MetabolitePilot™ 2.0 Alpha Software

Release Notes

RUO-IDV-03-1459-A

June 2014

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Introduction 1

The MetabolitePilot™ 2.0 software (Alpha version) is a tool for finding small-molecule metabolites using a variety of search algorithms. Other features include semi-automated structural elucidation, as well as correlation of previously generated results files.

Features

This version of the software provides the following functionality:

- High-throughput batch processing of exported Analyst® TF software text files and sample lists created using the WebMetabase software.
- Manual integration of analog data.
- Processing of SWATH™ acquisition data to obtain results.
- Post-processing assignment of ion types to metabolites, excluding protons.

Where to Get Help

- For general information and procedures related to the high-throughput batch feature, click the **Help** icon in the bottom left corner of the **High-Throughput Batch** workspace.
- For general information and procedures related to naming the .wiff files so that the exported file from the Analyst® TF software batch can be parsed appropriately, click the **Help** tab on the "Analyst" **Naming Conventions** dialog.
- For general information and procedures related to naming the .wiff files so that the sample lists created from the WebMetabase software protocol can be parsed appropriately, click the **Help** tab on the "WebMetabase" **Naming Conventions** dialog.
- For procedures and troubleshooting information for all other features, open the software and then click **Help > MetabolitePilot Help.**
- For general information and procedures related to a specific workspace, click **How Do I?** and then select the appropriate topic.
- For support, contact AB Sciex:
  - support@absciex.com
  - www.absciex.com

Requirements 2

- An English (US) version of the Microsoft Windows 7 (32-bit) operating system with SP1 is required.
- Microsoft Windows Installer version 3.1 or later must be installed.
- Microsoft .NET Framework version 4.0 or later must be installed.
- A licensed version of the WebMetabase software must be installed.
- Microsoft Word 2007 or later must be installed to create reports.
- Reporter 3.2 software must be installed.
- The user must be logged on to the computer as a Windows user with Administrator privileges to install the software.
  A license file is required to activate the MetabolitePilot™ software (Alpha version). Refer to *Activate the Software on page 6*.
- Dell OptiPlex 9010, or a later model provided by AB Sciex, is the recommended computer model.

File Compatibility

This version of the software supports:

- Data files created using the Analyst® TF software, version 1.5 or later.
- Results files created using the MetabolitePilot™ software, version 1.5.
- Correlation files created using the MetabolitePilot software, version 1.5.

Installation and Activation 3

Note: The user must be logged on to the computer as a Windows user with Administrator privileges to install the software.

Install the Software

Note: This procedure applies to the standard Windows extraction tool. Other extraction tools can be used but the steps might be different than those documented below.

1. Log on to the computer as a Windows user with Administrator privileges.
2. Download the **MetabolitePilot_2.0_Alpha.zip** file from the AB Sciex Web site.

   To prevent potential installation issues, it is recommended that you save the file to a location other than the computer desktop.
3. After the download completes, right-click the **MetabolitePilot_2.0_Alpha.zip** file.
4. Click **Extract All**.

   By default, the files are extracted to the **MetabolitePilot_2.0_Alpha** folder in the same location as **MetabolitePilot_2.0_Alpha.zip** was saved. A different location can be selected.
5. Browse to the extraction folder and then double-click the **MetabolitePilot.msi** file.
6. Follow the on-screen instructions.

Activate the Software

Note: Before activating the software, change the **User Account Control (UAC) Settings** to prevent issues with installing the license file. Refer to *Change the User Account Control (UAC) Settings on page 7*.

Tip! Internet access is required to obtain a license for the software. If the computer where the MetabolitePilot™ software is being installed does not have Internet access, then make a copy of the generated computer ID. On a computer with Internet access, go to http://licensing.absciex.com/activation/MetabolitePilot and then follow the instructions to obtain a license.

1. Double-click the MetabolitePilot 2.0 Alpha software desktop icon to open the MetabolitePilot software.

   The **MetabolitePilot™ Software Activation** dialog opens.
2. Type the license key from the license certificate in the appropriate field.
3. Click **Generate Computer ID**.

   This creates a unique identifier for the workstation.
4. Click **Copy ID to Clipboard**.
5. Click the http://licensing.absciex.com/activation/MetabolitePilot link.
6. Follow the instructions to obtain a license.
7. After the required information is submitted, a license file is sent to all of the e-mail addresses provided.
8. Close the browser window.
9. When the e-mail containing the license file is received, copy the license to the workstation desktop.
10. On the **MetabolitePilot™ Software Activation** dialog, click **Install License File**.
11. On the **Select the new license file to be installed** dialog, browse to and then select the license file.
12. Click **Open**.

    Both the **Select the new license file to be installed** and the **MetabolitePilot Software Activation** dialogs close. The MetabolitePilot 2.0 Alpha software opens.

Change the User Account Control (UAC) Settings

1. Click **Start > Control Panel.**
2. Click **User Accounts > Change User Account Control settings.**
3. On the **User Account Control Settings** dialog, move the slider bar to **Never notify me when** and then click **OK**.
4. Continue with *Activate the Software on page 6*.

Notes on Use 4

This software has not undergone extensive formal testing at this time. While the main functions of the software have been verified for correctness, the user might still encounter minor issues when using the software. AB Sciex assumes no liability or responsibility for any loss howsoever caused in connection with using this software.

In the released research version of the MetabolitePilot™ software, version 1.5, the **Analog - % Area** values are calculated based only on those analog peaks that are associated with MS peaks. Therefore, the sum of the **Analog - % Area** values of analog peaks associated with MS peaks is 100%.

In this alpha version of the MetabolitePilot software, version 2.0, the **Analog- % Area** values are calculated based on all analog peaks, regardless of whether or not they are associated with MS peaks. Therefore, the sum of the **Analog - % Area** values of analog peaks associated with MS peaks might be less than 100% because the % area values from analog peaks not associated with MS peaks are also included in the sum.

Known Issues and Limitations

Everyone should read this section of the Release Notes. This section applies specifically to issues that are known in the MetabolitePilot™ 2.0 Alpha software.

Note: The numbers in brackets are reference numbers for each issue or feature in our internal tracking system.

- Because an analog peak can be associated with one or more potential metabolites, it might be shown more than once in the Results Table. Multiple instances of a unique analog peak makes the % area values incorrect for all analog peaks in the MetabolitePilot software results. This issue will be resolved in the next release of the software. (MP-193)

Remove the Software 5

1. Log on to the computer as a Windows user with Administrator privileges.
2. Make sure that the MetabolitePilot™ 2.0 Alpha software is closed.
3. Click **Start > Control Panel > Programs and Features.**
4. Click **MetabolitePilot 2.0 Alpha**.
5. Click **Uninstall**.

   The license remains on the computer and is automatically used if the software is installed again.

Revision History

This log shows the revisions that took place during the preparation of this manual.

Revision	Reason for Change	Date
A	First release.	June 2014