Molecule Profiler Software 1.3.4.1 Release Notes

Introduction

The Molecule Profiler software 1.3.4.1 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, with the Analyst TF software 1.5 or later.
- X500 QTOF and ZenoTOF systems, with 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 1.3.4.1

This section gives a description of the changes in the Molecule Profiler software 1.3.4.1. To see the enhancements and corrected issues for an earlier 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 and enhancements:

Oligonucleotide Workflow

- The formulas used for the calculation of theoretical MS/MS fragments have been adjusted to make better matches with the most abundant fragments that are created by CID fragmentation.

  Note: Results files that were created in earlier versions of the Molecule Profiler software can be processed again to use the new theoretical MS/MS fragments during matching.

Fixed Issues

Oligonucleotide Workflow

The calculations for theoretical MS/MS fragments from CID fragmentation do not include fragments that contain a double bond. (MP-6104)

Related Documentation

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

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

Installation

Notes on Installation

- The Molecule Profiler software 1.3.4.1 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

Note: In the peptide workflow, processing parameter files that were created in an earlier version of Molecule Profiler can be out of date after the upgrade. Open the parameter file to make sure that all of parameters are correct, and then save the file again before use.

Note: During installation, the processing parameter templates are overwritten with the newest versions of the templates. The user must reset any preferred default values and then save the default settings.

Note: Results files created in earlier versions of Molecule Profiler will be automatically recalculated when opened in this version and some values can change. The **MSMS Peak Area Assigned (%)** values in the data table can be different than the values that are displayed in the histograms. To update the histogram with the new values, process the data again.

Use this procedure to upgrade from earlier versions of the Molecule Profiler software to the Molecule Profiler software version 1.3.4.1.

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 1.3.4.1.
2. Activate the Molecule Profiler software version 1.3.4.1. Refer to the section: Activate the Software.

Activate the Software

Note: To get the license, internet access is required. 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 from 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 License page.
3. Click **Install License**.
   The SCIEX OS Activation dialog opens.
4. Type the license key for the Molecule Profiler software in the applicable 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.
7. Follow the instructions to get the license.

   After the required information is submitted, a license file is sent to all of the e-mail addresses supplied.
8. Close the browser window.
9. When the e-mail that contains 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

Data Processing

- During data acquisition, if a user uses the Molecule Profiler software to process large quantities of data on the same computer, then the acquisition stops. To prevent this issue, do not process a large quantity of data during data acquisition, or process the data on a different computer.

Processing Method Issues

SWATH Acquisition MS/MS Reference Spectra

- During the extraction of reference spectra from SWATH acquisition data, the software proposes an extensive list of MS/MS spectral data. Some of the precursors related to the proposed MS/MS spectral data might have a low TOF MS peak intensity or a 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 filled. To fill 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 related to specific peak finding strategies might not be shown for some of the metabolites in the Results file. To make sure that all of the applicable 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) 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 that come from one or more antibody fragments with the same masses are not included in the list of other proposed names. Thus, the user cannot easily get access to them in the Interpretation view. (MP-1745)
- Different selections for **Source of Reference MS/MS Spectrum** (**Sample** or **Selected reference spectrum**) in the MS/MS Parameters of the Generic Parameters might show a different **MS/MS Similarity** score in the Details pane of the Results workspace. (MP-1839)

Grouping

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

Interpretation

- For ADC results, the **Load Sequence** option automatically adds the protein fragment sequence that is related to the name assigned during data processing. This also true when 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 of the fragments, and then clicks **Apply**, issues can occur. To prevent issues, make sure that the Fragments list contains at least one fragment, and then click **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)

Reports Issues

- Peptide or ADC workflows: Amino acid modifications that are present in assigned metabolite sequences and in sequences in the Fragments table are in square brackets in the software user interface. But, when an interpretation report is created for peptide and ADC results, the square brackets are not always included in the printed report. (MP-2186)

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Documentation

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