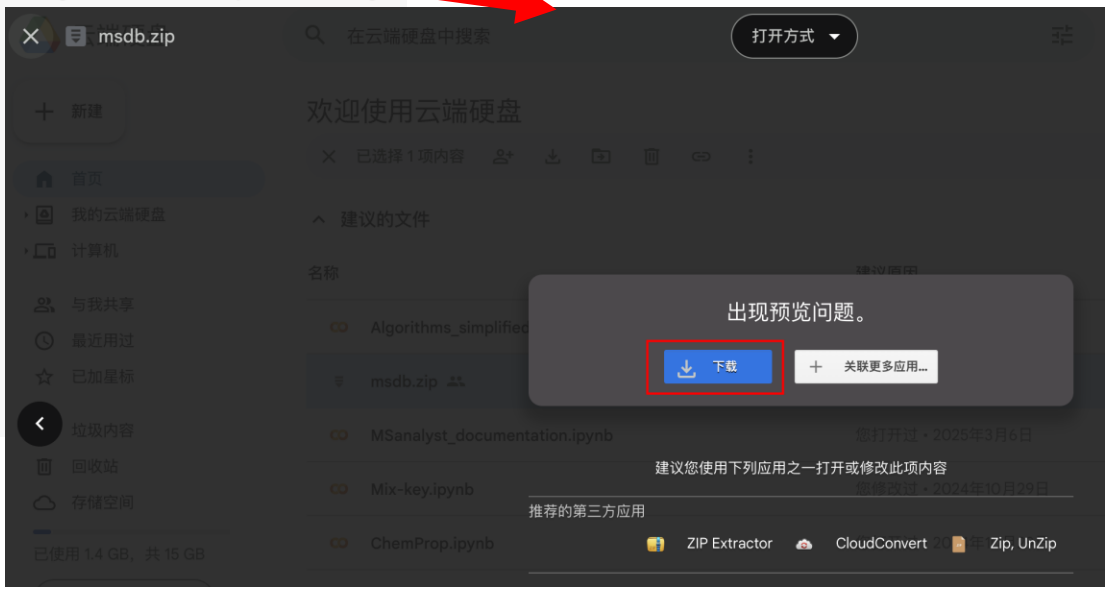
Installation

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

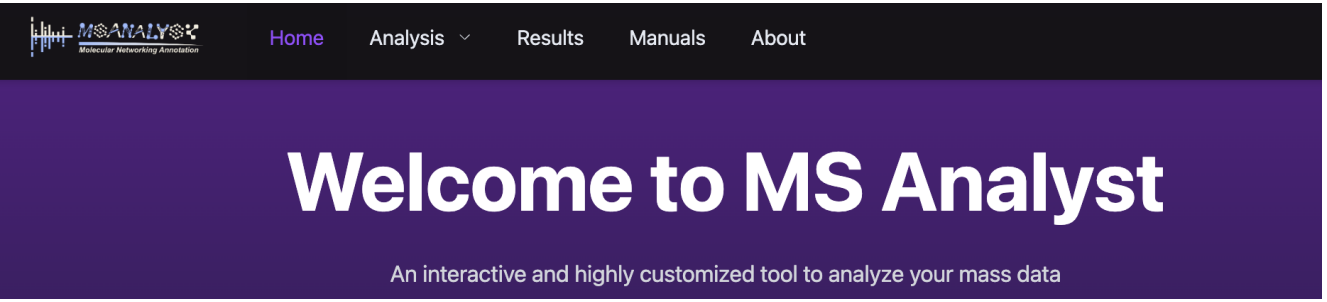
```
# Downloading msanalyst library using command or manually
wget --no-check-certificate 'https://drive.google.com/file/d/1w6HF3w1KIJlTz_QaVqqtN1BzkGDhDgzw/view?usp=sharing'

# 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
```

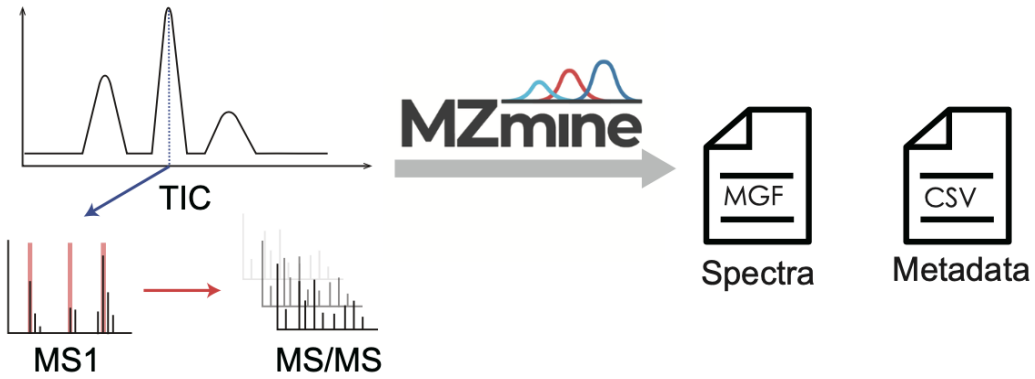


- **Or use the online version(https://msanalyst.net/)**



- **Data preprocessing**

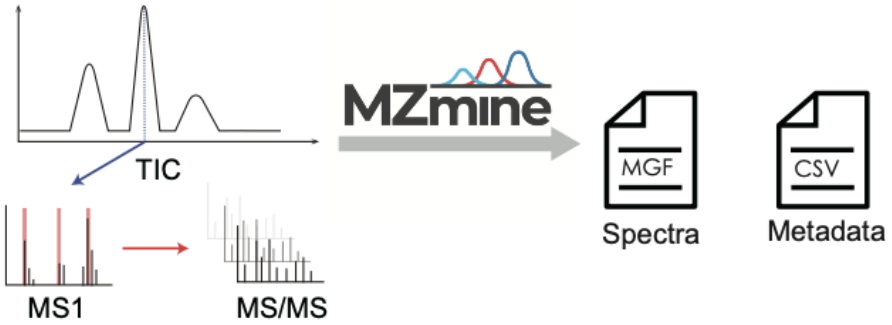
MZmine Untargeted LC-MS Workflow
https://mzmine.github.io/mzmine_documentation/workflows/lcmsworkflow/lcms-workflow.html

