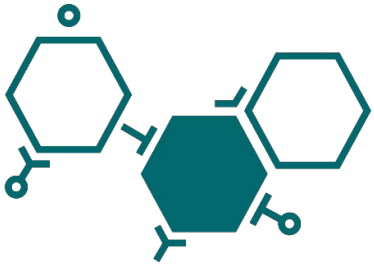

SpecSuite

SPECTROSCOPY SOFTWARE

SpecSuite Installation and User Manual

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SpecSuite

SpecSuite Software Version 1.1.11

Tutorial

8.0105.8053EN/ v2 / 2026-04-15

Metrohm Spectro, Inc.
Plainsboro Township, NJ 08536

This documentation is an original document.

This documentation has been prepared with great care. However, errors cannot be eliminated. Please send comments regarding possible errors to the address above.

Disclaimer
Deficiencies arising from circumstances that are not the responsibility of Metrohm, such as improper storage or improper use, etc., are expressly excluded from the warranty. Unauthorized modifications to the product (e.g., conversions or attachments) exclude any liability on the part of the manufacturer for resulting damage and its consequences. Instructions and notes in the Metrohm product documentation must be strictly followed. Otherwise, Metrohm's liability is excluded.

Contents

1. Overview

1.1 Introduction

The SpecSuite software is used with Metrohm laboratory i-Raman instruments and m-oem DIY Raman kits. SpecSuite can perform the following:

- Operate laboratory i-Raman instruments and DIY Raman kits to analyze samples
- Process and analyze the collected or imported spectra
- Perform identification and quantification of samples with proper licenses installed
- Generate, sign, and print reports
- Facilitate compliance with the FDA 21 CFR Part 11 code with proper licenses installed
- Administrate users and workflow
- Store data and track changes with an Audit Trail

1.2 Licensing

SpecSuite is a modular platform. Instrument functions and software modules can be freely combined. Instrument functions are available as license packages:

- **Basic** – Real-time data visualization and simple control over parameters like laser power, integration time, spectral averaging, and basic spectral processing.
- **Identification** – Supports creation of custom Raman libraries for identifying unknowns or verifying known substances.
- **Quantitative**– Facilitates the development and deployment of a prediction model for streamlined routine analysis.
- **Regulatory compliance** – Supports Audit Trail, electronic signatures, and other 21CFR Part 11 functionalities.
- **Libraries** – Licenses for Metrohm Raman spectral libraries are also available for use with the identification license.

Additional information on the licenses can be obtained from your local Metrohm sales organization.

Trial license

The initial installation of SpecSuite includes a 30-day trial license. This trial license includes all licensed modules, including 21CFR Part 11 compliance. Each time the software is opened, a message notifies the user of how much time remains on the license. The expiration date is also displayed on the License table in the Settings module.

2. Installation and Setup

2.1 System Requirements

Minimum System Requirements	
Operating system:	Windows 10 (1607) or later Windows 11 (x64) Windows Server 2016 or greater
CPU:	x64 processor – 1.4 GHz or faster
Memory (RAM):	4 GB or more
Disk:	20GB or more
Privileges:	Windows Administrator rights

Recommended System Requirements	
Operating system:	Windows 11 or Windows 10 (22H2) Windows Server 2022 or greater
CPU:	Multi-core processor at 2.0 GHz or faster
Memory (RAM):	8 GB or more
Disk:	SSD storage with 30+ GB free space
Privileges:	Windows Administrator rights

Database:

SpecSuite uses MS SQL Server 2022 for data storage. An Express edition of MS SQL Server 2022 is automatically installed during SpecSuite installation.

By default, a server named “ENTERPRISE” is created locally, and a database named ‘SpecSuiteDB’ is created on the server. IT users can create multiple databases. Each MS SQL Server Express database created on the server has a size limit of 10GB.

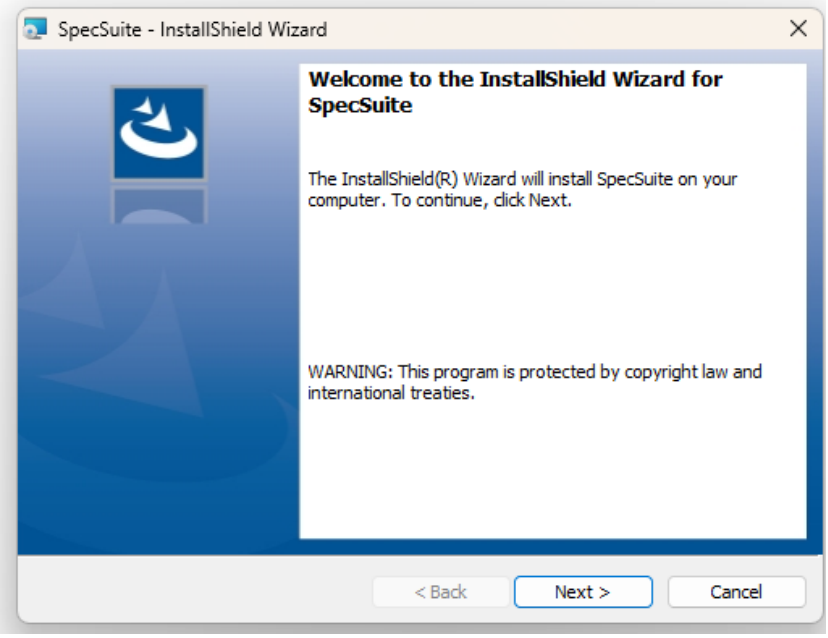
For addition information and installation requirements about MS SQL Server 2022 refer to Microsoft website SQL Server Installation Guide - SQL Server | Microsoft Learn

2.2 Installing SpecSuite

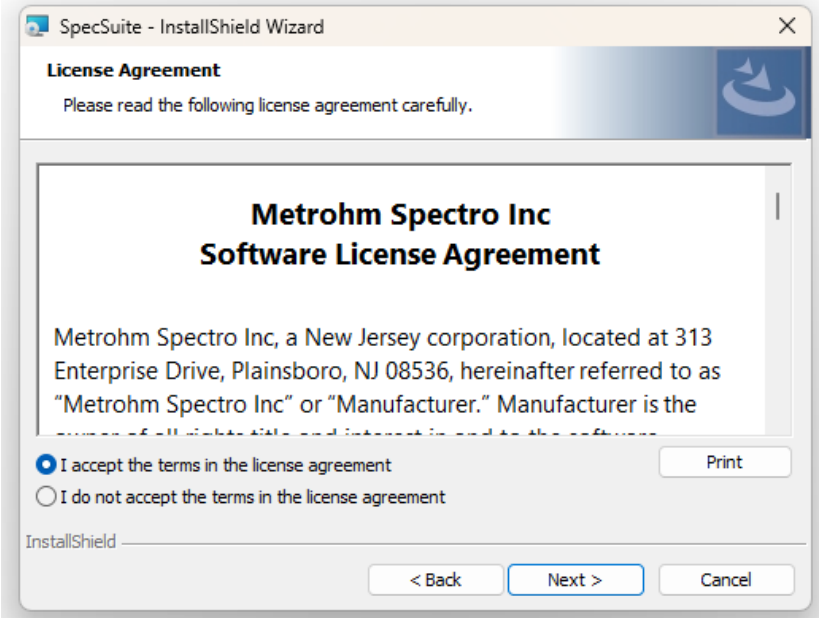
1. Ensure the system PC fulfills the minimum system requirements.
2. Ensure Windows administrative rights are granted before installing SpecSuite.
3. Download the compressed file for the release version of SpecSuite. Extract the files, then open the ‘SpecSuite_[version]’ folder. Right-click setup.exe and select Run as Administrator. The InstallShield Wizard for SpecSuite will appear.

NOTE: The location of the installation folder is not important, as the installer copies data to a temporary folder on the PC: C:\SQL2022TempFolder. Please consult with your IT department to confirm Write-access at this location.

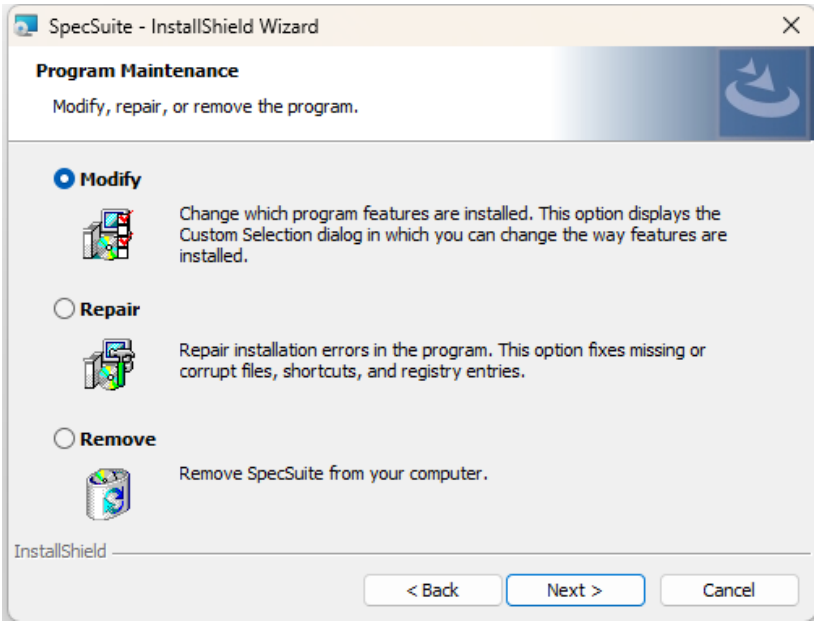
4. Click Next to continue the installation.



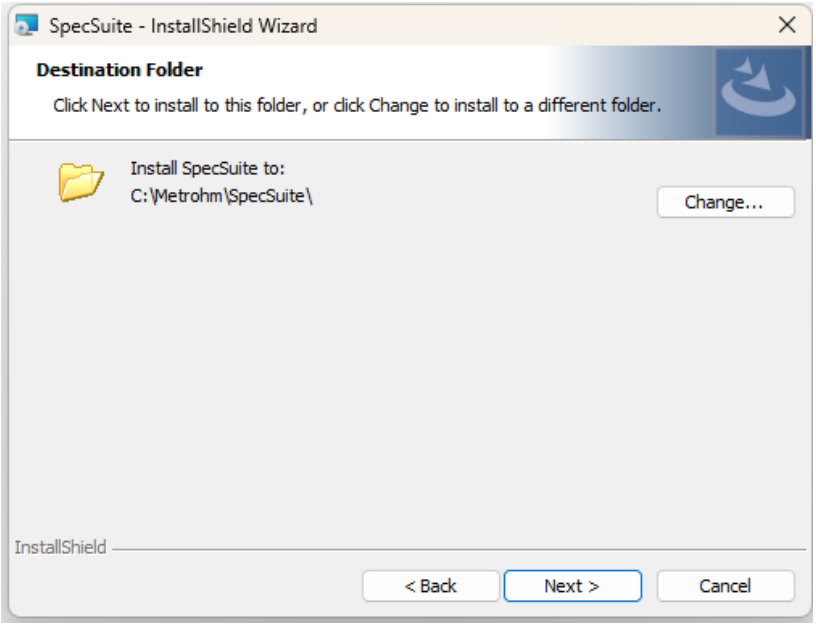
5. When the Metrohm Software License Agreement appears, choose “I accept the terms in the license agreement” then press Next.



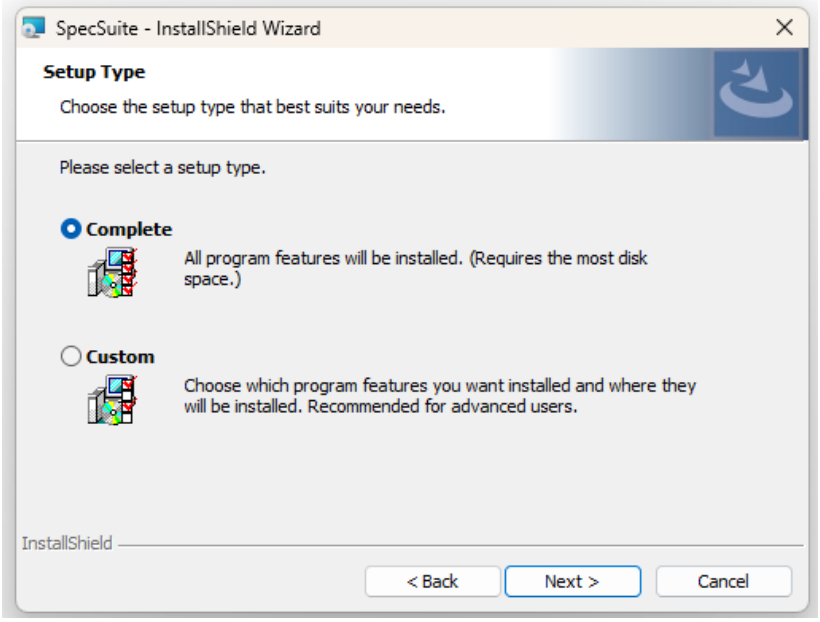
NOTE: If SpecSuite is already installed with the same version, the Program Maintenance options will appear. Select Modify or Repair, then Next to continue.



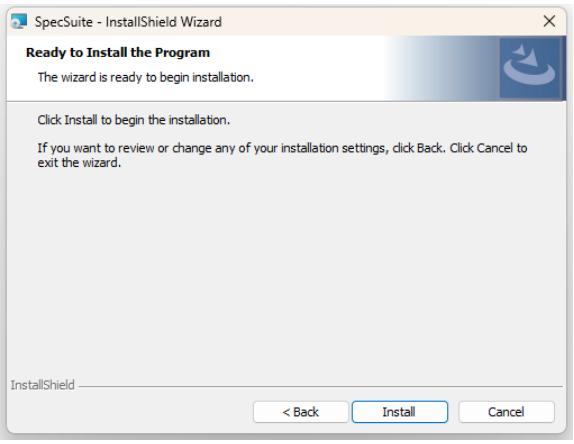
6. The installer will install SpecSuite to the default location: **C:\Metrohm\SpecSuite**. Use this default location and click Next.

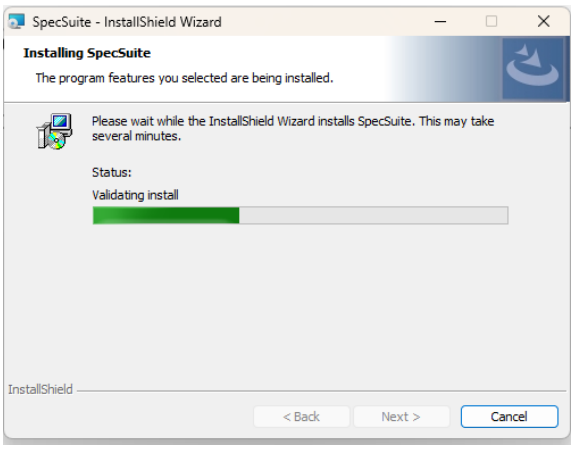


7. Under Setup Type, select Complete, then click Next.

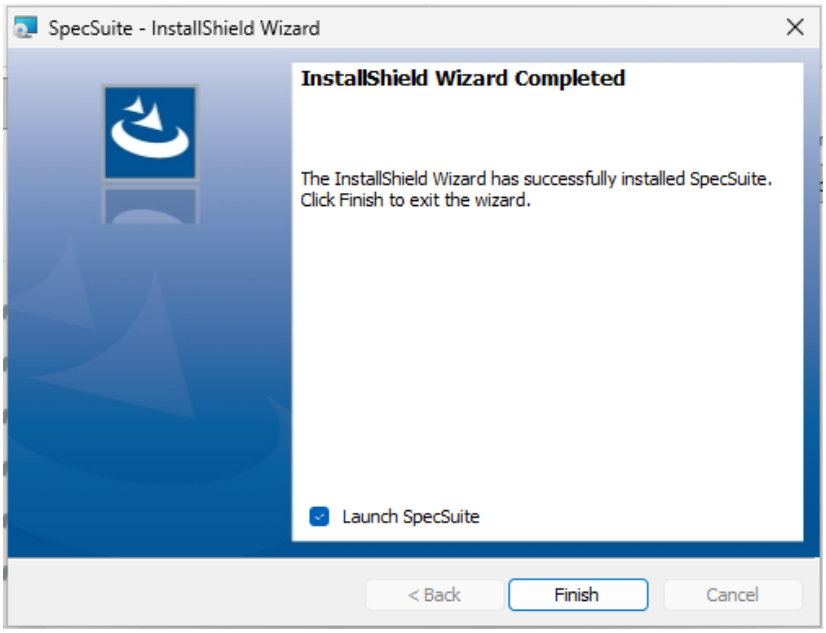


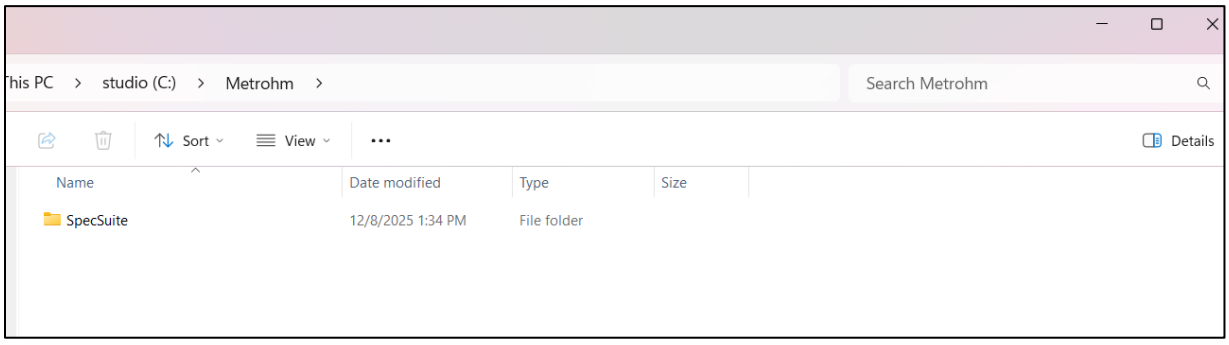
8. Click Install to begin installation. The installation should take approximately 1 minute.



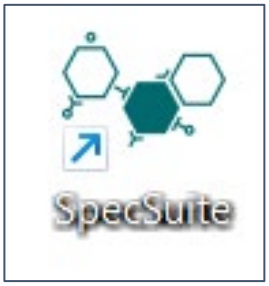


9. After the SpecSuite installation is completed, a message reporting successful installation will appear. Press Finish to close the installer. SpecSuite software is now successfully installed:





10. Locate the SpecSuite desktop icon and double-click to launch the SpecSuite software.

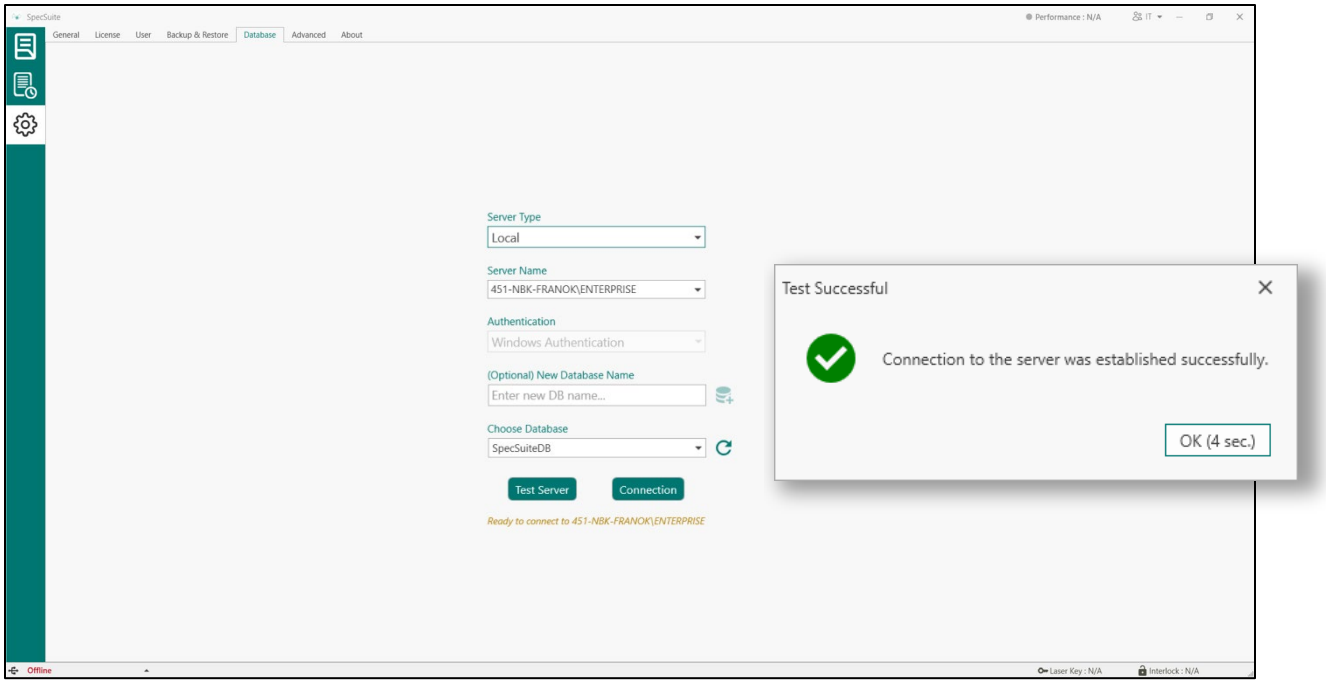


2.3 Setup Local SQL Express Database

During the SpecSuite installation, a local server named “ENTERPRISE” is automatically created. During the first startup of the software, a default database “SpecSuiteDB” will be created automatically on the ENTERPRISE server.

Check that this connection is successful:

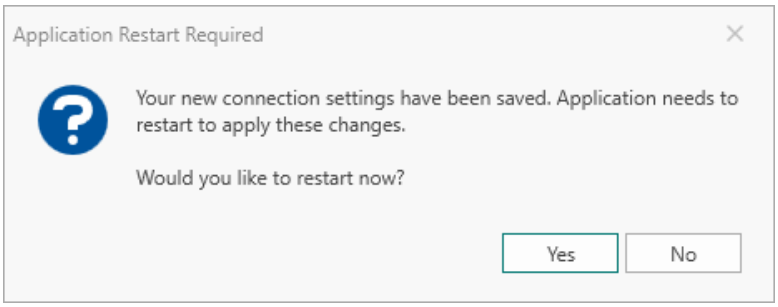
1. Log in to SpecSuite using the default IT account user name “IT”.
    a. For the first time login, use password 999999, then reset the password.
2. Go to Settings > Database.
3. Press Test Connection.
    a. The message "Connection to the server was established successfully" should appear:



To connect to a different local server

1. Log in to SpecSuite with an IT account.
2. Go to Settings > Database.
3. In the Server Name field, enter a known server name to connect to.
4. Press Test Connection to see if the Server is available.
5. If successful, press Connection.
    a. SpecSuite must restart to finish connecting to the new server.
6. Press Yes on the restart prompt.

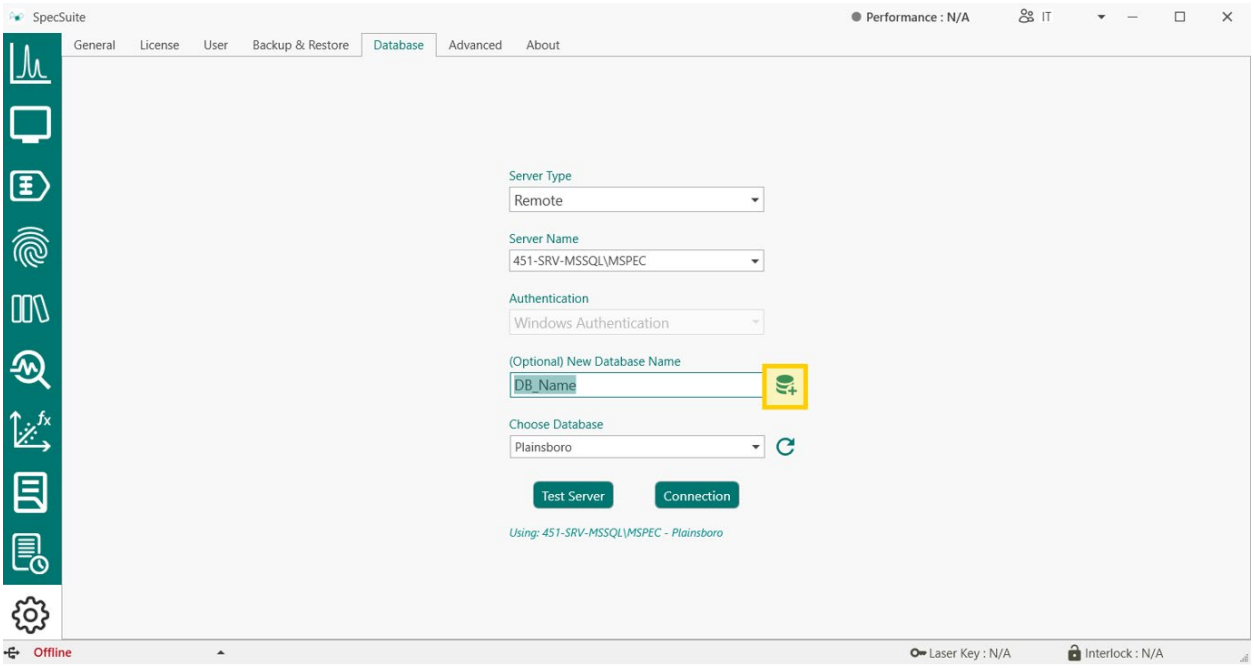
NOTE: SpecSuite is only compatible with MS SQL Server 2022. Performance on other versions is not guaranteed.



To create a new local database

In some cases, the user may not want to use the default database connection. SpecSuite allows users to create a new database inside the selected server.

1. Log in with an IT account.
2. Select Settings > Database tab.
3. Select the server instance where the database will be created.
4. Enter a new database name.
5. Press the Create New Database button:



6. Once a new database is created, choose the name from the Choose Database dropdown.
7. Click Connect.

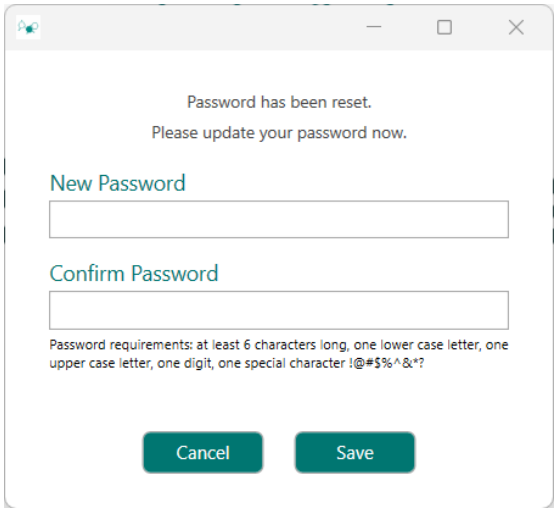
The default database uses an SQL Server Express database with a 10 GB storage limit.

2.4 First Time Login

Default Accounts

Username	Password
ADMIN	999999
IT	999999

After the first login, a password change dialog appears.



The password must be successfully changed to complete the login.

First Time Login

1. Open SpecSuite.
2. Enter username "ADMIN".
3. Enter password "999999".
4. Enter and **record** the new password for the ADMIN account.

2.5 Login Username and Password

On the login screen, enter the username and password for the account.

- Both credentials are case sensitive.
- The user can log in with the Login button or by pressing the Enter key.

If a password reset is required, the user will receive a prompt to update their password.

- Usernames are unique for all clients connected to the same database.
- A user can only be logged into one instance of SpecSuite.
    - If a user tries to log in to an account while this account is already logged in elsewhere, the new user will receive a notification that the account is already in use.

2.6 Software Setup

SpecSuite software must be installed before connecting to an i-Raman instrument or a DIY kit.

Import Licenses for SpecSuite and Metrohm Libraries

The license file for SpecSuite controls the modules available in the software and access to use Metrohm Libraries. The license file is tied to the serial number of the instrument for one-time activation. Licenses can be renewed or updated by importing a new license with the same or a different instrument SN. The instrument with the license's serial number must be connected to update a License.

Import License

1. Log in to SpecSuite with an ADMIN or IT account.
2. Select Settings.
3. Select License tab.
4. Select Load.
5. Locate the license file.
    a. *.lic file type
    b. Example: 195400102612001.Lic
6. Select Open.

Configure Probe (Ratio3)

In Hardware setup, the probe setup configures a Ratio3 file for the system.

The Ratio3 file corrects the shape and relative intensity of the spectra. It is needed for Performance Validation and should be used for all acquisitions.

Configure Probe

1. Turn on the instrument and connect it to the computer.
2. Log in to the ADMIN account.
3. Select Instrument.
4. Select Hardware Setup tab.
5. Select Probe to expand.

6. Enter Probe Name and Probe SN.
7. Select the Select button.
8. Locate the Ratio3 TXT file for your instrument and probe configuration.
    a. Ratio3 files are unique for each instrument and probe configuration. If a probe is changed, a new Ratio3 file must be loaded or created.
9. Select Save Probe.
10. Verify the Probe file is in the list, and the check mark is selected.

Import Performance Validation Reference file

The Performance Validation Reference (PVR) file is used to validate the instrument's performance. Instruments could be delivered with a PVR file designated for the instrument. This file should be imported to run validation.

If there are changes to the instrument or probe, a new PVR file may be required.

Import PVR file

1. Turn on the instrument and connect it to the computer.
2. Log in to the ADMIN account.
3. Select Instrument.
4. Select Performance.
5. Select Import PVR.
6. Locate the PVR file for your instrument and probe configuration.
    a. *.PVR file type
    b. Instrument SN, Probe SN, and time of creation are part of the file name
    c. Example: 19540010.26001-230105959-26-01-01.pvr
7. Select Open.
8. Select OK to clear the successful import message.

Import Metrohm Libraries (optional)

A license for the Metrohm Illicit and General Chemicals library is automatically installed with SpecSuite. The Metrohm Illicit and General Chemicals library package must be imported to display and activate it for use in measurements.

Additional libraries can be loaded using the same process but require additional licenses.

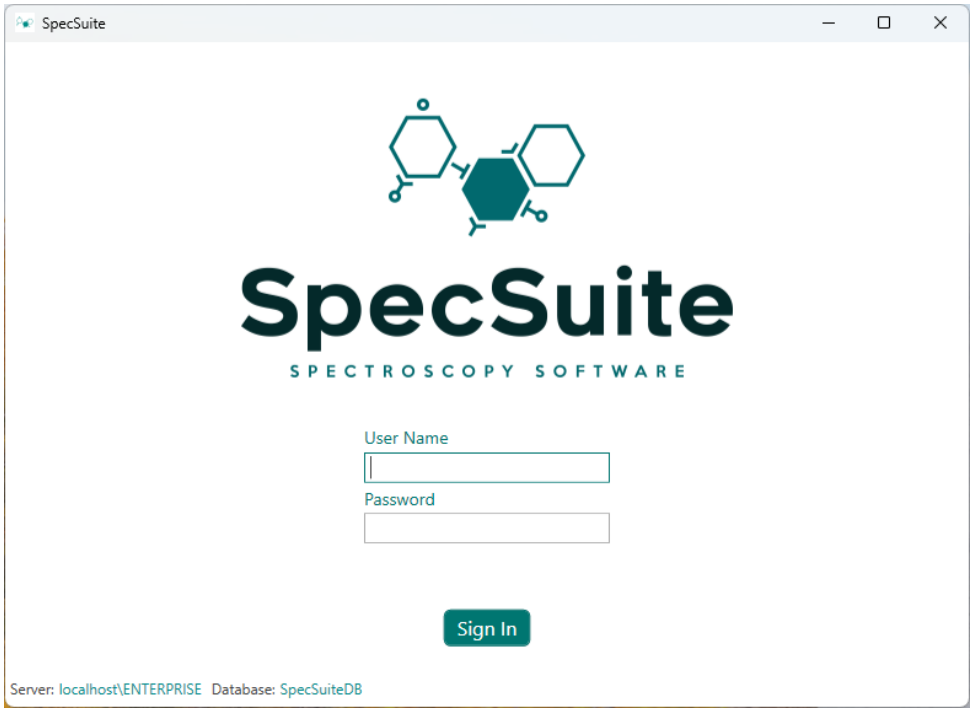
Install the Illicit and General Chemical library

1. Log in to the ADMIN account.
2. Select Library.
3. Select Import.
4. Locate the MSI_library_[Version]_Illicit and General Chemicals.zip file.
5. Select Open and wait for the package to finish importing.
6. Select OK to clear the successful import message.

Install the STContainer library

1. Login to the ADMIN account.
2. Select Library.
3. Select Import.
4. Locate the MSI_library_[Version]_STContainer file.
5. Select Open.
6. Wait for import.

3. SpecSuite Login Screen



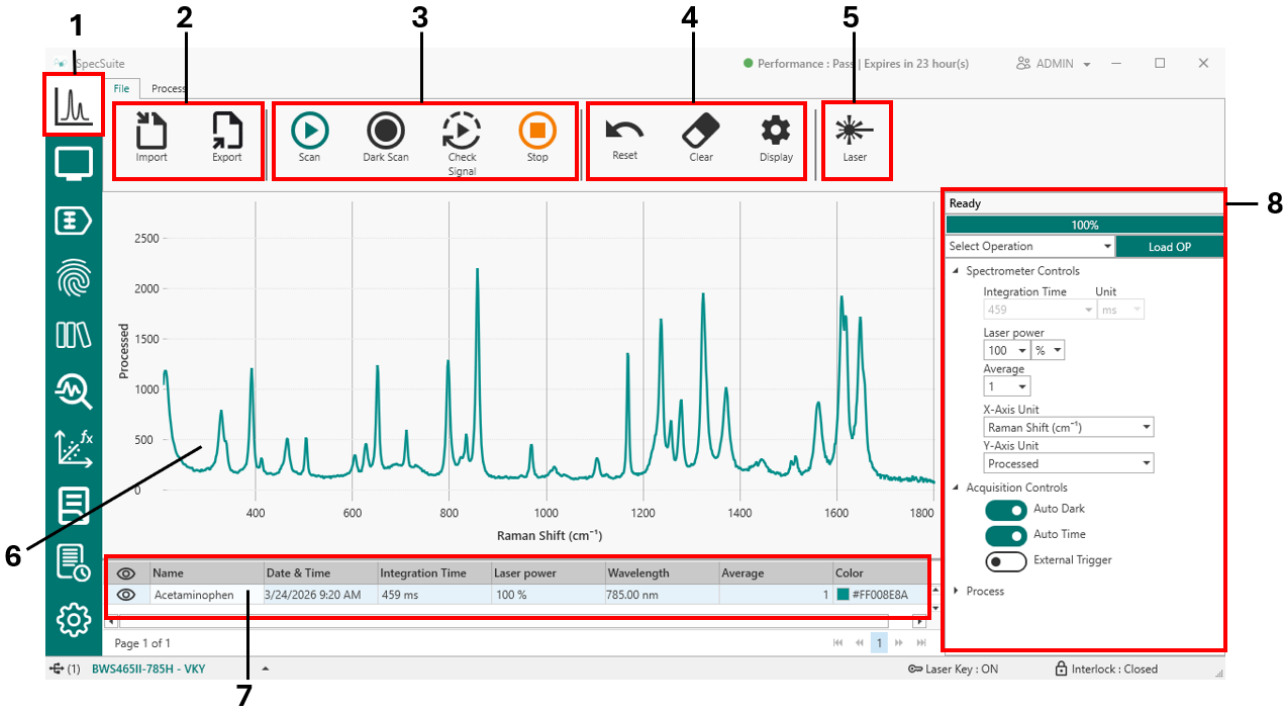
The Login window appears when SpecSuite is launched. After logging in, SpecSuite opens to different modules based on the user's account type. IT and Administrator account logins open to the Settings module. Developer account logins open to the Explore module, and Operator account logins open to the Operating Procedure module.

Refer to Section 2.4 and 2.5 for additional login information.

4. Explore

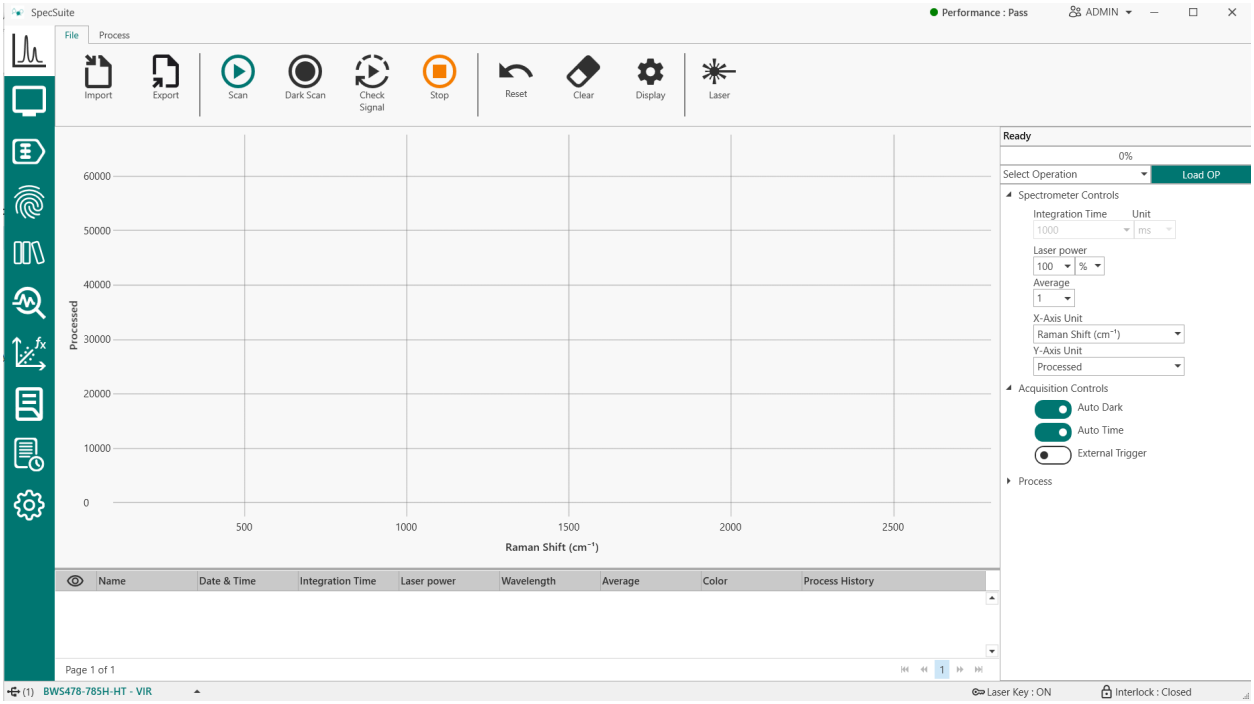
Explore is the most versatile module in SpecSuite, designed to collect and process data freely. Some applications for the explore workspace include:

- Experimenting with different data processing.
- Focusing the laser on a sample if using a probe stand or microscope.
- Viewing and processing existing data.



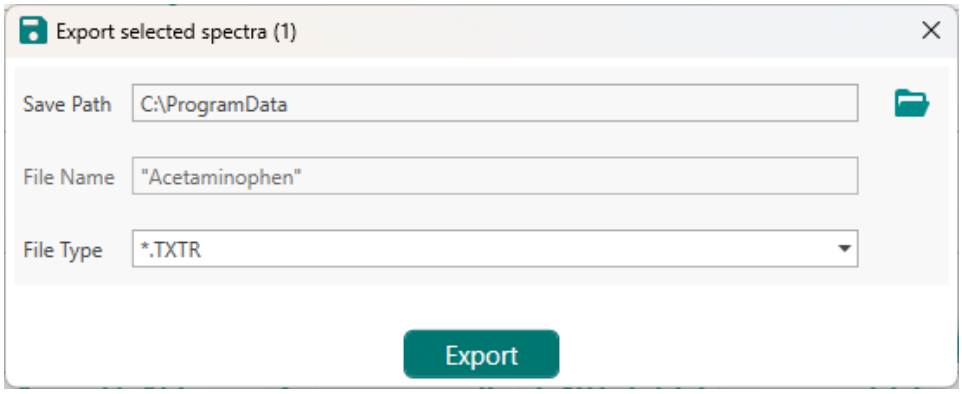
1	**Explore**	2	**Import and Export**
3	**Acquisition controls**	4	**Display controls**
5	**Laser controls**	6	**Spectrum plot**
7	**Data List**	8	**Acquisition control panel**

4.1 File Ribbon



In the top File ribbon, the user may:

- **Import** – Imports a file from the local hard drive of their computer. Imported data are not saved in the database.
    - Allowed file types are: .CSV, .TXTR, .TXT and .SPC.
- **Export** – Exports the selected spectral data file(s).



    - **Export file types are**: .TXTR, .CSV (Raw CSV), .CSV (Simple CSV), and .SPC (Simple SPC).

Export Spectral File Format Types:

TXTR

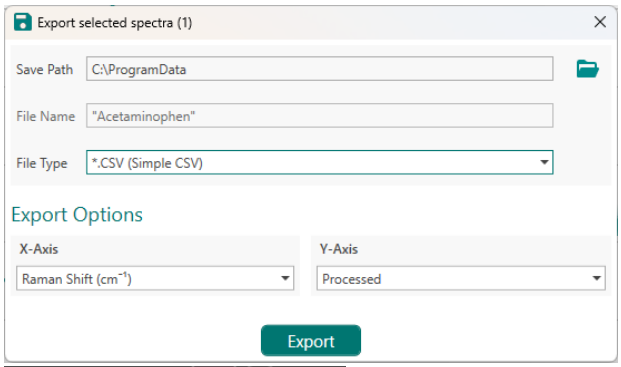
The TXTR file is a rich text format defined by Metrohm. It contains the most comprehensive information about the selected spectrum, including measurement metadata and all available x/y-axis information.

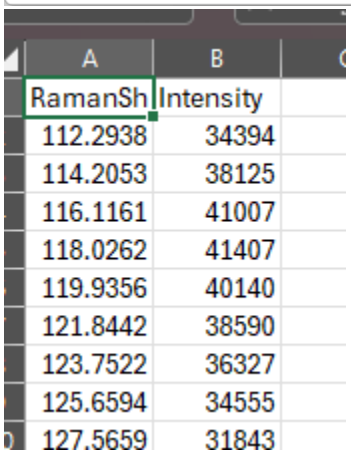
CSV (Raw CSV)

The Raw CSV file is a rich CSV format defined by Metrohm. It contains the same information as TXTR but is exported in CSV format.

