

# Agilent MassHunter Metabolite ID Software



## Installation and Getting Started Guide



**Agilent Technologies**

# Notices

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## Software Revision

This guide is valid for B.04.xx and higher revisions of the G2211 Agilent MassHunter Metabolite ID Software software, where xx refers to minor revisions of the software that do not affect the technical accuracy of this guide.

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## In This Guide...

This guide describes how to install (and uninstall) the Metabolite ID application and provides step-by-step instructions on how to work with the software, using example data files.

### **1 Installing Metabolite ID Software**

This chapter leads you through the process of installing the Metabolite ID software. It also describes how you can uninstall the software, if necessary.

### **2 Getting Started with Metabolite ID**

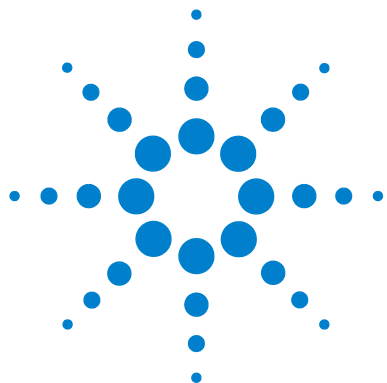
This chapter guides you step-by-step through some of the important features and functions of the Metabolite ID software.



# Content

|          |                                                     |           |
|----------|-----------------------------------------------------|-----------|
| <b>1</b> | <b>Installing Metabolite ID Software</b>            | <b>7</b>  |
|          | Prerequisites and Recommendations                   | 8         |
|          | To install the Metabolite ID program                | 9         |
|          | To configure Microsoft Excel 2010 for Metabolite ID | 13        |
|          | To remove the Metabolite ID program                 | 18        |
| <b>2</b> | <b>Getting Started with Metabolite ID</b>           | <b>21</b> |
|          | To start the Metabolite ID program                  | 22        |
|          | To set up a method and finding metabolites          | 24        |
|          | To review the results                               | 26        |
|          | To tune the method parameters                       | 28        |
|          | To work with Reference Compounds                    | 32        |
|          | To configure the display                            | 35        |
|          | To generate a report                                | 37        |





# 1

## Installing Metabolite ID Software

|                                                     |    |
|-----------------------------------------------------|----|
| Prerequisites and Recommendations                   | 8  |
| To install the Metabolite ID program                | 9  |
| To configure Microsoft Excel 2010 for Metabolite ID | 13 |
| To remove the Metabolite ID program                 | 18 |

This chapter leads you through the process of installing the Metabolite ID software. It also describes how you can uninstall the software, if necessary.



# Prerequisites and Recommendations

## PC Hardware

The following PC hardware is required to run the Metabolite ID application:

|             |                                                |
|-------------|------------------------------------------------|
| Display     | 1680 × 1050 recommended<br>1280 × 1024 minimum |
| CPU         | 3 GHz P4 class CPU<br>Dual-core recommended    |
| Main Memory | 4 GB recommended<br>2 GB minimum               |

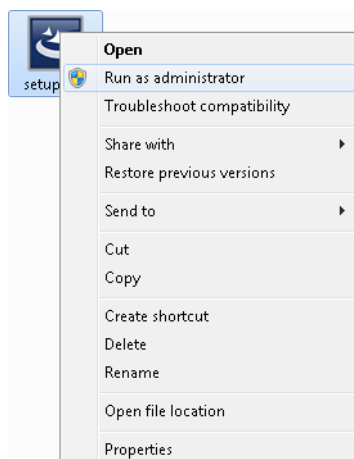
## Operating System and Software

The following software components are required to ensure that the Metabolite ID application can be installed and run:

|                  |                                                                                     |
|------------------|-------------------------------------------------------------------------------------|
| Operating System | Microsoft Windows® 7 64-bit system running as a 32-bit application                  |
|                  | Microsoft Windows® XP Professional with Service Pack 3 (or later) is also supported |
| For Reporting    | Microsoft Office 2010 or Microsoft Excel 2010 (US English)                          |

## To install the Metabolite ID program

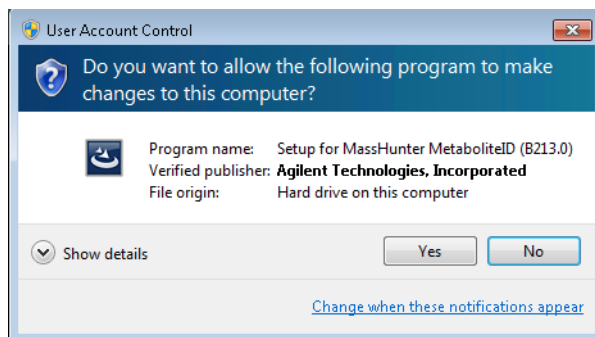
- 1 Insert the MassHunter Workstation Metabolite ID DVD into the DVD-ROM drive.
- 2 Open Windows Explorer.
- 3 Navigate to the DVD-ROM drive.
- 4 Right-click on **Setup** and select **Run as administrator** from the context menu (Figure 1).