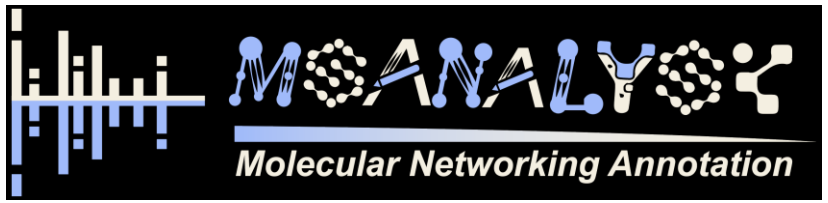


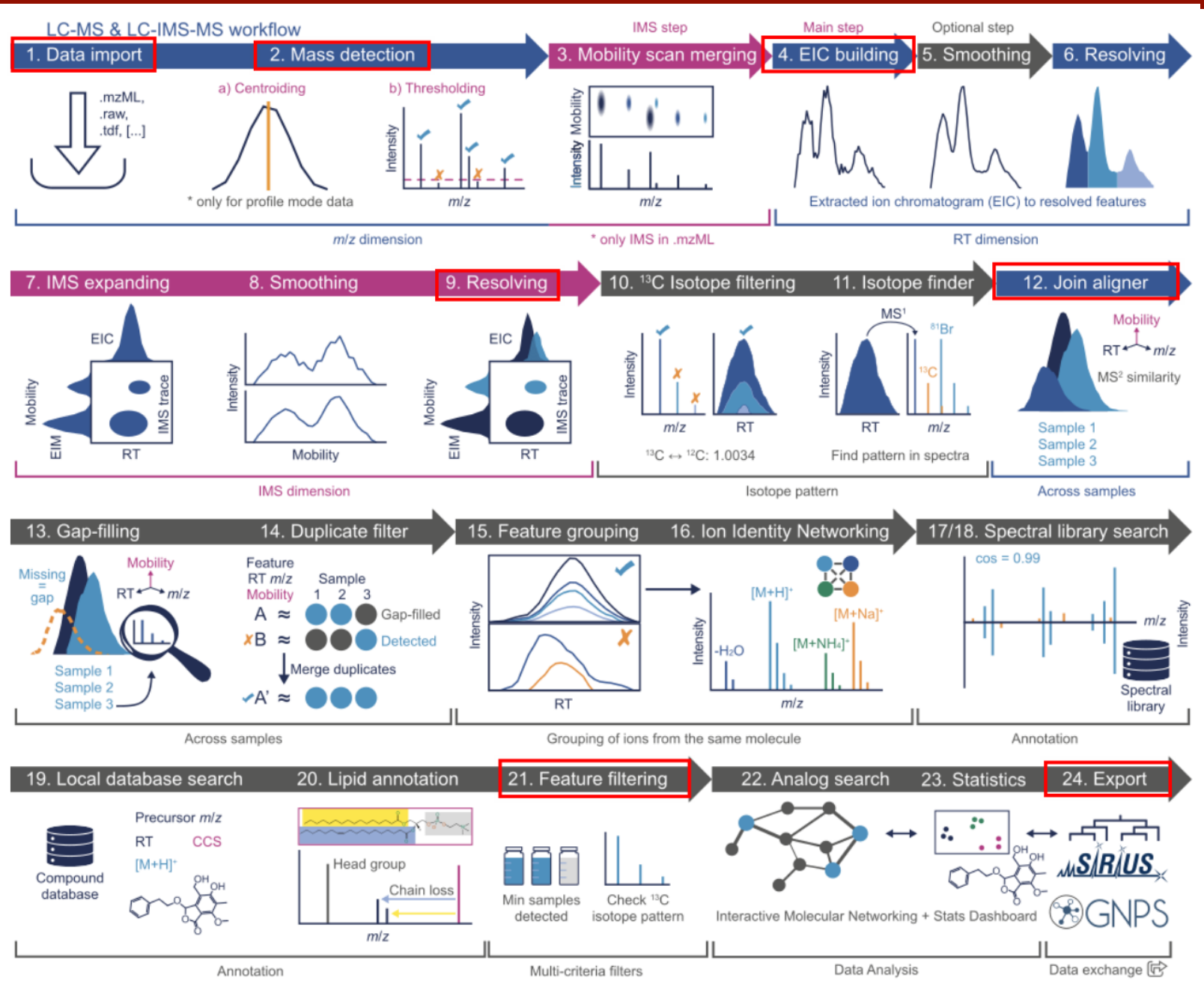
LC-MS data preprocessing

- **Data preprocessing**

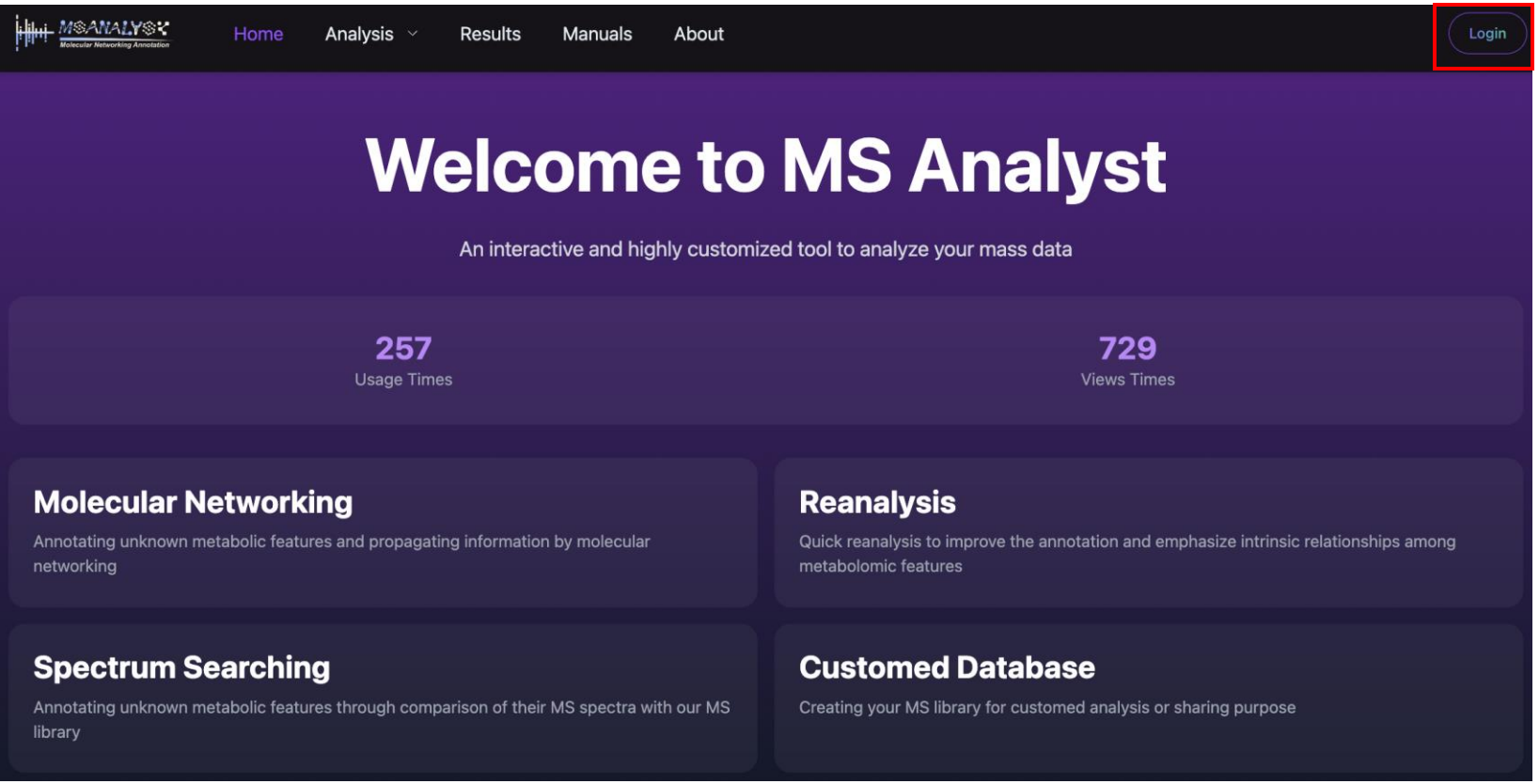
MZmine Untargeted LC-MS Workflow
https://mzmine.github.io/mzmine_documentation/workflows/lcmsworkflow/lcms-workflow.html