CSV (Simple CSV)

The Simple CSV file is a 2-column CSV format that contains the X-axis and Y-axis data in the units the user selects in the Export Options dropdowns.



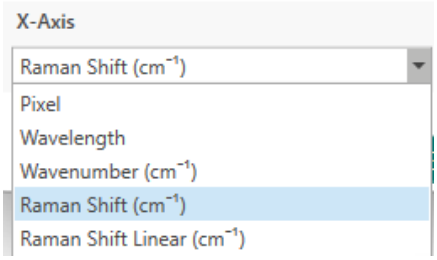


A	B
RamanSh	Intensity
112.2938	34394
114.2053	38125
116.1161	41007
118.0262	41407
119.9356	40140
121.8442	38590
123.7522	36327
125.6594	34555
127.5659	31843

The available X-axis types are:

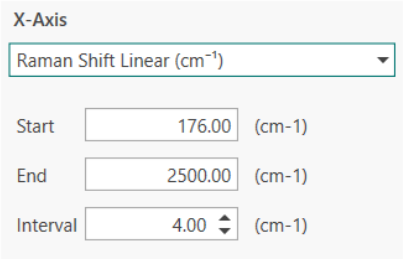
1. Pixel: When selected, the x-axis data will be arranged based on the instrument's detector pixel dimensions.

2. Wavelength (nm): When selected, the x-axis data will be interpolated from pixel to wavelength.
3. Wavenumber (cm^{-1}): When selected, the x-axis data will be interpolated from pixel to wavelength, then converted to absolute wavenumber.
4. Raman shift (cm^{-1}): When selected, x-axis data will be interpolated from pixel to wavelength, then converted to absolute wavenumber, then converted to Raman shift based on the instrument's laser wavelength with a default 4 cm^{-1} interpolation and default Raman shift range based on the instrument model.

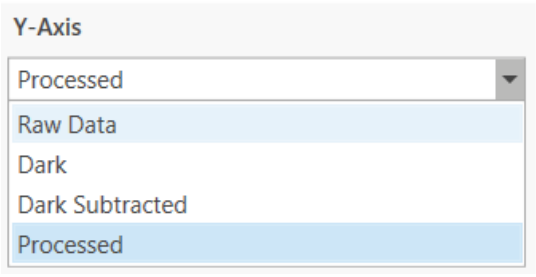


5. Raman Shift Linear (cm^{-1}): When selected, x-axis data will be interpolated from pixel to wavelength, then converted to absolute wavenumber, then converted to Raman shift based on the instrument's laser wavelength, with the start/finish Raman shift and interpolation interval set by the user in the Export Options dialog.

Export Options



The available Y-axis are:



1. Raw Data: Spectral intensity directly recorded on the detector, without any processing.

2. Dark: Spectral intensity recorded when the laser is turned off (with the same parameters as the laser-on scan) with no additional processing.

3. Dark Subtracted: Raw Data minus the Dark data.

4. Processed: Processed data is the relative intensity corrected spectra data with all the additional processing (smoothing, derivative, normalization, baseline correction) that the user applied on the spectra entry.

SPC (Simple SPC)

Simple SPC is a simple 2-column standard SPC format that follows the same axis convention as simple CSV.

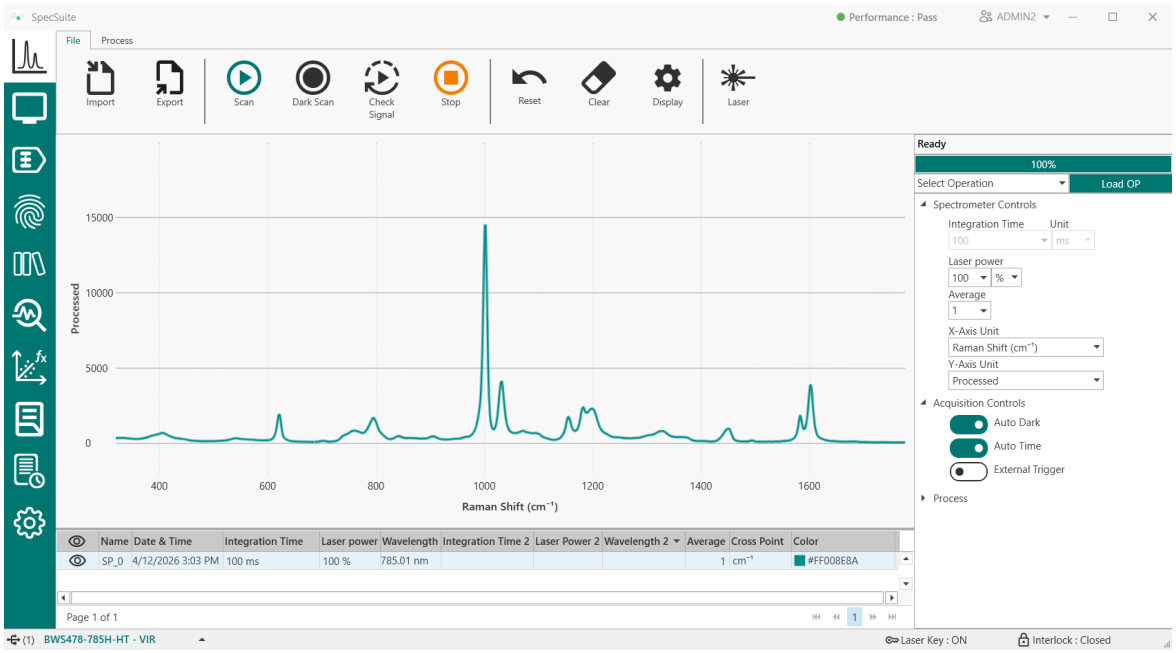
Simple CSV and Simple SPC files are not available for the i-Raman Duo.

Import Spectral File Format Types:

SpecSuite supports all file types mentioned in section 4.1.1 and all TXTR, CSV, and SPC file types from BWSpec 4.15. Multiple different file types can be imported simultaneously.

4.2 Acquisition Settings

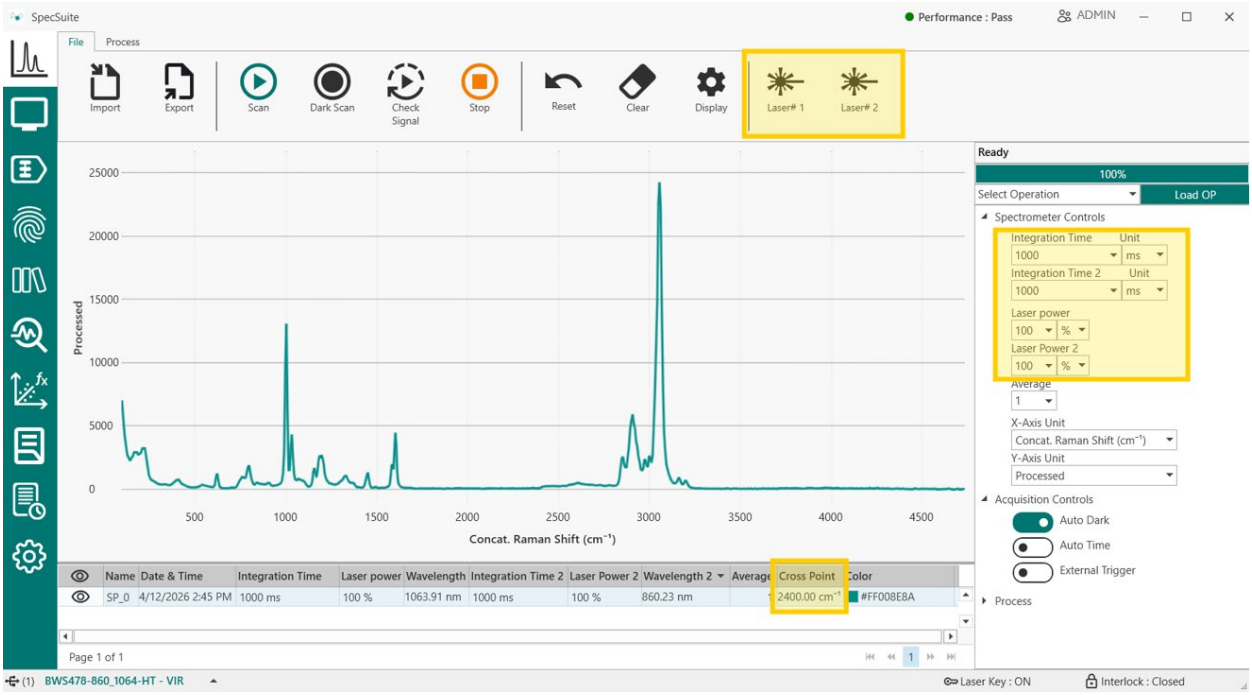
The Explore page allows the user to adjust acquisition parameters to fine-tune data collection.



Acquisition parameters are set in the right panel of the chart. Under Spectrometer Controls, the user can set:

- Integration Time (range depends on connected spectrometer) and Unit (ms, sec, min)
- Laser power (1- 100%)
- Average

When an i-Raman Duo or DIY Extended Range is connected, SpecSuite supports acquisitions with up to 2 lasers and 1 spectrometer to cover a wide Raman shift range. When two lasers are used, settings for both lasers will appear in the acquisition controls. Laser power and integration time may be different for both. When two lasers are enabled, a new column labeled "Cross Point" appears in the data list. The Cross Point is the point at which the spectra from each laser are concatenated together to form one full spectrum.



The units of each axis can be changed in the same panel.

X-axis options:

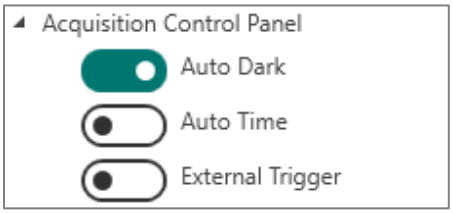
- Pixel
- Wavelength (nm)
- Wavenumber (cm^{-1})
- Raman Shift (cm^{-1})

Y-axis options:

- Raw Data
- Dark
- Dark Subtracted
- Processed

- Concatenated Raman Shift (cm^{-1})

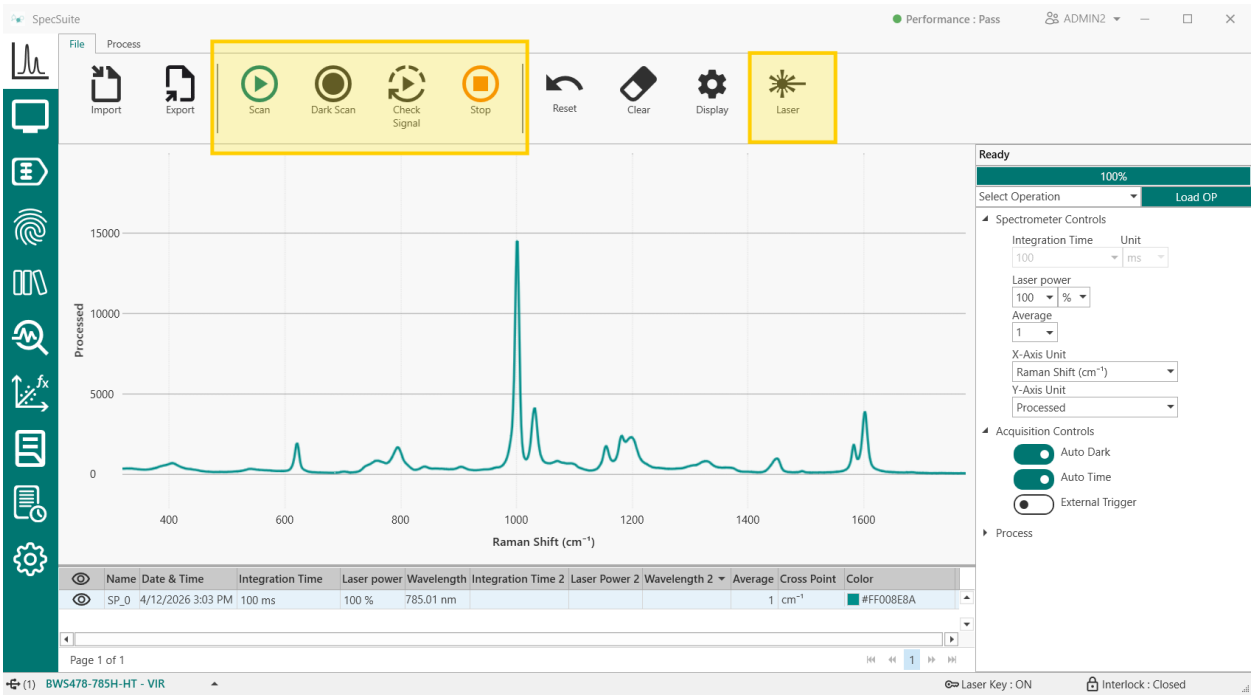
4.3 Acquisition Control Panel



The Acquisition Control Panel has additional controls:

- Auto Dark – When enabled, a dark scan is automatically collected after every data scan.
- Auto Time – The Integration Time can be set automatically to find the ideal exposure time to reach an intensity between 40,000 and 60,000 counts within a useful spectral range. When the Auto Time box is checked, the Integration Time field is disabled but displays the value from the most recent acquisition.
- External Trigger – When enabled, the trigger button on the probe will initiate the scan. To arm the trigger, the scan button must be pressed first. Then press the probe trigger to begin the acquisition.

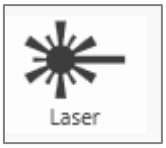
4.4 Acquisition Controls

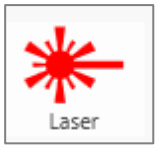


- **Scan** – When Scan is pressed, a spectrum is collected using the Integration Time, Laser Power, and Averages set in Spectrometer Controls, or automatically optimized if Auto Time is turned on. The scan appears in the data list below the chart, and a trace of the data appears in the chart area with the selected x- and y-axes units.
- **Dark Scan** – The Dark Scan button collects a spectrum using the same Integration Time as the current scan record. The laser is automatically turned off during a dark scan. This dark data is subtracted from the Scan data to produce the dark-subtracted spectrum. The dark data will be used for all subsequent acquisitions at the same integration time. When the integration time is changed, a new dark scan is required. In the Acquisition Control Panel, the user can enable Auto Dark, which automatically collects a dark scan after the data scan.
- **Check Signal** – The Check Signal button helps the user adjust the fiber probe position to maximize the signal. Pressing Check Signal will begin continuously taking data scans, replacing the previous results until the measurement is either paused or stopped. These Check Signal scans are not saved.
- **Pause** – The pause button appears during a multi-acquisition run. When pressed, it allows the current scan to finish before pausing all scans until the Scan button is pressed

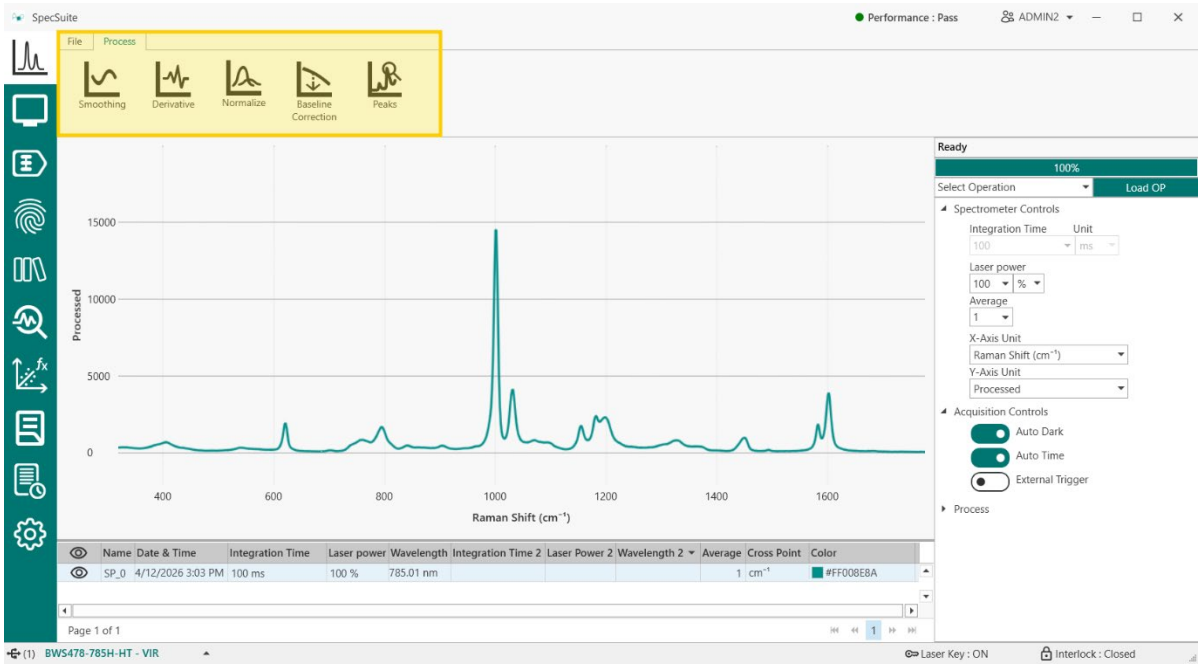
again. The next scan then starts immediately, ignoring any set delay (Interval) between scans.

- **Stop** – The stop button stops the current acquisition immediately. The canceled scan will not appear on the chart or in the data list. If Stop is pressed during a multi-acquisition, the entire acquisition will be canceled.
- **Laser** – The laser icon indicates when the laser is firing. The logo is black when the laser is not firing and red when it is firing. Hovering the mouse over the laser icon will display the laser wavelength. Pressing the laser button will turn it on and off. In case of emergency, the laser button can be used to turn the laser off during an acquisition.

Laser is NOT firing: 

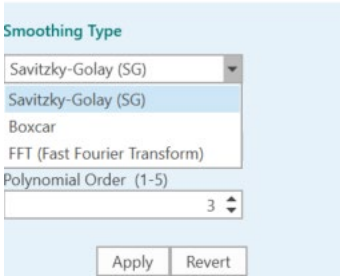
Laser IS firing: 

4.5 Process Ribbon



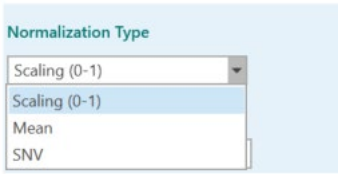
In the top Process ribbon, the user can enable the following Processing steps:

- **Smoothing –** Sets the type and parameters for smoothing the data. More info about smoothing can be found in section 6.2.



- **Derivative** – Sets the type of differentiation to use on the data and sets the order or other parameters.

Normalize – The intensity of the spectra is scaled so that spectra can be compared more easily. Normalization types are Scaling (0-1), Mean, and SNV.



Baseline Correction – A standard algorithm optimized for Raman spectra can correct the baseline of the data.

- **Peaks** – Peaks can be marked with their relevant values. The qualifications for peaks can be adjusted to include or exclude based on absolute intensity and other criteria.

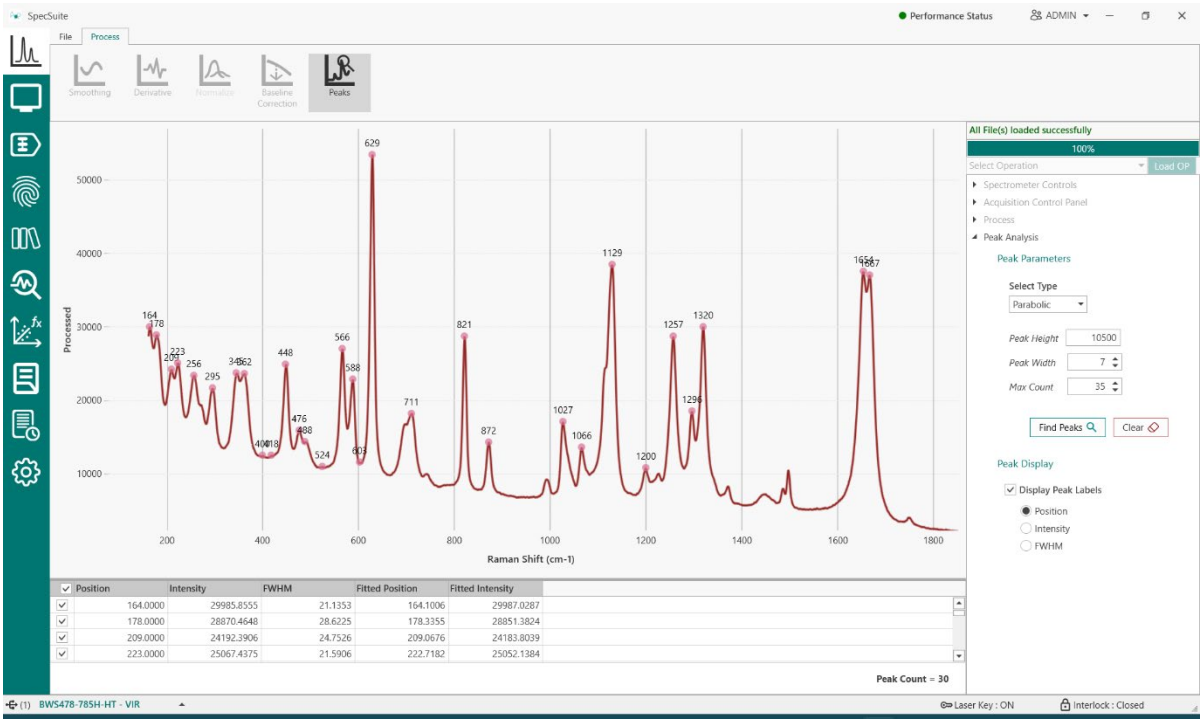
Processing actions are configured in the Process section of the right-side panel. Each processing step is recorded in the Process History column of the data table in the order in which they occur.

4.5.1 Peak Analysis

Information about a spectrum's peaks can be shown live in the Explore chart. Peak analysis can be performed for online and offline data.

It is highly recommended to apply baseline correction before performing Peak Analysis.

For more information about how the SpecSuite Peak Analysis feature works, see Appendix B.



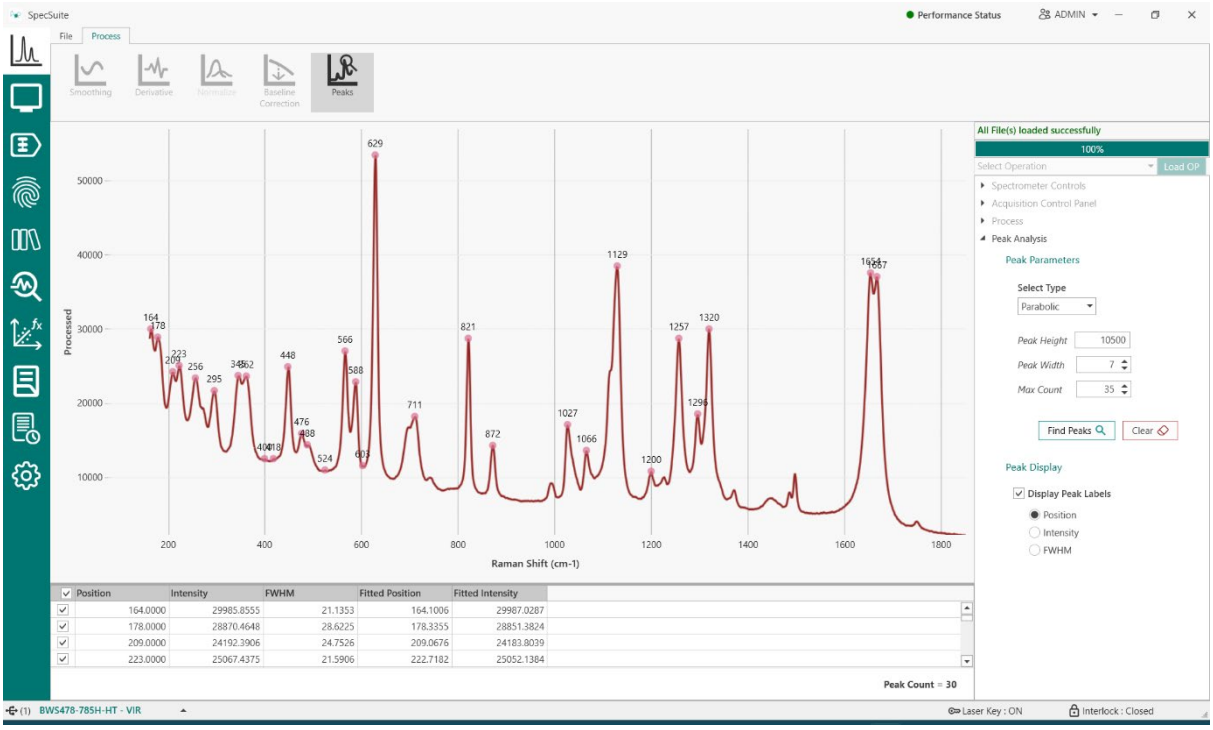
Selecting Peaks on the Process ribbon switches the Explore chart to the Peak Analysis view. The table beneath the chart will list the peaks in the selected spectrum. Position, Intensity, and FWHM are the default columns in the peak table. While the Peak Analysis view is open, File actions, Scan, Dark scan, Check Signal, Reference, Scale, Clear all, and Laser control are disabled.

Perform Peak Analysis

1. Select a spectrum from Data List.
2. Click Peaks to open the Peak Analysis view.
3. Configure Peak analysis settings in the right-side panel.
4. Press Find Peaks button to perform calculations.

Parameters can be adjusted to the right of the chart in the Peak Parameters section. Peak Type is the algorithm used to calculate which peaks are present.

- Peak analysis is applicable to the <u>ONE</u> active spectrum only
- Peak Type options include Data Points, Parabolic, and Curve Fit
    - For Data Points: Peak height is required
    - For Parabolic: Peak height and peak width are required
    - For Curve Fit: Peak height and peak width are required. Initial peaks are required. The user must specify the fit type, such as Gaussian, Lorentzian, or Voigt. If Voigt is selected, the user must also specify the Voigt ratio or use the default value 0.5.



Peak Display determines which peak information is displayed for the calculated peaks.

Checking the Display Peak Labels box displays annotations for calculated peaks in the chart.

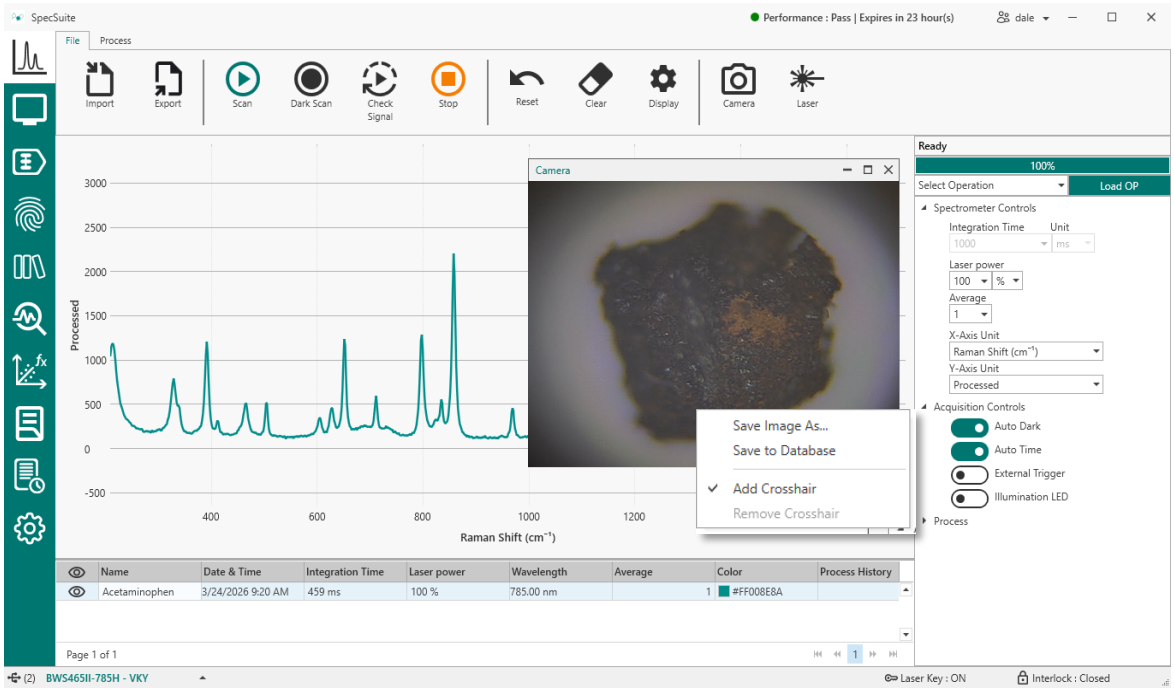
Right-clicking an unwanted peak in the table offers the option to delete it from the chart and table.

Clicking the Clear button resets the peak analysis view; peak annotations are removed, and the peak table is emptied.

4.6 Camera

When a camera is detected and enabled under Instrument -> Hardware setup, a camera icon will appear in the main Explore menu.

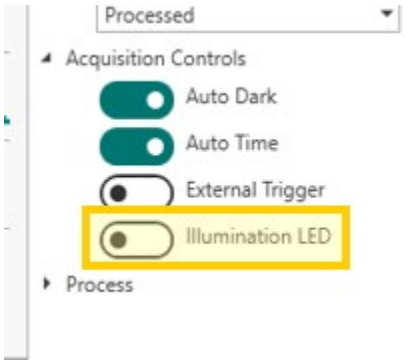
Click on the camera icon to open the camera configured in Hardware setup. This will open a window within the chart area that displays a live feed from the camera.



The right-click menu of the camera image allows the user to:

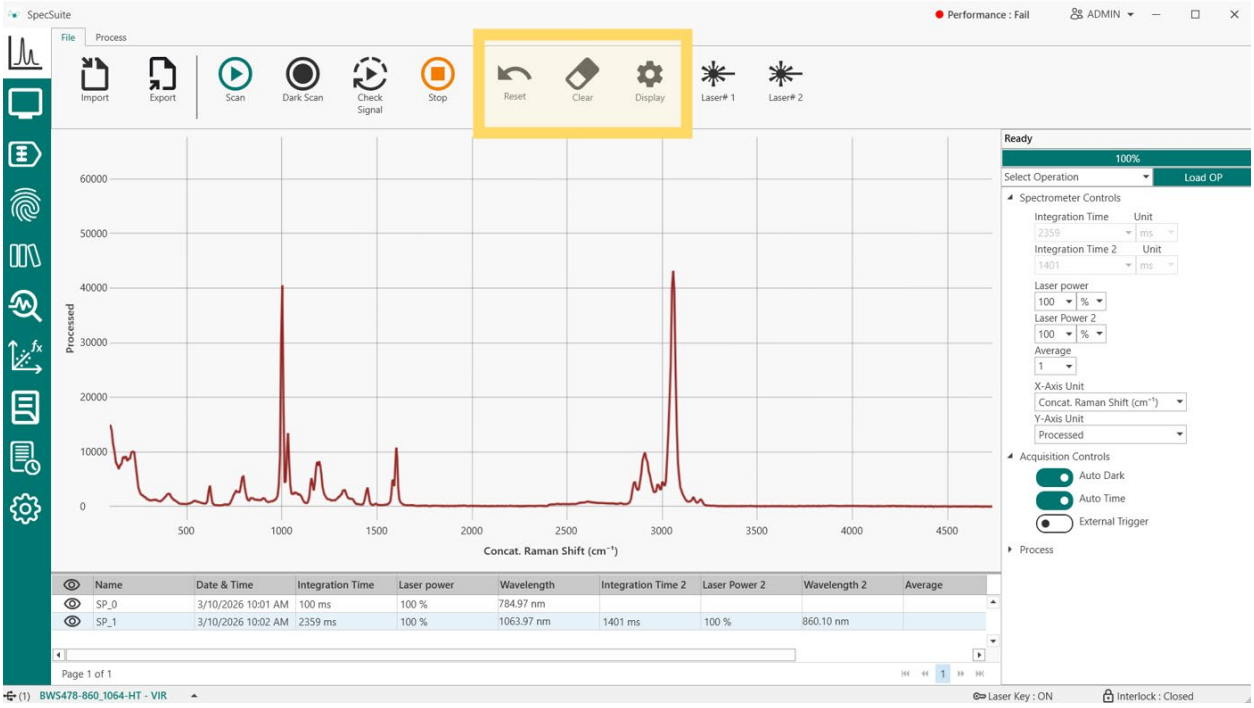
- Save the displayed image as a .PNG, .JPG or .BMP file (Save Image As…),
- Save up to 3 images to the selected spectrum record in the database (Save to Database), and
- Use the mouse to position crosshairs on the camera image (Add Crosshair) or remove them.

When a camera is checked under Hardware Setup, another toggle appears in the Acquisition Controls for Illumination LED. This allows the user to turn the microscope light on and off through the software.



4.7 Explore Chart

The explore chart provides tools for visualizing spectral data.



- **Reset** – Resets the x and y axes to the scaling set in the Scale window.
- **Clear** – Clears all the spectra from the chart and the table below.
- **Display** – Opens the Display window where the user can change the x and y axis scale to choose the size of the chart view. They can also set chart display options, such as the chart Legend.

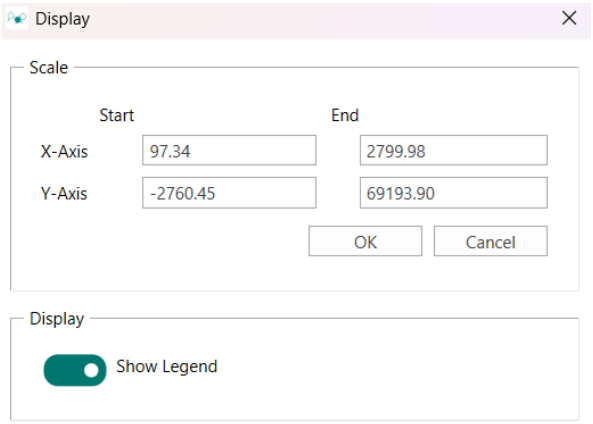
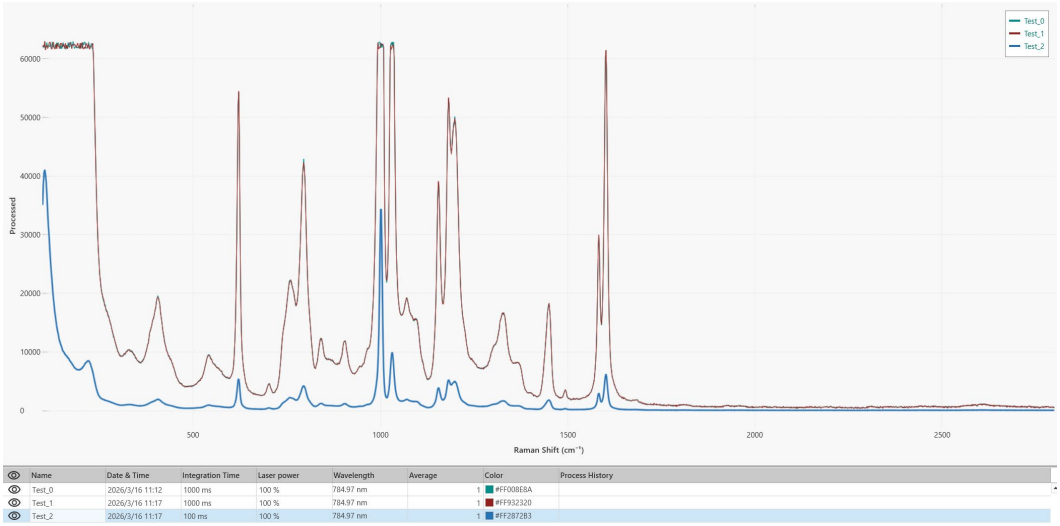
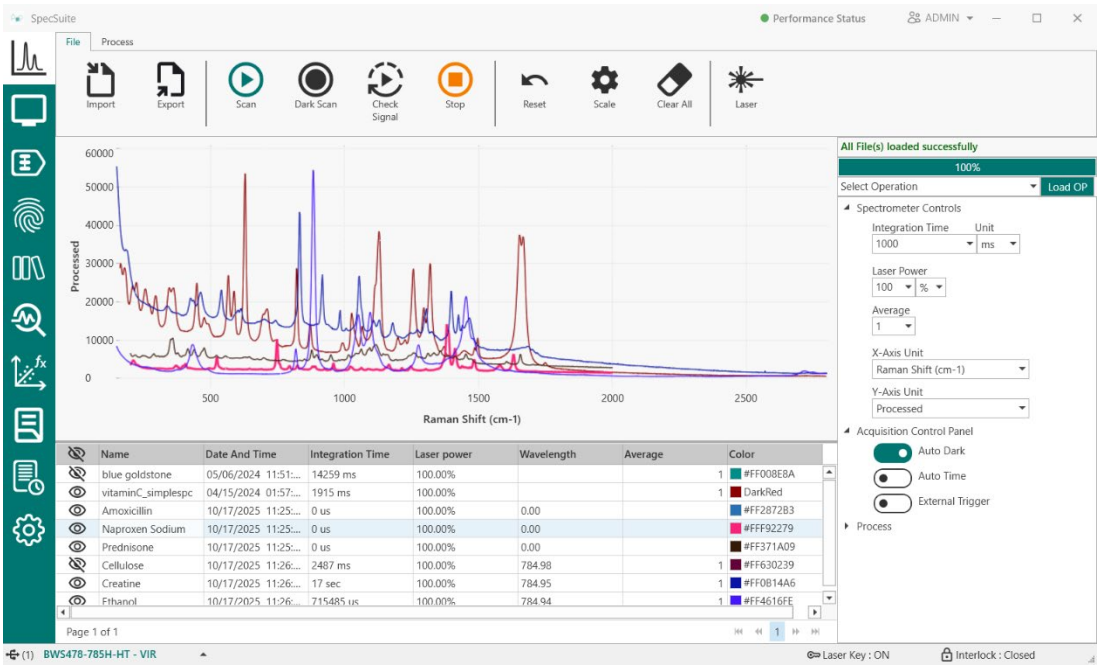


Chart Scale will reset if the X-axis unit and Y-axis units are changed. The chart legend will appear in the top-right corner of the screen.



4.8 Data List



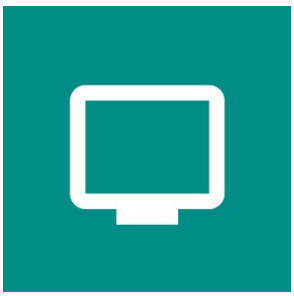
The Data List is the table of samples beneath the chart. By default, the columns in the data list are Visibility , Name, Date & Time, Integration Time, Laser power, Wavelength, Average, Color, and Process History.

	Name	Date & Time	Integration Time	Laser power	Wavelength	Average	Color	Process History
	Acetaminophen	4/13/2026 11:28 AM	3478 ms	100 %	784.98 nm	1	#FF008E8A	
	Acetone	4/13/2026 11:28 AM	392785 µs	100 %	784.94 nm	1	#FF932320	
	Aspirin	4/13/2026 11:28 AM	4227 ms	100 %	784.98 nm	1	#FF2872B3	
	Benzonitrile	4/13/2026 11:28 AM	250934 µs	100 %	784.98 nm	1	#FFE7352A	
	Cellulose	4/13/2026 11:28 AM	2487 ms	100 %	784.98 nm	1	#FF0C2B00	
	Creatine	4/13/2026 11:28 AM	17 sec	100 %	784.95 nm	1	#FF152320	
	Cyclohexane	4/13/2026 11:28 AM	1200 ms	100 %	1063.81 nm	1	#FFFA2560	
	Ethanol	4/13/2026 11:28 AM	715485 µs	100 %	784.94 nm	1	#FF211561	
	Methanol	4/13/2026 11:28 AM	2264 ms	100 %	784.98 nm	1	#FF6B0414	

Page 1 of 1

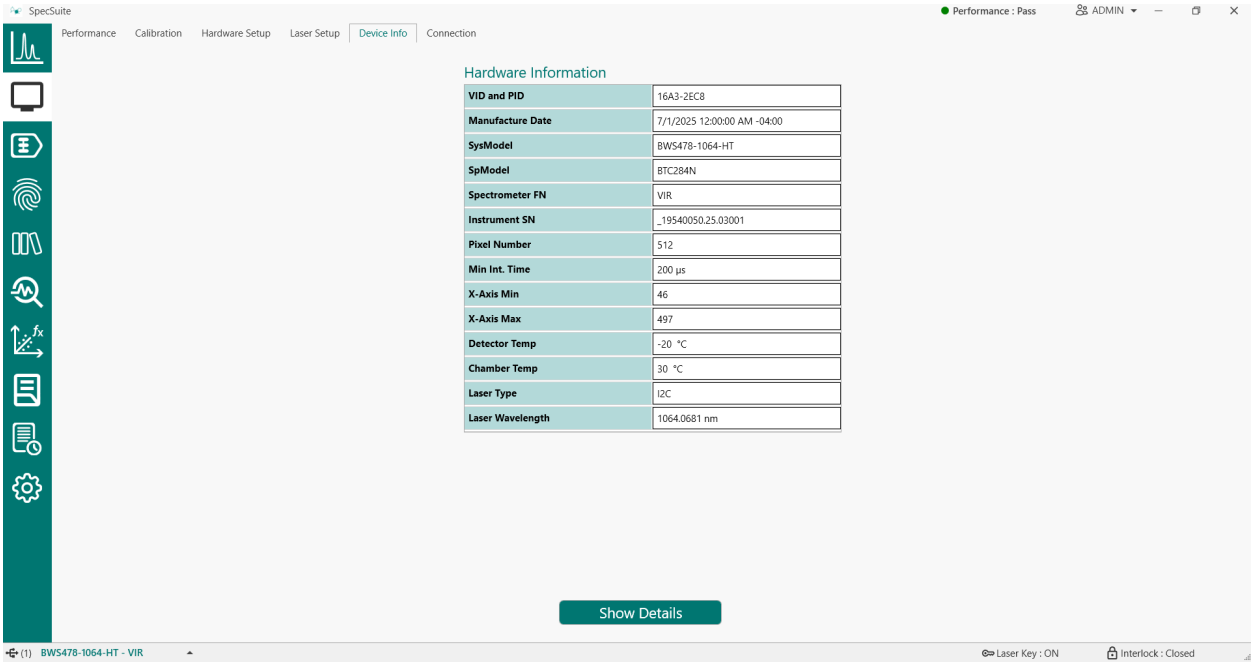
Some sample information may be edited here. The Name can be changed by clicking on the cell and typing. Changing the name of the data in the table updates the record in the database and automatically updates the name of the export data file.