**Figure 1** Setup context menu

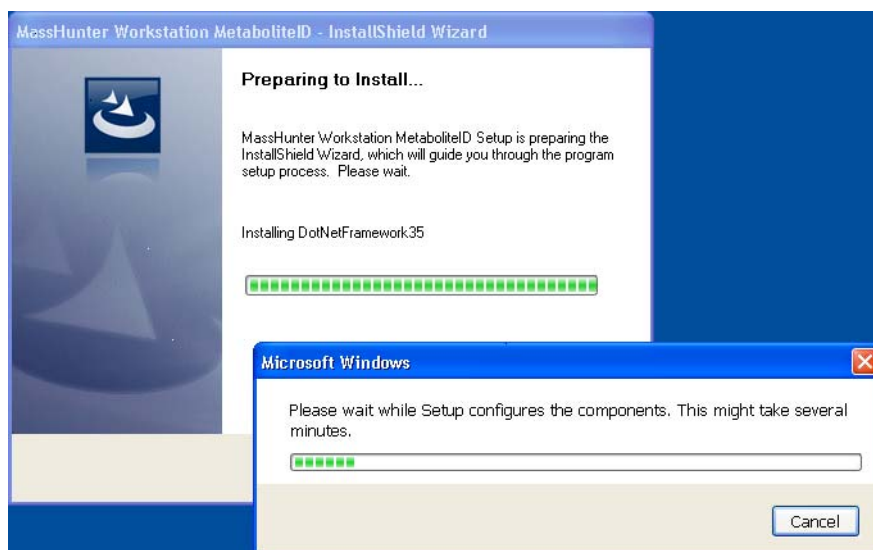
- 5 Click Yes in the User Account Control dialog box (Figure 2) to allow the installation program to make changes.

## 1 Installing Metabolite ID Software



**Figure 2** User Account Control dialog box

- 6** If the **NET 3.5** framework is not present, it is installed automatically (**Figure 3**).

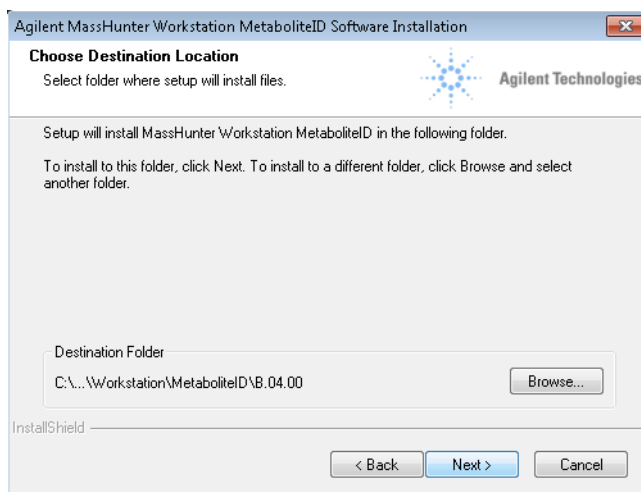


**Figure 3** NET Framework 3.5 component

When all necessary components have been installed, the MassHunter Workstation Metabolite ID Setup Welcome screen is displayed.

- 7** In the Welcome screen, click **Next**.
- 8** When you have read through the terms of the license agreement, mark the **I accept the terms in the License Agreement** check box and click **Next**.

The Destination Folder screen is displayed (Figure 4 on page 11), which allows you to select a folder for the Metabolite ID files.



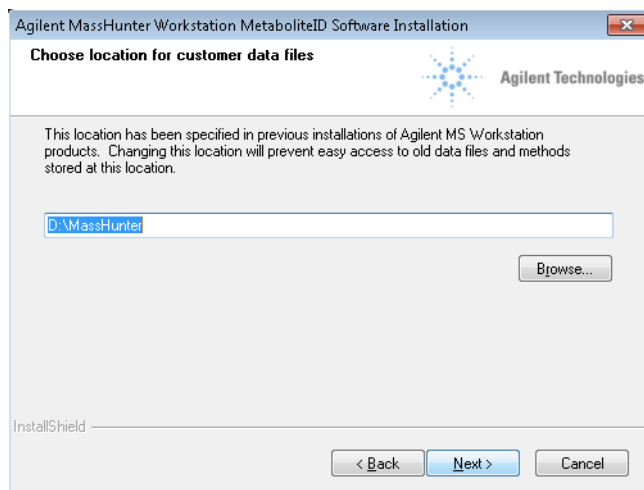
**Figure 4** Destination Folder screen

- 9 In the Destination Folder screen, click **Next** to accept the default folder, or click **Browse** and navigate to a destination folder of your choice.

If no other MassHunter application is already installed, the data files location screen is displayed (Figure 5 on page 12), which allows you to select a folder for your data files.

If another Masshunter application is installed, the directory information in the data files location screen is read-only.

## 1 Installing Metabolite ID Software



**Figure 5** Data files location screen

**10** Click **Install** to begin the installation process.

If you want to review your installation settings, click **Back** to return to the previous screen.

**11** When the installation has finished, click **Finish** to close the installation process.

The Metabolite ID application is now installed.

## To configure Microsoft Excel 2010 for Metabolite ID

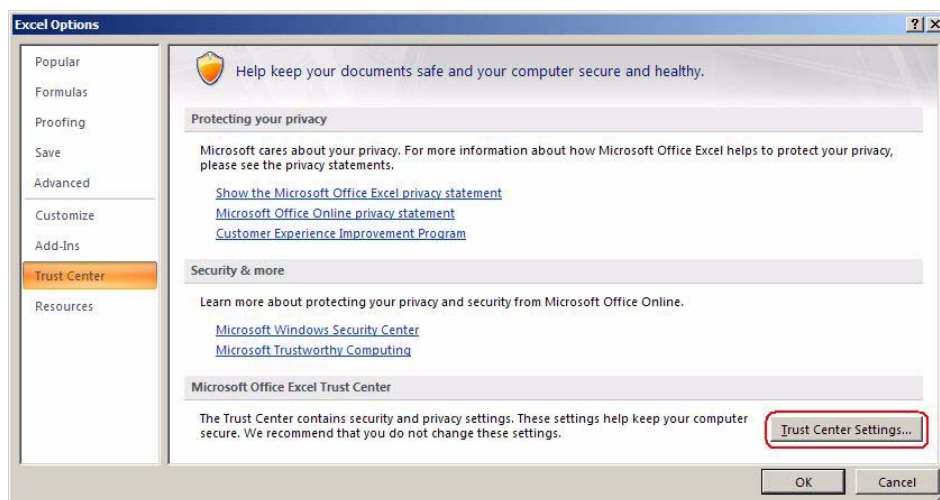
In order to use Microsoft Excel 2010 for Metabolite ID reporting, you must configure it to use the MassHunter Workstation Add-in.

