

Installation

- Installing the stand-alone version from github repository(<https://github.com/WenchYu/MSanalyst>)

```
# Downloading msanalyst library using command or manually
```

```
wget --no-check-certificate 'https://drive.google.com/file/d/1w6HF3w1KIJlTz_QaVqqtN1BzkGDhDgzv/view?usp=sharing'
```

```
# Cloning MSanalyst repository
```

```
git clone git@github.com:WenchYu/MSanalyst.git && cd MSanalyst
```

```
unzip msdb.zip -d ./ && rm msdb.zip
```

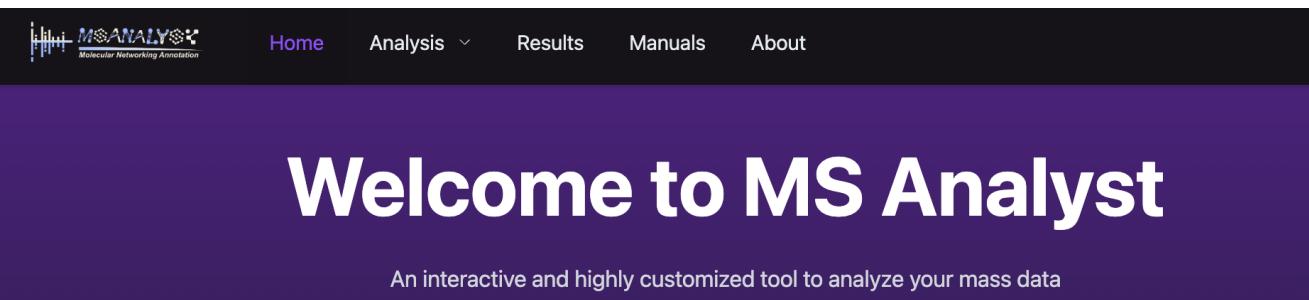
```
# Creating environment
```

```
conda create -n msanalyst python=3.8
```

```
conda activate msanalyst
```

```
pip install -r requirements.txt
```

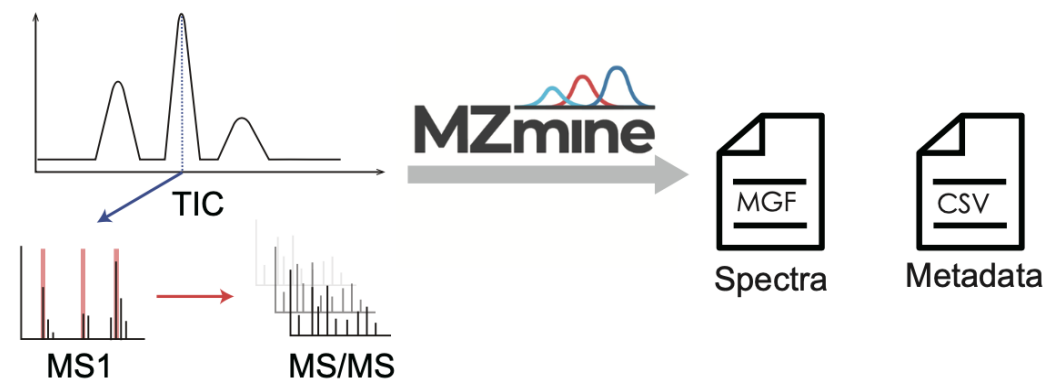
- Or use the online version(<https://msanalyst.net/>)



- Data preprocessing

MSmine Untargeted LC-MS Workflow

https://msmine.github.io/msmine_documentation/workflows/lcmsworkflow/lcms-workflow.html

