

ZhuLab

Lipid4DAnalyzer Help

Documentation, tutorial and configuration

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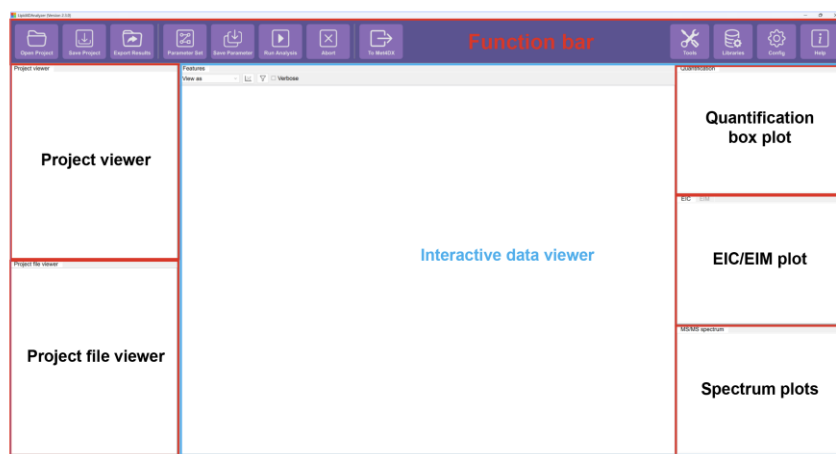
Lipid4DAnalyzer Documentation

Introduction

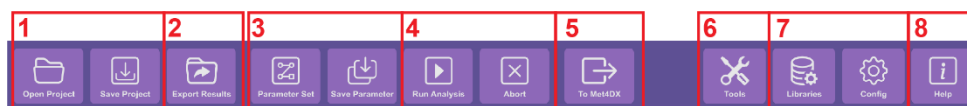
Lipid4DAnalyzer is part of Met4DX software. It is a fast, robust, and user-friendly mass spectrometry data processing tool for lipidomics data analysis by rebuilding the online version of Lipid4DAnalyzer (<http://lipid4danalyzer.zhulab.cn>).

Interface

Initial interface



Function bar



Project and data management

- 1) Open a previously saved project or save the current project to a file.
- 2) Export data for reading by Lipid4DAnalyzer from backend.

Data processing tools

- 3) Load a parameter set with defined data analysis workflow or save parameters of current data analysis workflow to a parameter set.
- 4) Submit experiments for data processing using the current data analysis workflow or abort the processing for all submitted experiments.

Go back to Met4DX

- 5) Go back to Met4DX for raw data processing

Other functions

- 6) Tools for lipidomics data analysis.
- 7) Config lipidomics library and Lipid4DAnalyzer software.

- 8) View helps documents, check logs and report bugs.

Parameter setting

Lipid4DAnalyzer provides the most used parameter sets in Zhulab for different data processing tasks, which is highly recommended for inexperienced users, and even for all users. To start a data processing workflow, one should load a parameter set first, modifying parameters later, and submit experiment for data processing at last.

Load a parameter set

A parameter set contains multiple steps for data processing, which will be shown in the analysis workflow viewer after loading a parameter set. For lipids identification, the corresponding instrument type should be selected. One can also provide the RT calibration table for scoring RT. Fragmentation rules can be applied accordingly.

Parameter Set

3D lipidomics positive (TOF)

3D lipidomics negative (TOF)

Left click

Peem configuration

Ion mode: ☒ Positive ☐ Negative

Instrument type: ☐ Agilent ☐ Bruker ☒ Sciex ☐ Shimadzu ☐ Waters

Library: ☒ 3D lipidomics (QTOF)

