ZhuLab

Lipid4DAnalyzer Help

Documentation, tutorial and configuration

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Contents

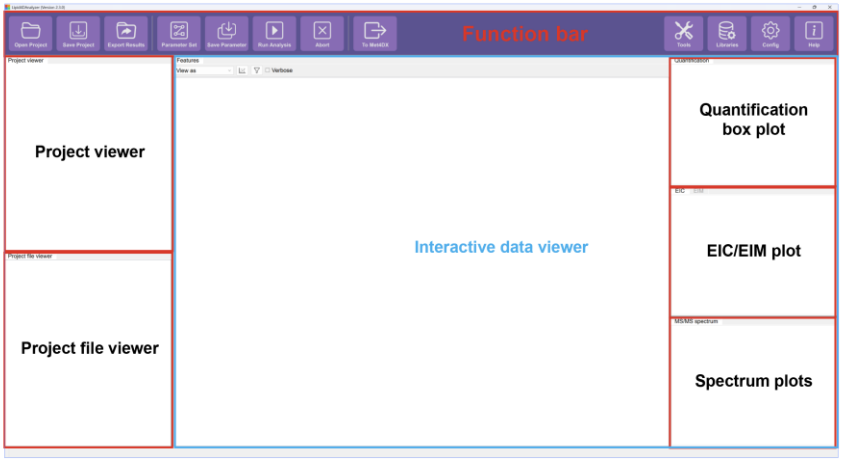
Lipid4DAnalyzer Documentation

Introduction

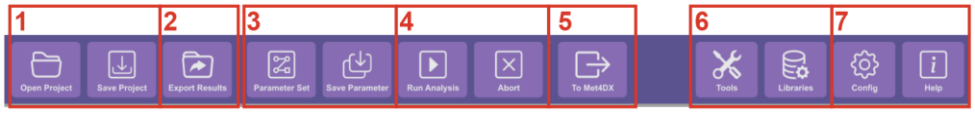
Lipid4DAnalyzer is part of Met4DX software. It is a fast, robust, and user-friendly mass spectrometry data processing tool for lipidomics data analysis by rebuilding the online version of Lipid4DAnalyzer (http://lipid4danalyzer.zhulab.cn).

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

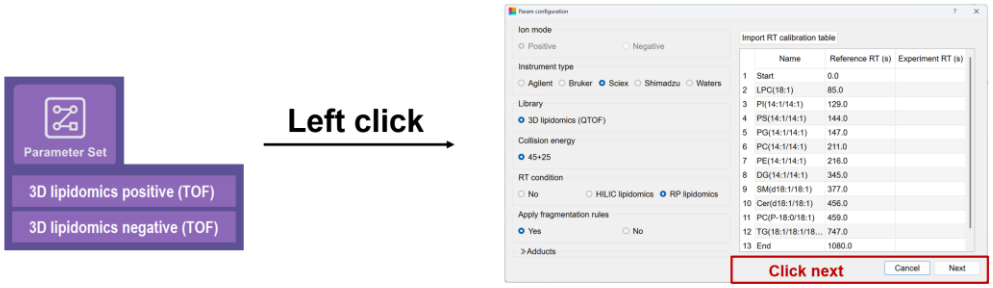
6) Config Met4DX software and lipidomics library.
7) View helps documents, check logs and report bugs.

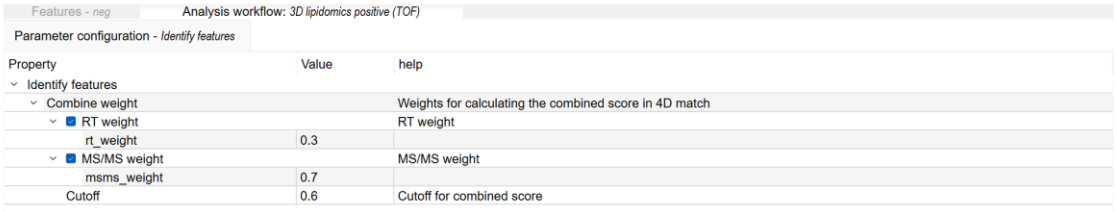
Parameter setting

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.