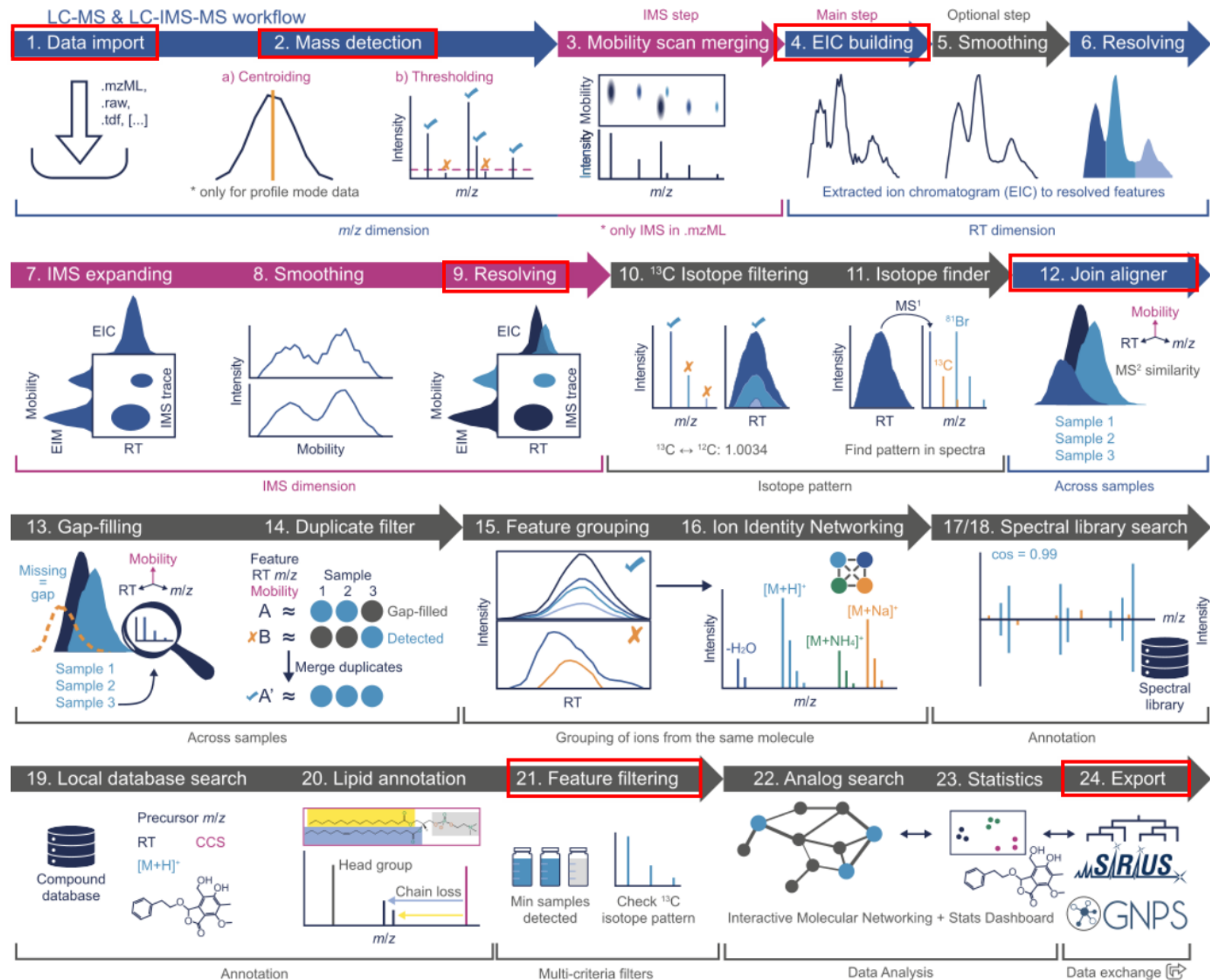
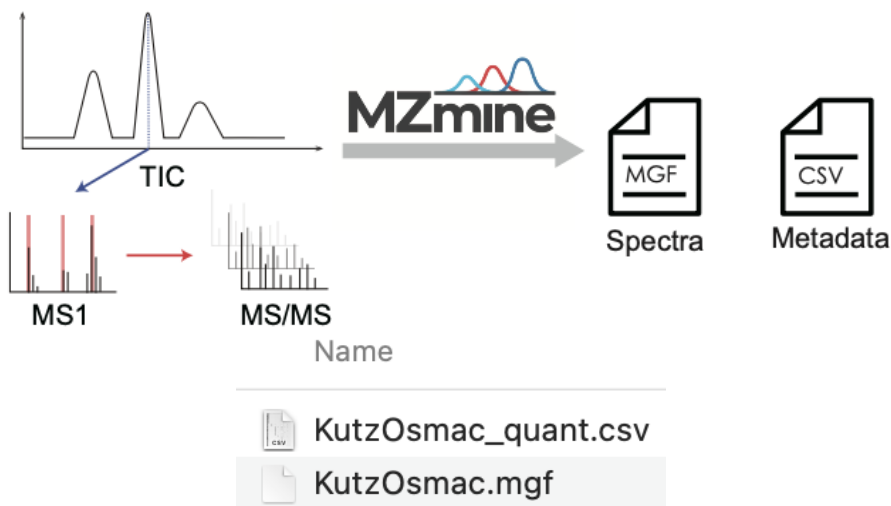