5. Instrument



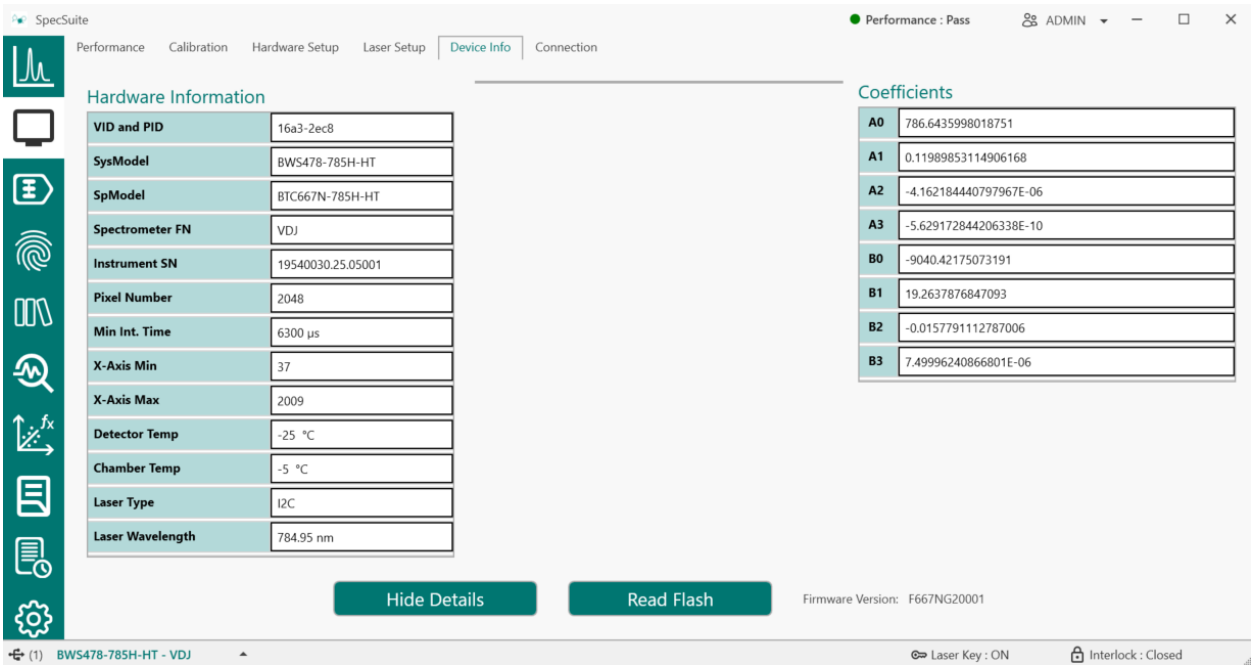
The Instrument module contains information about the connected system, spectrometer, and accessories currently connected to SpecSuite. From the Instrument module, the user may perform calibrations and create correction files to ensure the instrument is performing and collecting accurate data. For Operator and Developer level users, the Instrument module will not appear unless an instrument is connected.

5.1 Device Info



The Device Info tab displays the basic hardware information of the attached system or spectrometer:

- System Model
- SP model (Spectrometer Model)
- Spectrometer FN (Factory Number)
- Instrument SN
- Laser Type and Wavelength



Show Details reveals the entire contents of the EEPROM laid out in an easy-to-read way, including:

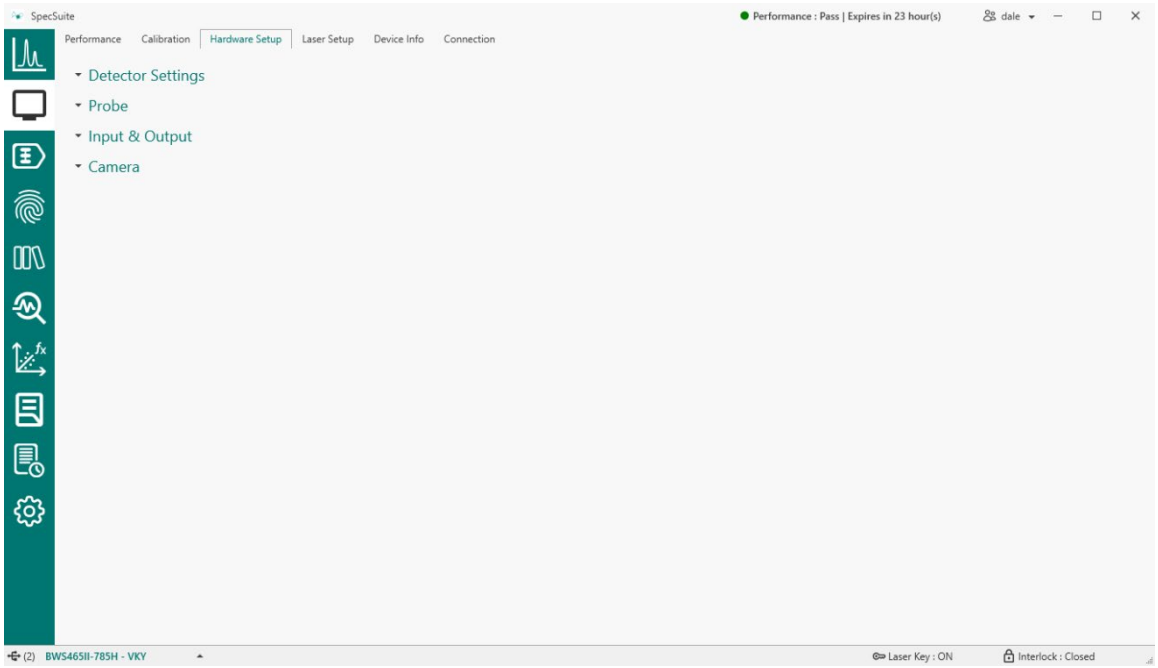
- Hardware Information
- Coefficients
- Firmware version – for BTC66xN series

Read Flash reads the EEPROM and refreshes the information displayed in the Device Info table, and resets all system/spectrometer settings to their defaults. The Read Flash button appears only when Detailed device info is shown.

Pressing Hide Details will show only Hardware info and hide the Read Flash option.

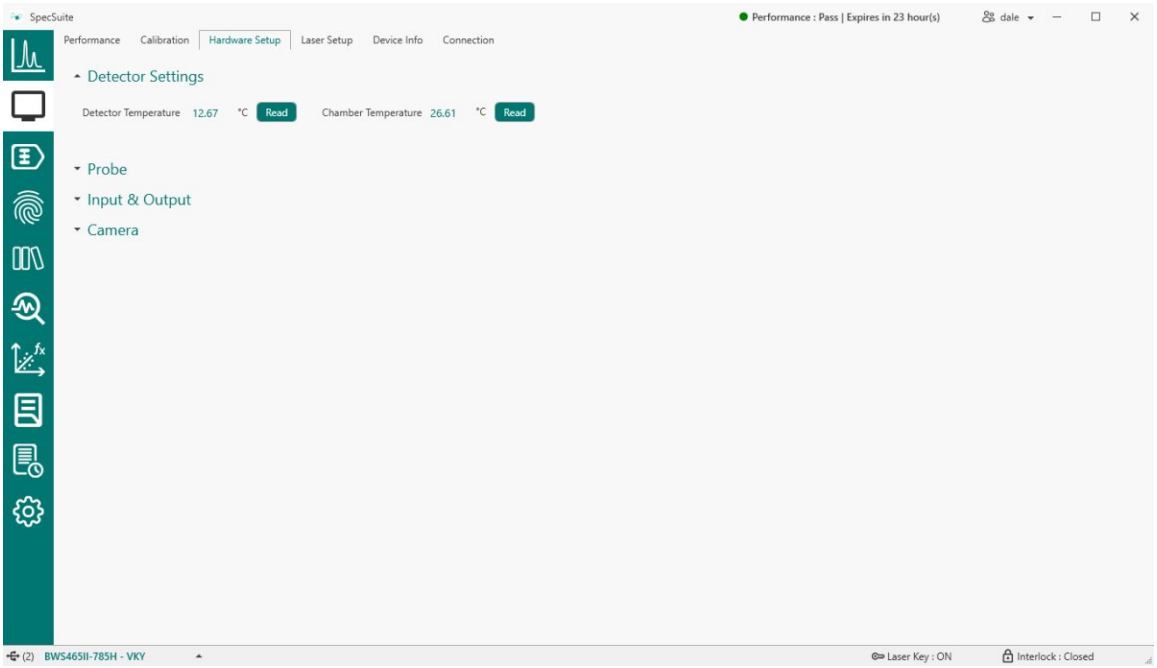
During Service, the instrument EEPROM might be adjusted.
It is recommended to click the Read Flash button to refresh the EEPROM information after service.

5.2 Hardware Setup



Hardware Setup contains options for Detector Settings, Probe, Input & Output, and Camera.

Detector Settings



Detector Temperature

The current detector temperature is displayed here. To update the current detector temperature, press Read.

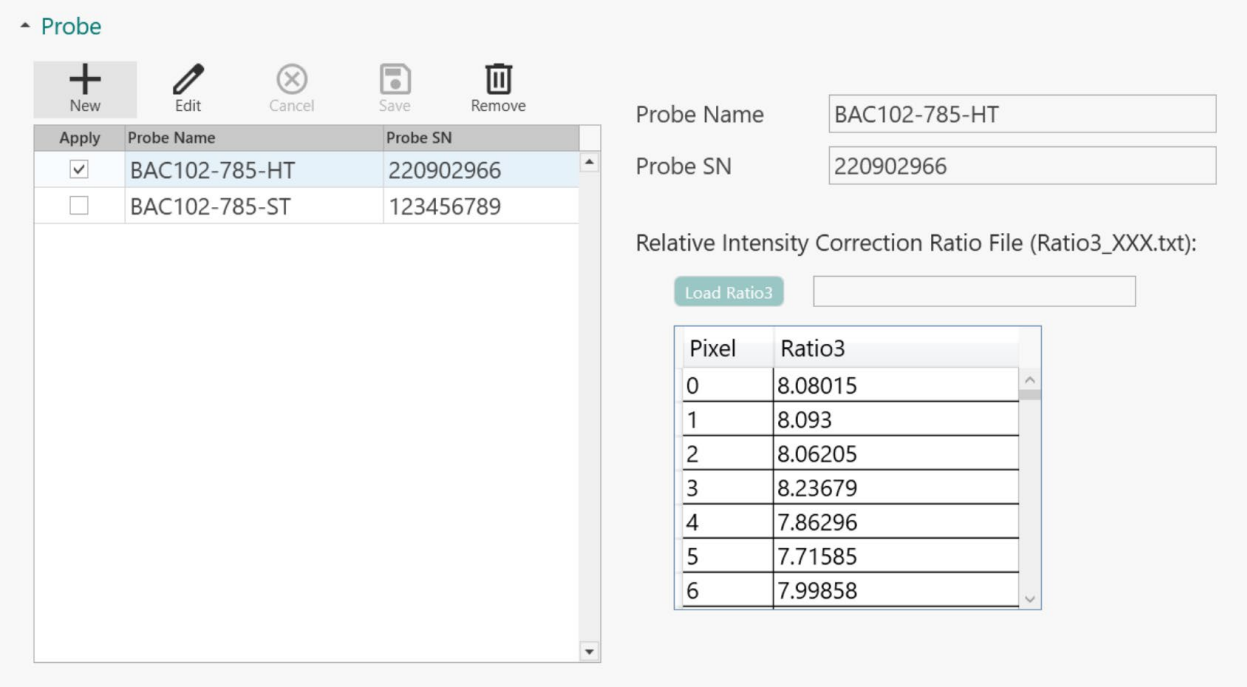
Chamber Temperature

The current chamber temperature is read and displayed here. To update the current temperature, press Read.

Check your instrument's user manual to see if it can display the temperature.

Probe

A probe must be set up before accurate data collection or performance verification can be performed. To create a new probe, a Ratio3.txt file for the connected device is required.



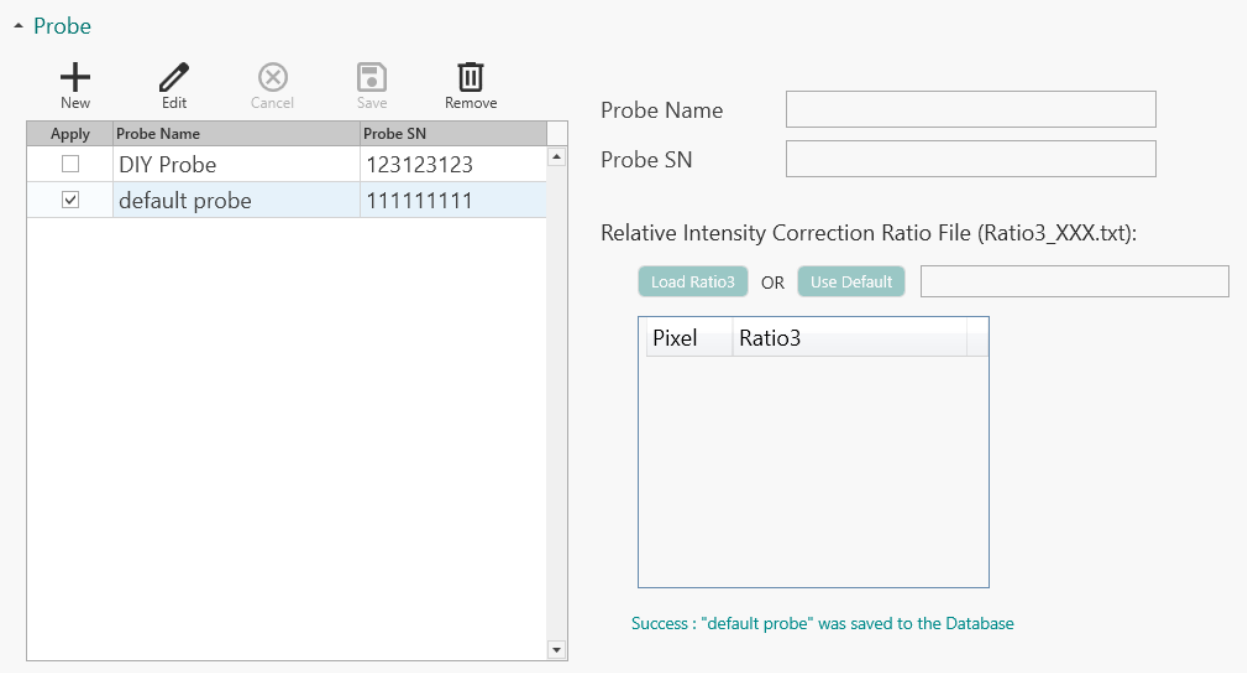
In the Probe list, the probe with the Apply checkbox checked will be applied to all data collected by the connected unit.

Add a probe

1. Above the Probe list, select New.
2. In the Probe Name section, enter a name for the probe and the serial number of the probe.

3. Select the Ratio3 file created for the instrument and probe combination.
    a. The contents of the Ratio file are displayed after the file is loaded.
    b. Instruments will have a Ratio3 file provided by Metrohm.
    c. If you do not have a Ratio3 file, request one from your local service representative.
    d. Experienced customers can follow the procedure in section 5.5.3 Relative Intensity Correction to create their own Ratio3 file. This process requires the appropriate Standard Reference Material to generate a Ratio3 relative intensity correction file.
4. Press Save to add the new probe to the Probe list.
    a. If any requirements are not met, an error will appear below the Save Probe button with information about why the probe was not saved.

For DIY setups, there is a button for the user to load a default Ratio3 with all 1s to create a probe record for functions that require a Ratio3 file, like Performance. Using the default Ratio3 file allows data to be collected without having intensity correction applied.
For i-Raman systems, this button is not shown, and the user must load a real Ratio3 file.



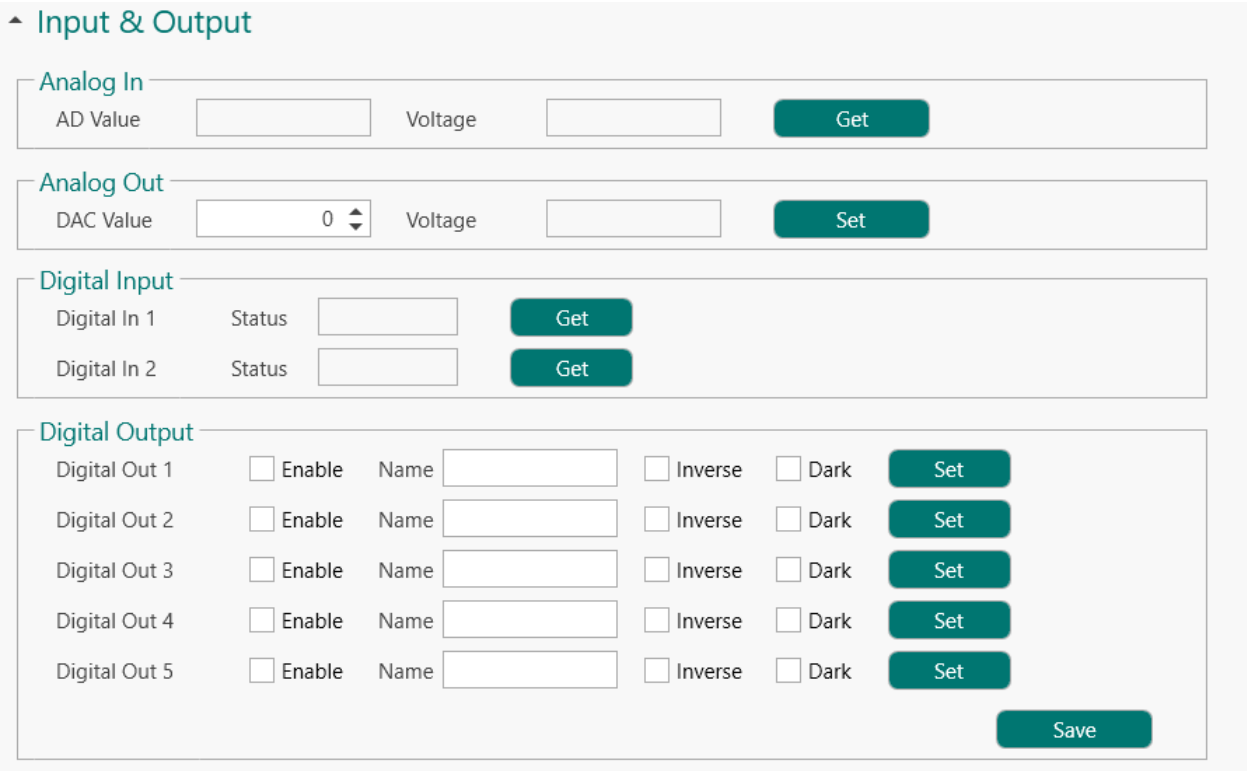
Delete a probe

There are two ways to delete a probe:

1. Select a probe, then press the Remove button.
   OR
2. Right-click on the probe entry and choose the Delete option.

In the Probe list, the probe with the Apply checkbox checked will be applied to all data collected by the connected unit.

Input & Output



Analog In value range and DAC value are defined in the spectrometer model's user manual.

Digital Inputs (read only)

- Digital Input 1 – Reads the laser key switch status
- Digital Input 2 – Reads the interlock status

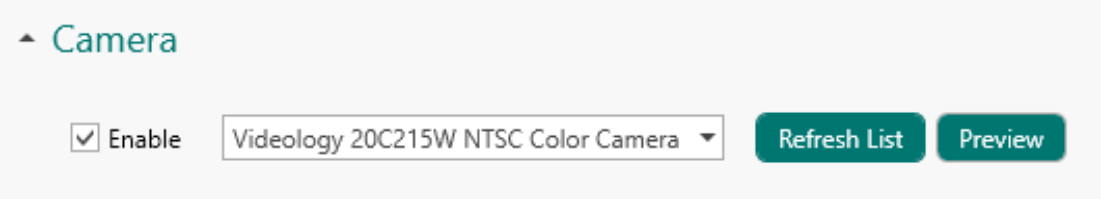
Digital Output (controllable)

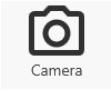
- Digital Output1 – Illumination LED for system enabled by default (inverse and dark unchecked)
- Digital Outputs 2-5 – User definable for DIY setups

Please consult the spectrometer user manual for your device for information about the specific Input and Output options for your hardware, or reach out to a Metrohm Service representative

Camera

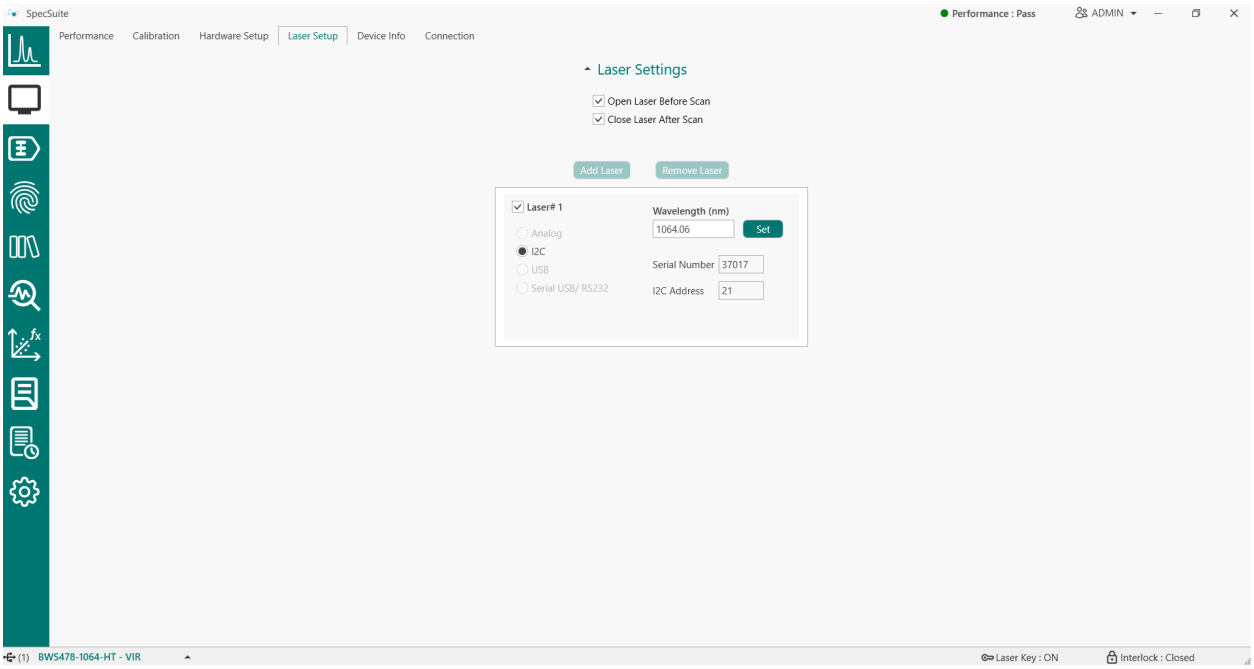
The camera section allows the user to select a BAC151C microscope camera or an alternate camera for image/video while taking a scan in Explore.



Users can click Refresh List to refresh the drop-down list of available camera modules connected to the PC. Users can also click Preview to open a preview of the camera feed. Once enabled, a camera icon 

appears in the top ribbon of the Explore module.

5.3 Laser Setup



The "Laser Setup" tab allows the user to view pre-set laser parameters, make adjustments to the laser configuration, or set up a laser manually. Lasers used in i-Raman systems are automatically detected and configured. **NOTE:** i-Raman systems do not allow another laser to be added or subtracted from a laser setup.

When a standalone laser device is connected, the user can add or remove a laser from this screen.

Add Laser – Adds a new laser to be configured for this instrument.

Remove Laser – Removes the laser from the configuration table for this instrument.

To allow SpecSuite to control a laser, a compatible laser must be used. The user may select the type of laser from the list:

Analog & I2C are for i-Raman systems and are automatically set by the software based on the connected i-Raman model.

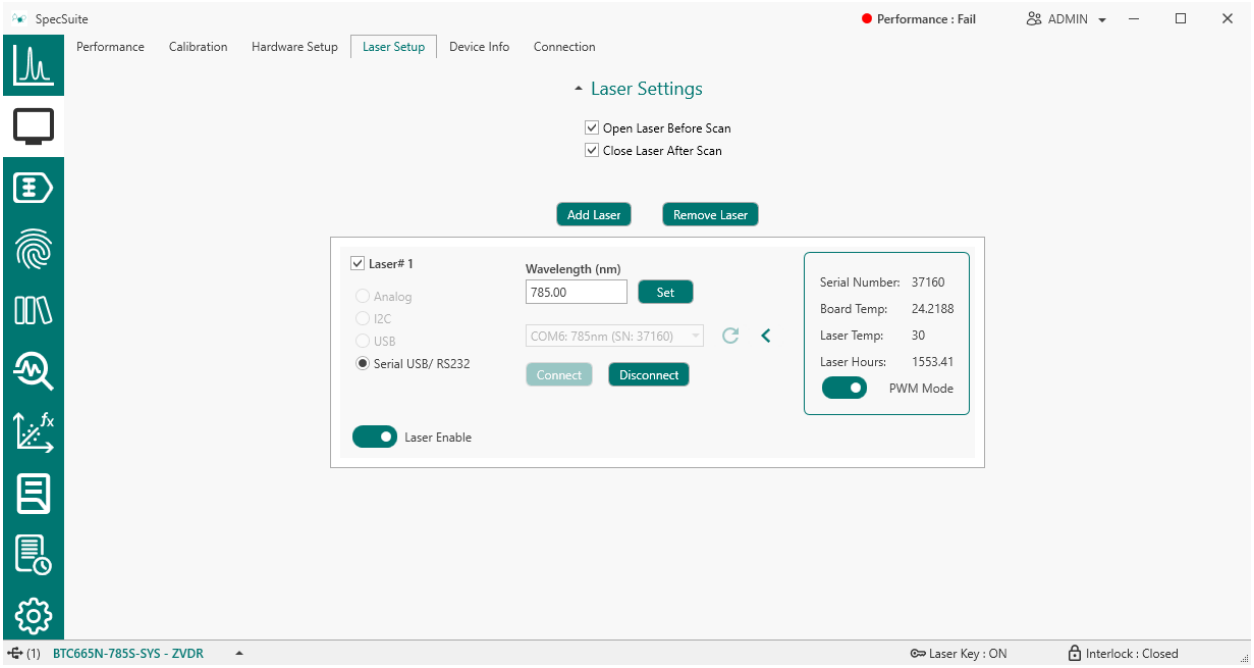
- **Analog** (for i-Raman system 532nm)

- **I2C** (for i-Raman NxG 785 and 1064, and i-Raman Plus 785)

USB and Serial USB/RS232 are reserved for DIY setup

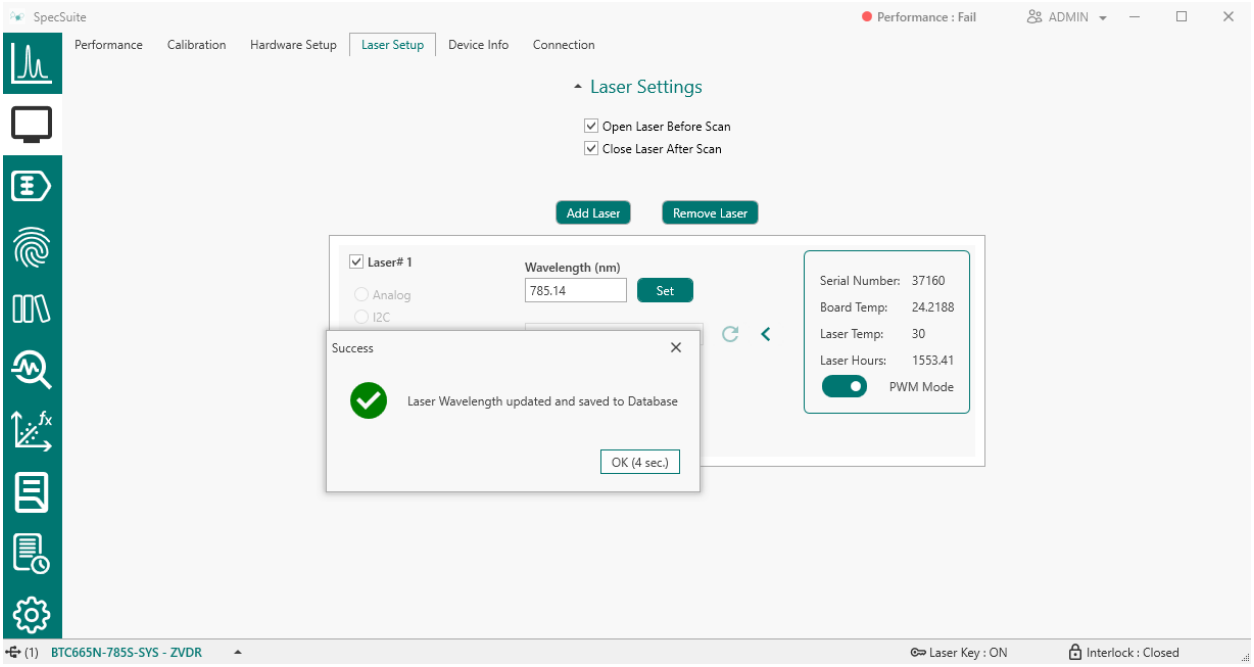
- **USB** (for DIY – GLM/Cleanlaze laser USB with the BWT driver)
- **Serial USB/RS232** (for DIY - IPS serial USB communication through COM port)

For **Serial USB/RS232**, the user will find the available IPS laser identified in the drop-down if the hardware is connected correctly. If no laser is available, check connections and troubleshoot by confirming operation in the laser user manual.
For an IPS laser, ensure that Laser Enable and PWM Control are selected while the Laser Enable signal is working on the laser device.



Only up to two lasers can be controlled by SpecSuite at one time. Add a second laser and input the laser wavelength to perform Raman Concatenation.

The user can manually set the laser wavelength. The Set button must be pressed for the laser setting to be saved. If the Wavelength has been set correctly, a message will appear saying "Laser Wavelength updated and saved to database".



The laser can be temporarily disabled but unchecking the box in the top left of the configured laser. This will stop control in the software without losing the configuration setting.

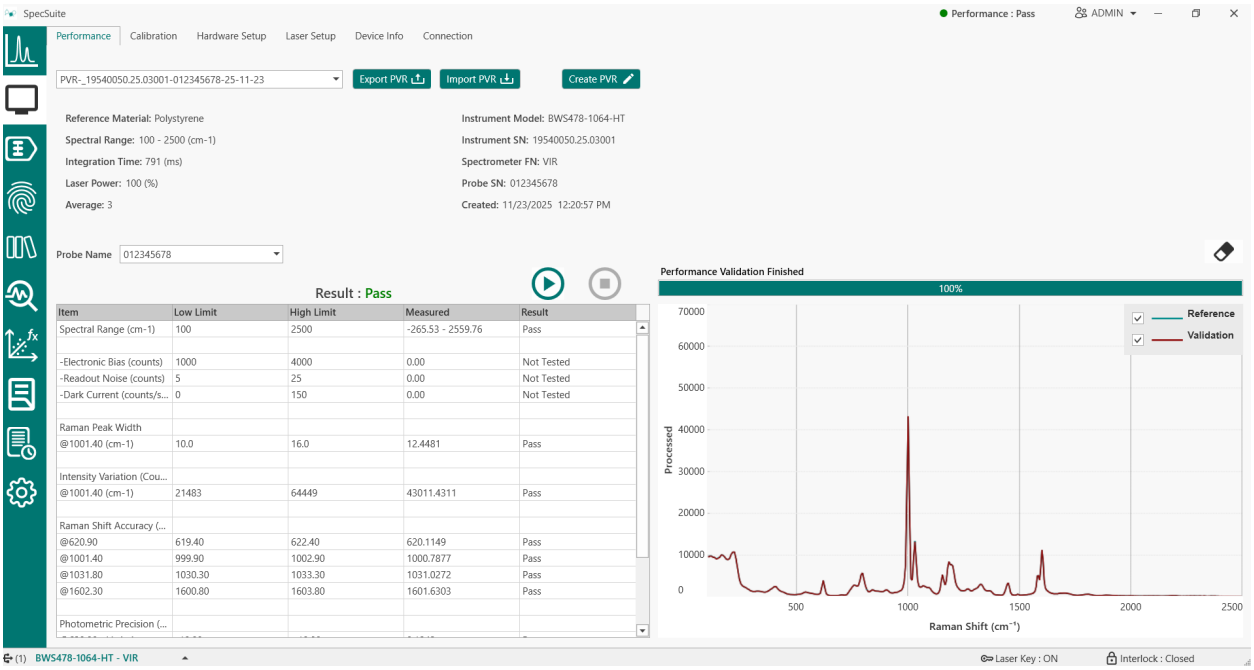
The Manual laser mode is intended to control the laser externally, while still being able to produce calibrated Raman data. Only the Laser Wavelength is required for input.

Other available Laser Settings:

Open Laser Before Scan – This setting is enabled by default. When this box is checked, the laser will automatically turn on before sample data is collected if it is not already on. When the box is unchecked, the laser will not automatically turn on if it is off when the scan starts. In this case, the laser must be manually turned on before the measurement is started.

Close Laser After Scan – This s is enabled by default. When this box is checked, the laser will automatically turn off after the sample data is collected. If the box is unchecked, the laser will continue firing even after the data scan is complete and remain so until the laser is manually turned off.

5.4 Performance



The Performance tab provides options to:

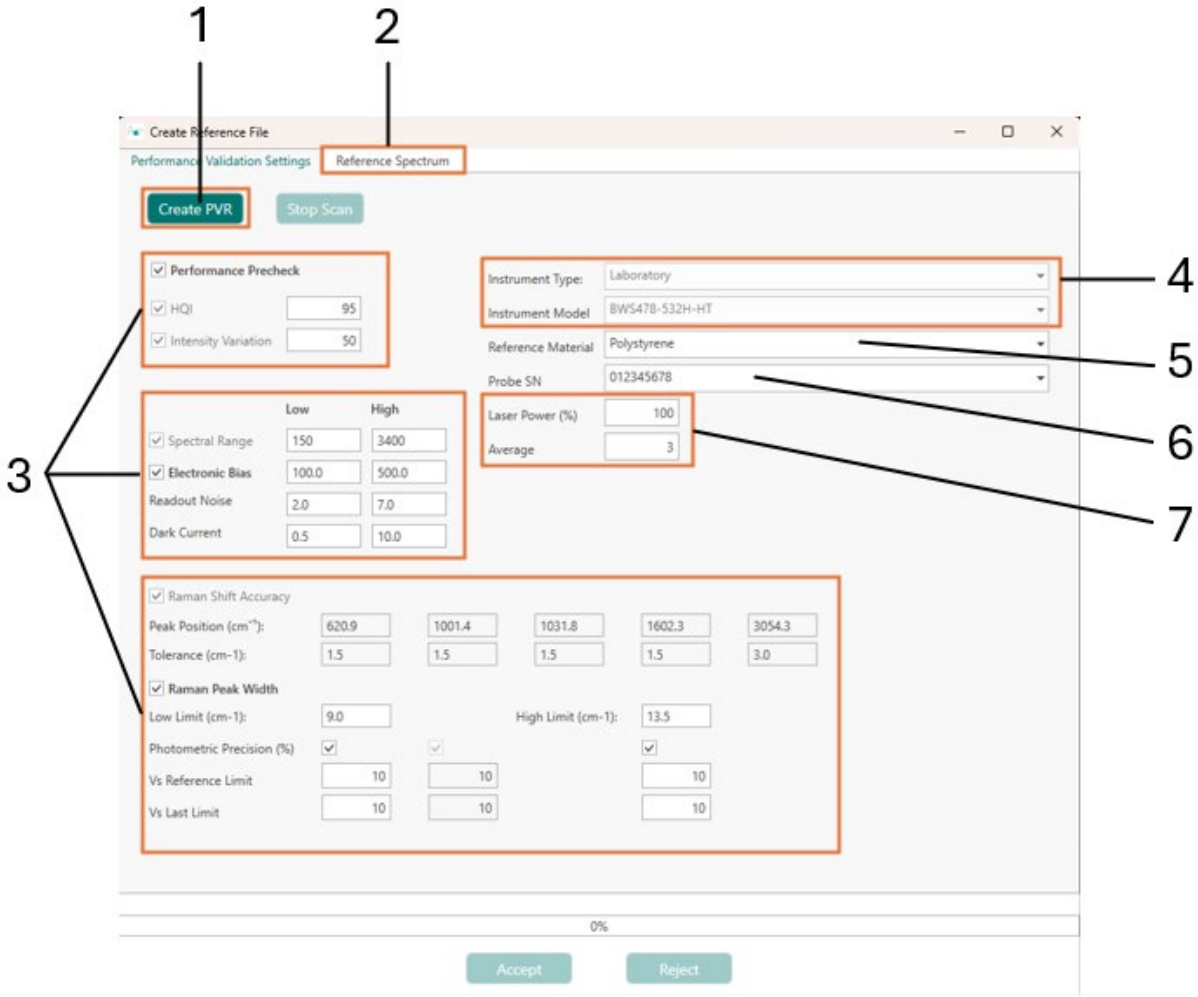
- Perform a Performance Validation (PV) to ensure the system is functioning correctly
- Create a new Performance Validation Reference (PVR) file if needed

The PVR file is unique for the instrument, probe, and material being sampled. If any of these parts change, a new PVR file should be created.

- If the reference material changes, a new PVR file should be made.
- If the system's hardware is changed or recalibrated, a new PVR file should be made.
- If a new probe is used, a PVR file for the specific instrument and probe combination should be used.

Even if the product is not used in a regulated environment, a performance validation should be performed routinely to ensure the instrument's reliability. i-Raman systems ship with a factory-created PVR file for instrument validation.

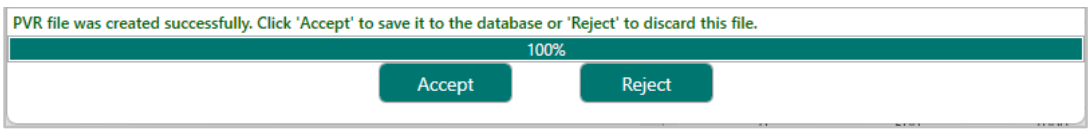
PVR File Creation



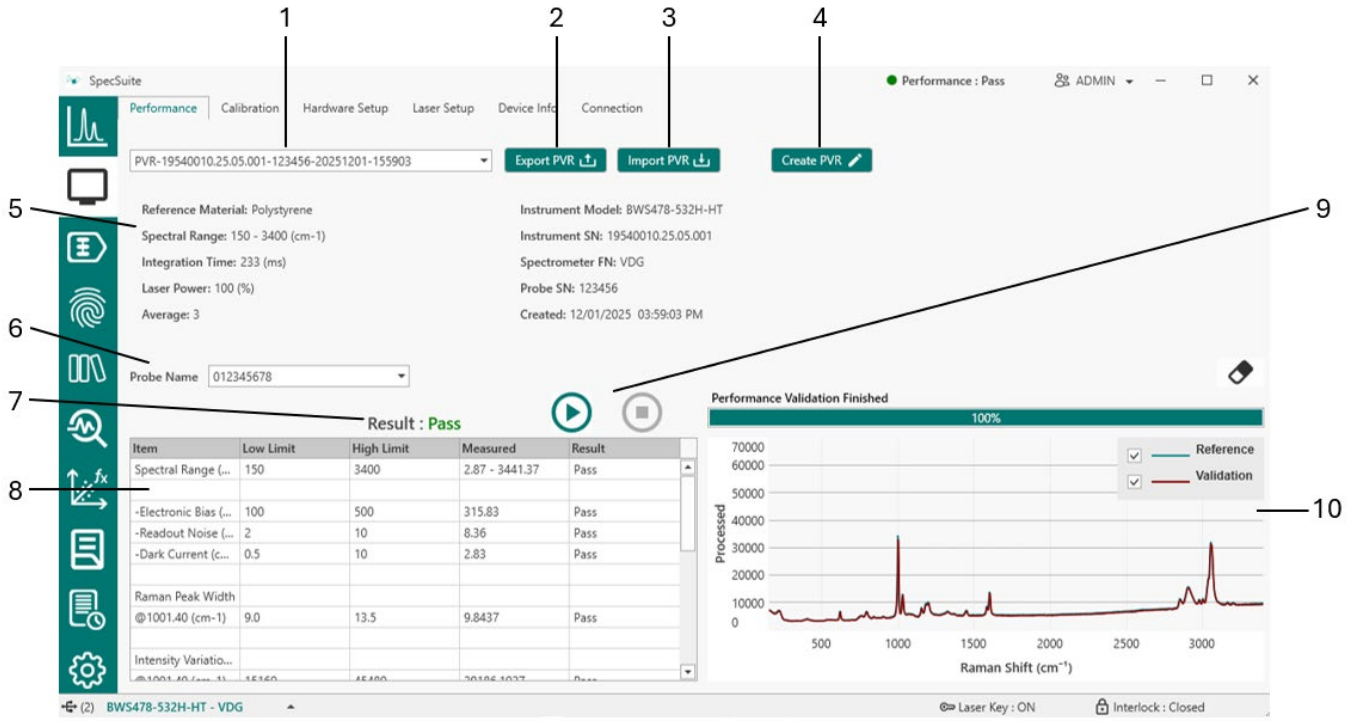
1	**Create PVR** Collect a spectrum and create a PVR file.	2	**Reference Spectrum** Displays the spectrum when the PVR file is created.
3	**Performance Settings** Settings used for the Performance Test. Default values are loaded based on the Instrument information.	4	**Instrument Information** Software automatically detects the connected instrument for this information.
5	**Reference Material** Test material to measure Raman shift calibration.	6	**Probe SN** Select the probe serial number from the list of created probes in Hardware Setup.
7	**Laser Power & Average**		

How to create a PVR file

1. In Instrument > Performance, click the ‘Create PVR' button, and the PVR creation window will appear.
   a. To create a PVR file, an instrument must be online.
   b. The connected system will automatically be identified and selected by the Instrument Type and Instrument Model fields (**4**).
2. Select the Reference Material used for the Reference file: Polystyrene, Acetaminophen, or Cyclohexane (**5**).
3. Select Probe by serial number (**6**).
   a. A probe must be created in Hardware setup prior to this operation.
4. Average and Laser Power can be set (**7**).
   a. Recommended defaults are 100% laser power and 3 averages.
5. All parameters are set to default values, but some can be changed (**3**).
   a. A Performance Precheck can be run to assess the instrument performance prior to creating the PVR file. If checked, the precheck will run: Dark1 and Dark2 (dark scans taken with the minimum integration time), and Dark(60s) scans. If not selected, these dark scans will be skipped to shorten the time to complete PVR file creation.
   b. If the box next to Electronic Bias is checked, the validation test will do a 60-second dark scan to assess the instrument performance. It is recommended to always create a PVR file with all testing options selected to fully validate the instrument's performance and ensure correct results.
6. Place the selected Reference Material in front of the sample probe and open the probe shutter.
7. Press Create PVR (**1**).
   a. During data collection, click the Stop button if the acquisition needs to be canceled.
   b. A progress bar and status message will appear under the Accept/Reject buttons to indicate the status of the PVR creation process.
8. The reference spectrum can be viewed by switching to the Reference Spectrum tab (**2**).
9. Press ‘Accept’ to save the PVR file.



