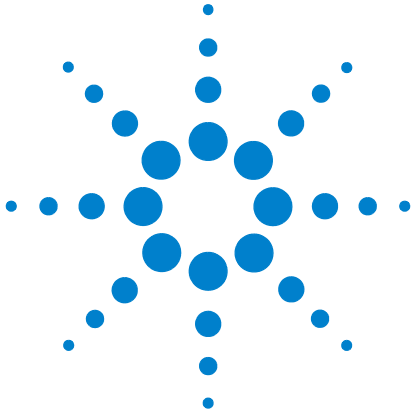

Agilent MassHunter Workstation Software Unknowns Analysis

Familiarization Guide

Agilent Technologies

Notices

Manual Part Number

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5301 Stevens Creek Boulevard
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Contents

In this Guide...

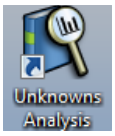
This guide presents step-by-step exercises to help you learn to use the Unknowns Analysis program. You can do these exercises with the demonstration analysis, method, and library files shipped with the system installation disk, or with data you acquire.

Before You Begin These Exercises

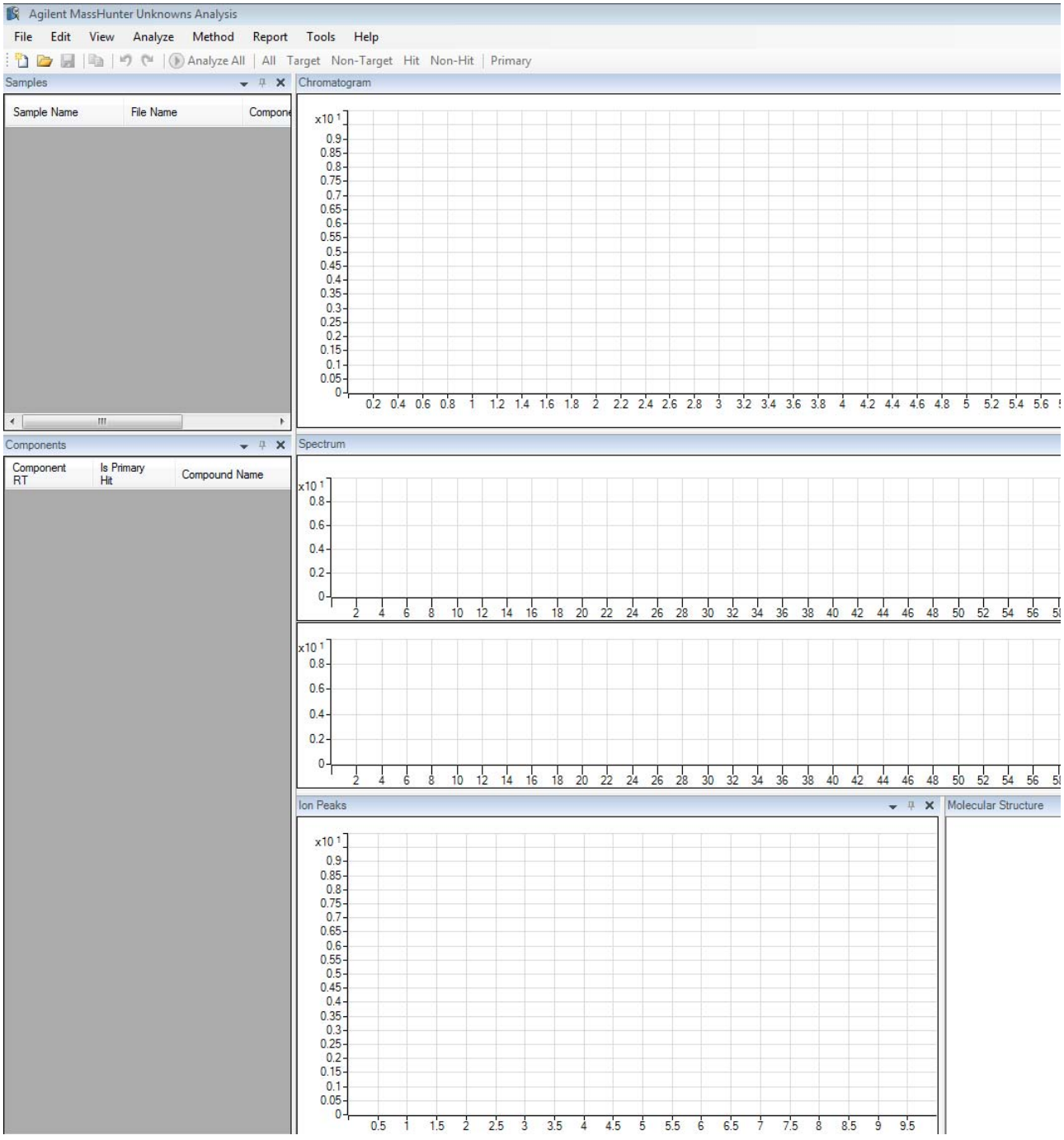
Copy files from the installation disk to your hard disk

