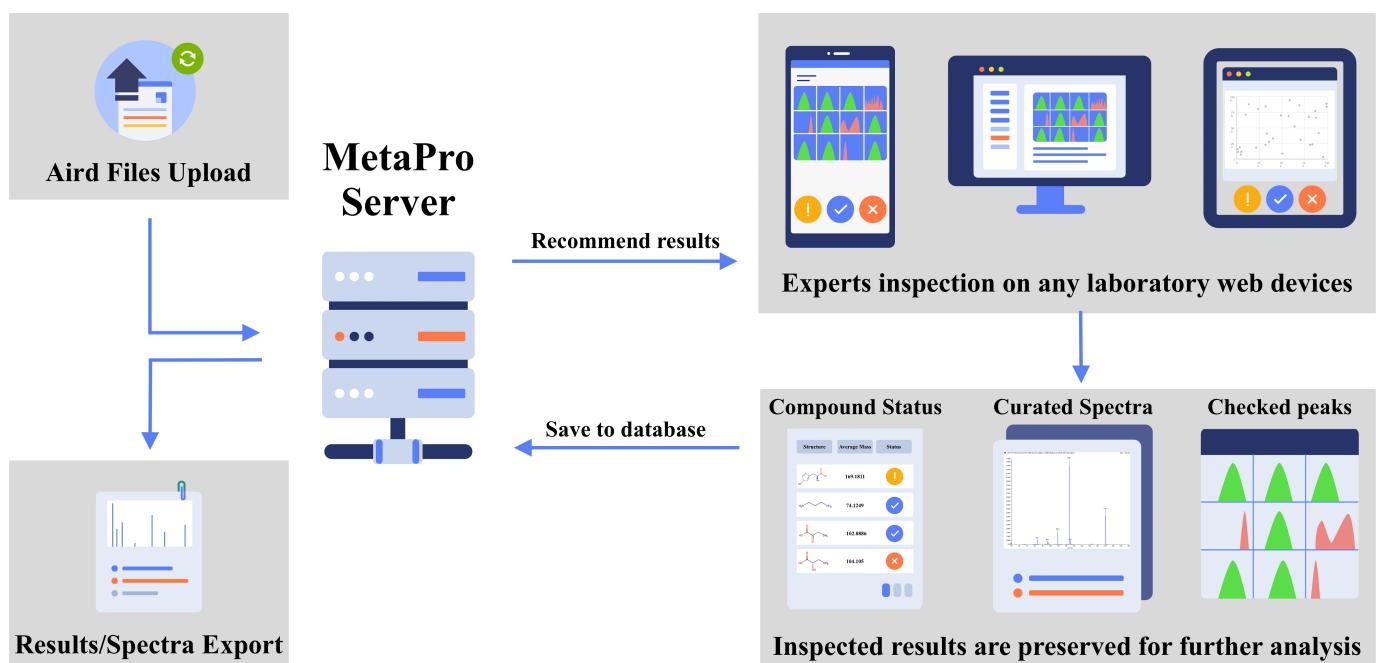


User Manual

Main Interface of MetaPro



Framework of MetaPro



Demo website

<http://47.88.77.176>

1 General Information

1.1 Scope of MetaPro

Currently mass spectrometry instruments are widely used in metabolomics studies, but software in this field usually have a lack of easily executed batch inspection and spectra curation ability. Besides, collaboration inconvenience on data processing also restrict analysis on efficiency.

MetaPro is a web-based stand-alone application for metabolomics MS data analysis, characterized by batch manual inspection and spectral library curation. MetaPro can perform accurate targeted compound detection on the input data and assure the result quality by batch manual inspection. Then, MetaPro can perform spectral library curation on the inspected results, which can improve the accuracy of further targeted analysis and promote the efficiency of manual inspection. The curated libraries and quantification results can be exported for further customized analysis.

1.2 System conception description

In MetaPro, we provide these main base compositon moduels:

[Batch](#) , [Compound](#) , [Experiment](#) , [Library](#) , [Method](#) , [Overview](#) , [Project](#) , [Spectrum](#) , [Task](#) .

The explanations for these base items are described below.

Item	Explanation
Batch	A batch is composed of some experimental files. A project can have a few batches.
Compound	A compound refers to a specific metabolite whose name, ID, m/z, RT and other information are stored in the database. Selected compounds could be used for conducting targeted analysis.
Experiment	An experiment is a basic analytical unit in the MetaPro. It represents the mass spectrometry data obtained from one sample. The actual storage mode of an experiment is an Aird format file under the user-defined document folder. A few experiments can be divided into one batch.
Library	A library contains a few compounds.
Method	All parameters used in the analysis steps are extracted into a method. Different parameters composition could be saved into different methods for convenient query.
Overview	An overview is the storage of the analyzed results. By checking a overview, multiple quality control operations can be achieved.
Project	A project can have a few batches. Each batch has a few experiments. Project is the largest unit where experiments could be organized.
Spectrum	A spectrum is correlated to a specific compound. Instrument type, collision energy, ionization mode and other description information of the mass spectrometry characteristics are stored in a spectrum.
Task	Task refers to a metabolomics analysis process needed to be done or undertaken. It's timely status and records could be seen in the task page.

1.3 Data restrictions

MetaPro currently only supports DDA mode data. The input for MetaPro should be converted vendor files (Aird files). The compound library should be given to the application in a specific format.

1.4 Data safety

MetaPro is a stand-alone application that can be deployed on your personal computer or high-performance server. All data will be saved on your local devices and will not be uploaded.

1.5 Contact us

If you have any questions, you can contact us through Github or csci@csibio.net.

2 Installation

2.1 System and hardware requirements

MetaPro is available for Windows 7 (or above), Linux and MacOS. The minimum and recommended system specifications are described in the following table.

Specifications	Minimum	Recommended
CPU	Intel Core i5 10–gen or AMD R5	Intel Core i9 12–gen or AMD R9 5900
Hard drive	50GB free space	2x data set size
RAM	16GB	64GB(Core i9–10gen), 128GB(Core i9–12gen)

2.2 Download

MetaPro

Installation packages for all the supported systems can be downloaded at [GitHub](#).

AirdPro

MetaPro uses AirdPro for Vendor MS file conversion.

AirdPro (version 1.1.0.0) can be freely downloaded at [GitHub](#).

Tutorial data

The tutorial data is a public metabolomics software benchmark dataset, published in Li, Zhucui, et al.

You can download the tutorial data at [GoogleDrive](#) and [OneDrive](#).

The data contains 2 datasets:

- **TripleTOF dataset**
 - 8 converted instrument data (16 files)
 - 2 library (internal standard library, analyte library)
- **QE HF dataset**
 - 10 converted instrument data (20 files)
 - 2 library (internal standard library, analyte library)

2.3 One-click installation

Extract MetaPro zip file to any directory you want.

Here we use INSTALLATION_PATH to represent your installation path, for example `C:\`

Windows

- Open INSTALLATION_PATH folder
- **start:** Right click `MetaproStart.bat`, run as administrator.

Successful operation:

The following operations appear in the terminal to indicate that the operation is successful:

```

MetaPro-server
2022-03-07 11:43:43.508 INFO 11656 --- [           main] org.quartz.core.SchedulerSignalerImpl : Initialized Scheduler Signaller of type: class org.quartz.core.SchedulerSignalerImpl
2022-03-07 11:43:43.508 INFO 11656 --- [           main] org.quartz.core.QuartzScheduler      : Quartz Scheduler v. 2.3.2 created.
2022-03-07 11:43:43.508 INFO 11656 --- [           main] org.quartz.simpl.RAMJobStore       : RAMJobStore initialized.
2022-03-07 11:43:43.509 INFO 11656 --- [           main] org.quartz.core.QuartzScheduler     : Quartz Scheduler (v2.3.2) 'quartzScheduler' with instanceId 'NON_CLUSTERED'
: Scheduler class: 'org.quartz.core.QuartzScheduler' - running locally.
NOT STARTED.
Currently in standby mode.
Number of jobs executed: 0
Using thread pool 'org.quartz.simpl.SimpleThreadPool' - with 10 threads.
Using job-store 'org.quartz.simpl.RAMJobStore' - which does not support persistence. and is not clustered.

2022-03-07 11:43:43.509 INFO 11656 --- [           main] org.quartz.impl.StdSchedulerFactory   : Quartz scheduler 'quartzScheduler' initialized from an externally provided properties instance.
2022-03-07 11:43:43.509 INFO 11656 --- [           main] org.quartz.impl.StdSchedulerFactory   : Quartz scheduler version: 2.3.2
2022-03-07 11:43:43.509 INFO 11656 --- [           main] org.quartz.core.QuartzScheduler       : JobFactory set to: org.springframework.scheduling.quartz.SpringBeanJobFactory@5c3e67b9
2022-03-07 11:43:43.554 INFO 11656 --- [           main] o.s.b.w.embedded.tomcat.TomcatWebServer: Tomcat started on port(s): 8080 (http) with context path ''
2022-03-07 11:43:43.555 INFO 11656 --- [           main] o.s.s.quartz.SchedulerFactoryBean     : Starting Quartz Scheduler now
2022-03-07 11:43:43.555 INFO 11656 --- [           main] org.quartz.core.QuartzScheduler       : Scheduler $NON_CLUSTERED started.
2022-03-07 11:43:43.560 INFO 11656 --- [           main] c.w.air.metapro.MetabolomicsApplication: Started MetabolomicsApplication in 2.921 seconds (JVM running for 3.172)

```

After successful startup, open a browser and connect to <localhost:8080>

- stop:** Right click [MetaProStop.bat](#), run as administrator
- uninstall:** Stop MetaPro and delete the installation folder.

MacOS

- Open a terminal

```
cd INSTALLATION_PATH
cd MetaproForMac
```

- start:**

```
1 bash MetaproStart.sh
```

Successful operation:

The following operations appear in the terminal to indicate that the operation is successful:

```
1 $ bash ./MetaproStart.sh
2 /Users/commands/MetaproForMac
3 ***** Start Redis *****
4 /Users/commands/MetaproForMac/redis
5 ***** Start MongoDB *****
6 /Users/commands/MetaproForMac/mongodb
7 ***** Start Metapro *****
8 about to fork child process, waiting until server is ready for connections.
9 forked process: 94332
10
11 $ child process started successfully, parent exiting
```

After successful startup, open a browser and connect to <localhost:8080>

- stop:**

```
1 bash MetaproStop.sh
```

- **uninstall:** Stop MetaPro and delete the installation folder.

Linux

- Open a terminal

```
cd INSTALLATION_PATH
cd MetaproForUbuntu
```

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- **start:**

```
1 bash MetaproStart.sh
```

Bash

Successful operation:

The following operations appear in the terminal to indicate that the operation is successful:

```
1 $ bash ./MetaproStart.sh
2 /home/commands/MetaproForMac
3 ***** Start Redis *****
4 /home/commands/MetaproForMac/redis
5 ***** Start MongoDB *****
6 /home/commands/MetaproForMac/mongodb
7 ***** Start Metapro *****
8 about to fork child process, waiting until server is ready for connections.
9 forked process: 94332
10
11 $ child process started successfully, parent exiting
```

Bash

After successful startup, open a browser and connect to localhost:8080

- **stop:**

```
1 bash MetaproStop.sh
```

Bash

- **uninstall:** Stop MetaPro and delete the installation folder.

