

# User Guide - Apus

Apu Pickup

# INTRODUCTION

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### Version: ApuPickup\_v202507

### Release Date: 2025.07.15

### OS: Windows 10 (x64) or Windows 11 (x64)

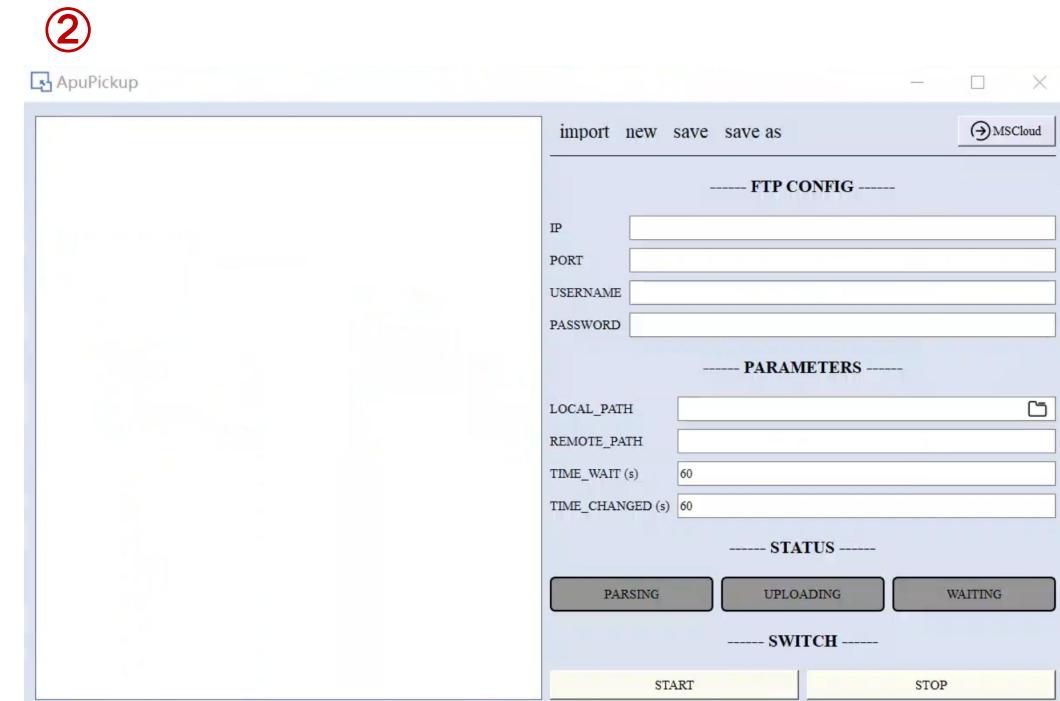
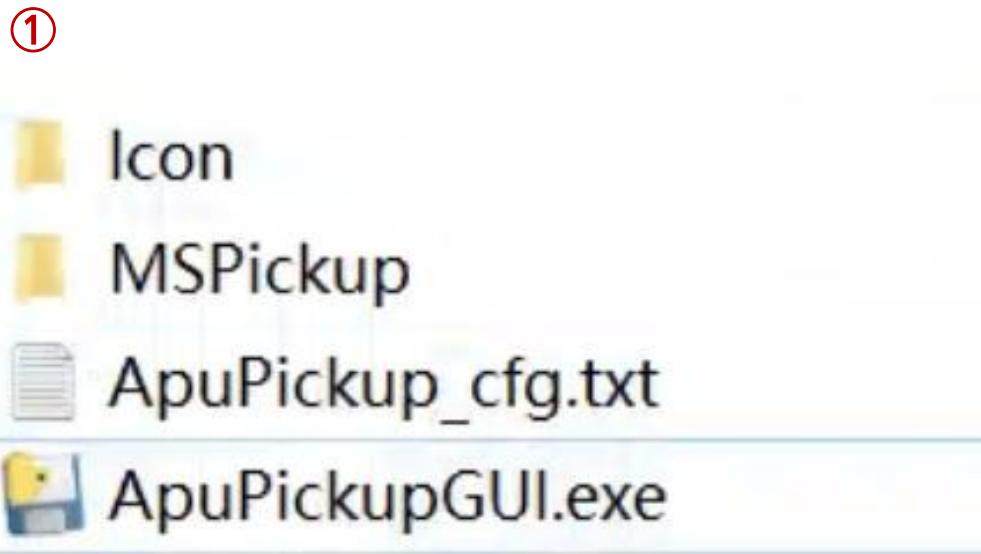
ApuPickup is a local client system within the Apus solution, responsible for the **automated aggregation** of raw data.

Deployed on the control computer of the LC-MS/MS instrument, its primary functions are:

1. **Real-time monitoring**: To continuously scan for and identify newly generated raw data files (e.g., .raw files).
2. **Automated data aggregation**: To securely transfer these new files to a central network-attached storage (NAS) server via the local area network (LAN).

# STEP-1

1. Download the ApuPickup installation package from github (<https://github.com/BUAA-LiuLab/Apus>) to **the control computer of the LC-MS/MS instrument**. (If you are only testing the software, it can be installed on any Windows computer that supports FTP)
2. Navigate to the “/ApuPickup\_v202507/” directory.
3. Execute **ApuPickupGUI.exe** to launch the application. This will open the main software interface.



## STEP-2

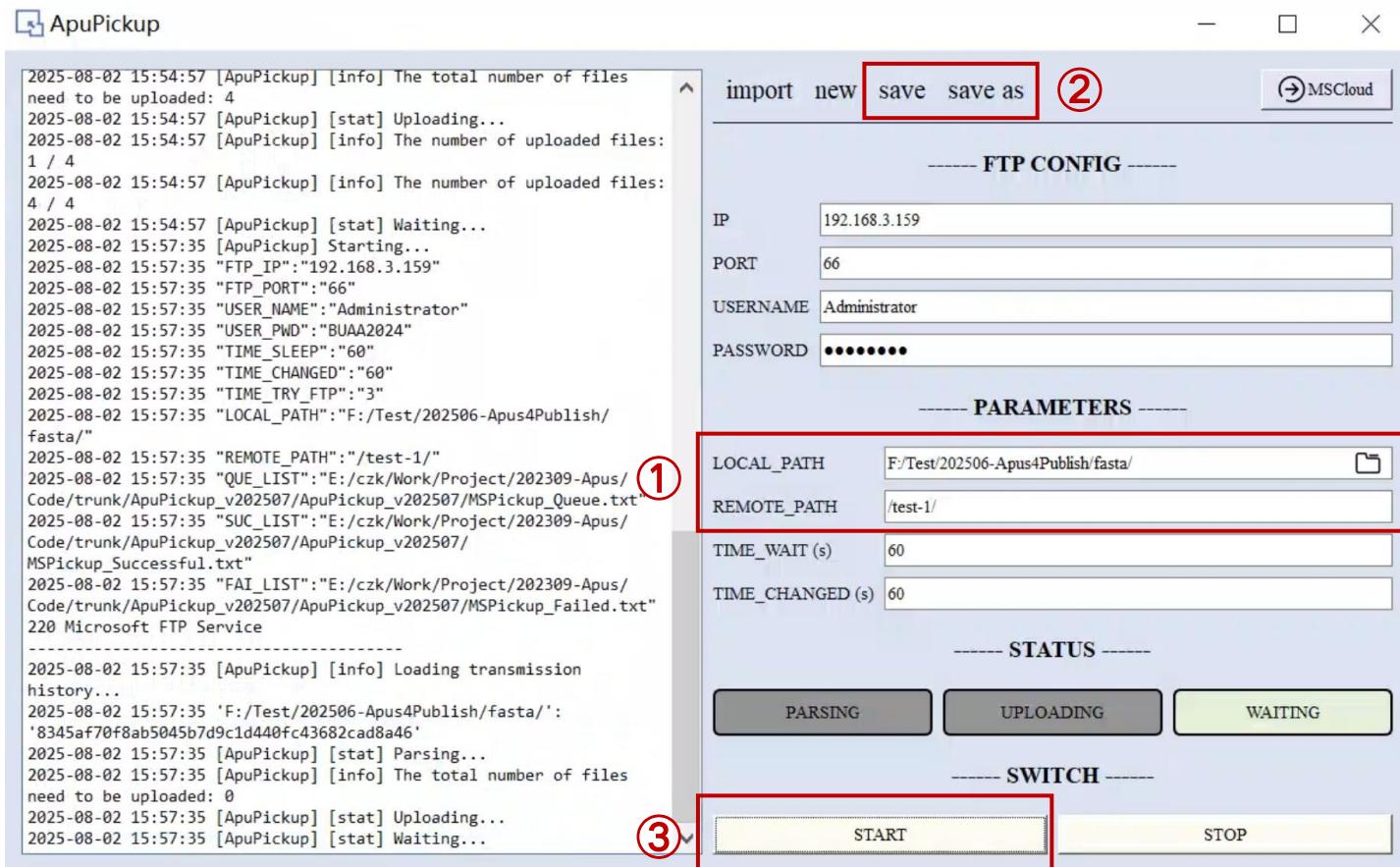
1. Use **IIS (Internet Information Services)** to establish an **FTP connection** between the local machine and the central NAS server. (If you are only testing the software, an FTP connection between any two computers on the same network is sufficient)
2. Input these **FTP configuration settings** into the software's interface. (The following figure is an example).

**----- FTP CONFIG -----**

IP	192.168.3.159
PORT	66
USERNAME	Administrator
PASSWORD	••••••••

# STEP-3

1. In the **LOCAL\_PATH** field, specify the directory path where the raw data files are generated.
2. In the **REMOTE\_PATH** field, specify the target directory path on the central NAS server designated for data storage.
3. Click **save** or **save as** to store the configuration settings locally as a file.
4. Click **START** to start the process. The software will then cycle through three operational states.



# ATTENTIONS

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1. ApuPickup operates based on the **File Transfer Protocol (FTP)**. Therefore, it is essential to ensure that the local machine and the central NAS server are **on the same local area network (LAN)** and that a **stable FTP connection** has been established between them.
2. ApuPickup features a **breakpoint resume mechanism** to handle network fluctuations, ensuring the integrity and stability of large-scale data transfers. A history of all transfer activities is recorded and saved as .pkl files within the **“/ApuPickup\_v202507/MSPickup/Uploaded Files/”** directory. Files that have already been successfully transferred will not be re-uploaded. To re-transmit any files, the **Uploaded Files** folder must be deleted.

ApuPioneer-DDA

# INTRODUCTION

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### Version: ApuPioneer-DDA\_v202507

### Release Date: 2025.07.15

### Computer configuration

CPU: Intel or AMD processor with 64-bit support, 2.3 GHz or faster processor with at least 2 cores is recommended

RAM: 16G or higher is recommended

ROM: for one raw MS data (1-2 G) or higher is recommended

OS: Windows 10 (x64) or Windows 11 (x64)

# INTRODUCTION

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ApuPioneer is an automated and parallel system for identification.

Its DDA mode uses the pFind open-search engine.

1. **Automation & parallelization:** The system automates the protein identification process. It runs tasks in parallel on multiple compute nodes.
2. **Real-time analysis:** ApuPioneer monitors a folder and automatically starts analyzing new raw files as they are transferred. You don't need to wait for all samples to be acquired.
3. **Simple to use:** The system uses optimized default parameters. Users only need to provide basic info, like the data path and database file, to start an analysis.

ApuPioneer's output follows the standard format of the search engine, including peptide-spectrum matches and protein inference results. These results can be used directly by the ApuHorizon system for quantification.

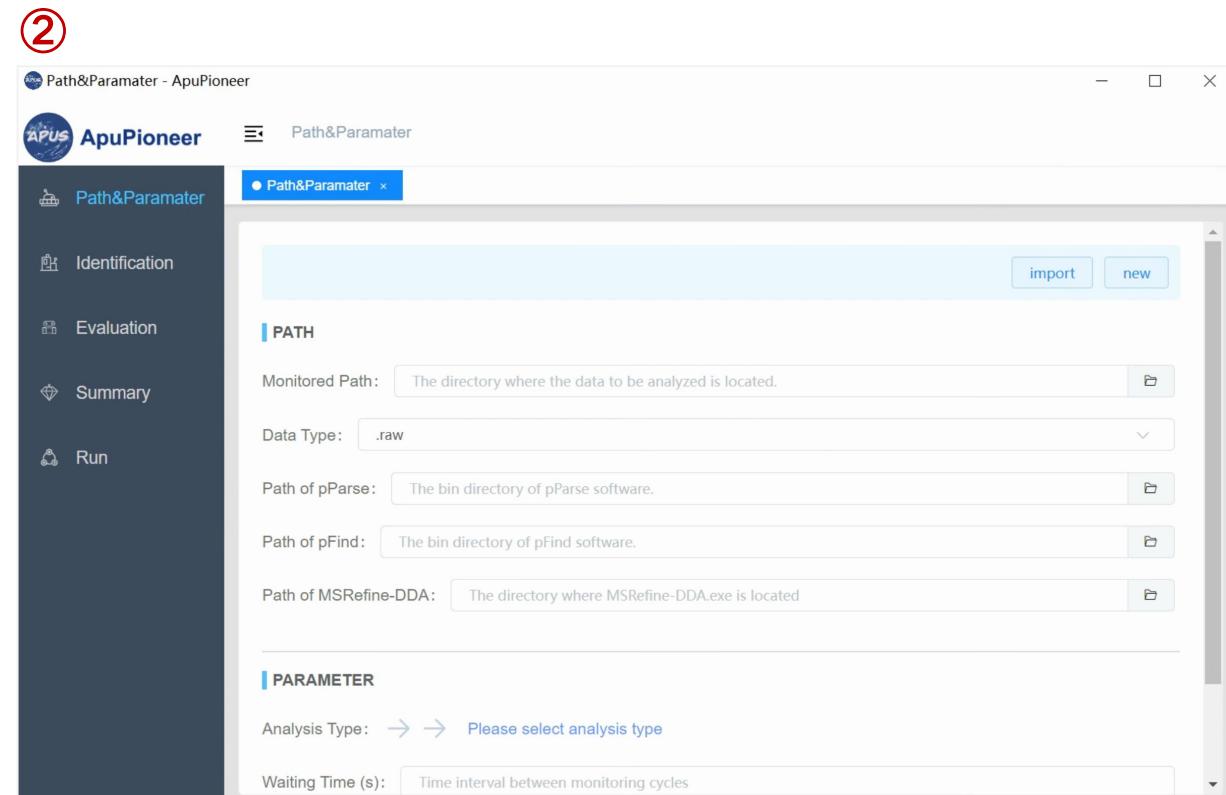
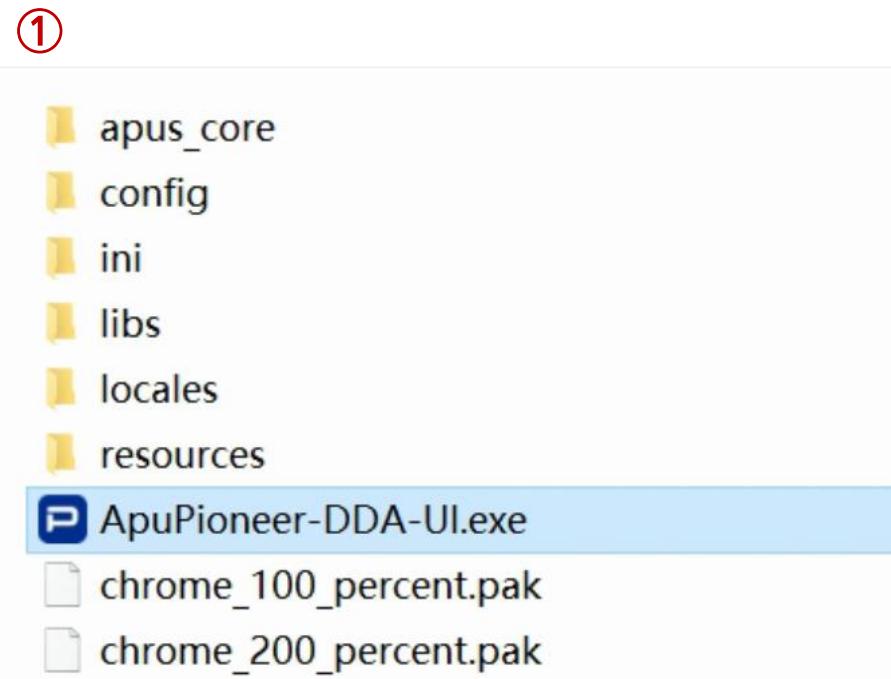
# STEP-1 Preparation

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1. **Install software:** Deploy ApuPioneer-DDA, pFind, and MSRefine-DDA on **every compute node** of your cluster.
  - Download ApuPioneer-DDA and MSRefine-DDA from [\*https://github.com/BUAA-LiuLab/Apus\*](https://github.com/BUAA-LiuLab/Apus).
  - Download pFind from [\*https://pfind.ict.ac.cn/se/pfind/#Downloads\*](https://pfind.ict.ac.cn/se/pfind/#Downloads).
2. **Get licenses:** Obtain the **licenses** for pFind and MSRefine-DDA by following the instructions in their manuals:
  - “/pFind3/pFind 3 UserGuide.pdf”
  - “/MSRefine-DDA\_v202407/Manual.for.MSRefine.pdf”
3. **Mount storage:** Use the **SMB** protocol to mount your data storage system to the local filesystem of the compute nodes, so it can be accessed like a local disk.

# STEP-2

1. Navigate to the “/ApuPioneer-DDA\_v202507/” directory.
2. Execute **ApuPioneer-DDA-UI.exe** to launch the application. This will open the main software interface.



# STEP-3 Path&Paramater

## 1. Fill in **data information**:

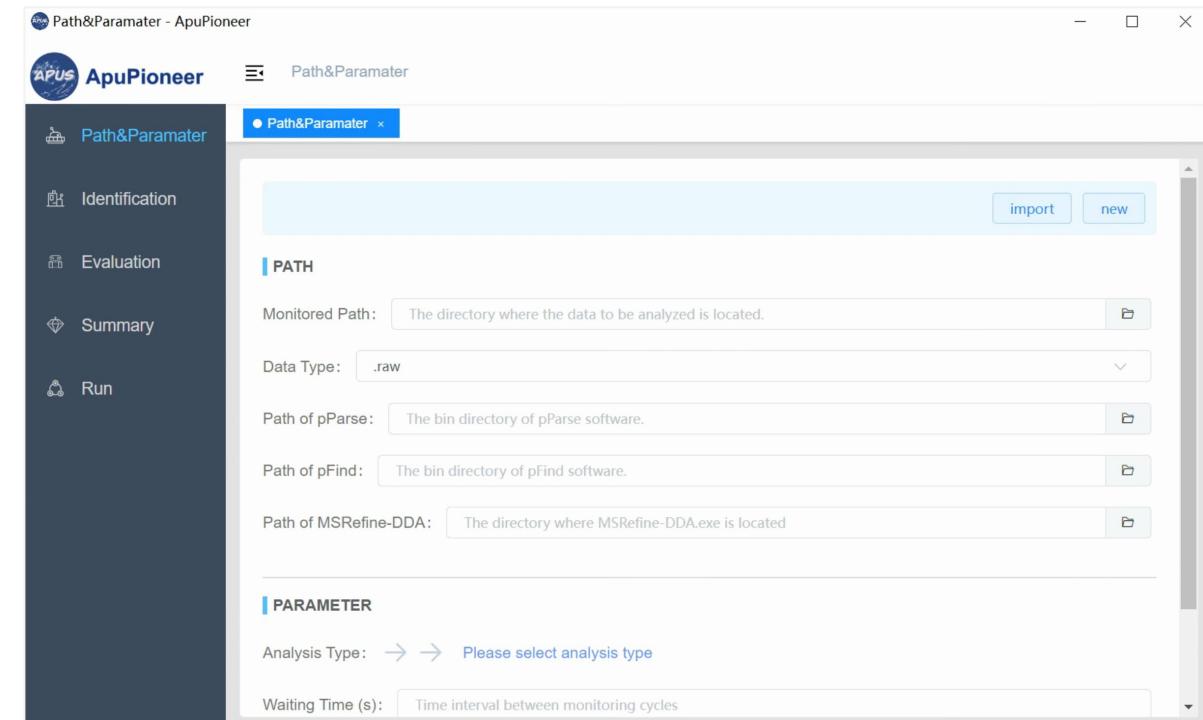
- Monitored path: The folder path where your MS data is stored.
- Data type: The format of your data files (e.g., .raw, .d, .wiff).