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 on the disk exactly, then the results obtained during these exercises will not match those shown in this guide.

Start the unknowns analysis software

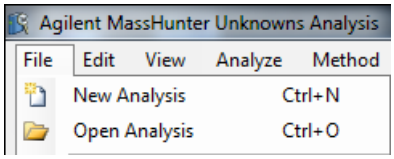
1 Select the **Unknowns Analysis** desktop icon, 

. Your start screen is blank as shown below.

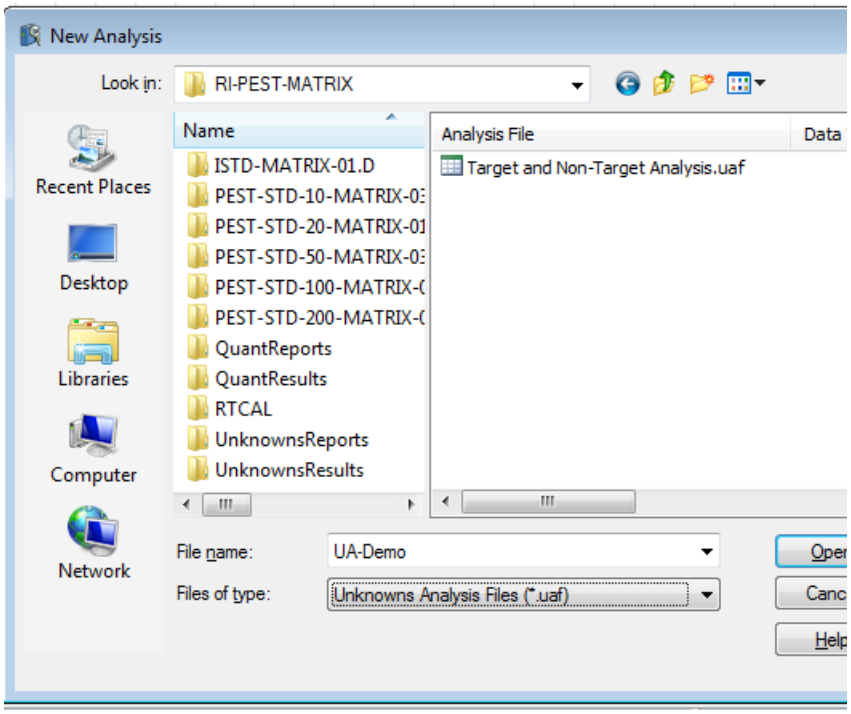


Create a New Analysis

1 From the menu bar, select **File > New Analysis**.