- 1 Start Microsoft Excel from the Windows **Start** menu or from the desktop.
- 2 Click the Office Button at the top left of the Microsoft Excel window.
- 3 Click the **Excel Options** button at the bottom right of the menu box.

The Excel Options dialog box is displayed.

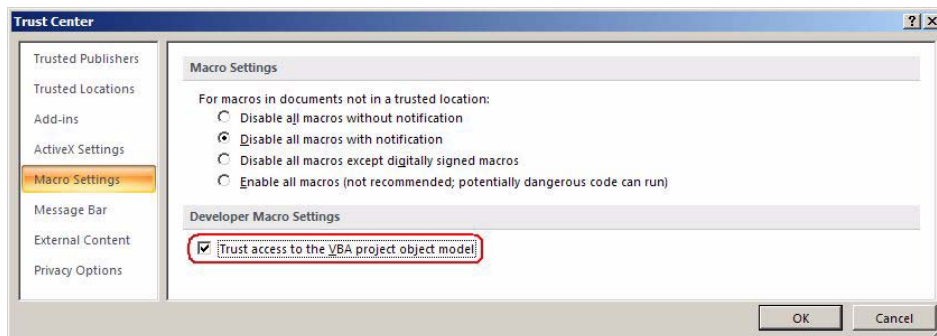
- 4 From the menu at the left of the dialog box, select **Trust Center**.
- 5 Click the **Trust Center Settings** button at the bottom right

The Trust Center Settings are displayed (Figure 6).



**Figure 6** Excel Options dialog box

- 6 From the menu at the left of the Trust Center Settings dialog box, select **Macro Settings**.
- 7 Mark the **Trust access to the VBA project object model** check box ☐.



**Figure 7** Trust Center Settings dialog box

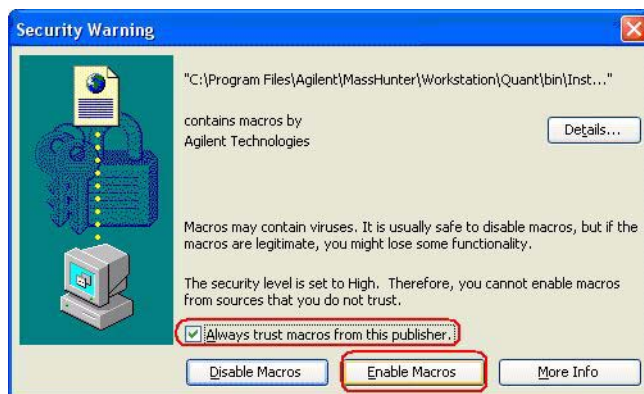
- 8** Mark the **Trust access to Visual Basic Project** and **Trust all installed add-ins and templates** check boxes.

The MassHunter Workstation Add-in uses the Microsoft Excel certificate technology to protect the Excel Add-in from modification. When **Trust access to Visual Basic Project** is enabled, Microsoft Excel can access the MassHunter Add-in and generate the workbook reports.

- 9** Click **OK** to close the Security dialog box.

Microsoft Excel is now ready to generate reports from Metabolite ID.

- 10** If you see a Windows security warning ([Figure 8](#) on page 15) the first time you generate a Metabolite ID report,
  - a** Mark the **Always trust macros from this publisher** check box, as in [Figure 8](#).
  - b** Click **Enable Macros** to enable the reporting macros and close the dialog box.

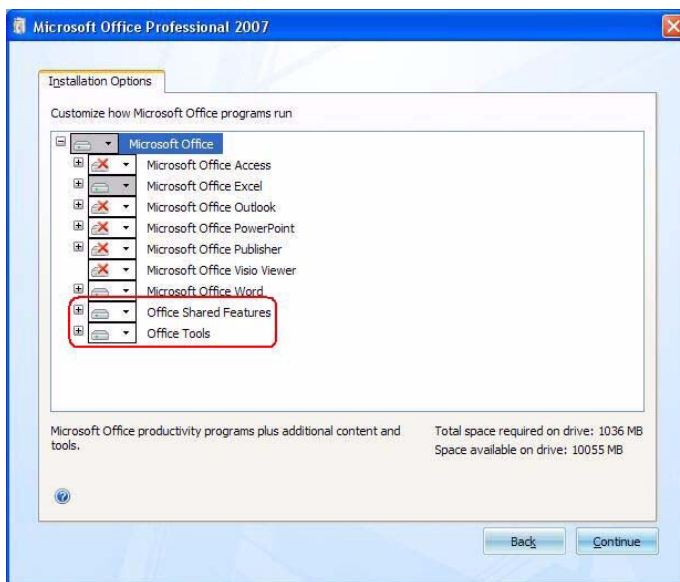


**Figure 8** Security warning from Certificate

### Custom installation of Office 2010

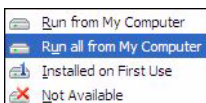
If you choose to do a custom installation of Office 2010, there are certain options that you must select in order to work with MassHunter Workstation. As a minimum you need to have Microsoft Office Excel, Office Shared Features and Office Tools set to **Run all from My Computer**. This is indicated by a white box containing a drive icon next to the text for these items (Figure 9 on page 16).

## 1 Installing Metabolite ID Software



**Figure 9** Microsoft Office 2010 Custom Installation Options

If these boxes are not white, click on the down arrow at the right of the icon. In the context menu that appears select the **Run all from My Computer** menu item.