## 2. Fill in **software paths**:

Enter the installation directory paths for pParse, pFind, and MSRefine-DDA. This should be the folder containing the main executable file (e.g., MSRefine-DDA.exe).

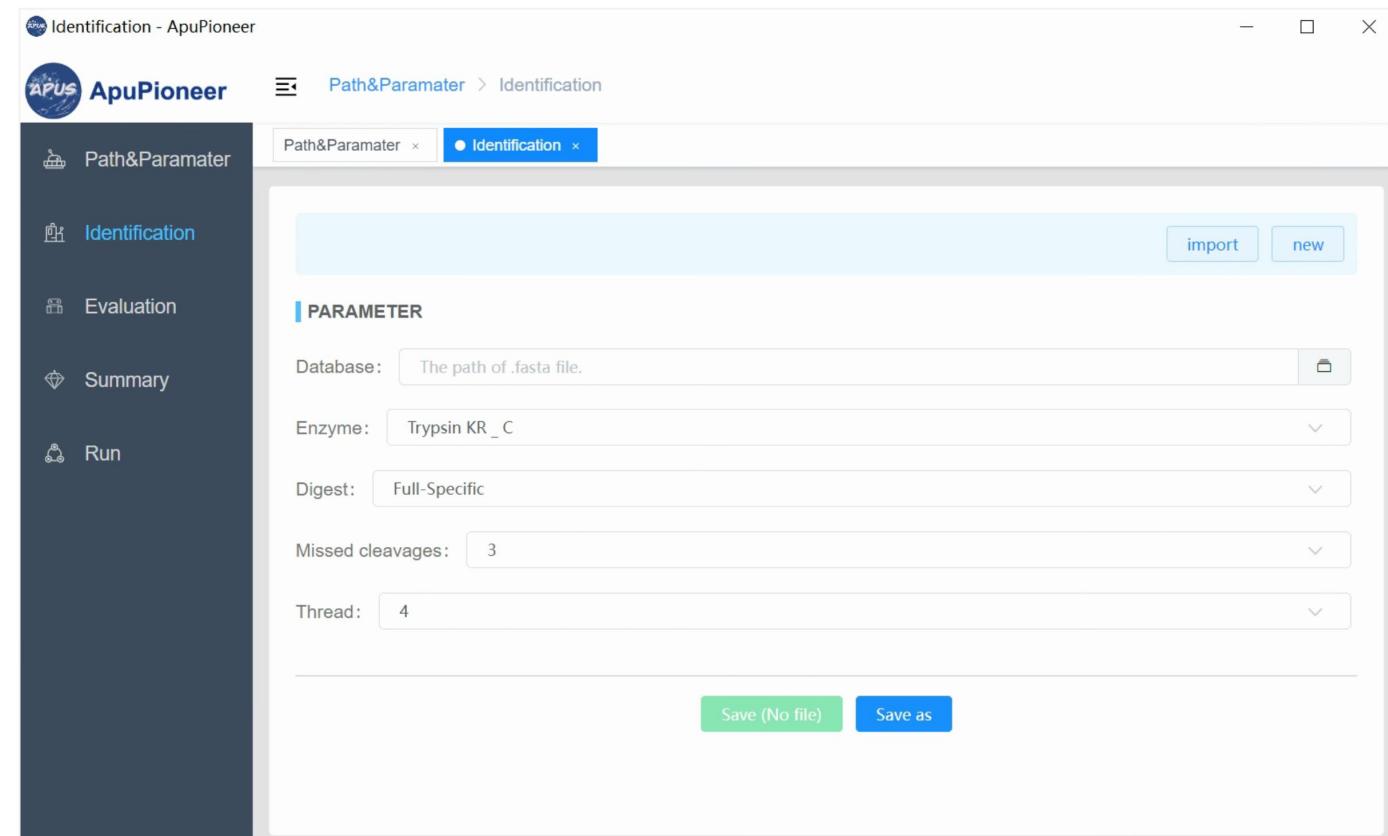
## 3. Fill in **analysis parameters**:

- Analysis type: "database search only" or "database search + quality control".
- Waiting time: The pause time between cycles of checking for new files.



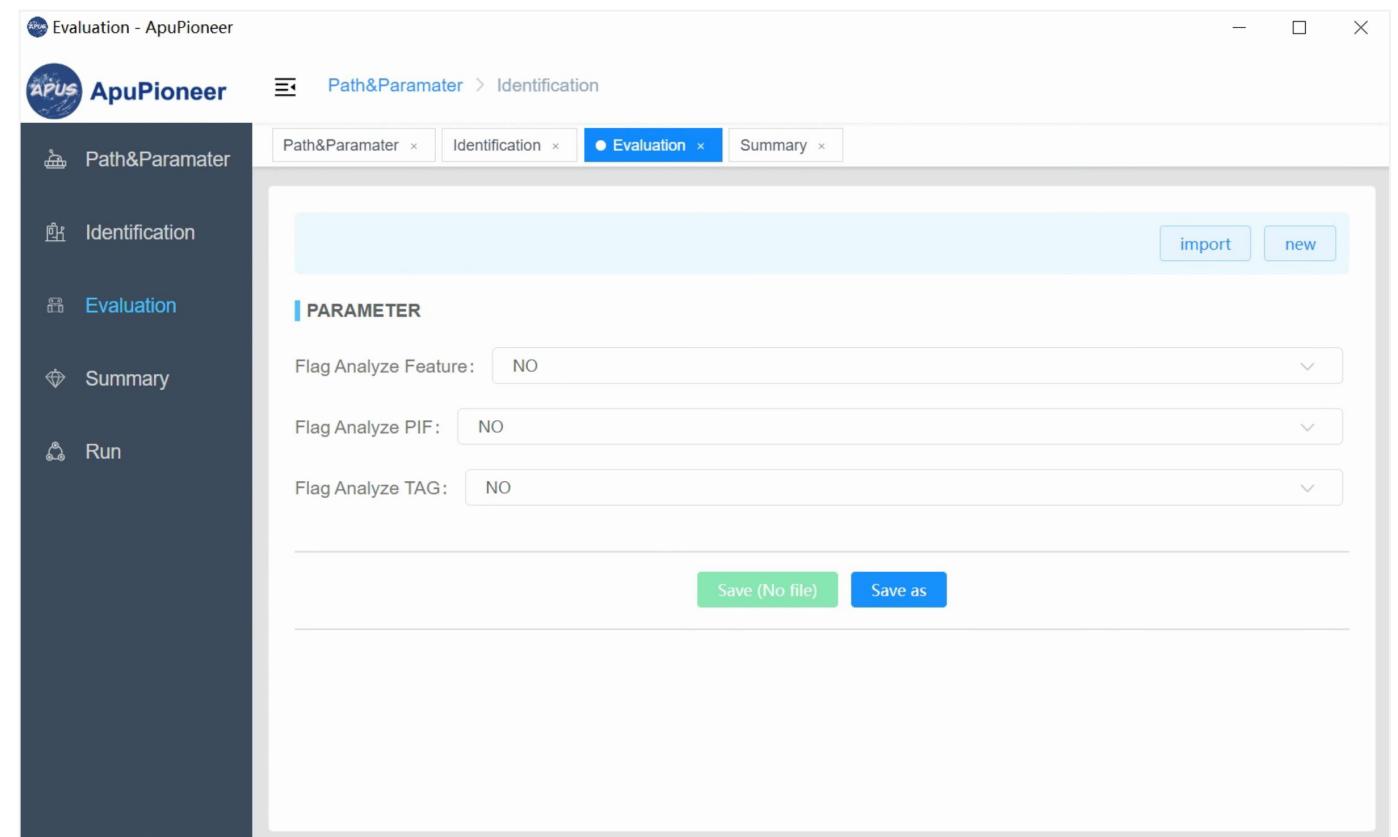
# STEP-4 Identification

- Fill in the following **search parameters** for DDA analysis. You can customize: Database, Enzyme, Digest, Missed cleavages, Thread
- **More advanced search parameters are already set to default.** You can view or edit them in the file: “/ApuPioneer-DDA\_v202507/config/pFind\_config.txt”



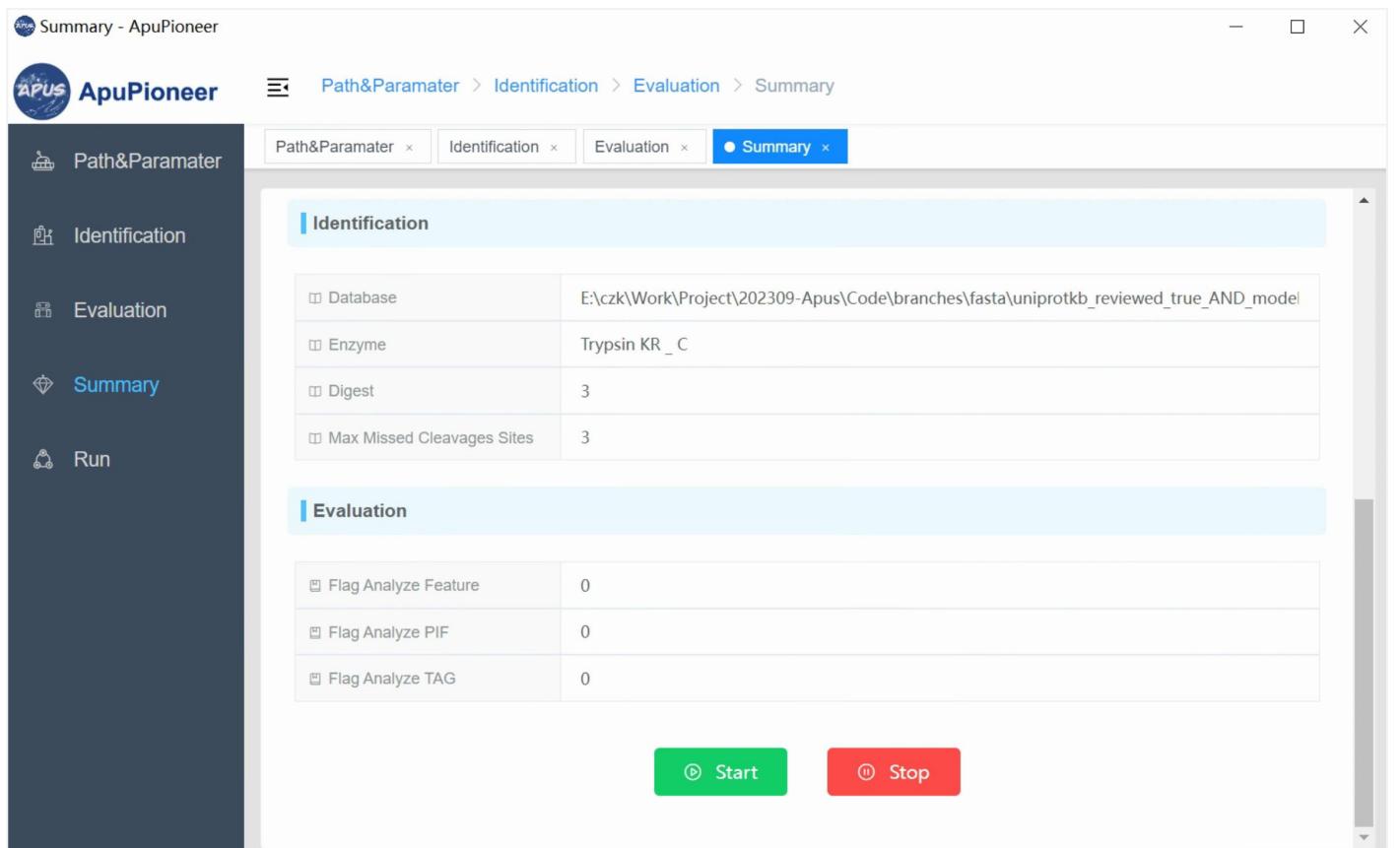
# STEP-5 Evaluation

- Fill in the following **parameters for quality control** in DDA analysis. You can configure: Flag Analyze Feature, Flag Analyze PIF, Flag Analyze TAG
- **More advanced MSRefine-DDA settings are already set to default.** You can view or edit them in the file: “/ApuPioneer-DDA\_v202507/config/MSRefine-DDA\_config.txt”.



# STEP-6 Summary

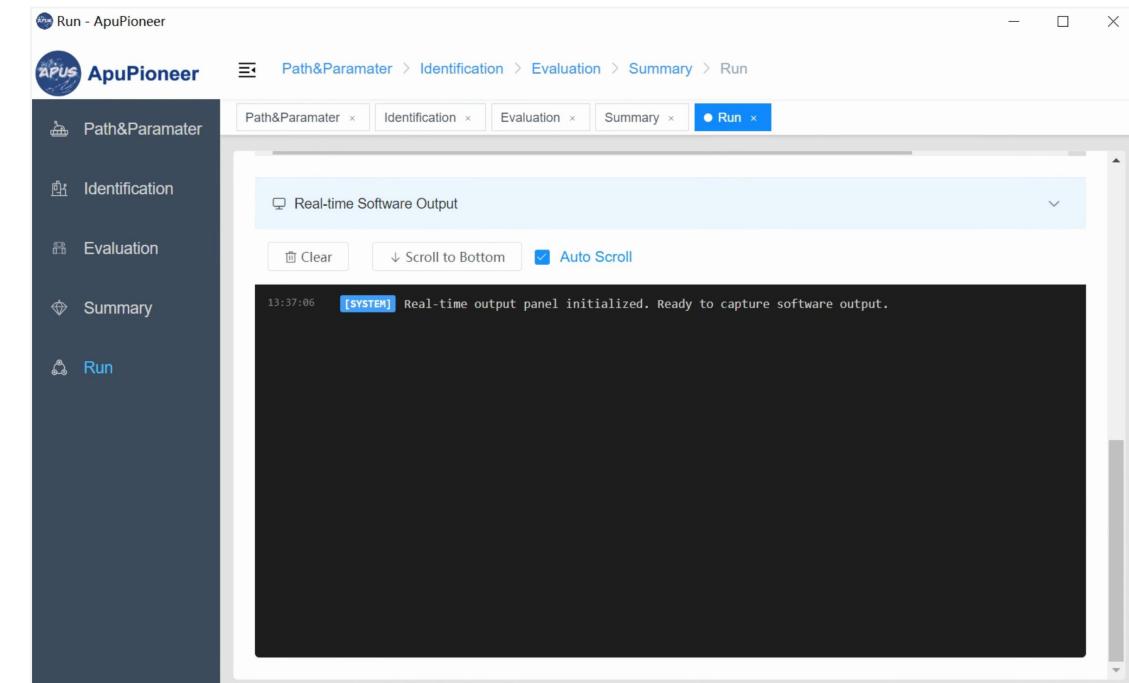
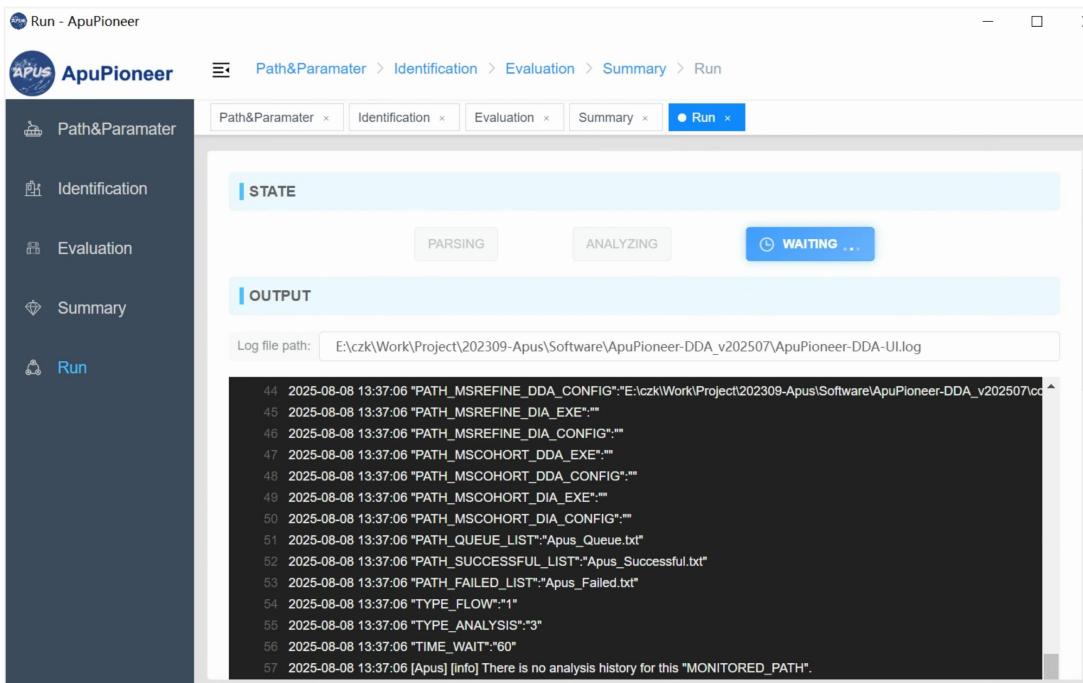
- 1. Review Configuration:** Navigate to the Summary page to review all previously configured parameters.
- 2. Start Process:** After verifying that all settings are correct, click the **Start** button to launch the application.



# STEP-7 Run

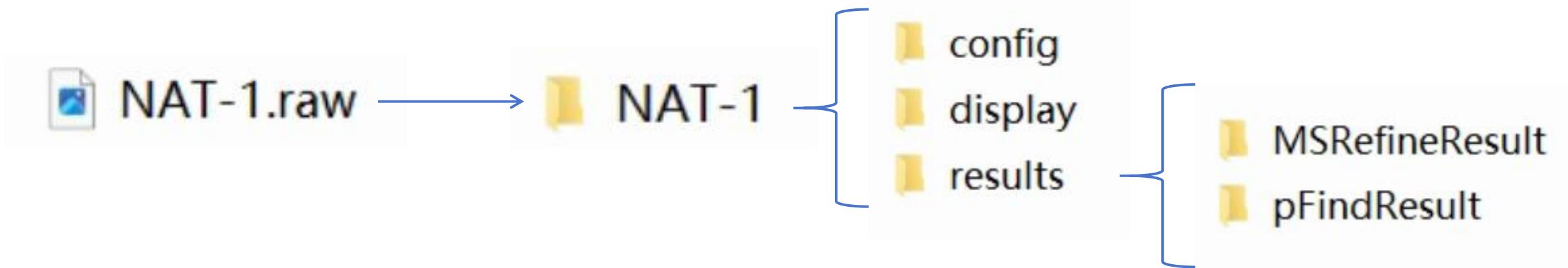
Go to the Run page to watch the program's progress.

- **STATE:** Shows the current status of the program's loop.
- **OUTPUT:** Here you can see live logs:
  1. Logs from ApuPioneer-DDA.
  2. More detailed logs from the tools it calls (like pFind).



