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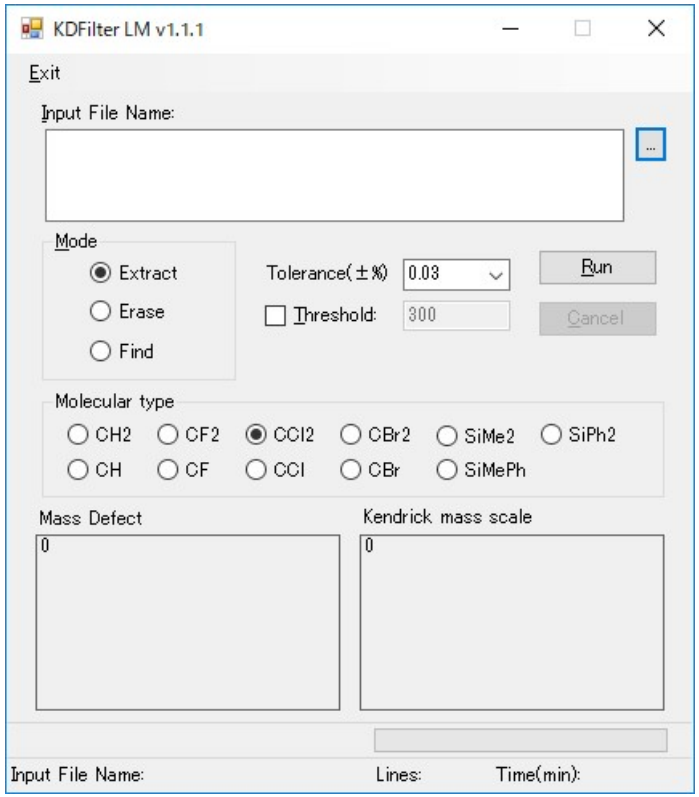
Reference: Hashimoto *et al.*(2013) Journal of Chromatography A, 1282, 183-189

What is a ‘KDF LM’?



Interface of a ‘KDF LM’.

This software can…

- directly read a netCDF file, which is a common format for MS data,
- and selectively extracts or removes mass spectrum matched a condition as follows,

$$Mrnd / Mobs \leq Mnom(U) / Mext(U) * (1 \pm tol)$$

where, Mrnd, Mobs, Mnom(U) and Mext(U) means rounded observed mass, observed mass, nominal and exact mass of a component unit, respectively. Allowable error is expressed by tol.,

- under various mass accuracy (mass resolution) conditions,
- and finally, output the result as netCDF.

Main settings for data extraction

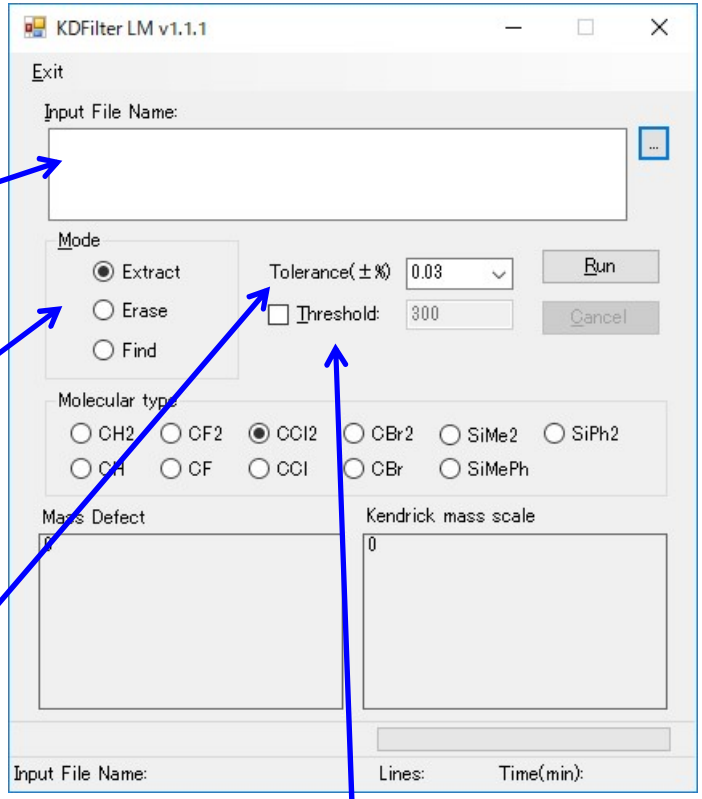
1) Input File Name*: choose filename(s) from the dialog box that will appear after right-clicking.

