

# Instructions of a 'ComEX'

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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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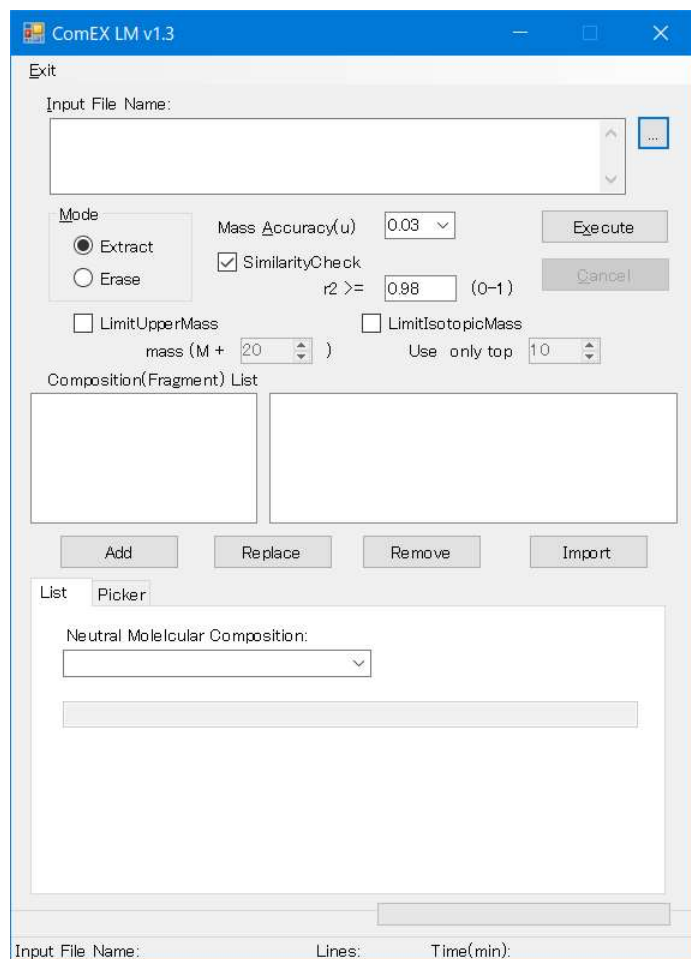
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# Extraction/removal of mass spectra based on composition formula



## ComEX software

This software can...

- ◆ Directly read netCDF (AIA formatted) files.
- ◆ Extract or remove mass spectra matched theoretical exact isotopic mass, which were automatically calculated from composition formula input, from whole data.
- ◆ Finally output result as a netCDF file.

ComEX interface

## Main settings for data extraction

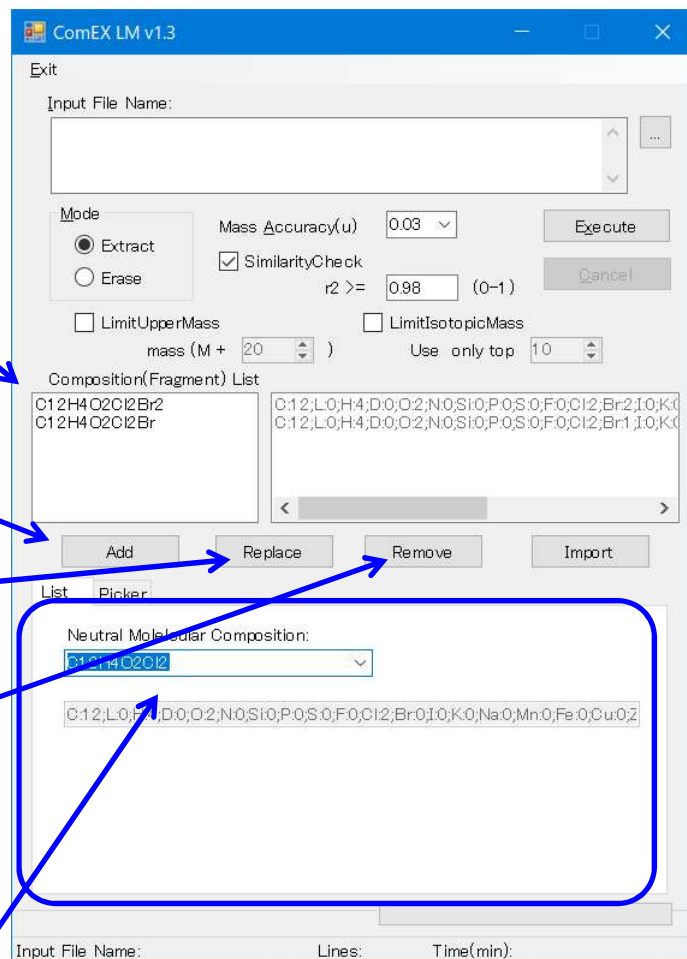
Formulas registered are listed in Composition (Fragment) List.

Add: Add a formula input on List or Picker tab to Compound List.

Replace: Replace a formula focused in Composition (Fragment) List with one input on List or Picker tab.

Remove: Delete a formula focused in Composition (Fragment) List

Neutral Molecular Composition: Choose Formula from the list or input it directly on List tab.



## 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.

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  $m/\Delta m$  6,000 @  $m/z$  300.)

4) **Similarity Check** (Isotopic Ratio Similarity): If only mass spectra matching the isotopic composition ratio are covered, be checked and input the coefficient of determination ( $r^2$ ).