2 In the **New Analysis** dialog box, navigate to the folder where you want to save the analysis. (**RI-PEST-MATRIX**)



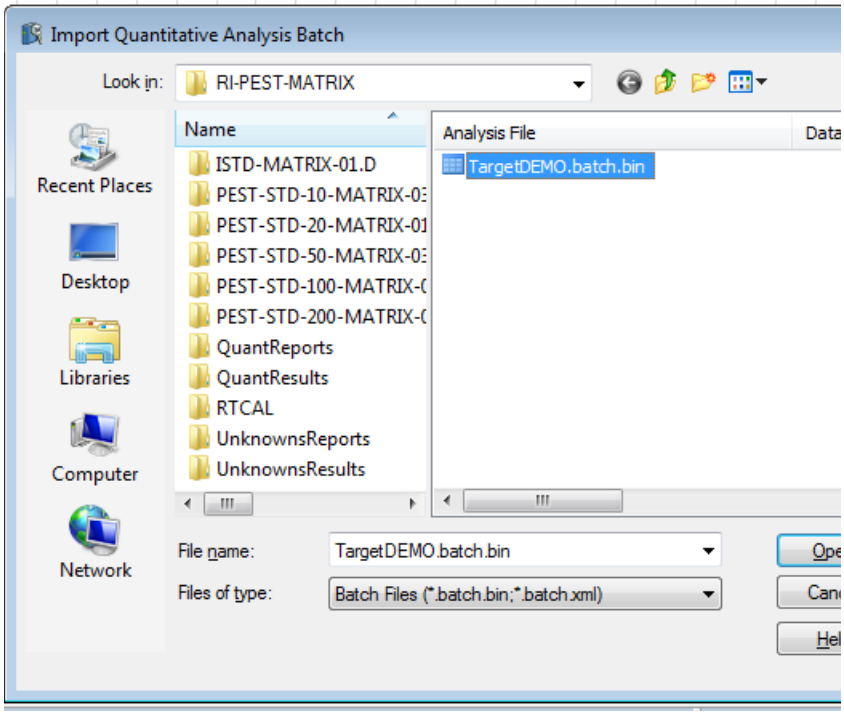
3 In the **File name** field, enter a name for your analysis. For this exercise use the file name, **UA-Demo.uaf**.

4 Select **Open**. The new analysis is created and opens with the name in the title bar.

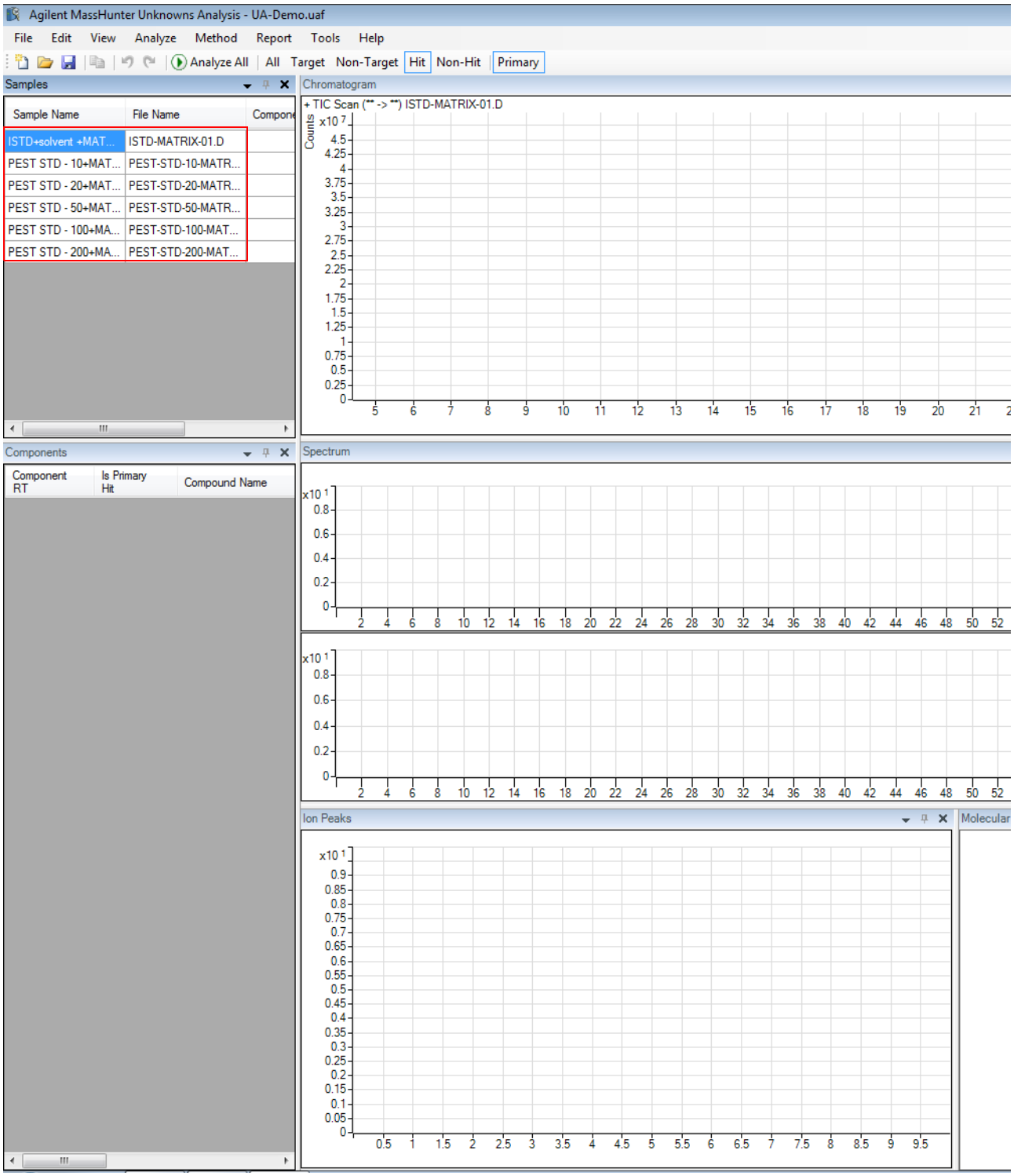
Import Data from a MassHunter Quantitative Analysis

