User Guide

SCIEX MS Data Converter Software 2.0.1

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Introduction 1

The SCIEX MS Data Converter software converts data that was acquired by a SCIEX mass spectrometer in the `wiff` and `wiff2` formats to the `mzml` format. The software can convert data directly or, to supply a peak list, it can process the data during the conversion.

Supported Scan Types

The SCIEX MS Data Converter software supports the conversion of data that was acquired with these scan types:

- Accurate mass systems: TOF MS, TOF MSMS, SWATH acquisition, MRM^{HR} algorithm, and ZT Scan
- Triple quadrupole systems: Neutral Loss, Precursor Ion, Product Ion, Q1, Q1 MI, Q3, Q3 MI, MRM, and Scheduled MRM (sMRM) algorithm
- LIT (QTRAP) systems: Enhanced Resolution (ER), Enhanced MS (EMS), Enhanced Product Ion (EPI), and MS^3

Supported Output Formats

`mzml` Format

The `mzml` format is the standard extended markup language (`xml`) format for mass spectrometry. This format is a combination of the older `mzxml` and `mzdata` formats. Data in the `mzml` format that is exported by the SCIEX MS Data Converter software obeys the version 1.1 specification for the `mzml` format. For more information about the `mzml` format, go to http://www.psidev.info/index.php?q=wiki/Mass_Spectrometry.

Note: The `xml` format uses much more file space than the `wiff` format. The software uses compression functions to decrease the file size, but the `mzml` output files that are created during the conversion of data in profile mode are many times larger than the original `wiff` data files.

Enhancements and Corrected Issues

- A new graphical user interface is available.
- Support was added for the `wiff2` format.
- Support was added for these nominal mass systems: SCIEX 4500 system, SCIEX 5500 system, SCIEX 5500+ system, SCIEX 6500 system, SCIEX 6500+ system, SCIEX 7500 system, and SCIEX 7500+ system.

- Support was added for these accurate mass systems: X500 QTOF system, ZenoTOF 7600+ system, and ZenoTOF 8600 system.
- Support was added for the Windows 11 operating system.
- MRM chromatograms that were acquired with nominal mass systems can be converted to the `mzml` format.
- Multiple samples in the same file can be selected.
- A new, better command line syntax is available.
- File compression can be turned on and off in the command line interface.
- The issues that occurred when `wiff1` files were opened or processed by the SCIEX Data API are corrected. (BLT-7361)
- The issue that caused an `ArgumentOutOfRangeException` to occur during the retrieval of experiment metadata with the SCIEX Data API when some `wiff` files with negative start times were opened is corrected. (SXOSLNT-6743)

Known Issues and Limitations

- ProteinPilot mode is not supported.

  All of the peak-finding options that are used in the Explorer workspace in the SCIEX OS software are available. The peak finder that is used by the ProteinPilot software is not compatible with this version of the SCIEX MS Data Converter software.
- Conversion to the Mascot generic format (`mgf`) is not supported.
- `wiff` files that do not have a related `scan` file are not supported.

  The Analyst software has an option to acquire data to a *flat* file format. In the flat file format, the `wiff` and `wiff.scan` files are put together. The flat file format is not supported by this version of the SCIEX MS Data Converter software.
- When data that was acquired in the Analyst software with the Scheduled MRM (sMRM) algorithm is converted, the XIC trace includes data points with zero values that are not in the schedule acquisition window. (ONYX-65077)

Installation 2

Requirements

Operating System Requirements

- Windows 10 (64 bit) or Windows 11
- .NET Desktop Runtime 8.0 (x64)
- Microsoft Visual C++ 2015-2022 Redistributable (x64), available at: https://learn.microsoft.com/en-us/cpp/windows/latest-supported-vc-redist?view=msvc-170. Select the **X64** option.

