



MetabolitePilot™ 2.0 Software

Release Notes



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The MetabolitePilot™ 2.0 software is a processing only software, used for the identification and characterization of metabolites. The software processes accurate-mass data, acquired from the SCIEX TripleTOF® series of instruments, using the Analyst® TF software, version 1.5 or later.

Related Documentation

The online Help for the MetabolitePilot™ software is installed automatically with the software and is available from the Start menu: **All Programs > SCIEX > MetabolitePilot**.

To access the online Help from within the MetabolitePilot™ software, users can press **F1** or click **Help** in the Menu bar.

Workflow-specific procedures are available through the **How Do I?** button in the upper-right corner of the workspace. When **How Do I?** is clicked, users can select the appropriate Help topic from the list provided.

Changes from Version 1.5 to Version 2.0

Note: Refer to [Issue Fixed in Version 2.0 of the MetabolitePilot Software on page 15](#) for a list of all of the previous issues that have been resolved with this release of the MetabolitePilot™ software.

Support for Data Generated by Previous Versions of the MetabolitePilot™ Software

- This release of the MetabolitePilot™ software does not support data generated by previous versions of the software (1.0 or 1.5). Only data generated by version 2.0 is supported.

Support for Peptide and Antibody Drug Conjugates (ADC) Data

- This release of the MetabolitePilot™ software enables users to characterize the MS/MS data for peptide and ADC compounds.

Support for Processing of SWATH® Acquisition Data

- This release of the MetabolitePilot™ software supports the processing of data acquired using SWATH® acquisition.

Enhanced Analog Data Processing

- With this release of the MetabolitePilot™ software, users can manually integrate analog data, use baseline subtraction, and modify retention time offsets to enhance the comparison between analog peaks and MS data.

Enhanced Batch Processing

- In this release of the MetabolitePilot™ software, the number of rows allowed in batches has increased to 200. Users also have the ability to review completed results files and the corresponding processing parameters while the batch is still processing.

Structure and Sequence Assignment

- This release of the MetabolitePilot™ software automatically proposes structures for small molecule metabolites and sequences for peptide catabolites.

Enhanced Processing Parameters

- Improvements have been made to the Processing Parameters workspace in this release of the MetabolitePilot™ software.

Support for Microsoft Windows 7, 64-bit Operating System

- This release of the MetabolitePilot™ software supports the 64-bit version of the Windows 7 operating system.

Note: The 32-bit version of the Microsoft Windows 7 operating system might be compatible. However, the software has not been extensively tested on a computer configured with this version.

Contact Us

SCIEX Support

- sciex.com/contact-us
- sciex.com/request-support

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- SCIEXUniversity

Technical Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the website at sciex.com.

Workstation Requirements

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The workstation must be configured with the following applications:

- English version of the 64-bit Microsoft Windows 7 operating system, with SP1

Note: The 32-bit version of the Microsoft Windows 7 operating system might be compatible. However, the software has not been extensively tested on a computer configured with this version.

- The AB SCIEX Reporter Template Suite 3.2. This application is not installed as part of the MetabolitePilot™ 2.0 software installation. To edit report templates, users must install this application separately, using the installation package included on the MetabolitePilot™ software installation DVD and in the **MetabolitePilot2.0.zip** installation file. Refer to [Install the AB SCIEX Reporter Template Suite 3.2 on page 17](#).
- Microsoft Office 2010 or 2013

Note: If a trial version of Microsoft Office is installed on the computer, then the full version of the Microsoft Office software must be activated before the trial period expires. The license can be purchased from your regional division of Microsoft or from an authorized distributor in your region.

Computer Requirements

Dell OptiPlex XE2 computer, with:

- An Intel Core I5-4570S processor (Quad core, 2.90 GHz, 6 MB with HD Graphics 4600)
- 32 GB DDR3 1600 Mhz SDRAM
- 2*2 TB HDD (RAID1)
- DVD+-RW

Note: Newer systems might become available. For more information, contact the local sales representative. Older computer models might be compatible. However, they have not been tested and might result in degraded performance.