1 From the menu bar, select **File > Import Quantitative Analysis**. The **Import Quantitative Analysis Batch** dialog box opens.

2 Navigate to **MassHunter/Data/R-PEST-MATRIX** and select **TargetDEMO.batch.bin**.

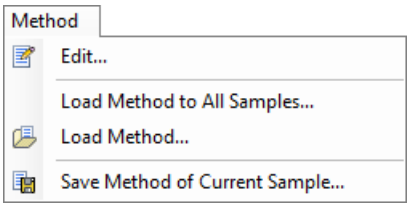


3 Select **Open**. The dialog box closes and the samples are added to the **Samples** table.

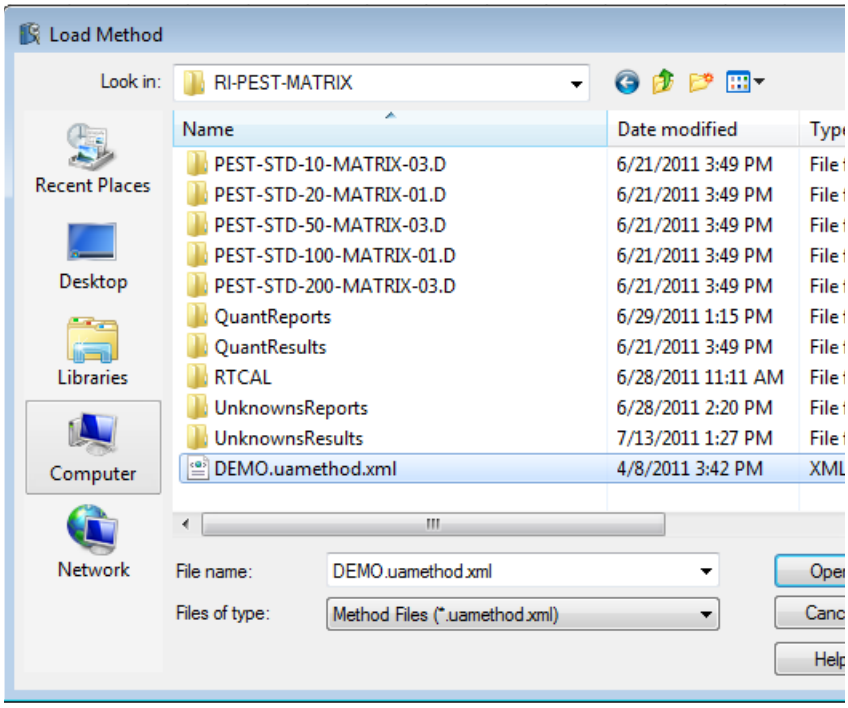


Load the Method

1 From the menu bar, select **Method > Load Method to All Samples**.



2 In the **Load Method** dialog box, navigate to **MassHunter/Data/RI-PEST-MATRIX** and select **DEMO.uamethod.xml**.



3 Select **Open**. The dialog box closes and the method is loaded to all the samples in your analysis.

Select a Library to Use for the Unknowns Analysis

1 From the menu bar, select **Method > Edit**. The **Method** dialog box opens in the view from which it was last closed. For this exercise, we will use the Standard view shown in Figure 1 If the Advanced dialog box opened as shown in Figure 2, select **Standard** to switch to the Standard view.