After successful startup, open the browser to enter: localhost:8080, enter MetaPro interface.

Browsers support: Modern browsers and IE11: IE11, Edge, Firefox, Chrome, Safari, Opera

2.4 Configuration

There are two important parameters in the configuration of MetaPro. The **analysis data directory** and the **result export directory**.

Analysis data directory

All files that need to be analyzed by MetaPro need to be placed under the analysis data directory according to the rules in section 4.1.1. MetaPro can quickly import multiple batches of experiments by monitoring the converted files in the **analysis data directory**. All results that need to be exported by MetaPro will be exported to the **result export directory**.

Both directories are automatically set during the installation process. Users can modify the path according to their requirements.

Default directories are summarized as follows:

```
[Windows]
# default analysis data directory
C://metapro//data
# default result export directory
C://metapro//export
```

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```
[MacOS]
# default analysis data directory
/Users/$USER/metapro/data
# default result export directory
/Users/$USER/metapro/export
```

```
[Ubuntu]
# default analysis data directory
/home/$USER/metapro/data
# default result export directory
/home/$USER/metapro/export
```

The way of changing default parameters is as follows:

1. Open the `config.properties` file in the installation directory of MetaPro.
2. Change the value of `directory` and `export`. `directory` is the analysis data directory and `export` is the result export directory.
3. Restart MetaPro.

2.5 Associated software

AirdPro

AirdPro (version 1.1.0.0) can be freely downloaded at [GitHub](#).

MetaPro uses AirdPro (version 1.1.0.0) for instrument vendor file conversion. Instrument data should be converted to Aird format (.aird, .json) before being loaded into MetaPro. Aird is a computational-oriented data format for rapid access of MS data. By rearranging, compressing, and indexing spectra data, Aird can significantly speed up data reading, and thus improve the efficiency of data analysis and inspection.

AirdPro supports the vendor files including `.raw`, `.wiff` and `.d` formats.

AirdPro runs on Windows system, limited by the system requirement of vendor APIs.

3 Page Introduction

3.1 Project management page

The screenshot shows the MetaPro application interface. On the left is a vertical sidebar with a dark background and white text, containing links for 'Project' (which is highlighted in blue), 'Library', 'Method', 'Task', and 'Help'. The main area has a light gray background. At the top, there's a search bar with fields for 'Project Name' and 'Owner', and buttons for 'Search', 'Reset', and 'Create Project'. Below the search bar is a table with the following data:

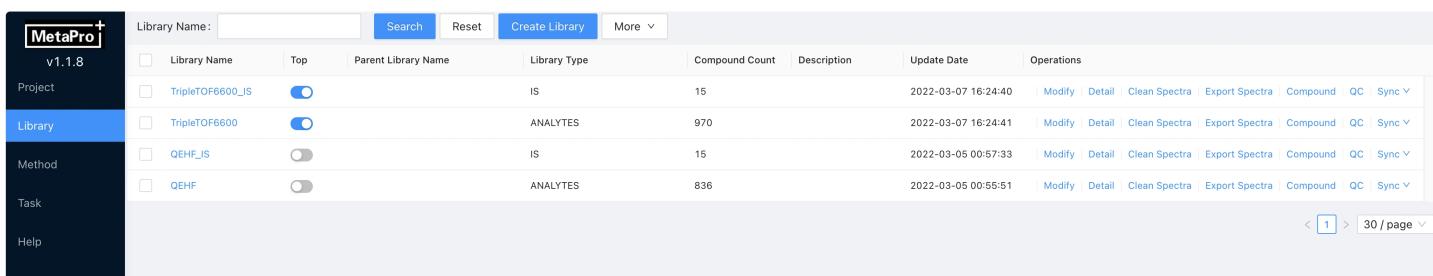
ID	Top	Project Name	Batch Count	Count	Overview Count	Size Ratio (Vendor:Aird)	Storage Saved	Owner	Description	Create Date	Operations
+ Show	<input checked="" type="checkbox"/>	5-2018-ACA	2	18	2	8880M : 4832M	4048M	Nico		2022-03-04 22:27:13	Scan Files List Target Analyze QC More
Total			2	18	2	8.9GB : 4.8GB					< 1 > 30 / page

This is the first page that users will see when they start the system. Users can create new projects by clicking on the Create Project button in the top column. Then, input the name, owner, and description information of the new project on this page, where delete, update and search options are also available. The project management page shows all the users' projects and their additional information, including batch numbers, experiment numbers, overview numbers, owner and create date. Storage space is shown with saved space because the use of Aird data format.

To add experimental files into a project, users need to categorize all the Aird files into a folder having the same name with the created project. The folder should be put under the repository of MetaPro. This folder must contain several sub-folders, which are considered to be batches under this project. Aird files must be put under the sub-folders rather than the folder having the same name with the created project. Subsequently, these Aird files and batches information can be read into the system through clicking on the "scan file" button. During this process, their brief information will be stored. Meanwhile, batch number and experiment number are automatically modified according to the actual file arrangement under the repository. Also, Users can check extracted ion chromatogram (EIC) in each experiment after the index is created in the system.

Clicking on the selected project will get access to its detailed information page, where its experiments information are fully displayed. Here, the experiment information is able to be updated, deleted, and modified.

3.2 Library management page



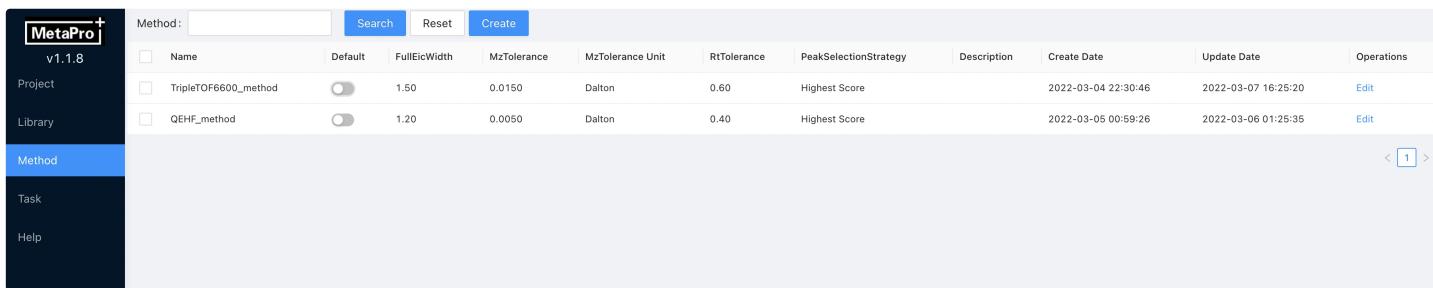
The screenshot shows the library management interface. On the left is a sidebar with buttons for Project, Library (which is selected), Method, Task, and Help. The main area has a header with 'Library Name' and buttons for 'Search', 'Reset', 'Create Library', and 'More'. Below is a table with columns: Library Name, Top, Parent Library Name, Library Type, Compound Count, Description, Update Date, and Operations. The table contains four rows of data:

Library Name	Top	Parent Library Name	Library Type	Compound Count	Description	Update Date	Operations
TripleTOF6600_IS	<input checked="" type="checkbox"/>		IS	15		2022-03-07 16:24:40	Modify Detail Clean Spectra Export Spectra Compound QC Sync
TripleTOF6600	<input checked="" type="checkbox"/>		ANALYTICS	970		2022-03-07 16:24:41	Modify Detail Clean Spectra Export Spectra Compound QC Sync
QEHF_IS	<input checked="" type="checkbox"/>		IS	15		2022-03-05 00:57:33	Modify Detail Clean Spectra Export Spectra Compound QC Sync
QEHF	<input checked="" type="checkbox"/>		ANALYTICS	836		2022-03-05 00:55:51	Modify Detail Clean Spectra Export Spectra Compound QC Sync

Pagination controls at the bottom right show page 1 of 30.

This page has the similar visualization hierarchical to the project management page. Creating, updating, modifying, deleting options toward compound libraries are available here. When creating a new library, MetaPro allows users to upload a formatted CSV file to fill the compounds information in this library. Clicking a library can check all the compounds that are included in this library.

3.3 Method management page



The screenshot shows the method management interface. On the left is a sidebar with buttons for Project, Library, Method (which is selected), Task, and Help. The main area has a header with 'Method' and buttons for 'Search', 'Reset', and 'Create'. Below is a table with columns: Name, Default, FullEicWidth, MzTolerance, MzToleranceUnit, RtTolerance, PeakSelectionStrategy, Description, Create Date, Update Date, and Operations. The table contains two rows of data:

Name	Default	FullEicWidth	MzTolerance	MzToleranceUnit	RtTolerance	PeakSelectionStrategy	Description	Create Date	Update Date	Operations
TripleTOF6600_method	<input checked="" type="checkbox"/>	1.50	0.0150	Dalton	0.60	Highest Score		2022-03-04 22:30:46	2022-03-07 16:25:20	Edit
QEHF_method	<input checked="" type="checkbox"/>	1.20	0.0050	Dalton	0.40	Highest Score		2022-03-05 00:59:26	2022-03-06 01:25:35	Edit

Pagination controls at the bottom right show page 1 of 1.

The contents shown here are the clustered parameters, which we call methods. When creating a new method, recommended parameters are preset in the method template. Noteworthy, created methods can be used to various projects, batches and experimental files. This design makes it easy to check parameter settings among different projects. Creating, viewing, deleting and modifying methods are operated on this page.

3.4 Task management page

Task Name	Task Status	Task Template	Cost Time(ms)	Create Date	Update Date
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	35957	2022-03-06 11:39:58	2022-03-06 11:40:34
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	58278	2022-03-06 11:26:58	2022-03-06 11:27:57
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	26029	2022-03-06 11:26:04	2022-03-06 11:26:29
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	23149	2022-03-06 01:51:32	2022-03-06 01:51:55
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	52918	2022-03-06 01:38:55	2022-03-06 01:39:48
BUILD_LIBRARY-BuildLibrary	Success	BUILD_LIBRARY	36535	2022-03-06 01:37:01	2022-03-06 01:37:38
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=batch	Success	TARGET_ANALYZE	15222	2022-03-06 01:33:31	2022-03-06 01:33:46
BUILD_LIBRARY-BuildLibrary	Success	BUILD_LIBRARY	54259	2022-03-06 01:29:19	2022-03-06 01:30:13
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	47299	2022-03-06 01:26:14	2022-03-06 01:27:02
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=batch	Success	TARGET_ANALYZE	2406	2022-03-06 01:00:29	2022-03-06 01:00:32
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	43149	2022-03-05 15:46:17	2022-03-05 15:57:00
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	40963	2022-03-05 14:28:06	2022-03-05 14:28:47
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=batch	Success	TARGET_ANALYZE	27849	2022-03-05 14:17:03	2022-03-05 14:17:31
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	4296	2022-03-05 14:03:51	2022-03-05 14:03:55
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	4346	2022-03-05 12:41:07	2022-03-05 12:43:11
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	3992	2022-03-05 12:18:02	2022-03-05 12:18:06
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=batch	Success	TARGET_ANALYZE	4505	2022-03-05 12:16:19	2022-03-05 12:16:23
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	42120	2022-03-05 12:09:23	2022-03-05 12:10:05
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	3978	2022-03-05 10:13:05	2022-03-05 10:13:09
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName=raw_batch	Success	TARGET_ANALYZE	3622	2022-03-05 10:07:42	2022-03-05 10:07:46

Task page presents the progress of **BUILD_LIBRARY** **SCAN_AND_UPDATE_EXPERIMENTS**. Users can check their execution status on this page. The execution log of each task can be viewed by clicking on the **+** button on each row. Time cost, created time, and updated dates are displayed for each task.

4 Step by step instructions

4.1 Data preparation

4.1.1 MS file preparation

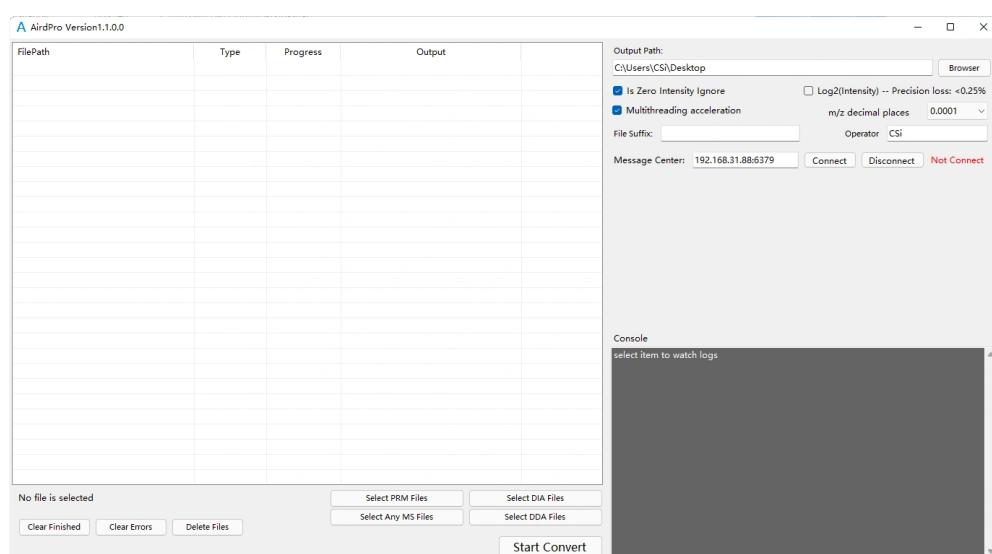
Step 1: File Conversion

MetaPro supports MS data acquired with the data-dependent acquisition (DDA) method. Vendor MS data should be converted to Aird format (.aird & .json) before being loaded into MetaPro.

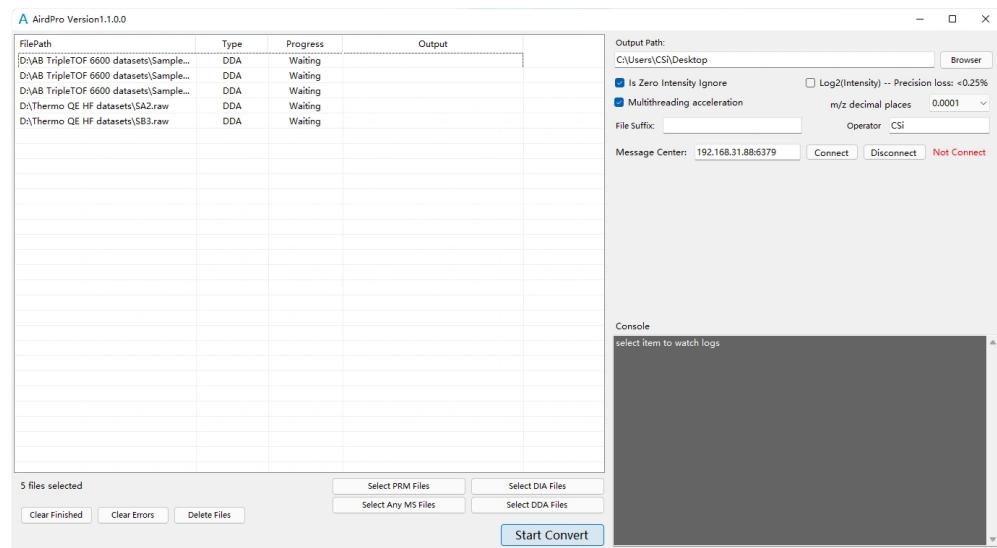
Introduction and download link of the file conversion software AirdPro is illustrated above in section 2.5.

1. Open AirdPro file converter

Open AirdPro by running AirdPro.exe in the installation directory. Users can create a desktop shortcut for easy access.



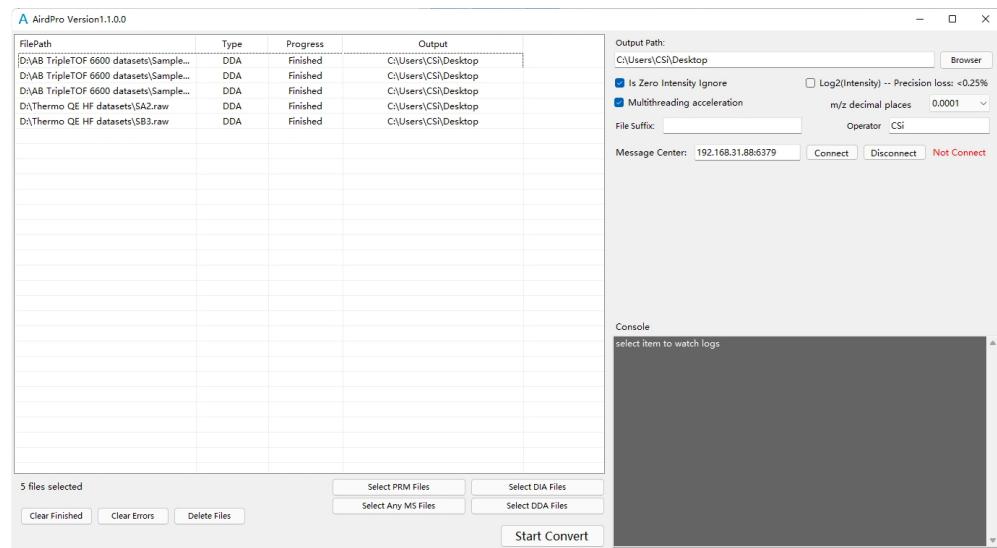
2. Select files for conversion in DDA mode



3. Select output folder

4. Start Convert

After file conversion, each MS file is converted to two converted files, end with .aird and .json.



For example:

```
# Thermo file
Original: file_name.raw
Converted: file_name.aird, file_name.json

# SCIEV file
Original: file_name.wiff, file_name.wiff.scan
Converted: file_name.aird, file_name.json
```

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Step 2: File directory arrangement

MetaPro enables efficient multi-batch files import by scanning folder structure under the previously set data repository (section 2.4).

For example, if we set the data directory as `repository=/usr/local/data`

The folder structure of different projects needs to be arranged as follows:

```
/usr/local/data
└── project-1
    └── batch-1
```

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```

    └── converted_file-1.aird
    └── converted_file-1.json
    └── converted_file-2.aird
    └── converted_file-2.json
    └── batch-2
        └── converted_file-3.aird
        └── converted_file-3.json
        └── converted_file-4.aird
        └── converted_file-4.json
    └── project-2
    └── ...

```

The first-level directory under the scan directory is the project name.

The second-level directory is the batch name.

Converted aird files should be placed into batch folders.

- **Note that:** If your project has only **ONE BATCH**, you also need to create a batch folder in the project directory and put the converted files in the batch folder.

4.1.2 Library preparation

The Library should be a .txt/.tsv format table formatted in the following template.

The first line at least needs to contain the `mz` and `rt` items. Other items are optional.

Example compound library

QE_lib											
complid	name	mz	rt	rtTolerance	structure2d	smiles	formula	inChI	avgMw	monoMw	description
1	C21H26N2S2	371.1617	18.85								
2	C25H31NO6	442.2233	17.66								
3	C14H17N3O2S	292.1118	3.01								
4	C27H31N7OS	502.2395	22.78								
5	C20H23NO4	342.1706	3.37								

Analyte Library

The analyte library is a list of compounds that you want to identify and quantify from the mass spectrometry data. MetaPro performs targeted data analysis based on this library.

If you do not have an analyte library, you can make your own analyte library based on the theoretical M/z and elution time of the compounds, download an open-source library, or modify analysis results of other software into an analyte library.

Internal Standard Library (Optional)

If you want to change the gradient of your experiment, for example, from 20min to 40min, the elution time of analytes would change and not elute at the RT value in the analyte library. In this circumstance, you can import a new analyte library with modified RT, or use an internal standard library.

- The internal standard library needs to be paired with the analyte library to correct the retention time of the analytes.
- The RT value in the internal standard library needs to be from the same gradient as the RT in the analyte library
- Compounds in internal standard library should have narrow and high-intensity chromatogram peaks.
- The compound number in the internal standard library should be about 10.

4.2 Start a targeted analysis task

4.2.1 Load file

1. Enter Project page, click `Create Project` at the top.

The screenshot shows the MetaPro software interface. On the left is a dark sidebar with options: Project (selected), Library, Method, Task, and Help. The main area has a header with fields for 'Project Name' (Please Input), 'Owner' (Please Input), 'Search', 'Reset', and 'Create Project' (highlighted with a red box). Below the header is a table with columns: ID, Top, Project Name, Batch Count, Count, Overview Count, Size Ratio (Vendor:Aird), Storage Saved, Owner, Description, Create Date, and Operations. A row for '5-2018-ACA' is shown with values: 2, 18, 2, 8880M : 4832M, 4048M, Nico, and a note '4.0GB (45.6% Size Out)'. At the bottom right are navigation buttons < 1 > 30 / page.

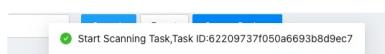
Then enter the **Project Name**. The project name should be the project name set in the **File directory arrangement** (section 4.1.1 Step 2). For example, if you set your project folder name as project-1, you need to name the **Project Name** as project-1.

Owner and **Description** are optional, fill in according to the demand.

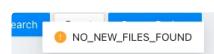
2. Click **Scan Files** to scan all converted Aird format files under the project file

The screenshot shows the MetaPro software interface. The sidebar is identical to the previous one. The main area has a header with fields for 'Project Name' (Please Input), 'Owner' (Please Input), 'Search', 'Reset', and 'Create Project'. Below the header is a table with columns: ID, Top, Project Name, Batch Count, Count, Overview Count, Size Ratio (Vendor:Aird), Storage Saved, Owner, Description, Create Date, and Operations. A row for '5-2018-ACA' is shown with values: 2, 18, 2, 8880M : 4832M, 4048M, Nico, and a note '4.0GB (45.6% Size Out)'. The 'Operations' column contains buttons: Scan Files (highlighted with a red box), List, Target Analyze, QC, and More. At the bottom right are navigation buttons < 1 > 30 / page.

If MetaPro finds new files in the project folder, MetaPro will start to load the files and pop a message as follows:



If find no new file or the folder is empty, MetaPro will pop up the following prompt box:



The file scanning progress can be find at the Task page.

