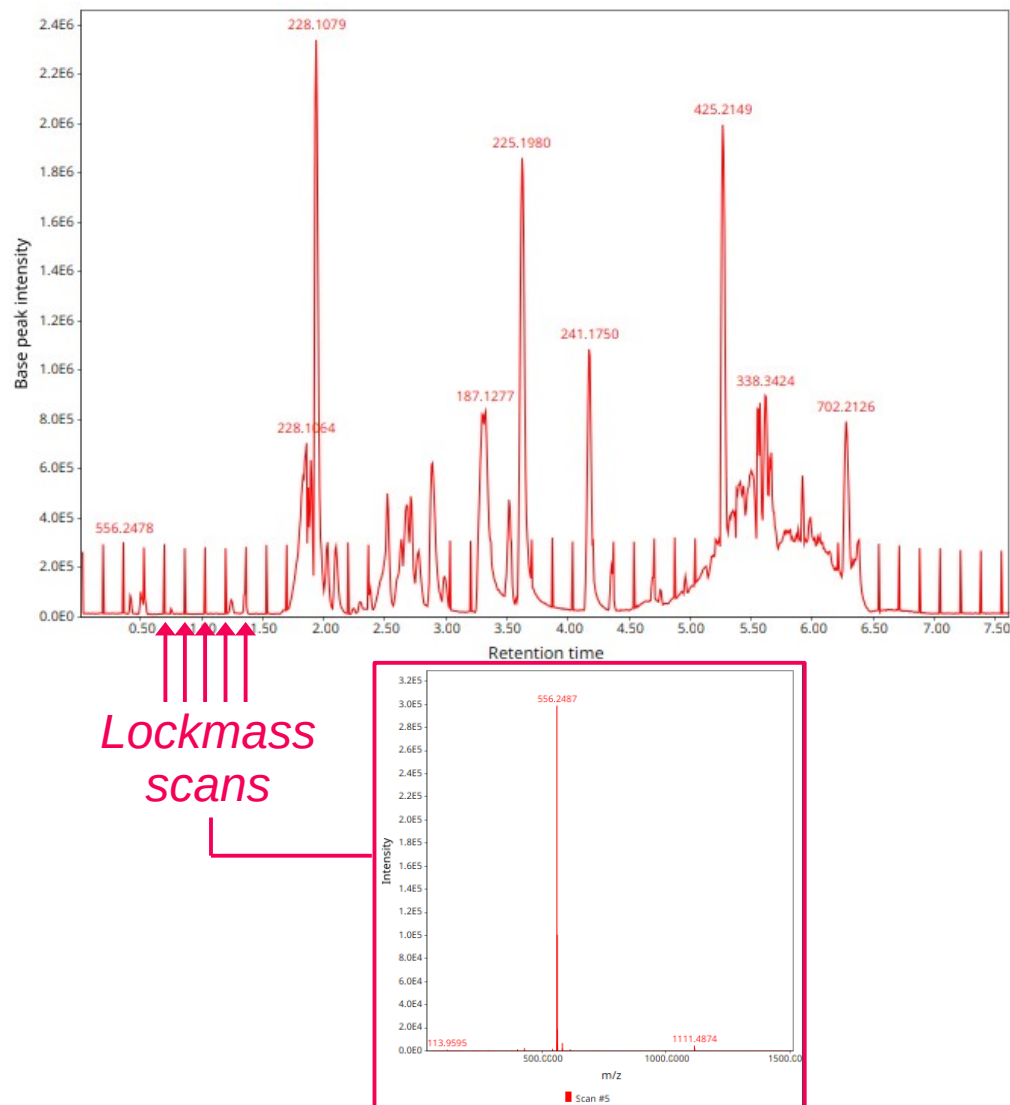
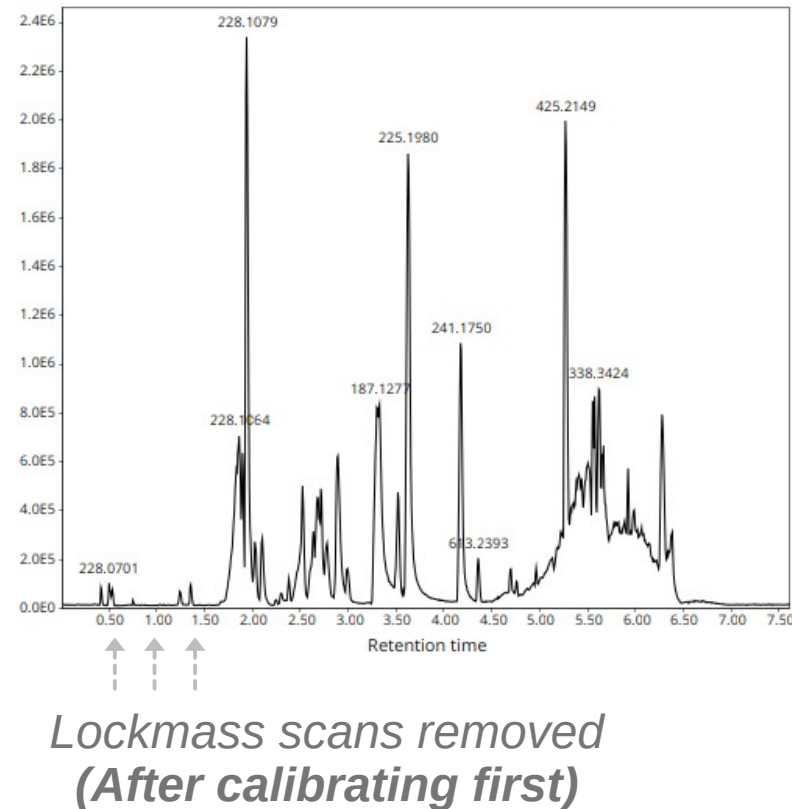