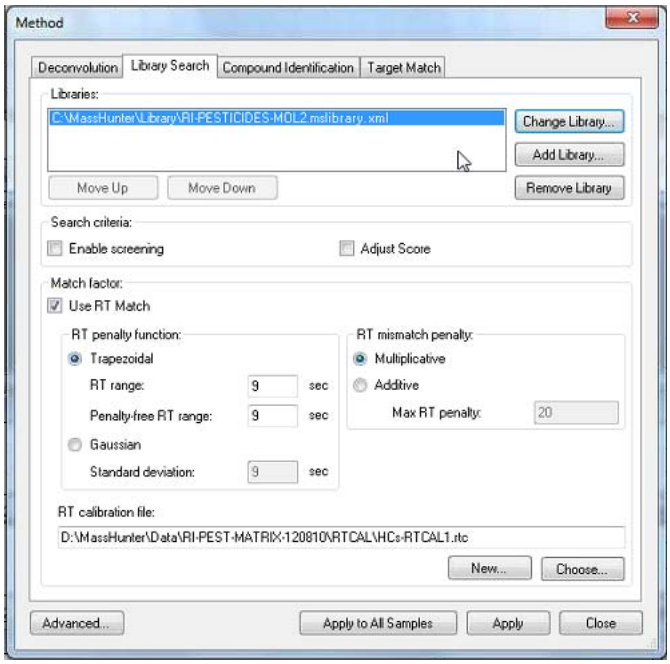


Figure 1 The **Method** dialog box, standard view

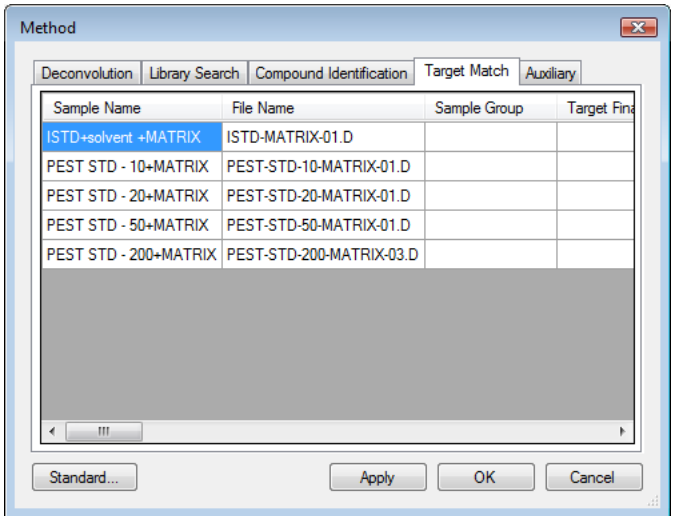


Figure 2 The **Method** dialog box, advanced view

2 Select the **Library Search** tab.

3 In the **Libraries** area, select **Change Library**.

4 In the **Open** dialog box, navigate to your **Data** folder and select **RI-PESTICIDES_MOL2.mslibrary.xml**.

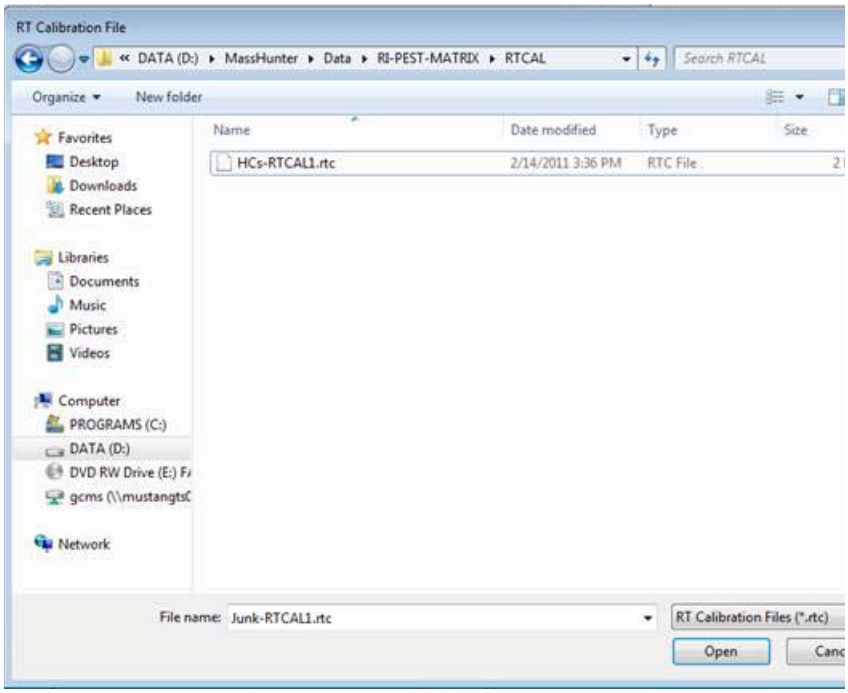
The Data folder was copied to your hard disk. See step 4 on page 6.

