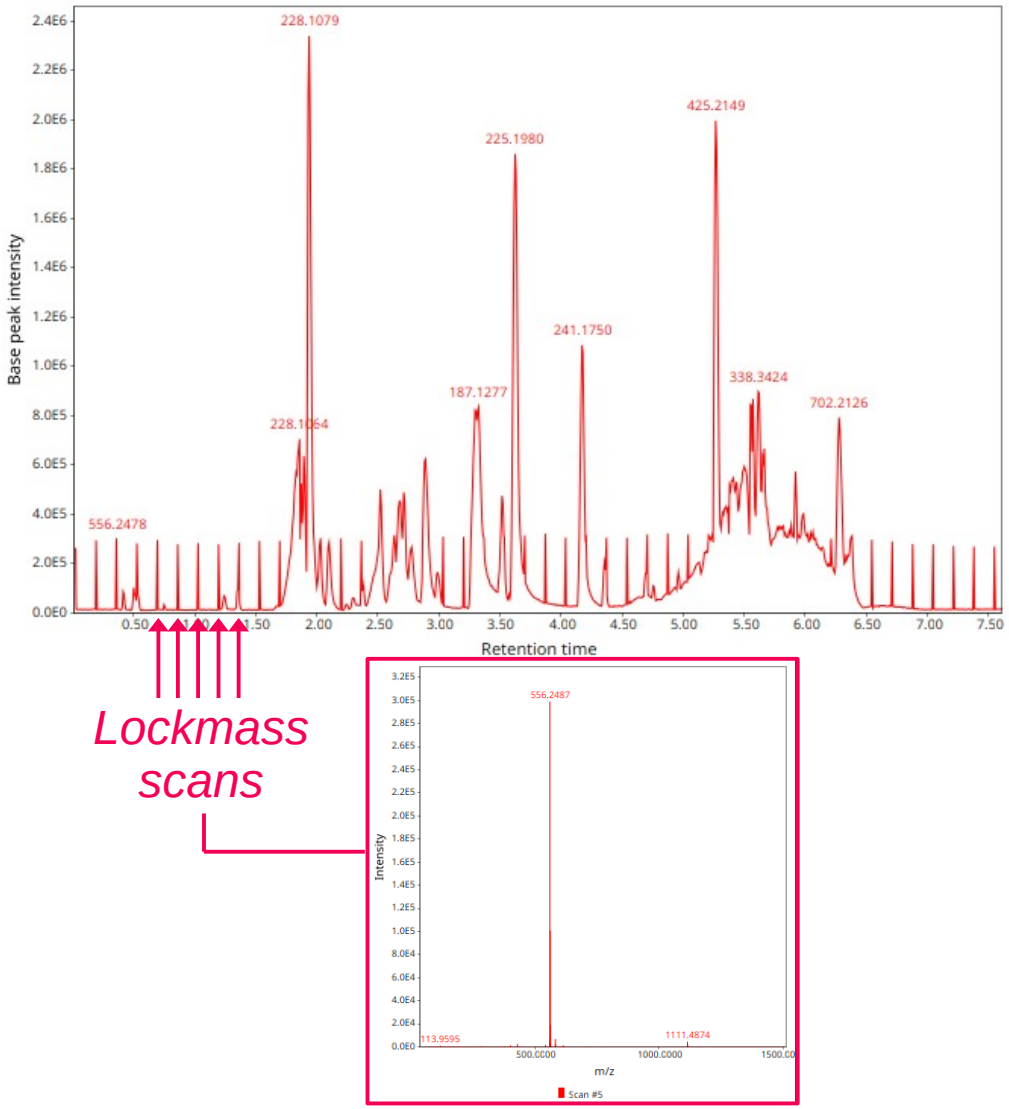
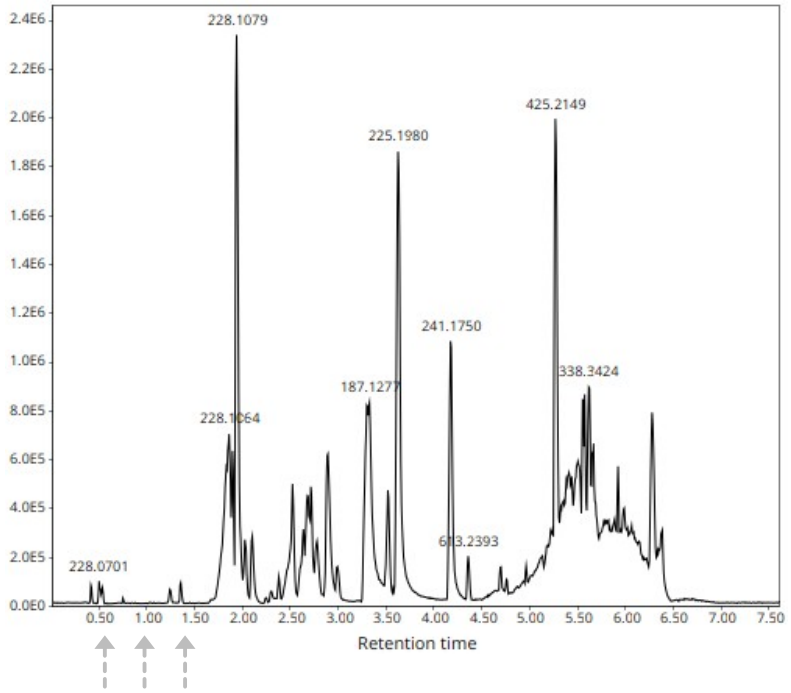
Improperly converted Waters dataset in MZMine:



Correctly converted Waters dataset:

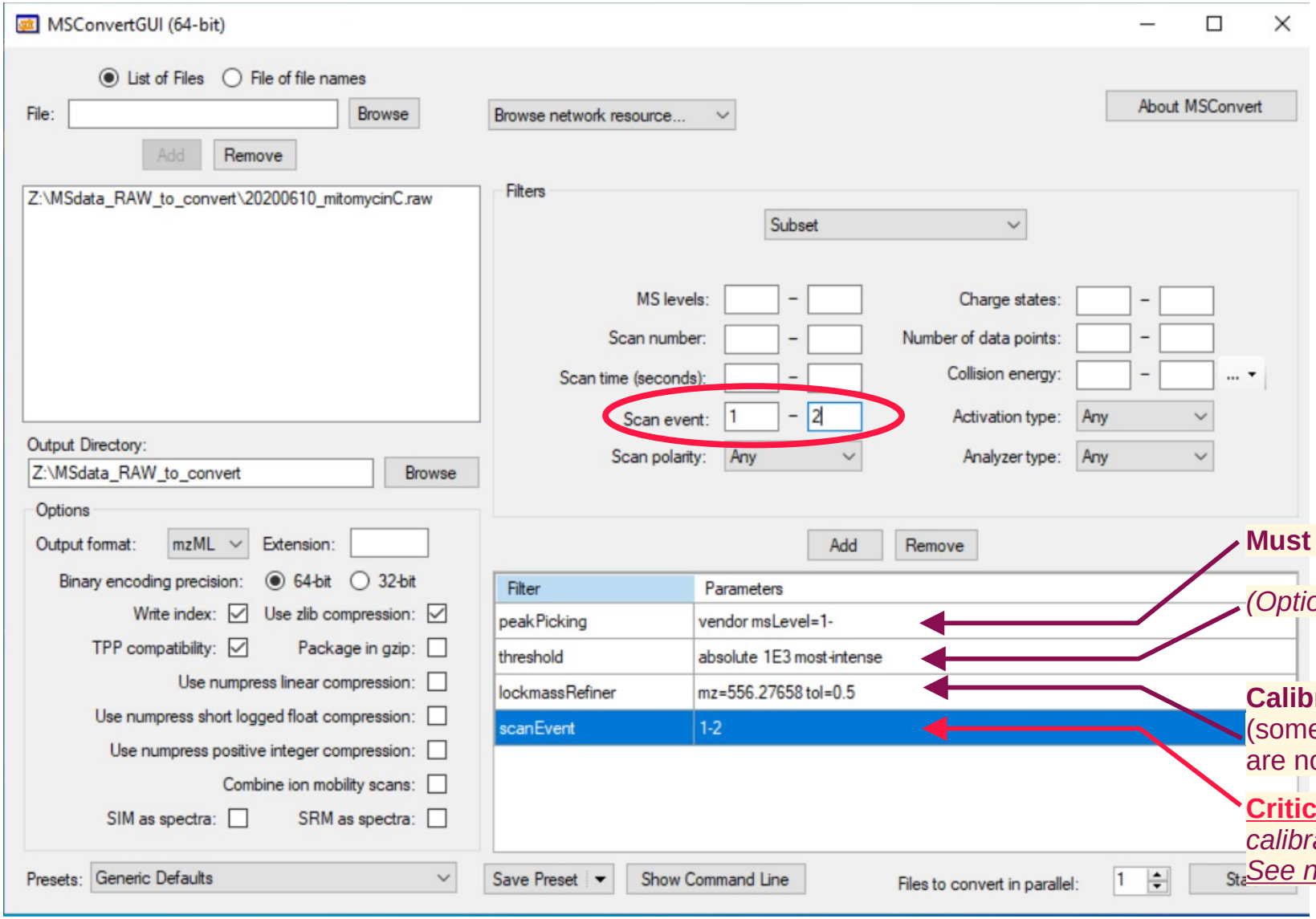


Lockmass scans removed
(After calibrating first)

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)



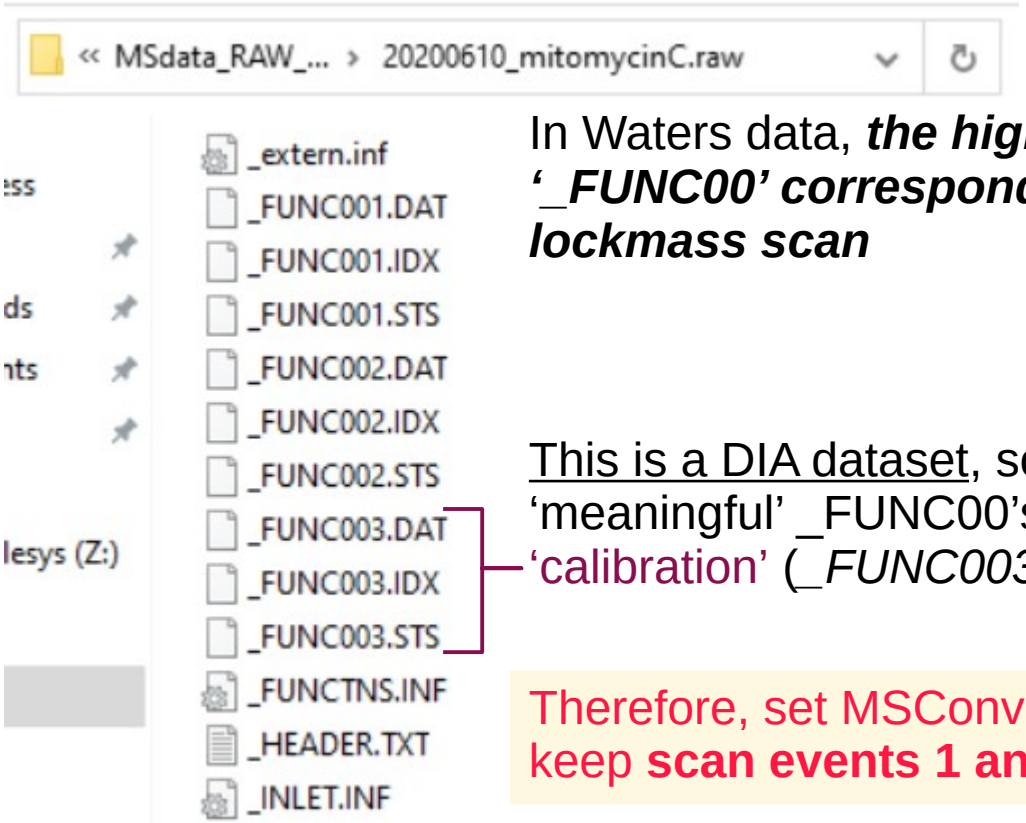
Must be first filter

(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***

<u>This is a DIA dataset</u>, 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 MS^2 precursors per MS^1 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