2) Mode*: choose one from “Extract”; only mass spectra matched conditions will be extracted as new data, “Erase”; only mass spectra NOT matched conditions will be extracted as new data, and “Find”; mass spectra matched conditions and the other mass spectra in the same data point will be extracted as new data

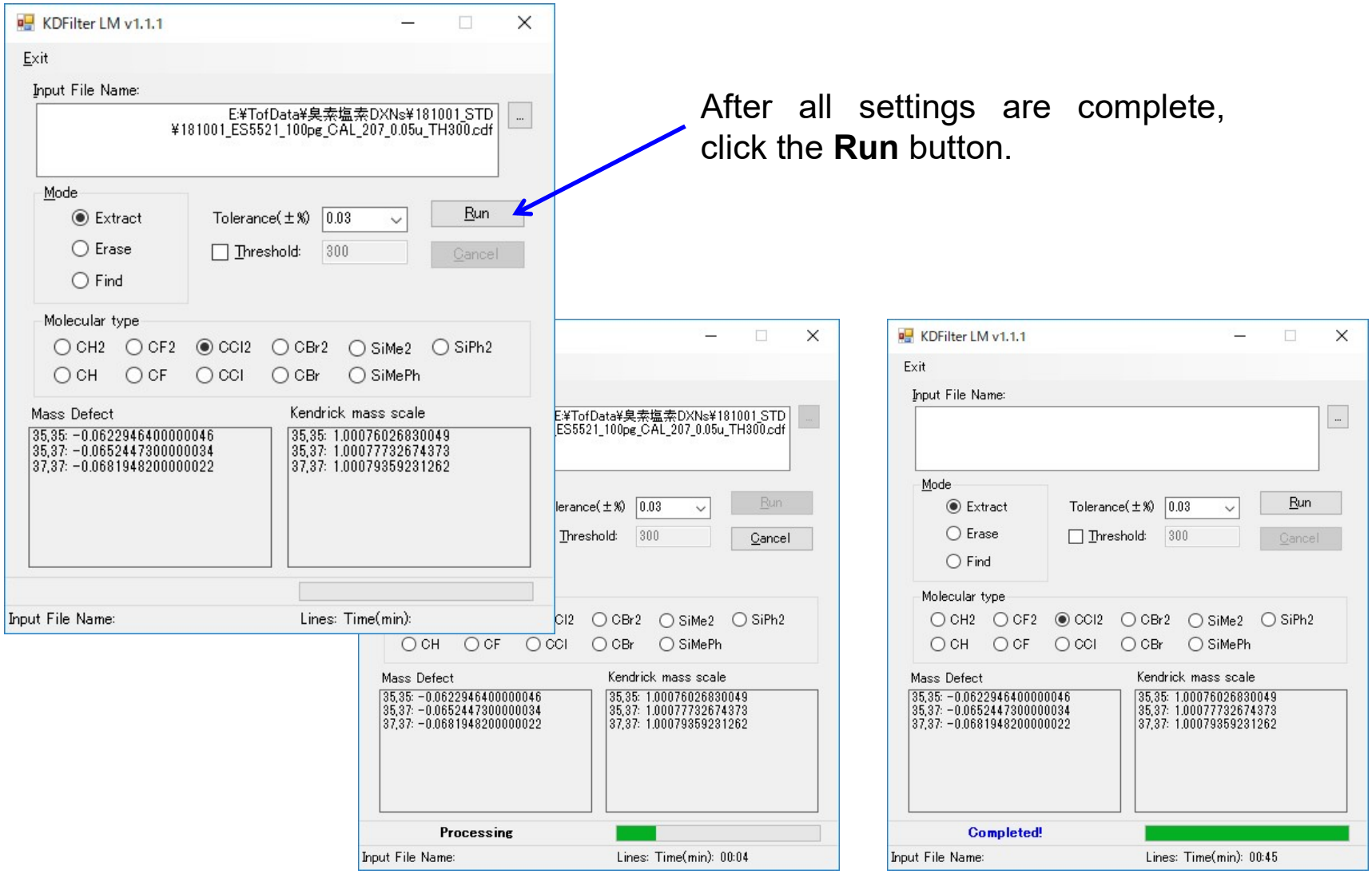
3) Tolerance*: choose a value from 0.001 to 1%.

4) Molecular type*: choose a unit of molecular type. (See **Technical Guide 1-3**.)

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



4) 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.)



