Lightnovo

Miraspec Flow software

User Manual

Version 0.1.4

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1. Introduction

1.1. Purpose of the Miraspec Flow software

Miraspec Flow is a software platform developed by Lightnovo to operate Raman spectroscopy instruments and perform analysis of the acquired spectral data. The software provides a unified environment for configuring measurements, acquiring Raman spectra, processing the data, and interpreting the results.

The primary purpose of Miraspec Flow is to support rapid and reliable chemical identification and analysis using Raman spectroscopy. It enables users to control spectrometer hardware, apply spectral preprocessing methods, compare measured spectra with reference libraries, and apply chemometric or machine-learning models for classification and quantification.

The software is designed for use in both research and industrial environments, where it facilitates consistent measurement procedures and efficient data analysis while reducing the need for manual processing of spectral data.

1.2. Overview of Miraspec Flow capabilities

Miraspec Flow provides a set of integrated tools for Raman spectrometer control, spectral processing, and chemical analysis. Key capabilities include:

Instrument control

The software allows users to configure and control connected Raman spectrometers. Measurement parameters such as laser power, integration time, detector gain, and number of accumulations can be adjusted to optimize spectral acquisition.

Advanced features of the software include acquisition of custom libraries, loading the libraries to the device, etc.

Spectral acquisition and visualization

Miraspec Flow enables real-time acquisition and display of Raman spectra. Users can monitor signal quality during measurement and perform repeated acquisitions when required.

Spectral preprocessing

The software includes several preprocessing functions used to improve spectral quality prior to analysis. These may include baseline correction, smoothing, normalization, and removal of spectral artifacts such as spikes.

Spectral library management and identification

Measured spectra can be compared with reference spectra stored in user-defined libraries. Similarity metrics are used to identify the most likely compound or material corresponding to the measured spectrum. In addition to user libraries, Miraspec supports Lightnovo libraries, as well third-party libraries such as RUFF database, ST Japan, etc.

Chemometric and multivariate analysis

Miraspec Flow supports multivariate analysis methods such as principal component analysis (PCA) and regression-based models. These tools enable classification of materials and quantitative estimation of component concentrations.

Data management and reporting

Measurement results, spectra, and analysis outputs can be stored, exported, and used for documentation or further processing. The data is kept in local Miraspec database.

1.3. Typical workflow in the system

A typical workflow in Miraspec Flow follows a sequence of steps from measurement configuration to final interpretation of results.

Instrument connection and configuration

The Raman spectrometer is connected to the computer running Miraspec Flow. The user configures measurement parameters such as laser power, exposure time, and number of spectral accumulations.

Spectral acquisition

The sample is placed in the measurement position and the Raman spectrum is acquired. The spectrum is displayed in real time, allowing the user to verify signal intensity and spectral quality.

Spectral preprocessing

The acquired spectrum is processed using preprocessing routines such as baseline correction, smoothing, or normalization to reduce noise and remove background effects.

Spectral analysis or identification

The processed spectrum is compared with reference spectra in a library or analyzed using chemometric models. The software calculates similarity scores or classification results to determine the most likely material or composition.

Result visualization and export

The identification result, processed spectra, and relevant analysis outputs are presented to the user. The results can be saved, exported, or included in reports for further use.

This workflow enables efficient transformation of raw Raman measurements into interpretable chemical information within a single software environment.

2. Safety Summary

This section provides important safety information for the operation of Miraspec Flow software and the Raman spectroscopy instruments it controls. Users must read and understand these guidelines before operating the system.

Detailed safety information is provided in *Appendix A – Detailed safety guidelines.*

2.1. General Safety Principles

Miraspec Flow software is designed to control Raman spectroscopy instruments and process spectral data. Safe operation of the software depends on the correct and responsible use of the connected hardware.

Users must follow the general safety rules below:

- Operate the system only according to the instructions provided in this manual.
- Ensure that the Raman spectrometer and associated hardware are installed correctly.
- Use the system only for its intended purpose of Raman spectral acquisition and analysis.
- Do not attempt to modify or bypass safety features of the instrument.
- Only trained personnel should operate the system.

Failure to follow these instructions may result in damage to equipment, incorrect analytical results, or potential safety hazards.

2.2. Laser Safety

Raman spectrometers typically use laser sources to excite the sample and generate Raman spectra. Laser radiation may pose a hazard to eyes and skin if not handled properly.

Users must observe the following precautions:

- Never look directly into the laser beam or optical path.
- Do not operate the spectrometer if protective covers or safety enclosures are removed.
- Avoid placing reflective materials in the laser beam path.
- Ensure that the instrument is operated in accordance with applicable laboratory laser safety procedures.

The classification and detailed safety requirements of the laser system depend on the specific spectrometer model used.

2.3. Electrical and Equipment Safety

The Raman spectrometer and associated devices require electrical power and may contain sensitive electronic components.

To ensure safe operation:

- Only connect devices using approved cables and interfaces.
- Ensure that power supplies are properly grounded.
- Do not open instrument housings unless instructed by qualified service personnel.
- Disconnect power before performing maintenance or hardware adjustments.

Improper handling of electrical equipment may result in equipment damage or personal injury.

2.4. Sample Handling Safety

Certain samples may pose chemical, biological, or thermal hazards when analyzed using Raman spectroscopy.

Users should ensure that:

- Samples are handled according to appropriate laboratory safety procedures.
- Hazardous materials are analyzed only in suitable laboratory environments.
- Samples that may degrade, burn, or react under laser illumination are handled with caution.

Users are responsible for following applicable safety regulations related to the materials being analyzed.

2.5. Intended Use

Miraspec Flow is intended for the control of Raman spectroscopy instruments and the analysis of Raman spectral data in research, industrial, or laboratory environments.

The software should not be used for purposes outside its intended scope, including medical diagnosis or safety-critical decision-making without proper validation.

2.6. Safety Symbols and Conventions

This manual may use the following symbols to highlight important information:

Warning

Indicates a potentially hazardous situation that could result in injury if not avoided.

Caution

Indicates a situation that could result in damage to equipment or loss of data.

Note

Provides additional information that may help improve system operation or understanding.

3. Getting Started

3.1. System requirements

Before installing and running Miraspec Flow, ensure that the computer system meets the minimum hardware and software requirements listed below. Meeting these requirements helps ensure stable operation of the software and reliable communication with connected Raman spectroscopy devices.

Supported Operating Systems

Miraspec Flow is designed to run on the following operating systems:

- Microsoft Windows 10 (64-bit)
- Microsoft Windows 11 (64-bit)

The system should have the latest recommended updates installed to ensure compatibility and security.

Hardware Requirements

The following hardware specifications are recommended for normal operation of the software.

Minimum Requirements

ComponentSpecificationOS: Windows 10 64-bit (version 1903 or later)
CPU: Intel Core i5 8th-gen / AMD Ryzen 5 3rd-gen · 4+ cores
RAM: 8 GB DDR4
GPU / Graphics: OpenGL 3.3 compatible (integrated GPU accepted)
Storage: 5 GB free (HDD)
Display: 1366 × 768
Ports: USB 2.0 or COM port (Raman device connection)

Recommended Requirements (smooth daily use)

ComponentSpecificationOS: Windows 11 64-bit (latest updates)
CPU: Intel Core i7 10th-gen+ / AMD Ryzen 7 5000+ · 6+ cores
RAM: 16 GB DDR4 or higher
GPU / Graphics: Dedicated GPU · OpenGL 4.5+ (NVIDIA or AMD)
Storage: 10 GB free on NVMe SSD
Display: 1920 × 1080 (Full HD) or higher
Ports: USB 3.0 or COM port

Higher system specifications may improve performance when working with large spectral datasets or complex analytical models.

Graphics Hardware

A dedicated graphics processing unit (GPU) is not required for normal operation of Miraspec Flow. The software can run using standard integrated graphics available on most modern computers.

Device Connectivity

To connect a Raman spectrometer to the computer, the system must provide the appropriate communication interfaces supported by the device. These may include:

- USB interface
- Ethernet connection (depending on the spectrometer model)

The required device drivers must be installed for the operating system to recognize the spectrometer hardware.

Disk Space for Data Storage

In addition to the software installation, sufficient disk space should be available for storing (these entities are stored in the database but the user can import them):

- project files
- spectral data
- spectral libraries
- trained models
- generated reports

Large measurement campaigns or extensive spectral libraries may require additional storage capacity.

Network Requirements (Optional)

Network connectivity may be required for certain system functions, such as software updates, remote support, or access to network-based databases or storage systems.

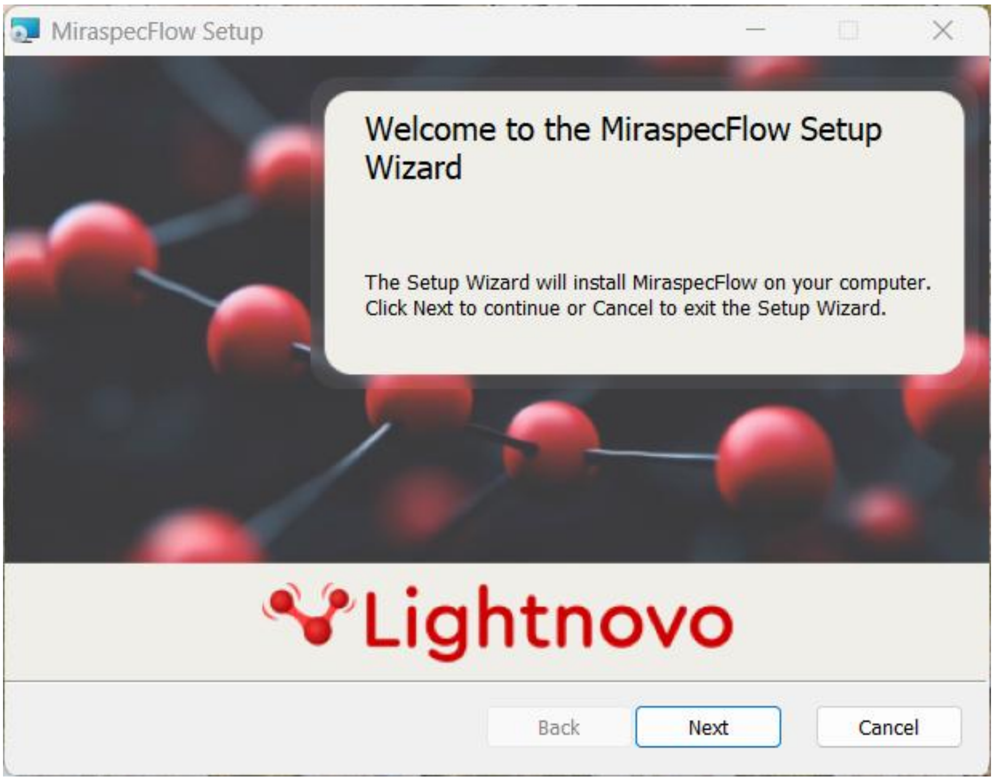
User Permissions

Installation of Miraspec Flow may require administrative privileges on the computer. After installation, normal system operation typically requires only standard user permissions unless administrative configuration tasks are performed.

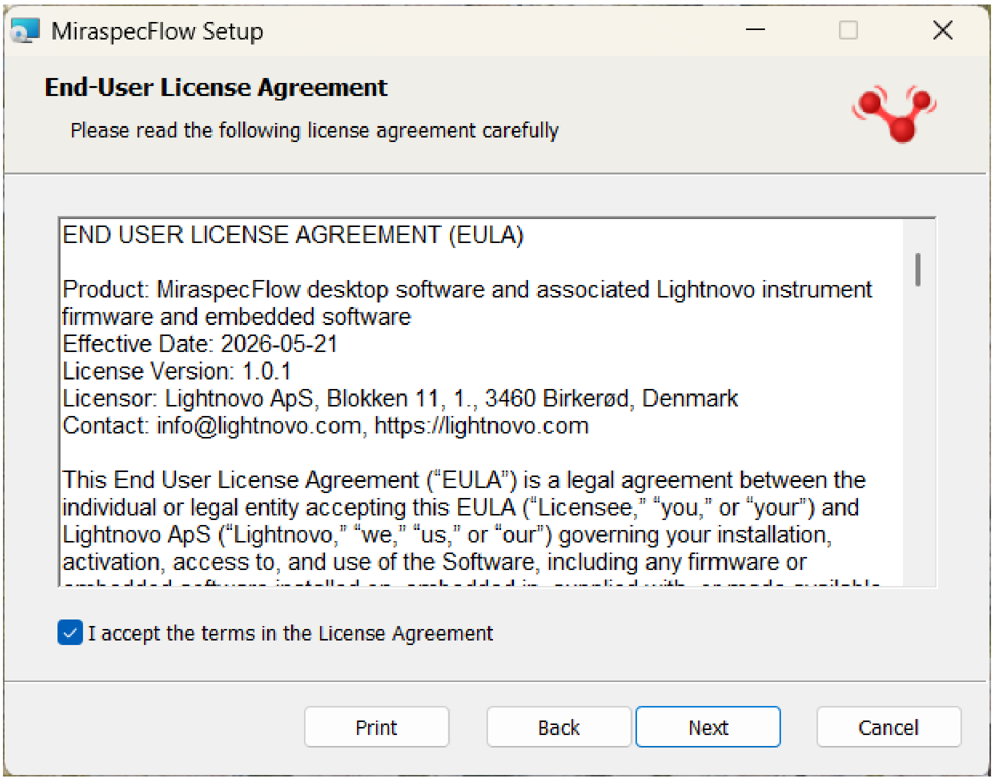
3.2. Software installation and licensing

Miraspec Flow is installed using the official installation package provided by Lightnovo. To install the software, run the installer and follow the instructions of the installation wizard. The installation process places the application files, required system components, and device communication drivers on the computer. Depending on the system configuration, administrative privileges may be required.

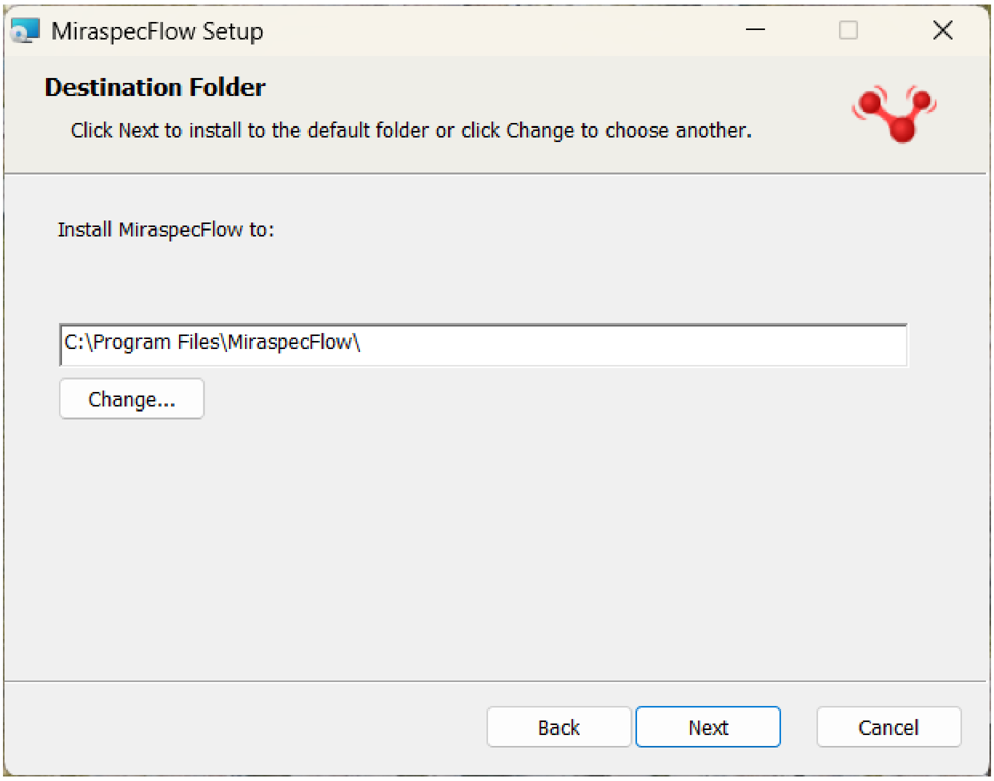
Launch the installer file and follow the steps of installer GUI.



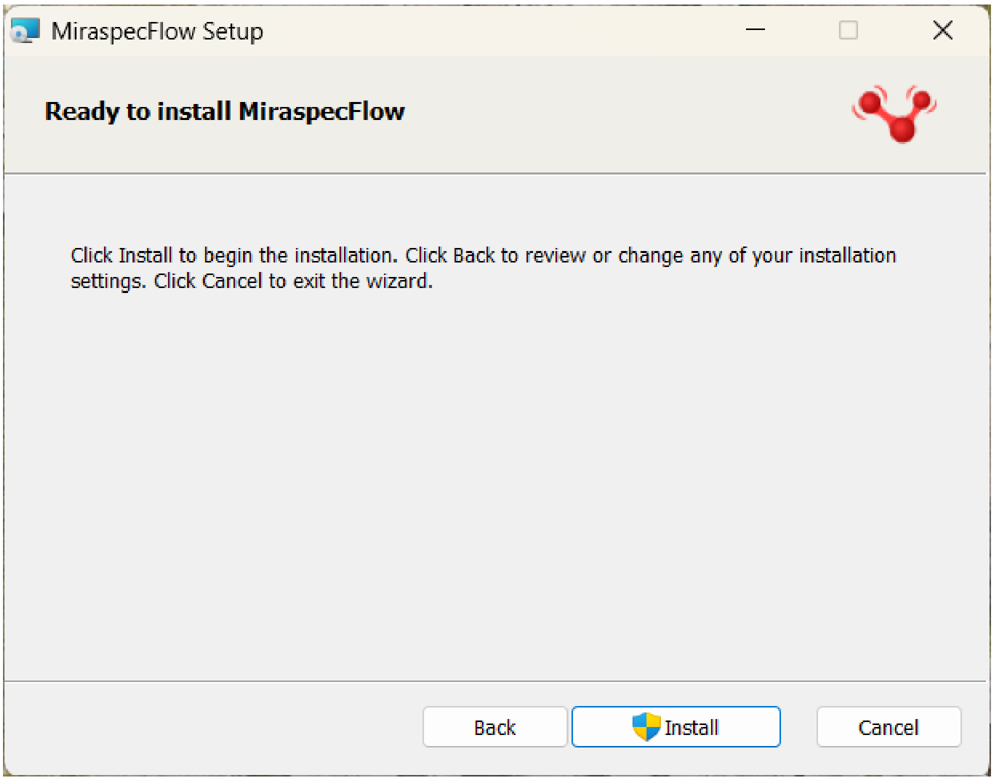
Read the license agreement and click on accept if you accept it:



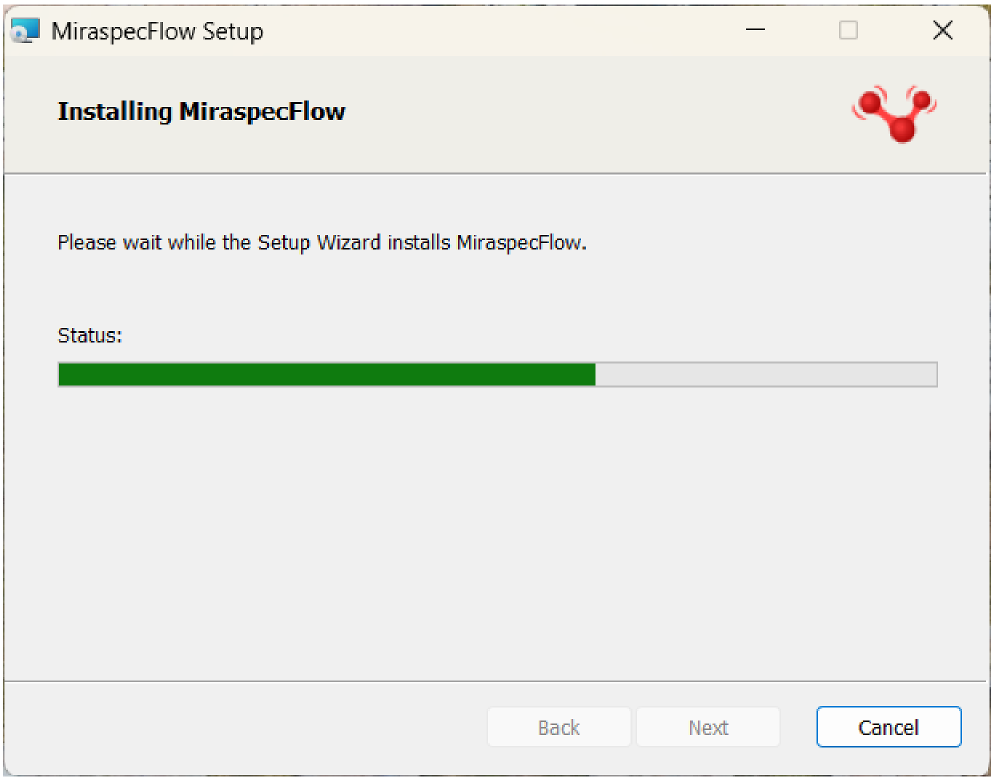
Choose destination folder



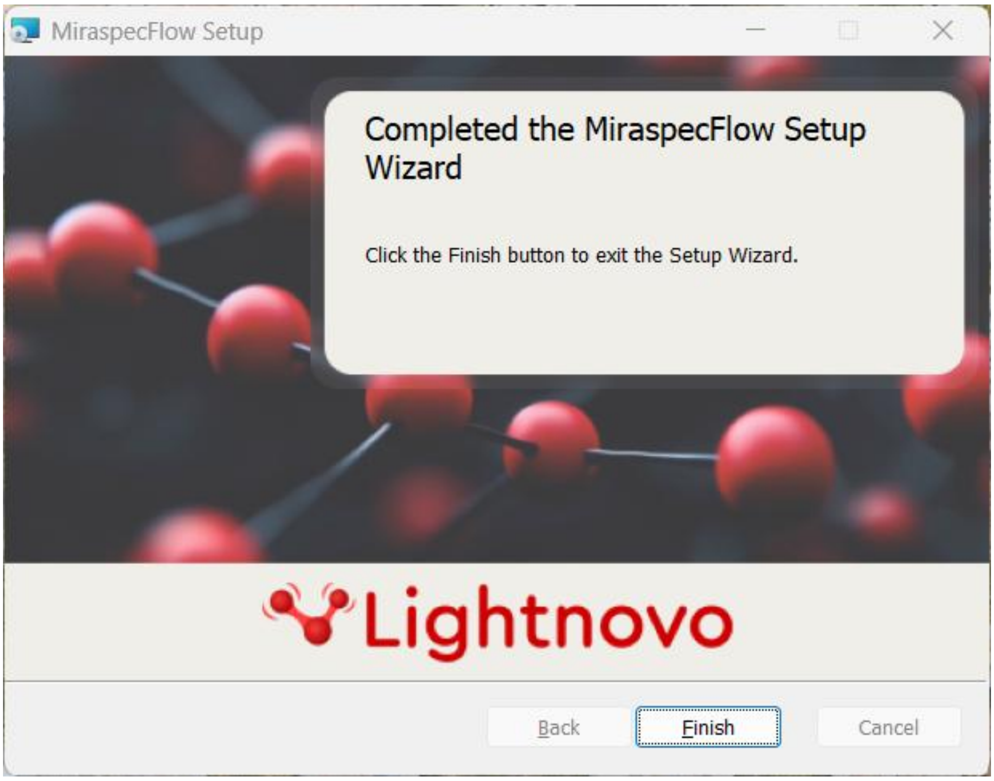
Install



Wait till installer is complete:



Installation is complete:



Click **Finish** to exit.

Miraspec Flow requires a valid software license for operation; license activation may be performed through the **Registration** section of the program settings using the license information provided with the software. The exact licensing and update procedures may vary depending on the system configuration and software version.

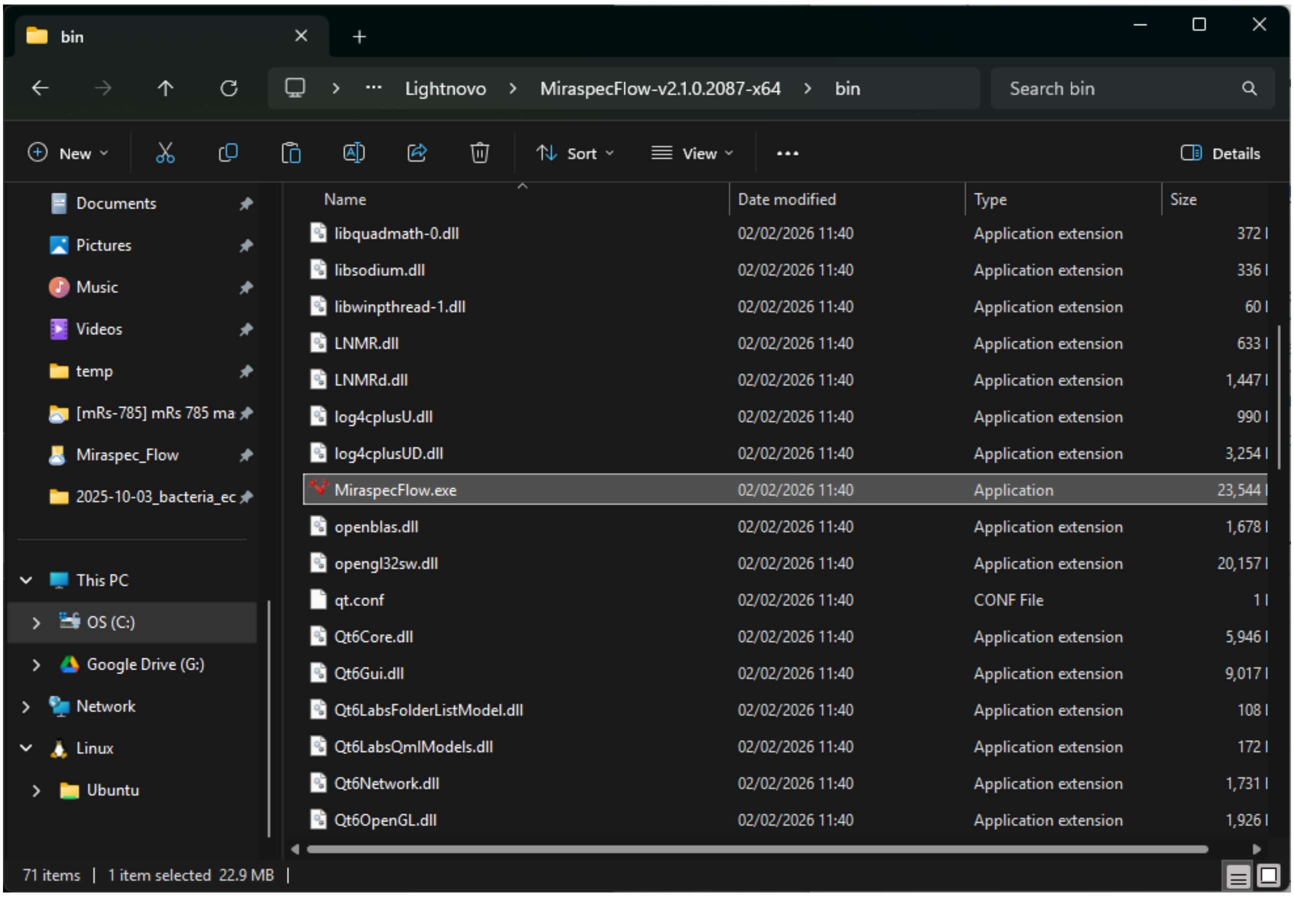
3.3. Starting the software

To start the Miraspec Flow software, locate the installation directory on the computer where the software has been installed. By default, the installation folder contains several subfolders, including the **bin** directory that holds the application executable files.

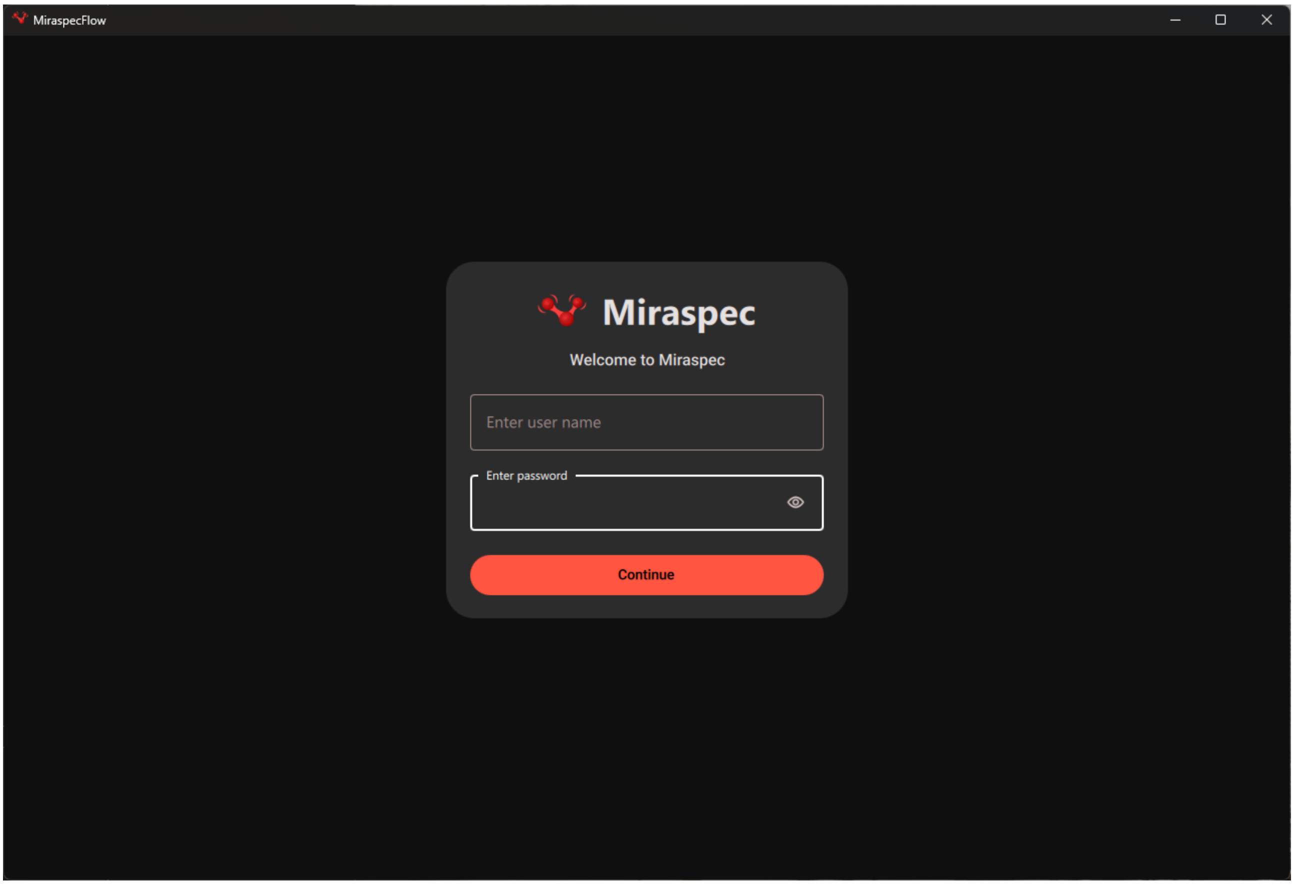
Open the installation folder and navigate to the **bin** subfolder. Inside this folder, locate the file **MiraspecFlow.exe**, which is the main executable file of the Miraspec Flow application.

Launch the software by double-clicking the **MiraspecFlow.exe** file. This action starts the Miraspec Flow application and initializes the system components required for operation, including configuration files, database connections, and available device interfaces.

As an alternative, the installer is also creating a desktop shortcut, double click on it to launch the software.



After the application starts, the **login window** is displayed. Users must authenticate using their assigned user credentials before accessing the system.

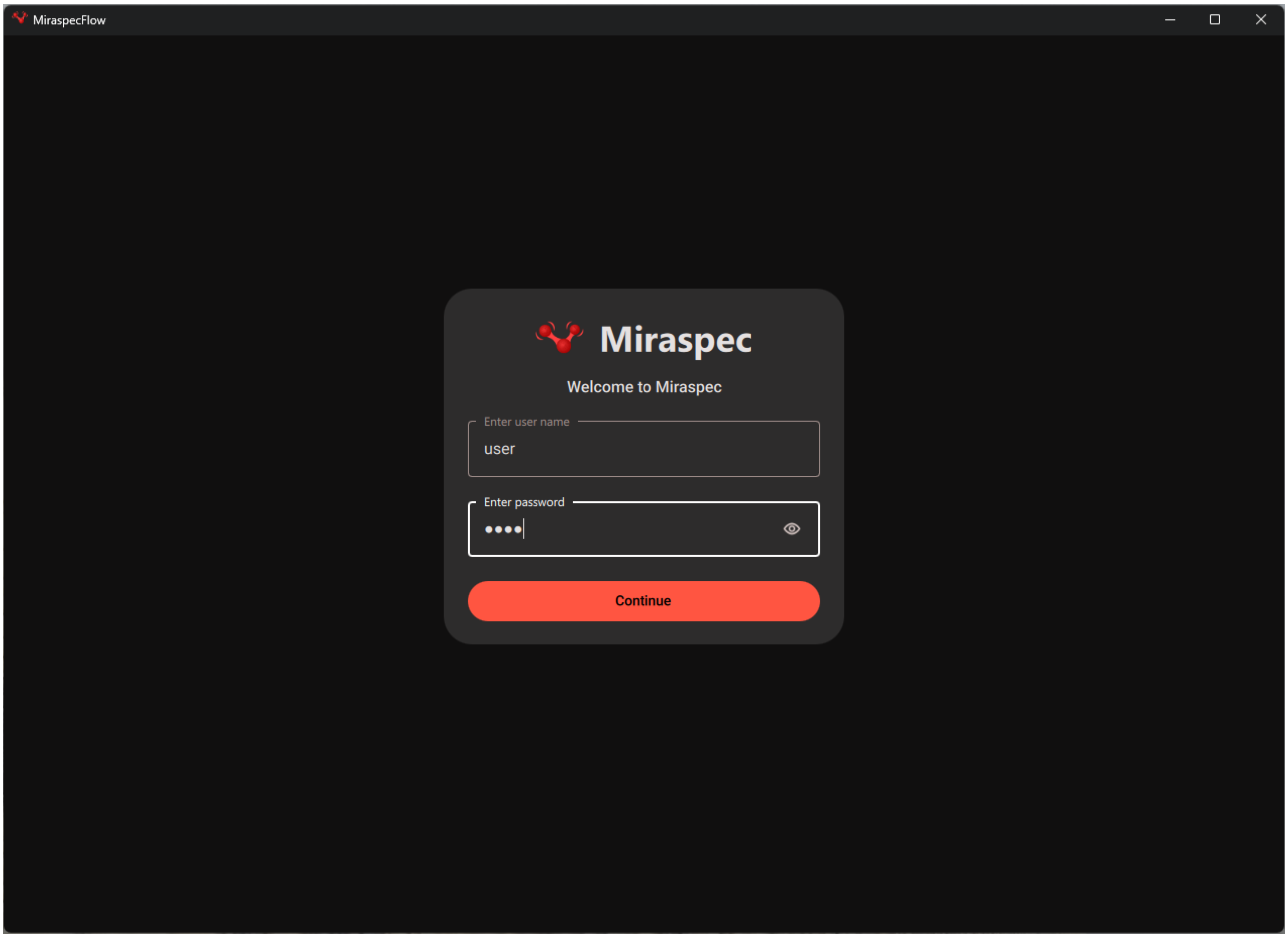


3.4. System login

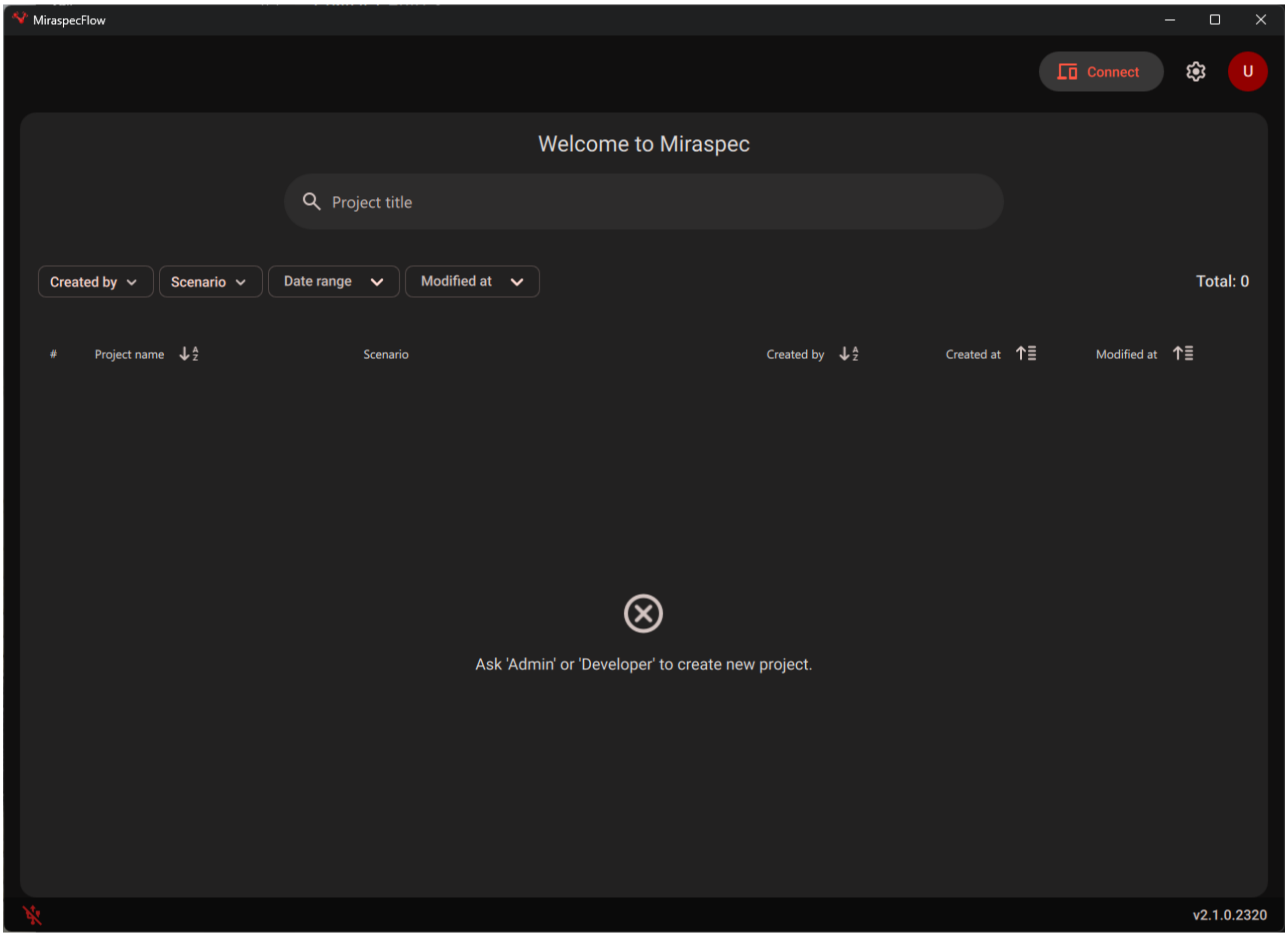
When Miraspec Flow is launched, the **login window** is displayed. Access to the system requires authentication using valid user credentials.

To log in to the system:

1. In the login window, enter your **username** in the Username field.
2. Enter your **password** in the Password field.
3. Click **Continue** to authenticate and access the software.

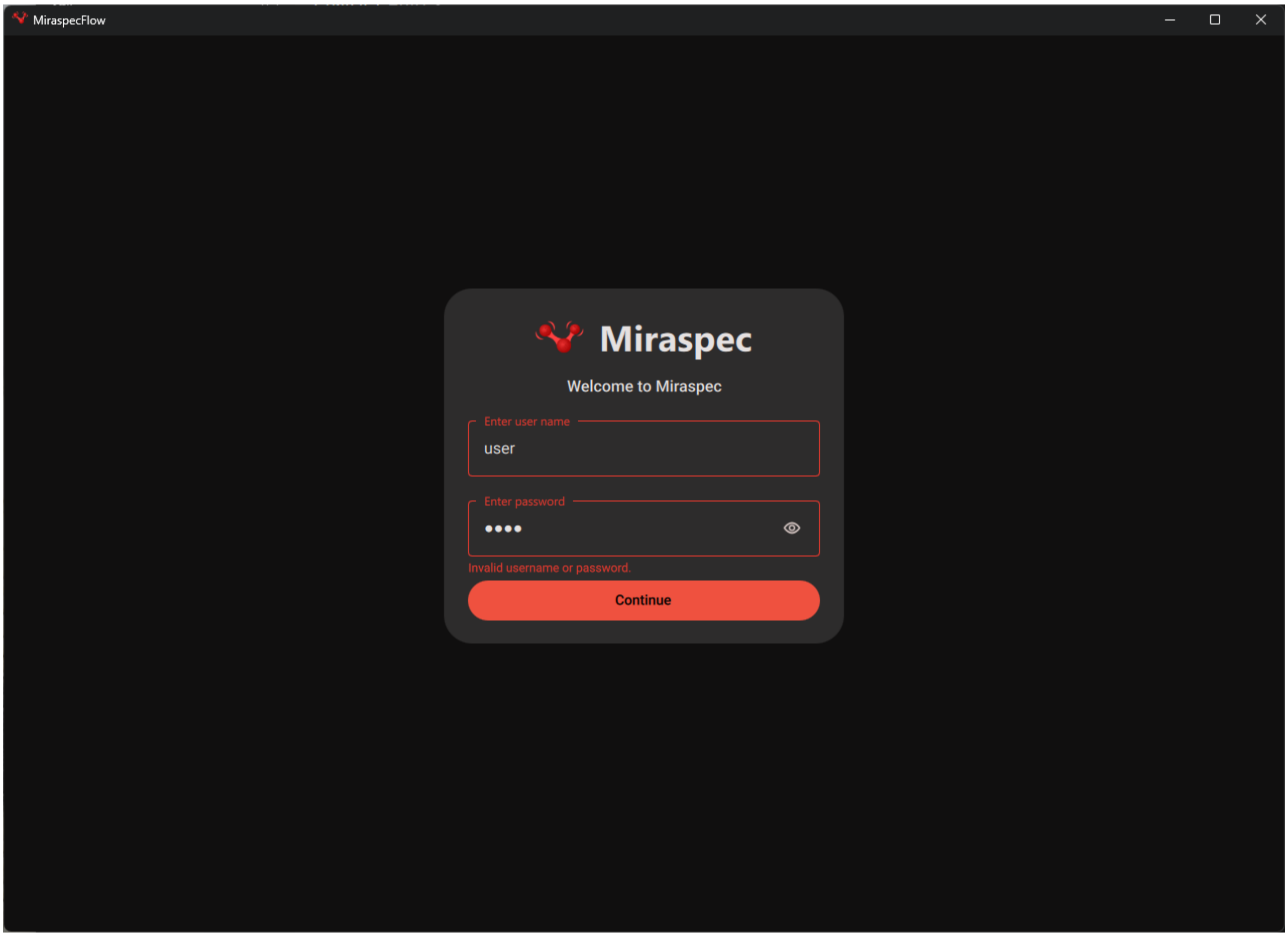


If the provided credentials are valid, the main application interface will be opened and the user will be granted access according to the permissions assigned to their account.



User roles and permissions determine which features and system functions are available to each user. For example, some users may have access only to measurement and analysis functions, while administrative users may also have permission to manage projects, models, and system settings.

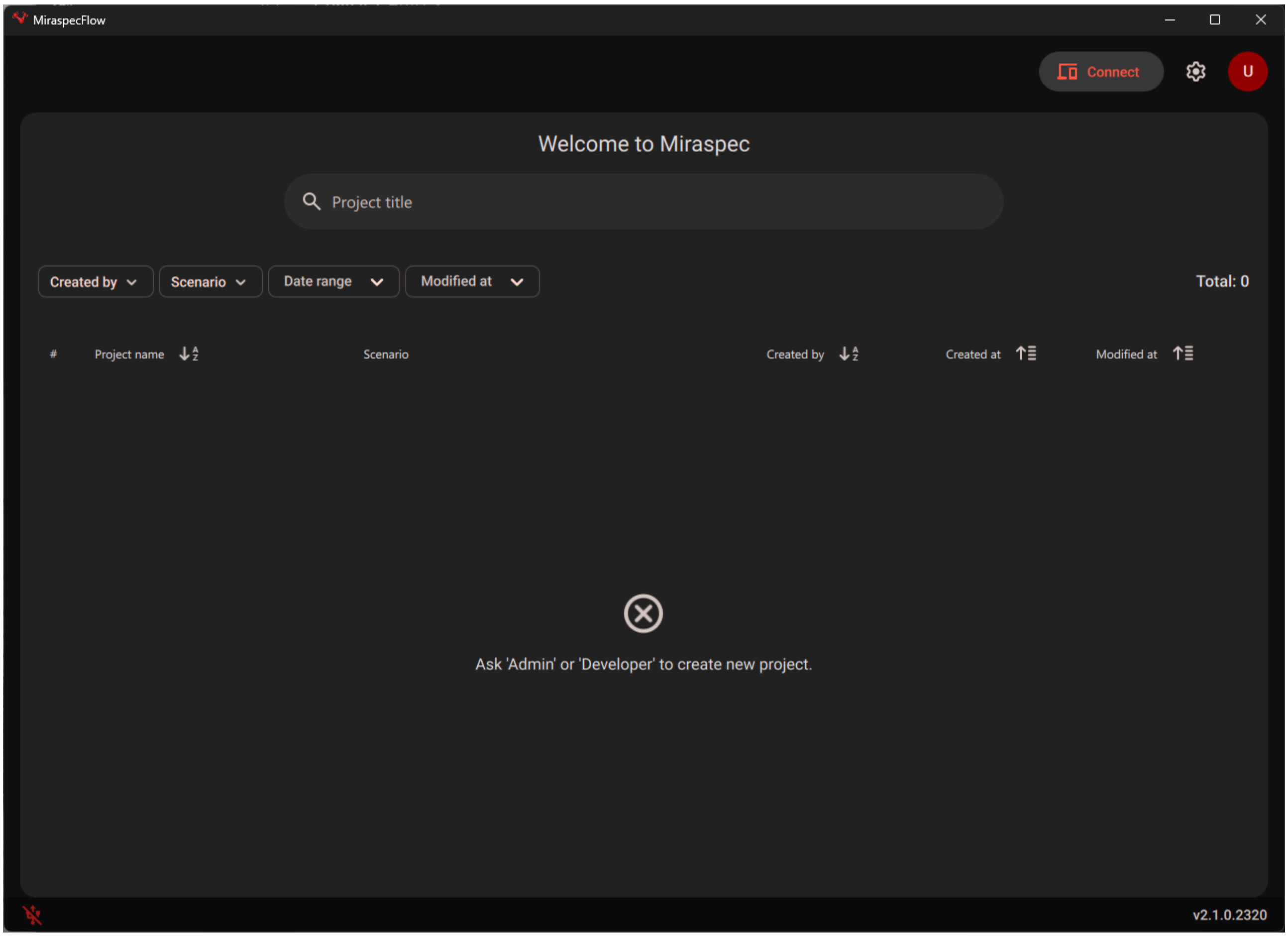
If the login attempt fails due to incorrect credentials, the system will display an error message and prompt the user to try again. This is allowed a limited number of attempts.



Users who have forgotten their password should contact the system administrator to reset their credentials.

3.5. User account information

User account information can be accessed by clicking on the user icon in the top right corner of the software window.



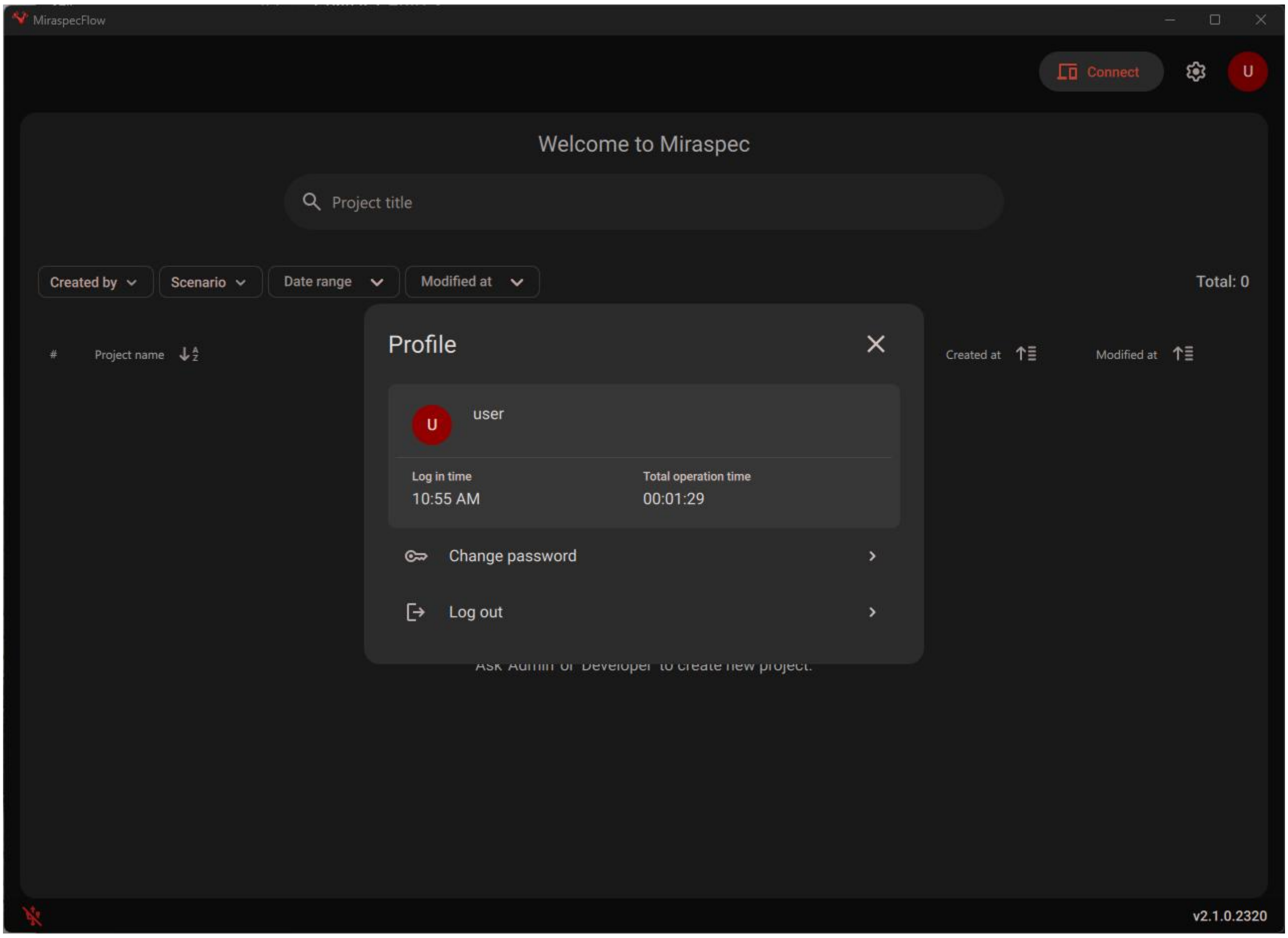
The profile pop-up window should appear.

It displays:

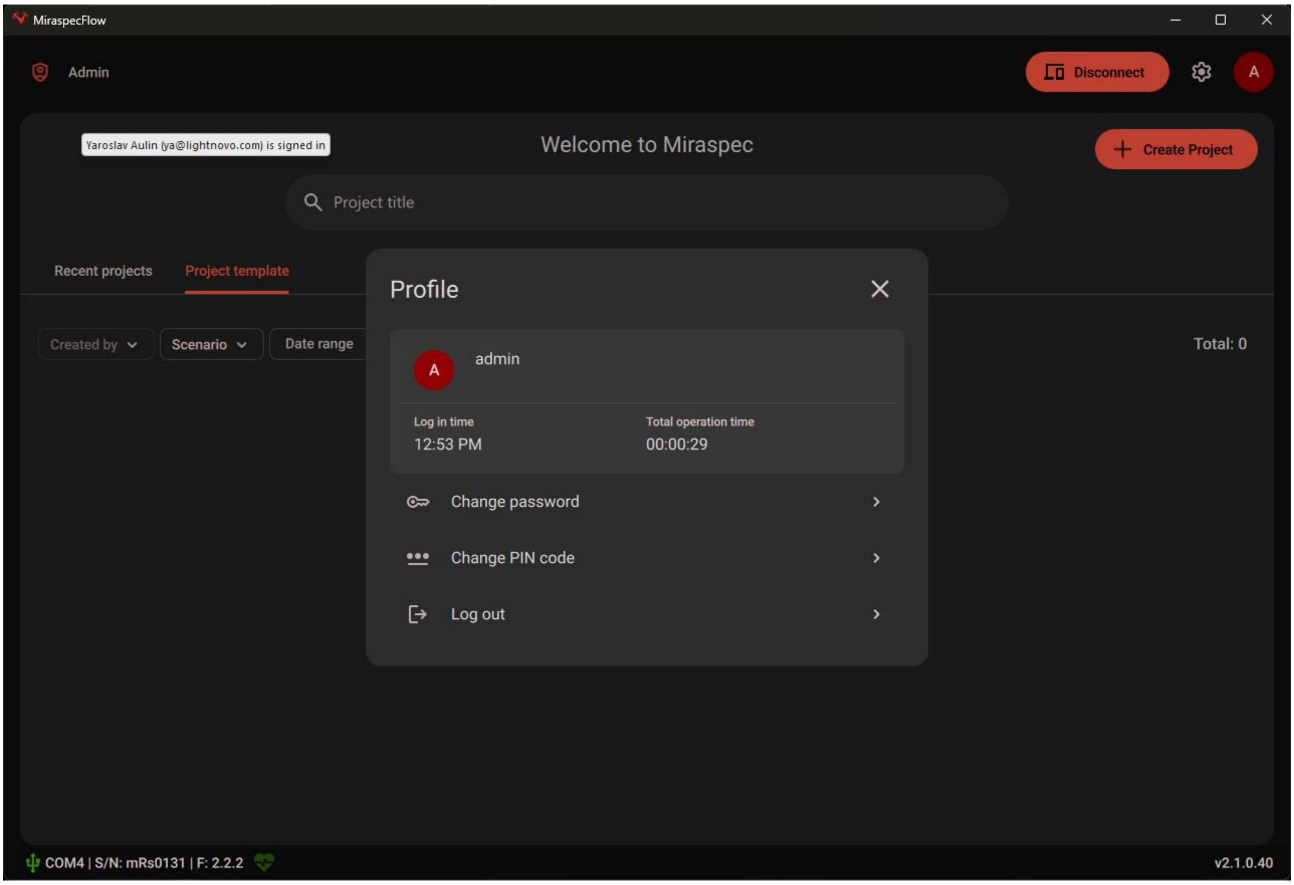
- User name
- Log in time
- Total operation time

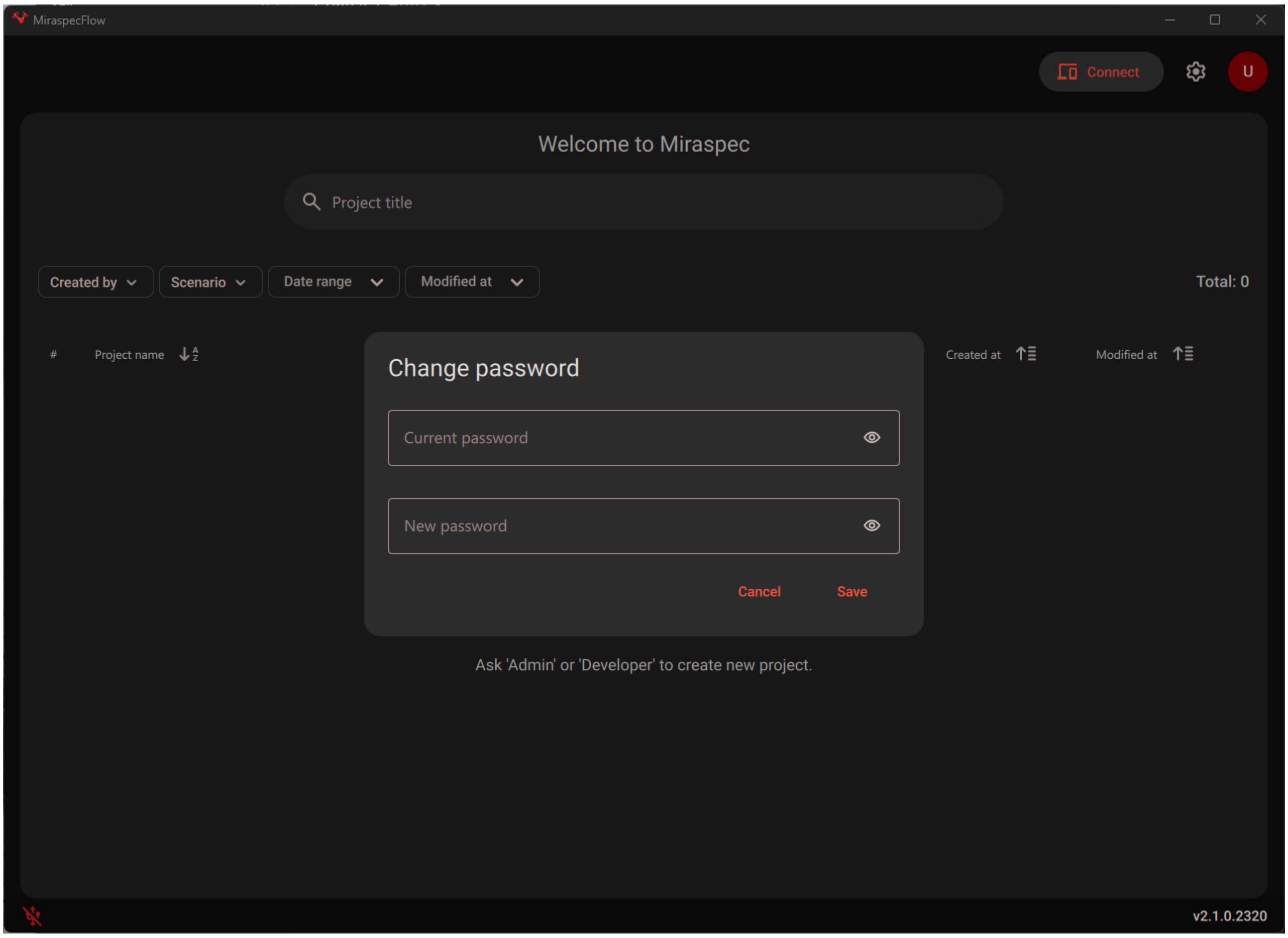
And has two functional buttons:

- Change password
- Log out

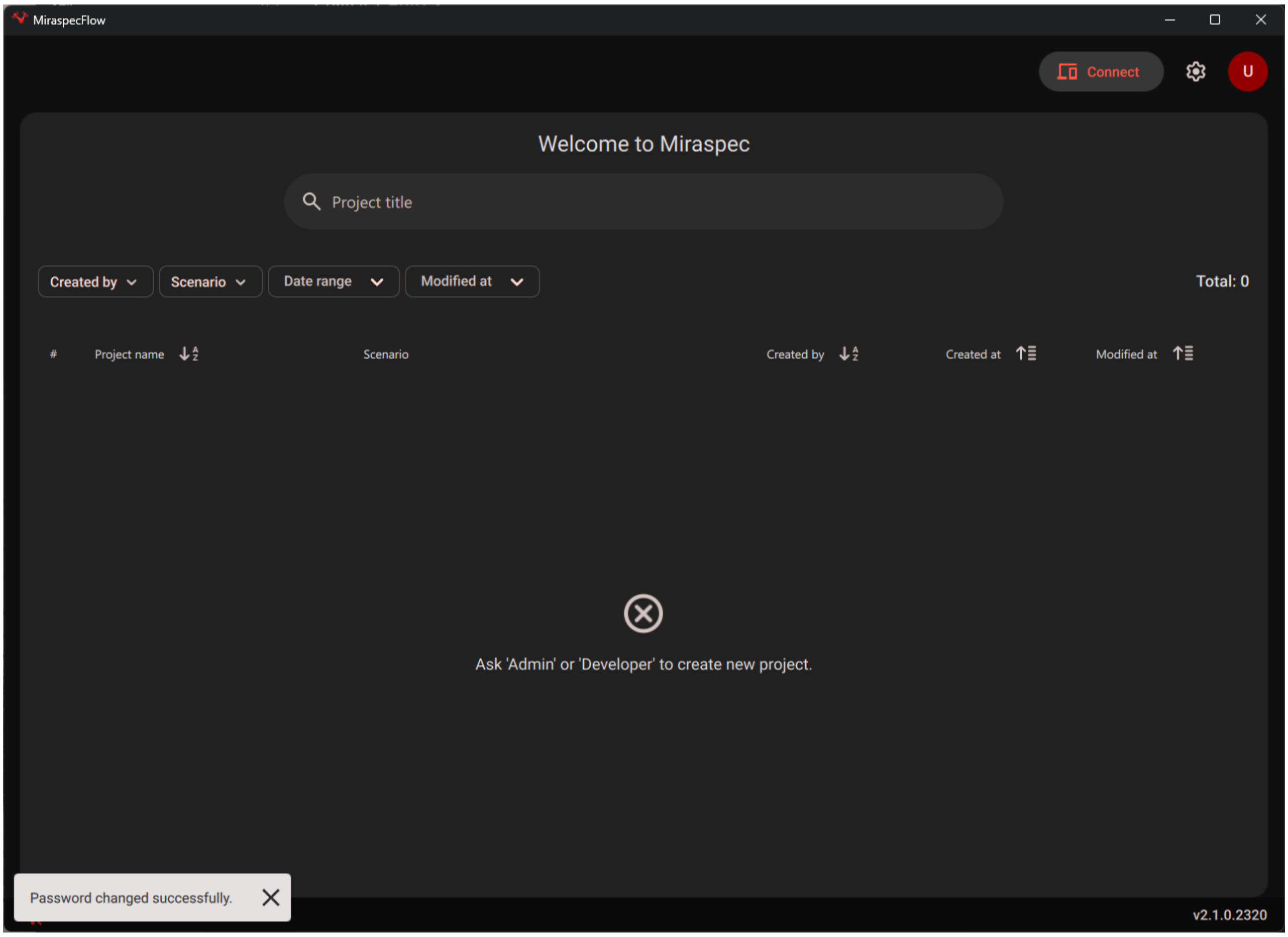


Upon clicking on Change password button the change password prompt window appearing asking to confirm current password and enter new password.

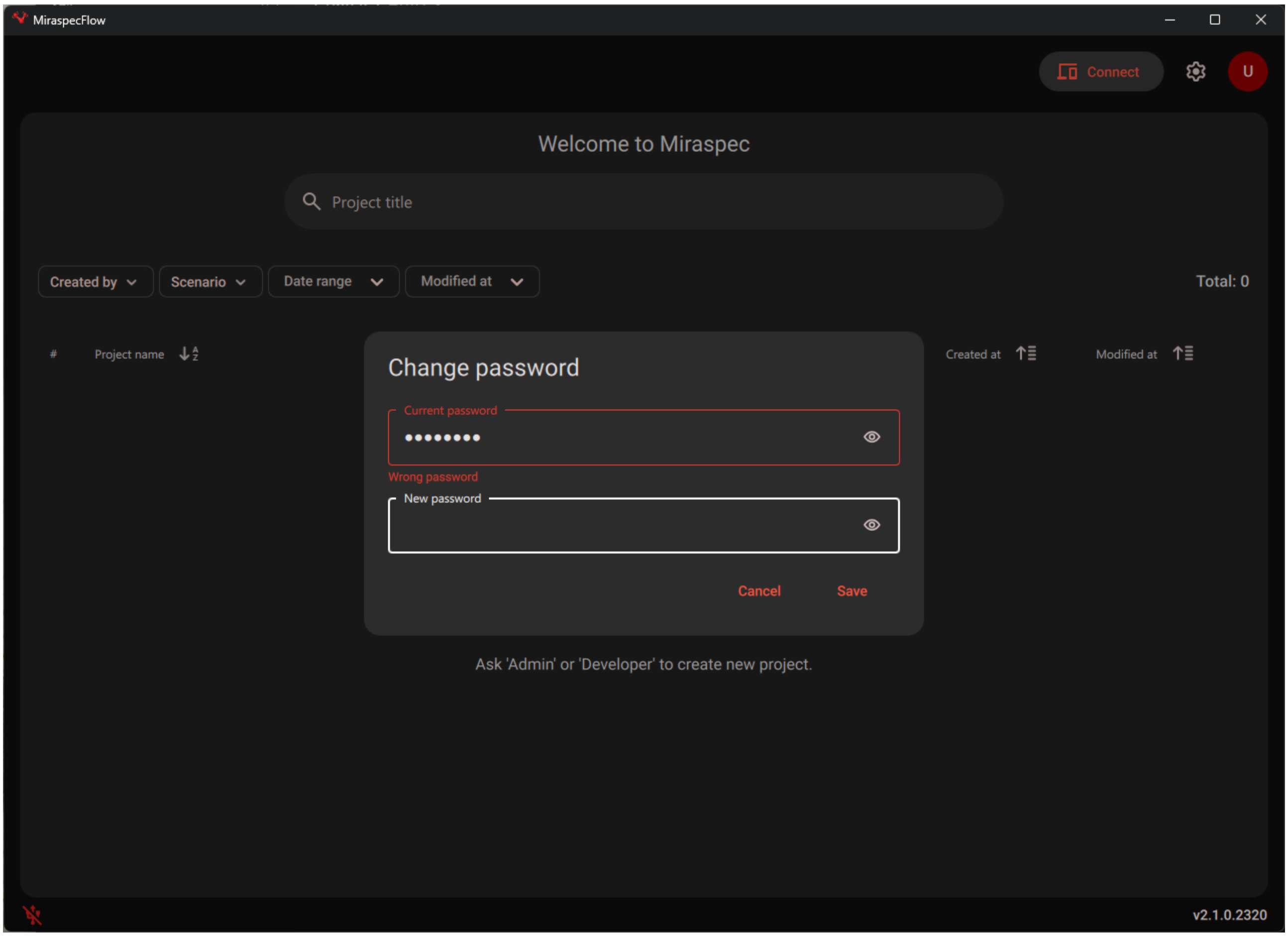




Enter current password and new desired password and click Save. If successful, password changed successfully pop-up message should appear.



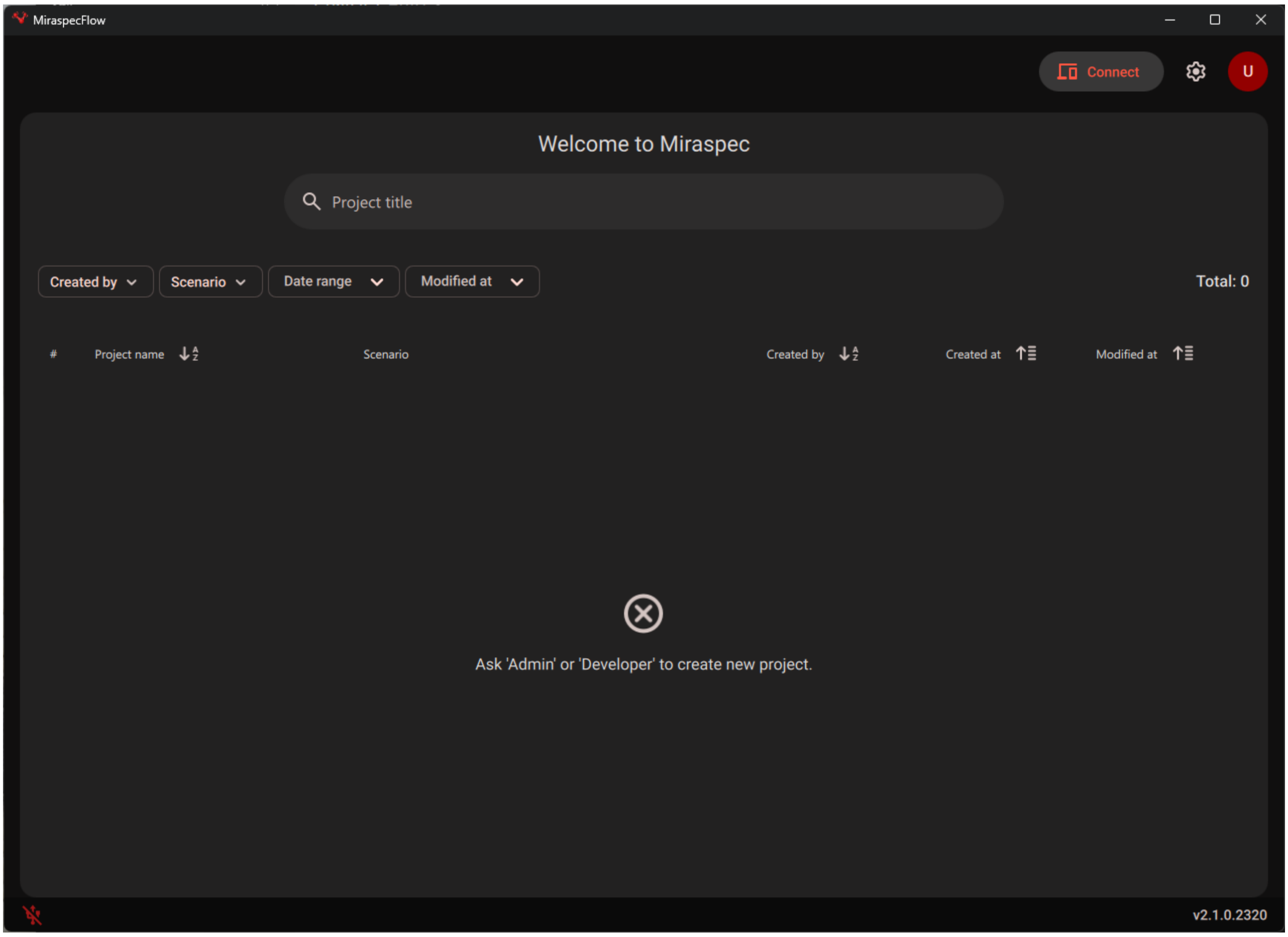
In case wrong current password is entered, the message should appear right a way in the login window:

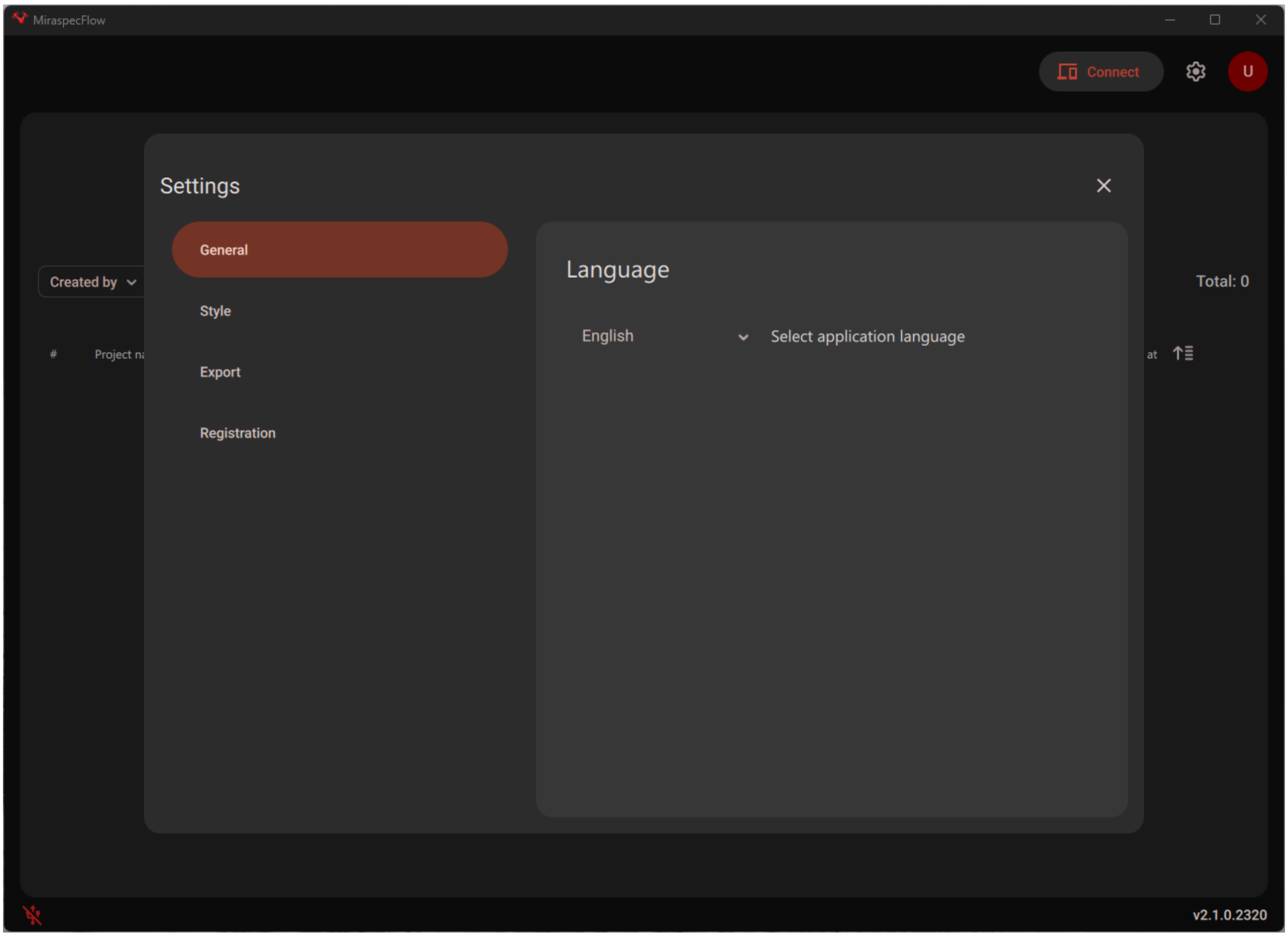


If you would like to cancel password change click on **Cancel**.

3.6. Program setting

Click on a gear icon to enter program settings sections. The Program Settings pop-up window should appear.





