Molecule Profiler 1.0.1 Software Release Notes

The Power of Precision

Introduction

The Molecule Profiler 1.0.1 software is a processing only software, used for the identification and characterization of metabolites.

The software processes accurate mass data, acquired from:

- TripleTOF systems, using the Analyst TF software, version 1.5 or later.
- TOF systems, using the SCIEX OS software.

Note: The numbers in parentheses are reference numbers for each issue or feature in the SCIEX internal tracking system.

New Features

The Molecule Profiler software builds upon the proven MetabolitePilot software. It includes these features:

- Support for the small molecule, peptide, oligonucleotide, and antibody drug conjugate (ADC) workflows.
- Integration with the SCIEX OS software.
- Ability to access the Explorer workspace in SCIEX OS.

Related Documentation

The documentation for the Molecule Profiler Software is installed automatically with the software and is available from the Start menu: **All Programs > SCIEX > SCIEX OS > Documentation**.

For step-by-step animations of basic procedures, open the Molecule Profiler Software and then click **Help > Show Me**.

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

Fixed Issues

This release fixes an issue where, after the Molecule Profiler software version 1.0 was installed, users were unable to view audit entries that related to existing Results Tables. (MP-3215)

Known Issues and Limitations

General Issues

Regional Setting

- Issues might occur if the Windows Region and Language are set to values other than **English (United States)**. (MP-3011)

Sample Information

- The sample information dialog cannot be closed by clicking the red Close box. To close the dialog, click **OK**. (MP-2979)

Copy Table

- The **Edit > Copy Selected Table** command is not available. Use the right-click menu to copy tables. (MP-2905)

MetabolitePilot Software Compatibility

- In the Results and Correlation workspace, the average mass column for data files created in the MetabolitePilot 2.0.4 software contains **0** instead of **N/A**. (MP-2371)

UV Data

- The software does not recognize or process UV data acquired by an X500 QTOF system. (MP-2185)

Processing Method Issues

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)

Product Ion and Neutral Losses Tab

(Peptide and oligonucleotide workflows) If the user opens a processing method that does not have a spectrum on the Product Ion and Neutral Losses tab, adds a spectrum, and then clicks the **Assign Fragments** button, the fragment table is not populated. To populate the table, change one of the filters, change it back, and then click **Assign Fragments**. (MP3071)

Batch Workspace Issues

Peak Finding

- 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)
- (Peptide workflow, SWATH acquisition data) If an isotope pattern is used for peak finding, then only the singly-charged form of the fragment ion formula is used. (MP-2007)

Results Workspace Issues

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 in the MS pane 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)

Scheduled MRM Algorithm

- MS/MS data is not shown after *Scheduled* MRM^{HR} algorithm data is processed, and it is not used to calculate the score. (MP-2976)
- For *Scheduled* MRM^{HR} algorithm data, the title for the MS/MS spectrum does not contain the correct precursor mass. (MP-2839)

Grouping

- When the grouping feature is used, the header of the Results Table is not updated properly after rows are deleted. (MP-2929)

Interpretation

- (Peptide workflow) 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)
- (Peptide workflow) 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)
- (Peptide workflow) 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.

- (Oligonucleotide workflow) If the user applies a filter to the Fragments list that hides all fragments, and then clicks **Apply**, issues can occur. To avoid issues, make sure that the Fragments list contains at least one fragment before clicking **Apply**. (MP-3024)
- (Oligonucleotide workflow) After a new MS/MS spectrum is added, and removal of interpretation data is confirmed, the **Assigned** check box is not cleared, and the sequence remains. The user can **Paste MS/MS** and **Assign Fragments**. (MP-3016)
- An error is shown if the **Prepare** button is clicked when no Results file is open. (MP-2935)
- (Peptide workflow) The Fragments table and Sequence pane get out of sync when the user goes from one candidate to another. To avoid this issue, work with a single candidate, rather than multiple candidates, in a session. (MP-3027)

Correlation Workspace Issues

- The total file size of all files used for correlation cannot exceed 4 GB. A Correlation Result file will not open if the total file size exceeds this limitation. To avoid issues, keep the number of large Results files used during correlation to a minimum. (MP-2161)

Reports Issues

- The Y-axis label is missing in the Compound-Specific Parameters section of the Isotope Pattern graph. (MP-3022)
- (Peptide and ADC workflows) 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)

Installation

Requirements

Workstation Requirements

- SCIEX Alpha Workstation 2020, with:
  - An Intel Core I5-8500 processor (6 core, 9 MB cache, 3.0 GHz, 4.1 GHz Turbo, with HD Graphics 630)
  - 32 GB (2 × 16 GB) 2666 MHz DDR4 UDIMM Non-ECC
  - 2*2 TB HDD (RAID1)
  - DVD±RW
- 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 × 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.