Install the SCIEX MS Data Converter Software

Prerequisites
• Remove earlier versions of the SCIEX MS Data Converter software

1. Log on to the computer as a Windows user with Administrator privileges.
2. Go to sciex.com/software-downloads, and then download the SCIEX MS Data Converter software to a local folder.

   Tip! To prevent installation issues, save the file to the local computer, in a different location than the desktop.
3. After the download is completed, right-click the `SciexMSDataConverterV2.0.1.zip` file, click **Extract All**, browse to and select the destination folder, and then click **Extract**.
4. Go to the extracted folder, and then double-click the `SCIEX.MSDataConverter.Extractor.exe` file.

   The SCIEX MS Data Converter Extractor opens.
5. Obey the on-screen instructions to complete the extraction.

Convert MS Data 3

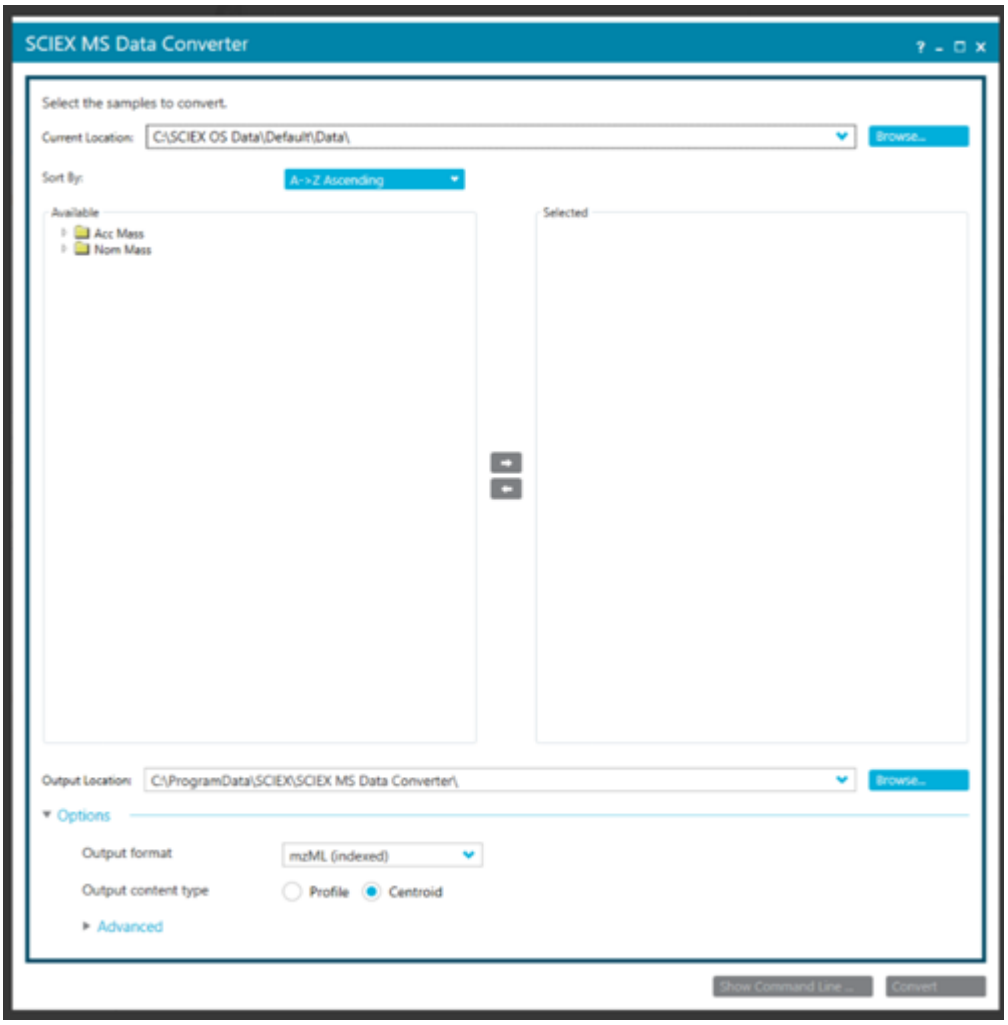
Use the Graphical User Interface

Use this procedure to use the graphical user interface to convert MS data.