Notes on Installation

- The MetabolitePilot™ 2.0 software is a new installation only. Upgrades to existing versions of the software are not supported.
- The user must be logged on to the computer as a user with Administrator privileges.
- The User Account Control settings must be set to **Never notify**. Refer to [Change the User Account Control \(UAC\) Settings on page 16](#).
- If using a zip file that contains the MetabolitePilot™ software installer, then extract all of the files from the zip file before running the installer from the location containing the extracted files. Errors will occur if the installer is run from within the zip file.
- If a DVD is used for the installation, then we recommend that customers copy all of the DVD contents to a local drive for storage. To prevent potential issues with installing the software, for example, if a repair is necessary, this locally-stored version must be used.
- The installer installs any required software that is not already installed on the system:
 - .NET Framework 3.5 with SP1
 - .NET Framework 4.5.1
 - Visual C++ 2010 Redistributable Package (x64)
 - Visual C++ 2010 Redistributable Package (x86)
 - Visual C++ 2013 Redistributable Package (x64)
 - Windows Installer 3.1
 - Microsoft Save as PDF Add-in

Install the MetabolitePilot™ Software

1. Read these release notes.
2. Log on to the computer as a Microsoft Windows user with administrator privileges.
3. Make sure that all of the applications are closed.

Installation

4. Install the MetabolitePilot™ software as described in [Table 3-1](#).

Table 3-1 Installation Instructions

To install from a file downloaded from the SCIEX website ...	To install from the MetabolitePilot™ software installation DVD ...
<p>Download the zip file from sciex.com/products/software/metabolitepilot-software.</p> <hr/> <p>Tip! To prevent potential installation issues, we recommend that the file is saved to a location other than the computer desktop.</p> <hr/>	<p>Load the MetabolitePilot™ software installation DVD in the DVD drive.</p>
<p>After the download is complete, right-click the MetabolitePilot2.0.zip.</p>	<p>If the installation does not start automatically, navigate to the DVD, open the Setup folder, and then double-click MetabolitePilotInstaller.exe.</p> <p>The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click Run.</p>
<p>Click Extract All.</p> <hr/> <p>Note: By default, the files are extracted to the MetabolitePilot2.0\Setup folder in the same location where the MetabolitePilot2.0.zip was saved.</p> <hr/>	<p>If any of the required software is not already installed, then the installer identifies the applications that will be installed.</p> <p>Click Install.</p> <hr/> <p>Note: Any end-user license agreements that are shown must be accepted to continue with the installation.</p> <hr/> <p>After the required software is installed, the MetabolitePilot 2.0 Setup dialog opens.</p> <p>The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click Run.</p>

Table 3-1 Installation Instructions (continued)

To install from a file downloaded from the SCIEX website ...	To install from the MetabolitePilot™ software installation DVD ...
<p>After the extraction is complete, browse to the extraction folder and then double-click MetabolitePilotInstaller.exe.</p> <p>The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click Run.</p>	—
<p>If any of the required software is not already installed, then the installer identifies the applications that will be installed.</p> <p>Click Install.</p> <hr/> <p>Note: Any end-user license agreements that are shown must be accepted to continue with the installation.</p> <hr/> <p>After the required software is installed, the MetabolitePilot 2.0 Setup dialog opens.</p> <p>The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click Run.</p>	—

5. Click **Next**.
The End-User License Agreement dialog opens.
6. Click **I Agree**.
The Destination Folder dialog opens.

Tip! The user can change the location of the software installation and the data folders before clicking **Next**.

7. Click **Next**.
The Ready to Install the Program dialog opens.
8. Click **Install**.
The Installing MetabolitePilot 2.0 dialog opens.
9. After the installation is complete, click **Finish**.

Installation

10. If a DVD was used to complete the installation, then back up the contents of the installation DVD to a local drive.

Note: The locally-stored installation files should be used if the software needs to be repaired.