You can view the loaded files by **List → Samples** or single click on the project name.

Sample list is presented as follows:

The screenshot shows the MetaPro software interface. The sidebar is identical. The main area has a header with a dropdown 'Total Batch Count:2, Current Batch: batch' (set to 'batch'), 'Sort', and 'More'. Below the header is a table with columns: Ordinal, Name, Sample Type, Description, and Operations. The table lists samples in two batches: Batch 0 (SampleA_1 to SampleA_4) and Batch 1 (SampleB_1 to SampleB_4). Each sample has 'Modify' and 'Search Data' buttons in the Operations column. At the bottom right are navigation buttons < 1 > 30 / page.

You can view the files in different batches by selecting Batch name at the top of this page.

4.2.2 Load library

Enter Library page, click **Create Library** at the top.

The screenshot shows the MetaPro software interface. The sidebar is identical. The main area has a header with a dropdown 'Library Name' (empty), 'Search', 'Reset', 'Create Library' (highlighted with a red box), and 'More'. Below the header is a table with columns: Library Name, Top, Parent Library Name, Library Type, Compound Count, Description, Update Date, and Operations. The table lists four libraries: 'TripleTOF6600_IS' (IS, 15 compounds, 2022-03-07 16:24:40), 'TripleTOF6600' (ANALYTICS, 970 compounds, 2022-03-07 16:24:41), 'QEHF_IS' (IS, 15 compounds, 2022-03-05 00:57:33), and 'QEHF' (ANALYTICS, 836 compounds, 2022-03-05 00:55:51). Each library has 'Modify', 'Detail', 'Clean Spectra', 'Export Spectra', 'Compound', 'QC', and 'Sync' buttons in the Operations column. At the bottom right are navigation buttons < 1 > 30 / page.

Input the **Library Name**, select the **Library Type**, and upload your library file at **Upload File**, click OK.

You must select a **Library Type** for this library. Select ANALYTES for the analyte library and IS for the internal standard library. If you forget to select library type, click **Modify** to set the library type before analyzing.

4.2.3 Set Method parameters

Enter Method page, click **Create** at the top.

Input the **Method Name**, and set the method parameters.

Update Method X

Name * Method: <input type="text" value="TripleTOF6600_method"/> Description: <input style="height: 100px;" type="text"/>	Peak Integration BaselineMethod: <input type="text" value="TOLERANCE"/> ▼ BaselineRtTolerance: <input type="text" value="0.4"/> FirstDerivativeCutoff: <input type="text" value="0.2"/>	EIC Noise Estimation EicNoiseEstimation: <input type="text" value="AMPLITUDE_EIC"/> ▼ NoiseAmplitude: <input type="text" value="100"/> NoisePercentage: <input type="text" value="20"/>
EIC Extraction FullEicWidth: <input type="text" value="1.5"/> minMzTolerance: <input type="text" value="0.015"/> Da MzTolerance: <input type="text" value="0.015"/> Da RtTolerance: <input type="text" value="0.6"/> Minutes	Peak Screening PeakNoiseEstimation: <input type="text" value="SLIDING_WINDOW_PE..."/> ▼ StnThreshold: <input type="text" value="1.0"/> minPeakHeight: <input type="text" value="500.0"/> minPeakWidth: <input type="text" value="0.02"/> minPeakPoints: <input type="text" value="7"/> maxNoiseRatio: <input type="text" value="0.5"/> minObviousness: <input type="text" value="1.0"/>	Peak Selection Strategy: <input type="text" value="HIGHEST_INTENSITY"/> ▼ LibrarySearchBinWidth: <input type="text" value="0.001"/> Da RtScoreWeight: <input type="text" value="1.0"/> MzScoreWeight: <input type="text" value="1.0"/> Ms1ForwardScoreWeight: <input type="text" value="1.0"/> Ms1ReverseScoreWeight: <input type="text" value="1.0"/> Ms1IsotopeScoreWeight: <input type="text" value="1.0"/> Ms2ForwardScoreWeight: <input type="text" value="1.0"/> Ms2ReverseScoreWeight: <input type="text" value="1.0"/>
EIC Smoothing SmoothMethod: <input type="text" value="GAUSS"/> ▼ SmoothPoints: <input type="text" value="5"/>	Batch Optimization labelRecommendation: <input type="text" value="RT_DISTRIBUTION"/> ▼ useNeighborDetection: <input checked="" type="checkbox"/>	Cancel Submit
Peak Selection PeakFindingMethod: <input type="text" value="PROPRO"/> ▼		

The parameters explanation is summarized below:

Workflow	Parameter name	Example value	Explanation
EIC Extraction	FullEicWidth	0.1	Extract EIC with RT width of 0.1 min
	minMzTolerance	0.001	If calculated M/z ppm tolerance is smaller than 0.001Da, extract EIC with a $\pm 0.001\text{Da}$ M/z window
	MzTolerance	10.0 ppm	Extract EIC with a $\pm 10\text{ppm}$ M/z window
	RtTolerance	0.05 Da	Extract EIC with a $\pm 0.05\text{Da}$ M/z window
EIC Smoothing	SmoothMethod	LINEAR	Smoothing with average intensity
		GAUSS	Smoothing with Gaussian-distributed weight
		SAVITZKY_GOLAY	Smoothing with Mexican-hat weight
		PROPRO_GAUSS	Smoothing by Gaussian regression weight
		NONE	Do not use smoothing
	SmoothPoints	5	5 point wide smooth window (center point, left 2 points and right 2 points; must be an odd number)
EIC Noise Estimation	EicNoiseEstimation	PROPRO_EIC	Estimate noise by signal local distribution
		AMPLITUDE_EIC	Bin all intensities in EIC with NoiseAmplitude. Consider the intensity of the highest frequency bin as noise intensity
		PERCENTAGE_EIC	Sort all intensities in EIC. Consider NoisePercentage percentile intensity as noise intensity
	NoiseAmplitude	100	Set the noise intensity amplitude width at 100
	NoisePercentage	20	Consider the 20% lowest intensity of the current EIC as the noise threshold
Peak Selection	PeakFindingMethod	PROPRO	Self-developed peak selection algorithm, used for smooth peak separation
		WAVELET	Maxican-hat regression, reproduced from XCMS,MZmine2, used for noisy peak selection
		LOCAL_MINIMUM	Analyze the first and second derivatives, reproduced from MZmine2, used for narrow peak selection
Peak Integration	BaselineMethod	TOLERANCE	Consider the minimum intensity with BaselineRtTolerance
		NONE	Do not use baseline detection
	BaselineRtTolerance	0.05	The RT width of baseline detection out of each side of the peak boundary
	FirstDerivativeCutoff	0.1	Set peak boundary at 0.1 times of max first derivative of each side
Peak Screening	PeakNoiseEstimation	SLIDING_WINDOW_PEAK	Estimate peak noise by sliding window out of peak boundary
		WAVELET_COEFF_PEAK	Estimate peak noise by Wavelet peak detection fitting performance
	StnThreshold	1	Minimum signal to noise ratio
	minPeakHeight	3000	Excluding peaks with apex intensity less than 3000
	minPeakWidth	0.02	Excluding peaks with RT width less than 0.02min
	minPeakPoints	7	Excluding peaks with less than 7 points
	maxNoiseRatio	0.5	Excluding peaks with noise signal ratio higher than 0.5
	minObviousness	0.7	Excluding peaks with obviousness less than 0.7
Peak Identification	Strategy	Nearest RT	Select the peak closest to the theoretical RT
		Highest Score	Select the peak with highest total score
		Highest Intensity	Select the peak with highest intensity
	LibrarySearchBinWidth	0.001Da	M/z tolerance used in spectral matching
	RtScoreWeight	1.0	The weight of RT accuracy score
	MzScoreWeight	1.0	The weight of M/z accuracy score
	Ms1ForwardScoreWeight	1.0	The weight of MS1 forward similarity score
	Ms1ReverseScoreWeight	1.0	The weight of MS1 reverse similarity score
	Ms1IsotopeScoreWeight	1.0	The weight of MS1 isotope intensity similarity score
	Ms2ForwardScoreWeight	1.0	The weight of MS2 forward similarity score
	Ms2ReverseScoreWeight	1.0	The weight of MS2 reverse similarity score
Batch Optimization	LabelRecommendation	RtDistribution	Recommend initial inspection labels by RT distibution of selected peaks
		EicAlignment	Align peaks in batch and recommend initial inspection labels by highest score
	useNeighborDetection	TRUE	Can only be used with EicAlignment recommendation method. Recommend initial inspection labels in consideration of the distribution of the neighbor compounds.

You can click [Edit](#) on the method page to change analysis parameters.

Suggestions:

- We recommend using different methods for data under different experimental conditions, such as different mass spectrometers.
- The optimized method should be less modified.

4.2.4 Start analysis

1. Enter Project page, click **Target Analyze** at the row end.

ID	Top	Project Name	Batch Count	Count	Overview Count	Size Ratio (Vendor-Aird)	Storage Saved	Owner	Description	Create Date	Operations
+ Show	5-2018-ACA		2	18	2	8880M : 4832M	4048M	Nico		2022-03-04 22:27:13	Scan Files List Target Analyze QC More
Total						8.9GB : 4.8GB	4.0GB (45.6% Size Out)				< 1 > 30 / page

2. Click **Edit** to change the libraries and method for batch targeted analysis.

Batch Name	Ins Lib	Ana Lib	Method	Operations
batch	TripleTOF6600_IS	TripleTOF6600	TripleTOF6600_method	Save Cancel
raw_batch	Not Select	QEHF	QEHF_method	Edit
	QEHF_IS			
	TripleTOF6600_IS			

Click **Save** to commit changes.

Multi-batch editing is also supported. You can select multiple batches by clicking on the checkboxes on the left. Then click **More → Edit**, and edit libraries and methods for multiple batches.

3. Click **Target Search** to start a targeted analysis. You can select multiple batches and click **Target Search** to submit multiple analysis tasks. MetaPro has a job queue and the tasks will be analyzed batch by batch.

The analysis progress can be viewed at the Task page.

TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName:raw_batch	Success	TARGET_ANALYZE	23149	2022-03-06 01:51:32	2022-03-06 01:51:55
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName:raw_batch	Success	TARGET_ANALYZE	52918	2022-03-06 01:38:55	2022-03-06 01:39:48
BUILD_LIBRARY-BuildLibrary	Success	BUILD_LIBRARY	36535	2022-03-06 01:37:01	2022-03-06 01:37:38
TARGET_ANALYZE-ProjectID:622221c1b7576771b65880f, BatchName:batch	Success	TARGET_ANALYZE	15222	2022-03-06 01:33:31	2022-03-06 01:33:46

Reverse Refresh

- 2022-03-06 01:33:46-Task Ended
- 2022-03-06 01:33:44-Extraction Finished
- 2022-03-06 01:33:42-IRT Success:y=99.898x+1.591 cost:33
- 2022-03-06 01:33:42-Success to read Aird data
- 2022-03-06 01:33:42-Begin to analyze batch SampleB_4
- 2022-03-06 01:33:42-Extraction Finished
- 2022-03-06 01:33:41-IRT Success:y=99.975x+0.473 cost:34
- 2022-03-06 01:33:41-Success to read Aird data
- 2022-03-06 01:33:41-Begin to analyze batch SampleB_3

Results can be found in QC page after the analysis process is finished.