Performing a Performance Validation



1	Select PVR	2	Export PVR
3	Import PVR	4	Create PVR
5	PVR settings Parameters of the selected PVR file	6	Probe Select Probe used for validation
7	Result area	8	Results table Detailed results for each parameter
9	Start / Stop	10	Spectra Shows the reference spectrum with the validation spectrum overlayed

The Pass/Fail result from the Performance Validation will update the Performance Indicator in the top bar of the SpecSuite window.

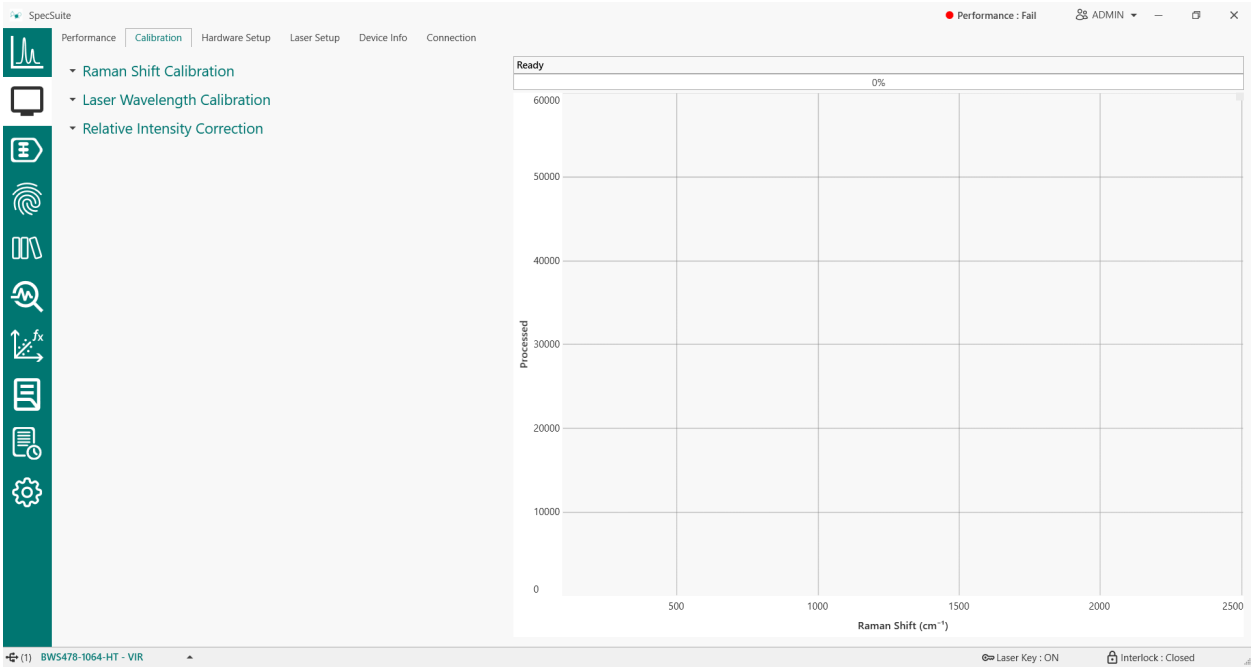
Pressing the Stop button will abort the Performance Validation (**9**).

A history of Performance Validations can be found in the Reports module. See section 11.4 Performance Validation Reports.

How to run a Performance Validation

1. Select a PVR file from the 'Select a PVR File…' dropdown (**1**).
    a. By default, the loaded PVR file will be the last used file.
    b. Only PVR files for the connected instrument will display.
2. Verify the selected PVR file's parameters are correct in the PVR setting section (**5**).
3. Select the active probe SN (**6**).
    a. The same probe used for pvr file creation should be used for performance validation.
4. Set up the instrument to measure the Reference Material.
5. Click the Start button (**9**).
    a. When the PVR file is using the full settings, the Performance Validation will run for approximately 90 seconds.
    b. A Pass or Fail result will appear in the Result area (**7**).
    c. The Results table (**8**), and the Reference spectrum and Performance spectrum (**10**) are created after the validation. The Results table contains detailed information about the Performance Validation results

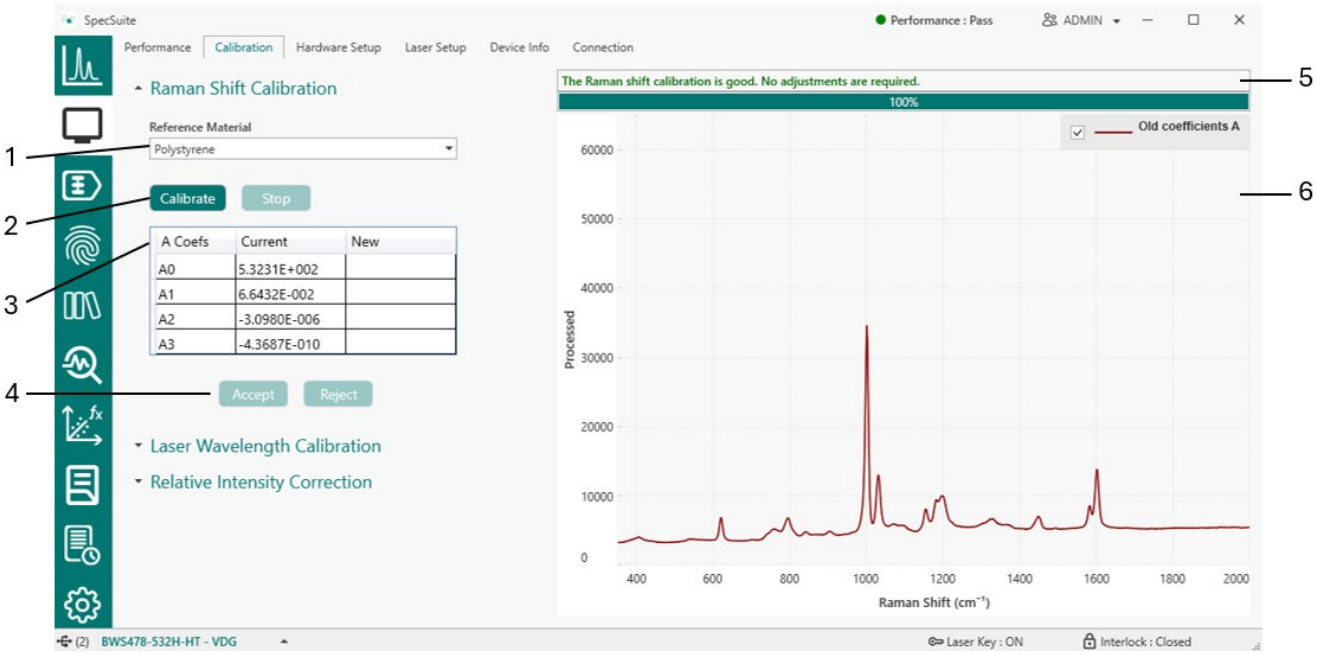
5.5 Calibration



The Calibration tab has several features available to make changes to the instrument's performance:

- Raman Shift Calibration
- Laser Wavelength Calibration
- Relative Intensity Correction

Raman Shift Calibration



1	Reference Material	2	Calibrate / Stop
3	A Coefficients	4	Accept / Reject
5	Result of Calibration	6	Calibration Spectrum Spectrum of reference material used for calibration

The Raman Shift calibration process uses polystyrene or cyclohexane as a reference material to generate calibration A-coefficients. The Polystyrene standard provided by Metrohm is recommended.

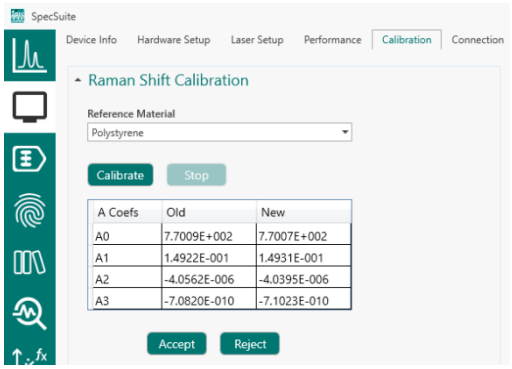
Raman Shift Calibration should be performed when a performance test fails due to one or more peak positions falling outside the range of specifications. If the Raman shift value is > 6cm^{-1}

from the specification, it is too large for the Raman shift calibration tool to correct, and the instrument may require service.

Once this calibration is successful, the user can choose to accept or reject the new calibration coefficients. Accepted coefficients will be saved to the database with other instrument-related parameters.

Run Raman Shift Calibration

1. Select Reference Material from the drop-down menu (**1**).
2. Set up the instrument to measure the Reference Material.
3. Select Calibrate (**2**).
4. Review the result of the calibration (**5**).
5. Select Accept or Reject (**4**).
    a. Accepted new coefficients will be saved to the database with other instrument-related parameters.



Laser Wavelength Calibration

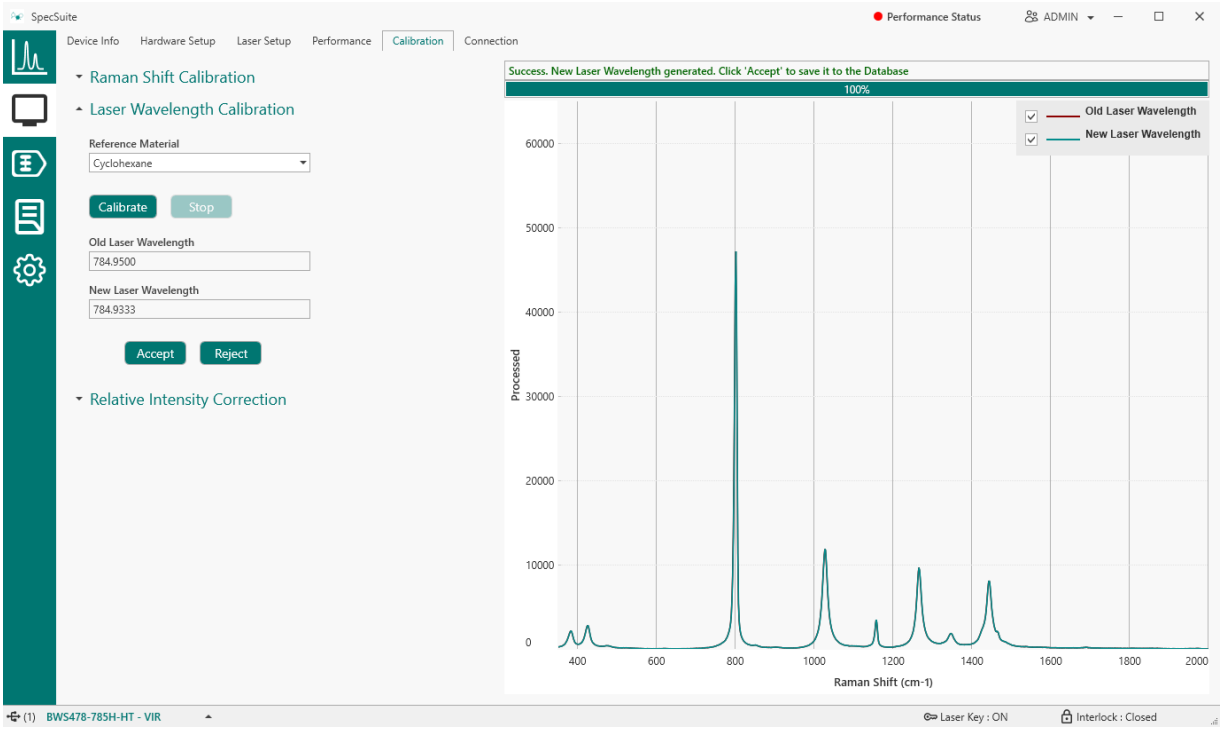
Laser wavelength calibration uses cyclohexane as a standard to calibrate the laser wavelength value. The cyclohexane peaks are used to determine the exact wavelength of the laser. Laser wavelength calibration should be done after installing a new laser.

Laser wavelength can also be entered manually in Hardware Setup > Laser Setup tab.

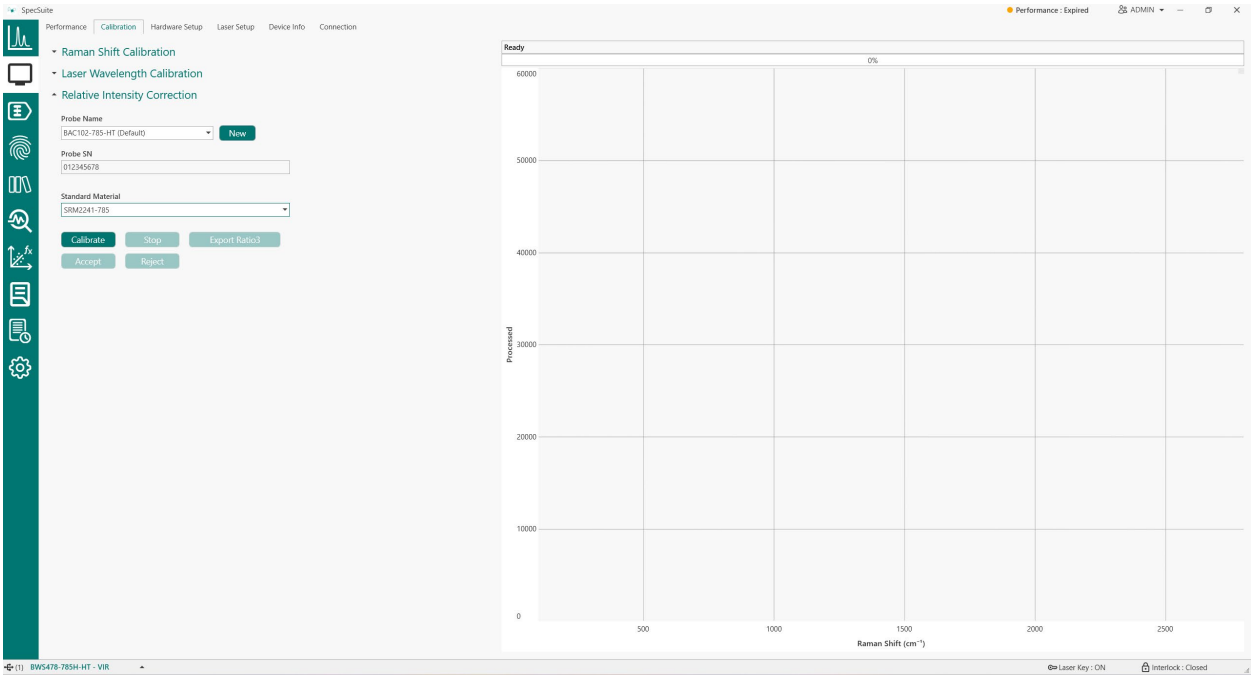
To run Laser Wavelength Calibration

1. Set up the instrument to sample cyclohexane.

2. Press Calibrate.
3. Select Accept to save the new wavelength value.
    a. Or Reject to not save the change.



Relative Intensity Correction



Metrohm's i-Raman systems ship with a factory-created relative intensity correction file.

The reference material required is determined by the laser wavelength of the instrument:

- 785nm: SRM 2241
- 532nm: SRM 2242a
- 1064nm: SRM 2244

The system will calibrate the Instrument and Probe with the standard.

To run Relative Intensity Correction with a new Probe

1. Set up the instrument to measure the corresponding reference material.
2. Click New, then enter a probe name
3. Select Standard Material from drop down menu.
4. Select Calibrate.
5. If the calibration is successful, click Accept.
6. Select Export the Ratio3.
7. Save the Ratio3 file.

a. The Ratio3 file can then be imported into SpecSuite as a Probe in Hardware Setup.

Users can also update an existing probe's calibration record by selecting the probe name from the drop-down menu, then following steps 3 to 7 listed above.

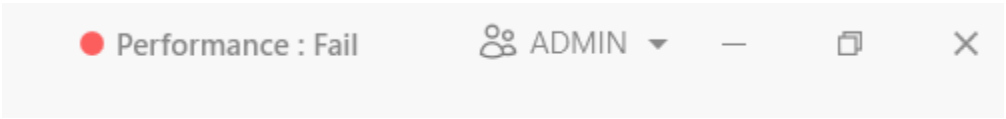
5.6 Instrument Status Messages

Around the top and bottom of the SpecSuite window, several status messages are displayed for easy monitoring.

Performance Status

At the top right of the SpecSuite window, a colored dot displays the result of the last Performance Validation.

- Red – Fail
- Green – Pass
- Yellow - Expired
- Gray – N/A, no instrument connected



If the Performance Validation Expiration setting is enabled, the approximate time until expiration will display after the status, as shown below. After that period, the status will become Expired, and a new Performance Validation is required.

Laser Key and Interlock

For an i-Raman system, both the Laser Key and Interlock statuses must be ON to take a scan.

The Laser Key and Interlock status are checked at the START of each scan.

If the Laser key is off, the laser button will not appear in the top bar, and the laser will not appear in the laser setup. A system cannot be treated or used as a lone spectrometer.

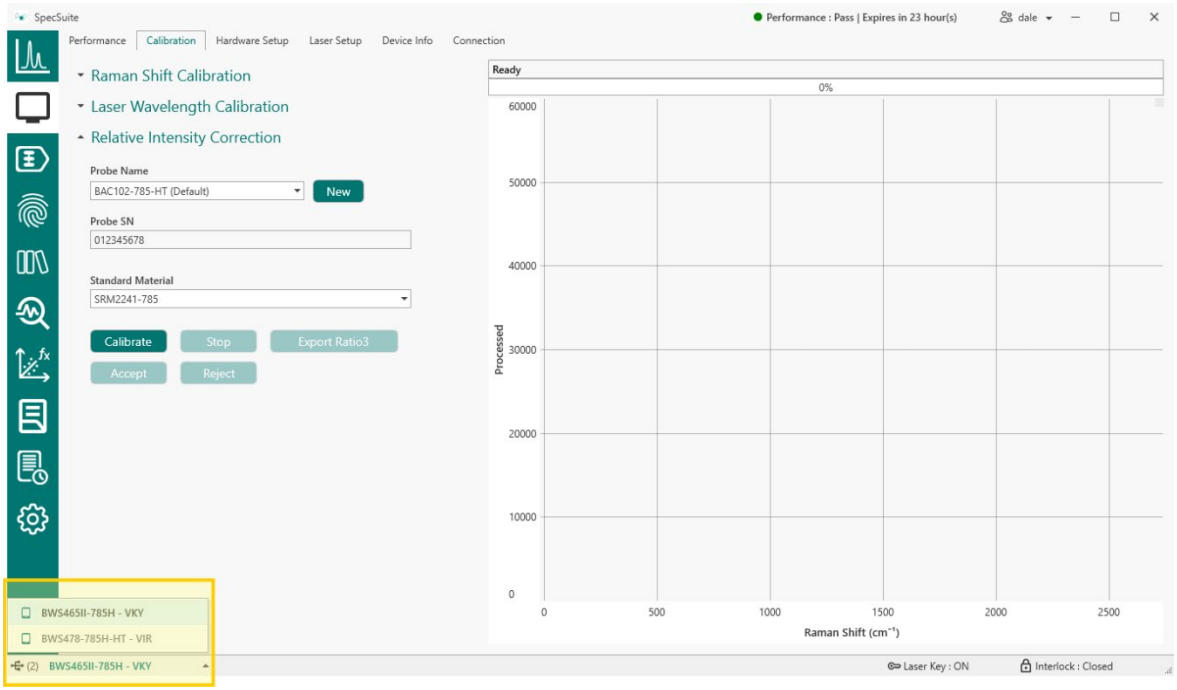
Interlock does not have a delay in turning the laser back on and will not affect the laser's availability.

It is recommended to set the laser key to ON before connecting the i-Raman instrument to the PC.

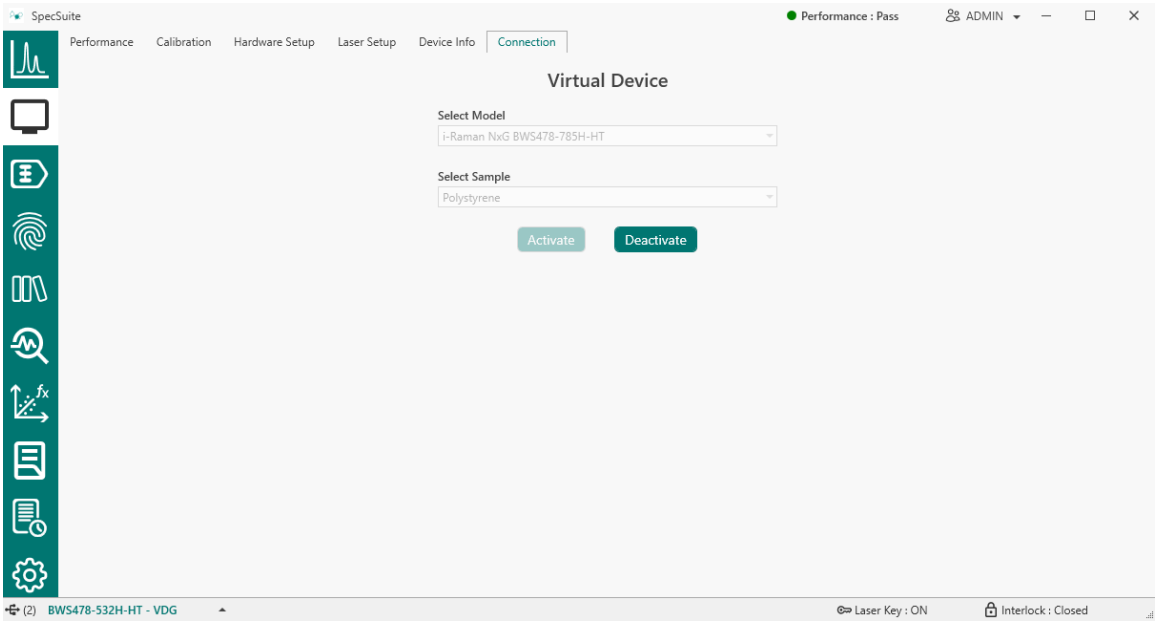
Turning the laser key on after connecting to the PC may cause the software to become unresponsive. Recycle the instrument power to reconnect and continue using the instrument.

Connected Instruments

The bottom left corner of the window shows the status of the connected instrument(s).



5.7 Virtual Device



NOTE: The Virtual Device tab will only appear when an Administrator or Service-level login is used.

Virtual Device connection enables all SpecSuite features without connecting a physical instrument. To enable a System or Spectrometer, check the Enable Virtual Device box, then select the desired system from the dropdown menu. Press Activate. SpecSuite will display the chosen system as Online (Virtual) in the bottom-left corner of the main window. Changes can be made using the Hardware Setup and Laser Setup tabs.

List of supported Virtual Devices:

- i-Raman NxG BWS478-785H-HT
- i-Raman NxG BWS478-785H-HT
- i-Raman NxG BWS478-785H-HT
- i-Raman Duo BWS478-860_1064-HT

List of available samples for each virtual device:

- Polystyrene
- Cyclohexane
- Acetone
- Acetaminophen

To enable a Virtual Device

1. Select the intended system from the dropdown menu.
2. Press Activate.
3. SpecSuite will identify the chosen system as Online with the displayed model ending in VIR in the bottom left of the main window. Changes can be made using the Hardware Setup and Laser Setup tabs.

6. OP (Operating Procedure)

The **OP Module** is a comprehensive module that allows users to define, configure, and manage spectroscopic analysis workflows. This module consists of three interconnected components:

- **OP**: Defines complete measurement workflows, including acquisition, processing, identification, routine analysis, and output settings.
- **Method**: Builds an analytical method based on available variables.
- **Variable**: Contains all the model variables created in the Model Module and user-created Basic variables.

6.1 OP

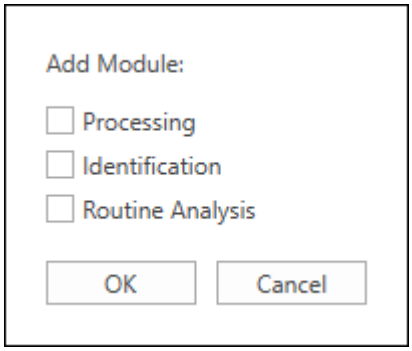
The Operating Procedure (OP) allows users to create and manage complete measurement workflows. An OP defines a full measurement procedure from data acquisition through processing to output generation.

Select an OP to view its contents in read-only

- **New** : Create new operations and methods.
- **Edit** : Modify existing configurations
- **Save** : Save the current operations or methods.
- **Archive** : Archive modules.
- **Withdraw** : Discards any changes made to the current OP.

6.2 Building an Operating Procedure

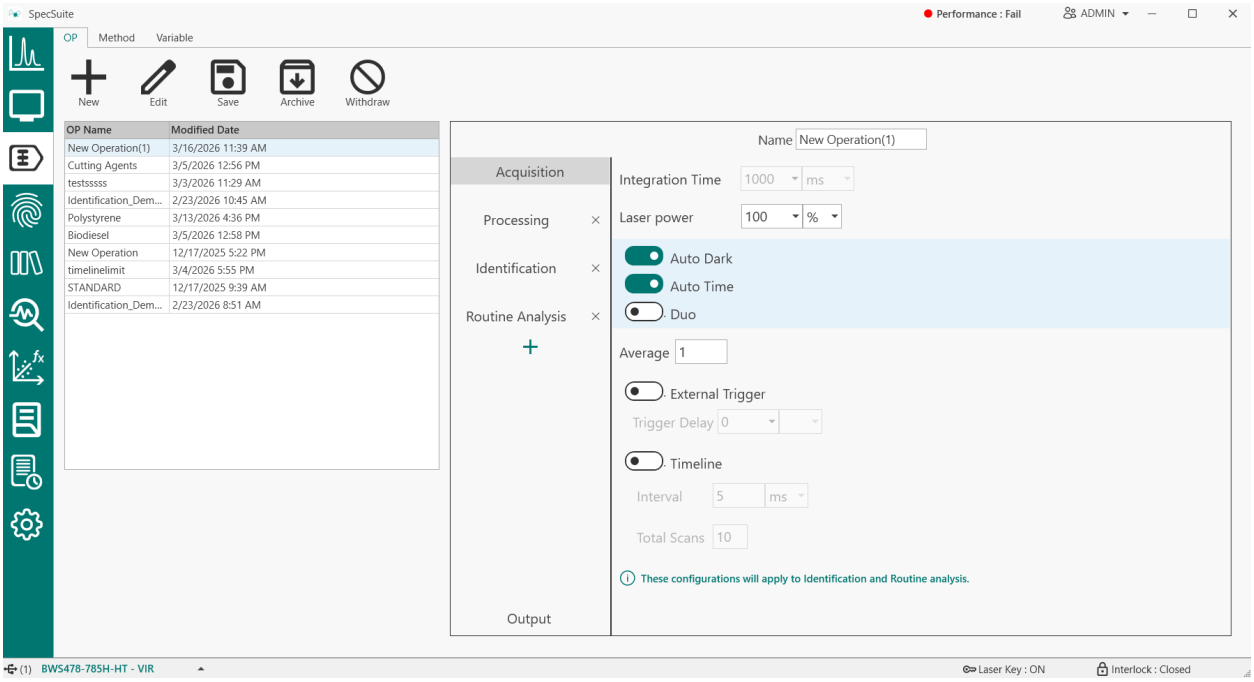
To create a New OP, press the New + button. On the right side of the page, the OP information can be viewed and edited.



OPs have two necessary components: Acquisition and Output. Other components can be added: Processing, Identification, and Routine Analysis.

Users can update the OP name at the top of the right section.

Acquisition

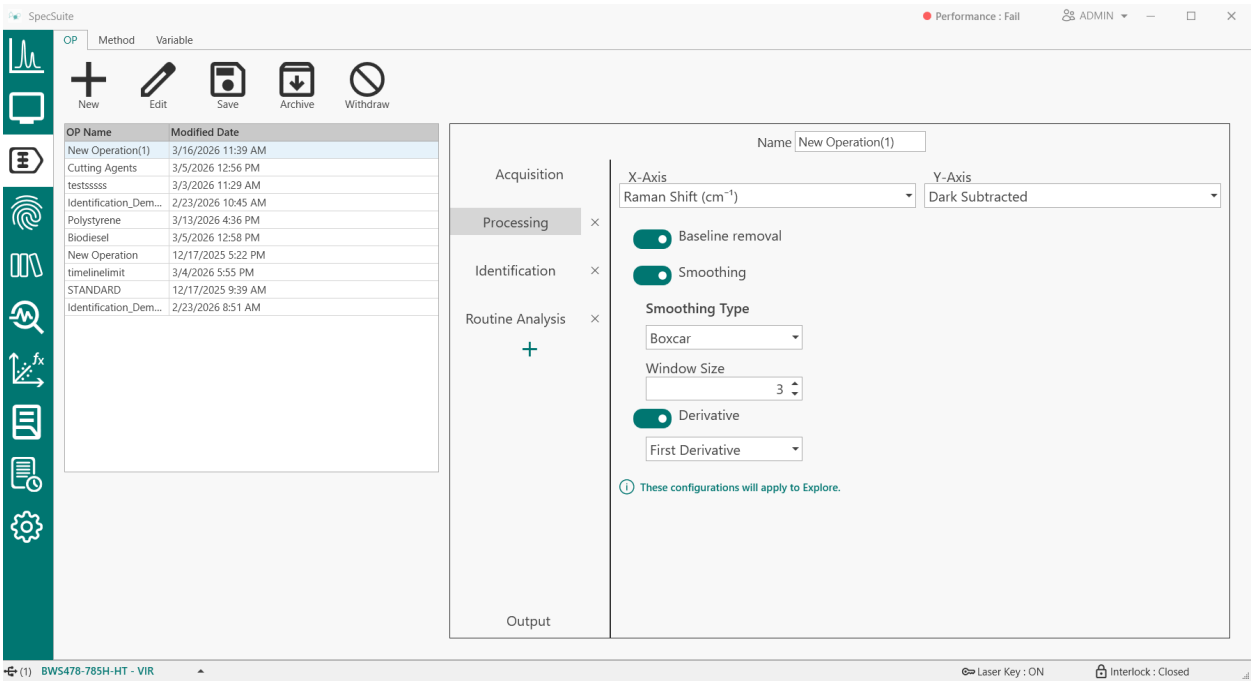


The following scan parameters can be set in the Acquisition section: Integration time, Laser Power, Average, Trigger, and Timeline.

Acquisition parameters are instrument independent, including laser wavelength, spectrometer type, etc. These parameters will apply to Explore, identification and Routine analysis modules.

- **Integration Time** – Controls the length of measurements. The limits will depend on the instrument's hardware.
- **Laser Power** – Adjusts the laser power from 1 to 100% in 1% increments.
- **Auto-Dark** – Collects a Dark spectrum scan (with the laser off) for each scan taken using the OP. If Auto-Dark is enabled in combination with Timeline, a dark scan is taken automatically for each acquisition.
- **Auto-Time** – The software will automatically optimize the integration time needed to achieve a maximum intensity between 40,000 and 60,000 counts.
- **Duo** – Optional item for i-Raman Duo operation. When enabled, additional settings for the 2nd laser can be adjusted, including "Integration Time 2" and "Laser Power 2".
- **Average** – specifies the number of data scans collected. All these scans are averaged to produce a single output spectrum. Spectral averaging is most often used to reduce noise in the spectrum.
- **External Trigger** - Allows the user to use the probe trigger to start a scan. The trigger delay is the time between pressing the trigger button and when the laser begins to fire.
- **Timeline** - Allows the user to collect multiple scans over a period without intervention. The first scan is taken immediately after Scan is pressed. The time interval between scans can be set, as well as the total number of scans to be collected. This feature is most helpful for measuring changes in a sample over time.

Processing



The Processing tab lets you apply data-processing algorithms to acquired spectra. These settings only apply to the Explore module visualization.

Processing Algorithms will apply to the selection of the X-axis and Y-axis defined in the operating procedure.

To add Processing:

1. Click the **+** button in the OP details panel.
2. Check **Processing** in the pop-up menu.
3. Click **OK.**
4. Configure spectral processing steps by enabling the toggle for each processing step.
5. Adjust the parameters for each enabled processing step.
6. Click "Save" to save the OP.

X-Axis and Y-Axis Conversion

X-Axis Options:

Pixel: The pixel index of the spectrometer.

Wavelength (nm): The wavelength of the spectrum.

Wavenumber (cm^{-1}): The wavenumber of the spectrum.

Raman Shift (cm^{-1}): The Raman shift of the spectrum, i.e., the wavenumber difference between the collected light and the laser light. Not interpolated.

Concatenated Raman shift (cm^{-1}): The Raman shift of the concatenated spectra.

Raman Shift Linear (cm-^{1}): The Raman shift of the spectrum, i.e., the wavenumber difference between the collected light and the laser light. Interpolated with 1 cm^{-1} intervals.

Note: For i-Raman Duo, or other 2-laser Raman systems, users must choose Concatenated Raman shift (cm^{-1}) in the processing module.

For all other devices, the Concatenated Raman Shift (cm-1) cannot be used in the OP's Processing module.

Y-Axis Options:

Raw: Original Spectrum Intensity

Dark: Dark Spectrum with laser turned off

Dark Subtracted: Raw Spectrum minus Dark Spectrum.

Processed: Raw Spectrum minus Dark Spectrum with relative intensity correction if a probe is enabled.

Baseline Removal

- Toggle On/Off
- Removes fluorescent background from Raman spectra.

Smoothing

- Toggle On/Off
- Smoothing Types:
- Savitzky-Golay (SG): Polynomial smoothing
    - Window Size: 5-99 (odd numbers only)
    - Polynomial Order: 1-5
- Boxcar: Moving average filter
    - Width: 3-99 (odd numbers only)
- FFT: Frequency domain filtering
    - Cutoff Frequency: 1-1024

Derivative

- Enable/Disable: Toggle switch
- Derivative Type: Savitzky-Golay
    - Derivative Order: 1-2
    - Window Size: 5-99 (odd numbers)
    - Polynomial Order: 1-5

Identification

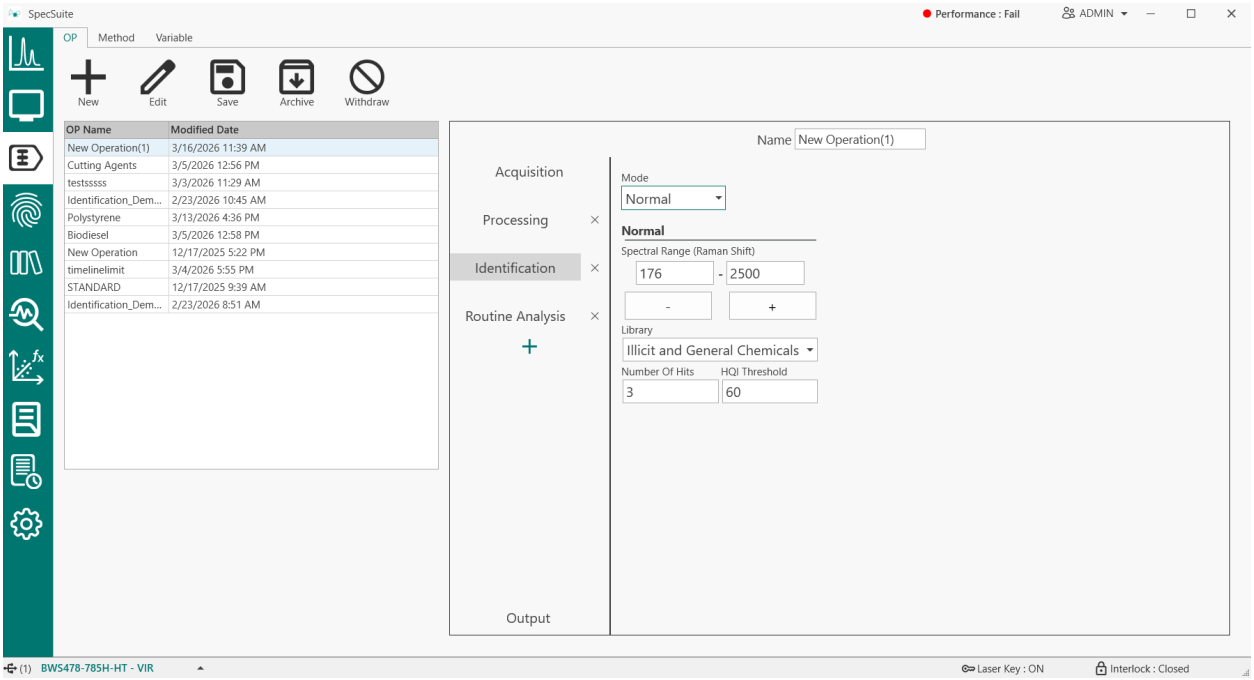
To use an OP in the Identification module, there must be an Identification setup included in the OP. If the OP does not have an identification section, it will not appear in the Identification OP selector. An OP can operate in one of three identification modes: Normal, ST, or Auto.

OPs with more than one ID mode or with multiple large libraries selected for matching take longer to complete acquisitions.

The configurations available in OP – Identification are the same as those in the Identification module's configuration panel.

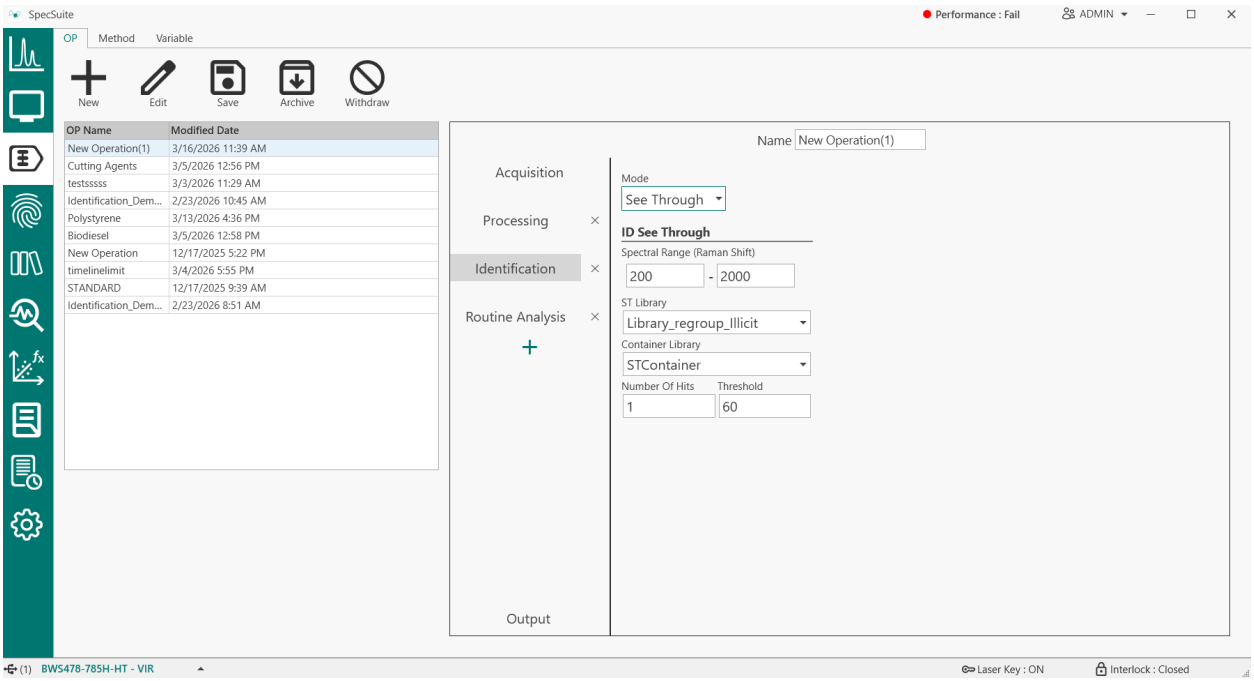
Here are the three OP identification modes the user can choose to configure.

Normal Mode



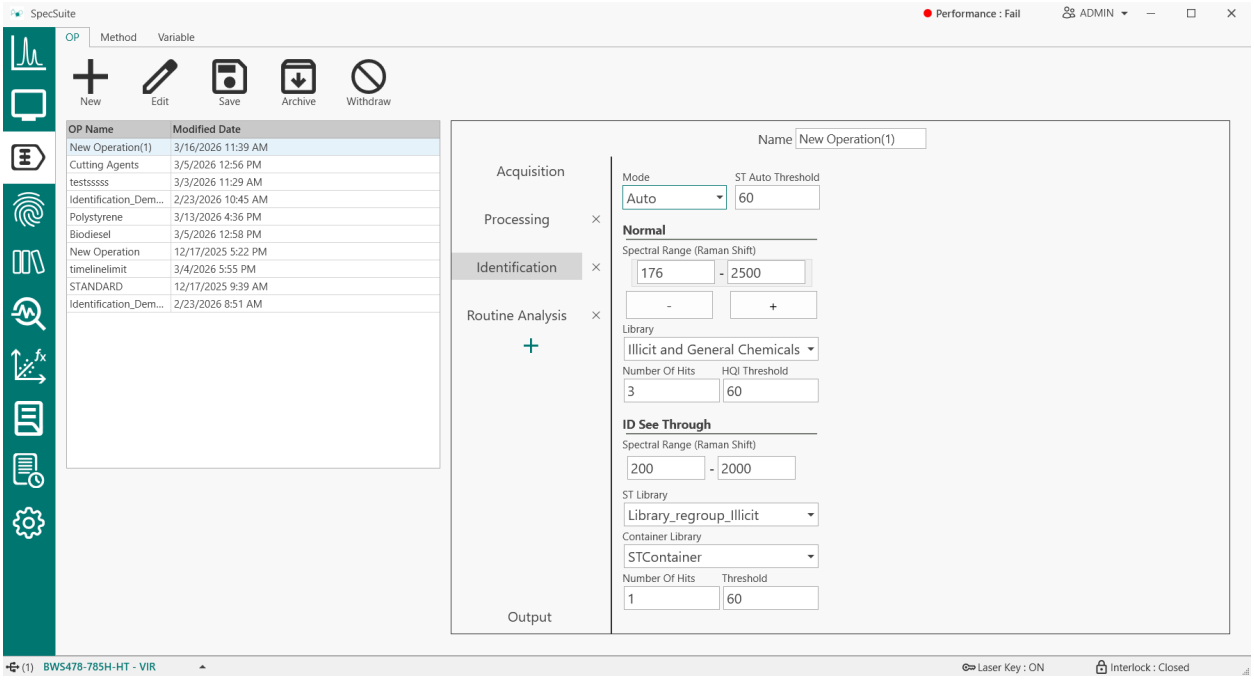
In Normal ID mode, the user can change the spectral range over which the data is processed, the spectral library used for matching, the number of hits, and the HQI threshold.