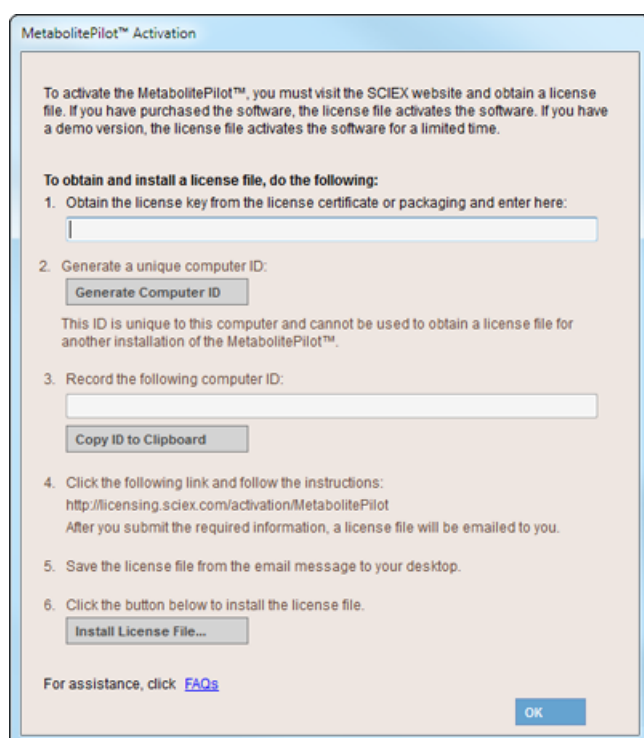
11. Continue with [Activation on page 10](#).

Activation

Note: 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.sciex.com/activation/MetabolitePilot> and then follow the instructions to obtain a license.

1. Double-click the MetabolitePilot™ software desktop icon.
The MetabolitePilot™ Activation dialog opens.

Figure 3-1 MetabolitePilot™ Activation Dialog



2. Type the license key from the license certificate (found in the MetabolitePilot™ software installation package) in the appropriate field.

Note: If the licence key is stored on the computer, then copy and paste the key in the field. If a license key is not available, then contact sciex.com/request-support.

3. Click **Generate Computer ID**.

This creates a unique identifier for the workstation.

4. Click **Copy ID to Clipboard**.

5. Click the <http://licensing.sciex.com/activation/MetabolitePilot> link.

6. Follow the instructions to obtain the license.

After the required information is submitted, a license file is sent to all of the e-mail addresses provided.

7. Close the browser window.

8. When the e-mail containing the license file is received, copy the license file to the workstation desktop.

9. In the MetabolitePilot™ Activation dialog, click **Install License File**.

10. In the Select the new license file to be installed dialog, browse to and then select the license file.

11. Click **Open**.

Both the Select the new license file to be installed and the MetabolitePilot™ Activation dialogs close, and the MetabolitePilot™ software opens.

Note: If a temporary license is being used, do not make any changes to the computer clock. Changes can void the temporary licence and a new license file will be required.

Known Issues and Limitations

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

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

Microsoft Windows 7 Operating System

- The Microsoft Windows 7 operating system might hide the C:\ProgramData folder. After installing the MetabolitePilot™ 2.0 software, make sure that all users can view the C:\ProgramData\SCIEX\MetabolitePilotData 2.0 folder. If the folder is not visible, then:
 1. In Windows Explorer, click **Organize > Folder and search options**. The Folder Options dialog opens.
 2. Select the **View** tab.
 3. Click **Hidden files and folder > Show hidden files, folders, or drives**.
 4. Click **Apply**.
 5. Click **OK**.

SWATH® Acquisition MS/MS Reference Spectra

- When extracting reference spectra from SWATH® acquisition data, an extensive list of MS/MS spectral data is proposed. Users should be aware that some of the precursors associated with the proposed MS/MS spectral data could have a low TOF MS peak intensity or low chromatographic peak intensity. (MP-1854)

Metabolite Name and Score

- For each metabolite, a list of possible MS identities is shown in the Name field of the Edit Name and Formula dialog. For ADC results, the MS identities resulting from one or more antibody fragments with identical masses are not included in the list of other proposed names and, therefore, are not conveniently accessible to the user in the Interpretation view. (MP-1745)
- The isotope pattern score and the MS isotope pattern highlight (orange) provide non-complementary information. (MP-1792)
 - The isotope pattern score shows the similarity between the experimental MS peaks and the isotope pattern of the formula and adduct assigned to the metabolite. In the absence of an assigned formula, the isotope pattern score shows the similarity between the experimental MS peaks and the isotope pattern of the reference compound formula using the adduct assigned to the metabolite.
 - The isotope pattern highlight on the MS panel shows the similarity of the isotope pattern to the reference compound using the primary ion type selected in the processing parameters.