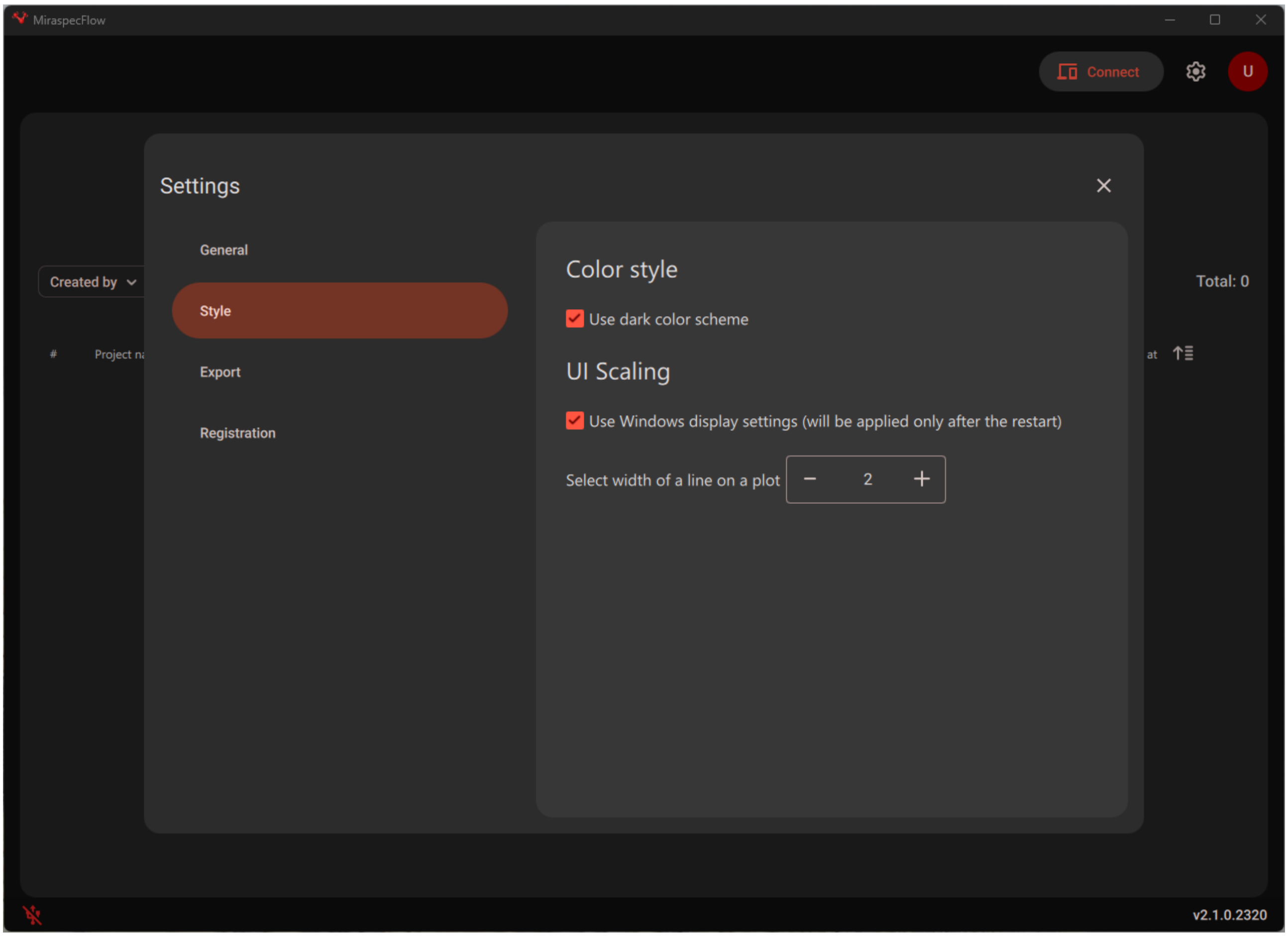
The program settings pop up window shows the following sections:

- General
- Style
- Export
- Registration

The general section allows to change the language of the software interface, default language and the only language available at the moment is English. Click on the arrow pointing down and choose your language from the menu.

Style section allows to change the visible appearance of the software:

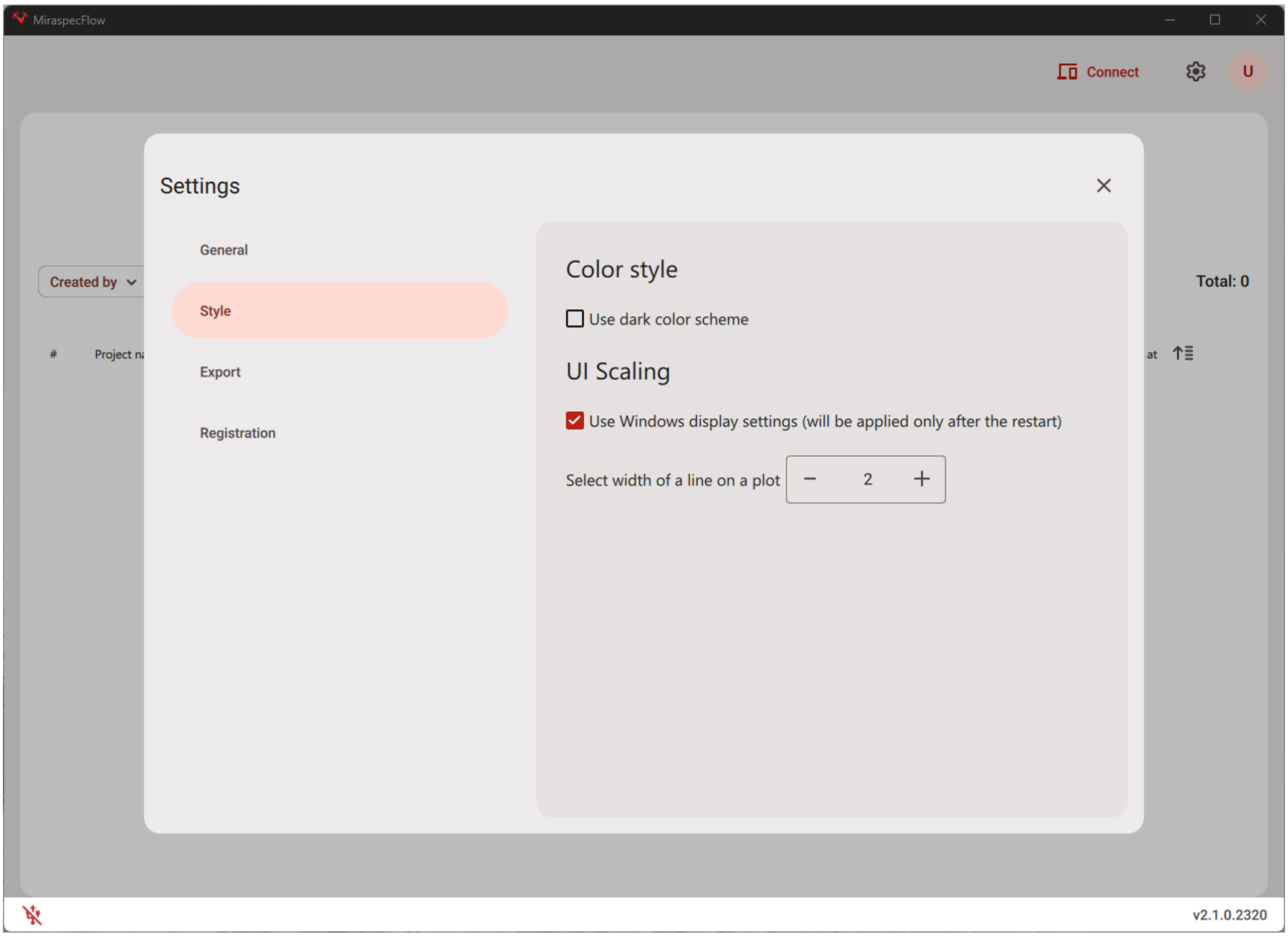
- Color style
- UI scaling



There are two options for color styling:

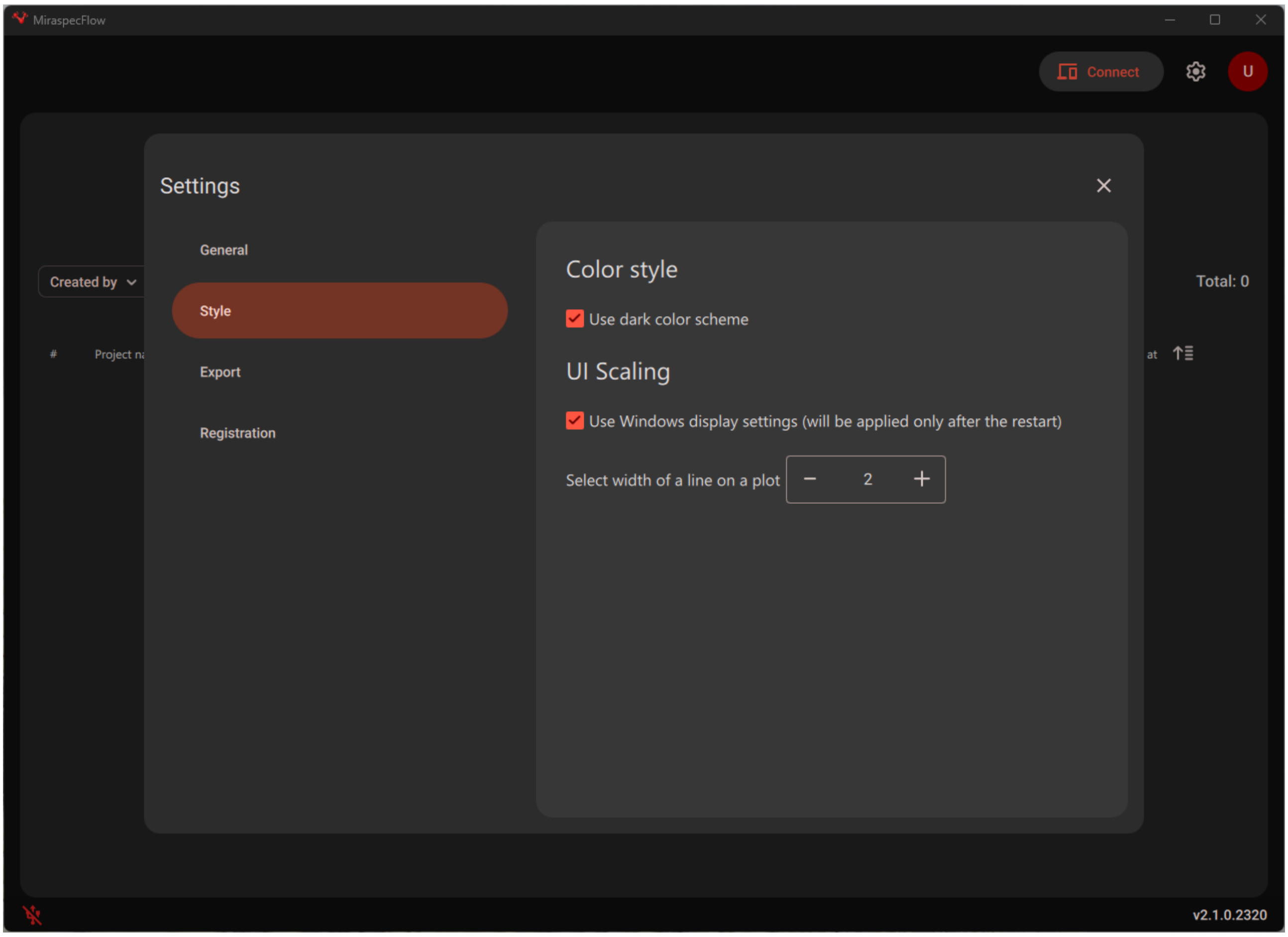
- dark color scheme
- light color scheme.

Untick the dark color scheme tick button to enable light color scheme.

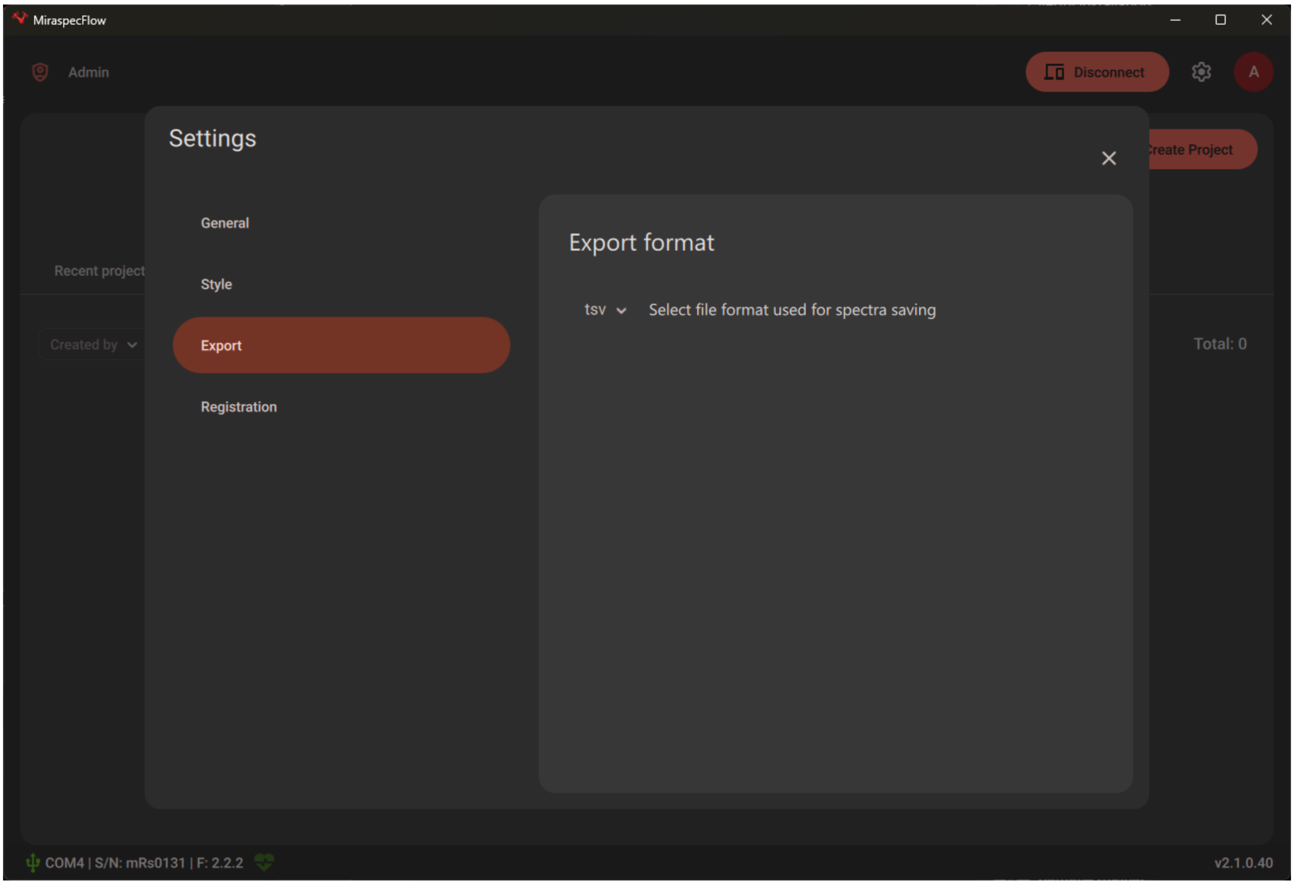


In practice light colour scheme might be more useful when taking the screenshots from the software for example for the reports etc.

The default value of UI scaling is 2. Click on the + and – buttons to adjust the UI scaling accordingly to match your preferences.

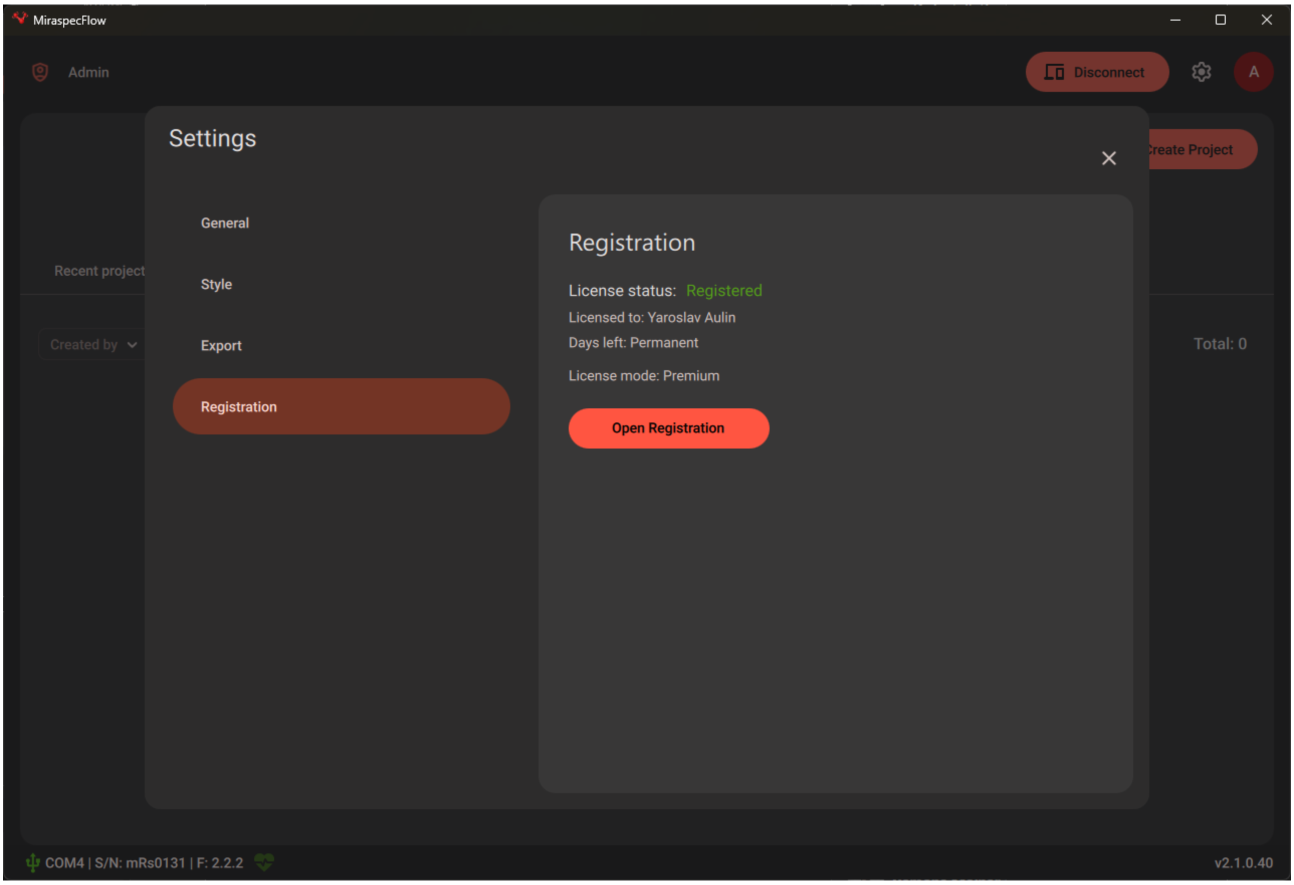


Export allows to choose default export format:



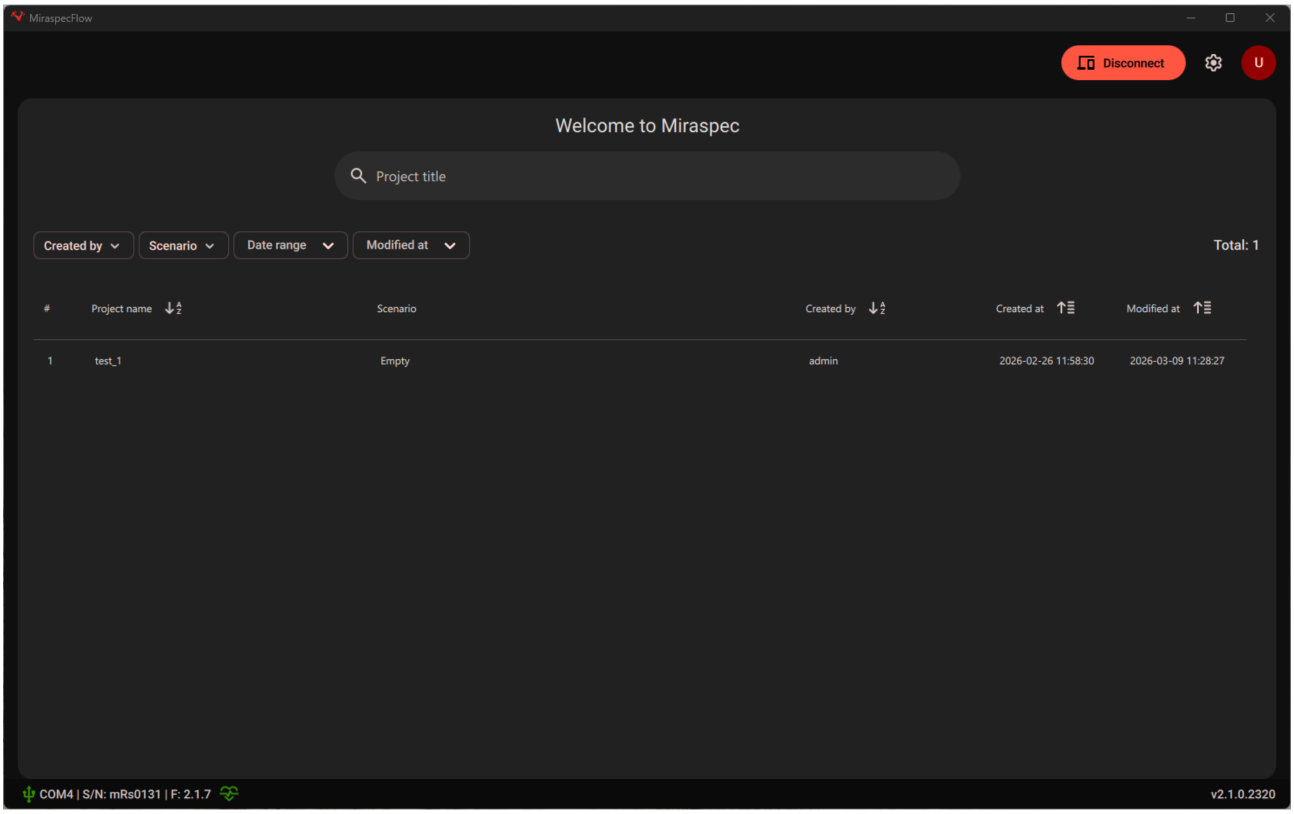
Available formats are .tsv, .jdx, .txt.

Registration section allows to check the registration status of the software:

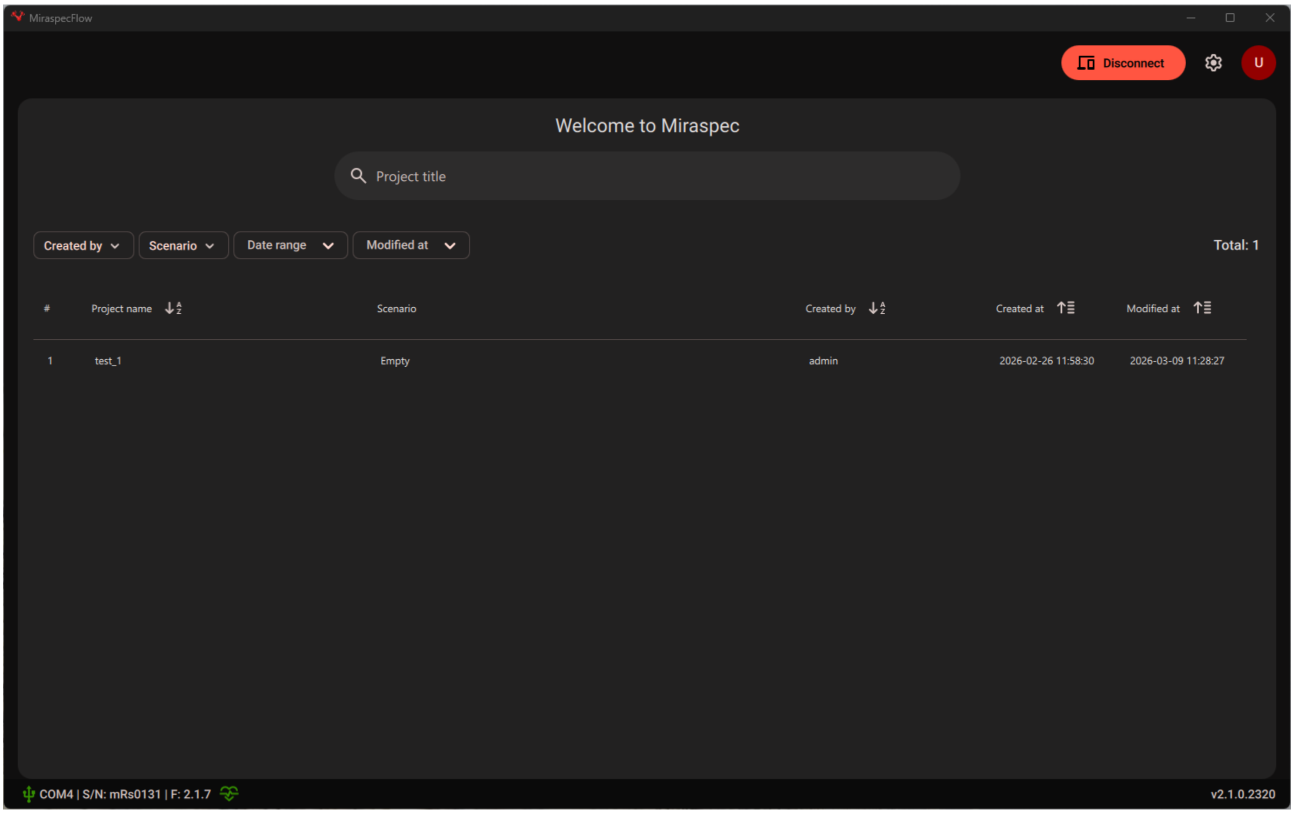


3.7. Interface overview and navigation

After the user logs in, the welcome to Miraspec screen is shown.



The bottom status bar contains information displaying the version of Miraspec Flow software in the right hand side:



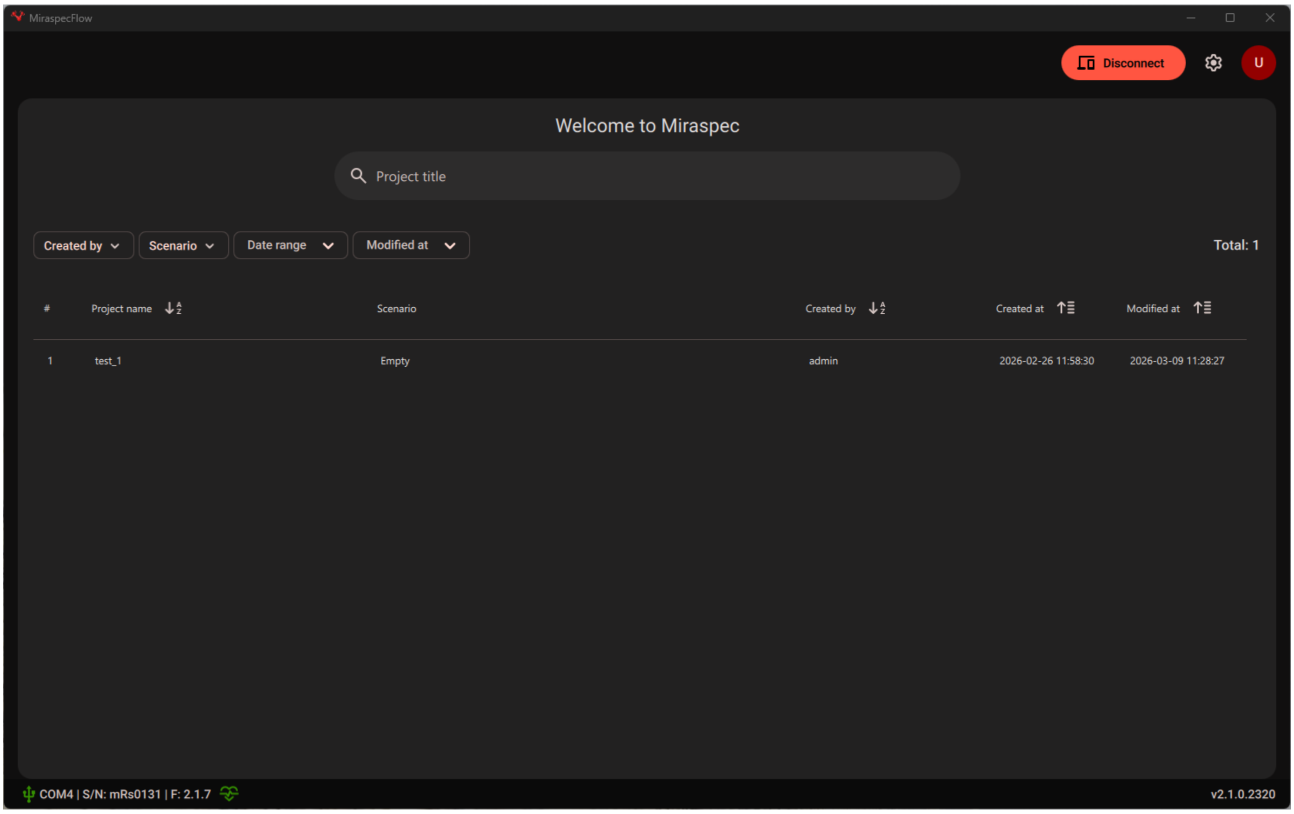
At the left hand side the status of the connected device is shown, indicating the following:

- COM port
- Device serial number
- Firmware version
- Health status of the device

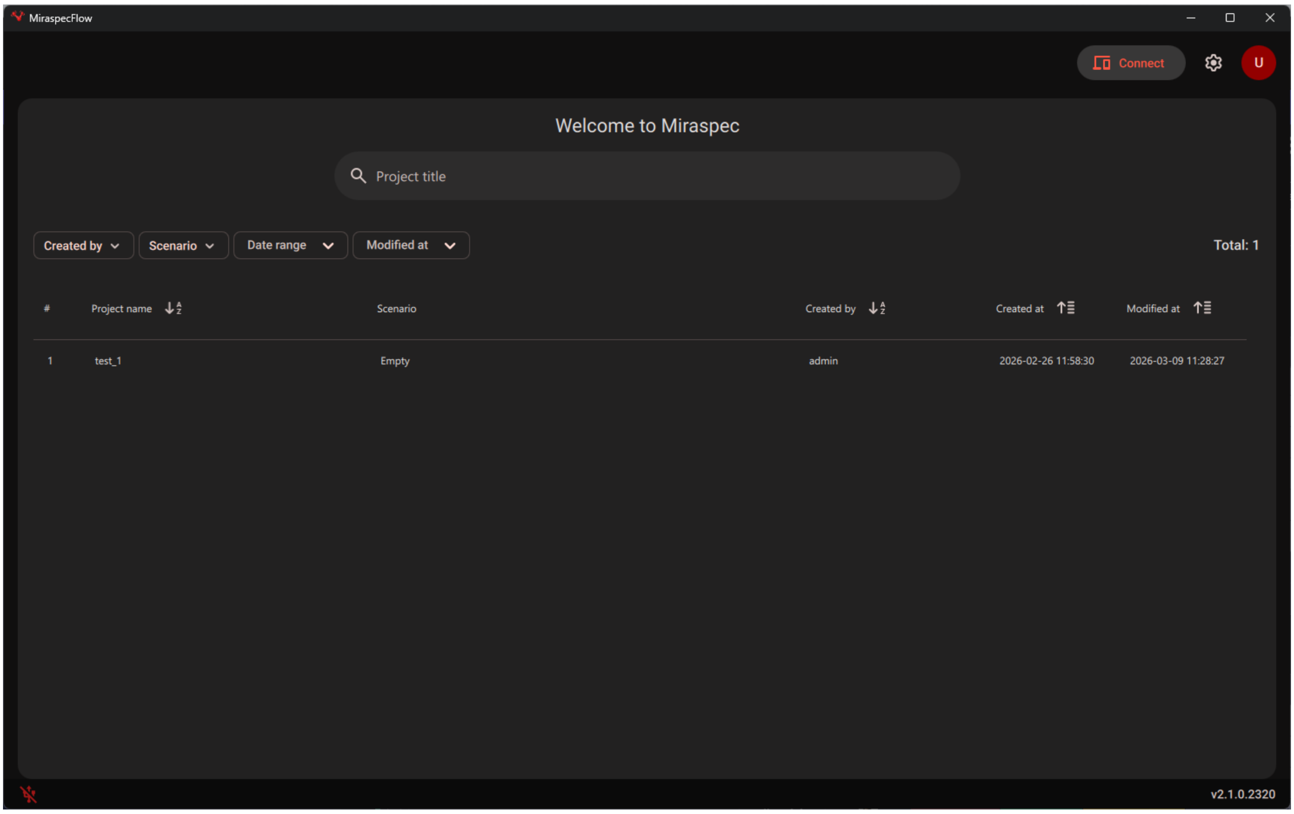
The health status of the device is indicated by the color of the heart:

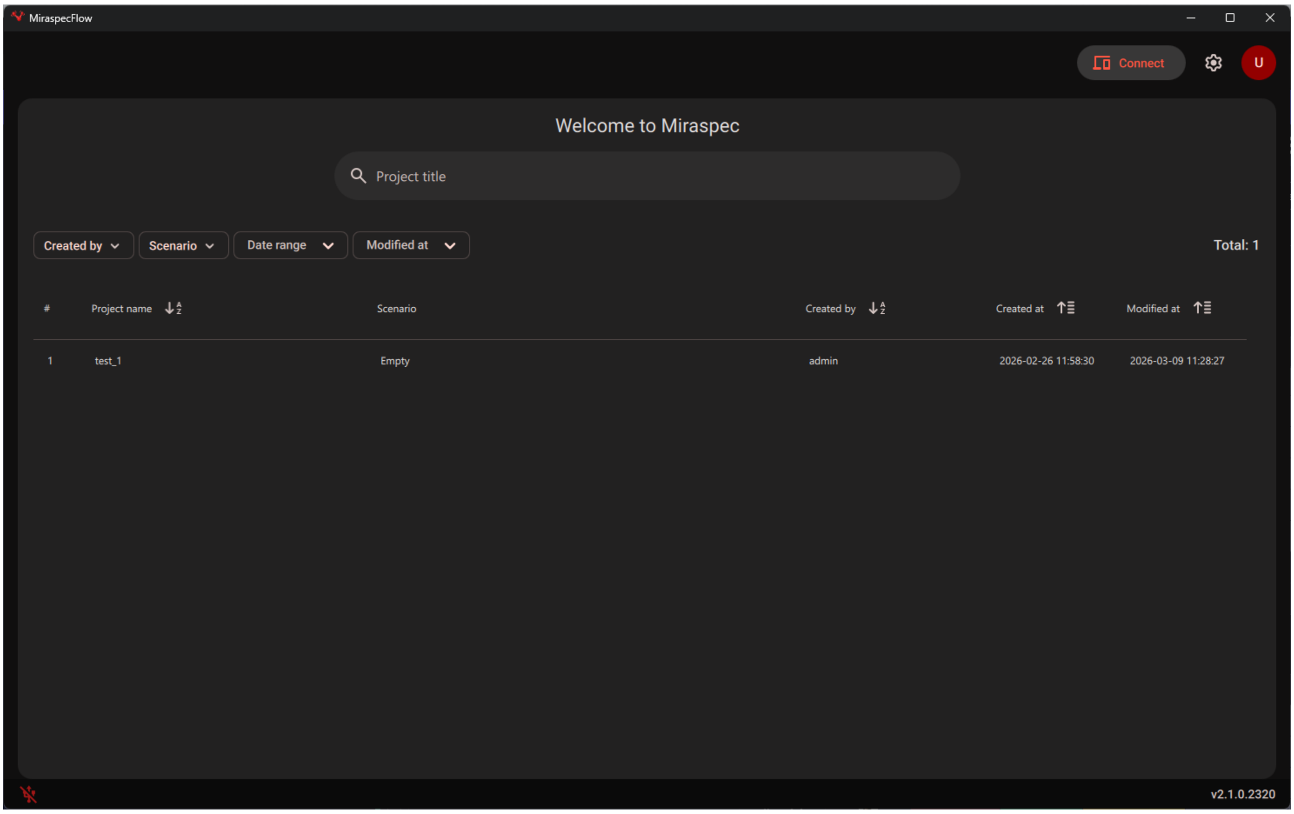
- Green – healthy
- Yellow – partly healthy
- Red – unhealthy

Connect/ disconnect button allow to connect or disconnect the device respectively.

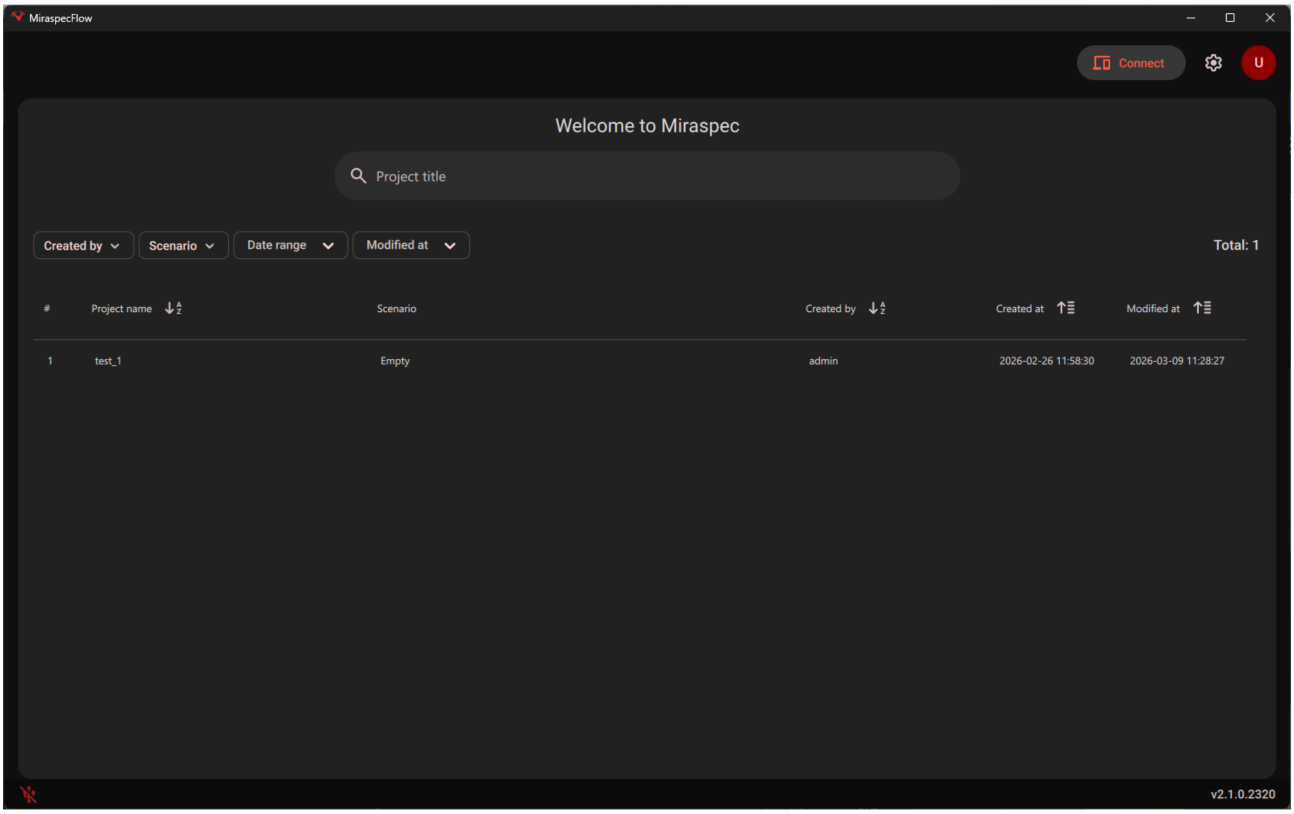


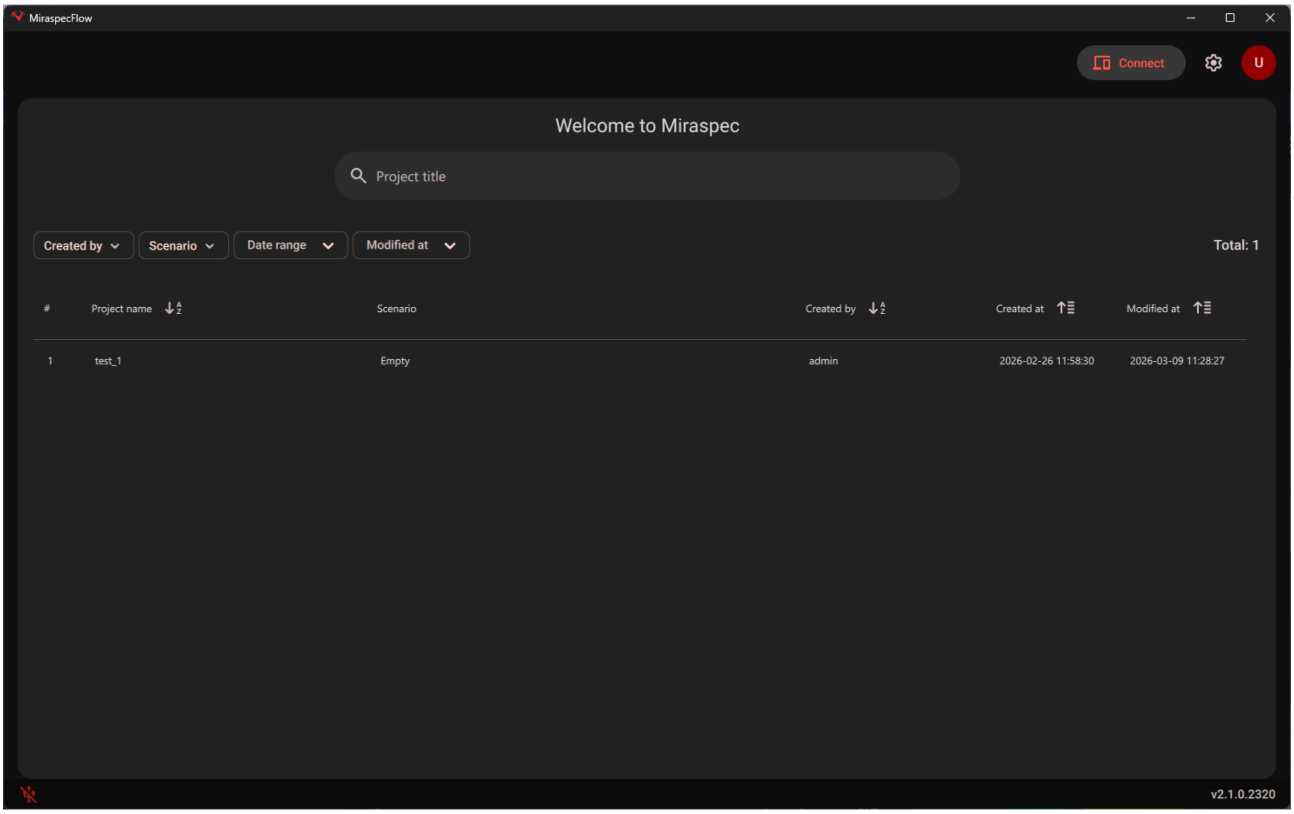
When the device is disconnected the USB connection icon changes colour to red. And the Disconnect button changes to Connect, by clicking on the connect button, one can connect the device.





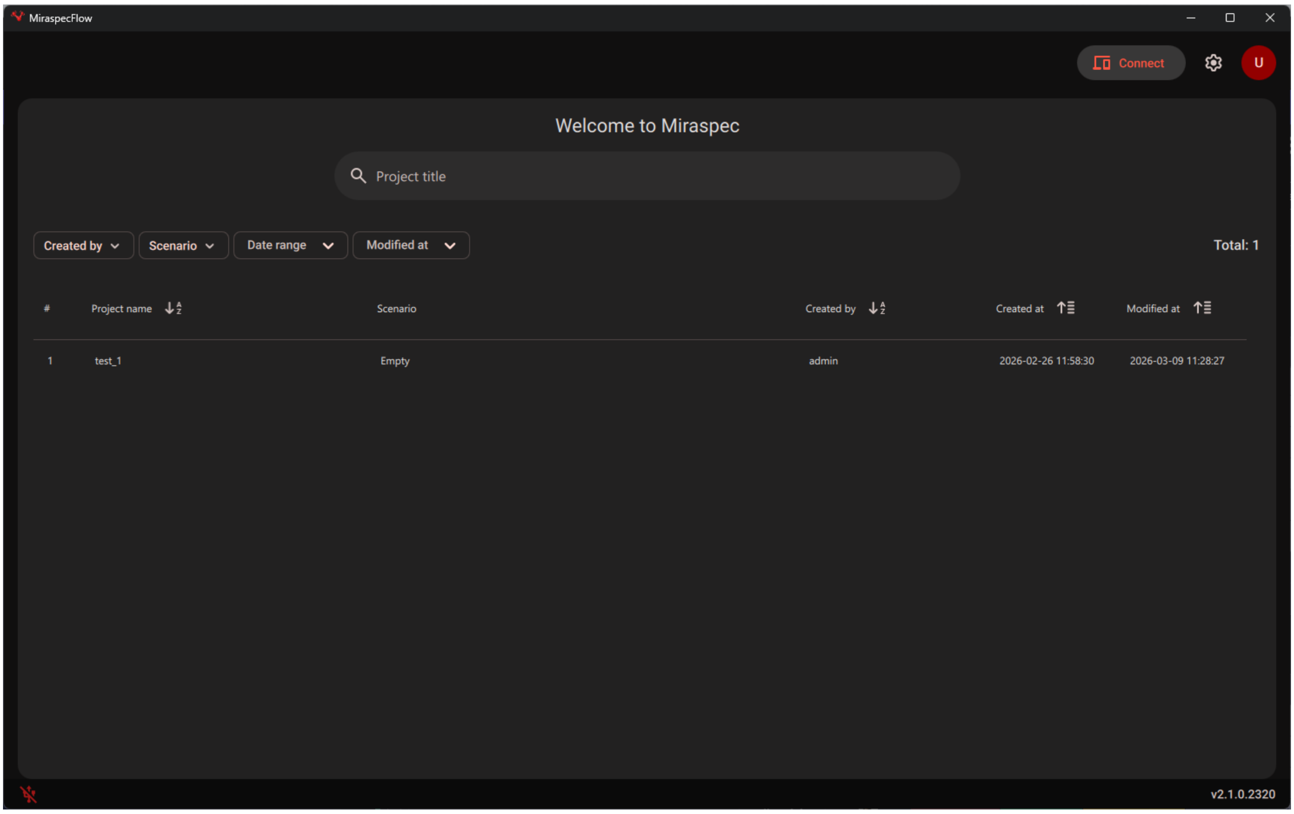
The gear icon allows to access Miraspec settings described in section 3.6 ***Program setting***.



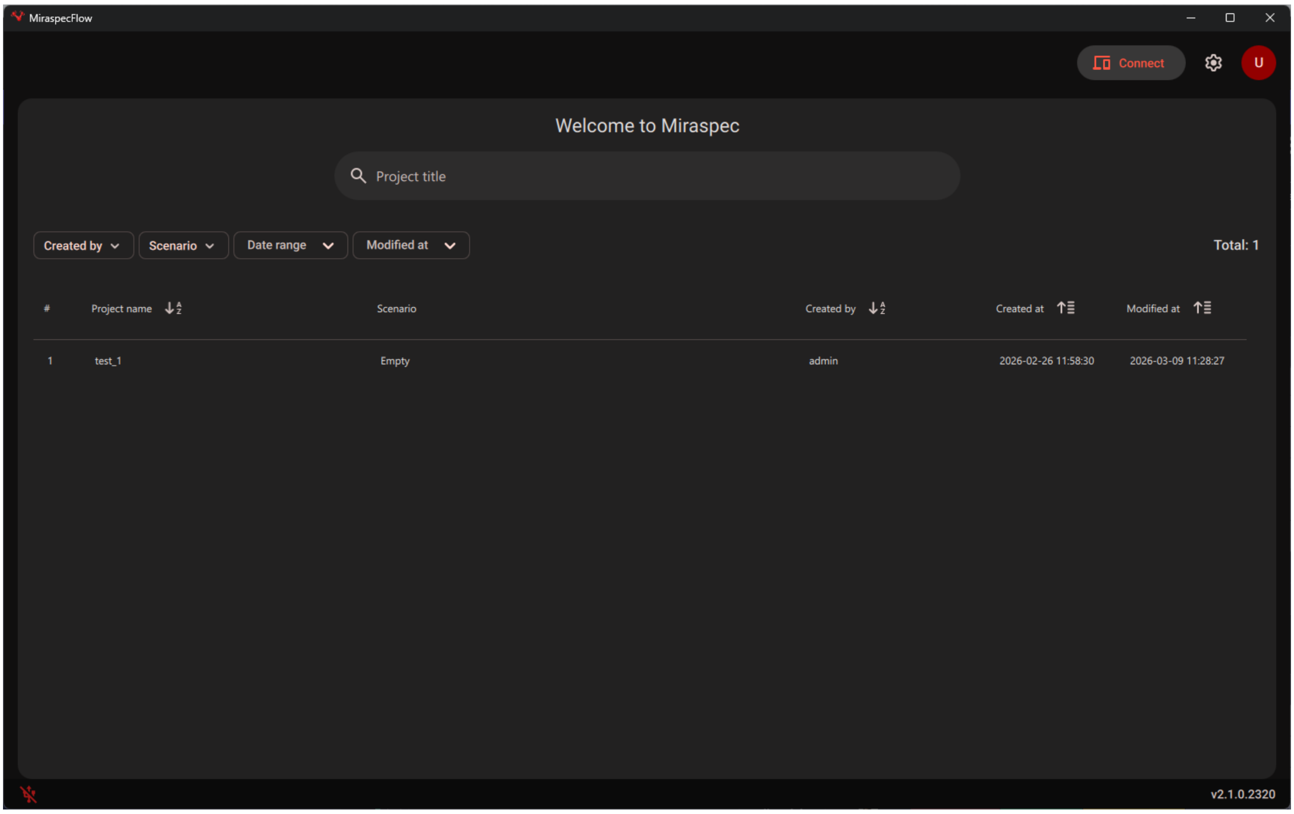


Clicking on the user icon settings allows to access user account information and change password, as well as log out from the system. This is described in section 3.5 ***User account information***.

Welcome to Miraspec screen contains the list of projects assigned to the user



The search bar above the list of projects allows to search for relevant projects as well as matching the proper filters, for example: created by specific user, search by scenario, creation date range and last modification date.



4. Projects and initial setup

Projects provide the primary organizational structure for measurements and analyses performed in Miraspec Flow. Each project contains the configuration settings, acquired spectra, processing parameters, analysis results, and related data associated with a specific measurement task or experimental study.

Using projects allows users to organize their work in a structured and reproducible manner. All information related to a measurement session—including device configuration, preprocessing steps, models used for analysis, and generated reports—can be stored and managed within a single project.

Before starting an experiment, users typically create a new project or open an existing one. Project templates may also be used to initialize projects with predefined settings, which helps ensure consistency across measurements and simplifies routine workflows.

Once a project is created or opened, users can configure the analysis scenario, connect the appropriate measurement device, and proceed to spectral acquisition and analysis.

The following sections describe how to create, open, and configure projects within Miraspec Flow.

4.1. Project history

The **Project History** section provides an overview of previously created and recently accessed projects in Miraspec Flow. This view allows users to quickly locate and reopen existing projects without manually browsing through project directories.

When the user logs into the system, the project history may display a list of recently used projects along with basic information such as the project name, scenario type, creator, and the date of creation or last modification. Selecting a project from this list opens the project and restores its associated data, including spectra, processing settings, models, and analysis results.

For new users or during the first use of the system, the project history may be empty until projects are created or opened. As projects are created and used over time, they will automatically appear in the history list.

The project history helps improve workflow efficiency by providing quick access to previously used projects and enabling users to continue working on ongoing experiments or analyses.

4.2. Creating a new project

A new project can be created to begin a new measurement or analysis workflow in Miraspec Flow. Creating a project initializes the project environment where spectra, processing steps, models, and analysis results will be stored and organized.

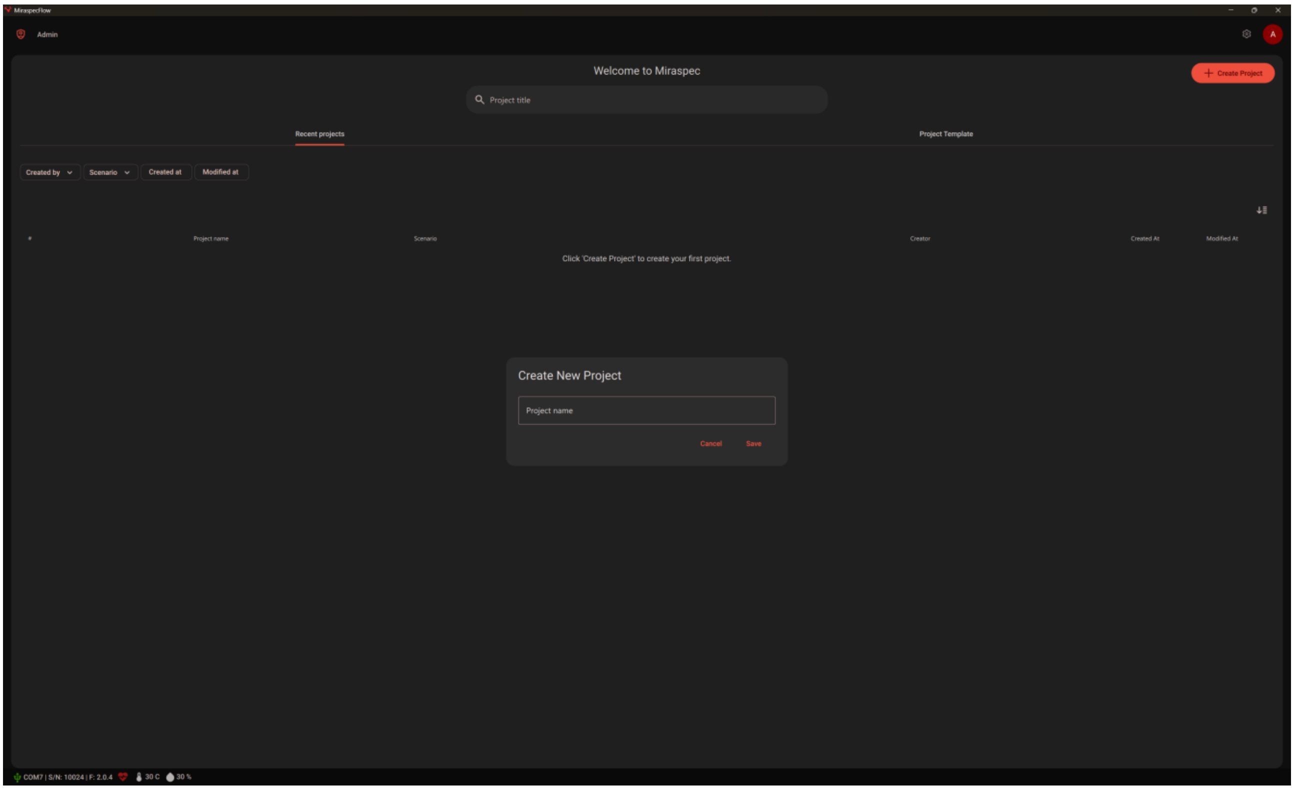
To create a new project, select the **Create Project** option in the project management interface. A dialog window will appear prompting the user to enter the project name and confirm the creation of the project.

After entering the desired project name, click **Save** to create the project. If the creation process is cancelled, the system will return to the previous screen without creating a new project.

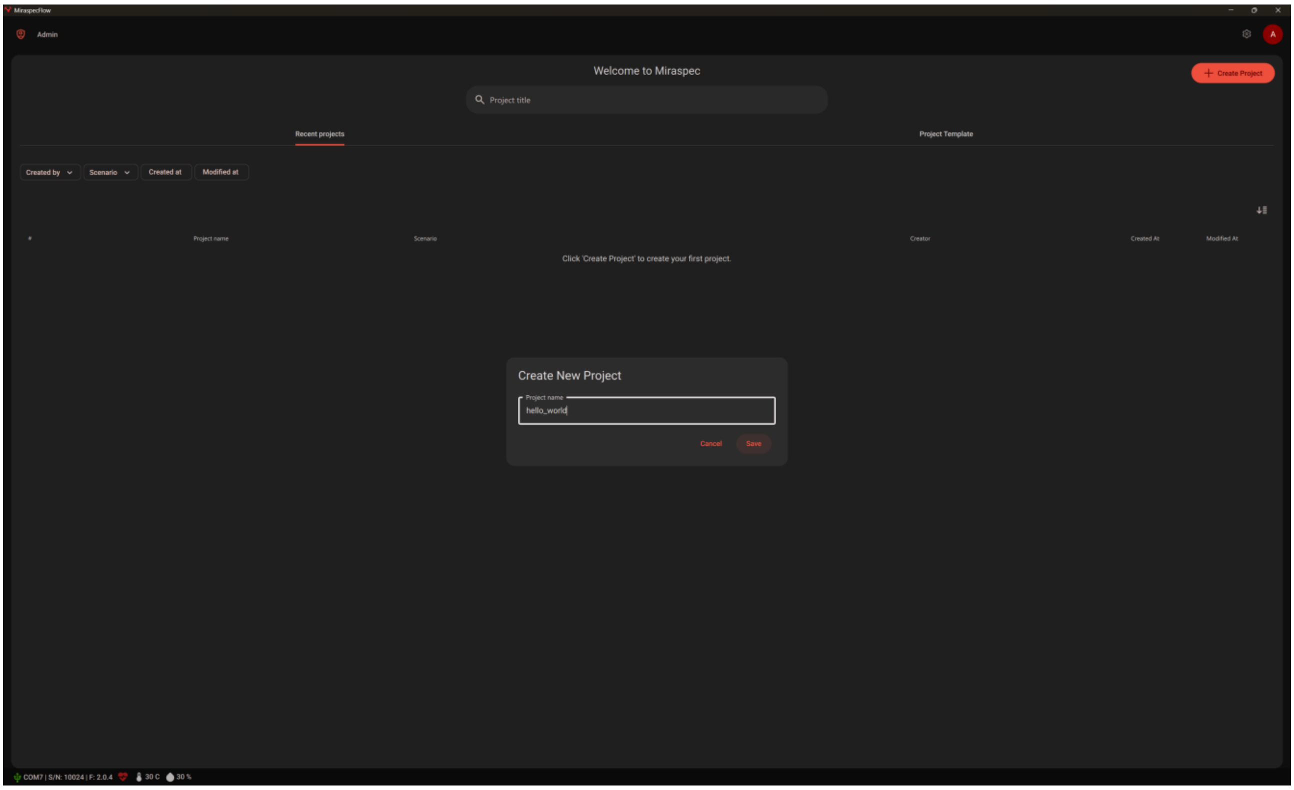
Once the project has been successfully created and the required configuration steps are completed, the system automatically proceeds to the **Experiment Workflow** section of the software. In this section, the user can connect the measurement device, configure acquisition parameters, and begin spectral measurements.

Creating a project ensures that all data and analysis results generated during the experiment workflow are organized and stored within a dedicated project environment.

Let’s create a new project. Click on create project red button in the top right corner of the software window.



Create new project prompt should appear. Let's call our first project hello_world.



Enter the project name and click save. In order to cancel click cancel. If we click save, there is next step to create scenario. This would be described further in the *Scenario Configuration* section.

4.3. Creating projects from templates

Miraspec Flow allows users to create new projects based on predefined **project templates**. Project templates contain saved configuration settings that can be reused to quickly initialize new projects with consistent parameters and workflows.

To create a project from a template, navigate to the **Project Templates** section and select the desired template from the list of available templates. Templates may include predefined settings such as the selected scenario, analysis type, and other configuration parameters used during spectral acquisition and analysis.

After selecting a template, the user can create a new project using the stored configuration. The user may be prompted to specify a project name before the project is created.

Once the project has been created from the template, the system proceeds directly to the **Experiment Workflow** section. In this environment, the user can connect the measurement device, configure acquisition parameters if necessary, and begin spectral acquisition.

Using project templates helps ensure consistency across experiments and simplifies the setup process for commonly used measurement workflows.

4.4. Opening saved projects

Previously created projects can be reopened to continue working with existing spectral data, processing results, models, and analysis outputs. Opening a saved project restores the project environment and provides access to all data and configurations associated with that project.

To open a saved project, select the desired project from the **project list** or **project history** displayed in the project management interface. Once selected, the project will be loaded into the system.

When a saved project is opened, the software loads the project data and displays the project workspace with its stored spectra, models, and analysis results. Unlike creating a new project, opening an existing project **does not automatically proceed to the Experiment Workflow**.

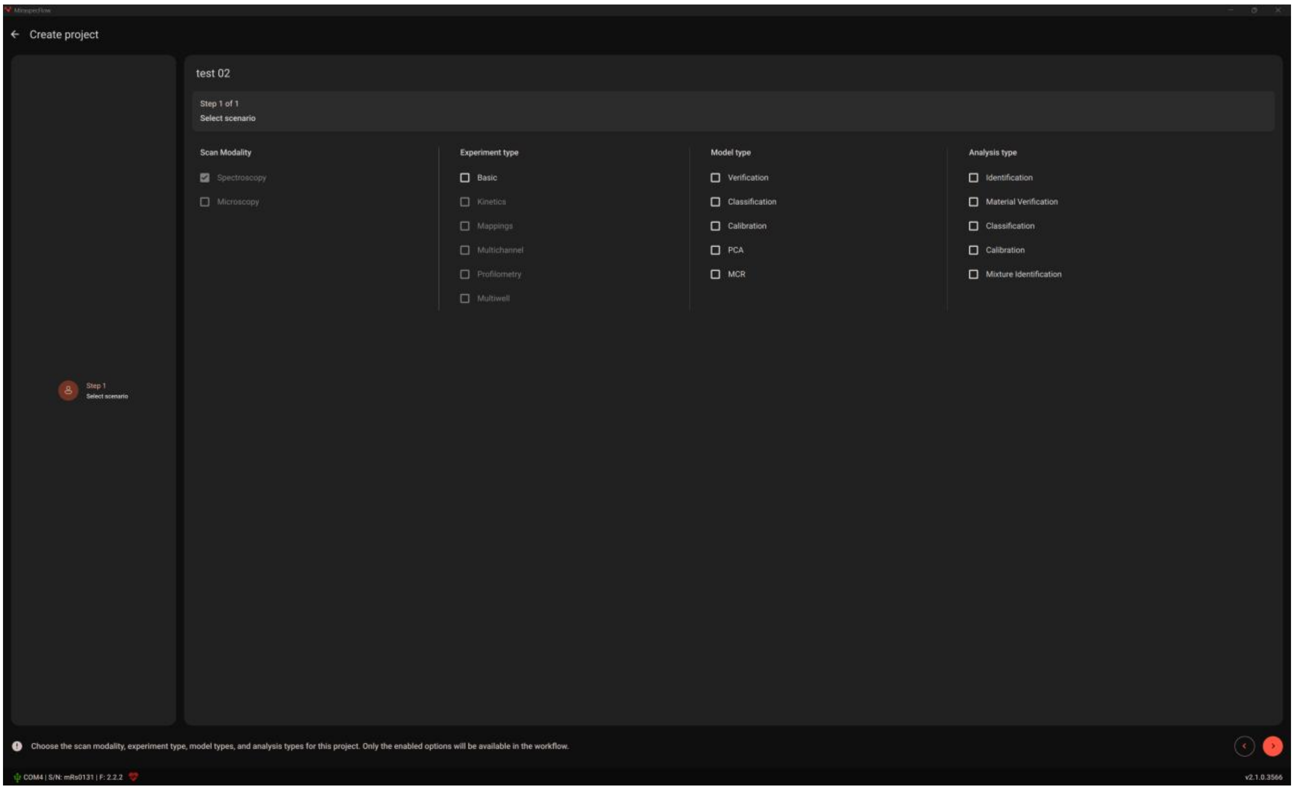
Instead, the user remains in the project environment and can navigate to the desired section of the workflow as needed. This approach allows users to review previously acquired data, continue analysis, modify project configurations, or perform additional measurements within the existing project.

4.5. Scenario Configuration

The **Scenario Configuration** section defines the analytical workflow that will be used within a project. During this step, users select the appropriate **model type** and **analysis type** that determine how spectral data will be processed, modeled, and analyzed throughout the experiment.

The selected scenario establishes the structure of the workflow and determines which tools and functions will be available in subsequent steps of the software. Depending on the selected configuration, the system prepares the appropriate environment for spectral acquisition, data processing, model creation, and analysis.

Choose scan modality for example Spectroscopy, experiment type for example basic, model type for example Verification Model and Analysis type for example Identification as shown below.



Then click Next red button in the bottom right corner of the screen. This way we proceed to step 2 – selection of device.

So, we click Next to proceed to the next step - Check connection.

The following sections describe how to select the model type and analysis type required for the intended application.

4.5.1. Model type

The **Model Type** setting defines the type of analytical model that will be used within the project. Selecting the appropriate model type determines the modeling tools and workflows that will be available during subsequent stages of the analysis.

Different model types support different analytical tasks. For example, models may be used to verify the identity of a known material, classify samples into predefined categories, or estimate the concentration of chemical components in a sample.

During scenario configuration, the user selects the model type that best matches the intended analytical objective. The selected model type determines the modeling methods and parameters that will be available in the **Models** section of the workflow.

Choosing the correct model type at the beginning of the project helps ensure that the appropriate modeling and analysis tools are available for the planned experiment.

4.5.2. Analysis type

The **Analysis Type** setting defines the method that will be used to interpret spectral data within the project. The selected analysis type determines how the processed spectra will be evaluated and what analytical tools will be available during the analysis stage of the workflow.

Different analysis types support different analytical objectives. For example, analysis methods may be used for identifying unknown materials, performing multivariate data exploration, classifying samples into predefined groups, or estimating chemical concentrations.

During scenario configuration, the user selects the analysis type that corresponds to the intended analytical task. The chosen analysis method determines which algorithms and analysis tools will be applied to the spectral data during the **Analysis** stage of the workflow.

Selecting the appropriate analysis type ensures that the software provides the correct analytical procedures for interpreting the acquired spectral measurements.

5. Device connection and status

5.1. Device connection

The devices are detected and connect automatically.

The user is also able to connect/ disconnect the device while inside the project.

In such case one needs to click on connect/disconnect button on the top right of the software window.

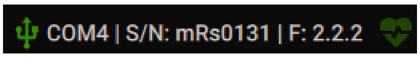
5.2. Device status

The **Device Status** section provides information about the current operational state of the connected spectrometer device. This information helps the user verify that the device is functioning correctly before starting spectral acquisition.

The device status may include parameters such as the device connection state, serial number, firmware version, and general device health indicators. Additional information such as temperature or environmental conditions reported by the device may also be displayed when available.

The status information is typically shown in the software interface or status bar, allowing the user to monitor the condition of the instrument during operation. If the device is properly connected and functioning normally, the system indicates that the device is ready for measurement.

The status of the device should also be shown in the status bar at the bottom left corner of the software window.



For example in our case the status bar says that the device is connected (green USB icon), the device’s serial number is mRs0131, firmware version is 2.2.2, the device is healthy.

If any issues are detected, such as a lost connection or abnormal device condition, the user should verify the hardware connection and device configuration before proceeding with the experiment workflow.

6. Experiment Workflow

The Experiment Workflow section describes the main operational environment used for spectral acquisition and measurement control in Miraspec Flow. This interface allows users to configure acquisition parameters, monitor the status of the connected device, capture Raman spectra, and visualize the measurement results in real time.

Within the experiment workflow, users can adjust measurement settings such as laser parameters, detector configuration, and acquisition sequences to optimize spectral quality for a given sample. The interface also provides tools for viewing previously acquired spectra, managing measurement history, and inspecting spectral data through interactive graphing and visualization features.

Before starting an experiment, a project must be created or opened and a compatible device must be connected to the system. Once these prerequisites are satisfied, the experiment interface enables users to initiate spectral acquisition and manage the measurement process.

The following sections describe the layout of the experiment interface, available parameter settings, device validation procedures, and the workflow used to capture and visualize Raman spectra.

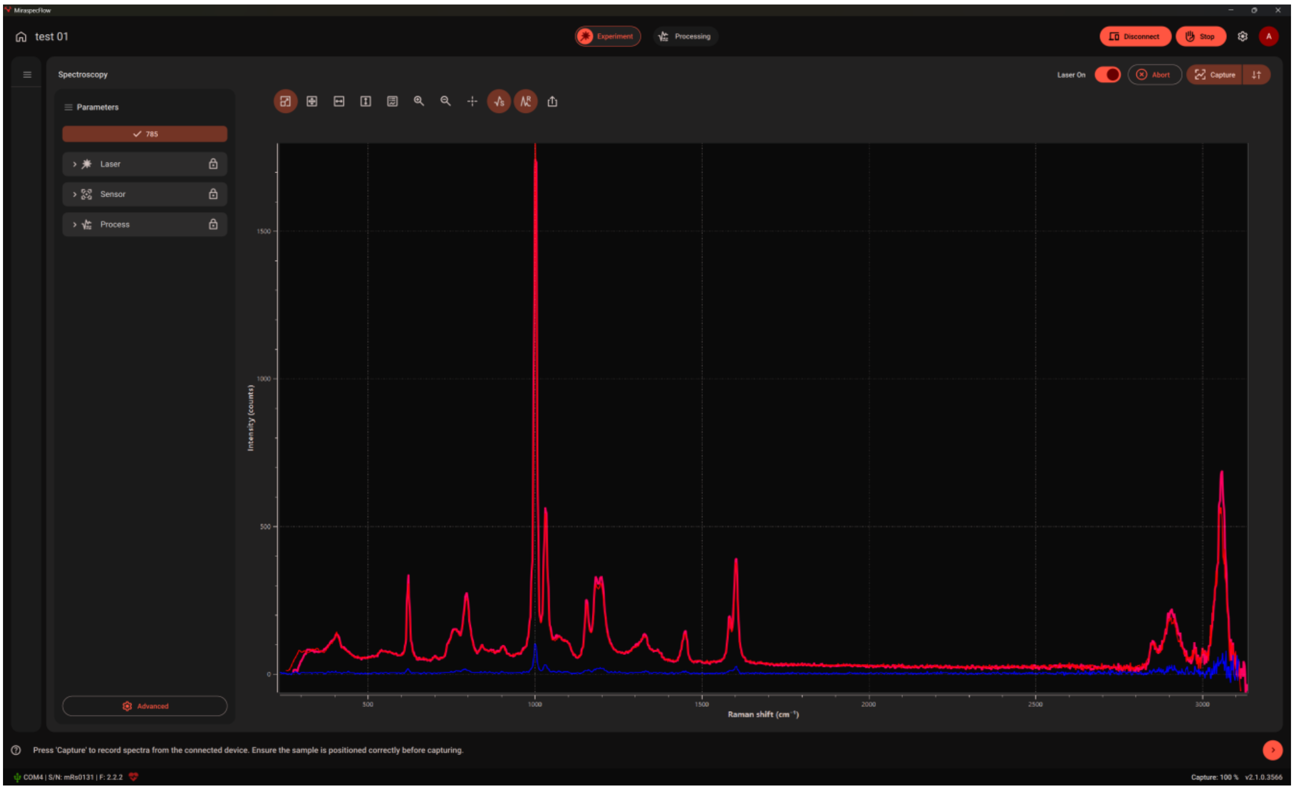
6.1. Experiment interface

The **Experiment Interface** provides the main working environment for spectral acquisition and measurement control in Miraspec Flow. In this interface, users can configure acquisition parameters, monitor the status of the connected device, capture spectra, and visualize measurement results in real time.

The experiment interface is typically organized into several functional areas. These include the **left panel**, which provides access to the dashboard, project data, and measurement history, the **parameters panel**, where acquisition settings such as laser, sensor, and processing parameters can be configured, and the **graph area**, where spectral data are displayed and monitored during measurements.

Using this interface, users can control the measurement process, adjust acquisition settings, and observe the resulting spectra as they are acquired. The interface also provides tools for managing recorded spectra and preparing data for further processing and analysis.

The experiment sections should show up which looks as follows in our case:



It shows the live data from the signal and reference channel of the miniRaman spectrometer in our case. As well as some settings and acquisition control buttons. Their functionality would be described in the next sections of this manual.

The following sections describe the main components of the experiment interface and explain how to configure measurement parameters, capture spectra, and work with spectral data within the experiment workflow.

6.2. Dashboard and project panels

The **Dashboard** and **Project** panels are located in the left section of the experiment interface and provide tools for managing spectral data within the current project.

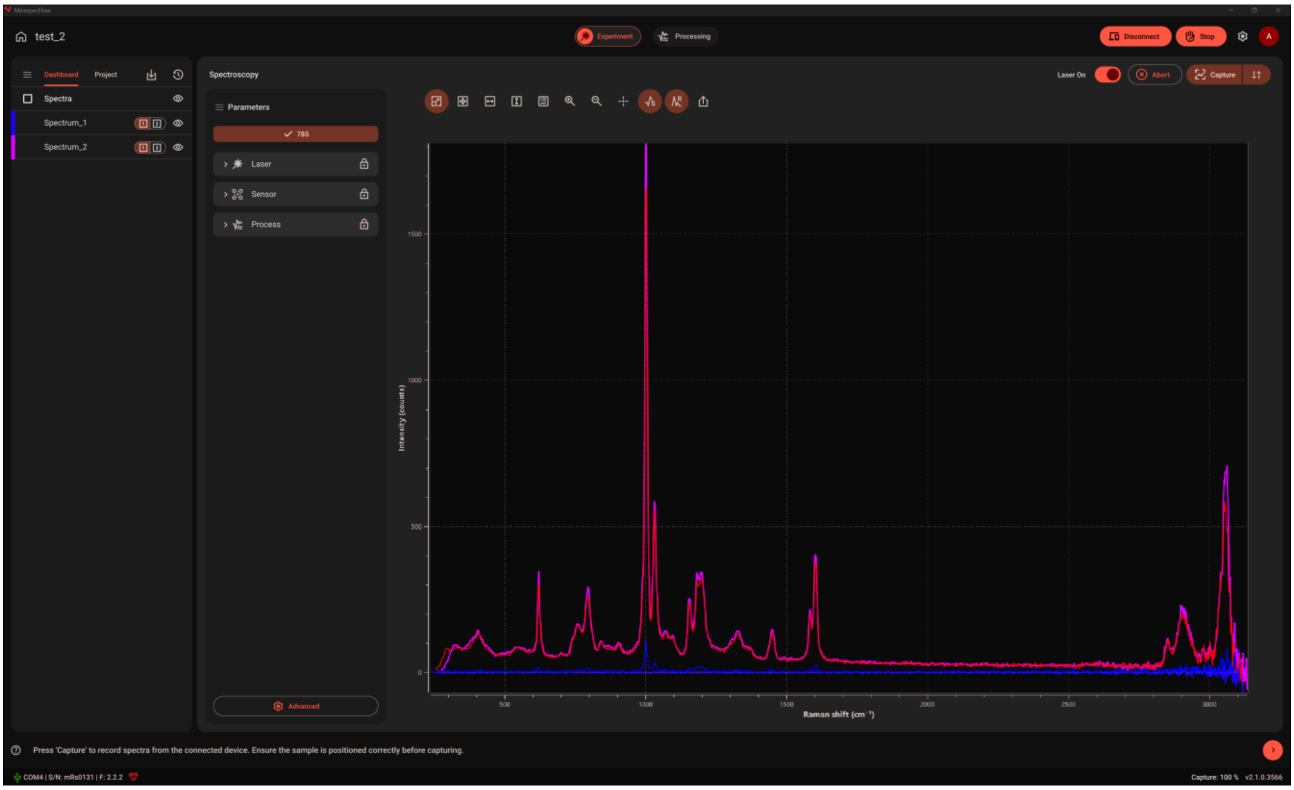
The **Dashboard** serves as the active workspace where users interact with spectra during the experiment and processing workflows. Spectra recorded during measurements or imported from external files appear in the Dashboard and can be displayed, compared, processed, or used for further analysis. Users can also perform operations such as exporting spectra, deleting them from the workspace, adding them to spectral libraries, or controlling their visibility in the graph.

The **Project** panel contains the complete set of data associated with the current project. This may include spectra, analytical models, and other project-related resources. Unlike the Dashboard, which is used as a working area, the Project panel acts as a structured repository where all project data are stored and organized.

