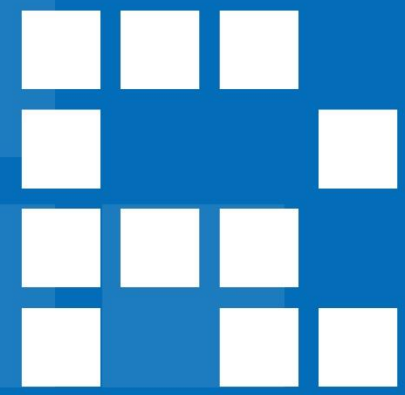


Rubikstation

USER MANUAL

Rubikstation

s t a t e m e n t

This manual is for the user to understand, use and maintain the standard data demonstration of the Rubikstation, rather than its own business and special purpose manuals.

The contents of this manual are subject to change without notice.

When this manual was published, it was considered accurate and complete after careful review. It is not responsible for possible errors and accidental or recurring injuries of the manual that cause concern.

In any case, it is not responsible for the use of this manual and equipment.

Contents

1 Rubikstation Introduce

Rubikstation is a self-developed network version chromatographic data workstation software for LC systems.

Users can remotely set and adjust the parameters of the liquid chromatography instrument to ensure the accuracy of the experiment. The software can automatically collect data generated during the experimental process, reduce human errors, and improve data accuracy. Rubikstation is equipped with powerful analytical tools to help users delve deeper into data and extract valuable scientific information. Users can quickly generate evaluation reports based on experimental results, providing support for research or production decisions.

The design of Rubikstation aims to simplify the chromatographic analysis process, improve work efficiency, and ensure the quality and reliability of data analysis. Through this software, researchers and industrial users can focus more on the experiment itself rather than the tedious operation process.

1.1 Features of Rubikstation

- Flexible Scalability: Rubikstation supports control over a large number of chromatographic instruments, using a standard browser/server (B/S) architecture to ensure system scalability and compatibility.
- Data interoperability: Rubikstation supports sharing, viewing, utilizing, and processing data, methods, and system resources among multiple users, while adhering to permission management, improving data flow and collaboration efficiency.
- Security Support: The system has powerful management functions that can meet the security requirements of different workflows.
- Audit Tracking: The system is capable of recording and saving detailed user operation information, including method applications, data operations, and system usage, to create and manage a complete audit tracking history.

- Flexible Report templates: Rubikstation allows users to customize report templates based on specific needs, supporting multiple project combinations to adapt to different reporting needs.
- Data Security: All data is stored in the server's database, ensuring the security and integrity of the data. At the same time, the system supports multiple data backup methods, including full backup, incremental backup, automatic backup, and manual backup, to meet the data protection needs in different scenarios.

2 Software Overview

This chapter provides a detailed introduction to the characteristics and components of Rubikstation. Currently applicable to:

- ◆ EClassical 3200L series liquid chromatography system;

2.1 Configuration Requirements

The system configuration and software and hardware requirements for the Rubikstation chromatographic data workstation are shown in the table below:

		Minimum Configuration	Recommended Configuration
windows	**Client**	**CPU:** i5-10500 / Ryzen 5 5500 **Graphic Card:** GTX 1060 **RAM：** 16GB **Operating System：** Windows 10 **Monitor：** 1920*1080 **Browser：** Edge 126.0.2592.68/ Chrome 123.0.6312.59	**CPU:** i5-12600 / Ryzen 5 7500 **Graphic Card:** GTX 1660S **RAM：** 32GB **Operating System：** Windows 11 **Monitor：** 2560*1440 **Browser：** Edge 126.0.2592.68/ Chrome 123.0.6312.59
	Server	**CPU:** Intel ® xeon ® E-2336 processor **RAM:** 16GB **Hard Disk:** 1T **Operating System：** windows server2022	**CPU:** Intel ® xeon ® E-2468 processor **RAM:** 32GB **Hard Disk:** 2T or above **Operating System：** windows server2022

Note: Please refer to the client requirements for the standalone version

2.2 Workstation Introduction

2.2.1 Workstation Deployment

The deployment of Rubikstation Network Edition Chromatographic Data Workstation shall be uniformly installed and deployed by the installation engineer for the customer in accordance with the 《Rubikstation Network Edition Chromatographic Data Workstation Deployment Guide》. Only after confirming the correct deployment can it be handed over to the customer for use.

Note: (1) Any abnormal phenomena that occur during the deployment process cannot be handed over to users for use.

(2) After the workstation is deployed correctly, it is necessary to inform the user of the workstation login address and make corresponding records.

2.2.2 User Login

After deploying the workstation environment, open the browser, access the workstation address, and enter the login page, as shown in Figure 2-1. The newly deployed workstation comes with a "superAdmin" user account and default password. After entering, log in to the workstation and set the user's account, password, and other information. Before delivering the workstation, the engineer needs to ensure that the management personnel modify the account password or delete the account before the delivery can be completed.

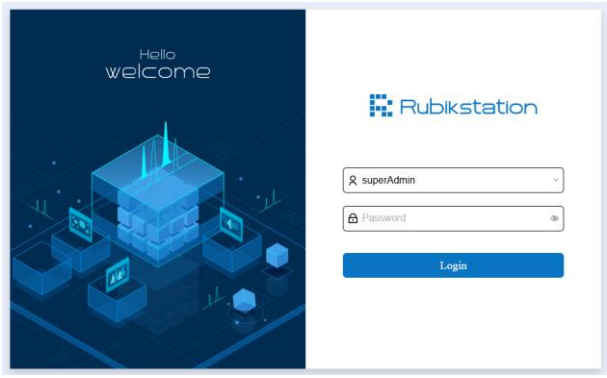


Figure 2-1 Login Page

2.2.3 User Management

After logging in, click on "User Management" on the dashboard to enter the user management page. On this page, users can be added, user information and permissions can be edited, user information can be viewed, and users can be deleted. As shown in Figure 2-2.

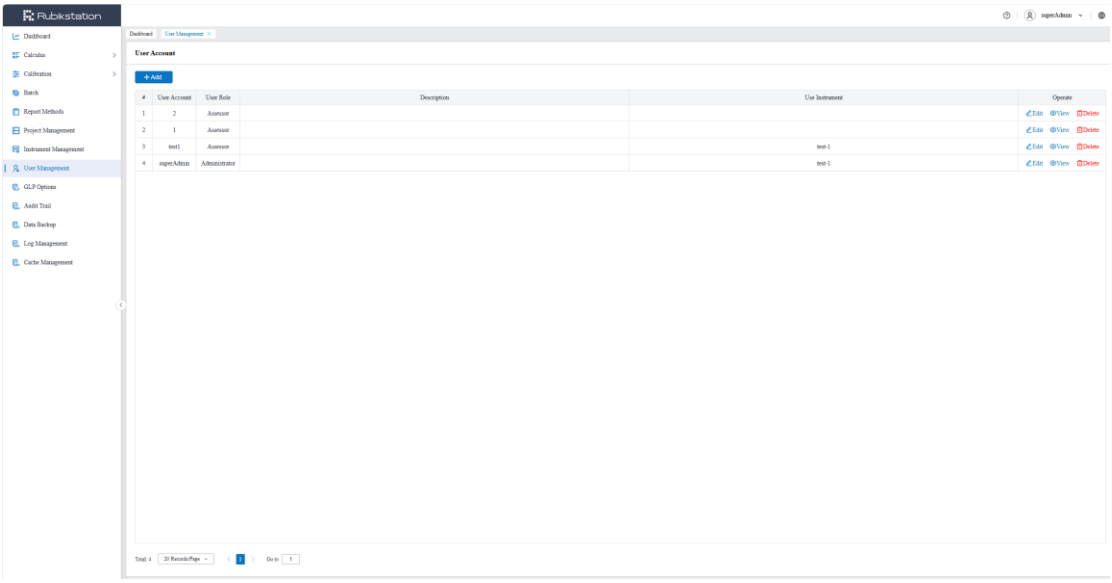


Figure 2-2 User Management

Click the "Edit" button to enter the "User Details" page, where you can set all permissions and other information for the user, as shown in Figure 2-3.

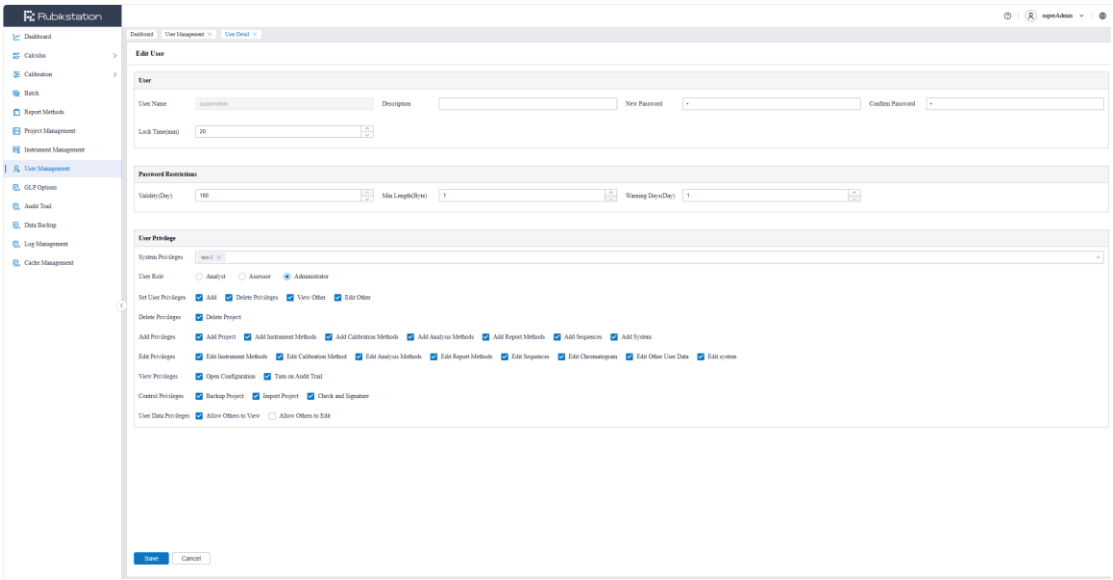


Figure 2-3 User Details

Users can edit user information in this module.

Password restrictions can impose certain restrictions on passwords.

"User permissions": Set usage permissions for users.

When creating new user roles using administrative permissions, access to software features can be set based on the roles.

2.2.4 Instrument Management

Click the "Instrument Management" button on the left side of the main page to enter the instrument configuration page, as shown in Figure 2-4. Click "New" to create a new instrument configuration module. The instrument module configured here can be directly called in subsequent use without the need for further configuration. Click "Edit" to edit the configuration and parameter information of existing instrument modules, such as adding instruments, filling in module names, entering instrument IP, Edge end IP, and other information, and then verifying the connection.

Click "Delete" to delete the current instrument module. It should be noted that if this module is in use, it cannot be deleted.

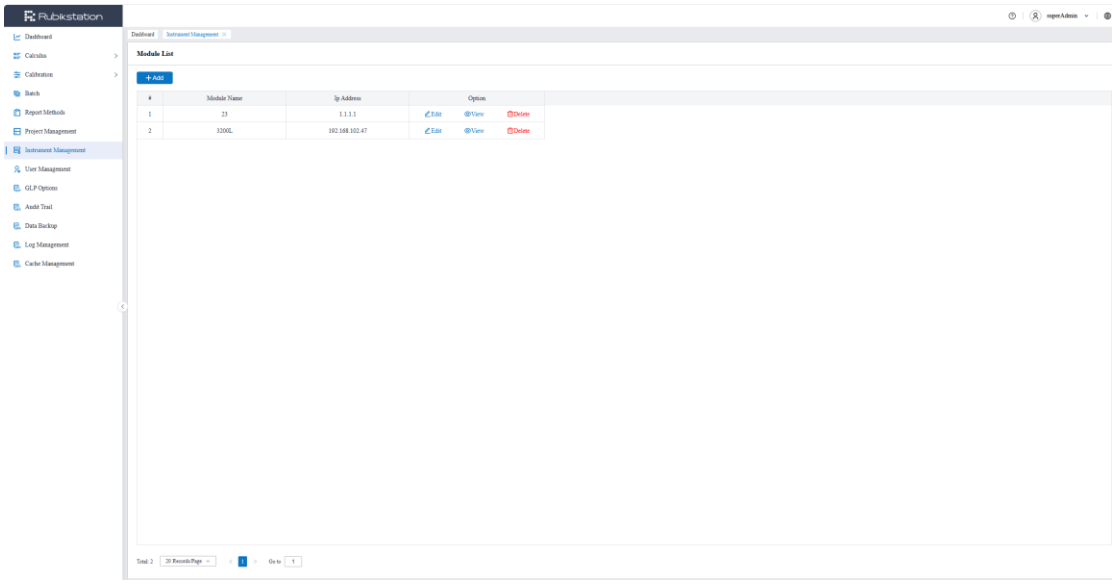


Figure 2-4 Instrument Management

Click "Edit" to modify the instrument parameters configured in the instrument module, and perform instrument connection verification, instrument configuration modification, etc.

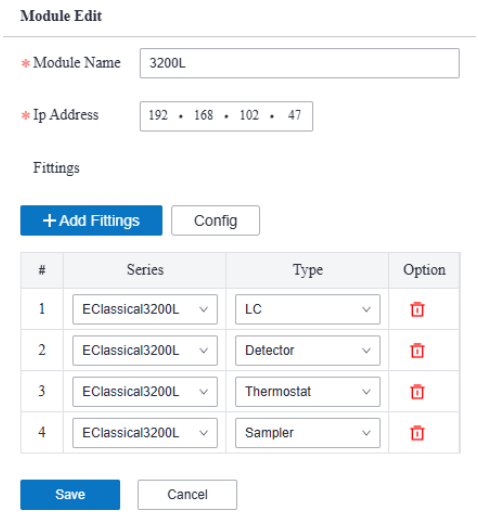


Figure 2-5 Instrument Editing

Click the "Configuration" button on the instrument editing page to edit the specific model, IP, and verification instrument connection of the configured instrument.

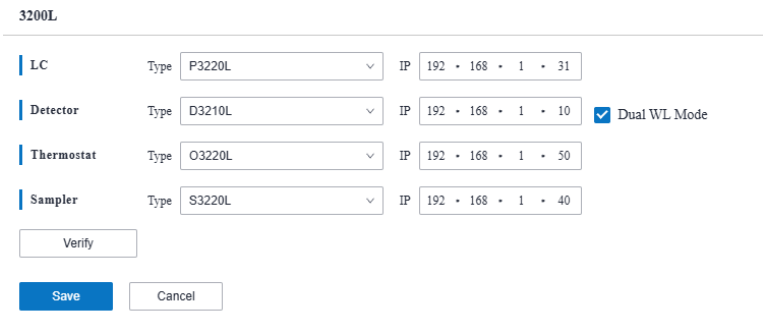


Figure 2-6 Instrument Configuration

Note: The configuration mode of other modules is the same.

2.2.5 Engineering Management

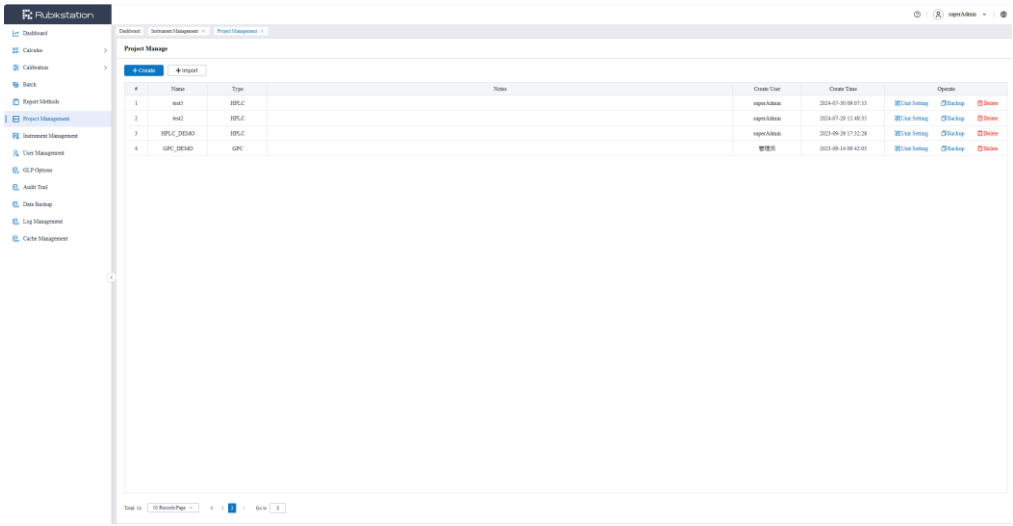


Figure 2-7 Engineering Management

Click "Engineering Management" to enter the engineering management page, which allows you to create, import, backup, delete projects, and modify the unit of the project. The page displays the project type, creator, and creation time, as shown in Figure 2-7.

- **New Project**

Click "Create" to create a new project. On the new project page, edit the project name, select the project type, add explanatory information (optional), and then click "OK" to save. Then you can see the newly created project on the "Engineering Management" page.

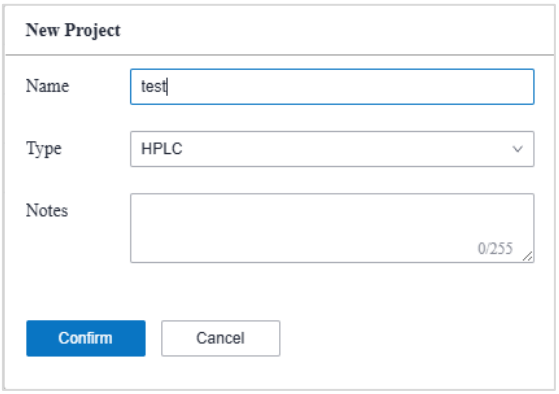


Figure 2-8 New Project

- **Import Project**

Click the "Import" button, select the path where the project is located in the pop-up window, select the project to be imported, then click "Open" and wait for the project to be imported.

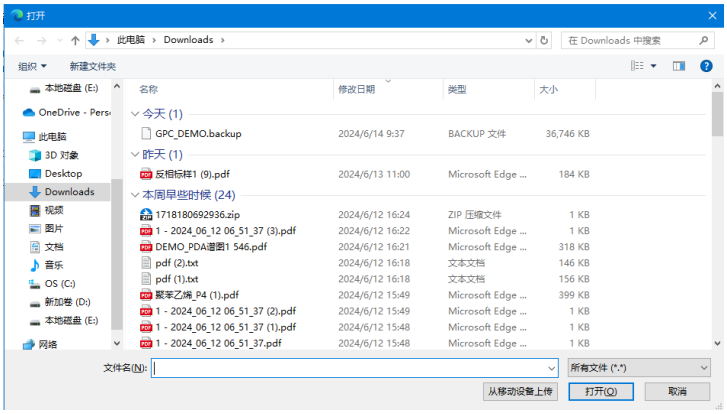


Figure 2-9 Selecting the Import Project

- **Unit Setting**

Click "Unit Setting" to set the basic unit, signal unit, coordinate axis unit, and other units of the current selected system.

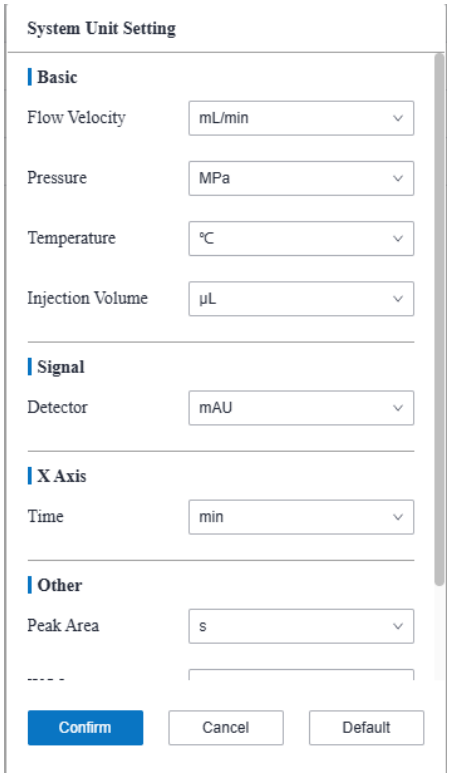


Figure 2-10 Unit Setting

2.2.6 GLP Options

Click on "GLP Options", and the user can select the desired option on the "GLP Options" page and click the "OK" button, as shown in 2-14.

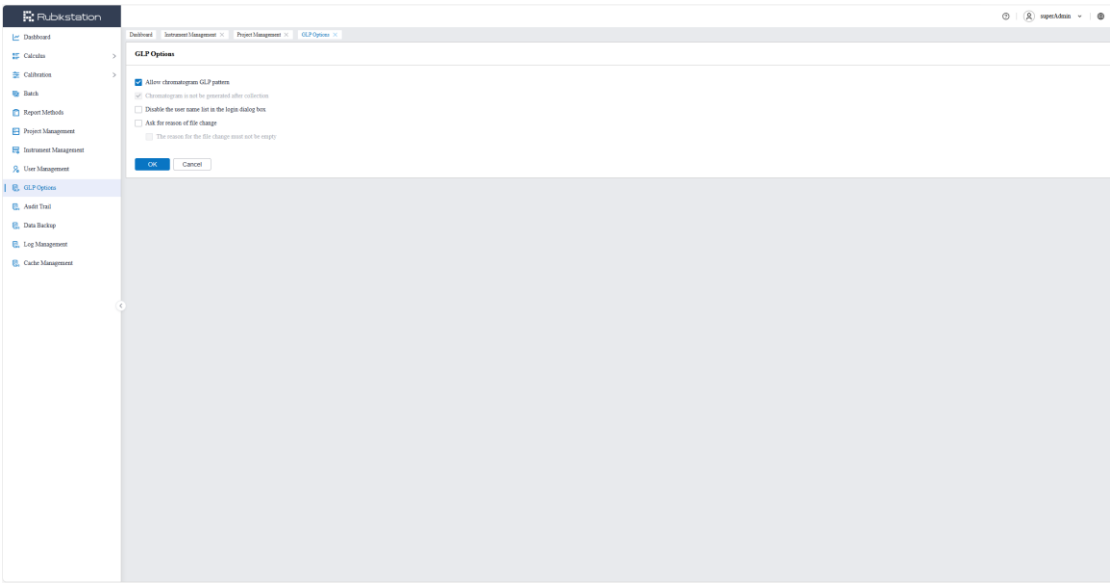


Figure 2-11 GLP Options

2.2.7 Audit Trail

Click "Audit Trail", and the audit trail page will be displayed on the right. Users can filter and view all operations on the workstation as needed, and export the results, as shown in Figure 2-12.

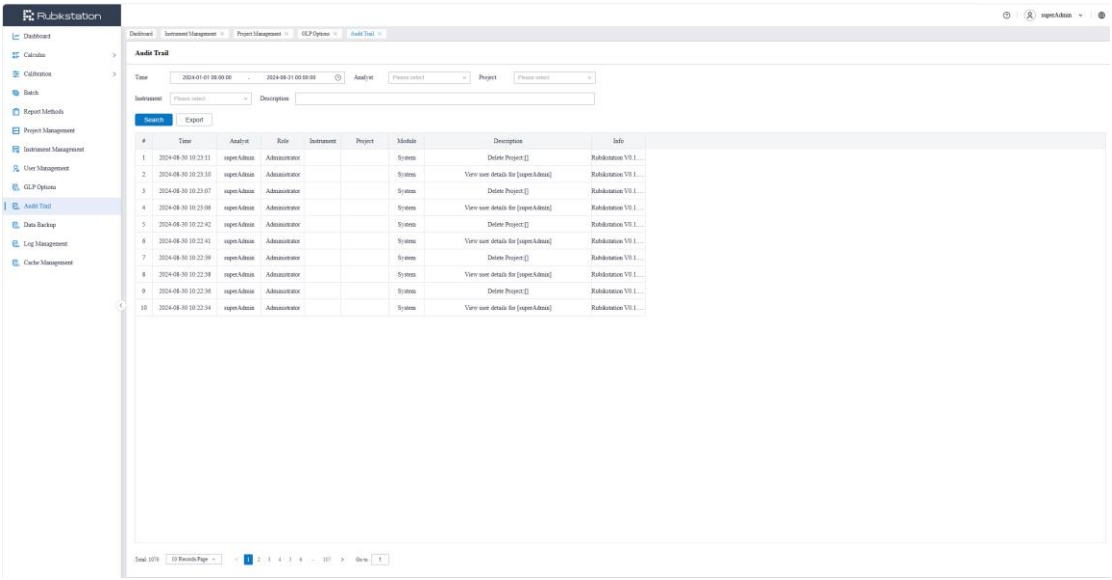


Figure 2-12 Audit Trail

2.2.8 Auxiliary Functions

There are several auxiliary function buttons in the upper right corner of the workstation. The first button is the "Help" button, which is used to view the help document of the workstation; The second button can view the personal information of the current logged in user, switch workstation themes, and log out of the current user; The third button can directly switch the language of the workstation. As shown in Figures 2-13.

