating reports.

   The report folder opens automatically when the report generation is complete.

   Alternatively, you can select **Menu > Open Report Folder** to view the newly generated report **best-hits.pdf**. The report opens in Adobe Reader.


Unknowns Analysis Report - Best Hits

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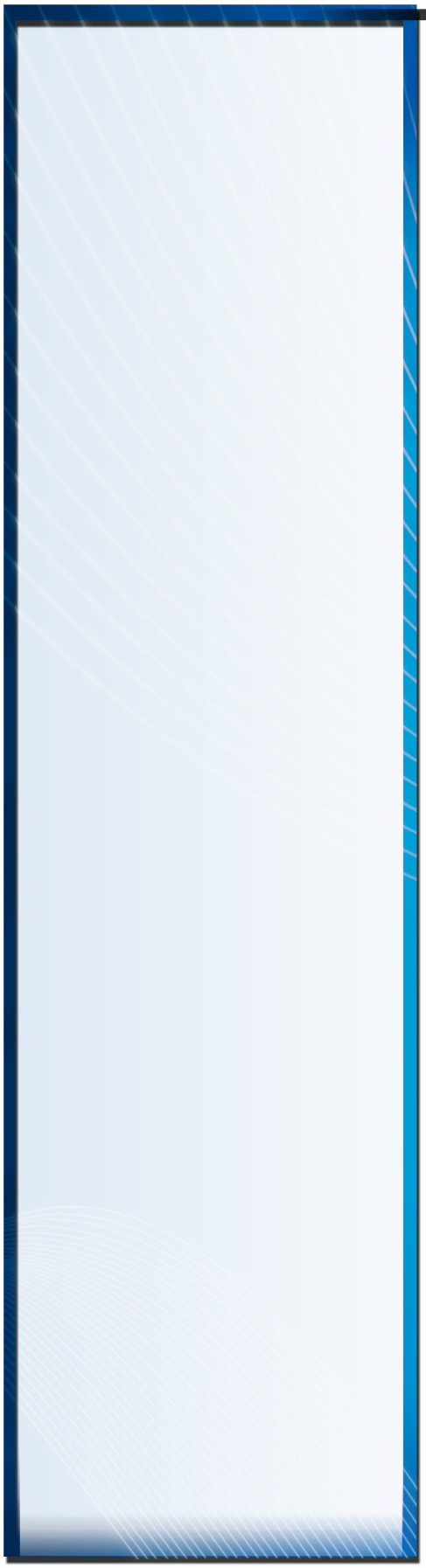
Batch Path	D:\MassHunter\Data\RI-PEST-MATRIX		
Analysis File Name	B482-deleledhits.uaf		
Analyst Name	suezhan1		
Analysis Time	9/17/2014 2:40:15 PM		
File Name	ISTD-MATRIX-01.D	Path Name	D:\MassHunter\Data\RI-PEST-MATRIX-120810
Sample Name	ISTD+solvent +MATRIX	Type	Sample
Acq. Method File	unknown ChemStation method	Acq. Method Path	
Acq. Date-Time	12/8/2010 1:15:51 PM	Acq. Operator	28HCs; PESTstds+25uL MATRIX
Instrument Name	WJB	Dil.	1

Component RT	Compound Name	Component Area	Match Factor	CAS#	Formula	Estimated Conc.
6.3300	4-Isopropylaniline	1537158.5	56.8	99-88-7	C9H13N	
7.2321	Promecarb artifact [5-isopropyl-3-methylphenol]	1133387.4	66.8	3228-03-3	C10H14O	
9.1645	Tetrahydrophthalimide, cis-1,2,3,6-	826266.1	82.1	27813-21-4	C8H9NO2	
9.5328	Cashmeran	3703229.1	73.2	33704-61-9	C14H22O	
10.9847	Diethyl phthalate	4538724.8	59.9	84-66-2	C12H14O4	
12.8049	4,4'-Dibromooctafluorobiphenyl	3198475.7	91.0	10386-84-2	C12Br2F8	
28.2691	Triphenyl phosphate	3314855.1	90.1	115-86-6	C18H15O4P	

8. Close the report.

9. To exit the program, select **File > Exit**.



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