

TOF-MS data conversion

imzML→imdx

If you use "Auto", the data may be too large, so specify the sampling interval.

In the case of profile data (.imzML)

The screenshot displays the IMDX Converter application window, which is divided into two main sections: **Input** and **Output**.

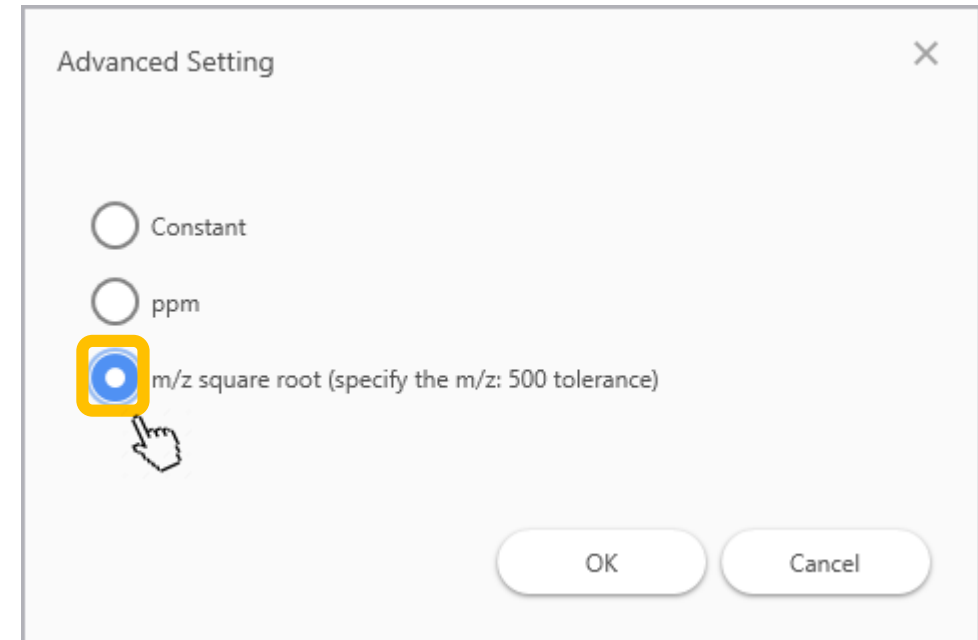
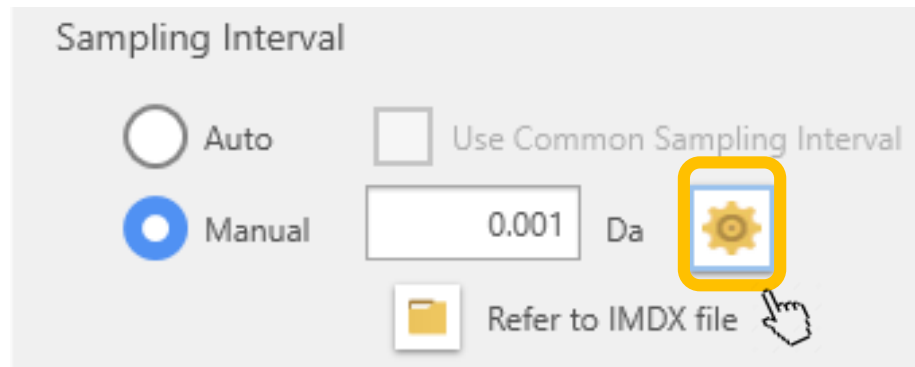
Input Section (KBD/imzML/analyze/RAW):

- Target Data:** Shows the source file path as `E:\Dropbox (Shimadzu)\Yamaguchi_data\data\imzml` and the file name as `With_location_file.imzML`. It also displays technical details: `Number of Pixels: 35(7, 5)`, `Pitch: 10.0, 10.0 [um]`, and `Measurement Range: m/z 0.999467134 - 4999.912109375`. Under the `m/z - Processed` section, the **Profile** radio button is selected and highlighted with a green box, while the **Centroid** radio button is unselected.
- Reference Image:** This section is currently empty, showing fields for `Folder:` and `File Name:`, and a `Preview:` area.