See-Through Mode



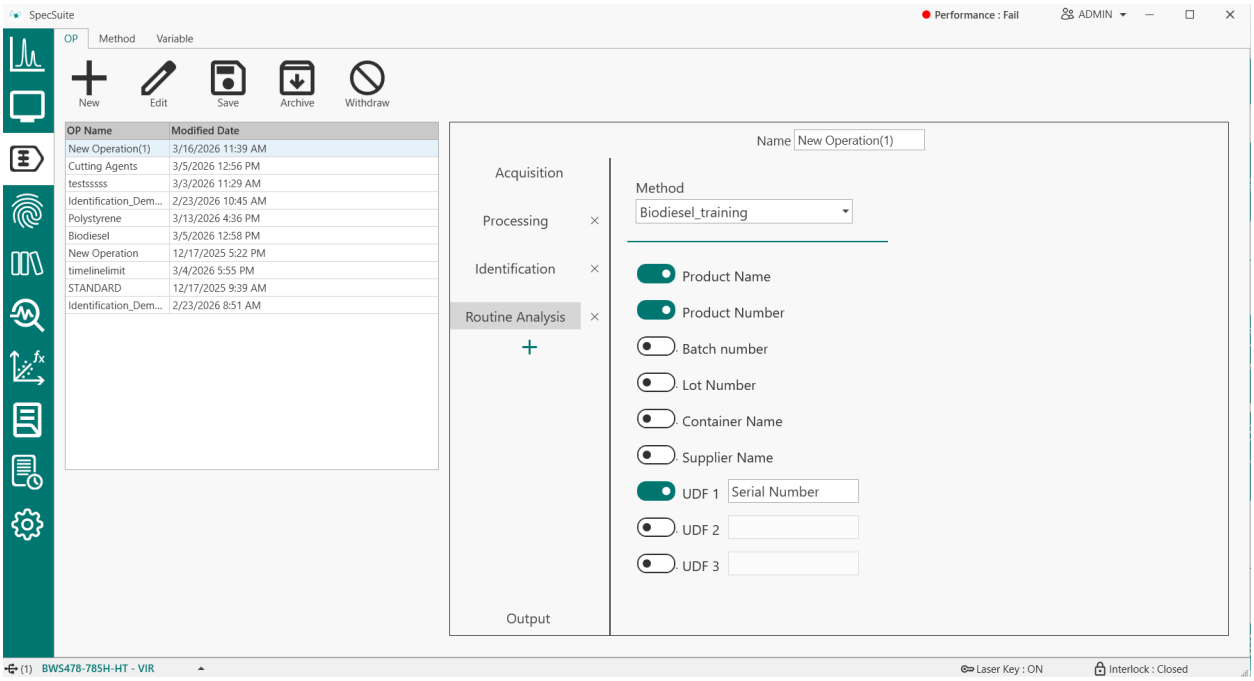
In See-Through ID mode, the user can configure spectral ranges, ST Library (Matched library), Number of Hits, and Threshold. To use See-Through mode, the default Container Library must be uploaded.

AUTO See-Through mode



In Auto See-Through Mode, user can configure both Normal mode settings and ST mode settings. Users can also configure Auto See-Through threshold, which will trigger the ST matching algorithm automatically by subtracting containers. Additional instructions on how to set up the Auto See-Through mode can be found in section 7.1 How to configure the Identification parameters

Routine Analysis



The Routine Analysis tab configures quantitative analysis workflows that combine mixture analysis and prediction models.

Configuration Areas:

1. Prediction Model Selection

- Select a Method to use in Routine Analysis. The Routine analysis will run the model/variable included in the Method.

2. Run Information Fields

Enable or disable these fields to track metadata during each routine analysis scan.

- Product Name
- Product Number
- Batch Number
- Lot Number

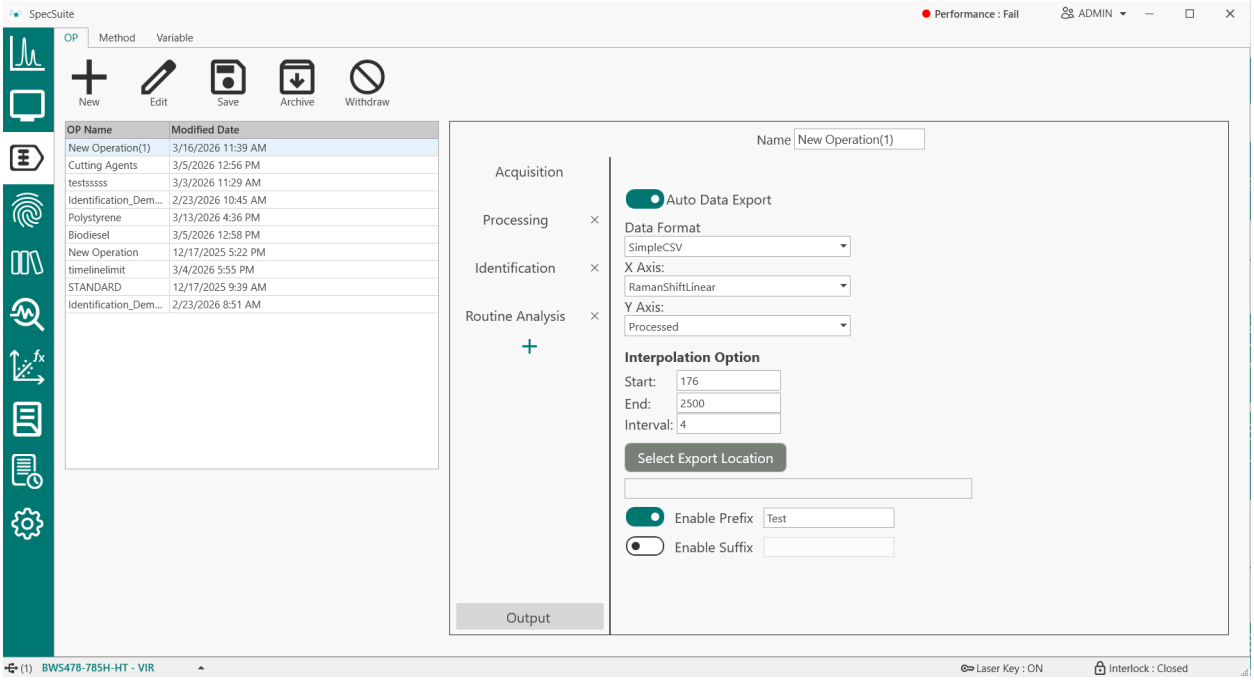
- Container Number

- Supplier Name

- User Defined Fields (UDF 1, 2, 3) (where user can define their own metadata)

The Sample Name is automatically generated by combining Product name, Run name, and Run Index. The user can input a maximum of 50 characters in ALL the fields listed above.

Output



The Output section defines how the data is saved after the OP completes.

Choose which file format the data is exported in. Choose from SPC, simple CSV, or simple SPC.

Choose which X-axis and Y-axis data is saved for simple CSV and simple SPC file types.

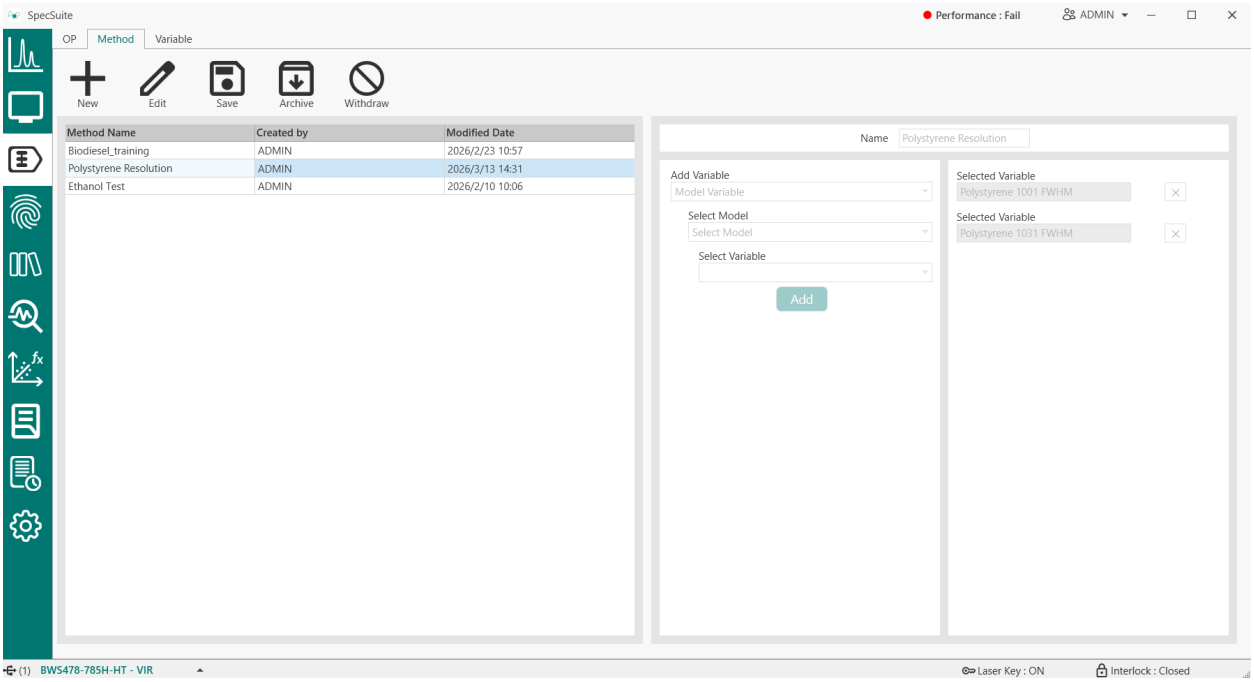
Output also allows the user to automatically save data collected with the OP in any module to a specified location.

The file name can include a prefix and/or suffix. Toggle the Enable Prefix and/or Enable Suffix options, then type the desired text in the field. The prefix and/or suffix will be separated from the rest of the file name with an underscore.

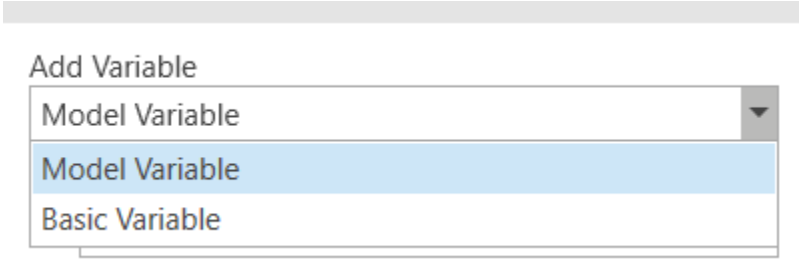
For example: prefix_scan name_suffix.

6.3 Method

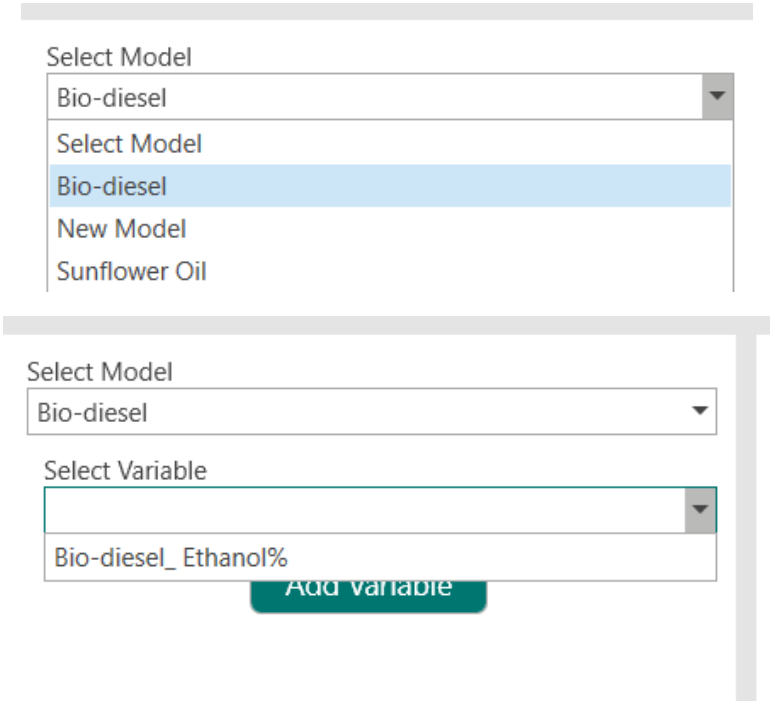
A Method allows the user to combine one or more variables into a single routine analysis measurement. The user can include both model variables and basic variables in the same method.



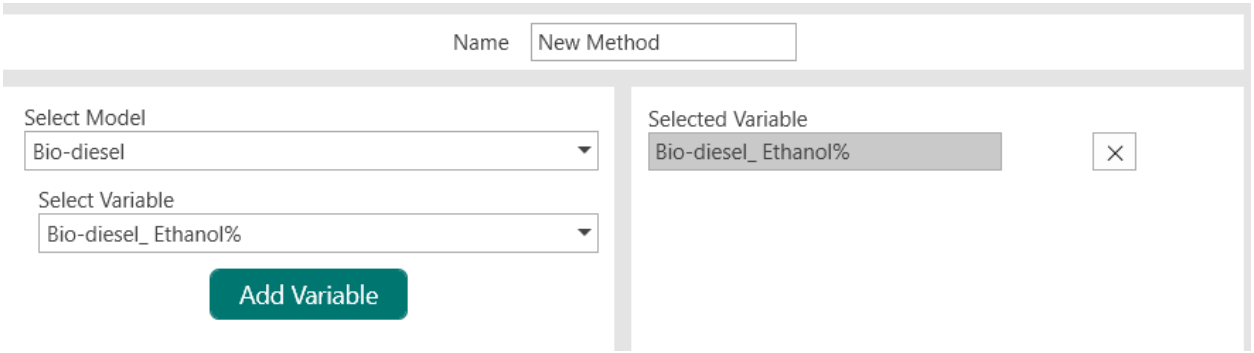
To build a new Method, click the “New” icon, then click “Edit”. Use the “Add Variable” drop-down and select whether to add a Model variable or a Basic Variable.



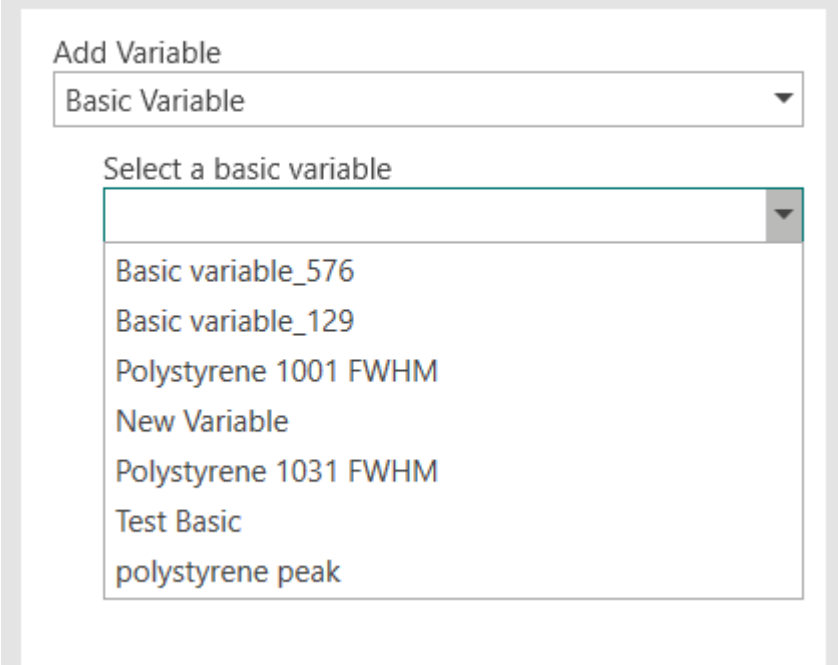
When the Model Variable is chosen, use the “Select Model" drop-down and the Select Variable drop-down to choose the variable.



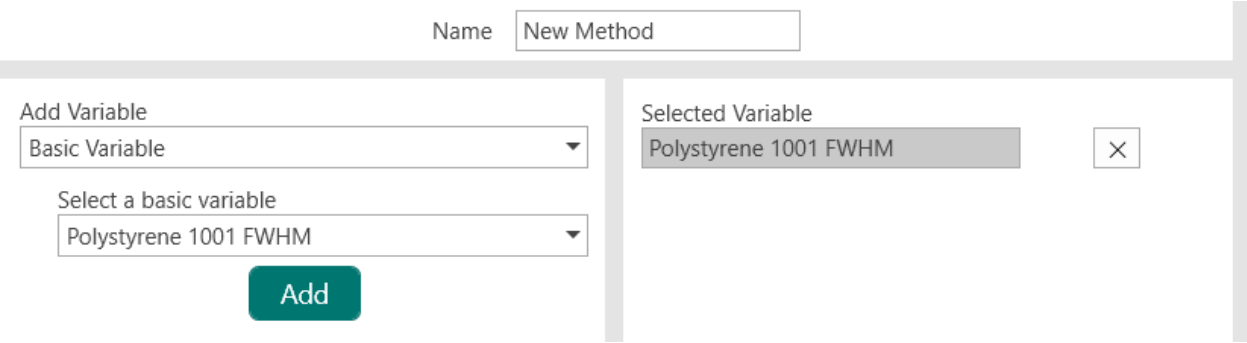
Click “Add Variable”. The selected variable is now added to the Selected Variable list on the right.



When Basic Variable is chosen, users can select the available basic variable from the drop-down list.



Click Add to add the basic variable to the Method.



The user can add up to 6 variables to a single method. The user can also click on the remove icon to remove a variable from the Selected Variable list.

Once all the variables are added to the Selected Variable list, click the "Save" button Save to save the method. A message indicating the method has been saved will appear.

6.4 Variables

Variables are items to be included in a Method and can be managed at the variable page.

The types of variables are:

- Basic Variable, which can be created, edited, and reviewed in the Explore page or the Variable page.
- Model Variable, which can be created and edited in the Model module by editing the "y1" field.

Basic Variable

Basic variables are peak analysis variables that can be derived from a specific spectrum. The user can define the processing steps, the spectral ranges used for each spectrum, and set the peak parameters for the Basic variable.

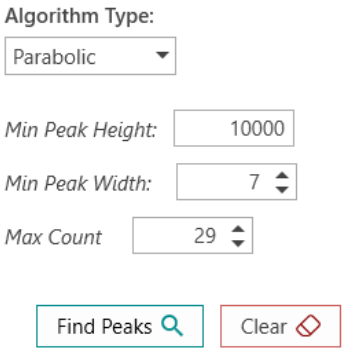
Creating a Basic Variable

The user can create the Basic variable from the Explore Page:

- Start peak analysis by clicking 

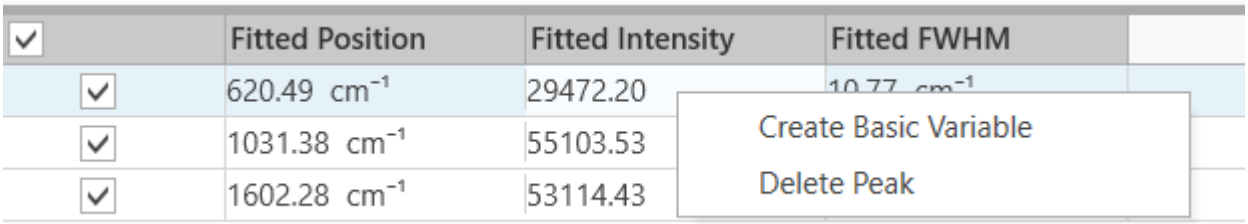
- Adjust the spectral Range 

- Select either Datapoint or Parabolic for initial peak analysis, adjust the min peak height and max peak counts, then click Find Peaks.

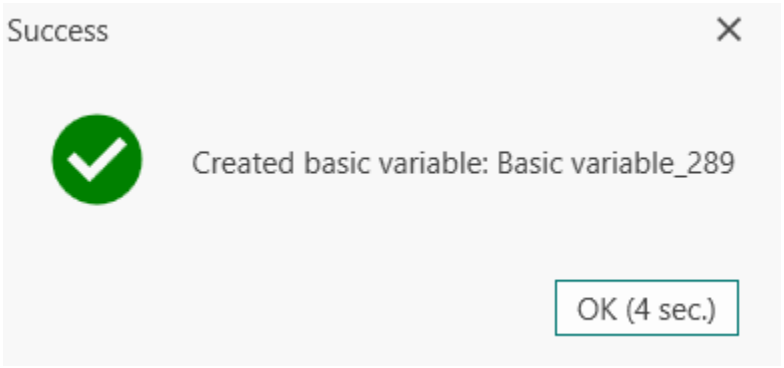


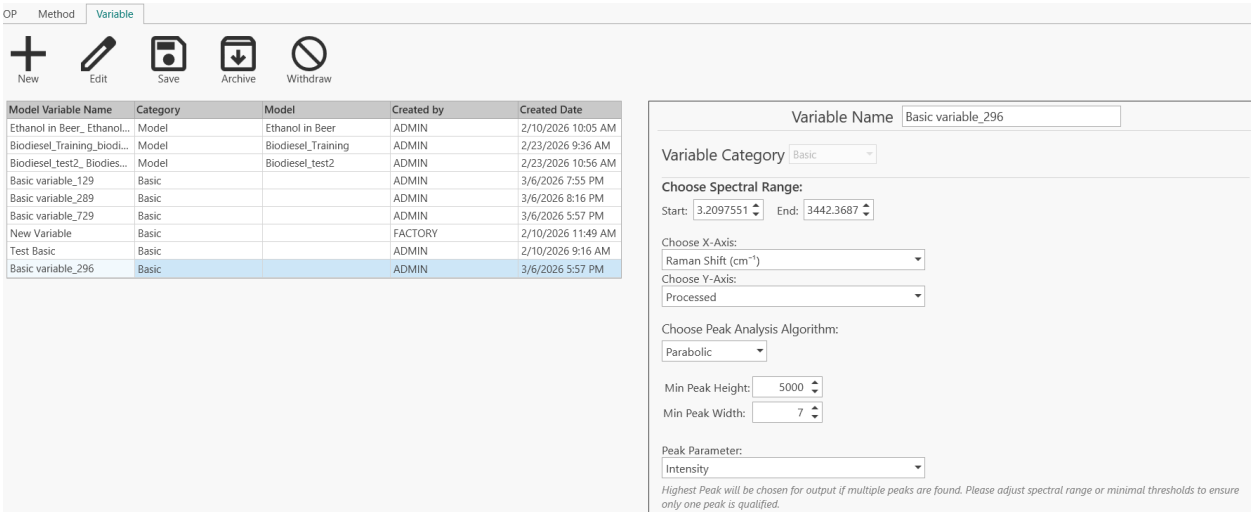
- (Optional) Switch to the Curve Fit algorithm and click Find Peaks. Note: the Curve Fit algorithm will only run when initial peaks are found through the Datapoint or Parabolic algorithms.

Once peaks are found, the user can view the peak list below the spectrum. Right-click on the cells in the "Fitted xxxx" column to create a basic variable.



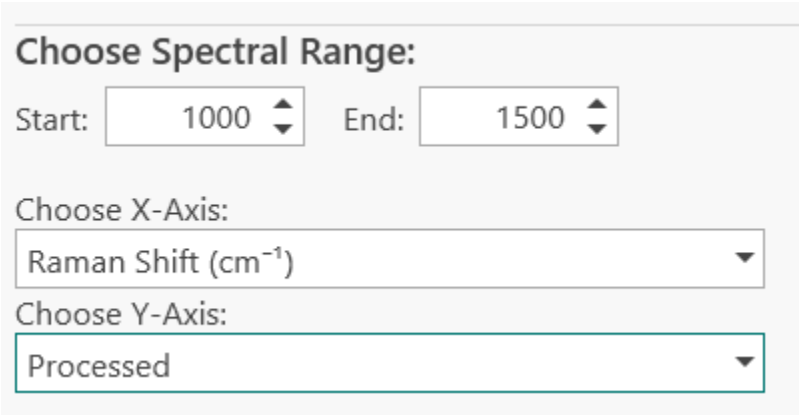
A Success message should pop up once the variable is created, and the variable will be added to the variable page.





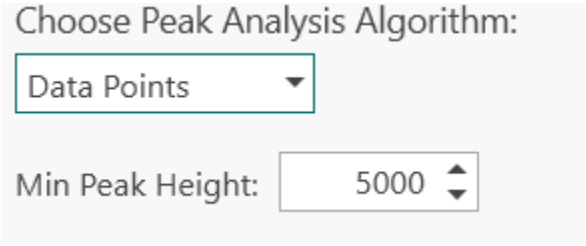
The user can also create a new basic variable from the Variable page:

1. Click on New  to open up the editing panel on the right.
2. Choose the Spectral Range, X-axis units, and Y-axis type



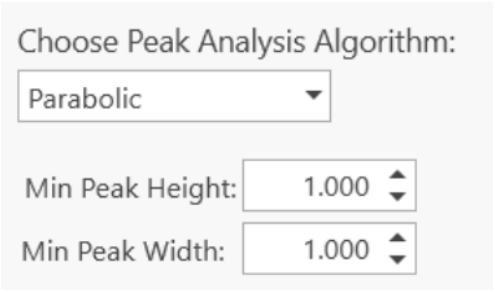
3. Select an algorithm from the Choose Peak Analysis Algorithm drop-down menu and provide the peak parameters:

   Choosing Datapoint:



   Users will need to provide the minimum peak height

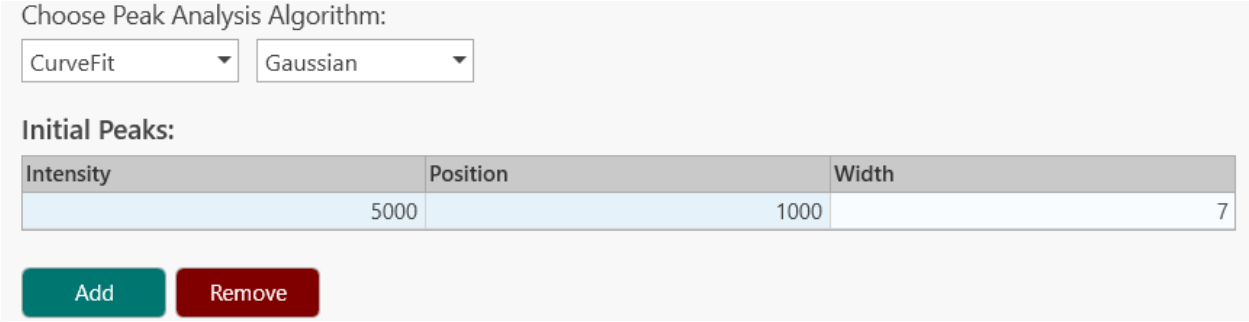
   Choosing Parabolic algorithm:



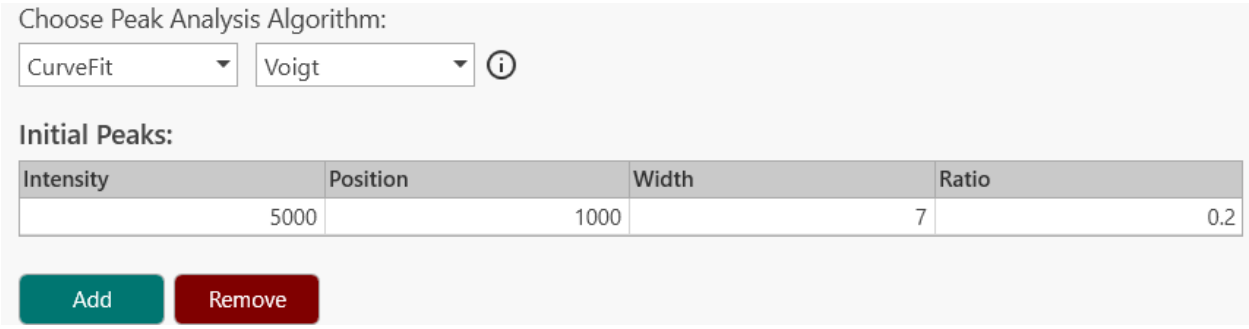
   Users will need to provide the appropriate minimum peak height and minimum peak width. The minimum peak width unit will use the same X-axis units selected in the Choose Spectral Range dialog.

Choosing Curve Fit

For either the Gaussian and Lorentzian Algorithms, users need to click Add, and define the initial peak intensity, position, and width. The initial peak parameters will be used to perform the fitting.



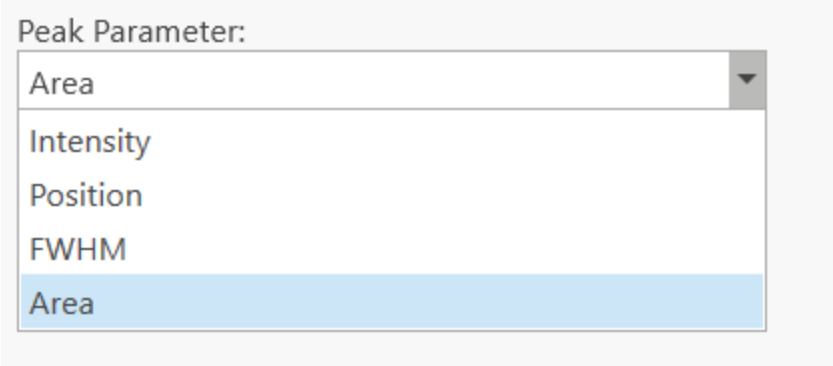
For the Voigt algorithm, users need to click Add, and define the initial peak intensity, position, width, and the ratio of the Lorentzian profile vs Gaussian profile. If the Ratio is 1, the peak will be fitted with a pure Lorentzian profile. If the Ratio is 0, the peak will be fitted with a pure Gaussian profile.



Multiple initial peaks can be added to improve the accuracy of the fitting results, but only one peak can be used to generate the peak parameters.

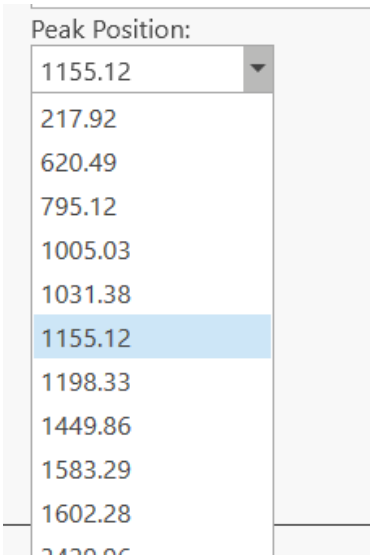
4. Select Peak position and Peak parameters as the basic variable

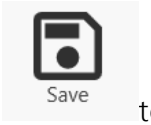
   Once the peak algorithm is defined, users can select the peak parameters (Intensity, Position, FWHM, Area) through the drop-down menu. This peak parameter value will serve as the output of this basic variable.



If Data Points or Parabolic is used for peak analysis, the highest-intensity peak will be selected as the output if multiple peaks are found. Users can use the spectral range and Min peak height to ensure only one peak is qualified.

If Curve fit is used for peak analysis, the user needs to identify the specific peak to output by selecting the labeled peak position through the drop-down menu. The available peak positions are derived from the initial peak labeled in the previous step, and the basic variable outputs the calculated peak value based on that label.



5. Click save 

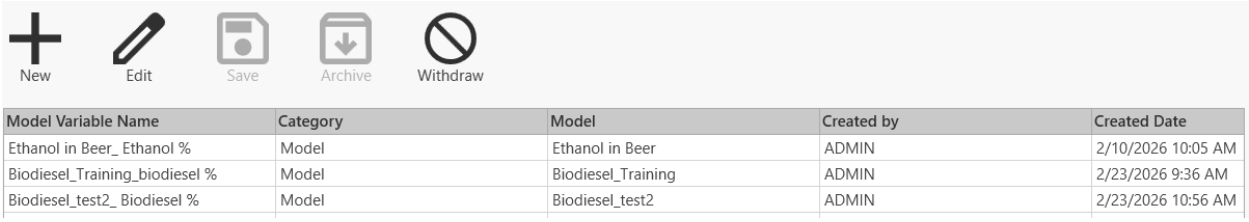
to save the basic variable settings.

Model Variable

Model variables are generated by building a model in the  Model module.

A model variable is automatically created when a model is saved. Variable names can be defined by changing label of the “y1” column for inputting reference values during the model-building process.

The variable page allows user to view available model variables. Users cannot edit model variables on the variable page; they must edit the model directly. See section 9 Model for details.



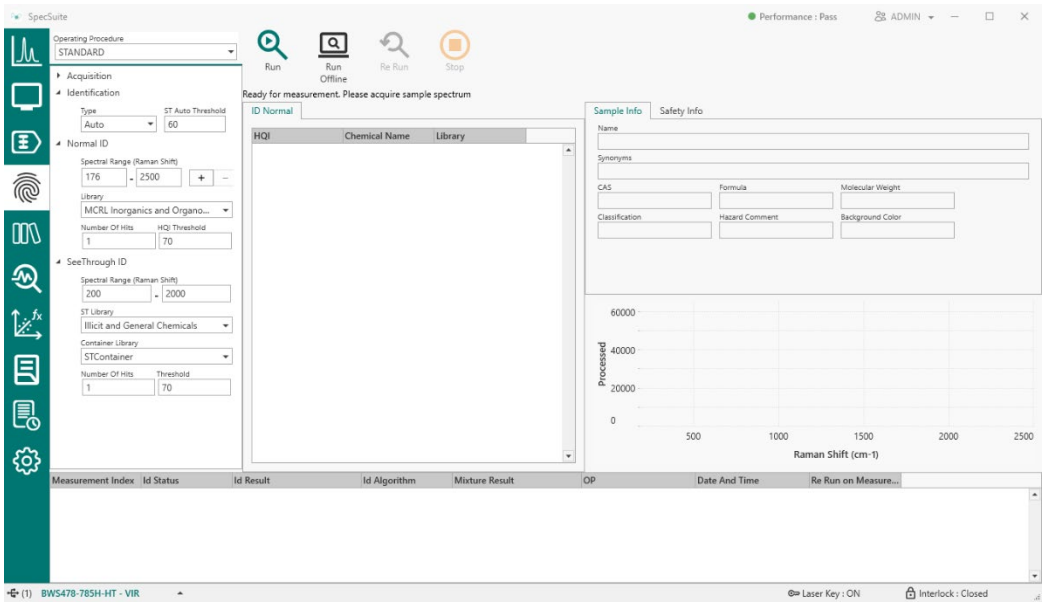
Model Variable Name	Category	Model	Created by	Created Date
Ethanol in Beer_ Ethanol %	Model	Ethanol in Beer	ADMIN	2/10/2026 10:05 AM
Biodiesel_Training_biodiesel %	Model	Biodiesel_Training	ADMIN	2/23/2026 9:36 AM
Biodiesel_test2_ Biodiesel %	Model	Biodiesel_test2	ADMIN	2/23/2026 10:56 AM

7. Identification

The Identification module is useful for qualitative sample identification using spectral libraries and multiple spectral-matching algorithms. Users can configure the identification parameters and choose different libraries for sample identification. It is intended for users of all levels, but must be activated with an ID License.

Identification can be performed online via a system connected to SpecSuite or offline using previously acquired spectral data. Data must be complete, meaning it includes both regular data and dark data. Data formats supported for Offline ID include CSV, TXTR, TXT, and SPC file formats.

7.1 Online ID



How to configure the identification parameters

1. **Acquisition:** Use this module to adjust laser power and integration time. Users can also check “Auto Time” to enable auto integration time.
2. **Identification:** Use this module to choose between the types of identification, including Auto, Normal, and See-through.
    a. Auto: When Auto is selected, the user can define an ST Auto threshold. The system will first perform Normal ID. If any container spectrum is identified and its HQI value exceeds the ST Auto Threshold, then See-Through ID is automatically executed.
    b. Normal: Normal ID uses a Hit Quality Index (HQI) to analyze the spectra and provide the highest HQI match result from the selected libraries.

c. See-Through: See-Through ID uses the STID algorithm to identify samples inside containers. Under See-Through, the selected container's spectrum is subtracted from the collected spectrum, and the resulting spectrum is analyzed for matches with materials from the selected ST Libraries.

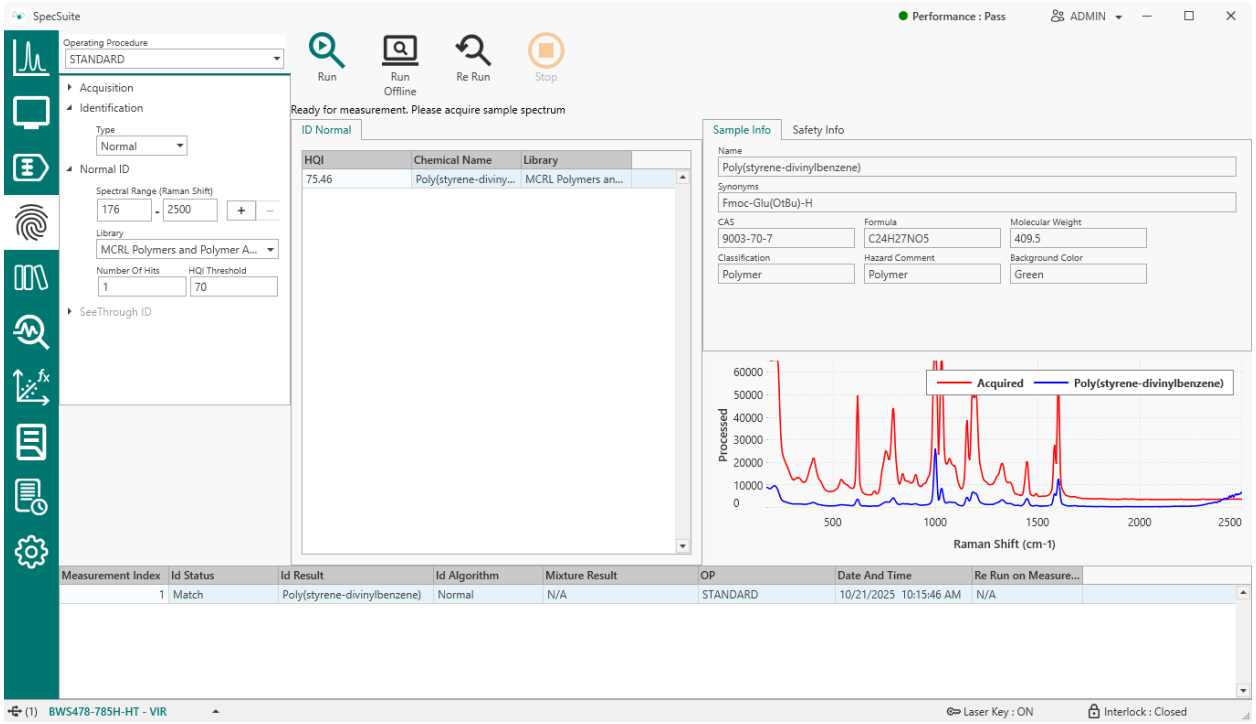
3. Normal ID:
    a. Spectral Range: The user can configure multiple separate spectral ranges by using the "Add" or "Subtract" features and selecting the spectral range by inputting the start/finish Raman Shift in wavenumbers. A default example is included in the Standard OP.
    b. Library: User can use the drop-down menu to select 1 or more libraries to use with the HQI match.
    c. Number of Hits: The maximum number of matching candidates the system will display. Maximum input is 99.
    d. HQI Threshold: The minimum matching threshold where a spectrum is considered a match. The HQI ranges from 0 to 100, with 100 indicating a perfect match.
4. See-Through ID:
    a. Spectral Range: The user can configure the spectral range by defining the start/finish Raman Shift in wavenumbers. A default example is included in the Standard OP.
    b. ST Library: The library used for spectral identification after the container spectrum is subtracted.
    c. Container Library: The library of container spectra.
    d. Container Material: The user can choose one container spectrum from the Container Library. This container spectrum will be subtracted from the measured spectrum before doing the See-Through matching.

How to perform an ONLINE ID

1. Verify proper setup

   a. The instrument is connected to SpecSuite.
   b. Online status is displayed in the lower left corner of the window.
   c. Performance status in the top right corner of the window is green , in valid standing.