Operating System Requirements

- Windows 10, 64-bit, operating system

Software Requirements

- SCIEX OS version 2.1.6

Notes on Installation

- The Molecule Profiler 1.0.1 software is a new installation only. Upgrades from the MetabolitePilot software are not supported.
- The user must be logged on to the computer as a user with Administrator privileges.
- When a zip file that contains the Molecule Profiler 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.

Install the Molecule Profiler Software

Prerequisites
• SCIEX OS version 2.1.6 is installed. • Molecule Profiler software version 1.0 is removed. • A Molecule Profiler license key is available. The license key might be distributed on a printed activation certificate, or in an e-mail from SCIEX Now. If the license key is missing, then contact a SCIEX sales representative.

1. Log on to the computer as a Microsoft Windows user with administrator privileges.
2. Make sure that SCIEX OS is closed.
3. Download the required zip file from sciex.com/software-support/software-downloads.

Tip! To prevent potential installation issues, save the file to a location other than the computer desktop and disconnect any external USB storage devices before starting the installation.

4. After the download is complete, right-click the downloaded file and then click **Extract All**.

   By default, the files are extracted to the location where the zip file was saved.

   Note: Accept any changes prompted by User Account Control during installation.

5. After the extraction is complete, browse to the extracted files and then double-click **MoleculeProfiler-AddOn.msi**.

   The Molecule Profiler 1.0.1 Setup Window opens.

6. Follow the on-screen instructions to complete the installation.

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

   The installation wizard installs the Molecule Profiler software.

   Note: Accept any end-user license agreements that are shown.

7. After the installation is completed, continue with the section: Activate the Software.

Activate the Software

Note: Internet access is required to obtain a license for the software. If the computer where the Molecule Profiler 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 sciex.com/request-support and then follow the instructions to obtain a license.

Note: Accept any changes prompted by User Account Control during activation.

1. Open SCIEX OS.

   Note: If SCIEX OS is not licensed, then the SCIEX OS Activation dialog opens. Go to step 4.

2. Open the Configuration workspace, and then go to the Licenses page.
3. Click **Install License**.

The SCIEX OS Activation dialog opens.

4. Type the license key in the appropriate field.

   The license key might be distributed on a printed activation certificate, or in an e-mail from SCIEX Now. If the license key is missing, then contact a SCIEX sales representative.

5. Click **Copy ID to Clipboard**.
6. Go to sciex.com/request-support and follow the instructions.
7. Follow the instructions to obtain the license.

   Note: Internet access is required to obtain the license. If the computer does not have Internet access, then make a copy of the generated computer ID. On a computer with Internet access, go to the licensing page of the SCIEX website and then follow the instructions to obtain a license.

   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 file to the workstation desktop.
10. In the SCIEX OS Activation dialog, click **Install License File**.
11. In the Select the new license file to be installed dialog, browse to and then select the license file.
12. Click **Open**.

    A confirmation dialog opens.

13. Click **OK**.

    Note: Close SCIEX OS and then open it again. The Molecule Profiler tile is added to the Home page.

Remove the Molecule Profiler Software

1. Log on to the computer as a Windows user with Administrator privileges.
2. Make sure that SCIEX OS closed.
3. 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.**

4. Select the Molecule Profiler software and then click **Uninstall**.

   The software is removed, with no user intervention required.

   The software is removed from the Installed Programs list, and the Molecule Profiler tile is removed from the SCIEX OS Home page.

Note: If the product is licensed, then the license file is not removed and can be used if the Molecule Profiler software is installed again.

Contact Us

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 Now Learning Hub

SCIEX 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 SCIEX website at sciex.com or contact us in one of the following ways:

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

CyberSecurity

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

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.

The latest versions of the documentation are available on the SCIEX website, at sciex.com/customer-documents.

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

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