Output Section (IMDX):

- Output Data:** The destination folder is set to `E:\Dropbox (Shimadzu)\Yamaguchi_data\data\imzml` and the output file name is `With_location_file`.
- Conversion Parameter:** This section contains several configuration options:
 - m/z Range:** The **All Areas (Auto Calculation During Conversion)** radio button is selected. The `m/z` range is set to `5 - 4999.912109375`.
 - Noise Cut:** The **None** radio button is selected.
 - Sampling Interval:** The **Manual** radio button is selected and highlighted with a yellow box. The interval is set to `0.001 Da`. The `Auto` and `Use Common Sampling Interval` options are unselected.
 - Mass Compensation:** The **Peak Setting** checkbox is unselected.
 - Intensity Correction:** The **Intensity Correction TOF** checkbox is checked.
 - Sample Information:** The **Polarity** and **Matrix** dropdown menus are both set to `Unknown`.
 - Comments:** A text area for entering additional information is present at the bottom.
- Downsampling:** This section is partially visible at the bottom of the interface.

Press the gear button to select “m/z square root”.



Enter the upper limit value (this is the sampling interval around m/z500 of the data to be converted)



This will convert the data without wasting time and data quality.

In the case of Centroid data (.imzML)

The screenshot displays the IMDX Converter application window, which is divided into two main panels: **Input** and **Output**.

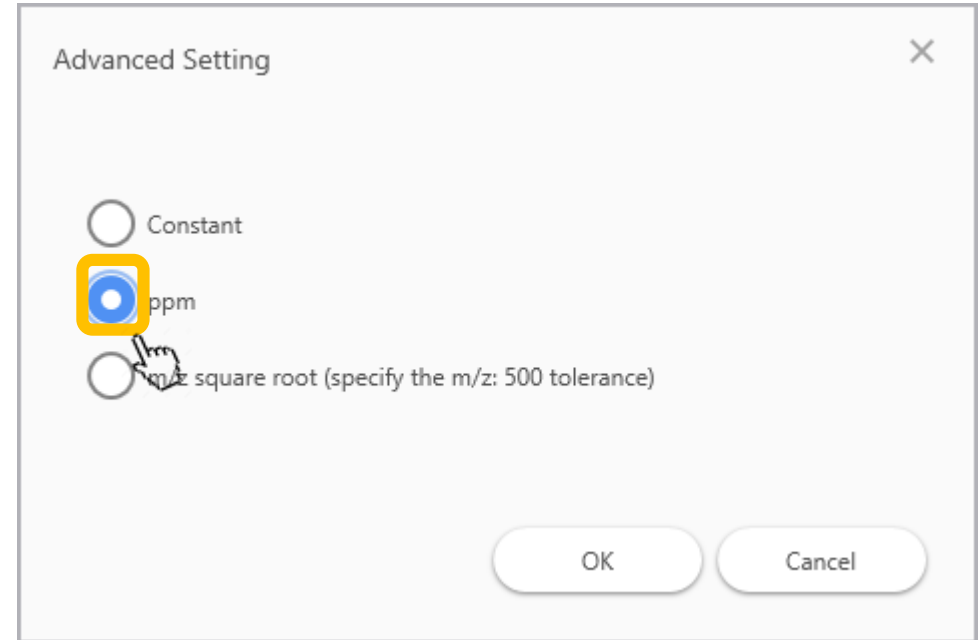
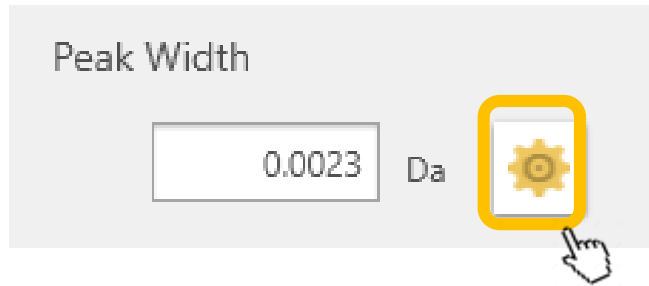
Input Panel (KBD/imzML/analyze/RAW):