Tip! The graphical user interface can be used to create commands for use in a Command Prompt window or batch. Set the parameters for the conversion, and then click **Show Command Line** to see and copy the related command.

1. Browse to the folder where the SCIEX MS Data Converter software was extracted, and then double-click the `SciexMSDataConverterUI.exe` file.

Figure 3-1 SCIEX MS Data Converter Software: Home Page



2. In the **Available** list, select the data files or samples to be converted, and then click  to add them to the **Selected** list.

Note: If the folder that contains the required data file is not shown in the **Available** list, then click **Browse** to browse to the correct folder.

3. In the **Output location** field, select the folder where the output file will be saved.

Note: If the required folder is not available in the list in the **Output location** field, then click **Browse** to browse to the folder.

4. In the **Output format** field, select one of these options:

   - **mzML**

- **mzML (indexed)**: `mzml` format with index data for spectral and chromatographic data

Note: Indexed `mzml` files let some software applications read in a random order more quickly.

5. In the **Output content type** field, select one of these options:
   - **Profile**: Include the full X-Y trace that was acquired by the mass spectrometer. The information content is not decreased.
   - **Centroid**: Include the centroid values for the peaks. The software uses the same peak finder as the Explorer workspace of the SCIEX OS software.
6. To set the advanced options for the conversion, click ▸ adjacent to **Advanced**, and then set the options that are shown in the table that follows:

Table 3-1 Advanced Options

Parameter	Description
Metric for Y-value	The metric to use for the centroid value for the peak. These options are available: • **Intensity sum above 50%** • **Area** • **Height** • **Intensity** • **Total Intensity Sum** (default) **Note:** This parameter is shown if **Output content type** is set to **Centroid**.
Isolated points	Keep peaks from single data points that have zero-intensity points before and after them. **Note:** This parameter is shown if **Output content type** is set to **Centroid**.

Table 3-1 Advanced Options (continued)

Parameter	Description
Smoothing	The level of smoothing to use. These options are available: • **Low**: Applicable to workflows with isotope clusters that are highly charged. • **Moderate** (default): Satisfactory for most workflows. **Note:** This parameter is shown if **Output content type** is set to **Centroid**.
Zero padding	Keep a zero-intensity point at the start and end of each peak.

Tip! To set the advanced options back to the default values, click **Reset**.

7. Click **Convert**.
   A dialog opens to show the progress of the conversion. When the conversion is completed, a message is shown.
8. Click **OK**.

Use the Command Line

This section gives the syntax for the `SciexMSDataConverter.exe` command that can be used in a Command Prompt window.

Tip! Use the graphical user interface to set the parameters for the conversion, and then click **Show Command Line** to see and copy the related command.

```
SciexMSDataConverter.exe <input> [options]
```

Table 3-2 Command Line Parameters

Parameter	Description
<input>	The path to the file to be converted, which includes the file name and extension. If the file is in the folder that contains the software files, then the path is not required. Example: `C:\Data\file.wiff` For `wiff` files that have a related `scan` file, include only the `wiff` file. Make sure that the related files are in the same folder as the `wiff` file. **Note:** The path must be a local path. The software does not support conversion across a network.
Options	
`--profile` | `--centroid`	The output content type. These options are available: • `--profile`: Include the full X-Y trace that was acquired by the mass spectrometer. The information content is not decreased. • `--centroid`: Include centroid values for the peaks. The software uses the same peak finder as the Explorer workspace of the SCIEX OS software.
`--output:` *<output>*	The output path, which includes the file name and extension. If the full path is not included, then the output file is saved in the folder that contains the input file. If the file name is not included, then the software uses the file name of the input file to create one. Example: `--output:C:\Data\file.mzml` **Note:** The output file cannot be saved in the folder that contains the software files. **Note:** The path must be a local path. The software does not support conversion across a network.
`--nocompression`	Do not compress spectral or chromatographic data.
`--mzMLIndexed`	Add index data for spectral and chromatographic data. **Note:** Indexed `mzml` files let some software applications read in a random order more quickly.