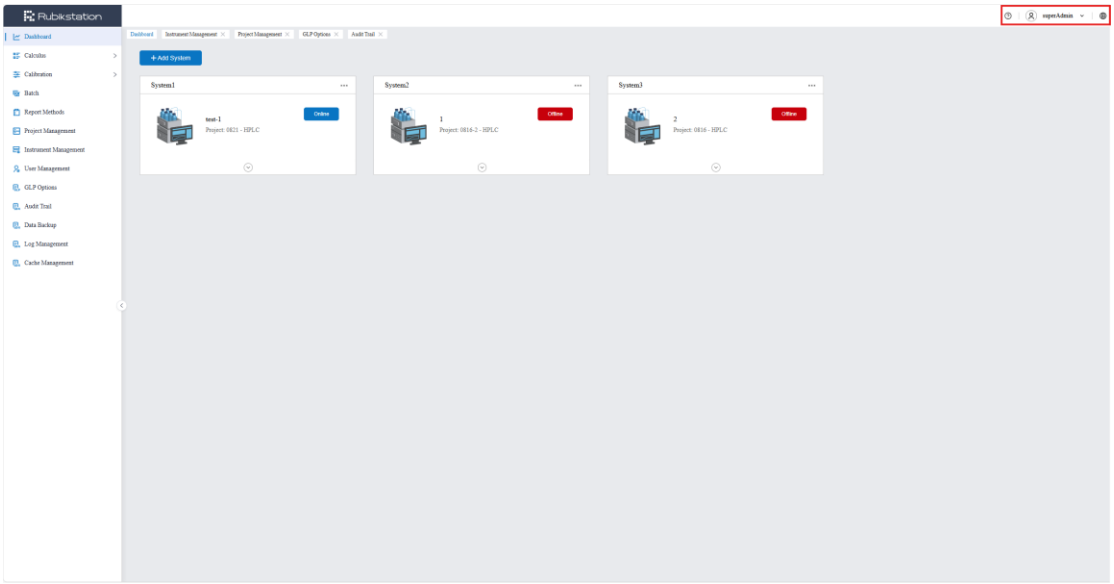


Figure 2-13 Auxiliary functions (1)

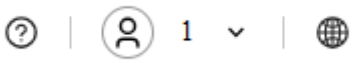


Figure 2-14 Auxiliary functions (2)

3 Dashboard

3.1 Dashboard

On the dashboard, you can create a system to view the current operating status of the system and the status of each system's configured instruments. As shown in Figure 3-1.

When there is an instrument connection failure in the system, the status behind the instrument

will display "failed", and the entire system will also display "offline" status; Display "online" status when all instruments are connected normally.

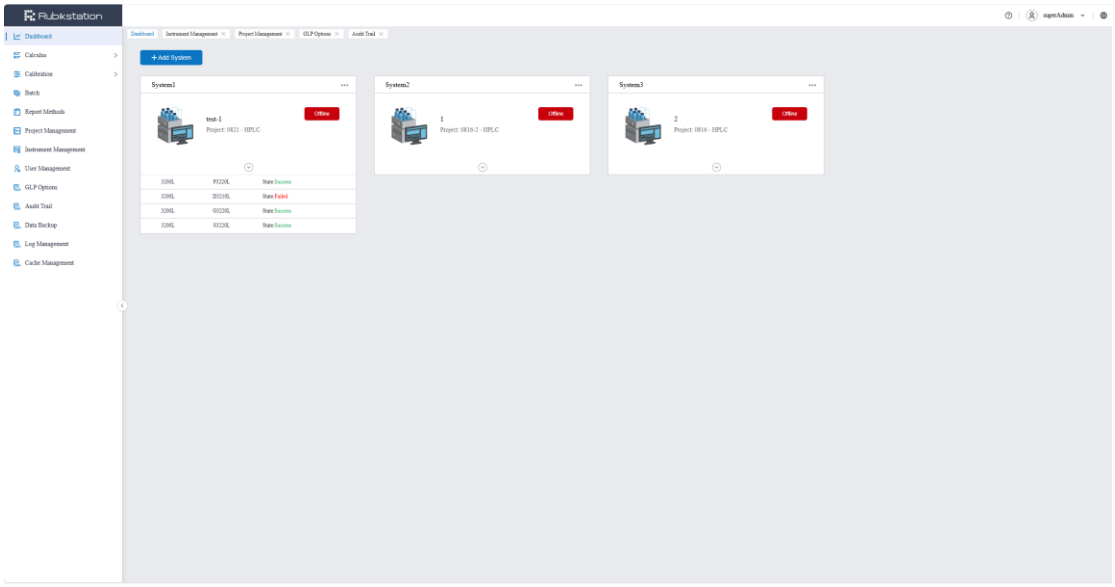


Figure 3-1 Dashboard (Offline)

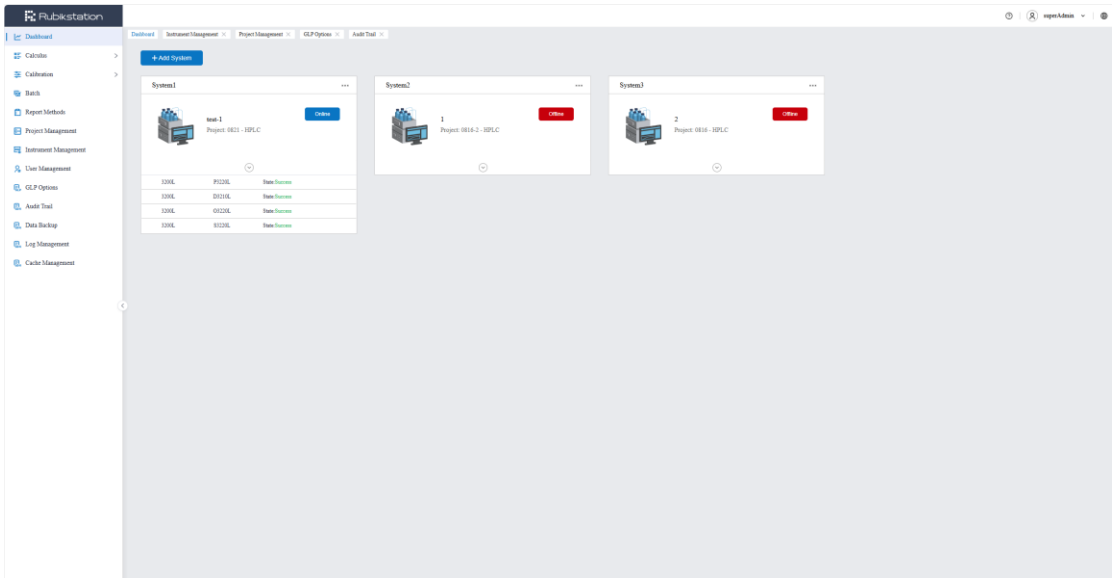


Figure 3-2 Dashboard (Online)

The "···" in the upper right corner of the system allows you to edit the instruments currently used in the system, edit the system name, select a project, and delete the system.

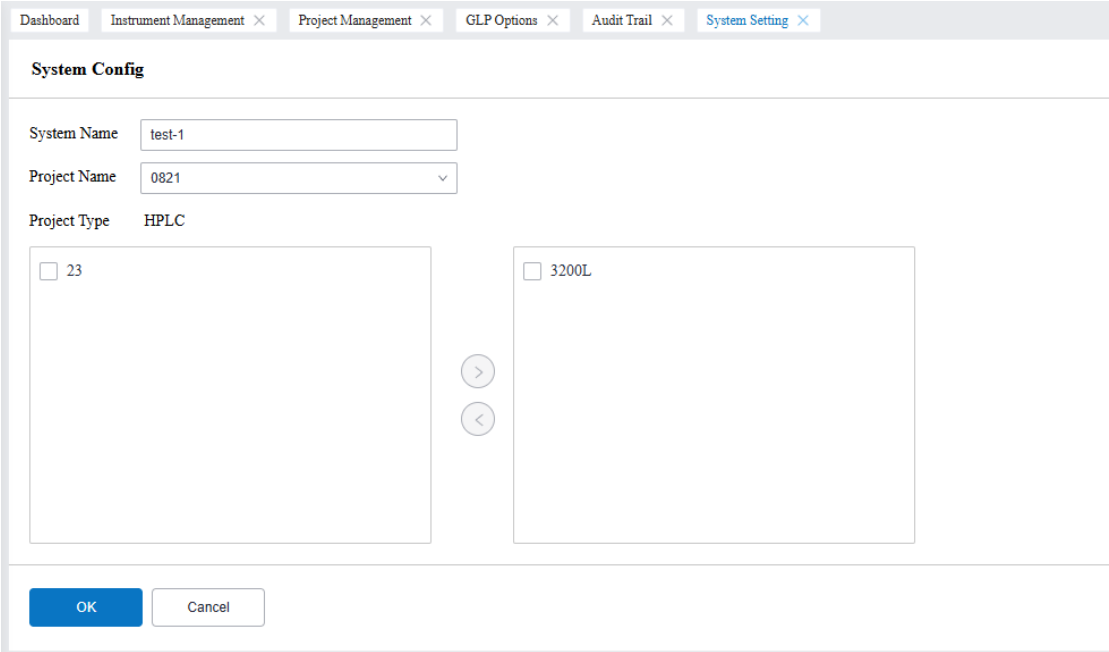


Figure 3-3 System Configuration

3.2 Instrument Method

3.2.1 LC Gradient Setting

The instrument method generally consists of four parts: LC gradient, detector, thermostat, and automatic sampler. Each section can be edited separately.

Taking 3200L binary high pressure as an example, modify the percentage of solvent in the mobile phase of pump A in the gradient table, and the percentage of solvent in the mobile phase of pump B can be automatically generated. The flow rate in the gradient table is the total flow rate of pumps A and B, as shown in Figure 3-4. The graph at the bottom left of the gradient table shows the flow velocity and the time-dependent curves of components A and B.

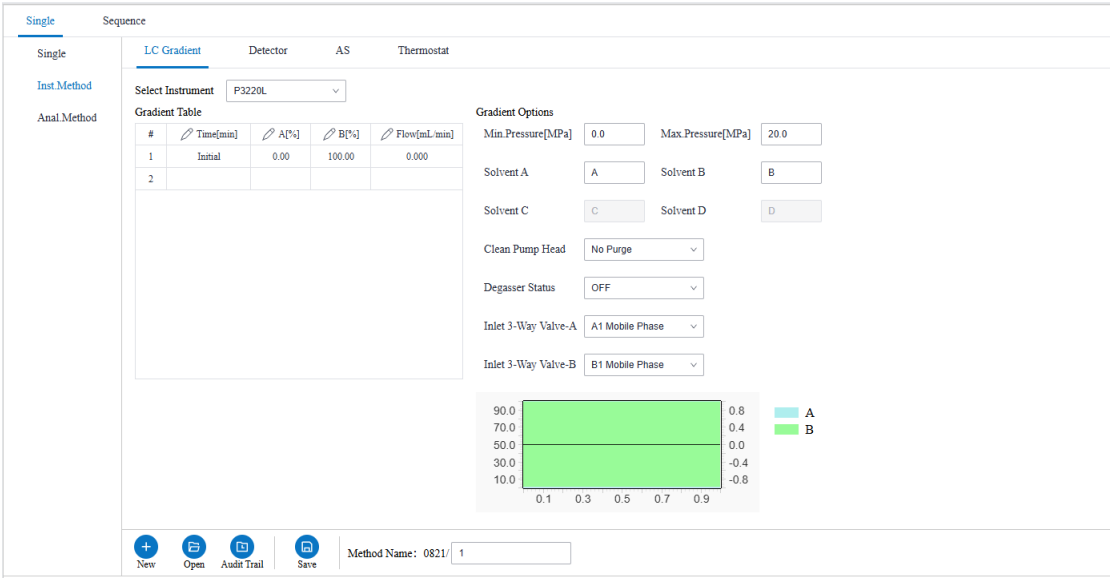


Figure 3-4 LC Gradient

- The "Gradient Options" dialog box in the gradient table allows you to set pump related functions such as maximum pressure, minimum pressure, solvent name, pump head cleaning status, deaerator status, and mobile phase inlet.

3.2.2 Detector Setting

Click on "Detector" in "Instrument Methods" to enter the detector settings dialog box, as shown in Figure 3-2. In the "Control Parameters" tab, you can set detector related parameters such as acquisition wavelength, acquisition frequency, response time, light source status, and detector temperature control; Click on 'Read Detector' to monitor the number of times the light source is turned on, running time, etc.

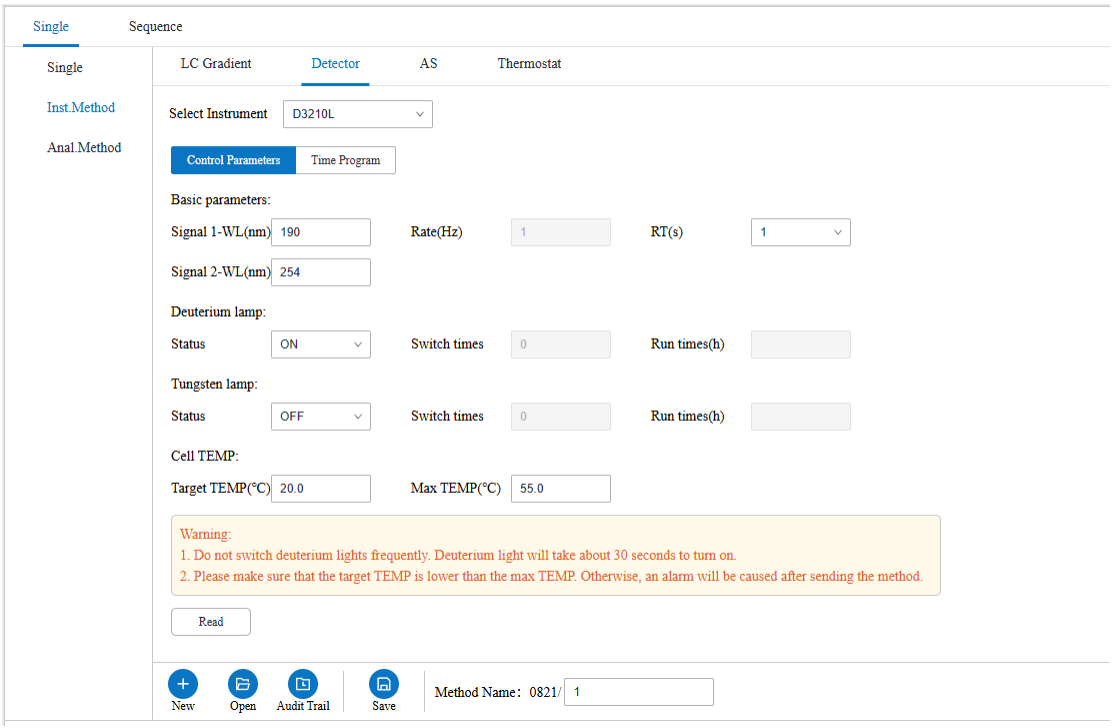


Figure 3-5 Detector Acquisition Condition Settings

The time wavelength program can be set in the "Time Program" tab, as shown in Figure 3-6.

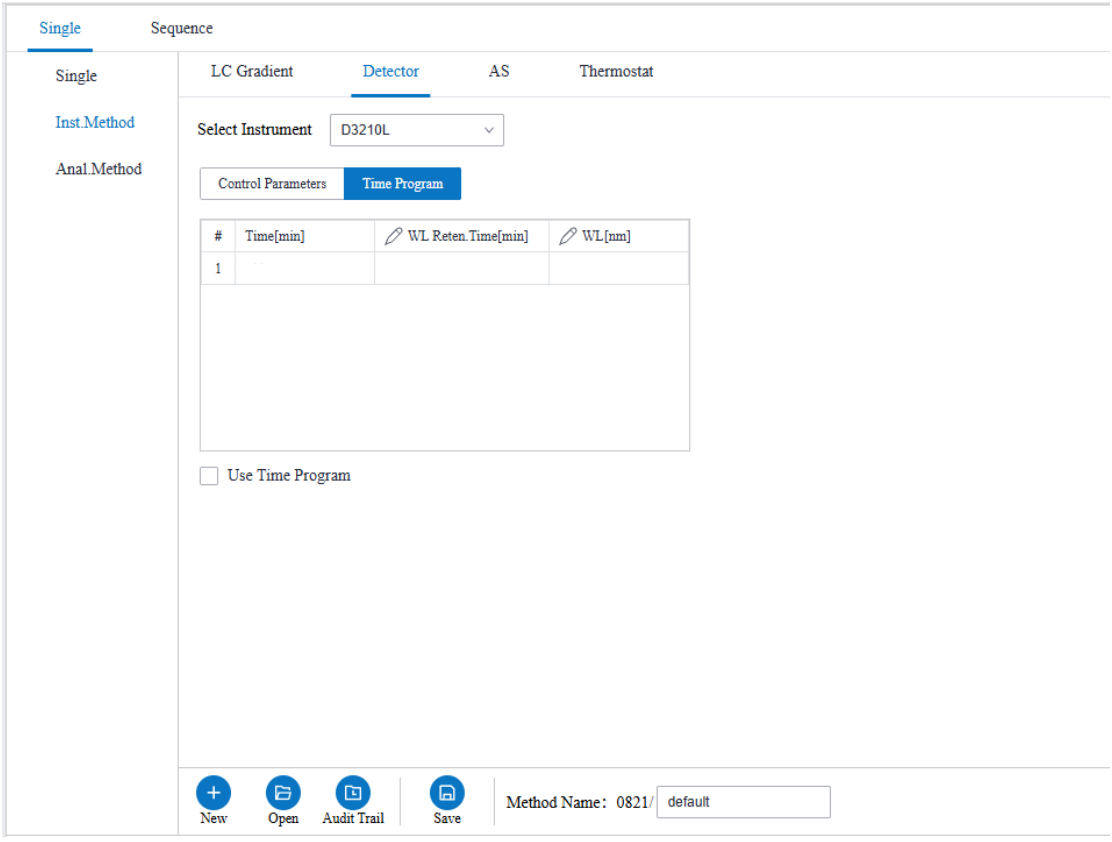


Figure 3-6 Time wavelength program settings

If the method is to be executed according to the set time program, it is necessary to check "Use time program".

3.2.3 Autosampler Setting

Click on "Automatic Sample Injector" in "Instrument Methods" to enter the detector settings dialog box, as shown in Figure 3-7. On the automatic injector page, basic parameters, injection parameters, cleaning parameters, etc. of the injector can be set.

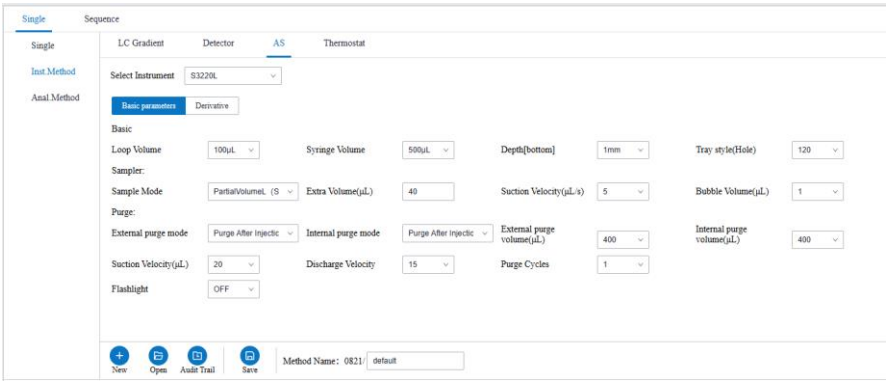


Figure 3-7 Autosampler Settings

If you need to use derivative functions, you need to check "Enable derivative functions".

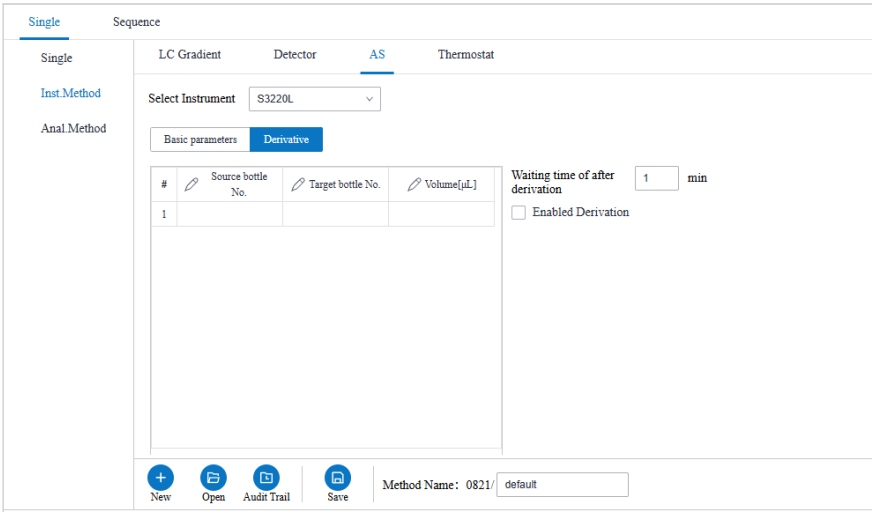


Figure 3-8 Derivative Settings

3.2.4 Thermostat Setting

Click on "Thermostat" in "Instrument Methods" to enter the thermostat settings dialog box, as shown in Figure 3-9. On the thermostat page, you can set the thermostat temperature, maximum alarm temperature, etc.

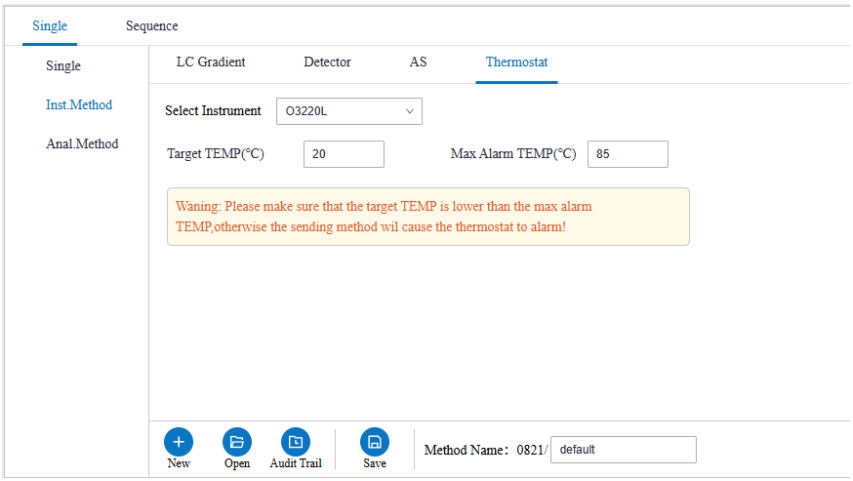


Figure 3-9 Thermostat Setting

3.3 Analysis Method

3.3.1 Measurement

Click on "Analysis Method" to enter the Analysis Method Settings dialog box. In the "Measurement" tab, you can describe the chromatographic analysis conditions, which will appear in the report description. Check "Enable Auto Stop" to set the running time of the method. When calculating column efficiency, it is necessary to set information such as column length and non retention time, as shown in Figure 3-10.

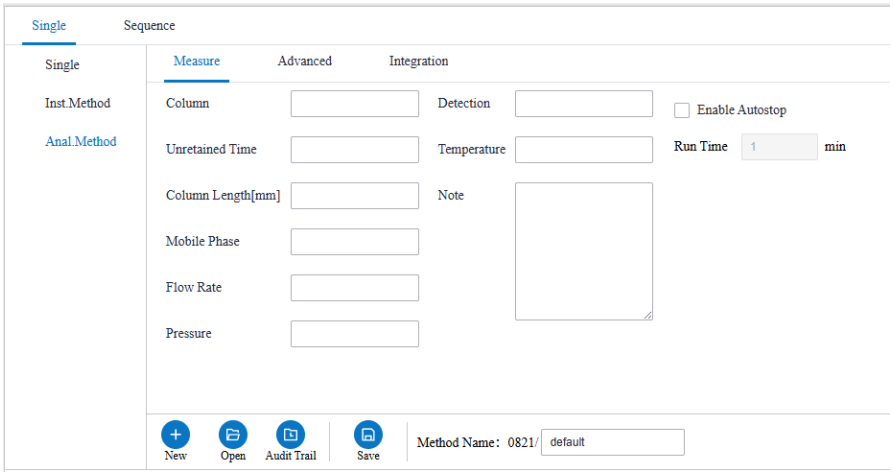


Figure 3-10 Analysis Method Setting Dialogue Box

3.3.2 Advanced

Click on the "Advanced" tab in the analysis method settings dialog box, as shown in Figure 3-11, to collect information such as pressure, flow rate, and temperature in the spectrum.

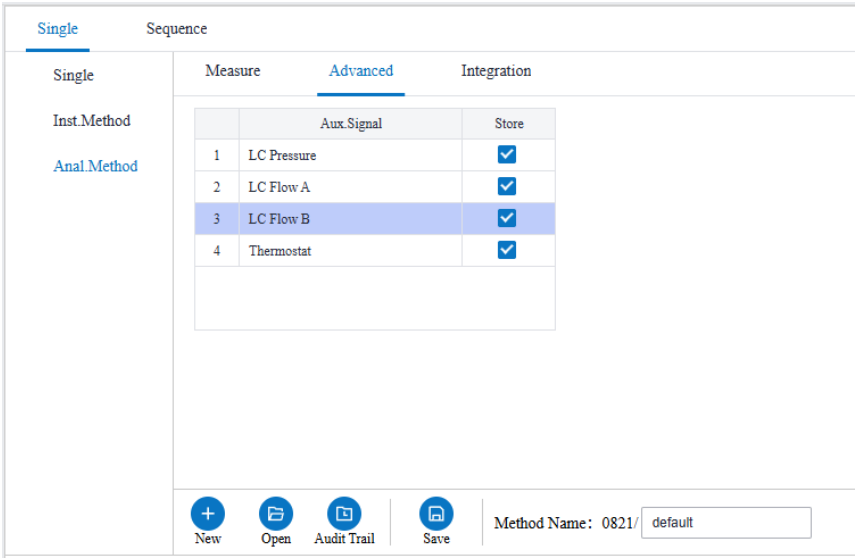


Figure 3-11 Advanced Condition Setting Dialogue Box

3.3.3 Integration

Click on the "Integration" tab in the analysis method settings dialog box to set the integral parameters for generating the graph, as shown in 3-12.

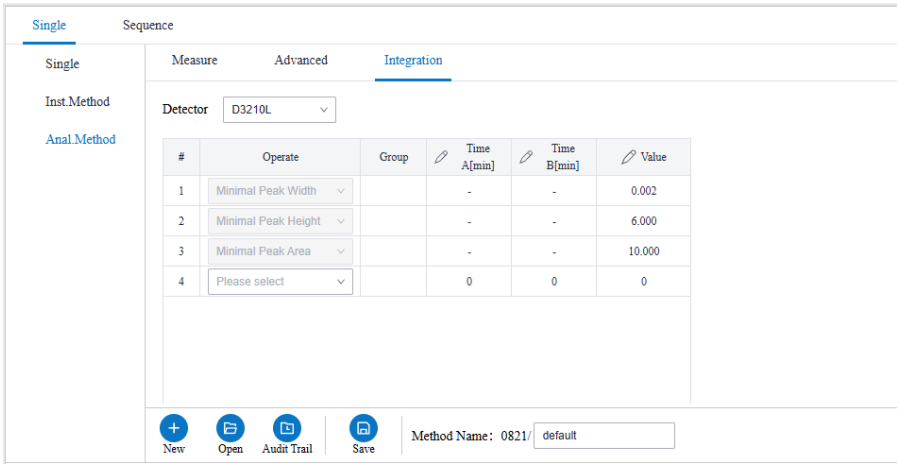


Figure 3-12 Integration Event Setting Dialogue Box

【Attention】

- **Integral events can only be selected from the "Chromatogram Operation" dropdown menu.**
- **Time A "is the start time of the event, and" Time B "is the end time of the event; If the integration time is a single point event similar to the "peak starting point", then "time A" is the peak retention time and "time B" is the starting point time.**

4 Analysis

4.1 Single Analysis

Single analysis "refers to the process of injecting, collecting, and storing data for a single sample.