Users can select spectra or models from the Project panel and add them to the Dashboard for further processing or analysis. This separation between the Dashboard and Project panels helps maintain an organized workflow while allowing users to focus on the data currently being analyzed.

In order to access the dashboard one should click on the three horizontal lines icon at the top left corner of the screen.

The dashboard should pop up. It will look as follows:



When we just start it should just be empty, without data with only one project hello_world showing up.

If some spectra were measured it should look as follows (the measurement procedure would be described in the following sections):

The Dashboard contains the spectra we are working with while the Project contains all the data. For example:

In order to export the spectra one should select the spectrum of interest for example polystyrene in our case:

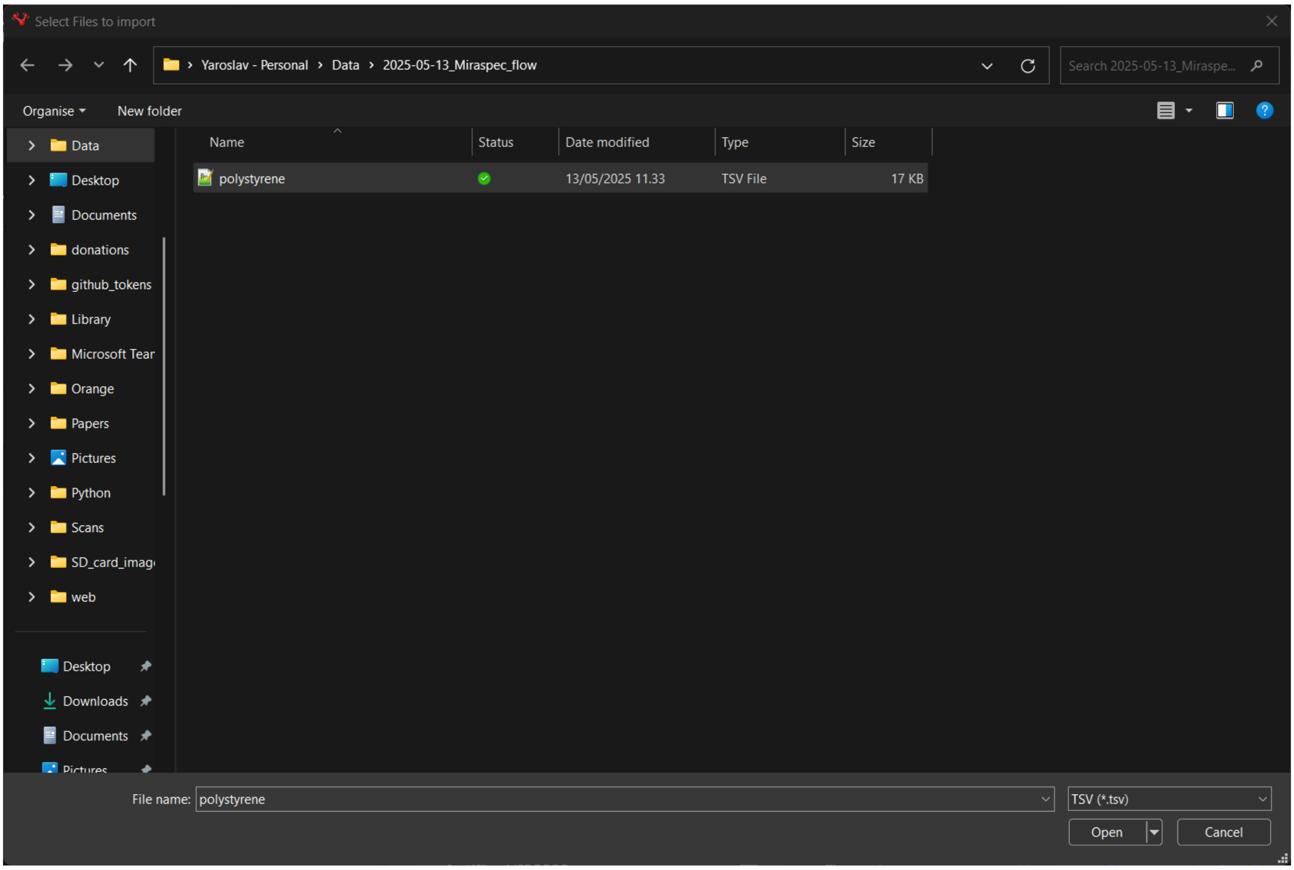
Then one should click on the icon with the up pointing arrow in the bottom right corner of the dashboard. The pop up window should show up. Select the folder where you would like to export your data and click Select folder button from the pop up window. It is also possible to save multiple spectra simultaneously. Now the data are saved into the folder you chose.

Note

Please note that it is possible to change the format of export under settings (gear icon).

In order to upload the data, click on the button with the down pointing arrow in the top right corner of the dashboard.

The pop up window should appear. Proceed to the folder of interest and select the files you would like to upload.

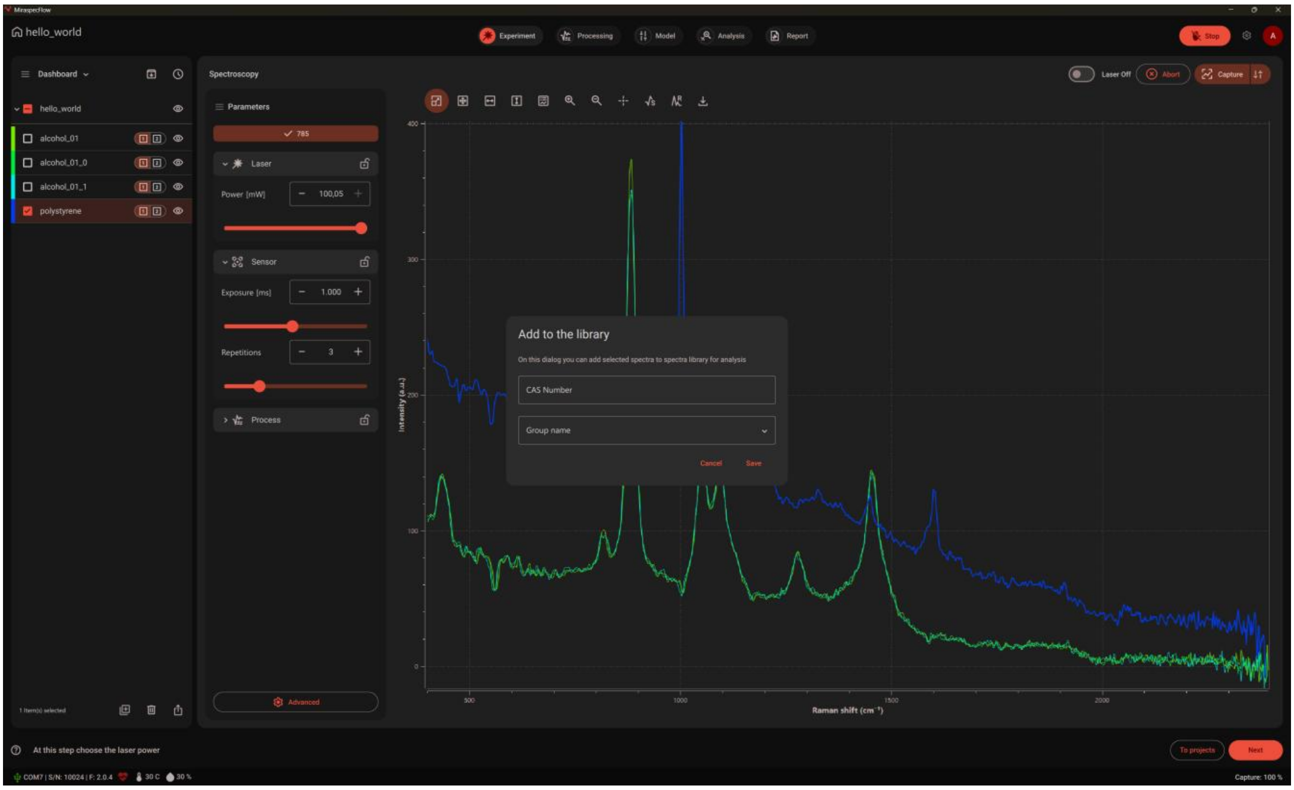


Now the new file is uploaded to the project.

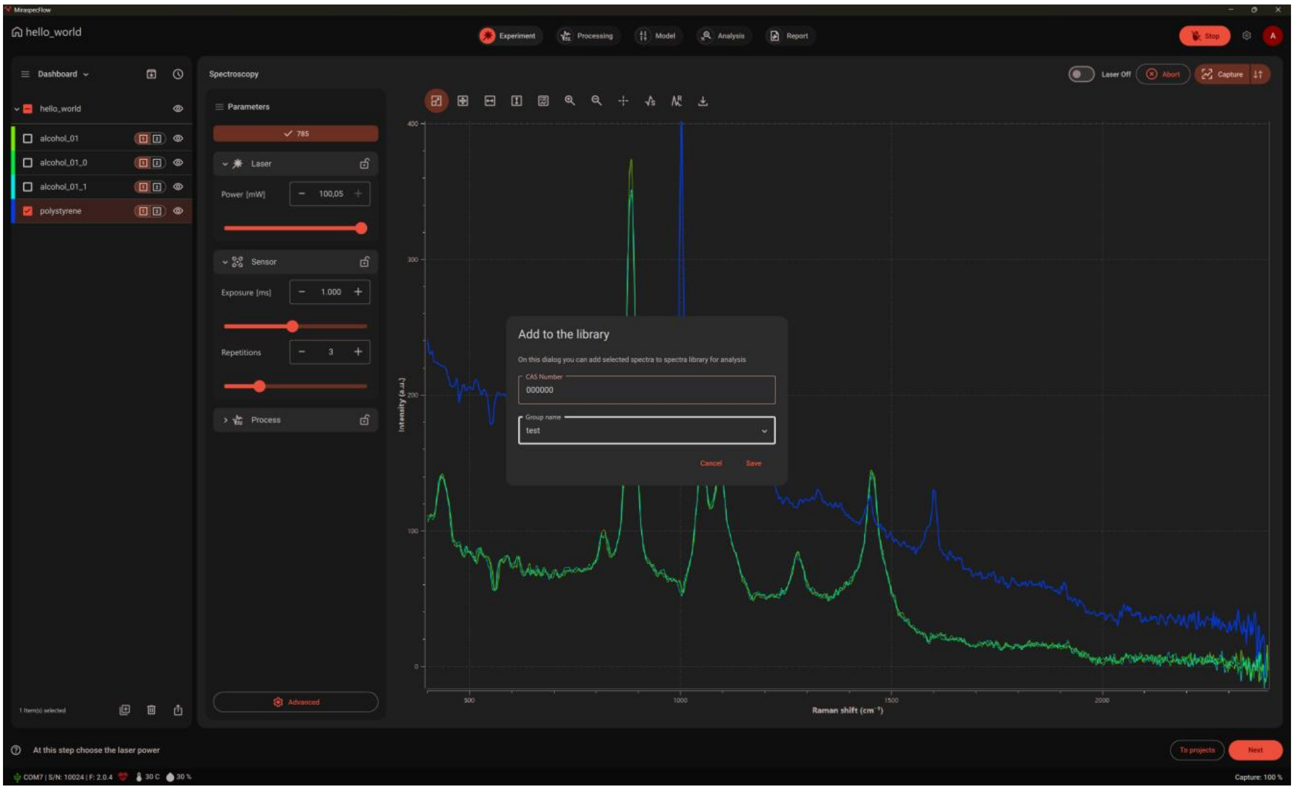
In order to delete the spectrum, select the spectrum you would like to delete (it is possible to delete multiple spectra, for example in our case we would like to delete two spectra). Spectra can be deleted from the Dashboard only, they are still present in Project.

Then click on the trash icon at the bottom of the dashboard. The spectra are deleted.

It is also possible to add the spectra to the library. Select the spectrum, then click on the icon with the plus at the bottom of the dashboard. A pop up window will appear.

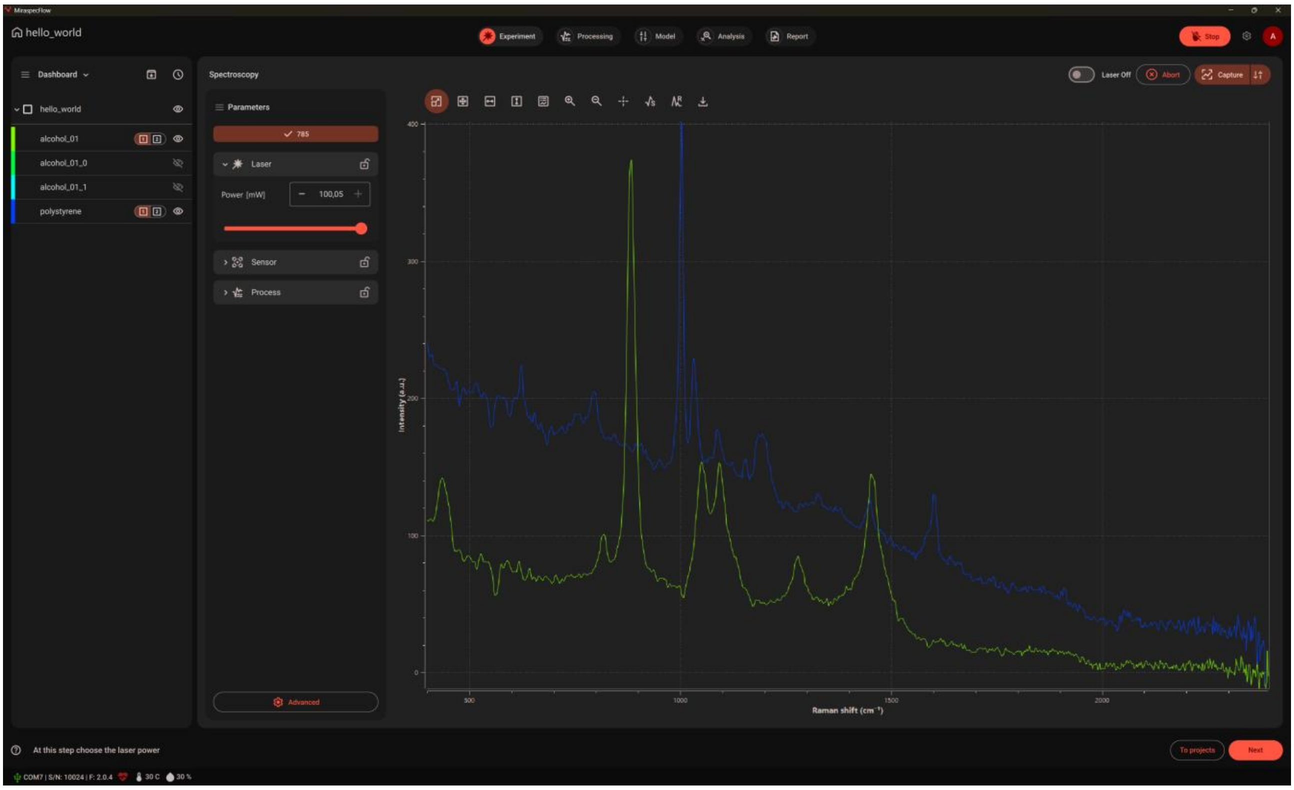


Enter the CAS number and choose the group or enter new group name. The CAS number is optional, the same for the group.

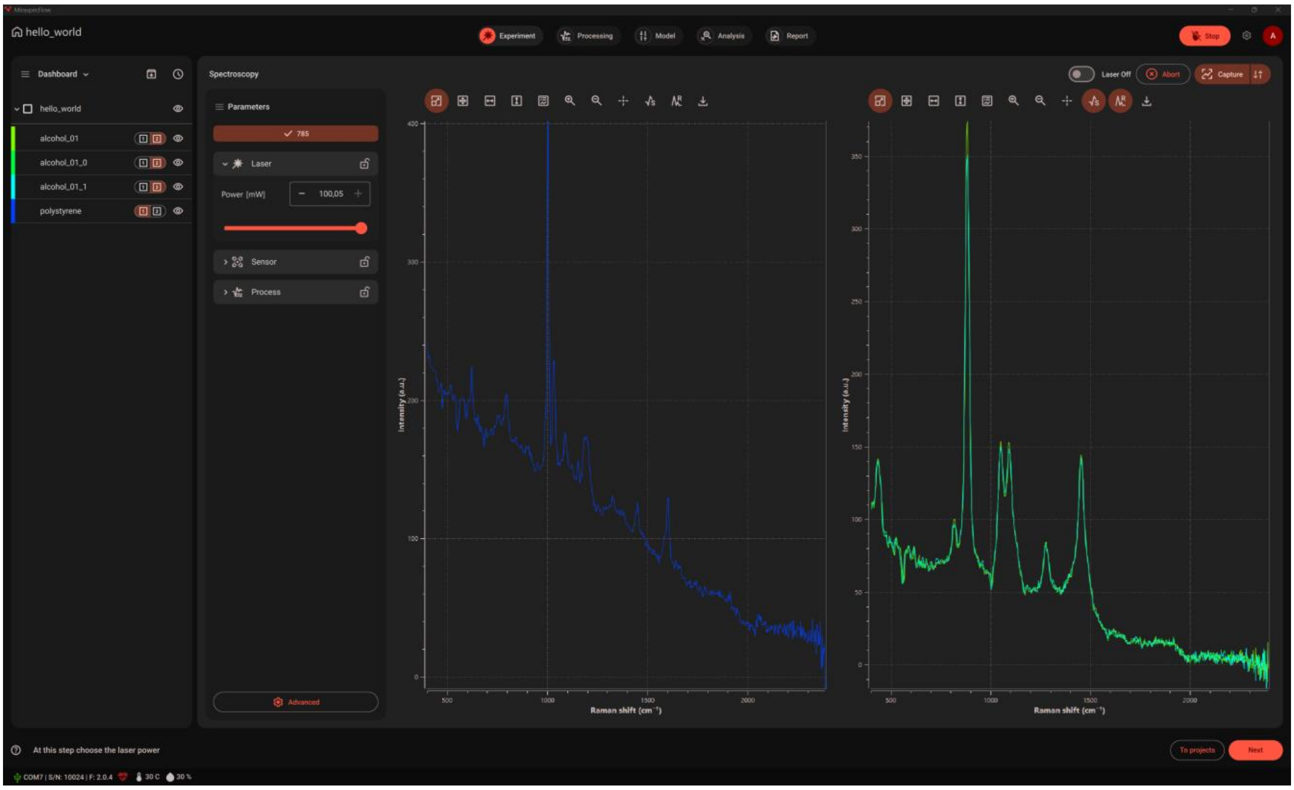


Click Save, now the spectrum should be added to the library. If you prefer to cancel, click Cancel.

In order to toggle between hide and show modes for the spectra click on the eye icon next to the spectrum. The hidden spectra won't be used in processing, data analysis, and so on.

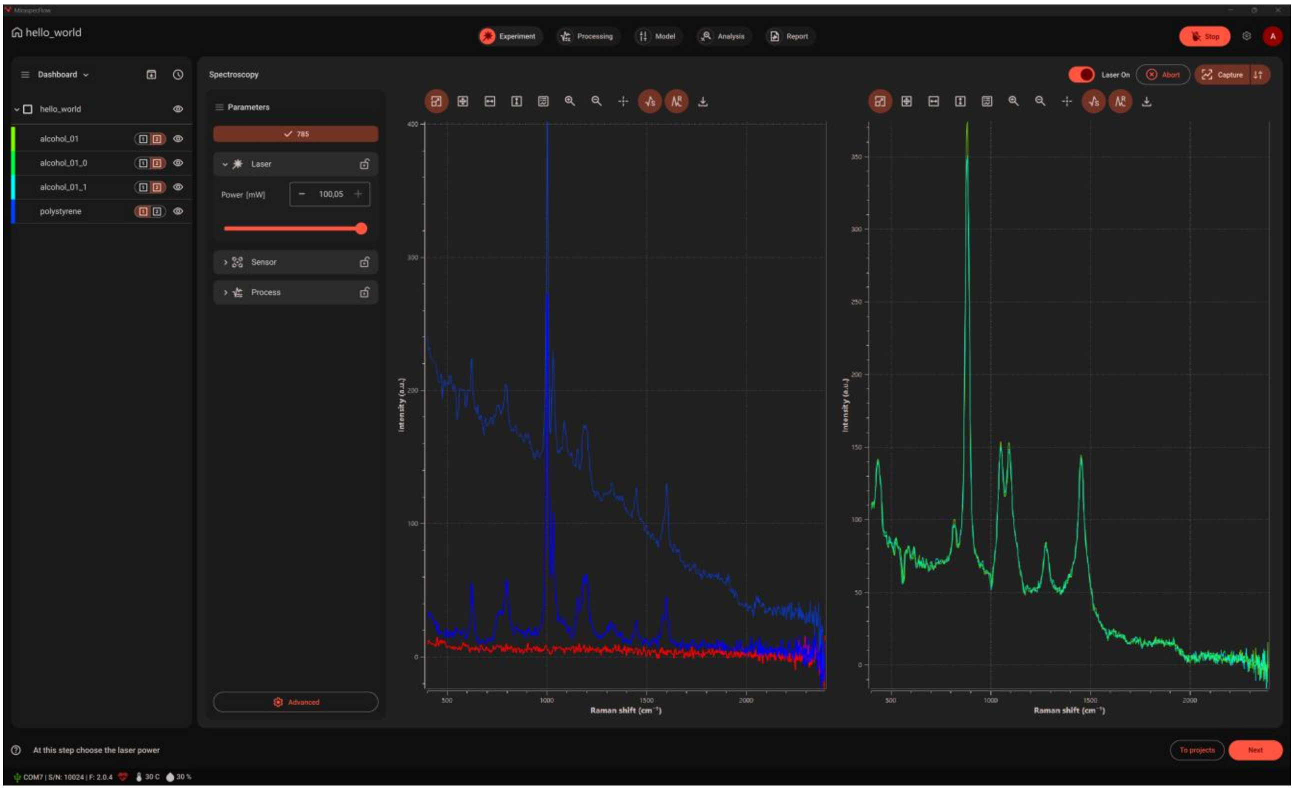


There is an option to split the graph into two graphs by clicking on the 1 and 2 buttons and assigning the specific spectrum to either 1 or 2 as in the example below:

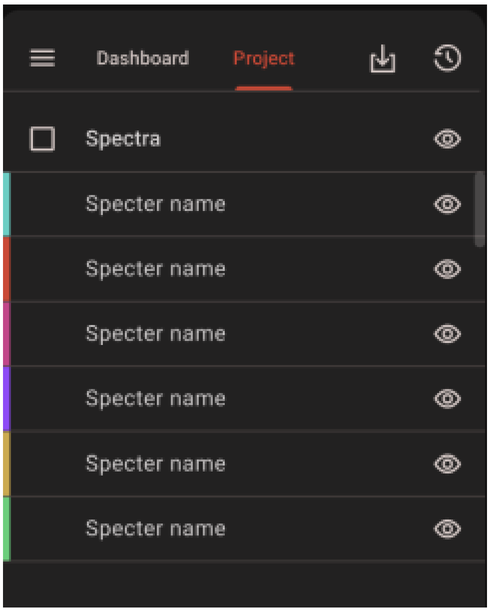


If all the spectra are at 1, only one graph is shown.

Live measurement data are shown in graph 1 only.



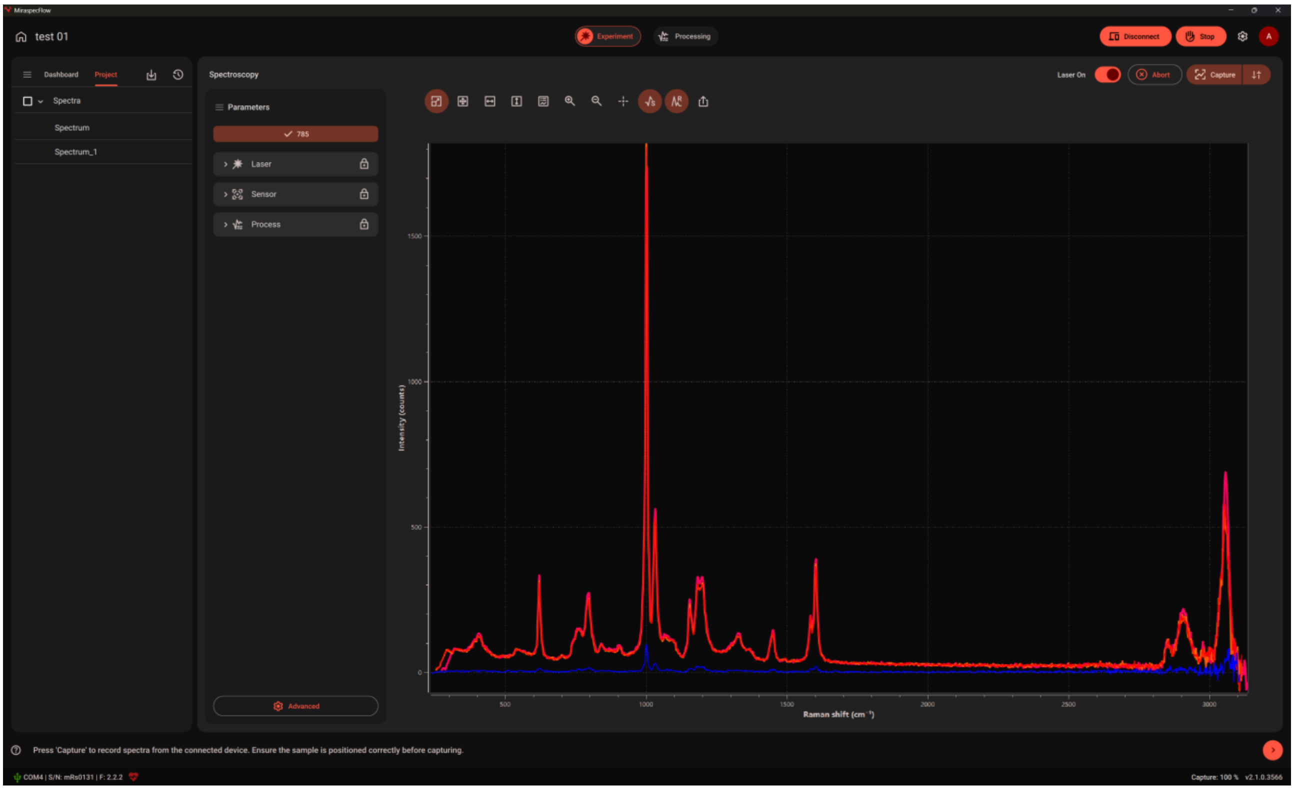
The Project tab is located in the left sidebar, next to the Dashboard tab. The user can switch between them depending on whether they want to work with the active workspace (Dashboard) or view and manage all data related to the current project (Project).



Purpose of the Project tab

The Project tab stores all spectra and models that the user has worked with within the current project:

- Spectra
- Verification Models
- Classification Models
- Calibration Models
- PCA Models
- MCR Models



These categories are displayed as collapsible groups, which can be expanded or collapsed for easier navigation, especially when working with large datasets.

Selecting elements (spectra and models)

Multiselect

Each item has a checkbox, allowing the user to select one or multiple elements.

Once at least one item is selected, an action bar appears at the bottom, which includes:

- number of selected items
- Add to Dashboard button
- Export button (download to local drive)
- Clear selection button (× icon)

Selection limitations based on the current page

On Experiment and Process pages

- selecting models is disabled (model checkboxes are inactive)
- only available spectra can be selected
- available spectra can be added to the Dashboard

On the Model page

- selecting spectra is disabled
- only available models can be selected
- available models can be added to the Dashboard

This ensures a consistent workflow and prevents the user from selecting unsupported item types on certain stages.

Adding items to the Dashboard

To add spectra or models from the Project tab to the Dashboard:

1) The user selects one or several items.
2) The action bar appears.
3) The user clicks **Add to Dashboard**.
4) The Project tab closes automatically.

Selected items do **not** disappear from Project — they remain stored there as part of the project data.

Exporting spectra and models

The user can export any selected spectra or models via multiselect:

1) Select items
2) Click the **Export** button
3) Save them to the local drive

This provides a convenient way to transfer project data or create backups.

6.3. History of spectra

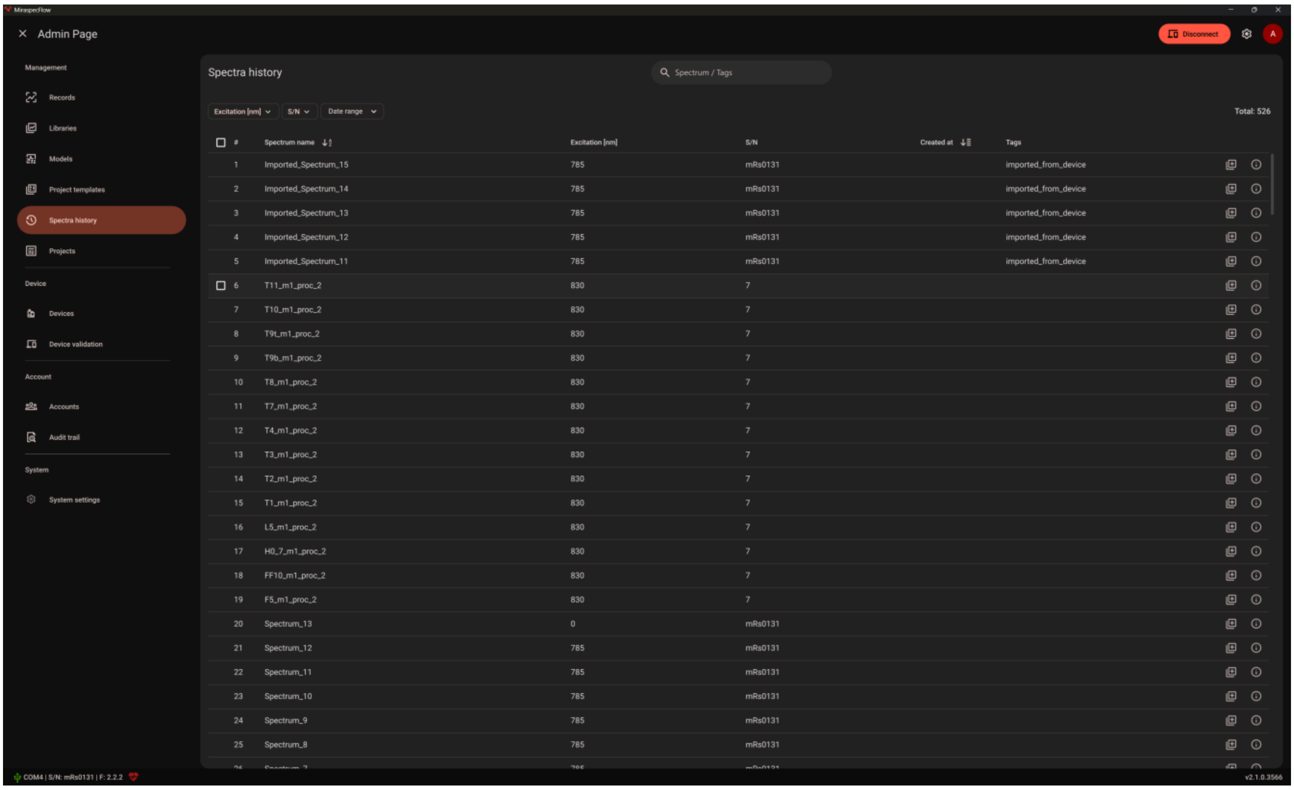
The **History of Spectra** section provides access to previously recorded spectral measurements within the current project or system history. This feature allows users to review earlier acquisitions and reuse spectral data for further processing, analysis, or comparison.

The spectra history typically displays a list of stored spectra along with associated information such as the spectrum name, acquisition date, device serial number, and other relevant metadata. Users can select spectra from the history and load them into the **Dashboard** for visualization or further analysis.

In addition to viewing previously recorded data, the history interface may allow users to export spectra, add selected spectra to a spectral library, or examine detailed metadata associated with each measurement.

The spectra history provides a convenient way to track previously acquired data and enables efficient reuse of spectral measurements during ongoing experiments or analysis workflows.

Clicking on clock icon in the top right corner of the dashboard shows the history of the project.



6.4. Parameter settings

The **Parameter Settings** section allows users to configure the measurement parameters used during spectral acquisition. These settings control various aspects of the spectrometer operation, including laser behavior, detector configuration, and data acquisition processes.

The parameters are organized into several categories to simplify navigation and configuration. Users can adjust settings related to the **laser**, **sensor**, and **data processing**, as well as access **advanced settings** when additional control over the device configuration is required.

Proper configuration of these parameters helps ensure optimal spectral quality and reliable measurement results. The following sections describe each group of parameters and explain how they influence the acquisition process.

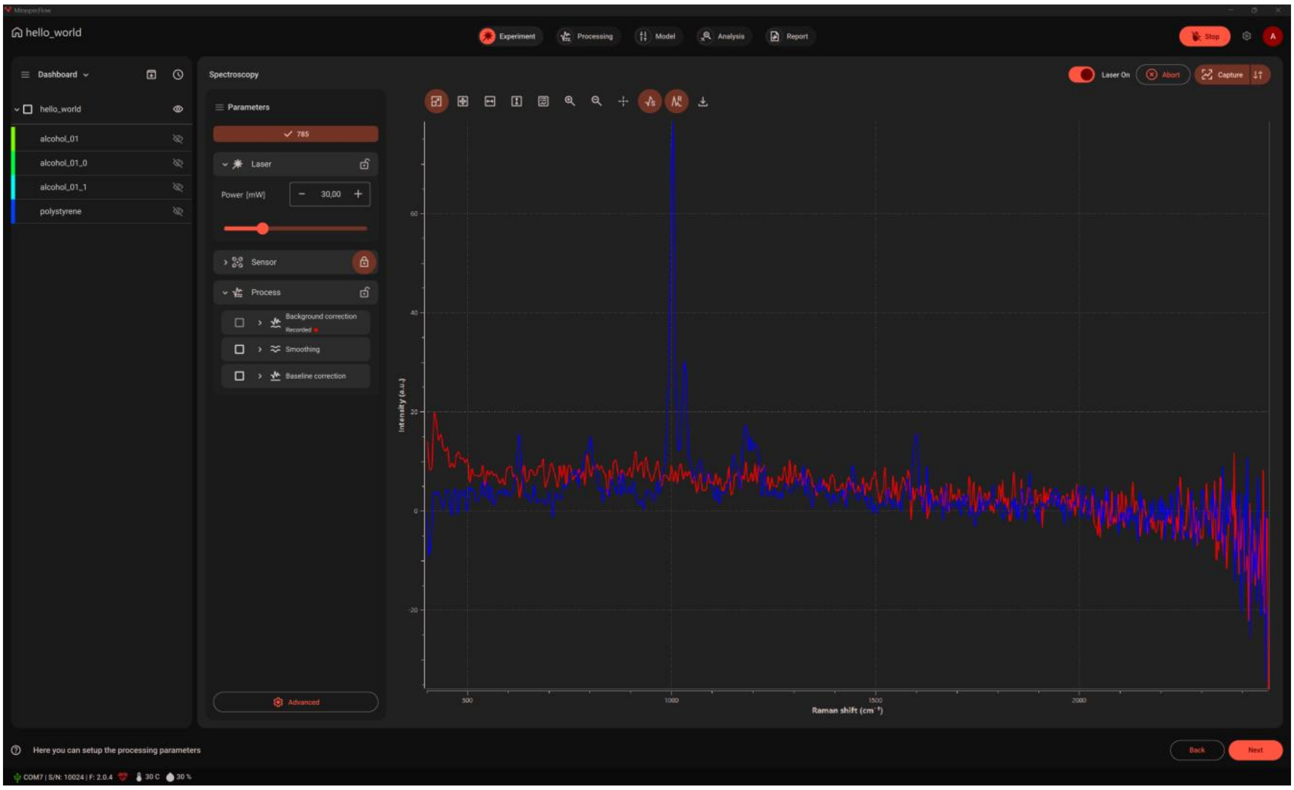
6.4.1. Laser

The **Laser** section contains parameters used to control the excitation laser of the Raman spectrometer. The laser provides the illumination required to generate Raman scattering from the sample, and its settings can significantly influence the intensity and quality of the measured spectrum.

Users can enable or disable the laser using the **Laser ON/OFF** control. When the laser is activated, the spectrometer begins illuminating the sample and spectral signals become visible in the graph display. For safety reasons, a confirmation message may appear when turning the laser on.

The laser section also allows adjustment of the **laser power**, which determines the intensity of the excitation light. Increasing the laser power generally increases the strength of the Raman signal, but excessive power may cause heating or degradation of sensitive samples. Users should therefore select laser power values appropriate for the sample being measured.

Proper adjustment of laser settings is important for obtaining high-quality spectral data while ensuring safe operation of the instrument.



6.4.2. Sensor

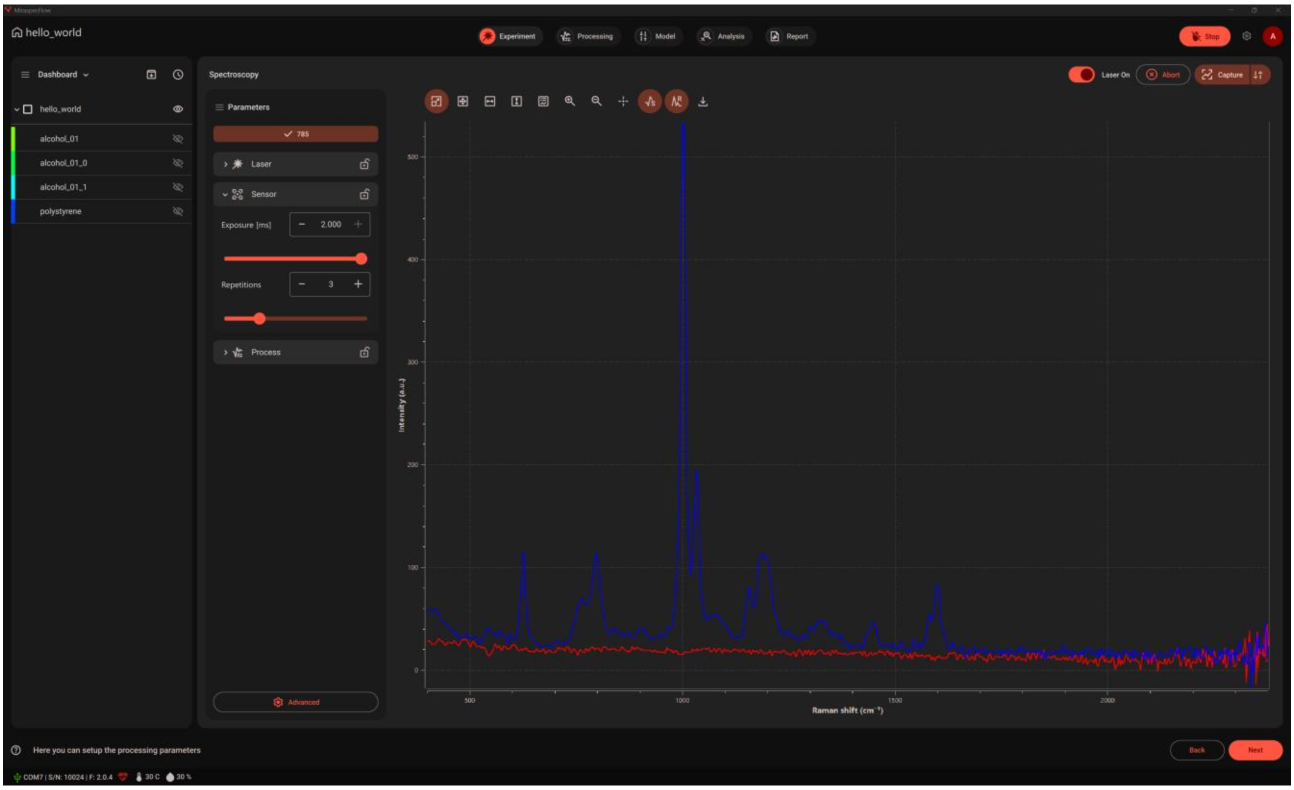
The **Sensor** section contains parameters that control the operation of the spectrometer detector during spectral acquisition. These settings determine how the detector collects and records the scattered light from the sample.

One of the primary parameters in this section is the **integration time** (or exposure time), which defines how long the detector collects light during a single measurement. Increasing the integration time generally increases the signal intensity but also increases the total acquisition time and may increase noise or risk detector saturation.

Another parameter is the **number of repetitions** (or accumulations), which specifies how many individual measurements are combined to produce a final spectrum. Averaging multiple repetitions can improve the signal-to-noise ratio by reducing random noise in the measured signal.

Adjusting sensor parameters allows users to optimize measurement conditions for different sample types and experimental requirements. Proper configuration of these settings helps achieve a balance between signal intensity, acquisition time, and spectral quality.

In the sensor section one can control the exposure time and the number of repetitions. Let's try to change the exposure time from 1000 ms to 2000 ms. The signal would grow up twice, and the acquisition would take twice as long. This is also reflected in live spectrum.



The number of repetition is relevant when we capture the spectrum

6.4.3. Process

The **Processing** section contains parameters that control the preprocessing of spectral data during acquisition. These settings determine how the raw spectral signal is prepared before being displayed or used for further analysis.

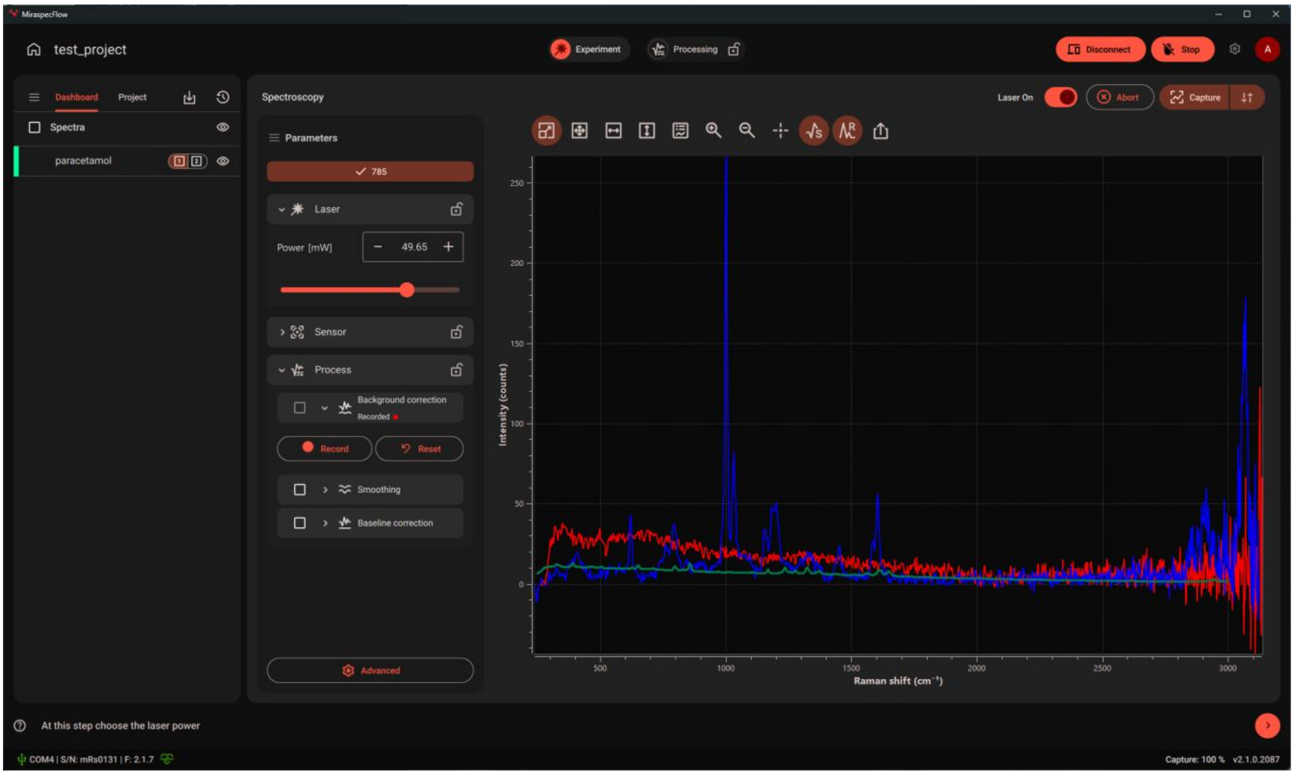
Preprocessing operations may include steps such as smoothing, baseline correction, normalization, or other signal processing methods designed to improve spectral quality. These operations help reduce noise, remove background effects, and make the spectral data more suitable for comparison, modeling, and analysis.

Depending on the configuration of the system, users may enable or disable specific preprocessing steps and adjust their parameters. The applied processing settings affect how spectra are displayed in the graph and how they are used in subsequent analysis procedures.

Proper configuration of processing parameters helps ensure that the spectral data are clear, consistent, and suitable for reliable interpretation.

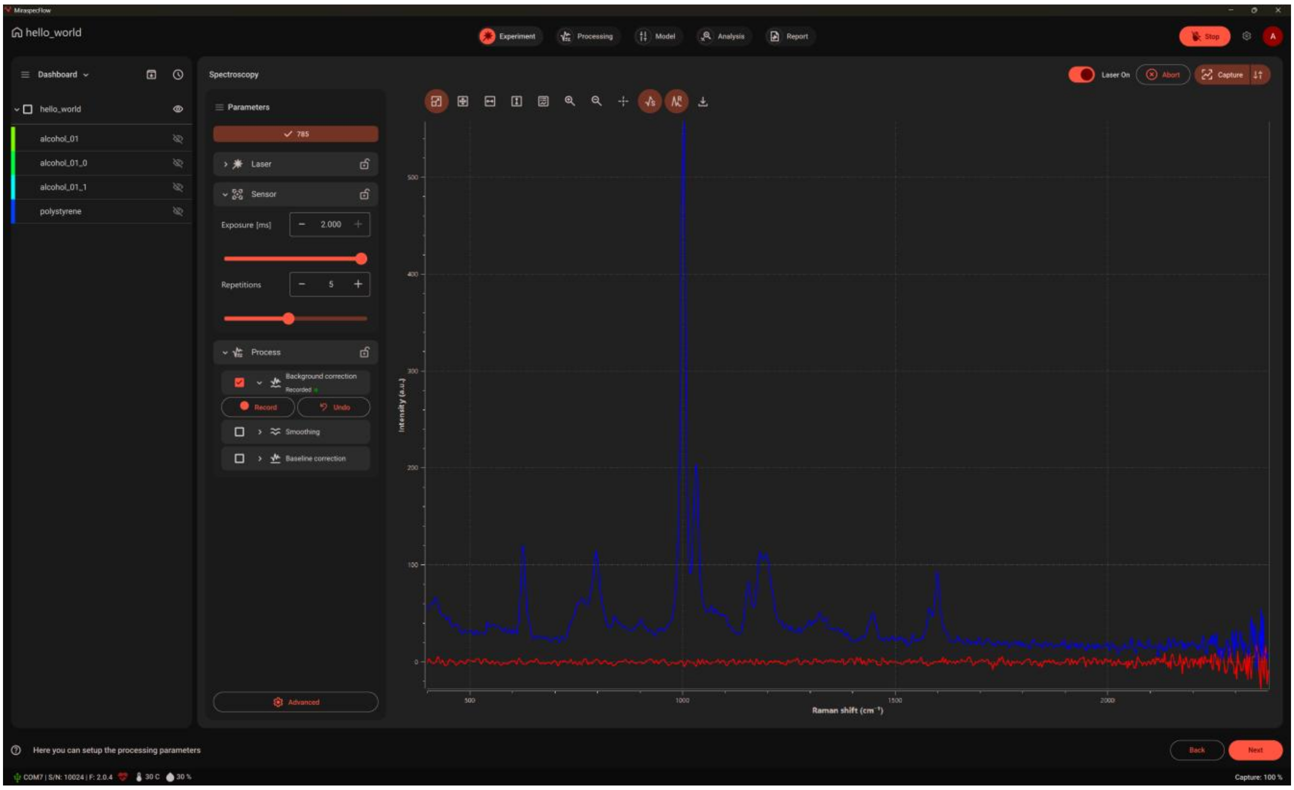
The process section has the following subsections: background correction, smoothing and baseline correction.

Background should be taken when the laser is on and there is no sample in the laser beam.

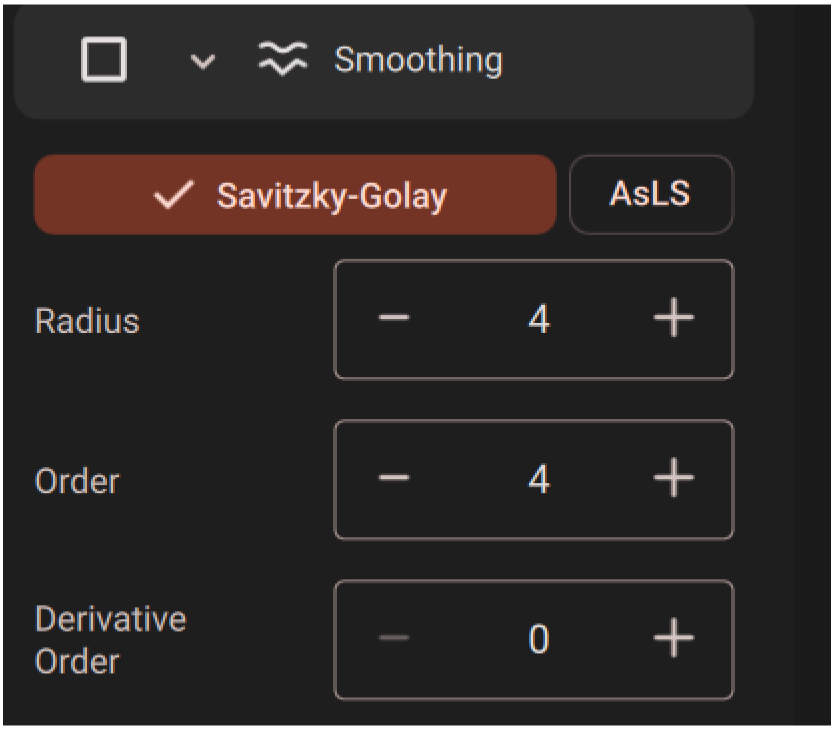


Click on Record to record background signal. The background would be acquired. When the background is being acquired it is displayed as gray spectrum, then when it is acquired it disappears. When the background is recorded the recorded indicator switches from red to green. There is always an option to Reset background acquisition.

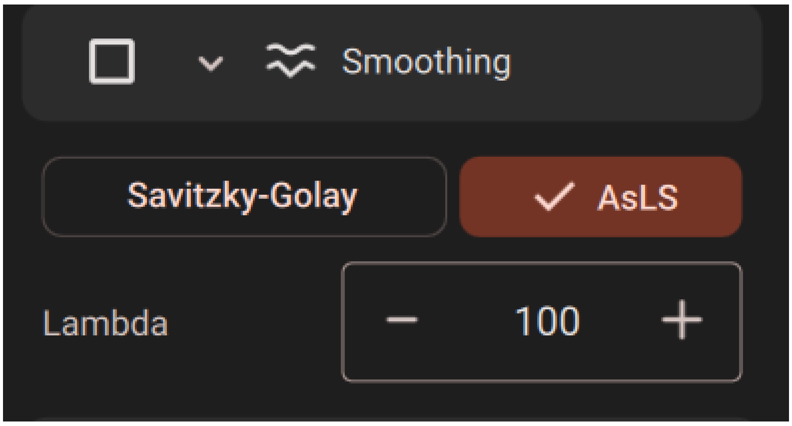
In order to apply background correction, click on background correction checkbox. Let's see what happens. It basically brings the baseline to zero as shown in the figure below.



Next goes the smoothing subsection. You have an option to perform the smoothing on the go. There are two options for smoothing: Savitzky Golay and Asymmetric Least Squares(AsLS). In Savitzky Golay one needs to specify the Radius, Order and Derivative order as shown below.



And in case of AsLS it's just one parameter Lambda.



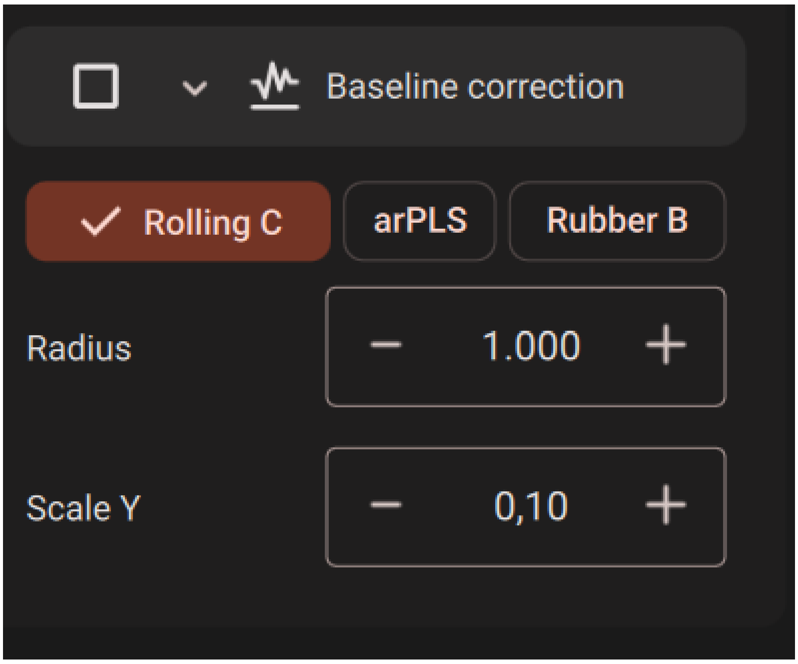
In order to demonstrate how the smoothing works let's record three spectra of a sample (alcohol in a plastic bottle): no smoothing, Savitzky Golay smoothing with parameters 10, 4, 0, and AsLS (Asymmetric Least Squares) with the parameter equal to 200. Let's not forget to enable checkbox for smoothing.

As we can see, the smoothened spectra have reduced noise but as well broadened spectral features.

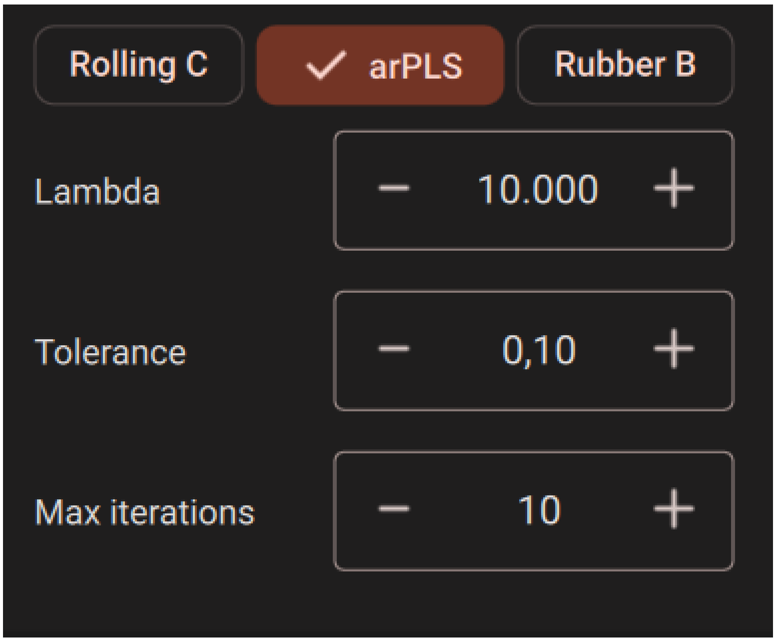
Let's disable smoothing for now by unchecking the checkbox and let's proceed to the next sub-section – baseline correction.

There are three options for baseline correction: Rolling circle, arPLS (Adaptive Reweighted Penalized Least Squares) and Rubber Band.

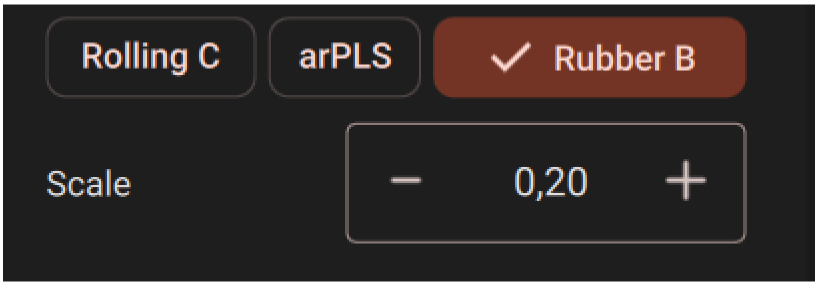
Rolling circle has two settings: Radius and Scale Y



ArPLS has three parameters: Lambda, Tolerance, and Max Iterations.



While Rubber band has only one parameter – scale.



Baseline subtraction removes broad features in the spectra and is typically used to remove fluorescence background. Baseline subtraction should not be confused with background subtraction described above.

Let's capture to spectra of the same sample without baseline subtraction, and with baseline subtraction (Rubberband with scale 0.2). The result is clearly demonstrated in the figure below (red – no baseline subtraction, blue – baseline subtracted).

6.4.4. Advanced settings

The **Advanced Settings** section provides additional configuration options for controlling specialized parameters of the spectrometer and acquisition process. These settings offer extended control over device behavior and measurement conditions beyond the standard laser and sensor parameters.

Advanced settings may include parameters related to device calibration, acquisition timing, signal handling, or other instrument-specific configuration options. The availability of these parameters may depend on the connected device and system configuration.

Because these settings can influence the performance and operation of the spectrometer, they are typically intended for experienced users or administrators. Incorrect configuration of advanced parameters may affect measurement quality or device operation.

Users should modify advanced settings only when necessary and with an understanding of their impact on the measurement process.

The advanced settings tab is available for users with proper access credentials. It is accessible upon clicking on Advanced button with the gear at the bottom of the Parameters panel and allows to change advanced settings such as Intensity units (counts or percents), modify the wavenumber range, change stability reference settings (for miniRaman devices). It also allows to perform device validation (will be described in the next section).

6.5. Device validation

The **Device Validation** step allows the user to verify that the connected spectrometer is functioning correctly before starting spectral acquisition. Validation ensures that the instrument meets the required operational conditions and is ready for reliable measurements.

During the validation process, the system performs checks on the device and evaluates key parameters that indicate whether the instrument is operating within acceptable limits. The results of these checks are displayed in the validation interface.

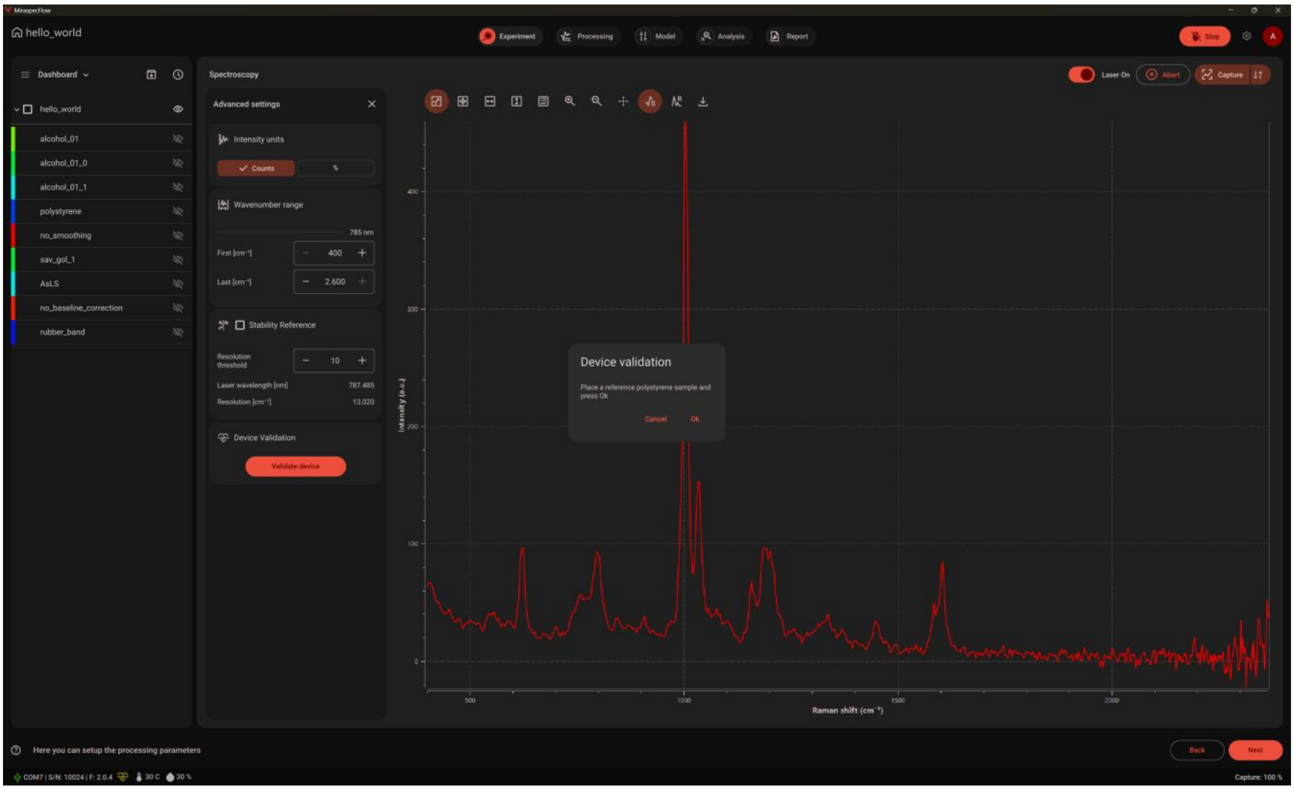
The validation result typically indicates one of the following statuses:

- **Ready** – the device meets the required conditions and can be used for measurements.
- **Partially Ready** – some parameters may require attention, but the device may still be usable depending on the situation.
- **Not Ready** – the device does not meet the required conditions and should not be used until the issue is resolved.

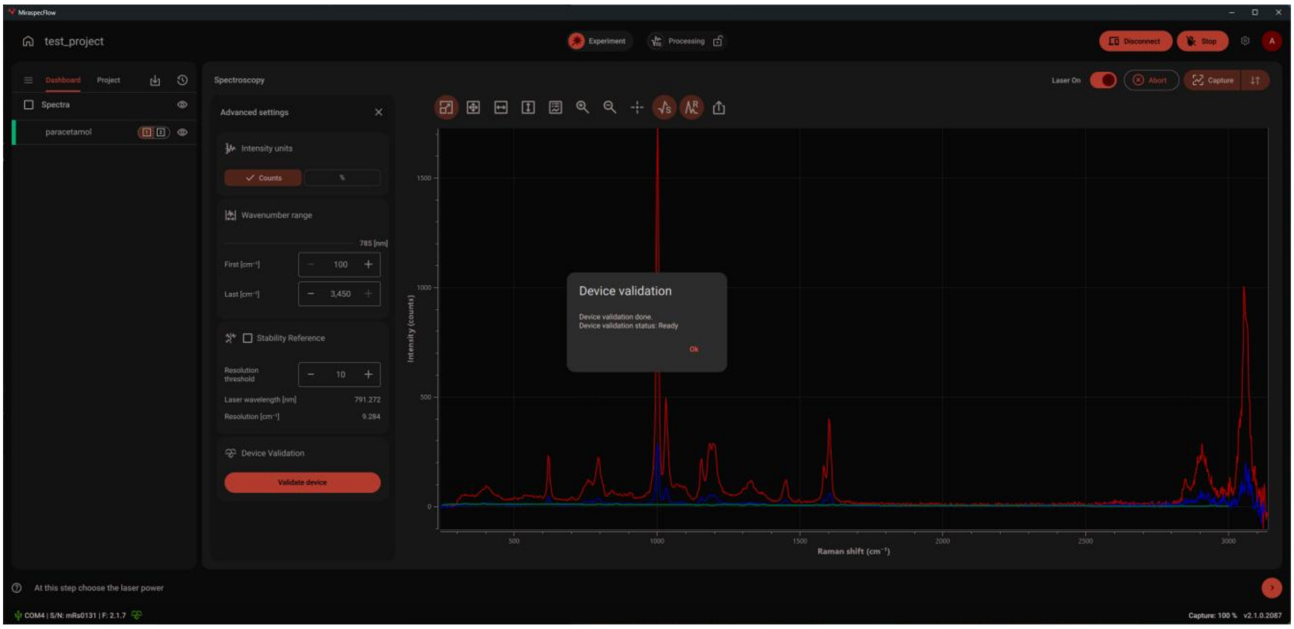
If the device is not ready, the user should verify the hardware connection, device configuration, and environmental conditions before attempting validation again.

Performing device validation helps ensure reliable operation of the spectrometer and improves the quality and consistency of spectral measurements.

Device validation procedure could be invoked from the Advanced settings of the Parameters tab. In order to perform validation one needs to click on the Validate device button. Upon clicking the button a pop up window appears asking to place a reference polystyrene sample in the laser beam path. Place the sample and click OK to proceed. In order to cancel, click cancel.



The spectral acquisition starts and the software is performing the validation of the device upon acquisition.



The validation is done, device status should be ready. The heart icon at the bottom of the screen should change to green.

If the validation is performed, clicking on the heart shows the validation report.

6.6. Capture workflow

The **Capture Workflow** section describes the process used to acquire Raman spectra during an experiment. Once the device is connected, validated, and the acquisition parameters have been configured, the user can begin spectral measurements.

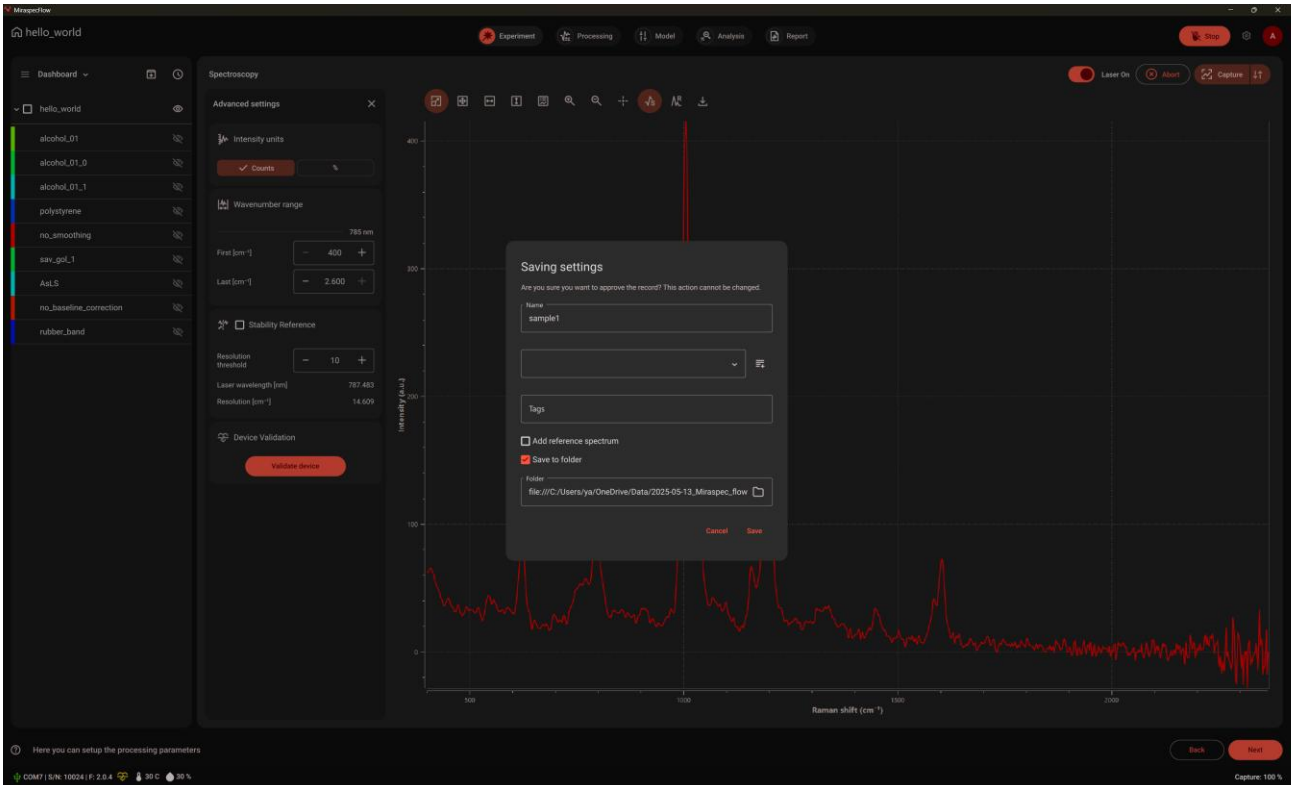
To capture a spectrum, the user initiates the acquisition process using the **Start Capture** or equivalent control in the experiment interface. When acquisition begins, the spectrometer collects light scattered from the sample and records the spectral signal according to the configured laser and sensor parameters.

During acquisition, the spectrum is displayed in the **graph area** of the interface, allowing the user to monitor the signal in real time. The displayed spectrum may be updated continuously as new measurements are recorded.

After the acquisition is completed, the resulting spectrum is stored within the current project and added to the **Dashboard**, where it can be viewed, processed, or used for further analysis. Multiple spectra can be acquired during a session, enabling comparison between different samples or measurement conditions.

The capture workflow enables users to efficiently acquire spectral data and prepare it for subsequent processing, modeling, and analysis within the project environment.

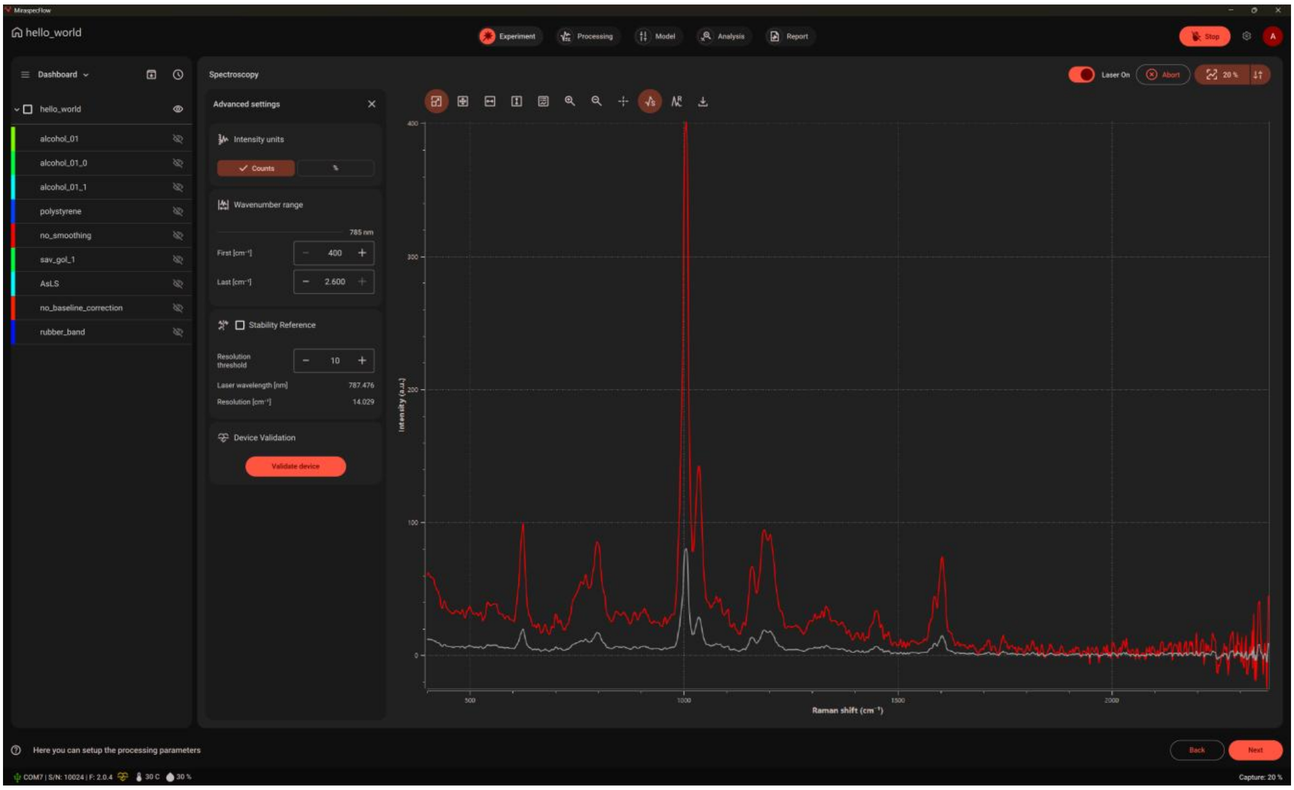
Saving settings could be accessed by clicking on the button with toggle switches next to the capture button. Here you have an option to name the sample, add tags, add reference sample and automatically save to a specified folder.



Input the savings settings, click on Save to save the saving settings, otherwise click cancel.

In order to capture, click capture button. The acquisition progress in percents would be shown on the capture button right away as shown below.

Through this dialog it is possible to specify the name of the files, add tags, upload the name list of files in .txt format, as well as do additional operations such as crop NaNs, add reference spectra, and choose the destination folder.



While capturing, the spectrum is grey, when it is captured, it changes its colour.

Abort button

The abort button allows to abort live capture; it is located to the left of the capture button and has a diagonal cross icon.

Stop button

Stop button is an emergency stop button located in the top right corner of the software window. It automatically shuts down the laser.

6.7. Graph tools and visualization options

The **Graph Tools and Visualization Options** section describes the tools available for interacting with and customizing the display of spectral data in the experiment interface. These tools help users inspect spectral features, compare measurements, and adjust the graphical representation of spectra for clearer interpretation.

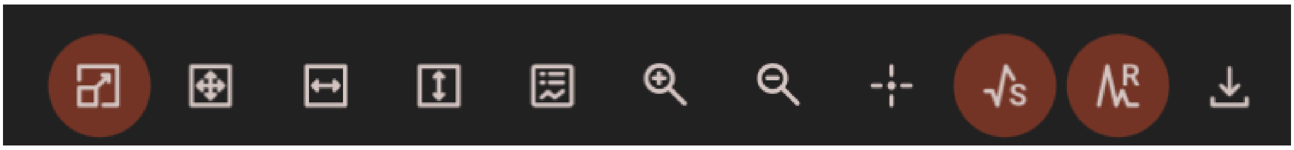
The graph interface allows users to **zoom in and out** of specific spectral regions to examine peaks in greater detail. Users can also **pan across the spectrum** to explore different parts of the Raman shift range.

Multiple spectra can be displayed simultaneously in the graph, enabling **comparison between measurements**. Users may toggle the visibility of individual spectra to focus on selected data or reduce visual clutter.

Additional visualization options may include:

- **Resetting the graph view** to the default display range
- **Showing or hiding selected spectra** in the graph
- **Viewing spectral values** at specific points along the spectrum
- **Adjusting axis scaling** for improved visualization of spectral features

On top of the graph there are 11 buttons.



They have the following functionality:

1 Automatically scale to window
2 Zoom to window XY
3 Zoom to window X
4 Zoom to window Y
5 Show legend
Here is an example of the plot with the legend.

