

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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Our contact information;

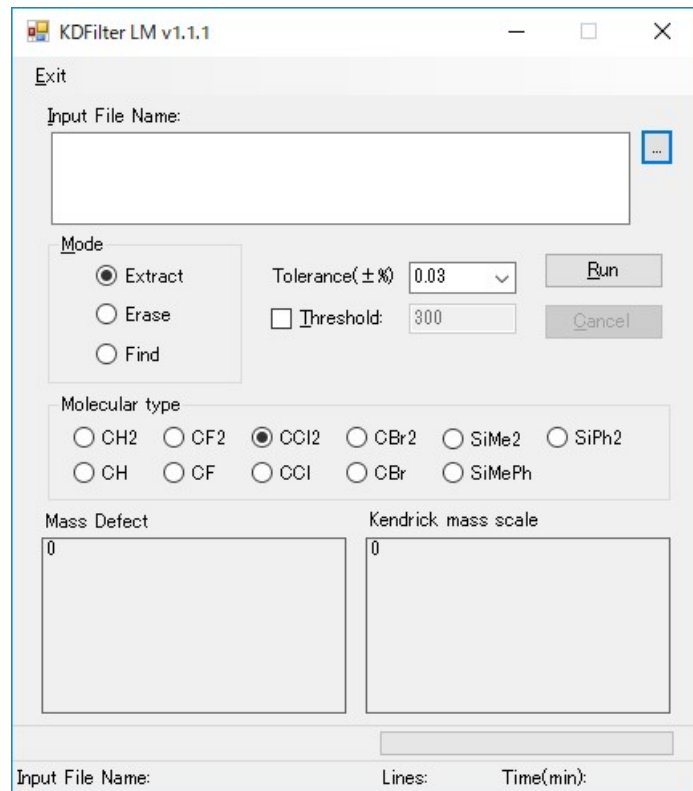
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Reference: Hashimoto *et al.*(2013) Journal of Chromatography A, 1282, 183-189

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.

The screenshot shows the 'KDFilter LM v1.1.1' dialog box. It has a title bar with standard window controls. The main area contains several sections: 'Exit' at the top, 'Input File Name:' with a text box and a browse button (...), 'Mode' with three radio buttons (Extract, Erase, Find), 'Tolerance(±%)' with a dropdown menu showing '0.03', a checkbox for 'Threshold' with a value of '300', 'Molecular type' with two rows of radio buttons (CH2, CF2, CCl2, CBr2, SiMe2, SiPh2 and CH, CF, CCl, CBr, SiMePh), 'Mass Defect' and 'Kendrick mass scale' each with a large empty box, and 'Input File Name:', 'Lines:', and 'Time(min):' at the bottom. Blue arrows point from the text instructions to the 'Input File Name' text box, the 'Extract' radio button, the 'Tolerance' dropdown, and the 'Threshold' checkbox.

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.)

KDFilter LM v1.1.1

Exit

Input File Name:

E:\TofData\臭素塩素DXNs\181001_STD
¥181001_ES5521_100pg_CAL_207_0.05u_TH300.cdf

Mode

☒ Extract ☐ Erase ☐ Find

Tolerance(±%) 0.03

☐ Threshold: 300

Run Cancel

Molecular type

☐ CH₂ ☐ CF₂ ☒ CCl₂ ☐ CBr₂ ☐ SiMe₂ ☐ SiPh₂

☐ CH ☐ CF ☐ CCl ☐ CBr ☐ SiMePh

Mass Defect

35.35: -0.0622946400000046
35.37: -0.0652447300000034
37.37: -0.0681948200000022

Kendrick mass scale

35.35: 1.00076026830049
35.37: 1.0007732674373
37.37: 1.00079359231262

Input File Name:

Lines: Time(min):

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

KDFilter LM v1.1.1

Exit

Input File Name:

E:\TofData\臭素塩素DXNs\181001_STD
ES5521_100pg_CAL_207_0.05u_TH300.cdf

Mode

☒ Extract ☐ Erase ☐ Find

Tolerance(±%) 0.03

☐ Threshold: 300

Run Cancel

Molecular type

☐ CH₂ ☐ CF₂ ☒ CCl₂ ☐ CBr₂ ☐ SiMe₂ ☐ SiPh₂

☐ CH ☐ CF ☐ CCl ☐ CBr ☐ SiMePh

Mass Defect

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37.37: -0.0681948200000022

Kendrick mass scale

35.35: 1.00076026830049
35.37: 1.0007732674373
37.37: 1.00079359231262

Processing

Input File Name:

Lines: Time(min): 00:04

Running program
Elapsed time is displayed.