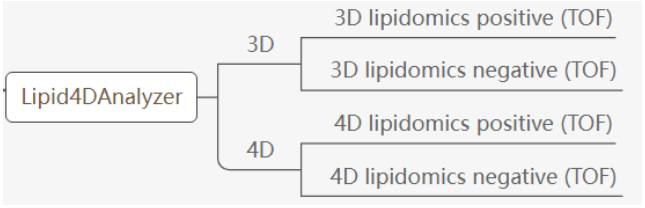
Load a parameter set

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.





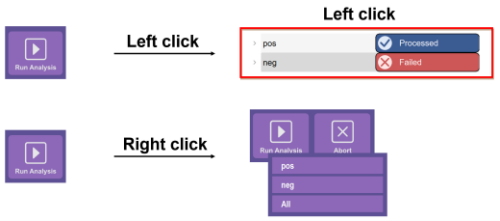
Parameter sets



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 filed experiment.

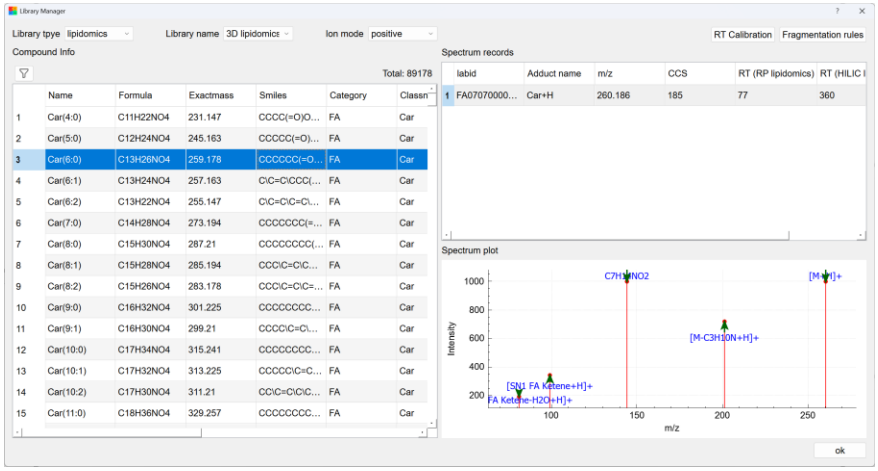
NOTE:

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

Other functions

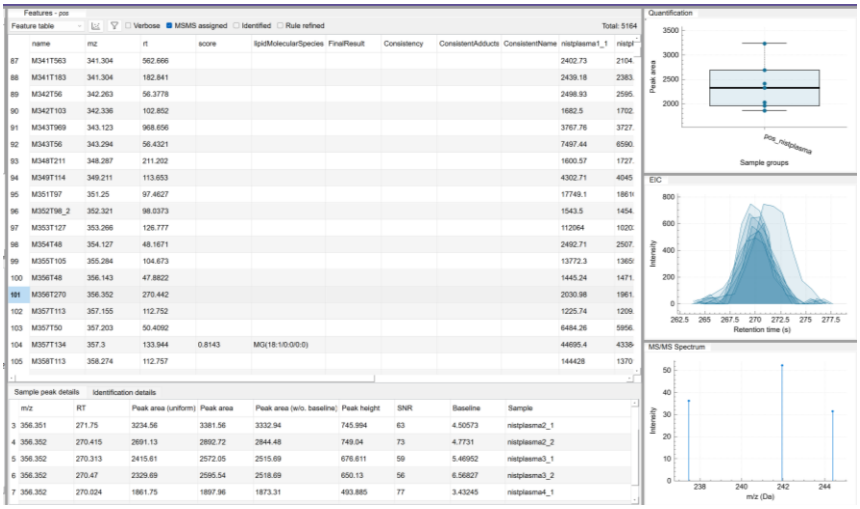
Library configuration

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.