6 Zoom in
7 Zoom out
8 Show tracer lines to track position and intensity of peaks

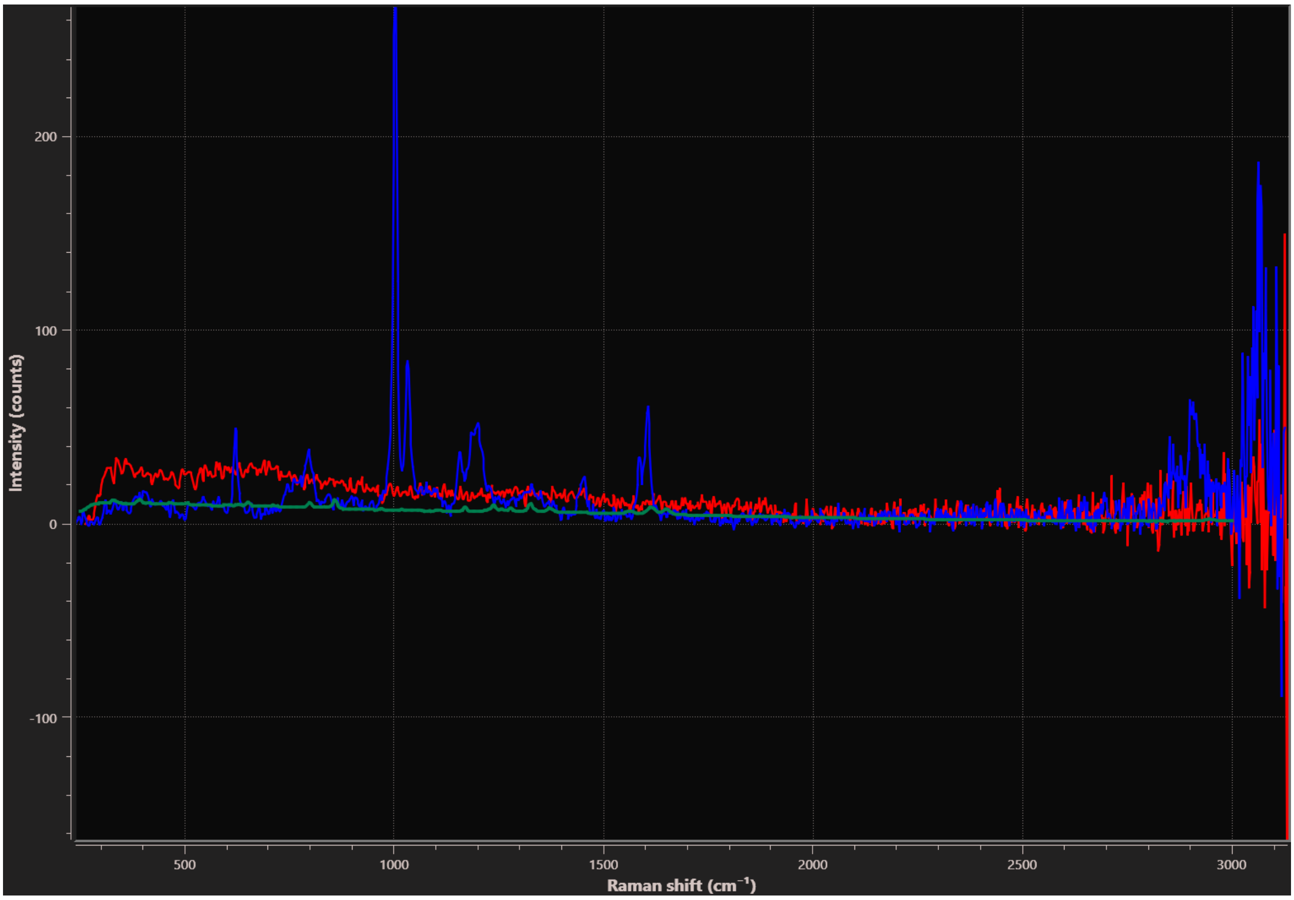
9 Show/hide signal spectrum

10 Show/hide reference spectrum

11 Save as .png.

This option takes a screenshot of the graph and saves it to a specified .png file on the hard drive.

Here's an example of such a screenshot.



These visualization tools allow users to analyze spectral data more effectively and support interpretation of measurement results during the experiment workflow.

7. Data processing

The Data Processing section describes the methods used in Miraspec Flow to prepare acquired Raman spectra for analysis. Raw spectral data often contain background signals, noise, or measurement artifacts that may affect the accuracy of identification or quantitative analysis. To address these effects, the software provides a set of preprocessing tools that improve spectral quality and ensure consistent analytical results.

Data processing typically involves a sequence of operations applied to the raw spectrum, such as cropping the spectral range, removing spikes caused by detector artifacts, smoothing high-frequency noise, correcting baseline distortions, and normalizing signal intensity. These preprocessing steps help reduce unwanted variations in the spectral data while preserving the chemical information contained in the Raman signal.

In Miraspec Flow, preprocessing operations can be configured and applied as part of the analysis workflow. The processing pipeline allows users to visualize both the original and processed spectra, making it possible to evaluate the effect of each processing step.

The Processing section of the workflow is shown below. Only visible spectra are processed.

The following sections describe the available preprocessing methods and explain how they are used to transform raw spectral measurements into data suitable for subsequent analysis and modeling.

7.1. Overview of the processing pipeline

The **Processing Pipeline** defines the sequence of preprocessing operations applied to spectral data before analysis or model development. These operations are designed to improve spectral quality by reducing measurement artifacts and standardizing the data for consistent interpretation.

Raw spectra acquired during measurements may contain noise, baseline distortions, or other artifacts that can affect the reliability of analytical results. The processing pipeline applies a series of configurable steps to correct these effects and prepare the spectra for further analysis.

Typical preprocessing operations in the pipeline may include:

- **Cropping**, which limits the spectral range to the region of interest
- **Spike removal**, which eliminates sharp intensity spikes caused by detector artifacts
- **Smoothing**, which reduces high-frequency noise in the spectrum
- **Baseline correction**, which removes background signals such as fluorescence
- **Normalization**, which scales spectral intensity to allow consistent comparison between spectra

Each step in the processing pipeline can be configured according to the requirements of the analysis. Users can observe the effect of preprocessing directly in the spectral visualization interface by comparing raw and processed spectra.

A properly configured processing pipeline helps ensure that spectral data are clean, consistent, and suitable for reliable modeling and analysis.

7.2. Crop

The **Crop** operation is used to restrict the spectral data to a specific Raman shift range. Cropping allows users to remove portions of the spectrum that are not relevant for analysis, such as regions containing noise, background signals, or areas outside the useful spectral range of the measurement.

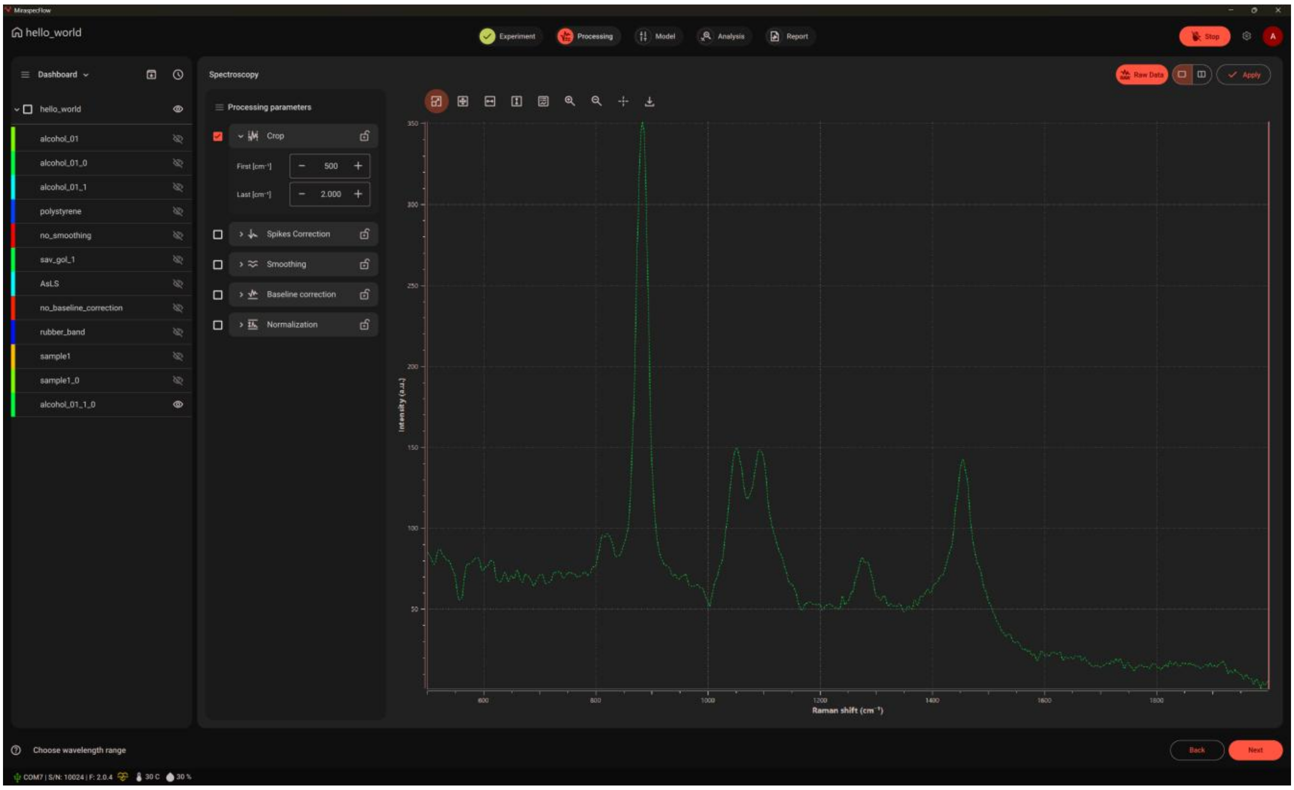
By selecting an appropriate range of Raman shift values, users can focus the analysis on the spectral region that contains meaningful information about the sample. This helps improve the quality of subsequent processing and analytical procedures.

During the cropping step, the user defines the **minimum** and **maximum** Raman shift values that determine the boundaries of the retained spectral region. Data points outside this range are excluded from further processing and analysis.

Let's crop the spectrum in the range 500..2000 cm^{-1}. To do so we enter proper first and last wavenumbers, enable crop checkbox and click apply. The cropped spectrum appears.

Note

Note that after this procedure the original spectrum would be hidden.



Cropping is often used as an initial preprocessing step in the processing pipeline to eliminate unwanted spectral regions and reduce the size of the dataset before applying additional preprocessing operations.

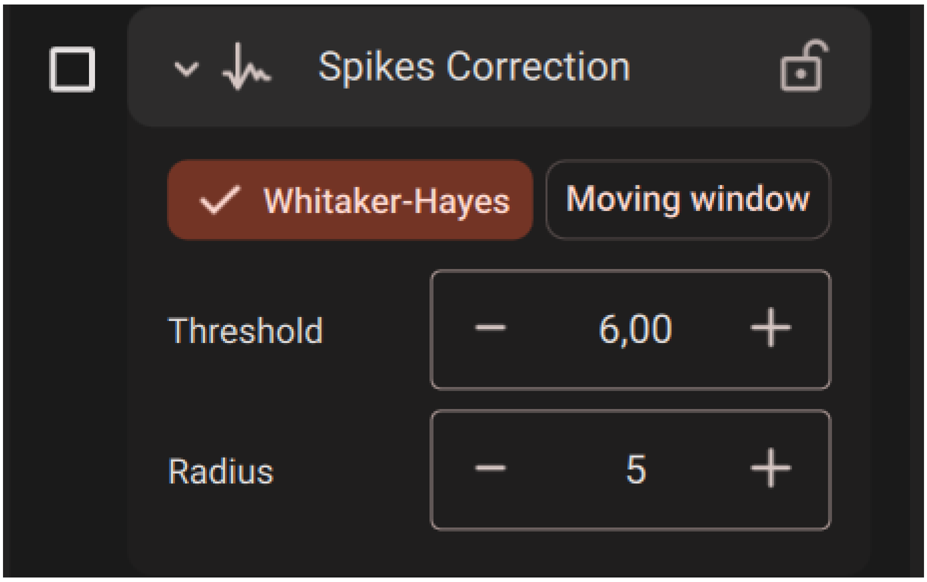
7.3. Spikes correction

The **Spike Correction** operation is used to detect and remove sharp, isolated spikes that may appear in spectral data. These spikes are typically caused by detector artifacts, cosmic rays, or other transient disturbances during spectral acquisition.

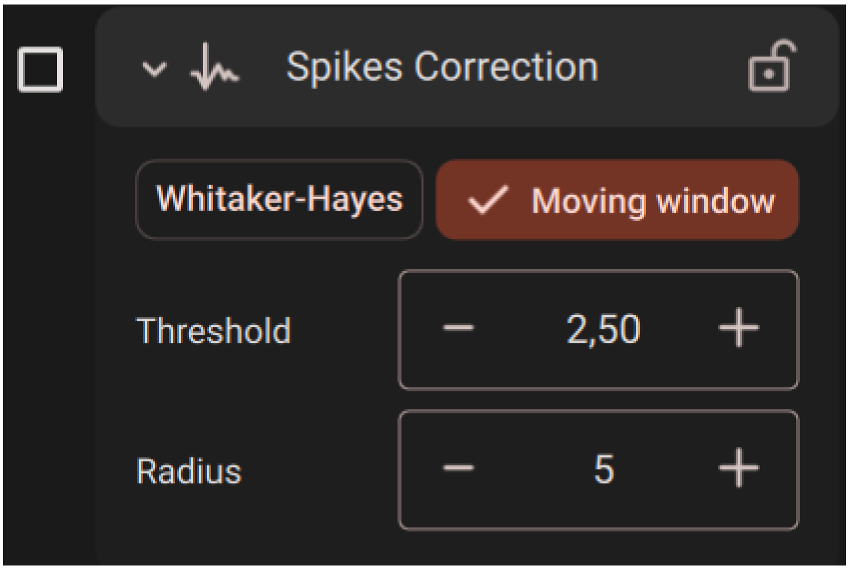
Spike artifacts appear as narrow, high-intensity peaks that do not represent actual Raman signals. If not corrected, these artifacts can interfere with preprocessing, modeling, and analysis procedures.

During spike correction, the software automatically identifies abnormal intensity points that deviate significantly from neighboring spectral values. Once detected, these spikes are corrected by replacing the affected data points using interpolation or smoothing based on the surrounding spectral values.

Let's now apply the spikes correction algorithm to the cropped spectrum. There are two options for spikes correction: Whitaker-Hayes and Moving window. The Whitaker-Hayes algorithm has two parameters: threshold and radius:

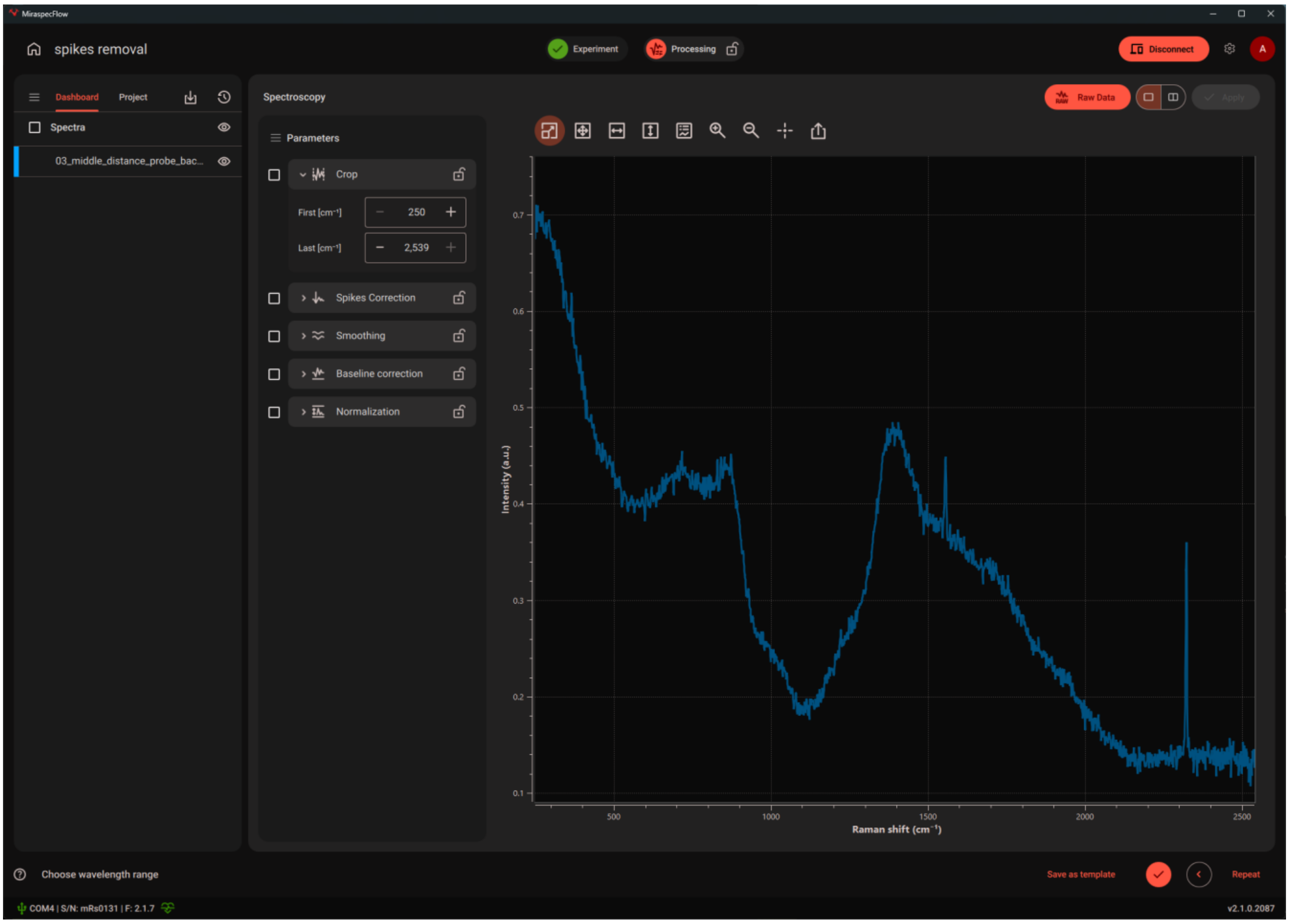


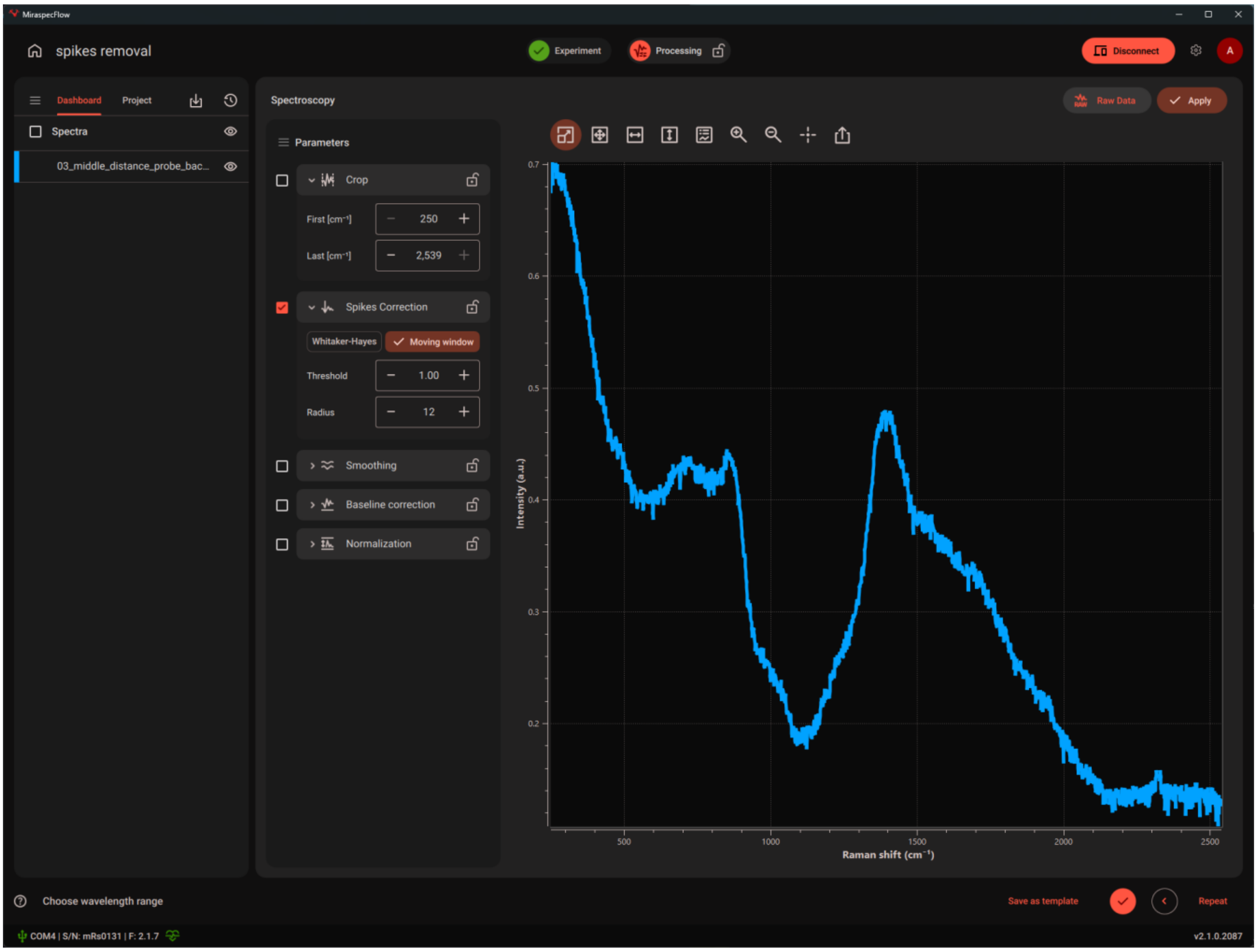
same goes for the moving window – again two parameters – threshold and radius:



Let's choose Whitaker-Hayes with threshold 2.5 and radius 5, we check the checkbox, and click apply.

The result is saved in a new spectrum. As we can see the spikes are completely removed from the spectrum while spectral shape maintains intact.





Applying spike correction helps improve spectral quality and ensures that the data used for further processing and analysis more accurately represent the true Raman signal of the sample.

7.4. Smoothing

The **Smoothing** operation is used to reduce high-frequency noise present in spectral data. Noise may arise from detector fluctuations, environmental conditions, or other measurement-related factors that affect the stability of the recorded signal.

Smoothing algorithms process the spectral data by averaging neighboring data points to produce a cleaner and more stable signal while preserving the overall shape of the spectral peaks. This helps improve the clarity of the spectrum and makes characteristic Raman features easier to interpret.

Common smoothing methods operate by applying a moving window across the spectrum and calculating adjusted intensity values based on surrounding points. The size of the smoothing window determines the degree of noise reduction: larger windows provide stronger smoothing but may also reduce the sharpness of spectral peaks.

There are two options for smoothing: Savitzky-Golay and AsLS (Asymmetric Least Squares). Savitzky Golay has 3 parameters: radius, order, and derivative order. AsLS has only one parameter lambda.

Let’s apply AsLS with lambda equal to 5. The smoothing option allows for live monitoring of resulting spectrum while changing the parameter without saving it.

We check the checkbox and click apply. As a result, we get much smoother spectrum:

Proper smoothing can enhance spectral readability and improve the reliability of subsequent data analysis, but excessive smoothing should be avoided because it may distort important spectral features.

7.5. Baseline correction

The **Baseline Correction** operation is used to remove background signals from a Raman spectrum. These background signals are often caused by fluorescence or other sources of broad spectral intensity that can distort the true Raman signal.

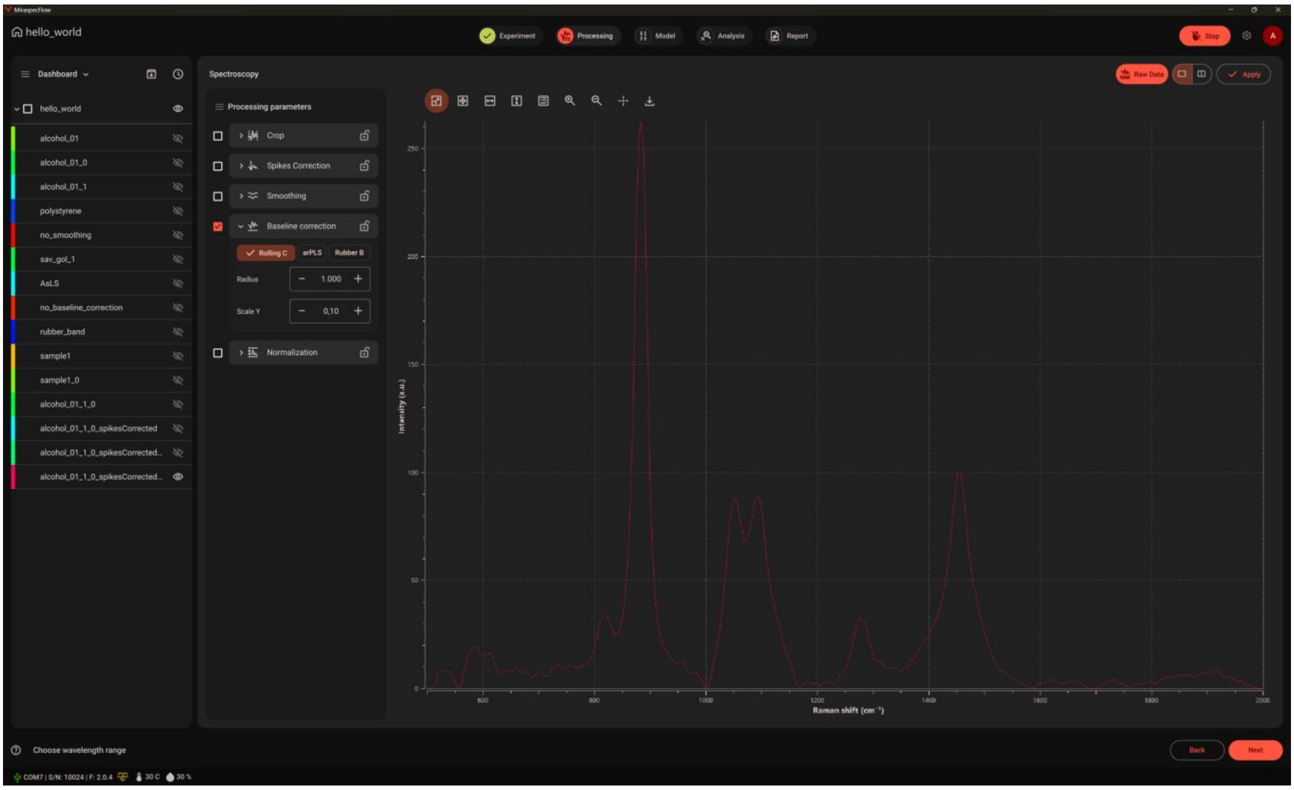
In many measurements, the recorded spectrum may contain a slowly varying background that shifts the entire spectrum upward. Baseline correction identifies this background trend and subtracts it from the spectrum, allowing the true Raman peaks to be more clearly observed.

During this step, the software estimates the baseline using an appropriate mathematical method and adjusts the spectral intensities accordingly. The resulting spectrum has a corrected baseline where the background contribution is minimized.

There are three options for the baseline correction: Rolling circle with parameters Radius and Scale Y, ArPLS with three parameters: Lambda, tolerance and max iterations, and Rubber band with one scale parameter. Let’s apply Rolling circle algorithm with Radius equal to 1000 and scale equal to 0.1. And again the behaviour of the algorithm can be monitored live as we change the parameters.

We click apply to save the spectrum in the dashboard.

As you can see the spectrum processed in such a way does not contain broad residual fluorescence background.



Applying baseline correction improves the visibility of spectral features and helps ensure that the data used for modeling and analysis more accurately represent the chemical information contained in the Raman signal.

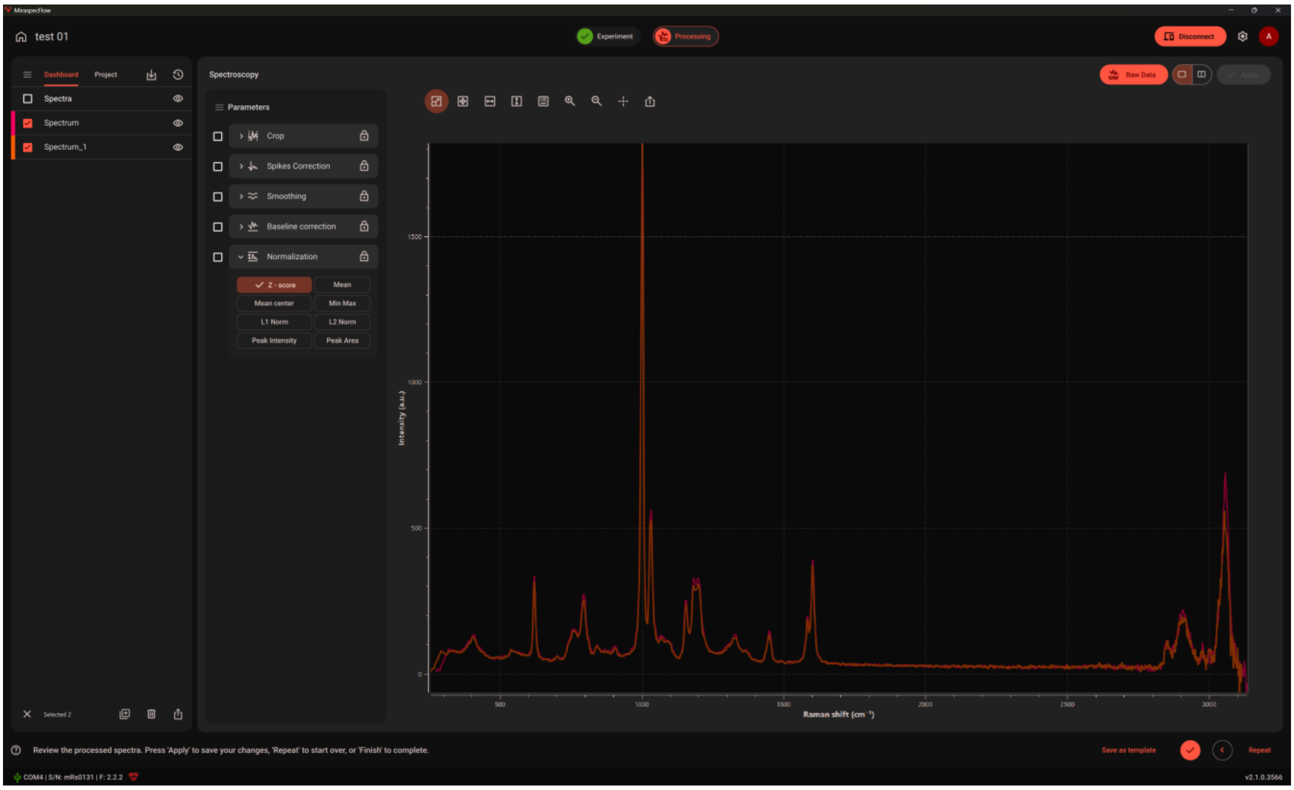
7.6. Normalization

The **Normalization** operation is used to scale spectral intensity values so that spectra can be compared consistently. Differences in measurement conditions, such as variations in laser power, integration time, or sample positioning, may cause overall intensity differences between spectra even when the chemical composition of the samples is similar.

Normalization adjusts the intensity values of the spectrum according to a selected scaling method. This process preserves the relative shape and position of the spectral peaks while bringing spectra to a comparable intensity scale.

By applying normalization, users can reduce variability caused by measurement conditions and focus on the spectral features that reflect differences in sample composition. This step is particularly important when comparing multiple spectra, training analytical models, or performing multivariate analysis.

The last option of the processing toolbox is normalisation. There are 6 options on how we can normalize the data: Z-score, mean, mean centre, min max L1 norm, and L2 norm Peak intensity and peak area normalization.



Proper normalization improves the consistency of spectral datasets and helps ensure more reliable results in subsequent analysis and modeling procedures.

7.7. Raw versus processed data visualization

The **Raw versus Processed Data Visualization** feature allows users to compare the original spectral data with the processed spectrum after preprocessing steps have been applied. This comparison helps users evaluate the effect of the processing pipeline and verify that the applied operations improve spectral quality without distorting important spectral features.

In the visualization interface, both the **raw spectrum** and the **processed spectrum** can be displayed simultaneously in the graph area. This allows users to observe how preprocessing steps such as cropping, spike correction, smoothing, baseline correction, and normalization modify the spectral signal.

By comparing raw and processed data, users can identify improvements such as reduced noise, corrected baseline drift, or removal of artifacts. At the same time, this comparison helps ensure that the characteristic Raman peaks remain intact and accurately represent the sample's chemical information.

Sometimes it is useful to display the raw and processed data on two separate graphs. To switch between one and two graphs mode we need to click on the button to the left of the apply button. Two graph representation looks as follows (first processed data, then the raw data):

There is an option to hide/show raw data. In order to do so one must click on the Raw Data red button to the left of the button to switch between one and two graphs representation. The result is as follows:

The ability to visualize both versions of the spectrum provides an important quality control step during preprocessing and helps users optimize the processing pipeline for reliable analysis.

8. Models

Models in Miraspec Flow are used to interpret Raman spectral data and support automated identification, classification, and quantitative analysis of measured samples. A model represents a mathematical or statistical relationship derived from reference spectral data and is used to analyze new measurements acquired during experiments.

Depending on the analytical task, different types of models may be applied. These may include models designed for material verification, classification of unknown samples, or calibration models used for quantitative estimation of chemical concentrations. Each model is constructed using reference spectra and appropriate preprocessing steps to ensure reliable analytical performance.

Model development typically involves selecting relevant training data, applying preprocessing methods, and evaluating the performance of the resulting model. Once created, models can be stored within the system and reused for routine analysis across multiple projects.

The following sections describe the different types of models available in Miraspec Flow and outline the process of training, evaluating, and applying these models within the software.

8.1. Overview of model types

Miraspec Flow supports several types of analytical models designed to interpret Raman spectral data for different analytical tasks. These models use reference spectral data and statistical or machine-learning methods to analyze newly acquired spectra and produce identification, classification, or quantitative results.

Each model type is intended for a specific analytical objective and may use different mathematical approaches depending on the nature of the analysis.

The primary model types available in Miraspec Flow include:

Verification Models

Verification models are used to confirm whether a measured spectrum corresponds to a specific known material. In this approach, the measured spectrum is compared with a reference model representing the expected spectral characteristics of a particular compound or material. The model determines whether the sample matches the reference within predefined acceptance criteria.

Verification models are commonly used in quality control applications where the objective is to confirm the identity of a known substance.

Classification Models

Classification models are designed to assign an unknown sample to one of several predefined classes or categories. These models are trained using spectral data representing different materials or sample types. When a new spectrum is analyzed, the model evaluates its similarity to the training data and determines the most probable class.

Classification models are useful for identifying unknown materials from a library of known substances.

Calibration Models

Calibration models are used for quantitative analysis, where the goal is to estimate the concentration of one or more components in a sample. These models are developed using spectral measurements of reference samples with known concentrations. Statistical regression methods are applied to establish the relationship between spectral features and concentration values.

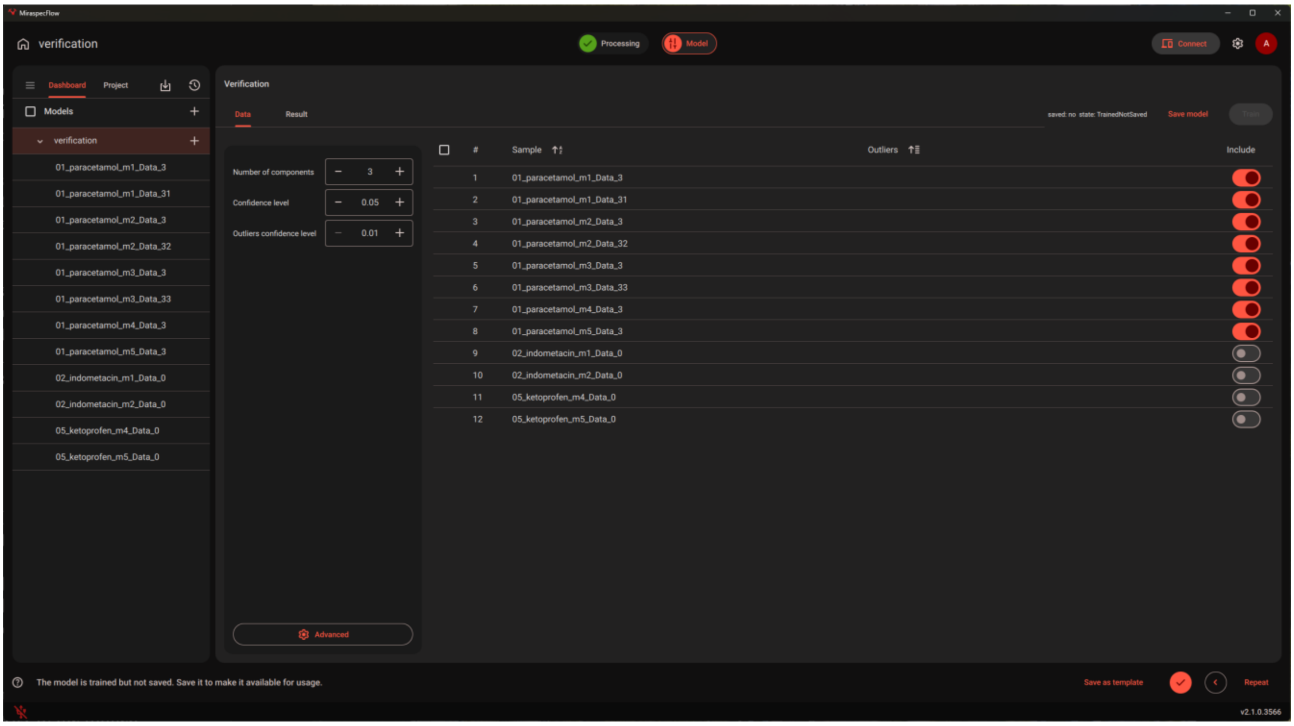
Calibration models enable the estimation of component concentrations in unknown samples based on their measured spectra.

Miraspec Flow supports several analysis models commonly used in Raman spectroscopy and chemometrics. These methods include identification through spectral comparison, principal component analysis (PCA) for exploratory analysis, classification methods for assigning samples to predefined categories, multivariate curve resolution (MCR) for resolving mixed spectral contributions, and calibration techniques for quantitative analysis.

8.2. Verification model

The **Verification Model** is used to confirm whether a measured spectrum corresponds to a specific known material. This type of model is typically applied in quality control or material verification tasks where the goal is to determine whether a sample matches a predefined reference.

A verification model is created using reference spectra that represent the expected spectral characteristics of a particular compound or material. During model training, the software analyzes the selected spectra and establishes criteria that define acceptable similarity between the reference spectra and future measurements.



Once the model has been trained and saved, it can be applied to newly acquired spectra. When a spectrum is analyzed using a verification model, the system compares the measured spectrum with the reference model and determines whether the sample passes or fails the verification criteria.

The result of the verification process typically indicates whether the measured sample is consistent with the reference material used to build the model. This approach is commonly used in applications where confirming the identity of a known substance is required.

8.3. Classification model

The **Classification Model** is used to assign an unknown spectrum to one of several predefined classes based on its spectral characteristics. This type of model is commonly used for identifying materials or categorizing samples into groups with similar chemical composition.

A classification model is created by training the system using a dataset of spectra that have been labeled according to their corresponding classes. During training, the software analyzes the spectral features of each class and learns patterns that allow it to distinguish between different sample categories.

After training, the model can be applied to new spectra acquired during experiments. When a spectrum is analyzed using the classification model, the system evaluates its similarity to the trained classes and determines the most probable class assignment.

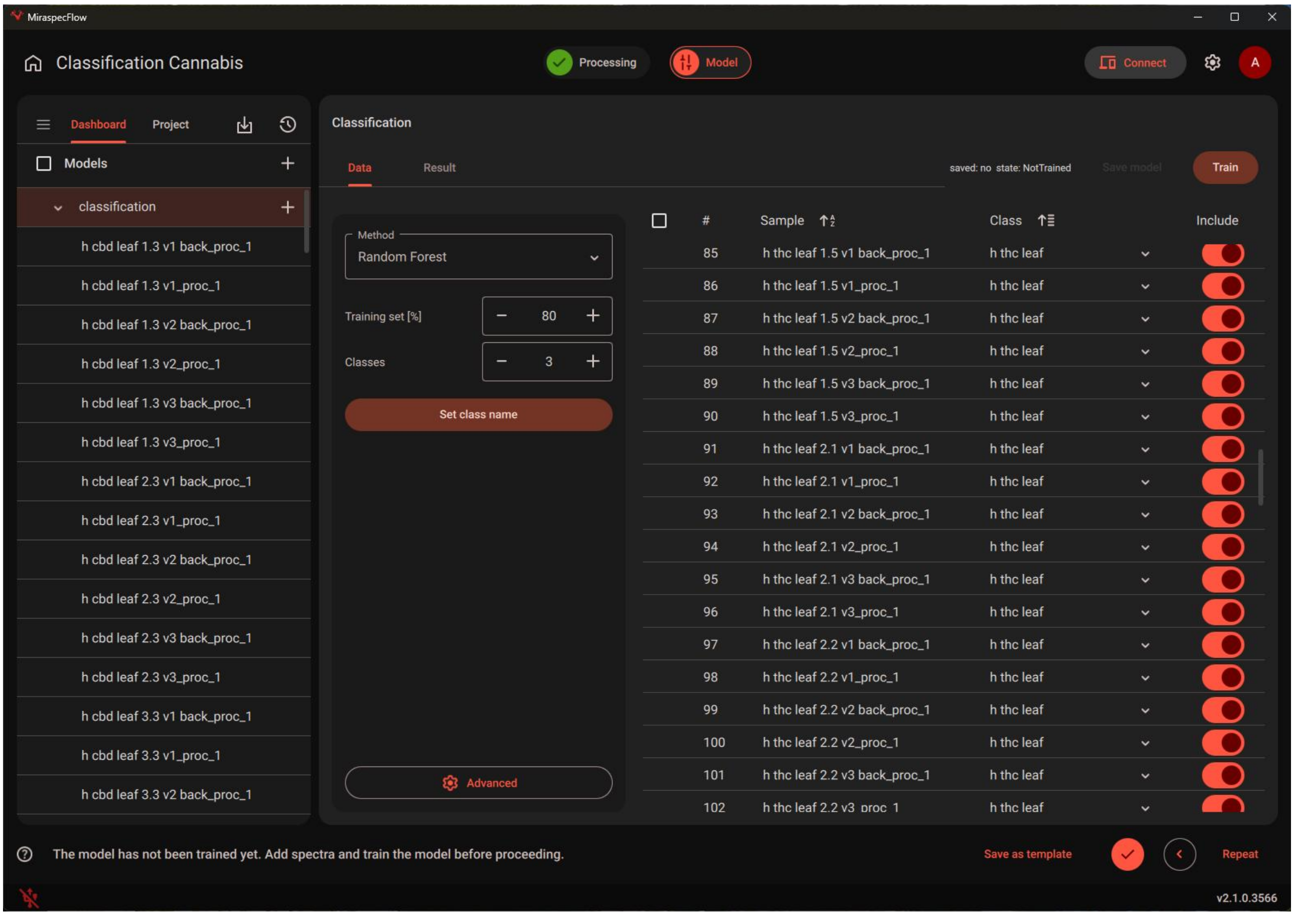
The classification results may include additional performance metrics such as **accuracy**, **precision**, **recall**, and **F1 score**, which help assess the quality of the trained model. These metrics are typically calculated during model training and validation using separate training and test datasets.

Classification models are particularly useful when working with datasets that contain multiple material types and when automated identification of unknown samples is required.

We will show the classification model on the example of cannabis dataset. There are three classes – THC rich, CBD rich and mixed cannabis leaves.

First, you need to create a new project and choose Classification Model, then proceed to the next step and load the data in the dashboard. After that you can apply some data processing, for example we will crop the data in the range 600 – 1600 cm^{-1}, apply baseline correction (Rubber Band with Smooth radius 3 and Scale 1.0) as well as normalization (MinMax).

Then we click Apply and proceed to the next step by clicking on the arrow at the bottom right of the Miraspec software window. This way we proceed to the Model step. We need to label all the spectra. For this specific dataset we will have 3 classes THC, CBD and MIX. We choose Random forest model under the classificatory, as well as training set 80% for the train-test split. The classes can be named by clicking on the Set Class Name red button.

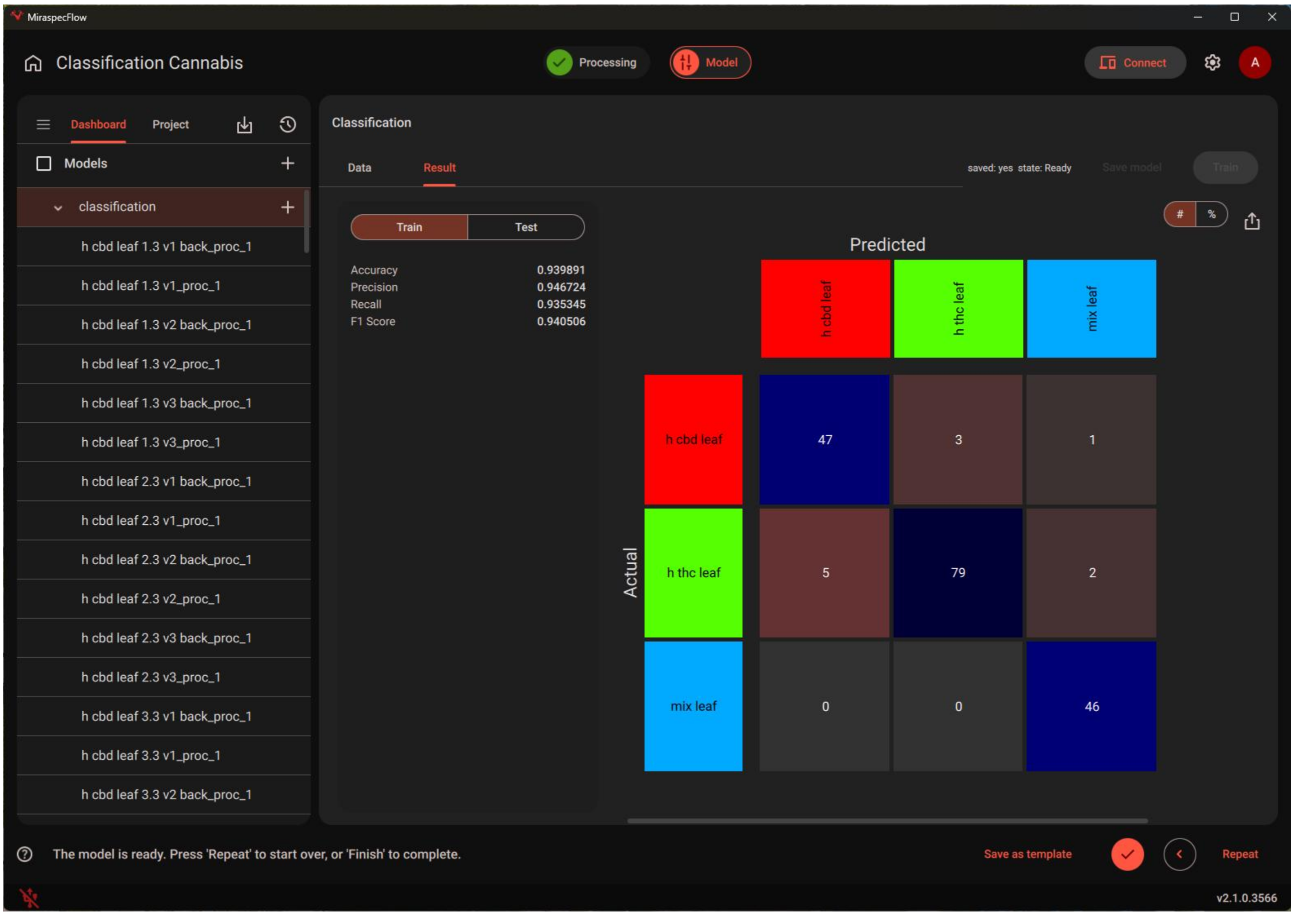


We click on Train button to train the model.

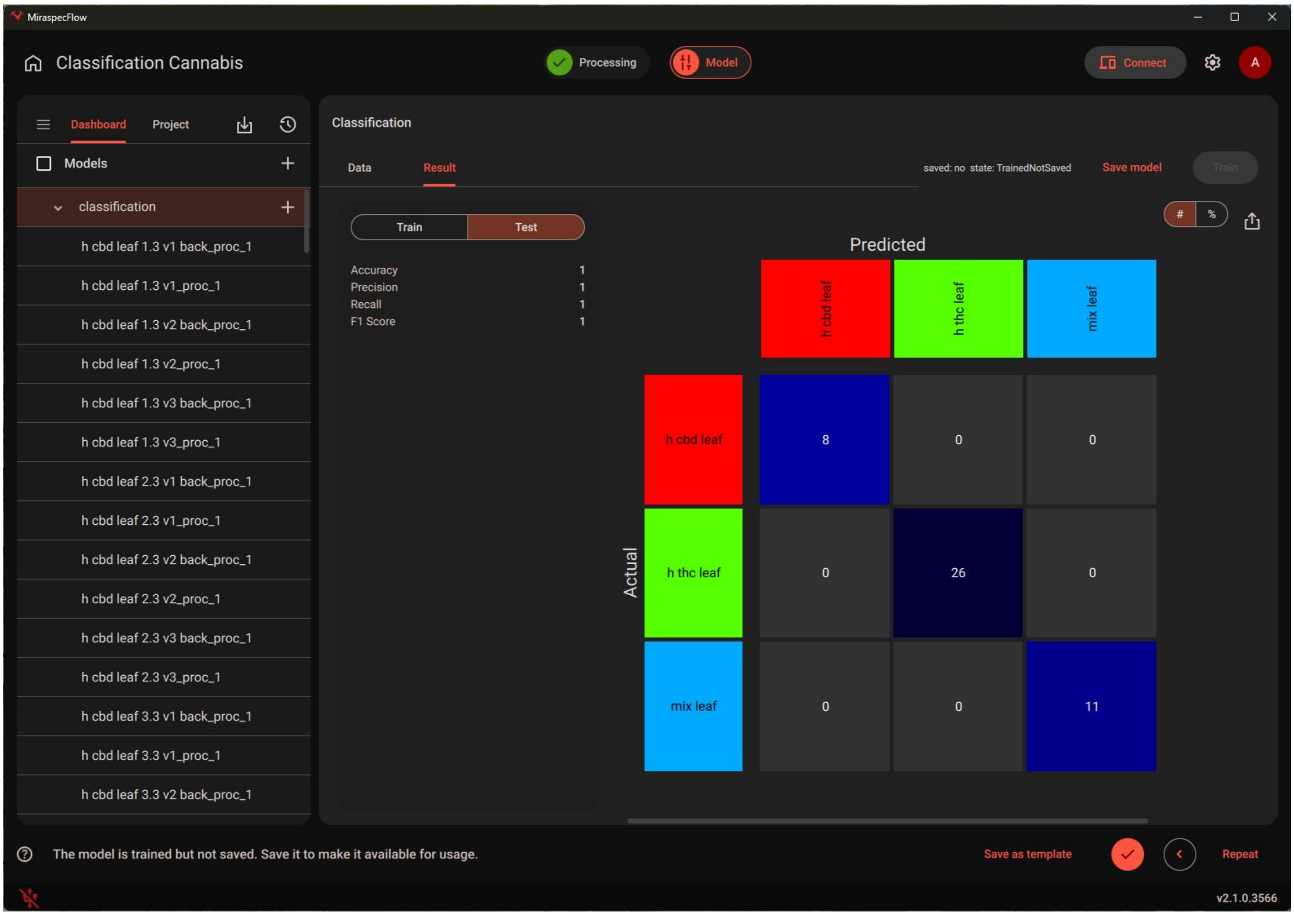
The confusion result is immediately shown as a confusion matrix, as well as such parameters as accuracy, precision, recall and F1 score are shown in the right panel.

We can switch between the results for the train and test datasets by clicking on the corresponding buttons in the right panel.

For example the result for the train dataset is shown below:



And here's the result for the test dataset:



Then, we should save the model by clicking on Save model button.

After that we can proceed to analysis. The analysis step will be described in the next section.

8.4. Calibration model

The **Calibration Model** is used for quantitative analysis of spectral data. This type of model allows the estimation of the concentration of one or more chemical components in a sample based on its measured Raman spectrum.

Calibration models are developed using a set of reference spectra obtained from samples with known concentrations of the target component. During model training, the software analyzes the relationship between spectral features and the corresponding concentration values to establish a predictive mathematical model.

Once the model has been trained and validated, it can be applied to new spectra acquired during experiments. The system uses the trained model to estimate the concentration of the target component in unknown samples.

Calibration models often rely on regression methods, such as **Partial Least Squares (PLS)**, to identify correlations between spectral intensity patterns and concentration values. During model development, the system may evaluate parameters such as the number of factors, prediction error, and variance explained by the model.

The performance of a calibration model is typically assessed using statistical metrics that compare predicted values with known reference values. These metrics help determine the accuracy and reliability of the model for quantitative analysis.

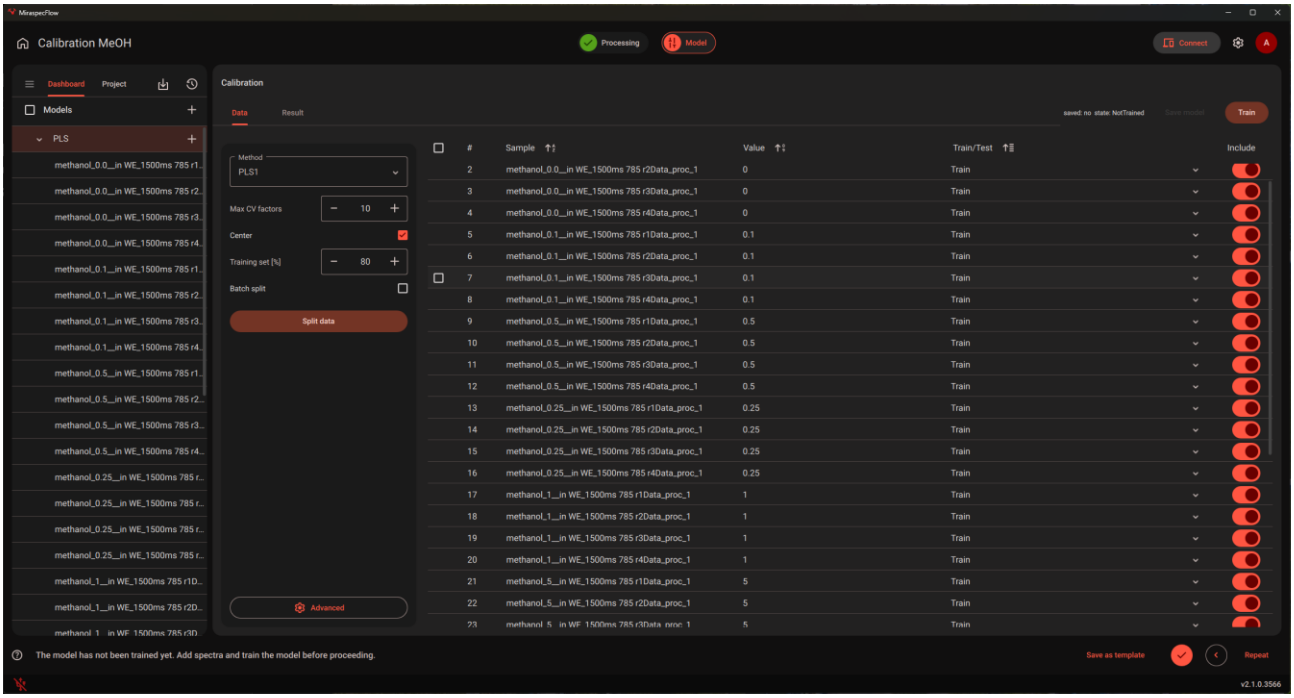
Calibration models are widely used in applications where precise measurement of chemical composition or concentration is required.

We will show how to build the calibration model on the example of the methanol in vodka dataset.

First, we need to create a project with Calibration model, then we load the data, and apply preprocessing, for example Crop, baseline correction, and normalization as shown below:

We click Apply, then we click next in order to proceed.

At this point we need to select the calibration model. For example let's choose PLS1 as classificatior, 10 as max CV factor, use Center option and 80 % as train-test split. We click Split data, then we need to properly label all the spectra with proper concentrations of methanol as denoted in the file names. This gives the results for train and test dataset as the plot of Nominal versus Predicted values. Additional information such as optimal number of factors, number of factors, PRESS, explained variance Xcal and explained variance Ycal, as well as RMSECV, F, and p parameters are displayed inside the right panel. We can switch between Train and Test datasets by clicking on the corresponding buttons.



The results for the train dataset look as follows:

And for the test dataset as follows:

In addition to prediction plot, it is also possible to display RMSE plot, prediction error, and prediction error samples plots:

In order to save the model we click on Save

8.5. PCA

Principal Component Analysis (PCA) is a multivariate statistical method used to explore patterns and relationships within spectral datasets. PCA reduces the dimensionality of the data while preserving the most significant variations present in the spectra.

In Raman spectroscopy, each spectrum may contain hundreds or thousands of intensity values corresponding to different Raman shift positions. PCA transforms these correlated variables into a smaller set of new variables called **principal components**, which capture the dominant variations in the dataset.

The first principal component represents the direction of the largest variance in the data. Each subsequent component represents additional variance while remaining mathematically independent from the previous components.

PCA is commonly used for **exploratory data analysis**, visualization of spectral similarities, and detection of patterns or clusters within spectral datasets. The results of PCA analysis are typically displayed as:

- **Scores plots**, which show the relationships between samples in the reduced component space
- **Loadings plots**, which indicate which spectral regions contribute most strongly to each principal component

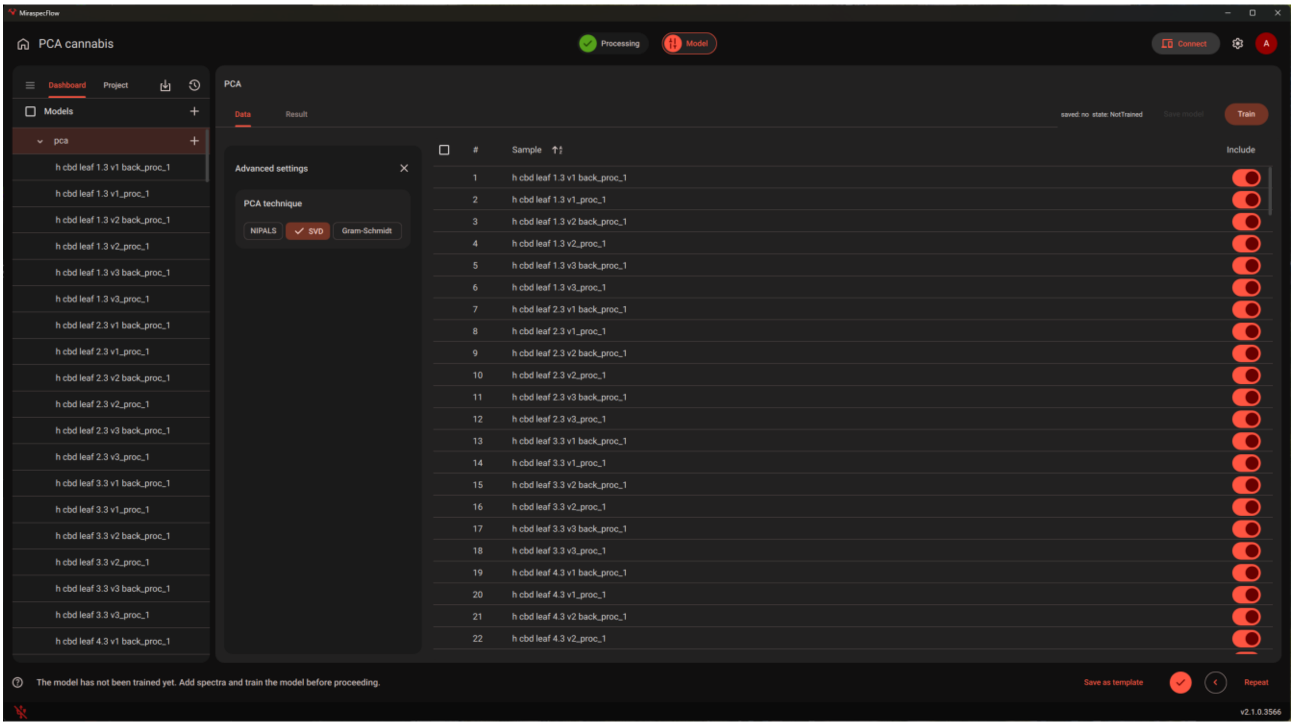
By examining these plots, users can identify groups of similar samples, detect outliers, and better understand the underlying structure of the spectral data.

PCA does not perform classification by itself but provides valuable insight into the structure and variability of the dataset, which can support further modeling and analysis.

We will show how to perform PCA on the example of cannabis dataset. We need to create a new project: PCA. Then we load the cannabis data in the dashboard.

At the next step we apply preprocessing: crop, baseline correction and normalization as shown below and click Apply. This results in the following processed spectral dataset:

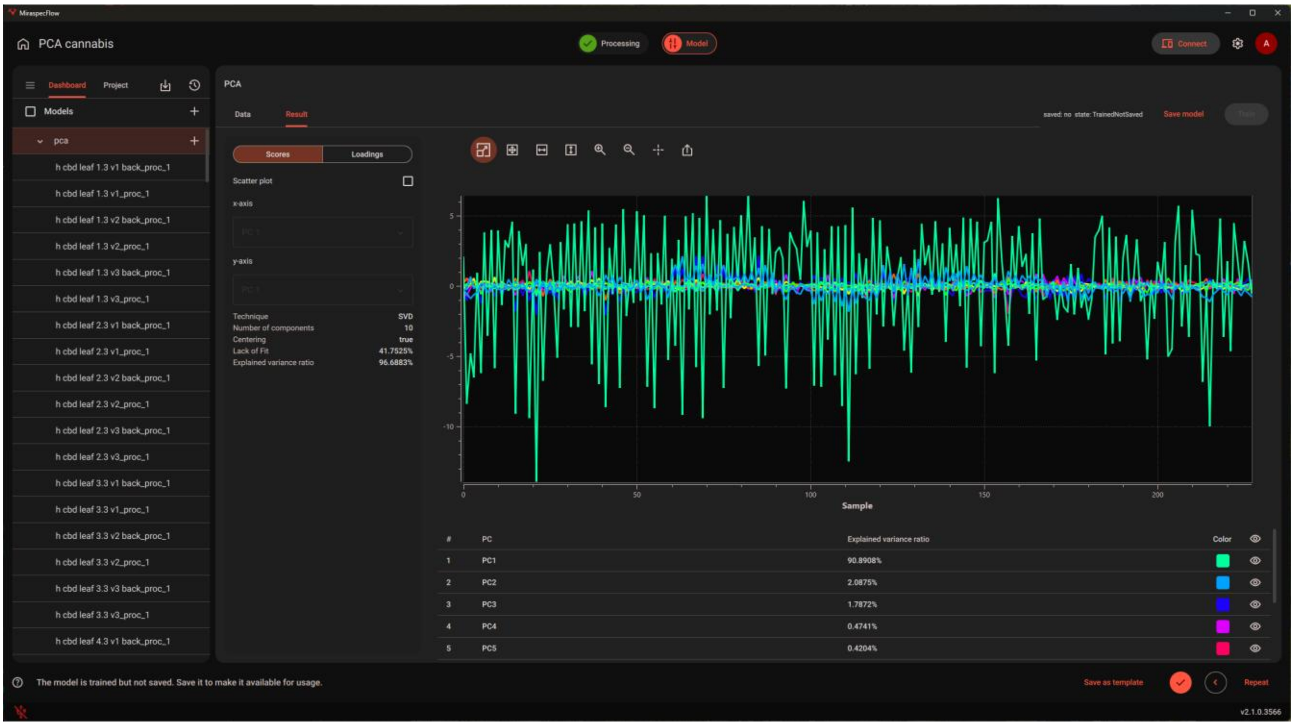
Under advanced settings we can choose PCA technique: NIPALS, SVD or Gram-Schmidt:



We choose number of PCA components as 10 and click Run PCA by clicking on Train. This performs the PCA and gives the result.

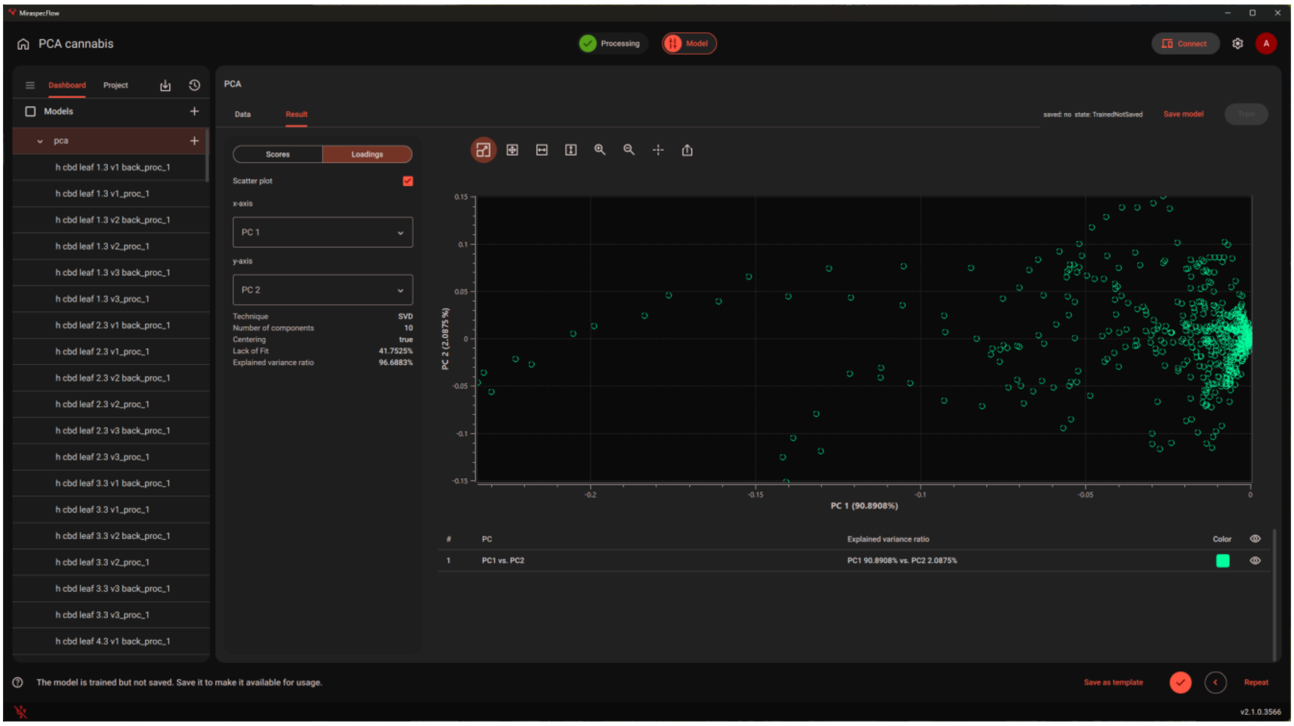
We can switch between PCA scores and loadings.

Scores:



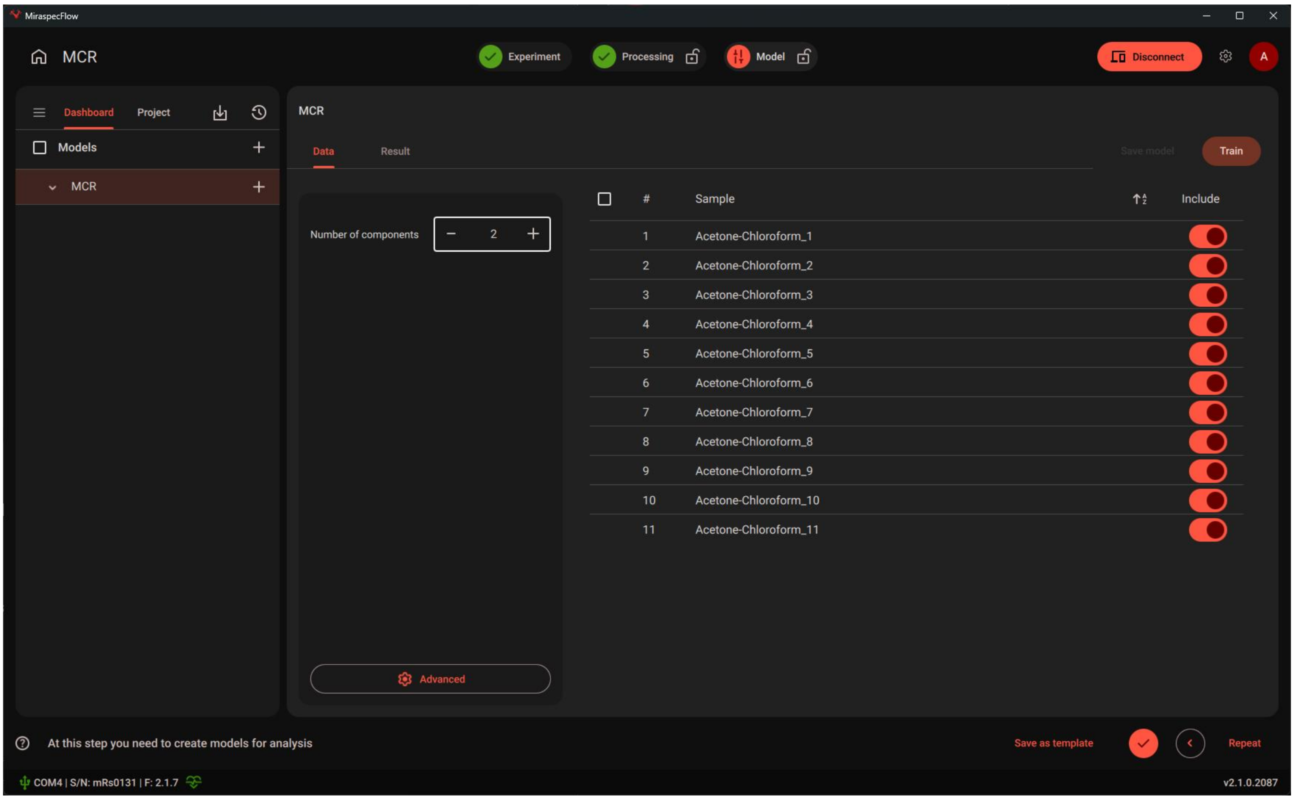
Loadings:

Scatter plot



8.6. MCR

Create new project, choose model type MCR. We will show it on example of acetone chloroform data.



Number of components 2.

Results - resolved spectra of the components:

As well as concentrations of the components in each sample:

Multivariate Curve Resolution (MCR) is a chemometric analysis method used to decompose complex spectral datasets into contributions from individual chemical components. This technique is particularly useful for analyzing mixtures where the measured spectrum contains overlapping signals from multiple substances.

MCR separates the measured spectral data into two main elements: the estimated spectra of the underlying components and their corresponding concentration profiles across the dataset. By analyzing the variation in the spectral data, the method identifies patterns that correspond to individual chemical species present in the samples.

During MCR analysis, the user specifies the number of components expected in the dataset. The software then applies an iterative algorithm to estimate the spectral signatures of these components and determine their relative contributions to each measured spectrum.

The results of MCR analysis are typically presented as:

- **Resolved component spectra**, representing the estimated spectral signatures of the individual components
- **Concentration profiles**, showing the relative abundance of each component in the analyzed samples

MCR is particularly useful when studying mixtures of substances or when it is necessary to identify hidden spectral components that are not easily distinguishable in the original spectra.

8.7. Model training and evaluation

The **Model Training and Evaluation** section describes the process used to create analytical models and assess their performance in Miraspec Flow. Model training involves using a set of reference spectra to build a mathematical model that can later be applied to analyze new spectral measurements.

During the training process, the system analyzes the spectral data and extracts relevant features that allow the model to distinguish between different materials or estimate chemical concentrations. The training dataset typically consists of spectra with known labels or known concentration values, depending on the type of model being developed.

To evaluate model performance, the dataset is often divided into **training** and **test** subsets. The training subset is used to construct the model, while the test subset is used to evaluate how well the model performs on previously unseen data. This approach helps assess the model’s ability to generalize to new measurements.

Several evaluation metrics may be used to assess model quality. For classification models, common metrics include **accuracy**, **precision**, **recall**, and **F1 score**. For calibration models, evaluation may involve comparing predicted concentration values with known reference values and calculating statistical indicators such as prediction error or variance explained by the model.

After training and evaluation, the model can be saved and stored within the system. Saved models can be reused in future projects to analyze new spectra and automate identification, classification, or quantitative analysis tasks.

9. Analysis

The Analysis section describes the methods available in Miraspec Flow for interpreting processed Raman spectral data. These analytical tools allow users to identify materials, classify unknown samples, explore relationships between spectra, and estimate the concentration of chemical components.

After spectral acquisition and preprocessing, the processed data can be analyzed using one or more analytical techniques provided by the software. Depending on the analytical objective, the user may perform qualitative identification, multivariate classification, exploratory data analysis, or quantitative calibration.

The following sections describe the available analysis methods and explain how they are applied to processed spectral data within the software.

9.1. Identification

The **Identification** analysis method is used to determine the identity of an unknown sample by comparing its Raman spectrum with reference spectra stored in a spectral library. This method is commonly used for qualitative analysis, where the objective is to identify the material present in a sample.

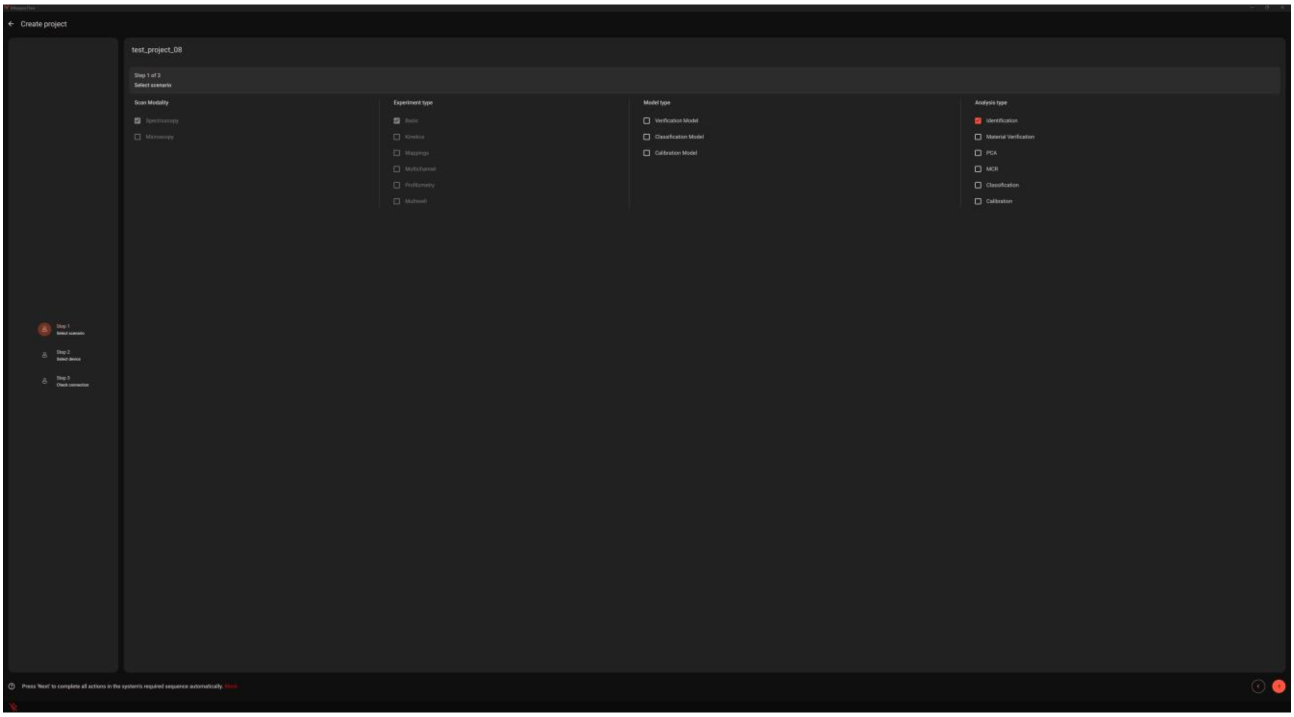
During identification, the processed spectrum of the measured sample is compared with spectra in the selected reference library. The software calculates a similarity score between the measured spectrum and each library spectrum using a defined comparison method. The results are then ranked according to their similarity to the measured spectrum.