KDFilter LM v1.1.1

Exit

Input File Name:

E:\TofData\臭素塩素DXNs\181001_STD
ES5521_100pg_CAL_207_0.05u_TH300.cdf

Mode

☒ Extract ☐ Erase ☐ Find

Tolerance(±%) 0.03

☐ Threshold: 300

Run Cancel

Molecular type

☐ CH₂ ☐ CF₂ ☒ CCl₂ ☐ CBr₂ ☐ SiMe₂ ☐ SiPh₂

☐ CH ☐ CF ☐ CCl ☐ CBr ☐ SiMePh

Mass Defect

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37.37: -0.0681948200000022

Kendrick mass scale

35.35: 1.00076026830049
35.37: 1.0007732674373
37.37: 1.00079359231262

Completed!

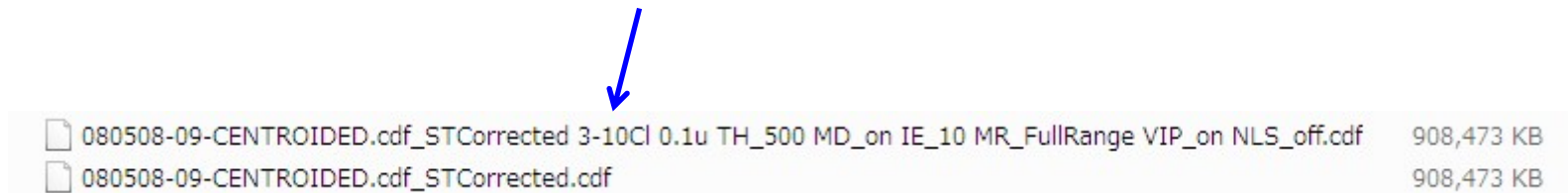
Input File Name:



Lines: Time(min): 00:45

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.



 080508-09-CENTROIDED.cdf_STCorrected 3-10Cl 0.1u TH_500 MD_on IE_10 MR_FullRange VIP_on NLS_off.cdf	908,473 KB
 080508-09-CENTROIDED.cdf_STCorrected.cdf	908,473 KB

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.

	^1H	^4He	...	^{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)

$$\text{CH}_2 = 0.01565006414$$

$$\text{CCl}_2(^{35}\text{Cl} * 2) = -0.06229464$$

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

$$\text{CCl}_2(^{35}\text{Cl}^{37}\text{Cl}) = -0.06524473$$

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

$$\text{CCl}_2(^{37}\text{Cl} * 2) = -0.06819482$$

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 CH₂ can be used to define the Kendrick mass, for example CO₂, H₂, H₂O, 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 defined 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: $\text{nominal-mass-F} / \text{exact-mass-F}$

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

ex)