During the analysis process, all MetaPro functions are not affected.

4. Result management.

- [View] Click + button of project in Project page

ID	Top	Project Name	Batch Count	Overview Count	Size Ratio (Vendor:Aird)	Storage Saved	Owner	Description	Create Date	Operations
5-2018-ACA	<input checked="" type="checkbox"/>		2	18	2	8880M : 4832M	4048M	Nico	2022-03-04 22:27:13	Scan Files List Target Analyze QC More

Show 5-2018-ACA

- batch
 - 2022-03-04 22:37:29-----Ins Lib: TripleTOF6600_IS-----Ana Lib: TripleTOF6600-----Method: TripleTOF6600_method
- raw_batch
 - 2022-03-05 15:56:17-----Ins Lib: QEHF_IS-----Ana Lib: QEHF-----Method: QEHF_method

Total 2 18 2 8.9GB : 4.8GB **4.0GB (45.6% Size Out)**

- [View & Delete] Click [List](#) → [Overview List](#)

Batch Name:	id	Batch Name	Project Name	Is Target	Delete	Ana Lib	Ins Lib	Method Name	Create Date
raw_batch	<input checked="" type="checkbox"/>	raw_batch	5-2018-ACA	Target	Delete	QEHF	QEHF_IS	QEHF_method	2022-03-05 15:56:17
batch	<input type="checkbox"/>	batch	5-2018-ACA	Target	Delete	TripleTOF6600	TripleTOF6600_IS	TripleTOF6600_method	2022-03-04 22:37:29

Show raw_batch

Total 2 18 2 8.9GB : 4.8GB **4.0GB (45.6% Size Out)**

4.3 Use batch QC inspection page for targeted analysis

4.3.1 Access the batch QC inspection page

If the targeted analysis process has been finished, then you can view the quantification results on the batch inspection interface.

Enter project page and click on QC on the project that you want to view.

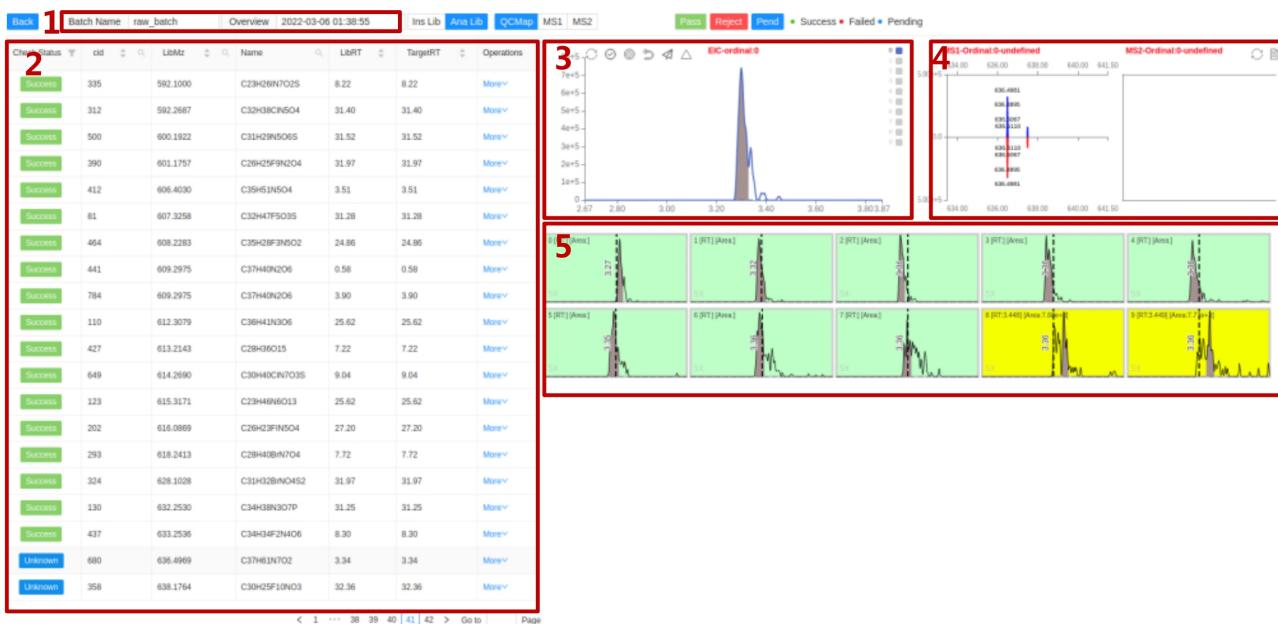
ID	Top	Project Name	Batch Count	Overview Count	Size Ratio (Vendor:Aird)	Storage Saved	Owner	Description	Create Date	Operations
5-2018-ACA	<input checked="" type="checkbox"/>		2	18	2	8880M : 4832M	4048M	Nico	2022-03-04 22:27:13	Scan Files List Target Analyze QC More

Show 5-2018-ACA

Total 2 18 2 8.9GB : 4.8GB **4.0GB (45.6% Size Out)**

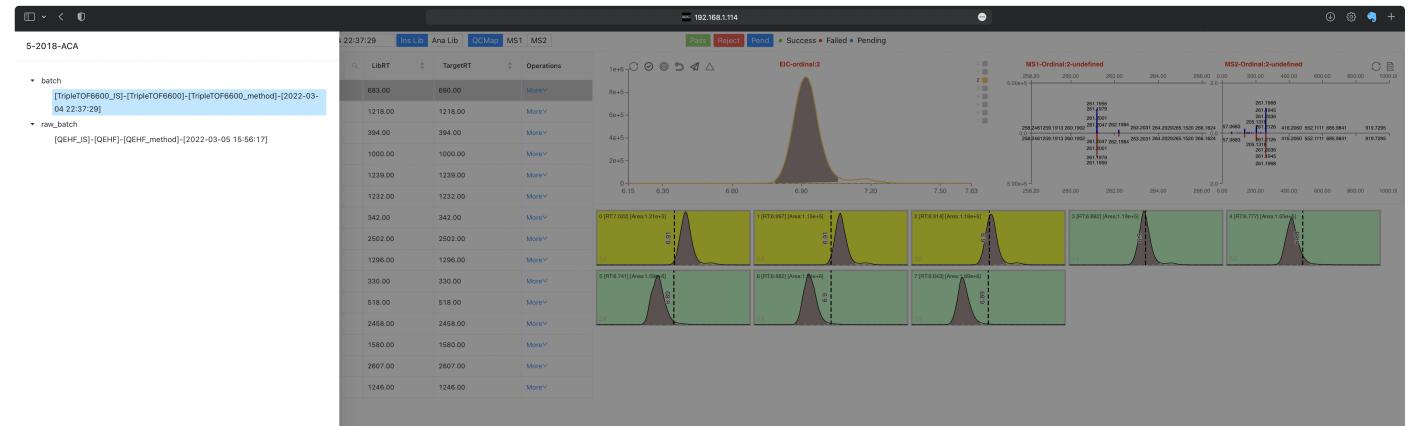
4.3.2 Batch Quality Control inspection interface

This is the main inspection page on samples in a batch. It includes different function modules as labeled.



1. Overview switch module

Click on the [Batch Name](#) or [Overview](#) dialog on the left top. You will see the following interface. You can change the current overview to another by clicking on a specific overview.



2. Compound switch module

- [Check Status](#) represents for the current check status of compounds. It has Success, Failed, Unknown status.

Success	13	205.0975	C11H12N2O2	3.34	3.34	More▼	Reset TargetRT
Unknown	3	292.1118	C14H17N3O2S	3.01	3.01	More▼	Reset Integration Params
Failed	12	312.1234	C18H17NO4	23.36	23.36	More▼	1e+5
Success	14	338.0867	C15H20BrN3O	3.32	3.32	More▼	5e+4

Shortcuts

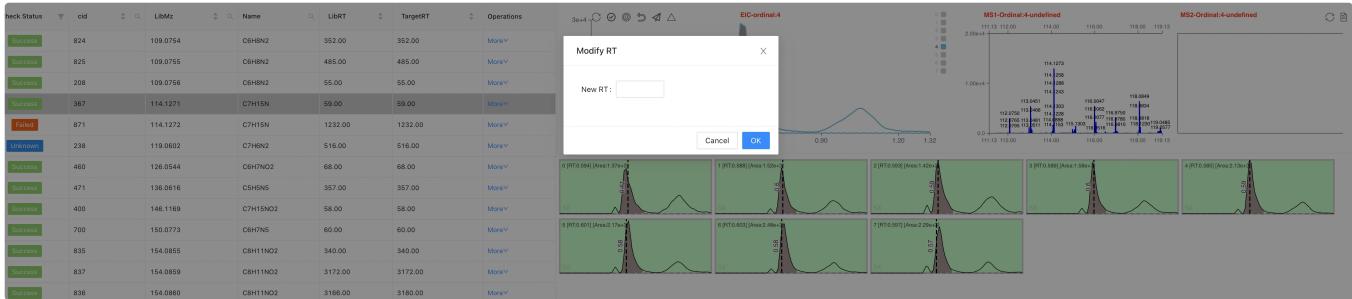
- Arrow keys: switch compound; switch page

2. Control the check status of the current compound, **Space** and **Enter**: Success, **BackSpace**: Failed

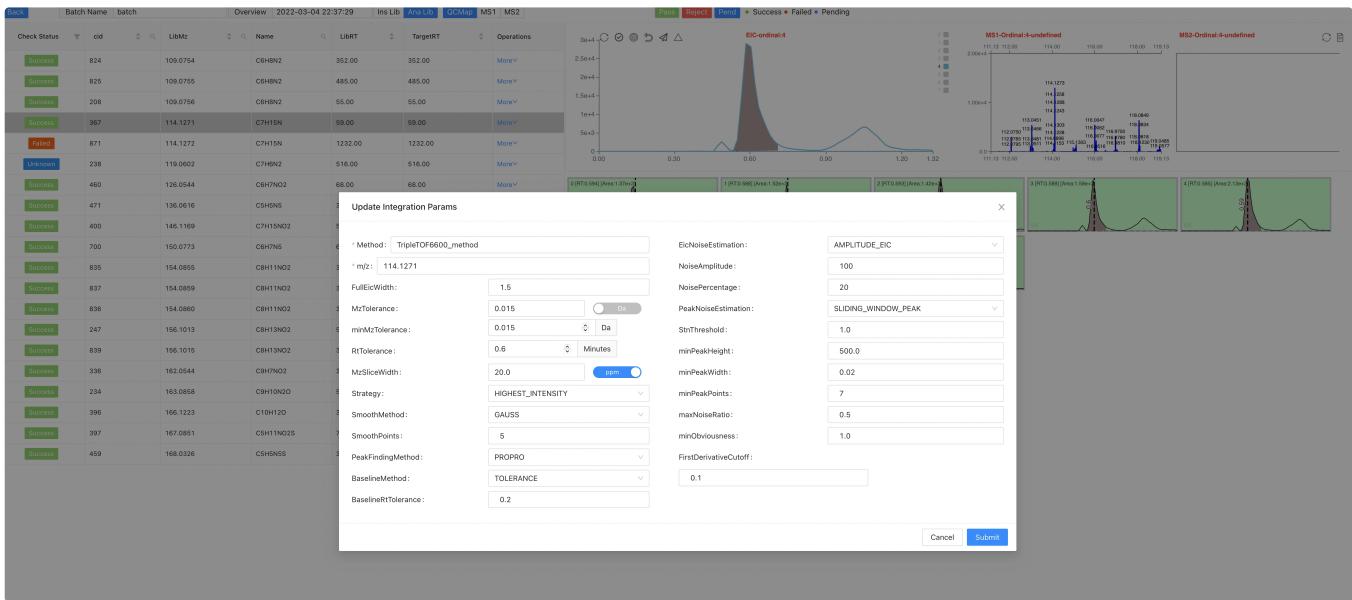
3. **Double click** on each row to change RT value

- Click on the "more", users can **Reset integration params** and **Reset TargetRT** of a compound.