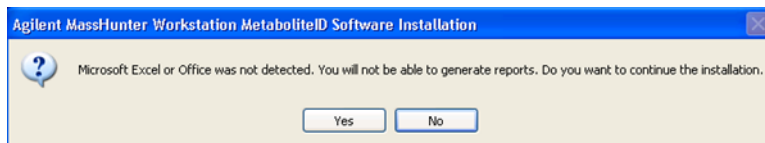


**Figure 10** Context menu

Do this for each of the three necessary components. You can add additional Microsoft Office components such as Word, PowerPoint or Publisher as you desire.

### Non-existent or incomplete installation of Office 2010

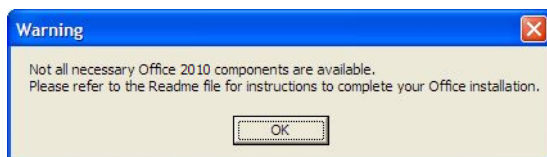
If no valid Excel installation has been detected, a warning message as shown in [Figure 11](#) is displayed during installation of MassHunter Metabolite ID. If you do not want to use reporting functionality on this PC, click **OK** to continue to the next step.



**Figure 11** MassHunter Metabolite ID warning that Microsoft Office was not detected

If you want to use reporting functionality on this PC, you need to cancel the Metabolite ID installation and install Office first. Once this is completed, you can restart the Metabolite ID installation.

If an Office 2010 installation has been detected but some of the necessary Office components are not available, a warning message is displayed as shown in [Figure 12](#). If you do not want to use reporting functionality on this PC, click **OK** to continue to the next step.



**Figure 12** MassHunter Metabolite ID warning that Microsoft Office 2010 is incomplete

If you want to use reporting functionality on this PC, you need to cancel the installation and modify your Office 2010 installation to include the components as shown [“Custom installation of Office 2010”](#) on page 15. Once this is completed, you can restart the Metabolite ID installation.

### Error on generating the first report

After Excel 2010 or Microsoft Office 2010 has been installed, the message shown in might appear when you generate your *first* report.

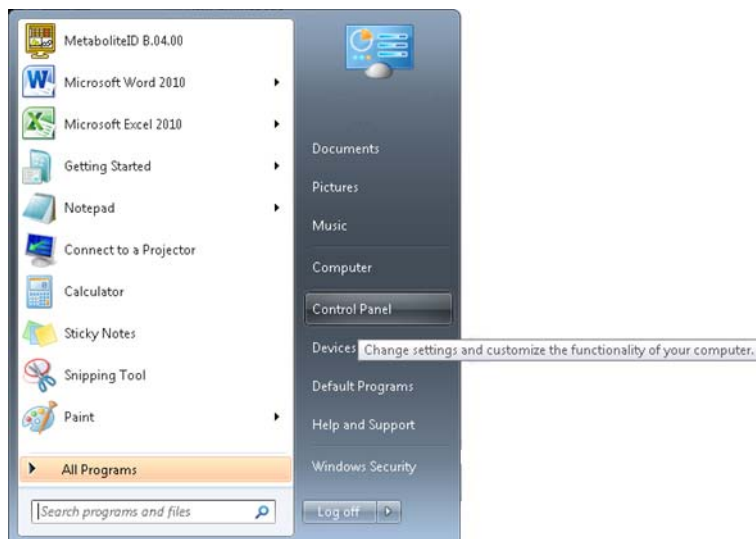


**Figure 13** MassHunter Addin message

Click **Yes** to start the installation of the Add-in.

## To remove the Metabolite ID program

- 1 Click the Windows **Start** button.
- 2 From the Start menu, select **Control Panel** (Figure 14).



**Figure 14** Starting the Control Panel

3 From the Control Panel, select **Programs and Features** (Figure 15).

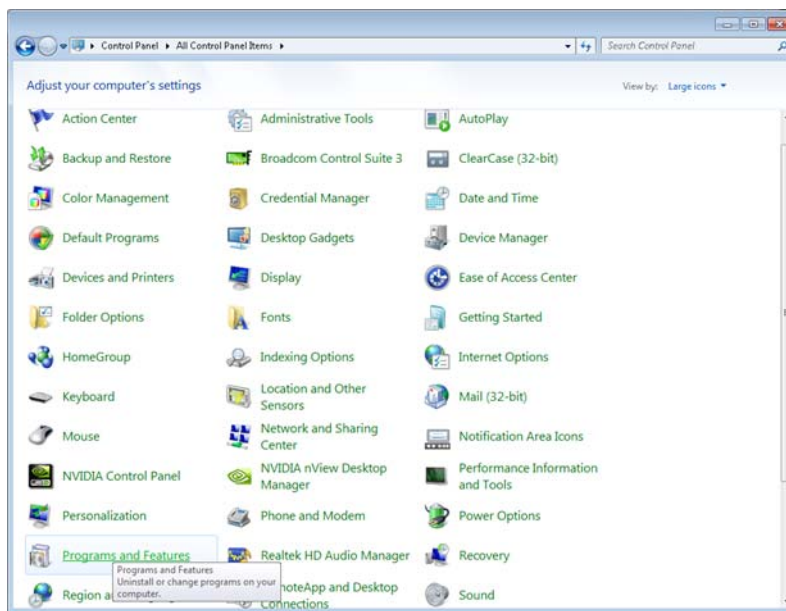


Figure 15 Selecting Programs and Features

4 From the list of currently installed programs, select **Agilent MassHunter Workstation Metabolite ID B.04.00** and click **Uninstall**. (Figure 16)

