MetabolitePilot™ 2.0.4 Software

Release Notes

MP

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Contents

Introduction 1

The MetabolitePilot™ 2.0.4 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 higher.

- The SCIEX X500 QTOF series of instruments, using SCIEX OS.

Changes from Version 2.0.3 to Version 2.0.4

Support for the Microsoft Windows 10, 64-bit operating system.

Operating System Support

This version of the MetabolitePilot™ software is compatible with the Microsoft Windows 7 and the Microsoft Windows 10, 64-bit operating systems. Cybersecurity support is included for the Windows 10, 64-bit operating systems.

Note: Cybersecurity support is not included for the Microsoft Windows 7 operating system.

Note: While it is a widely acknowledged good practice to use antivirus software, these applications might affect system performance. Set the anti-virus software to not scan during data processing or data review to avoid affecting system performance.

Workstation 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 1600Mhz SDRAM
  - 2*2Tb HDD (RAID1)
  - DVD+-RW
  - English version of Microsoft Windows 7, 64-bit operating system, with SP1 **or** English version of the Microsoft Windows 10, 64-bit operating system
  - Microsoft Office 2010 or 2013 (64-bit) or 2016 (64-bit)

    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.

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.

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.

Note: To view the changes in the software and fixed issues for previous versions of the MetabolitePilot™ software, refer to the *Release Notes* for previous versions.

Notes on Documentation

This version of the document supercedes all previous versions of this document.

To view this document electronically, Adobe Acrobat Reader is required. To download the latest version, go to https://get.adobe.com/reader.

To request a free, printed version of this document, contact sciex.com/contact-us.

Contact Us

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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

- SCIEX**University**

CyberSecurity

For the latest guidance on cybersecurity for SCIEX products, visit sciex.com/productsecurity.

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.

Installation 2

Notes on Installation

- The MetabolitePilot™ 2.0.4 software is a new installation only. Upgrades from existing versions of the software are not supported. If version 2.0, 2.0.2, or 2.0.3 of the MetabolitePilot™ software is installed, then it must be removed before version 2.0.4 can be installed. Refer to Remove the MetabolitePilot™ Software. However, other versions of the MetabolitePilot™ software (1.0 and 1.5) can exist on the same computer.

- The user must be logged on to the computer as a user with Administrator privileges.

- When a zip file that contains the MetabolitePilot™ software installer is being used, 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 the following software if it is not already installed on the system:
    - .NET Framework 3.5 with SP1, if required
    - .NET Framework 4.5.1, if required
    - Microsoft Visual C++ 2010 Redistributable Package (x64)
    - Microsoft Visual C++ 2010 Redistributable Package (x86)
    - Microsoft Visual C++ 2013 Redistributable Package (x64)
    - Microsoft Visual Studio 2010 Tools for Office Runtime (x64)
    - AB SCIEX Reporter Template Suite 3.2
    - Microsoft Save as PDF Add-in for 2007 Microsoft Office programs
    - Microsoft Office 2010 Primary Interop Assemblies

Install the MetabolitePilot™ Software

1. Read these release notes.

2. Log on to the computer as a Microsoft Windows user with administrator privileges.

Installation

3. Make sure that all of the applications are closed.

> **Note:** If the MetabolitePilot™ 2.0, 2.0.2, or 2.0.3 software was installed, then remove the software before installing version 2.0.4.

4. Install the MetabolitePilot™ software. Refer to Table 2-1.

Table 2-1 Installation Instructions

To install from a file downloaded from the SCIEX website …	To install from the MetabolitePilot™ software installation DVD …
Download the zip file from https://sciex.com/products/software/metabolitepilot-software. **Tip!** To prevent potential installation issues, we recommend that the file is saved to a location other than the computer desktop.	Load the MetabolitePilot™ software installation DVD in the DVD drive.
After the download is complete, right-click the zip file.	If the installation does not start automatically, then navigate to the DVD, open the **Setup** folder, and double-click **MetabolitePilotInstaller.exe**. The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click **Run**.

Table 2-1 Installation Instructions (continued)

To install from a file downloaded from the SCIEX website ...	To install from the MetabolitePilot™ software installation DVD ...
Click **Extract All**.	If any of the required software is not already installed, then the installer identifies the applications that will be installed.
Note: The files are extracted to the same location where the zip was saved.	Click **Install**.
Note: Accept any changes prompted by User Account Control during installation.	**Note:** Any end-user license agreements that are shown must be accepted to continue with the installation.
	Note: Accept any changes prompted by User Account Control during installation.
	After the required software is installed, the MetabolitePilot™ 2.0.4 Setup dialog opens.
	The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click **Run**.