4.1.1 Single Analysis Setting

The operation steps are as follows:

1) Click on "Single Setting" to display the Single Setting dialog box, as shown in Figure 4-1. Fill in relevant information such as spectrum name, sample ID, sample name, total amount, dilution, internal scalar, injection bottle number, injection volume, and whether to use an automatic sampler in the single analysis dialog box.

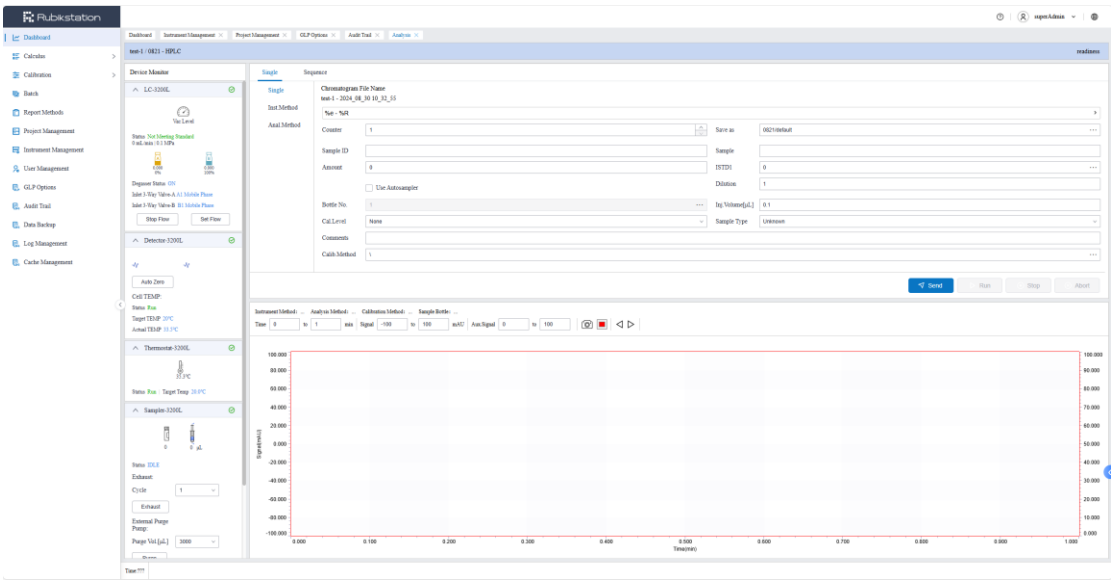


Figure 4-1 Single Analysis Dialogue Box

- Sample ID "is the sample identification number used to distinguish the sample.
- The "sample name" can be used to set sample description information.
- The "total amount" refers to the total amount of the sample used in calibration calculations, and the units used should be consistent with those in the calibration file, with a default value

of 0. In the internal standard method, the input value for "total amount" is the sample size without the addition of internal standard.

- “内 The 'internal scalar' refers to the amount of internal standard added in the internal standard method, and the unit should be consistent with the unit in the calibration file. The default value is 0.
- Dilution "is the dilution factor of the sample, and the result calculated using the calibration file will be automatically multiplied by the corresponding dilution factor to obtain the final calculation result, which will appear in the report table with a default value of 1.
- The "injection volume" is the injection volume of the sample, with a default value of 0. When calculating with a calibration file, the software automatically corrects the proportionality coefficient between the sample injection volume and the injection volume in the calibration file.
- The "calibration standard" is the level of the calibration standard. The spectrum obtained after activation will be automatically saved in the corresponding subdirectories of the calibration file and cannot be changed during the method operation.
- The "instrument method" and "analysis method" will run according to the currently selected method.

4.1.2 Operation of Single Analysis

Click the "Send Method" button, wait for the baseline balance to stabilize the readings of each instrument component, then click "Run" to perform a single sample analysis.

Note: When 'Do you want to use the automatic sampler' is not selected, the software will not send injection instructions to the automatic sampler.

4.2 Sequence Analysis

"Sequence" is the process of automatically conducting multiple, multi method, and multi sample analyses.

By using sequences, each sample can be automatically injected and data can be collected and analyzed according to the specific method used for that sample. Each sample in the sequence can be analyzed using different analytical methods, and different settings of chromatographic conditions and parameters can be used.

Sequence Group: Multiple sequences can be stored in one sequence group as needed, that is, multiple sequences can be called simultaneously for analysis, reducing the workload of sequence editing.

Note: If the injection method for "sequence" and "sequence group" is "standard" or "unknown" and there is no automatic sampler in the system, an external injection trigger signal must be received before analysis can begin. Otherwise, analysis will not be run.

4.2.1 Settings for Sequence Analysis

The sequence and sequence group need to be established and saved in the same way as the instrument method and analysis method before they can be used.

1. The setup and operation of sequence analysis can be carried out according to the following steps:

1) Click on "Sequence" to enter the sequence analysis window, as shown in Figure 4-2.

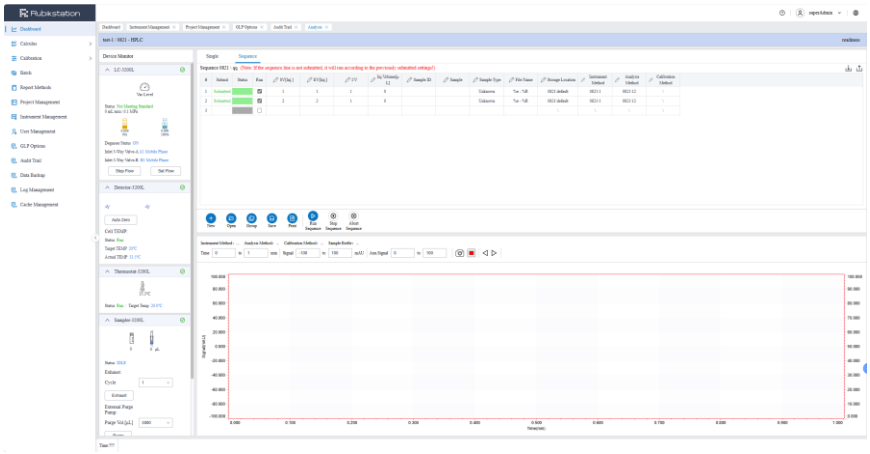


Figure 4-2 Sequence Analysis

2) Fill in the starting bottle number, ending bottle number, injection frequency, injection

volume, sample ID, sample name, sample type, spectrum name, instrument method, analysis method, calibration method, etc. in sequence in the sequence analysis dialog box, as shown in Figure 4-3.

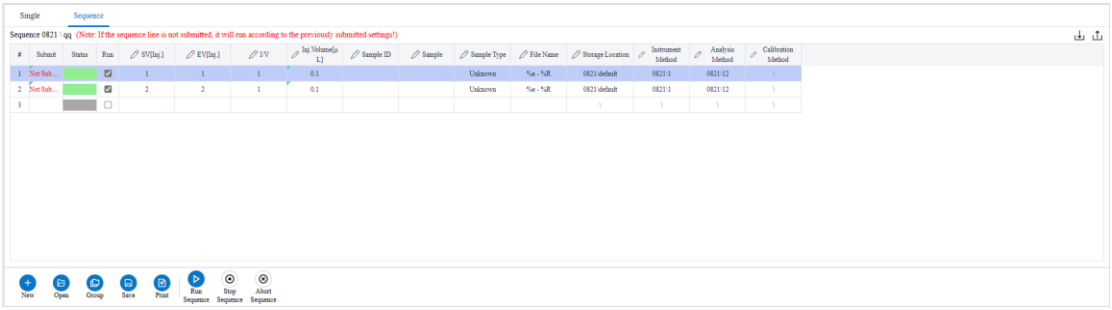


Figure 4-3 Editing Sequence

3) After completing the sequence editing, click the "Save" button, enter the sequence name, and save the sequence.

2. The editing method for "sequence group" is as follows:

1) Edit sequence group

Click on "Open Group" on the "Sequence" page, and a sequence group editing page as shown in Figure 4-4 will pop up. Click on "Add Sequence Group" in this pop-up window, then enter the name of the sequence group in the pop-up window and click "OK". At this time, the newly added sequence group name will be displayed in the sequence group list. Clicking the "+" after it will display all saved sequence lists. After clicking the sequence that needs to be added to the sequence group in the sequence list, click the OK button to return to the sequence group list page. After selecting the sequence group, click OK to display the current sequence group on the sequence analysis page, as shown in Figure 4-5.

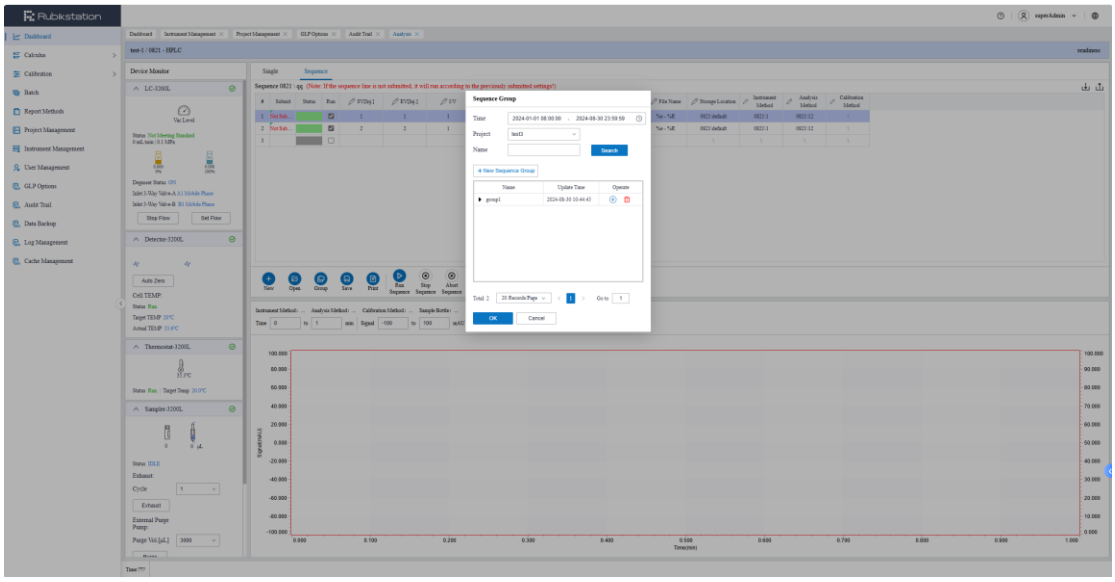


Figure 4-4 Edit Sequence Group

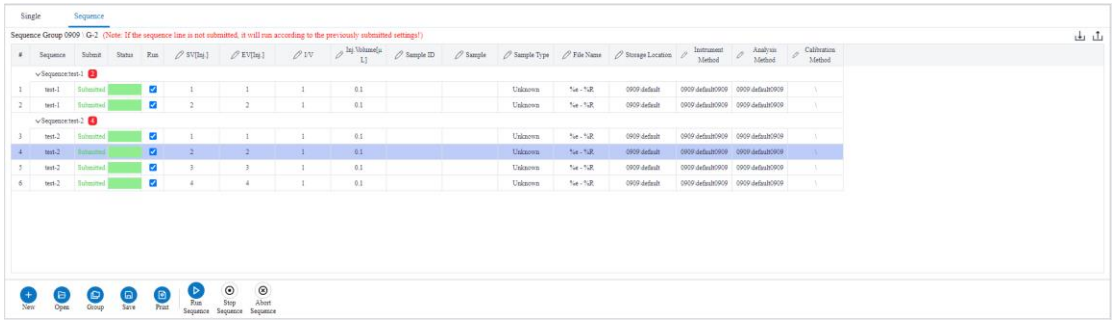


Figure 4-5 shows the sequence group

4.2.2 Operation of Sequence Analysis

1）After editing the sequence, if there is a problem with the sequence, it will display  in the "status" of the problem line. If there is no problem with the sequence, it will display  in the "status" of the problem line.

2）Click on  , and the selected sequence will start running.

1) After the sequence analysis is completed, the corresponding sequence state changes. The sequence runs in orange, the completed sequence is displayed in gray, and the reset state sequence is displayed in white.

2) If you want to run the sequence again, simply select the completed sequence and click "Reset".

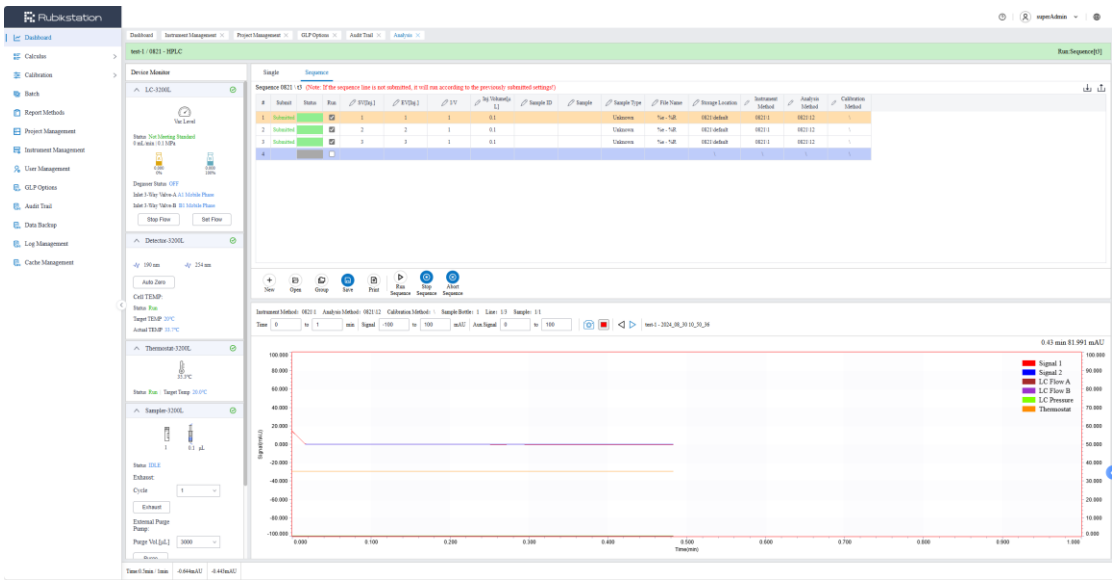


Figure 4-6 Running Sequence

Note: The operation and status of the sequence group are consistent with the sequence.

5 Data Acquisition

Data acquisition is the process of recording and storing the response signals of the detector. During the data acquisition process, the detector converts all response signals from analog signals to digital signals, which are then transmitted to the workstation and stored in the signal data file. This chapter provides a detailed introduction to the data collection function and related operations.

5.1 Data Acquisition Interface

After logging into the workstation, you can directly enter the data collection interface. As shown in Figure 5-1.

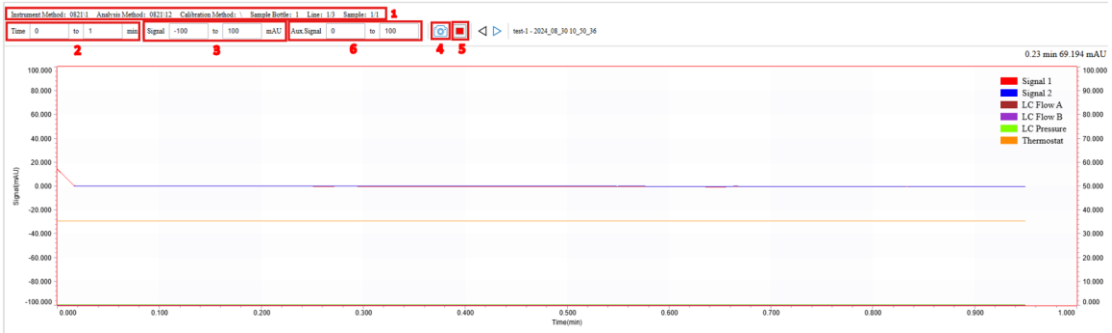


Figure 5-1 Data Collection Interface

#	Description
1	The displayed information includes instrument methods, analysis methods, calibration methods, injection bottles, and other relevant details from this operation
2	Used for setting the timeline of the data collection interface
3	Used for setting the signal axis of the data acquisition interface
4	During the data collection process, this function displays the chromatogram from the beginning of the analysis until clicking this button, allowing you to check peak area, peak height, and other information during the analysis process
5	This function is used to change the color of the detector signal according to requirements
6	coordinate axis of auxiliary signals, which can read the auxiliary signal values during the data acquisition process, such as real-time flow rate, pressure, column temperature, etc.
7	Right click on "Auxiliary Signal Settings" on the data acquisition interface to display the pump flow rate, column temperature, and pump pressure signal lines; Right click on the data to switch back and forth between "Set Background Spectrum" and "Close Background Spectrum"

5.1.1 Device Monitor

In the device monitor, the operating status of the instrument can be viewed, and in addition, its parameter values can be adjusted by directly entering values in the functional units of the monitor.

The "Device Monitor" in the analysis column is shown in Figure 5-2.

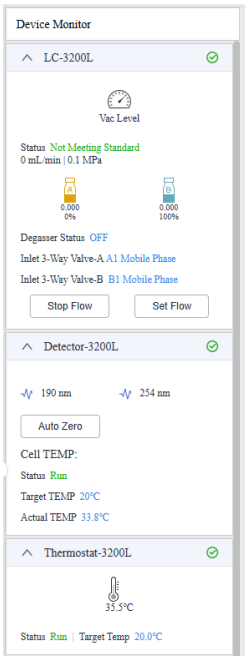


Figure 5-2 Device Monitor

Pump: The pump flow rate and pressure changes can be observed at any time, and parameter settings and flow rate setting operations can be performed.

Autosampler: Perform operations such as syringe exhaust, cleaning, and column derivatization.

Thermostat: Display set temperature and real-time temperature changes.

Detector: Display deuterium lamp, tungsten lamp energy changes, status (on/off), temperature display, and enable baseline zeroing operation.

5.2 Beginning of Data Acquisition

In a single analysis, after clicking "Send Method" and the baseline runs smoothly, click "Run" to collect data. As shown in Figure 5-3.

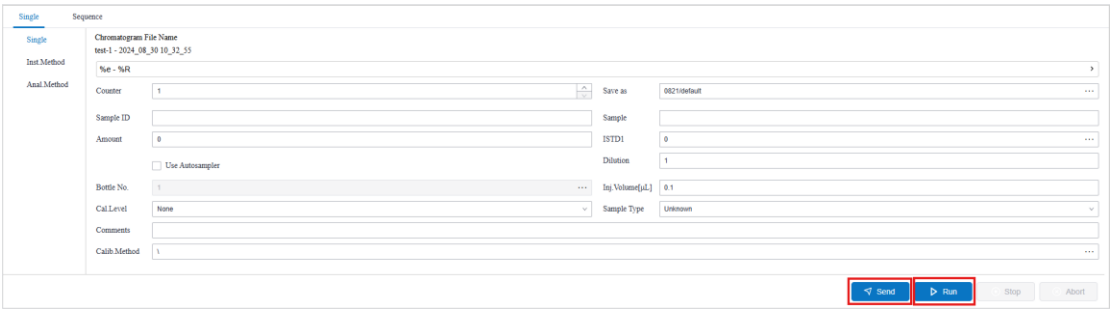


Figure 5-3 Single Analysis - Start of Data Acquisition

In sequence analysis, first click on option 1 to send the method. After the baseline runs smoothly, click on option 2 or 3 to run the sequence. As shown in Figure 5-4.

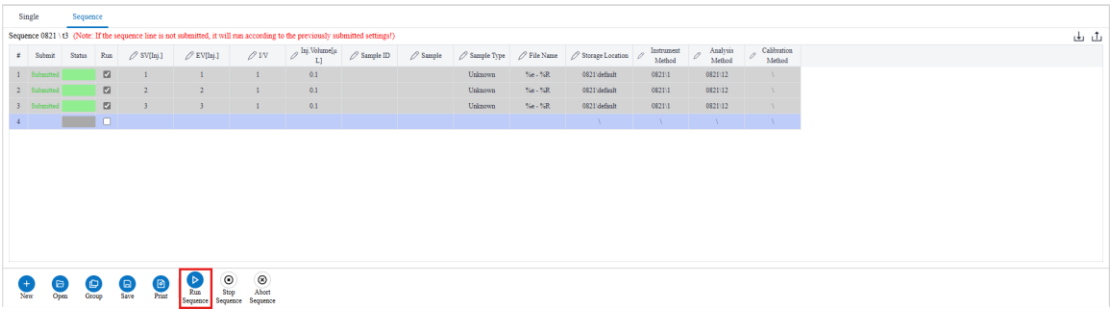


Figure 5-4 Sequence Operation - Start of Data Acquisition

5.3 End of Data Acquisition

Data Acquisition can be stopped by the following methods:

- When the "Running Time" of the detector set in the "Analysis Method" is reached, data collection will be automatically terminated.
- In a single analysis, click 'Stop' to end data collection and save the data at the same time.

  Click 'Abandon' to stop data collection and not save the data this time.
- In sequence analysis, click "Stop" to stop the data collection and save the data after completing the current running analysis. Click 'Stop' twice to immediately end data collection and save this data.

  Click 'Abandon' to stop data collection and not save the data this time.

5.4 Set background chromatogram

- Operation: Blank area in the "Data Collection" section ->Right click ->Click "Set Background Image" ->In the pop-up "Chromatogram List" window ->Select the chromatogram as the background chromatogram ->Click OK.
- Application: Display as a comparison chart during the analysis and operation process.
- Close background chromatogram: Blank section of "Data Collection" → Right click → Close background chromatogram

5.5 Setting Analysis Time (During Analysis)

When the analysis is not running, the analysis time is set in the analysis method, see 3.3.1 for details.

During the analysis of operational status, most of the parameter settings for instrument and analysis methods will be locked and cannot be modified. If the automatic stop function is enabled in the analysis method, only the running time in the analysis method can be edited and saved. If you need to modify the collection time of the spectrum during analysis, you can directly modify the "running time" in the analysis method used for the analysis. After saving, the collection section will automatically update the analysis time. As shown in Figures 5-5 and 5-6.

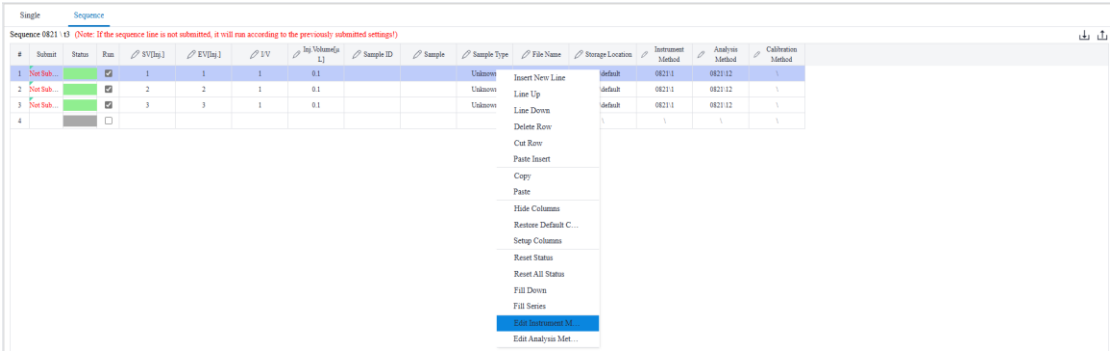


Figure 5-5 Editing and Analysis Method during Sequence Operation

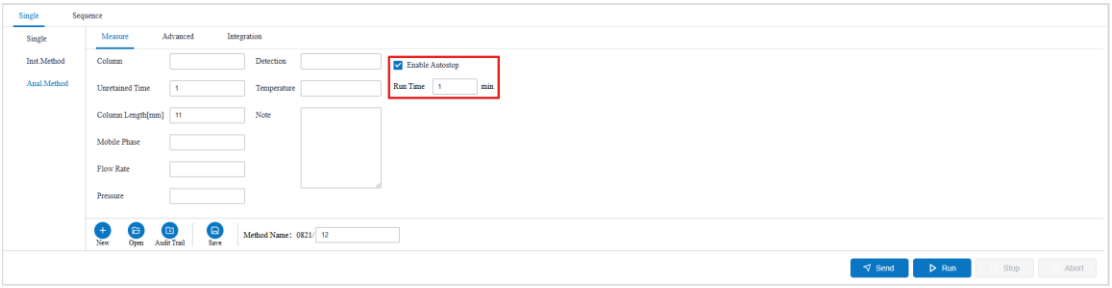


Figure 5-6 Change in running time

6 Data Processing

Data processing includes HPLC data processing, GPC data processing, and PDA spectra, and the processing of different spectra requires the use of corresponding data processing pages. It should be noted that the conventional processing functions of PDA spectra and the data processing of HPLC spectra are both on the HPLC data processing page, while the unique functions of PDA spectra are on the PDA spectra page.

6.1 HPLC Data Processing

6.1.1 View Chromatogram

Click on "Data Processing" - "HPLC Data Processing" in the workstation to enter the HPLC data processing page. The chromatograms of all projects are displayed on the left side of the page, and the chromatograms, chromatogram result information, and chromatogram processing tools are displayed on the right side. As shown in Figure 6-1.