5 Select **Open**. The dialog box closes and the library is added to the **Libraries** list in the **Method** dialog box. (see Figure 1 on page 12).

6 In the **RT Calibration File** area, select **Choose**.

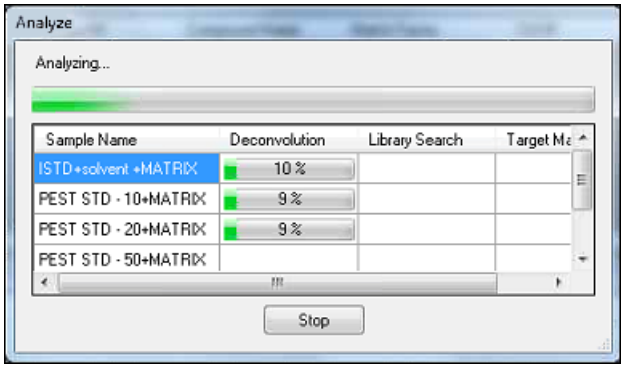
7 In the **RT Calibration File** dialog box, navigate to your **DATA** folder and select **HCs-RTCal1.rtc**.

8 In the **Method** dialog box, select **Apply to All Samples** and then **Close**.



Analyze and Review Results

1 From the menu bar, select **Analyze > Analyze All** or Analyze All.



2 From the menu bar, select **View > Layout > All-Extended**.

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

4 Select one of the following toolbar buttons:

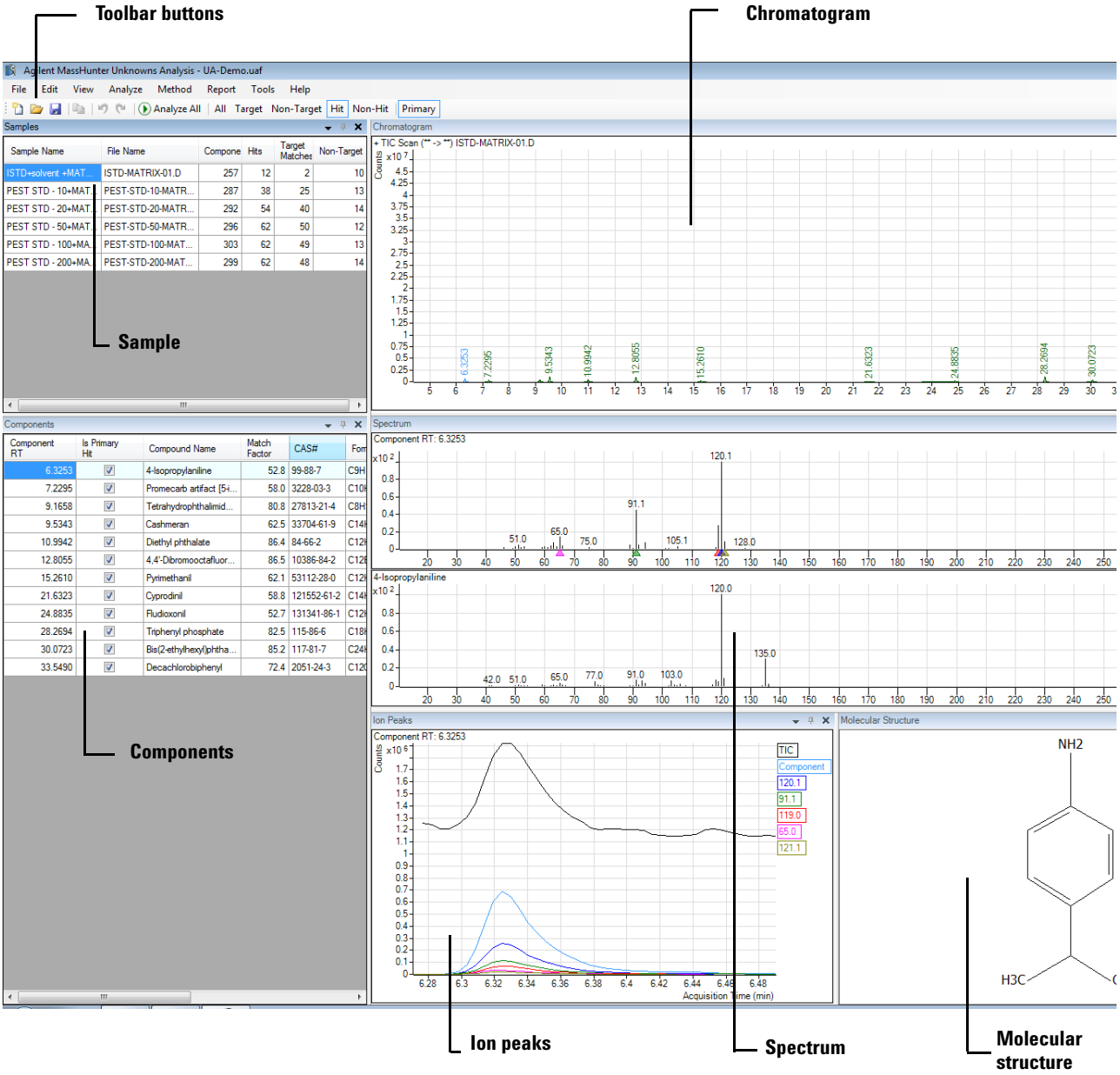
- **All** - Select to view all the peaks
- **Target** - Select to view the peaks that are also in the quantitation batch
- **Non Target** - Select to view the peaks that are not in quantitation batch
- **Hit** - Select to view the peaks that are also in the library
- **Non-Hit** - Select to view the peaks that are not in the library
- **Primary** - Select to view the best match.