$$\text{CH}_2 = 0.9988833864$$

$$\text{CCl}_2(^{35}\text{Cl} * 2) = 1.000760268$$

$$\text{CBr}(^{79}\text{Br}) = 1.000898201$$

$$\text{CCl}_2(^{35}\text{Cl}^{37}\text{Cl}) = 1.000777326$$

$$\text{CBr}(^{81}\text{Br}) = 1.000900912$$

$$\text{CCl}_2(^{37}\text{Cl} * 2) = 1.000793592$$

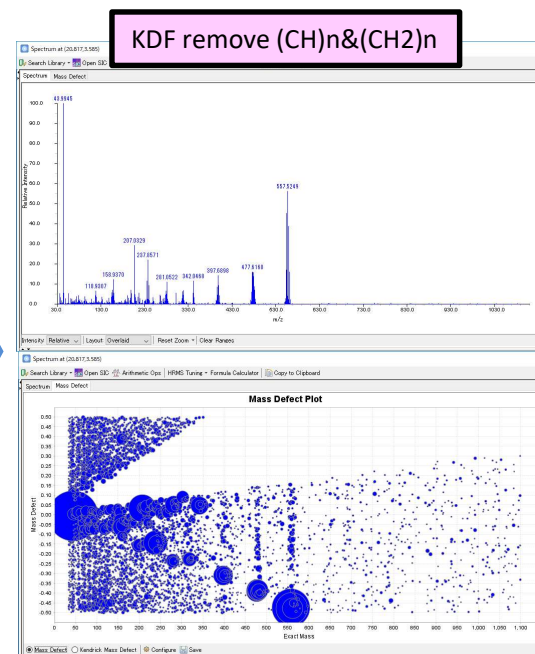
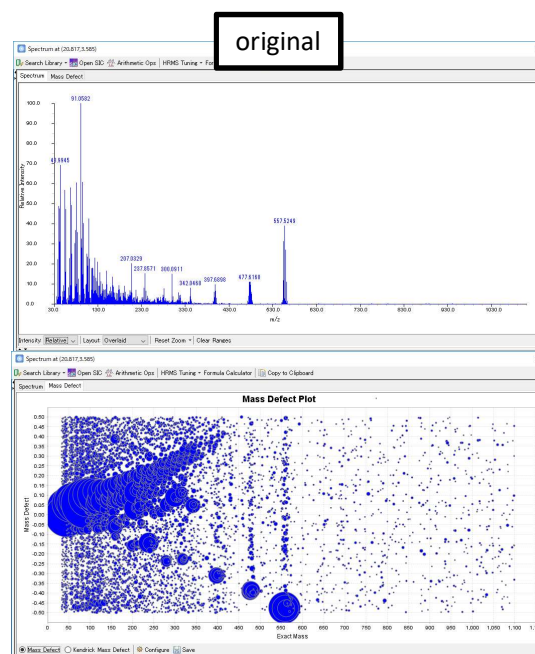
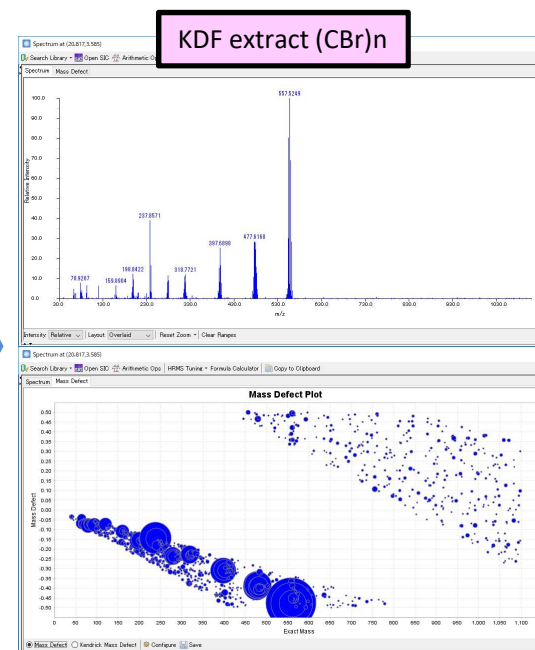
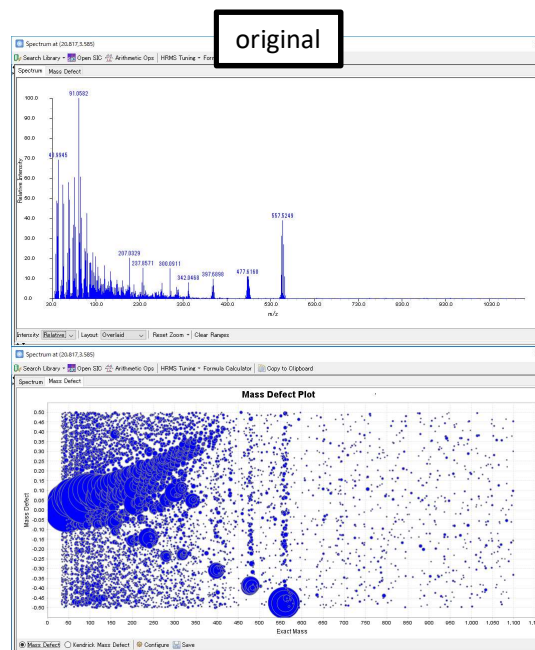
examples of result

mass spectra

mass defect plot

mass spectra

mass defect plot



February 15, 2019