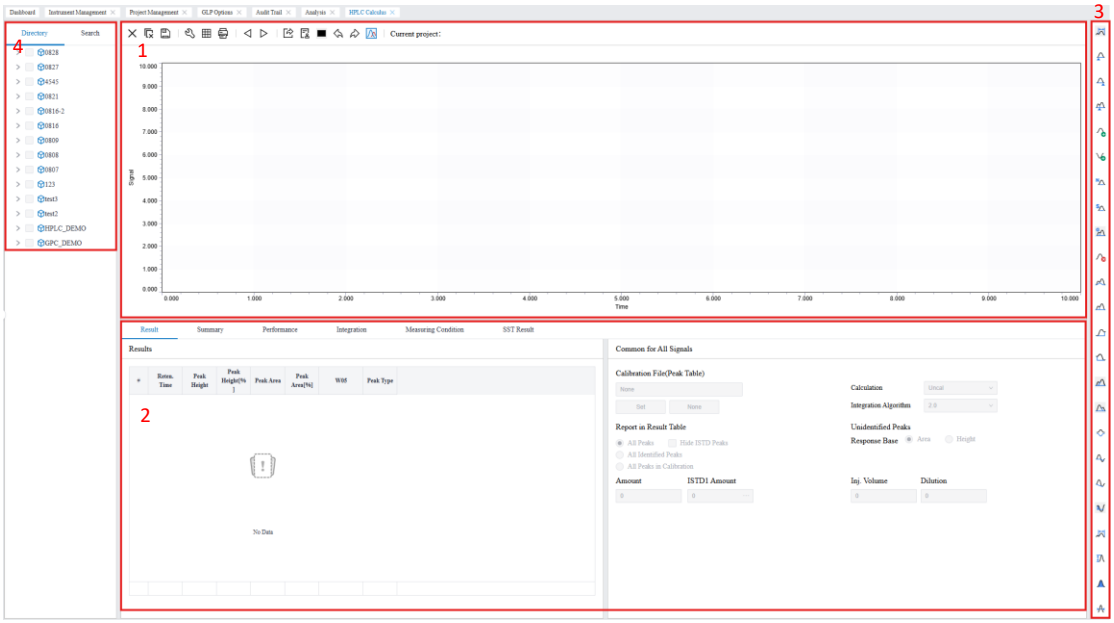


Figure 6-1 Chromatogram Window

#	Description
1	The chromatogram display area can be selected for zooming in, and the corresponding functions about chromatogram display can be displayed by right clicking.
2	Display chromatographic column, method, integration information, chromatographic peak information, etc.
3	Chromatogram integration tool
4	List of chromatograms

Open Chromatogram: Click on the chromatogram name in the chromatogram list on the left; As shown in Figure 6-2.

Overlay Chromatogram: In the toolbar above the chromatogram display area, make the overlay button light up, and then click on the chromatogram on the left side to overlay and display the clicked chromatogram.

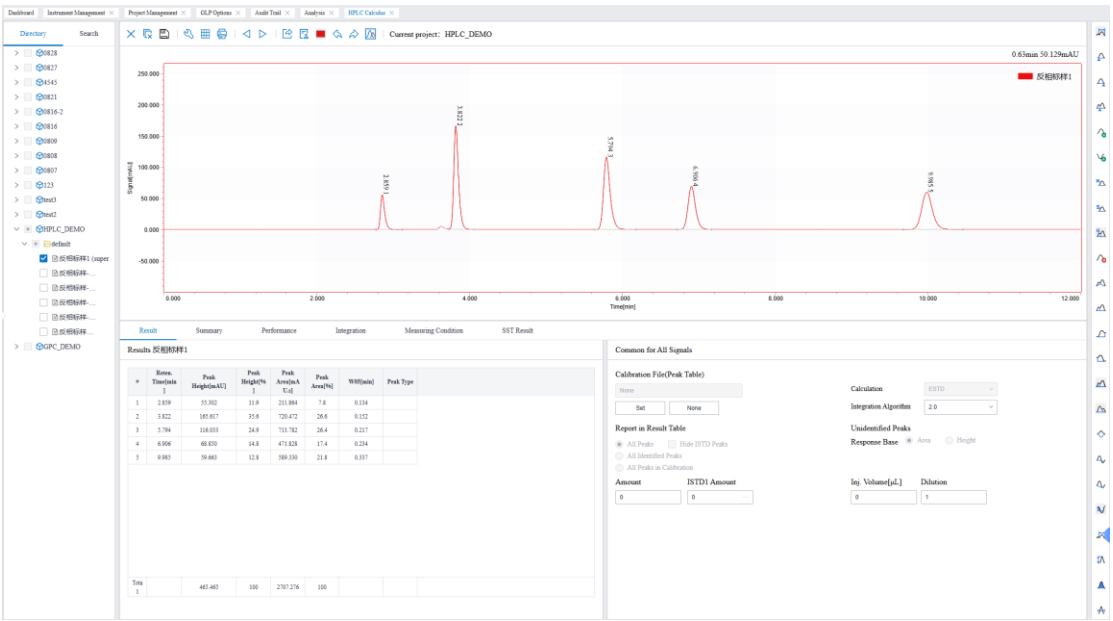


Figure 6-2 Stacked Chromatogram

6.1.2 Integration Setting

Integral is the process of identifying peaks in a signal and calculating their magnitude. Integral is essential for viewing, qualitative and quantitative calculations, peak purity calculations (PDA spectra), and other data results of the tested substance.

6.1.2.1 Manual Integration

The integration tool can be used to perform various operations on peaks, such as adding peaks, modifying the starting and ending points of peaks, or removing unnecessary peaks. When the collected spectrum is integrated according to the integration setting in the analysis method but satisfactory integration results are not obtained, it is convenient for users to adjust and use it.

Open the chromatogram to be processed in the "Data Processing" window, and manually change the chromatogram parameters using the commands on the right side of the menu. The sub menu commands under the main menu in the chromatogram window can be used to adjust the chromatogram.

Manually move the starting and ending points of the peak. Click on the  in the points column to change the starting point of the points. Click on  to change the endpoint of the integral, as shown in Figures 6-3 and 6-4.

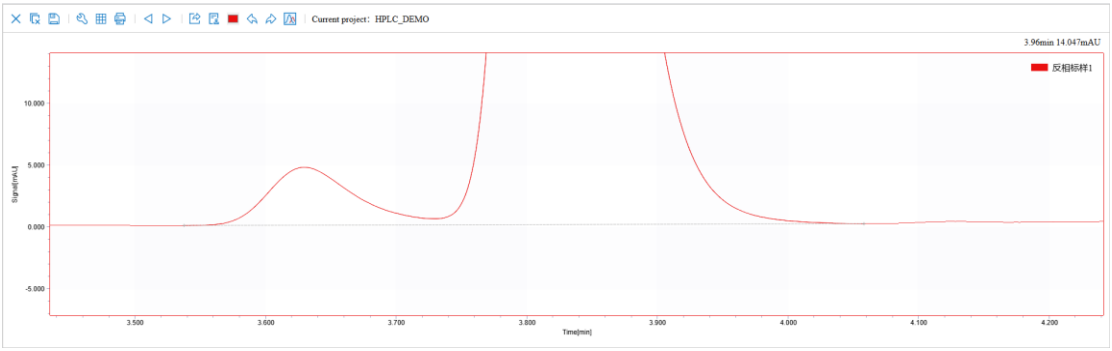


Figure 6-3 Before Manual Integral Change

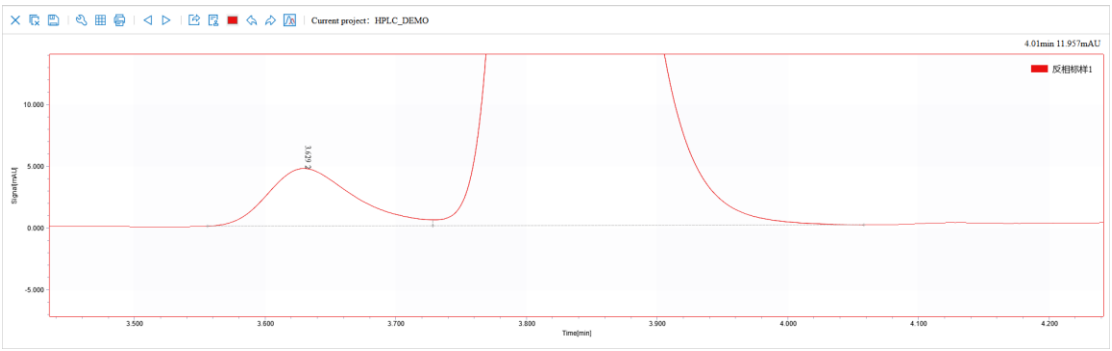


Figure 6-4 After Manual Integral Change

The manual points menu commands are shown in Table 1 below:

	Overall Peak Width
	Set the integration starting point of a single peak, and the adjusted parameters can be displayed in the integration table of the chromatogram
	Set the integration point of a single peak, the adjusted parameters can be displayed in the integration table of the chromatogram
	Demarcation point
	Add a positive peak
	Add a negative peak
	Mandatory naming of selected peaks
	Label solvent peak
	Assign all peaks in the selected interval to the set group
	Delete peaks and do not integrate the peaks in the selected area
	Peak-valley separation, separate a single peak by setting the start and end points of the peak-valley separation area
	Vertical separation, draw a vertical line to all peaks in the selected area to separate a single peak
	Horizontally forward, the baseline will be forced forward in the selected area and separate chromatographic peaks vertically
	Horizontally backward, the baseline in the selected area will be forced backward and vertical separation of chromatographic peaks
	Front tangent
	Back tangent
	Change the negative peaks in the specified area to positive peaks

6.1.2.2 Integral Results

Below the display area of the chromatogram, there are various information tables for the chromatogram, including result table, summary table, performance table, integration table, measurement conditions, and SST table. As the integration results are adjusted, the corresponding results will be displayed in various tables, as shown in Figure 6-5.

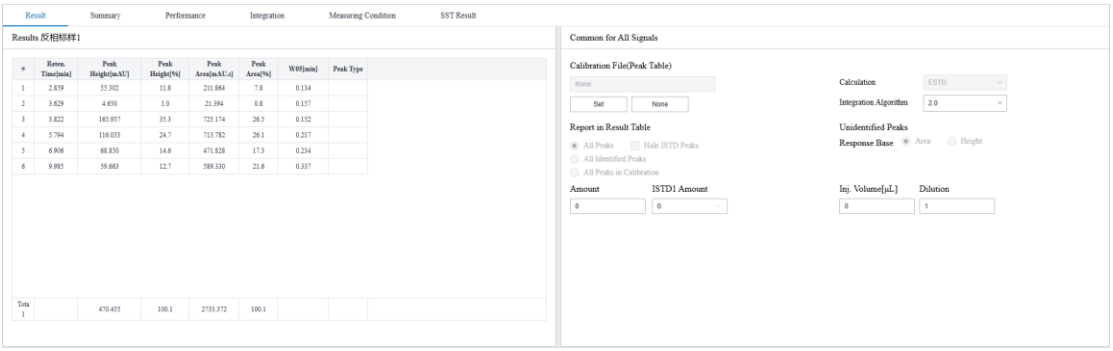


Figure 6-5 Results View

Right click the mouse in the "Results Table" and "Summary Table" to set the queue, as shown in Figure 6-6.

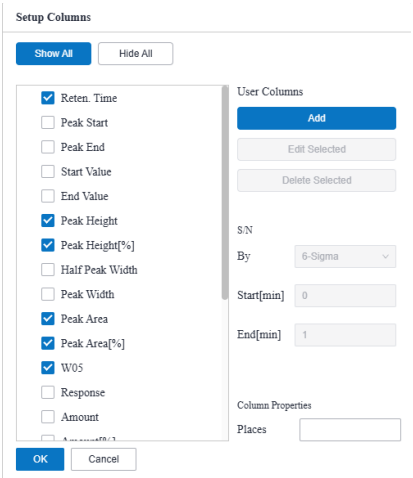


Figure 6-6 Setting Queue

6.1.3 Subtract Background Chromatogram

The mobile phase under gradient conditions may cause baseline instability, affect integration

results, and even lead to inaccurate quantification. To eliminate baseline issues, the spectrum of the empty run gradient can be used as the background chromatogram, and the normal sample chromatogram can be calculated after deducting the background chromatogram.

Specific operation: Data processing → Measurement conditions → (Deduction) settings → Select background spectrum from the chromatogram list → Confirm. As shown in Figure 6-7.

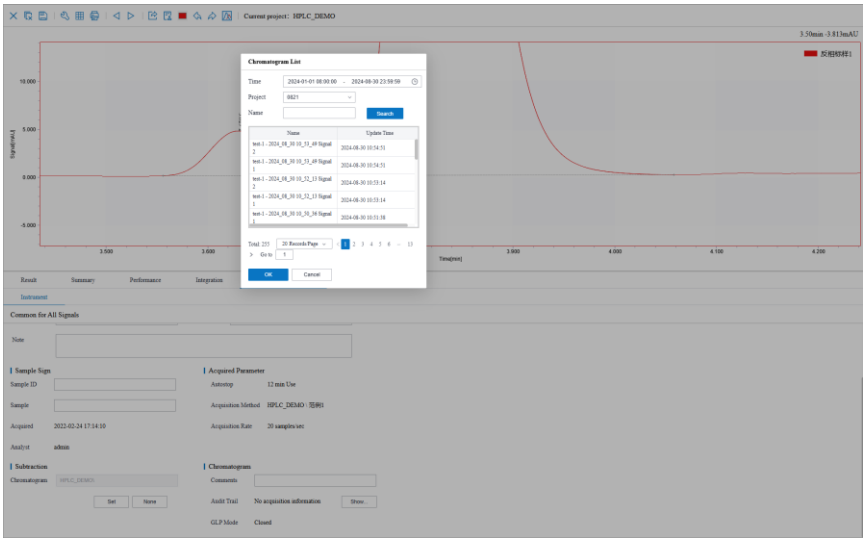


Figure 6-7 Subtract background chromatogram

6.1.4 Calculation of noise and drift

After opening a chromatogram, right-click in the chromatogram area, click on "Noise/Drift", select a calculation method, and then choose the calculation area. The calculated noise/drift results will automatically appear in the result table below the window. As shown in Figure 6-9.

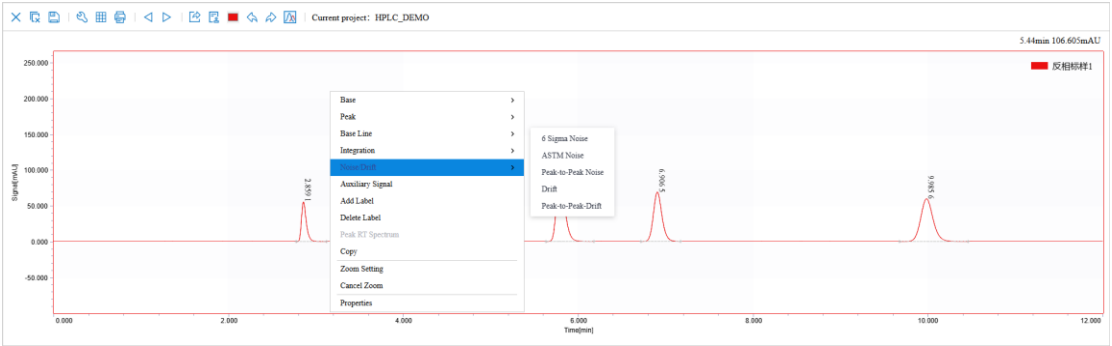
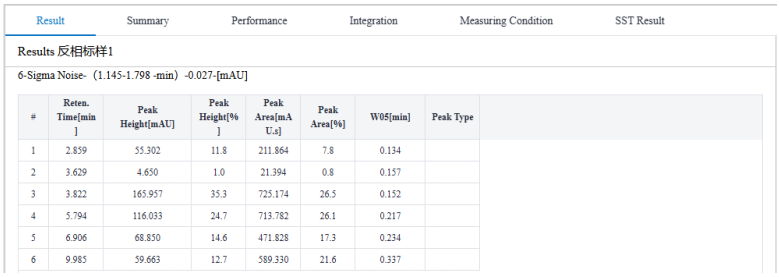


Figure 6-8 Noise and Drift



#	Reten. Time[min]	Peak Height[mAU]	Peak Height[%]	Peak Area[mAU.s]	Peak Area[%]	W05[min]	Peak Type
1	2.859	55.302	11.8	211.864	7.8	0.134	
2	3.629	4.650	1.0	21.394	0.8	0.157	
3	3.822	165.957	35.3	725.174	26.5	0.152	
4	5.794	116.033	24.7	713.782	26.1	0.217	
5	6.906	68.850	14.6	471.828	17.3	0.234	
6	9.985	59.663	12.7	589.330	21.6	0.337	

Figure 6-9 Calculation of Noise and Drift

6.1.5 Summary Table

Click on the "Summary" tab below the chromatogram to view the calculation results of the calibrated peaks in the summary table, as shown in Figure 6-10. If no calibration file is set or no peak is recognized, no data will be displayed in the summary table.

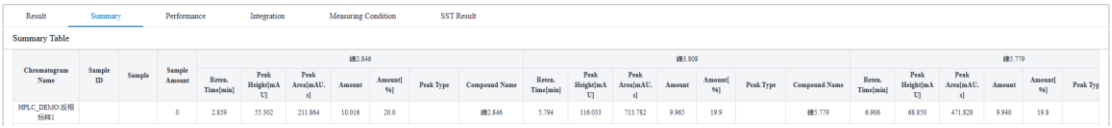


Figure 6-10 Summary Table

The calibration peaks of the superimposed spectra will also be displayed in the summary table. If it is necessary to compare the same peak results of different spectra, it can be viewed through the summary table.

6.1.6 Performance Table

Add non retention time and column length to the "Analysis Method" and select the corresponding "Standard Method". The "Performance Table" below the chromatogram will display the various performance parameters of the chromatographic column, as shown in Figure 6-11.

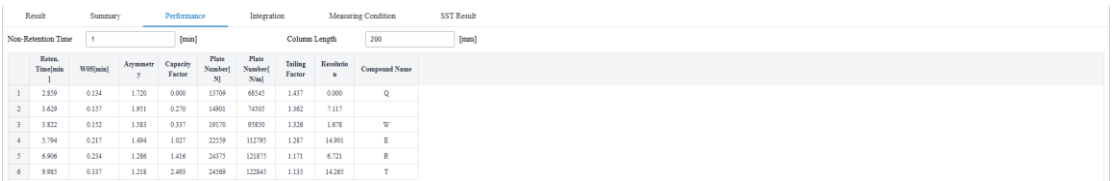


Figure 6-11 Performance Table

6.1.7 Measurement Condition

The "Measurement Conditions" tab below the chromatogram displays all measurement method information, as shown in Figure 6-12.

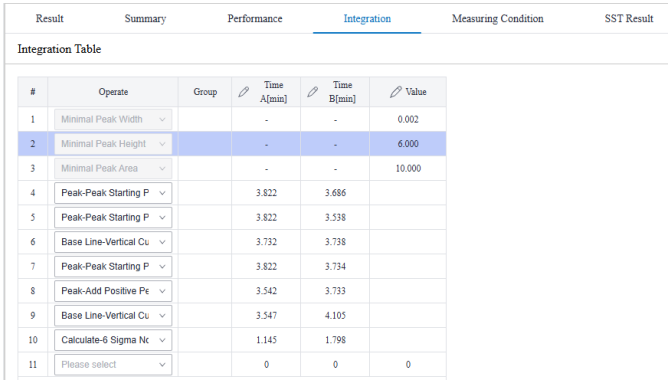


Figure 6-12 Measurement Conditions Tab

6.1.8 SST

SST (System Suitability Test) is commonly used to monitor the performance of methods.

1) Open the spectrum that requires SST result calculation on the data processing page, and set the calibration file for each spectrum separately to correctly identify the peaks that need to be calculated;

2) Click on "SST Results" in the Results section to switch to the SST Results page, right-click anywhere under "All SST Results" on the left, and click "Update from Calibration" in the pop-up tool window. The workstation will automatically update the information of the identified peaks in the currently open spectrum on the left; As shown in Figure 6-13;

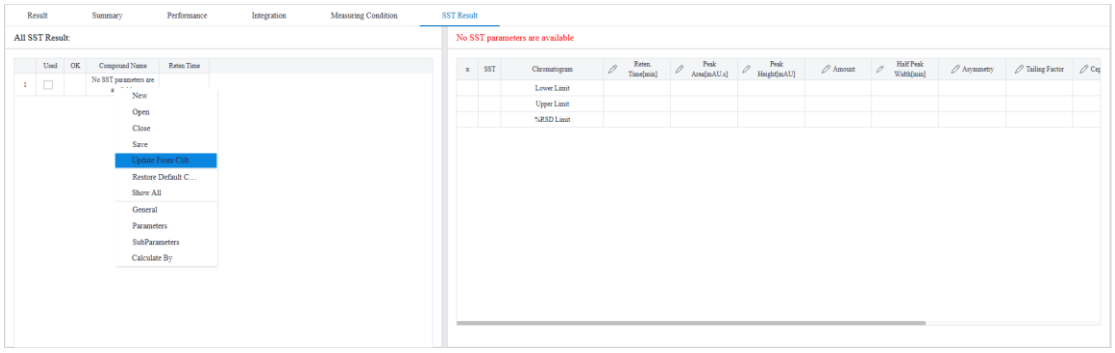


Figure 6-13 Update from Calibration

3) Select the peaks that need to be used for calculation from the peaks identified on the left, and display the selected peaks in the table on the right;

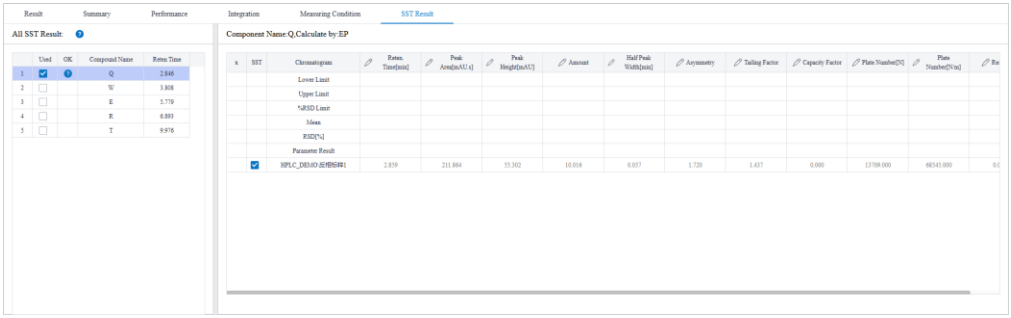


Figure 6-14 Loading Identification Substances

4) Then right-click on the table on the right and select "Parameters". Set the SST calculation related properties in the pop-up SST properties window, check the parameters to be calculated, and set the calculation standards. As shown in Figure 6-15; After clicking the confirm button, the selected parameters "retention time" and "peak area" in the table on the right side of the SST result table will become editable; As shown in Figure 6-18;

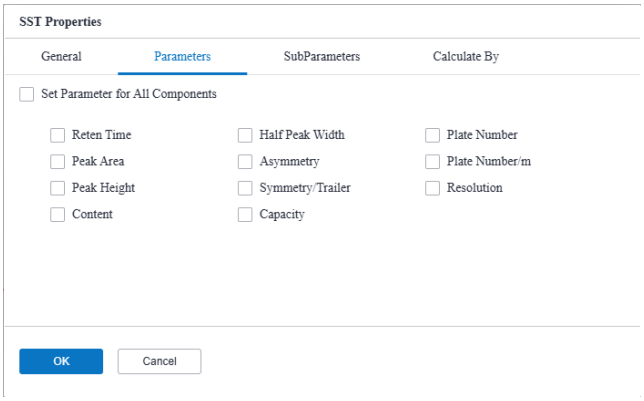


Figure 6-15 Setting SST Parameters (1)

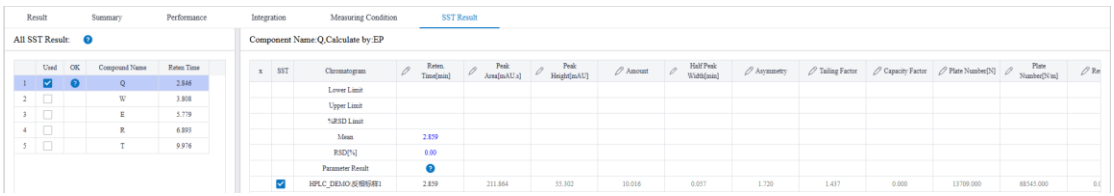


Figure 6-16 Setting SST Parameters (2)

5) After entering the values of "upper limit", "lower limit", and "% RSD limit" in the parameter section of the SST result table on the right, the workstation automatically calculates the average value, RSD%, and parameter results; The parameters that meet the criteria are displayed in green, while those that do not meet the criteria are displayed in red; As shown in Figure 6-17;

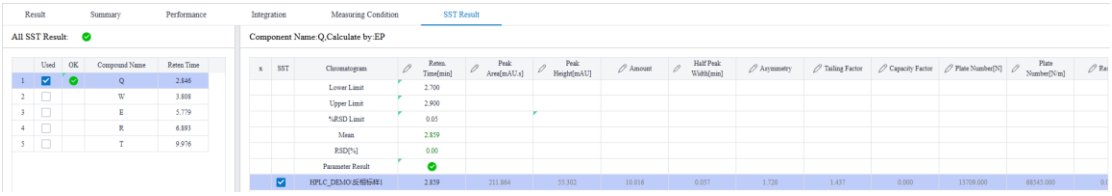


Figure 6-17 SST Calculation Results

6) After setting the parameters, right-click on the SST result table on the right and click "Save". Set the SST file name in the pop-up window and click "OK"; As shown in Figure 6-18;

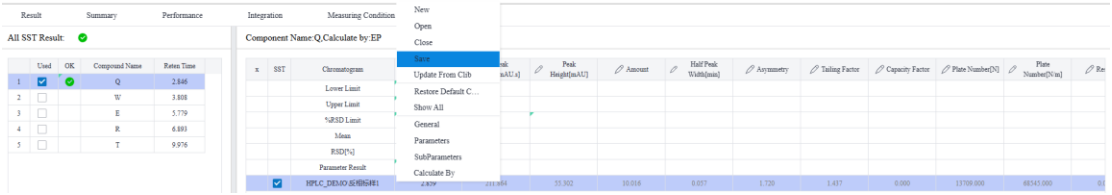


Figure 6-18 SST file saving

The SST result function is powerful, and there is no need to copy the test data into an EXCEL spreadsheet for further calculation, making it convenient for customers to use.