Table 2-1 Installation Instructions (continued)

To install from a file downloaded from the SCIEX website ...	To install from the MetabolitePilot™ software installation DVD ...
After the extraction is complete, browse to the extraction folder and then double-click **MetabolitePilotInstaller.exe**. The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click **Run**.	—
If any of the required software is not already installed, then the installer identifies the applications that will be installed. Click **Install**. --- **Note:** Any end-user license agreements that are shown must be accepted to continue with the installation. --- After the required software is installed, the MetabolitePilot™ 2.0.4 Setup dialog opens. The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click **Run**.	—

5. Click **Next**.

   The End-User License Agreement dialog opens.

6. Click **I Agree**.

   The Destination Folder dialog opens.

   Note: Installation of the Data folder in the C:\Users folder is prohibited.

   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™ 2.0.4 dialog opens.

9. After the installation is complete, click **Finish**.

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.

   Note: If the MetabolitePilot™ 2.0, 2.0.2, or 2.0.3 software was installed and licensed, then a new license file is not required. Version 2.0.4 can be used with the version 2.0 license file.

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 2-1 MetabolitePilot^{TM} Activation Dialog
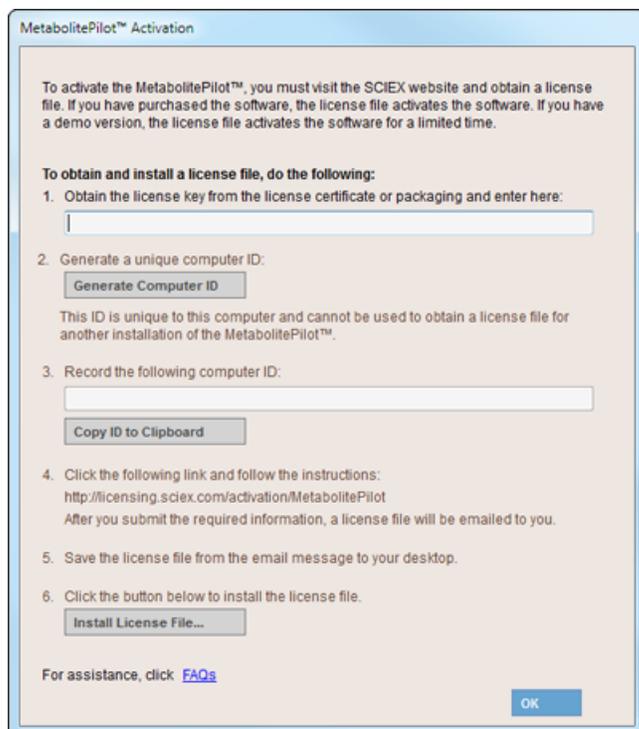
2. Type the license key from the license certificate (found in the MetabolitePilot^{TM} software installation package) in the appropriate field.

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.

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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.

Note: SCIEXNow login credentials are required to obtain the license key.

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, then 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 3

Everyone should read this section of the Release Notes.

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

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)

- For a multi-chain sequence, the Sequence Coverage in the Assignment summary might show a value that is greater than the total number of residues in the sequence. This might be caused by the software counting some of the residues multiple times. As a workaround, the value can be assumed to be all of the residues in the sequence having an MS/MS ion evidence in the Fragments table. (MP-2166)

  Note: Sequence Coverage is not used to rank the Sequence Candidates.

Correlation

- The Correlation Results file has a size limitation of 4GB, which is the maximum size for a SQL Compact Edition Database. A Correlation Result file will not open if the file size exceeds this limitation. As a workaround, keep the number of large Results files used during correlation to a minimum. (MP-2161)

Peak Finding Strategies

- When more than one peak finding strategy is used to process a data file, the chromatograms associated with specific peak finding strategies might not be shown for some of the metabolites in the Results file. To make sure that all of the appropriate chromatograms are shown, increase the **Maximum number of unexpected metabolites** on the MS Parameters tab of the Generic Parameters. (MP-2011)

Amino Acid Modifications

Known Issues and Limitations

- Amino acid modifications that are present in assigned metabolite sequences and in sequences in the Fragments table are enclosed in square brackets in the software user interface. However, when an interpretation report is generated for peptide and ADC results, the square brackets are not always included in the printed report. (MP-2031)

Remove the MetabolitePilot™ Software 4

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.

2. Do one of the following:

   - For Microsoft Windows 7 operating systems, click **Start > Control Panel > Programs and Features**.

   - For Microsoft Windows 10 operating systems, click **Start > Windows System > 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

   - Microsoft .NET Framework, versions 3.5 and 4.5.1, if installed

   - Microsoft Visual C++ 2010 Redistributable Package (x64)

   - Microsoft Visual C++ 2010 Redistributable Package (x86)

   - Microsoft Visual C++ 2013 Redistributable Package (x64)

   - Microsoft Visual Studio 2010 Tools for Office Runtime (x64)

   - Microsoft Save as PDF Add-in for 2007 Microsoft Office programs

   - Microsoft Office 2010 Primary Interop Assemblies