- The isotope pattern score shown on the Details pane for a metabolite can vary for the same metabolite (with identical XIC and MS peaks), depending on the peak finding strategy used to process the data. (MP-1832)
 - For metabolites found by the Predicted Metabolite peak finding strategy, the isotope pattern score shows the similarity between the experimental MS peaks and the isotope pattern of the formula and adduct assigned to the metabolite.
 - For metabolites found by a peak finding strategy other than the Predicted Metabolite peak finding strategy, the isotope patterns score shows the similarity between the experimental MS peaks and the isotope pattern of the reference compound formula, using the adduct assigned to the metabolite.
- For the same wiff file, there might be a variation in the MS/MS Similarity score in the Details pane of the Results workspace, depending on the Source of Reference MS/MS Spectrum selected (Sample or Selected reference spectrum) in the MS/MS Parameters of the Generic processing parameters. (MP-1839)

Structure and Sequence Assignment

- For small molecule results, the structures and ranking proposed by the software through the Generate option have not been validated for metabolites assigned with multiple biotransformations. (MP-1938)
- For large, complex peptide data, the time required by the software to propose potential sequence candidates through the Generate option and the time required to review the MS/MS ion annotation for the proposed candidate is extensive. (MP-1692, MP-1712)

Interpretation

- Because of the restrictive representation of the sequence for cyclopeptide, the interpretation of the MS/MS spectrum only assigns a subset of the fragmentation ions. (MP-923)
- For peptide and Antibody Drug Conjugates (ADC) results, some of the MS/MS peaks that are successfully assigned, as shown in the Fragments tables, are incorrectly identified as x or are missing the ✓ in the peak label on the MS/MS spectrum. The ✓ on the MS/MS spectrum indicates that the peak has been assigned a formula. (MP-1559, MP-1771)
- The ion names for the MS/MS peaks assigned as ion fragments arising from three or more broken bonds on a multi-chain sequence are incomplete and show only a portion of the actual a- or b- type cleavages involved in generating the fragments. (MP-1777)
- For ADC results, the Load Sequence option populates the protein fragment sequence associated with the name assigned during data processing even if the name of the metabolite has been modified using the Edit Name and Formula option. As a workaround, the sequence of interest can be typed in the Metabolite Sequence pane. (MP-1957)

Remove the MetabolitePilot™ Software

5

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Click **Start > Control Panel > Programs and Features**.

Tip! If the control panel components are shown by **Category**, then click **Start > Control Panel > Programs > Programs and Features > Uninstall a program**.

3. Select the MetabolitePilot™ software and then click **Uninstall**.

The software is removed, with no user intervention required.

During the removal, the software name is removed from the Installed Programs list, the shortcut to the MetabolitePilot™ software is removed from the desktop, and the shortcuts to the software and the user documentation are removed from the Start menu.

The following components remain on the computer:

- The C:\ProgramData\SCIEX\MetabolitePilotData 2.0 folder, which contains MetabolitePilot™ software project data.
- The C:\ProgramData\SCIEX\ElementalCalculator folder, which contains any custom residues and modifications.
- If the product is licensed, then the C:\Program Files\SCIEX\MetabolitePilot 2.0 folder, which contains the license file, remains on the computer.
- AB SCIEX Reporter Template Suite 3.2, if manually installed by the customer
- Microsoft .NET Framework, versions 3.5 and 4.5.1.
- Visual C++ 2010 Redistributable Package (x64)
- Visual C++ 2013 Redistributable Package (x86)
- Visual C++ 2013 Redistributable Package (x64)
- Windows Installer 3.1 or later
- Microsoft Save as PDF Add-in

Issue Fixed in Version 2.0 of the MetabolitePilot™ Software

A

Note: The following issue has been fixed with the release of version 2.0 of the MetabolitePilot™ software.