6.2 GPC Data Processing

6.2.1 GPC Mode Usage

The project saved after selecting "GPC" in the "Project Type" of the created project is called a GPC project. The analysis performed using this project is called GPC analysis, and the chromatogram obtained from the analysis is also a GPC chromatogram.

6.2.2 GPC Basic Theory

Gel Permeation Chromatography (GPC) or Size Exclusion Chromatography (SEC) is a liquid chromatography technique for measuring the molecular weight distribution of polymers. Polymer samples containing different molecular sizes are separated on a chromatographic column. In this chromatographic separation mode, different molecules are separated based on their size, with larger molecules being eluted first and smaller molecules being eluted later. Select a standard substance with appropriate molecular weight, draw a calibration curve of molecular weight size and elution volume, and calculate the molecular weight distribution.

6.2.2.1 Narrow Distribution Standard Calibration

When a standard substance with a narrow molecular weight distribution can be obtained, narrow distribution standard calibration is the most commonly used calibration method, by plotting the calibration curve based on the peak position molecular weight and the retention time of the highest point of the chromatographic peak.

6.2.2.2 Flow Velocity Correction

The elution volume is calculated by flow rate and retention time, and small changes in flow rate will have a significant impact on the accuracy of molecular weight test results. Select a small molecular weight sample (flow rate marker) and add it to the standard or sample to make the retention time in different chromatograms more accurate.

6.2.2.3 Universal Calibration

The separation of polymer molecules on a chromatographic column depends on the size of the molecules, not their molecular weight. The size of polymer molecules is not only related to their molecular weight, but also to their configuration (linear, dendritic, and star shaped) and conformation (solvent and temperature dependent). If the K and alpha values of the polymer are known, the Mark-Houwink equation can be used to calculate the molecular weight of molecules

with the same size.

6.2.3 GPC Integral Settings

Click on the "Integral" tab in the analysis method settings dialog box to set the integral parameters for generating the graph, as shown in Figure 6-19.

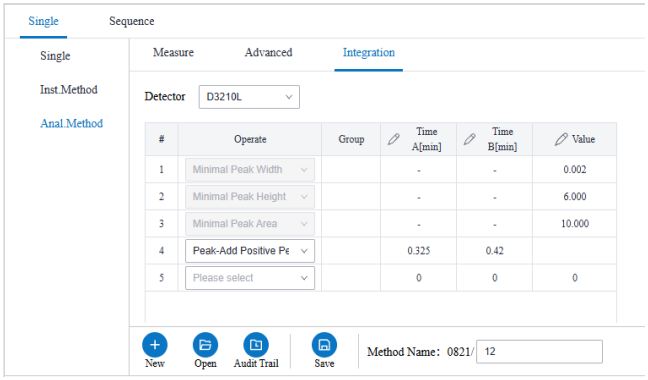


Figure 6-19 Integral Event Setting

The GPC mode "Analysis Method Setting Integral" and the standard mode "Analysis Method Setting Integral" are similar, but have the following three differences:

1) The way GPC pattern recognizes solvent peaks is different from the standard pattern. GPC pattern marks all peaks that appear in the selected interval as solvent peaks. Once marked as a solvent peak, this peak will be removed from the GPC result table.

2) Add flow rate marker 

function, GPC mode can set a peak for flow rate correction calculation. There is only one peak in the entire chromatogram that can be labeled as the flow rate labeled peak.

【Attention】 If the GPC calibration option window selects "Use flow rate correction", the flow rate marker peak must be marked, otherwise the flow rate correction function will not work.

3) The group function  is not available in GPC mode. To obtain the average values of

different molecular weight distributions of polymers, the "delete peak" and "add positive peak" functions are used to integrate multiple peaks into a single peak.

6.2.3 Analysis

3.2.3.1 Single Analysis

In the single analysis dialog box, K and alpha values can be entered, which can be used to input the Mark-Houwink equation for universal calibration. 14.1 and 0.7 are the K and α values of linear polystyrene in tetrahydrofuran solvent at 25℃, respectively. Users can read the appropriate K and alpha values by clicking on Read K & Alpha. Other settings are the same as those in standard mode.

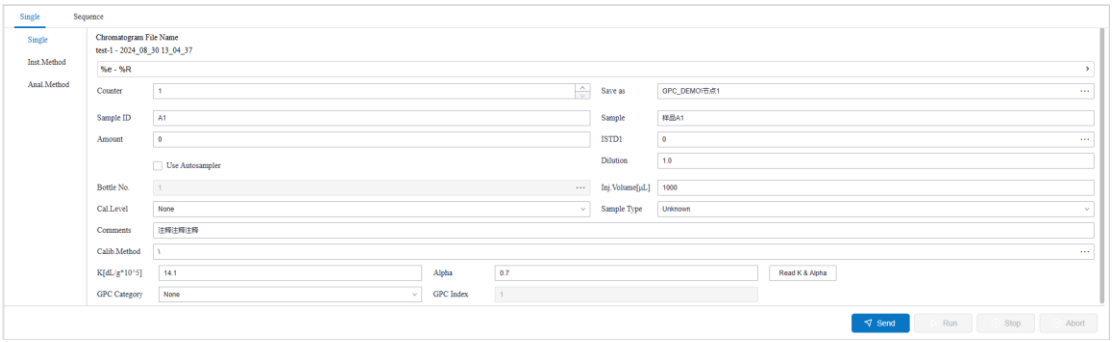


Figure 6-20 Single Analysis

In the data processing window, if you select the corresponding file through the "Directory" menu to open the chromatogram, the K value and alpha value will be opened together.

3.2.3.2 Sequence Analysis

In the sequence analysis window of GPC mode, input columns for K value and α value have been added. The GPC standard type and GPC standard number are used for automatic recalibration of GPC during sequence operation.

Other settings are the same as standard mode.

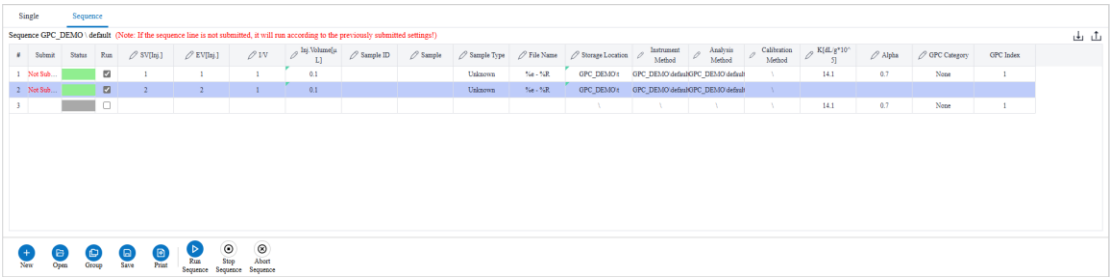


Figure 6-21 Sequence Analysis

6.2.4 GPC Data Processing Window

In the GPC data analysis window, chromatograms, molecular weight distributions, or cumulative molecular weight distribution tables can be selectively displayed (with GPC calibration set).

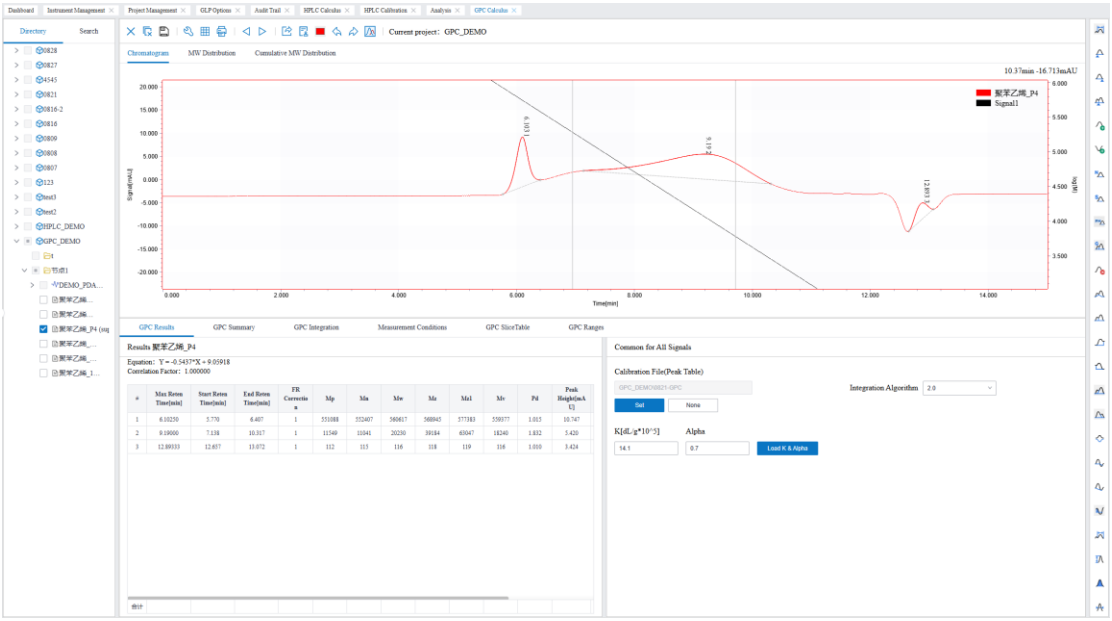


Figure 6-22 Chromatogram Window

The GPC results, GPC summary, GPC integral, measurement conditions, GPC slice table, and GPC range can all be displayed below the window.

6.2.4.1 Chromatogram

The GPC chromatogram can be viewed in the GPC data processing window in the same way as HPLC data processing.

6.2.4.2 MW Distribution

The MW distribution map displays the molecular weight distribution of the selected peak. Click on the row where the peak is located in the "GPC Results" to select the peak. The retention time of the peak is displayed in the upper right corner of the image, as shown in Figure 6-23.

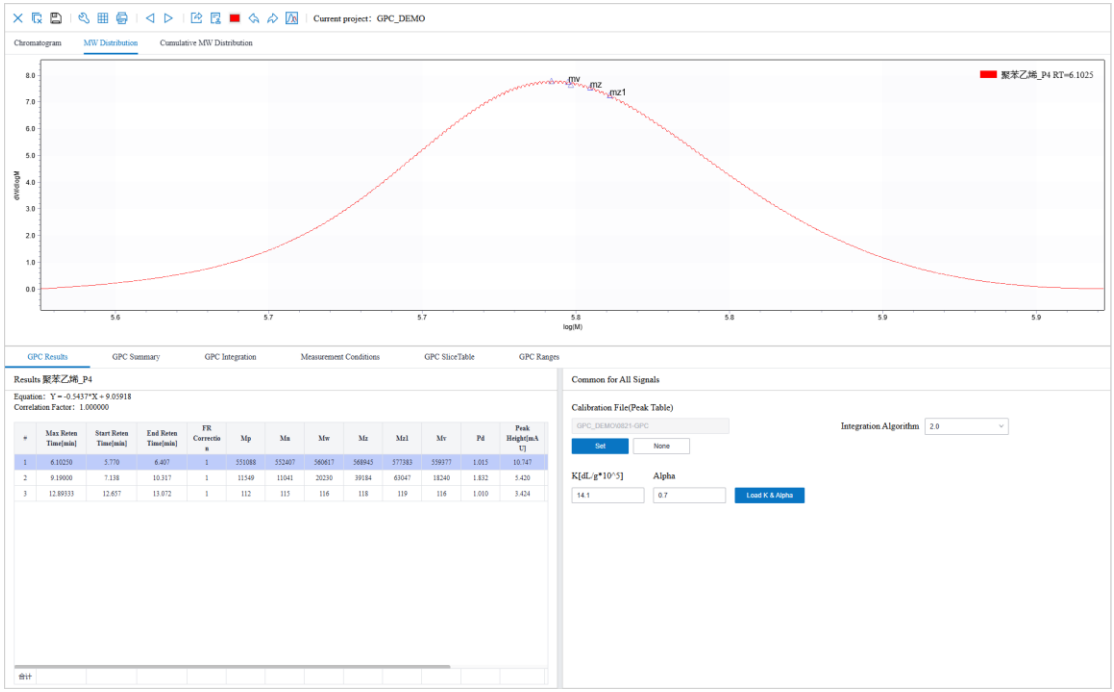


Figure 6-23 Chromatogram-MW Distribution

6.2.4.3 MW cumulative distribution

MW cumulative distribution displays the cumulative molecular weight distribution (%) of the selected peak. Click on the row where the peak is located in the "GPC Results" to select the peak.

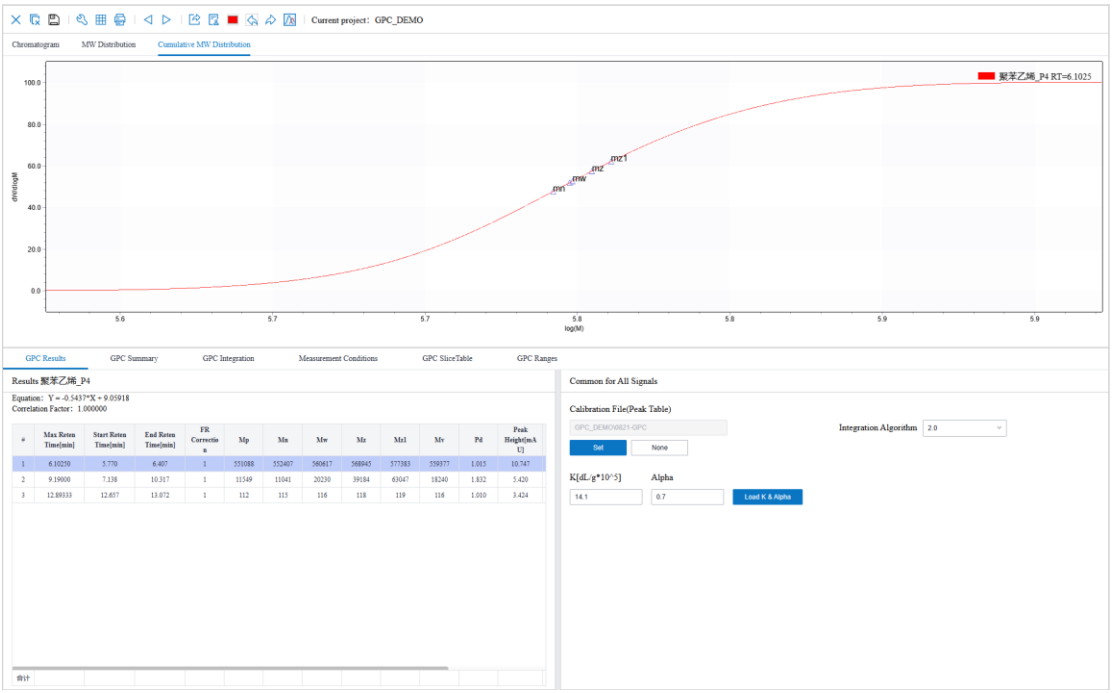


Figure 6-24 Chromatogram-Cumulative MW Distribution

6.2.4.4 GPC Results

On the right side of the GPC result table, you can choose whether to add a calibration file.

1） None means that the calibration curve is not added, and all molecular weight results in the results table show NA.

2）The Set function can select the saved calibration curve, and all molecular weight results in the result table are displayed normally.

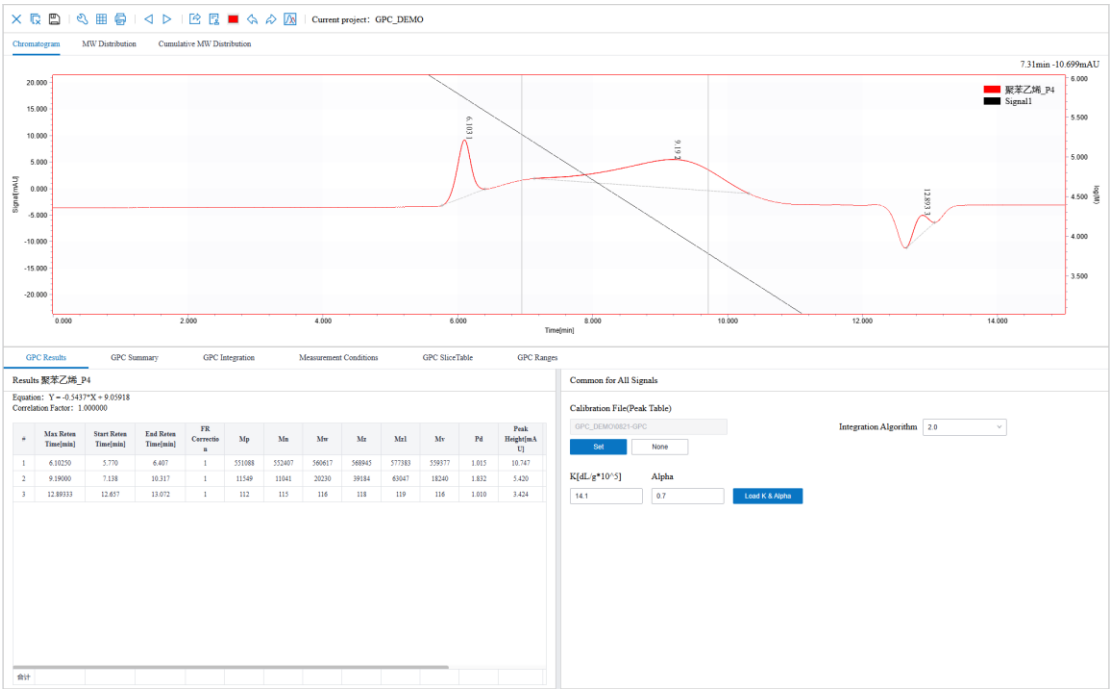


Figure 6-25 GPC Results Table

- Max.RT : Retention time of peak maximum;
- Start RT : Retention time of peak integration start;
- End RT : Retention time of peak integration end;
- Mp : Molecular Weight at peak maximum;
- Mn : Molecular Weight number average;
- Mw : Molecular Weight weight average;
- Mz : Molecular Weight Z average;
- Mz1 : Molecular Weight Z+1 average;
- Mv : Molecular Weight viscosity average;
- PD :Polydispersity;
- Flow Rate Correction : Flow rate correction factor;

Other parameters are the same as standard mode parameters.

6.2.4.5 GPC Summary

The GPC Summary table contains parameters for all peaks, and the table queue can be set by right-clicking.

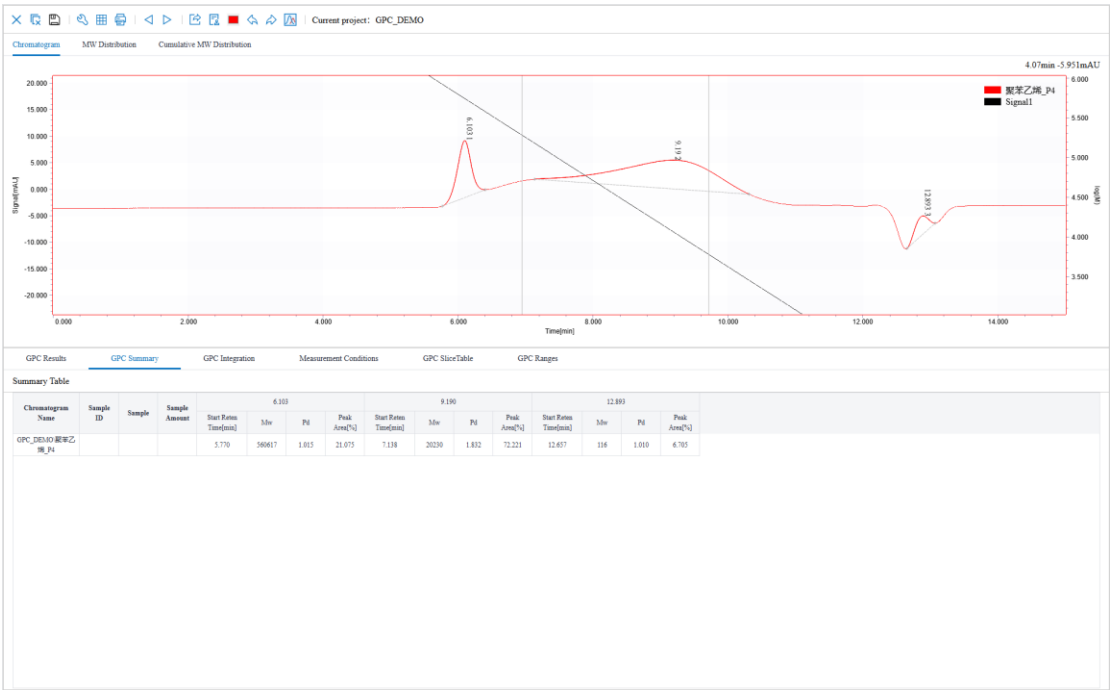


Figure 6-26 GPC Summary table

6.2.4.6 GPC Integration

GPC integration can display or edit all operations on chromatographic peaks, all operations can be added directly in the table, or in the chromatogram window using the integration tool button on the right to add.

Most operations are the same as in standard mode, see 6.2.3 for differences.

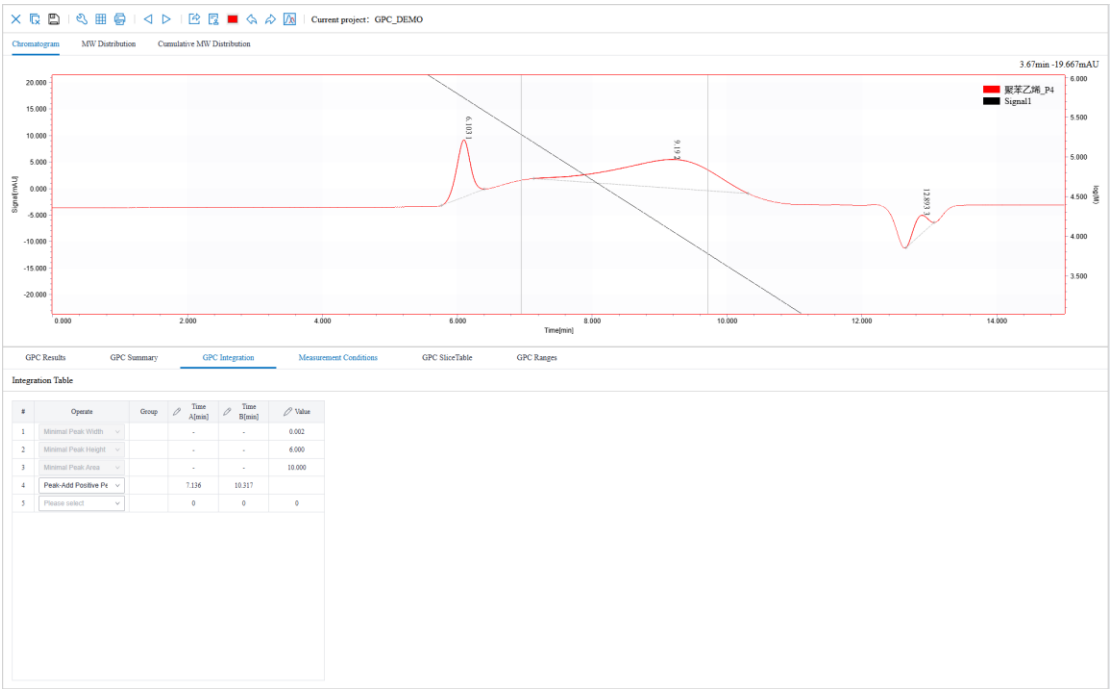


Figure 6-27 GPC Integration table

6.2.4.7 Measurement Conditions

The content of the measurement conditions is the same as that of the standard mode, see 6.1.7.

6.2.4.8 GPC Slice Table

The GPC slice table displays cumulative molecular weight distribution results for selected peaks.

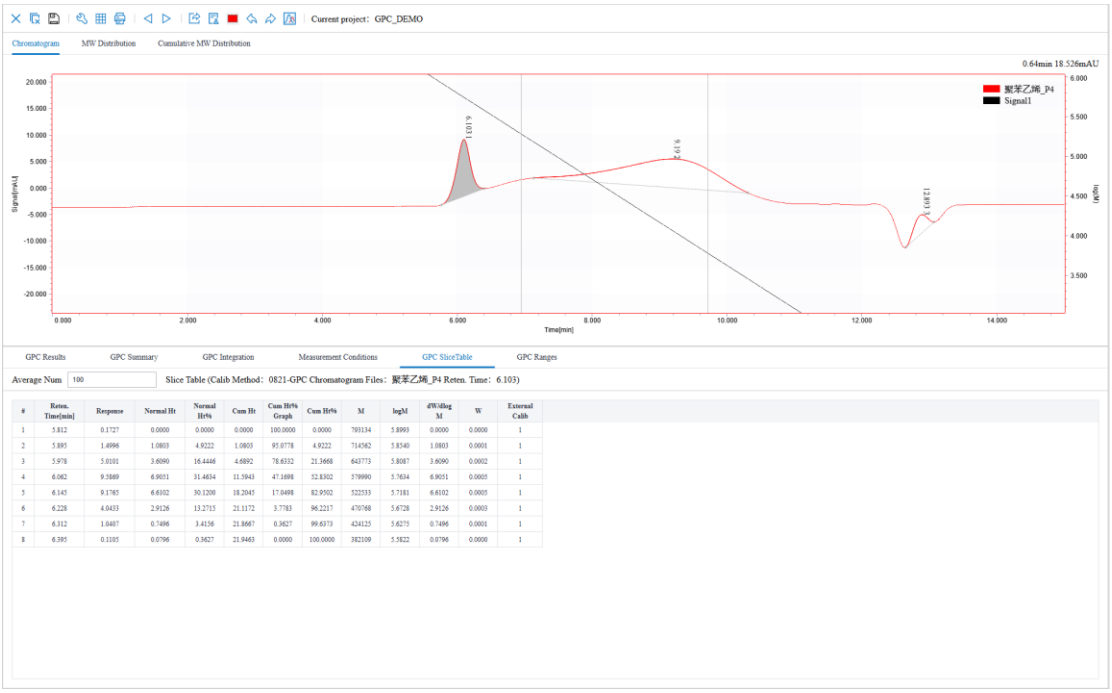


Figure 6-28 GPC Slice table

The average number depends on the integration interval and peak width set in the "GPC Integration" table, ranging from 1 to 100.