Only reference spectra with similarity scores above a defined threshold are typically considered valid matches. The results are displayed as a list of candidate materials, along with their corresponding similarity values.

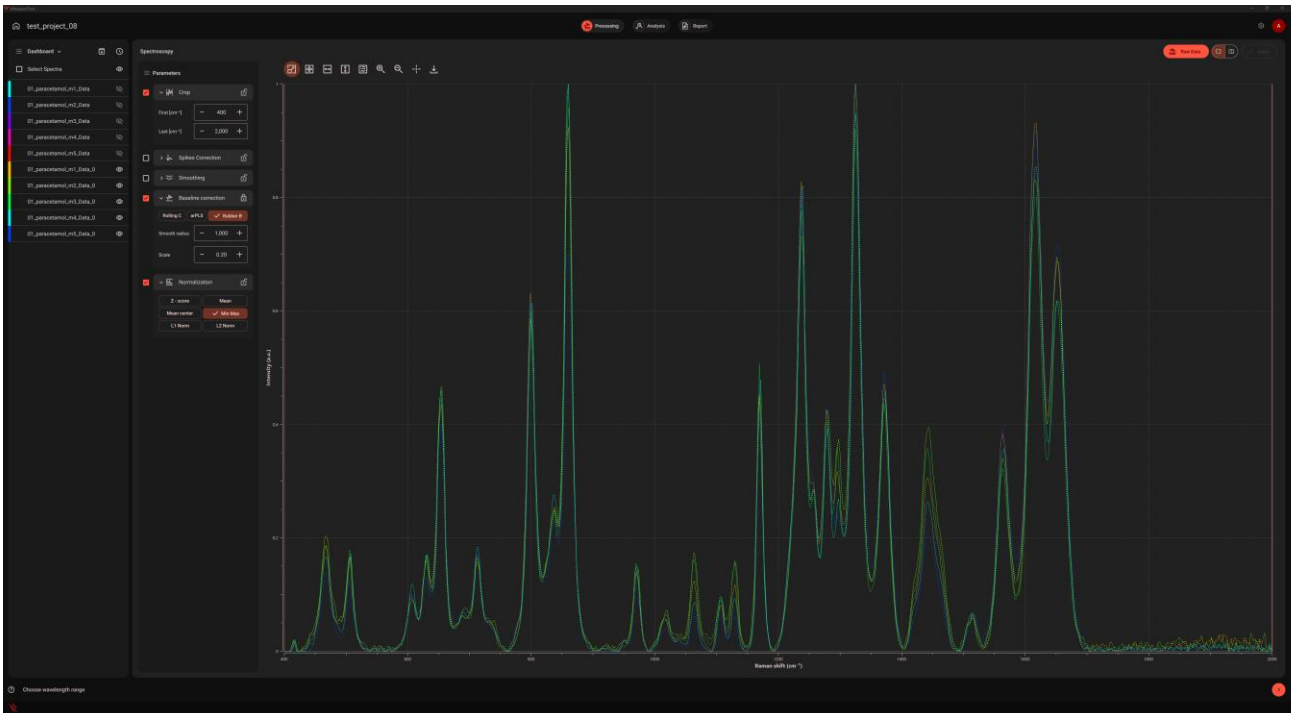
Users can review the identification results by comparing the measured spectrum with the matched library spectra. This visual comparison helps verify the identification and assess the quality of the match.

The identification method is widely used in applications where rapid determination of the chemical identity of a sample is required.

For the identification create a new project, choose analysis type identification and proceed to Next step:



Upload the data for example we use paracetamol dataset, apply some preprocessing for instance crop in the range 400.. 2000 cm^{-1}, baseline correction and minmax normalization and click apply:



Click on next to proceed to data analysis. Choose library for identification, for example we will use ST Japan.

Go to Advanced settings to set the spectral range, identification threshold and the method of HQI calculation, for example Pearson correlation, SEC (Squared Euclidian Cosine), SFDEC (Squared First-Derivative Euclidean Cosine), there is also an option to use segmented HQI.

In this example we will use standard Pearson correlation:

Click Identify button in the top right corner of the software window to identify the spectra.

You can then see the results of identification:

The table underneath the graph shows best matches for the experimental spectra from the library spectra which fall above the HQI threshold value.

Note

Please note that acetaminophen is another name of paracetamol and eventually is the same compound.

We can switch between the spectra by clicking on the names of the data files underneath the graph and see the corresponding identification results and the spectra of the library compounds shown.

Click on next to proceed to reports.

9.2. Classification

The **Classification** analysis method is used to assign measured spectra to predefined classes using a trained classification model. This method allows the automated identification of sample categories based on their spectral characteristics.

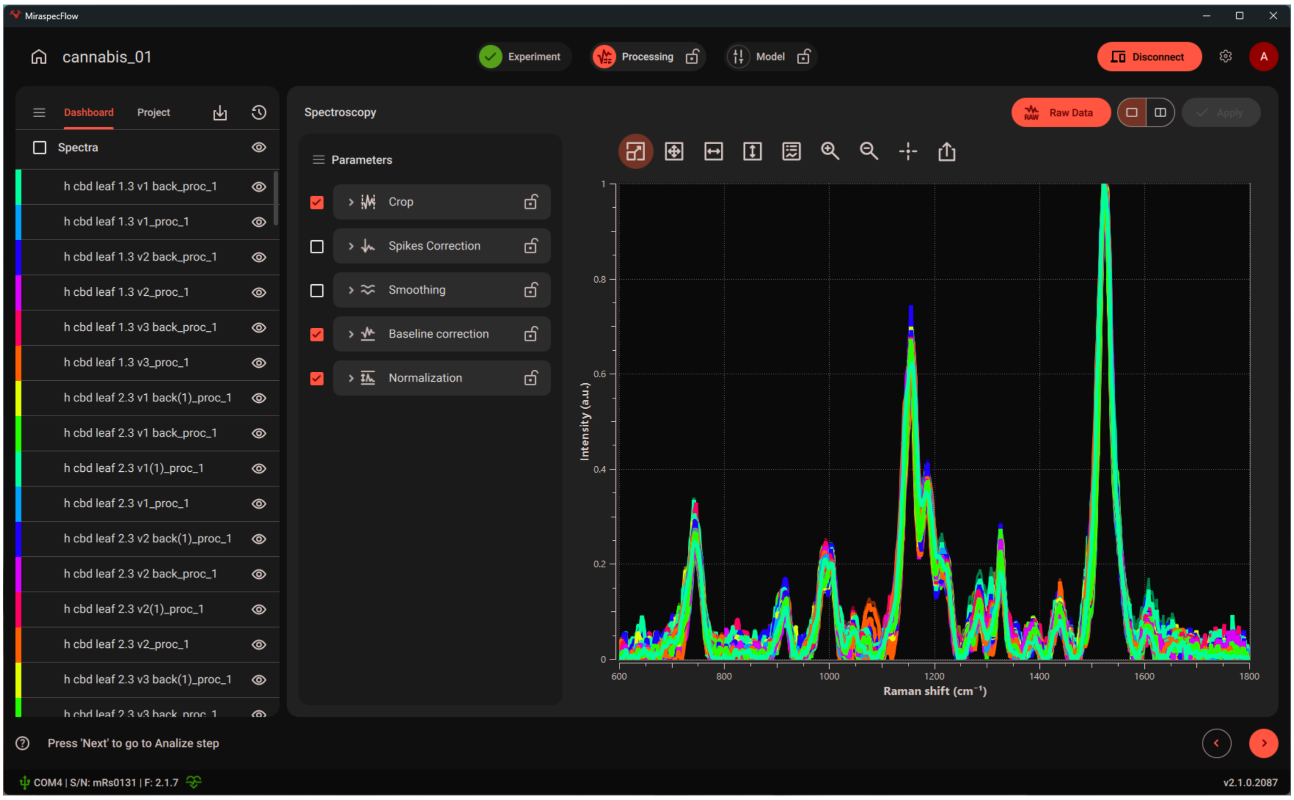
During classification analysis, the processed spectrum of a sample is evaluated using a previously trained classification model. The model analyzes the spectral features and determines the most probable class to which the sample belongs. The classification result indicates the predicted class together with additional information about the model performance.

Classification models are typically trained using labeled spectral datasets representing different materials or sample types. During analysis, the trained model compares the measured spectrum with the learned patterns from the training data and assigns the spectrum to the closest matching class.

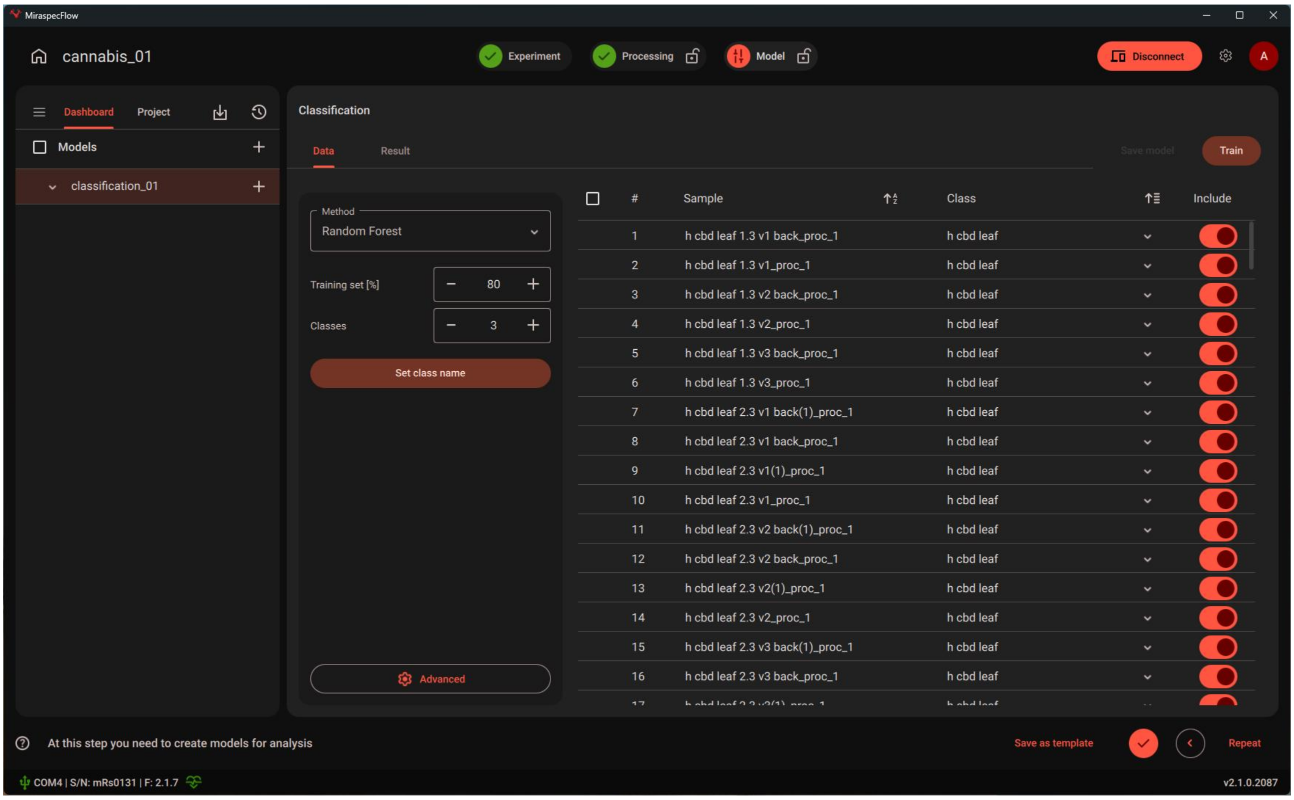
The classification results may also include evaluation metrics such as **accuracy**, **precision**, **recall**, and **F1 score**, which reflect the overall performance of the model during training and testing.

Classification analysis is useful in applications where multiple material types must be distinguished automatically, such as identification of substances within a predefined set of known classes.

We can perform classification on the same cannabis dataset. We choose the project with classification model, load the data, then apply preprocessing to crop, remove the baseline and perform min max normalization.



We proceed to next. We add classification model, choose random forest model with 3 classes (cbd leaf, thc leaf and mixed).

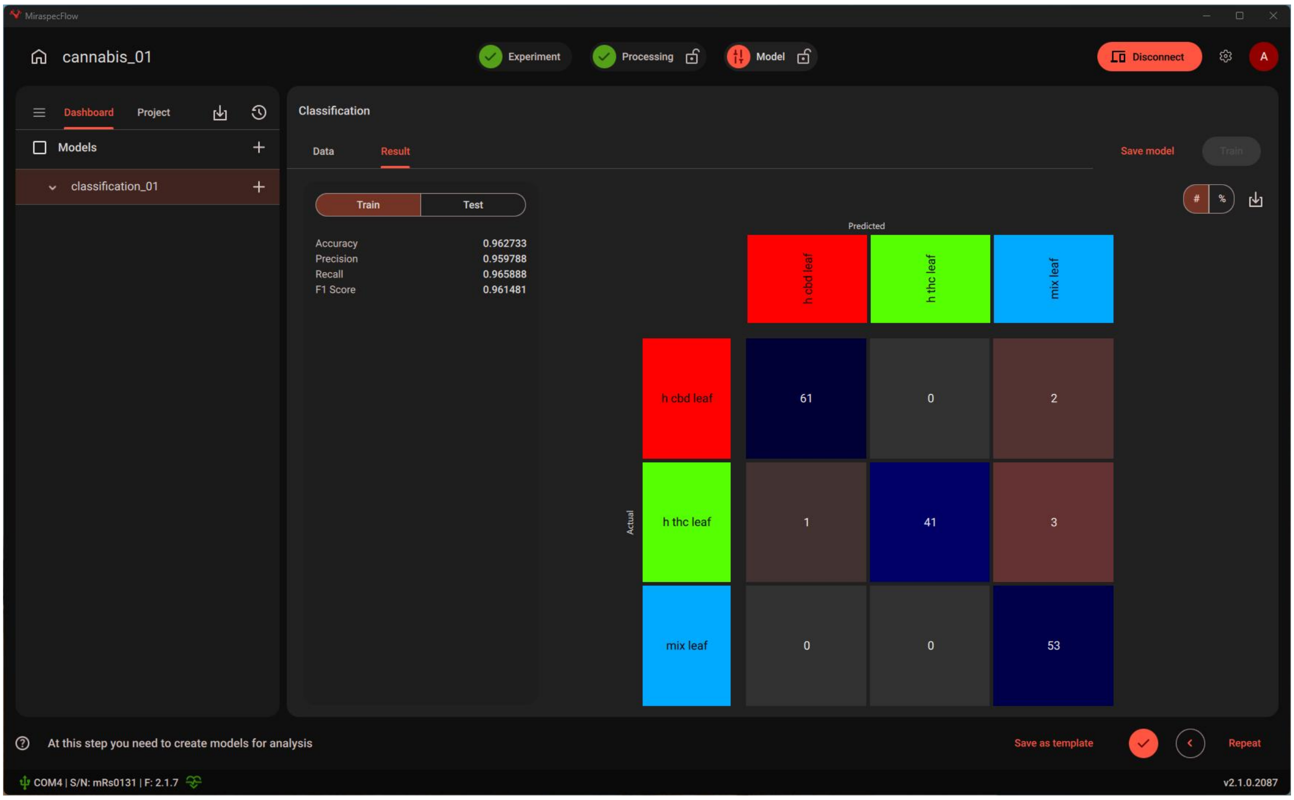


The classes have to be properly assigned to the spectra.

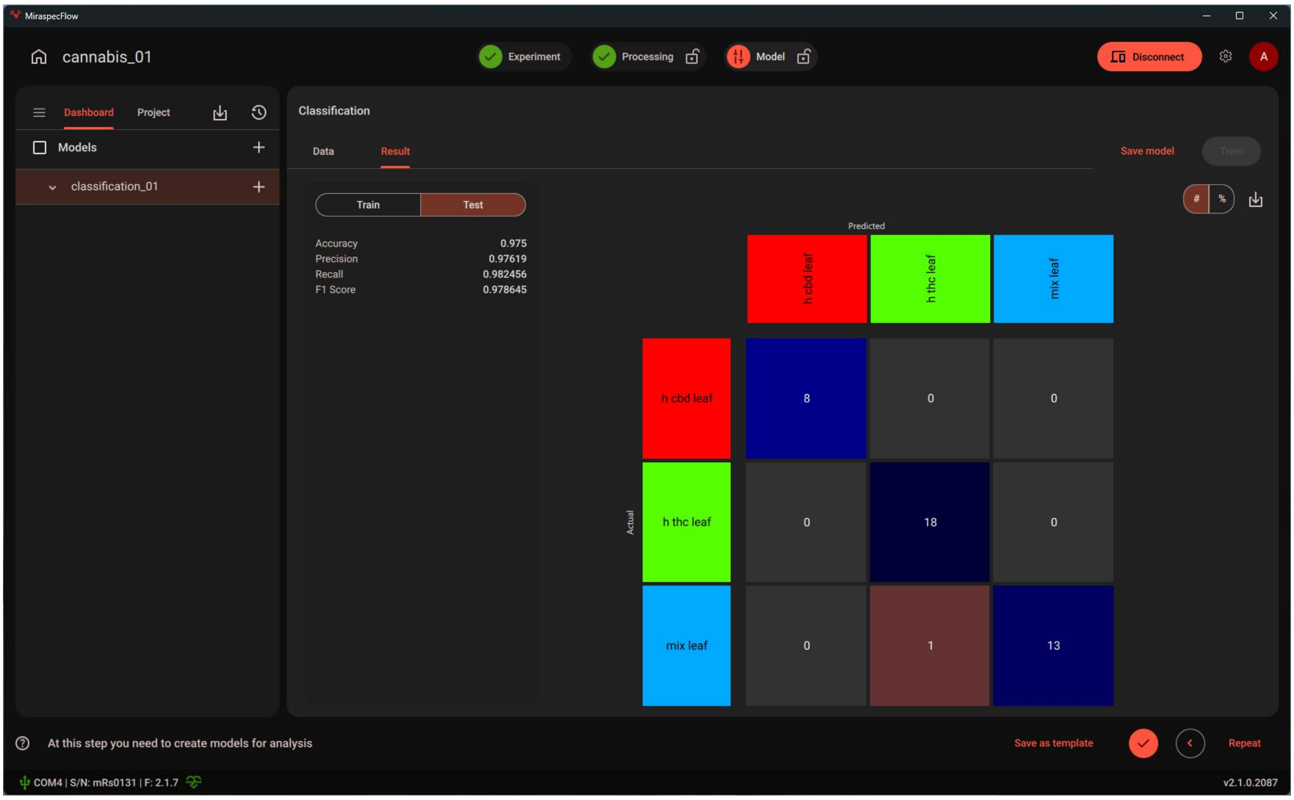
Click on train the model to train the model.

As a result, the confusion matrices for train and test datasets are provided.

Train:



Test:



In the results pannel the parameters such as Accuracy, Precision, Recall, and F1 score are displayed.

9.3. Calibration

The **Calibration** analysis method is used to estimate the concentration of a specific chemical component in a sample based on its Raman spectrum. This approach relies on a previously trained calibration model that describes the relationship between spectral features and known concentration values.

During calibration analysis, the processed spectrum of a sample is evaluated using the selected calibration model. The model analyzes the spectral data and predicts the concentration of the target component according to the relationships established during model training.

Calibration models are typically developed using reference spectra obtained from samples with known concentrations. Regression techniques, such as **Partial Least Squares (PLS)**, are commonly used to construct these models by identifying correlations between spectral intensities and concentration values.

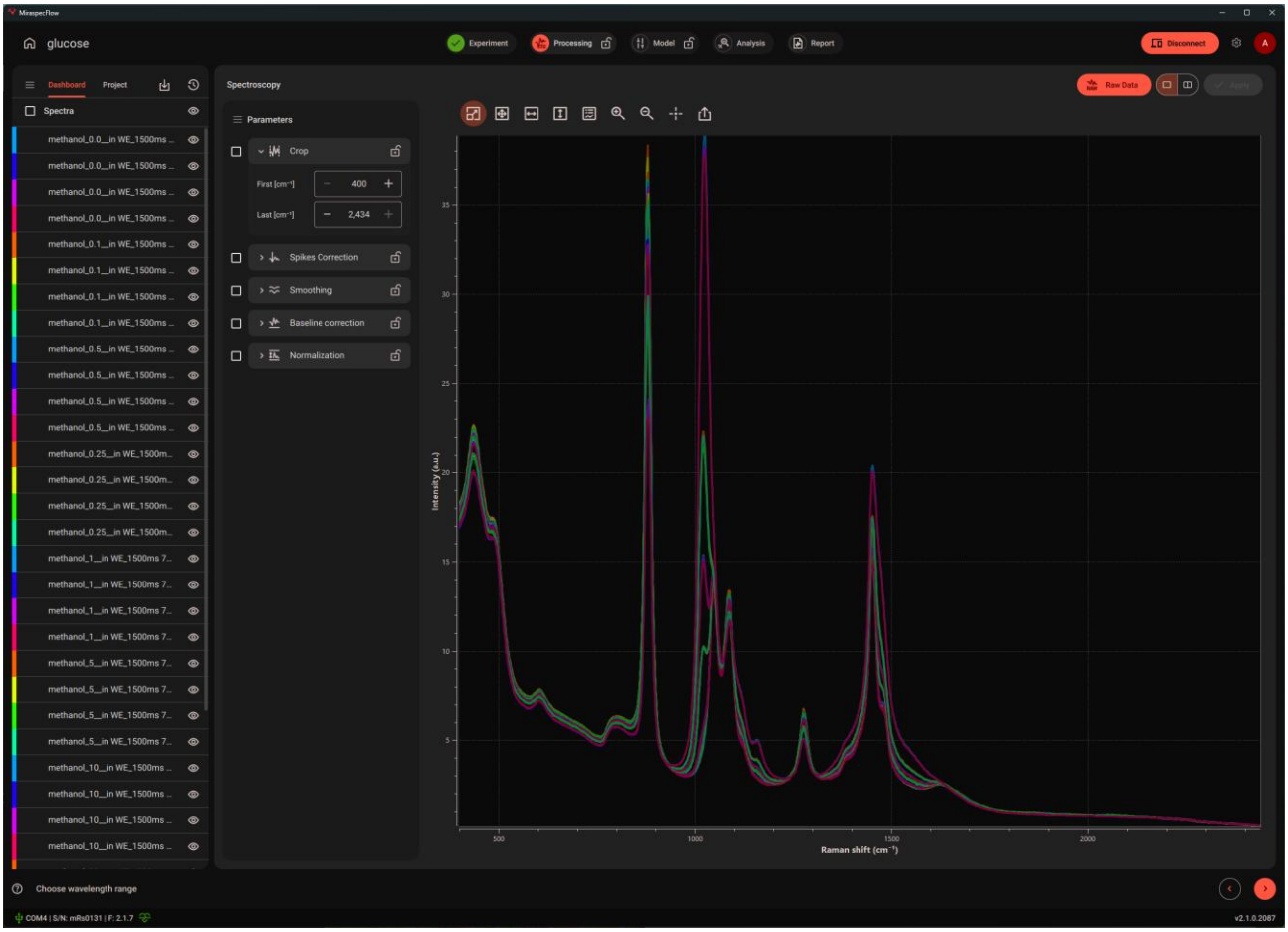
The results of calibration analysis may include:

- predicted concentration values for the analyzed samples
- graphical comparison of predicted and reference values
- statistical indicators that describe the quality of the calibration model

Calibration analysis is widely used in quantitative spectroscopy applications where accurate estimation of chemical concentrations is required.

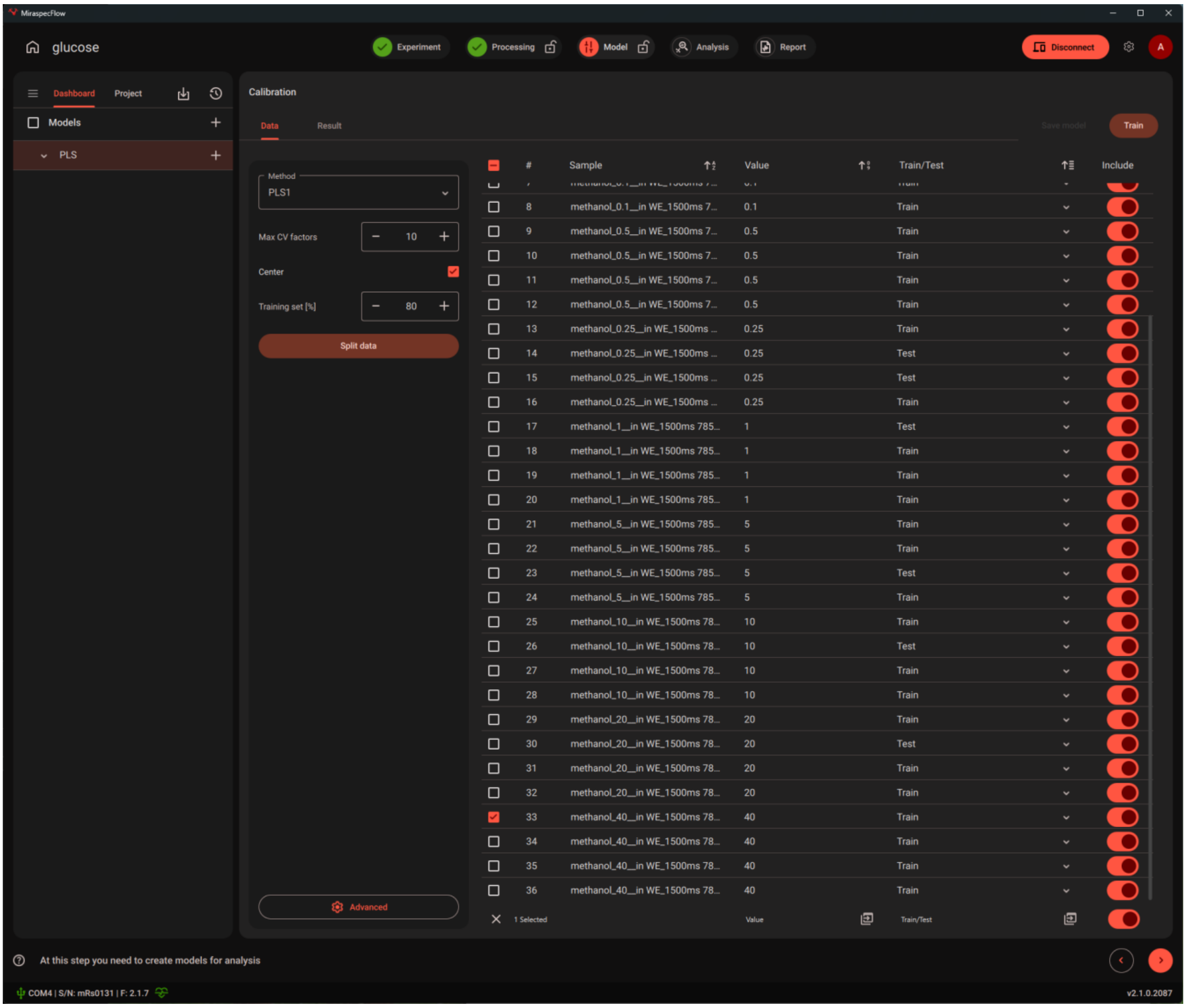
We will demonstrate calibration model on methanol in vodka dataset.

We create the project with calibration model and load the data:



We apply some preprocessing (cropping to spectral range 900..1250, baseline correction).

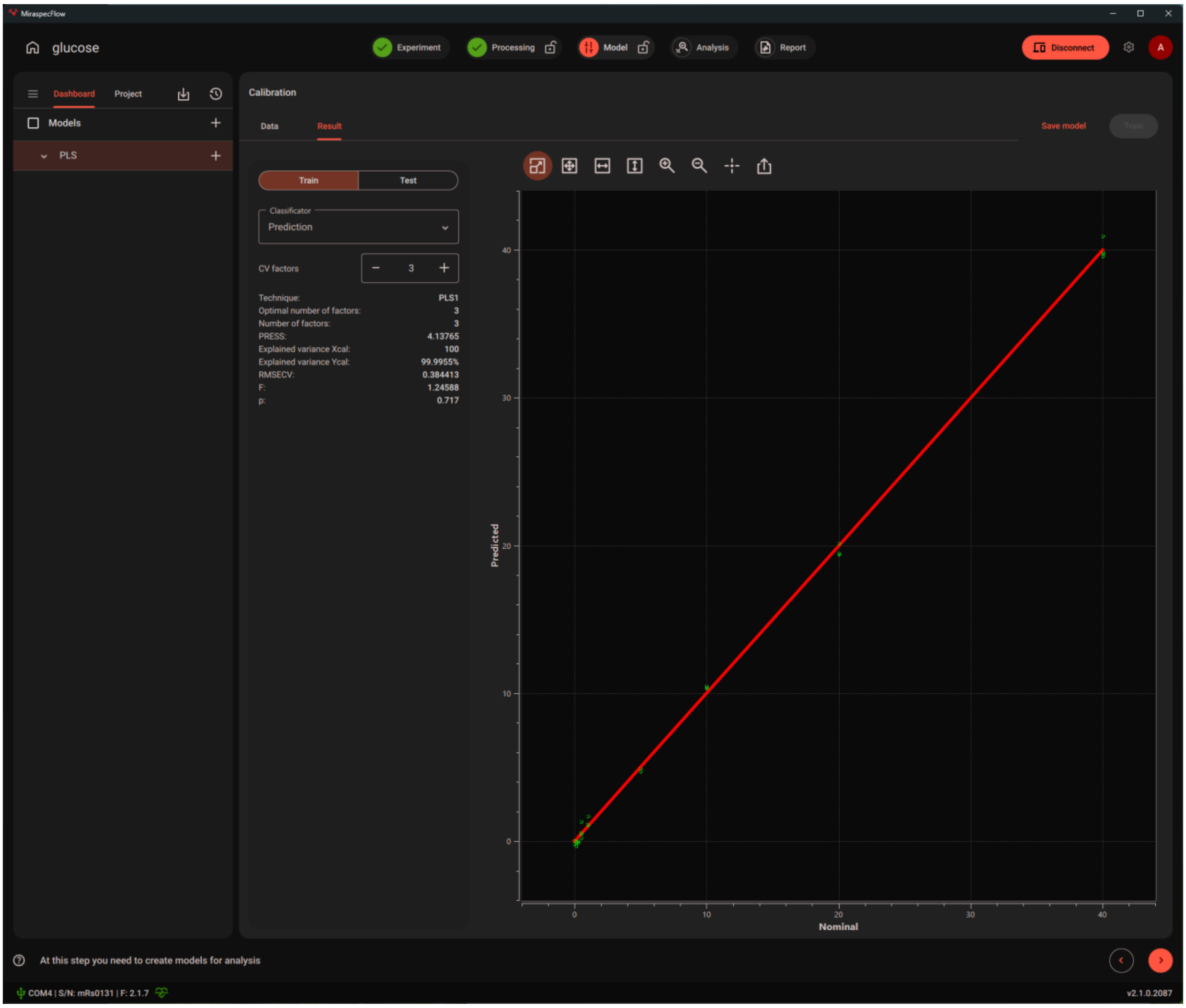
We choose PLS model, method PLS1, number of factors 10 and specify the concentrations under value.



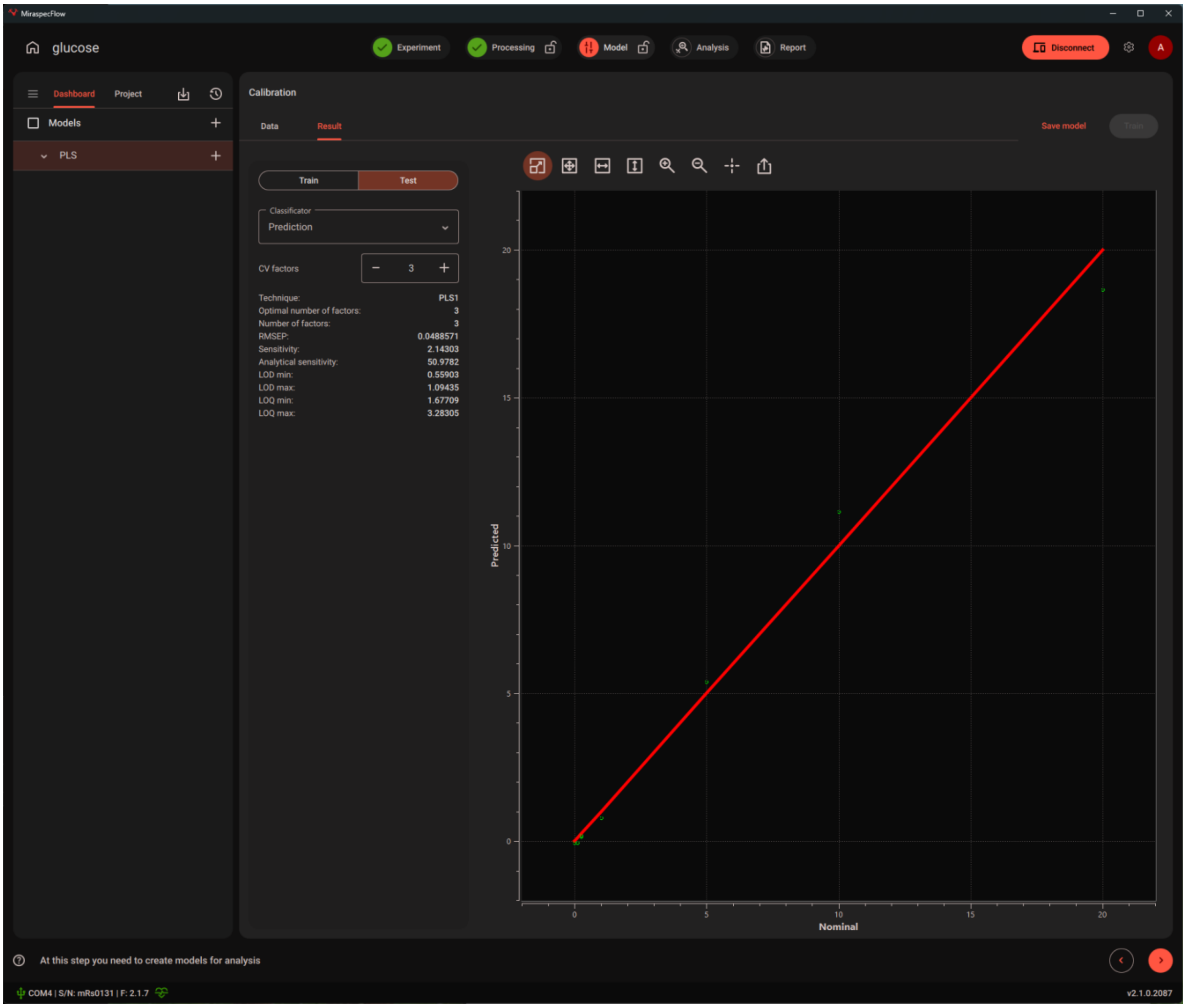
Then we train the model by clicking on the Train button.

The results are displayed for train and test datasets.

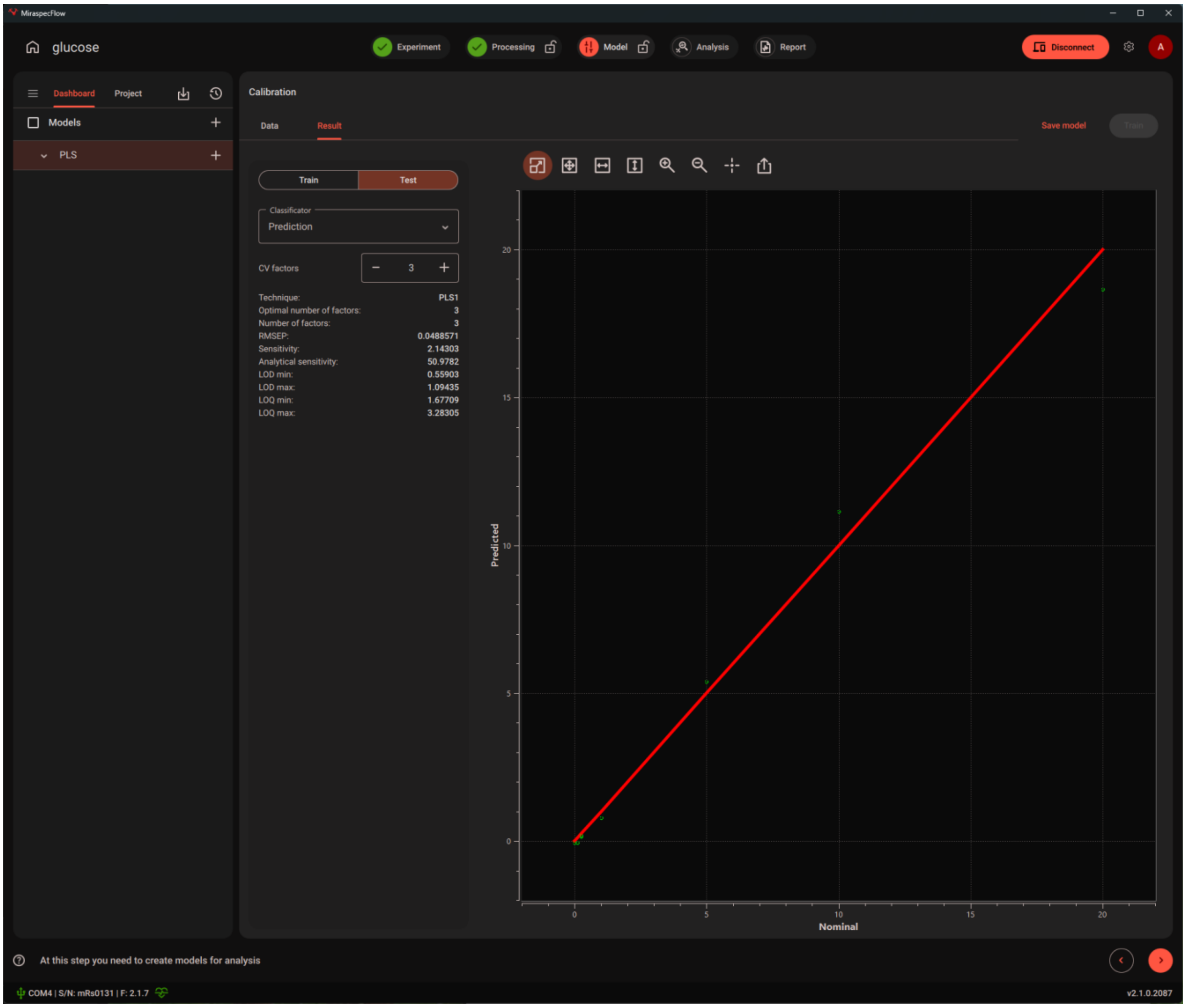
Train:


MiraspecFlow
glucose
Experiment
Processing
Model
Analysis
Report
Disconnect
Dashboard
Project
Models
PLS
Calibration
Data
Result
Save model
Train
Train
Test
Classificator
Prediction
CV factors
3
Technique: PLS1
Optimal number of factors: 3
Number of factors: 3
PRESS: 4.13765
Explained variance Xcal: 100
Explained variance Ycal: 99.9955%
RMSECV: 0.384413
F: 1.24588
p: 0.717
Predicted
Nominal
At this step you need to create models for analysis
COM4 | S/N: mRs0131 | F: 2.1.7
v2.1.0.2087

Test:


MiraspecFlow
glucose
Experiment
Processing
Model
Analysis
Report
Disconnect
Dashboard
Project
Models
PLS
Calibration
Data
Result
Save model
Train
Train
Test
Classificator
Prediction
CV factors
3
Technique: PLS1
Optimal number of factors: 3
Number of factors: 3
RMSEP: 0.0488571
Sensitivity: 2.14303
Analytical sensitivity: 50.9782
LOD min: 0.55903
LOD max: 1.09435
LOQ min: 1.67709
LOQ max: 3.28305
Predicted
Nominal
At this step you need to create models for analysis
COM4 | S/N: mRs0131 | F: 2.1.7
v2.1.0.2087

Test results tab also displays calculated results for the ranges of limit of detection (LOD) and for the limit of quantification (LOQ).



Then we can save the model by clicking on save model. By clicking next we can proceed to analysis step.

9.4. Verification

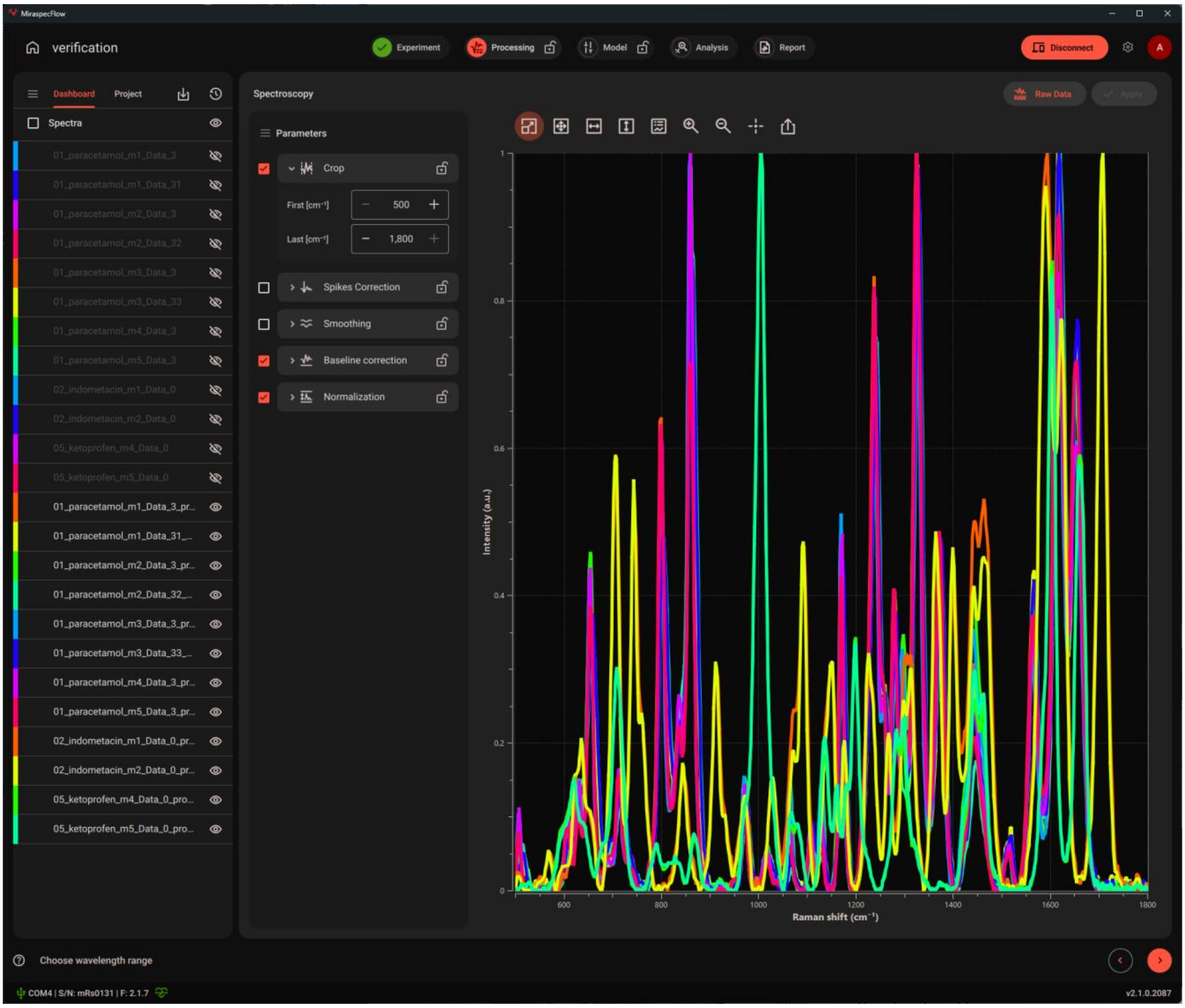
The **Verification** analysis method is used to confirm whether a measured spectrum corresponds to a specific known material. This method evaluates whether a sample matches the spectral characteristics defined by a previously trained verification model.

During verification analysis, the processed spectrum of the sample is compared with the reference model. The model calculates similarity measures between the measured spectrum and the reference spectra used to construct the model. Based on predefined acceptance criteria, the system determines whether the sample passes or fails the verification test.

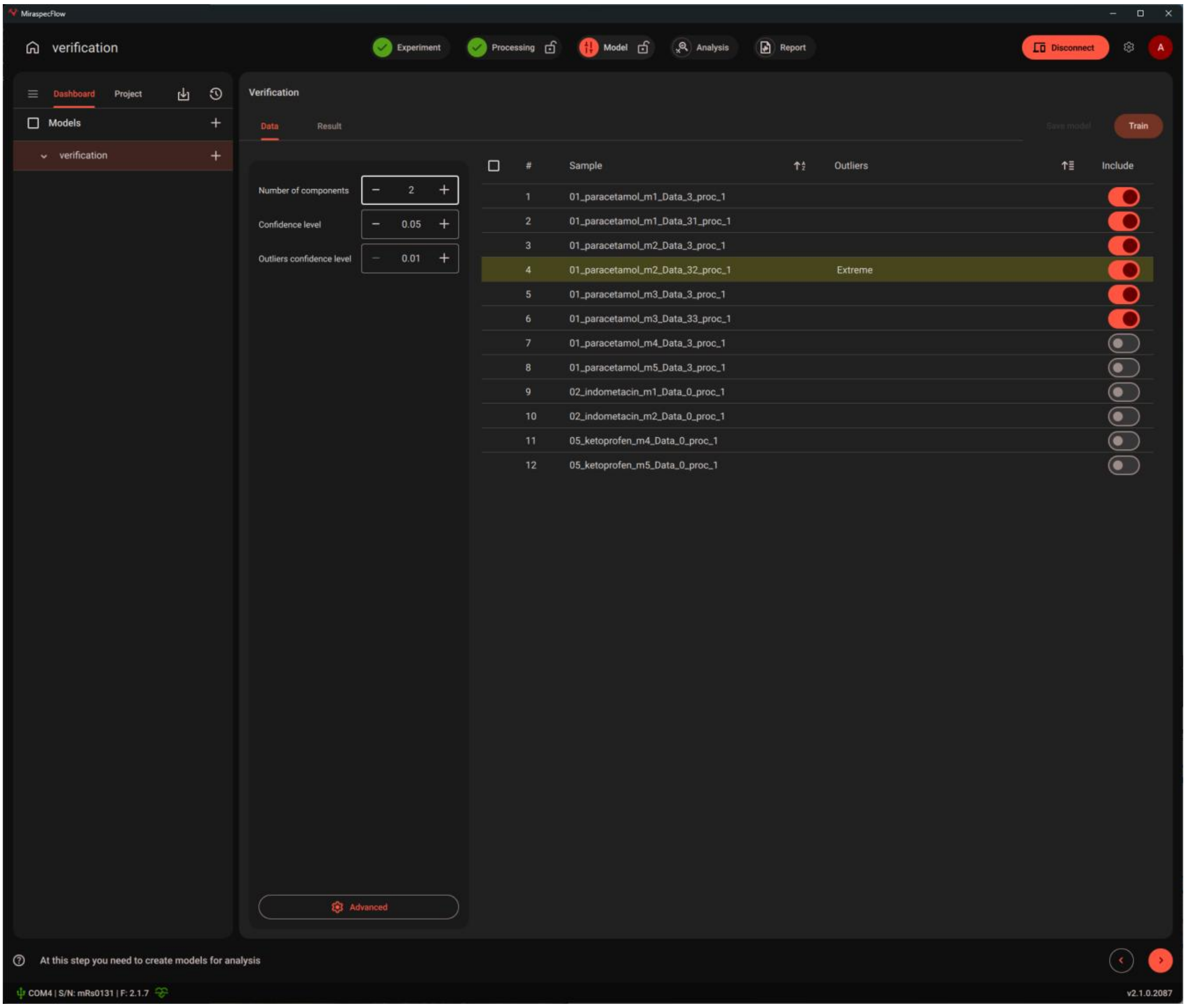
The verification result typically indicates whether the sample is consistent with the reference material represented by the model. If the similarity between the measured spectrum and the reference model falls within the acceptable range, the sample is considered verified. If the similarity falls outside the defined criteria, the sample fails the verification.

Verification analysis is commonly used in quality control applications where the objective is to confirm the identity of a known substance rather than classify an unknown sample.

We choose new project, model type: verification, analysis type: material verification. Then we click next and load the data (pharmaceutical powders). Crop 500..1800, baseline correction, minmax normalization, click apply

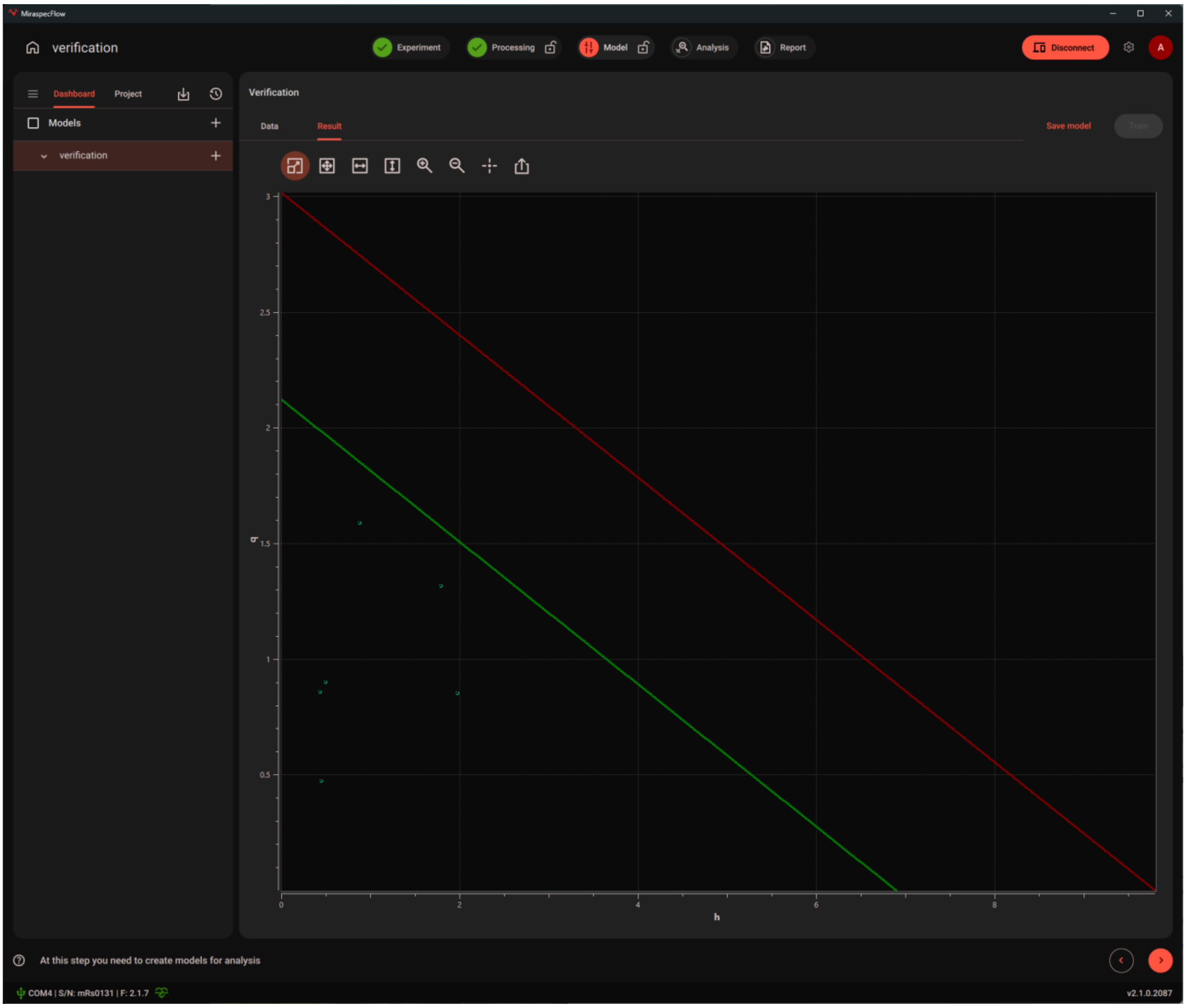


We choose which paracetamol spectra to include into the model.



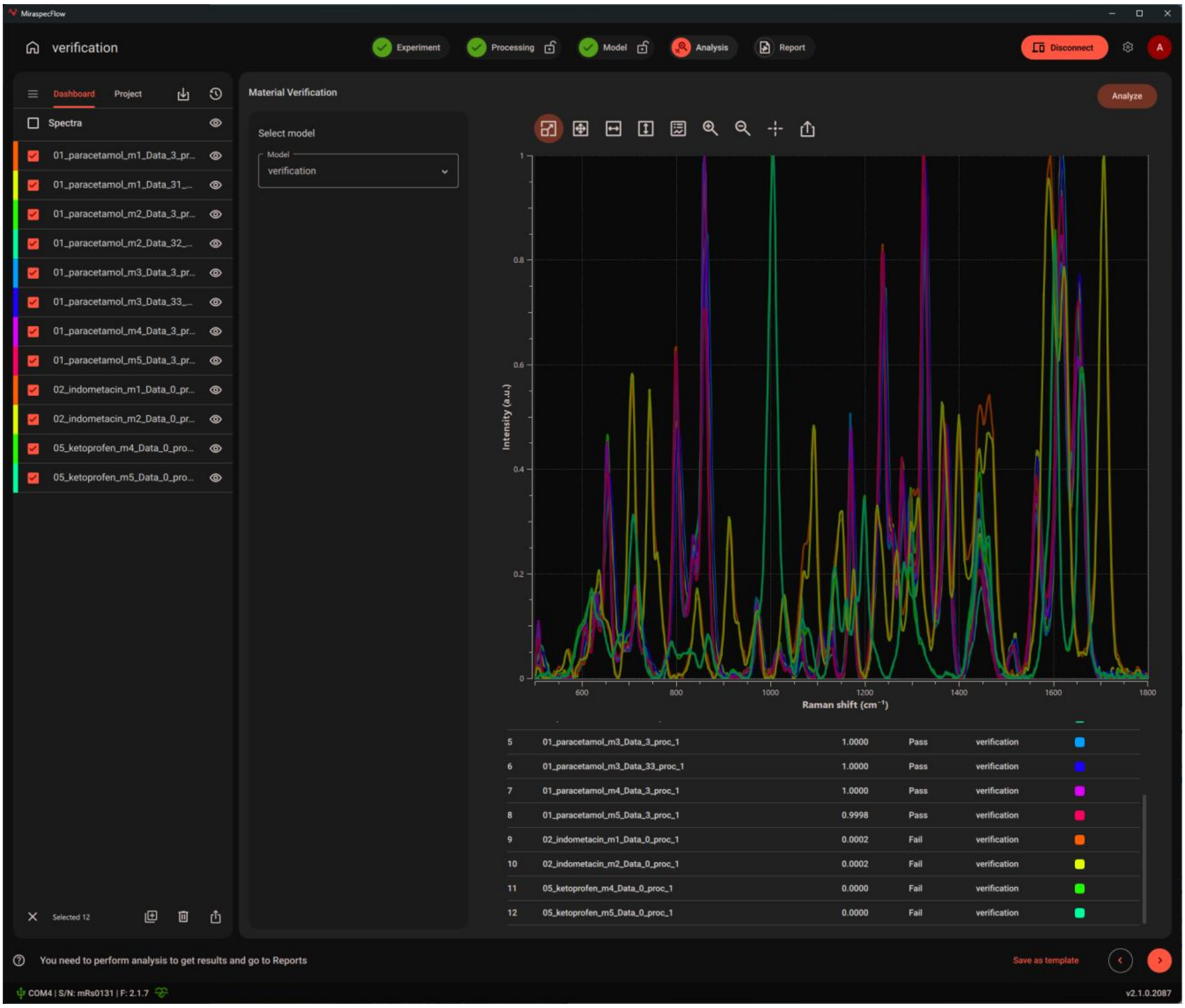
And then click on train.

The result is displayed as follows:



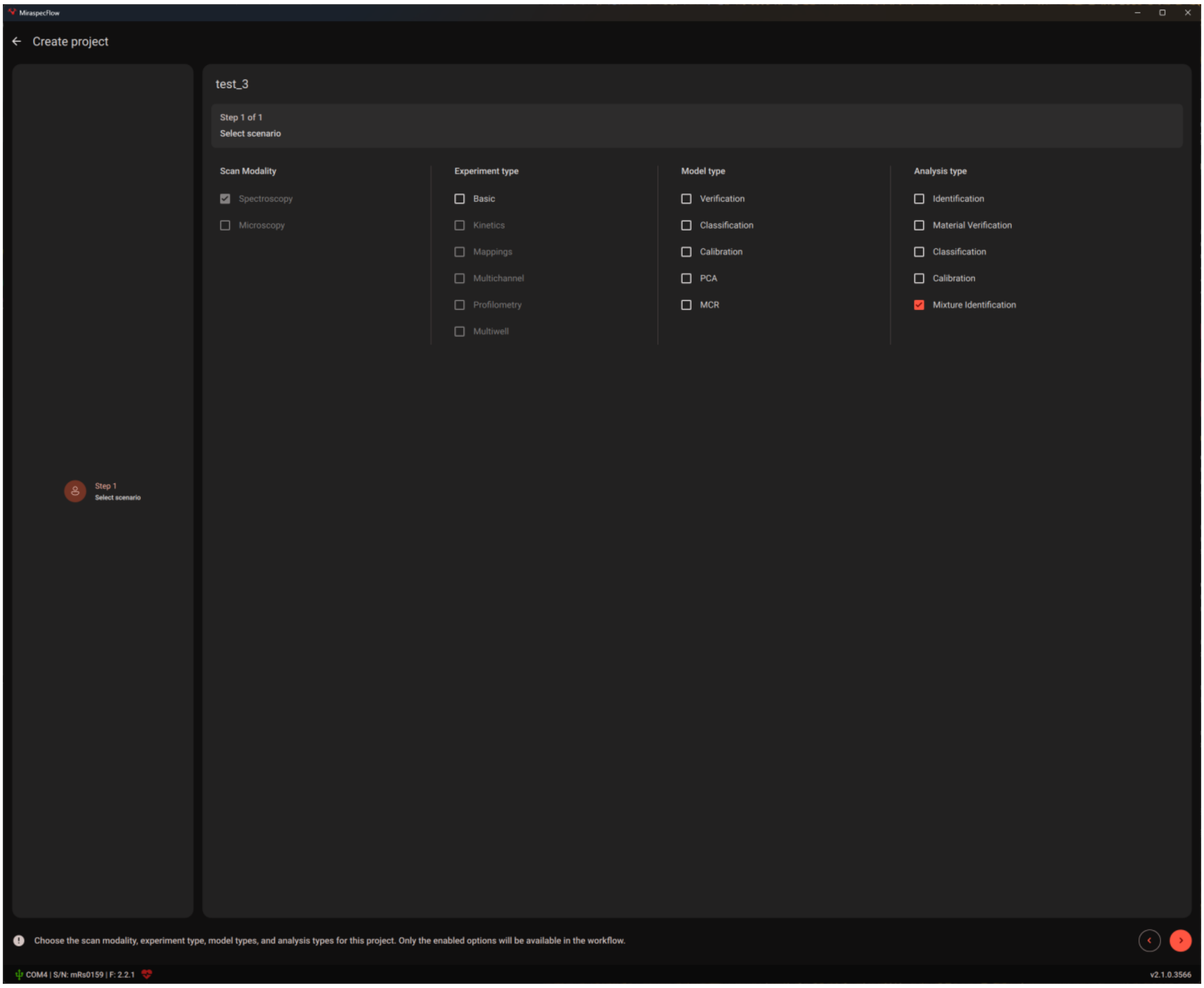
Then we save the model and proceed to next step – analysis.

We click on analyse and as we can see paracetamol spectra pass verification while indomethacin and ketoprofen spectra fail to pass the test (this is expected since those spectra are not the spectra of paracetamol).

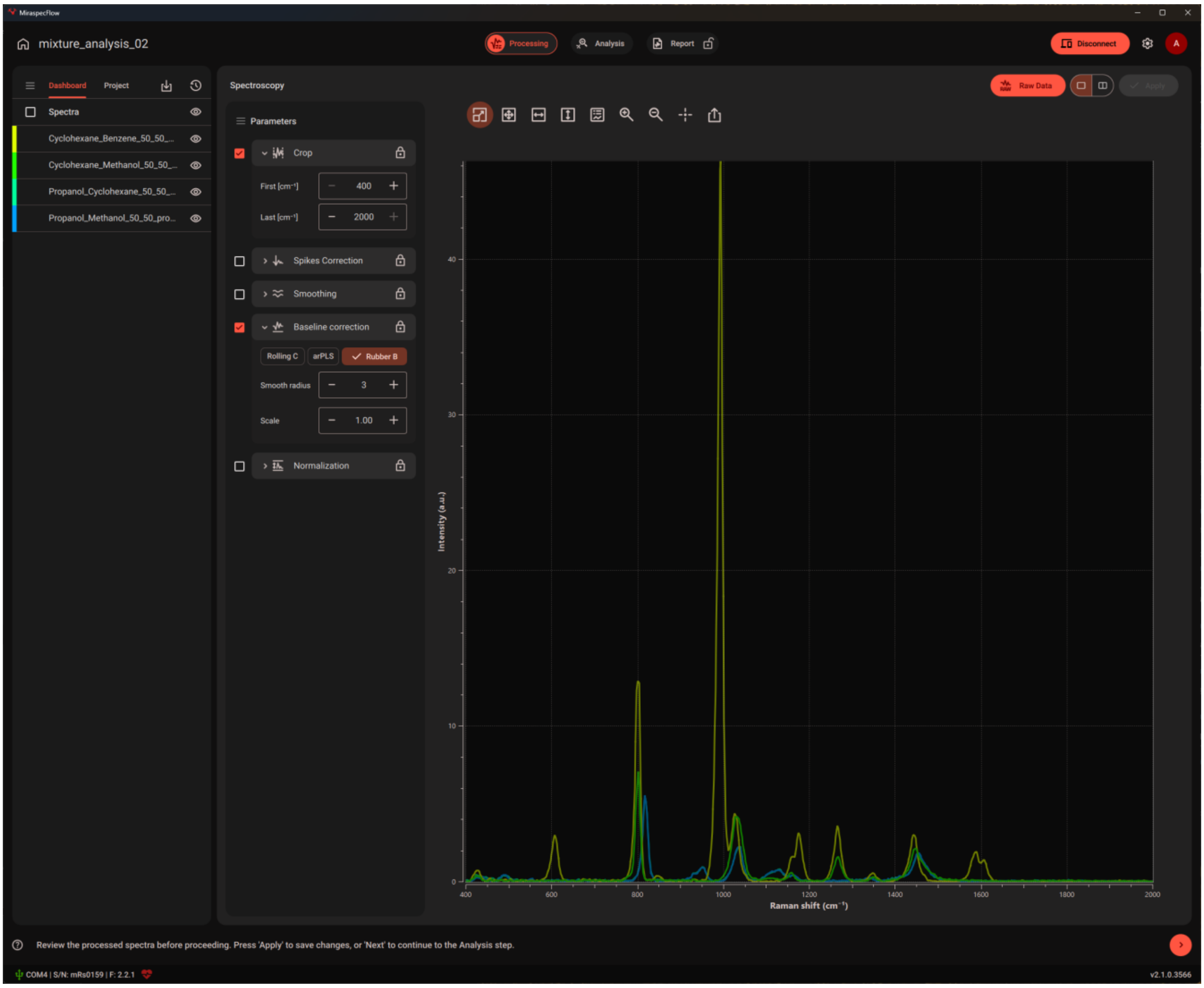


9.5. Mixture Identification

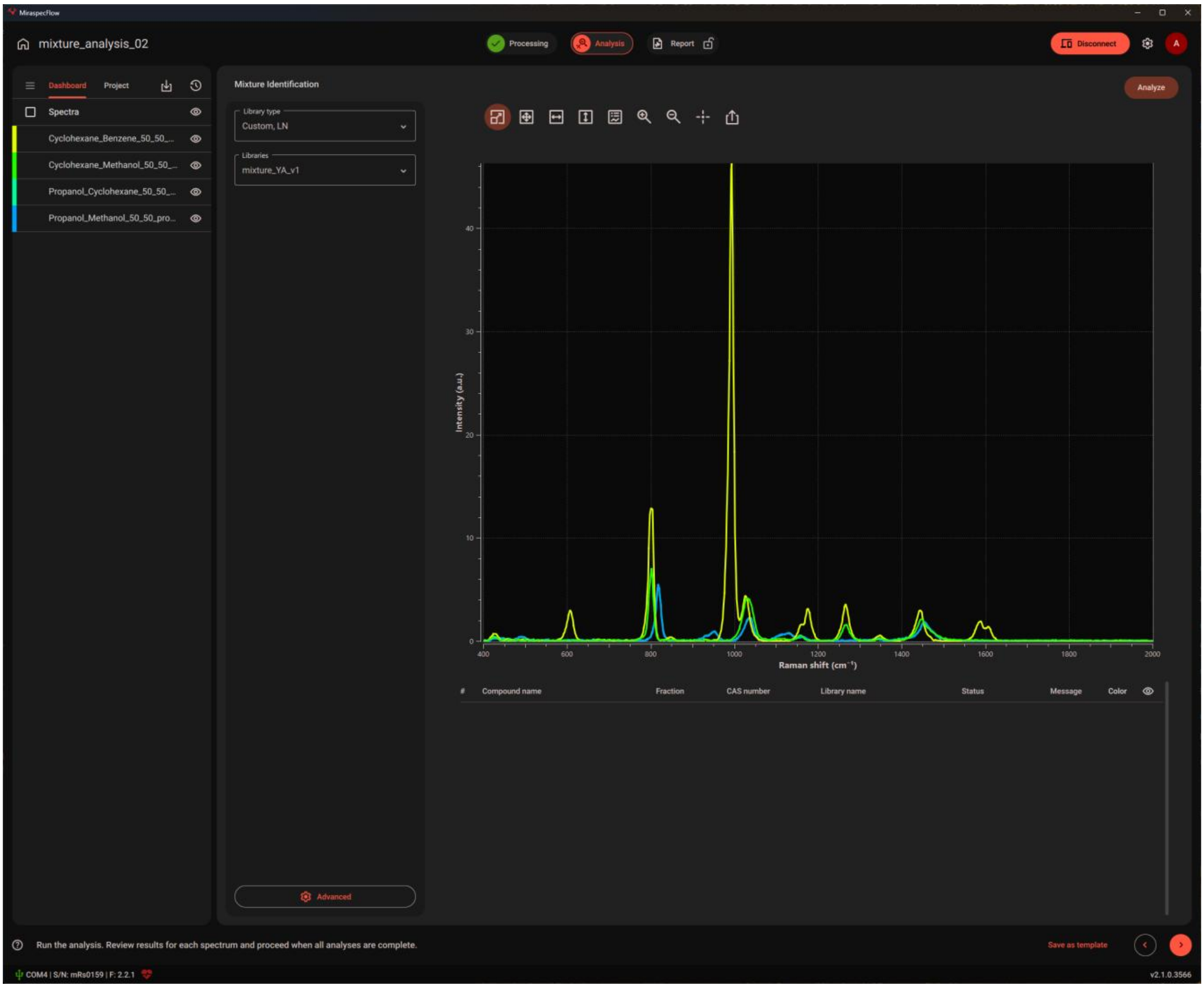
Create a project with mixture identification:



Upload the files to analyze, go through preprocessing step if necessary:



Select the library and click analyze:



The results of analysis will appear:

10. Reports

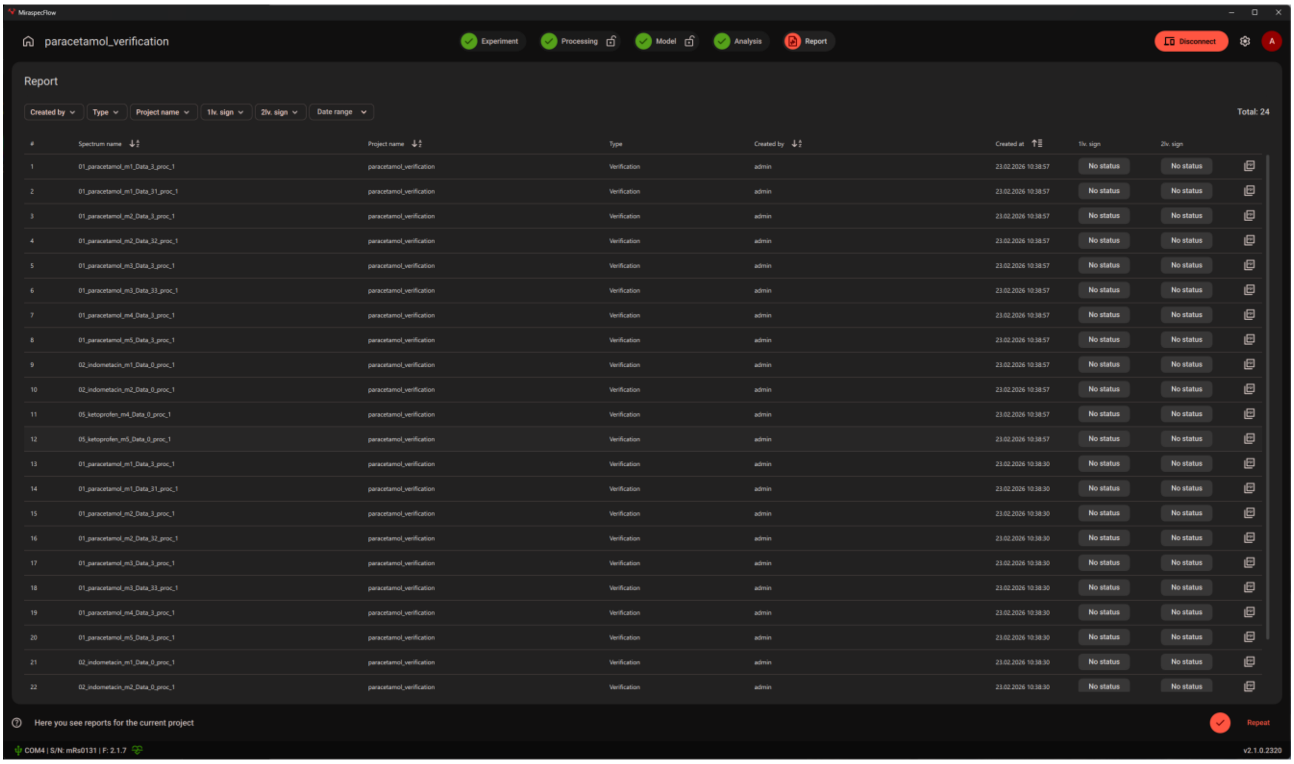
The Reports section describes the tools available in Miraspec Flow for generating and managing analytical reports based on measurement results and spectral analyses. Reports provide a structured summary of the experiment, including relevant spectral data, analysis results, and associated metadata.

Reports can be generated after completing spectral acquisition and analysis. The report may include information such as project details, measurement parameters, processed spectra, identification or classification results, and other analytical outputs produced during the experiment workflow.

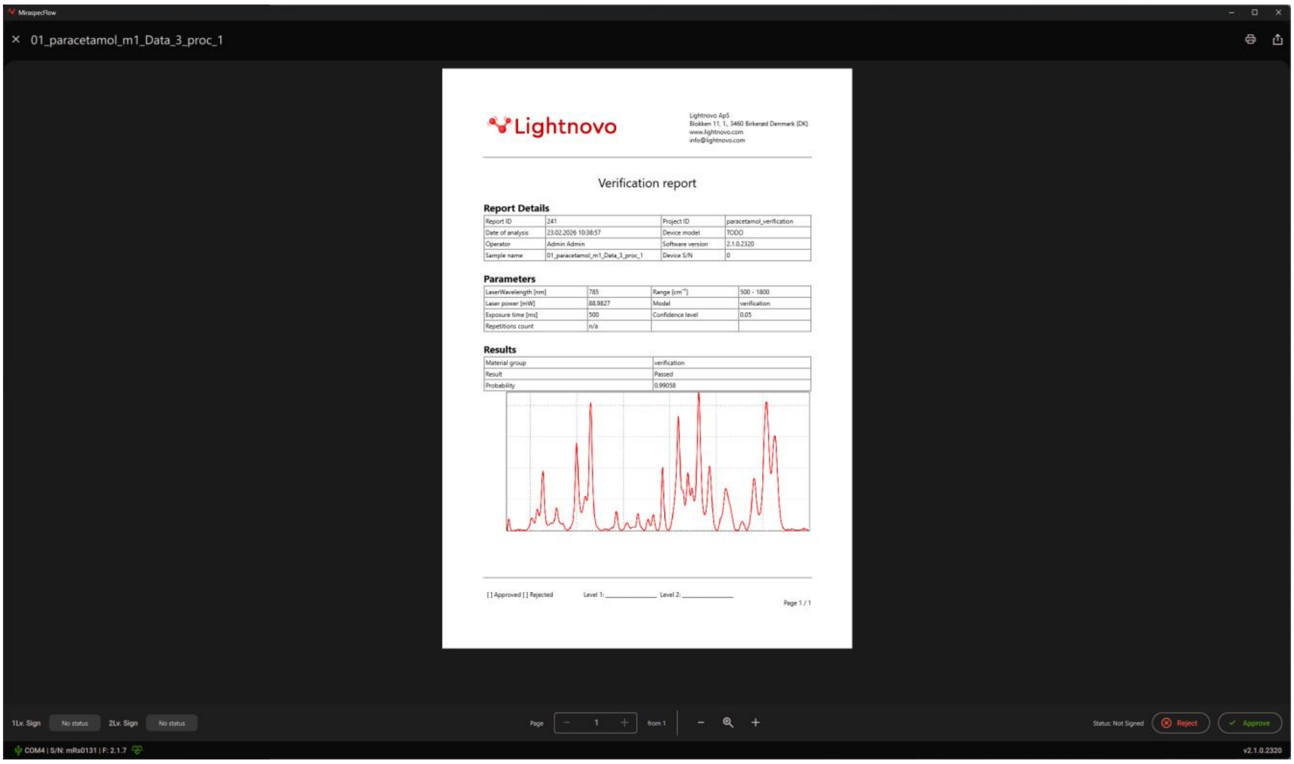
Miraspec Flow provides functionality for reviewing reports within the software and, where applicable, managing an approval workflow. This enables authorized users to verify analytical results before reports are finalized or shared.

Completed reports can be exported or printed for documentation, record keeping, or further analysis. The reporting functionality helps ensure that experimental results are documented in a consistent and traceable format.

For example after verification model is used the reports are created.



Then the user can click on pdf icon to view a report. For example:



The user who has proper credentials has also an option to approve or reject the report.