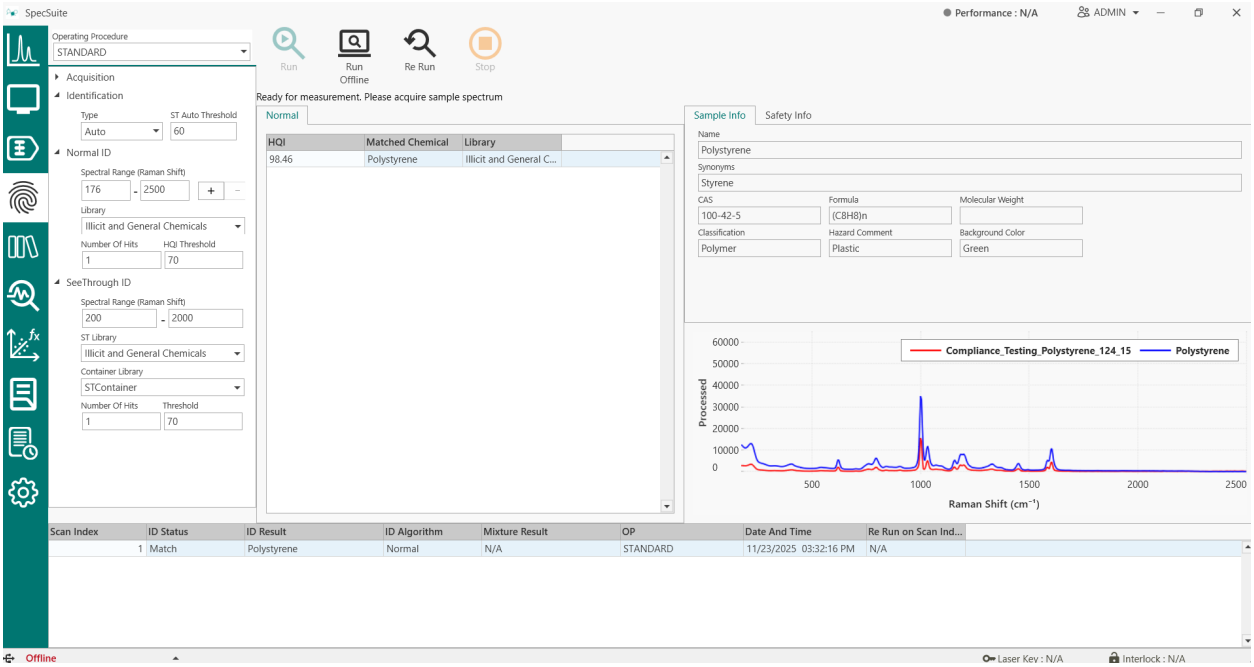
2. Select Identification Module  .
3. Select a dropdown to choose an Operating Procedure.
   a. The identification Details will populate below the OP selection.
   b. The ID types will appear according to the chosen OP.
      i. Normal mode will show Normal ID.
      ii. ST mode will show See-Through ID.
      iii. AUTO mode will show Normal and ST.
   c. The library options will show the available libraries for matching.
4. Review the ID Details.
   a. Only Developers and Administrators can adjust ID-related OP settings from the details panel.
   b. ID parameters may be adjusted.
   c. Other parts of the OP must be edited in the OP module.
5. The software is now properly configured to run the ID.
   a. Verify the sample is correctly positioned for acquisition.
   b. Ensure the probe shutter is open.
6. Press the Run button to begin the ID acquisition.
   a. While scanning, press the Stop button to stop the scan at any point.
   b. The scan data will appear in the chart. In the Sample List table, the Result column(s) will say “In progress…” while the matching algorithm runs.



7. Review your results.
    a. ID results will appear in the result table in the middle of the screen with applicable matching statistics. Normal and ST results will show the HQI value.
    b. The spectrum chart will display the acquired spectrum overlaid with the spectrum selected in the result table.
    c. Switching to the sample info tab will display information for the chemical selected in the results table: name, synonyms, CAS, Classification, Formula, Molecular weight, NFPA Diamond, and GHS information.
    d. The ID record is saved in the database, and an entry is added to the bottom scan list on screen.
    e. Selecting any entries from the scan list will update the info shown in the Result table, Sample Info, Safety Info, and the spectrum chart.

All Online ID results and spectra are automatically saved in the connected database. The user can use the Report module to review and e-sign the identification report.

7.2 Offline ID



Identification can be run without a system online or on previously collected data. **Offline ID records are NOT saved in the database.**

How to perform an OFFLINE ID:

1. Select the Identification Module.
2. Select a dropdown to choose an Operating Procedure.
    a. The identification Details will populate below the OP selection.
    b. **For Offline ID**, the acquisition settings for the OP will be ignored. Only the library matching settings will be applied to the data.
3. Review the ID Details.
    a. Only Developers and Administrators can adjust ID related OP settings from the details panel.
    b. ID parameters may be adjusted.
4. Select the Run Offline button.

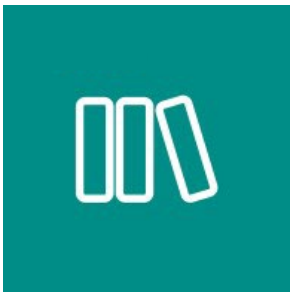
5. Select the file to run the ID on, then press Open.
    a. The identification will start right away.
    b. Multiple records of different file types can be selected for the sample spectrum. When using See-through Mode, only 1 record can be selected for the container spectrum.
    c. Allowed file types: CSV, TXTR, TXT, and SPC.
6. The scan data will appear in the chart, and in the Sample List table. The Result column(s) will say "In progress…" while the matching algorithm runs.
7. Review your results.
    a. ID results will appear in the result table with applicable matching statistics.
    b. Normal and ST results will show HQI value.
    c. The spectrum chart will display the ID result spectrum overlayed with the chemical spectrum selected in the result table.
    d. Switching to the sample info tab will display information for the chemical selected in the results table: name, synonyms, CAS, Classification, Formula, Molecular weight, NFPA Diamond, and GHS information.

7.3 Re Run

The user can click the "Re Run" button 

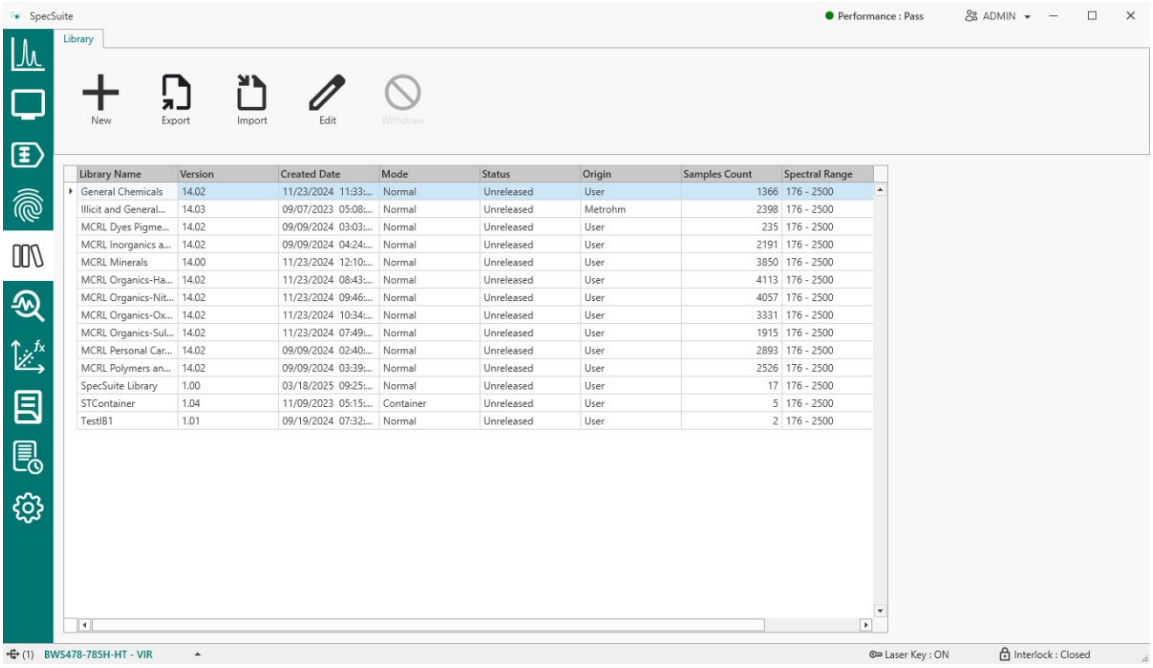
to redo the identification of the currently selected scan. Re-run records are **not** saved in the database and are for viewing only.

8. Library



The Library module contains all the tools needed to view, create, and share user-created libraries. Metrohm-licensed libraries are also stored here, with limited permissions. The Library module opens to the Library List. The Library module is only included with the ID license.

8.1 Library List



The library list is a table for viewing the available spectral libraries in the SpecSuite database.

Information about each library is available in the library table. Some examples are Library Name, Version, Created date and time, Mode, Status, Origin, and Sample Count.

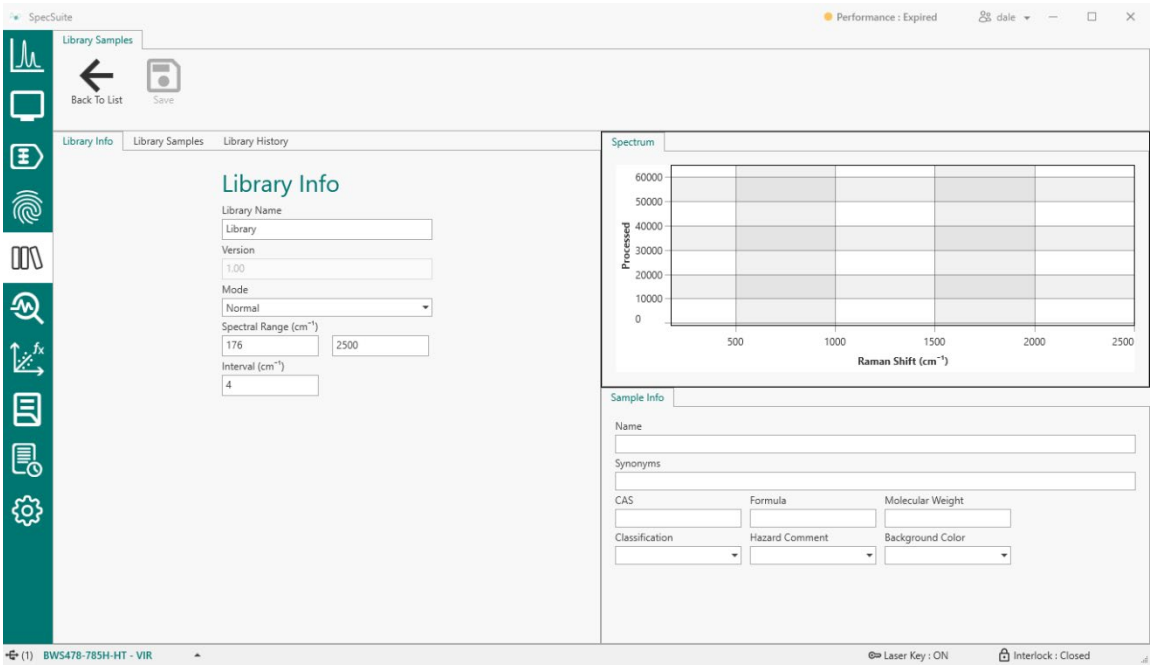
In the library ribbon, there are options for the libraries in the library list below:

- New – Creates a library
- Export – Saves the selected library in a *.zip file format to make it portable. Library packages are compatible with SpecSuite and Metrohm TacticID-1064 ST.
- Import – A user-created library can be imported either from the database or from the computer hard drive in the form of a Library package *.zip file. Purchased Metrohm Libraries can also be imported using this feature.

- **Edit** – A user can select a library out of the list and then choose Edit, or they can open a library for editing by double-clicking the library entry.
- **Withdraw** – The changes made to a library are saved temporarily. Pressing Withdraw will discard all changes made to the library since the last save. While a library is temporarily saved, library ribbon functions other than Withdraw or Edit are disabled.

8.2 Creating a New Library

A new library can be created by pressing the 'New' button on the Library List view. The Library Info screen will be displayed.



Only users with a Developer or Administrator account can create libraries. A library can only be saved if it contains at least one spectrum.

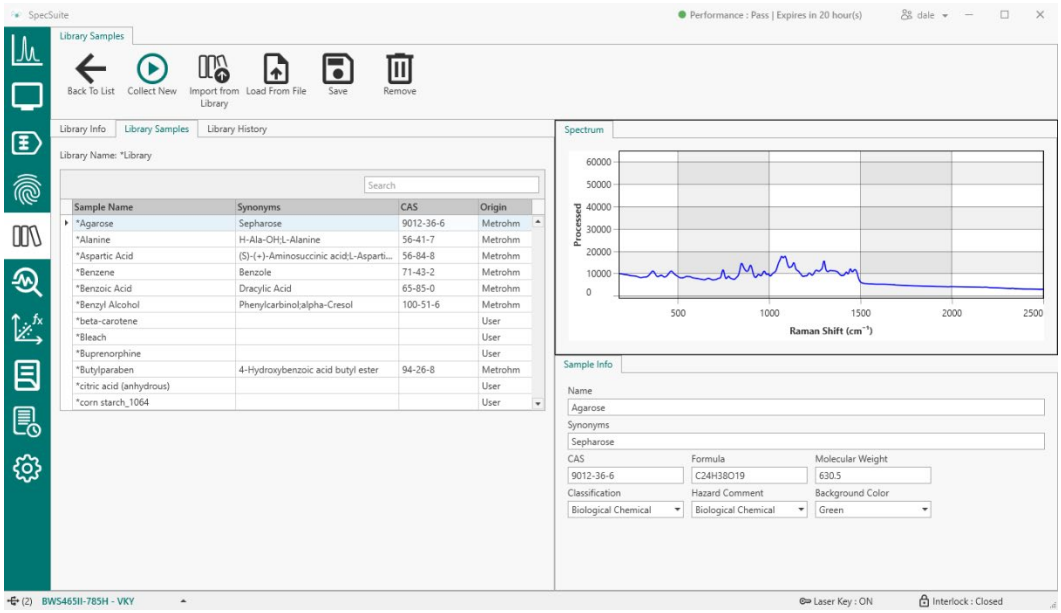
On the Library Info screen, a Library Name can be entered.

Library naming rules:

- A maximum of 40 characters can be entered as the library name. Once saved, the library name cannot be changed.
- Library names cannot contain the following symbols: /\:*?><|.
- A space character is not allowed at the start of the library name.
- A library name cannot match one of the reserved Metrohm Library names.
    - Reserved Metrohm Library names include:
        - Illicit and General Chemicals
        - MCRL Inorganics and Organometallics
        - MCRL Organics
        - MCRL Personal Care Products
        - MCRL Polymers and Polymer Additives
        - MCRL Dyes Pigments and Stains
        - MCRL Minerals
        - MCRL Pesticides
        - MCRL Biochemicals
        - MCRL API
        - General Chemicals
        - CWA
        - EXP
    - If a new Metrohm Library is imported and there is already an existing user library with a matching name, the user library will be appended with '-C' to avoid duplicate library names.
        - Example: 'Material' would be updated to 'Material-C'

In the Mode dropdown, users can choose to create a Container library. Container libraries can only be selected as the Container Library when performing SeeThrough ID.

8.3 Adding Samples



On the Library Samples tab, samples can be added from:

- An existing library.
- A local file.
- Collecting a spectrum with an online instrument.

Samples can be removed from the library by:

1. Select the sample(s) to be removed.
2. Press the Remove button.

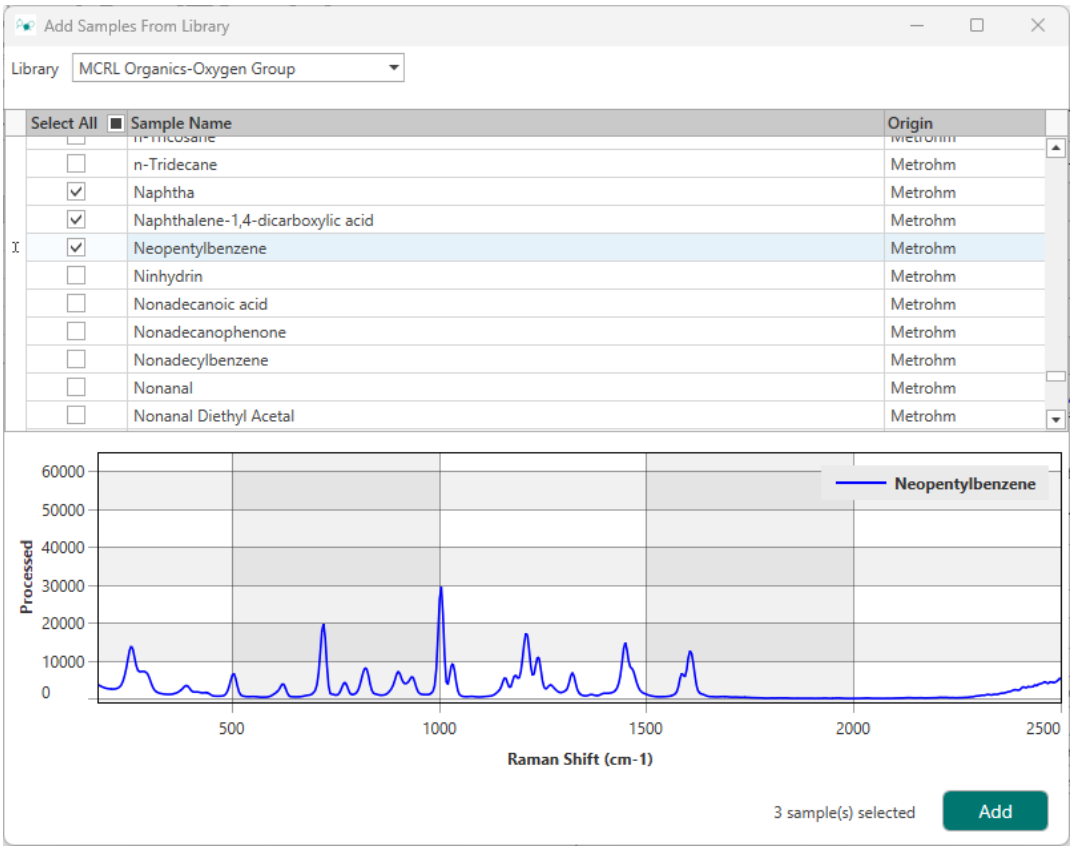
The process of removing samples is recorded in the Library History.

All samples within a library must have unique names. A warning message will appear if a sample is given a non-unique name. A library cannot be saved when two samples have duplicate names.

To save a library, it must contain at least one sample.

Import from Library

Samples from a Metrohm licensed library can be used to create a user library. The samples can be edited once regrouped into a user library.



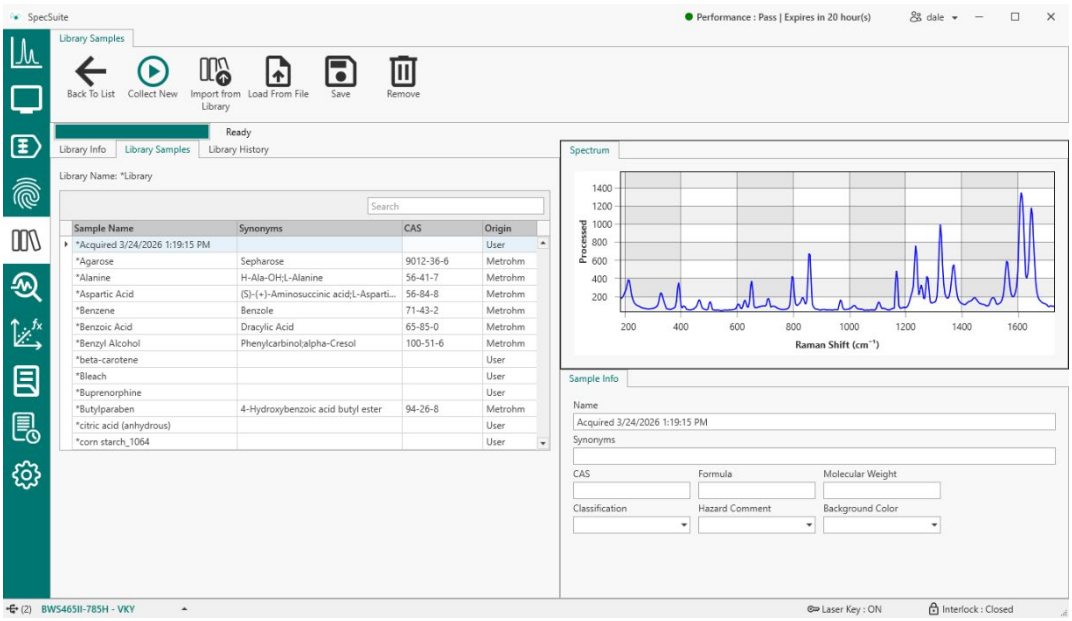
1. Press the Import from Library button.
2. From the Library dropdown, select which library to add samples from.
    a. Select the sample(s) to be added to the library by checking the box next to each sample.
3. Press the Add button.
    a. Note that samples can only be selected from one library at a time.
    b. Changing the library selection will clear the current sample selection.

Load from File

Sample files saved to the computer can be selected to add to a library.

1. Press the Load from File button.
    a. A file browser window appears.
2. Choose the file(s) to load and press Open.
    a. The samples will be loaded into the library.

Collect New

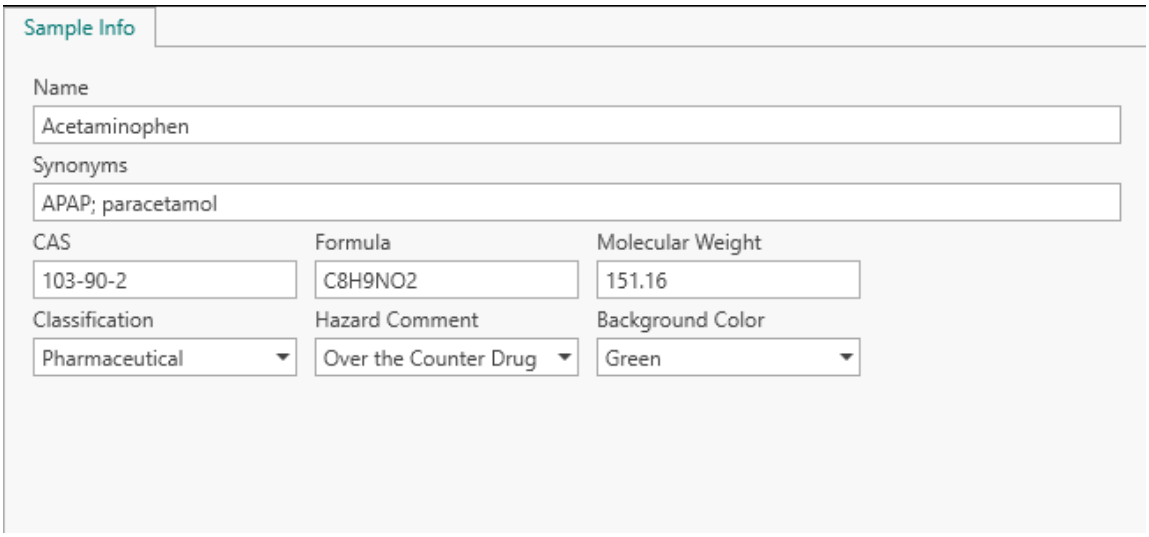


Press the Collect New button to acquire new library spectrum from an Online system. The acquisition is collected using the Standard OP, which cannot be changed.

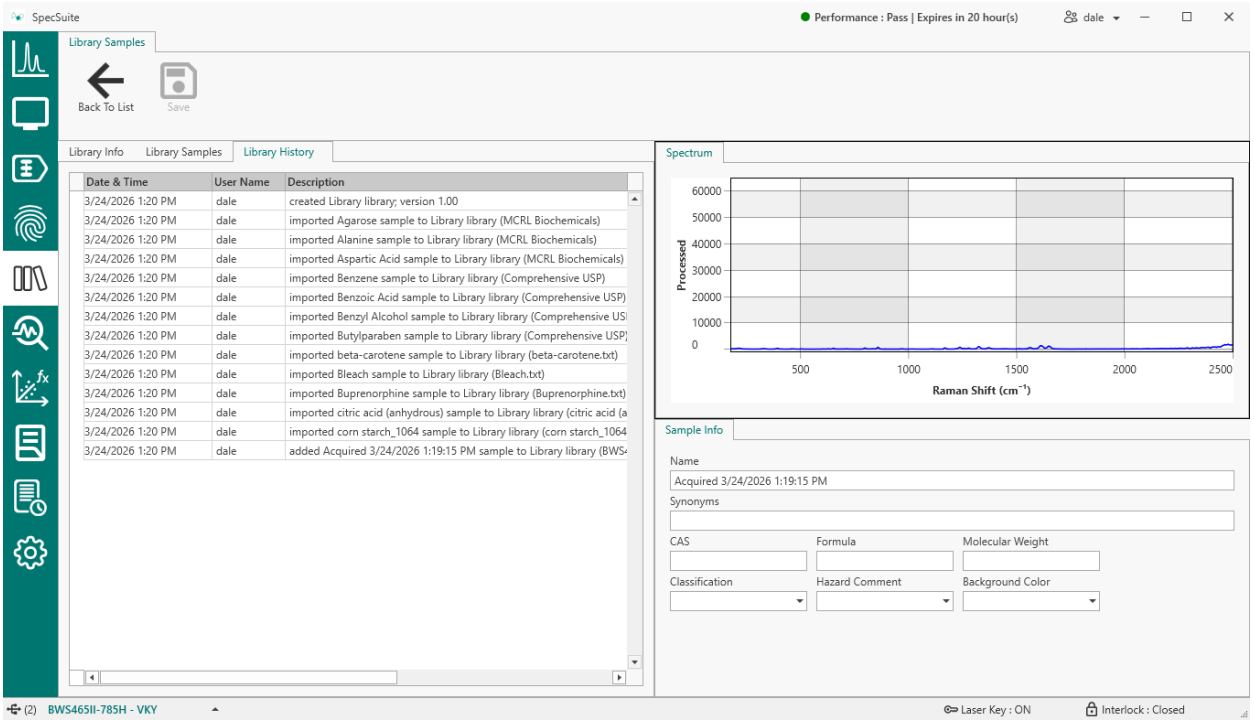
Library Samples Info

Detailed library sample information can be edited for each user-created library sample entry, such as:

- Sample Name
- Synonyms
- CAS number
- Formula
- Molecular Weight
- Classification
- Hazard Comment
- Background Color



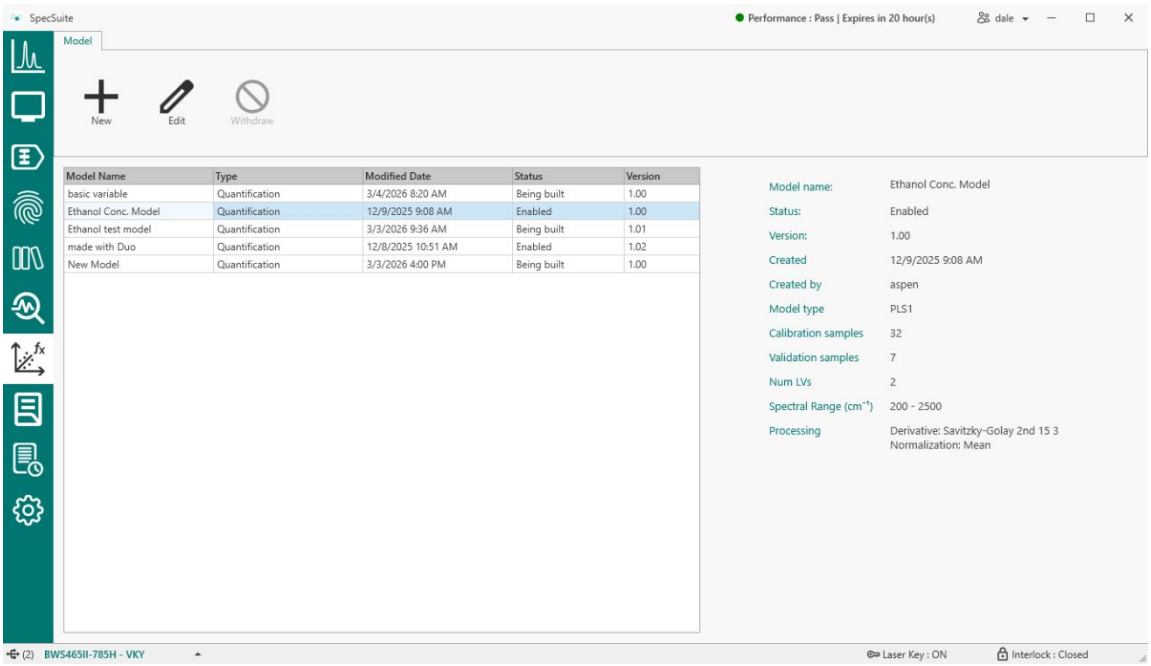
8.4 Library History



Each library contains its own history record. The Library History allows the user to see all actions performed on a library and who performed them. The same records are also included in the Audit Trail.

9. Model

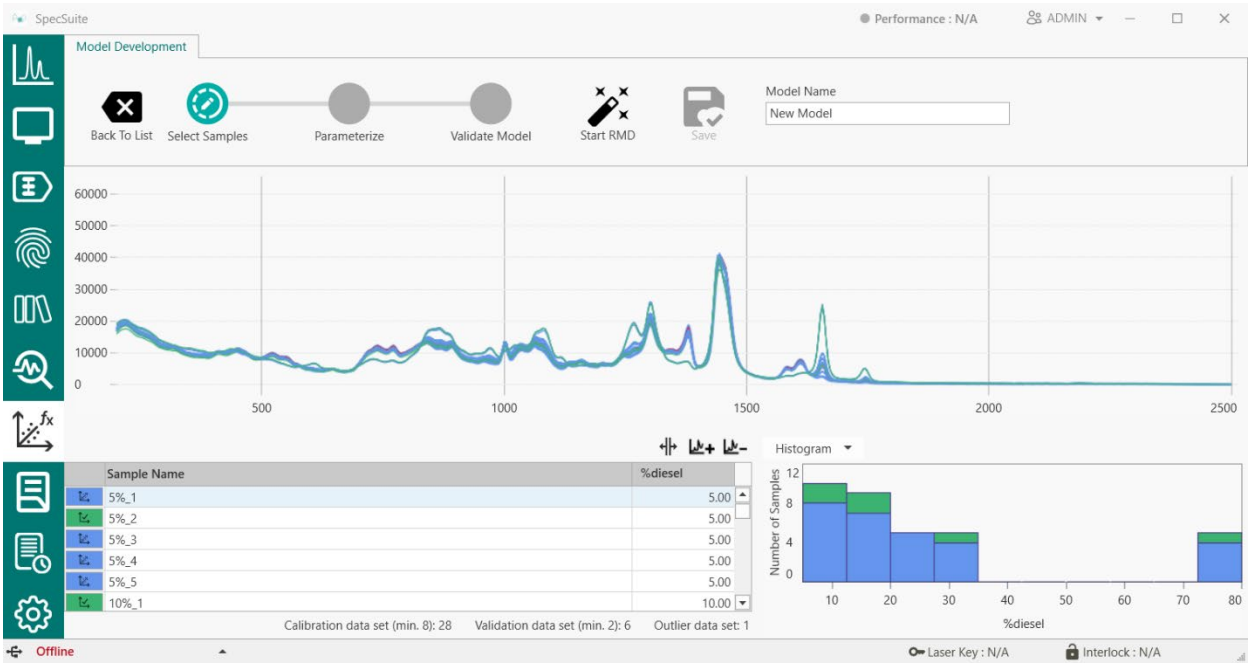
Quantitative chemometric analysis tools are a part of SpecSuite. The Model module currently supports PLS1 quantification.



Click New or Edit to start a model-building or editing session. There are 3 main steps to building a successful model:

1. Select Samples.
2. Parameterize the Model.
3. Build and Validate the Model.

9.1 Select Samples



Adding Samples

The sample table is located in the lower left of the Build screen. Above the sample table, there are 2 icons that are used to add and remove samples to the model:

adds new spectra to the data set.

- A file browser opens for the user to select files from their local PC.
    - Allowed formats are: CSV, TXTR, TXT, and SPC.

removes the selected spectra from the data set.

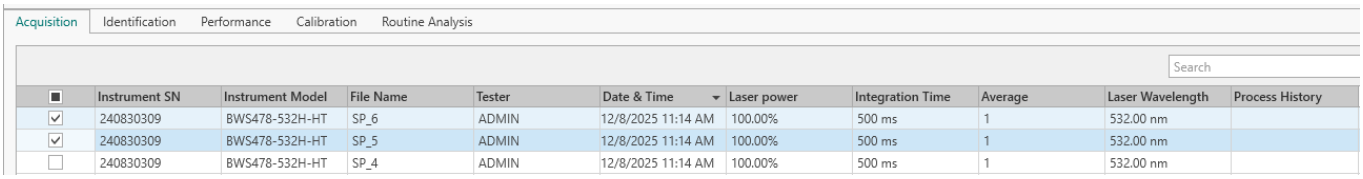
- Selecting a row in the sample table will highlight it on the XY chart, just like in Explore.
- On the spectral chart, selecting a trace on the XY chart will select the sample in the sample table.
    - Data can be selected visually to be classified as an outlier or not to be used.

Database samples can also be used for model building. First, the sample must be moved to Explore. The sample can then be moved to the model-building stage.

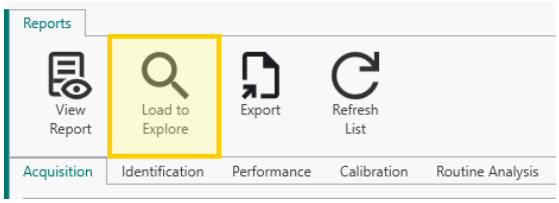
Load Samples from database:

1. Go to Reports.

2. Select Samples.

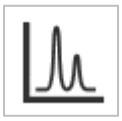


3. Select 'Load to Explore'.



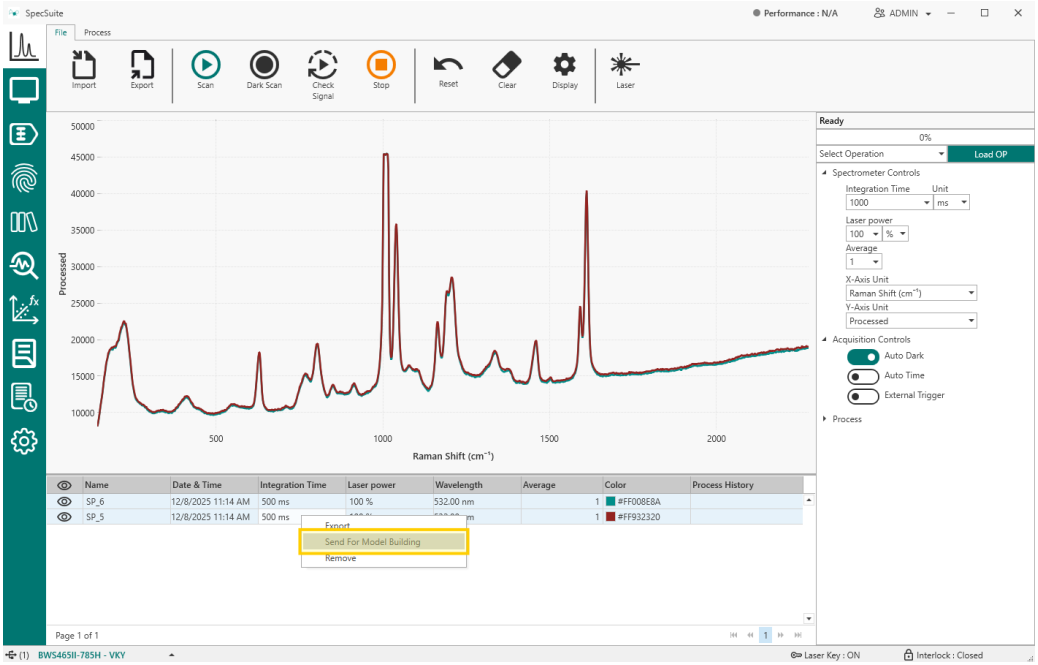
4. Select Model.

5. Create a new model or edit an existing model.
6. Go to Explore.



7. Right-click on the selected samples.

8. Choose ‘Send for Model Building.

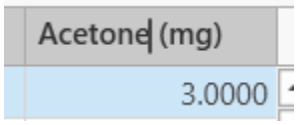


a. Selected samples are moved to model.

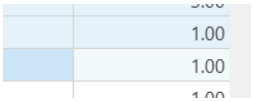
Input y-data

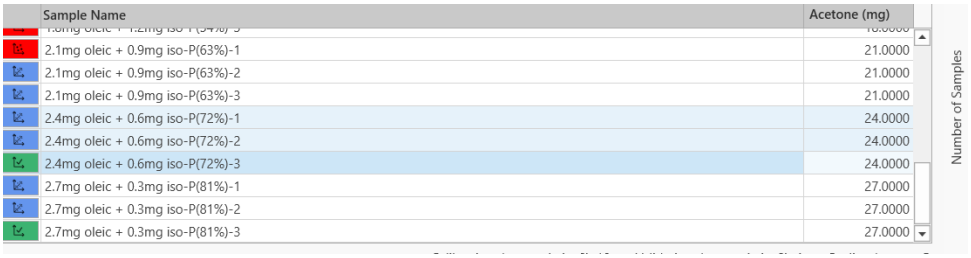
In the Sample table, the model variable is listed in the right-most column. The model variable name “y1” in the column header and the reference values for the model listed in this column can be set next.

- The variable name can be changed by typing it directly in the column header.
    - The variable name should include the name of the compound and the unit of measure for the best visual and report representations.



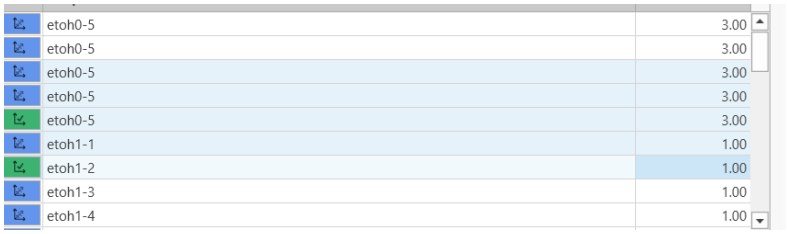
The reference value for each sample can be set manually by typing into the table. There are multiple ways to update the y1 variable value:

1. Manually updating each cell, then using the keyboard/mouse to navigate to the next one.
2. Several values can be updated to the same value at once with the following methods:
    a. Hold CTRL Key or SHIFT Key to allow multiple row selection
    b. Select multiple y1 cells by left-clicking on them. Make sure that at the end of the selection, the y1 cell is highlighted with the lighter blue color
        i. 

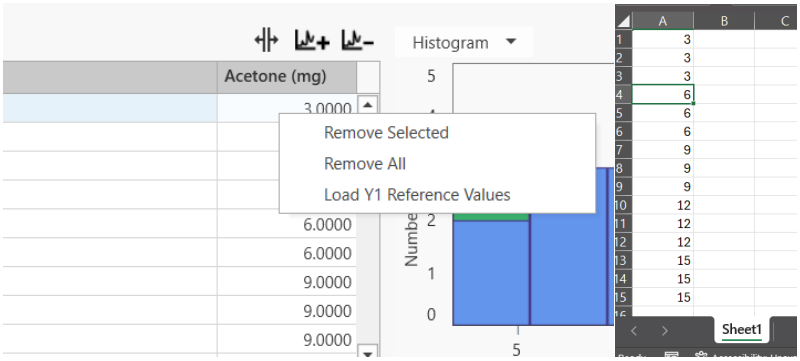
    c. Release CTRL or SHIFT key, multiple rows are still selected as shown below
        i. 

    d. ENTER the desired value for the variable from the keyboard, then press “ENTER”. All the selected y1 cells will be updated.

Note: If you select the Sample Name cells while highlighting, the y1 value will not be updated. Make sure to click from y cell to y cell.



3. Users can also quickly update the y-values by right-clicking on the table and selecting 'Load Y1 Reference Values'.
    a. A file browser will open, allowing users to load a CSV file containing the reference values.
    b. The CSV file should contain a single column of variable values in the same sequence as the samples included in the model.

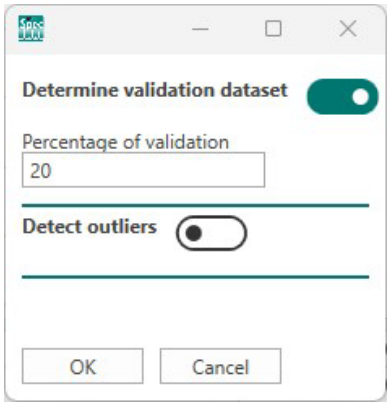


Where you right-click to import Y1 Reference Values is where the values will begin to populate from. If you want to import values for all y1 variables, make sure to right-click the top row.

For example, when a user clicks in the second row to load the y values, it will put the first value from the file in the y1 value column .CSV file in the second row, and then it will continue with rows down until there are no more reference values in the file or no more rows to set the values. Check your reference values before moving forward.

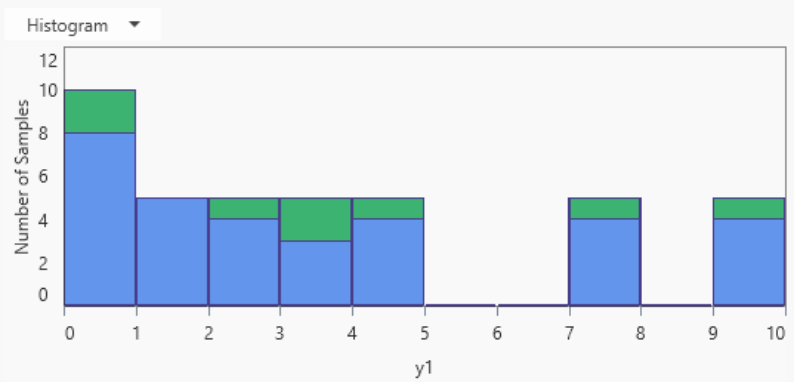
Split the Data

Splits Dataset – This function can automatically split the dataset. In the pop-up panel, the percentage of validation spectra can be defined. There is also a toggle to detect spectral Outliers during the sample selection process.

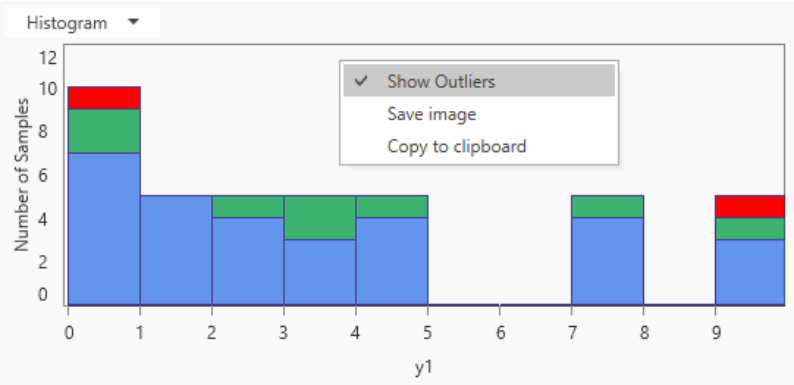


Spectra can also be manually designated as Validation, Calibration, Outlier, or Not Used. The designation can be manually adjusted by clicking the icon directly to the left of the sample name.

To the right of the sample table is the Histogram. The Histogram shows the distribution of calibration and validation samples across the range of y-values. The Histogram view can be switched to another using the dropdown menu above the chart.