# STEP-8 View analysis results

- Enter "Monitored Path" and view the data analysis results in the **folder with the same name as the MS data file**.



# ATTENTIONS

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1. Always click **Save** or **Save As** before leaving a page.
2. ApuPioneer keeps a record of processed files to run efficiently and prevent re-running completed tasks if the analysis is interrupted. It saves two types of history:
  1. **Local History**: Stored in the “`/ApuPioneer-DDA_v202507/AP_LocalHistory/`” folder (as `.pkl` files).
  2. **Global History**: Stored in the “`/Monitored Path/AP_GlobalHistory.txt`” file.
3. **To re-analyze all data in a folder from the beginning, you must delete the old history files first:**
  1. Delete the `AP_LocalHistory` folder.
  2. Delete the `AP_GlobalHistory.txt` file.

ApuPioneer-DIA

# INTRODUCTION

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### Version: ApuPioneer-DIA\_v202507

### Release Date: 2025.07.15

### Computer configuration

CPU: Intel or AMD processor with 64-bit support, 2.3 GHz or faster processor with at least 2 cores is recommended

RAM: 16G or higher is recommended

ROM: for one raw MS data (1-2 G) or higher is recommended

OS: Windows 10 (x64) or Windows 11 (x64)

# INTRODUCTION

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ApuPioneer is an automated and parallel system for identification.

Its DIA mode defaults to **DIA-NN**.

1. **Automation & parallelization**: The system automates the protein identification process. It runs tasks in parallel on multiple compute nodes.
2. **Real-time analysis**: ApuPioneer monitors a folder and automatically starts analyzing new raw files as they are transferred. You don't need to wait for all samples to be acquired.
3. **Simple to use**: The system uses optimized default parameters. Users only need to provide basic info, like the data path and database file, to start an analysis.

ApuPioneer's output follows the standard format of the search engine, including peptide-spectrum matches and protein inference results. These results can be used directly by the ApuHorizon system for quantification.

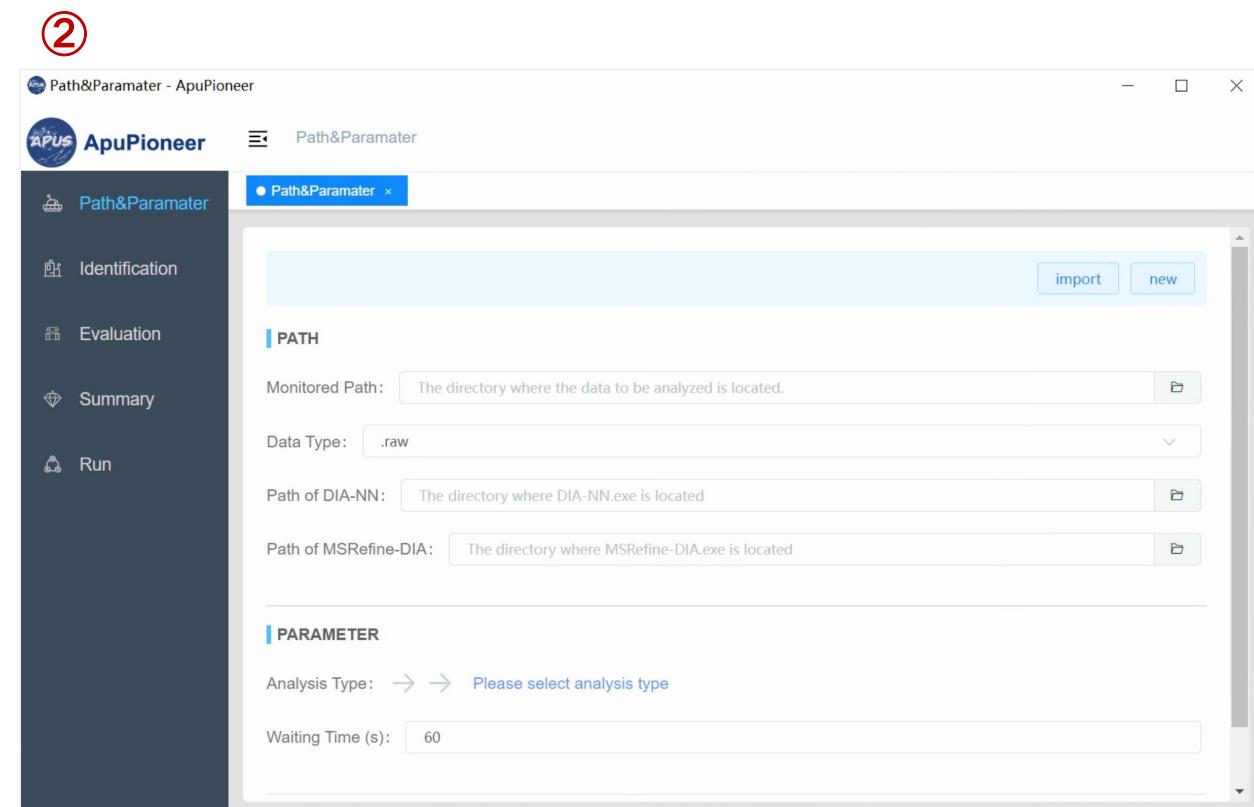
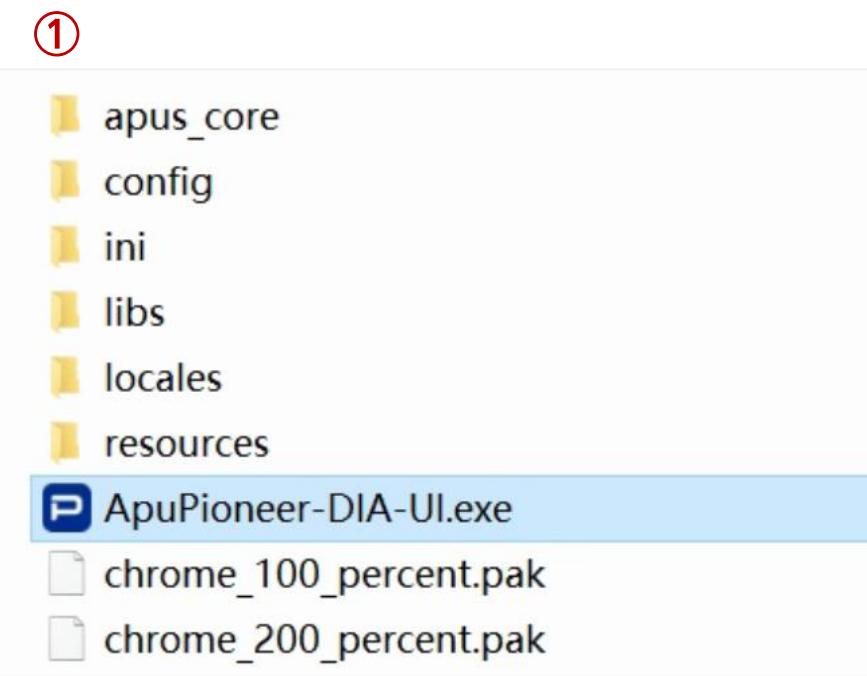
# STEP-1 Preparation

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1. **Install software:** Deploy ApuPioneer-DIA, DIA-NN, and MSRefine-DIA on all **compute nodes** of your cluster.
  - Download ApuPioneer-DIA and MSRefine-DIA from <https://github.com/BUAA-LiuLab/Apus>.
  - Download DIA-NN from <https://github.com/vdemichev/DiaNN>.
2. **Mount storage:** Use the **SMB** protocol to mount your data storage system to the local filesystem of the compute nodes, so it can be accessed like a local disk.

# STEP-2

1. Navigate to the “/ApuPioneer-DIA\_v202507/” directory.
2. Execute **ApuPioneer-DIA-UI.exe** to launch the application. This will open the main software interface.



# STEP-3 Path&Paramater

## 1. Fill in **data information**:

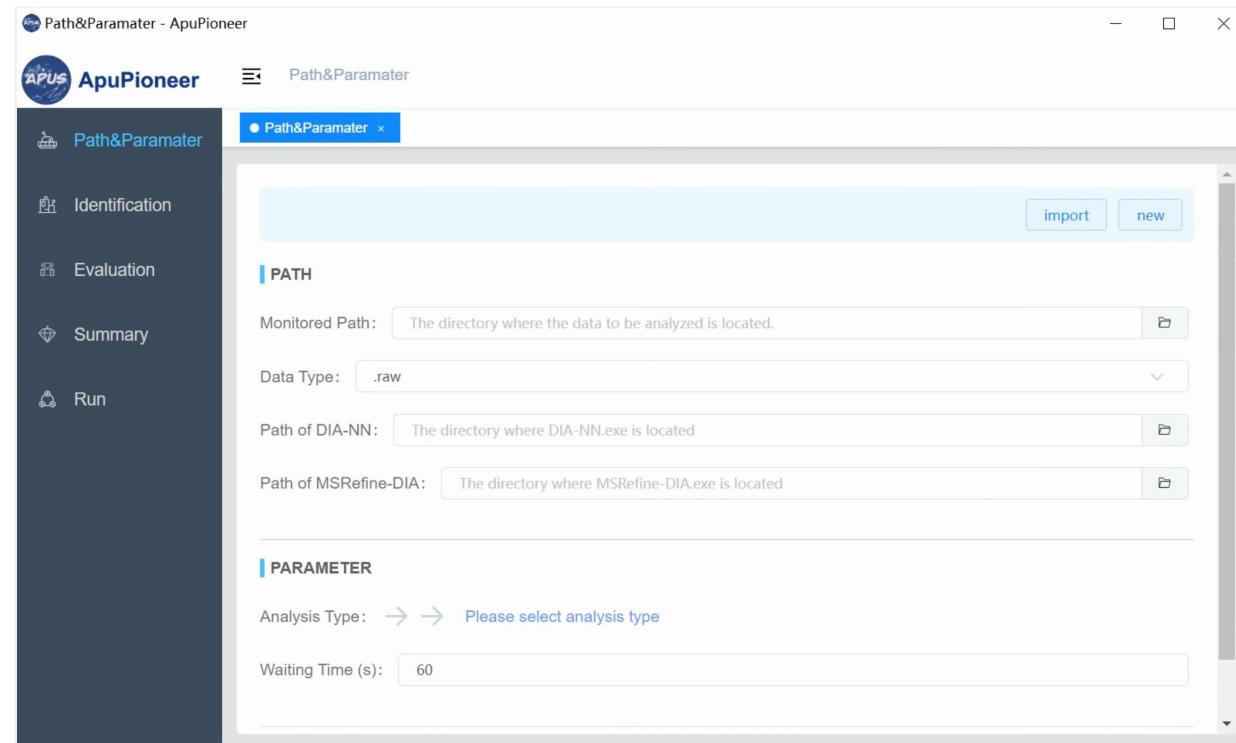
- Monitored path: The folder path where your MS data is stored.
- Data type: The format of your data files (e.g., .raw, .d, .wiff).

## 2. Fill in **software paths**:

Enter the installation directory paths for DIA-NN and MSRefine-DIA. This should be the folder containing the main executable file (e.g., MSRefine-DIA.exe).

## 3. Fill in **analysis parameters**:

- Analysis type: "database search only" or "database search + quality control".
- Waiting time: The pause time between cycles of checking for new files.



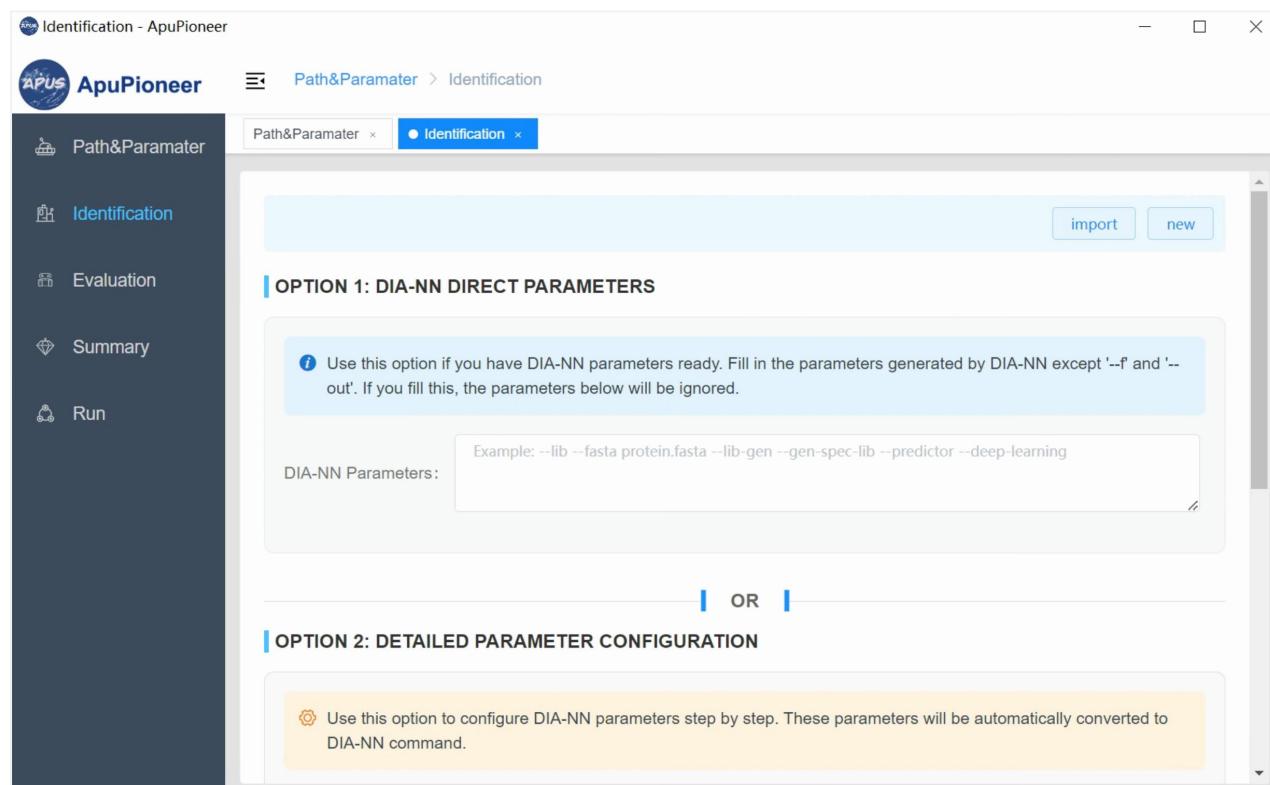
# STEP-4 Identification

Configure **search parameters** for ApuPioneer-DIA.

1. Many search parameters are preset with optimized default values. Users only need to specify essential parameters, such as the FASTA Database and Library-free Search options, to run the analysis.
2. Notably, for DIA mode, besides setting common DIA-NN parameters via the GUI, **ApuPioneer allows users to input a full command-line argument string.**

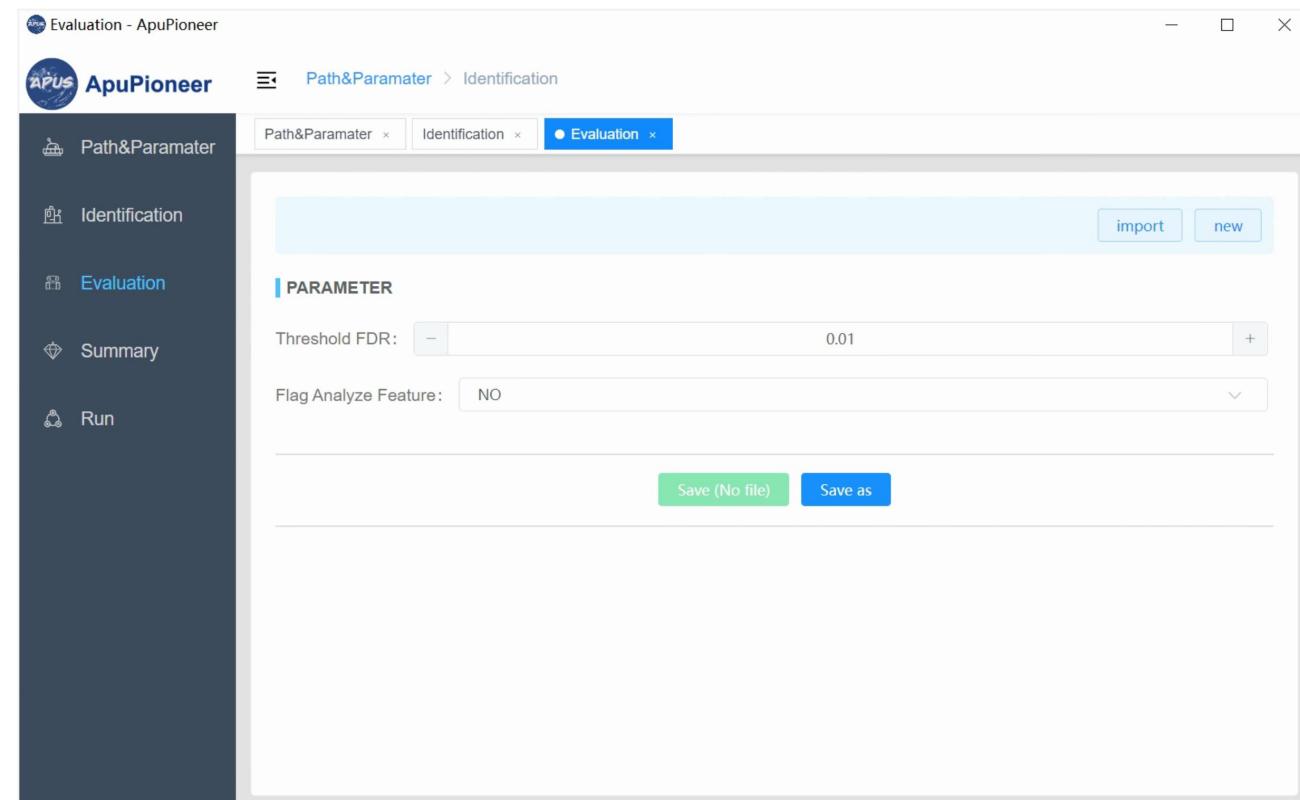
This string should be generated from the native DIA-NN interface, excluding the `--f` and `--out` arguments.

This feature provides fine-grained control over the identification process.