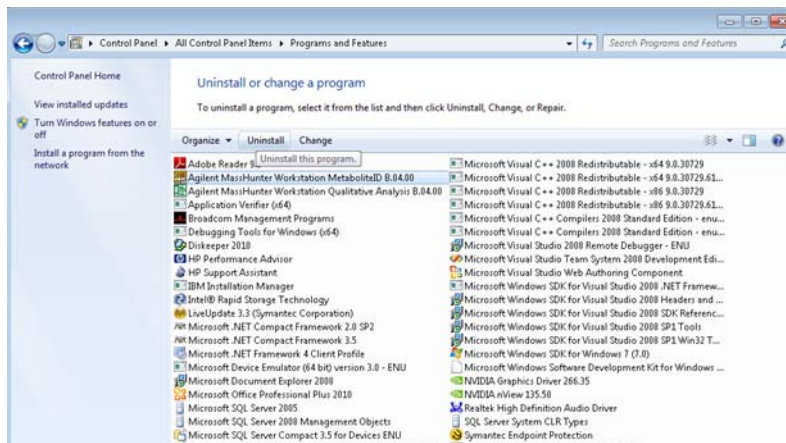
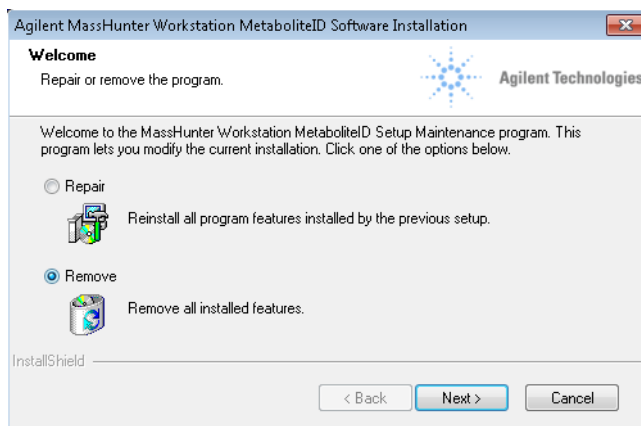
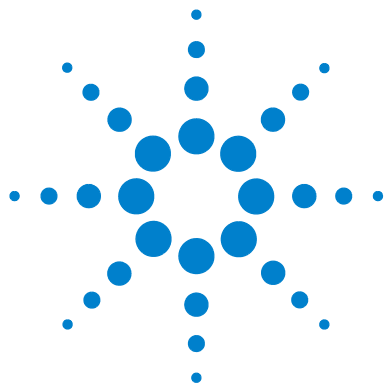


Figure 16 Uninstalling Metabolite ID B.04.00

5 Click **Remove** to remove the Metabolite ID application (Figure 17).



**Figure 17** Remove the Metabolite ID software



## 2 Getting Started with Metabolite ID

- To start the Metabolite ID program 22
- To set up a method and finding metabolites 24
- To review the results 26
- To tune the method parameters 28
- To work with Reference Compounds 32
- To configure the display 35
- To generate a report 37

This chapter guides you step-by-step through some of the important features and functions of the Metabolite ID software. The exercises in this chapter make use of demonstration data files to illustrate the operation of the application. The nefazodone demonstration data files will be used to detect the main metabolites only. When you have worked through the exercises, you will be ready to use Metabolite ID with your own data.

### Before you begin

- Make sure that the Metabolite ID application is installed as in [Chapter 1](#), “Installing Metabolite ID Software”.
- Make sure that Microsoft Excel is configured for Metabolite ID reporting as in [Chapter 1](#), “Installing Metabolite ID Software”.
- The nefazodone demonstration data files are available in the Data folder on the DVD-ROM. You can either use them directly from the DVD-ROM or copy them to a local folder on your hard disk.



## To start the Metabolite ID program

In this exercise, you start the Metabolite ID software and load a set of demonstration data files into the Worklist.

- 1 On the Windows desktop, click  to start the Metabolite ID application.

If you do not find the shortcut on the desktop, start the application from the Start menu:

**Start > Programs > Agilent > MassHunter Workstation > Metabolite ID**

- 2 In the **Application Startup** panel, click **New Session**.
- 3 In the **New Session** dialog box, specify a name for your session, for example, DemoSession1.

We recommend that you save the session in the default location, but if you wish, you can specify an alternative location for your session.

- 4 Click **Save** to save the session.

Because there are no data files associated with the session, the **Edit Worklist** dialog box is displayed to allow you to specify the data files for the session.

- 5 In the **Edit Worklist** dialog box, click **Add ...** to display the **Open** file selection dialog box.
- 6 Navigate to the directory where the demonstration files are located, and select **Nefazodone-2GHz-demo-control.d** and **Nefazodone-2GHz-demo-metabolite.d**.
- 7 Click **Open** to load the files into the worklist.

Note that the files are highlighted in the worklist with an orange background. This is because both files have the sample type **Metabolite**.

- 8 In the **Sample Type** field of the **Nefazodone-2GHz-demo-control.d** sample, click the down arrow and select **Control** from the list.

Note that the highlighting denoting the error condition is removed.

- 9 Click **OK** to load the data files.
- 10 Note the status display at the bottom right of the workspace.

The session is **Inconsistent** because no method has yet been applied, and is flagged as **Not saved**.

- 11** In the **Chromatograms & Spectra** window, you now see the total ion chromatograms (**TIC**) and base peak chromatograms (**BPC**) of the two data files that you loaded.

If you do not see the **TICs** and **BPCs**, click the first combo box in the **Chromatograms & Spectra** toolbar and select **Overview**.

- 12** Click the  icon in the main toolbar, and note that the session is now flagged as **Saved**.

If you do not see the main toolbar, because the application window does not fill the screen, click the bottom right corner of the application window and drag the mouse to expand the window.

## To set up a method and finding metabolites

In this exercise, you set up the essential method parameters.

- 1 Restore the default layout of the windows.

**View > Restore Default Layout**

- 2 In the **Method Editor**, at the top left of the workspace, ensure that the **Parent Compound** pane is displayed.

Note the  icon in the toolbar and against the fields **Name**, **Molecular Formula** and the mass field. These fields are required.