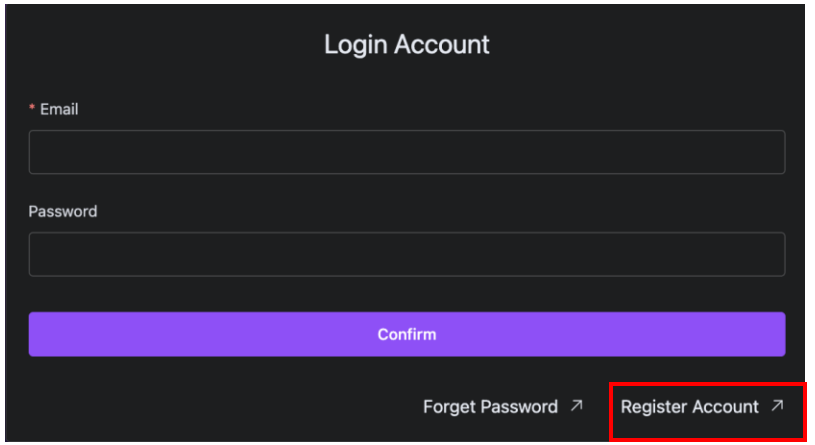


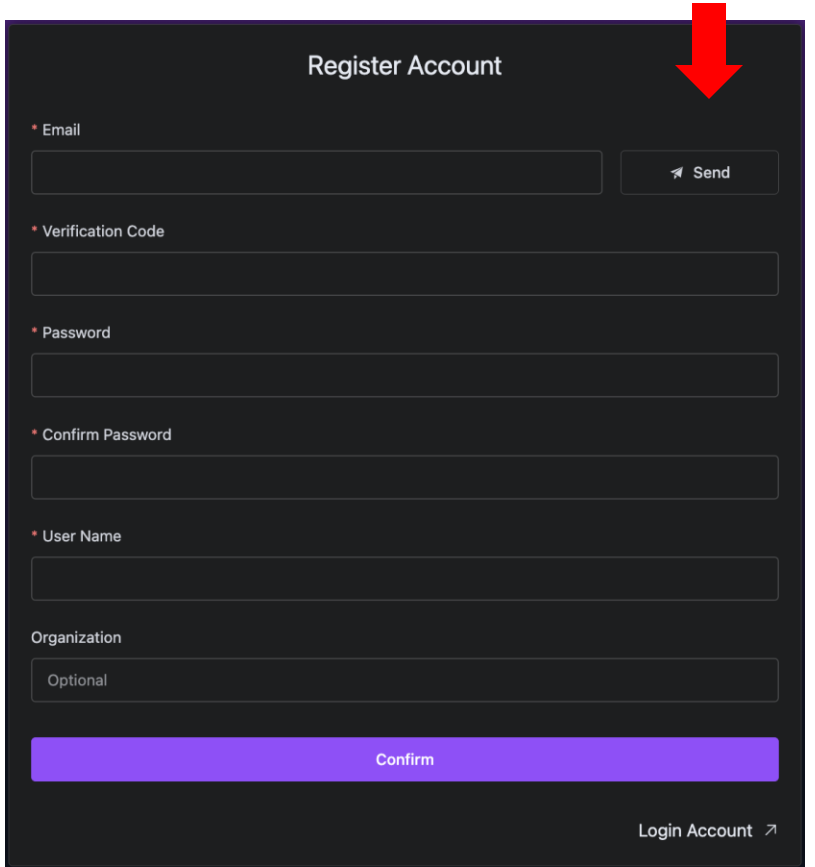




The MSanalyst homepage







Homepage

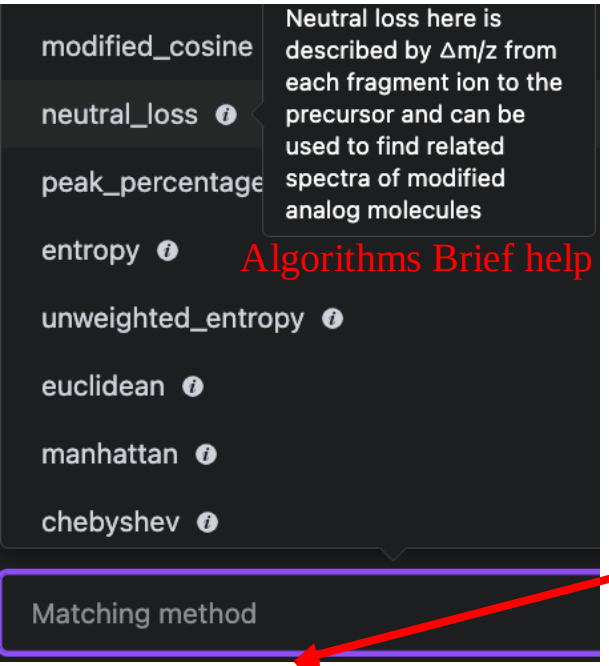
- Linkage: https://msanalyst.net/
- Four modules: Molecular Networking, Reanalysis, Spectrum Searching, and Customed Database