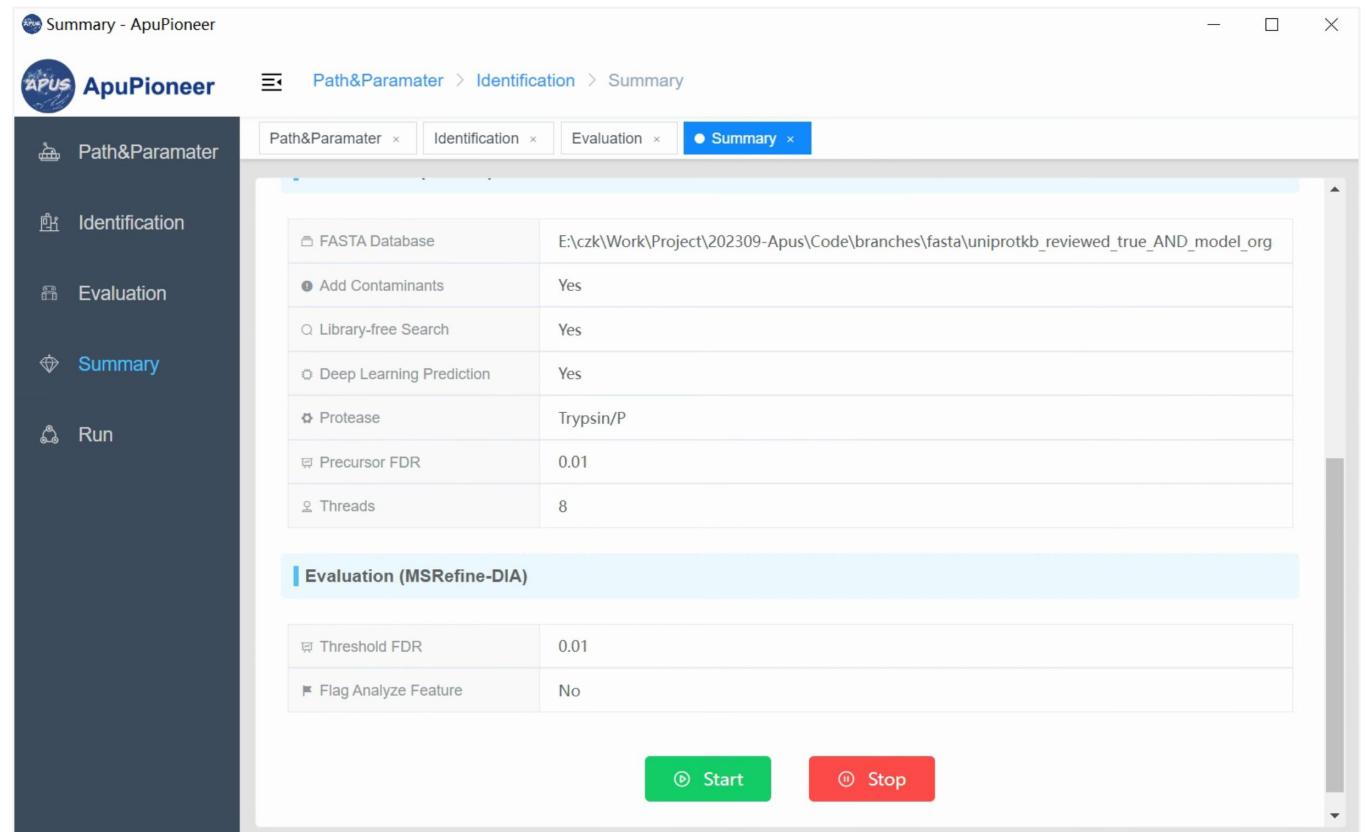
# STEP-5 Evaluation

- Fill in the following **parameters for quality control** in DIA analysis. You can configure: Threshold FDR, Flag Analyze Feature.
- **More advanced MSRefine-DIA settings are already set to default.** You can view or edit them in the file: “/ApuPioneer-DIA\_v202507/config/MSRefine-DIA\_config.txt”.



# STEP-6 Summary

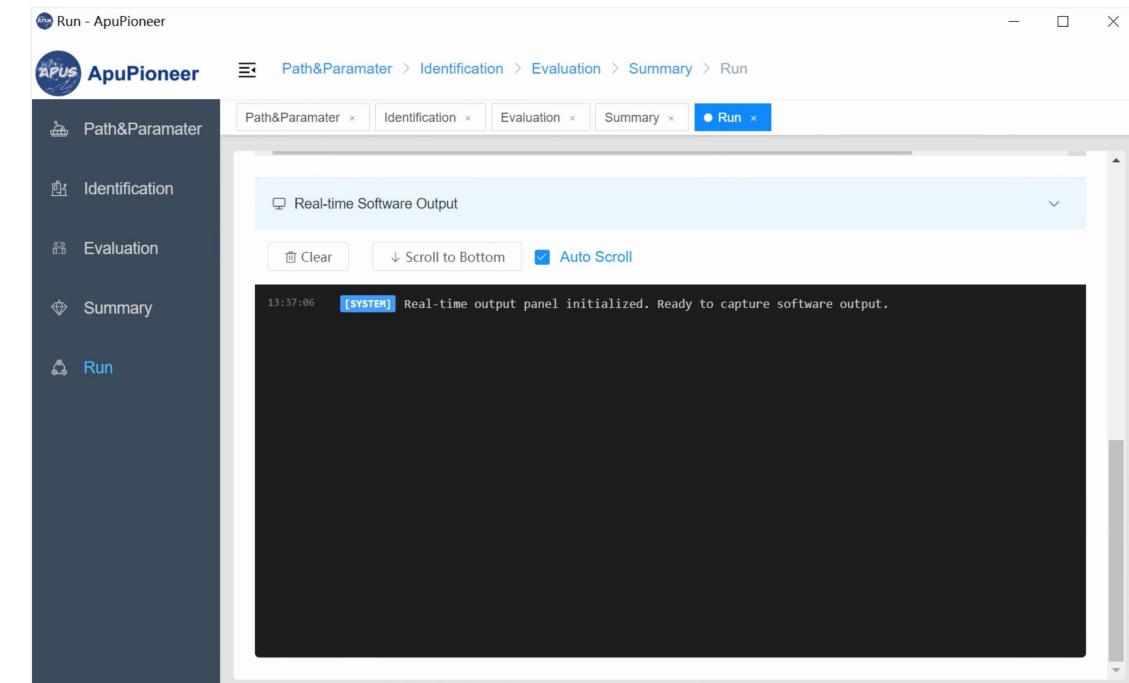
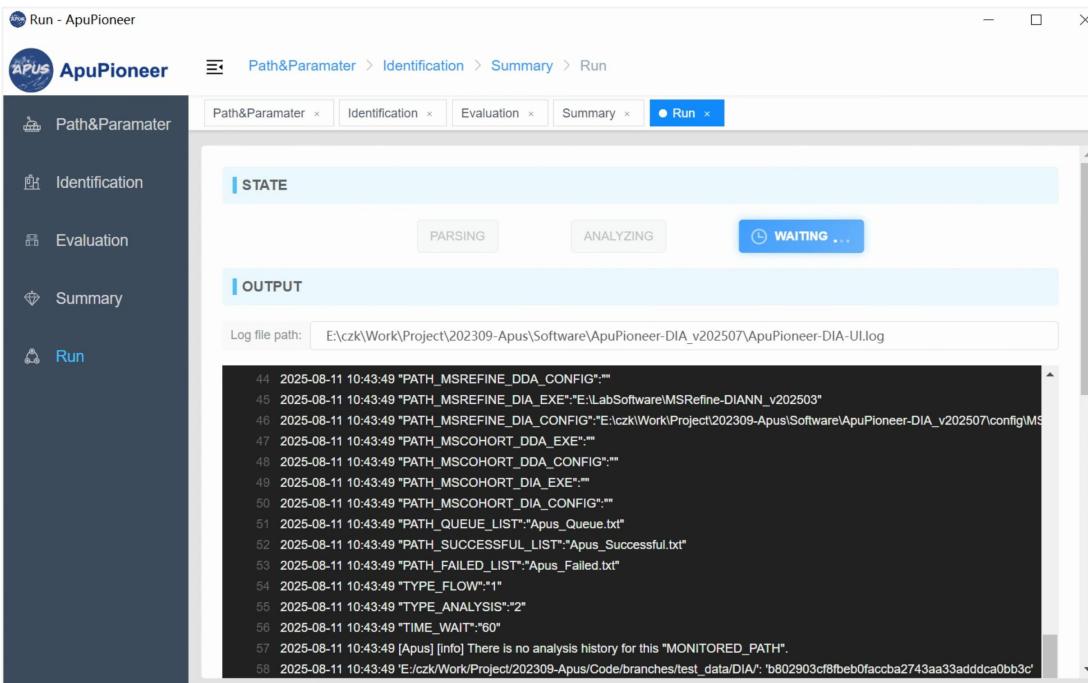
- Review configuration:** Navigate to the Summary page to review all previously configured parameters.
- Start process:** After verifying that all settings are correct, click the **Start** button to launch the application.



# STEP-7 Run

Go to the Run page to watch the program's progress.

- **STATE:** Shows the current status of the program's loop.
- **OUTPUT:** Here you can see live logs:
  1. Logs from ApuPioneer-DIA.
  2. More detailed logs from the tools it calls (like DIA-NN)



# STEP-8 View analysis results

- Enter "Monitored Path" and view the data analysis results in the **folder with the same name as the MS data file**.



# ATTENTIONS

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1. Always click **Save** or **Save As** before leaving a page.
2. ApuPioneer keeps a record of processed files to run efficiently and prevent re-running completed tasks if the analysis is interrupted. It saves two types of history:
  1. **Local History**: Stored in the “`/ApuPioneer-DIA_v202507/AP_LocalHistory/`” folder (as .pkl files).
  2. **Global History**: Stored in the “`/Monitored Path/AP_GlobalHistory.txt`” file.
3. **To re-analyze all data in a folder from the beginning, you must delete the old history files first:**
  1. Delete the AP\_LocalHistory folder.
  2. Delete the AP\_GlobalHistory.txt file.

# ApuHorizon-DDA

# INTRODUCTION

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### Version: ApuHorizon-DDA\_v202507

### Release Date: 2025.07.15

### Computer configuration

CPU: Intel or AMD processor, 32 cores or higher is recommended

RAM: 256GB or higher is recommended

ROM: 1TB or higher high-speed NVMe SSD is recommended

OS: Windows 10 (x64) or Windows 11 (x64)

# INTRODUCTION

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**ApuHorizon:** The protein quantification system of Apus.

It is deployed on a dedicated server with substantial memory to handle the high-throughput quantification of a large cohort comprising hundreds to thousands of samples.

- **Input:** Receives identification results from ApuPioneer.
- **Process:** Performs LFQ using a proven engine (defaults to **pQuant** for DDA mode).
- **Output:** Generates a result file detailing analyte abundances per sample.
- **Integration:** Output is ready for immediate use in ApuInsight (for bioinformatics).

# STEP-1 Preparation

---

1. **Install software:** Deploy ApuHorizon-DDA, pQuant, and MSCohort-DDA on the quantification server with substantial memory.
  - Download them from [\*https://github.com/BUAA-LiuLab/Apus\*](https://github.com/BUAA-LiuLab/Apus).
2. **Get licenses:** Refer to “/pQuant-pGlycoQuant\_v202407/Manual for pQuant.pdf” to obtain the pQuant license.
3. **Mount storage:** Use the **SMB** protocol to mount your data storage system to the local filesystem of the compute nodes, so it can be accessed like a local disk.

# STEP-2

1. Navigate to the “/ApuHorizon-DDA\_v202507/” directory.
2. Execute **ApuHorizon-DDA-UI.exe** to launch the application. This will open the main software interface.

①

The screenshot shows a Windows File Explorer window. The path is 'C:\Program Files\ApuHorizon-DDA\_v202507'. The contents of the folder are:

- apus\_core
- config
- ini
- libs
- locales
- resources
- ApuHorizon-DDA-UI.exe** (highlighted in blue)
- chrome\_100\_percent.pak
- chrome\_200\_percent.pak

②

The screenshot shows the ApuHorizon software interface. The title bar says 'Path&Parameter - ApuHorizon'. The left sidebar has the following options:

- Path&Parameterer (selected)
- Quantification
- Evaluation
- Summary
- Run

The main panel is titled 'Path&Parameterer'. It contains the following fields:

- PATH**
  - Monitored Path: The directory where the data to be analyzed is located. (Input field with a browse button)
  - Data Type: .raw (Input field)
  - Path of pQuant: The directory where Quant.exe is located (Input field with a browse button)
  - Path of MSCohort-DDA: The directory where MSCohort-DDA.exe is located (Input field with a browse button)
- PARAMETER**
  - Analysis Type: → → No analysis selected (Input field)

At the bottom right are 'Save (No file)' and 'Save as' buttons.

# STEP-3 Path&Paramater

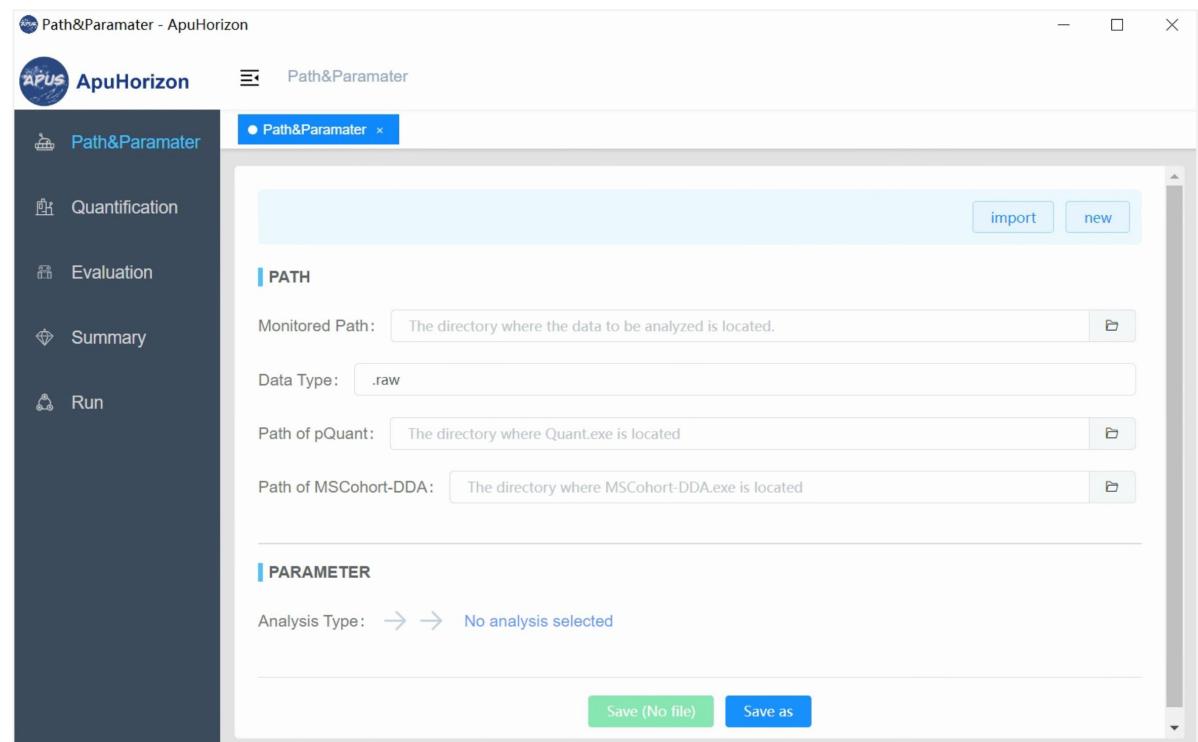
## 1. Fill in **data information**:

- Monitored path: The folder path where your MS data is stored.
- Data type: The format of your data files (e.g., .raw, .d, .wiff).

## 2. Fill in **software paths**:

Enter the installation directory paths for pQuant and MSCohort-DDA. This should be the folder containing the main executable file (e.g., MSCohort-DDA.exe).

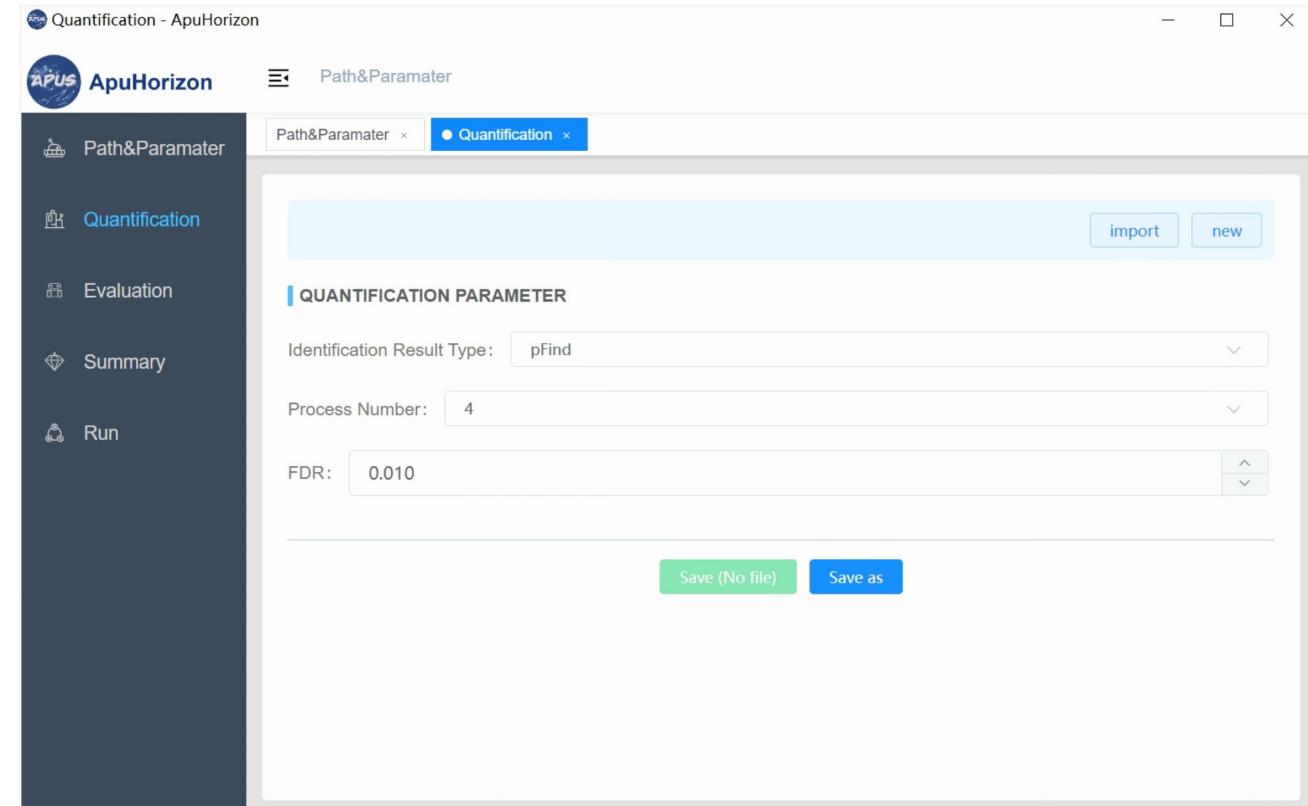
## 3. Fill in **analysis type**: "quantification only" or "quantification + quality control".



# STEP-4 Quantification

Configure the **quantification parameters** for DDA analysis.