Click on **Reset TargetRT**



Click on **Reset integration params**



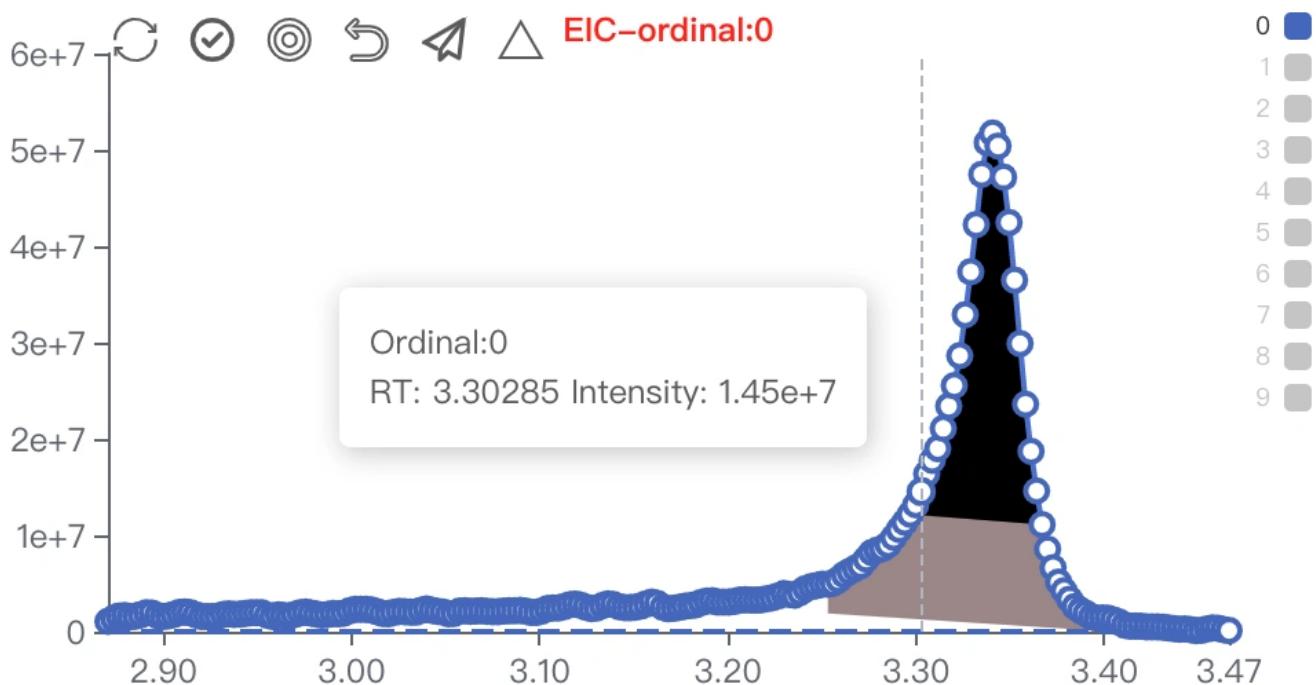
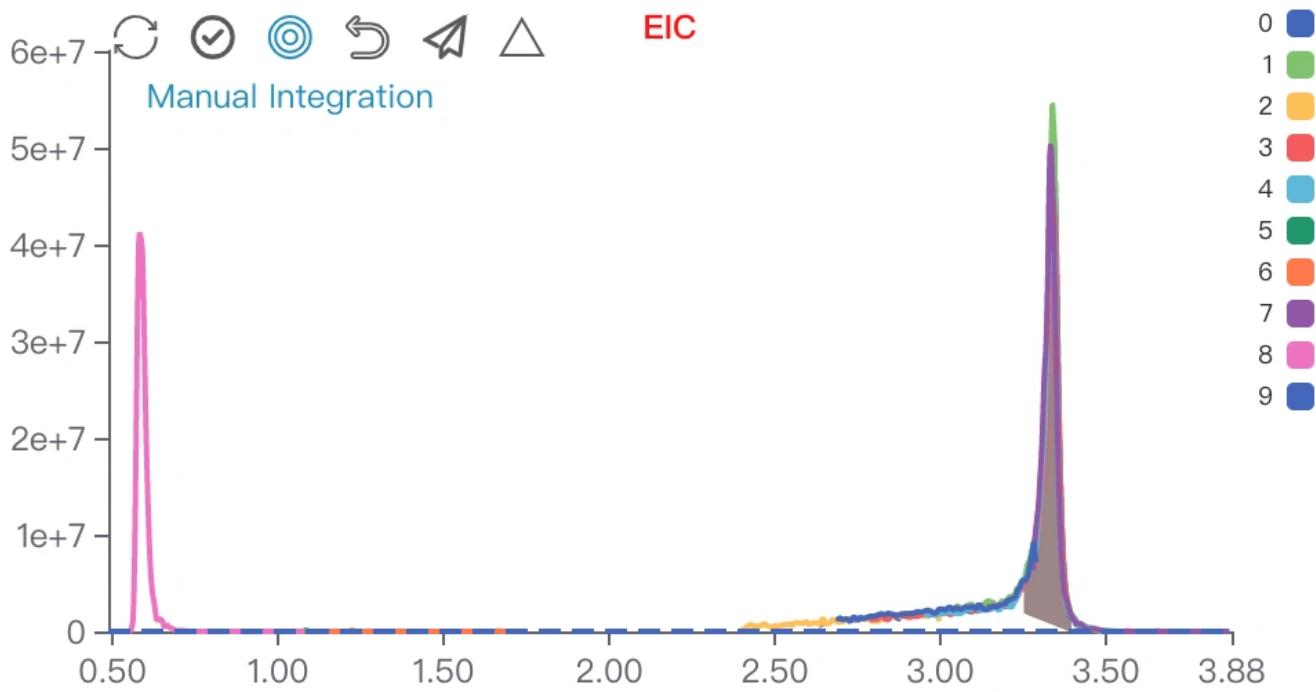
3. Manual inspection module

The buttons on the top are: **Restore**, **Select All/UnSelect**, **Manual Integration**, **Reselect**, **Submit**, **Batch Submit**

Restore : Restore the current module to its initial status.

Select All/UnSelect : View all the sample peaks in this batch/Cancel view all the peaks.

Manual Integration : Enter manual integration mode on the selected peak. You can choose two data points (start, end) to modify the peak shape.



Reselect : Click this to rechoose the data points.

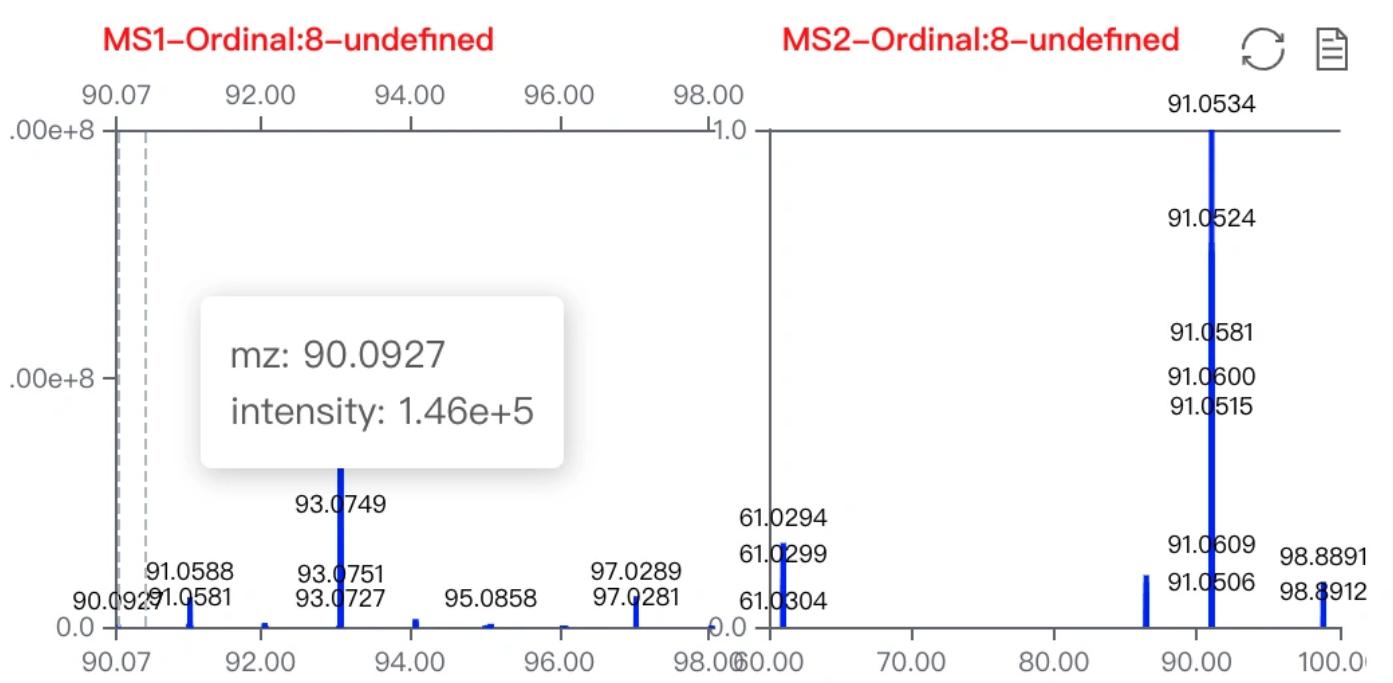
Submit : Submit the modified peak shape to database.

Batch Submit : Apply the modified peak RT range to all samples in this batch. Used for integrating multiple peaks on an EIC.