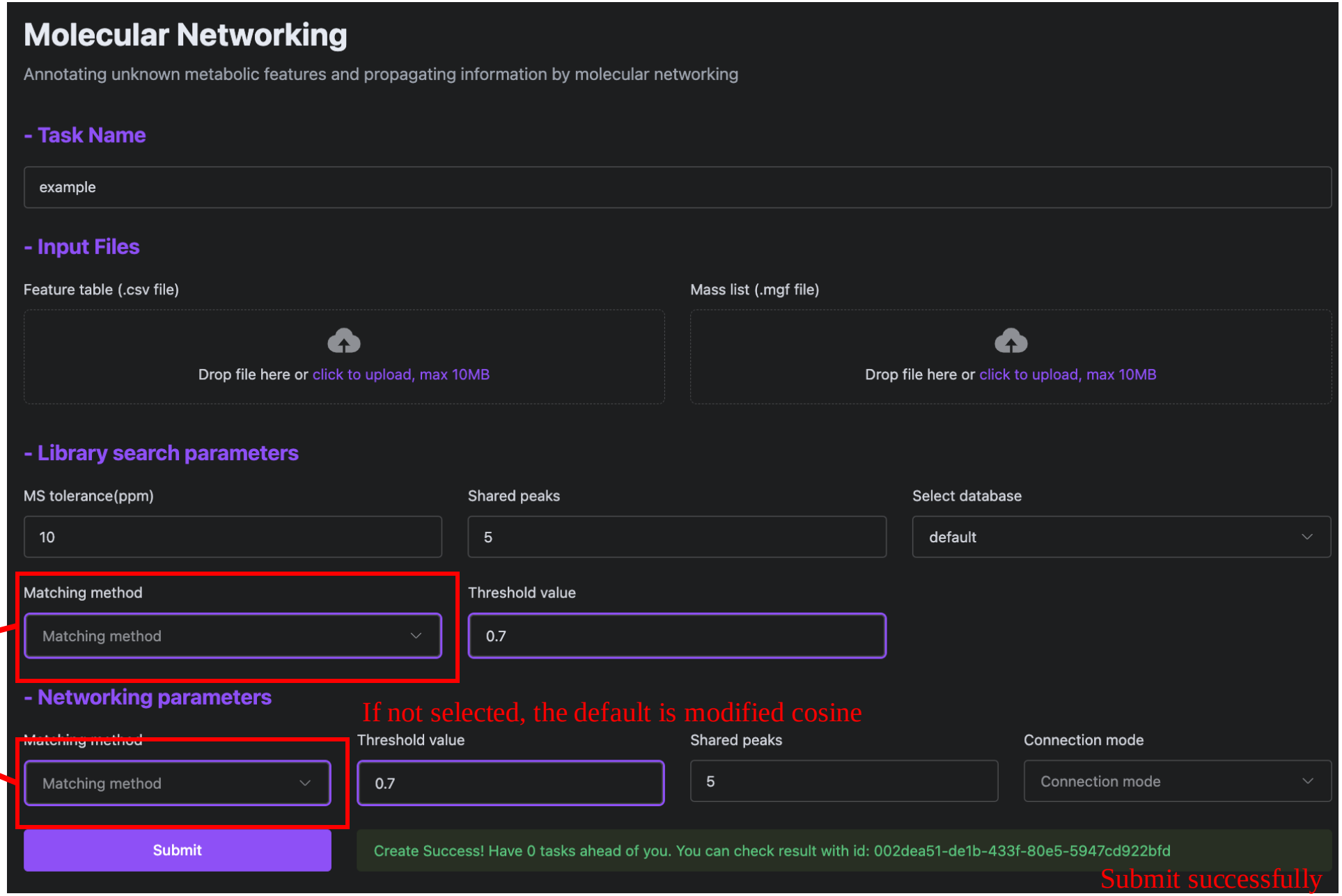
Molecular Networking

Molecular networking

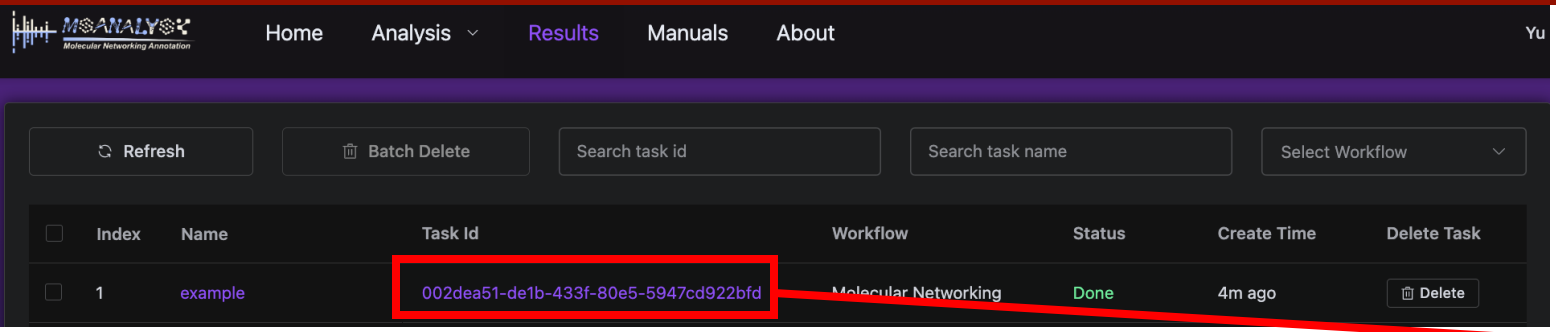
Annotating unknown metabolic features

- Upload files
- Set parameters
- Submit



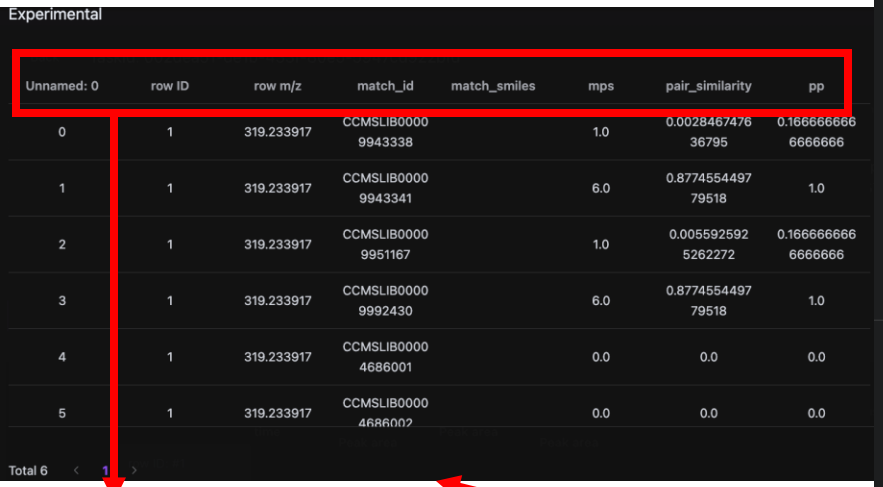


Molecular Networking

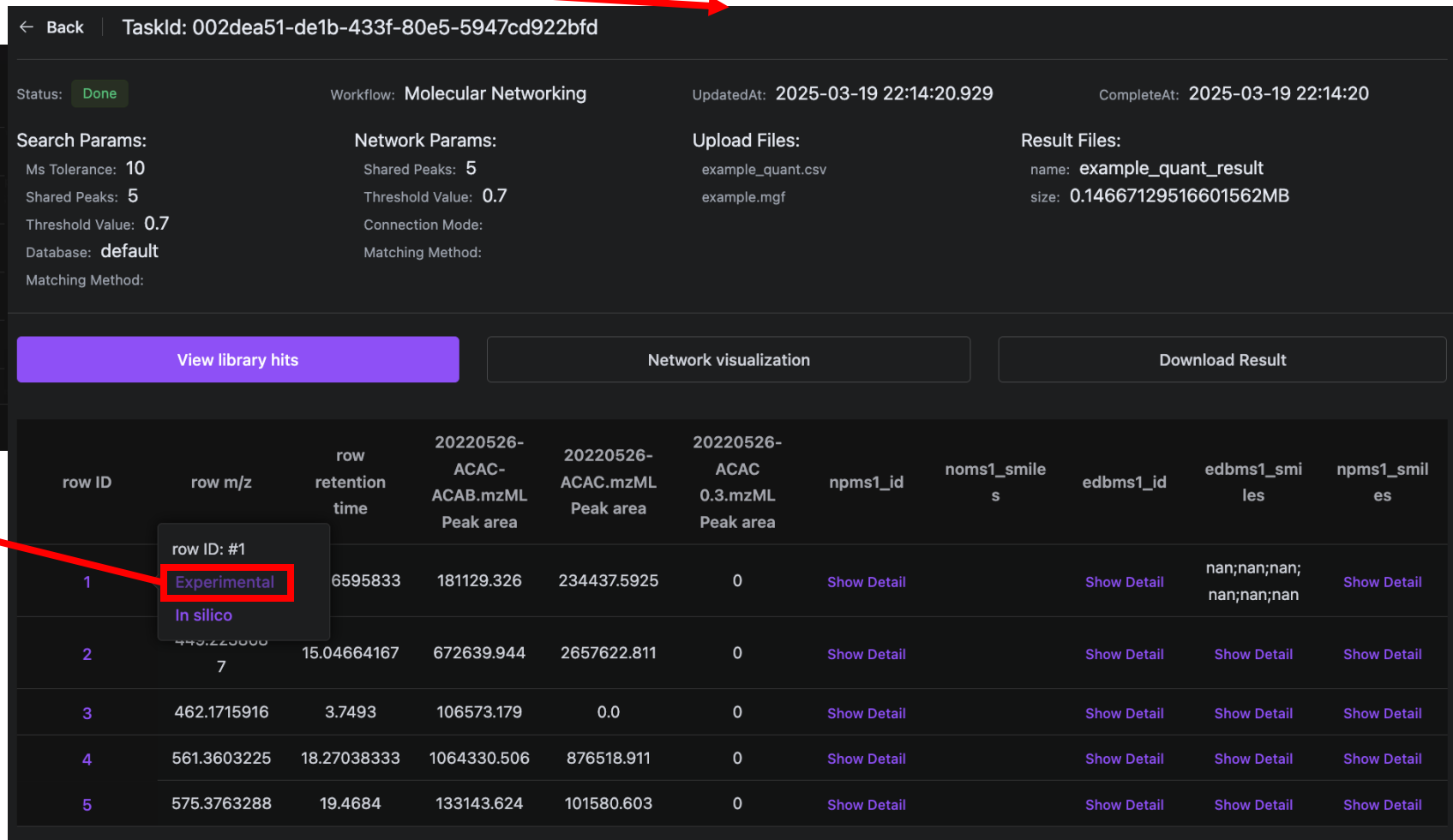


Molecular networking result page