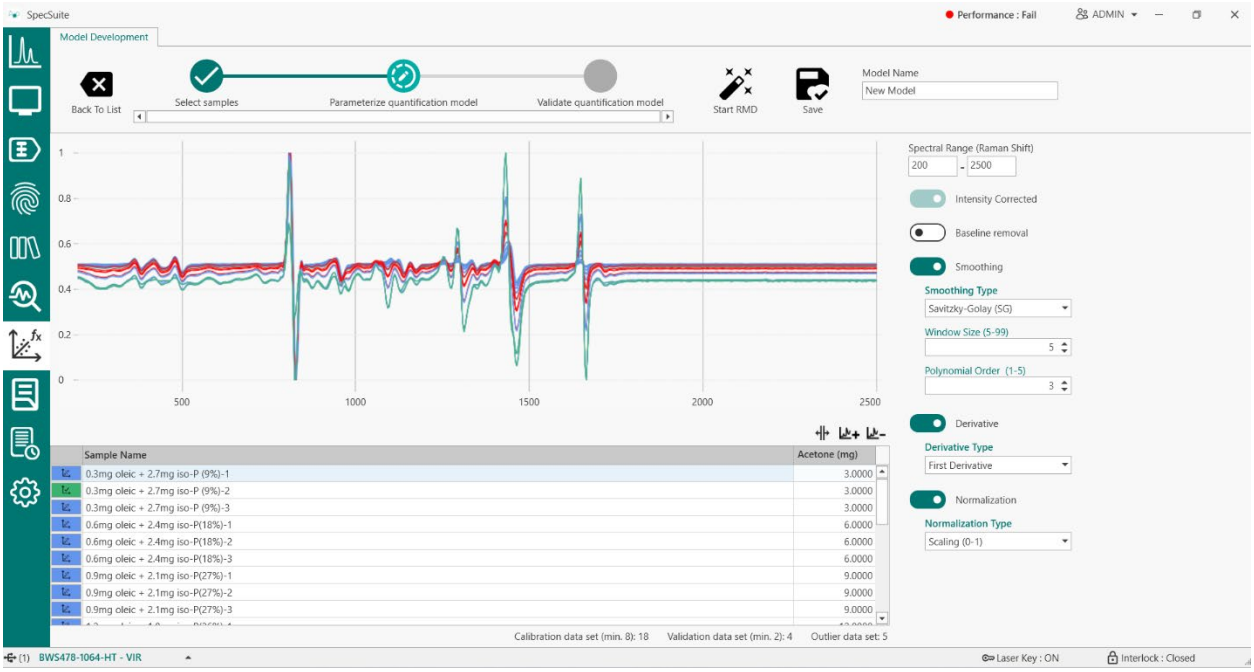
By default, the Outliers are not included on the histogram, but can be added by right-clicking on the histogram chart and selecting 'Show Outliers'.



After the samples are added and split, the user may continue to the second step, which is to parameterize the Model.

The parameterization step can be skipped by selecting the Raman Model Developer (RMD) option, which automatically generates the model using the recommended settings. **At least 10 spectra must be added to the model before the model can be built.**

9.2 Parameterize the Model



Data Processing:

- Range selection
- Smoothing
- Derivative
- Baseline removal
- Normalization: scaling (0-1); mean; SNV

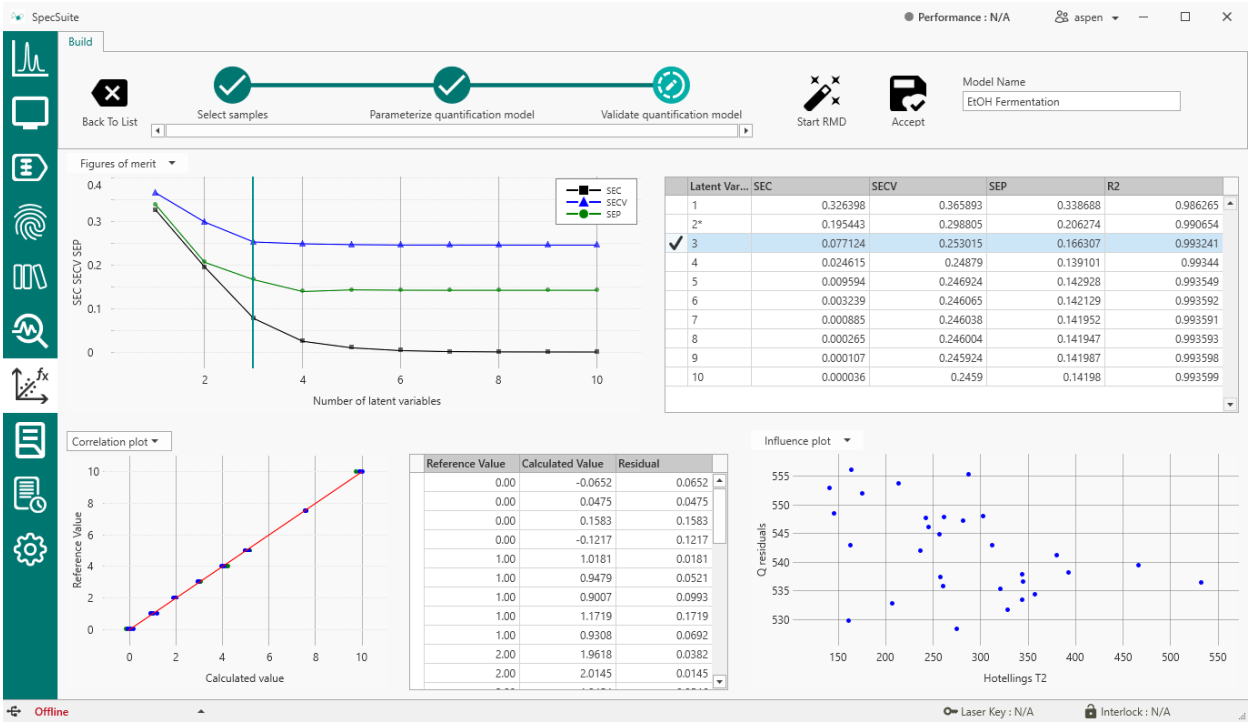
Users can use the toggle button to manually turn processing steps on or off. The exact functions of each processing step are described in chapter 3.5 and chapter 5.2.2.

9.3 Build and Validate the Model

After the model parameters are set, the user can click on the 'Validate quantification Model'

step to generate the model using the custom parameters set in step 2.

The model will be built, and the final Model Validation page appears.



Terms:

SEC: Standard error of calibration

SECV: Standard error of cross-validation

SEP: Standard error of prediction

R^2: Coefficient of determination

Criteria - Iterates model parameters to find results in a close SEC: SEP ratio and a high R^2 value.

This is the information displayed in the Model validation screen:

Diagrams:

- Figures of merit: SEC, SECV, SEP

- Correlation plot: Reference Vs. Predicted
- Influence plot: Q residual Vs. Hotelling's T2
- Loadings plot
- Score plot

Tables:

- Figures of merit for all latent variables
- Figures of merit of individual samples: residuals

The software automatically selects the one with the closest SEC and SEP values.

Reading the Loading Plot

A loading plot tells you which Raman shift regions matter the most for your model and how they matter.

Large peaks = important wavelengths

- Where you see **big upward or downward spikes**, those Raman shift points **strongly influence the model**.

- Example from the plot above:
  The **~950–1100 cm^{-1} region** has large peaks → **this region explains real chemical differences**.
- Big **positive** or **negative** values both mean "important."
  The sign simply tells the direction of the correlation.

You care most about these regions for model building. These are where chemical signals live.

Flat or very small values = unimportant / noise

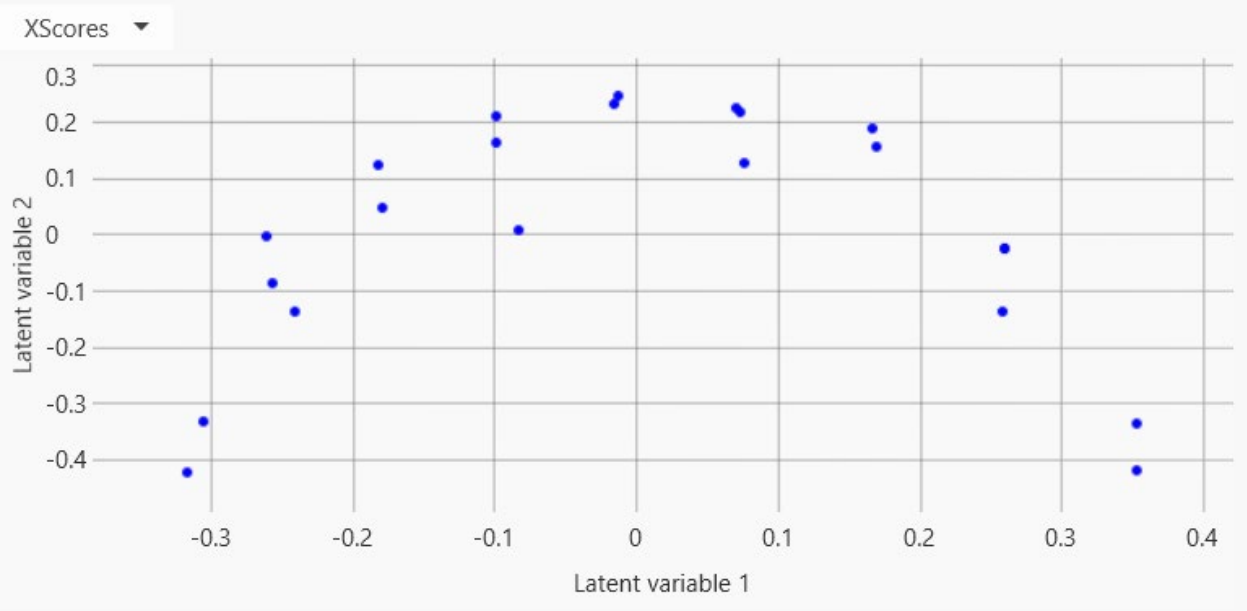
- Regions where the line is flat (near zero) mean:
  - The model sees **no meaningful chemical variation**
  - Likely just **noise**
  - These wavelengths can be **ignored** or de-weighted

Each LV curve tells you what each factor is doing

- LV1 usually captures the strongest chemical variation
- LV2 captures the next strongest pattern
- Higher LVs (LV7–LV10) start to look like random wiggles → **mostly noise**

Reading the Score Plot

A PLS **score plot** is a map showing how your samples relate to each other after the model has compressed the spectrum into a few "latent variables" (LVs).



In the case above, the axes are:

- **LV1 (horizontal)** = the strongest direction of variation in the spectra
- **LV2 (vertical)** = the second strongest direction of variation

Each **blue dot = one sample**.

Samples close together = similar spectra

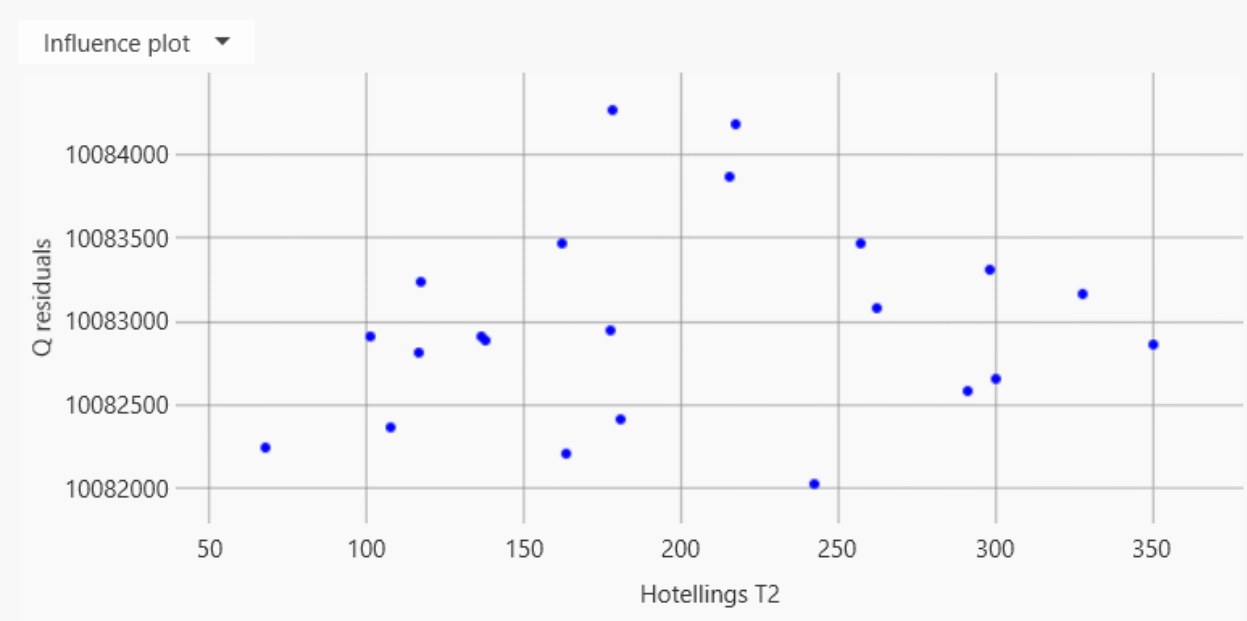
Points that are close together have **very similar chemical signatures**.

Samples far apart = different spectra

Points that are far away have different spectral characteristics or different chemical compositions.

If a sample is isolated → it may be an **outlier**, a contaminated sample, or something fundamentally different.

Reading the Influence Plot



An influence plot combines:

- **Hotelling's T^2** (x-axis)

  • Hotelling's T^2 represents how far a sample is from the model center (in the score space).

  High T^2 = sample is an **extreme but still modeled** point.

- **Q-Residuals** (y-axis)
- Q-residuals represent how much of a sample's spectral information is **NOT explained by the model**.
  This is the "leftover noise or unexplained structure."

  High Q-residual = poor model fit.

The Example Influence Plot above shows:

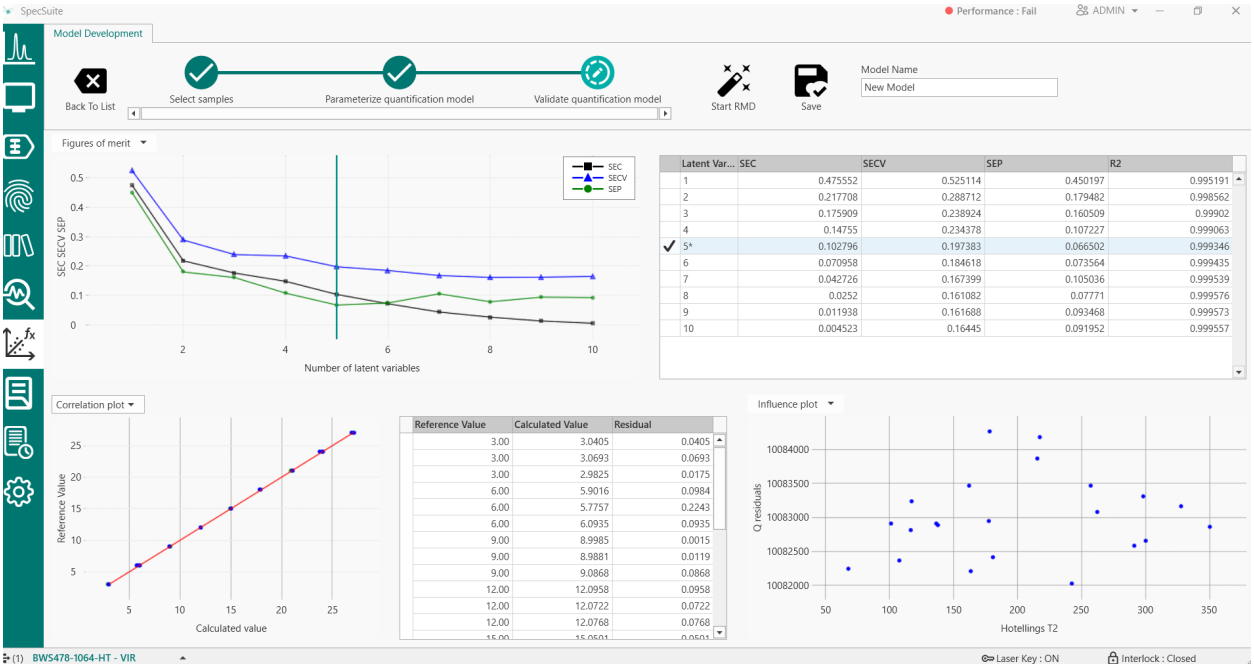
- The points cluster in a horizontal band, with no one point extremely far up or far right.
- Q-residuals are extremely close together → model explains all samples similarly well.
- T^2 ranges from ~50 to ~350, but none are extreme.
- No outliers in the model

- Model is stable, and all samples are described by the model without large leftover error
- Consistent measurement/processing conditions with little variation in Q-residuals.

9.4 Start RMD (Raman Model Development)

Once the sample variable values are labeled, the user may press Start RMD. This will automatically split the dataset, parameterize the model and generate the model using default optimized parameters.

If custom parameters have been set in Step 2, they will be overwritten when Start RMD is pressed

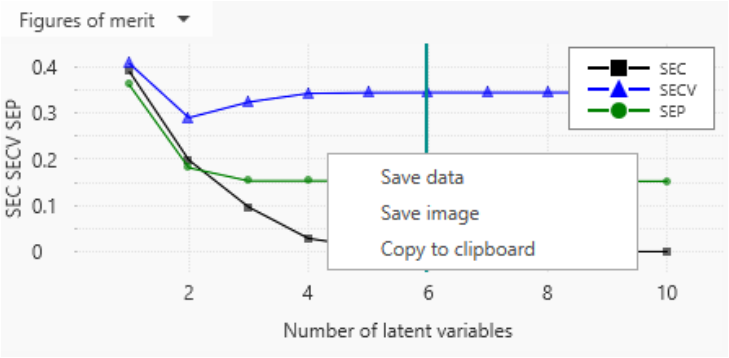


9.5 Exporting Model Data

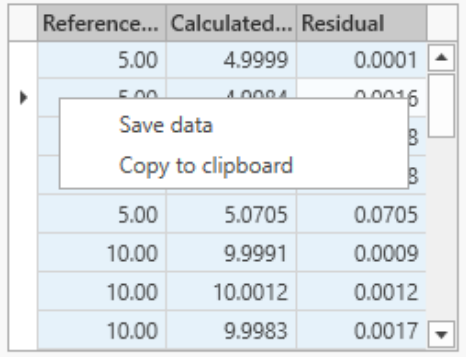
At all points of the model-building process, all charts and tables (except the Sample table) can be copied, saved, and exported.

- **For charts**: Right-click the chart to choose either to save data, image, or copy to clipboard.
- **For tables:** Use CTRL/SHIFT select function, then right click on the data to save or copy to the clipboard.

Save Charts:

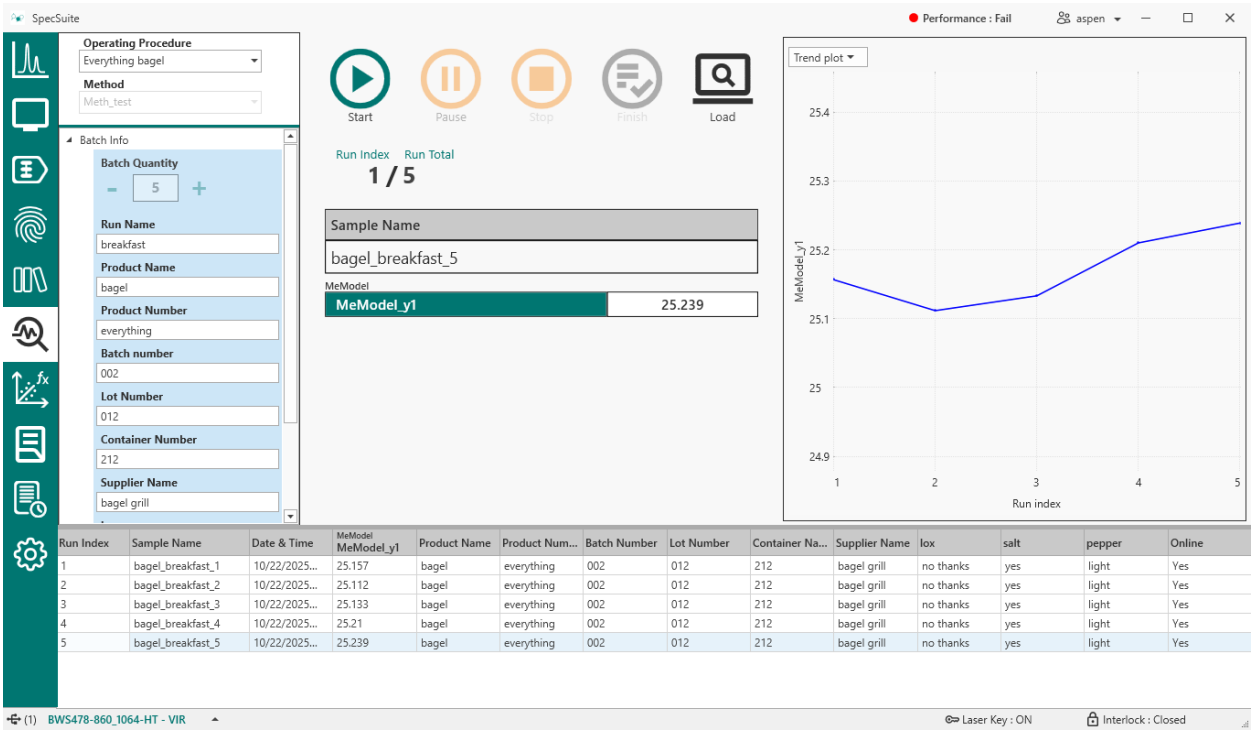


Save Tables:



10. Routine Analysis

Routine Analysis is a quick way to run qualitative or quantitative analyses of chemicals using an existing model and method. Routine analysis requires the setup of an operating procedure before it can be used. The following are instructions on how to correctly set up and perform a Routine Analysis.



10.1 Preparation

Three things need to be set up before using the Routine Analysis module.

Create a **Variable** → Make a **Method** → Build an **OP** → *Routine Analysis*

1. Create a **Variable**

Variables are either created automatically when a model is created or can be created manually as a Basic Variable. Follow the instructions in the Model section for detailed model creation, or the instructions in the Basic Variable section.

2. Build a **Method**

   Methods are set up within the OP Module. Refer to the OP Methods section.

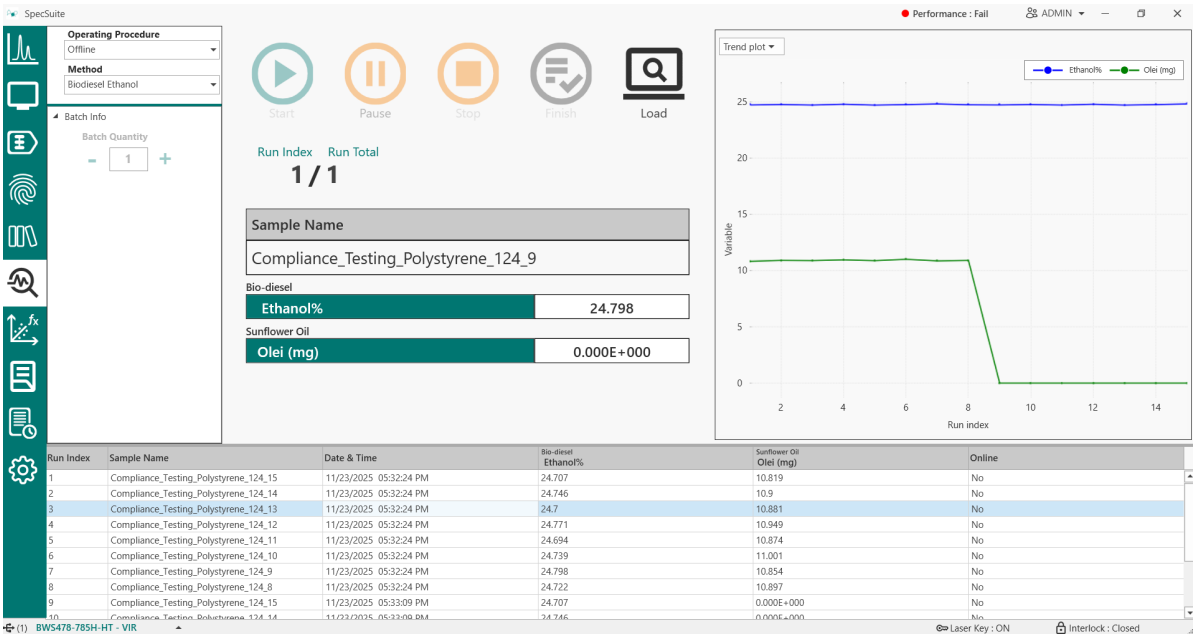
3. Build an **OP**

   To use Routine Analysis, an OP must be configured with a **Routine Analysis module enabled**. Only one method can be selected in an OP, but each Method can contain multiple variables.

Offline Routine Analysis

Offline Routine Analysis provides a testing environment for Developer and Administrator-level users to test the Method created. CSV, simple CSV or simple SPC data can be loaded to make predictions. Multiple data files can be loaded at once.

Once loaded, the system will automatically process the data using the selected algorithms and generate the prediction result on screen. Offline routine analysis data is not saved to the database.



10.2 Basic Operations

Metadata input

On the left panel, Developers and Operators can input metadata that are pre-configured in the operating procedure:

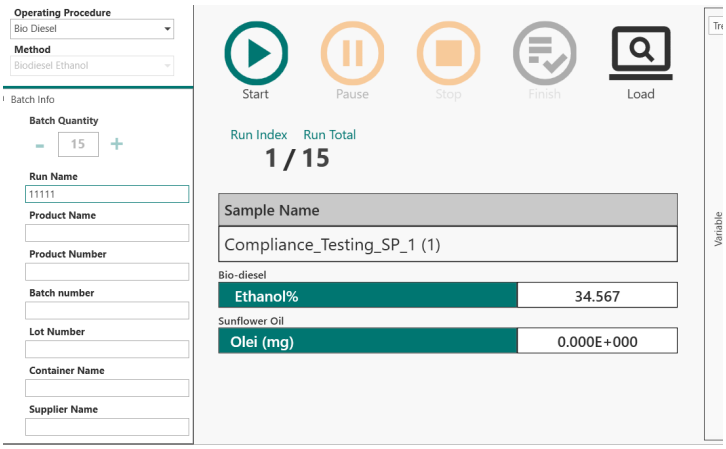
Batch Quantity:

Batch quantity can be increased or decreased by hitting the + or – icon or typed in by keyboard. The maximum batch quantity per run is 5000.

Run Name:

Run Name is a unique run identifier that must be entered before starting a run. The Run Name field supports a maximum of 50 characters, including letters and numbers. If the Run Name field is empty, the "Start" button will be greyed out.

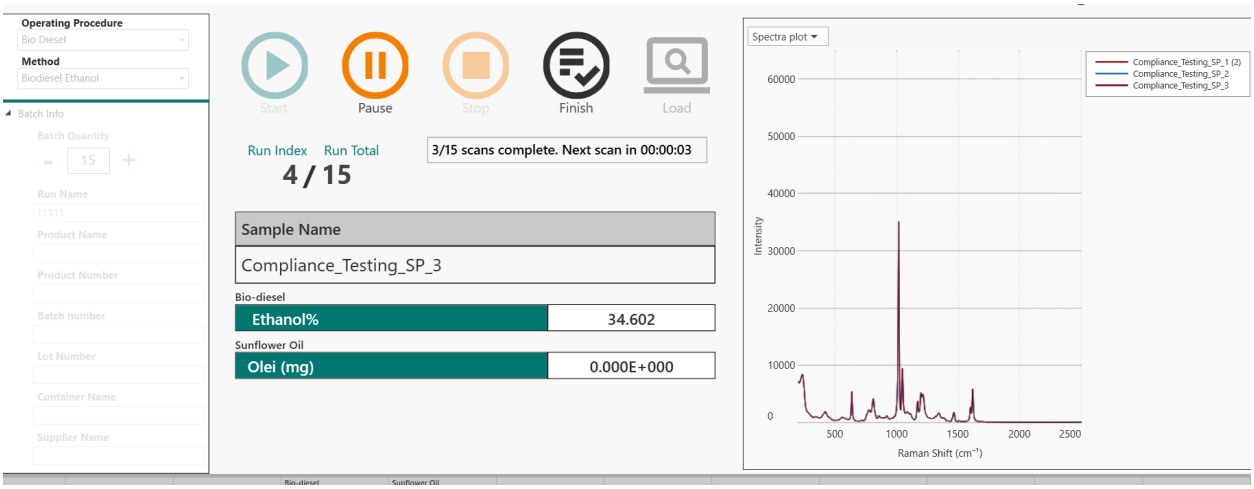
Users can add metadata fields, such as product names, to the routine analysis if they are defined in the operating procedure. Users can also use a barcode scanner to directly scan the barcode into a specific metadata field.



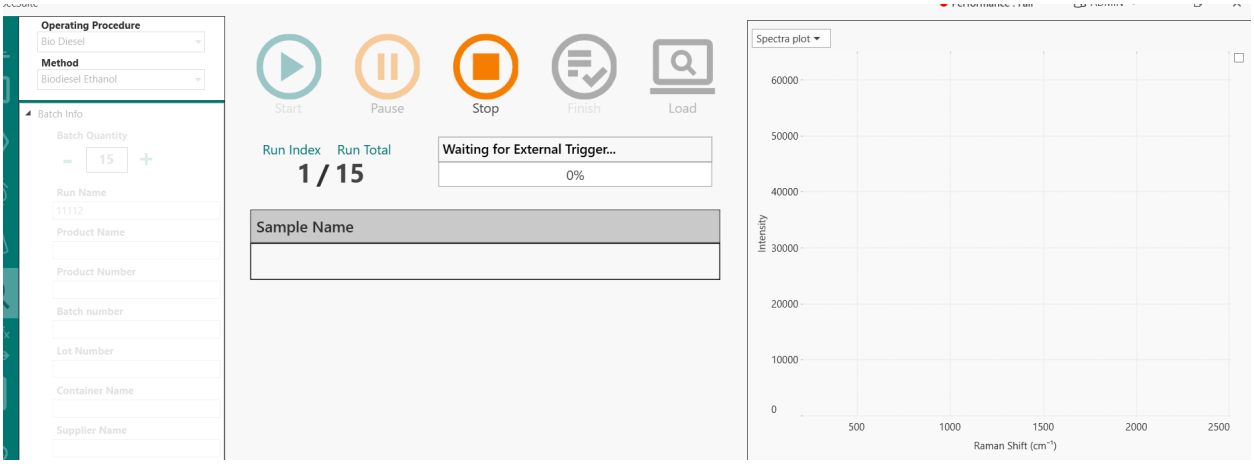
Start a Run

- **Start** – When the Start button is pressed, a spectrum is collected using the Integration Time, Laser Power, and Averages set in the selected Operating Procedure.

If the timeline is enabled in the operating procedure, the next scan will automatically start at the interval defined in the OP. There will also be a timer counting down to the next scan.



If the external trigger is enabled in the OP, the user must press the external trigger on the probe body to start the measurement after clicking Start.

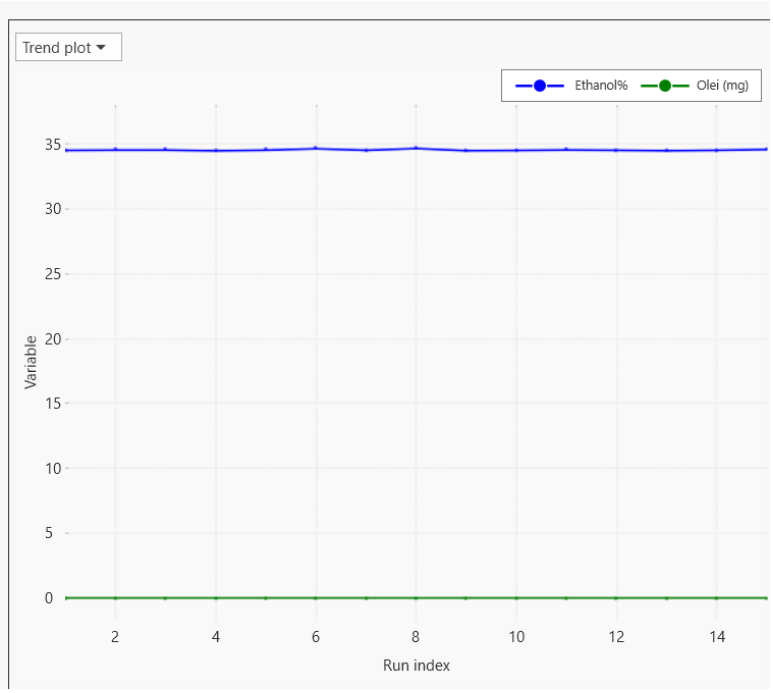


- **Pause** – The pause button will appear during a multi-acquisition run. Pausing will allow the current scan to complete, then all scans will be paused until the Scan button is pressed again. The next scan will immediately begin regardless of any set delay (Interval) between scans.
- **Stop** – The stop button will immediately halt the acquisition being collected. The cancelled scan will not appear on the chart or in the data list. If Stop is pressed during a multi-acquisition, the entire acquisition will be canceled.

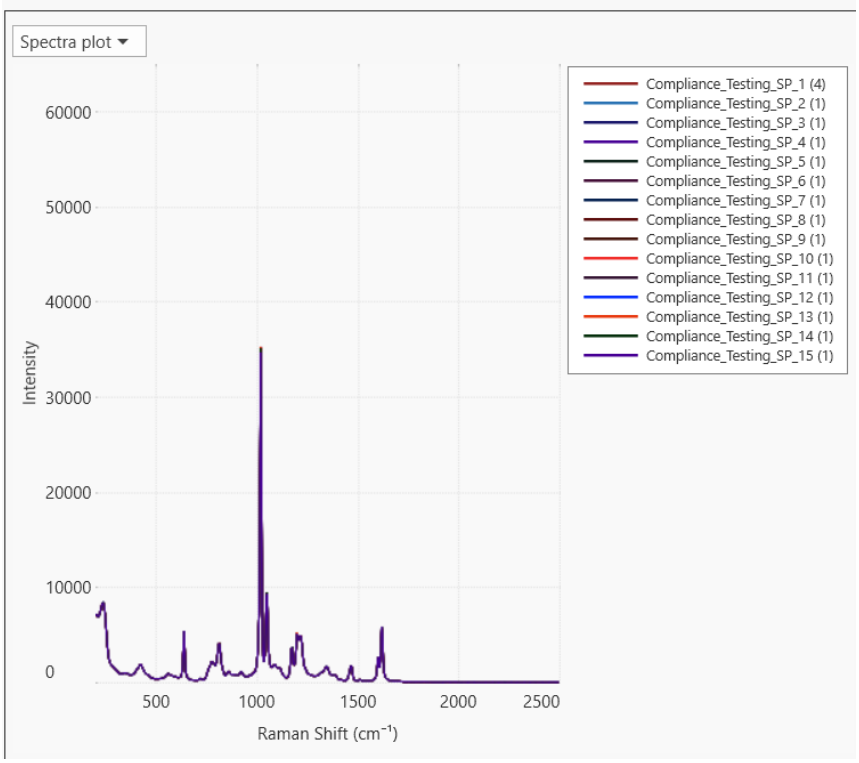
- **Finish** – The Finish button completes the current run.
- **Load** – Loads offline files to perform an analysis on.

10.3 Spectra Plot and Trend Plot

Users can view the multivariable trend plot directly on the right side of the screen.



Users can also click on the drop-down menu and switch the spectra plot. Both plots will be updated live during the routine analysis.



The sample list of a specific Routine Analysis run can be found in the table at the bottom of the screen. The routine analysis record cannot be changed once it has been generated. Each specific run will refresh the spectra plot, trend plot, and the sample list.

Run Index	Sample Name	Date & Time	Bio-diesel Ethanol%	Sunflower Oil Olei (mg)	Product Name	Product Number	Batch number	Lot Number	Container Name	Supplier Name	Online
1	Compliance_Testing...	11/23/2025 05:49:0...	34.524	0.000E+000							Yes
2	Compliance_Testing...	11/23/2025 05:49:0...	34.544	0.000E+000							Yes
3	Compliance_Testing...	11/23/2025 05:49:1...	34.545	0.000E+000							Yes
4	Compliance_Testing...	11/23/2025 05:49:1...	34.49	0.000E+000							Yes
5	Compliance_Testing...	11/23/2025 05:49:2...	34.54	0.000E+000							Yes
6	Compliance_Testing...	11/23/2025 05:49:3...	34.649	0.000E+000							Yes
7	Compliance_Testing...	11/23/2025 05:49:3...	34.53	0.000E+000							Yes
8	Compliance_Testing...	11/23/2025 05:49:4...	34.667	0.000E+000							Yes
9	Compliance_Testing...	11/23/2025 05:49:4...	34.499	0.000E+000							Yes

11. Reports

The Reports tab keeps records of all the contents of the database. Here you can see a list of all scans collected in Explore, identification, Routine analyses, Performance, and Calibrations.

For each type of report, the options in the Reports ribbon are the same:

- **View Report** – Loads offline files to perform a routine on.
- **E-signature** – Virtually sign and date reports.
- **Load to Explore** – Data from the selected records open to the Explore module
- **Export** – Export the specific report in pdf format, or its associated spectra file.
- **Refresh list**– Refresh the report table to display the latest changes.

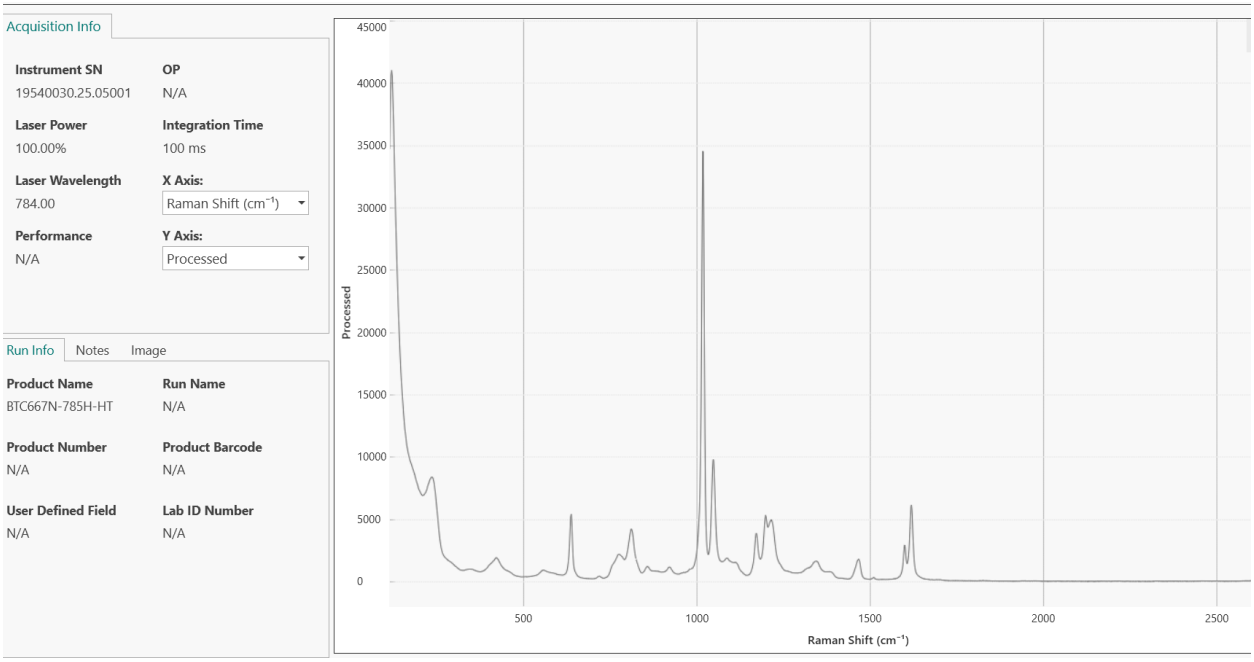
The Report pages is separated into 5 tabs:

- Acquisition Reports
- Identification Reports
- Routine Analysis Reports
- Performance Validation Reports
- Calibration Report

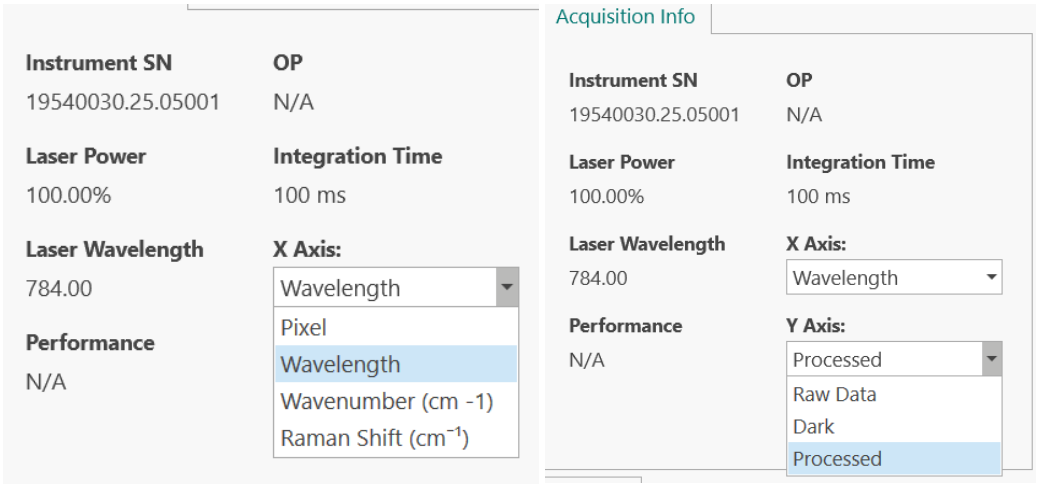
11.1 Acquisition Reports

The Acquisition Report Tab includes all online measurements collected in the Explore, Identification, Routine Analysis, Performance, and Calibration modules. It serves as a general

lookup table for users to search all the scanned samples. Users can select a specific entry and view the detailed instrument acquisition info:

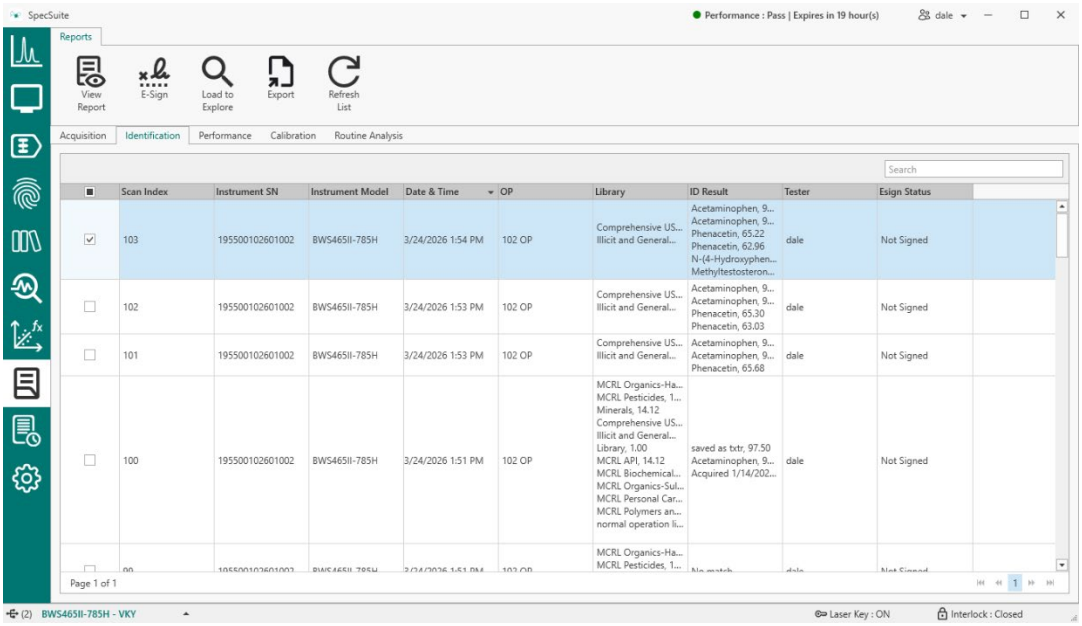


The left panel shows the spectrum-acquisition parameters for instruments, including laser power, integration time, and laser wavelength. Users can also use the drop-down field to select different X-axis and Y-axis to view the spectrum on the right.