Analog Data

- **Issue:** When the Time offset from MS in the Chromatographic Data of the Generic processing parameters was set to a large negative value, any channel other than channel 1 might have an incorrect starting time.

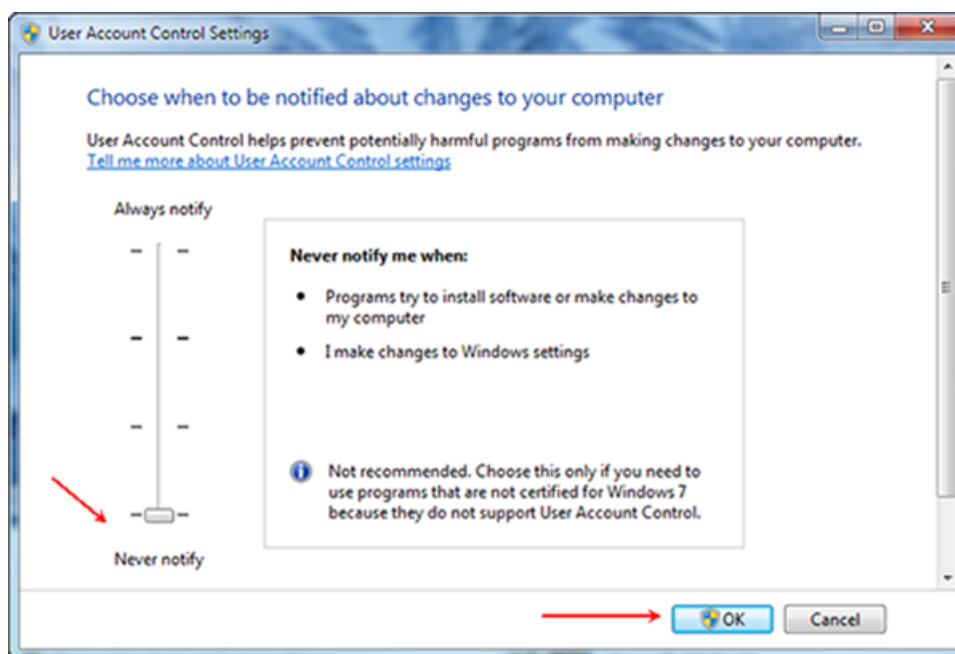
Resolution: Version 2.0 of the MetabolitePilot™ software only allows a Time offset from MS value between 2.00 min and –2.00 min.

Change the User Account Control (UAC) Settings

B

1. Click **Start > Control Panel**.
2. Click **User Accounts > Change User Account Control settings**.
The User Account Control Settings dialog opens.
3. Move the slide bar to the **Never notify** setting and then click **OK**.

Figure B-1 User Account Control Settings Dialog



Install the AB SCIEX Reporter Template Suite 3.2

C

1. Log on to the computer as a Microsoft Windows user with administrator privileges.
2. Do one of the following:
 - If a MetabolitePilot™ software installation DVD is available, then load the DVD in the DVD drive.
 - If the MetabolitePilot2.0.zip file was downloaded from the SCIEX website, then navigate to the extraction folder.
3. Navigate to the **ReporterEditing** folder and then open the appropriate CDImage folder, depending on the configuration of the computer.
 - If the computer is configured with the 64-bit version of the Microsoft Windows 7 operating system, then open the **CDImage_x64** folder.
 - If the computer is configured with the 32-bit version of the Microsoft Windows 7 operating system, then open the **CDImage_x86** folder.
4. Double-click **setup.exe**.

The License Agreement dialog opens.
5. Select the **I accept the terms in the License Agreement** check box and then click **Install**.

The Installing AB SCIEX Reporter Template Suite 3.2 dialog opens.
6. After the installation is complete, click **Finish**.

Revision History

Revision	Description	Date
A	First release of document.	March 2017