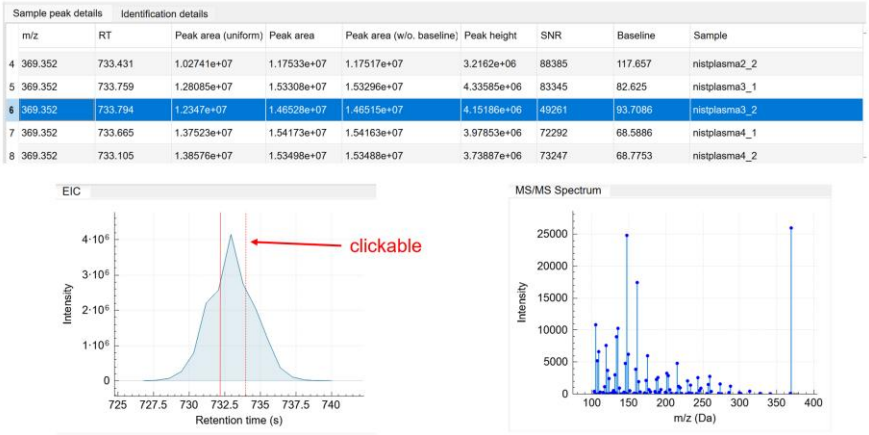


The panels in the right column show the corresponding figures as follows:

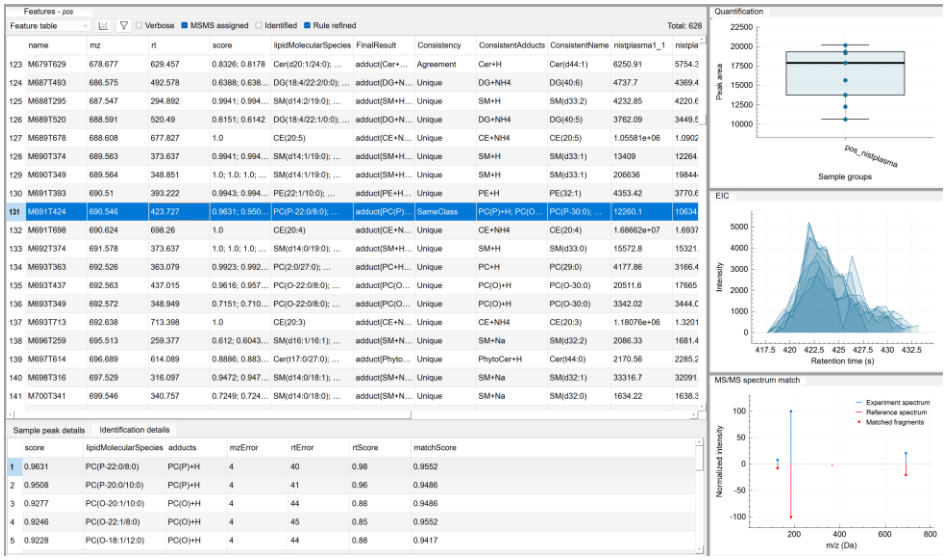
1) Quantification: The box plot of the peak area of different sample
2) EIC/EIM: EICs/EIMs of the peaks for belonging to the corresponding feature
3) MS/MS spectrum: MS/MS spectrum assigned to the feature

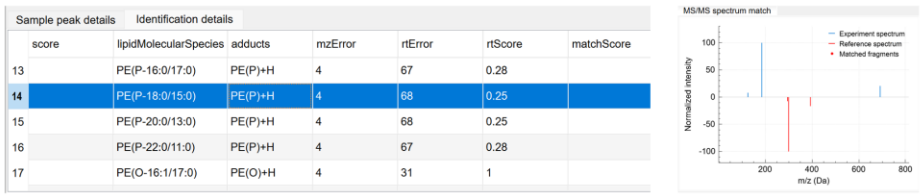
Clicking the peaks in 'sample peak details' panel will change the figures in the right column

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.



