Instructions of a ‘CBEx64 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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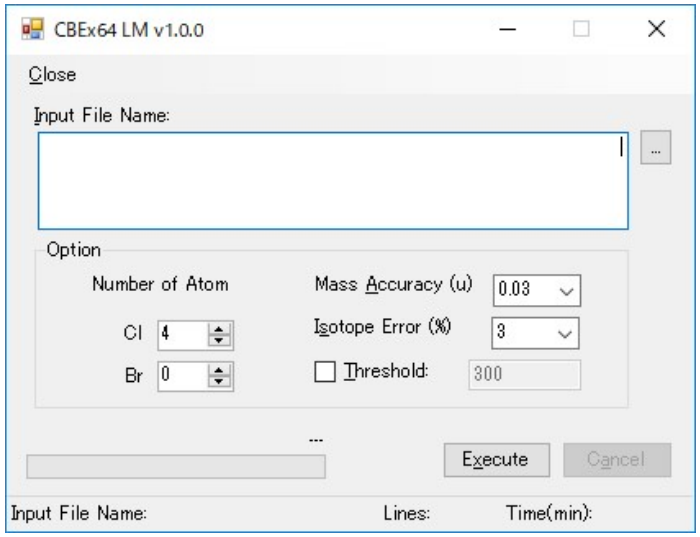
Reference: Hashimoto *et al.*(2013) Journal of Chromatography A, 1282, 183-189

What is a ‘CBEx64 LM’?



Interface of a ‘CBEx64 LM’.

This software can…

- directly read a netCDF file, which is a common format for MS data,
- and extract mass spectra that have a chlorine or bromine isotopic profile from all the data without setting a target mass number,
- under various mass accuracy (mass resolution) conditions,
- and finally, output the result as netCDF.

Main settings for data extraction

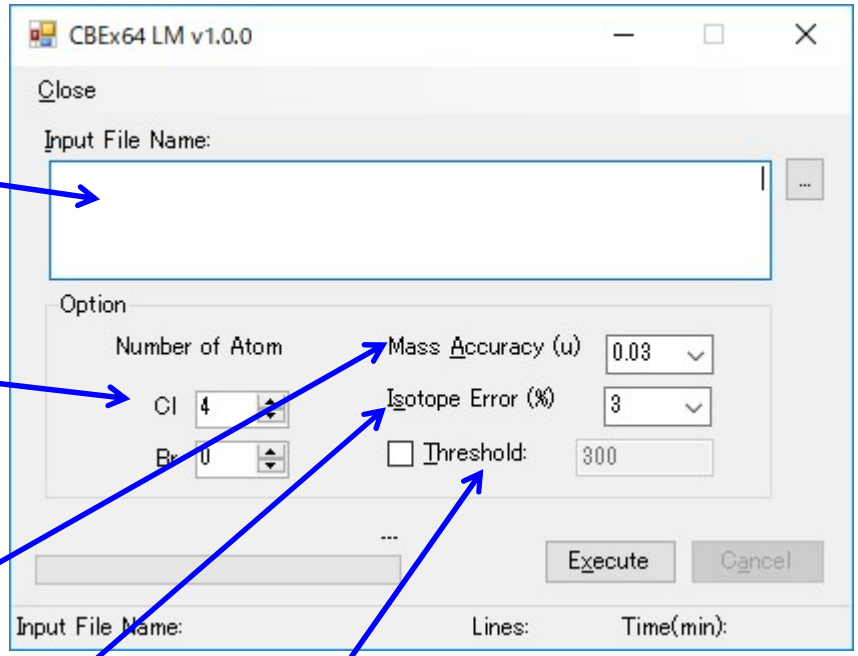
1) Input File Name*: choose filename(s) from the dialog box that will appear after right-clicking.

2) Number of Atom*: choose the Cl or Br mode. (The Cl and Br mode will extract mass spectra containing Cl and Br atom(s) from the input data, respectively.)