- 3 In the **Name** field of the **Parent Compound** pane, type Nefazodone.
- 4 Click the **Browse** button to display the **Open** file selection dialog box.
- 5 Navigate to the directory where the demonstration files are located and select **Nefazodone.mol**.

The structure is displayed in the **Preview** panel, and the molecular formula and mass are shown in the **Information** group.

- 6 Click **Open** to enter the molecular formula, mass, structure file and structure into the **Parent Compound** pane.

The  icons indicate that these values have been changed, but the method has not been saved (see the status line).

### NOTE

If no molecular structure file is available for the compound you are studying, you can enter the molecular formula in the **Molecular Formula** field; the mass is calculated automatically.

- 7 Click the combo box in the **Method Editor** toolbar and select **Biotransformations** from the list.

The default list of biotransformations can be edited: you can delete biotransformations that are not relevant, and add new biotransformations to the list.

- 8 Place the cursor on the split between the **Method Editor** and the **Metabolites Browser** and move the split to the right so that you can see the six buttons below the **Biotransformations Repository** table.
- 9 Click the **Select Phase 1** button to select all phase 1 biotransformations.
- 10 Ensure that the **Restrict to possible** check box is marked.

The **Restrict to possible** check box ensures that biotransformations that involve the loss of an element that is not in the parent compound are not selected.

- 11 Click the combo box in the **Method Editor** toolbar again and select **Identification Criteria** from the list.

The **Identification Criteria** pane allows you to specify the algorithms that are used to find metabolite candidates. It also allow you to assign a relevance to each of the algorithms.

- 12 Leave the contents of the **Identification Criteria** pane unchanged.

- 13 Click the combo box in the **Method Editor** toolbar again and select **Find Compounds by Molecular Features** from the list.

The Molecular Features Extractor is one of the most important algorithms for finding compounds.

- 14 Select the **Compound Filters** tab.

- 15 Ensure that the **Relative height** check box is marked and set the value to 1.5%.

- 16 In the main toolbar, click **Find Metabolites**.

Note the timeline as each of the algorithms is applied. The algorithms take different amounts of time to complete.

- 17 When all processes are complete, note the status line:

- the number of metabolite candidates is displayed; the first number is the number of metabolite candidates in the table, the second number is the total number of metabolite candidates found.
- the session is Consistent, because the method has been applied.
- the session has not been saved.

- 18 Click the  icon in the main toolbar, and note that the session is now flagged as **Saved**.

## To review the results

The **Metabolites Browser**, at the top right of the workspace, contains the complete details of all the metabolite candidates, both qualified (shown with a green background) and unqualified (shown with a red background). You can use this set of tables to review your results and refine your method.

- 1 Click the first combo box in the **Metabolites Browser** toolbar to display the list of all sections available in the **Metabolites Browser**.
- 2 Select **Short Summary** from the list.

The **Short Summary** displays only the qualification flags for each of the sections in the table, except the **Metabolites** section. By default, the **Metabolites** section is fixed; when you use the horizontal scroll bar, only the sections to the right of the **Metabolites** section are scrolled.

- 3 Click the second combo box in the **Metabolites Browser** toolbar, select **Overall** and click **OK**.

This filter allows you to display only those metabolite candidates that have been qualified by selected algorithms. The **Overall** filter displays only those metabolite candidates that have satisfied the total qualification conditions. Now, the number of metabolite candidates in the table is much less than the total number.

- 4 Note that, by default, the metabolite candidates are displayed in order of increasing retention time.
- 5 Click in the header of the **Name** column, and note that the order changes to alphabetical by name.
- 6 Click in the header of the **RT** (retention time) column to restore the original order.
- 7 From the Filter combo box, deselect **Overall** and select **EIC Compound Search**. Click **OK**.

The **EIC Compound Search** filter displays only those metabolite candidates that have been qualified by the EIC Compound Search algorithm.

- 8 Scroll down the table until the parent compound (Nefazodone) is displayed.

The parent compound is also highlighted with a white background. Note that two parent compounds are present in the table, one from the control sample and one from the metabolites sample.

Note that the table contains metabolite candidates that arise only from the metabolites sample, and parent candidates that may arise from the parent compound sample, the control sample or the metabolites sample. Parent compound candidates that do not arise from the metabolites sample are flagged by the warning icon, . They do not count to the number of metabolite candidates, and can be filtered out using the **Show Control Sample Compounds** command from the context menu.

- 9 Select the first metabolite candidate in the **Metabolites Browser**.
- 10 Use the  and  buttons in the **Metabolites Browser** toolbar to move through the table.

You can also use the navigation keypad on your keyboard to navigate through the table.

Note that, as you move through the table, the **Fragments** table is updated for each metabolite candidate.

## To tune the method parameters

The default method parameters returned about 37 metabolite candidates. This exercise shows you how you can refine the method to reduce the number of metabolite candidates to a more manageable number.

- 1 From the filtered **Metabolites Browser** table, note the retention time of Nefazodone.
- 2 In the **Method Editor** toolbar, select **Find Compounds by Molecular Features** from the combo box drop-down list.
- 3 Select the **Compound Filters** tab.
- 4 In the **Compound location** group, mark the **Restrict retention time to** check box and type 1-12 in the field.
- 5 Select the **Mass Filters** tab.
- 6 Mark the **Filter mass list** check box and type 125-650 in the **Source of masses** field.

Restricting the retention time and mass range in this way removes unlikely metabolite candidates from the table.

- 7 Select the **Ion Species** tab.
- 8 In the **Allowed ion species** group, deselect everything except **+H** in the **Positive Ions** panel and **-H** in the **Negative Ions** panel.
- 9 Click **Find Metabolites** and note that the number of metabolite candidates found has reduced to about 15.
- 10 In the **Metabolites Browser**, change the filter to **None (Show all metabolites)** and click **OK**.
- 11 In the **Method Editor** toolbar, select **Molecular Formula Assignment** from the combo box drop-down list.
- 12 In the **Setup element limits and max mass** group, ensure that the **Use** option is selected.
- 13 From the **Use** combo box, select **Phase I** biotransformations.