- Target Data:**
 - Folder: E:\Dropbox (Shimadzu)\Yamaguchi_data\demo_data_etc\DemoData\IMDX
 - File Name: Liver_Slide9_9AA_200-600_A_2.5x_1_AREA01_centroid.imzML
 - Number of Pixels: 8260(140, 59)
 - Pitch: 50.0, 50.0 [um]
 - Measurement Range: m/z 200.334898147 - 599.630586581
 - m/z: Processed
 - Profile
 - Centroid
- Reference Image:**
 - Folder: (empty)
 - File Name: (empty)
 - Preview: (empty)

Output Panel (IMDX):

- Output Data:**
 - Folder: E:\Dropbox (Shimadzu)\Yamaguchi_data\demo_data_etc\DemoData\IMDX
 - File Name: Liver_Slide9_9AA_200-600_A_2.5x_1_AREA01_centroid
- Conversion Parameter:**
 - m/z Range:**
 - All Areas (Auto Calculation During Conversion)
 - m/z: 200.334898147 - 599.630586581
 - Noise Cut:**
 - None
 - Cut Below Specified Percentage: 10 %
 - Peak Width:** 0.0023 Da
 - Downsampling:** Bin Size: 1
- Mass Compensation:**
 - Peak Setting
- Intensity Correction:**
 - Intensity Correction TOF
- Sample Information:**
 - Polarity: Unknown
 - Matrix: Unknown
- Comments:** (empty text area)


Press the gear button to select "ppm".



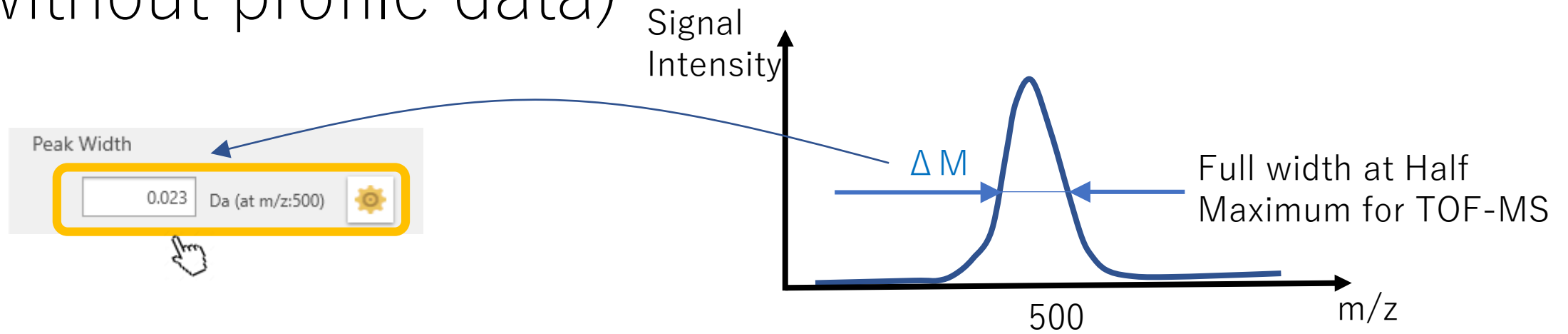
Enter the resolving power in ppm.

For example,
100 ppm when the resolution is 10,000
20 ppm when the resolution is 50,000

Peak Width

 ppm 

Enter the peak width ΔM around m/z 500 of the data to be converted (cannot be confirmed without profile data)



mass resolving power : $M/\Delta M$

- If the measurement range does not include m/z 500,
1. find $R = M/\Delta M$ (this M can be any m/z).
 2. $\Delta M @ m/z 500 = 500/R$