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


Features - pos
Feature table
Verbose
MSMS assigned
Identified
Rule refined
Total: 628
name mz rt score lipidMolecularSpecies FinalResult Consistency ConsistentAdducts ConsistentName nistplasma1_1 nistpla
123 M679T629 678.677 629.457 0.8326; 0.8178 Cer(d20:1/24:0); ... adduct[Cer+... Agreement Cer+H Cer(d44:1) 6250.91 5754.3
124 M687T493 686.575 492.578 0.6388; 0.638... DG(18:4/22:2/0:0); ... adduct[DG+N... Unique DG+NH4 DG(40:6) 4737.7 4369.4
125 M688T295 687.547 294.892 0.9941; 0.994... SM(d14:2/19:0); ... adduct[SM+H... Unique SM+H SM(d33:2) 4232.85 4220.6
126 M689T520 688.591 520.49 0.6151; 0.6142 DG(18:4/22:1/0:0); ... adduct[DG+N... Unique DG+NH4 DG(40:5) 3762.09 3449.6
127 M689T678 688.608 677.827 1.0 CE(20:5) adduct[CE+N... Unique CE+NH4 CE(20:5) 1.05581e+06 1.0902
128 M690T374 689.563 373.637 0.9941; 0.994... SM(d14:1/19:0); ... adduct[SM+H... Unique SM+H SM(d33:1) 13409 12264.
129 M690T349 689.564 348.851 1.0; 1.0; 1.0; ... SM(d14:1/19:0); ... adduct[SM+H... Unique SM+H SM(d33:1) 206636 19844.
130 M691T393 690.51 393.222 0.9943; 0.994... PE(22:1/10:0); ... adduct[PE+H... Unique PE+H PE(32:1) 4353.42 3770.6
131 M691T424 690.546 423.727 0.9631; 0.950... PC(P-22:0/8:0); ... adduct[PC(P)... SameClass PC(P)+H; PC(O... PC(P-30:0); ... 12260.1 10634
132 M691T698 690.624 698.26 1.0 CE(20:4) adduct[CE+N... Unique CE+NH4 CE(20:4) 1.68662e+07 1.6937
133 M692T374 691.578 373.637 1.0; 1.0; 1.0; ... SM(d14:0/19:0); ... adduct[SM+H... Unique SM+H SM(d33:0) 15572.8 15321.
134 M693T363 692.526 363.079 0.9923; 0.992... PC(2:0/27:0); ... adduct[PC+H... Unique PC+H PC(29:0) 4177.86 3166.4
135 M693T437 692.563 437.015 0.9616; 0.957... PC(O-22:0/8:0); ... adduct[PC(O... Unique PC(O)+H PC(O-30:0) 20511.6 17665
136 M693T349 692.572 348.949 0.7151; 0.710... PC(O-22:0/8:0); ... adduct[PC(O... Unique PC(O)+H PC(O-30:0) 3342.02 3444.0
137 M693T713 692.638 713.398 1.0 CE(20:3) adduct[CE+N... Unique CE+NH4 CE(20:3) 1.18076e+06 1.3201
138 M696T259 695.513 259.377 0.612; 0.6043... SM(d16:1/16:1); ... adduct[SM+N... Unique SM+Na SM(d32:2) 2086.33 1681.4
139 M697T614 696.689 614.089 0.8886; 0.883... Cer(t17:0/27:0); ... adduct[Phyto... Unique PhytoCer+H Cer(t44:0) 2170.56 2285.2
140 M698T316 697.529 316.097 0.9472; 0.947... SM(d14:0/18:1); ... adduct[SM+N... Unique SM+Na SM(d32:1) 33316.7 32091.
141 M700T341 699.546 340.757 0.7249; 0.724... SM(d14:0/18:0); ... adduct[SM+N... Unique SM+Na SM(d32:0) 1634.22 1638.3
Sample peak details
Identification details
score lipidMolecularSpecies adducts mzError rtError rtScore matchScore
1 0.9631 PC(P-22:0/8:0) PC(P)+H 4 40 0.98 0.9552
2 0.9508 PC(P-20:0/10:0) PC(P)+H 4 41 0.96 0.9486
3 0.9277 PC(O-20:1/10:0) PC(O)+H 4 44 0.88 0.9486
4 0.9246 PC(O-22:1/8:0) PC(O)+H 4 45 0.85 0.9552
5 0.9228 PC(O-18:1/12:0) PC(O)+H 4 44 0.88 0.9417
Quantification
Peak area
Sample groups
EIC
Intensity
Retention time (s)
MS/MS spectrum match
Experiment spectrum
Reference spectrum
Matched fragments
Normalized intensity
m/z (Da)


Sample peak details
Identification details
score lipidMolecularSpecies adducts mzError rtError rtScore matchScore
13 PE(P-16:0/17:0) PE(P)+H 4 67 0.28
14 PE(P-18:0/15:0) PE(P)+H 4 68 0.25
15 PE(P-20:0/13:0) PE(P)+H 4 68 0.25
16 PE(P-22:0/11:0) PE(P)+H 4 67 0.28
17 PE(O-16:1/17:0) PE(O)+H 4 31 1
MS/MS spectrum match
Experiment spectrum
Reference spectrum
Matched fragments
Normalized intensity
m/z (Da)