As you switch from the default **Phase I and II** to **Phase I**, note the changes to the limits in the **Elements and limits** group.

- 14 Switch to the **Mass Defect Filter** pane of the **Method Editor**.
- 15 In the **Setup tolerance** group, select the **Use** option, and select **Phase I** from the combo box drop-down list.

**16** Switch to the **Identification Criteria** pane of the **Method Editor**.

**17** Mark the **Molecular formula assignment** check box.

This switches on the calculation of formulas. Formula calculation is switched off by default to save computation time.

**18** Click **Find Metabolites** in the main toolbar.

**19** Note the  icons in the **Warning** column of the **Metabolites Browser**. When you place the cursor over the icon, the text box gives you more information.

**20** Click the **Processing Logbook** tab at the bottom of the **Metabolites Browser** window.

The processing logbook give you complete information about the operation of each of the algorithms in the metabolite search. Each time **Find Metabolites** is run, a new set of reports is produced.

**21** Return to the **Metabolites Browser**.

**22** Navigate through the list of metabolite candidates, and note that, for all those metabolite candidates for which molecular formulas have been generated, the **Formulas** window is updated with the molecular formulas generated for the compound.

**23** Apply the **Overall** filter to the **Metabolites Browser**, and select the **Hydroxylation** at 8.439 minutes.

**24** In the **Chromatograms & Spectra** window, position the cursor on one of the plots, for example, TIC, and click the right mouse button to display the plot context menu.

**25** Select the **Color** menu item and select a different color for the plot. Click OK to close the color selection dialog box.

**26** Display the plot context menu for the same plot again and select the **Dash Style** menu item.

**27** Select **Dash** from the menu and note how the line style changes.

**28** Select **Reset Plot Style** from the context menu to reset the plot to its default color and style.

**29** Select **Result** from the first combo box drop-down list of the **Chromatograms & Spectra** window.

The Result view shows the extracted compound chromatograms (ECC) and extracted ion chromatograms (EIC) for the selected metabolite candidate. To the right of the chromatograms is the spectrum of the metabolite candidate.

- 30** Using the right mouse button, draw a box around the main peaks in the spectrum at  $m/z$  486.2270.

This action allows you to zoom in on a part of the spectrum.

- 31** Press and hold down the **CTRL** key on your keyboard, then double-click the **CIP** legend at the top of the spectrum window to zoom in to the calculated isotope pattern peaks.

You can now see the comparison between the calculated isotope pattern for the molecular formula  $C_{25}H_{32}ClN_5O_3$  and the acquired isotope pattern.

- 32** In the **Formula** window, ensure that **Formula** is selected in the combo box,

and that the  button is activated to display all three levels of the **Formula** table.

The third-level table in the **Formula** window contains details of the isotope pattern calculation for the currently selected formula. Note that there may be more than one possible formula for any selected group of ions.

- 33** In the **Chromatograms & Spectra** window, select **Fragments** from the first combo box drop-down list.

The MS/MS spectra for the parent compound and the metabolite candidate are shown in the window. By clicking on one of the legends, you can highlight the relevant spectrum.

- 34** In the **Fragments** window, scroll down to the peak at  $m/z$  274.1548 and select it.

Note that the related peaks in the **Fragments** window are highlighted; the mass shift between parent and metabolite candidate is also shown.

- 35** From the **View** menu, select **Fragment Loss**.

The **Fragment Loss** window shows a matrix of the mass differences between all the peaks in a mass spectrum. As you navigate through the metabolite candidates, the **Fragment Loss** window is updated.

- 36** In the **Fragment Loss** toolbar, click **Settings**.

- 37** In the **Fragment Search** group, enter a **Mass Precision** of 10 mDa

- 38** In the **Formula** column of the table, type O and click in the **Color** column. Note that the mass of oxygen is entered in the **Mass** column.

If you prefer, you can enter a mass difference into the **Mass** column. If you enter a mass, however, the formula is not calculated automatically.

**39** In the **Color** column, select a color (for example, a pale blue) from the drop-down list and click OK

**40** Now, when you navigate through the list of metabolite candidates, all differences of O in the spectra are highlighted.

**41** From the **View** menu, select **Fragment Overview**.

The **Fragment Overview** is a configurable three-dimensional display of all fragments in all metabolite candidates. Each of the circles represents a fragment peak. The size and color of the circle indicates the abundance of the peak. For more details of the **Fragment Overview**, refer to the online help.

**42** Select **Restore Default** Layout from the **View** menu, and save the session.

## To work with Reference Compounds

In this exercise, you learn how to use the software to search a database of reference compounds and review the search results. The demonstration files include a database for use with this exercise.

- 1 In the **Method Editor**, select **Identification Criteria** and mark the **Reference Compound Search** check box.

This switches on the search of one or more databases for reference compounds that match each metabolite candidate.

- 2 Select the **Reference Compound Search** section of the **Method Editor** and select the **Compound Sources** tab.
- 3 Clear the check boxes against all existing data sources.
- 4 Click **Add** to display the **Open Compound Source** dialog box.
- 5 From the **Files of type** combo box at the bottom of the dialog box, select **SDF Files (\*.sdf)**.

### NOTE

Metabolite ID B.04.00 supports the following file formats:

\*.mol, \*.sdf, \*.csv and \*.cdb. The \*.cdb format replaces the \*.mtl format, which is no longer supported. \*.mtl databases can be converted to \*.cdb using the **MTLtoCDBConvert.exe** tool, which must be launched from the following locations:

Windows 7: **C:\Program Files (x86)\Agilent\MassHunter\Workstation\PCDL\Bin**

Windows XP: **C:\Program Files\Agilent\MassHunter\Workstation\PCDL\Bin**

- 
- 6 Navigate to the directory where the demonstration files are located, select **nef\_prediction.sdf** and click **Open**.
  - 7 Click **Find Metabolites** in the main toolbar.