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



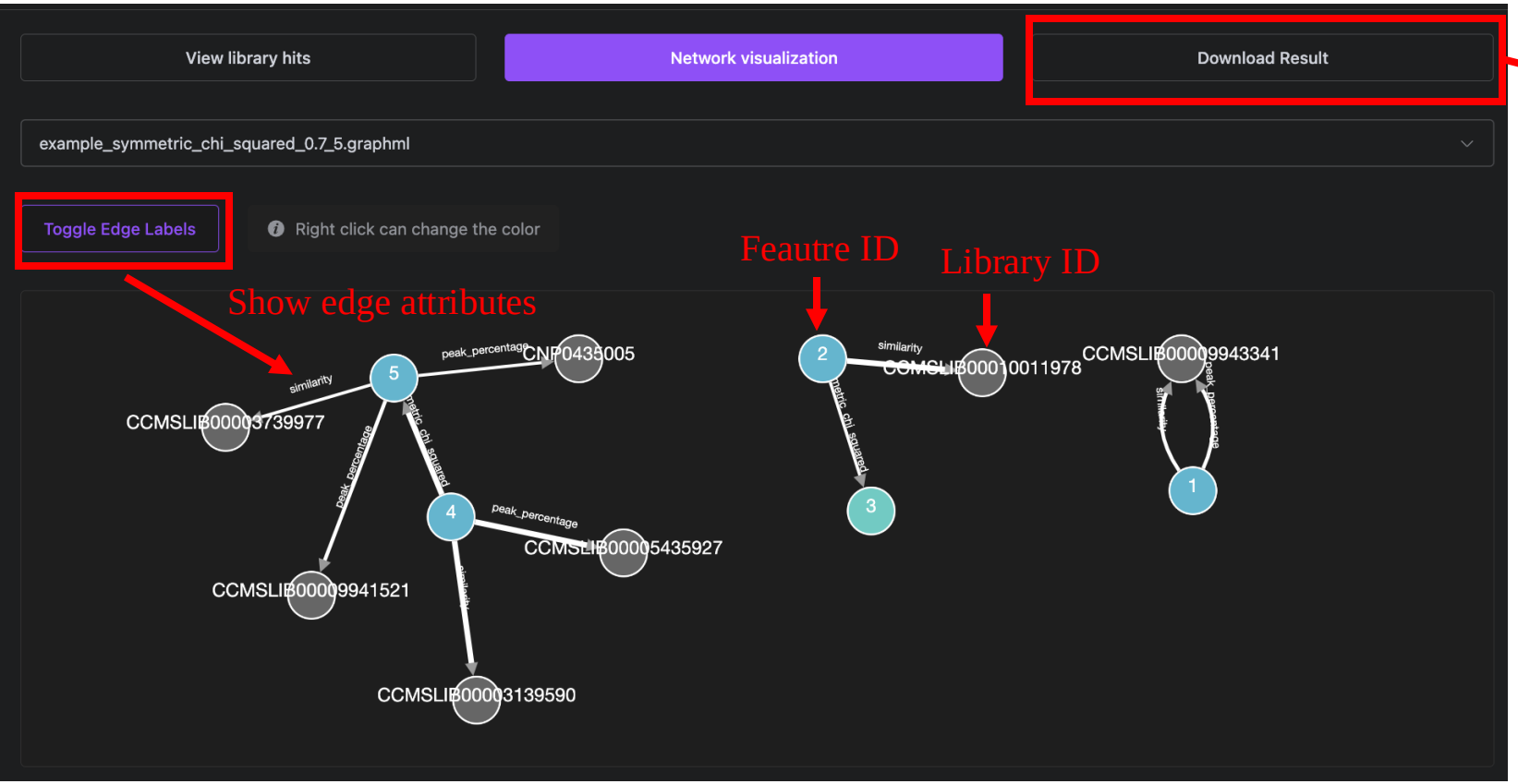
Detailed information of comparison
Row ID: Feature ID in query spectral file
Row m/z: Precursor m/z
match_id: Hits id in the library
match_smiles: Hits structure
mps: Number of matched peaks
pair_similarity: spectral similarity
pp: peak percentage score