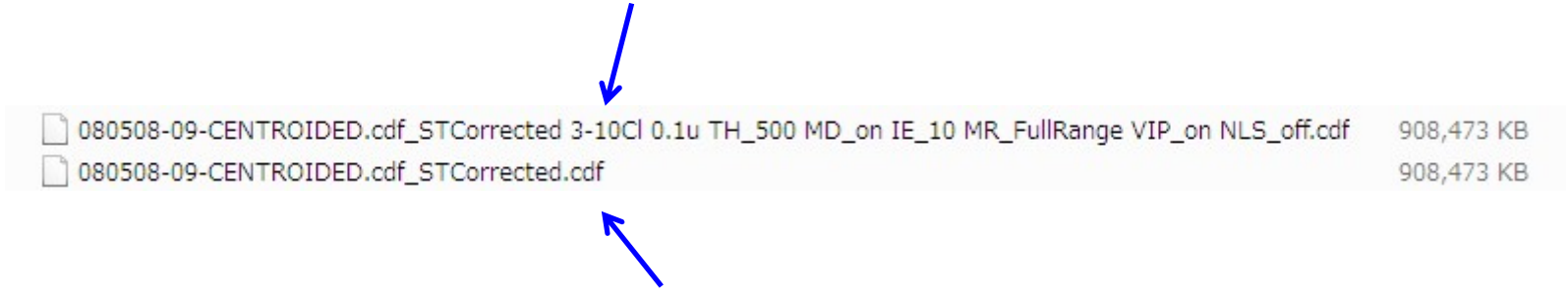
After all settings are complete, click the **Run** button.

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: Mass deficiency

Mass excess (Mass defect):

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

— from Wikipedia

Mass deficiency:

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

	^{1}H	^{4}He	...	^{12}C	^{14}N	^{16}O	...	^{35}Cl	...	^{79}Br
nominal	1	4		12	14	16		35		79
exact	1.007825	4.0026		12	14.003074	15.9949		34.96885268		78.9183371
Difference.	+0.007825	+0026		±0	+0.003074	-0.0051		-0.03114732		-0.0816629

ex)

CH_2 = 0.01565006414

$CCl_2(^{35}Cl*2)$ = -0.06229464

$CCl_2(^{35}Cl^{37}Cl)$ = -0.06524473

$CCl_2(^{37}Cl*2)$ = -0.06819482

$CBr(^{79}Br)$ = -0.081662899

$CBr(^{81}Br)$ = -0.08370940

2: Kendrick mass

Kendrick mass:

The Kendrick mass is defined by setting the mass of a chosen molecular fragment, typically CH2, to an integer value in atomic mass units.....

— from Wikipedia

To convert an IUPAC mass of a particular compound to the Kendrick mass, the equation

$$\text{Kendrick-mass} = \text{IUPAC-mass} \times \frac{14.00000}{14.01565}$$

Other groups of atoms in addition to CH_2 can be used define the Kendrick mass, for example CO_2, H_2, H_2O, and O. In this case, the Kendrick mass for a family of compounds F is given by

$$\text{Kendrick-mass-(F)} = (\text{observed-mass}) \times \frac{\text{nominal-mass-F}}{\text{exact-mass-F}}$$

where, nominal-mass-F/ exact-mass-F is define as **Kendrick mass Scale**.

3: Kendrick mass scale

Kendrick mass deficiency(KMD):

The Kendrick mass defect is defined as the exact Kendrick mass subtracted from the nominal (integer) Kendrick mass:

$$\text{Kendrick-mass-defect} = \text{nominal-Kendrick-mass} - \text{Kendrick-mass}$$

or

$$\text{Kendrick-mass-defect} = \text{nominal-mass} - \text{Kendrick-exact-mass}$$

Kendrick mass scale: nominal-mass-F / exact-mass-F

Kendrick mass scale is typical and constant against each isotopic homologous compound (F).

ex)

CH_2 = 0.9988833864

$CCl_2(^{35}Cl*2)$ = 1.000760268
$CCl_2(^{35}Cl^{37}Cl)$ = 1.000777326
$CCl_2(^{37}Cl*2)$ = 1.000793592