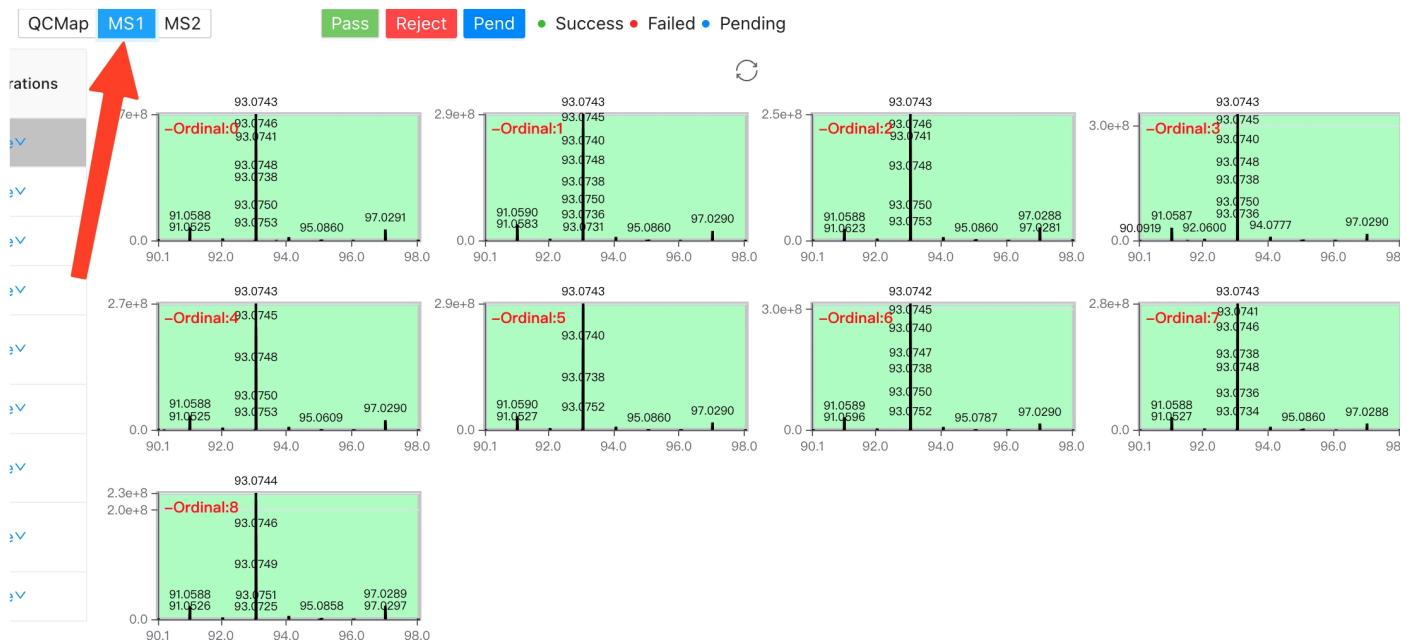
Click on **Manual Integration**, you can choose two data points to conduct manual integration functions. First left and then right.

4. Spectrum viewer of [MS1](#) and [MS2](#)

This is changed according to the sample you choose on the batch inspection module.



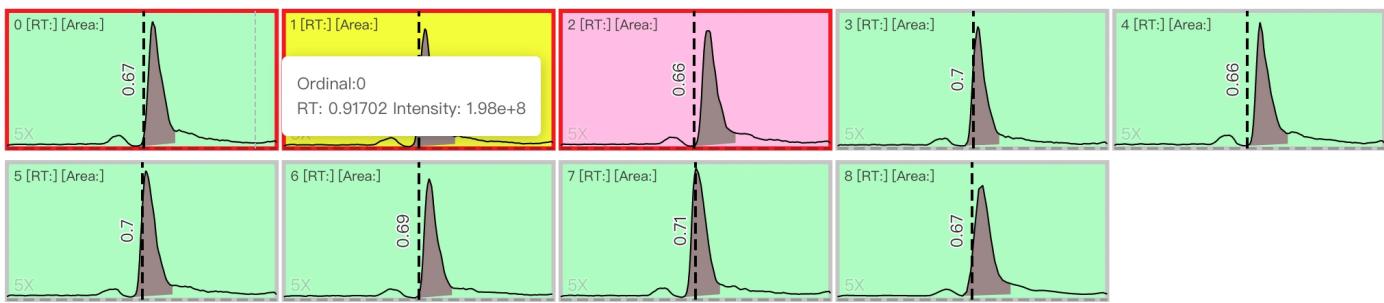
This is the Spectrum viewer towards all the **MS1** and **MS2**. Click on the pointed label to switch pages.



Shortcuts

1. keyboard **1**, **2**, **3** : switch check status
2. **A** : choose all the samples
3. **ESC** : cancel check all
5. Peak shape batch inspection

Users can choose multi-samples to change their status. Red represents for rejection. Yellow represents for unknown. Green represents for pass. The shortcuts are **1**, **2**, **3**. Keyboard **A** is to choose all the samples. If the status of a sample is labeled in yellow or red, its quantification result area will be set to 0.



4.3.3 QC inspection interface shortcuts conclusion

1. Compound switch module
 1. Arrow keys: switch compound; switch page
 2. Control the check status of the current compound, and : Success, : Failed
 3. on each row to change RT value
2. Peak shape batch inspection
 1. keyboard , , : switch check status
 2. : choose all the samples
 3. : cancel check all
3. Manual integration module
 1. : submit manual integration results
 2. : refresh the current page

4.4 Spectral Library Curation

4.4.1 Build Library

Choose inspected overview to conduct library curation process on a specific project.

Project Name:		<input type="text" value="Please Input"/>	Owner:	<input type="text" value="Please Input"/>	Search	Reset	Create Project	More ▾
ID	Top	Project Name	Batch Count	Count	Overview Count			
-	Show	5-2018-ACA	1	8	10			
Build Library								
batch <ul style="list-style-type: none"> <input checked="" type="checkbox"/> 2022-03-04 14:50:47----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:29:39----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:22:20----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:15:28----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:13:02----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:09:49----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:07:44----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:07:11----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:04:34----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-03 23:33:23----Library: undefined----Method: TripleTOF6600 								

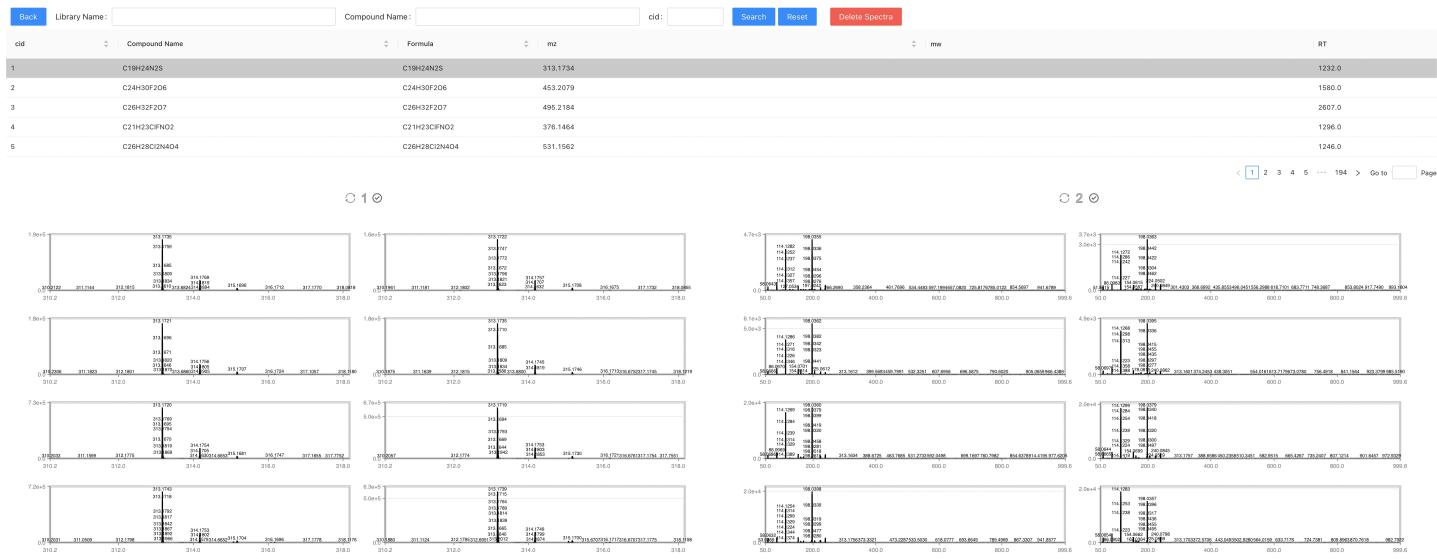
This will generate a Library Building task and you can check it on the task list. The process automatically chooses all the inspected and passed spectra to save them into the database. If you saw the task status is finished, you can conduct library QC on the curated library.

4.4.2 Library QC

After build library task has been finished on a inspected library. This library will have collected spectra waiting for inspection. Click on the **QC** button to view the spectra inside this library.

Library Name	Compound Count	Description	Update Date	Operations
TripleTOF6600_IS	15		2022-03-07 16:24:40	Modify Detail Clean Spectra Export Spectra Compound QC Sync
TripleTOF6600	970	ANALYTES	2022-03-07 16:24:41	Modify Detail Clean Spectra Export Spectra Compound QC Sync
QEHF_IS	15	IS	2022-03-05 00:57:33	Modify Detail Clean Spectra Export Spectra Compound QC Sync
QEHF	836	ANALYTES	2022-03-05 00:55:51	Modify Detail Clean Spectra Export Spectra Compound QC Sync

Enter the library QC interface you will see a page like that.



On this page you can see all the spectra collected on this compound. You can multi-choose to delete low-quality spectra.

Shortcuts:

1. Arrow keys: switch compound; switch page
2. **Del** : Delete the selected spectra.

4.5 Export

4.5.1 Export quantification reports

Project Name : Please Input Owner: Please Input Search Reset Create Project More ▾

ID	Top	Project Name	Batch Count	Count	Overview Count	Build Library
-	Show <input type="checkbox"/>	5-2018-ACA	1	8	10	Export Report
batch <ul style="list-style-type: none"> <input checked="" type="checkbox"/> 2022-03-04 14:50:47----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:29:39----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:22:20----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:15:28----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:13:02----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:09:49----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:07:44----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:07:11----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-04 00:04:34----Library: undefined----Method: TripleTOF6600 <input type="checkbox"/> 2022-03-03 23:33:23----Library: undefined----Method: TripleTOF6600 						

First, choose a project on the project page, click on the [+ Export Report](#) . It will let users input the output file name towards a specific overview. The quantification results of this overview will be exported into the given [.xlsx](#) file.