Collision energy: ☒ 45+25

RT condition: ☐ No ☒ HILIC lipidomics ☐ RP lipidomics

Apply fragmentation rules: ☒ Yes ☐ No

> Adducts

Import RT calibration table

	Name	Reference RT (s)	Experiment RT (s)
1	Start	0.0	
2	LPC(18:1)	85.0	
3	PC(14:1/14:1)	129.0	
4	PS(14:1/14:1)	144.0	
5	PC(14:1/14:1)	147.0	
6	PC(14:1/14:1)	211.0	
7	PE(14:1/14:1)	216.0	
8	DG(14:1/14:1)	345.0	
9	SM(18:1/18:1)	377.0	
10	Cer(18:1/18:1)	456.0	
11	PCIP-18.0/18:1	459.0	
12	TG(18:1/18:1/18:1)	747.0	
13	End	1080.0	

Click next

Analysis workflow: 3D lipidomics positive (TOF)

Parameter configuration - Identify features

Property	Value	help
Identify features		
Combine weight		Weights for calculating the combined score in 4D match
RT weight		RT weight
rt_weight	0.3	
MS/MS weight		MS/MS weight
mmsms_weight	0.7	
Cutoff	0.6	Cutoff for combined score

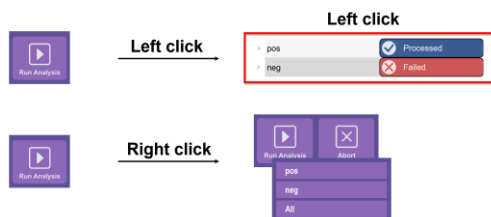
Parameter sets

3D	TOF	3D lipidomics positive (TOF)
		3D lipidomics negative (TOF)
	Orbitrap	3D lipidomics positive (Orbitrap)
		3D lipidomics negative (Orbitrap)
4D	TOF	4D lipidomics positive (TOF)
		4D lipidomics negative (TOF)

Data processing

Run analysis

- 1) Left click "Run Analysis": submit all experiments for processing using the selected analysis workflow.
- 2) Right click "Run Analysis": submit a single/all experiment(s) for data processing with selected analysis workflow.



After submission, the experiments in project viewer will show the corresponding processing status.

- Processing current processing experiment.
- Submitted submitted experiment, waiting for processing.
- Processed already processed experiment.
- Failed failed experiment.

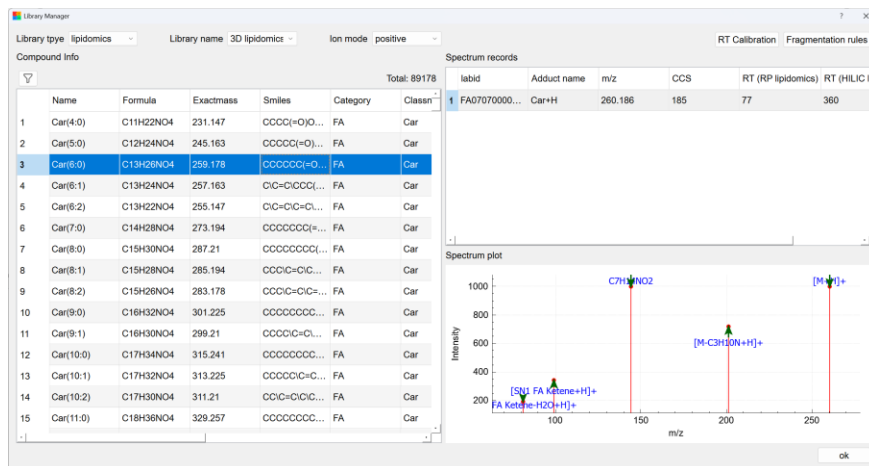
NOTE:

- Please make sure the running experiments of the same ion mode with the selected parameter set.

