Molecule Profiler Software 1.3.1 Release Notes

Introduction

The Molecule Profiler software 1.3.1 is processing-only software, used for the identification and characterization of parent molecules and their metabolites or impurities.

The software processes accurate mass data, acquired from the following systems:

- TripleTOF systems, using the Analyst TF software, version 1.5 or later.
- X500 QTOF and ZenoTOF 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 in Version 1.3.1

This section gives a description of the changes in the Molecule Profiler software 1.3.1. To see the enhancements and fixed issues for a previous version of the Molecule Profiler software, refer to the document: *Release Notes* that came with that version of the software.

New Features and Enhancements

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

- New biotransformation sets with lipid-specific modifications
- A dedicated processing parameter template for ionizable lipid molecule analysis
- Performance improvements in small molecule or lipid workflows that include:
  - Data in a batch is processed faster
  - During data review, users can move between the Results and Interpretation views faster
  - Data is loaded faster when users move to different rows in the Potential Metabolites table
- Small molecule and lipid workflows: The ability to copy MS/MS data from Explorer and paste it in the Molecule Profiler software. The MS/MS spectrum is automatically centroid prior to pasting.
- The small molecule biotransformation database is expanded to enable the prediction of automatic structures

Note: Because of the updates to the biotransformation database, we recommend that users make new processing parameter templates to process data.

- The support for multiply-charged MS/MS fragments in the small molecule and lipid workflows
- Improvements to the Mass Defect tab in Processing Parameters
- The support for multi-row selection in the Potential Metabolites table in the Results workspace
- An increase to 60 in the maximum allowable AA limit in the ADC workflow

Fixed Issues

The values in the **Maximum number of bonds to break** and **Maximum number of C-C bonds to break** fields that are used to generate data are shown incorrectly in the printed report. The data generated in the report is correct. (MP-3802)

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

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**.

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

Installation

Notes on Installation

- The Molecule Profiler software 1.3.1 is installed as part of the SCIEX OS software, and activated with a version 1.3.1 license. For installation instructions and requirements for the SCIEX OS software, refer to the document: *SCIEX OS Software Installation Guide*. To activate the Molecule Profiler software, refer to the section: Activate the Software.
- The Molecule Profiler software is removed with the SCIEX OS software. For instructions, refer to the document: *SCIEX OS Software Installation Guide*.
- To upgrade from an earlier version of the Molecule Profiler software, install the SCIEX OS software. The earlier version is removed and the new version is installed. Refer to the section: Upgrade the Software.

Upgrade the Software

Use this procedure to upgrade from earlier versions of the Molecule Profiler software to the Molecule Profiler software version 1.3.1.

Note: A Molecule Profiler software 1.3.1 license is required.

1. Install the SCIEX OS software Refer to the document: *SCIEX OS Software Installation Guide*.
   The installation program installs the SCIEX OS software and upgrades the Molecule Profiler software to version 1.3.1.
2. Activate the Molecule Profiler software version 1.3.1. Refer to the section: Activate the Software.

Activate the Software

Note: Internet access is required to get 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 get a license.

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

1. Open the SCIEX OS software.

   Note: If the SCIEX OS software 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 for the Molecule Profiler software 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.

   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**.
    The Select the new license file to be installed dialog opens.
11. Browse to and then select the license file.

12. Click **Open**.
    A confirmation dialog opens.
13. Click **OK**.

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

Known Issues and Limitations

General Issues

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)

Data Processing

- During data acquisition, if a user uses the Molecule Profiler software to process large amounts of data on the same computer, then the acquisition will stop. To prevent this issue, do not process large amount of data during data acquisition, or process the data on a separate computer.

Processing Method Issues

Processing Parameter Templates

During the installation of version 1.3.1, the processing parameter templates are overwritten with the most current versions of the templates. The user must reset any preferred default values and then save the default settings. (MP-4029)

SWATH Acquisition MS/MS Reference Spectra

- When extracting reference spectra from SWATH acquisition data, the software proposes an extensive list of MS/MS spectral data. Users should be aware that some of the precursors associated with the proposed MS/MS spectral data might 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, then the fragment table is not populated. To populate the table, change one of the filters, change it back, and then click **Assign Fragments**. (MP-3071)

Batch Workspace Issues

Peak Finding

- If more than one peak finding strategy is used to process a data file, then 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)

Scheduled MRM (sMRM) Algorithm Data Processing

- MS/MS data is not shown and it is not used to calculate the score. (MP-2976)

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, thus, 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 uses the adduct assigned to the metabolite to show the similarity between the experimental MS peaks and the isotope pattern of the reference compound formula.
    - The isotope pattern highlighted in the MS pane uses the primary ion type selected in the processing parameters to show the similarity of the isotope pattern to the reference compound.
- 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 that was 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 uses the adduct assigned to the metabolite to show the similarity between the experimental MS peaks and the isotope pattern of the reference compound formula.
- 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 large, complex peptide data, the time required by the software to propose potential sequence candidates with the **Generate** option and the time required to review the MS/MS ion annotation for the proposed candidate is extensive. (MP-1692, MP-1712)
- For lipid impurities containing only an n-alkyl chain loss, for example a loss of n-butyl, the proposed structure candidates are not scored correctly. As a result, proposed candidates will all have a rank of 1. Use the **Assigned Score** value as a guide for selecting a structure. (MP-5112)

Grouping

- When the grouping feature is used, the header of the Results Table is not updated properly after rows are deleted. As a workaround, click **Save**, ungroup the data, and then group the data again. The correct number is then shown. (MP-2929)

Interpretation

- 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 missing the ✓ in the peak label on the MS/MS spectrum. (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 used to generate 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 changed with the **Edit Name and Formula** option. As a workaround, the sequence of interest can be typed in the Metabolite Sequence pane. (MP-1957)

- Oligonucleotide workflow: If the user applies a filter to the Fragments list that hides all fragments, and then clicks **Apply**, issues can occur. To prevent 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 stays. The user can **Paste MS/MS** and **Assign Fragments**. (MP-3016)
- Peptide workflow: The Fragments table and Sequence pane get out of sync when the user goes from one candidate to another. To prevent this issue, work with a single candidate, rather than multiple candidates, in a session. (MP-3027)
- For multi-chain peptides, the sequence coverage reported can be incorrect because it might include fragments that have undergone limited fragmentation and have a mass similar to a precursor ion with neutral losses. Clear the **Use** check box to get the correct sequence coverage for these specific fragments. (MP-3711)
- Peptide or oligonucleotide workflow: The sequence coverage for a selected row is not shown above the MS/MS graph when the user moves between the Results view and the Interpretation view. As a workaround, click **Assign** or select a different row and then re-select the required row. (MP-5155)

Reports Issues

- Peptide or 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-2186)

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