$CBr(^{79}Br)$ = 1.000898201
$CBr(^{81}Br)$ = 1.000900912

Technical guides

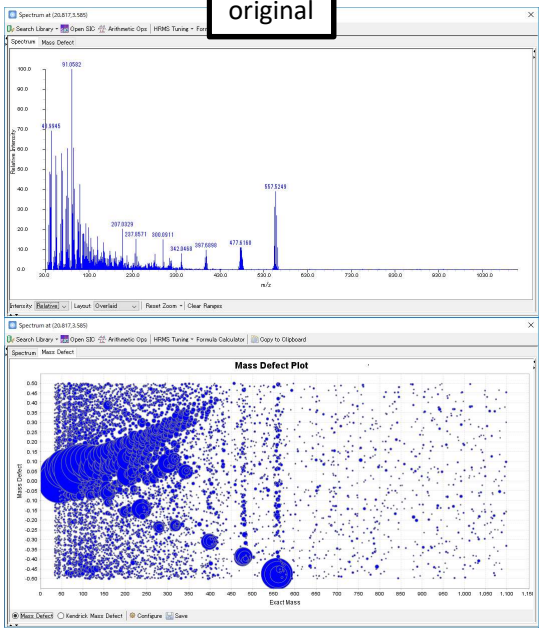
examples of result

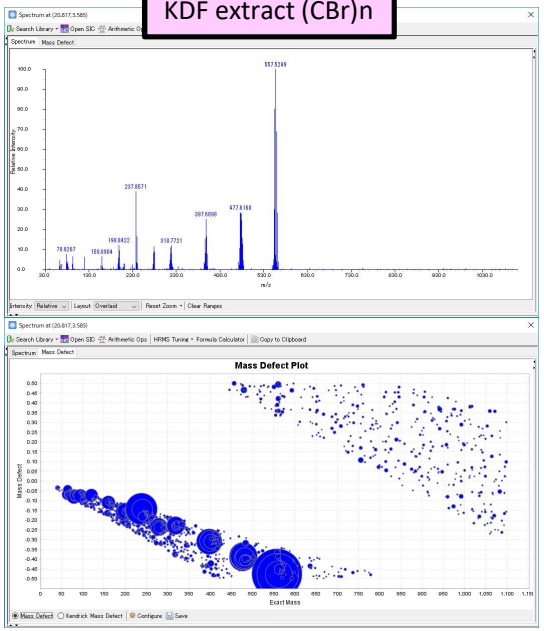
original

KDF extract (CBr)n

mass spectra

mass defect plot



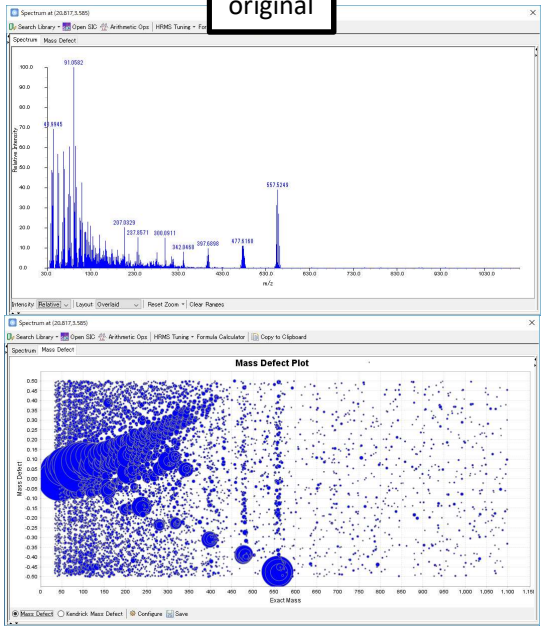


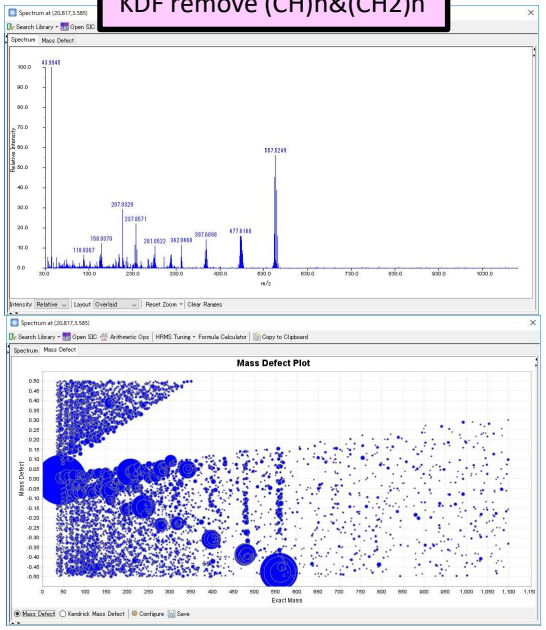
original

KDF remove (CH)n&(CH2)n

mass spectra

mass defect plot





February 15, 2019