LC-MS data preprocessing

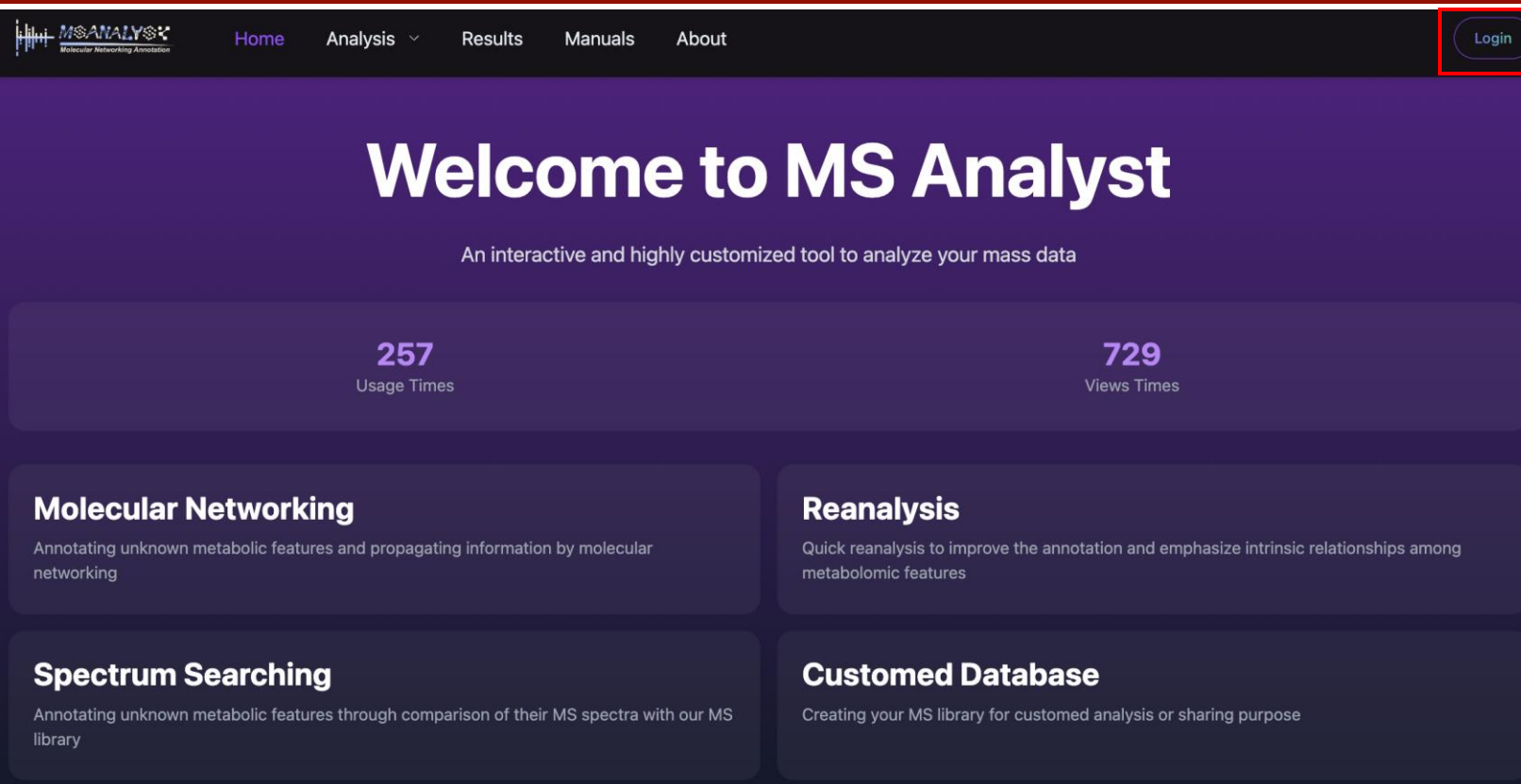
• Data preprocessing

MZmine Untargeted LC-MS Workflow

https://mzmine.github.io/mzmine_documentation/workflows/lcmsworkflow/lcms-workflow.html



The MSAnalyst homepage



The screenshot shows the MSAnalyst homepage with a dark purple header and main content area. The header contains the MSANALYST logo and navigation links: Home, Analysis, Results, Manuals, and About. A 'Login' button is highlighted with a red box and a red arrow pointing to the right. The main content area features a large 'Welcome to MS Analyst' heading, a subtitle 'An interactive and highly customized tool to analyze your mass data', and two statistics: '257 Usage Times' and '729 Views Times'. Below these are four modules: Molecular Networking, Reanalysis, Spectrum Searching, and Customized Database, each with a brief description.