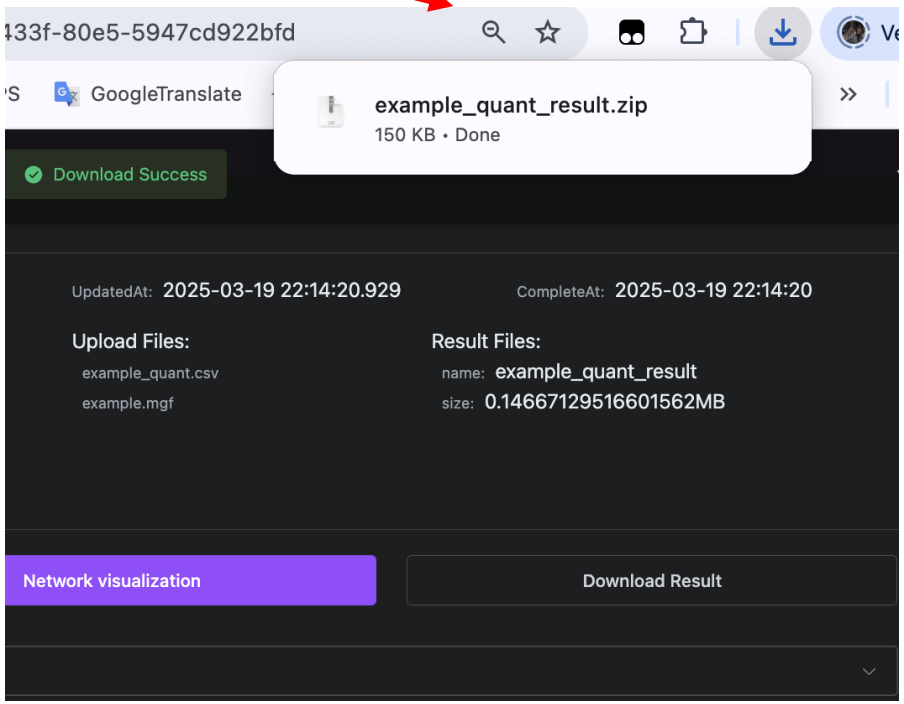


Molecular Networking

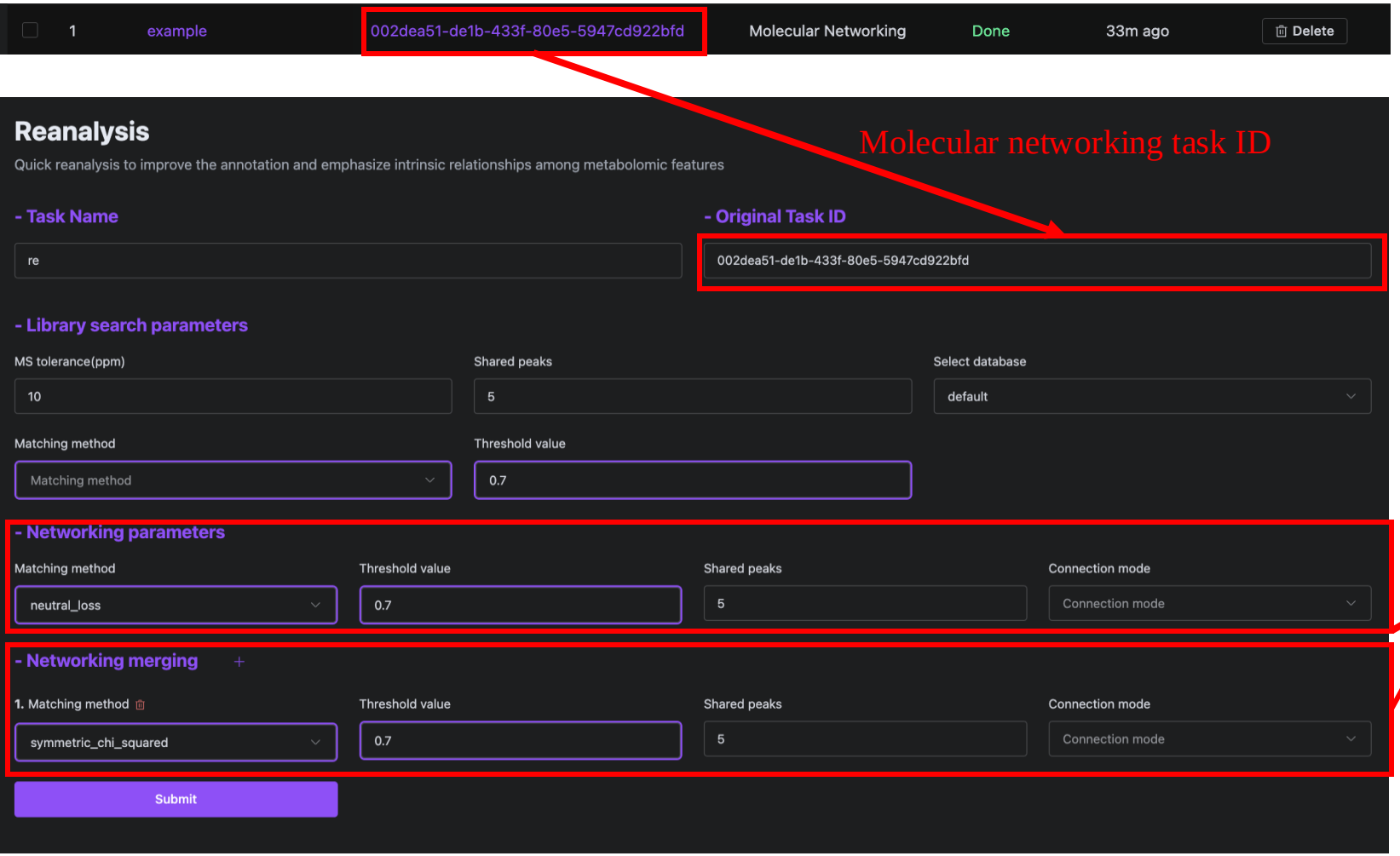
Molecular networking result page

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





Reanalysis