- RT : Retention time of the slice (averaged);
- Response : Slice peak height(averaged);
- Norm. Ht: Normalized slice height(summed);
- Norm. Ht%: Percentage of the slice height from total of all slices height(summed to give total 100%);
- Cum. Ht: Cumulative slice height(averaged);
- Cum. Ht%: Cumulative percentage of the slice height from the total of all slices heights(averaged);
- Cum. Ht% Graph: Cumulative percentage of the slice height from the total of all heights in the inverse order(increasing with increasing)(averaged);
- M: The molecular weight corresponding to the slice retention time(averaged);
- Log M: The logarithm of the molecular weight corresponding to the slice retention time(averaged);
- dW/d log M: Normalized distribution of slice molecular weights used for the graph in the MW

Distribution tab;

- W: Normalized slice height used for molecular weight distribution calculation;
- Outside Calibration: Flag marking whether the slice is inside or outside of the used calibration retention time range. Outside of the range gives value 1, while inside the range gives value0.

6.2.4.9 GPC Ranges

The GPC Range table is used to calculate area percentages that define a range of molecular weights, or to calculate average molecular weights that define a range of area percentages. The type of range (whether percentage or molecular weight) can be chosen arbitrarily.

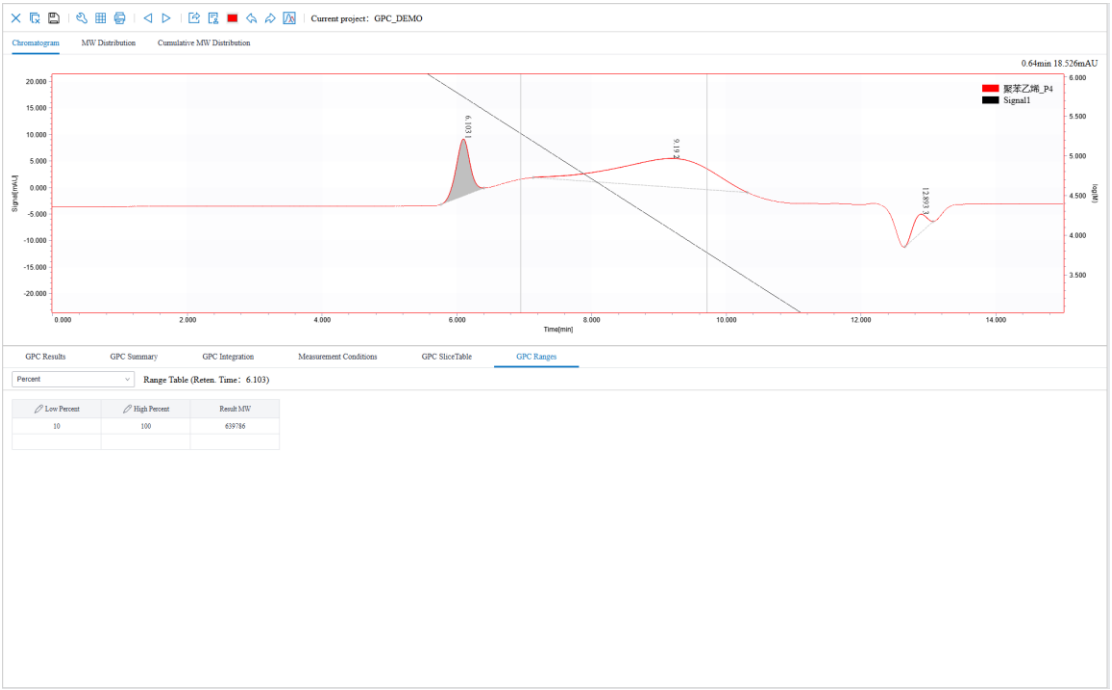


Figure 6-29 GPC Ranges

For example, when the average molecular weight of 10% of the final peak area needs to be calculated, the low and high percentages are set to 90 and 100, respectively. Multiple ranges of the same type can also be set.

6.3 PDA Module

The PDA module is an independent module designed specifically for use with diode array detectors. Below is a brief introduction to the PDA module:

6.3.1 Module Configuration

The configuration method of the PDA module is the same as that of conventional instruments, only requiring the instrument management to select the PDA detector when adding instruments, and then use the PDA detector as the detector for subsequent analysis. Refer to the configuration of the conventional instrument management system for specific steps.

6.3.2 Method Settings

6.3.2.1 Instrument Method Setting

The PDA instrument method is the same as the conventional instrument method setting, but it is necessary to pay attention to the choice of chromatogram output format when setting detector parameters. The default option is 2D output, that is, it does not contain chromatogram, 3D chromatogram and other information, and 2D or 3D output can be automatically selected according to demand.

6.3.2.2 Analytical Method Setting

The analytical method Settings are the same as the general Settings.

6.3.3 Data analysis

6.3.3.1 2D Chromatogram Analysis (conventional Chromatogram)

The chromatogram stored in the 2D chromatogram mode of the PDA is consistent with the conventional chromatogram, and the data processing method is also consistent, see Section 6.1 for

details.

6.3.3.2 3D Chromatogram Analysis (PDA Chromatogram interface)

(1) PDA chromatogram interface

Click "PDA chromatogram " under "Data processing" to open the PDA chromatogram page, as shown in Figure 6-30. By default, this interface only opens chromatogram, spectrogram, contour view and peak purity spectrum view. Click the button in the upper left corner to open the chromatogram list, select the PDA chromatogram and click OK to open the display.

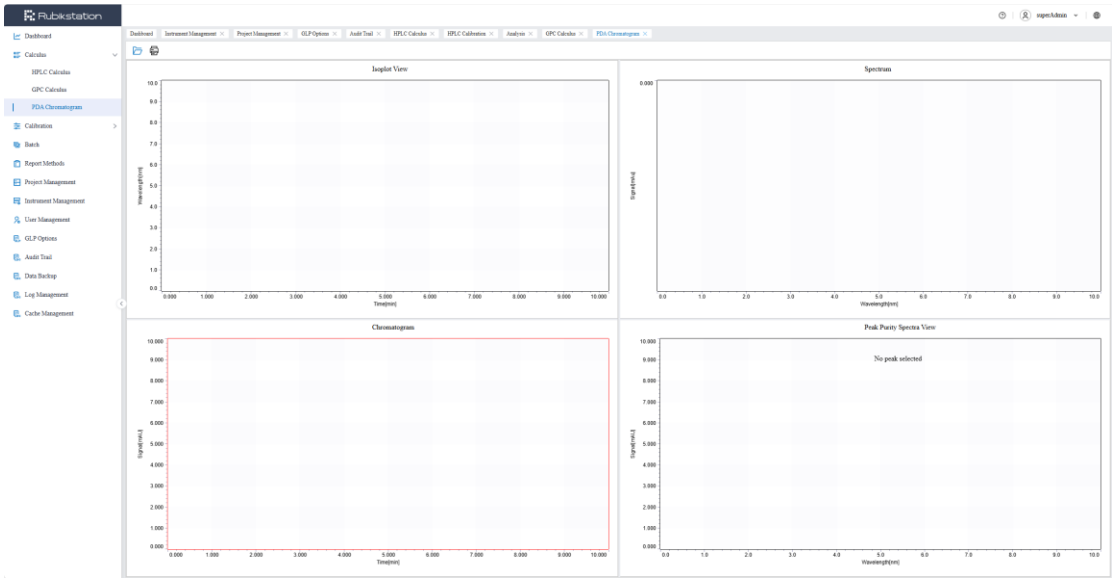


Figure 6-30 PDA chromatogram screen

(2) 3D view

After opening the PDA chromatogram, right-click in the "Chromatogram" area - select "Show 3D View" to open the "3D View" interface (Figure 6-31). The 3D view interface is displayed, as shown in Figure 6-32.

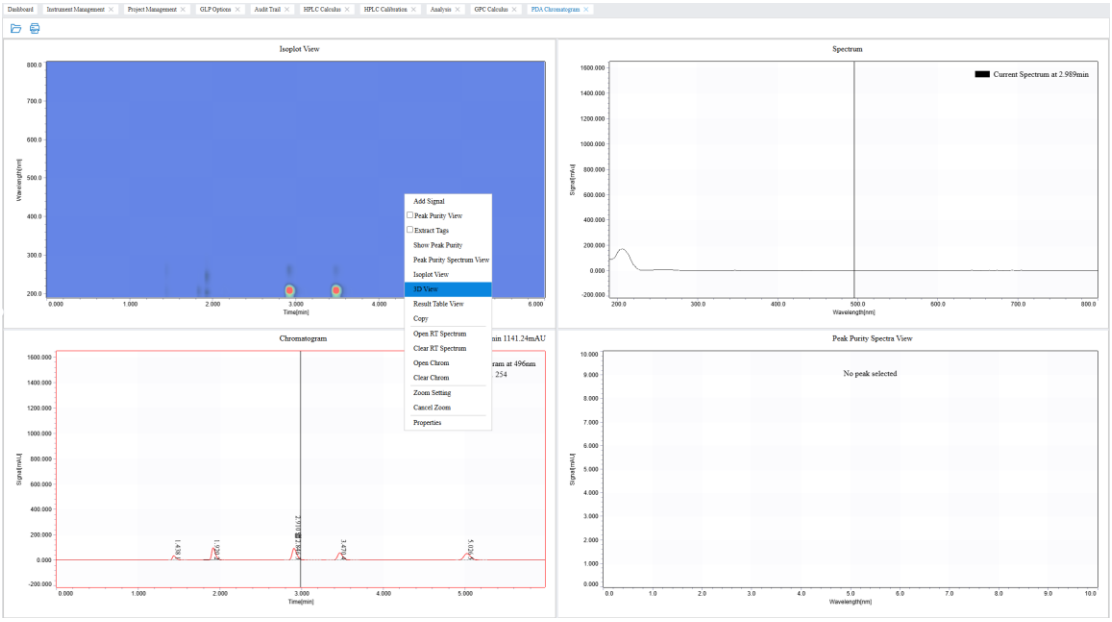


Figure 6-31 Opening the 3D view screen

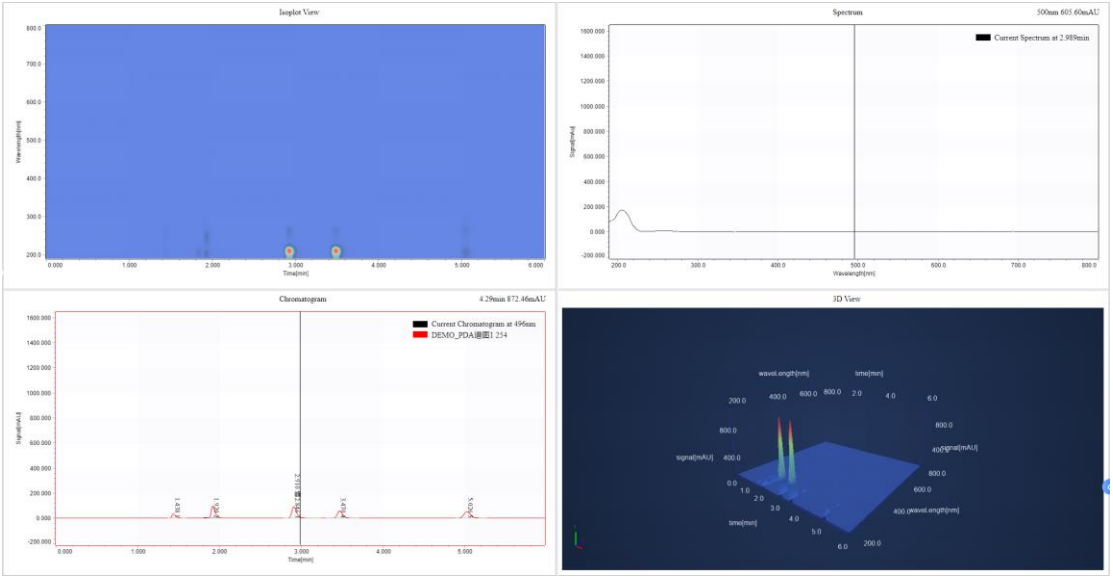


Figure 6-32 3D view screen

(3) Peak purity spectrum view

Drag the mark line in the "Chromatogram" area to move to the selected peak, and then right-click in the "Chromatogram" area and select Show peak purity spectrum to open.

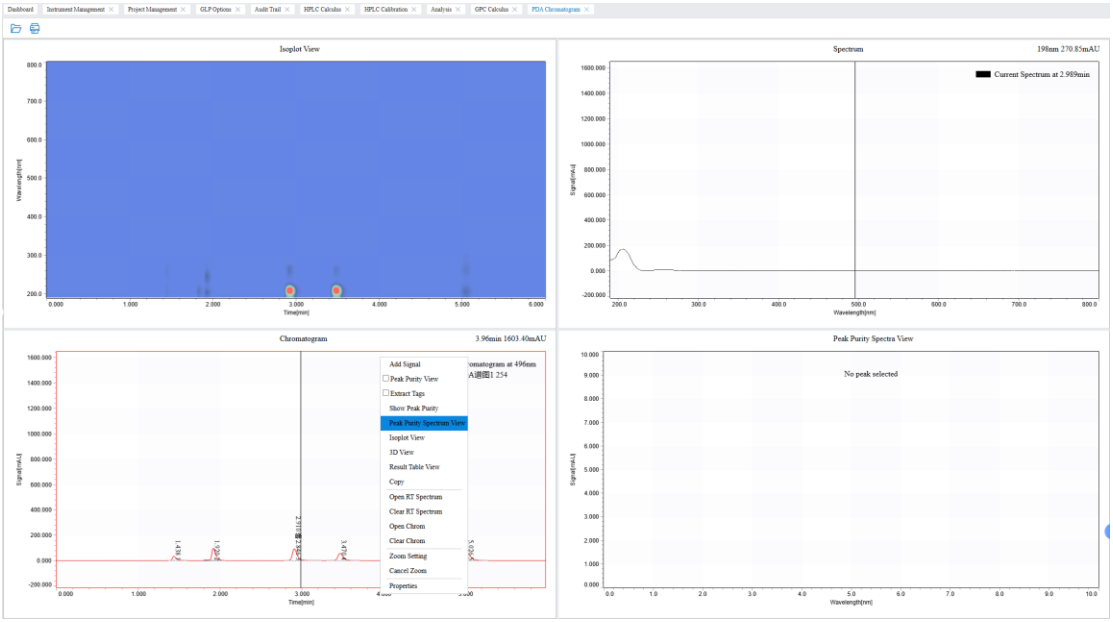


Figure 6-33 Show Peak purity spectra

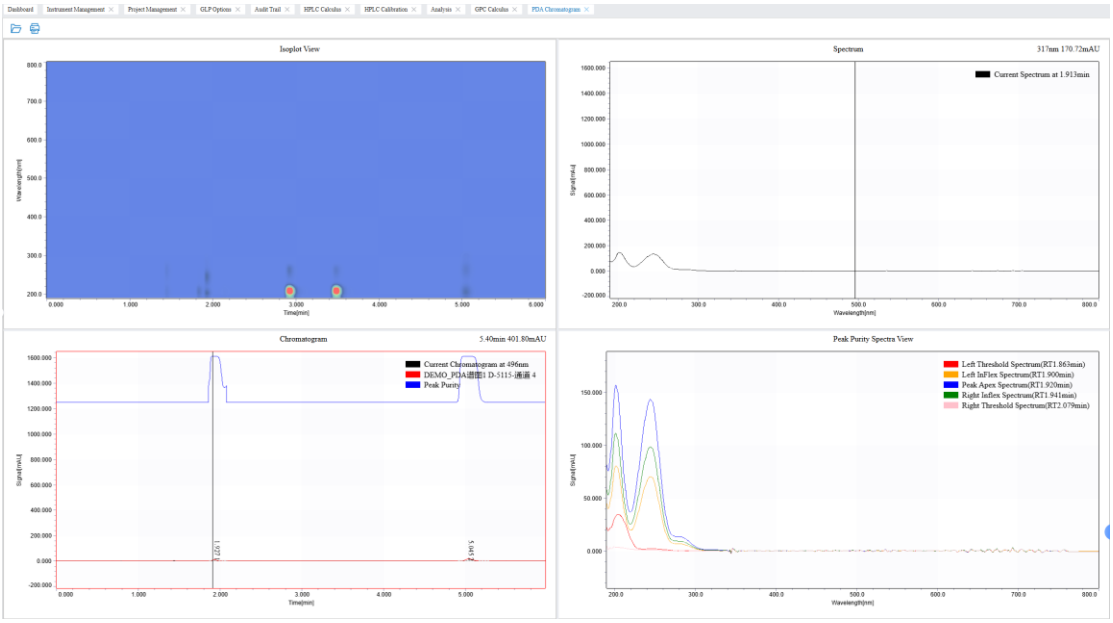


Figure 6-34 Peak purity spectrogram

(4) Peak purity curve

Right-click in the Chromatogram area and select Peak Purity Curve to display the peak purity curve in the chromatogram, as shown in Figure 6-35 and 6-36.

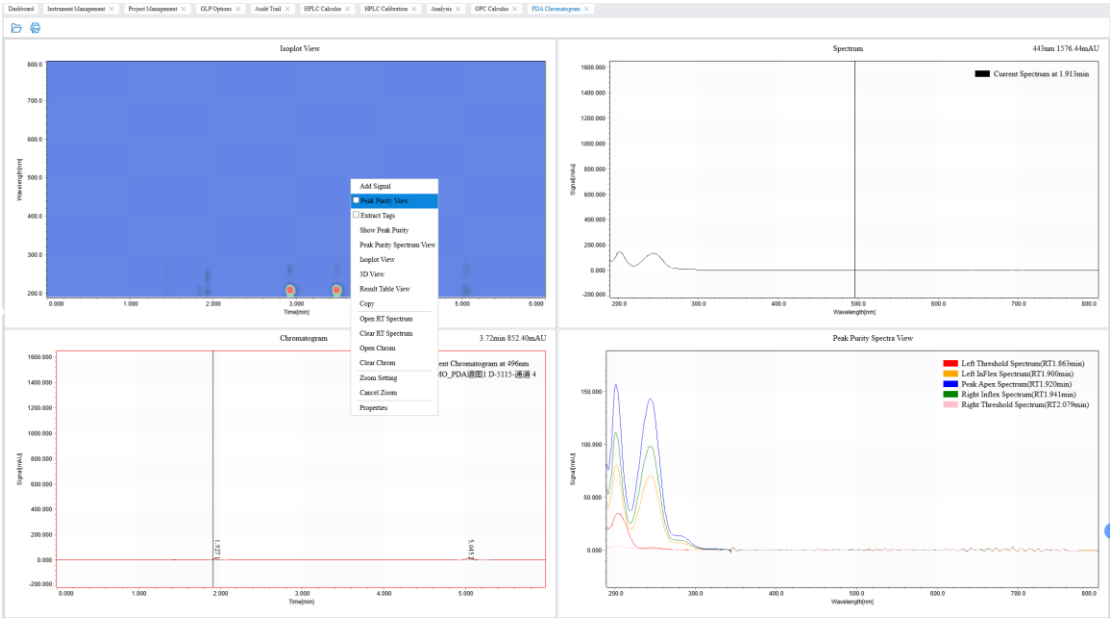


Figure 6-35 Shows the peak purity curve

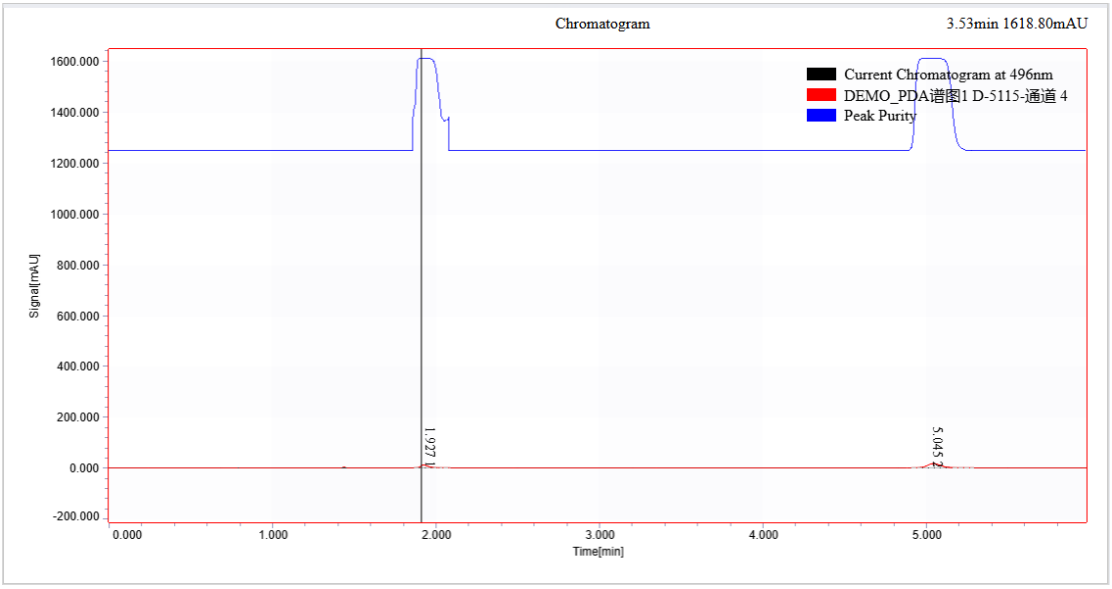


Figure 6-36 Peak purity curve

(5) Peak purity view

Right-click in the "Chromatogram" area and click "Show Peak Purity" to display the peak purity view in the lower right area, as shown in Figure 6-37.

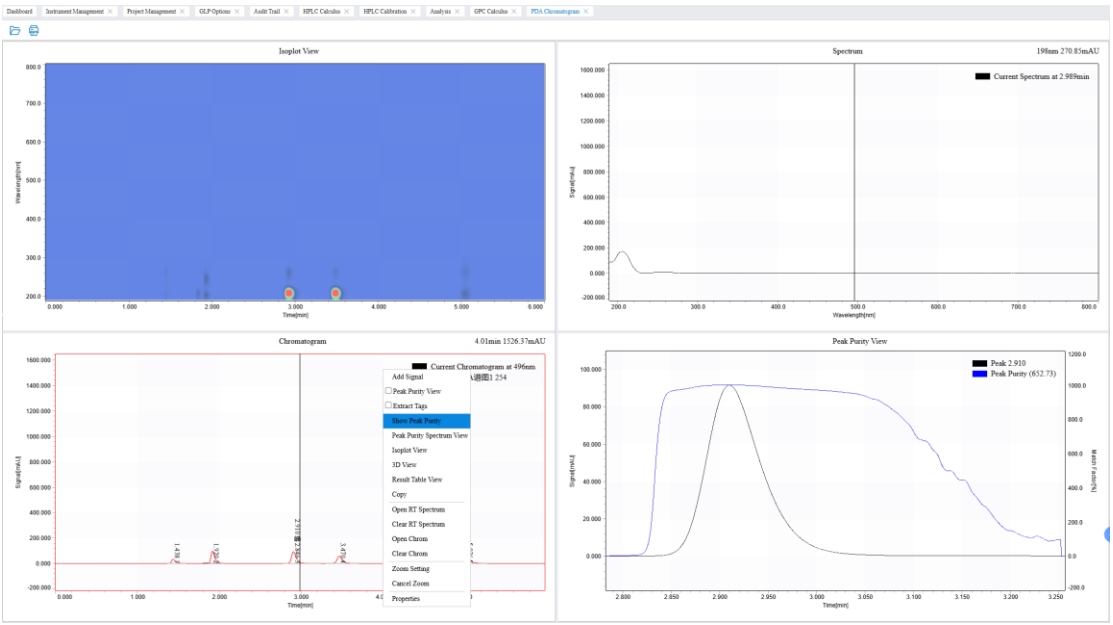


Figure 6-37 Peak purity view

(6) Add chromatogram signal

Right-click in the Chromatogram area and choose Add Signal to bring up the Add Chromatogram Signal window, as shown in Figure 6-38. In this window, you can set the wavelength, reference, and so on to add chromatogram.

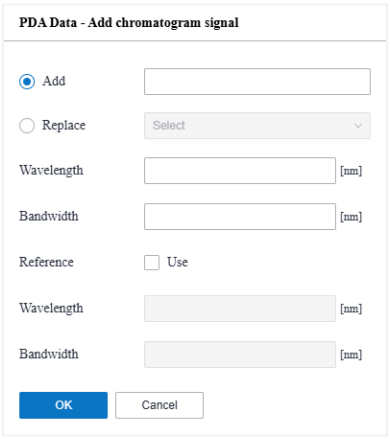


Figure 6-38 Add chromatogram signal

(7) Properties

Right-click in the "Chromatogram" area or "Spectrogram" area and select the "Properties" option to bring up the "Properties" setting window, as shown in Figure 6-39. In this window, you can set axis parameters and so on.

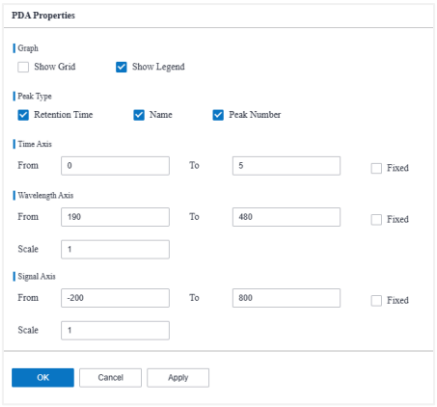


Figure 6-39 Properties window

(8) Spectrum Library

Right-click in the "spectrum chart" area to pop up the spectrum library related options. It includes the functions of creating a new library, opening the library, adding to the library, searching in the library, etc. As shown in Figure 6-40.