MSANALYST
Molecular Networking Annotation

Home Analysis Results Manuals About

Login

Welcome to MS Analyst

An interactive and highly customized tool to analyze your mass data

257 Usage Times

729 Views Times

Molecular Networking

Annotating unknown metabolic features and propagating information by molecular networking

Reanalysis

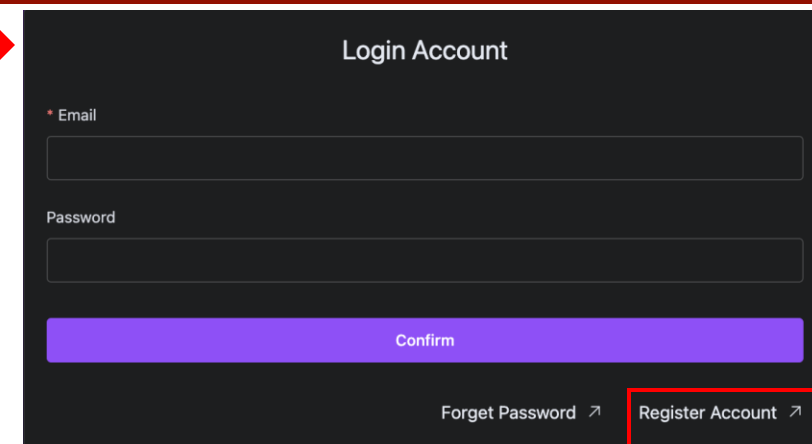
Quick reanalysis to improve the annotation and emphasize intrinsic relationships among metabolomic features

Spectrum Searching

Annotating unknown metabolic features through comparison of their MS spectra with our MS library

Customized Database

Creating your MS library for customized analysis or sharing purpose



The screenshot shows the 'Login Account' form. It has a dark background with white text. The form includes fields for 'Email' and 'Password', both marked with an asterisk. Below the password field is a 'Confirm' button. At the bottom right, there are links for 'Forget Password' and 'Register Account', both with external link icons.

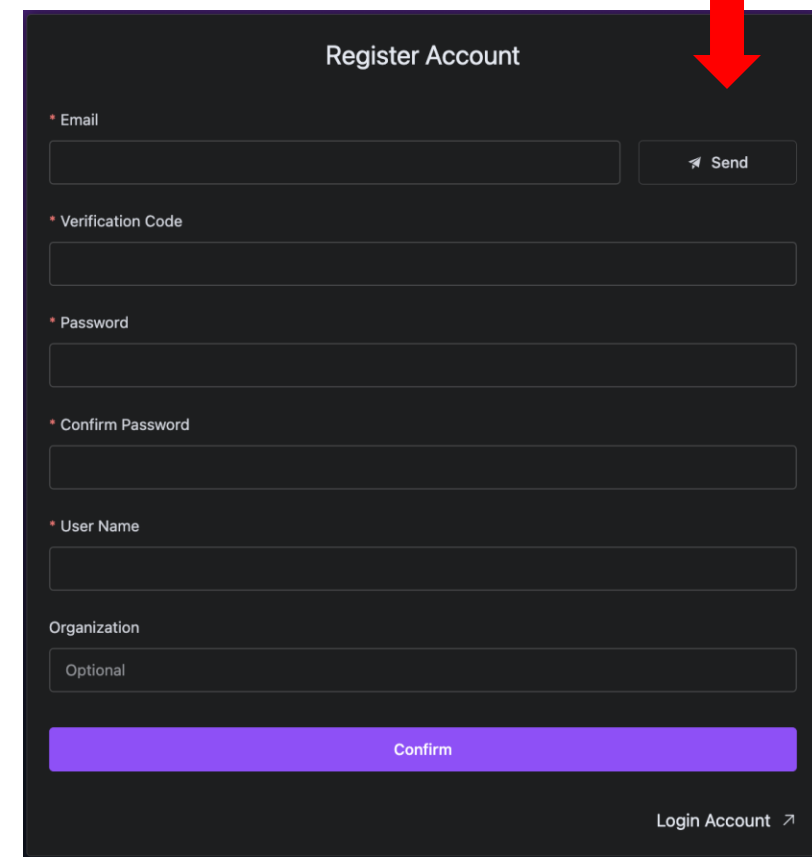
Login Account

* Email

Password

Confirm

Forget Password [↗](#) [Register Account](#) [↗](#)