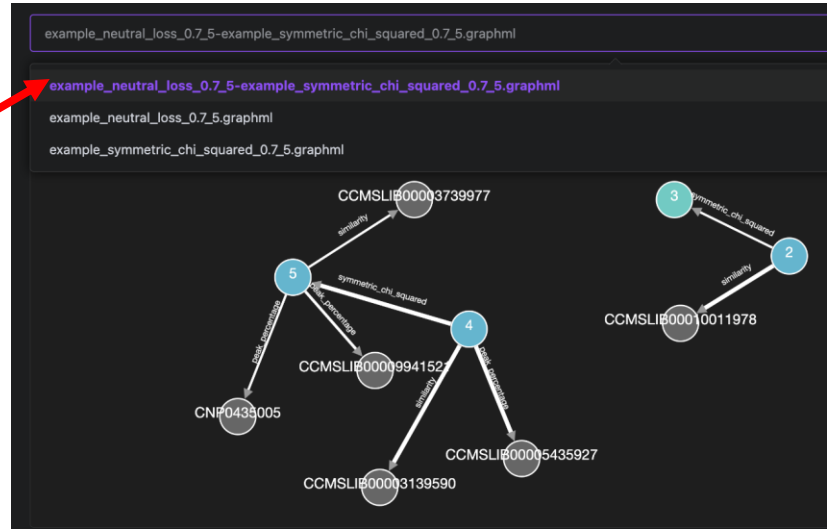
Reanalysis

Quick adjustment of thresholds and algorithms

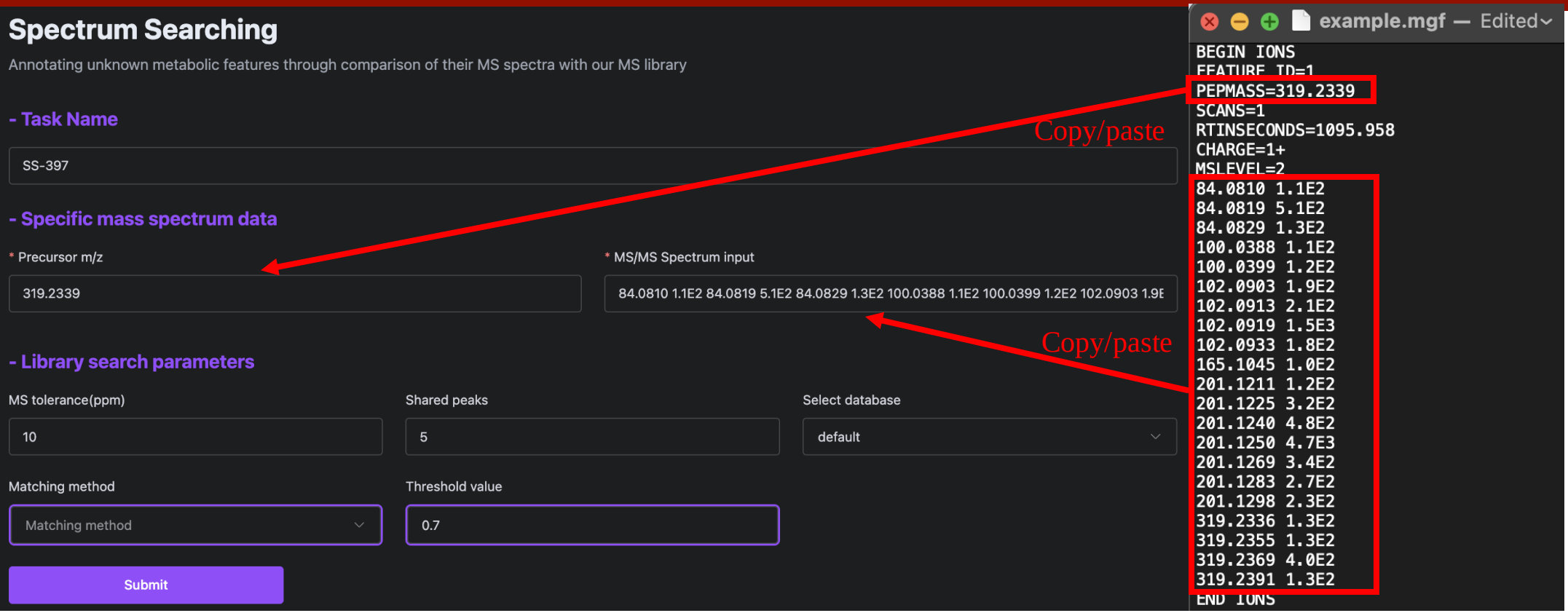
- Type in the molecular networking task ID
- Set thresholds and algorithms