Other functions

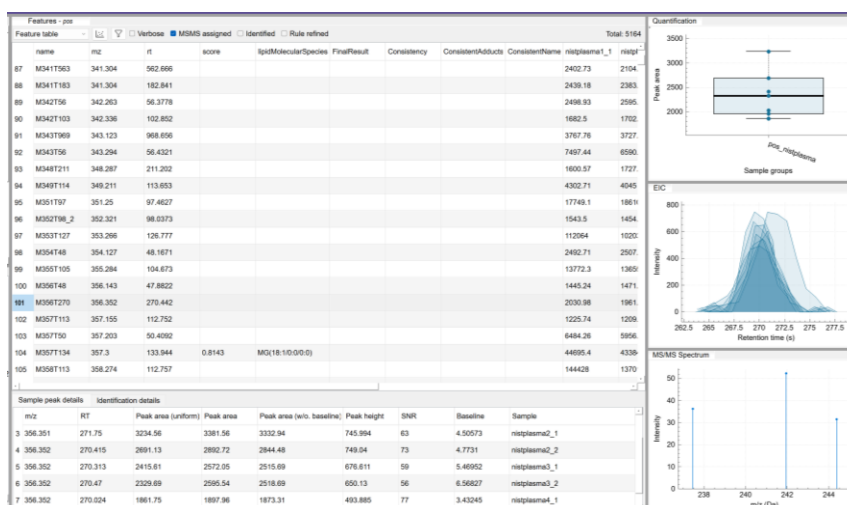
Library configuration

The lipids records in the library can be viewed in the library configuration. The reference RT calibration table and fragmentation rules can be checked by clicking the corresponding button.



Interactive data viewer

The interactive data viewer will load data from Met4DX for viewing by Lipid4DAnalyzer once the project is opened, which may take some time. One can check the general information for the features by selecting one line of the feature table. The details of the peaks from corresponding sample and identification results can be found in the lower panels via 'sample peak details' and 'identification details', respectively.

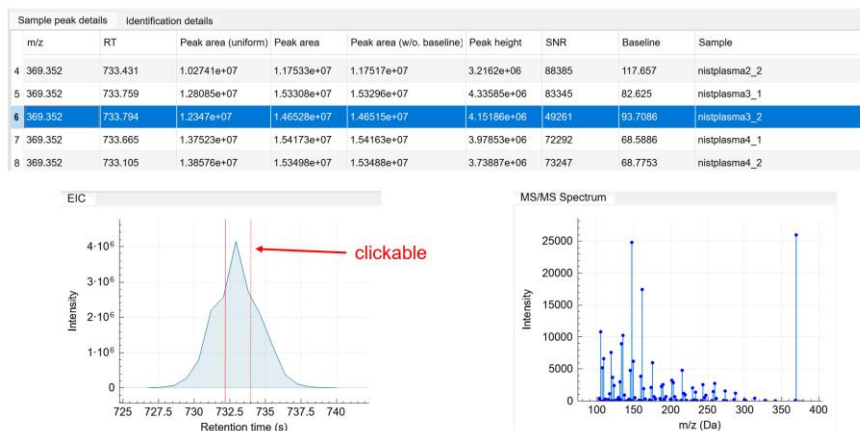


The panels in the right column show the corresponding figures as follows:

- 1) Quantification: The box plot of the peak area of different sample
- 2) EIC/EIM: EICs/EIMs of the peaks for belonging to the corresponding feature
- 3) MS/MS spectrum: MS/MS spectrum assigned to the feature

Clicking the peaks in 'sample peak details' panel will change the figures in the right column

- 1) EIC/EIM: EICs/EIMs of the peak. The red lines show the position where MS/MS spectrum was found. The corresponding MS/MS spectrum can be shown by clicking the line.
- 2) MS/MS spectrum: MS/MS spectrum under the peak. The MS/MS spectrum at the position of the solid red line in the EIC/EIM panel is shown by default.



When the identification work is done, the 'MS/MS spectrum' panel of the identified features will be changed to 'MS/MS spectrum match' to show the mirror plot of the final identification and the 'identification details' panel is shown for checking the identification details. Clicking each identification, the corresponding mirror plot of identification is shown in the MS/MS spectrum match panel