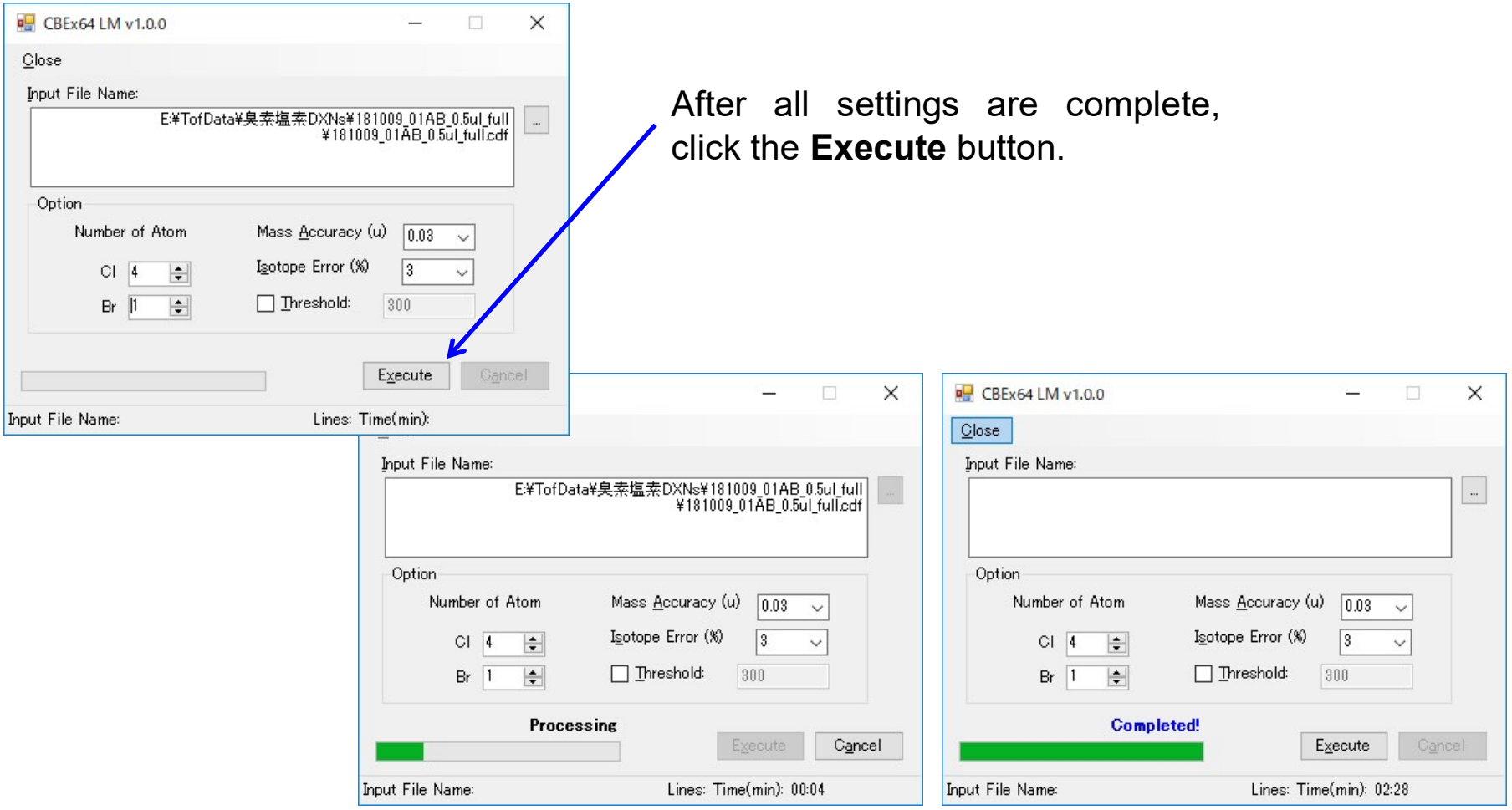
3) Mass Accuracy*: choose a value from 1 to 0.001u. (This parameter will determine the accuracy of the mass, e.g., MA: 0.05u is equivalent to a mass resolution of m/Δm 6,000 @ m/z 300.)

4) Isotope Error*: input an integer from 0 to 99. (See **Step iii** in **Technical Guide 1**.)

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



5) 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.)

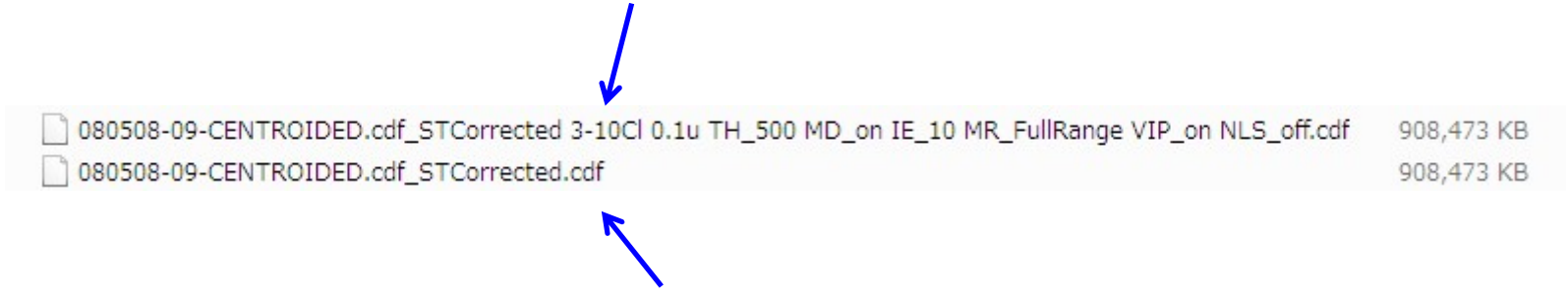


Running program
Elapsed time is displayed.