Networking merging

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



Spectrum Searching

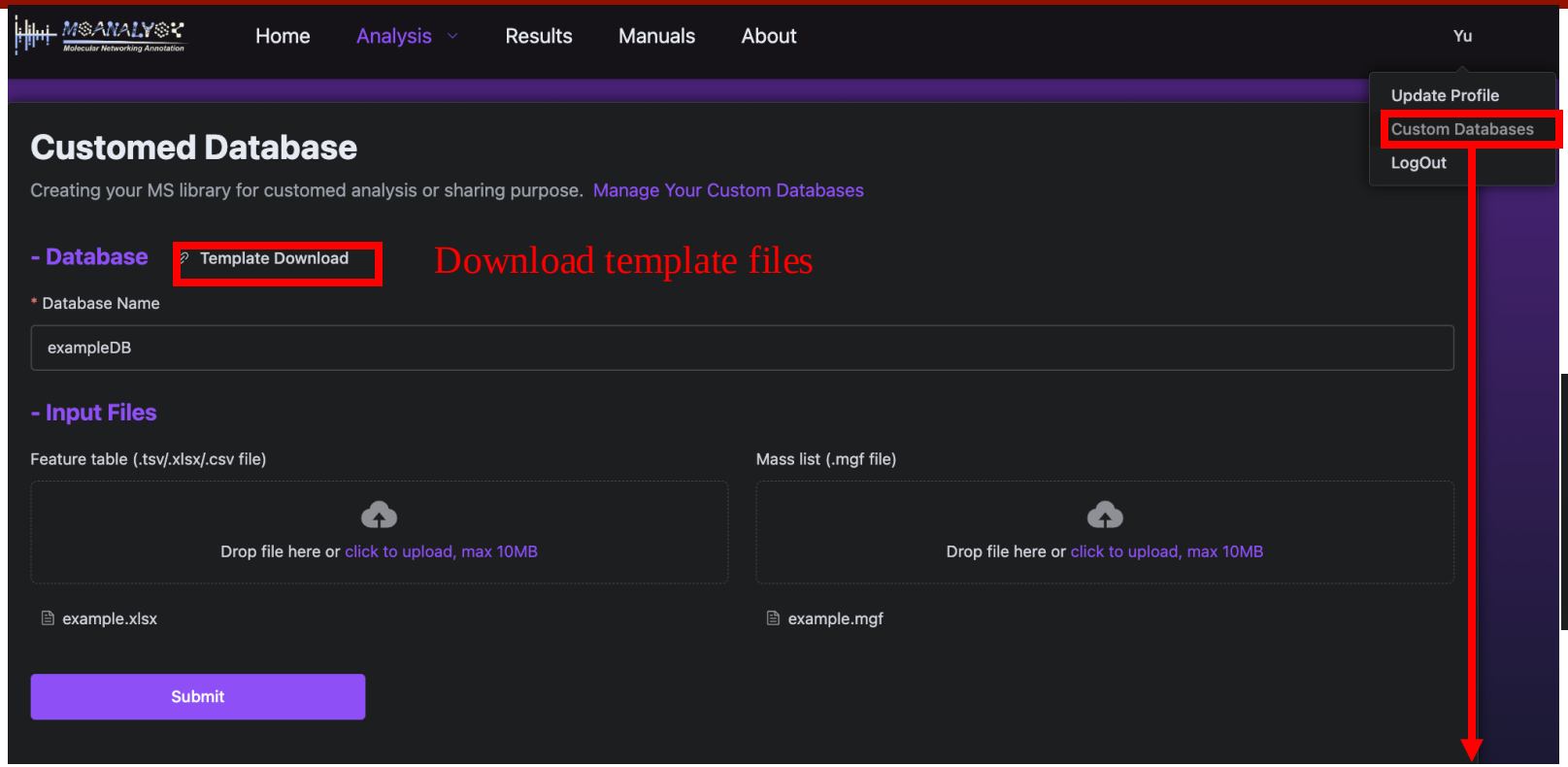


Spectrum Searching

Search specific spectrum against entire library of MSanalyst

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

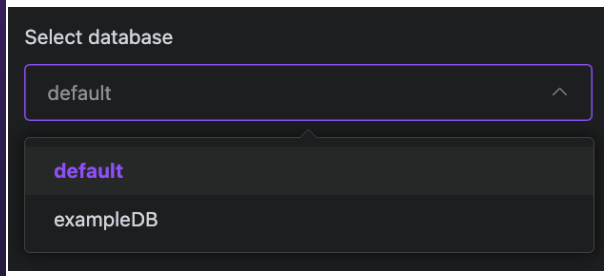
Customed Database



Customed Database

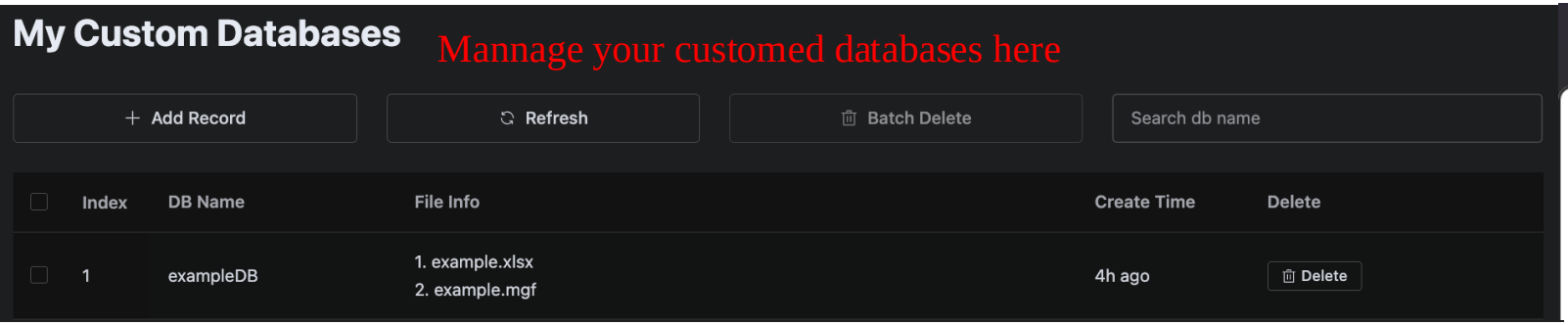
Create customed spectral database for search purpose

- 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



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
```



example.xlsx — Open with Microsoft Excel

compound_name	feature_ID	smiles	collector	adduct	organism
at-1	1	(C(COC3=(	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)((	Yu	M+H	*Aspergillus*
at-5	5	1C(O)=C3(	Yu	M+H	*Aspergillus*