The following sections describe how to generate reports, review report content, manage approval or rejection workflows, and export reports from the system.

10.1. Report generation

The **Report Generation** section describes the process of creating reports that summarize the results of spectral measurements and analyses performed in Miraspec Flow. Reports provide a structured representation of the experiment, including relevant data, analysis outcomes, and associated metadata.

Reports can be generated after completing an analysis step within the experiment workflow. Depending on the type of analysis performed, the report may include information such as project details, measurement parameters, processed spectra, model results, and identification or verification outcomes.

When a report is generated, the system collects the relevant information from the current project and analysis results and compiles it into a structured document. The generated report is stored in the system and becomes available for viewing, approval, export, or printing.

Reports help ensure that analytical results are documented in a consistent and traceable format, supporting record keeping, quality control, and further review of experimental outcomes.

10.2. Viewing reports

The **Viewing Reports** section describes how users can access and review reports generated within the Miraspec Flow system. Reports provide a detailed summary of spectral measurements, analysis results, and associated project information.

Generated reports are stored in the system and can be accessed through the **Records** section or other report management interfaces available to authorized users. The report list typically displays key information such as the report name, associated project, analysis type, creator, and the date of creation.

To view a report, users can select the corresponding entry from the report list and open it in the report viewer. Reports are typically displayed in **PDF format**, allowing users to review the document in a structured layout that includes graphical results, tables, and relevant metadata.

From the report viewer, users may also perform additional actions such as exporting the report, printing the document, or proceeding with approval procedures if such workflows are enabled.

Viewing reports allows users to review analytical results and verify that the reported information accurately reflects the performed measurements and analyses.

10.3. Approval and rejection workflow

The **Approval and Rejection Workflow** section describes the process by which authorized users can review and validate reports generated in Miraspec Flow. This workflow ensures that analytical results are verified before being finalized or distributed.

After a report is generated, it may require review by users with appropriate permissions. During the review process, the report can be examined to confirm that the measurement data, analysis results, and associated information are correct and complete.

Authorized users may then perform one of the following actions:

- **Approve the report**, confirming that the results are valid and the report can be accepted as an official record.
- **Reject the report**, indicating that the results require further review, correction, or repetition of the analysis.

The approval status of each report is recorded in the system and may include information such as the user who performed the action and the date of approval or rejection. In some cases, multiple levels of approval may be implemented depending on system configuration and organizational procedures.

The approval workflow helps ensure data integrity, traceability of analytical results, and proper quality control within the system.

10.4. Exporting and printing reports

The **Exporting and Printing Reports** section describes the options available for saving and distributing reports generated in Miraspec Flow. Reports can be exported or printed for documentation, sharing, or archival purposes.

After opening a report in the report viewer, users can export the document to a local storage location. Reports are exported in **PDF format**, which preserves the layout, graphical elements, and metadata contained in the report. Exported reports can be stored for record keeping or shared with other users and external stakeholders.

In addition to exporting, users can also print reports directly from the report viewer using the standard printing functionality of the operating system. This allows users to produce physical copies of reports when required for documentation, review, or regulatory compliance.

Providing options to export and print reports ensures that analytical results can be easily documented and distributed in a consistent and accessible format.

11. Administration (Admin page)

11.1. Admin page - control centre of the system

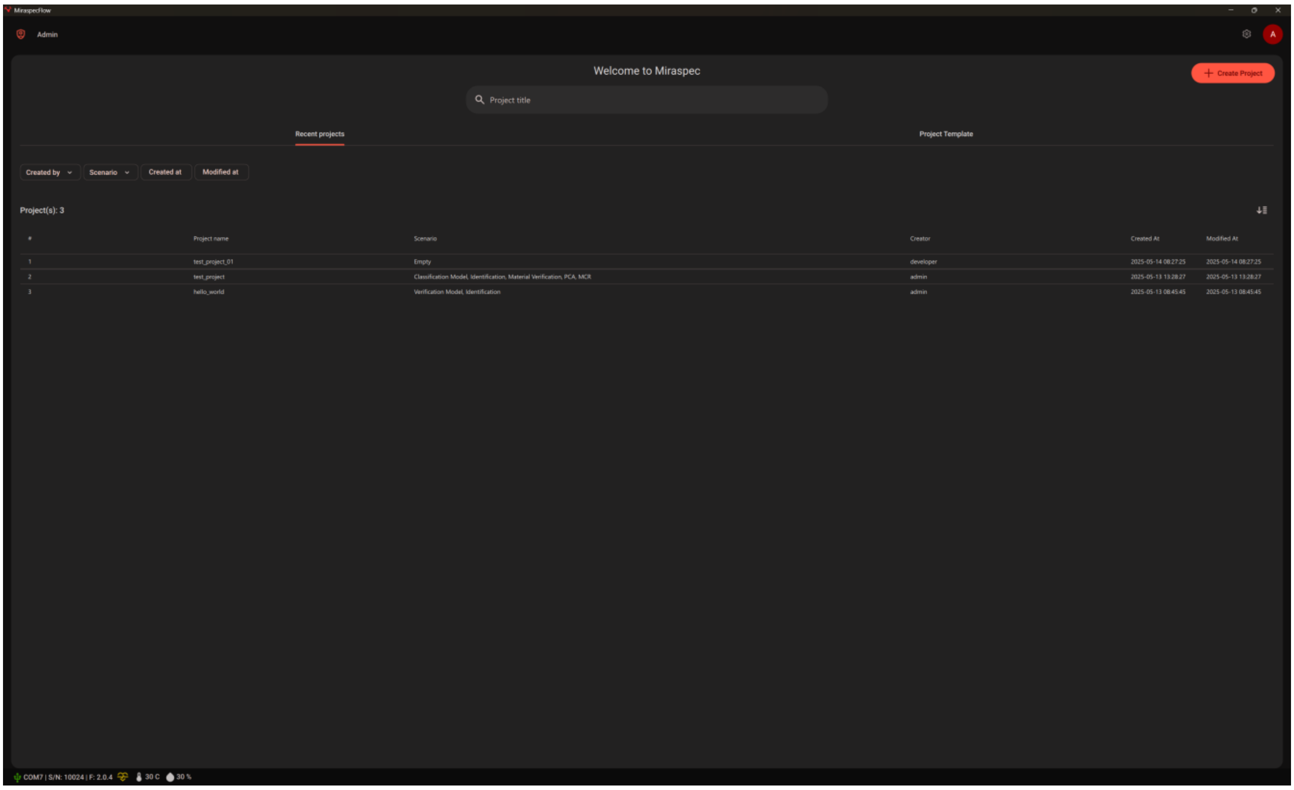
The Admin page functions as the central management interface of the system. It provides administrators with tools to configure, organize, and maintain all key elements required for the operation of the software. Through this interface, users with administrative privileges can manage system data, create and organize projects, maintain spectral libraries, configure connected devices, and administer user accounts and permissions.

From the Admin page, administrators can create, modify, or delete projects, ensuring that experimental data and analyses are organized according to specific applications or research activities. The interface also allows management of spectral libraries, including uploading new reference spectra, updating existing entries, and organizing library structures used for material identification.

In addition, the Admin page provides controls for device management, enabling the configuration and monitoring of connected spectrometers or other supported hardware components. Administrators can also manage user accounts, assign roles, and define access permissions to ensure that users have appropriate levels of access to system features and data.

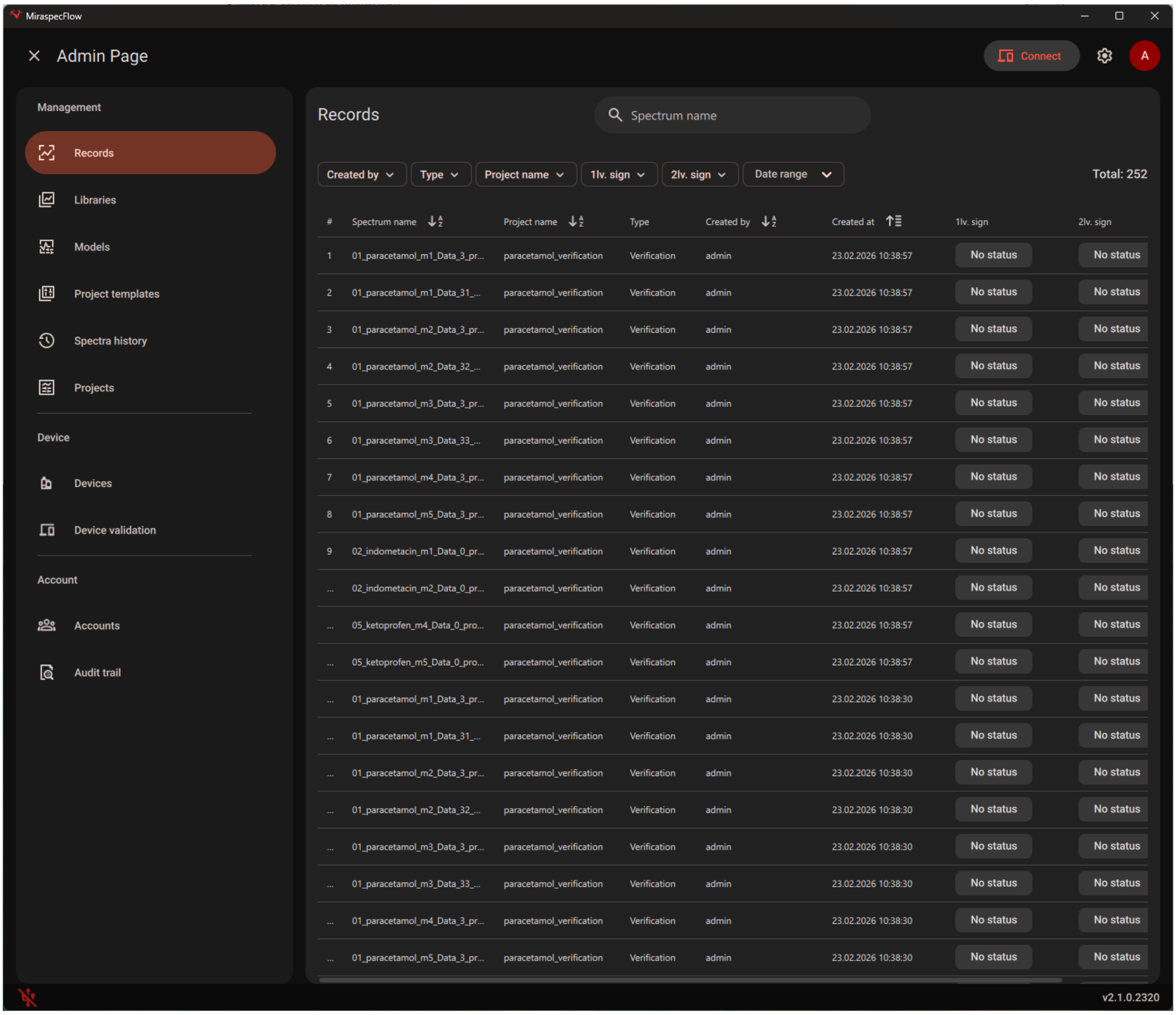
Overall, the Admin page serves as the central control point for system configuration, resource management, and user administration, ensuring that the platform operates in a structured and secure manner.

Upon logging in into administrator account the following page is shown:



It shows two tabs with the list of projects and the list of project templates

Click on the shield icon to access the admin page.



Features available from the Admin Page:

- Records — working with internal records.
- Library Management — creating new libraries, importing/exporting, and editing content.
- Models — adding signatures to reports.
- Project Templates - viewing project templates.
- Spectra history — viewing the history of collected spectra.
- Projects — viewing projects and changing their names.
- Devices — managing libraries on connected devices.
- Device validation — viewing validation status and results for the device.
- Accounts — creating, editing, and managing user accounts
- Audit trail — system activity log.

11.2. User administration

The User Administration section provides tools for managing user accounts and access permissions within the Miraspec Flow system. These features allow administrators to control who can access the software and what actions each user is allowed to perform.

Administrators can create and manage user accounts, assign roles, and configure permissions to ensure that users have appropriate levels of access to system functions and data. Proper management of user accounts helps maintain system security, data integrity, and traceability of actions performed within the software.

The following sections describe how to manage user accounts and configure roles and permissions.

11.2.1. Accounts

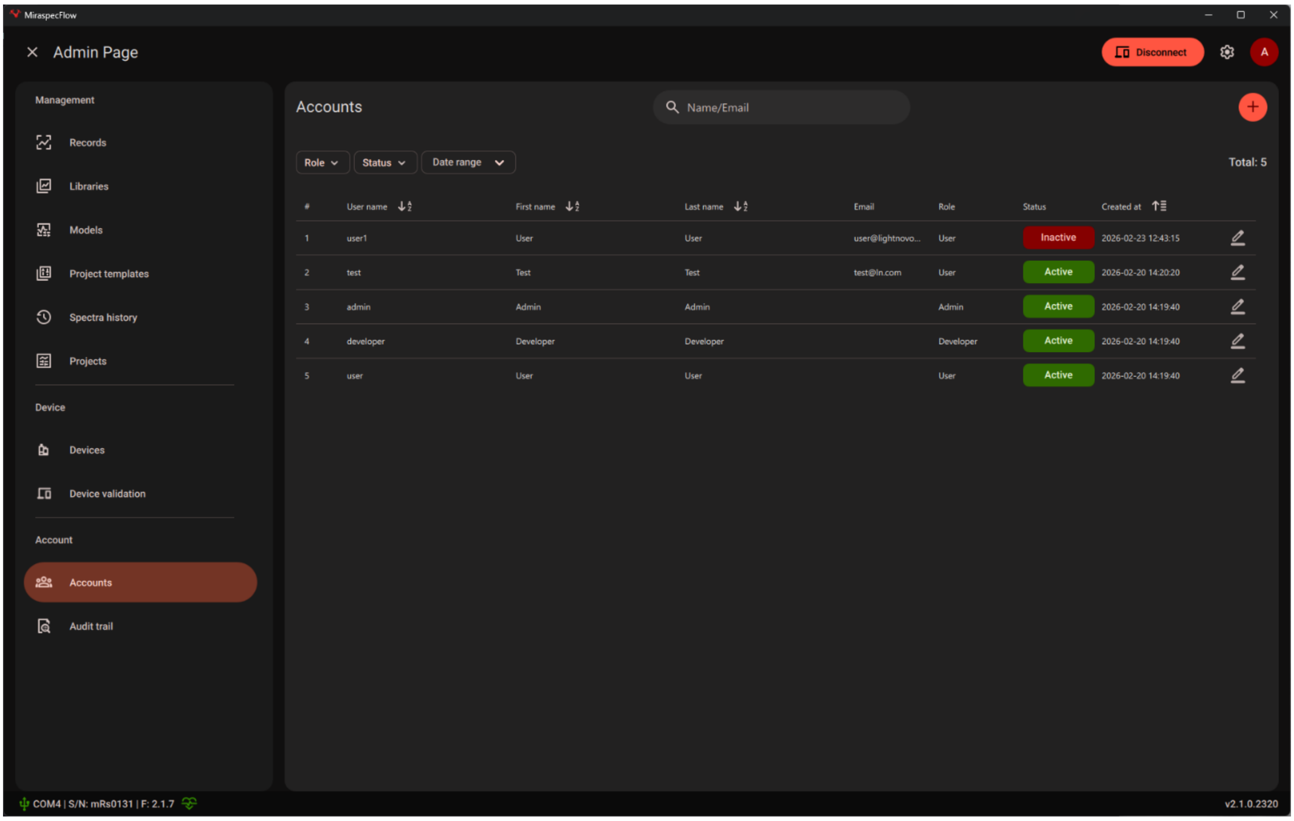
The **Accounts** section allows administrators to manage user accounts within the Miraspec Flow system. User accounts control access to the software and determine which system functions are available to each user.

Administrators can create new accounts, modify existing user information, and manage account status. Each account contains information such as the user name, role, and account status.

When creating a new user account, the administrator must provide the required user information and assign an appropriate role. The role determines the level of access granted to the user and the actions they are permitted to perform within the system.

User accounts can also be updated if changes are required, such as modifying user details or resetting a password. If a user no longer requires access to the system, the account can be deactivated. Deactivated accounts remain in the system for record-keeping purposes but cannot be used to log in.

Proper management of user accounts helps ensure system security, controlled access to data, and traceability of user actions.



11.2.2. Roles and permissions

The **Roles and Permissions** section defines the access rights associated with different user roles in Miraspec Flow. Roles determine which system features a user can access and which actions they are authorized to perform.

The system supports several predefined roles with different levels of access. Typical roles include **Administrator**, **Developer**, and **User**.

- **Administrator**
  Administrators have full access to the system. They can manage user accounts, configure system settings, administer projects and libraries, and perform device management tasks. Administrators are responsible for maintaining system operation and managing access control.
- **Developer**
  Developers have extended access to advanced system functions. In addition to standard user operations, developers can configure scenarios, create or modify analytical models, and manage spectral libraries used for analysis.
- **User**
  Standard users perform routine tasks such as acquiring spectra, processing data, running analyses, and generating reports according to predefined workflows. Users typically cannot modify system configuration, create new scenarios, or manage user accounts.

Assigning appropriate roles ensures that users have access only to the functions required for their tasks, which helps maintain system integrity and proper workflow control.

11.3. Data management

The Data Management section provides tools for organizing and maintaining the data resources used within Miraspec Flow. These resources include spectral libraries, analytical models, and stored measurement data.

Administrators can use the data management functions to manage reference spectra, maintain model libraries, and review historical spectral data generated during experiments. Proper data management helps ensure that analytical resources remain organized, accessible, and consistent across different projects and users.

The following sections describe how to manage spectral libraries, analytical models, and stored spectra within the system.

11.3.1. Library management

The **Library Management** section provides tools for creating, organizing, and maintaining spectral libraries used within Miraspec Flow. Spectral libraries contain reference spectra that can be used for material identification, comparison, and model development.

Administrators can create new libraries, modify existing libraries, and manage the spectra stored within them. Libraries may contain reference spectra obtained from experimental measurements or imported from external spectral databases.

Typical library management operations include:

- creating new spectral libraries
- editing library information
- importing or exporting libraries
- adding spectra to an existing library
- removing spectra from a library

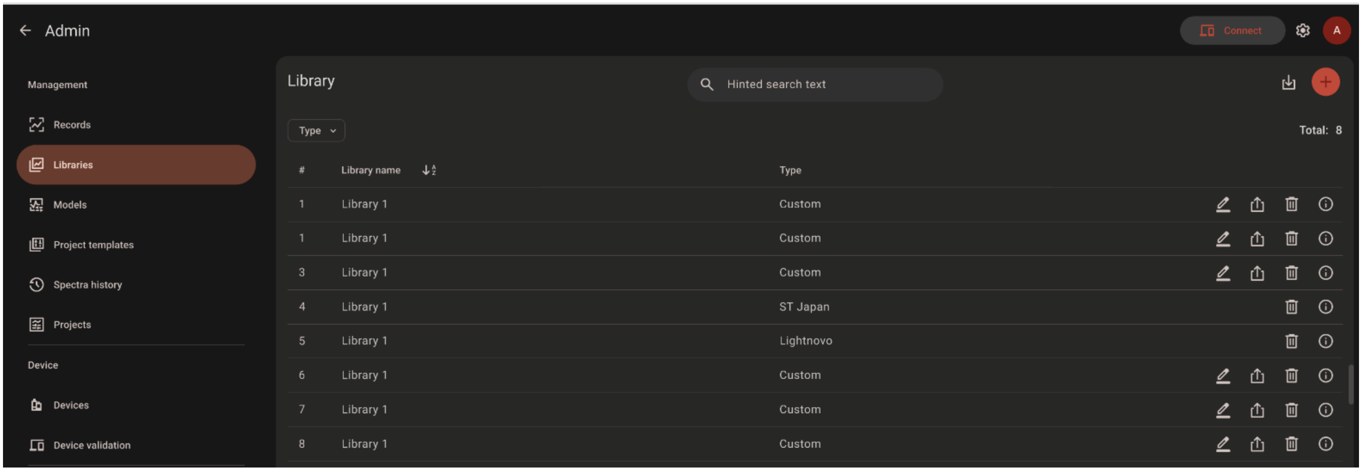
Libraries can also be organized into categories or groups to facilitate easier navigation and selection during spectral analysis.

Users can view detailed information about the spectra stored in a library, including metadata such as spectrum name, chemical identifier (for example CAS number), and other associated information. Spectra can be renamed, updated, or removed when necessary to maintain the accuracy and relevance of the library.

Proper management of spectral libraries helps ensure reliable identification results and supports consistent analytical workflows across different projects.

Through this tab, users can organize internal and external libraries, apply search and filtering, and access spectrum information for further analysis.

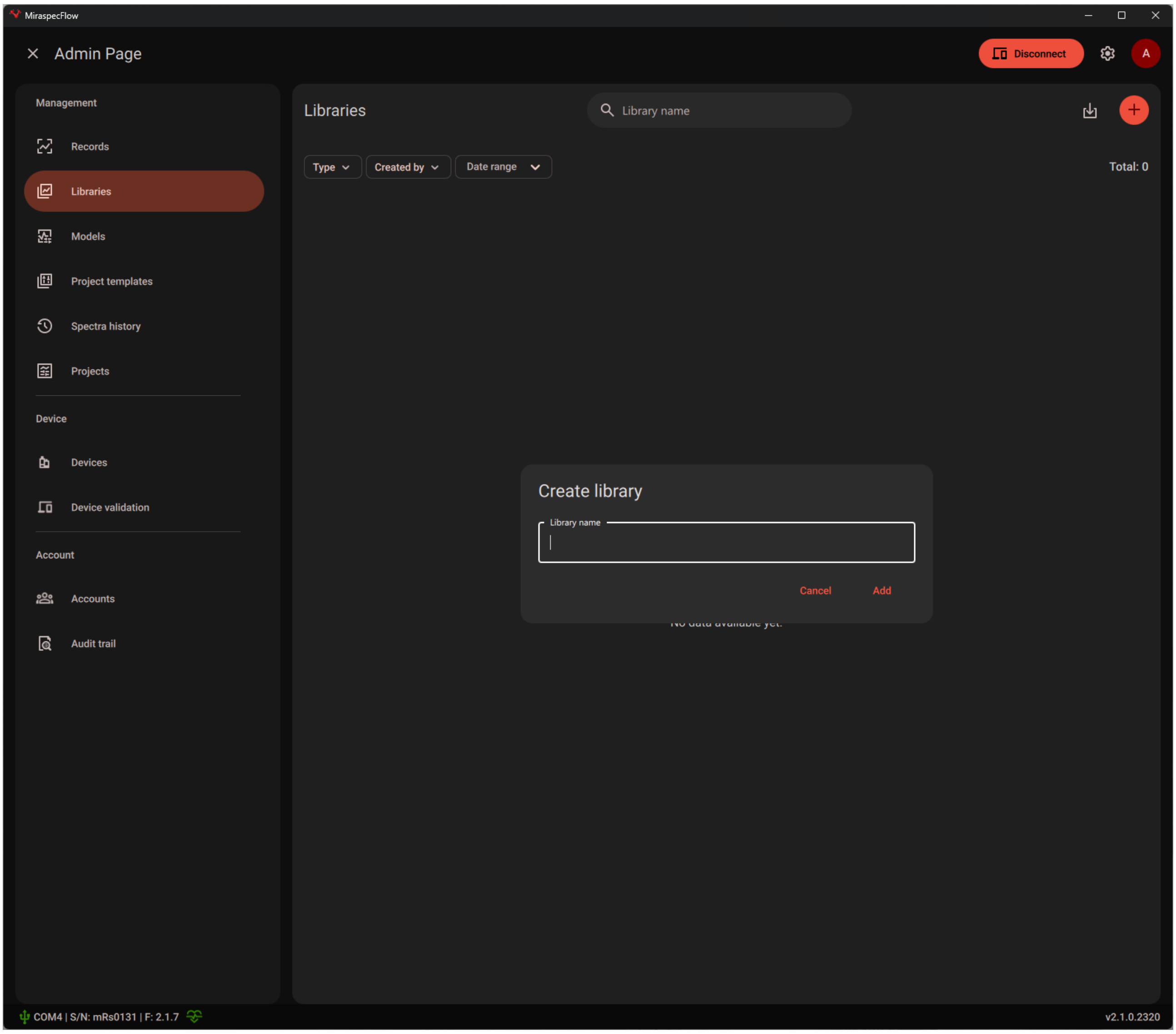
This functionality ensures efficient handling of spectral data and provides a foundation for accurate identification, comparison, and use of libraries in projects.



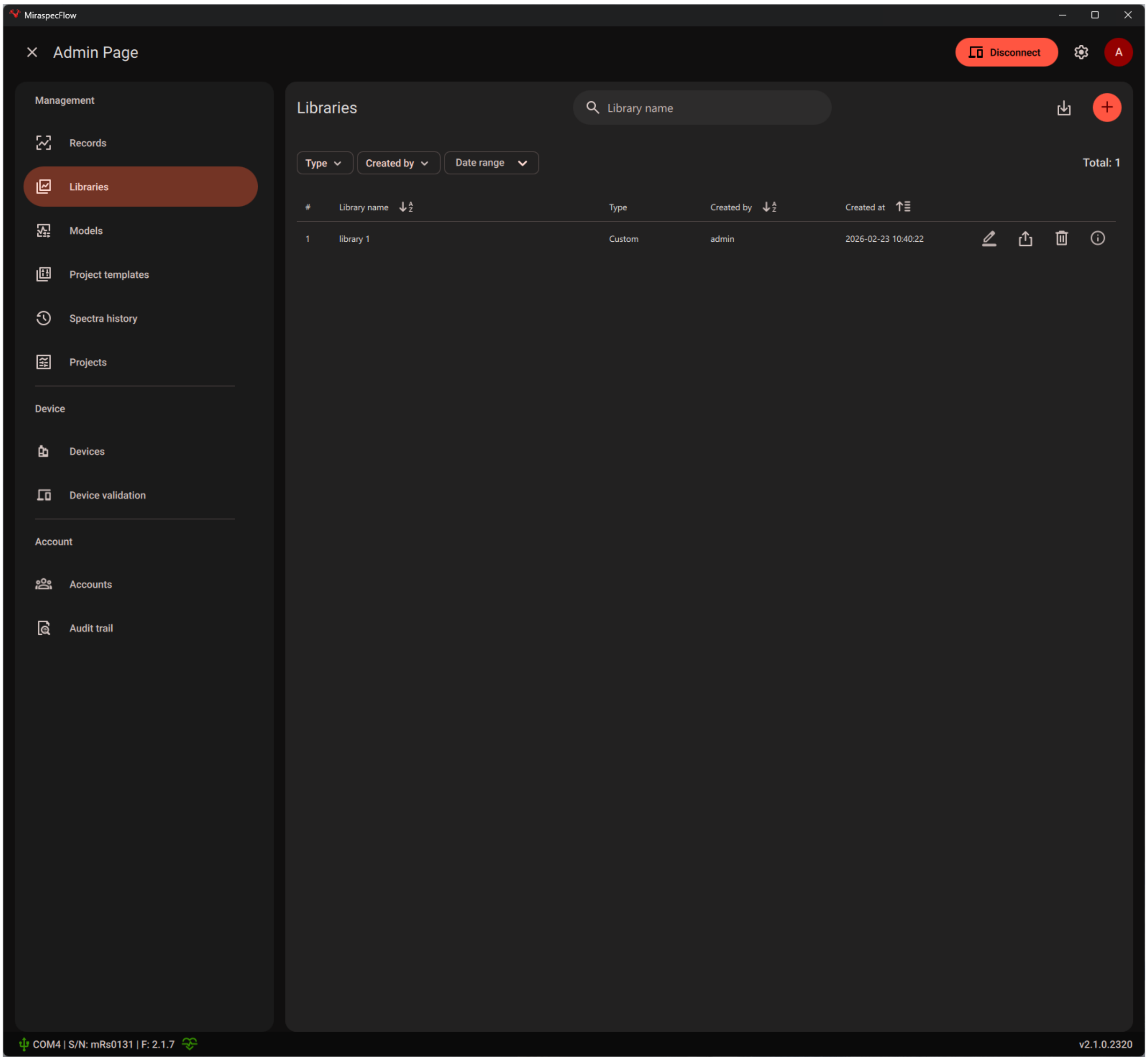
Core functionality

- Create library – add a new library manually.
- Edit library – update the library name or attributes.
- Import library – upload an existing library into the system.
- Export library: - export library to the device or PC
- Delete library – with confirmation via the Delete? dialog.
- View library details (Spectra)

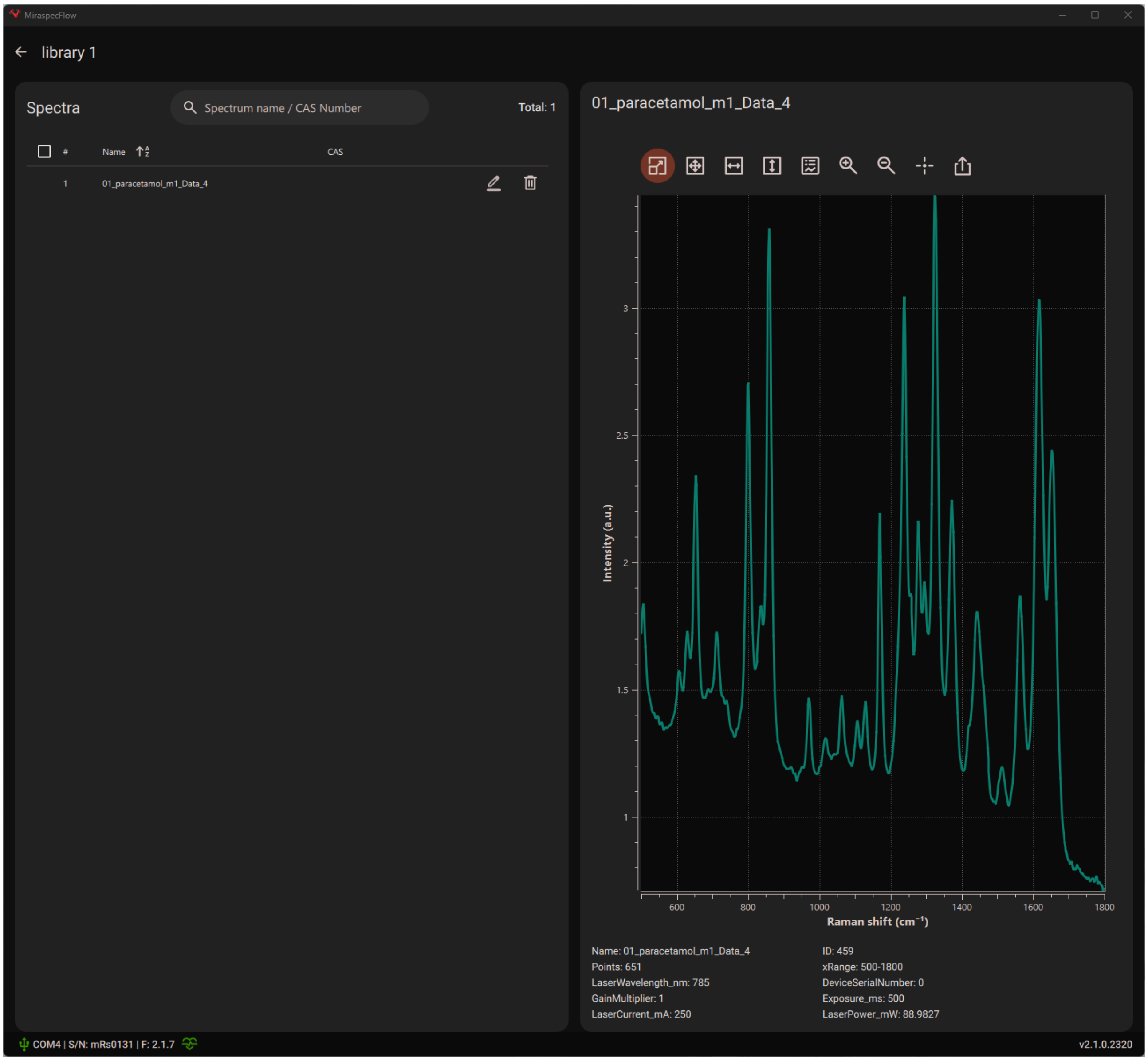
Create library – to create the library click on plus icon.



Then the user can eventually add spectra to the library while working on a particular project.

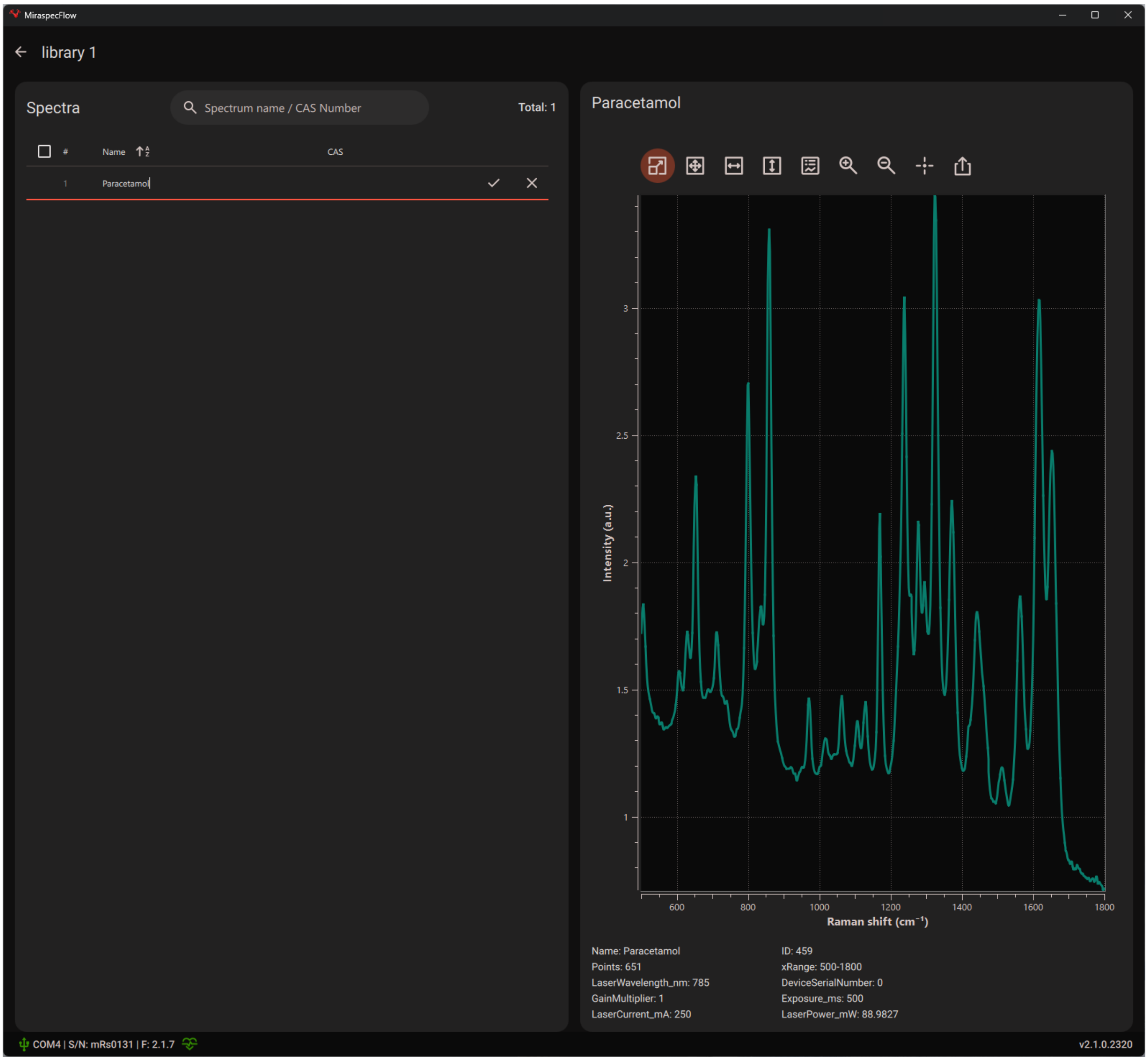


Click on info button to view the spectra in the library.



Here you can rename the spectra in the library as well as remove the spectra from the library.

Example on how to rename the spectra:



Search and filter

The user can search libraries by name and apply filters for easier navigation within the list.

Available tools:

- Search bar – enter a library name to find it in the table.
- Filter chips – filter libraries by name and by type (Custom, Lightnovo, STJapan). Clicking a chip opens a dropdown list where one or multiple options can be selected.
- Reset button – clears all applied filters and shows the full list of libraries.
- Sorting – change the order of display by library name (ascending or descending).

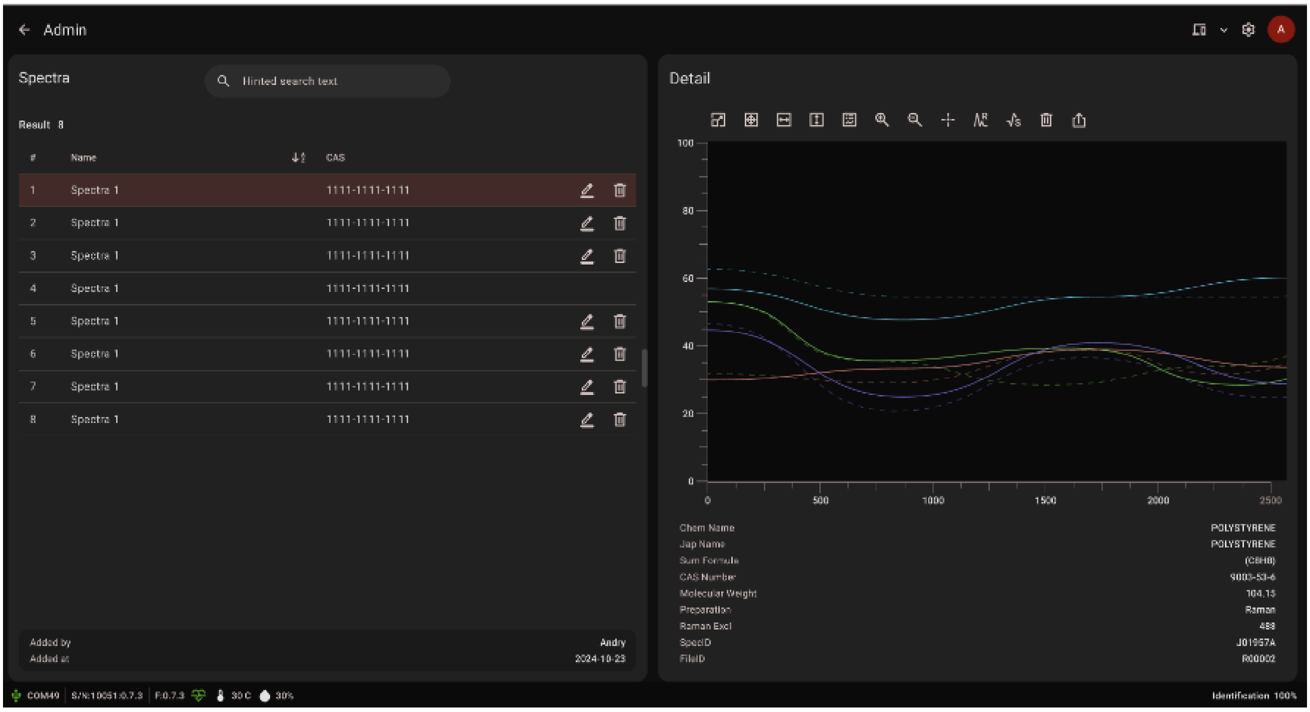
Goal: provide quick search and convenient navigation through libraries in the table.

View library details (Spectra)

The user can view detailed information about a library by clicking the Info button in the Library management table row.

This action opens the Spectra page, which displays:

- a table with all spectra contained in the library,
- the ability to edit a spectrum name and CAS number, or delete a spectrum,
- search, filtering, and sorting tools,
- additional library metadata (creator, creation date) displayed below the table,
- an interactive spectra plot occupying approximately 50% of the screen,
- a metadata block below the graph that updates when a spectrum is selected in the table.



11.3.2. Models

The **Models** section provides administrative tools for managing analytical models stored in the Miraspec Flow system. Models are used to interpret spectral data and may include verification, classification, calibration, PCA, or MCR models created within different projects.

Administrators can view the list of available models and access detailed information about each model, including its name, type, associated project, creator, and creation date. This section allows administrators to maintain an organized repository of models used for analysis across the system.

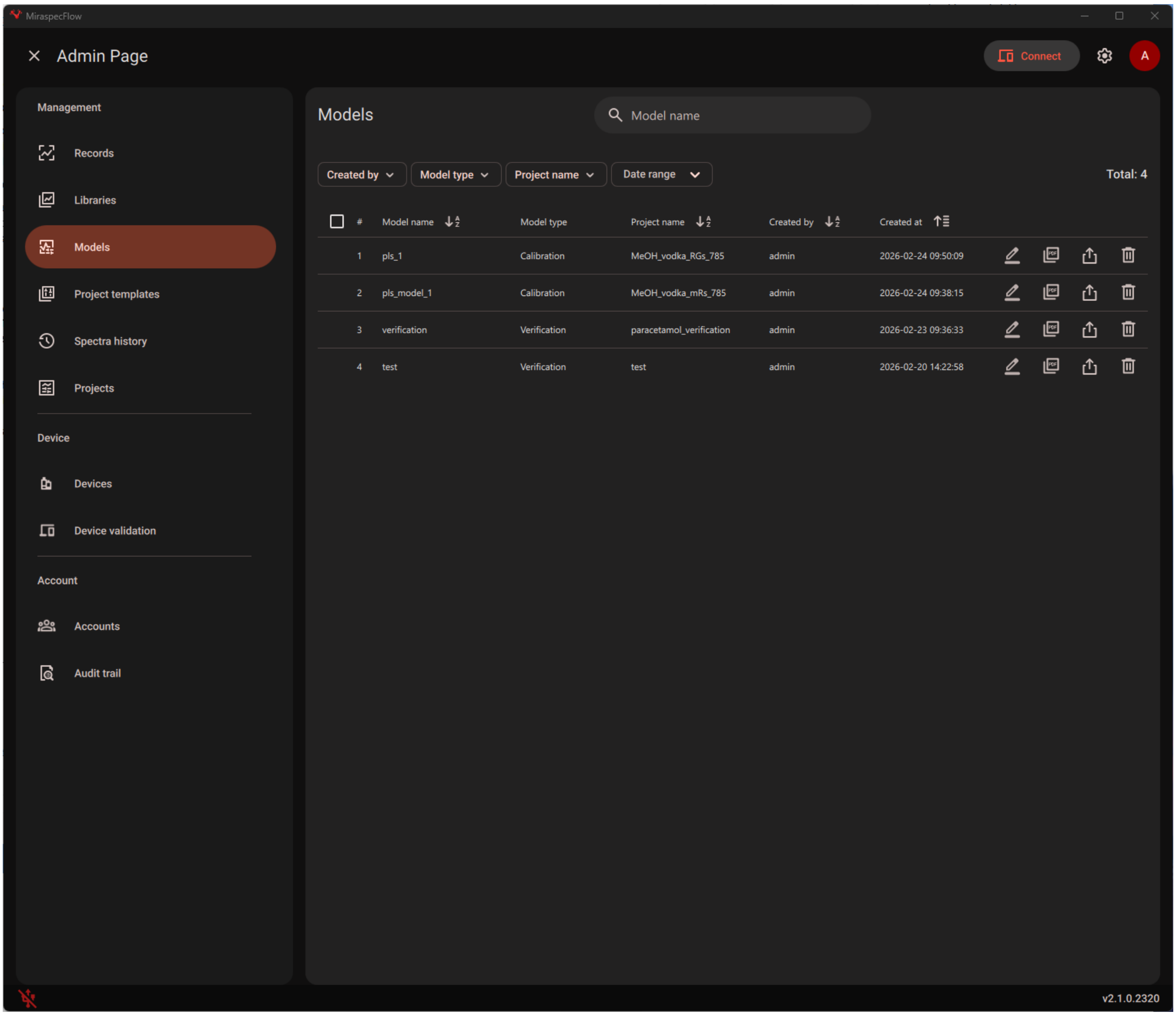
Typical model management operations include:

- viewing model details
- renaming models
- exporting models for external use or backup
- removing outdated or unused models

Detailed information about a model can be opened in a report view, which may include model parameters, training results, and evaluation metrics. These reports can be exported or printed for documentation purposes.

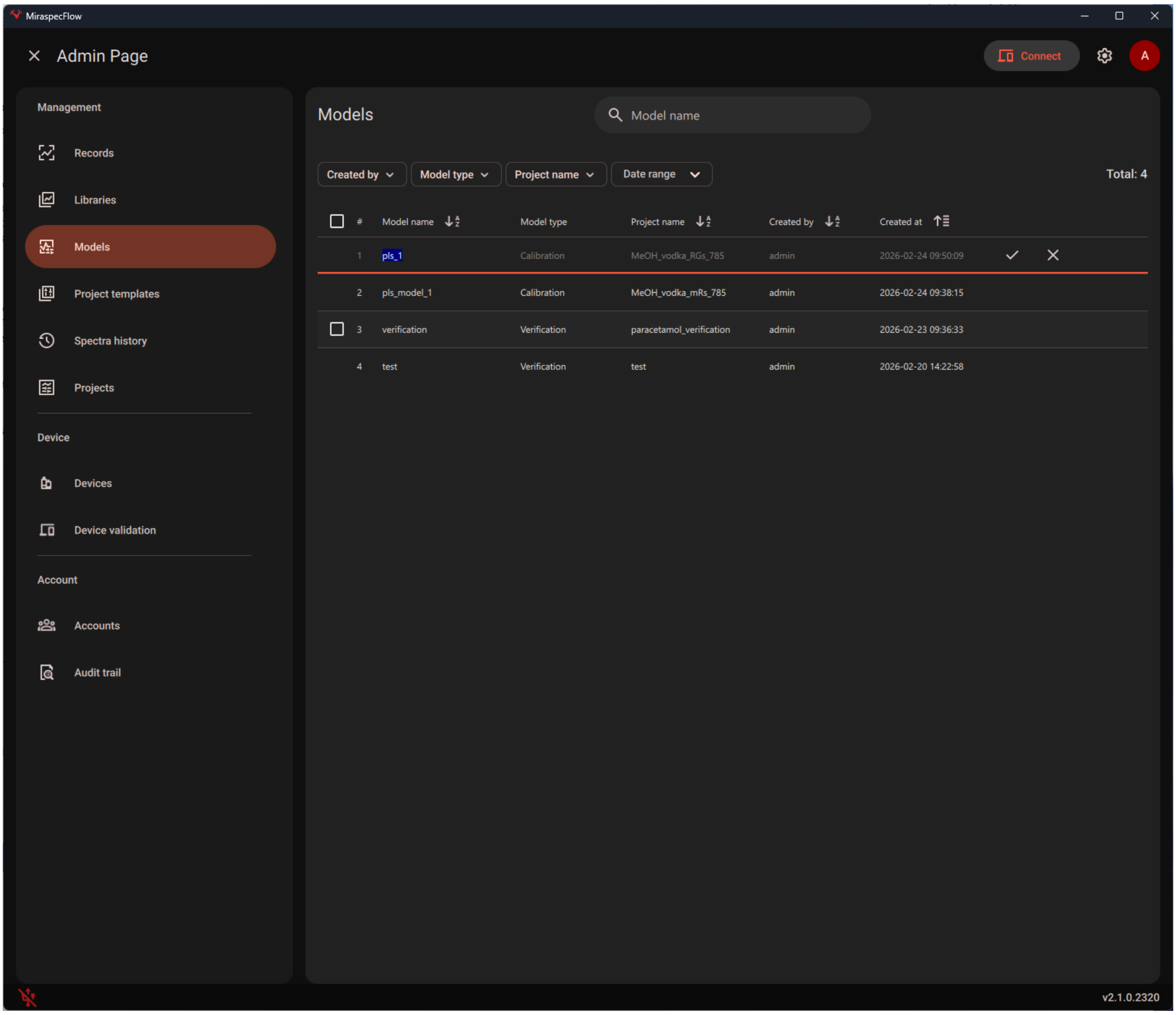
Search, filtering, and sorting tools are available to help users quickly locate models based on criteria such as model type, project name, author, or creation date.

Proper management of analytical models ensures that only validated and up-to-date models are available for use in spectral analysis workflows.

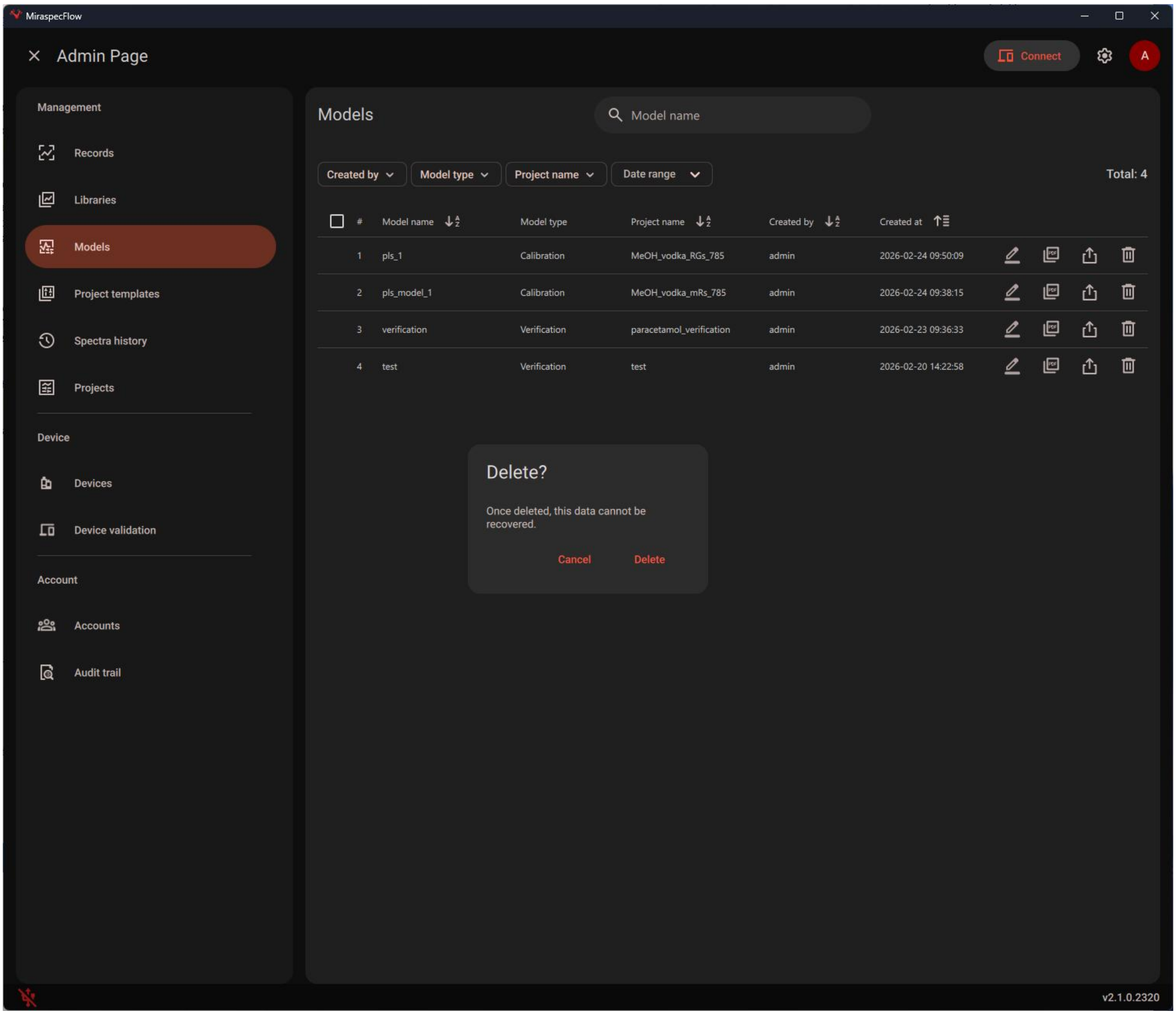


Core functionality:

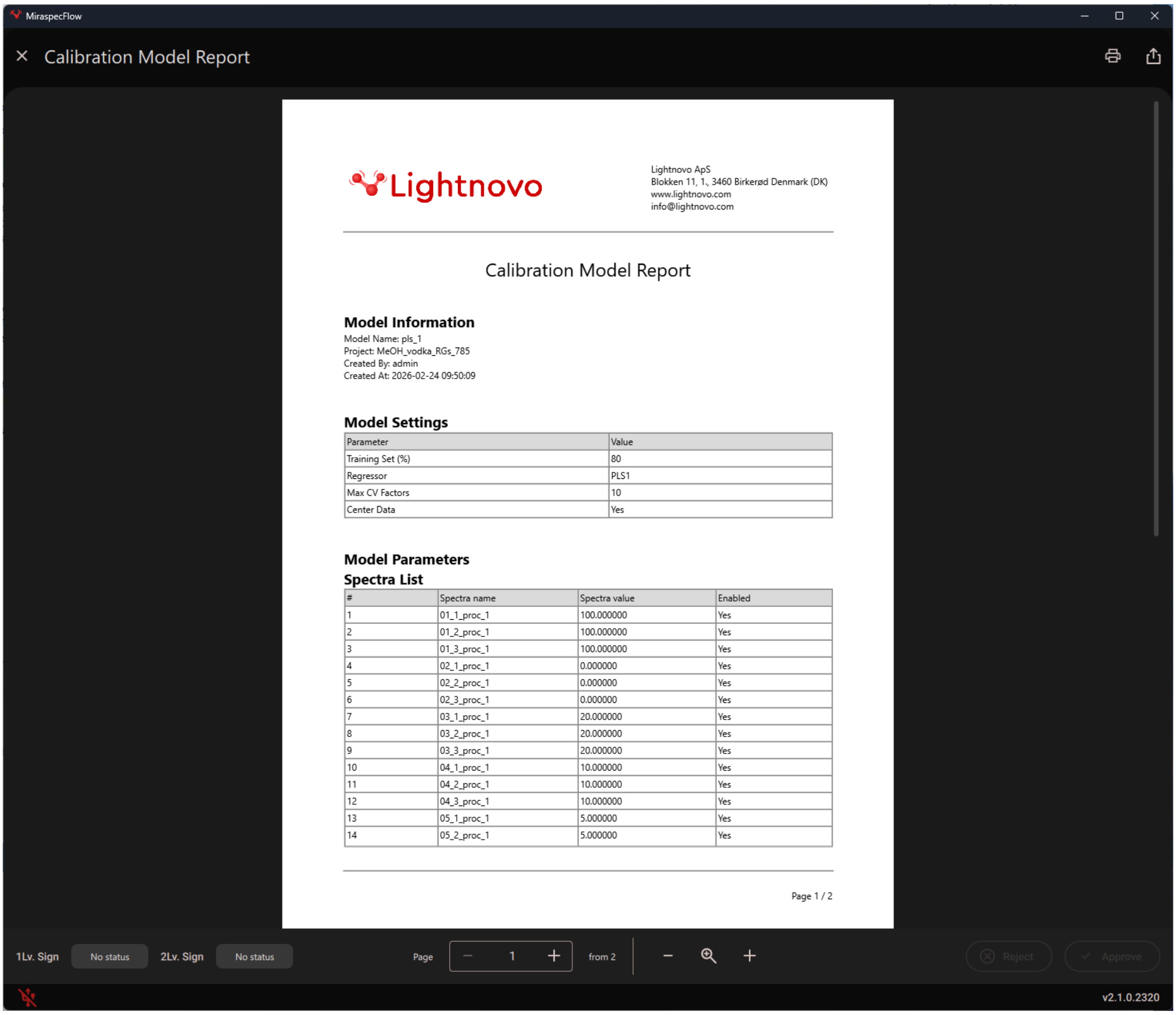
- Edit model – change the model name.



- Delete model – permanently remove the model from the system.



- View model – open the PDF file with detailed information, export or print it.



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Calibration Model Report

Model Information

Model Name: pls_1
Project: MeOH_vodka_RGs_785
Created By: admin
Created At: 2026-02-24 09:50:09

Model Settings

Parameter	Value
Training Set (%)	80
Regressor	PLS1
Max CV Factors	10
Center Data	Yes

Model Parameters

Spectra List

#	Spectra name	Spectra value	Enabled
1	01_1_proc_1	100.000000	Yes
2	01_2_proc_1	100.000000	Yes
3	01_3_proc_1	100.000000	Yes
4	02_1_proc_1	0.000000	Yes
5	02_2_proc_1	0.000000	Yes
6	02_3_proc_1	0.000000	Yes
7	03_1_proc_1	20.000000	Yes
8	03_2_proc_1	20.000000	Yes
9	03_3_proc_1	20.000000	Yes
10	04_1_proc_1	10.000000	Yes
11	04_2_proc_1	10.000000	Yes
12	04_3_proc_1	10.000000	Yes
13	05_1_proc_1	5.000000	Yes
14	05_2_proc_1	5.000000	Yes

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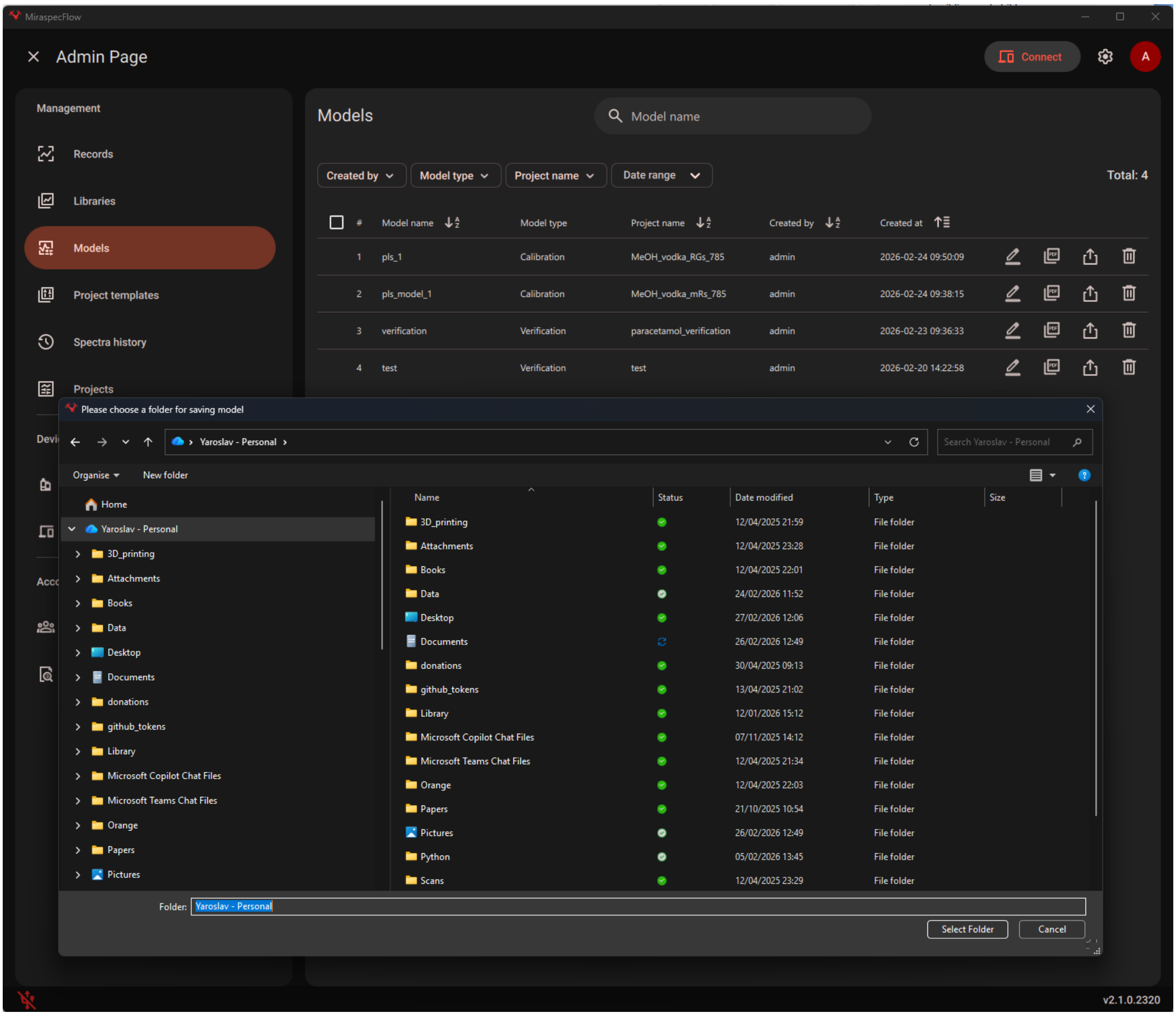
Save model – the model can be saved on the local drive by clicking up arrow icon



Search, sorting and filter

The user can search models by name and apply filters for easier navigation within the list.

Available tools:

- Search bar – enter a model name to find it in the table.
- Filter chips – filter models by: Model type, Project name, Created by, Date range
- Reset filters – clears all applied filters and shows the full list of models. The button appears only when at least one filter is active.
- Sorting – changes the display order in the table by:Model name, Project name, Created by, Created at (ascending or descending order).

11.3.3. Spectra history

The **Spectra History** section provides tools for viewing and managing the history of spectra acquired or imported into the Miraspec Flow system. This section allows administrators to review previously recorded spectral data and access associated metadata such as spectrum name, device serial number, acquisition date, and other measurement parameters.

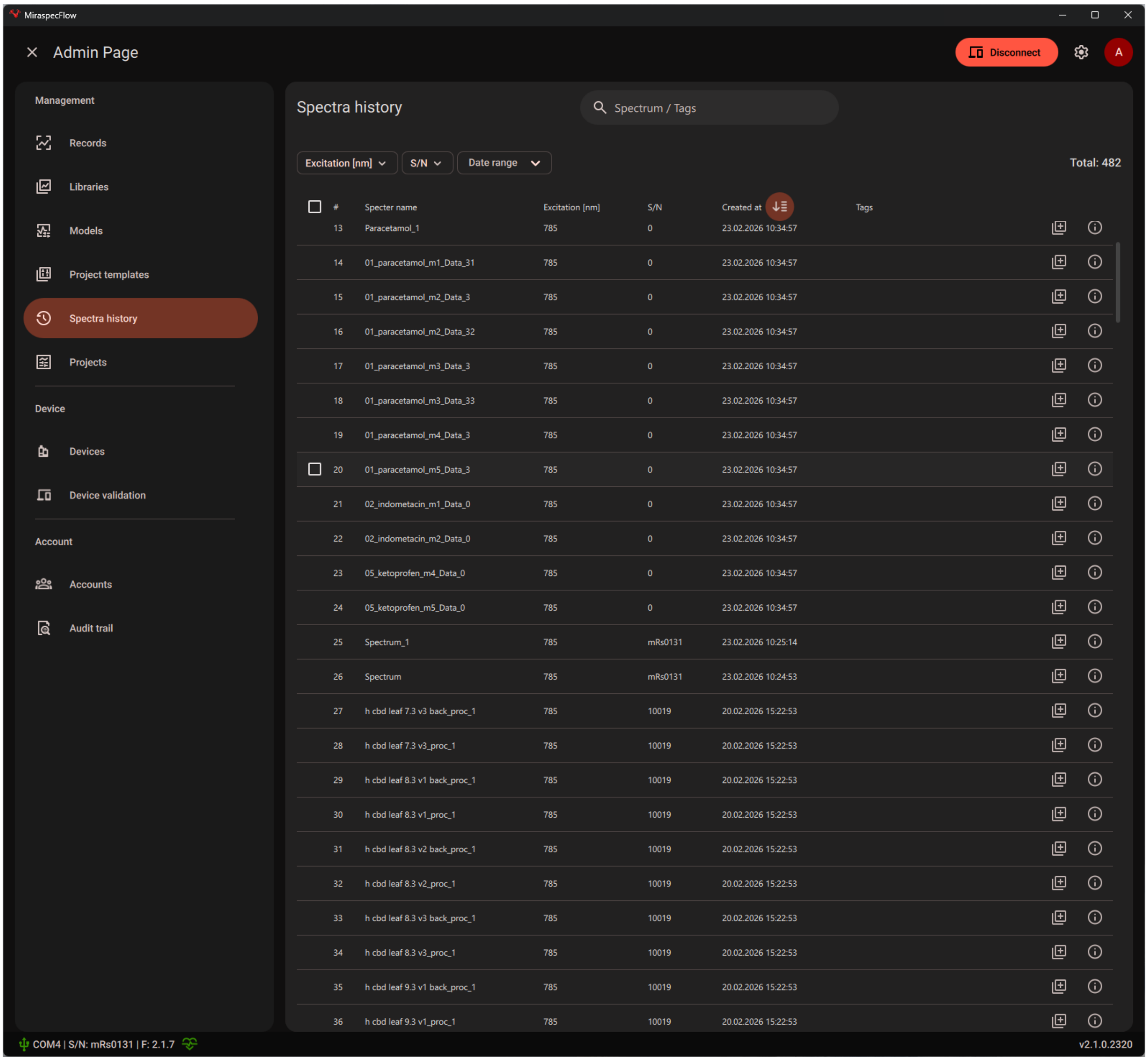
The spectra history provides a centralized record of spectral measurements collected during experiments. This helps users track previously acquired data and reuse spectra for further analysis, model development, or library creation.

Typical operations available in this section include:

- viewing stored spectra and associated metadata
- previewing spectral data in graphical form
- exporting spectra to external files
- adding selected spectra to a spectral library
- removing spectra from the history if necessary

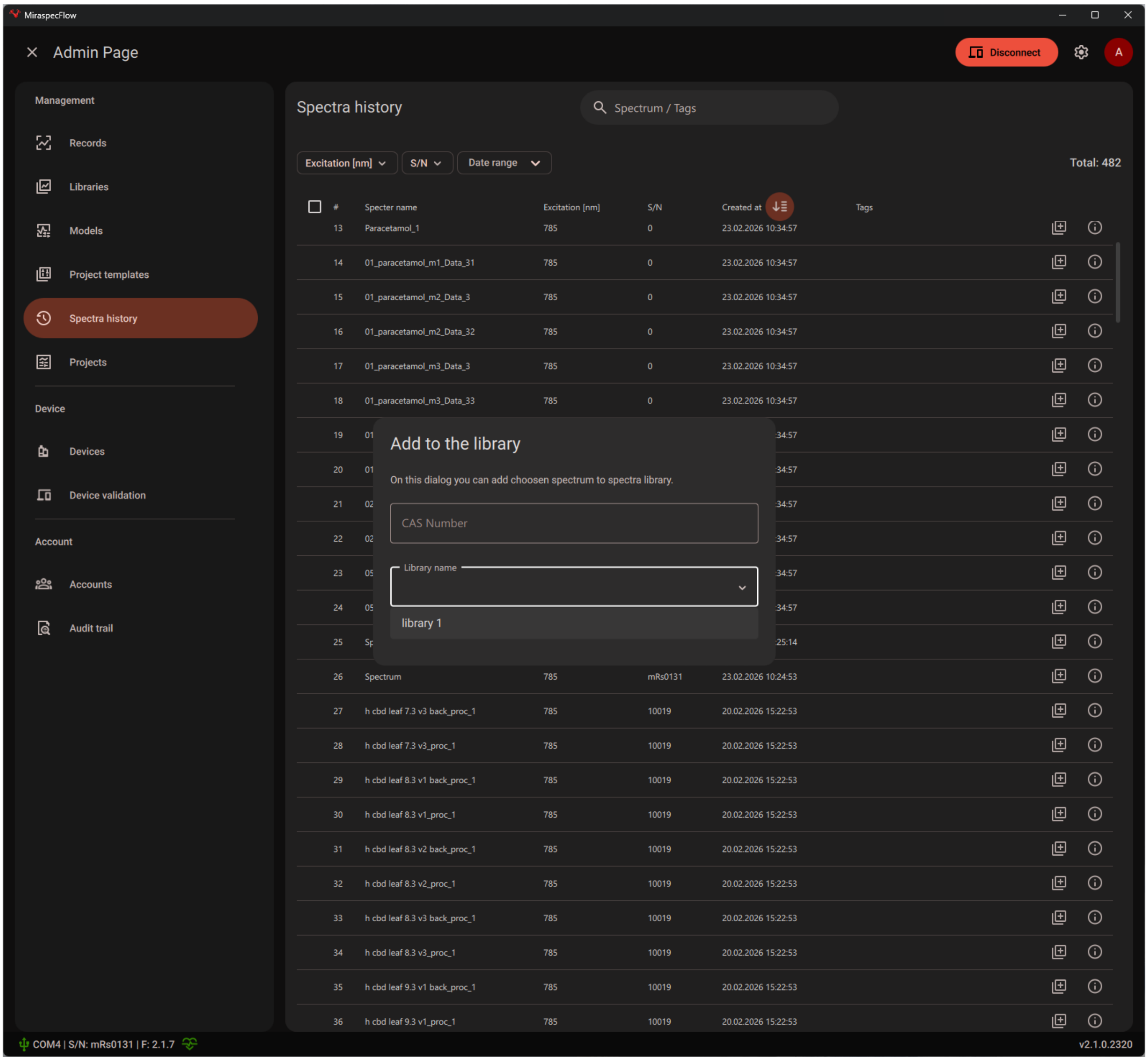
Search, filtering, and sorting tools are available to help users locate specific spectra based on attributes such as spectrum name, acquisition date, or device identifier.

Maintaining a well-organized spectra history allows users to efficiently access previously collected data and supports traceability of spectral measurements across different projects and experiments.



Core functionality

- Add to Library by clicking on plus icon the spectrum can be added to the library. The user should specify library name and CAS number (optional).



By clicking on the i icon the user can preview the spectra.

- Export Spectra

Select the spectrum, then you should be able to save the spectrum on the drive by clicking the icon with up arrow appearing at the bottom of the software window.

- Spectrum Preview

Search, Sorting and Filter

The user can search spectra by name and apply filters for easier navigation within the list.

Available tools:

- Search bar – enter a spectrum name to find it in the table.
- Filter chips – filter spectra by N/m, S/N, and Date range.
- Clicking a chip opens a dropdown list where one or multiple options can be selected.
- Reset filters – clears all active filters and restores the full list of spectra.
- Sorting – changes the display order in the table by Specter name (A–Z / Z–A) or Created at (newest / oldest).

- At the top of the table, the number of found results is displayed, and after resetting filters, Total shows the overall number of spectra.

11.4. Project management

The Project Management section provides administrative tools for organizing and maintaining projects within the Miraspec Flow system. Projects are used to group related measurements, processing configurations, analysis results, and reports associated with specific experimental tasks.

Administrators can create, modify, or remove projects and manage project templates used to standardize measurement workflows. Proper project management helps maintain an organized structure for experimental data and ensures consistency across different users and applications.

The following sections describe how to manage projects and project templates within the system.

11.4.1. Projects

The **Projects** section provides administrative tools for managing projects stored within the Miraspec Flow system. Projects serve as the primary organizational units for experimental work and contain related spectra, processing configurations, models, analysis results, and reports.

Through the Projects interface, administrators can view the list of all projects created in the system and access key information such as the project name, associated scenario, creator, and creation date. This section allows administrators to maintain an organized project structure and manage project ownership when multiple users are working within the system.

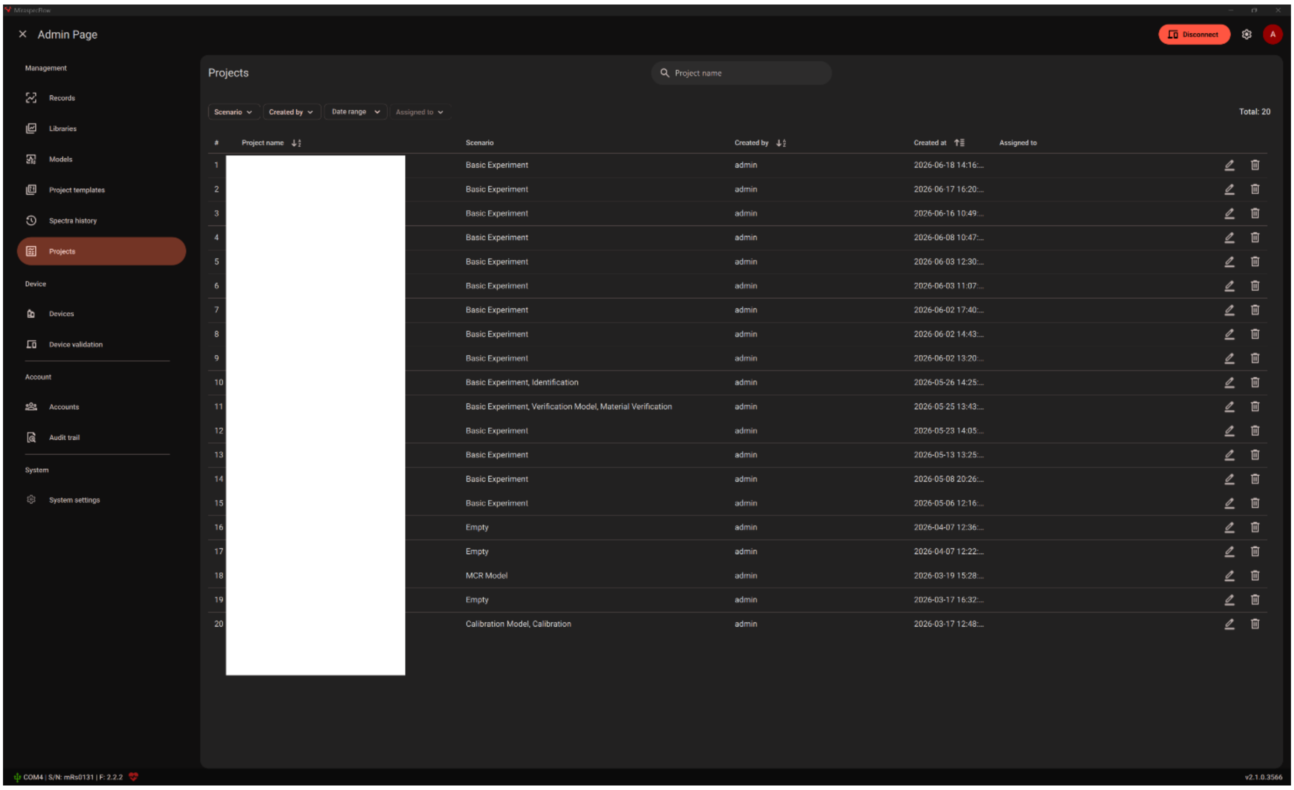
Typical operations available in this section include:

- viewing the list of existing projects
- renaming project titles
- assigning projects to different users
- deleting projects that are no longer required

Search, filtering, and sorting tools are available to help locate projects quickly based on attributes such as project name, scenario, creator, or creation date.