Completed process

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

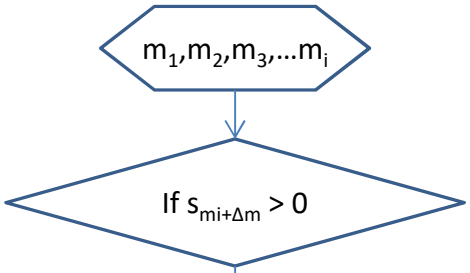
Output file: The file name is automatically created by appending the parameters used for the processing.



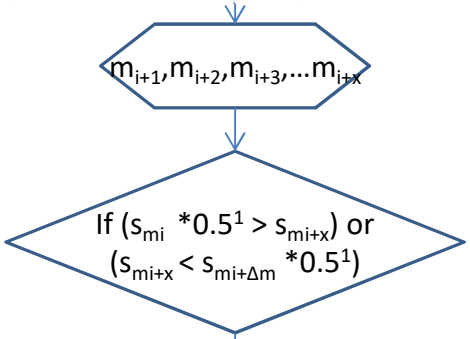
Input file: The file must be formatted in netCDF.

1: Process of isotopic pattern detection

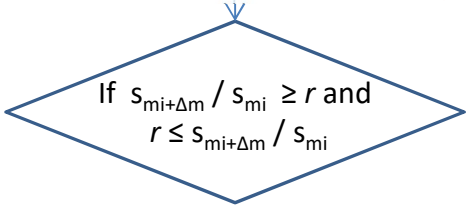
i) Mass spectra that are Δm, (2* Δm), (3* Δm)… (n* Δm) larger than m_i are searched about a mass spectrum (m_i).

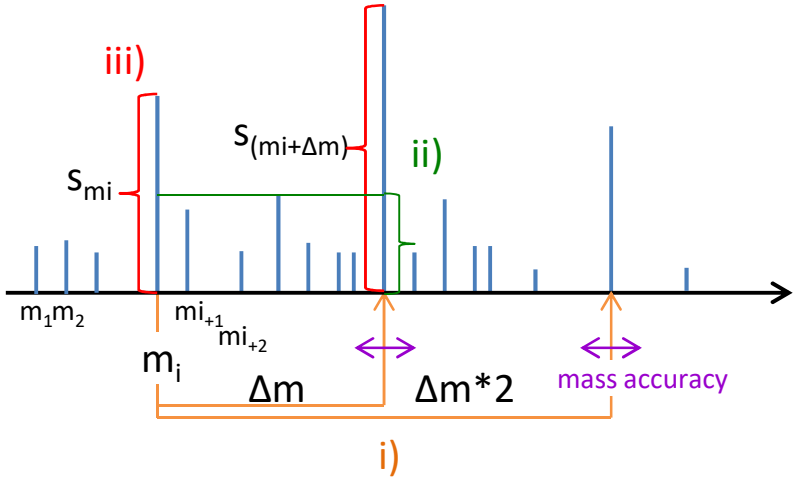


ii) If they are found, then mass spectra between the masses, m_i and m_i+ *n*Δ m, are checked to see if they are smaller than mass spectra found in step i. (This step is an alternative)



iii) If they satisfy the previous condition, finally the ratio of (m_i+ *n*Δ m) to m_i spectrum intensities is compared with its theoretical isotopic ratio.





Δm:

^{37}Cl (36.965903) – ^{35}Cl (34.968853)
= 1.99705

^{81}Br (80.916291) – ^{79}Br(78.918338)
= 1.997953

s_{mi}: signal intensity of mass spectra at m_i

r: isotopic ratio of (M+2) to M

No. of Cl	*r*
1	0.3196
2	0.6392
3	0.9588
4	1.2784
5	1.5980
6	1.9176
7	2.2372
8	2.5568
9	2.8764
10	3.1960

No. of Br	*r*
1	0.9728
2	1.9456
3	2.9184
4	3.8912
5	4.8640
6	5.8368
7	6.8096
8	7.7824
9	8.7552
10	9.7280

1 The factor, 0.5, is regarded as moderate for finding an isotopic pattern of Cl or Br at trace level.

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