5 From the **Components** table, select a component from the **Component RT** column.

6 View the **Spectrum**, **Ion 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.

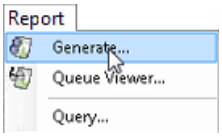
The **Molecular Structure** is from the library.



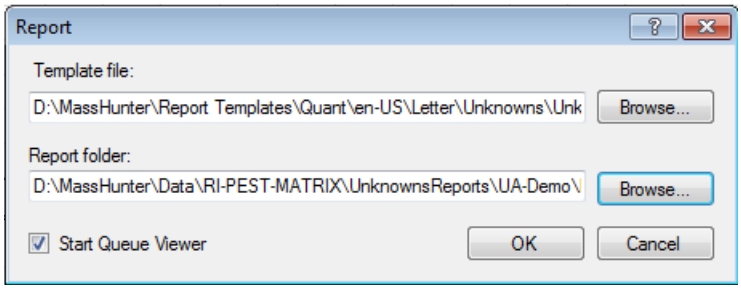
7 To save the analysis, select **File > Save Analysis**.

Generate a Report

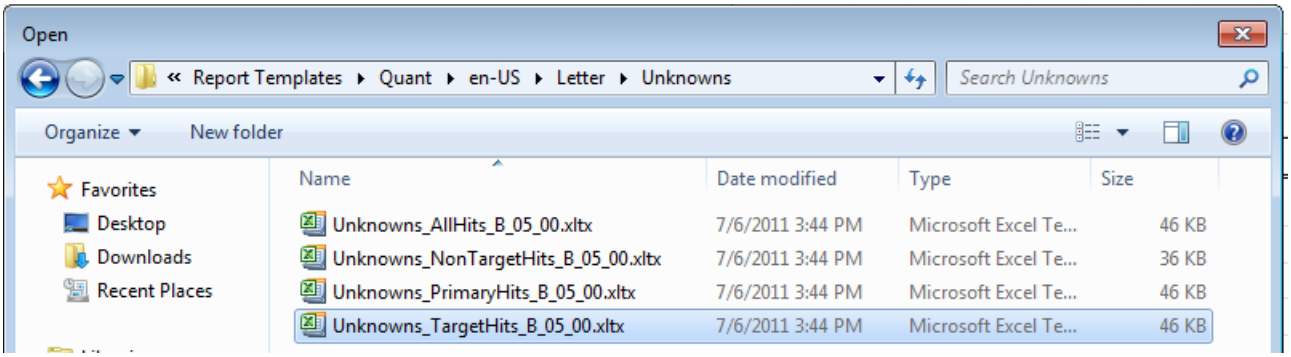
1 From the menu bar, select **Report > Generate**.



