Instructions of a ‘MDF LM’

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Read me first

This program was developed for study purposes, so please be forewarned that you are using it at your own risk. We are not able to provide compensation for any damage it might cause.

The program requires a Microsoft Windows 10 or later "64 bit" environment. It also needs installing a netCDF4 (64bit) run time liberally. The liberally can be obtained from unidata web site (https://www.unidata.ucar.edu/software/netcdf/).

BE SURE TO BACK UP YOUR INPUT DATA BEFORE USING THIS PROGRAM.

Please let us know if you have any special requirements or suggestions. We will consider them for inclusion in our development process.

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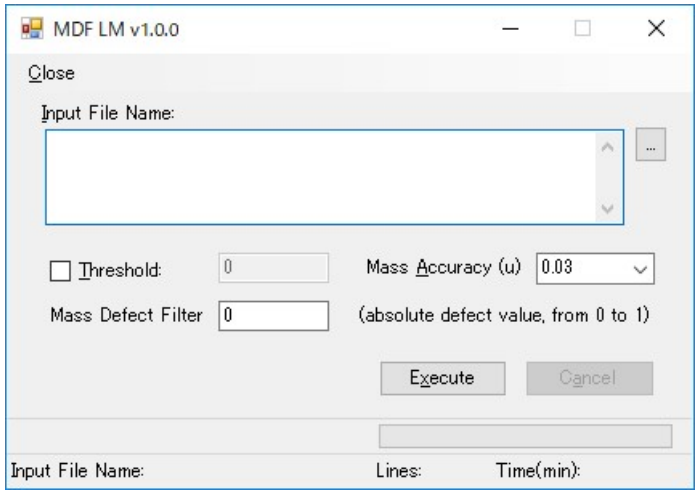
Reference: Hashimoto *et al.*(2013) Journal of Chromatography A, 1282, 183-189

What is a “MDF LM”?



Interface of a “MDF LM”

This software can…

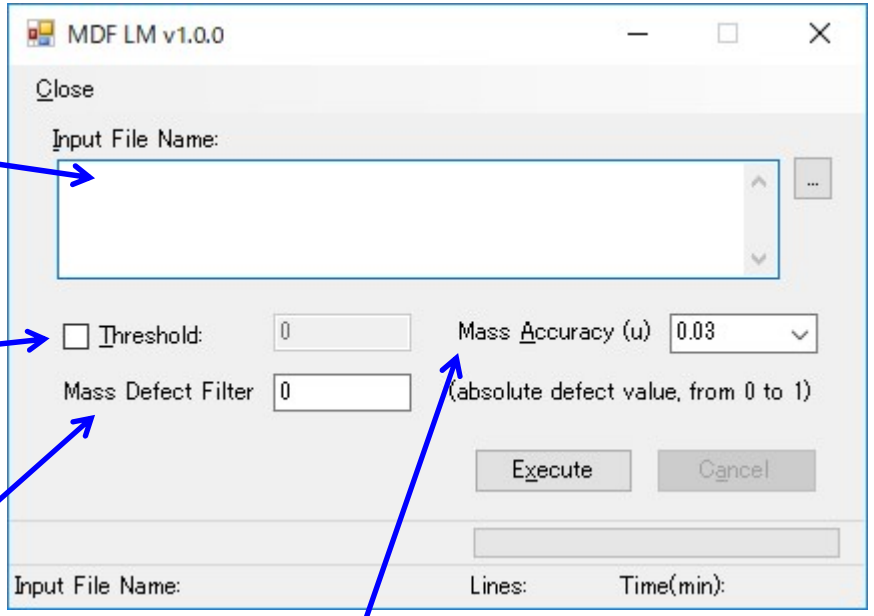
- directly read a netCDF file, which is a common format for MS data,
- and extract mass spectra in range of mass defects,
- under various mass accuracy (mass resolution) conditions,
- and finally, output the result as netCDF.

Main settings for data extraction

1) Input File Name*: choose filename(s) from the dialog box that will appear after right-clicking.

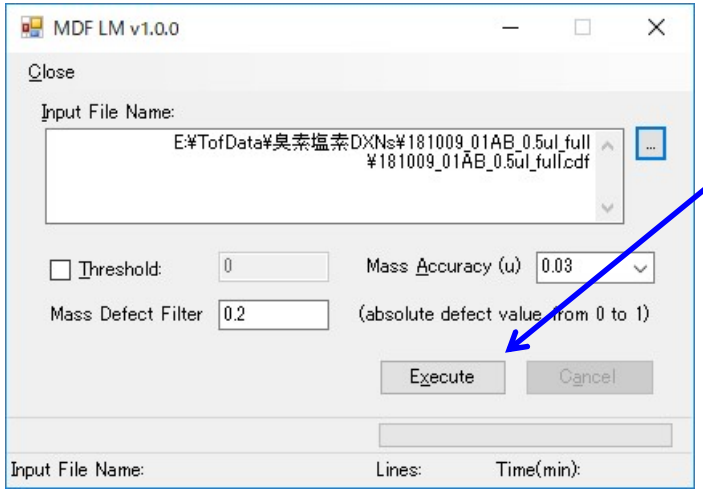
3) Threshold: check and input an integer from 0 to 1,000,000 if needed. Recommended values are 500, 1,000 or 3,000 depending on the situation. (Commas are not required.)

2) Mass Defect Filter*: The value must be from 0 to 1. (See **Technical Guide 1**.)