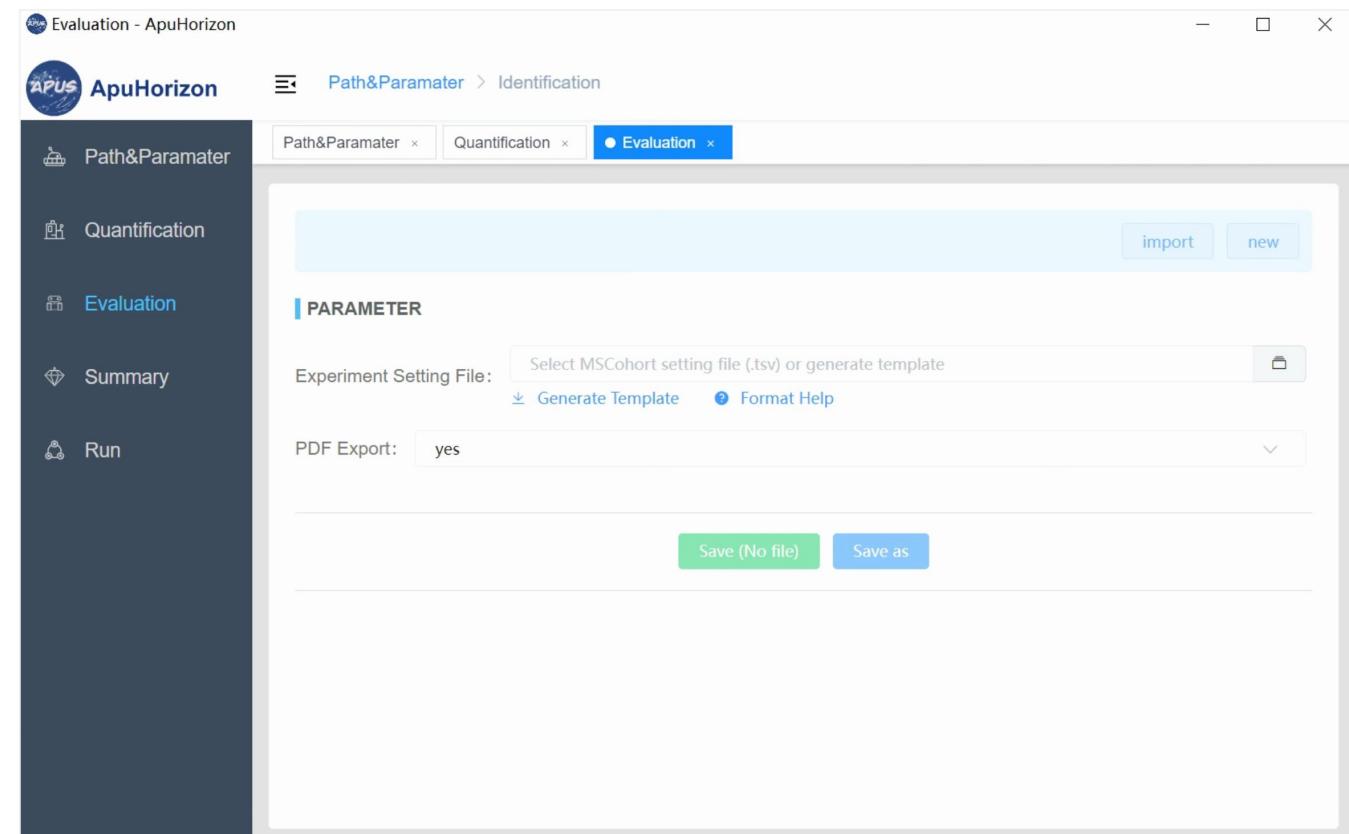
- The system is pre-loaded with numerous default parameters and automatically locates the identification result files.
- For more specific quantification parameters, please refer to the configuration file at "/ApuHorizon-DDA\_v202507/config/pQuant\_config.txt".



# STEP-5 Evaluation

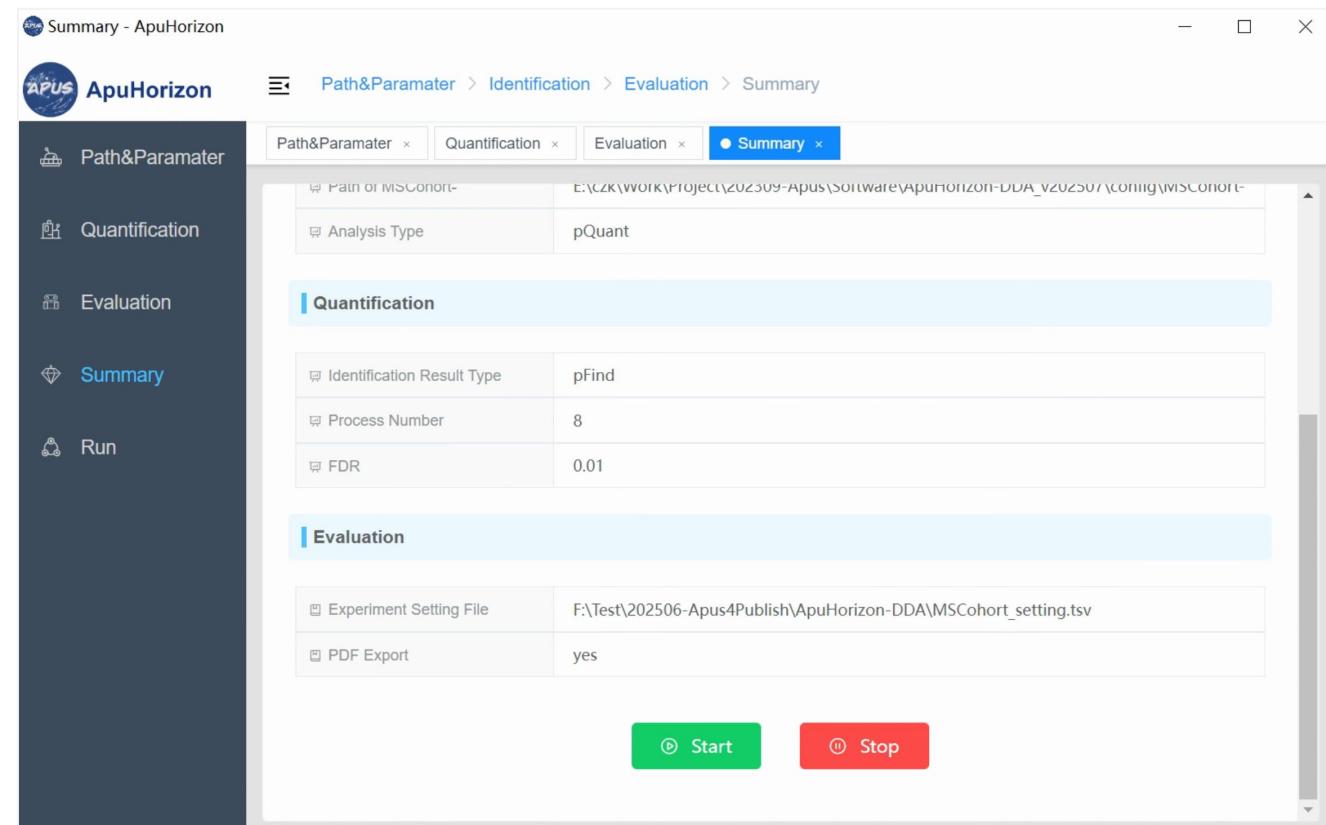
Fill in the following **MSCohort-DDA parameters** for quality control.

More advanced **MSCohort-DDA settings** are already set to default. You can view or edit them in the file: “/ApuHorizon-DDA\_v202507/config/MSCohort-DDA\_config.txt”.



# STEP-6 Summary

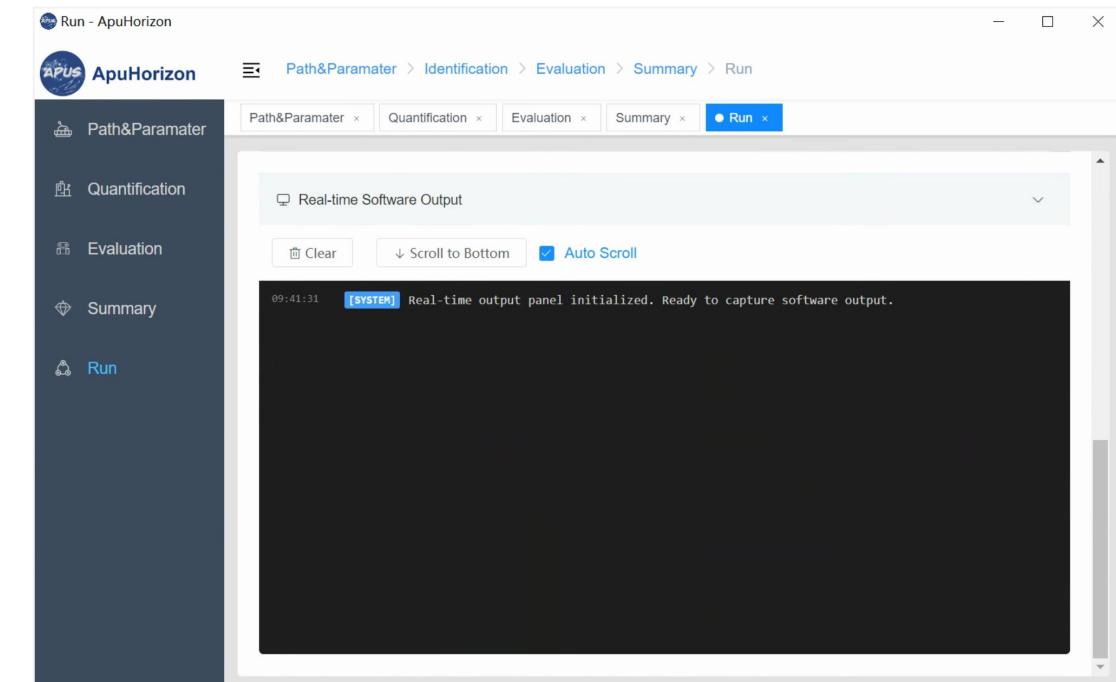
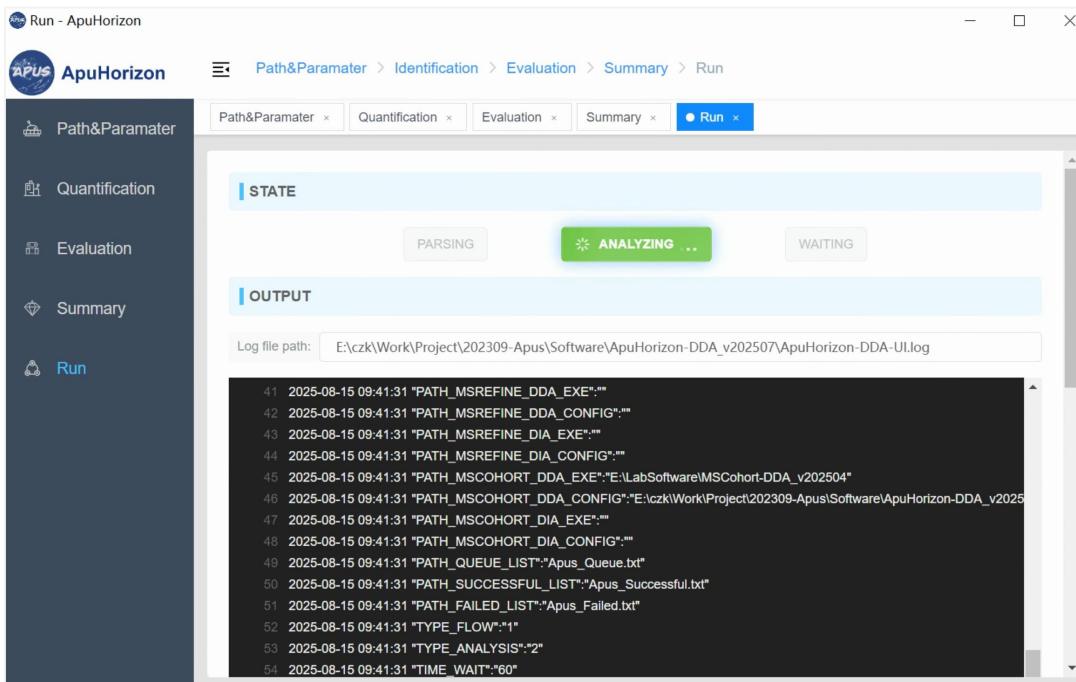
- Review configuration:** Navigate to the Summary page to review all previously configured parameters.
- Start process:** After verifying that all settings are correct, click the **Start** button to launch the application.



# STEP-7 Run

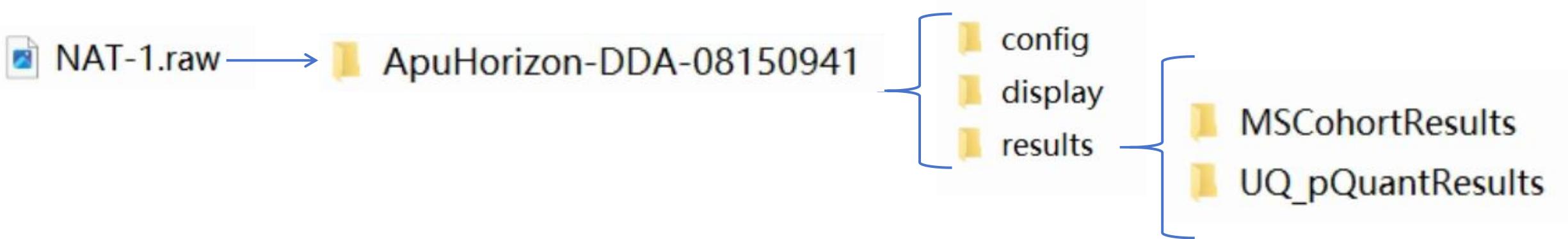
Go to the Run page to watch the program's progress.

- **STATE:** Shows the current status of the program's loop.
- **OUTPUT:** Here you can see live logs:
  1. Logs from ApuHorizon-DDA.
  2. More detailed logs from the tools it calls (like pQuant).



# STEP-8 View analysis results

- Navigate to "Monitored Path" and view the data analysis results in the folder named **ApuHorizon-DDA+[Timestamp]**.



# ATTENTIONS

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1. Always click **Save** or **Save As** before leaving a page.
2. ApuHorizon automatically locates the analysis results from ApuPioneer. **Do not manually rename the identification result folder, as this will prevent the analysis from running correctly.**

ApuHorizon-DIA

# INTRODUCTION

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### Version: ApuHorizon-DIA\_v202507

### Release Date: 2025.07.15

### Computer configuration

CPU: Intel or AMD processor, 32 cores or higher is recommended

RAM: 256GB or higher is recommended

ROM: 1TB or higher high-speed NVMe SSD is recommended

OS: Windows 10 (x64) or Windows 11 (x64)

# INTRODUCTION

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**ApuHorizon:** The protein quantification system of Apus.

It is deployed on a dedicated server with substantial memory to handle the high-throughput quantification of a large cohort comprising hundreds to thousands of samples.

- **Input:** Receives identification results from ApuPioneer.
- **Process:** Performs LFQ using a proven engine (defaults to **DIA-NN** for DIA mode).
- **Output:** Generates a result file detailing analyte abundances per sample.
- **Integration:** Output is ready for immediate use in ApuInsight (for bioinformatics).

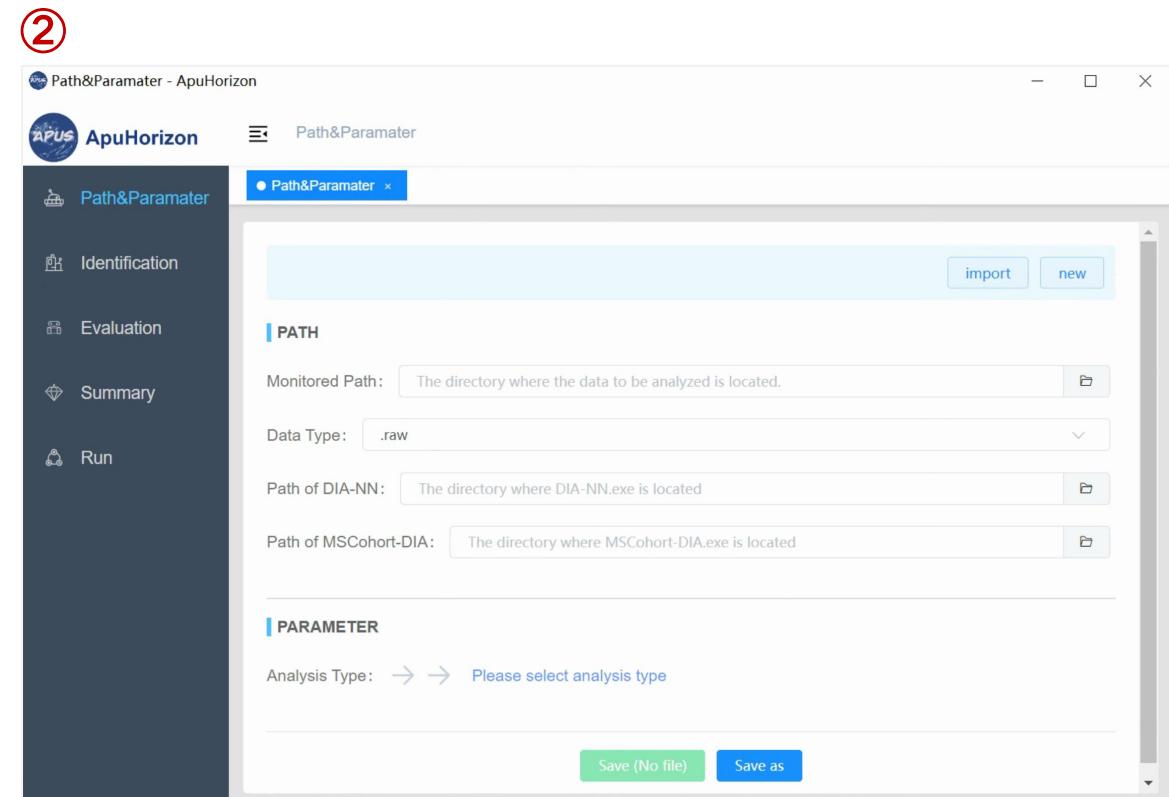
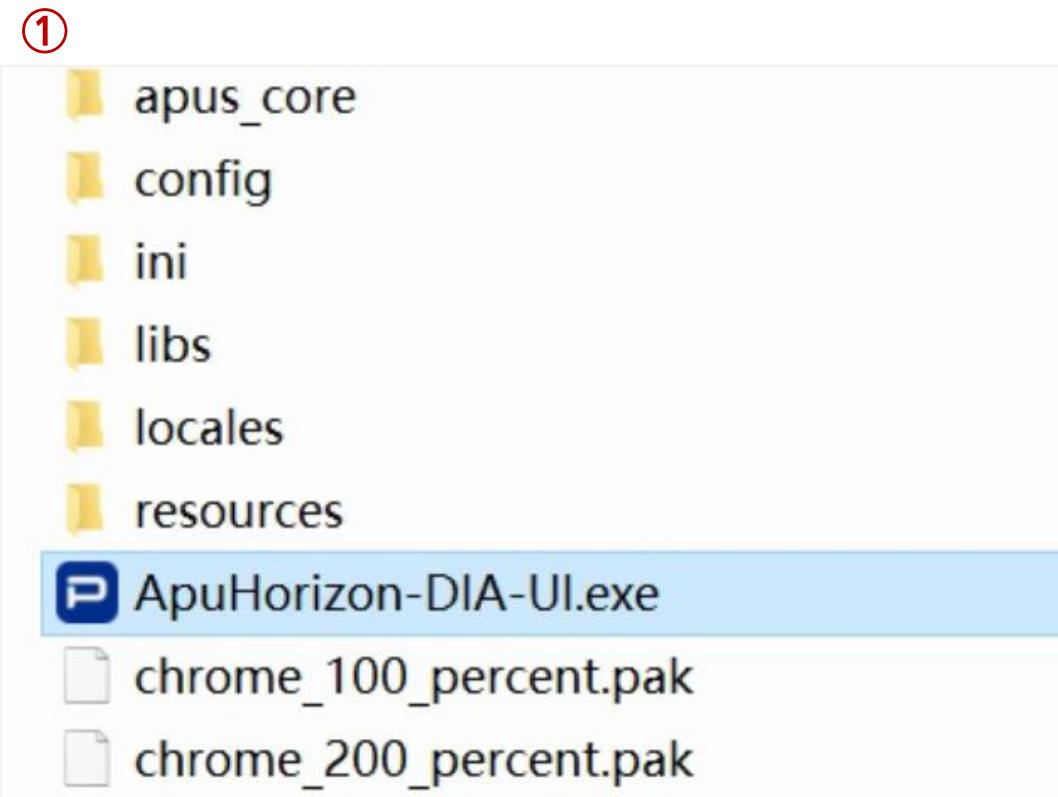
# STEP-1 Preparation

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1. **Install software:** Deploy ApuHorizon-DIA, DIA-NN, and MSCohort-DIA on the quantitative analysis server.
  - Download ApuHorizon-DIA and MSCohort-DIA from <https://github.com/BUAA-LiuLab/Apus>.
  - Download DIA-NN from <https://github.com/vdemichev/DiaNN>.
2. **Mount storage:** Use the **SMB** protocol to mount your data storage system to the local filesystem of the compute nodes, so it can be accessed like a local disk.