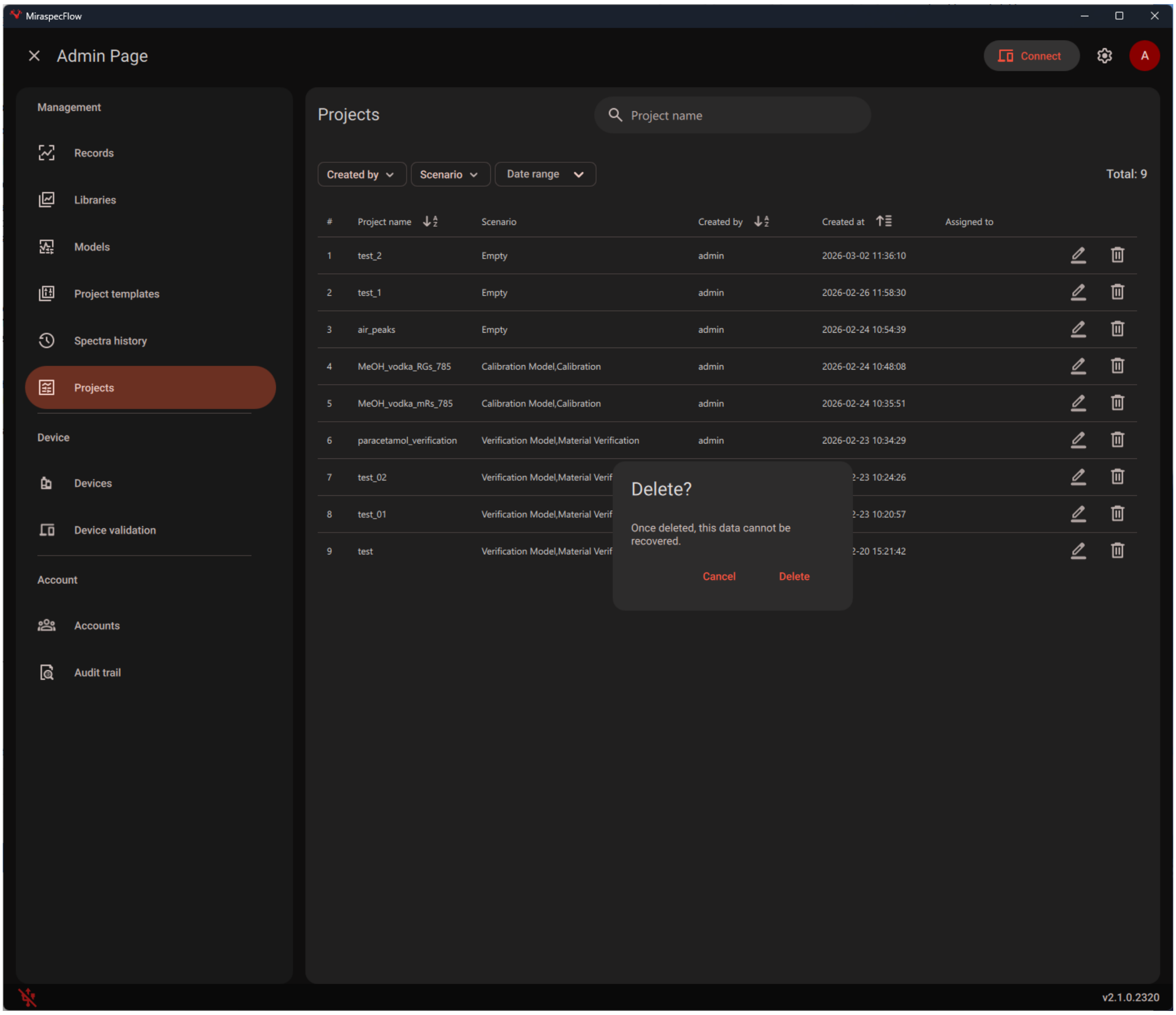
Proper project management helps maintain a clear organization of experimental data and ensures that projects remain accessible and properly assigned to responsible users within the system.

Through this tab, projects in the system can be organized, quickly found, and kept in order. This functionality ensures efficient interaction with projects and provides a foundation for transparent teamwork, control, and further analysis. .



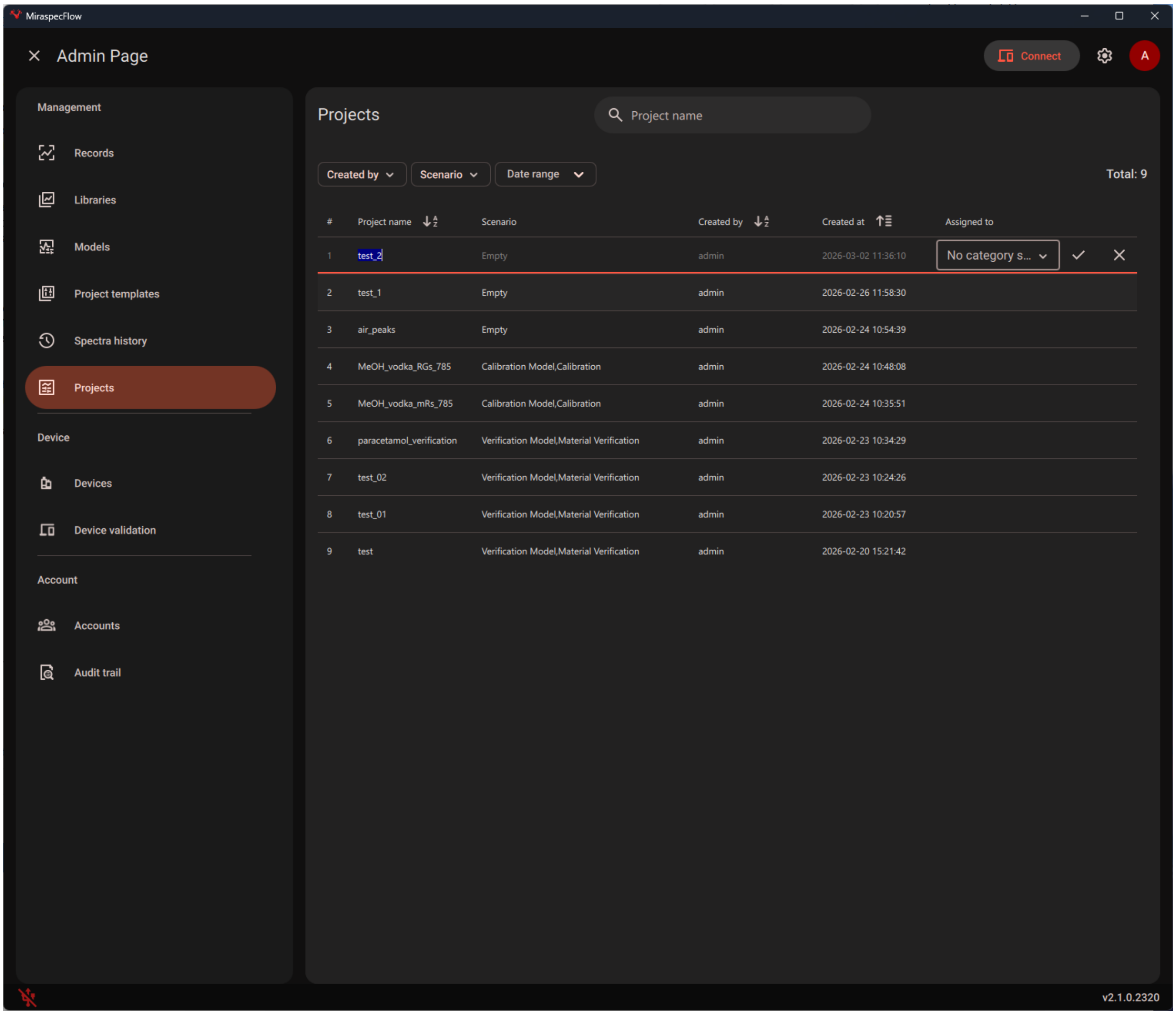
Core functionality

- Delete Project – by clicking on trash bin icon the project can be deleted

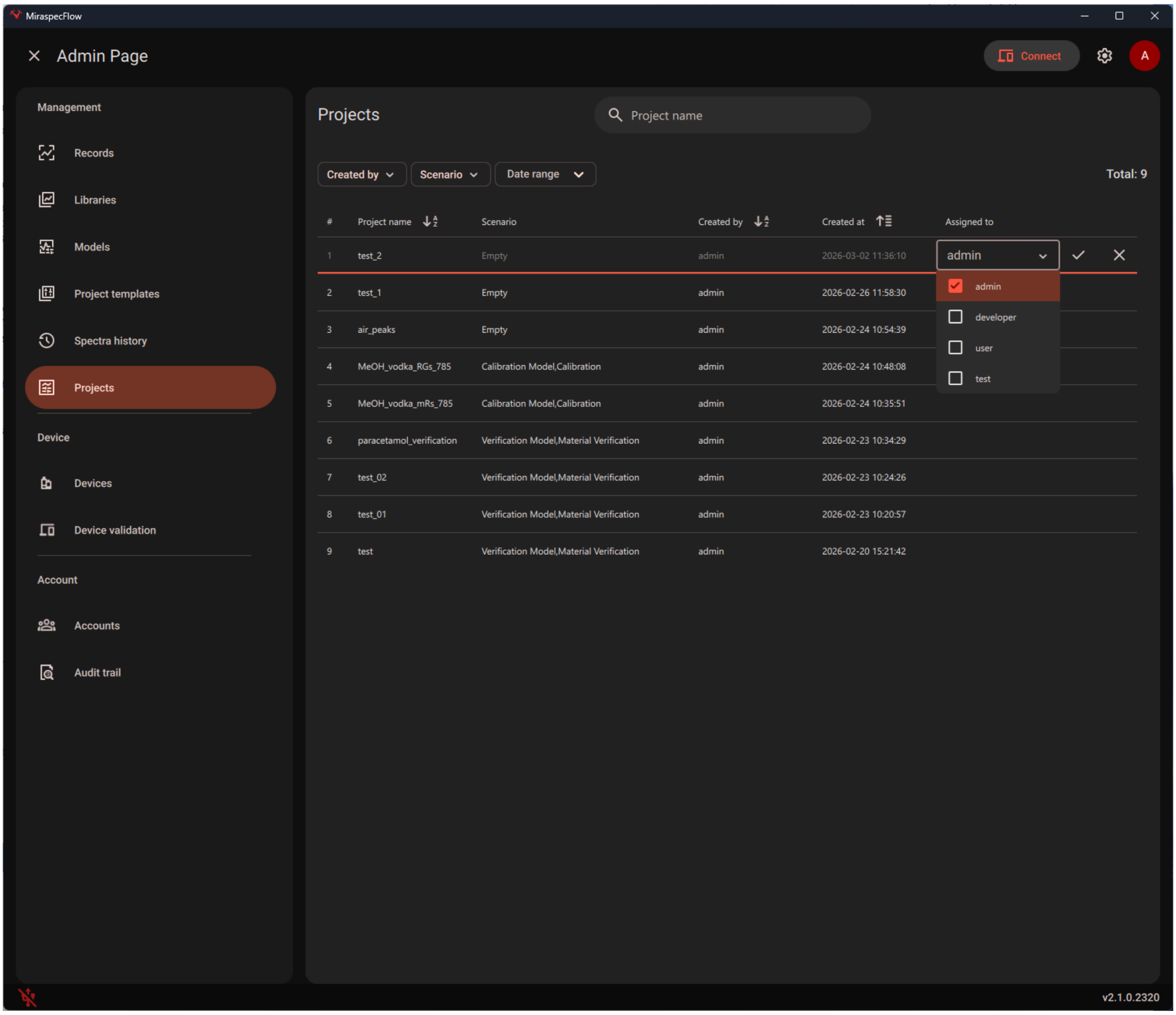


- Assign Project and Rename Project – click on edit icon:

The project can be renamed:



as well as assigned to a specific user:



Click on V to confirm.

Search, Sorting & Filters

The user can search projects by name and apply filters for easier navigation within the list.

Available tools:

- Search bar – enter a project name to find it in the table.
- Filter chips – filter projects by name, scenario, and author (Scenario, Created by, Date range). Clicking a chip opens a dropdown list where one or multiple options can be selected, and a search field is available inside the list.
- Reset filters button – clears all applied filters and shows the full list of projects.
- Sorting – change the display order by Project name,Created by, Created at (ascending or descending).
- Result counter – shows the number of projects found after applying search or filters.

11.4.2. Project templates

The **Project Templates** section provides tools for managing reusable project configurations in Miraspec Flow. Project templates allow users to create new projects based on predefined settings, which helps standardize experimental workflows and reduces the time required to configure new projects.

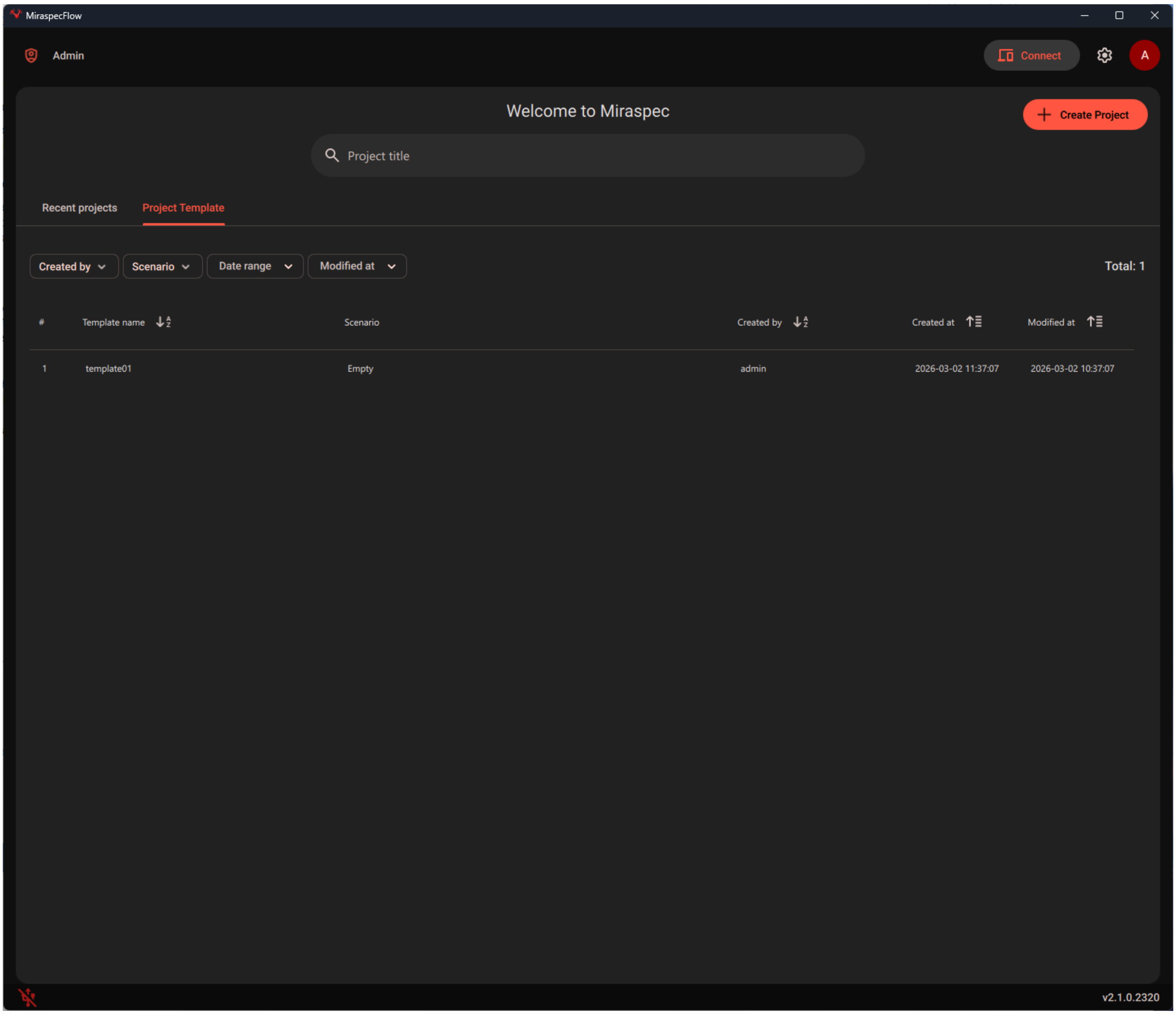
A project template contains the configuration of a project without the associated measurement data. This may include the selected scenario, analysis type, processing settings, and other configuration parameters used during spectral acquisition and analysis.

Administrators can view and manage the list of available project templates and perform typical operations such as:

- creating new project templates from existing projects
- renaming template entries
- viewing template configuration details
- exporting template information for documentation
- deleting templates that are no longer required

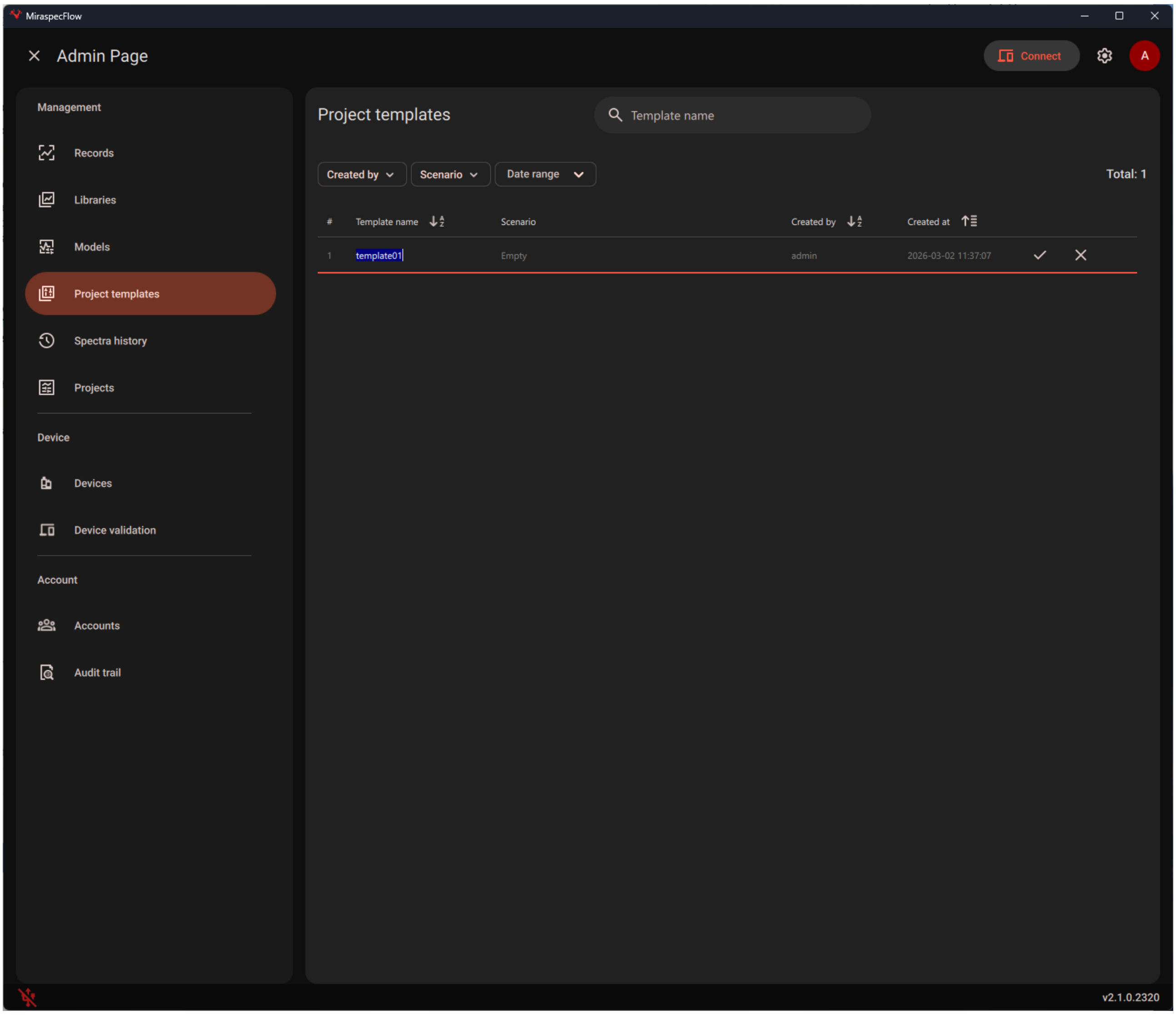
Search, filtering, and sorting tools are available to help users locate templates based on attributes such as template name, scenario, creator, or creation date.

Using project templates ensures consistency across experiments and simplifies the creation of new projects that follow established measurement and analysis procedures.

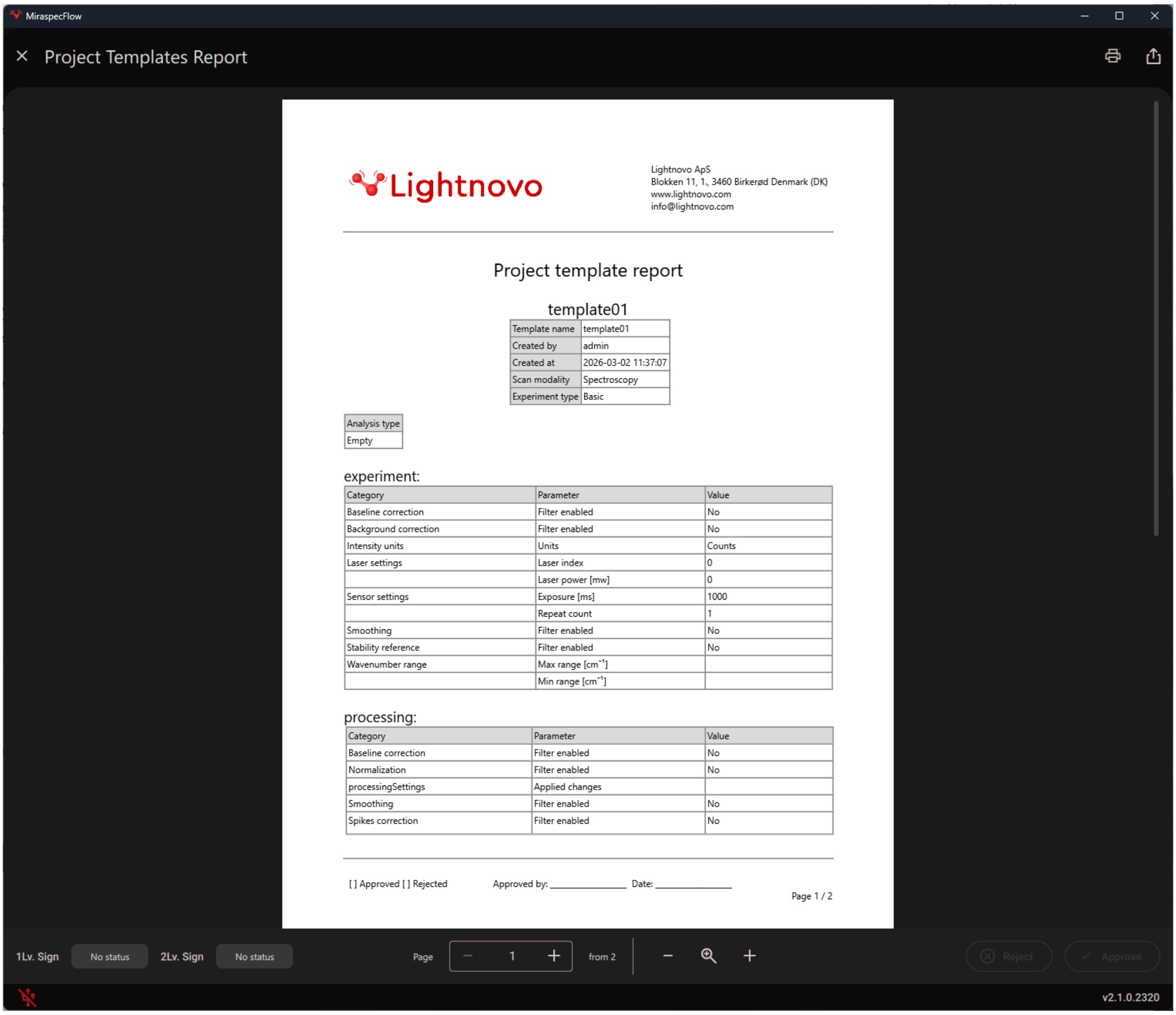


Core functionality

- Edit template name



- View report with settings



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Project template report

template01

Template name	template01
Created by	admin
Created at	2026-03-02 11:37:07
Scan modality	Spectroscopy
Experiment type	Basic

Analysis type
Empty

experiment:

Category	Parameter	Value
Baseline correction	Filter enabled	No
Background correction	Filter enabled	No
Intensity units	Units	Counts
Laser settings	Laser index	0
	Laser power [mw]	0
Sensor settings	Exposure [ms]	1000
	Repeat count	1
Smoothing	Filter enabled	No
Stability reference	Filter enabled	No
Wavenumber range	Max range [cm^{-1}]	
	Min range [cm^{-1}]	

processing:

Category	Parameter	Value
Baseline correction	Filter enabled	No
Normalization	Filter enabled	No
processingSettings	Applied changes	
Smoothing	Filter enabled	No
Spikes correction	Filter enabled	No

[ ] Approved [ ] Rejected Approved by: _____________ Date: _____________

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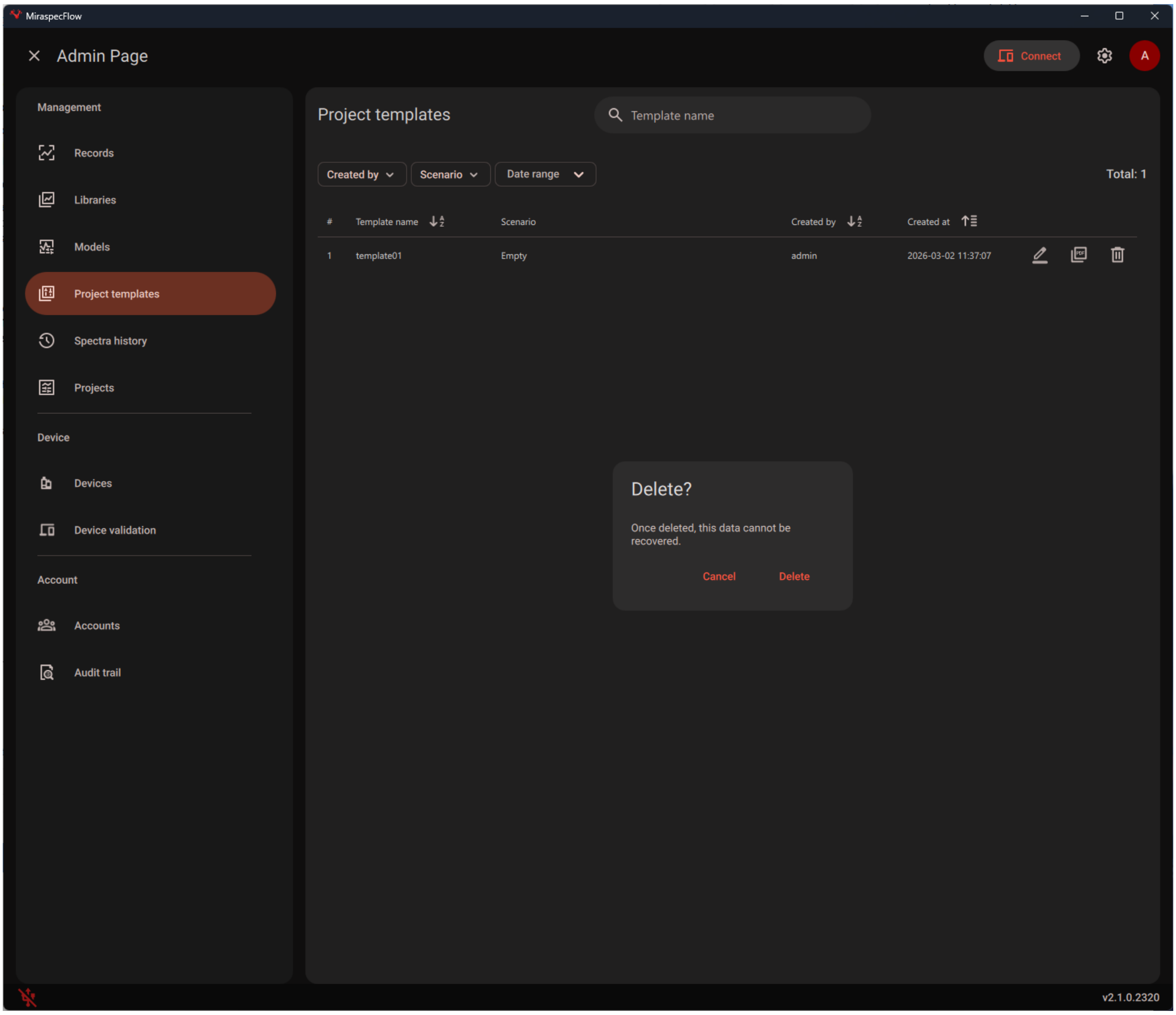
- Delete project template



Search, sorting and filter

The user can search templates by name and apply filters for easier navigation within the list.

Available tools:

- Search bar – enter a template name to find it in the table.
- Filter chips – filter templates by name (Template name), scenario (Scenario), creator (Created by), and date range (Date range).
- Reset filters button – clears all applied filters and displays the full list of templates.
- Sorting – change the display order by template name (Template name), creator (Created by), or creation date (Created at), in ascending or descending order.
- Search results – when filters are applied, the number of found results is shown (Result). After resetting filters, the total number of templates is displayed (Total).

Goal: provide quick search and convenient navigation through templates in the table.

11.5. Device management

The Device Management section provides administrative tools for configuring and maintaining the spectrometer devices used with Miraspec Flow. These tools allow administrators to manage connected instruments, verify device availability, and ensure that the system is properly configured for spectral acquisition.

Through the device management interface, administrators can register devices, review device status, and perform validation procedures to confirm that the instruments are functioning correctly. Proper device management helps ensure reliable communication between the software and connected hardware.

The following sections describe how to manage devices and perform device validation within the system.

11.5.1. Devices

The **Devices** section provides tools for viewing and managing spectrometer devices that are connected to the Miraspec Flow system. This section allows administrators to monitor device status, review device information, and perform administrative actions related to connected hardware.

The Devices interface displays a list of devices that are currently connected to the system as well as devices that have been previously used. For each device, the system typically displays information such as the device serial number, connection status, assigned user, and the date of the last synchronization.

Typical operations available in this section include:

- viewing the list of connected and previously connected devices
- monitoring the current connection status of each device
- assigning or modifying the user associated with a device
- synchronizing data between the device and the system
- accessing detailed device information, such as available libraries and stored spectra
- initiating firmware updates when available

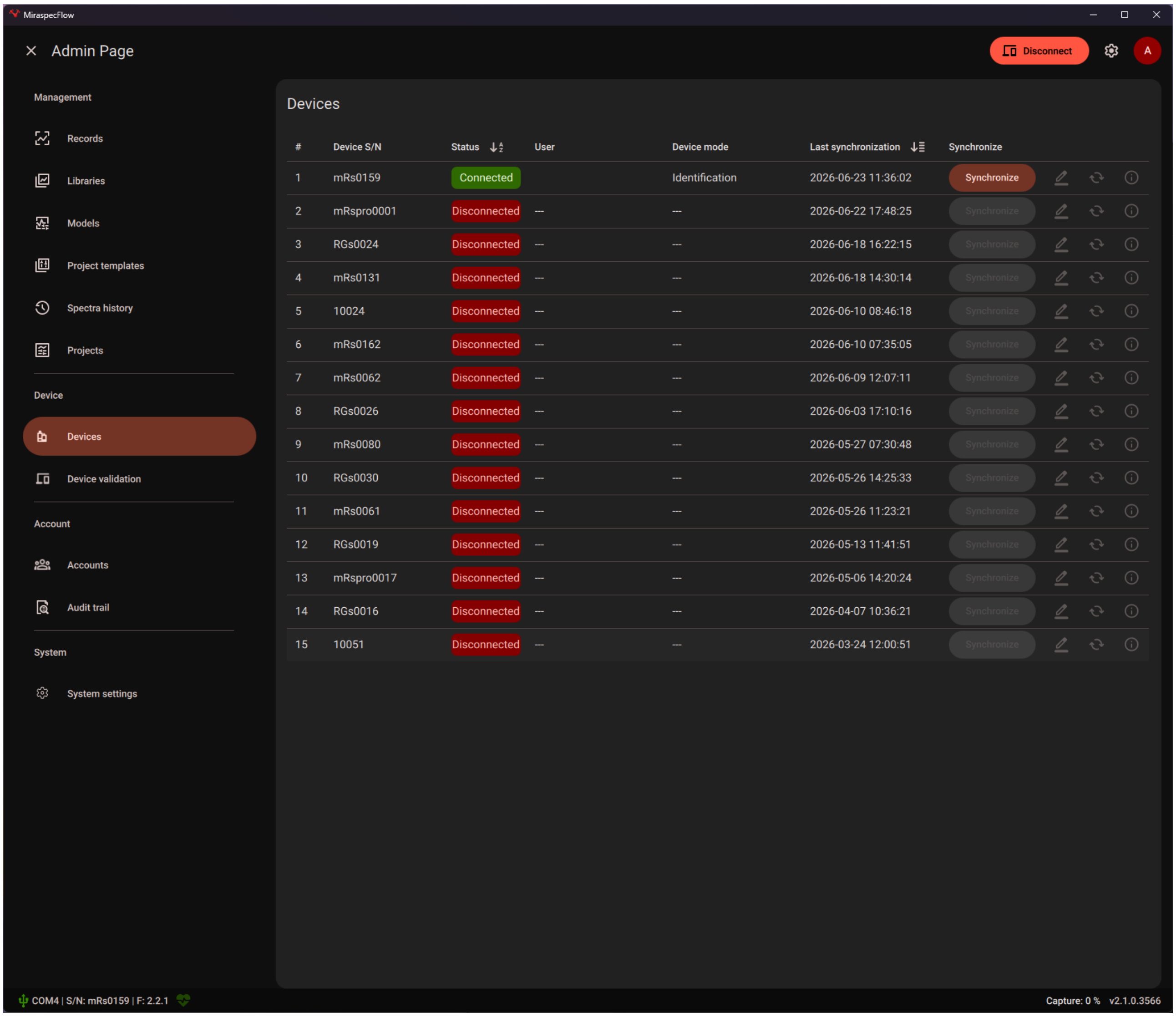
If a device is disconnected, certain actions such as synchronization or editing device settings may be unavailable until the device is reconnected.

The Devices section provides administrators with a centralized interface for managing hardware resources and ensuring proper communication between the software and connected spectrometer devices.

Through this tab, users can initiate data synchronization with a connected device, edit device information (such as assigned user), and access detailed device information, including available libraries, their type, and the number of spectra stored. Users can also hide or delete specific libraries directly on the device.

This functionality ensures efficient control of connected hardware, provides transparency in device usage, and enables reliable synchronization of spectral data for further processing and analysis.

Goal: provide users with a convenient tool for monitoring and managing connected devices, simplify the data synchronization process, and ensure the accuracy and integrity of information used for analytics and library management.



Core functionality

The Devices page provides full control over all devices that have been connected to the system.

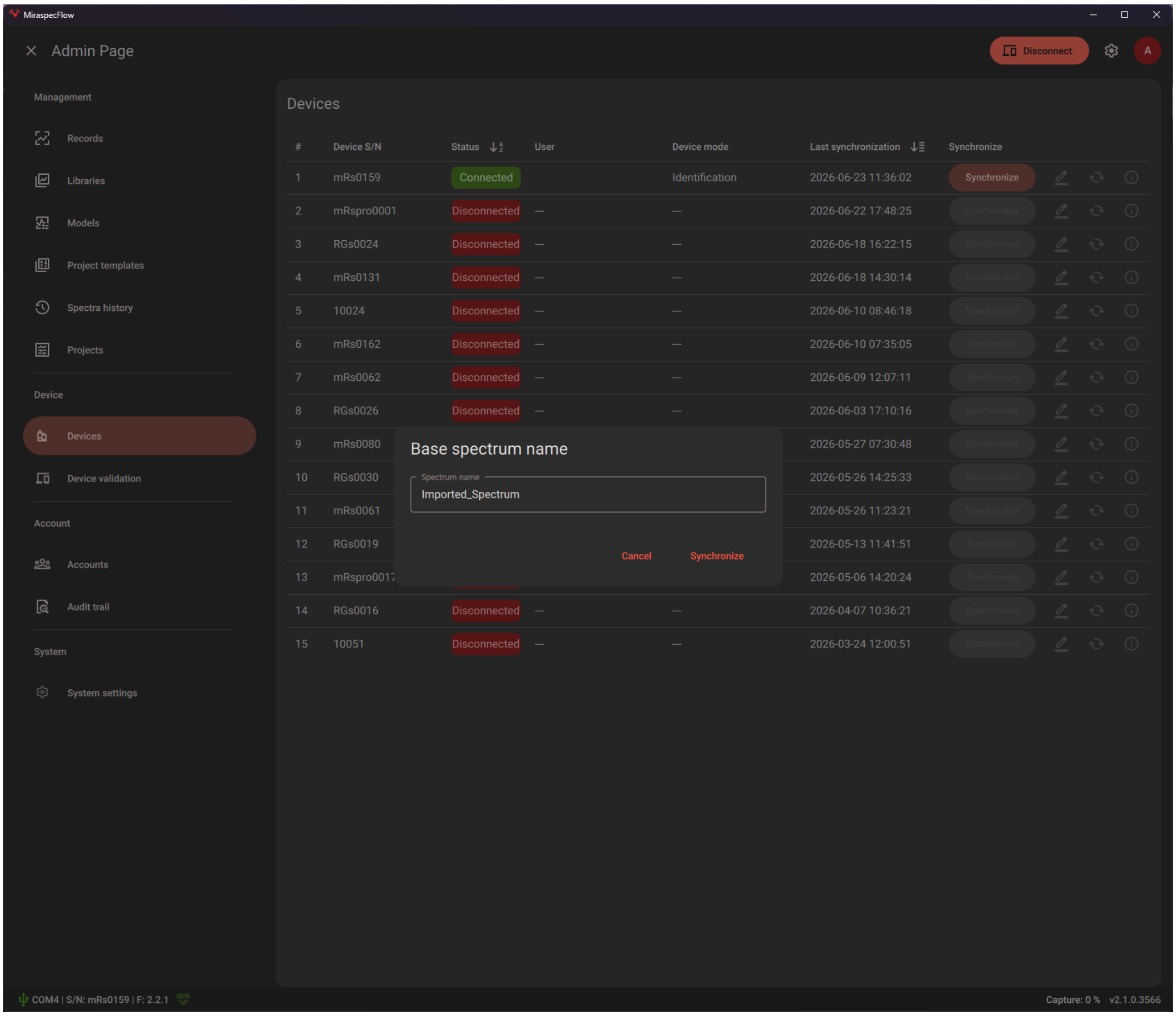
Through this page, the user can:

- Synchronize data with the device;
- Change the user assigned to the device.
- Info – a button that opens detailed information about the device

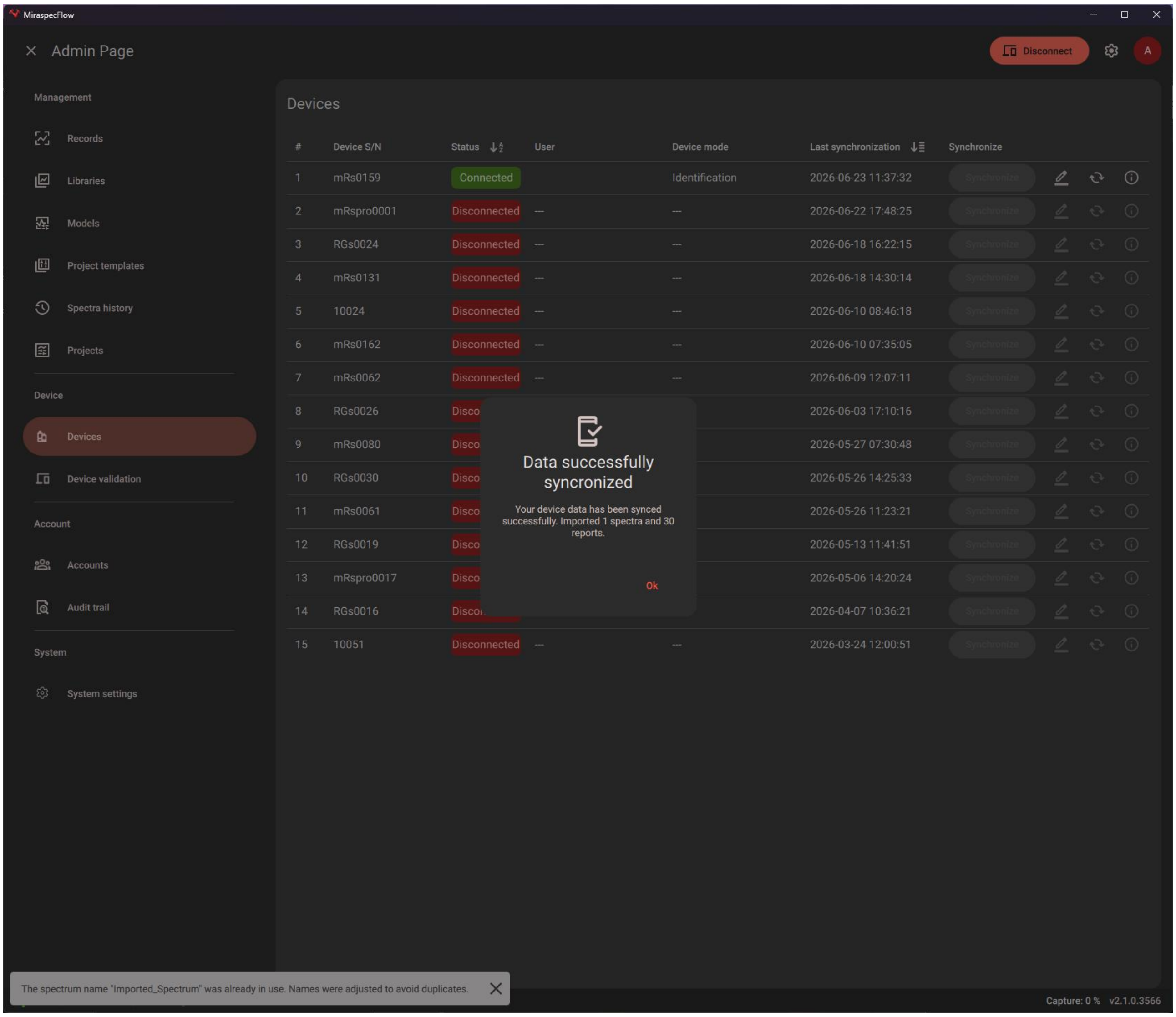
- Update Firmware

In order to perform synchronization click on Synchronize button corresponding to the connected device.

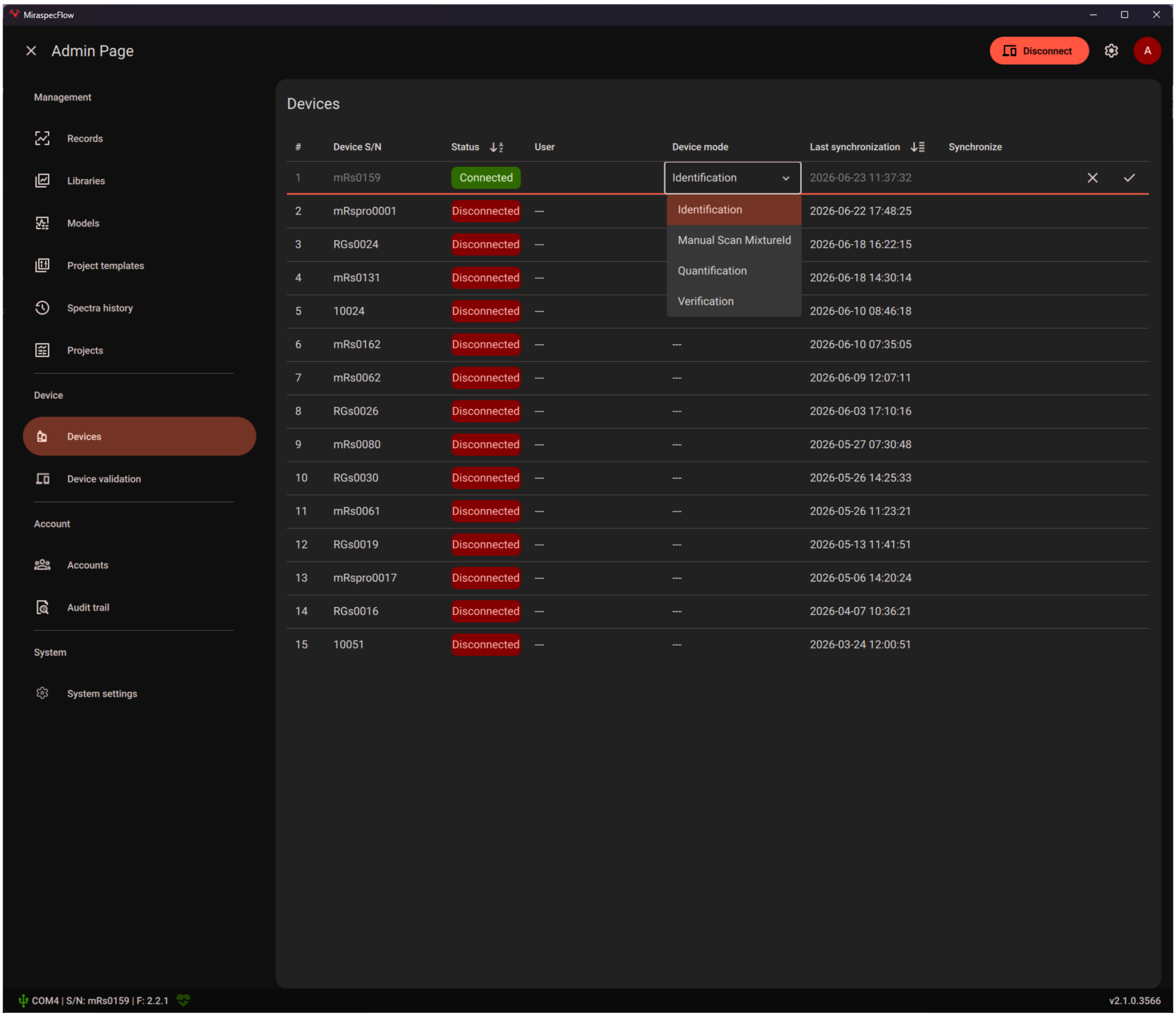
Enter base spectrum name.



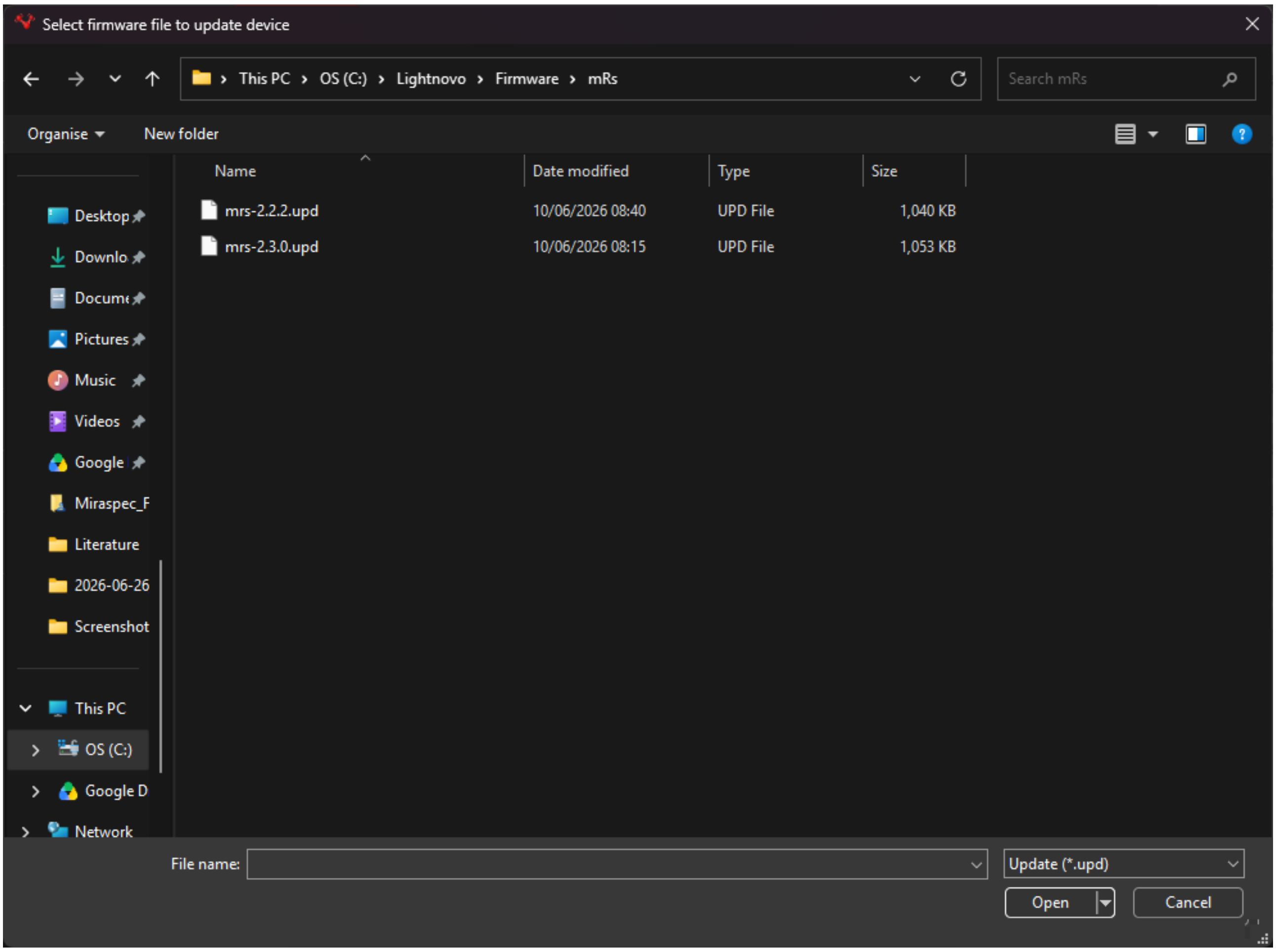
Then click Synchronize, the data are now transferred to the Miraspec flow software.



Clicking on Edit button allows to choose the device mode from available options:

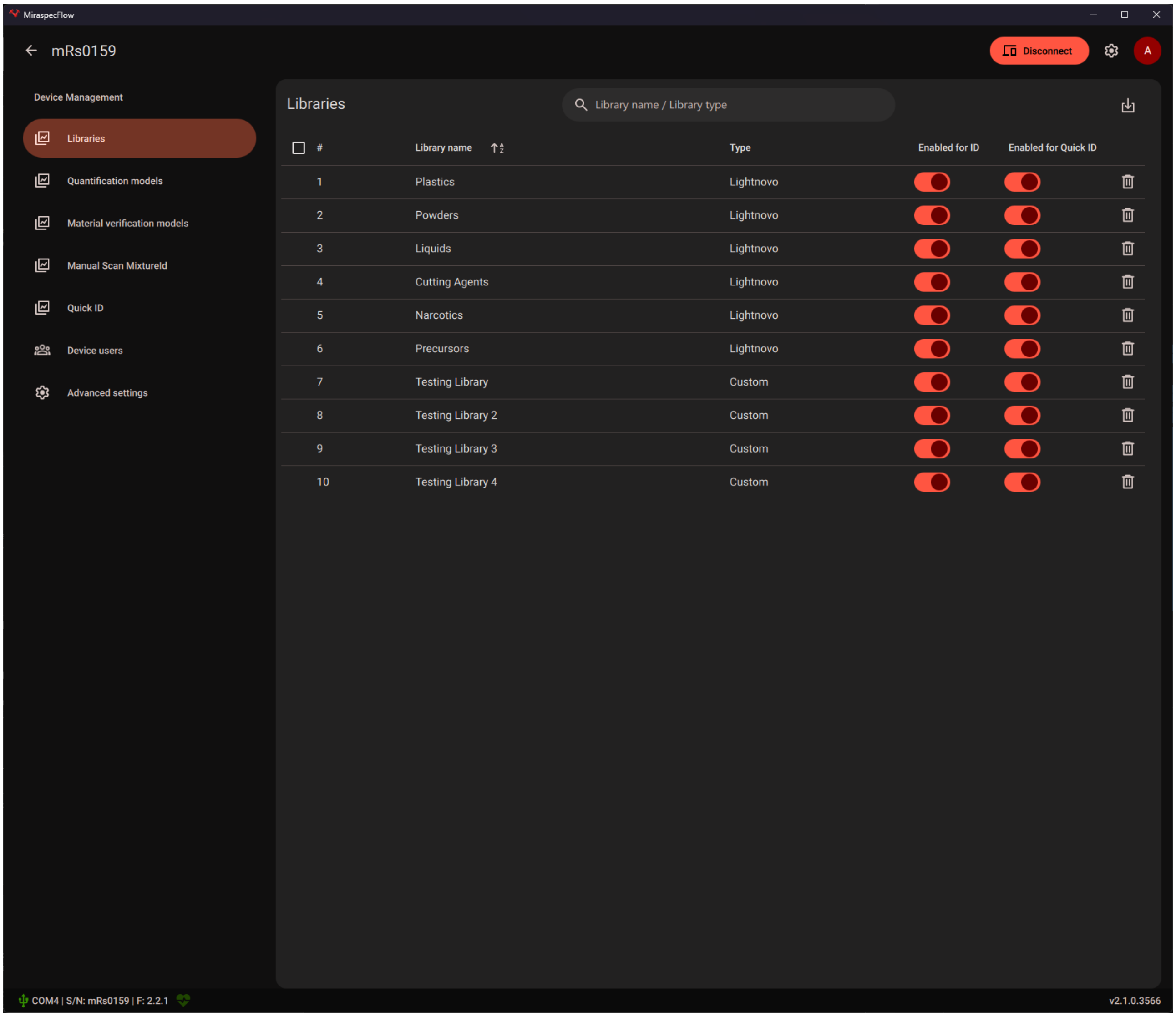


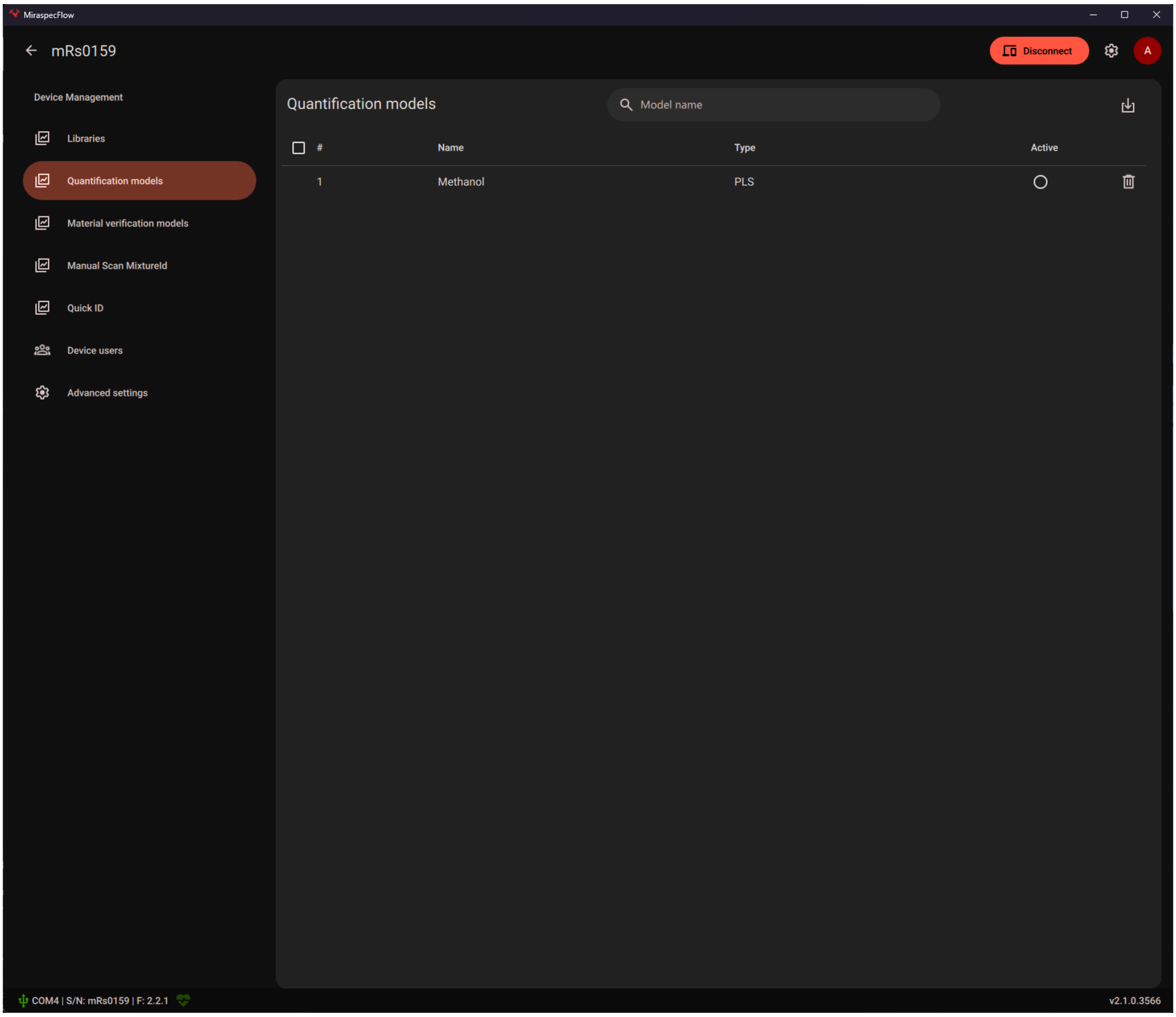
In order to update the firware one should click on cycling arrows icon and choose the firmware update file using file dialog prompt which will pop up. You will need .upd files from Lightnovo stored locally on your computer to perform firmware updates.

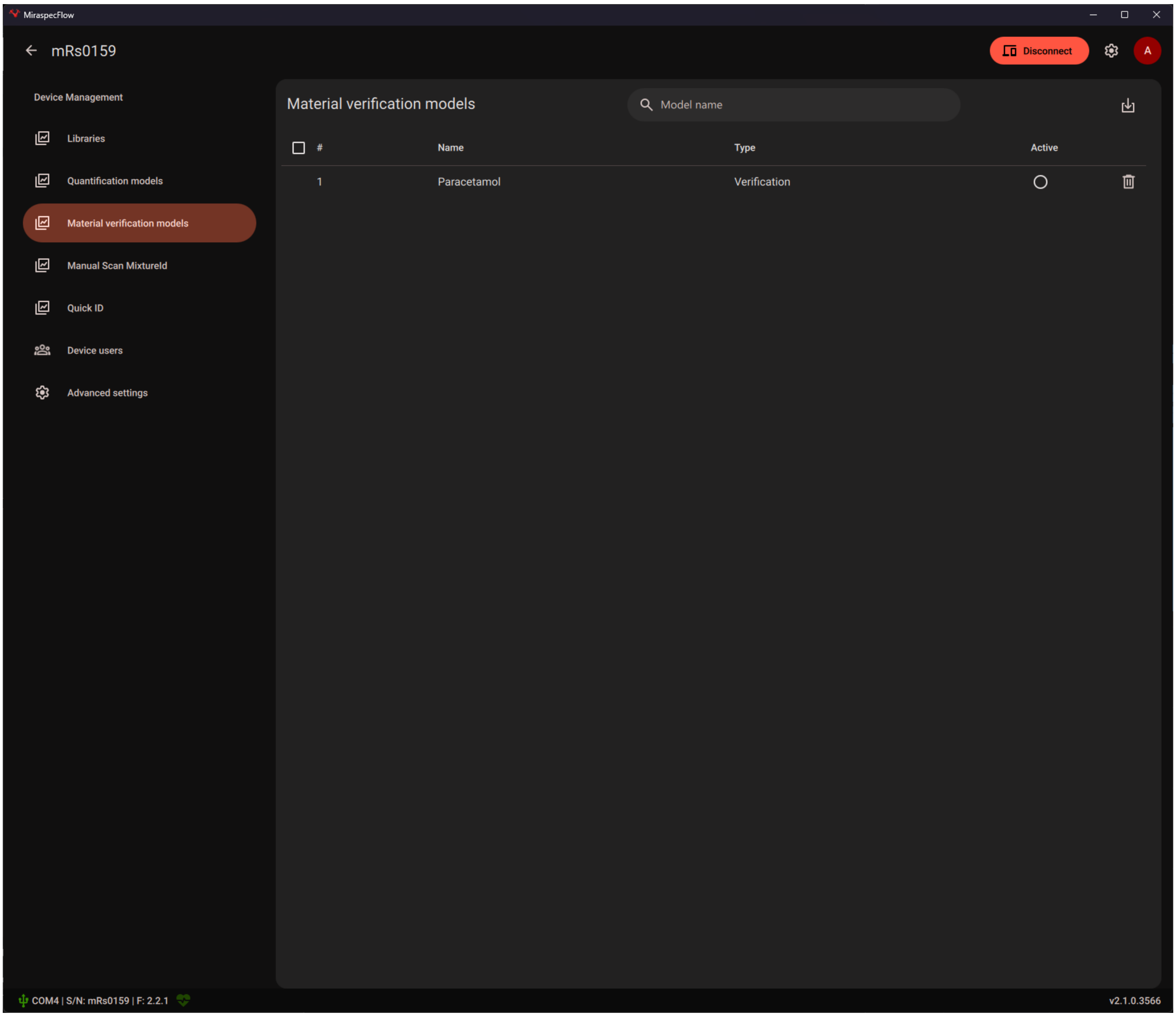


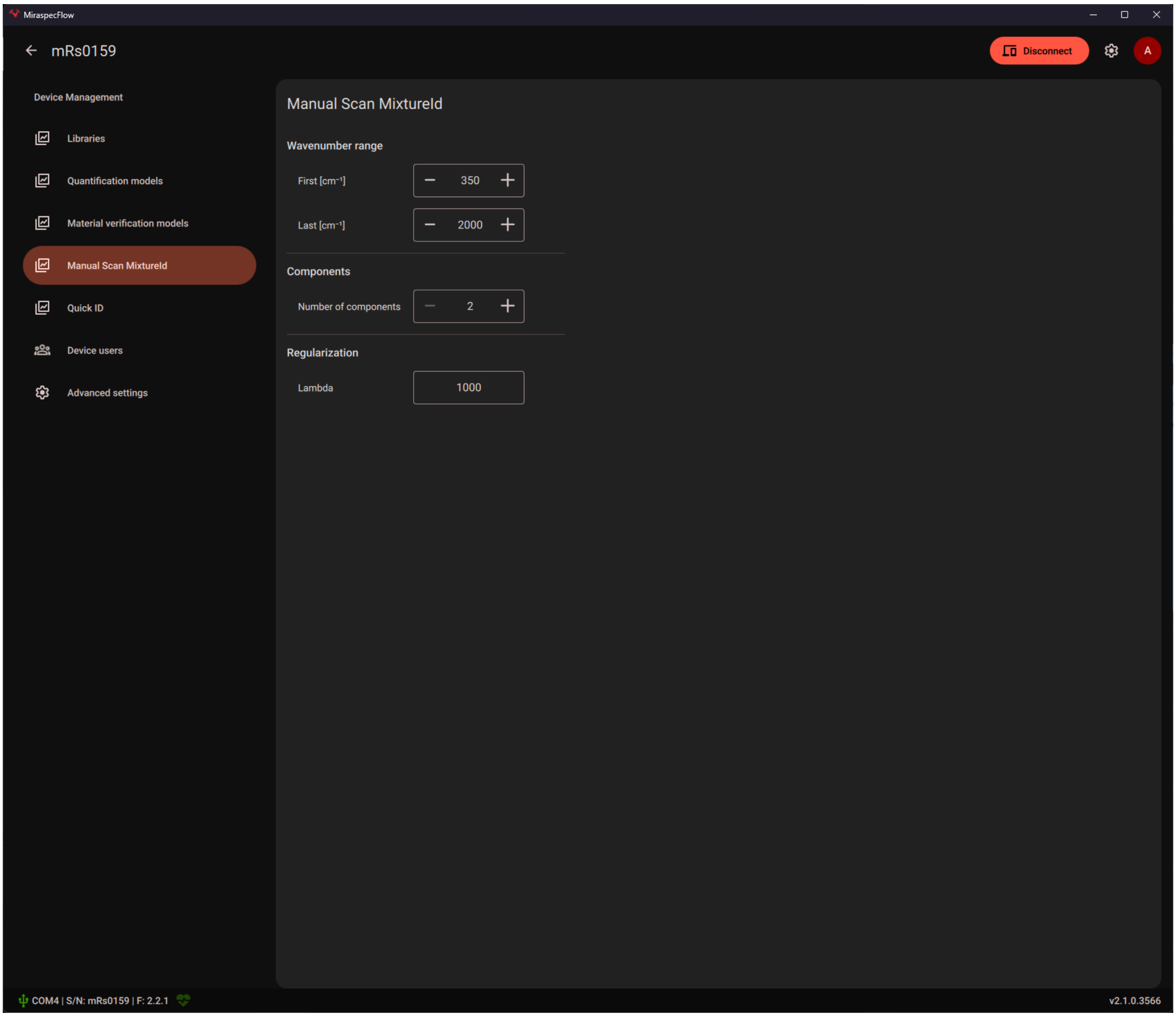
Clicking on the info button allows:

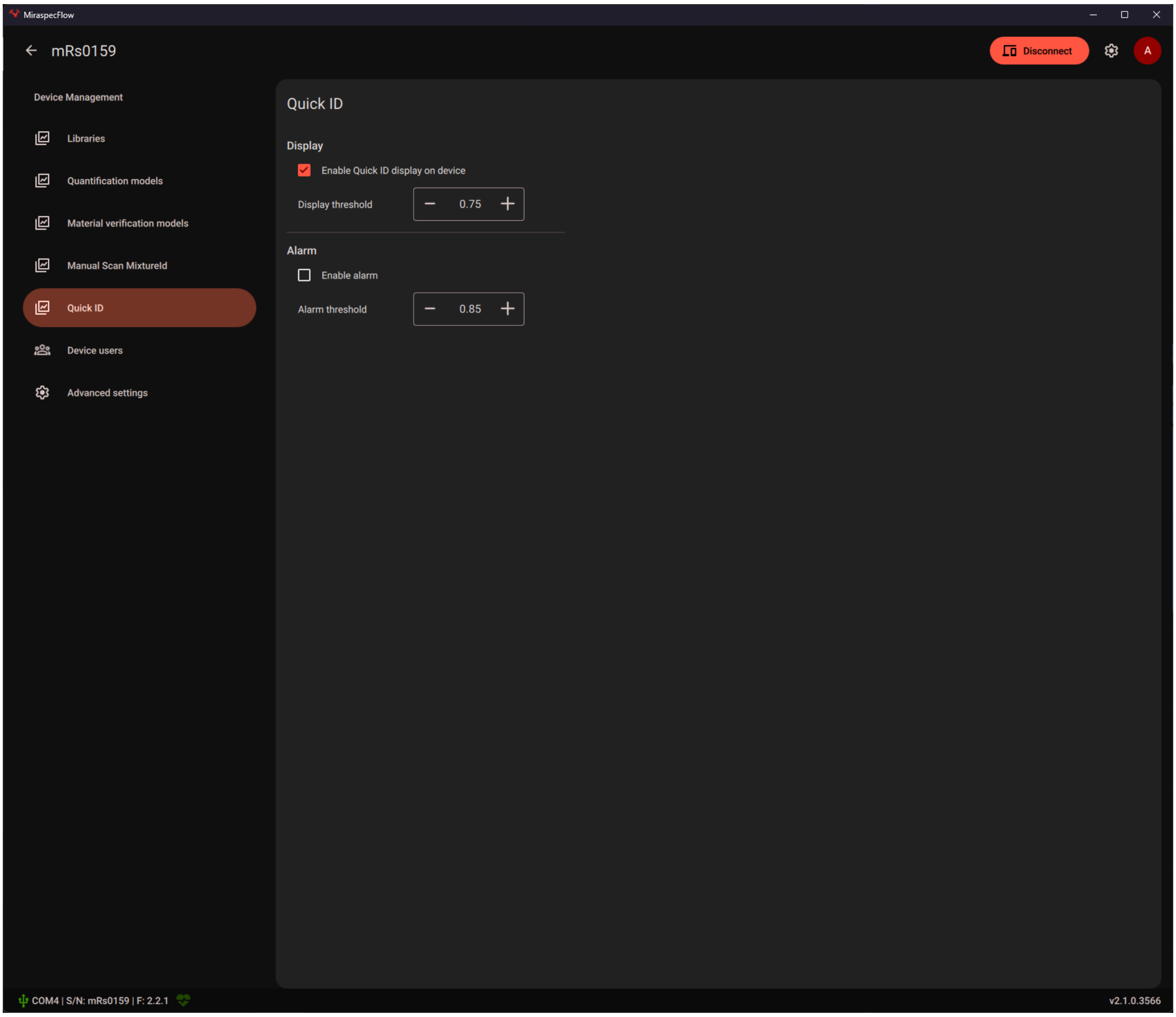
- To see the spectral libraries on the device as well as to upload new libraries,
- To see the quantification models on the device and to upload new quantification models
- To see the material verification models on the device and to upload new verification models
- Adjust manual scan MixtureID settings
- Adjust QuickID settings
- Add/remove device users
- As well as change advanced settings: colour scheme on the device, auto exposure settings, fluorescence correction settings, Raman background correctrion setings, etc.

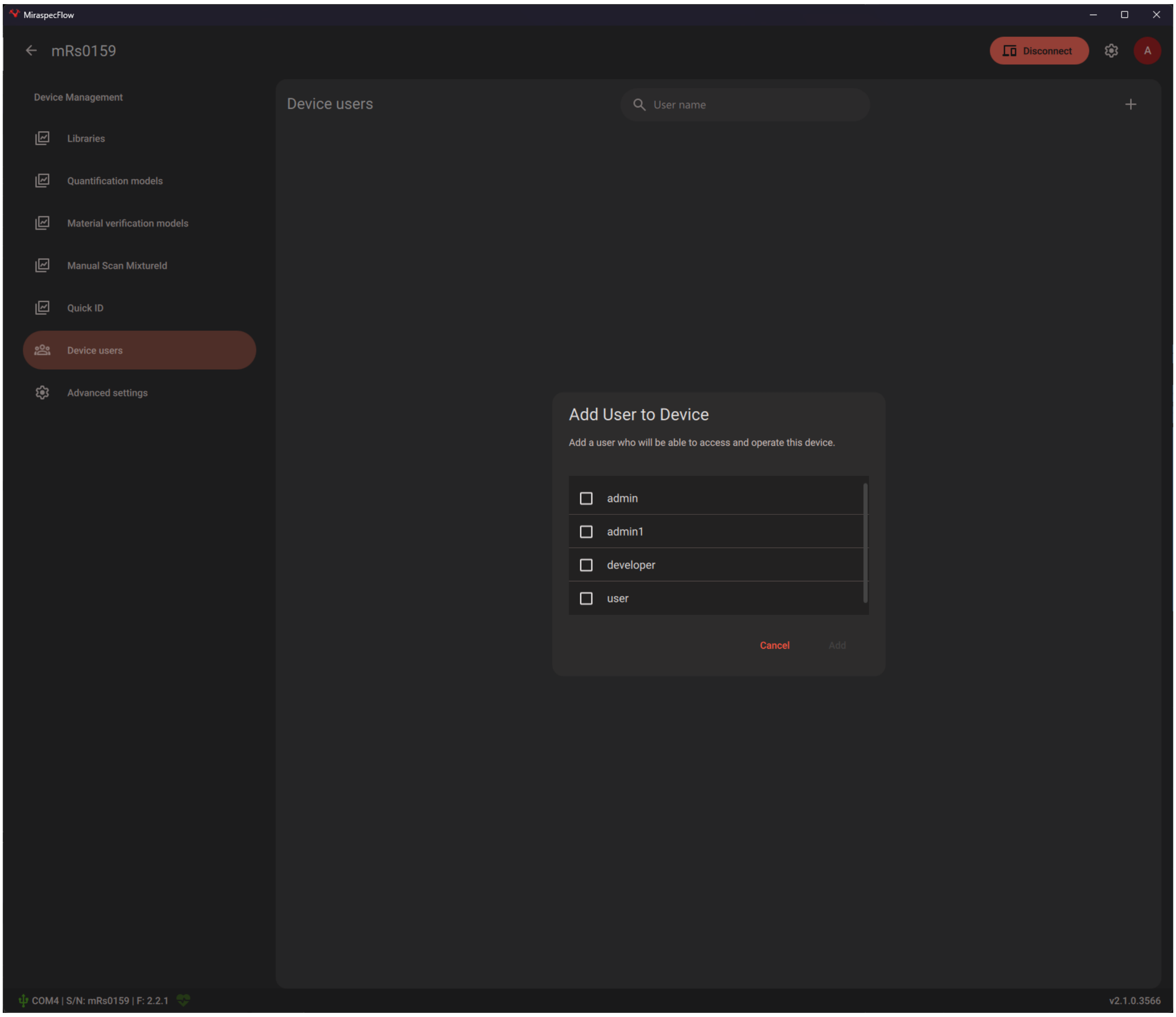


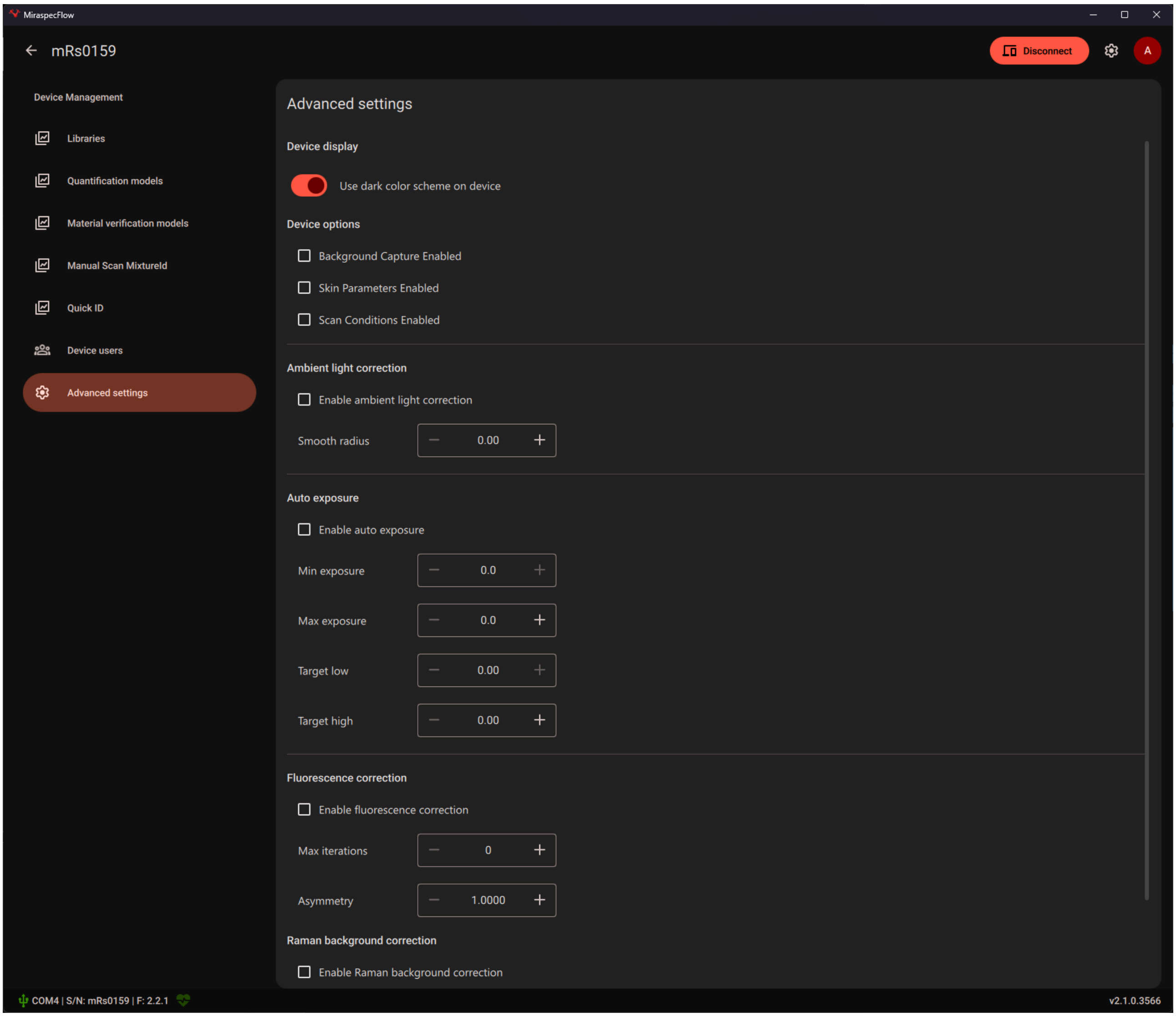

MiraspecFlow
mRs0159
Disconnect
A
Device Management
Libraries
Quantification models
Material verification models
Manual Scan MixtureId
Quick ID
Device users
Advanced settings
Quantification models
Model name
#
Name
Type
Active
1
Methanol
PLS
COM4 | S/N: mRs0159 | F: 2.2.1
v2.1.0.3566


MiraspecFlow
mRs0159
Disconnect
A
Device Management
Libraries
Quantification models
Material verification models
Manual Scan MixtureId
Quick ID
Device users
Advanced settings
Material verification models
Model name
#
Name
Type
Active
1
Paracetamol
Verification
COM4 | S/N: mRs0159 | F: 2.2.1
v2.1.0.3566


MiraspecFlow
mRs0159
Disconnect
A
Device Management
Libraries
Quantification models
Material verification models
Manual Scan MixtureId
Quick ID
Device users
Advanced settings
Manual Scan MixtureId
Wavenumber range
First [cm⁻¹]
350
Last [cm⁻¹]
2000
Components
Number of components
2
Regularization
Lambda
1000
COM4 | S/N: mRs0159 | F: 2.2.1
v2.1.0.3566


MiraspecFlow
mRs0159
Disconnect
A
Device Management
Libraries
Quantification models
Material verification models
Manual Scan MixtureId
Quick ID
Device users
Advanced settings
Quick ID
Display
Enable Quick ID display on device
Display threshold
0.75
Alarm
Enable alarm
Alarm threshold
0.85
COM4 | S/N: mRs0159 | F: 2.2.1
v2.1.0.3566


MiraspecFlow
mRs0159
Disconnect
A
Device Management
Libraries
Quantification models
Material verification models
Manual Scan MixtureId
Quick ID
Device users
Advanced settings
Device users
User name
Add User to Device
Add a user who will be able to access and operate this device.
admin
admin1
developer
user
Cancel
Add
COM4 | S/N: mRs0159 | F: 2.2.1
v2.1.0.3566



The Devices table displays all information about currently connected and previously connected devices.