Note that the **Structure Workspace** at the bottom right of the workspace now contains a structure.

- 8 In the **Metabolites Browser**, select the **Hydroxylation** metabolite candidate at 8.439 minutes.
- 9 From the **View** menu, select **Reference Compound Browser**.

The **Reference Compound Browser** lists all the reference compounds in the database that match the selected metabolite candidate (in this case, the hydroxylated compound).

The compound shown in the **Structure Workspace** is highlighted in the table; this is the currently selected reference compound for the hydroxylated metabolite.

The **Included** column of the **Reference Compound Browser** shows which reference compounds are included in the report (currently only the selected reference compound). You can include other compounds in the report by marking the appropriate **Included** check boxes

- 10 Click the  tool in the **Reference Compound Browser** toolbar to autosize all the columns.
- 11 Double-click in the three rows below the selected reference compound in the table.
- 12 Close the **Reference Compound Browser**; note that the **Structure Workspace** now contains the three additional reference compounds that you double-clicked in the **Reference Compound Browser**.

You can also add compounds to the **Structure workspace** using the **Reference Compound Browser's** toolbar or context menu.

The selected reference compound is highlighted in the **Structure Workspace**.

You can use the **Structure Workspace** to compare the different reference compounds and select the most appropriate one based on the MS and MS/MS spectral data.

- 13 Click the  tool in the main toolbar of the **Structure workspace** to display the annotation panes of the reference compounds.

The lower (gray) pane shows the information about the reference compound from the database. You cannot edit this information.

The upper pane allows you to include additional information; text that you add here is saved with the metabolite ID results (but is not added to the database).

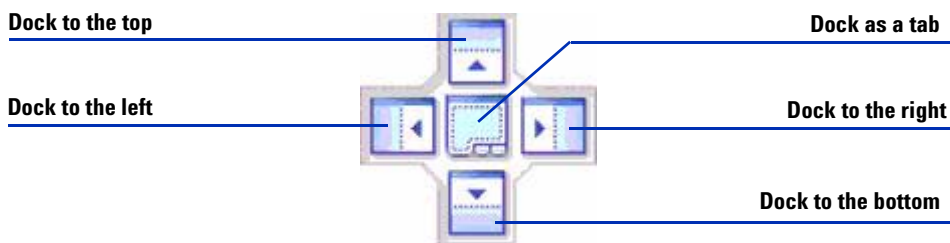
**14** Use the tools in the individual reference compound windows to:

- change the selection of reference compound
- reject the compound so that it is not reported
- close the reference compound window

For further information on using the Metabolite ID software to find the metabolites of nefazodone, see the *Getting Started Supplement*.

## To configure the display

In this exercise, you learn how to use the docking tool (Figure 18) to dock and undock windows, and how to save a display configuration.



**Figure 18** Docking tool for Metabolite ID windows

- 1 Position the left mouse button in the title bar of the **Chromatograms & Spectra** window, and click and drag the window up towards the centre of the workspace.

Note how the window expands as you move it.

- 2 Position the left mouse button in the title bar of the **Chromatograms & Spectra** window again, and click and drag the window down and to the right until the cursor is in the left arrow of the docking tool.
- 3 Release the mouse button and note how the window docks to the left of the **Structure** window.

### NOTE

You can also toggle the status of a window between docked and floating by double-clicking in the title bar. If you want to move a floating window freely around the workspace without docking it, press and hold the **Ctrl** key while you are moving the window.

- 4 Position the left mouse button in the title bar of the **Fragments** window, and click and drag the window upwards a short distance until the cursor is in the centre tile of the docking tool.
- 5 Release the mouse button and note how the **Fragments** window becomes a tab of the **Formulas** window.

You can now manipulate these tabbed windows as a single unit.

- 6 Select **Fragment Loss** from the **View** menu, and dock the **Fragment Loss** window as a third tab in the **Formulas** window.
- 7 Select **MFE Compounds** from the **View** menu to display the **MFE Compounds** window.
- 8 Dock the **MFE Compounds** window as a third tab of the **Metabolites Browser**.  
Note that the **MFE Compounds** tab is inserted as the first tab in the window.
- 9 Select the **MFE Compounds** tab and drag it to the right to lock it as the last tab.
- 10 If you wish, do the same for the **Processing Logbook** tab so that the tab order becomes **Metabolites Browser - MFE Compounds - Processing Logbook**.
- 11 From the **View** menu, select **Save Layout**.
- 12 In the **Save Layout** dialog box, enter a name for the layout, for example, `MyView1`, and click **Save**.
- 13 Restore the default layout (**View > Restore Default Layout**).
- 14 Select **Load Layout** from the **View** menu, and load the layout you just saved.

You can set up and save as many layouts as you wish.

## To generate a report

In this exercise, you generate a report from one of the default templates, and view it on the screen.

- 1 From the **Report** menu, select **Generate Report** to display the **Report Selection** dialog box.
- 2 In the **Method Report** group, ensure that the **Generate** check box is cleared to ensure that a method report is not generated.
- 3 Click the **New** button.
- 4 From the **Open** dialog box, select either **A4** or **Letter**, depending on your paper size, and click **Open**.
- 5 From the list of report templates, select **Detailed.midresult.xlt** and click **Open**.
- 6 In the **Printer** column, display the drop-down list and select **<None>**.
- 7 Click **OK** to generate the report.

The report is generated as an Excel file, and is saved by default in a report subfolder in the session folder.





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## **In This Book**

This guide describes how to install and uninstall the Metabolite ID application, and contains step-by-step instructions on how to work with the software.

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