# STEP-2

1. Navigate to the “/ApuHorizon-DIA\_v202507/” directory.
2. Execute **ApuHorizon-DIA-UI.exe** to launch the application. This will open the main software interface.



# STEP-3 Path&Paramater

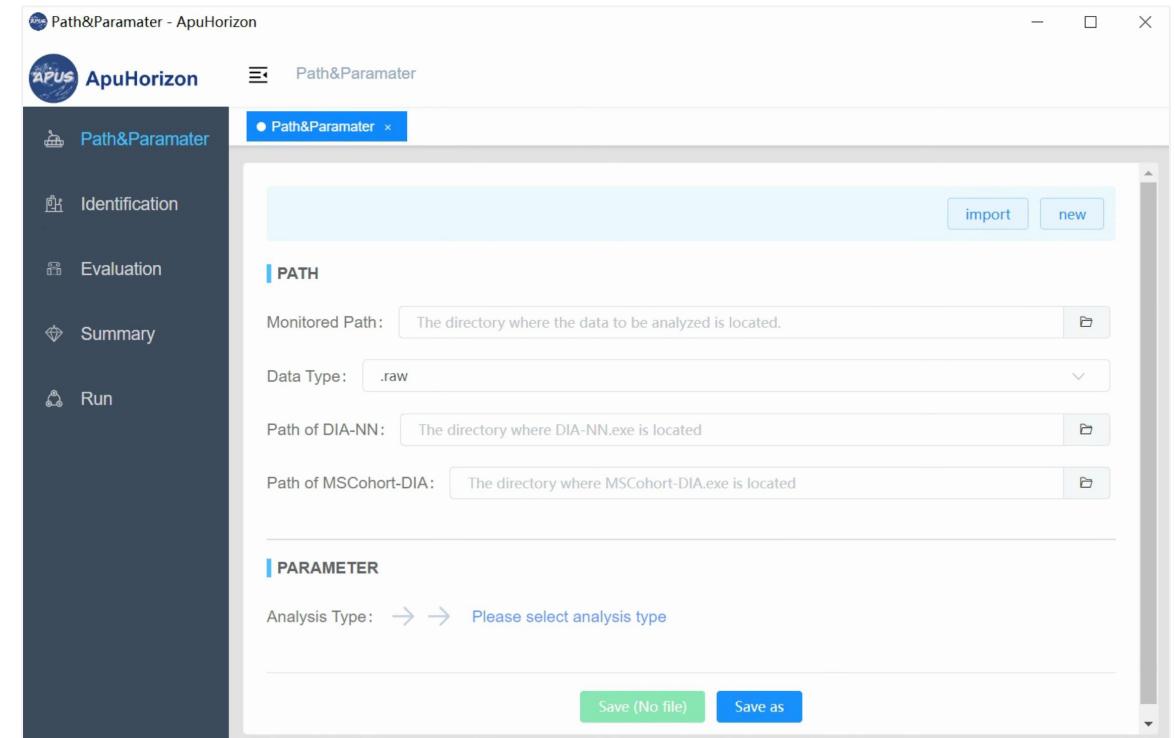
## 1. Fill in **data information**:

- Monitored path: The folder path where your MS data is stored.
- Data type: The format of your data files (e.g., .raw, .d, .wiff).

## 2. Fill in **software paths**:

Enter the installation directory paths for DIA-NN and MSCohort-DIA. This should be the folder containing the main executable file (e.g., MSCohort-DIA.exe).

## 3. Fill in **analysis type**: "quantification only" or "quantification + quality control".



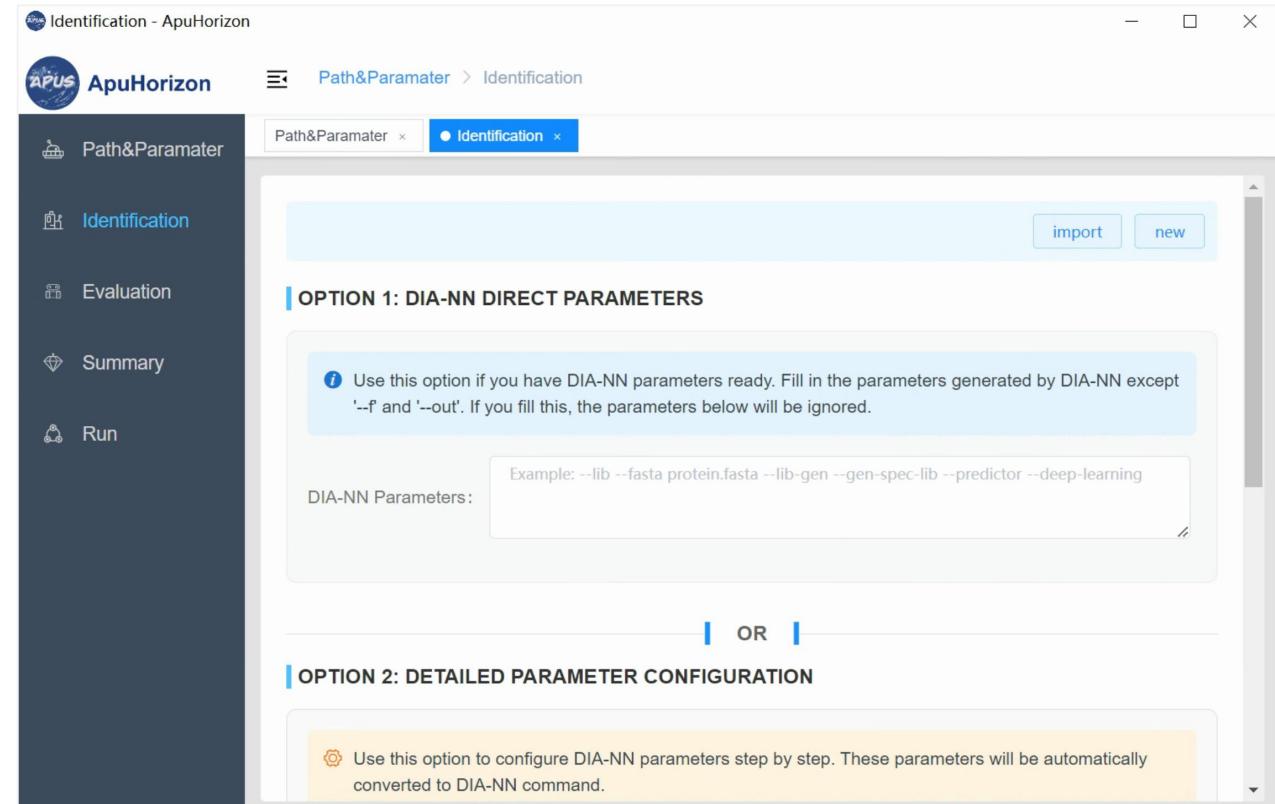
# STEP-4 Quantification

Configure DIA-NN Parameters for DIA quantification.

1. Many parameters are preset with optimized default values. Users only need to specify some essential parameters to run the analysis.
2. Notably, for DIA mode, besides setting common DIA-NN parameters via the GUI, ApuHorizon allows users to input a full command-line argument string.

This string should be generated from the native DIA-NN interface, excluding the `--f` and `--out` arguments.

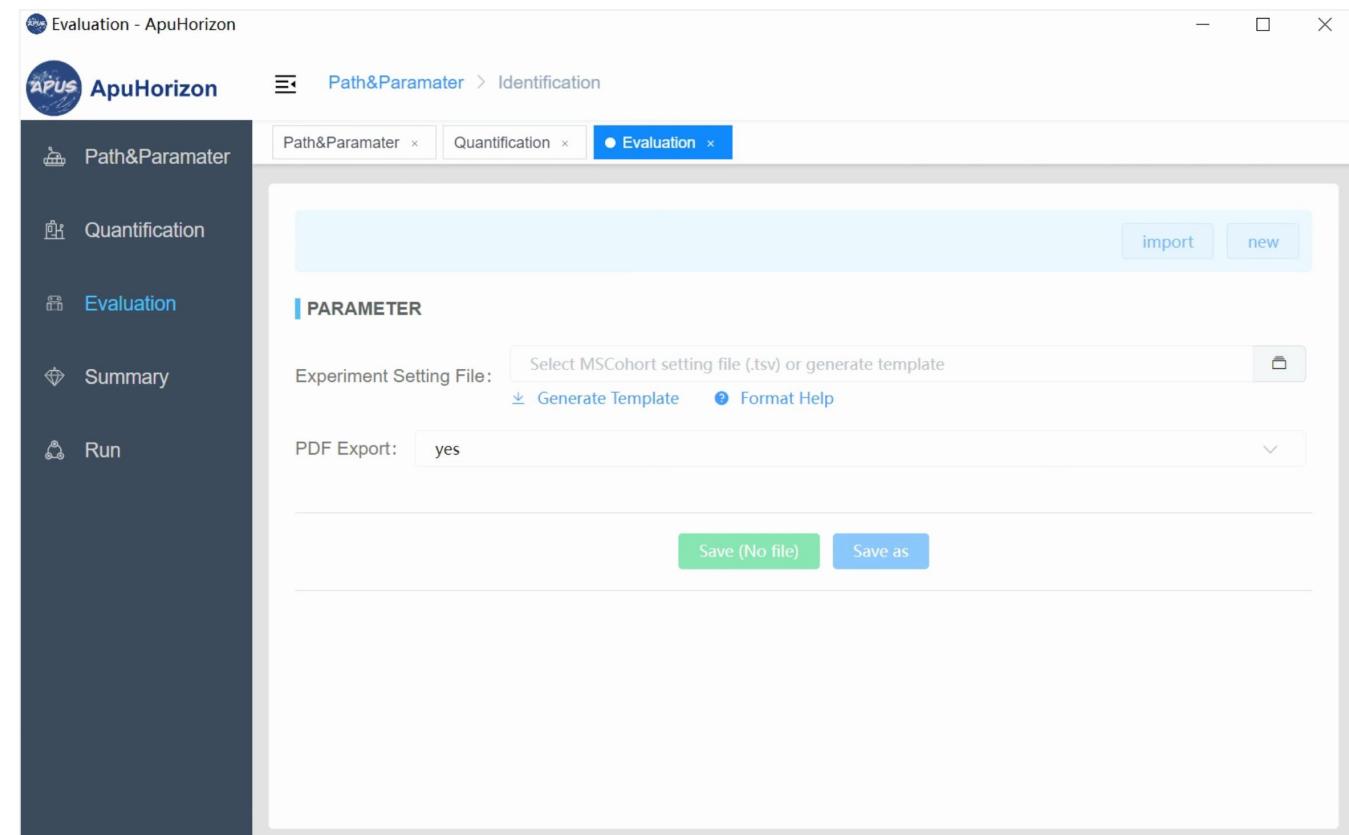
This feature provides fine-grained control over the quantification process.



# STEP-5 Evaluation

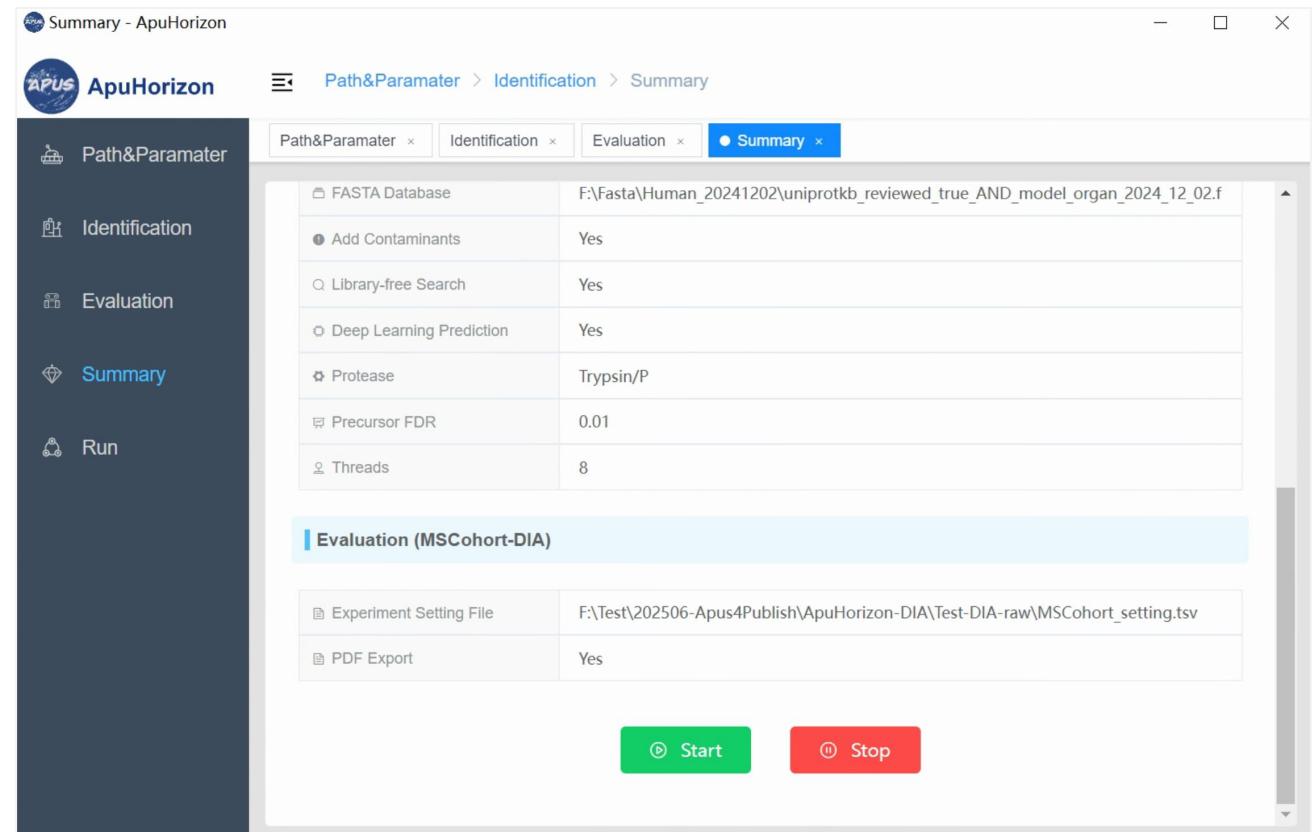
Fill in the following **MSCohort-DIA parameters** for quality control.

More advanced **MSCohort-DIA settings are already set to default**. You can view or edit them in the file: “/ApuHorizon-DIA\_v202507/config/MSCohort-DIA\_cfg.txt”.



# STEP-6 Summary

- Review configuration:** Navigate to the Summary page to review all previously configured parameters.
- Start process:** After verifying that all settings are correct, click the **Start** button to launch the application.



# STEP-7 Run

Go to the Run page to watch the program's progress.

- **STATE:** Shows the current status of the program's loop.
- **OUTPUT:** Here you can see live logs:
  1. Logs from ApuHorizon-DIA.
  2. More detailed logs from the tools it calls (like DIA-NN).

The screenshot shows the ApuHorizon software interface. The main window title is "Run - ApuHorizon". The left sidebar has tabs for "Path&Parameter", "Identification", "Evaluation", "Summary", and "Run". The "Run" tab is selected. The main area has two sections: "STATE" and "OUTPUT". The "STATE" section shows three buttons: "PARSING", "ANALYZING ...", and "WAITING". The "OUTPUT" section shows a log file path: "E:\czk\Work\Project\202309-Apus\Software\ApuHorizon-DIA\_v202507\ApuHorizon-DIA-UI.log". Below this, there is a scrollable text area displaying log entries from line 45 to 58. The log entries include various system messages and file paths related to the DIA-NN analysis.

```
45 2025-08-15 15:09:59 "PATH_MSCOHORT_DDA_EXE": ""
46 2025-08-15 15:09:59 "PATH_MSCOHORT_DDA_CONFIG": ""
47 2025-08-15 15:09:59 "PATH_MSCOHORT_DIA_EXE": "E:\LabSoftware\MSCohort-DIANN_v202504"
48 2025-08-15 15:09:59 "PATH_MSCOHORT_DIA_CONFIG": "E:\czk\Work\Project\202309-Apus\Software\ApuHorizon-DIA_v202507\ApuHorizon-DIA-UI.log"
49 2025-08-15 15:09:59 "PATH_QUEUE_LIST": "Apus_Queue.txt"
50 2025-08-15 15:09:59 "PATH_SUCCESSFUL_LIST": "Apus_Successful.txt"
51 2025-08-15 15:09:59 "PATH_FAILED_LIST": "Apus_Failed.txt"
52 2025-08-15 15:09:59 "TYPE_FLOW": "1"
53 2025-08-15 15:09:59 "TYPE_ANALYSIS": "2"
54 2025-08-15 15:09:59 "TIME_WAIT": "60"
55 2025-08-15 15:09:59 [Apus] [stat] Reading parameters...
56 2025-08-15 15:09:59 [Apus] [stat] Parsing folder...
57 2025-08-15 15:10:00 [Apus] [info] The total number of files need to be analyzed: 3
58 2025-08-15 15:10:01 [Apus] [stat] Data detected, automatic analysis begins!
```

The screenshot shows the ApuHorizon software interface. The main window title is "Run - ApuHorizon". The left sidebar has tabs for "Path&Parameter", "Identification", "Evaluation", "Summary", and "Run". The "Run" tab is selected. The main area has a section titled "Real-time Software Output" with a status indicator "Running". Below this are buttons for "Clear", "Scroll to Bottom", and "Auto Scroll". A scrollable text area displays log entries from 15:10:02 to 15:10:22. The log entries are categorized by tool: DIA-NN and camprotR. The DIA-NN logs mention optimising mass accuracy and generating a library. The camprotR logs show the loading of FASTA files, processing, and assembling elution groups.

```
15:10:02 [INFO] DIA-NN will optimise the mass accuracy automatically using the first run in the experiment. This is useful primarily for quick initial analyses, when it is not yet known which mass accuracy setting works best for a particular acquisition scheme.
WARNING: it is strongly recommended to first generate an in silico-predicted library in a separate pipeline step and then use it to process the raw data, now without activating FASTA digest
15:10:02 [INFO] 3 files will be processed
[0:00] Loading FASTA
F:\Fasta\Human_20241202\uniprotkb_reviewed_true_AND_model_organ_2024_12_02.fasta
15:10:04 [INFO] [0:02] Loading FASTA camprotR_240512_cRAP_20190401_full_tags.fasta
15:10:05 [INFO] [0:02] Processing FASTA
15:10:10 [INFO] [0:07] Assembling elution groups
15:10:14 [INFO] [0:11] 4302395 precursors generated
15:10:14 [INFO] [0:11] Gene names missing for some isoforms
15:10:14 [INFO] [0:11] Library contains 20522 proteins, and 20284 genes
15:10:16 [INFO] [0:13] Encoding peptides for spectra and RTs prediction
15:10:22 [INFO] [0:20] Predicting spectra and IMs
```

# STEP-8 View analysis results

- Navigate to "Monitored Path" and view the data analysis results in the folder named **ApuHorizon-DIA+[Timestamp]**.