Table 3-2 Command Line Parameters (continued)

Parameter	Description
`--overwrite`	If the file name is found, then overwrite the file. **Note:** If the file name is found and this parameter is not used, then a new file is created with a number added to the end of the file name.
`--skipExisting`	If the file name is found, then do not overwrite the file, and do not convert the sample.
`--sample:<n>`	Convert the sample with the index <*n*>. If this option is not used, then all of the samples are converted. To convert the first sample: `--sample:1`
`--centroidMetric:<value>`	Select the metric to use for the centroid value for the peak. These options are available: • `IntensitySumAbove50Percent` • `Area` • `Height` • `Intensity` • `TotalIntensitySum` (default) **Note:** This parameter is applicable if the `--centroid` option is used.
`--centroidSmooth:<value>`	Select the level of smoothing to use. These options are available: • `Moderate` (default): Satisfactory for most workflows. • `Low`: Applicable to workflows with isotope clusters that are highly charged. **Note:** This parameter is applicable if the `--centroid` option is used.
`--centroidScaleFactor:<n>`	Multiply the metric for the centroid value for the peak by <*n*>. If the downstream software requires peak values (for example, Area) to be more than 1.0, then use this option. **Note:** This parameter is applicable if the `--centroid` option is used.
`--zeroPadding`	Keep a zero-intensity point at the start and end of each peak.

Table 3-2 Command Line Parameters (continued)

Parameter	Description
`--include IsolatedPoints`	Keep peaks from single data points that have zero-intensity points before and after them. **Note:** This parameter is applicable if the `--centroid` option is used.

Use a Batch

Use this procedure to convert MS data with a batch file.

Note: The procedure uses an example batch file: `Example batch file.bat`.

1. Create a text file with a `bat` extension. For example, `Example batch file.bat`.

   Note: If the computer is configured to hide file extensions for known file types, then, in File Explorer, open the View tab, and then click **Options**. Open the View tab, and then clear the **Hide extensions for known file types** check box.

2. Add the commands to the batch file. For help with command creation, refer to the section: Use the Command Line.

   Tip! At the end of the batch file, include a `pause` command, to keep the command window open after the batch is completed.

   ```
   SciexMSDataConverter.exe C:\Data\file.wiff
        --output:C:\Data\file.mzml --sample:1
   pause
   ```

   This example batch converts the first sample in the `file.wiff` file to an `mzml` file with the same file name but a different extension.

   To convert multiple input files in the same batch file, include multiple conversion commands.

Tip! On a computer with multiple cores, multiple conversions can be done in parallel to decrease processing time. Start each conversion as a separate instance, as shown in the example that follows.

```
start "<instance1>" /i SciexMSDataConverter.exe C:\Data\file.wiff
     --output:C:\Data\file1.mzml --sample:1
timeout 10
start "<instance2>" /i SciexMSDataConverter.exe C:\Data\file.wiff
     --output:C:\Data\file5.mzml --sample:5
timeout 10
start "<instance3>" /i SciexMSDataConverter.exe C:\Data\file.wiff
     --output:C:\Data\file7.mzml --sample:7timeout 10
start "<instance4>" /i SciexMSDataConverter.exe C:\Data\file.wiff
     --output:C:\Data\file10.mzml --sample:10
timeout 10
pause
```

Where *<instance1>* to *<instance4>* are user-defined names for the different instances of the software.

3. Save the batch file.
4. Copy the batch file to the folder that contains the SCIEX MS Data Converter software.
5. Double-click the batch file to start it.

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