It is the main tool for managing devices, monitoring their status, and accessing available actions (synchronization, user editing, viewing detailed information).

- # – sequential number of the record in the table.
- Device SN – the device's serial number. Used for device identification.
- Status – the connection status of the device:
    - Connected (green indicator) – the device is active, all functions are available.
    - Disconnected (red indicator) – the device is inactive, functions are unavailable.
- User – the user assigned to the device. This value can be changed via editing (available only for Connected devices).
- Last synchronization – the date and time of the last data synchronization with the device.
- Synchronize – a button to start the data synchronization process (active only for Connected devices).
- Edit – an edit button that allows reassigning the user associated with the device.

- The Update Firmware functionality allows the user to update the firmware of a connected device to the latest version.
- Info – a button that opens detailed information about the device (libraries, number of spectra, etc.).

If the device status is Disconnected, all functions (Synchronize, Edit, Info) are disabled until the device is connected again.

11.5.2. Device validation

The **Device Validation** section provides tools for reviewing the results of validation procedures performed on spectrometer devices connected to the Miraspec Flow system. Device validation is used to verify that an instrument is operating within acceptable performance parameters before it is used for spectral measurements.

This section displays a list of validation records generated during previous validation procedures. Each record typically includes information such as the device serial number, the user who performed the validation, the date of the validation, and the resulting device status.

Possible validation statuses may include:

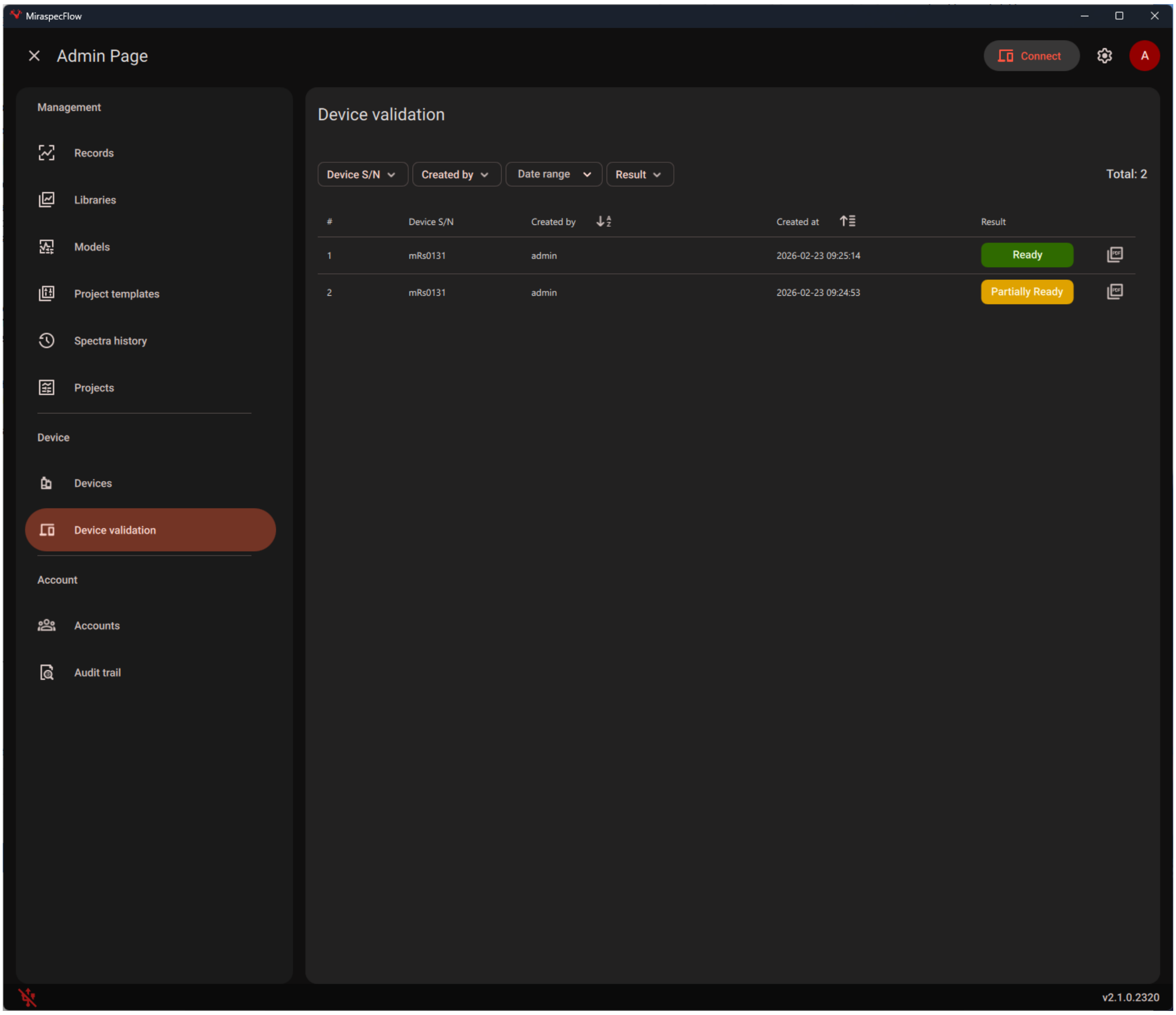
- **Ready** – the device meets the required performance criteria and is suitable for use.
- **Partially Ready** – some parameters may require attention or verification.
- **Not Ready** – the device does not meet the required criteria and may require maintenance or recalibration.

Users can open detailed validation reports to review the results of the validation procedure. These reports may include measurement results, graphical data, and information about the validation conditions. Validation reports can typically be viewed, exported, or printed for documentation and quality control purposes.

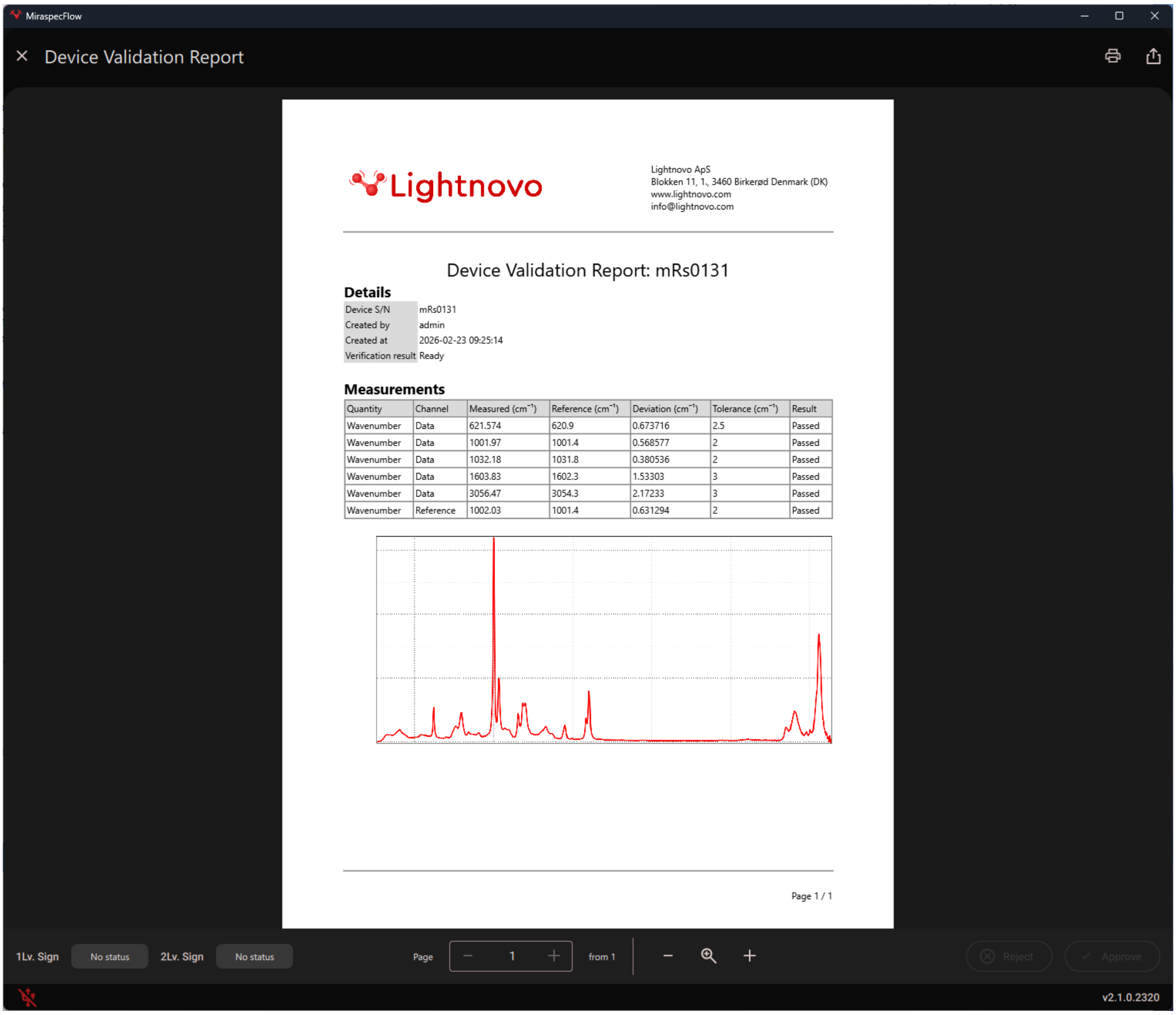
Filtering and sorting tools are available to help users locate validation records based on attributes such as device serial number, user, validation date, or validation result.

Maintaining a record of device validation helps ensure instrument reliability and supports quality assurance and compliance requirements.

Through this tab, users can apply filters to quickly find the needed record and open a PDF report for detailed analysis of the validation results. The main functionality includes the ability to view the full PDF report in a modal window with options to download or print it. This provides convenient access to an official document containing all measurements, deviations, and graphical data. Such an approach simplifies device quality control, enables tracking of their technical condition, and forms a reliable basis for inspection, audit, and technical documentation.



By clicking on pdf icon one can view the validation report:



Core functionality

- PDF Report Viewing
- Filters

Available tools:

- Filter chips – filter records by Device SN, Created by, Date range, and Result.
- Clicking a chip opens a dropdown list where one or multiple options can be selected.
- Reset filters – clears all active filters and restores the full list. After resetting, the total count is displayed as Total, replacing the previous Result count.
- Sorting – changes the order of display by Created by or Created at (ascending or descending).

11.6. System monitoring

The System Monitoring section provides tools for reviewing system activity and maintaining traceability of operations performed within Miraspec Flow. These tools allow administrators to monitor system records and review audit information related to user actions and system events.

System monitoring helps ensure transparency, accountability, and proper management of data and system resources. By reviewing system records and audit trails, administrators can track important events such as user activity, project modifications, and configuration changes.

The following sections describe how to access system records and review the audit trail within the system.

11.6.1. Records

The **Records** section provides access to reports generated during spectral analysis and experiment workflows in Miraspec Flow. These records contain documented results of analyses performed within projects and serve as an official record of system activity and analytical outcomes.

Each record typically includes information such as the report name, associated project, analysis type, user who generated the report, and the date and time of creation. Reports may also include processed spectra, identification results, model outputs, and other relevant analytical information.

Users can open a record to view the report in a document format, typically presented as a PDF file. From this view, the report can be reviewed in detail and may be exported or printed for documentation purposes.

In environments where report approval is required, records may also include information about the approval status, such as whether the report has been approved or rejected by authorized users.

Search, filtering, and sorting tools are available to help locate specific records based on criteria such as report name, project name, creator, analysis type, or creation date.

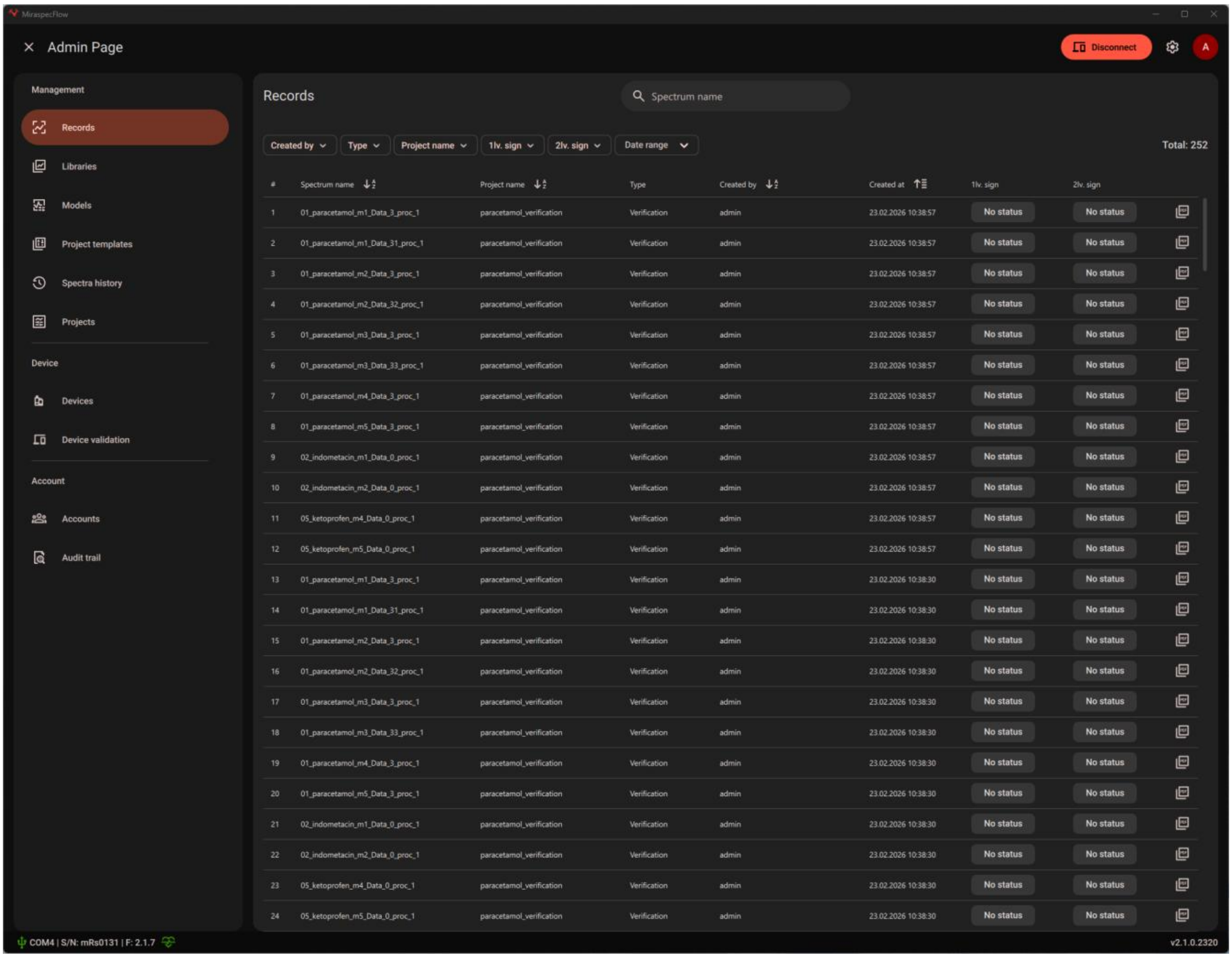
Maintaining records of generated reports ensures traceability of analytical results and supports documentation and quality control procedures.

The Records tab is used for centralized management of created reports containing the results of spectroscopic analysis.

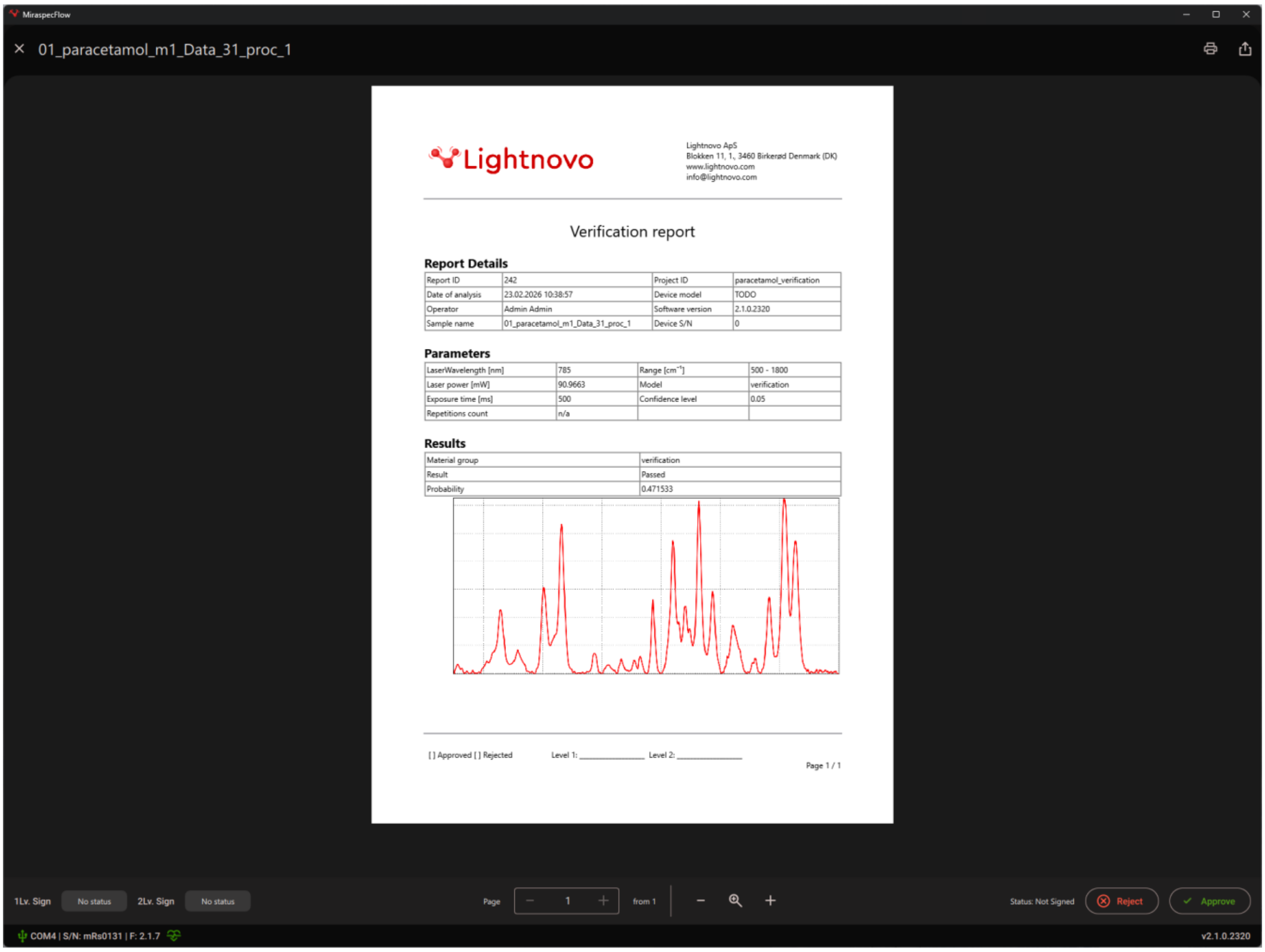
It allows users to view the list of all saved reports, apply search, filtering, and sorting by various parameters (type, user, date, signature status).

Each report can be opened in PDF format for detailed review, signing, exporting, or printing.

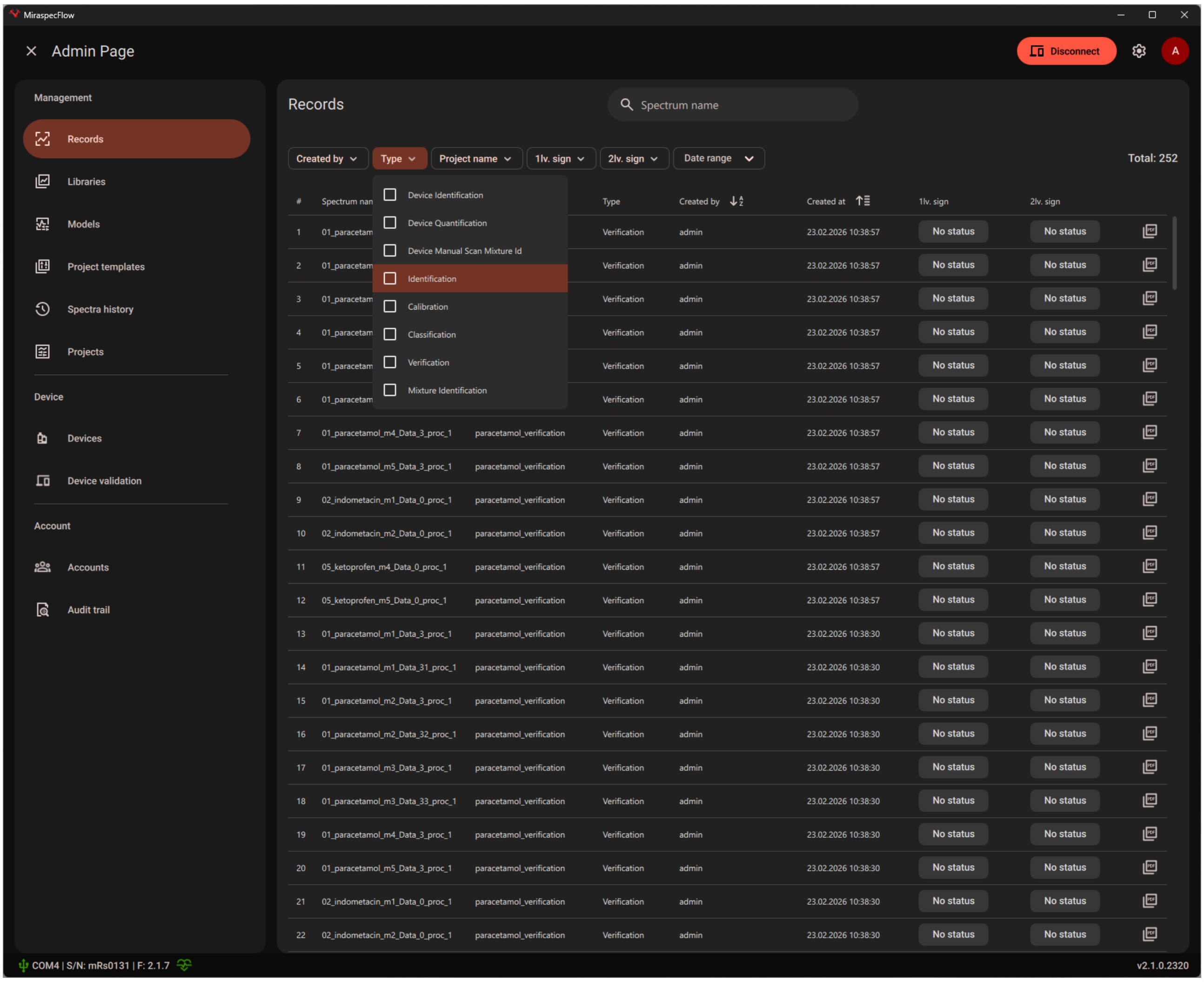
This tab ensures transparent control over all generated reports, simplifies the verification process, and supports the full approval workflow across multiple signature levels.



The user can click on pdf icon to view the report:



Example of filtering by type of project



Core functionality

View report – open the PDF file in a modal window for detailed review, with the ability to sign it once (Approve or Reject), export, or print the document.

Search and filter

The user can search reports by name and apply filters for easier navigation within the table.
Available tools:

- Search bar – enter a spectrum or project name to find the desired report in the table.
- Filter chips – filter reports by Type, Created by, Date range, 1Lv. Sign, and 2Lv. Sign. Clicking a chip opens a dropdown list where one or multiple options can be selected.
- Reset filters – clears all active filters and displays the full list of reports.
- Sorting – changes the display order by Specter name, Project name, Created by, or Created at (ascending or descending).

Goal: provide quick search and convenient navigation through reports in the table.

11.6.2. Audit trail

The **Audit Trail** section provides a record of system events and user activities performed within the Miraspec Flow system. The audit trail helps ensure transparency and traceability of actions carried out by users, supporting system monitoring, troubleshooting, and compliance with internal quality procedures.

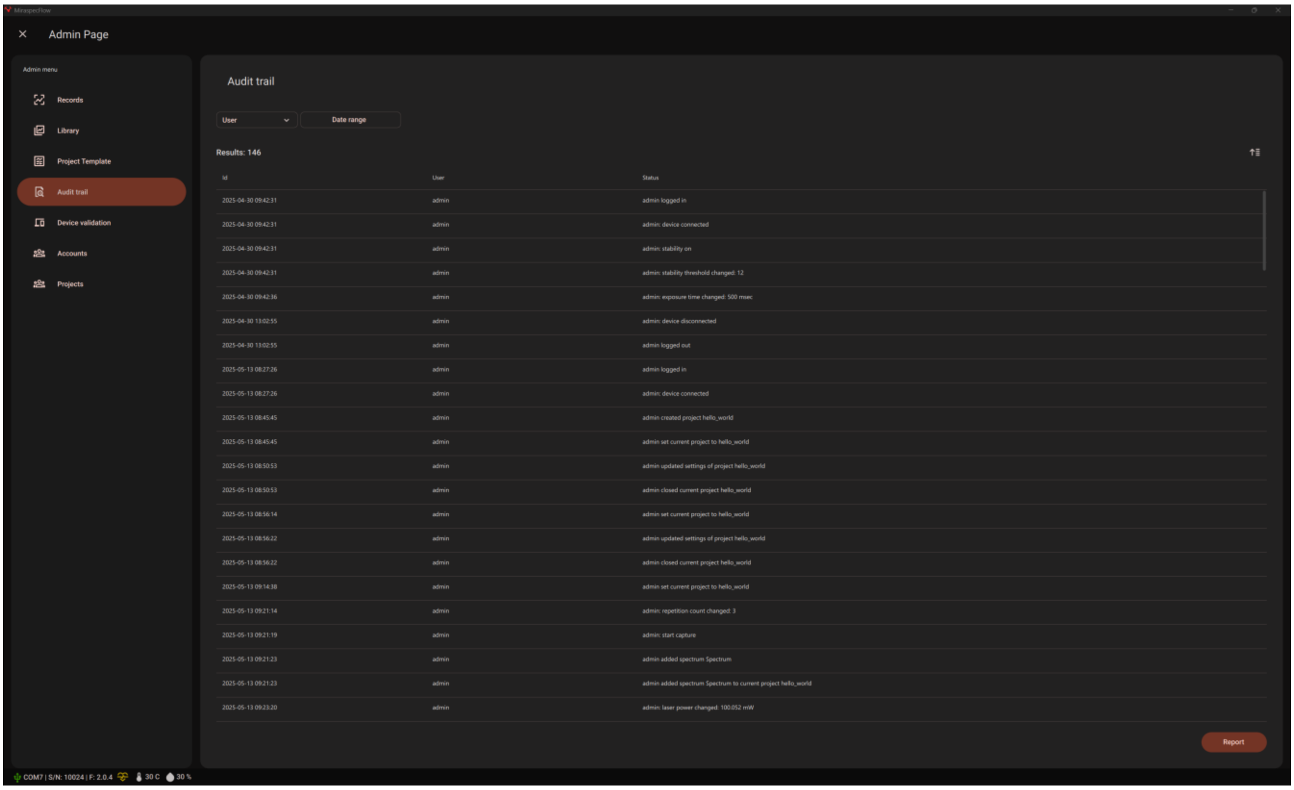
Each audit trail entry typically includes information such as the date and time of the event, the user who performed the action, and a description of the activity. Recorded events may include actions such as user logins, project creation or modification, model updates, report generation, or changes to system settings.

Administrators can review the audit trail to monitor system usage and track changes made within the software. Search, filtering, and sorting tools are available to help locate specific events based on criteria such as user name, event type, or date range.

The audit trail records can also be exported as a report, allowing administrators to generate documentation of system activity for auditing or review purposes.

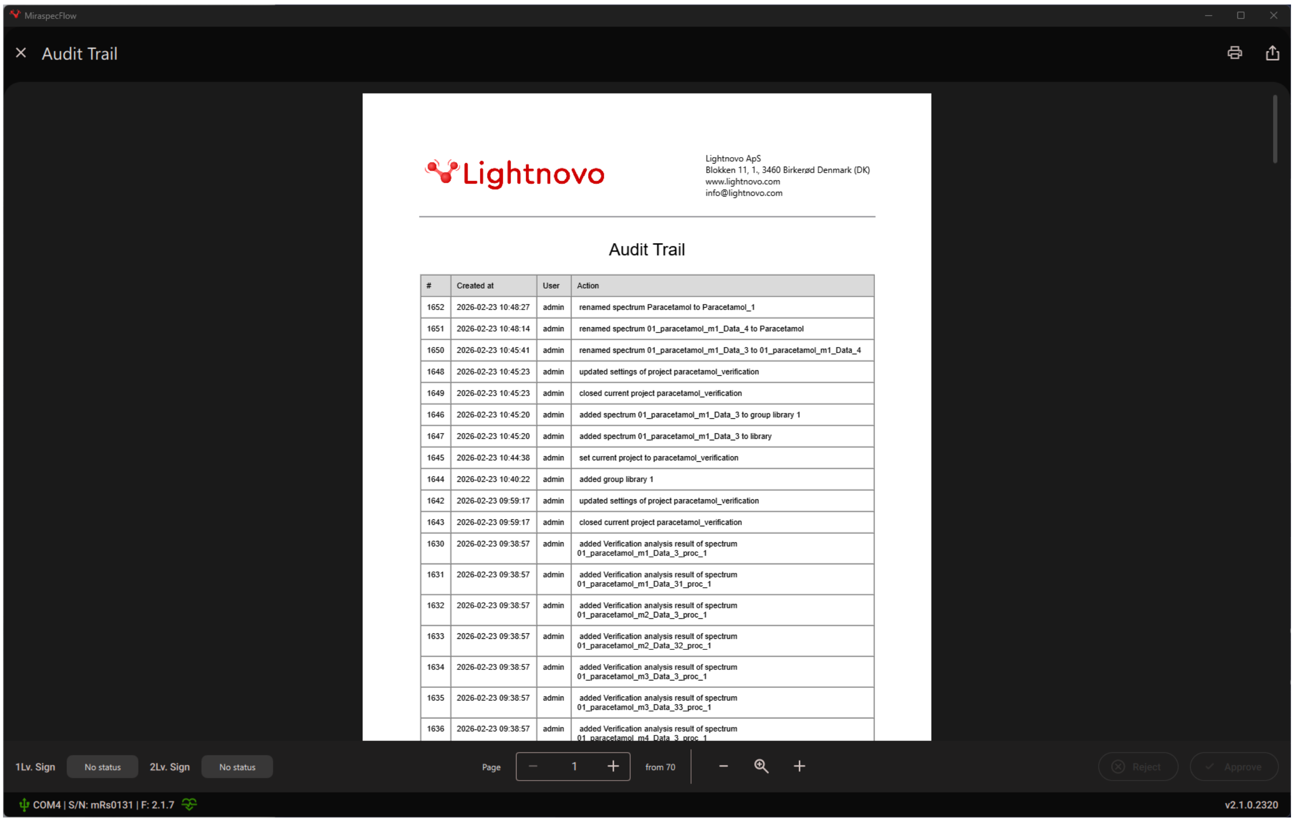
Maintaining an audit trail helps ensure accountability of user actions and supports secure and reliable operation of the Miraspec Flow system.

The Audit trail tab is used for centralized tracking of user actions within the system. It allows viewing the history of events, including the date, user, and performed action. Through this tab, administrators can monitor changes made to data or settings, filter records by date or user, and analyze system activity. This functionality ensures workflow transparency, enhances security, and helps investigate possible errors or improper actions.



Core functionality

Open Report – generate and open a document containing detailed information about all recorded user actions in the system, including date, time, user name, and description of each action. The report is displayed in a printable PDF format with company details and can be used for audit and compliance purposes.



#	Created at	User	Action
1652	2026-02-23 10:48:27	admin	renamed spectrum Paracetamol to Paracetamol_1
1651	2026-02-23 10:48:14	admin	renamed spectrum 01_paracetamol_m1_Data_4 to Paracetamol
1650	2026-02-23 10:45:41	admin	renamed spectrum 01_paracetamol_m1_Data_3 to 01_paracetamol_m1_Data_4
1648	2026-02-23 10:45:23	admin	updated settings of project paracetamol_verification
1649	2026-02-23 10:45:23	admin	closed current project paracetamol_verification
1646	2026-02-23 10:45:20	admin	added spectrum 01_paracetamol_m1_Data_3 to group library 1
1647	2026-02-23 10:45:20	admin	added spectrum 01_paracetamol_m1_Data_3 to library
1645	2026-02-23 10:44:38	admin	set current project to paracetamol_verification
1644	2026-02-23 10:40:22	admin	added group library 1
1642	2026-02-23 09:59:17	admin	updated settings of project paracetamol_verification
1643	2026-02-23 09:59:17	admin	closed current project paracetamol_verification
1630	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m1_Data_3_proc_1
1631	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m1_Data_31_proc_1
1632	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m2_Data_3_proc_1
1633	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m2_Data_32_proc_1
1634	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m3_Data_3_proc_1
1635	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m3_Data_33_proc_1
1636	2026-02-23 09:38:57	admin	added Verification analysis result of spectrum 01_paracetamol_m4_Data_3_proc_1

By clicking on the top right arrow, one can save the report to a .pdf file on the drive.

12. Troubleshooting

This section provides guidance for diagnosing and resolving common issues that may occur when using Miraspec Flow. The problems described below represent typical situations related to device connectivity, spectral acquisition, model operation, and system configuration.

If an issue cannot be resolved using the steps described in this section, users should contact the system administrator or technical support.

12.1. Device Not Detected

In some cases, the connected Raman spectrometer may not appear in the list of available devices within the software.

Possible causes include incorrect hardware connections, missing device drivers, or the device not being powered on.

To resolve this issue:

- Ensure that the spectrometer is properly connected to the computer using the correct communication interface (such as USB or Bluetooth).
- Verify that the device is powered on.
- Confirm that the required device drivers are installed.
- Restart the Miraspec Flow software and attempt to detect the device again.
- If necessary, reconnect the device and restart the computer.

If the device still cannot be detected, contact the system administrator or device manufacturer for further assistance.

12.2. No Spectrum Acquired

If spectral acquisition is started but no spectrum appears in the visualization window, the issue may be related to device configuration, measurement parameters, or sample positioning.

Possible solutions include:

- Verify that the device connection has been successfully established.
- Confirm that the laser and detector settings are correctly configured.
- Check that the sample is properly positioned in the measurement area.
- Ensure that integration time and acquisition parameters are appropriate for the sample.
- Verify that the laser is enabled and operating correctly.

If the issue persists, restart the experiment workflow and attempt to acquire the spectrum again.

12.3. Saturated Detector

Detector saturation occurs when the measured signal intensity exceeds the dynamic range of the detector. This can result in distorted spectral data and inaccurate analytical results.

To resolve detector saturation:

- Reduce the laser power used during measurement.
- Decrease the integration time.
- Reduce the number of accumulations if applicable.
- Ensure that the sample is not positioned too close to the excitation source.

After adjusting the acquisition parameters, repeat the spectral measurement to confirm that the detector signal is within the acceptable range.

12.4. Model Not Loading

In some cases, a model may fail to load or become unavailable during analysis.

Possible causes include missing model files, incorrect project configuration, or compatibility issues between the model and the current software environment.

To address this problem:

- Verify that the model exists in the system model library.
- Confirm that the model is associated with the current project or analysis scenario.
- Ensure that the required preprocessing steps match those used during model training.
- Reload the project or restart the software if necessary.

If the model continues to fail to load, the model may need to be recreated or restored from a backup.

12.5. Database Errors

Miraspec Flow stores project data, spectra, and analysis results in the system database. Errors related to database access may prevent the software from loading projects or saving new data.

Possible solutions include:

- Restart the Miraspec Flow application.
- Verify that the database service is running.
- Ensure that the user has the necessary permissions to access the project database.
- Check that sufficient disk space is available on the system.

If database errors persist, contact the system administrator for assistance with database maintenance or recovery.

12.6. General Troubleshooting Recommendations

When troubleshooting system issues, the following general steps may help resolve unexpected problems:

- Restart the Miraspec Flow application.
- Verify that the spectrometer and associated hardware are properly connected and powered on.
- Confirm that the correct project and device configuration are selected.
- Check that the latest software updates and device drivers are installed.

If the issue cannot be resolved using these steps, users should consult technical support and provide detailed information about the problem, including any error messages displayed by the software.

12.7. Contacting Technical Support

If a problem cannot be resolved using the troubleshooting steps described above, users should contact **Lightnovo technical support** for assistance.

When submitting a support request, please include the following information to help the support team diagnose the issue efficiently:

- **Customer name or organization**
- **Serial number of the Raman spectrometer device**
- **Miraspec software version**
- **Devic firmware version**
- **Detailed description of the issue**, including the actions performed before the problem occurred
- **Screenshots of the software interface** showing the issue or any error messages displayed
- **System information for the computer running Miraspec Flow**, including:
  - operating system and version
  - processor type
  - amount of installed RAM
  - graphics hardware (if applicable)

Providing complete information about the system configuration and the observed behavior helps reduce the time required to identify and resolve the problem.

If possible, include the project files or relevant measurement data associated with the issue to assist with further analysis.

Appendix A – Detailed safety guidelines

This appendix provides detailed safety information for the operation of Miraspec Flow and the Raman spectroscopy instruments controlled by the software. These guidelines supplement the *Safety Summary* described in Section 2 of this manual.

Users must follow all applicable laboratory safety procedures and local regulations when operating Raman spectroscopy equipment.

A.1 General Safety Guidelines

Miraspec Flow is designed to operate Raman spectroscopy instruments and perform spectral analysis. Safe system operation requires proper handling of both the software and the associated measurement hardware.

To ensure safe use of the system:

- Operate the software only as described in this manual.
- Ensure that the Raman spectrometer is installed and configured according to the manufacturer's instructions.
- Do not bypass or disable safety mechanisms of the instrument.
- Only trained and authorized personnel should operate the system.
- Ensure that the operating environment is suitable for laboratory instrumentation.

Improper use of the system may lead to equipment damage, incorrect analytical results, or potential safety hazards.

A.2 Laser Safety

Raman spectroscopy instruments use laser radiation to excite molecular vibrations in the sample. Laser radiation can pose hazards to eyes and skin if appropriate precautions are not followed.

Users should observe the following laser safety guidelines:

- Never look directly into the laser beam or optical path.
- Avoid exposure of eyes or skin to direct or reflected laser radiation.
- Do not operate the instrument with protective covers or safety enclosures removed.
- Avoid placing reflective materials in the optical path.
- Follow laboratory laser safety procedures appropriate for the laser classification of the instrument.

The laser classification and associated safety requirements depend on the specific spectrometer model being used.

A.3 Electrical Safety

Raman spectrometers and associated devices require electrical power and contain sensitive electronic components.

To reduce the risk of electrical hazards:

- Ensure that all power connections are properly grounded.
- Use only approved power supplies and cables.
- Do not open instrument housings unless instructed by qualified service personnel.
- Disconnect power before performing maintenance or hardware adjustments.
- Do not operate equipment that appears damaged or malfunctioning.

If electrical problems are suspected, disconnect the system and contact qualified technical support.

A.4 Sample Safety

Certain materials may present chemical, biological, or thermal hazards during analysis.

When handling samples for Raman measurement:

- Follow appropriate laboratory safety procedures for the materials being analyzed.
- Use protective equipment when handling hazardous substances.
- Ensure that samples are compatible with laser illumination.
- Be aware that some materials may heat, degrade, or react when exposed to laser radiation.

Users are responsible for ensuring that sample handling complies with applicable safety regulations and laboratory practices.

A.5 Instrument Handling and Operation

Proper handling of the Raman spectrometer and associated hardware is important for both safety and instrument reliability.

Users should observe the following guidelines:

- Ensure that the instrument is placed on a stable surface.
- Do not block ventilation openings of the device.
- Avoid exposing the instrument to excessive humidity, dust, or vibration.
- Do not attempt to modify or repair the instrument without authorization.

Routine maintenance should only be performed by qualified personnel

A.6 Environmental Conditions

The operating environment may affect both the safety and performance of the instrument.

Recommended environmental conditions include:

- stable room temperature
- moderate humidity levels
- minimal dust and contamination
- protection from direct sunlight

Extreme environmental conditions may affect instrument performance or cause equipment damage.

A.7 Software Safety Considerations

While Miraspec Flow itself does not generate physical hazards, improper configuration of measurement parameters may affect instrument operation or measurement quality.

Users should:

- verify acquisition parameters before starting measurements
- avoid excessively high laser power for sensitive samples
- ensure that measurement settings are appropriate for the sample type

Incorrect settings may lead to sample damage or unreliable results.

A.8 Emergency Situations

If an unsafe condition or equipment malfunction occurs:

1. Stop the measurement immediately.
2. Turn off the spectrometer if necessary.
3. Disconnect power if there is a risk of electrical hazard.
4. Inform the system administrator or responsible personnel.

Do not continue operation until the issue has been properly resolved.

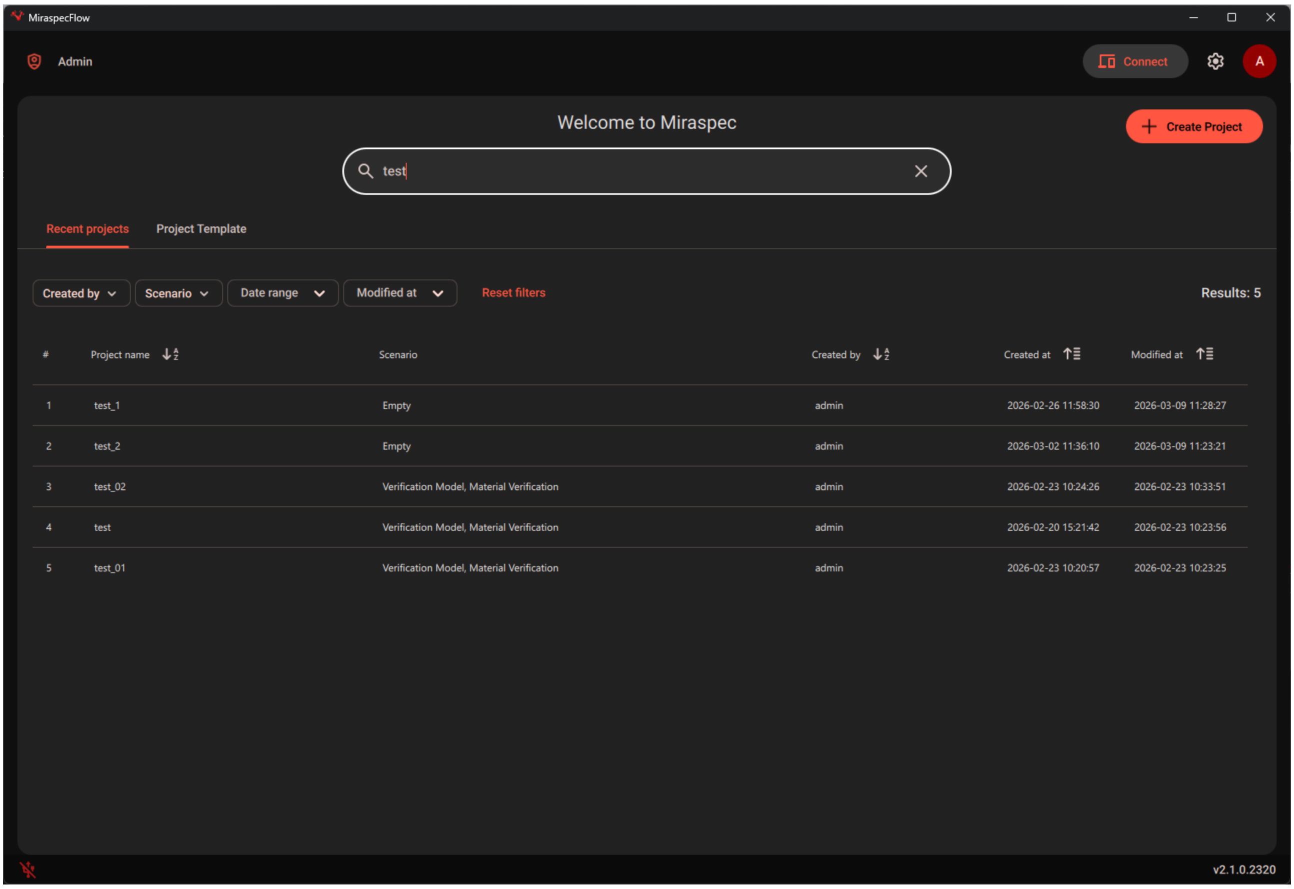
A.9 Responsibility of the User

Users are responsible for operating the system in accordance with the instructions provided in this manual and with applicable laboratory safety regulations.

Lightnovo assumes no responsibility for damage or injury resulting from improper use of the software or associated hardware.

Appendix B - Search function

The search function in Miraspec Flow allows users to quickly locate projects, models, spectra, reports, and other system resources. Search and filtering tools are available throughout different sections of the software interface, helping users navigate large datasets and manage information efficiently.



The search interface includes a **search bar**, **filter controls**, and **sorting options** that allow users to narrow down the displayed results according to specific criteria.

B.1 Searching for Items

The search bar allows users to locate items by entering a name or part of a name. This functionality is available in several parts of the software, including project lists, model libraries, spectra records, and administrative tables.

To perform a search:

1. Locate the **search bar** at the top of the relevant page.
2. Enter the full name or part of the name of the item you wish to find.
3. The system automatically filters the displayed results based on the entered text.

For example, entering a keyword such as **"test"** will display all projects, spectra, or records whose names contain that keyword.

This feature helps users quickly locate specific items without manually browsing through the entire list.

B.2 Filtering Results

In addition to keyword search, Miraspec Flow provides filter options that allow users to narrow results according to specific parameters.

Common filtering options may include:

- **Scenario or model type**
- **User who created the item**
- **Date of creation or modification**
- **Item status or category**

Filters are typically available as selectable filter controls or dropdown menus. Users can select one or multiple filtering criteria to refine the displayed results.

For example, users may filter projects to show only those created by a specific user or associated with a particular analysis scenario.

B.3 Filtering by User

Items stored in the system may also be filtered by the user who created or modified them.

To filter items by user:

1. Select the **Created by** filter option.
2. Choose one or more users from the available list.
3. The system updates the displayed results to show only items associated with the selected users.

This feature is particularly useful in multi-user environments where projects and datasets are created by different operators.

B.4 Filtering by Date

Users can also filter items based on their creation or modification dates.

To filter by date:

1. Select the **Created at** or **Modified at** filter option.
2. Specify the desired date or date range.
3. The system will display only items that fall within the selected time period.

Date-based filtering helps users locate recently created or modified items and track project activity over time.

B.5 Sorting Results

In addition to search and filtering, many tables in Miraspec Flow support sorting options. Users can change the order in which items are displayed based on different attributes.

Typical sorting options include:

- item name
- creator
- creation date
- modification date

Sorting can usually be applied in **ascending or descending order**, allowing users to organize information according to their needs.

B.6 Resetting Filters

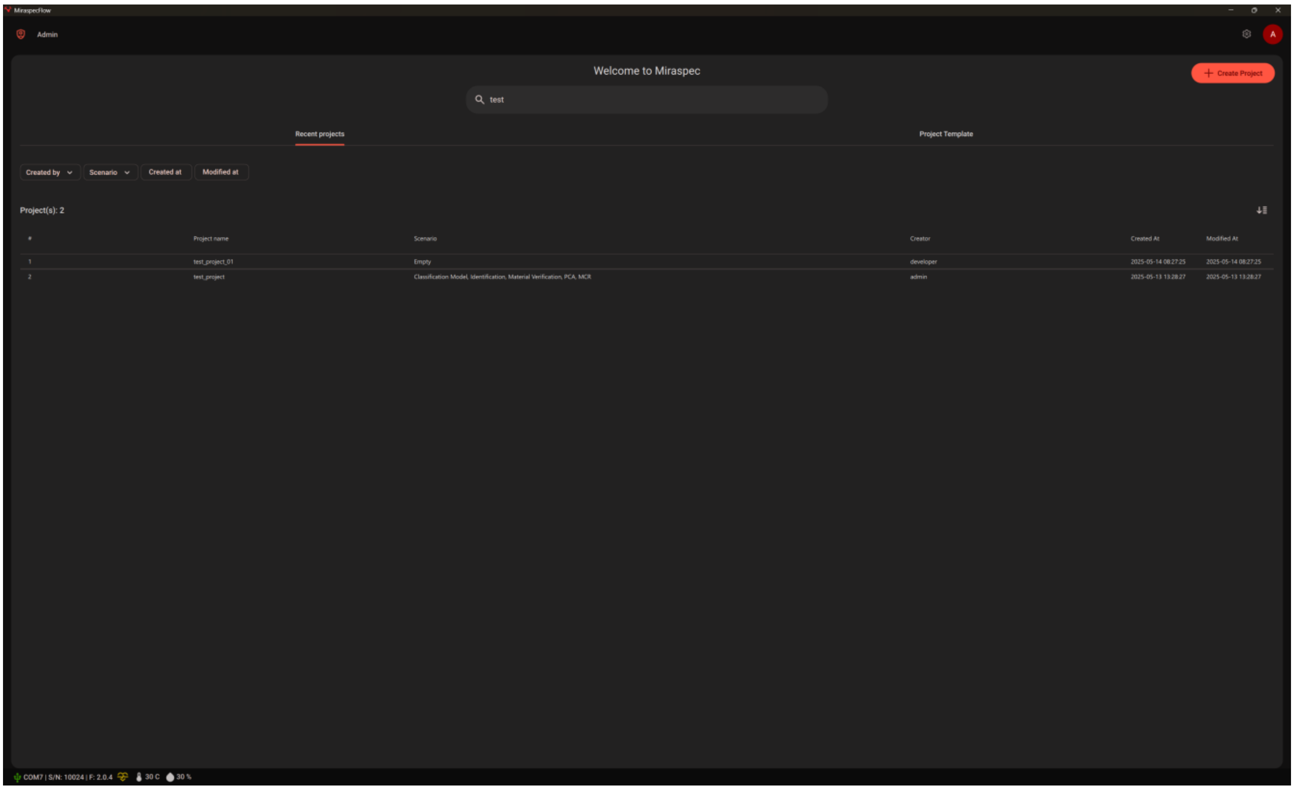
When filters are applied, only a subset of the available data may be displayed. To return to the full list of items, users can reset the active filters.

This can typically be done by selecting the **Reset Filters** option, which clears all active search terms and filtering criteria.

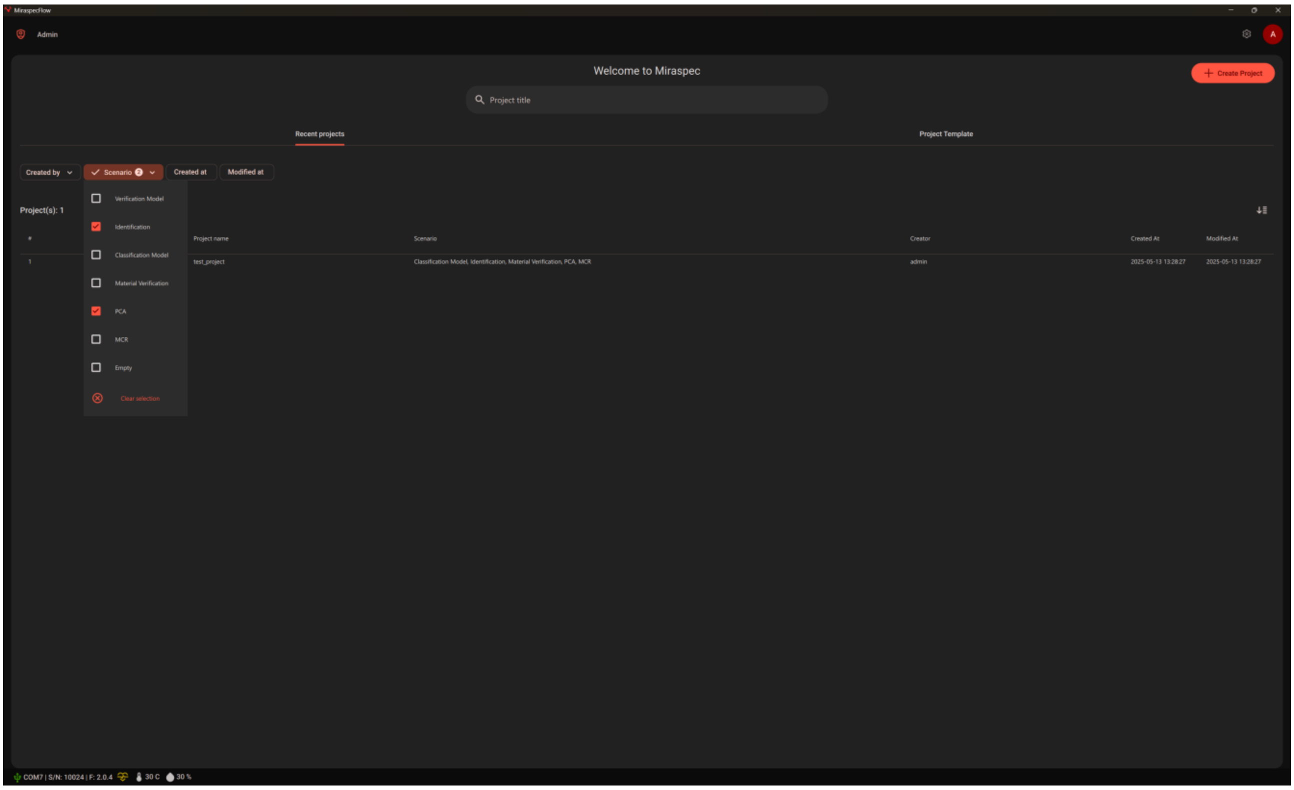
After resetting filters, the system displays the complete list of available items again.

B.7 Examples of using search and filtration function

In order to search for projects type the project name or part of project name in the search bar of the Welcome to Miraspec page. For example, let's search for all the projects containing the word "test". We type test in the search bar and only the corresponding projects are displayed now.

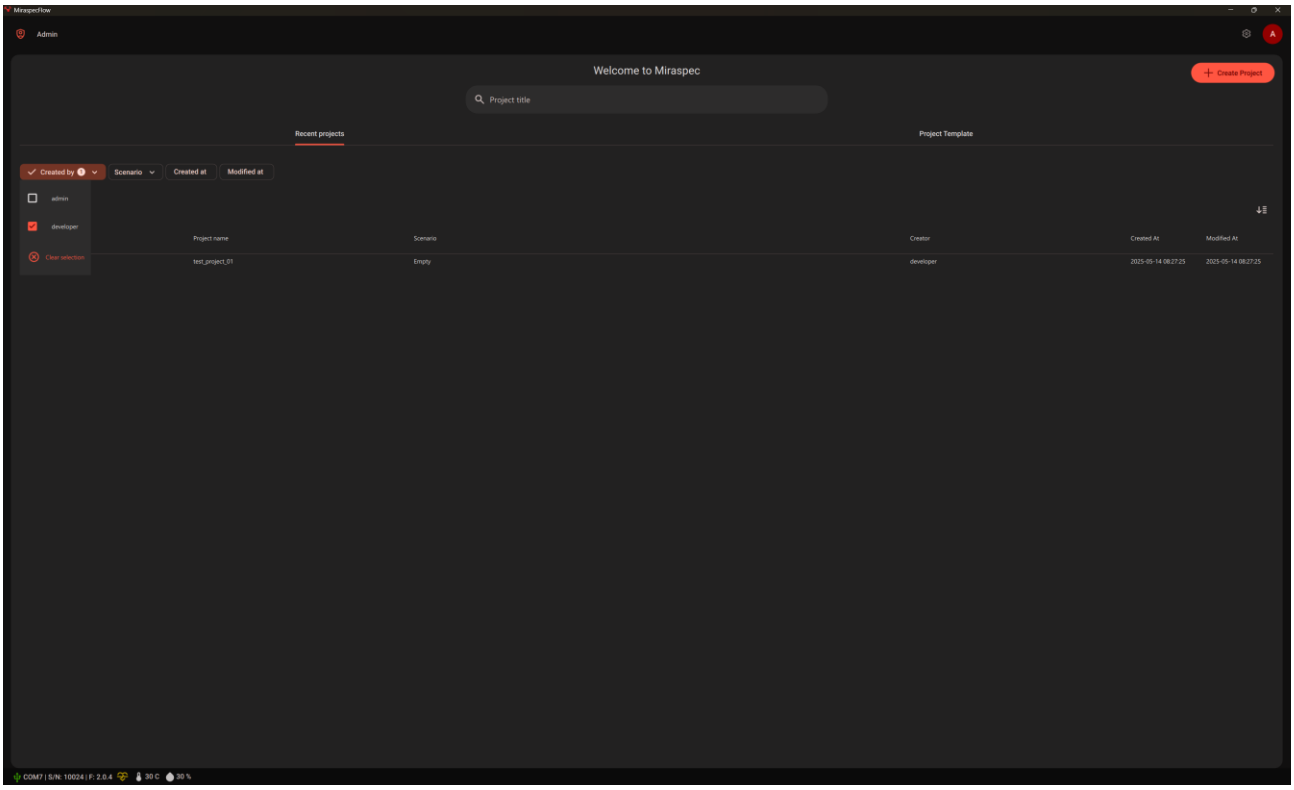


To choose the models corresponding to a certain scenario, click on Scenario button and select from the list of scenarios and models you are interested in.

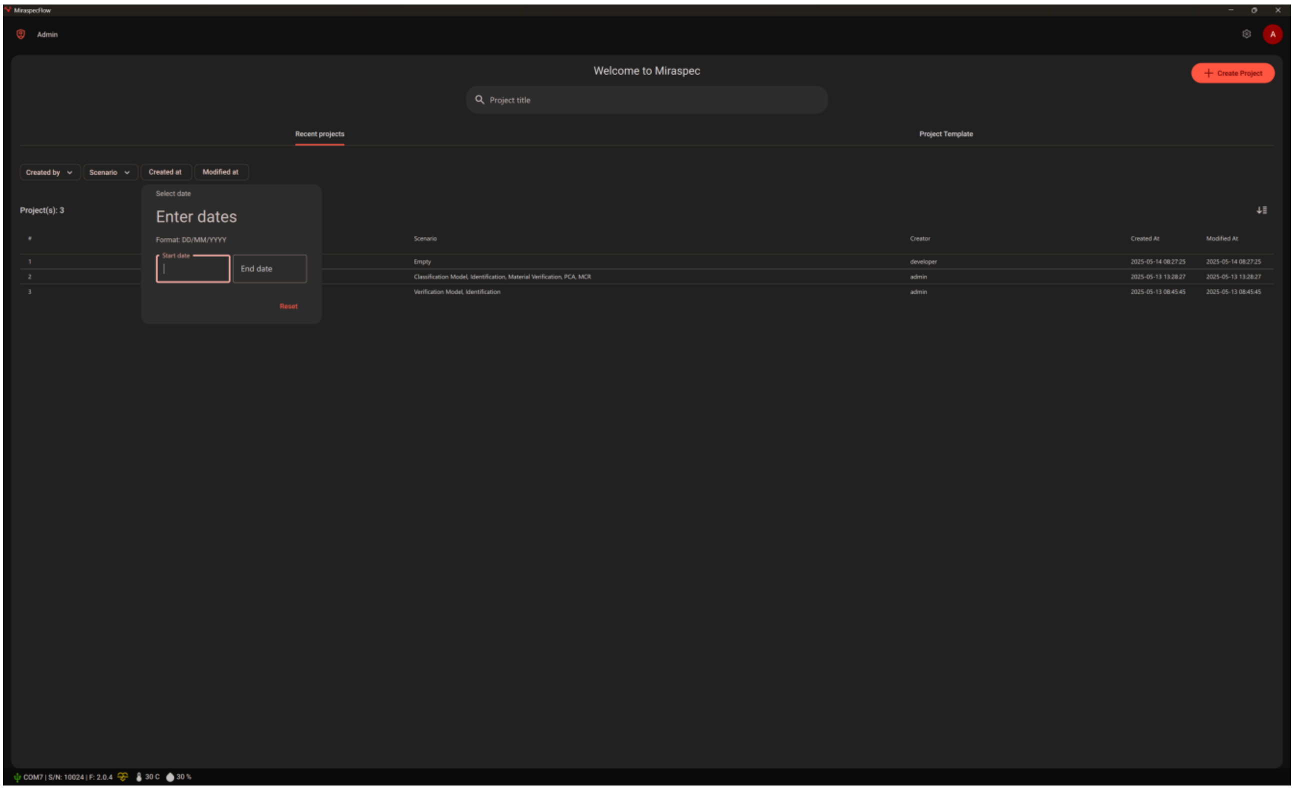


Filtration by data, user, status

There is also an option to filter by the user who created the project. Click on Created by and choose the user/users of interest.



There is also an option to search by date. Click on created at or modified at and corresponding projects would appear in the list of projects.


Welcome to Miraspec
Project title
Create Project
Recent projects
Project Template
Created by
Scenario
Created at
Modified at
Project(s): 3
Select date
Enter dates
Format: DD/MM/YYYY
Start date
End date
Reset

Appendix C – File formats

Miraspec Flow supports exporting and importing spectral data and analysis results in several commonly used file formats. These formats allow users to share data, perform further analysis in external software, or archive measurement results for documentation purposes. Supported export formats include:

- **TSV (Tab-Separated Values)**, which stores spectral data in a structured tabular format with metadata included in the file header;
- **JDX (JCAMP-DX)**, a standard format widely used for exchanging spectroscopic data between scientific software systems;
- **TXT (Text File)**, a plain text format containing spectral values that can be easily imported into data analysis tools or spreadsheets.

Users can select the preferred export format in the software settings depending on their workflow and compatibility requirements with external applications.

Appendix D – Database

D.1 Database Overview

Miraspec Flow uses an internal database to store information required for the operation of the system. The database allows the software to organize and retrieve data efficiently while maintaining data consistency and access control.

The database may store various types of information, including:

- user accounts and authentication data
- roles and permission settings
- spectral libraries and reference spectra
- trained analytical models
- project metadata and experiment records
- device configuration information
- system logs and audit records

By centralizing this information, the database supports reliable operation of the software and ensures that data can be accessed and managed across different projects and users.

D.2 Data Management

The database is managed automatically by Miraspec Flow during normal operation. Users typically do not need to interact directly with the database structure.

When users perform actions in the software, such as creating projects, uploading reference spectra, training models, or generating reports, the relevant information is stored and organized within the database.

Administrative users may manage certain database contents through the **Admin page**, where they can:

- manage user accounts and permissions
- maintain spectral libraries
- manage analytical models
- review experiment history and system records

These functions allow administrators to control how data is organized and accessed within the system.

D.3 Data Integrity and Backup

To prevent loss of important data, it is recommended that the database be included in regular system backup procedures. Backup strategies may depend on the specific system configuration and organizational policies.

Regular backups help ensure that critical data such as projects, spectral libraries, and trained models can be restored in case of hardware failure, software issues, or accidental data deletion.

System administrators should establish appropriate backup procedures for the database and related system files.

D.4 Database Access

Direct modification of the database outside the Miraspec Flow application is not recommended. Manual changes to database files or tables may result in data inconsistencies or software malfunction.

If database maintenance, migration, or recovery is required, it should be performed by qualified system administrators or by Lightnovo technical support.

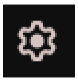
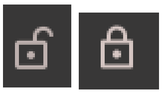
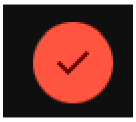
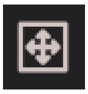
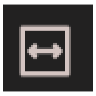
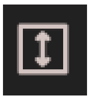
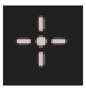
D.5 System Logs and Audit Records

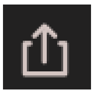
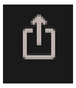
The database may also store system logs and audit records that track important system events. These records may include:

- user login activity
- project modifications
- model creation or updates
- system configuration changes

Audit records support system monitoring, troubleshooting, and traceability of actions performed within the software.

Appendix E – Table of UI icons

Icon	Description
	Home icon
	Settings icon
	Show panel/hide panel icon
	Lock icon
	Step forward/ step backward icons
	Finish icon
Graph icons	
	1 plot/2 plots
	Autoscaling icon
	Fit to window icon
	Fit horizontally icon
	Fit vertically icon
	Show legend icon
	Zoom in icon
	Zoom out icon
	Show tracer lines icon

Icon	Description
	Save graph icon
Spectral processing icons	
	Crop icon
	Spikes correction icon
	Smoothing icon
	Baseline correction icon
	Normalization icon
Dashboard/project icons – take screenshots	
	Upload spectra icon
	History icon
	Show/hide icon
	Add to dashboard
	Save icon
	Delete icon

Appendix F – Glossary

This glossary provides definitions of key terms used in Miraspec Flow and in Raman spectroscopy data analysis. The terms described below help clarify the concepts related to spectral acquisition, preprocessing, modeling, and analysis.

Accumulations

The number of repeated spectral measurements combined to produce a single spectrum. Averaging multiple accumulations can improve the signal-to-noise ratio by reducing random noise.

Baseline Correction

A preprocessing method used to remove background signals or fluorescence from a Raman spectrum. Baseline correction adjusts the spectral baseline so that the resulting spectrum more accurately represents the Raman signal of the sample.

Calibration Model

A mathematical model used for quantitative analysis. Calibration models are created using reference spectra from samples with known concentrations and are used to estimate the concentration of components in unknown samples.

Chemometrics

The application of statistical and mathematical methods to chemical data. In spectroscopy, chemometric methods are used to analyze complex spectral datasets and extract meaningful chemical information.

Classification Model

A type of analytical model used to assign an unknown spectrum to one of several predefined classes or material categories based on spectral features.

Detector

The optical sensor in a spectrometer that converts incoming light into an electrical signal that can be measured and processed by the software.

Integration Time

The duration for which the detector collects light during spectral acquisition. Increasing the integration time generally increases signal intensity but may also increase noise or risk detector saturation.

Library Search

A method used to identify unknown materials by comparing a measured spectrum with spectra stored in a reference spectral library.

MCR (Multivariate Curve Resolution)

A chemometric method used to separate overlapping spectral contributions in complex mixtures. MCR decomposes measured spectra into individual component spectra and their corresponding concentration profiles.

Normalization

A preprocessing step used to scale spectral intensity values so that spectra can be compared consistently. Normalization reduces variability caused by differences in measurement conditions or signal intensity.

PCA (Principal Component Analysis)

A statistical technique used to reduce the dimensionality of spectral data while preserving the most important variance in the dataset. PCA is commonly used for exploratory data analysis, visualization of spectral relationships, and identification of patterns in spectral datasets.

Preprocessing

A set of data processing operations applied to raw spectra before analysis. Preprocessing helps remove measurement artifacts and improves the reliability of subsequent modeling and analysis.

Raman Effect

A physical phenomenon in which incident light interacts with molecular vibrations in a sample and is scattered with a shift in wavelength. This shift provides information about the molecular structure of the material.

Raman Shift

The difference in wavelength or frequency between the incident laser light and the scattered light produced by the Raman effect. Raman shifts are typically expressed in **wavenumbers (cm^{-1})** and represent vibrational energy levels of molecules.

Raman Spectrum

A plot showing the intensity of scattered light as a function of Raman shift. The spectrum provides information about the molecular structure and chemical composition of a sample.

Reference Spectrum

A spectrum obtained from a known material and stored for comparison or model training. Reference spectra are commonly used in spectral libraries and model development.

Signal-to-Noise Ratio (SNR)

A measure of the strength of the Raman signal relative to background noise. Higher signal-to-noise ratios generally indicate higher quality spectral data.

Spectral Library

A collection of reference spectra representing known materials or compounds. Spectral libraries are used for comparison and identification of unknown samples.

Spectral Preprocessing

A set of mathematical operations applied to raw spectral data to improve quality and prepare the data for analysis. Common preprocessing steps include spike removal, smoothing, baseline correction, and normalization.

Spike Removal

A preprocessing technique used to remove sharp, isolated intensity spikes in a spectrum, which are typically caused by detector artifacts or cosmic rays.

Verification Model

A model used to confirm whether a measured spectrum corresponds to a specific known material by comparing the spectrum with a predefined reference model.

Wavenumber

A unit commonly used in spectroscopy, expressed in **cm^{-1}**, representing the reciprocal of wavelength. Wavenumbers are used to describe Raman shifts and vibrational energy levels.

Appendix G – Troubleshooting Guide

G.1 Device Not Detected

Problem
The spectrometer does not appear in the list of available devices.

Possible causes

- The device is not connected to the computer.
- Required device drivers are not installed.
- The USB or network connection is not functioning.
- The device is powered off.

Recommended actions

1. Verify that the spectrometer is powered on.
2. Check that the USB or Ethernet cable is properly connected.
3. Confirm that the device drivers are installed.
4. Restart Miraspec Flow and attempt device detection again.
5. If necessary, reconnect the device and restart the computer.

G.2 Unable to Establish Device Connection

Problem
The device appears in the device list but the connection cannot be established.

Possible causes

- Another application is using the device.
- The device communication interface is blocked.
- The device firmware is incompatible with the software version.

Recommended actions

1. Close other applications that may be accessing the spectrometer.
2. Click the **Reconnect** button in the device connection interface.
3. Disconnect and reconnect the device cable.
4. Restart Miraspec Flow and attempt to reconnect the device.

G.3 No Spectrum Acquired

Problem
The acquisition process starts but no spectrum is displayed.

Possible causes

- The laser is turned off.
- Integration time is set too low.

- The sample is not positioned correctly in the optical path.
- The detector is not receiving signal.

Recommended actions

1. Ensure that the laser is enabled.
2. Increase the integration time.
3. Verify that the sample is placed correctly in the measurement position.
4. Check that the spectrometer device is functioning normally.

G.4 Saturated Detector

Problem

The measured spectrum shows saturated intensity values.

Possible causes

- Laser power is too high.
- Integration time is too long.
- The sample produces a very strong Raman signal.

Recommended actions

1. Reduce the laser power.
2. Decrease the integration time.
3. Reduce the number of accumulations if applicable.
4. Reacquire the spectrum after adjusting parameters.

G.5 Poor Signal-to-Noise Ratio

Problem

The acquired spectrum contains excessive noise.

Possible causes

- Integration time is too short.
- Laser power is too low.
- Sample signal is weak.
- Environmental light interference.

Recommended actions

1. Increase the integration time.
2. Increase the number of repetitions or accumulations.
3. Verify that the sample is properly aligned with the laser beam.
4. Minimize ambient light in the measurement environment.

G.6 Model Not Loading

Problem
A stored analytical model cannot be loaded in the software.

Possible causes

- The model file is corrupted.
- The model was created using a different software version.
- The project does not contain the required preprocessing configuration.

Recommended actions

1. Verify that the model file exists and is accessible.
2. Ensure the software version supports the model.
3. Reload the project or import the model again if necessary.

G.7 Database or Data Storage Issues

Problem
Project data, spectra, or models cannot be accessed.

Possible causes

- The database connection failed.
- Project files are missing or corrupted.
- Insufficient storage space.

Recommended actions

1. Restart the Miraspec Flow application.
2. Verify that the project directory exists.
3. Ensure sufficient disk space is available.
4. Restore project data from a backup if available.

G.8 General Troubleshooting Recommendations

If an issue occurs during operation:

1. Verify that the device is properly connected and powered.
2. Confirm that the correct device is selected in the software.
3. Check acquisition parameters such as laser power and integration time.
4. Restart the software application.
5. Restart the computer if the problem persists.

These steps resolve many common operational issues.

Appendix H - System Requirements

H.1 Minimum System Requirements

Component	Specification
OS	Windows 10 64-bit (version 1903 or later)
CPU	Intel Core i5 8th-gen / AMD Ryzen 5 3rd-gen, 4+ cores
RAM	8 GB DDR4
GPU / Graphics	OpenGL 3.3 compatible (integrated GPU accepted)
Storage	5 GB free (HDD)
Display	1366 × 768
Ports	USB 2.0 or COM port (Raman device connection)

H.2 Recommended System Requirements

Component	Specification
OS	Windows 11 64-bit (latest updates)
CPU	Intel Core i7 10th-gen or newer / AMD Ryzen 7 5000 series or newer, 6+ cores
RAM	16 GB DDR4 or higher
GPU / Graphics	Dedicated GPU with OpenGL 4.5+ support (NVIDIA or AMD)
Storage	10 GB free on NVMe SSD
Display	1920 × 1080 (Full HD) or higher
Ports	USB 3.0 or COM port

Appendix I - Contacting Technical Support

If the problem cannot be resolved using the troubleshooting recommendations, contact Lightnovo technical support.

When contacting support, please provide the following information:

- Customer or organization name
- Instrument model and serial number
- Screenshots illustrating the issue
- A detailed description of the problem
- Miraspec software version
- Computer specifications (operating system, RAM, processor, and storage)

Providing this information helps the support team diagnose and resolve the issue more efficiently.

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