# ATTENTIONS

---

1. Always click **Save** or **Save As** before leaving a page. If you don't, your changes will be lost.
2. ApuHorizon automatically locates the analysis results from ApuPioneer. **Do not manually rename the identification result folder, as this will prevent the analysis from running correctly.**

# ApuMonitor

# INTRODUCTION

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### Version: ApuMonitor\_v202511

### Release Date: 2025.11.15

### OS: Windows 10 (x64) or Windows 11 (x64)

# INTRODUCTION

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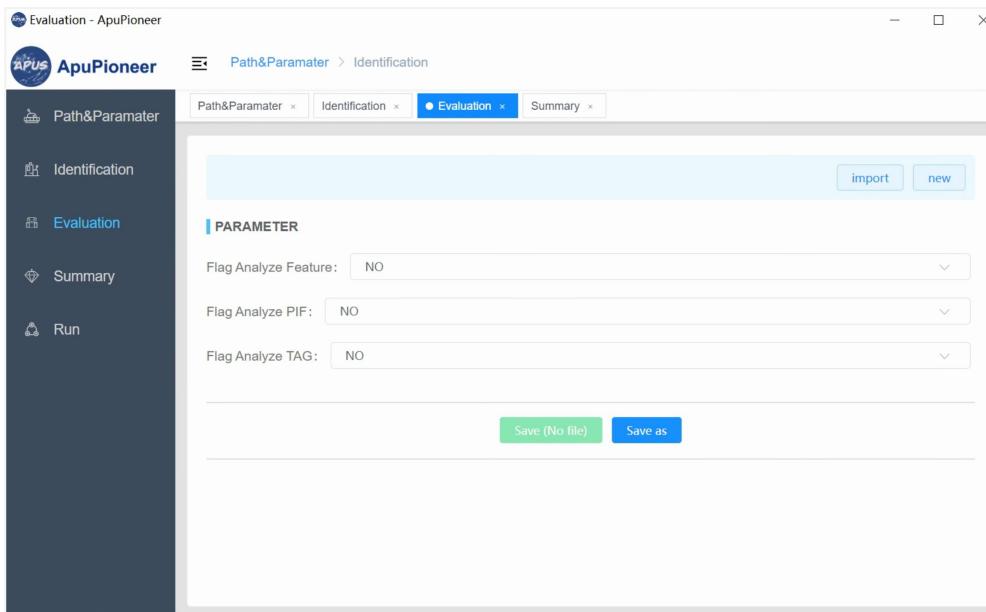
**ApuMonitor** is the integrated quality control system of Apus. It operates automatically in the background to assess the quality and stability of your proteomics experiments in real time.

## Key Features:

- **Intra-experiment QC:** Generates a detailed QC report for each individual sample run right after protein identification is complete.
- **Inter-experiment QC:** Produces a cohort-level QC report after quantification, allowing you to assess the consistency across all samples in your study.
- **Real-Time Monitoring and Early Warning:** Stay in control of your experiment with a web-based dashboard that visualizes key performance metrics in real time. Building on this live monitoring, an early-warning system automatically dispatches email alerts if any metric violates a user-defined threshold or if an instrument becomes inactive, allowing you to intervene immediately and prevent data loss.

# Function-1: Intra-experiment QC

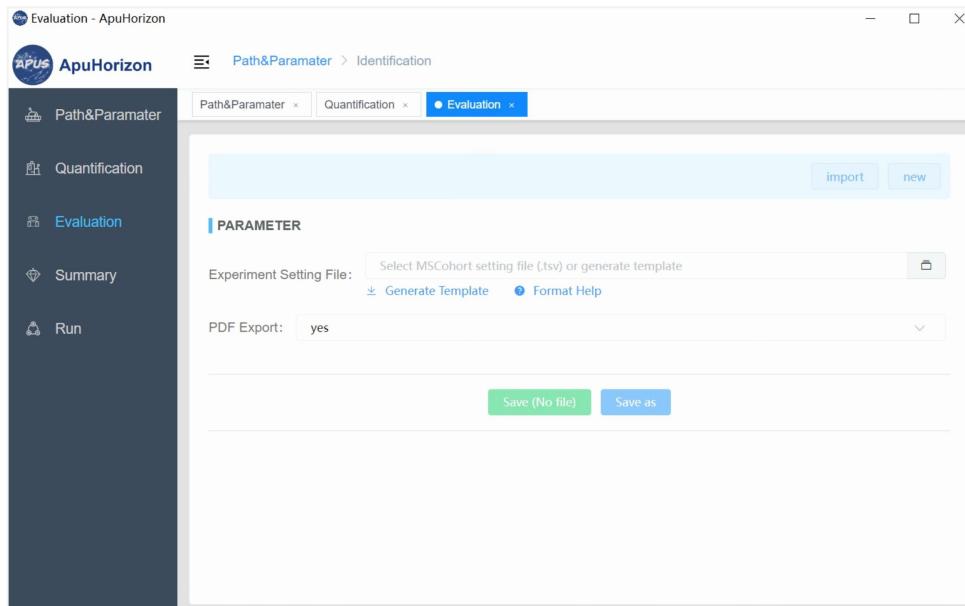
- When performing identification analysis with ApuPioneer, users can select the "database search + QC" mode and configure its parameters on the **Evaluation** interface.
- The system will then automatically perform intra-experiment QC for each dataset upon the completion of database searching. **This process tracks QC metrics throughout data aggregation and identification**, ultimately generating a QC report for each individual sample.
- View the result file “Analysis\_Report.html” under this path: “\results\MSRefineResult”



picture	2025/4/2 22:28
Analysis_Report.html	2025/4/2 22:28
INFO_Chromatography.txt	2025/4/2 22:28
INFO_Cycle_MS1.txt	2025/4/2 22:27
INFO_Cycle_MS2.txt	2025/4/2 22:27
INFO_Feature.txt	2025/4/2 22:25
INFO_ID.txt	2025/4/2 22:28
INFO_Mass_Deviation.txt	2025/4/2 22:25
INFO_MS1.txt	2025/4/2 22:27
INFO_MS1_PEAKS.txt	2025/4/2 22:27
INFO_MS2.txt	2025/4/2 22:27
INFO_MS2_PEAKS.txt	2025/4/2 22:27
INFO_peptides.txt	2025/4/2 22:28
INFO_Scans.txt	2025/4/2 22:28
INFO_Summary.txt	2025/4/2 22:28

# Function-2: Inter-experiment QC

- When performing quantification analysis with ApuHorizon, users can select the "quantification + QC" mode and configure parameters on the Evaluation interface.
- After ApuHorizon completes quantification for the entire cohort, ApuMonitor automatically extracts 23 inter-experiment QC metrics, evaluates the quality of the entire cohort, and generates a cross-experiment QC report.
- View the result file “Cohort Analysis Report.html” under this path: “\results\MS Cohort Result”



iRT_Visual	2025/4/9 12:05
model_train	2025/4/9 12:05
picture	2025/4/9 12:05
tmp_file	2025/4/9 12:06
txt	2025/4/12 18:07
Cohort Analysis Report.html	2025/4/9 12:05
Cohort Analysis Report.pdf	2025/4/9 12:06

## Function-3: Real-Time Monitoring and Early Warning

---

To enable proactive quality management, ApuMonitor features a visualization dashboard and an automated early-warning system.

- **Real-Time Monitoring:** The dashboard, accessible from any web-enabled device, allows researchers to monitor a set of key QC metrics that reflect the LC-MS/MS instrument status and identification depth in real time.
- **Early Warning:** The early-warning system allows researchers to set custom thresholds for QC metrics of particular interest. If any metric violates its user-defined threshold, or if the system detects prolonged instrument inactivity, ApuMonitor automatically dispatches an email alert to designated addresses, prompting timely intervention on potential issues.

The following section outlines the procedure for using ApuMonitor to achieve proactive quality management.

# STEP-1 Preparation

---

**Important Note:** Due to differences in key quality control metrics, ApuMonitor provides separate software packages and MySQL database files for DDA and DIA analyses. Please ensure you download and use the version that matches your experiment type. **This guide will use the ApuMonitor-DIA workflow as an example.**

## 1. Deploy Software:

- ApuMonitor should be deployed on a dedicated monitoring computer.
- Download the ApuMonitor-DIA package from <https://github.com/BUAA-LiuLab/Apus>.

## 2. Mount storage:

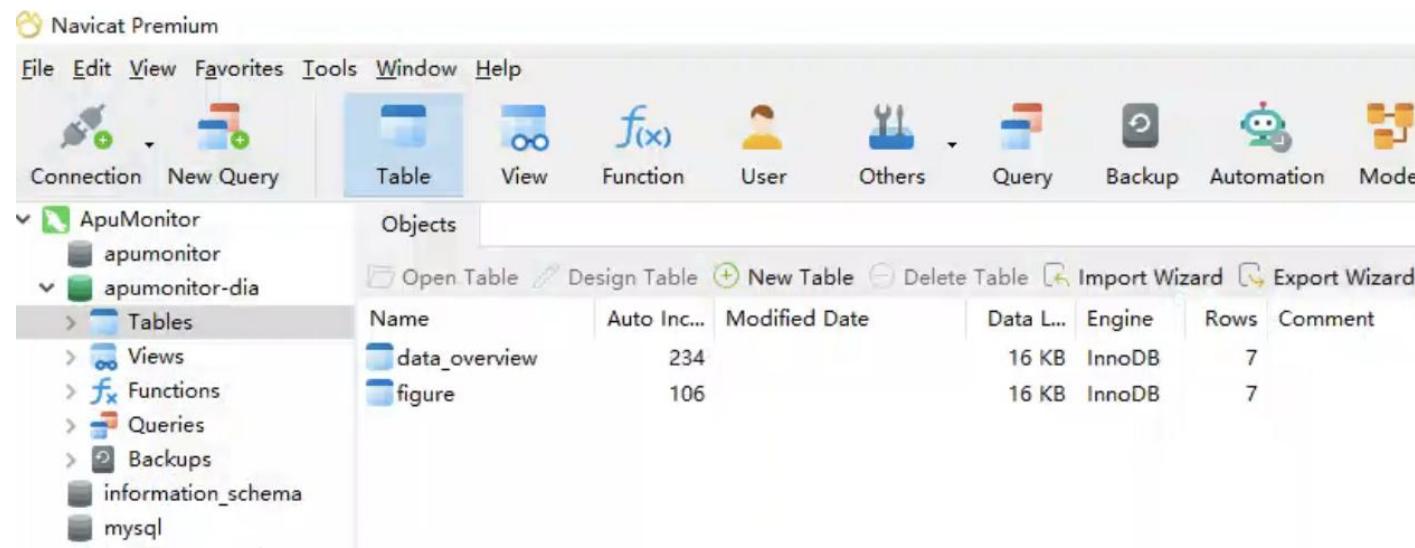
- Use the **SMB** protocol to mount your data storage system to the local filesystem of the compute nodes, so it can be accessed like a local disk.

## 3. MySQL Database:

- Install **MySQL** on a computer that is on the same network as the data storage system.
- Install a **graphical database management tool**, such as **Navicat**.

# STEP-2 MySQL Configuration

1. **New Connection:** In your MySQL tool, create a new server connection.
2. **New Database:** Within the connection, create a new database with the following properties:
  - Name: apumonitor-dia
  - Character Set: utf8mb3
  - Collation: utf8mb3\_general\_ci
3. **Import Schema:** Right-click the apumonitor database and execute the “apumonitor-dia.sql” file located in your ApuMonitor-DIA folder.
4. **Verify:** After importing, confirm that the data\_overview and figure tables are present in the apumonitor database.



# STEP-3 Dashboard Configuration

## 1. Install FineReport and Import Template:

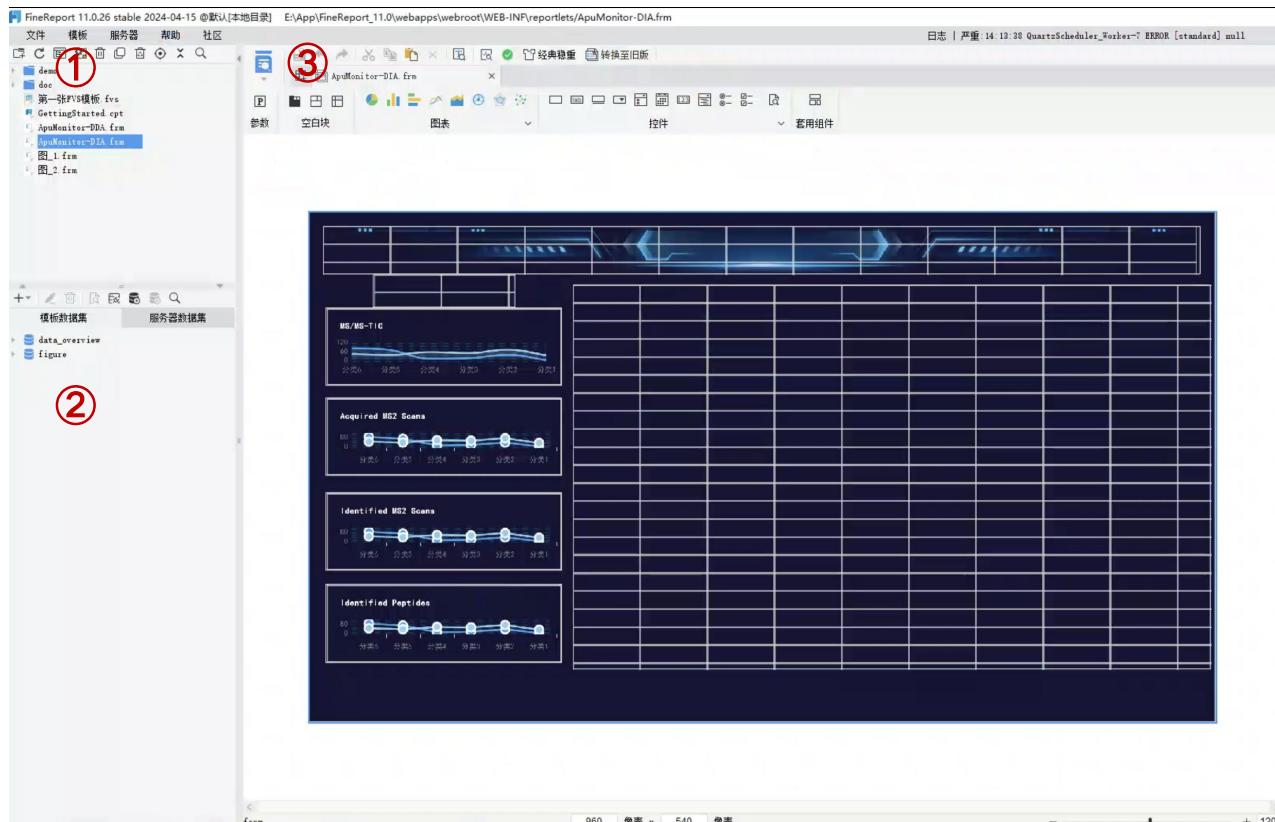
- Download the FineReport reporting tool (v11.0 is recommended).
- Create a new project and import the “ApuMonitor-DIA.frm” template.

## 2. Connect to Database:

- Within FineReport, establish a data connection to the MySQL database you configured previously.

## 3. Launch Dashboard:

- Open the report. It will be rendered as a web report in your default browser.



# STEP-4 ApuMonitor Basic Configuration

## 1. Launch the Application:

- Navigate to the ApuMonitor-DIA\_v202511 directory.
- Double-click ApuMonitor-DIA\_UI.exe to start the application.

## 2. Fill in **Basic Configuration**:

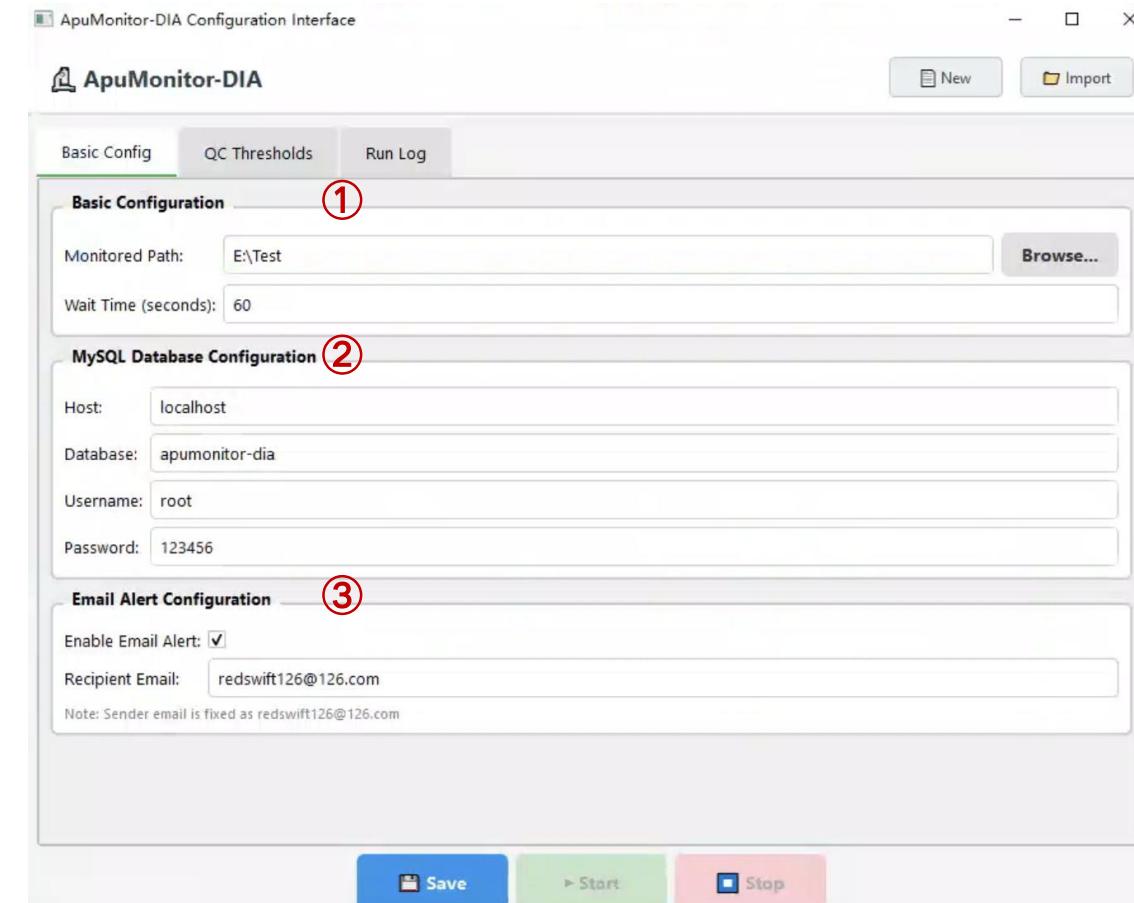
- Monitored path: Where MS data is stored.
- Wait time: The pause time between cycles of checking for new files.

## 3. Fill in **MySQL Database Configuration**:

- Including Host, database name, username, and password.

## 4. Fill in **Email Alert Configuration**:

- To enable the alert feature and receive emails, please check the box and enter your email address.



