Molecule Profiler 1.2 Software Release Notes

Introduction

The Molecule Profiler 1.2 software is processing-only software, used for the identification and characterization of parent molecules and their metabolites.

The software processes accurate mass data, acquired from:

- 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.

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.

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 SCIEX OS. When **How Do I?** is clicked, users can select the appropriate Help topic from the list provided.

New in Version 1.2

New Features and Enhancements

Sequence Information on the Interpretation Pane (Peptide Workflow)

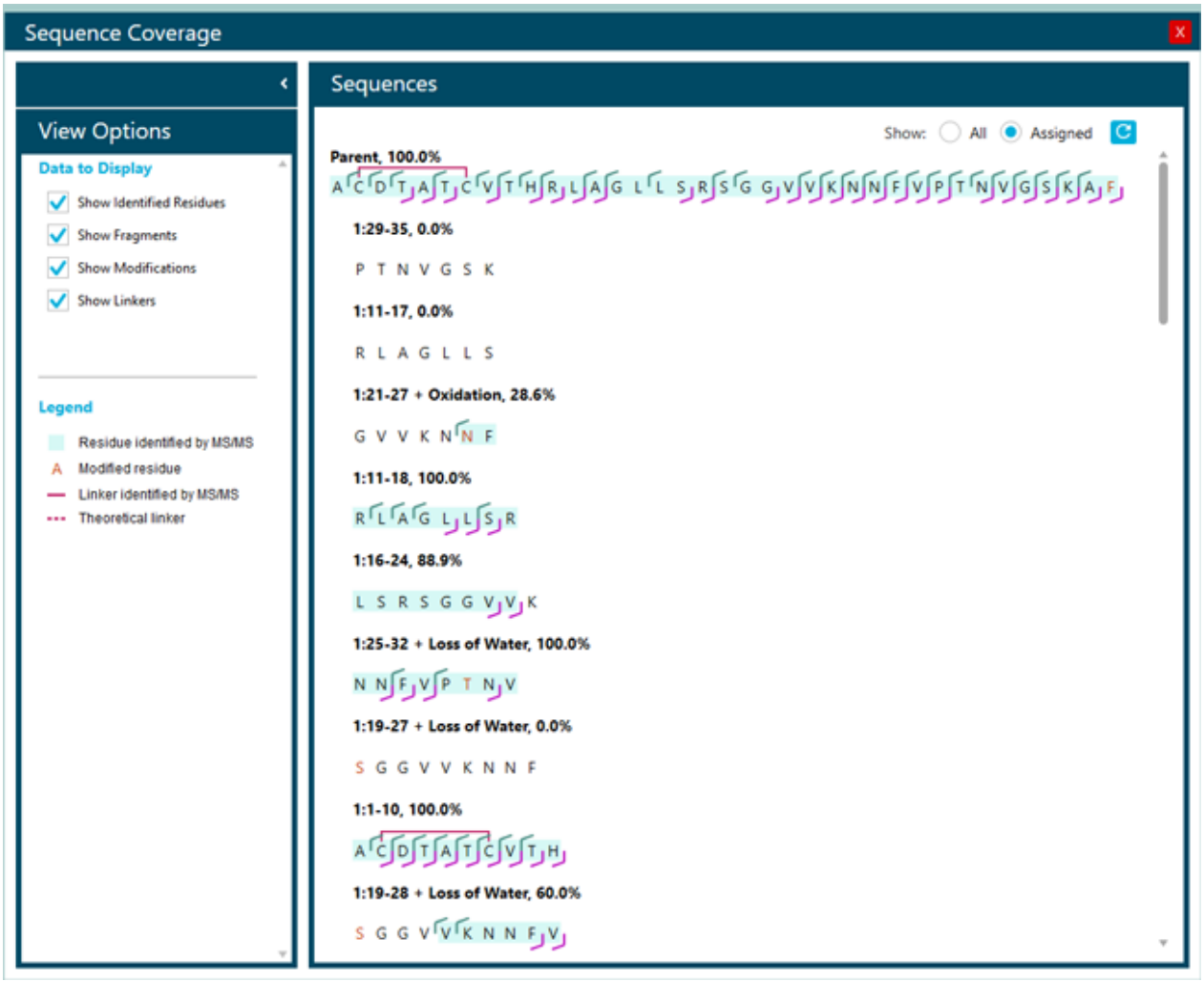
Fragment sequence information is now shown at the top of the MS/MS graph pane, to let the user assess fragment sequence coverage. The fragmentation positions and indexes are represented on the sequence by ticks and numbers, respectively. The sequence is updated dynamically when the user applies a change, such as changing the parent formula, or excluding

fragments from use. The user can copy and paste the sequence and the spectrum, either separately, or combined in a single figure.

Sequence Coverage is available in the Peptide and Oligonucleotide Workflows

The Sequences pane shows the cumulative sequence coverage across charge states of the same molecule.

Figure 1 Sequence Coverage Dialog



Note: Sequence Coverage is not used to rank the sequence candidates.

Support for Multiple Local Languages

The software user interface now supports Japanese, Chinese, Korean, Spanish, French, Italian, German, and Portuguese.

Support for SQLite

(All workflows) Because Microsoft has retired the SQL CE database, result and correlation files are stored in SQLite format. Existing results and correlation files will be updated automatically.

New report templates

New report templates are available under Molecule Profiler resources at sciex.com/software-support/software-downloads. Download and extract the zip files to the desktop, and then copy the files to `C:\ProgramData\SCIEX\Molecule Profiler Data\Report Templates`. If any of the existing report templates have been changed and the default report name kept, then those reports will be overwritten when the new reports are copied to the folder. To keep the customized reports, save the reports using a different name and then copy the new templates.

Fixed Issues

- Peptide workflow: For a multi-chain sequence, the **Sequence Coverage** in the Assignment summary might have shown a value that is greater than the total number of residues in the sequence. This issue might have been caused by the software counting some of the residues multiple times. (MP-2166)

Installation

Notes on Installation

- The Molecule Profiler 1.2 software is installed as part of the SCIEX OS 3.0 software, and activated with a version 1.2 license. For installation instructions and requirements for SCIEX OS, 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 is removed with the SCIEX OS 3.0 software. For instructions, refer to the document: *SCIEX OS Software Installation Guide*.
- To upgrade from an earlier version of Molecule Profiler, install SCIEX OS 3.0. 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 to the Molecule Profiler software version 1.2.

Note: A Molecule Profiler 1.2 software license is required.

1. Install SCIEX OS version 3.0. Refer to the document: *SCIEX OS Software Installation Guide*.
   The installation program installs SCIEX OS 3.0 and upgrades the Molecule Profiler software to version 1.2.

2. Activate the Molecule Profiler software version 1.2. Refer to the section: Activate the Software.

Activate the Software

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.

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 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**.
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.

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)

Data Processing

- During data acquisition, if a user processes large amounts of data on the same computer using the Molecule Profiler software, 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

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**. (MP-3071)

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)

MRM^{HR} Algorithm

- MS/MS data is not shown after MRM^{HR} algorithm data is processed, and it is not used to calculate the score. (MP-2976)

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 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)
- 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)
- 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 obtain the correct sequence coverage for these specific fragments. (MP-3711)

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)
- 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)

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(GEN-IDV-09-10816-D)

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AB Sciex Pte. Ltd.
Blk33, #04-06 Marsiling Industrial Estate Road 3
Woodlands Central Industrial Estate, Singapore 739256