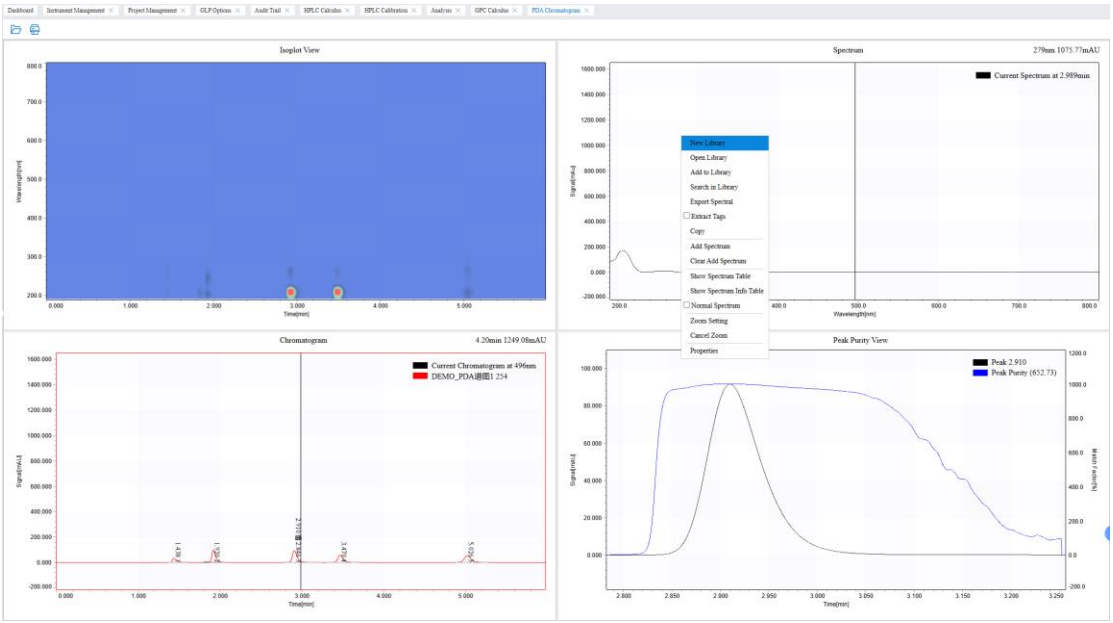


Figure 6-40 Right-click in the Spectrum area

(9) Spectrum library view

This view displays spectrogram information for the spectrum library that has been opened. In this view, the spectrum name and comments can be changed. If "Show spectrum" is checked, the spectrum diagram corresponding to the library spectrum and the current chromatogram can be displayed in the spectrum diagram view at the same time. Figure 6-41 shows the diagram.

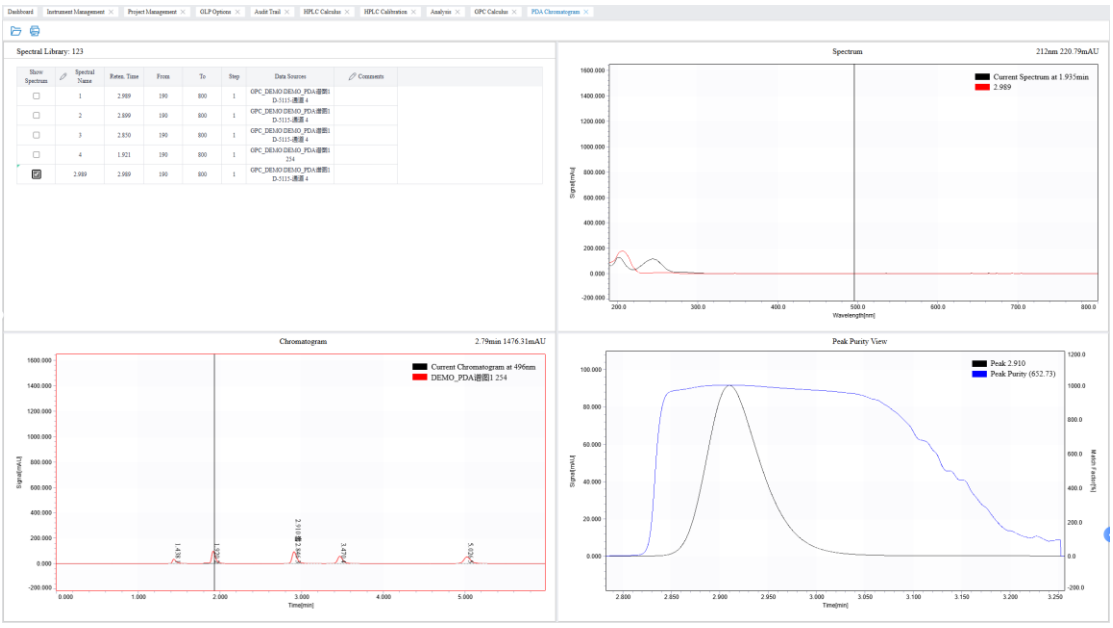


Figure 6-41 Spectrum library view

(10) Spectrum Library search results view

This view displays spectrum library search results. As shown in Figure 6-42.

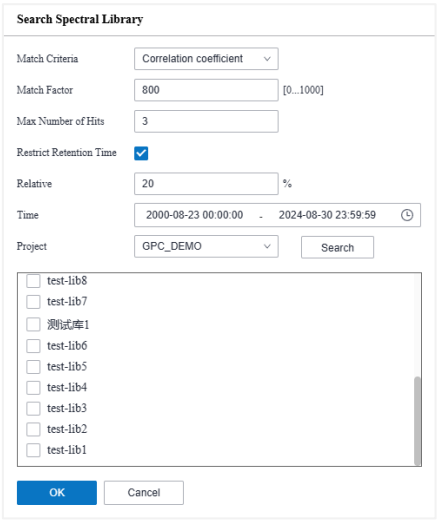


Figure 6-42 Spectrum Library search list

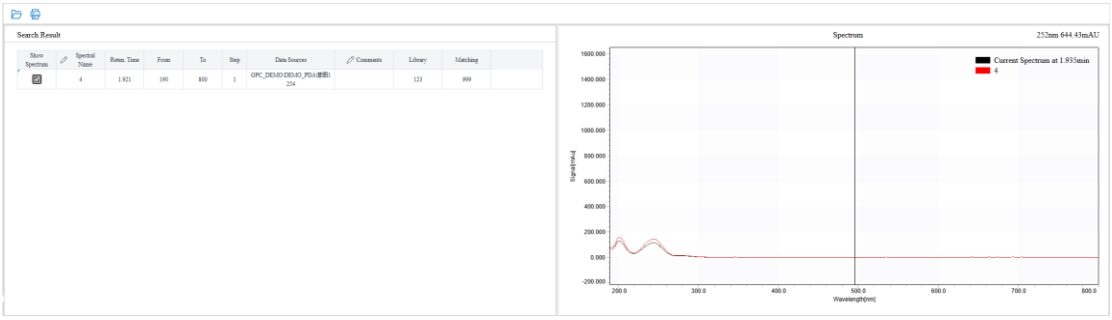


Figure 6-43 Spectrum library search results view

7 Calibrate

Calibration involves setting up the calibration file with calling the calibration file

7.1 Percentage Method

This method requires that all compounds in the sample are eluded and integrated by the mobile phase, and the response factors of all components (that is, the same peak area of the same content or the same peak height, in general, this method is used when the universal detector is used) are exactly the same. The percentage method can be used to quickly approximate the relative content of each component. This method is mainly used to estimate the relative content of impurities or degraded compounds in a pure substance.

7.2 Normalization method

This method requires that all compounds in the sample have been elided and integrated, and that the response factors for all components are known. In the normalization method, the response factor is used for peak area or peak height to compensate for variations in detector sensitivity for different sample components.

The formula used to calculate the compound content:$x\% = \frac{Response_x \cdot RF_x}{\sum(Response \cdot RF)} \times 100\%$

$Response_x$: The area or height of peak X

RF_x : Response factor of peak X

$\sum(Response \cdot RF)$: The sum of the response values of the area or height of all peaks

Advantages: simple, the accuracy of the sample size and the change of operating conditions have little influence on the determination results.

Note: in the percentage method and normalization method, when the peak area is used as the quantitative basis, all peaks are required to peak and baseline separation; When the peak height is used as the quantitative basis, the peak shape is required to be better (peak trailing factor is between

0.95 and 1.05).

7.3 External standard method

This method is the most commonly used and most basic method for determining the concentration of an unknown sample. $y = ax + bA$ standard solution of known concentration (a pure product of the compound to be tested) is prepared, injected into the liquid chromatography and analyzed in the same volume of each standard solution, and then the concentration is plotted with the peak response value. A calibration curve is obtained. See Figure 7-1.

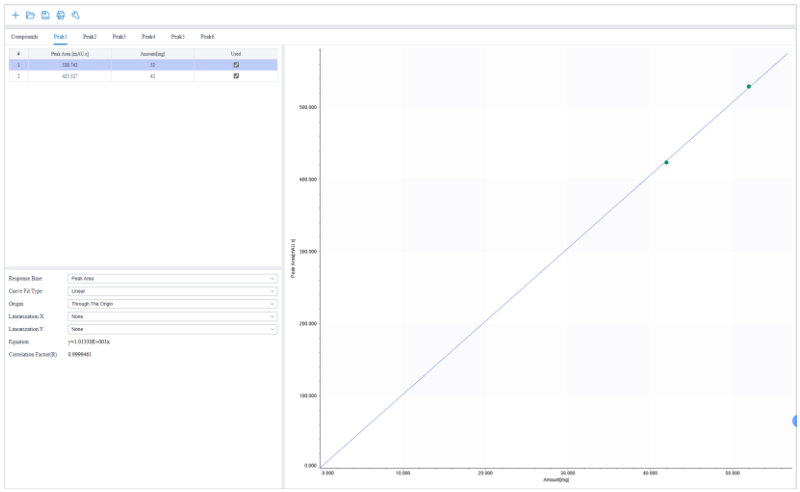


Figure 7-1 Calibration curve of the external label

7.3.1 Making calibration curve

Before making calibration curves, the chromatogram of the standard product used for calibration should be pretreated to remove unnecessary peaks and correct integration conditions.

(1) Open the calibration page

Click "HPLC" calibration under "Calibration" to open the HPLC calibration page. On the left side of the calibration page is the chromatogram list, and on the right side is the calibration summary table and calibration curve and other information. See Figure 7-2.

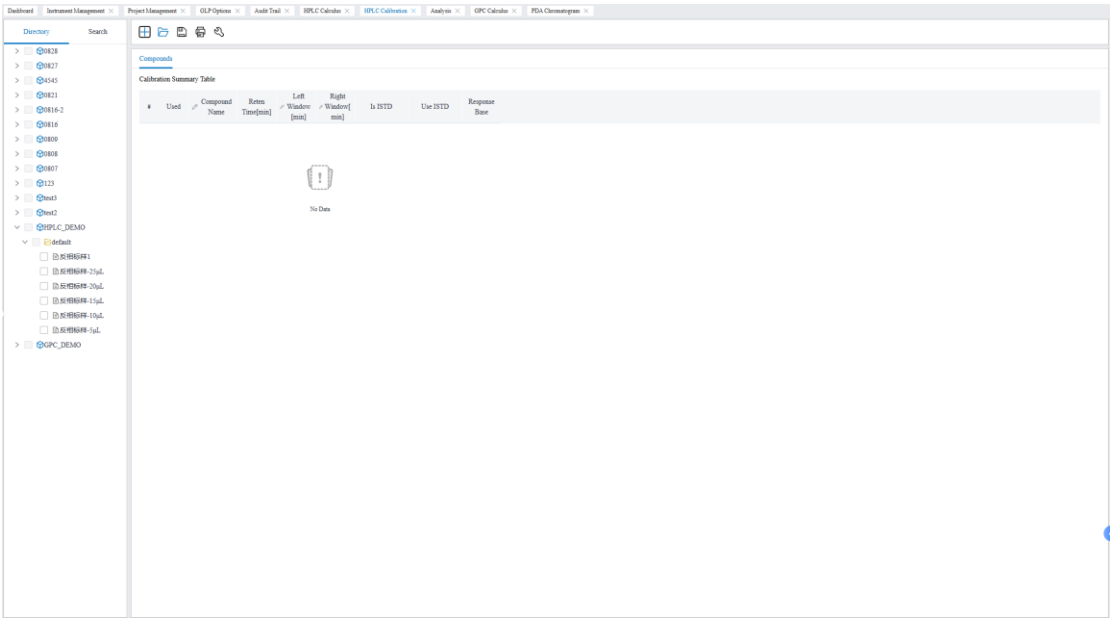


Figure 7-2 The Calibration window is displayed

(2) Unit Settings

Click the button in the calibration window to set the calibration response, response unit and decimal number;  As shown in Figure 7-3.

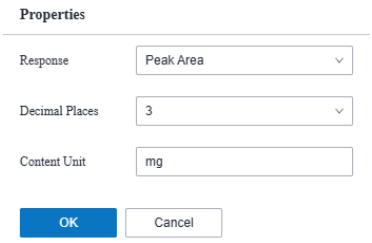


Figure 7-3 Calibration unit Settings

(3) Open the pre-processed standard spectrum in the left chromatogram list, and all integral peaks of the standard spectrum will be displayed in the calibration summary table on the right, as shown in Figure 7-4.

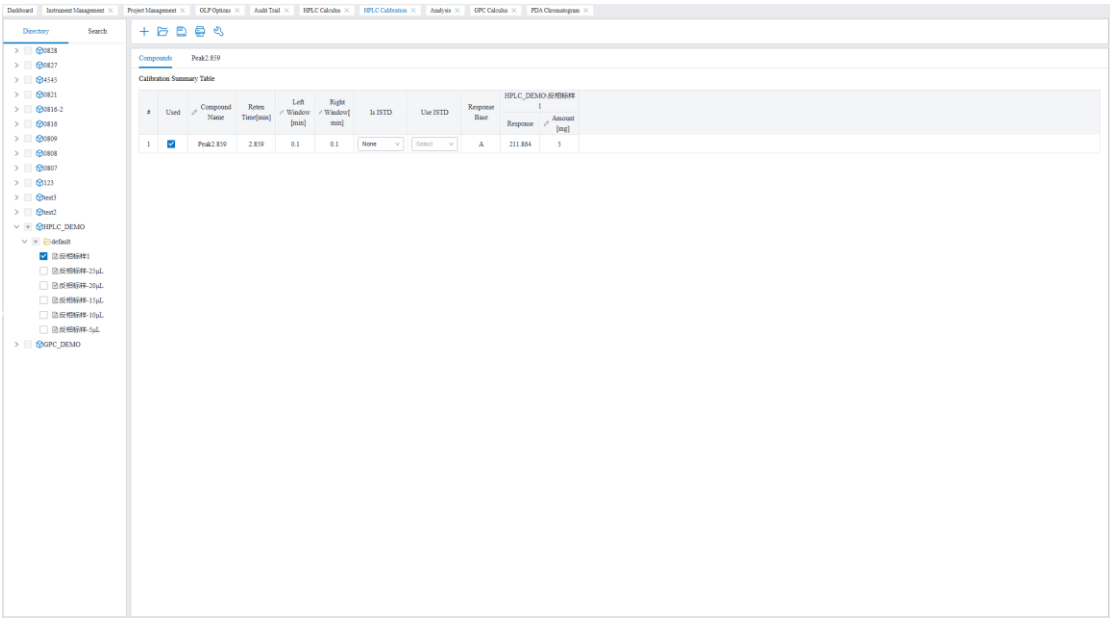


Figure 7-4 Open the first calibration spectrum

(4) Select the calibration peak you want to use in the Calibration Summary Table. The name of the calibration peak is "Peak + retention time" by default. The response is based on the peak area or peak height.

(5) Repeat steps (3) - (4) until the files needed for calibration are added.

(6) After setting the calibration point, you can view the calibration curve in the TAB of the corresponding compound and set the calibration method of the calibration curve, as shown in Figure 7-5. If the column of "Used" of a calibration point in the information table on the upper left is left blank, the calibration point will be displayed as a circle in the calibration table, and the calibration point data will not be calculated when the curve is calculated.

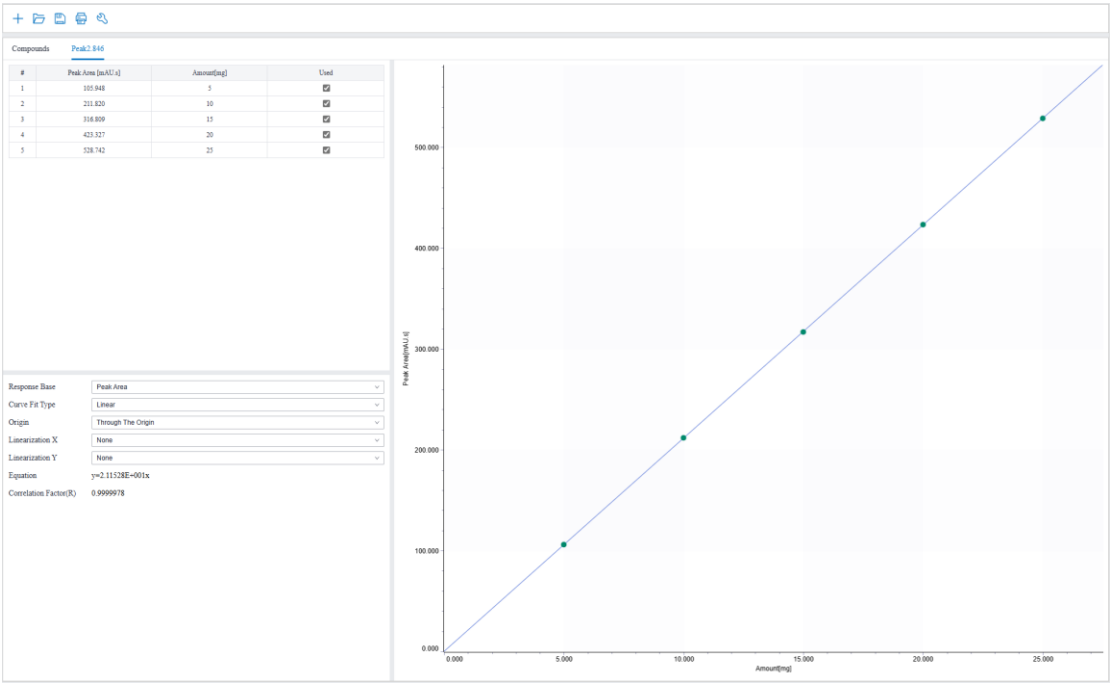


Figure 7-5 Calibration curve - Individual substance

After the calibration curve is finished, click the icon of the "Calibration" window menu to save the standard curve.

7.3.2 Use of calibration curve

(1) Open the chromatogram of the test sample and choose whether to modify the integration condition as needed.

(2) In the right half of the "Result" TAB, click "Setting" in the "Calibration file" column to select the calibration file, and select the type of calibration file and set other calibration parameters in the "Calculation" column.

(3) After the setting, the quantitative calculation results of each substance in the sample corresponding to the calibration curve will be displayed in the "Result" TAB and "Summary" TAB, as shown in Figure 7-6.

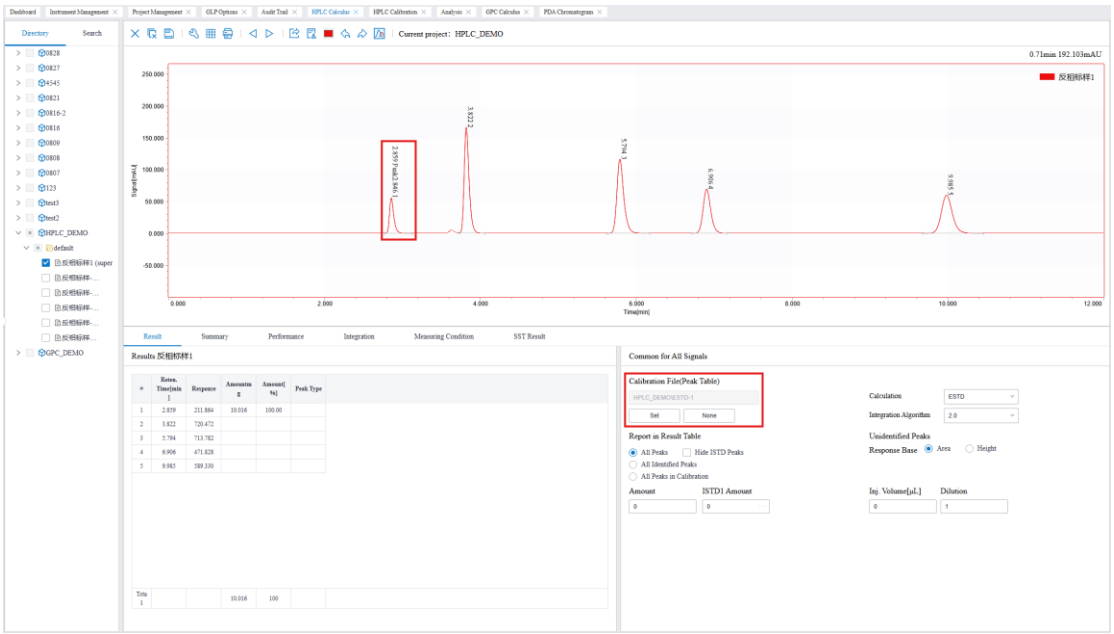


Figure 7-6 External standard method - Use of calibration file

After setting the calibration curve, click Save chromatogram.

7.4 Internal standard method

7.4.1 Overview

Internal standard method refers to the addition of a known content of a component to the standard sample and sample to produce a uniform factor, the component is the internal standard. The compound used as the internal standard should be chemically similar to the compound being corrected, with a similar retention time, but can be completely separated on the chromatogram.

This internal standard method does not require high sampling repeatability for the chromatogram. There are two steps to calculate the ratio of the corrected content of a specific compound in an unknown sample:

1. Correction

Each point in the correction curve is composed of the calculated value of the content ratio and response value ratio of a peak in the correction table.

Content ratio: the content of the compound of this grade divided by the content of the internal standard

Response value ratio: The area of the class compound divided by the area of the inner standard

2. Unknown sample

The ratio of the response value of the unknown compound divided by the response value of the unknown sample to the response value of the unknown sample, the amount of the unknown sample is obtained by the above calibration curve.

7.4.2 Production of calibration curve

The steps of making calibration curves by internal standard method are the same as the first five steps of external standard method, the difference lies in the sixth step.

For steps 1 to 5, please refer to Steps (1) to (5) of the external standard method, as detailed in 7.3.1.

(6) After the calibration point is set, set the items "for ISTD" and "Use ISTD" in the calibration summary table, set the peak of the internal standard to "for ISTD", and the summit of the measured substance will automatically set "Use ISTD"; Check the calibration curve in the TAB of the corresponding compound and set the calibration method of the calibration curve, as shown in Figure 7-7.

After the calibration curve is made, click the icon of the "Calibration" window menu to save the made standard curve.

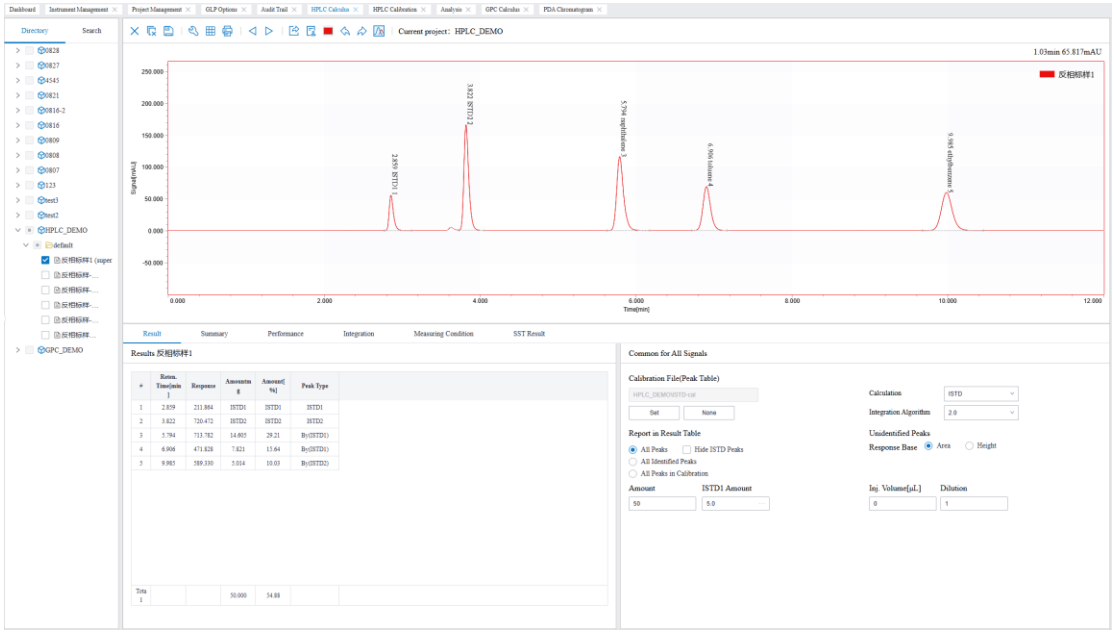


Figure 7-7 Internal standard method - Calibration file

【 Note 】 When making the internal standard calibration curve, only one of the correction substances can be set as the internal standard.

7.4.3 Use of calibration curve

The invoking method of the internal standard calibration curve is basically the same as that of the external standard method. The difference is that after invoking the internal standard calibration curve, parameters such as the content and total amount of the internal standard need to be set on the data processing page, as shown in Figure 7-8. When using the internal standard calibration file, it is necessary to set "Calculation" in the lower right area of data processing, select "ISTD", and then fill in the values of "total amount", "ISTD amount", "sample volume" and "dilution". After correctly filling in, the workstation will automatically calculate the peak content of the measured substance and other related parameter results.