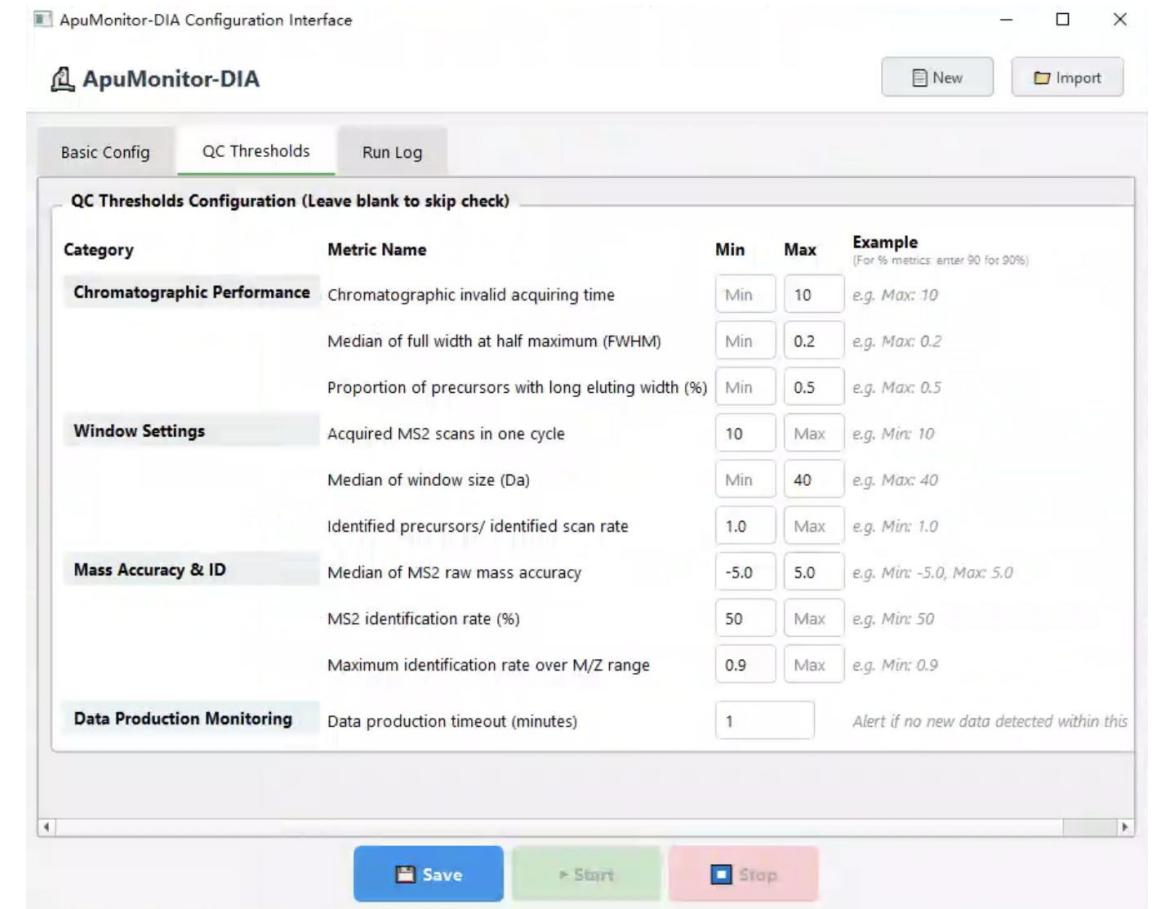
# STEP-5 QC Thresholds Configuration (Optional)

## 1. Set Metric Thresholds:

- Define a maximum or minimum value for any QC metric of interest.
- ApuMonitor will send an email alert if a metric from a new run exceeds its defined threshold.

## 2. Set Instrument Inactivity Timeout:

- Specify a time limit (e.g., in hours).
- ApuMonitor will send an email alert if the time interval between newly acquired data files exceeds this limit.

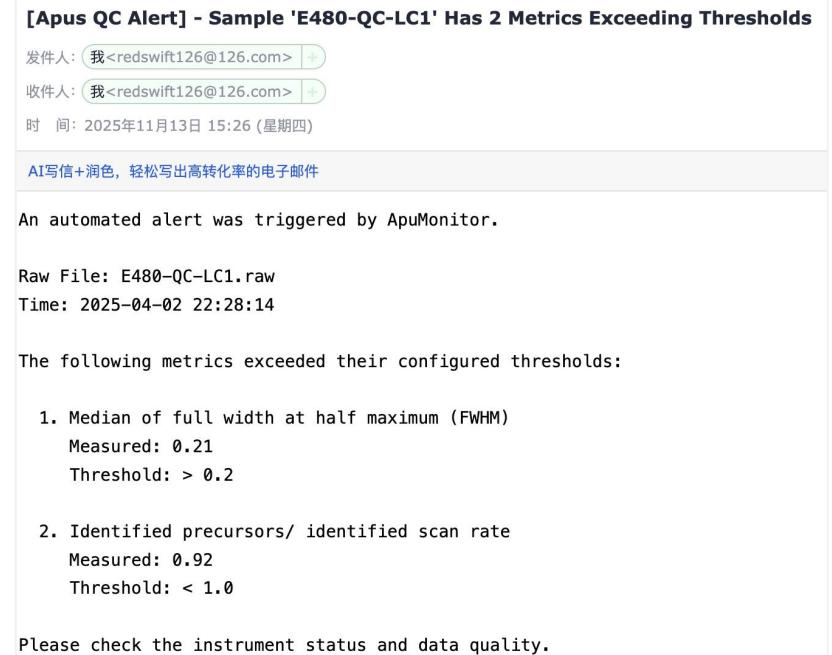
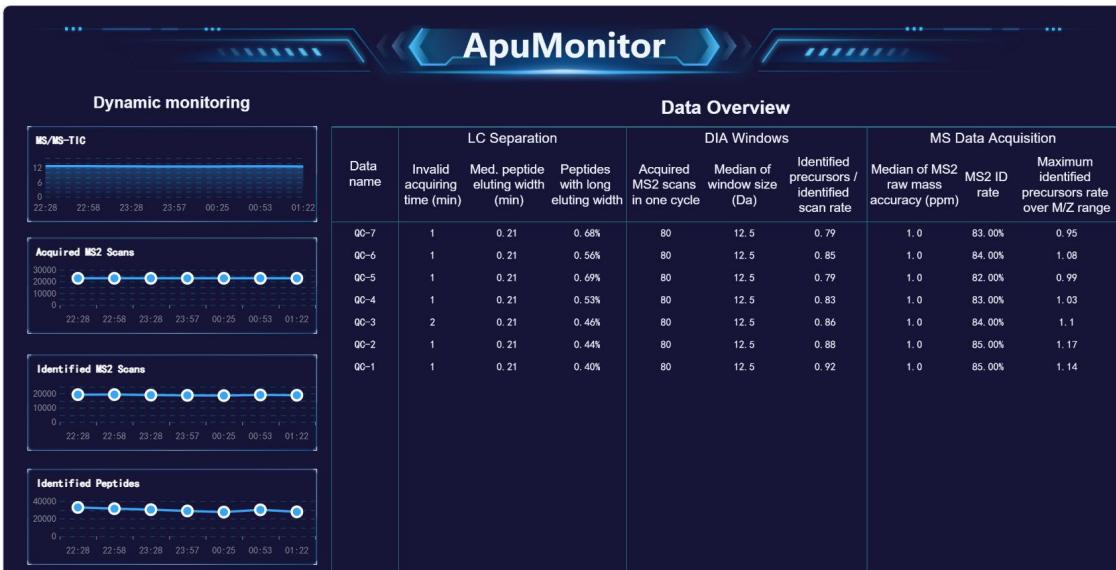


# STEP-6 Run

- Save Parameters:** Click the “Save” button to store your configuration.
- Start the Process:** Click the “Start” button to launch the ApuMonitor background service.

Once ApuMonitor is running, it will perform the following actions automatically:

- Database Sync:** New QC metrics are continuously uploaded to the MySQL database.
- Live Dashboard:** The web dashboard auto-refreshes every 10 minutes to display the latest data.
- Email Alerts:** You will receive an immediate email alert if any QC threshold is violated or if the instrument is inactive.



**ApulInsight**

# INTRODUCTION

### Version: ApulInsight\_v202507

### Release Date: 2025.07.15

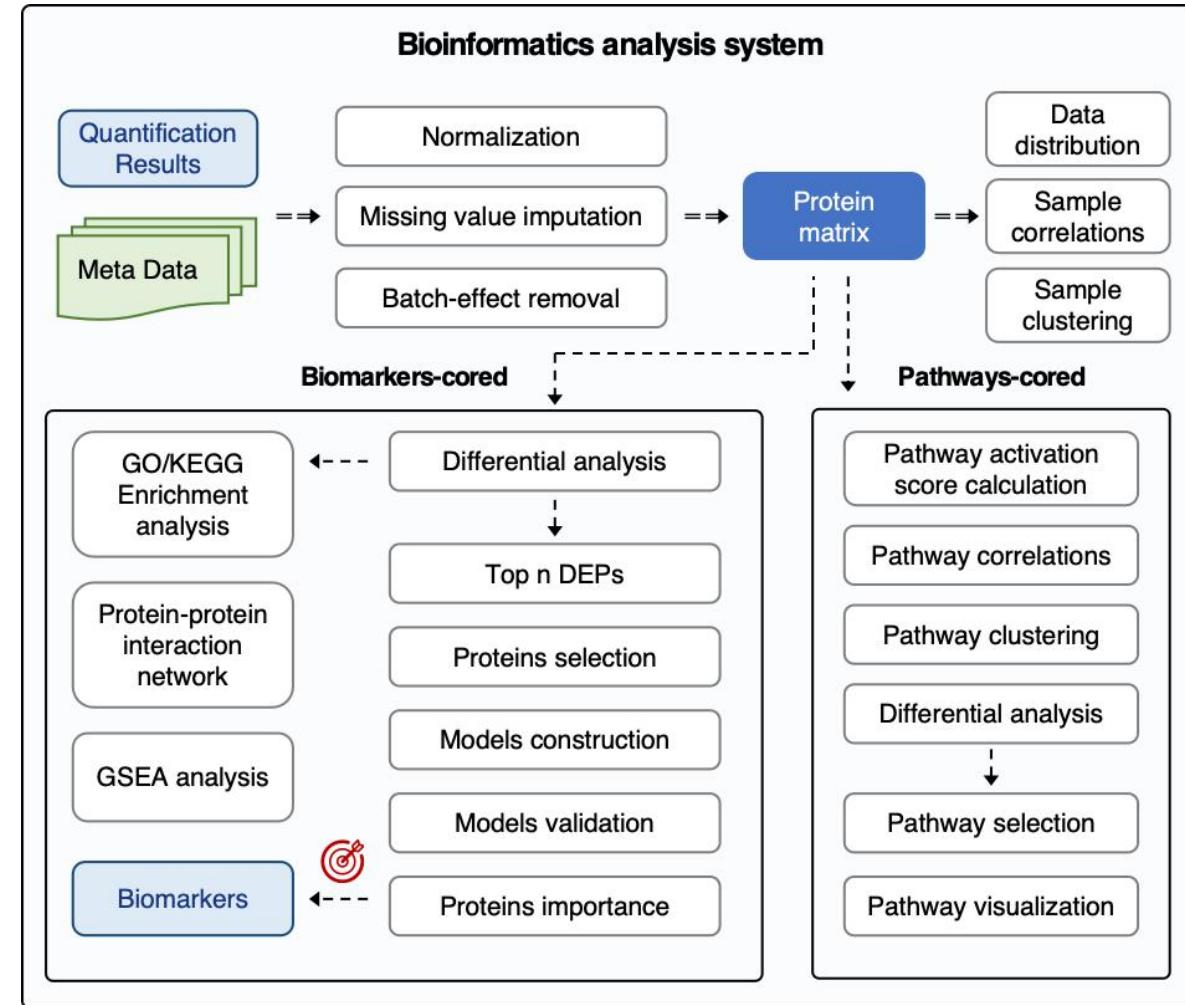
### OS: Windows 10 (x64) or Windows 11 (x64)

**ApulInsight** is an automated bioinformatics workflow for large-cohort proteomics analysis. Users only need to provide a metadata file based on the protein quantification file. Subsequently, the automated analysis process can be initiated.

We developed two workflows to meet the needs of large-cohort proteomics analysis.

(1) Biomarker-cored workflow

(2) Pathway-cored workflow



# STEP-1 Install

---

1. Download the installation package of Apulnsight from [\*https://github.com/BUAA-LiuLab/Apus\*](https://github.com/BUAA-LiuLab/Apus).
2. Enter the “Apulnsight\_v202507” directory
3. Click on “**install.exe**” to install, and after completion, a folder named “**proteomicAnalysis**” will be generated, containing all contents such as scripts, dependency packages, configuration files, etc.

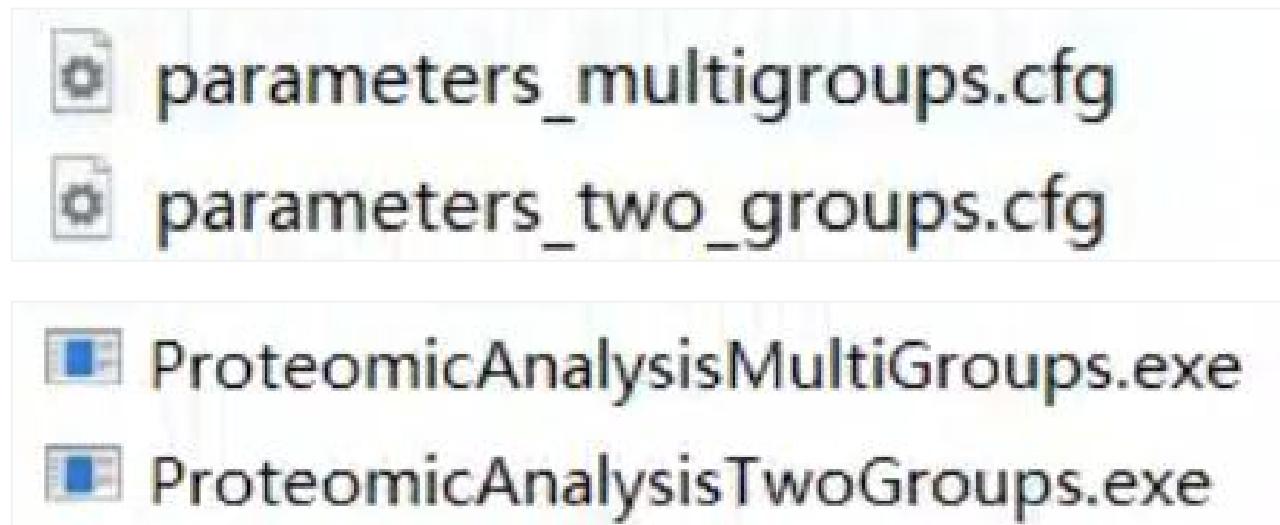
# STEP-2 Fill in the configuration file

---

**Configuration files and their corresponding exe programs are categorized into two types:**

1. Two groups analysis: The configuration file is "parameters\_two\_groups.cfg", and the program is "ProteomicAnalysisMultiGroups.exe"
2. Multiple group analysis: The configuration file is "parameters\_multigroups.cfg", and the program is "ProteomicAnalysisTwoGroups.exe"

According to the specific analysis task, fill in the configuration file (see the file "ApuInsight-Parameter Description.docx" for detailed parameter explanations)



# STEP-3 Fill in meta information

1. The filename must be exactly "metadata.xlsx".
2. The file must contain four columns: **Sample**, **Condition**, **Batch**, and **PairedID**, corresponding to sample names, group labels, batch information, and pairing information, respectively.
  - The Condition value should be an abbreviation derived from the Sample name (e.g., for Sample "CTRL1" / "MSA1", the Condition would be "CTRL" / "MSA").
3. If batch information is available, fill it in the Batch column; otherwise, leave it blank.
4. For paired differential analysis, provide IDs in the PairedID column. The format should be the Condition value followed by a number (e.g., "CTRL\_1", "MSA\_1"). Paired samples must share the same numeric suffix. If this analysis is not needed, leave the column blank.
5. Avoid using special characters such as hyphens (-) in the file to prevent potential errors.
- The image on the right is a simple example.

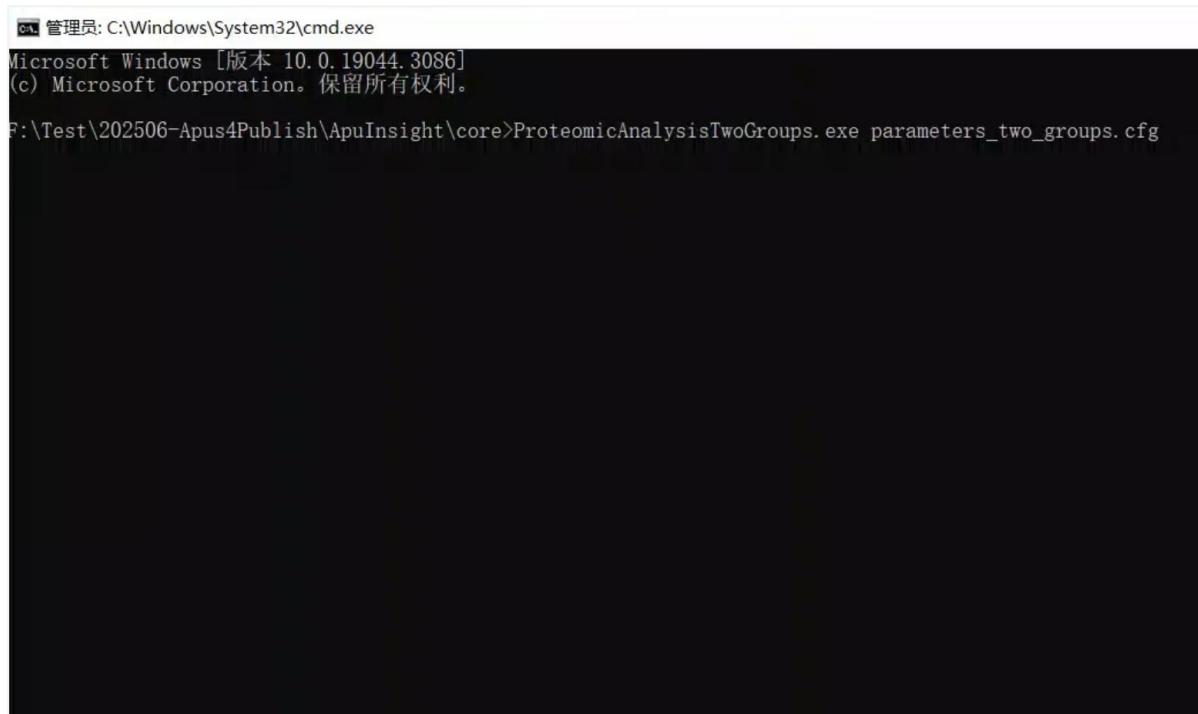
	A	B	C	D
1	Sample	Condition	Batch	PairedID
2	NAT_1	NAT		
3	NAT_2	NAT		
4	NAT_3	NAT		
5	NAT_4	NAT		
6	NAT_5	NAT		
7	T_1	T		
8	T_2	T		
9	T_3	T		
10	T_4	T		
11	T_5	T		

# STEP-4 Run

After filling in the parameter configuration file and metadata.xlsx, run the program exe in cmd, followed by the corresponding cfg file name.

Example: **ProteomicAnalysisTwoGroups.exe parameters\_two\_groups.comg**

After waiting for the completion of the run, view the analysis results in the custom result output directory.



```
管理员: C:\Windows\System32\cmd.exe
Microsoft Windows [版本 10.0.19044.3086]
(c) Microsoft Corporation。保留所有权利。
F:\Test\202506-Apus4Publish\ApuInsight\core>ProteomicAnalysisTwoGroups.exe parameters_two_groups.cfg
```

 data_overview	2025/4/7 23:11
 data_preprocessing	2025/4/7 23:11
 differential_expression_analysis	2025/4/7 23:11
 functional_analysis	2025/4/7 23:15
 log	2025/4/7 23:11
 pathway_activity_analysis	2025/4/7 23:16
 pathway_activity_analysis_2025-04-07...	2025/4/7 23:16
 proteomics_analysis_2025-04-07_23...	2025/4/7 23:15