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

## Main settings for data extraction

5) **Limit Upper Mass:** Enter x as the difference ( $M+x$ ) from the monoisotopic mass for the upper limit of the isotopic mass of the mass spectrum to be extracted (deleted).

6) **Limit Isotopic Mass:** Limit the number of isotope mass spectra to be extracted (deleted) to the number of isotope mass spectra entered from the top of theoretical existence values.

ComEX LM v1.3

Exit

Input File Name:

Mode: ☒ Extract ☐ Erase

Mass Accuracy(u): 0.03

☒ SimilarityCheck  $r2 \geq 0.98$  (0-1)

☒ LimitUpperMass mass (M + 20)

☒ LimitIsotopicMass Use only top 10

Composition(Fragment) List

C12H4O2Cl2Br2	C:12;L:0;H:4;D:0;O:2;N:0;S:0;P:0;S:0;F:0;Cl:2;Br:2;I:0;K:0
C12H4O2Cl2Br	C:12;L:0;H:4;D:0;O:2;N:0;S:0;P:0;S:0;F:0;Cl:2;Br:1;I:0;K:0

Add Replace Remove Import

List Picker

Elements

C 0	F 0	Fe 0	Ag 0
H 0	Cl 0	Cu 0	Mn 0
O 0	Br 0	As 0	I 0
N 0	P 0	Hg 0	
S 0	Si 0	Pb 0	D 0
K 0	Na 0	Zn 0	L(13C) 0

Input File Name: Lines: Time(min):

## Main settings for data extraction

ComEX LM v1.3

Exit

Input File Name:

Mode

☒ Extract

☐ Erase

Mass Accuracy(u) 0.03

☒ SimilarityCheck

r2 >= 0.98 (0-1)

☒ LimitUpperMass

mass (M + 20 )

☒ LimitIsotopicMass

Use only top 10

Composition(Fragment) List

C12H4O2Cl2Br2  
C12H4O2Cl2Br

C:12;L:0;H:4;D:0;O:2;N:0;S:0;P:0;S:0;F:0;Cl:2;Br:2;I:0;K:0  
C:12;L:0;H:4;D:0;O:2;N:0;S:0;P:0;S:0;F:0;Cl:2;Br:1;I:0;K:0

Add Replace Remove Import

List Picker

Elements

C 0	F 0	Fe 0	Ag 0
H 0	Cl 0	Cu 0	Mn 0
O 0	Br 0	As 0	I 0
N 0	P 0	Hg 0	
S 0	Si 0	Pb 0	D 0
K 0	Na 0	Zn 0	L(13C) 0

Input File Name: Lines: Time(min):

You can also make a formula by set numbers of each element on Picker tab.

ComEX LM v1.3

Exit

Input File Name: G:\TestData\181009\_01 AB\_0.5ul.cdf

Mode  
☒ Extract  
☐ Erase

Mass Accuracy(u) 0.03

☒ SimilarityCheck  
 r2 >= 0.98 (0-1)

☒ LimitUpperMass  
 mass (M + 20 )

☒ LimitIsotopicMass  
 Use only top 10

Composition(Fragment) List  
 C12H4O2Cl2Br2  
 C12H4O2Cl2Br

Add Replace Remove Import

List Picker

Elements

C 0	F 0	Fe 0	Ag 0
H 0	Cl 0	Cu 0	Mn 0
O 0	Br 0	As 0	I 0
N 0	P 0	Hg 0	D 0
S 0	Si 0	Pb 0	L(13C) 0
K 0	Na 0	Zn 0	

Input File Name: Lines: Time(min):

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

ComEX LM v1.3

Exit

Input File Name: G:\TestData\181009\_01 AB\_0.5ul.cdf

Accuracy(u) 0.03

☒ SimilarityCheck  
 r2 >= 0.98 (0-1)

☒ LimitIsotopicMass  
 Use only top 10

Composition(Fragment) List  
 C12;L0;H4;D0;O2;N0;Si0;P0;S0;F0;Cl2;Br2;I0;K0  
 C12;L0;H4;D0;O2;N0;Si0;P0;S0;F0;Cl2;Br1;I0;K0

Replace Remove Import

Processing

N 0	P 0	Hg 0	
S 0	Si 0	Pb 0	D 0
K 0	Na 0	Zn 0	L(13C) 0

Input File Name: 1009\_01 AB\_0.5ul.cdf Lines: Time(min): 00:03

ComEX LM v1.3

Exit

Input File Name:

Mode  
☒ Extract  
☐ Erase

Mass Accuracy(u) 0.03

☒ SimilarityCheck  
 r2 >= 0.98 (0-1)

☒ LimitUpperMass  
 mass (M + 20 )

☒ LimitIsotopicMass  
 Use only top 10

Composition(Fragment) List  
 C12H4O2Cl2Br2  
 C12H4O2Cl2Br

Add Replace Remove Import

List Picker

Elements

C 0	F 0	Fe 0	Ag 0
H 0	Cl 0	Cu 0	Mn 0
O 0	Br 0	As 0	I 0
N 0	P 0	Hg 0	D 0
S 0	Si 0	Pb 0	L(13C) 0
K 0	Na 0	Zn 0	

Completed!

Input File Name: 1009\_01 AB\_0.5ul.cdf Lines: Time(min): 00:48

Running program  
Elapsed time is displayed.

Completed process



Sep. 16, 2020