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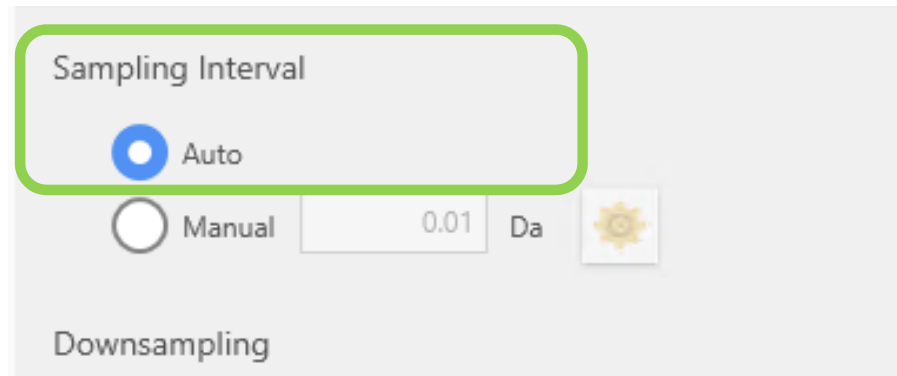
IMDX Converter

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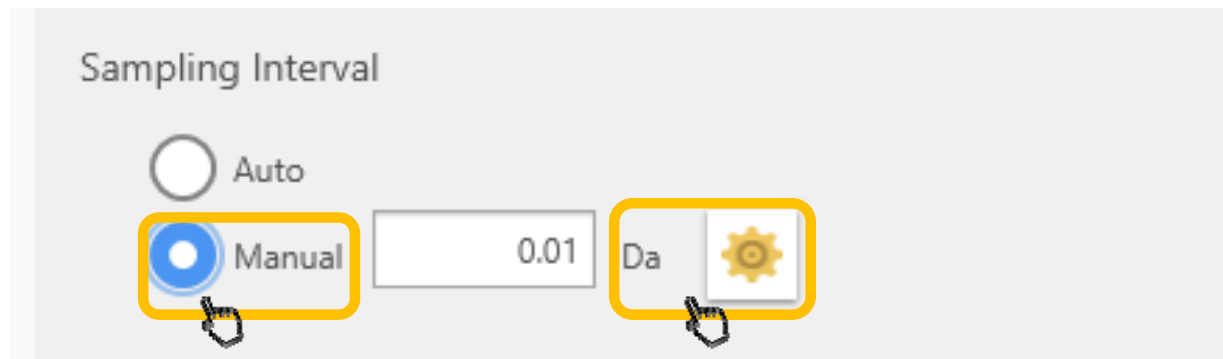
Select "Manual" and you can now type in a value. Click on the cog icon to change the units in "Advanced Settings".

Advanced settings

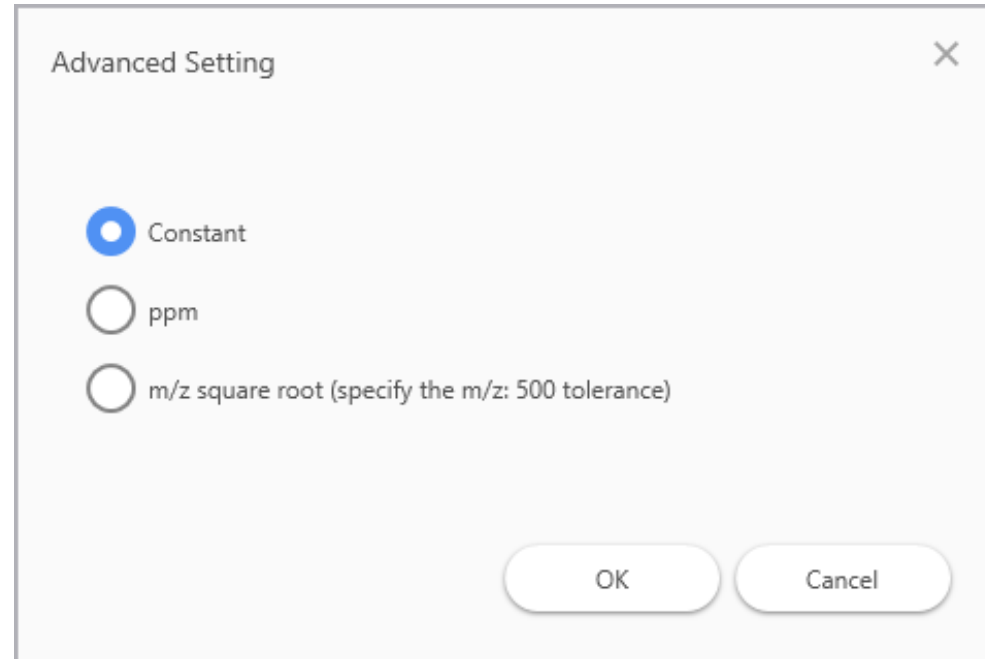Advanced Setting   ×

○ Constant

○ ppm

○ m/z square root (specify the m/z: 500 tolerance)
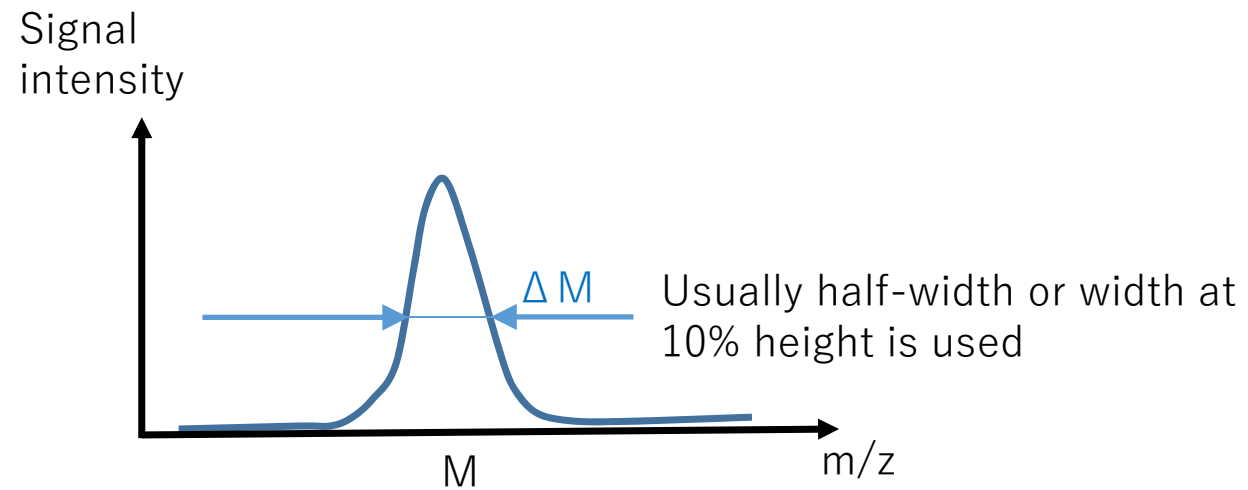
OK   Cancel

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/(mass resolution x 10)
  - e.g. if mass resolution = 50,000, then 1/(50,000 x10) = 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: $M/\Delta M$