2 In the **Report** dialog box, under **Template file** select **Browse**.



3 In the **Open** dialog box, browse to **MassHunter > Report Templates>Quant>en-US>Letter>Unknowns**. For this exercise select **Unknows_TargetHits_B-05_00.xltx**.

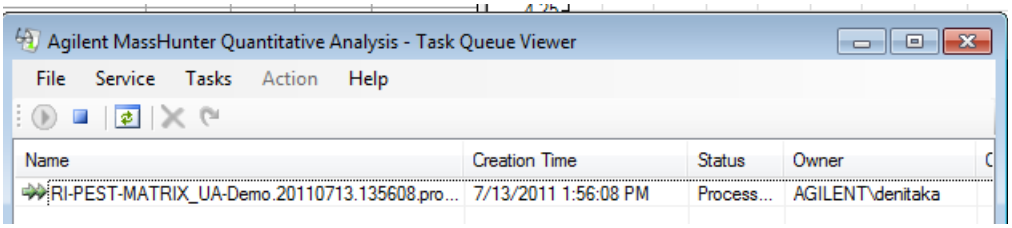


4 In the **Report** dialog box, under **Report folder** select **Browse.**

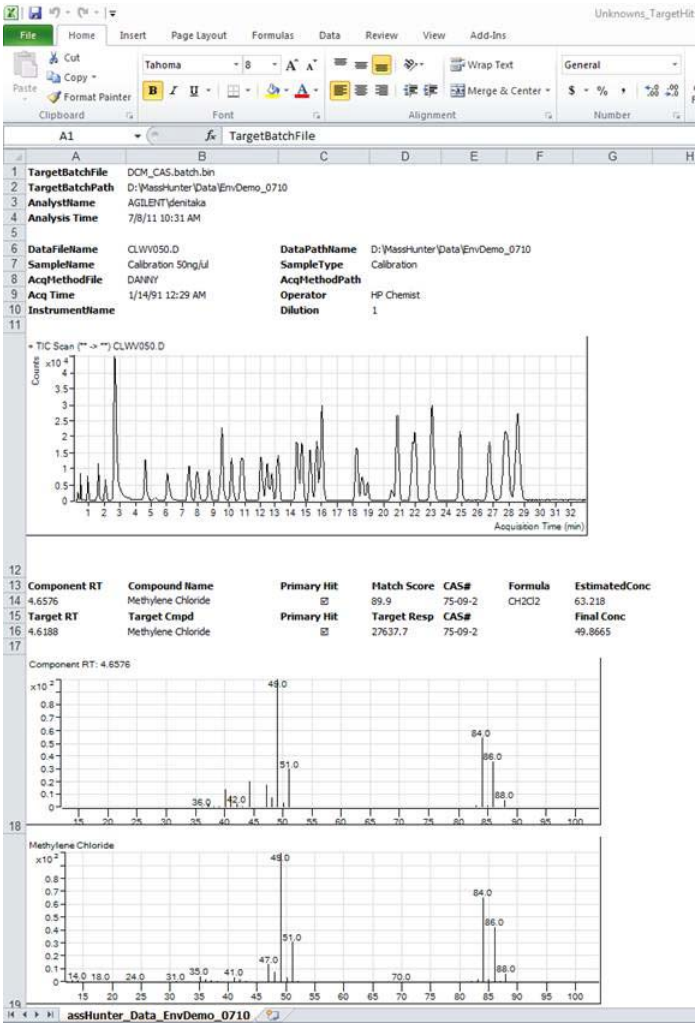
5 In the **Open** dialog box, browse to where you want to store your report and select **Open**. The default location is the same place the analysis is stored.

6 In the **Report** dialog box, select **OK**.

7 The **Task Queue Viewer** is displayed.



8 When the task is complete, in the **Task Queue** viewer select **Action > Open Unknowns TargetHits_B_05_00.xls**. The report opens in Excel. You can use the normal Excel features to print, save, or modify the report.



9 Close the report.

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

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