

Problems with IMDX files that have been converted from imzML

1. The file is too big
2. Peaks disappear
3. Masses shift

The sampling interval may be the issue

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2. Peaks disappear
3. Masses shift

It is possible that an appropriate sampling interval has not been set.

IMDX Converter

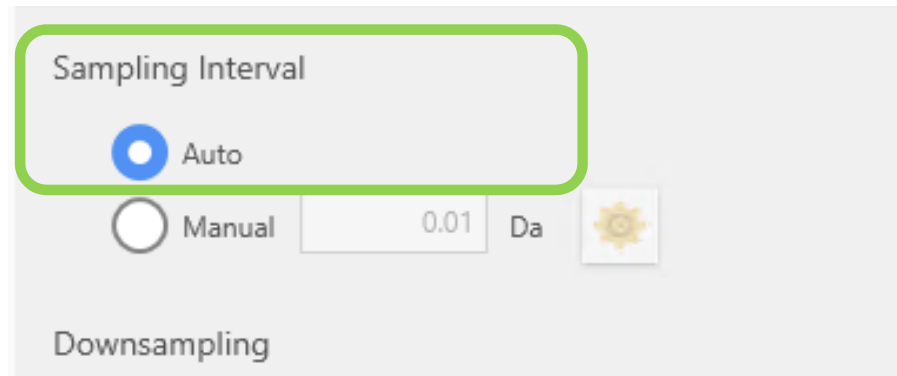
The screenshot displays the IMDX Converter software interface, which is divided into several sections:

- Input (KBD/imzML/analyze):**
 - Target Data:** Shows folder (C:\temp), file name (test.imzML), number of pixels (44220(220, 201)), pitch (30.0, 30.0 [um]), and measurement range (m/z 687.952941894 - 899.994995118). The spectrum type is set to "Profile" (highlighted with a green box).
 - Reference Image:** Includes fields for folder and file name, and a preview area.
- Output (IMDX):**
 - Output Data:** Shows folder (C:\temp) and file name (test).
 - Conversion Parameter:**
 - m/z Range:** Options include "All Areas (Auto Calculation During Conversion)" (selected) and "m/z" with a range of 687.952941894 - 899.994995118.
 - Noise Cut:** Options include "None" (selected) and "Cut Below Specified Percentage" (10 %).
 - Sampling Interval:** Options include "Auto" (selected) and "Manual" (0.01 Da, highlighted with a green box).
 - Downsampling:** Bin Size is set to 1.
 - Mass Compensation:** Includes a "Peak Setting" checkbox.
 - Intensity Correction:** Includes an "Intensity Correction TOF" checkbox.
 - Sample Information:** Includes dropdowns for Polarity (Unknown) and Matrix (Unknown), and a "Comments" text area.
- Conversion List:** A table with columns: No., Input File Name, Measurement Range, Output Destination Folder, Output File Name, and m/z Range.

Buttons for "Add to Conversion List" and "Run Convert" are visible at the bottom right.

If the spectrum type is set as "Profile", then "Sampling Interval" settings can be applied.

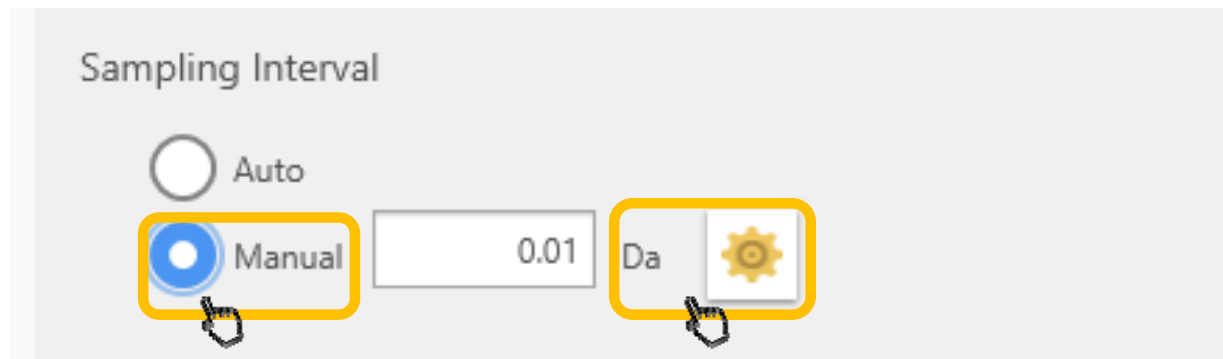
The default sampling interval setting is “Auto”



However, depending on the imzML file, this can result in problems such as:

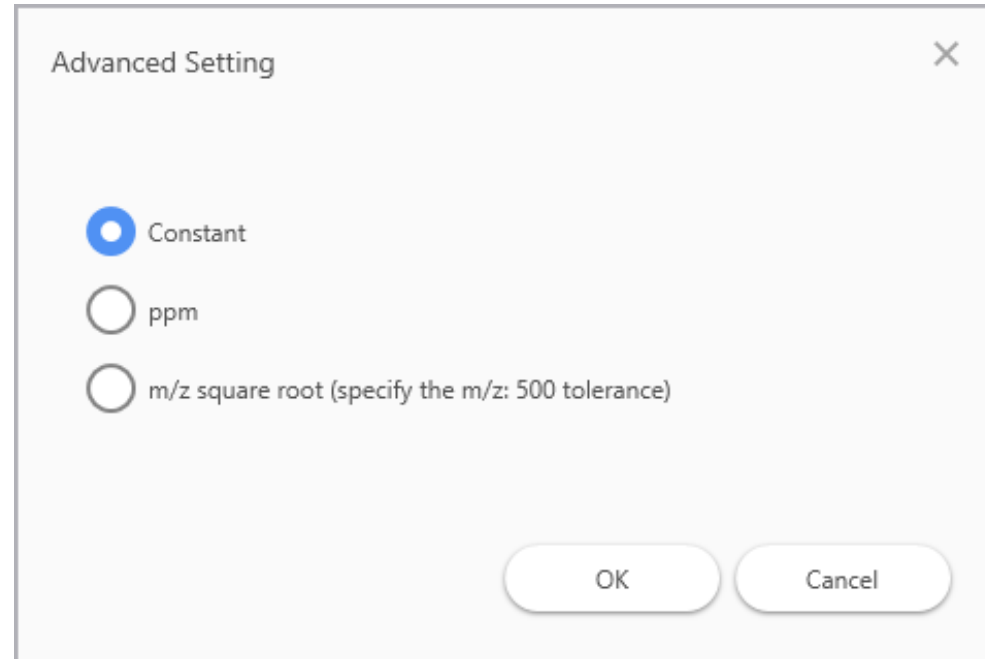
1. File size is too big -> Sampling interval is too small
2. Peaks disappear -> Sampling interval is too big
3. Masses are not aligned -> Sampling interval is too big

Choose the “Manual” setting for the sampling interval



Select “Manual” and you can now type in a value. Click on the cog icon to change the units in “Advanced Settings”.

Advanced settings

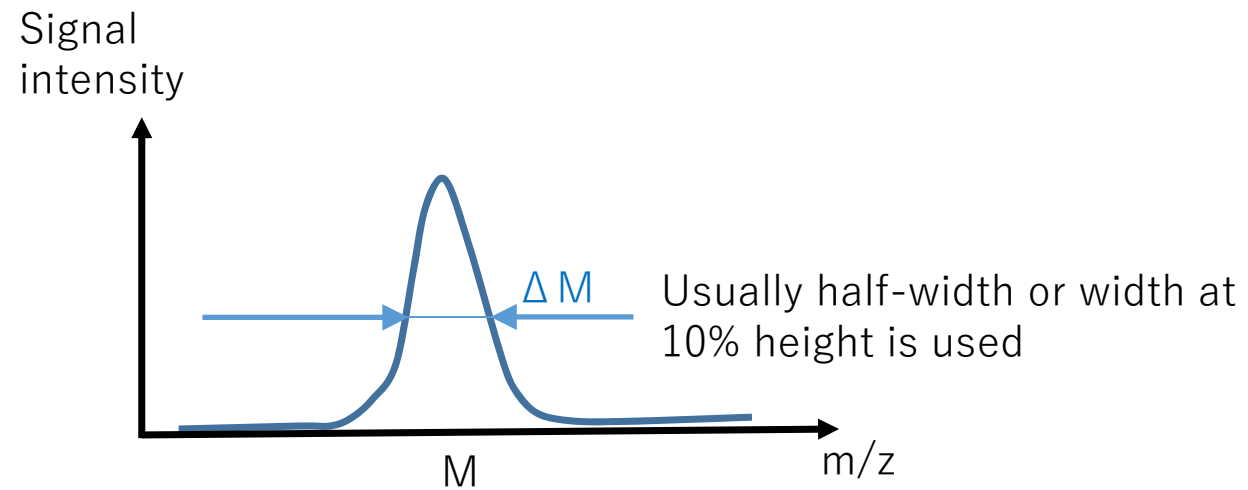


FT-ICR: ppm
Orbitrap, TOF: m/z square root
Other: Constant
are recommended.

Approximate sampling interval (10 points/peak)

- Constant (files tend to become large)
 - e.g. target peak is m/z 500 with peak width 1 Da: 0.1 Da
- ppm
 - $1/(\text{mass resolution} \times 10)$
 - e.g. if mass resolution = 50,000, then $1/(50,000 \times 10) = 2/1,000,000 = 2$ ppm
- m/z square root
 - In this software, the width in Da of a peak at m/z 500 is specified.
 - e.g. target peak is m/z 500 with peak width 1 Da: 0.1 Da
 - The sampling interval changes in proportion to the square root of m/z .

Calculation of mass resolution



Mass resolution: $M/\Delta M$