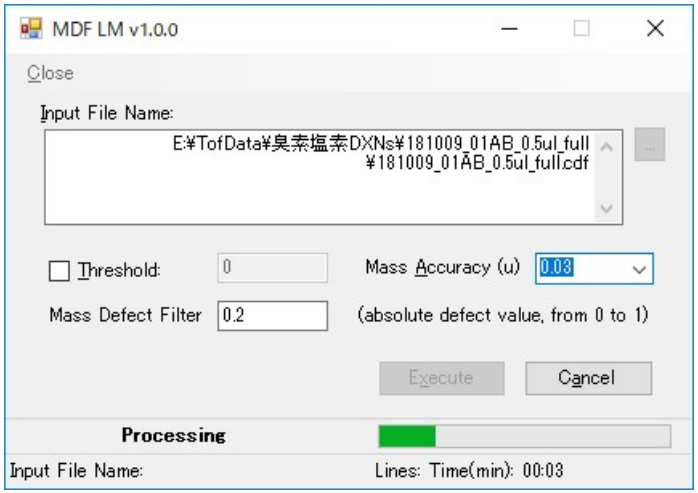


4) Mass Accuracy*: choose a value from 1 to 0.001u. (This parameter will determine the accuracy of the mass, e.g., MA: 0.05u is equivalent to a mass resolution of m/Δm 6,000 @ m/z 300.)

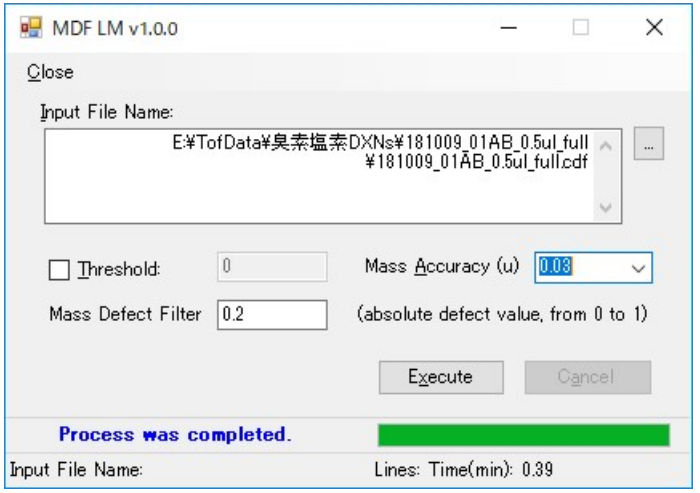
*all fields followed by an asterisk must be filled in.



After all settings are complete, click the **Execute** button.



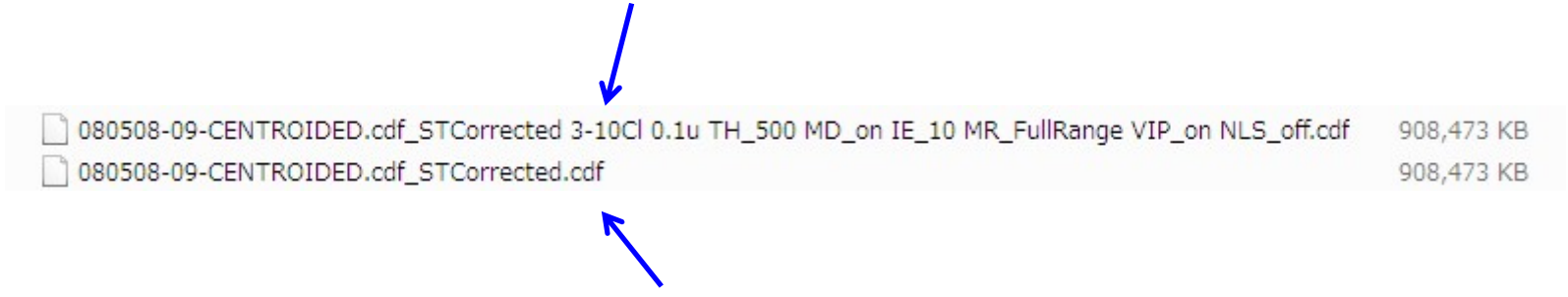
Running program
Elapsed time is displayed.



Completed process

If the process has successfully completed, an output file, formatted as netCDF, is created in the same folder as the input file.

Output file: The file name is automatically created by appending the parameters used for the processing.



Input file: The file must be formatted in netCDF.

1: Filter using mass deficiency

Mass excess (Mass defect):

The mass excess of a nuclide is the difference between its actual mass and its mass number in atomic mass units. .....

— from Wikipedia

Mass deficiency:

Mass deficiency is a state where the mass excess is negative. (actual mass < mass number) N and atoms whose mass number exceeds ^{12}C exhibit mass deficiency .

Mass deficiency is used for simple data filtration before Cl or Br isotopic pattern checking.

Specifically, mass spectra showing mass deficiency within a 0 to -0.2 range are left in the data and the other spectra are removed from the data.

	^{1}H	^{4}He	...	^{12}C	^{14}N	^{16}O	...	^{35}Cl	...	^{79}Br
Atom No.	1	4		12	14	16		35		79
Exact mass	1.007825	4.0026		12	14.003074	15.9949		34.96885268		78.9183371
defference	+0.007825	+0026		±0	+0.003074	-0.0051		-0.03114732		-0.0816629

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