Improperly converted Waters dataset in MZMine:



Correctly converted Waters dataset:



Chromatogram creation will result in this error:

[11:07:07 AM]: Unhandled exception java.lang.IllegalArgumentException: Scans not sorted in retention time dimension! Ca

(Tested in MZMine 4.2)

MSConvertGUI (64-bit)

☒ List of Files ☐ File of file names

File: Browse

Z:\MSdata_RAW_to_convert\20200610_mitomycinC.raw

Filters

Subset

MS levels: - Charge states: -

Scan number: - Number of data points: -

Scan time (seconds): - Collision energy: - ...

Scan event: 1 - 2 Activation type: Any

Scan polarity: Any Analyzer type: Any

Output Directory: Z:\MSdata_RAW_to_convert

Options

Output format: mzML Extension:

Binary encoding precision: ☒ 64-bit ☐ 32-bit

Write index: ☒ Use zlib compression: ☒

TPP compatibility: ☒ Package in gzip: ☐

Use numpress linear compression: ☐

Use numpress short logged float compression: ☐

Use numpress positive integer compression: ☐

Combine ion mobility scans: ☐

SIM as spectra: ☐ SRM as spectra: ☐

Filter	Parameters
peakPicking	vendor msLevel=1-
threshold	absolute 1E3 most-intense
lockmassRefiner	mz=556.27658 tol=0.5
scanEvent	1-2

Presets: Generic Defaults

Files to convert in parallel: 1

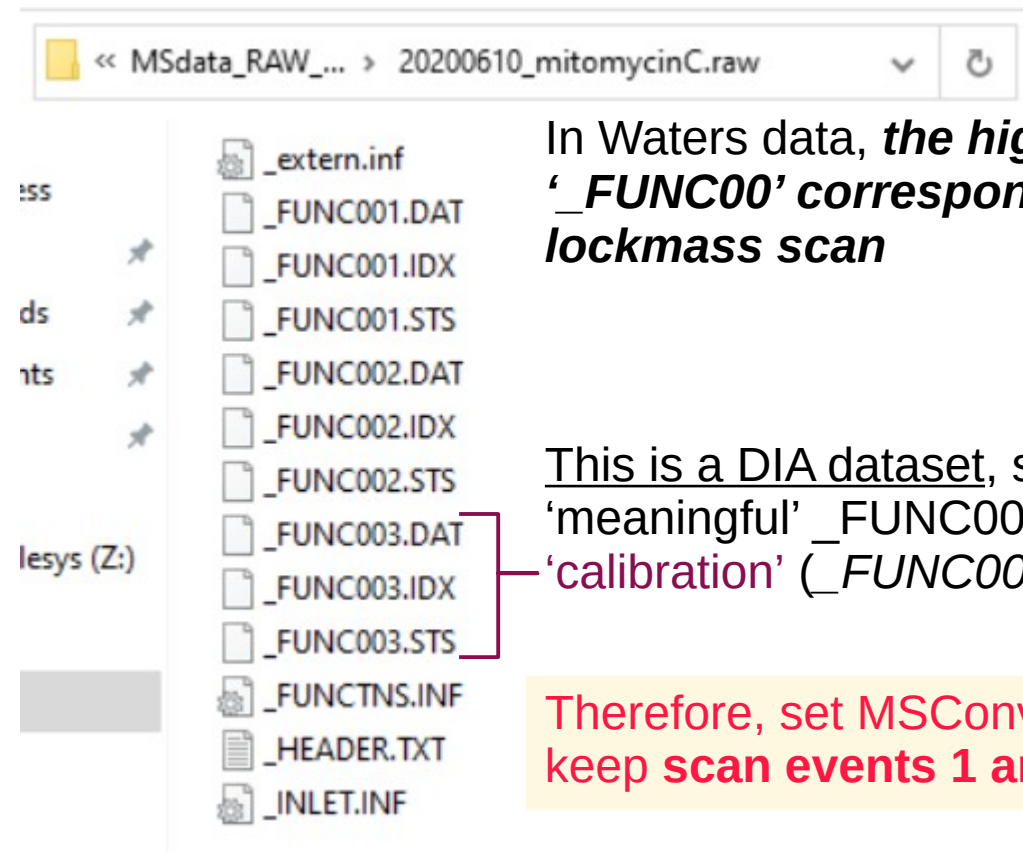
Must be first filter

(Optional)

Calibrate data using LeuEnk
(sometimes Waters .RAW files
are not calibrated)

Critical. Discards lockmass
calibration scans*

See next slide for more info



In Waters data, *the highest number* '**_FUNC00**' corresponds to the **lockmass scan**

This is a DIA dataset, so there's two 'meaningful' _FUNC00's **plus** one for '**calibration**' (_FUNC003)

Therefore, set MSConvert to only keep **scan events 1 and 2**

If converting a DDA dataset with 3 selected MS² precursors per MS¹ scan, then:

Scan event 1 = MS1

Scan event 2 = MS2

Scan event 3 = MS2

Scan event 4 = MS2

Scan event 5 = **calibration**

Remove scan event 5