Confirm the fields to export



Project Name	5-2018-ACA-Backup
Output file name	5-2018-ACA-Backup_raw_batch
.xlsx	

Example exported file look like

CompoundName	CompID	Type	Status	Sample_A_1_Mz	Sample_A_1_Rt	Sample_A_1_Area	Sample_A_2_Mz	Sample_A_2_Rt	Sample_A_2_Area	Sample_A_3_Mz	Sample_A_3_Rt	Sample_A_3_Area	Sample_A_4_Mz	Sample_A_4_Rt	Sample_A_4_Area	Sample_B_1_Mz	Sample_B_1_Rt	Sample_B_1_Area	Sample_B_2_Mz	Sample_B_2_Rt	Sample_B_2_Area	Sample_B_3_Mz	Sample_B_3_Rt	Sample_B_3_Area	Sample_B_4_Mz	Sample_B_4_Rt	Sample_B_4_Area	validID	avrgMz	avrgRt	avrgStDev																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C9H9N3O ⁸⁸⁷	ANALYTES Success	192.0817	6.66295	13015.74	192.0799	6.7082	10954.16	192.0779	6.727033	13340.81	192.0778	6.780767	15013.64	192.0782	6.960333	17278.98	192.0779	7.012133	18711.25	192.0779	7.096767	19590.86	192.076	7.20035	18042.73	8	192.0784	6.893567	15743.52																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C9H9N3O ⁸⁸⁸	ANALYTES Success	192.0744	20.01887	5009.287	192.0741	20.058847	5899.855	192.0739	20.57453	6911.056	192.0726	20.57453	7198.194	192.0725	20.53878	8002.349	192.0722	20.52193	7984.935	192.0739	20.5249	7963.751	192.0719	20.52232	7661.36	8	192.0732	20.55799	17078.849																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C21H20N ⁸⁸⁹	ANALYTES Success	377.1576	22.42792	35651.22	377.1589	22.495	35240.09	377.1609	22.60683	37074.3	377.1584	22.66123	38638.55	377.1606	22.8478	41933.7	377.1581	22.9201	40834.35	377.1571	23.00573	46207.22	377.1571	23.09098	46513.66	8	377.159	22.75695	40261.27																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C26H33N ⁸⁹⁰	ANALYTES Success	392.2585	28.52035	2034205	392.2588	28.67196	21791.3	392.2566	28.70877	230549.4	392.2582	28.76733	237467.2	392.2562	29.0024	230630.1	392.2591	29.1087	223874.1	392.2587	29.2	24490.1	392.2567	29.29575	244351.3	8	392.2584	28.8963	229623																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C8H11NO ⁸⁹¹	ANALYTES Success	248.0493	1.963	287.183	248.0493	1.96167	1.96179	248.0493	1.96179	1749.4	248.051	1.96183	1567.5	248.0498	2.06265	230549.8	248.051	2.07975	2103.376	248.053	2.08265	134.0	248.051	2.08463	248.051	2.08265	271.136	8	248.050	2.07776	1888.202																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C10H10NO ⁸⁹²	ANALYTES Success	248.0494	1.9632	1.96157	248.0494	1.96167	1.96179	248.0494	1.96179	1824.7	248.051	1.96183	1567.5	248.0498	2.06265	230549.8	248.051	2.07975	2103.376	248.053	2.08265	134.0	248.050	2.07776	248.051	2.08265	271.136	8	248.0489	2.07776	1888.202																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C29H31N ⁸⁹³	ANALYTES Success	694.2649	18.4108	1488937	694.2649	18.52127	1540074	694.2644	18.72195	1521.47	694.2647	18.82464	1744.928	694.2644	18.92464	1744.929	694.2644	19.02464	1744.929	694.2644	19.12464	1744.929	694.2644	19.22464	1744.929	694.2644	19.32464	1744.929	694.2644	19.42464	1744.929	694.2644	19.52464	1744.929	694.2644	19.62464	1744.929	694.2644	19.72464	1744.929	694.2644	19.82464	1744.929	694.2644	19.92464	1744.929	694.2644	20.02464	1744.929	694.2644	20.12464	1744.929	694.2644	20.22464	1744.929	694.2644	20.32464	1744.929	694.2644	20.42464	1744.929	694.2644	20.52464	1744.929	694.2644	20.62464	1744.929	694.2644	20.72464	1744.929	694.2644	20.82464	1744.929	694.2644	20.92464	1744.929	694.2644	21.02464	1744.929	694.2644	21.12464	1744.929	694.2644	21.22464	1744.929	694.2644	21.32464	1744.929	694.2644	21.42464	1744.929	694.2644	21.52464	1744.929	694.2644	21.62464	1744.929	694.2644	21.72464	1744.929	694.2644	21.82464	1744.929	694.2644	21.92464	1744.929	694.2644	22.02464	1744.929	694.2644	22.12464	1744.929	694.2644	22.22464	1744.929	694.2644	22.32464	1744.929	694.2644	22.42464	1744.929	694.2644	22.52464	1744.929	694.2644	22.62464	1744.929	694.2644	22.72464	1744.929	694.2644	22.82464	1744.929	694.2644	22.92464	1744.929	694.2644	23.02464	1744.929	694.2644	23.12464	1744.929	694.2644	23.22464	1744.929	694.2644	23.32464	1744.929	694.2644	23.42464	1744.929	694.2644	23.52464	1744.929	694.2644	23.62464	1744.929	694.2644	23.72464	1744.929	694.2644	23.82464	1744.929	694.2644	23.92464	1744.929	694.2644	24.02464	1744.929	694.2644	24.12464	1744.929	694.2644	24.22464	1744.929	694.2644	24.32464	1744.929	694.2644	24.42464	1744.929	694.2644	24.52464	1744.929	694.2644	24.62464	1744.929	694.2644	24.72464	1744.929	694.2644	24.82464	1744.929	694.2644	24.92464	1744.929	694.2644	25.02464	1744.929	694.2644	25.12464	1744.929	694.2644	25.22464	1744.929	694.2644	25.32464	1744.929	694.2644	25.42464	1744.929	694.2644	25.52464	1744.929	694.2644	25.62464	1744.929	694.2644	25.72464	1744.929	694.2644	25.82464	1744.929	694.2644	25.92464	1744.929	694.2644	26.02464	1744.929	694.2644	26.12464	1744.929	694.2644	26.22464	1744.929	694.2644	26.32464	1744.929	694.2644	26.42464	1744.929	694.2644	26.52464	1744.929	694.2644	26.62464	1744.929	694.2644	26.72464	1744.929	694.2644	26.82464	1744.929	694.2644	26.92464	1744.929	694.2644	27.02464	1744.929	694.2644	27.12464	1744.929	694.2644	27.22464	1744.929	694.2644	27.32464	1744.929	694.2644	27.42464	1744.929	694.2644	27.52464	1744.929	694.2644	27.62464	1744.929	694.2644	27.72464	1744.929	694.2644	27.82464	1744.929	694.2644	27.92464	1744.929	694.2644	28.02464	1744.929	694.2644	28.12464	1744.929	694.2644	28.22464	1744.929	694.2644	28.32464	1744.929	694.2644	28.42464	1744.929	694.2644	28.52464	1744.929	694.2644	28.62464	1744.929	694.2644	28.72464	1744.929	694.2644	28.82464	1744.929	694.2644	28.92464	1744.929	694.2644	29.02464	1744.929	694.2644	29.12464	1744.929	694.2644	29.22464	1744.929	694.2644	29.32464	1744.929	694.2644	29.42464	1744.929	694.2644	29.52464	1744.929	694.2644	29.62464	1744.929	694.2644	29.72464	1744.929	694.2644	29.82464	1744.929	694.2644	29.92464	1744.929	694.2644	30.02464	1744.929	694.2644	30.12464	1744.929	694.2644	30.22464	1744.929	694.2644	30.32464	1744.929	694.2644	30.42464	1744.929	694.2644	30.52464	1744.929	694.2644	30.62464	1744.929	694.2644	30.72464	1744.929	694.2644	30.82464	1744.929	694.2644	30.92464	1744.929	694.2644	31.02464	1744.929	694.2644	31.12464	1744.929	694.2644	31.22464	1744.929	694.2644	31.32464	1744.929	694.2644	31.42464	1744.929	694.2644	31.52464	1744.929	694.2644	31.62464	1744.929	694.2644	31.72464	1744.929	694.2644	31.82464	1744.929	694.2644	31.92464	1744.929	694.2644	32.02464	1744.929	694.2644	32.12464	1744.929	694.2644	32.22464	1744.929	694.2644	32.32464	1744.929	694.2644	32.42464	1744.929	694.2644	32.52464	1744.929	694.2644	32.62464	1744.929	694.2644	32.72464	1744.929	694.2644	32.82464	1744.929	694.2644	32.92464	1744.929	694.2644	33.02464	1744.929	694.2644	33.12464	1744.929	694.2644	33.22464	1744.929	694.2644	33.32464	1744.929	694.2644	33.42464	1744.929	694.2644	33.52464	1744.929	694.2644	33.62464	1744.929	694.2644	33.72464	1744.929	694.2644	33.82464	1744.929	694.2644	33.92464	1744.929	694.2644	34.02464	1744.929	694.2644	34.12464	1744.929	694.2644	34.22464	1744.929	694.2644	34.32464	1744.929	694.2644	34.42464	1744.929	694.2644	34.52464	1744.929	694.2644	34.62464	1744.929	694.2644	34.72464	1744.929	694.2644	34.82464	1744.929	694.2644	34.92464	1744.929	694.2644	35.02464	1744.929	694.2644	35.12464	1744.929	694.2644	35.22464	1744.929	694.2644	35.32464	1744.929	694.2644	35.42464	1744.929	694.2644	35.52464	1744.929	694.2644	35.62464	1744.929	694.2644	35.72464	1744.929	694.2644	35.82464	1744.929	694.2644	35.92464	1744.929	694.2644	36.02464	1744.929	694.2644	36.12464	1744.929	694.2644	36.22464	1744.929	694.2644	36.32464	1744.929	694.2644	36.4246

Supplementary

Performance Optimization

- NOTE: This step has relatively complicated operations. Users who need to perform high-throughput inspection analysis on the server can perform performance optimization according to the following description.

MetaPro uses in-memory caching technology to speed up the analysis of MS data.

In the manual inspection process, each time the user changes the integration parameters, MetaPro needs to re-analyze all files in the current batch. Most of the analysis time is spent reading the files, about `1 second` per file on the tutorial dataset. If a user is inspecting a batch with `10 data files` and wants to change the integration parameter of a compound, without memory caching, it will take `10 seconds` to load files and re-analysis the compound within `1 second`. MetaPro accelerates repeated reading of files through caching technology. In the case of sufficient memory, MetaPro can load the file from disk only once when recalculating the first compound, save the file reading time for the inspection of other compounds, and achieve efficient batch manual quality control.

Considering the performance of most users' computers, we configure a small amount of cache in the default installation. Users can change the cache configuration themselves to achieve faster response and higher inspection efficiency.

The configuration file is located at `INSTALLATION_PATH/libs/config/ehcache.xml`

```
1  <?xml version="1.0" encoding="UTF-8"?>
2  <ehcache xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
3      xsi:noNamespaceSchemaLocation="http://ehcache.org/ehcache.xsd"
4      updateCheck="false">
5      <diskStore path="java.io.tmpdir/Tmp_EhCache"/>
6      <defaultCache eternal="false" maxElementsInMemory="100"
7          overflowToDisk="false" diskPersistent="false" timeToIdleSeconds="0"
8          timeToLiveSeconds="600" memoryStoreEvictionPolicy="LRU"/>
9      <cache name="expMsCycle" eternal="false" maxElementsInMemory="10"
10         overflowToDisk="false" diskPersistent="false"
11         timeToIdleSeconds="0" timeToLiveSeconds="0"
12         memoryStoreEvictionPolicy="LFU"/>
13
14      <cache name="resultQCInfo" eternal="false" maxElementsInMemory="10"
15         overflowToDisk="false" diskPersistent="false"
16         timeToIdleSeconds="0" timeToLiveSeconds="0"
17         memoryStoreEvictionPolicy="LFU"/>
18  </ehcache>
```

Users can moderately increase the value of `maxElementsInMemory` at line 9, according to the computer memory size. This value means the max number of cached files. If the memory size is big enough, `maxElementsInMemory` should be larger than the number of files in each batch. If not, try separating data into multiple batches to avoid disk reading.

Save the config file, restart MetaPro and enjoy.