The screenshot shows the 'Register Account' form. It has a dark background with white text. The form includes fields for 'Email', 'Verification Code', 'Password', and 'Confirm Password', all marked with an asterisk. There is also a 'User Name' field and an 'Organization' field with a placeholder 'Optional'. A 'Send' button is next to the email field. At the bottom, there is a 'Confirm' button and a link to 'Login Account'.

Register Account

* Email [↗ Send](#)

* Verification Code

* Password

* Confirm Password

* User Name

Organization
Optional

Confirm

[Login Account](#) [↗](#)

Homepage

- Linkage: <https://msanalyst.net/>
- Four modules: Molecular Networking, Reanalysis, Spectrum Searching, and Customized Database

Molecular Networking

Molecular networking

Annotating unknown metabolic features

- Upload files
- Set parameters
- Submit

modified_cosine

neutral_loss ⓘ

peak_percentage

entropy ⓘ

unweighted_entropy ⓘ

euclidean ⓘ

manhattan ⓘ

chebyshev ⓘ

Matching method

Neutral loss here is described by $\Delta m/z$ from each fragment ion to the precursor and can be used to find related spectra of modified analog molecules

Algorithms Brief help

Molecular Networking

Annotating unknown metabolic features and propagating information by molecular networking

- Task Name

example

- Input Files

Feature table (.csv file)



Drop file here or [click to upload](#), max 10MB

Mass list (.mgf file)



Drop file here or [click to upload](#), max 10MB

- Library search parameters

MS tolerance(ppm)

10

Shared peaks

5

Select database

default

Matching method

Matching method

Threshold value

0.7

- Networking parameters

Matching method

Matching method

Threshold value

0.7

Shared peaks

5

Connection mode

Connection mode

Submit

Create Success! Have 0 tasks ahead of you. You can check result with id: 002dea51-de1b-433f-80e5-5947cd922bfd

Submit successfully

Molecular Networking

MSANALYZER

Molecular Networking Annotation

Home

Analysis

Results

Manuals

About

Yu

Refresh

Batch Delete

Search task id

Search task name

Select Workflow

<input type="checkbox"/>	Index	Name	Task Id	Workflow	Status	Create Time	Delete Task
<input type="checkbox"/>	1	example	002dea51-de1b-433f-80e5-5947cd922bfd	Molecular Networking	Done	4m ago	Delete

Molecular networking result page

- Find specific task name and id
- View library hits**
Show the overall annotation of metabolic features within the sample

Experimental

Unnamed: 0	row ID	row m/z	match_id	match_smiles	mps	pair_similarity	pp
0	1	319.233917	CCMSLIB0000 9943338		1.0	0.0028467476 36795	0.16666666 6666666
1	1	319.233917	CCMSLIB0000 9943341		6.0	0.8774554497 79518	1.0
2	1	319.233917	CCMSLIB0000 9951167		1.0	0.005592592 5262272	0.16666666 6666666
3	1	319.233917	CCMSLIB0000 9992430		6.0	0.8774554497 79518	1.0
4	1	319.233917	CCMSLIB0000 4686001		0.0	0.0	0.0
5	1	319.233917	CCMSLIB0000 4686002		0.0	0.0	0.0

Total 6

Back

TaskId: 002dea51-de1b-433f-80e5-5947cd922bfd

Status: Done

Workflow: Molecular Networking

UpdatedAt: 2025-03-19 22:14:20.929

CompleteAt: 2025-03-19 22:14:20

Search Params:

Network Params:

Upload Files:

Result Files:

Ms Tolerance: 10

Shared Peaks: 5

Threshold Value: 0.7

Database: default

Matching Method:

Shared Peaks: 5

Threshold Value: 0.7

Connection Mode:

Matching Method:

example_quant.csv

example.mgf

name: example_quant_result

size: 0.14667129516601562MB

View library hits

Network visualization

Download Result

row ID	row m/z	row retention time	20220526-ACAC-ACAB.mzML Peak area	20220526-ACAC.mzML Peak area	20220526-ACAC 0.3.mzML Peak area	npms1_id	noms1_smiles	edbms1_id	edbms1_smiles	npms1_smiles
1	319.233917	6.595833	181129.326	234437.5925	0	Show Detail	Show Detail	nan;nan;nan;nan;nan;nan	Show Detail	
2	449.22380007	15.04664167	672639.944	2657622.811	0	Show Detail	Show Detail	Show Detail	Show Detail	
3	462.1715916	3.7493	106573.179	0.0	0	Show Detail	Show Detail	Show Detail	Show Detail	
4	561.3603225	18.27038333	1064330.506	876518.911	0	Show Detail	Show Detail	Show Detail	Show Detail	
5	575.3763288	19.4684	133143.624	101580.603	0	Show Detail	Show Detail	Show Detail	Show Detail	

Detailed information of comparison

Row ID: Feature ID in query spectral file

Row m/z: Precursor m/z

match_id: Hits id in the library

match_smiles: Hits structure

mps: Number of matched peaks

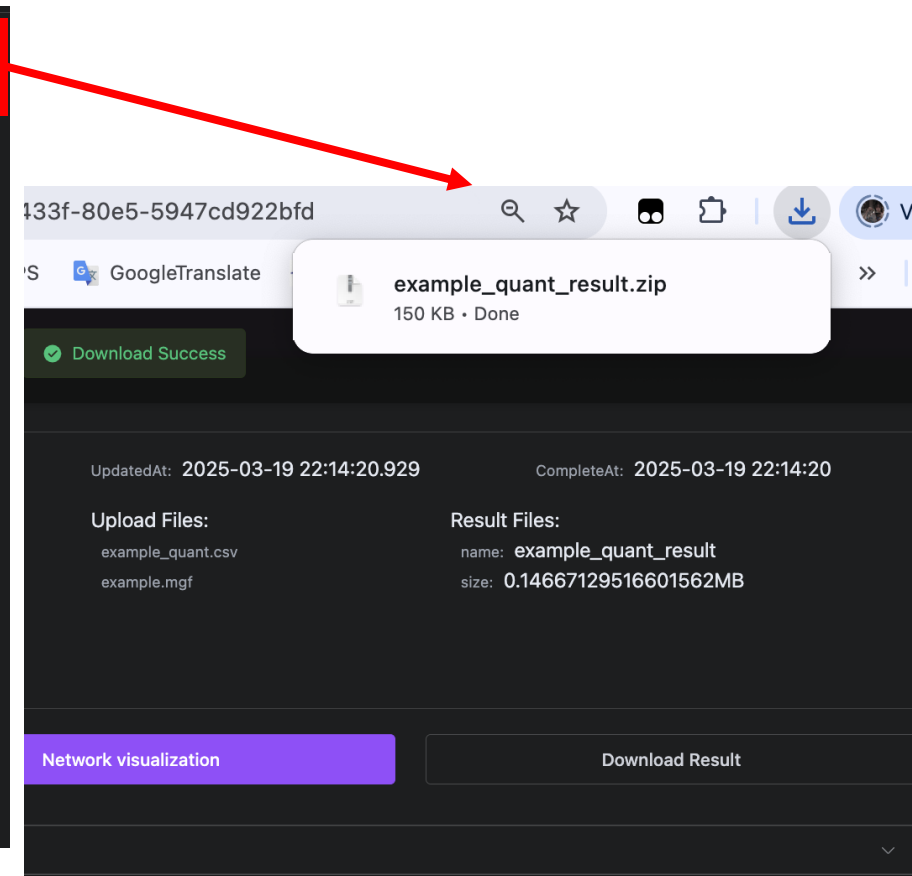
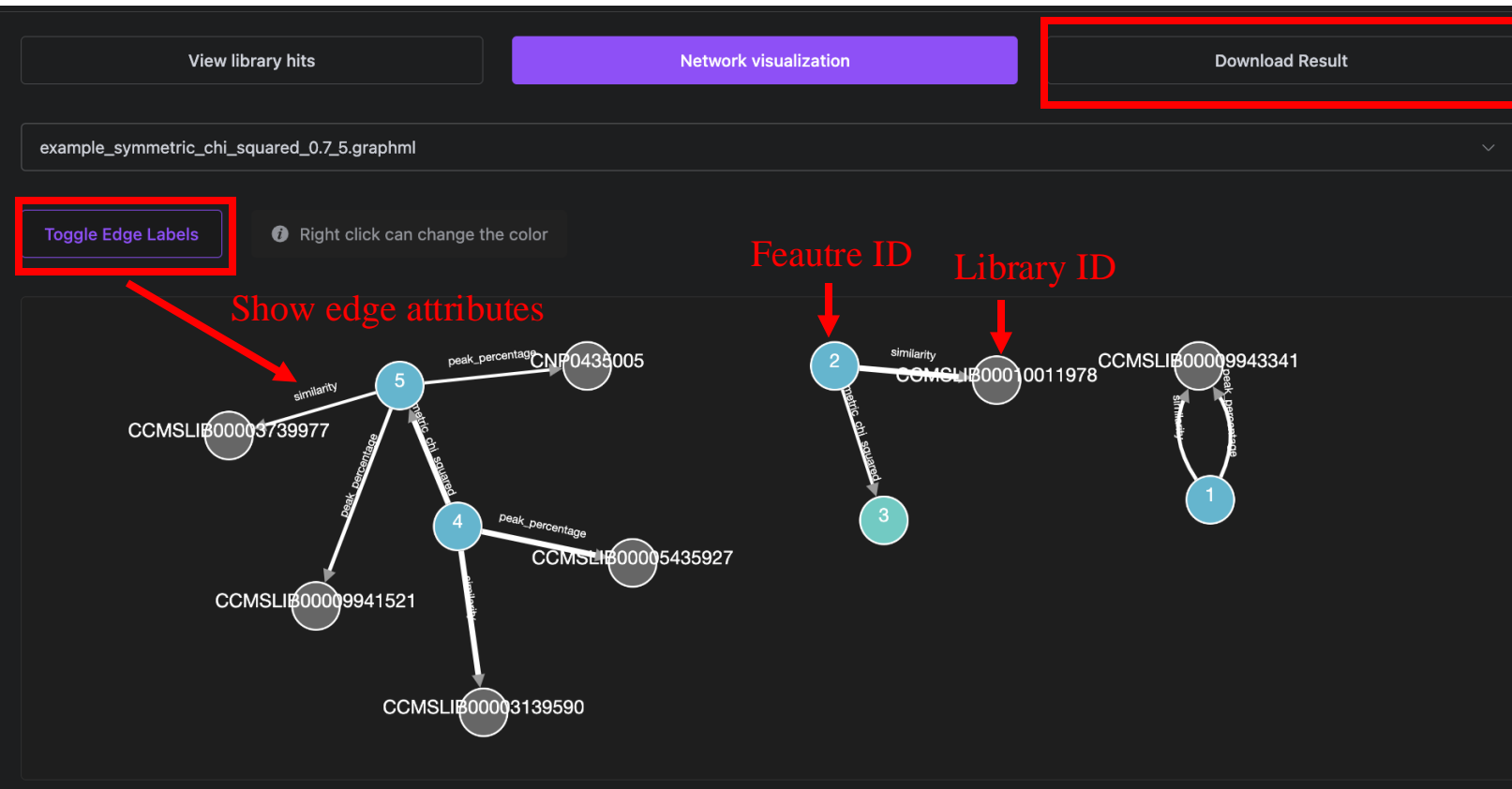
pair_similarity: spectral similarity