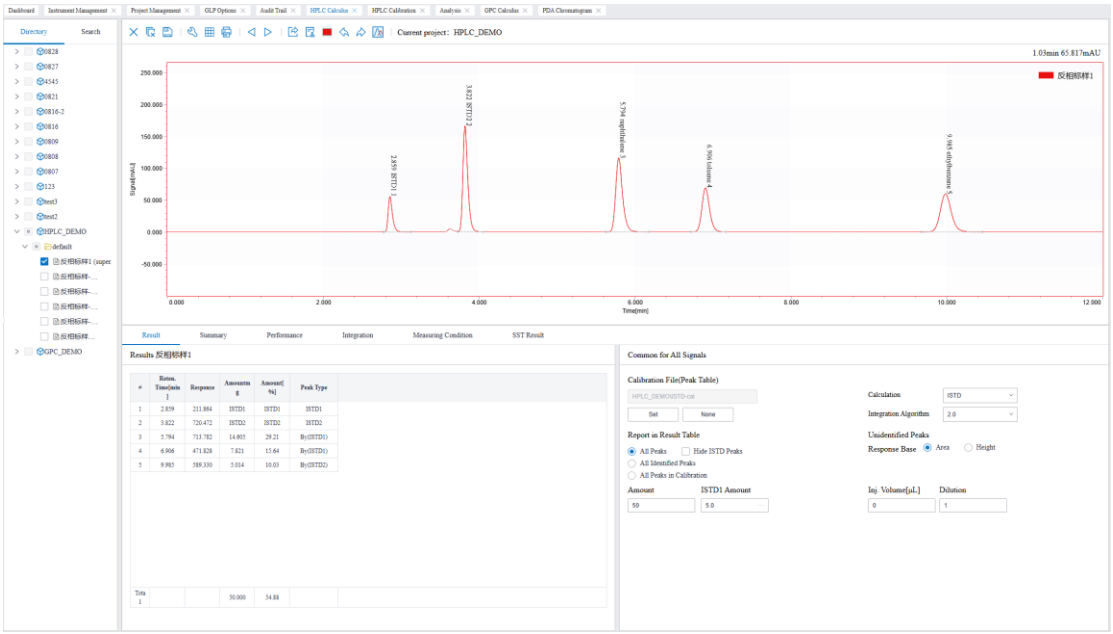


Figure 7-8 Internal standard method - Use of calibration file

If only "ISTD" is selected in "Calculation" and no parameters such as content are set, the corresponding result such as content will not be calculated in the result table, and a prompt message will be displayed on the right under the content, as shown in Figure 7-9.

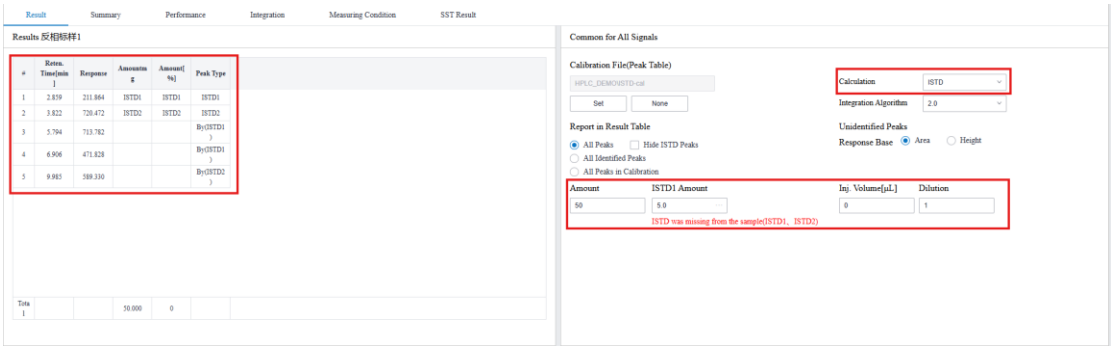


Figure 7-9 Internal standard method - No parameter is filled in

Once the calibration curve is set, click Save chromatogram.

7.5 Quantitative Calculation (GPC)

Quantitative calculations are performed using the GPC calibration curve, which is used to calculate the molecular weight distribution of the polymer sample.

7.5.1 Opening of calibration window

Click "GPC Calibration" in the following table of "Calibration" to enter the GPC calibration window, which is used to make, modify and display the calibration curve. In the image area of the calibration curve window, the chromatogram of the last opened standard sample and the calibration curve are displayed at the same time, as shown in Figure 7-8.

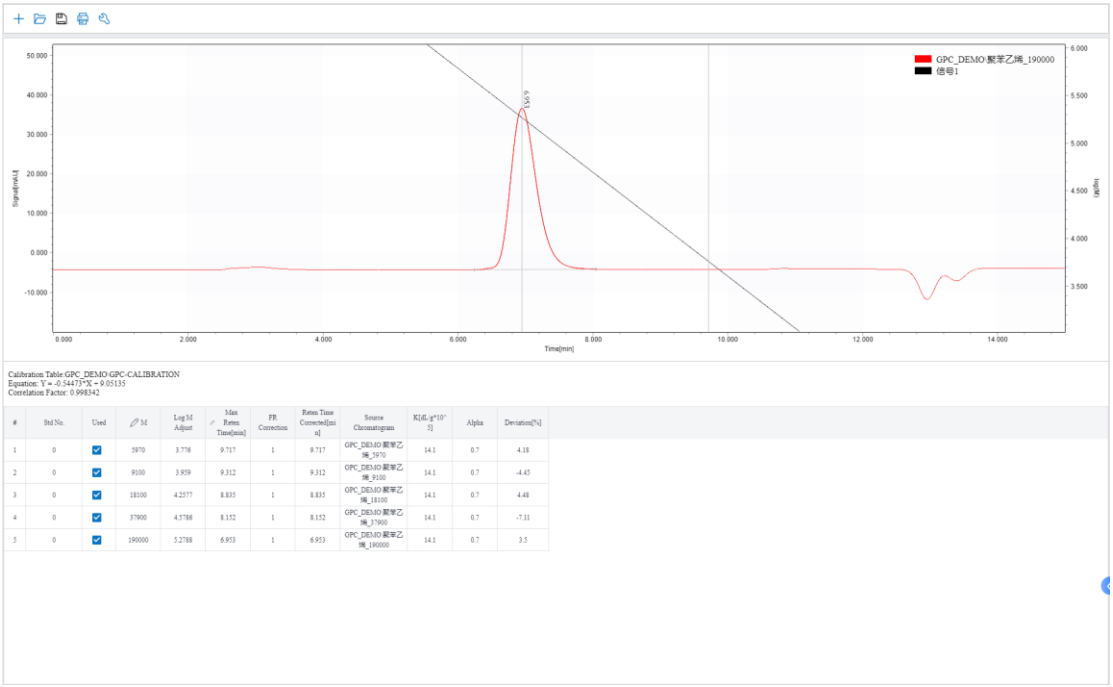


Figure 7-10 GPC Calibration Curve window

7.5.2 GPC Calibration Options

Under the Calibration window, click the button and the "GPC Calibration Options" dialog box will appear, which contains additional options such as calibration type, K value, alpha value, etc.

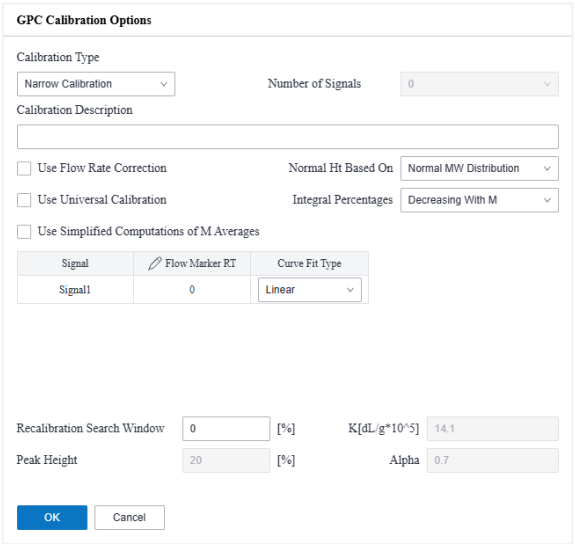


Figure 7-11 GPC Calibration options Settings

7.5.2.1 Calibration Type

The calibration type is narrow-peak calibration.

7.5.2.2 Use Flow correction

If a flow marker peak is set, selecting "Use Flow Correction" will correct the calibration curve and calculation.

7.5.2.3 Use a Universal Calibration

Selecting "Use Universal Calibration" will correct the calibration curve and calculations according to the Mark-Houwink equation.

Note: With or without this option, the α value is only used to calculate the visco-average molecular weight.

7.5.2.4 Simplified calculation using M mean

Select "Simplified calculation using the M mean", then the M mean will be calculated using the simplified method instead of the standard method.

[Note] The difference between the simplified calculation method of M mean and the standard calculation method only exists in nonlinear calibration.

7.5.2.5 Number of signals

It determines the number of signals used to draw the standard curve, and this number automatically increases with the number of signals used to make the chromatogram of the

calibration curve.

7.5.2.6 Flow marking RT

When using flow rate correction, the flow marker RT needs to be set for flow rate correction.

7.5.2.7 Type of curve fitting

The curve fitting type is used to set the standard curve fitting type, which can be selected from the table.

7.5.2.8 Recalibrate the search

Set the maximum standard deviation (%) of the peak retention time of the standard sample from the stored data to be used for recalibration.

7.5.2.9 Peak height

Peak height (%) is only applicable if the calibration type is selected for linear calculation, determining the position of the points used to draw the calibration curve.

7.5.3 Calibration curve Making - Narrow peak calibration

If the molecular weight distribution of the standard is narrow (dispersion coefficient < 1.2), select the narrow-peak calibration type. Draw a calibration curve by the retention time of the peak peak and the known peak molecular weight. If no peak molecular weight is available, the square root of the product of weight mean molecular weight and number mean molecular weight can be substituted.

1） All standard spectrograms are preprocessed to remove unwanted peaks and modify integral conditions.

2） Open the calibration window, click the button, set the parameter of "GPC Calibration

options", and select "Narrow peak Calibration" as the calibration type.

3） Click on the chromatogram file to open the first processed standard spectrogram.

4） Select the calibration peak you want to use in the calibration table below and enter the M-value of the calibration peak.

5） Repeat steps 3) and 4), add the standard chromatogram in turn, and the standard level is automatically upgraded.

6） After all the standard spectra have been added, the correction curve will automatically appear.

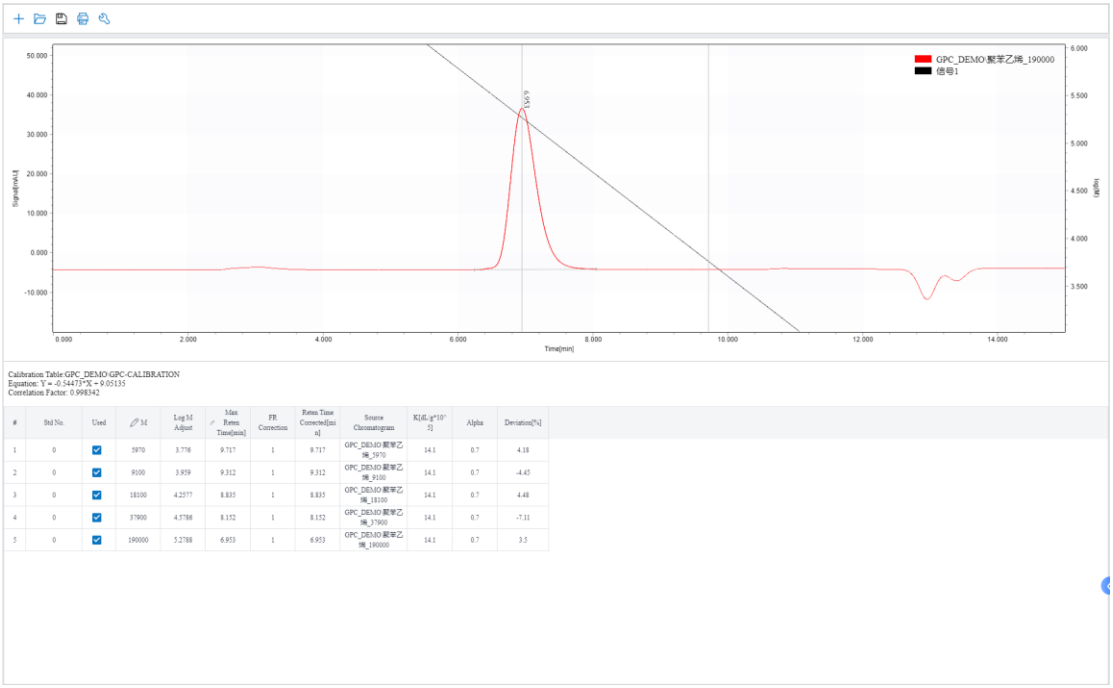


Figure 7-12 Narrow peak calibration curve

8 Report

8.1 Report Settings

Click "Report" on the main page of workstation to enter the report setting page. By default, there are 4 report templates on this page. The report templates are divided into two formats:.docx

and.xlsx; You can download, edit and upload the report template. As shown in Figure 8-1.

The downloaded template can be opened using Word or Excel, as shown in Figure 8-2; Edit, delete, add, save, etc. according to the user's needs, and upload the edited file again in the workstation, as shown in Figure 8-3. The uploaded report template can be invoked on all report printing pages to export the report.

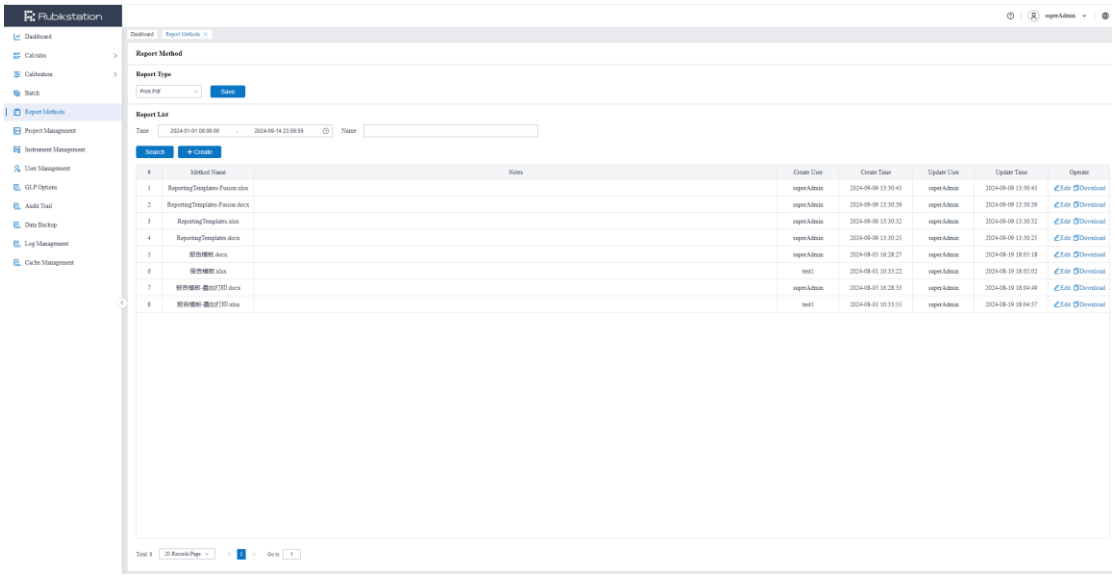


Figure 8-1 Report Settings window

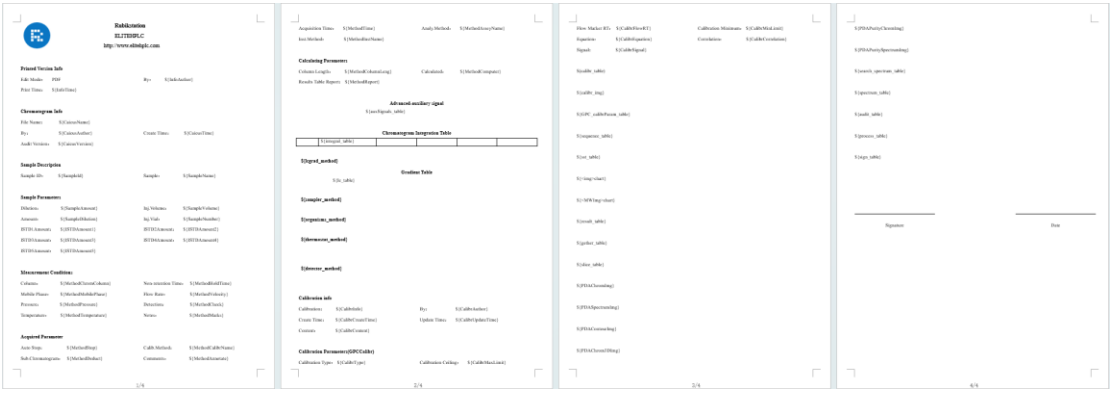


Figure 8-2 Edit report template

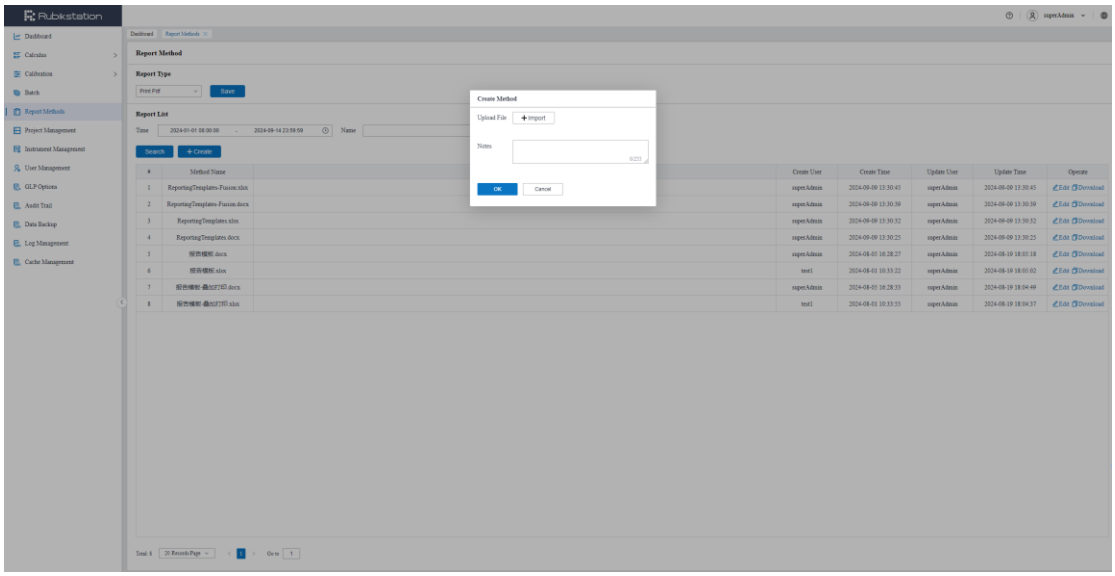


Figure 8-3 Report Settings window

[Note]

- **When you print a report, the contents in the report are printed in the order listed in the report template. You can adjust the order in the report template.**
- **There are four report DEMO files in the workstation. Do not overwrite or replace the DEMO file with another report. After creating a new report file in the workstation, upload the user's report template in the new report file, and do not overwrite the DEMO file in the workstation.**
- **The report PDF file is saved to the file download path set by the browser by default. If necessary, you can set the browser file download path.**

8.2 Outputting a Report

Upload report templates, including HPLC data processing, GPC data processing, PDA chromatogram, HPLC calibration, GPC calibration and batch processing, can be invoked on all

output report pages of the workstation.

In addition to batch processing, the report output of other pages need to click the button first, select the required report template in the pop-up window, and then click "OK" to print the PDF  file directly to the file download address set by the browser.

9 Batch Processing

The batch processing page is used to batch process the integration of spectrograms, batch export reports, batch set up spectrogram calibration files and preview functions.

9.1 Batch integration and calibration

Click "Batch Processing" on the home page of the workstation to open the batch processing page, and display the chromatogram diagram list on the left side of the page. You can select the corresponding project and chromatogram diagram according to your needs, as shown in Figure 9-1.

The analysis method, calibration method and report method for processing the chromatogram can be selected on the upper right side. During batch processing, the chromatogram will be output data batch processing according to the analysis method and calibration method selected here, and then output according to the selected report.

The middle part of the right side can choose the output mode, including exporting PDF, exporting data, if the option is checked, when clicking "OK" button, it will output the report according to the selected mode, if not selected, it will not output the report.

At the bottom of the right side there are preview, confirm, cancel three buttons, click the preview button can jump to the batch processing preview page, the whole page is basically consistent with data processing; On the left side, the list of spectra selected in the batch processing is displayed. When one or more spectra are opened, integration processing will be performed according to the analysis method and calibration method selected in the batch processing. On the batch processing page, you can check whether the integration and calibration processing results of the selected method meet the requirements, and you can directly adjust and save the integration of the selected analysis method on the preview page, as shown in Figure 9-2.

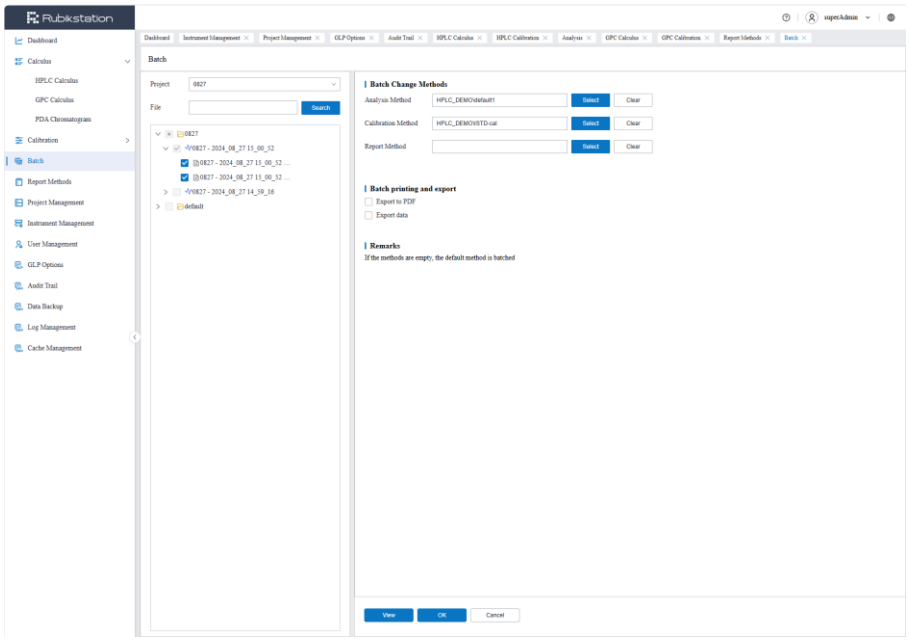


Figure 9-1 Batch processing page

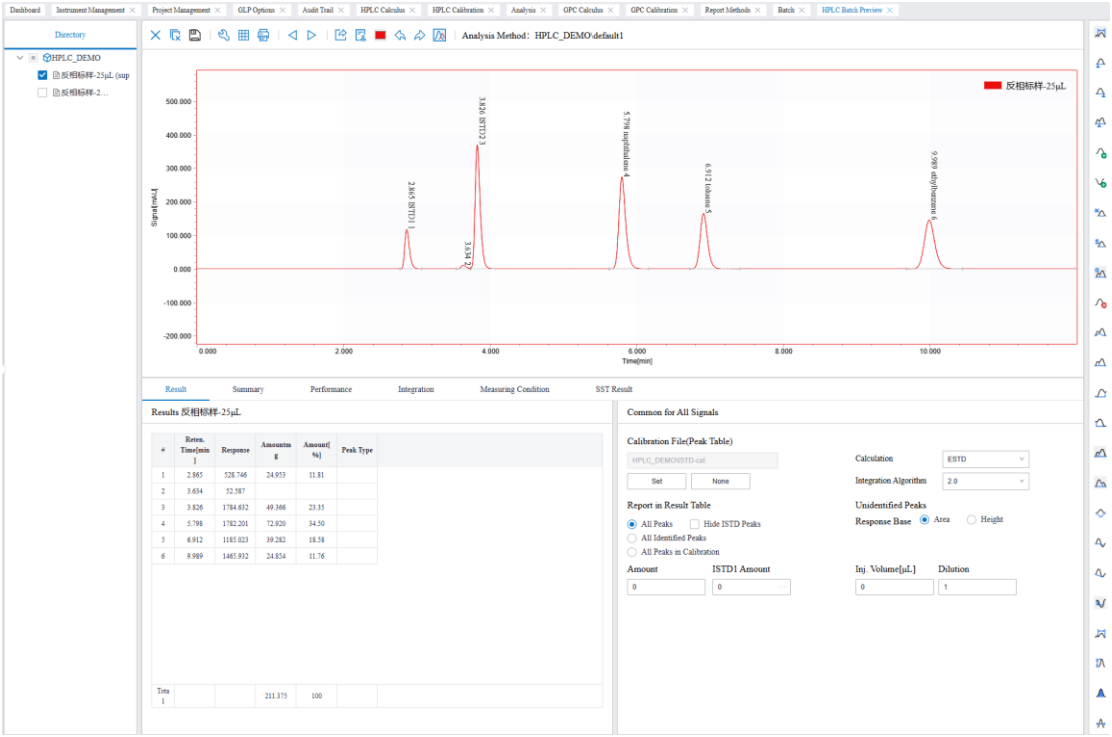


Figure 9-2 Batch preview page

[Note]

◆ **The batch preview page is not a data processing page, and processing actions such as integral changes are not saved to the**

chromatogram.

◆ **Click the "Save" button on the batch preview page to save the analysis method. Only after returning to the batch page and clicking the "OK" button, the spectral graph will be integrated and saved according to the integral Settings in the integration method.**

Appendix

Safety Information

- ***General safety information***

The following general safety matters must be followed at all stages of instrument operation, maintenance and repair. Failure to follow the special warnings elsewhere in this manual will violate the safety standards for the design, manufacture and use of the instrument, and we shall not be liable for any damage caused by the user's failure to comply with these requirements.

- ***Safety Standards***

This instrument is a Class I safety equipment (that is, provides protective grounding end), and is manufactured and tested according to national safety standards.

Safety Sign

Signs	Instructions
	For equipment marked with this symbol, users should refer to the instruction manual to avoid injury to the operator and damage to the instrument.
[Warnings]	Warn you of situations that could result in injury or death. Do not operate beyond the warning unless you have fully understood and met the required conditions.
【 Be careful 】	Warning you of conditions that may result in data loss or damage to the equipment, do not exceed caution unless you have fully understood and

	met the required conditions.
【 Note 】	Warning you may cause the experimental data is not ideal or the instrument does not work properly, unless you have fully understood and met the required conditions, do not operate beyond the scope of attention.