pp: peak percentage score

Molecular Networking

Molecular networking result page

- **Network visualization**
Visualizing the generated molecular network
- **Download result**



Reanalysis

Reanalysis

Quick reanalysis to improve the annotation and emphasize intrinsic relationships among metabolomic features

- Task Name

- Original Task ID

- Library search parameters

MS tolerance(ppm)

Shared peaks

Select database

Matching method

Threshold value

- Networking parameters

Matching method

Threshold value

Shared peaks

Connection mode

- Networking merging +

1. Matching method

Threshold value

Shared peaks

Connection mode

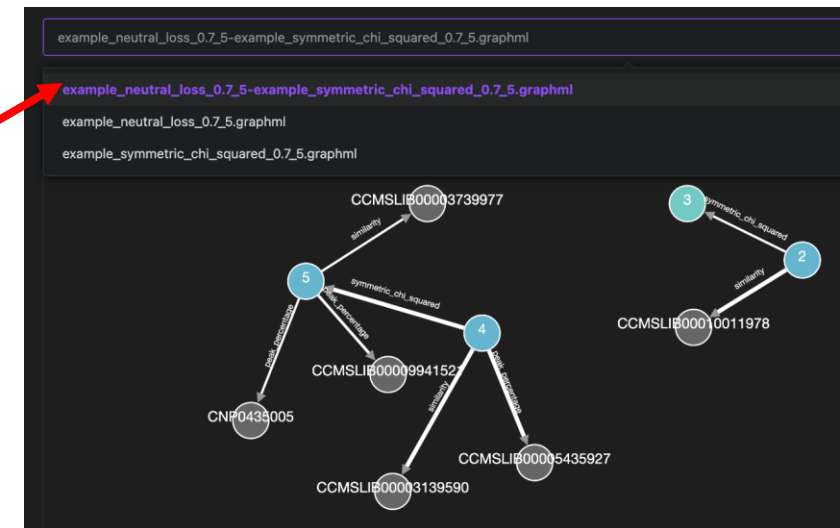
Reanalysis

Quick adjustment of thresholds and algorithms

- Type in the molecular networking task ID
- Set thresholds and algorithms

Networking merging

If additional molecular network generation parameters are set, different molecular networks will be merged while generating separate molecular networks.



Spectrum Searching

Spectrum Searching

Annotating unknown metabolic features through comparison of their MS spectra with our MS library

- Task Name

- Specific mass spectrum data

*** Precursor m/z**

*** MS/MS Spectrum input**

- Library search parameters

MS tolerance(ppm)

Shared peaks

Select database

Matching method

Threshold value

example.mgf — Edited

```
BEGIN IONS
FEATURE TD=1
PEPMASS=319.2339
SCANS=1
RTINSECONDS=1095.958
CHARGE=1+
MSLEVEL=2
84.0810 1.1E2
84.0819 5.1E2
84.0829 1.3E2
100.0388 1.1E2
100.0399 1.2E2
102.0903 1.9E2
102.0913 2.1E2
102.0919 1.5E3
102.0933 1.8E2
165.1045 1.0E2
201.1211 1.2E2
201.1225 3.2E2
201.1240 4.8E2
201.1250 4.7E3
201.1269 3.4E2
201.1283 2.7E2
201.1298 2.3E2
319.2336 1.3E2
319.2355 1.3E2
319.2369 4.0E2
319.2391 1.3E2
END IONS
```

Spectrum Searching

Search specific spectrum against entire library of MSAnalyst

- When you only enter precursor m/z, search at ms1 level
- When you only enter precursor m/z and ms/ms spectrum, search at ms2 level

Customed Database

Customed Database

Creating your MS library for customed analysis or sharing purpose. [Manage Your Custom Databases](#)

- Database [Template Download](#) **Download template files**

* Database Name

exampleDB

- Input Files

Feature table (.tsv/.xlsx/.csv file)

Drop file here or [click to upload](#), max 10MB

example.xlsx

Submit

Mass list (.mgf file)

Drop file here or [click to upload](#), max 10MB

example.mgf

Yu

Update Profile

Custom Databases

LogOut

Customed Database

Create customed spectral database for search purpose

- Please make sure the format is consistent with the following files and the feature_ID in csv and mgf should correspond one to one
- Once generated, the database can be selected

Select database

default

default

exampleDB

example.mgf

```
BEGIN IONS
FEATURE_ID=1
PEPMASS=319.2339
SCANS=1
RTINSECONDS=1095.958
CHARGE=1+
MSLEVEL=2
84.0810 1.1E2
84.0819 5.1E2
84.0829 1.3E2
100.0388 1.1E2
100.0399 1.2E2
102.0903 1.9E2
102.0913 2.1E2
102.0919 1.5E3
102.0923 1.8E3
```

My Custom Databases

Mannage your customed databases here

+ Add Record

↻ Refresh

🗑 Batch Delete

Search db name

<input type="checkbox"/>	Index	DB Name	File Info	Create Time	Delete
<input type="checkbox"/>	1	exampleDB	1. example.xlsx 2. example.mgf	4h ago	<div>🗑 Delete</div>

example.xlsx

Open with Microsoft Excel

compound_name	feature_ID	smiles	collector	adduct	organism
at-1	1	[C(COC3=C	Yu	M+H	Aspergillus
at-2	2	NC1=C/C2=	Yu	M+H	Aspergillus
at-3	3	NC1=C/C2=	Yu	M+H	Aspergillus
at-4	4	:[C@](O)(O	Yu	M+H	Aspergillus
at-5	5	1C(O)=C3	Yu	M+H	Aspergillus