The Acquisition table is for filtering and displaying only. Users cannot generate or e-sign a PDF report in the Acquisition tab.

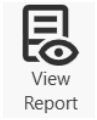
11.2 Identification Reports

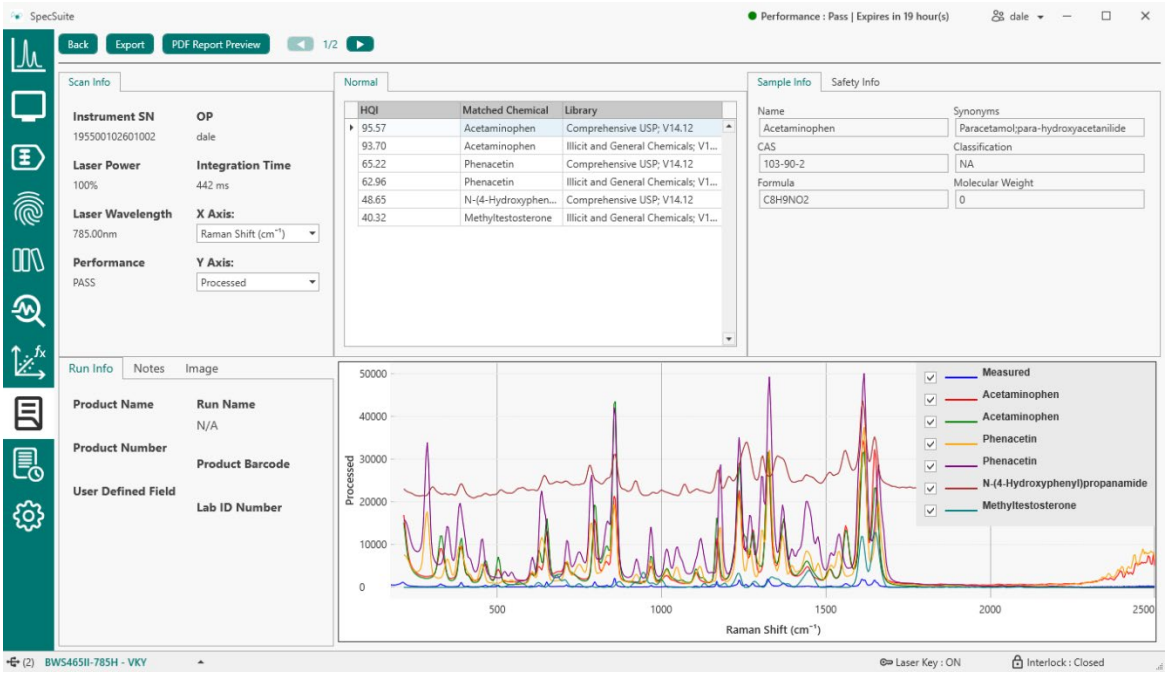


After an identification run, the record is saved in the database and will appear in the Identification Tab of the Report Module. ID reports can be viewed, signed, printed, and exported.

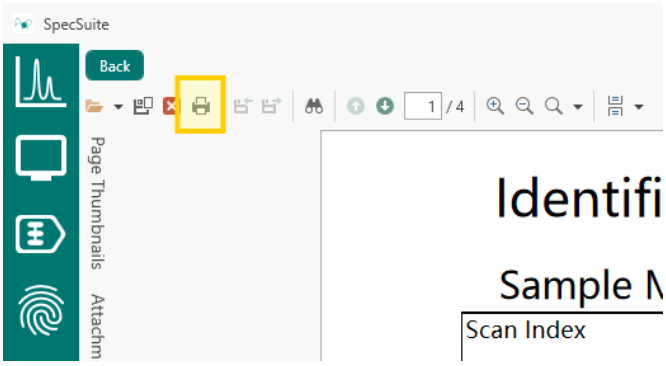
ID records can be filtered by Scan Index, Instrument SN, Instrument Model, Tester, OP, Library, ID result, and Date and time. Additional Columns can be added, such as Laser power, Integration time, Scan average, laser wavelength, probe SN, ID mode, container library, container spectrum, Tester's E-sign status, Approver's E-sign status, and E-sign Date and time.

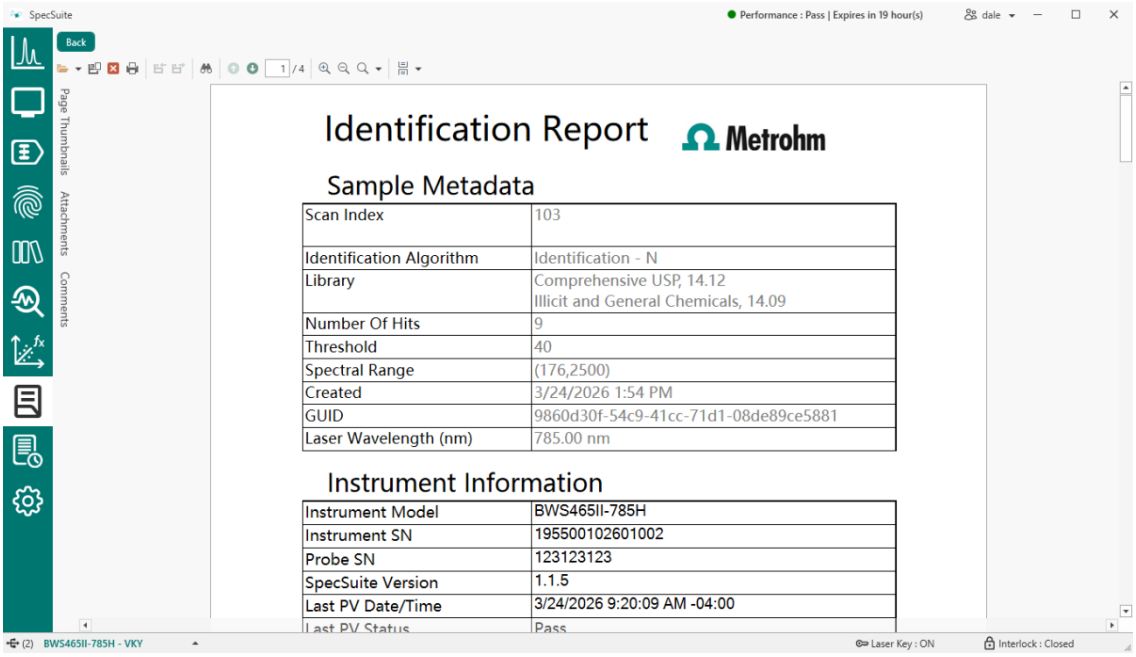
Users can select 1 or multiple ID report entries and click View Report to view the details.





Click on “PDF Report Preview” to preview a PDF report, which can be saved or sent to a physical printer through the PDF report widgets.





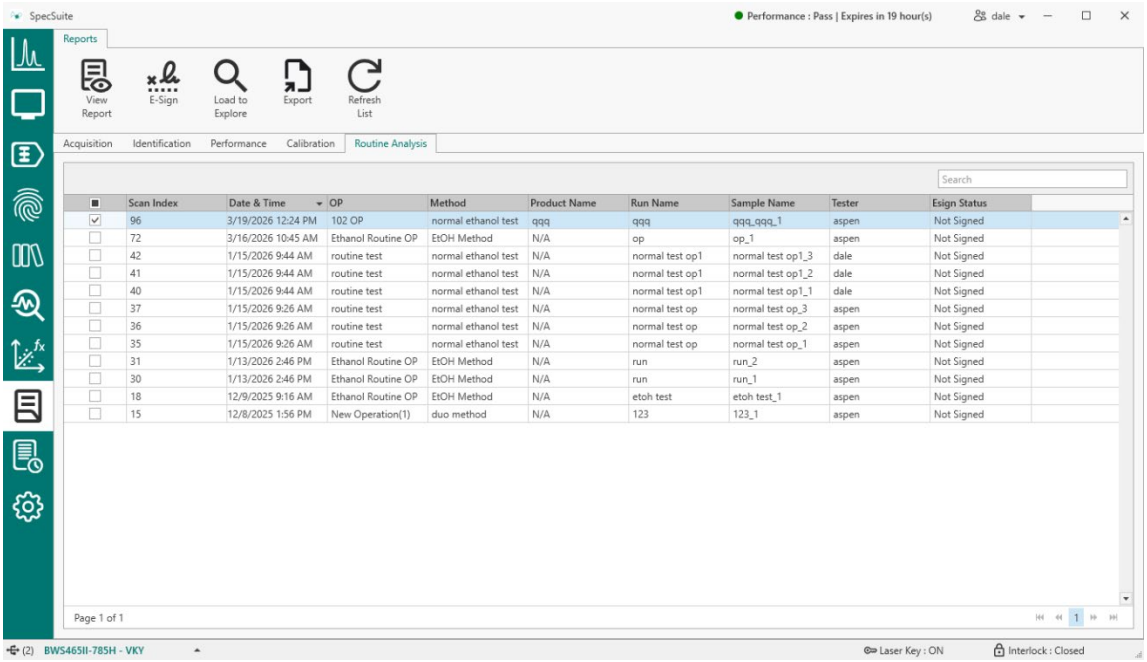
11.3 Routine Analysis Reports

After a Routine Analysis is run in the Routine Tab, the record is saved to the database and appears on the Routine Analysis page of the Report tab. Routine Analysis reports can be viewed, signed, printed, and exported.

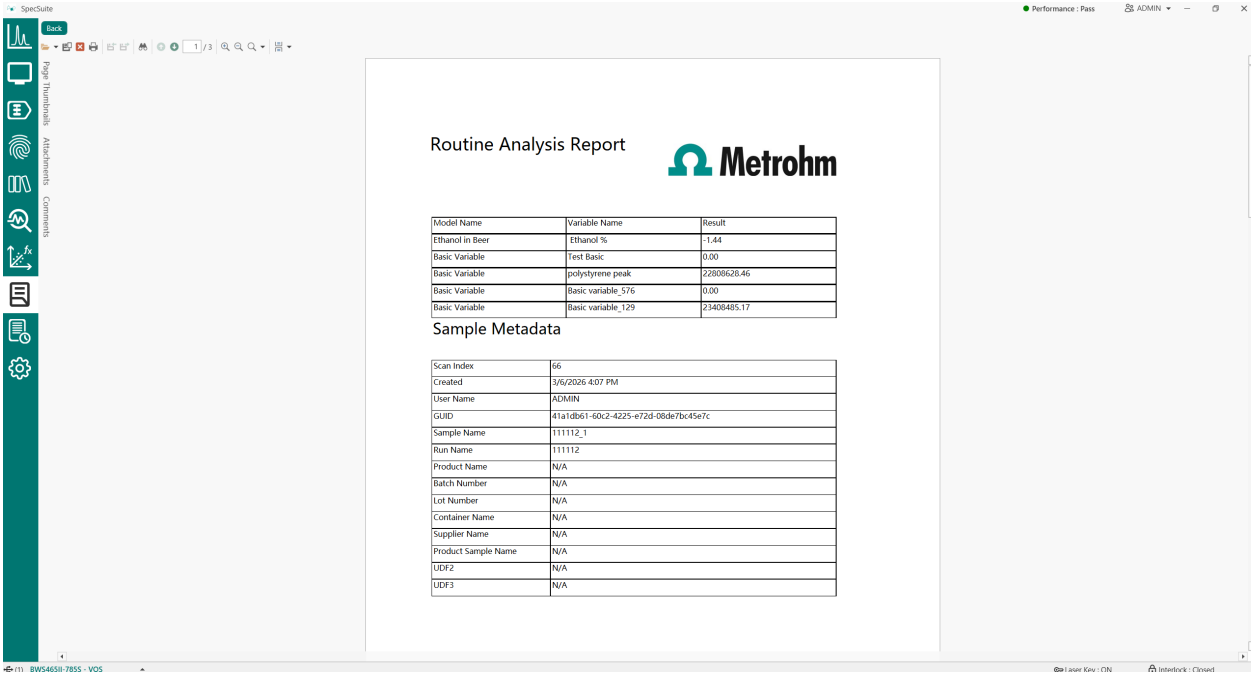
Routine Analysis records can be filtered by

- User Name
- Date & Time
- OP (Operating Procedure)
- Method Name
- Run Name
- Sample Name
- Laser Power
- Integration Time
- Number of Averages
- Laser Wavelength
- Probe Serial Number
- Last Validation ID

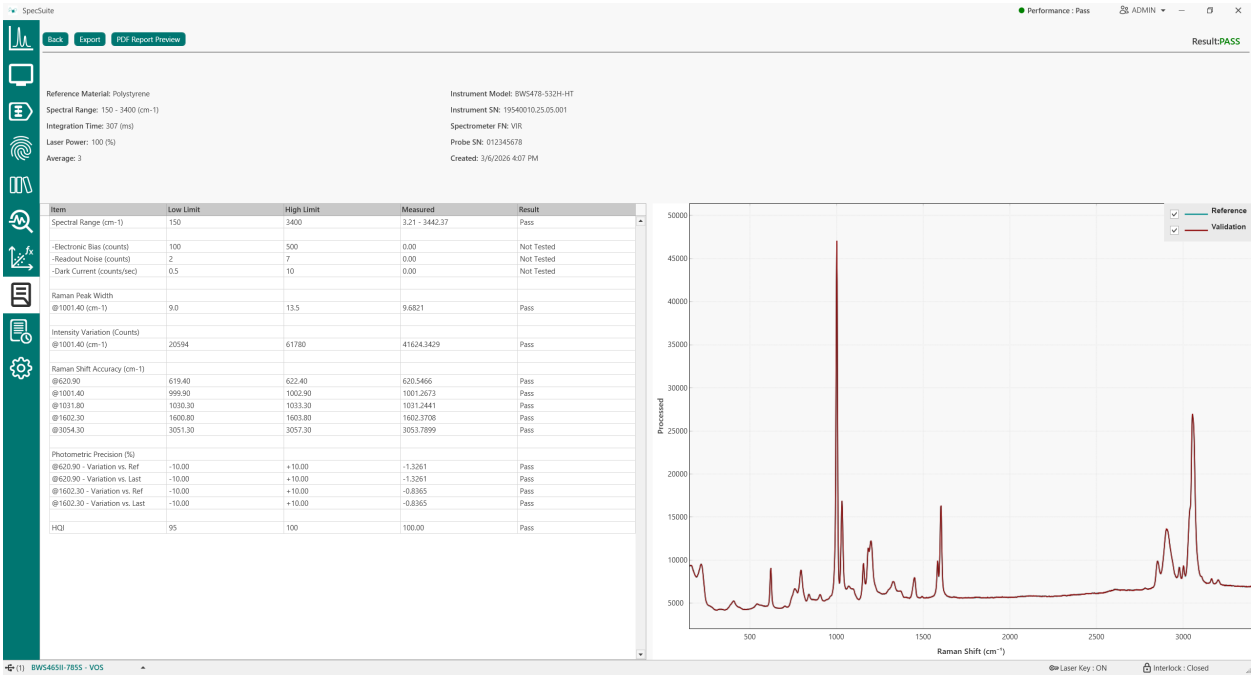
- Tester E-sign status
- Approver E-sign status
- E-Sign Date and Time
- Method Variable Names and Values



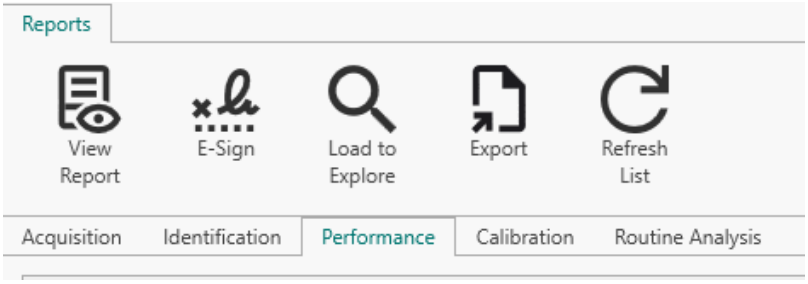
Users can select a routine analysis report using the checkbox, then click View report, and a PDF Routine Analysis report will be displayed. Users can then use the PDF widget to save the report as a PDF file or send it to a printer.


SpecSuite
Performance : Pass
ADMIN
Back
Page Thumbnails
Attachments
Comments
Routine Analysis Report
Metrohm
Model Name | Variable Name | Result
Ethanol in Beer | Ethanol % | -1.44
Basic Variable | Test Basic | 0.00
Basic Variable | polystyrene peak | 22808628.46
Basic Variable | Basic variable_576 | 0.00
Basic Variable | Basic variable_129 | 23408485.17
Sample Metadata
Scan Index | 66
Created | 3/6/2026 4:07 PM
User Name | ADMIN
GUID | 41a1db61-60c2-4225-e72d-08de7bc45e7c
Sample Name | 111112_1
Run Name | 111112
Product Name | N/A
Batch Number | N/A
Lot Number | N/A
Container Name | N/A
Supplier Name | N/A
Product Sample Name | N/A
UDF2 | N/A
UDF3 | N/A
BWS465II-7855 - VOS
Laser Key : ON
Interlock : Closed

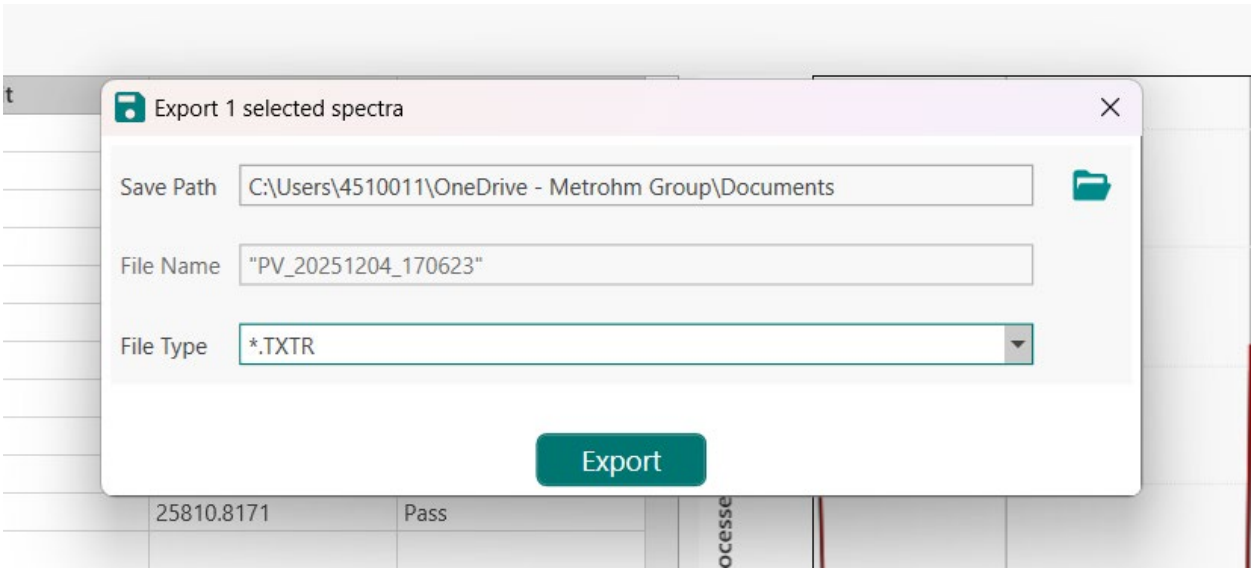
11.4 Performance Validation Reports



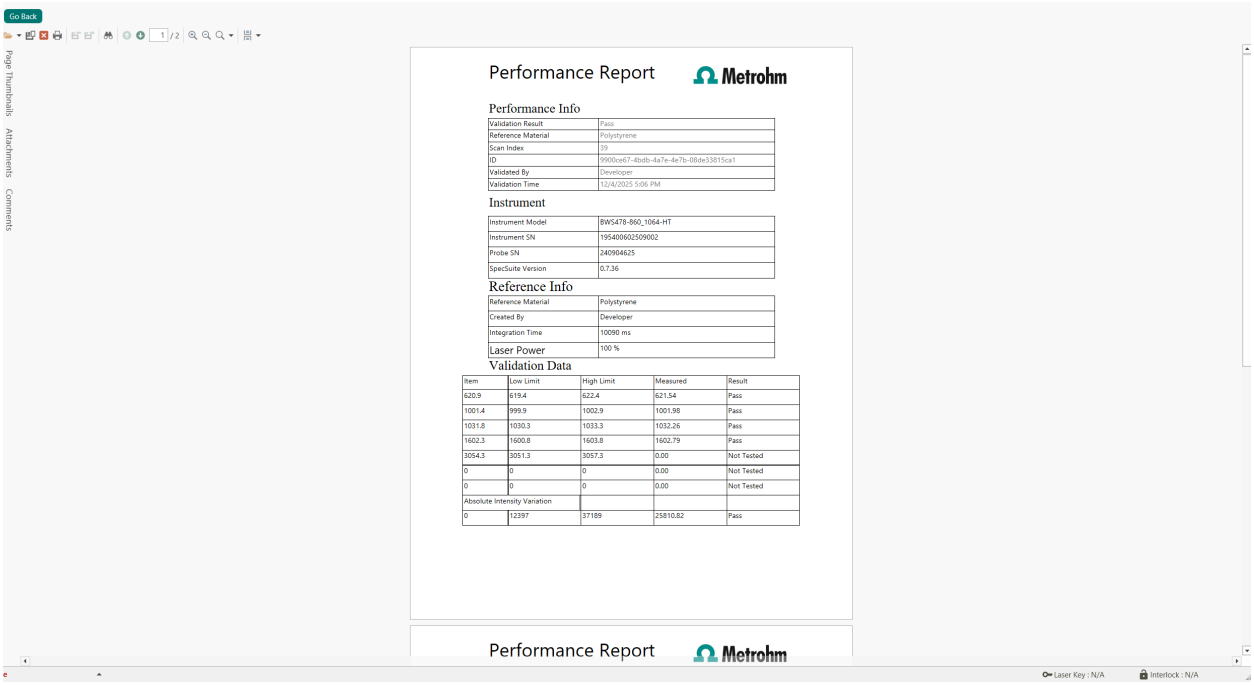
Performance Validation Records can be viewed at all user levels. Users can select the specific performance validation records from the table, then click View Report to view the detailed pass/fail results of each item.



Users can then click the Export button to export selected performance validation spectra in the CSV, simple CSV and simple SPC formats.



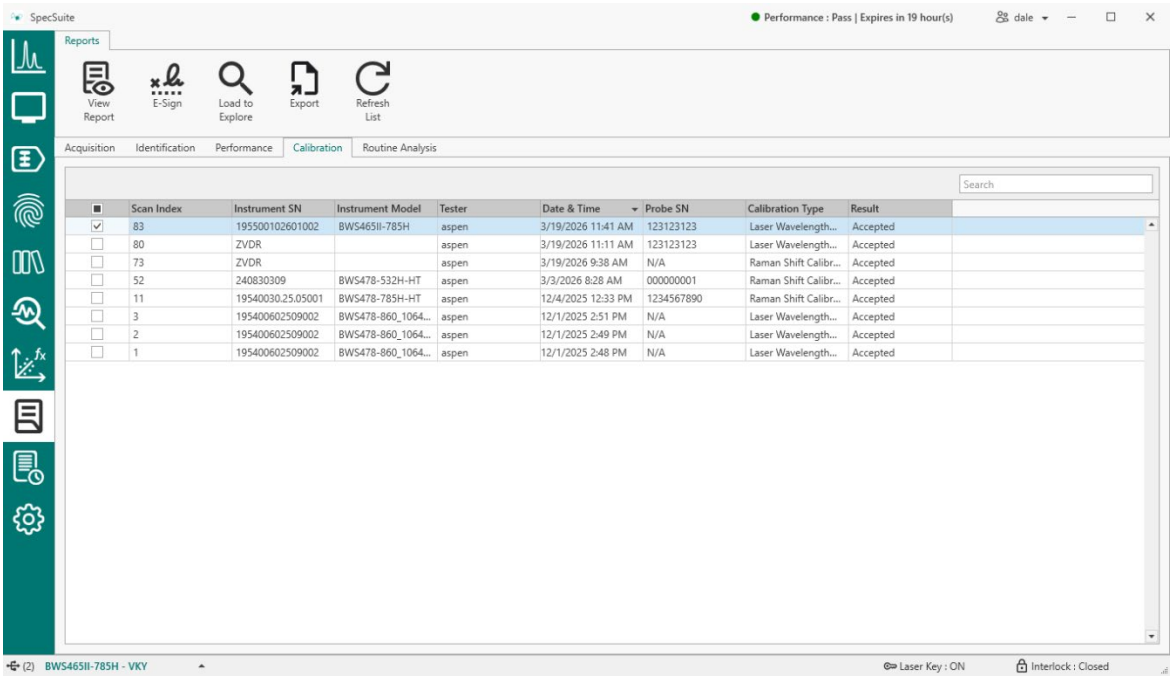
Click on “PDF Report Preview” to preview PDF reports.



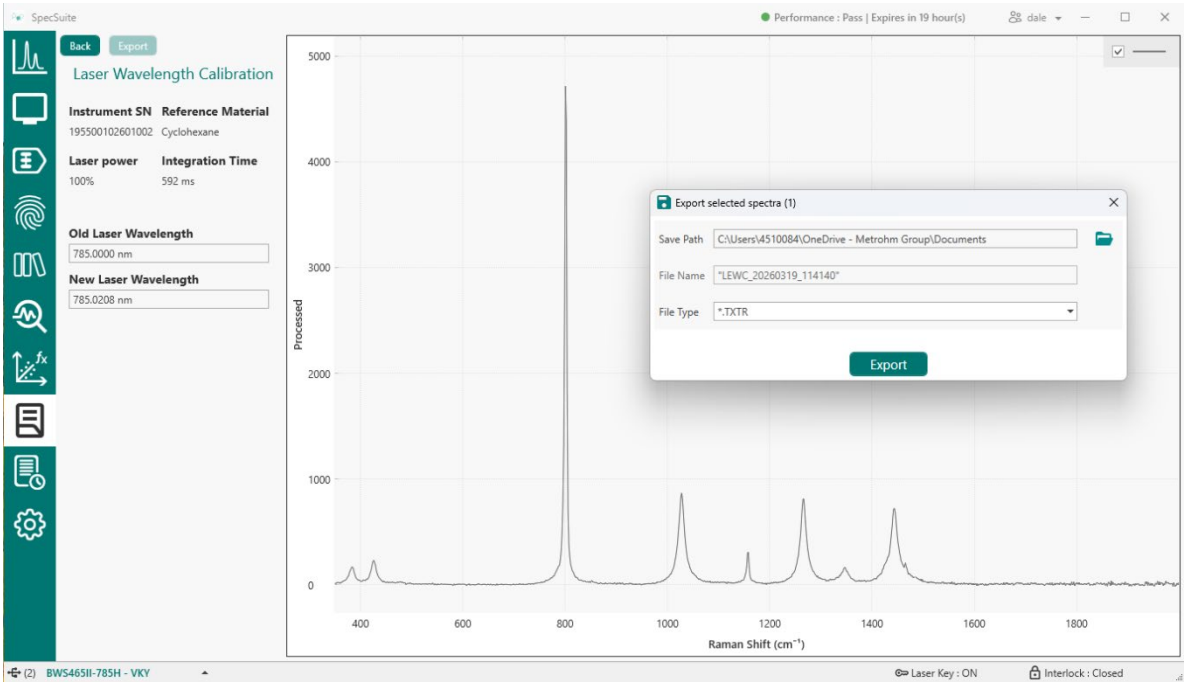
Click “Back” to return to the previous screen.

11.5 Calibration records

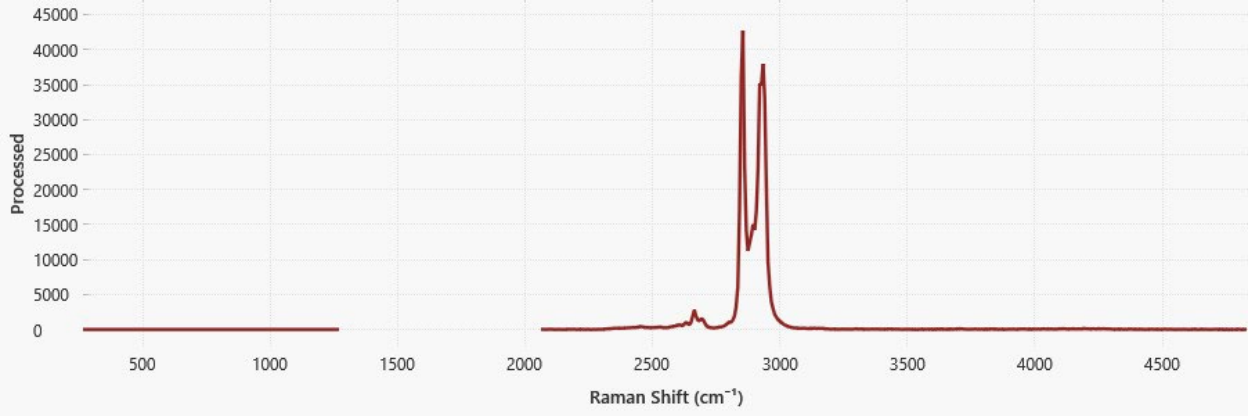
All previously accepted calibration records will be saved in the “Calibration" tab. Users can select and view the detailed calibration data during Raman Shift Calibration, Laser Wavelength Calibration, and Relative Intensity Calibration.



Calibration data can be exported in CSV, Simple CSV, or Simple SPC files.



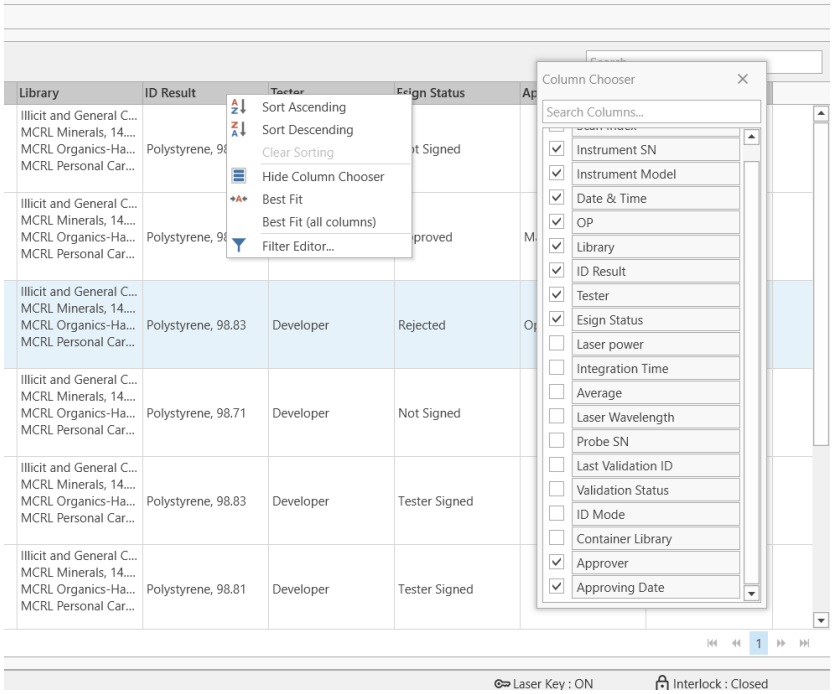
Note: For Calibrations performed on an i-Raman DUO system, Load to Explore will appear with a gap as shown below. This is not an error. DUO system calibrations use a smaller useful range that excludes data in this region.



11.6 E-Signatures

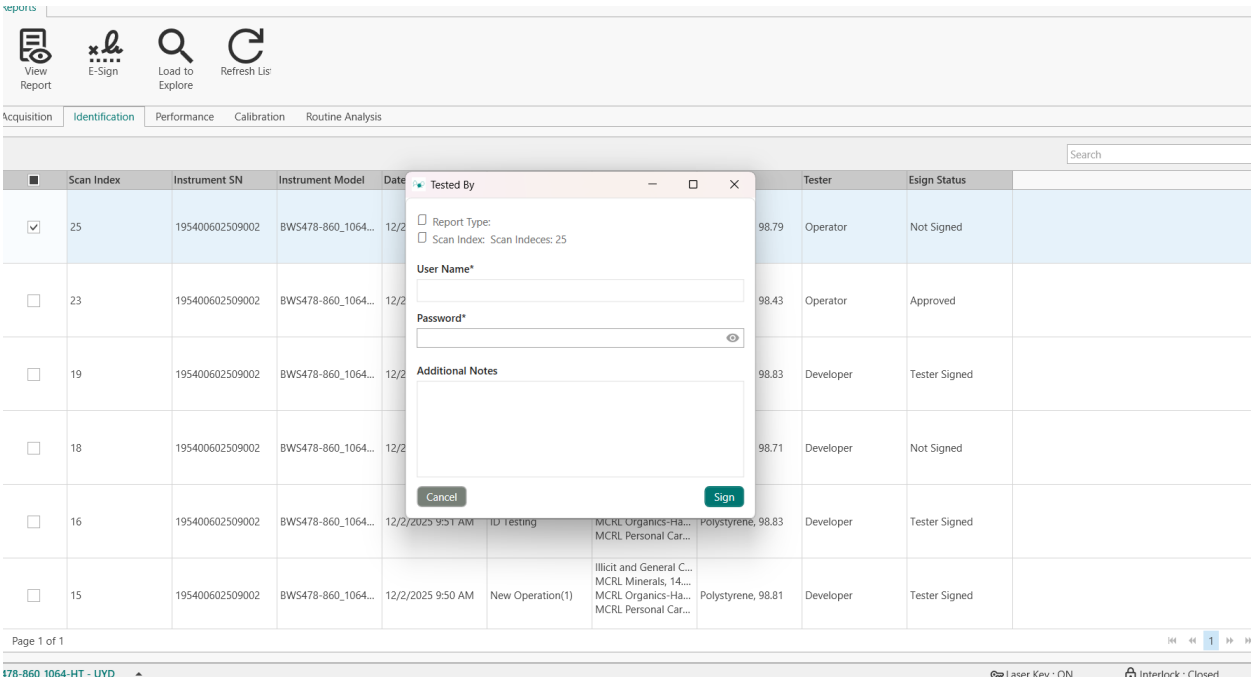
User accounts with Developer, Operator, and Lab Managers privileges are allowed to sign Identification, Routine Analysis, and Performance Validation records.

The person who executed the measurement will be shown under the “Tester” column, and the person who approves/rejects the record will be shown under the “Approver” column. Users can right-click the column to view column choosers and enable/disable additional columns.

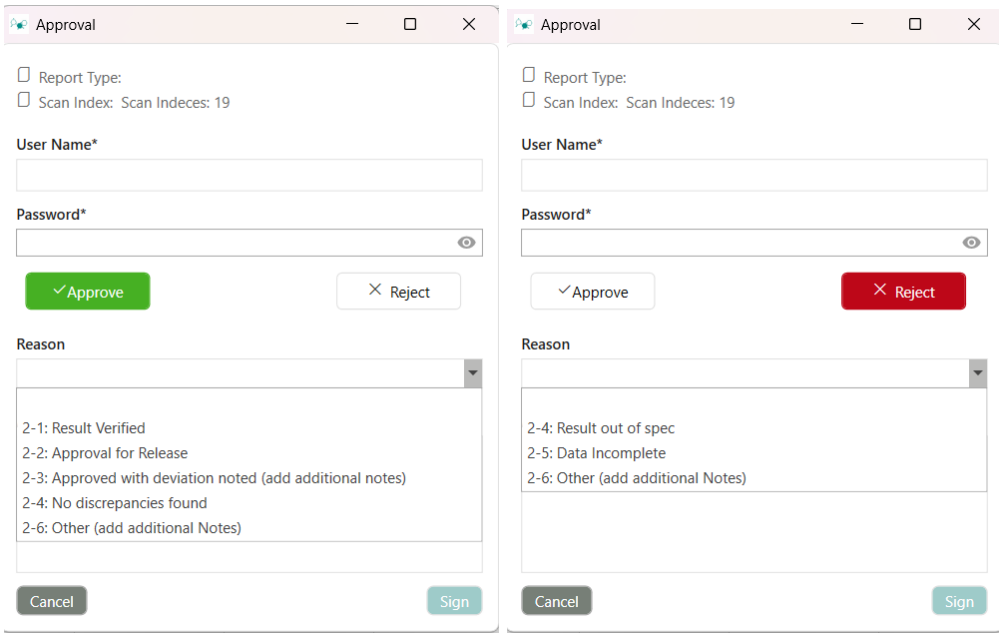


To sign a record, select the record from the list and click on 

. The tester can sign the record through the pop-up window. The Tester must enter their username and password, then click Sign. The E-sign status will change to “Tester Signed.”



Once the Tester signs their own record, another person (typically a lab manager) can Approve or Reject it. During the approval process, the approver can choose either “Approve” or “Reject” and select a reason based on the drop-down list.



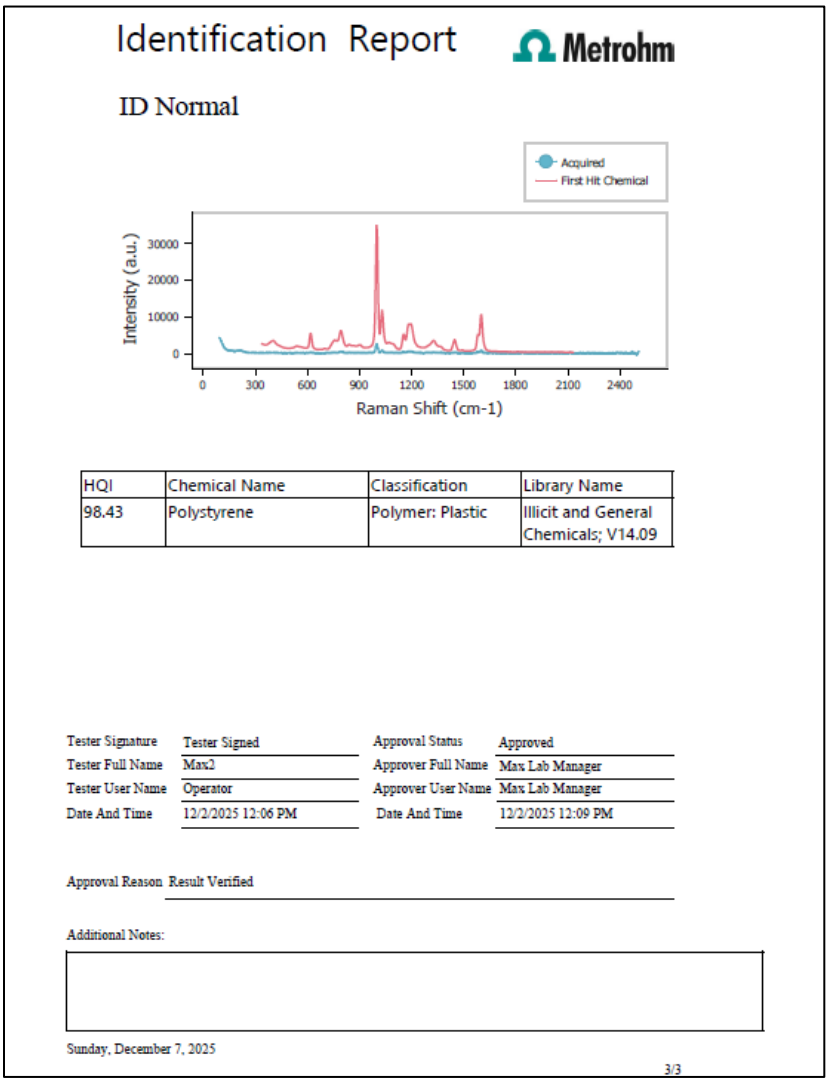
E-sign rules:

1. The same user (Tester) who executed the identification, performance validation or routine analysis scan must sign the record first. Non-testers cannot sign the record first.

2. Users must sign in with the same credentials as their login credentials.
3. Testers cannot approve or reject the record.
4. The same user cannot sign the record twice.
5. Operator-level users cannot approve or reject the report.

Administrators and IT users cannot sign any records.

After the user has signed the report, the E-sign status, Full name, Username and Signing Date and time will be shown in the report PDF.



Identification Report

Metrohm

ID Normal

HQI	Chemical Name	Classification	Library Name
98.43	Polystyrene	Polymer: Plastic	Illicit and General Chemicals; V14.09

Tester Signature	Tester Signed	Approval Status	Approved
Tester Full Name	Max2	Approver Full Name	Max Lab Manager
Tester User Name	Operator	Approver User Name	Max Lab Manager
Date And Time	12/2/2025 12:06 PM	Date And Time	12/2/2025 12:09 PM

Approval Reason Result Verified

Additional Notes:

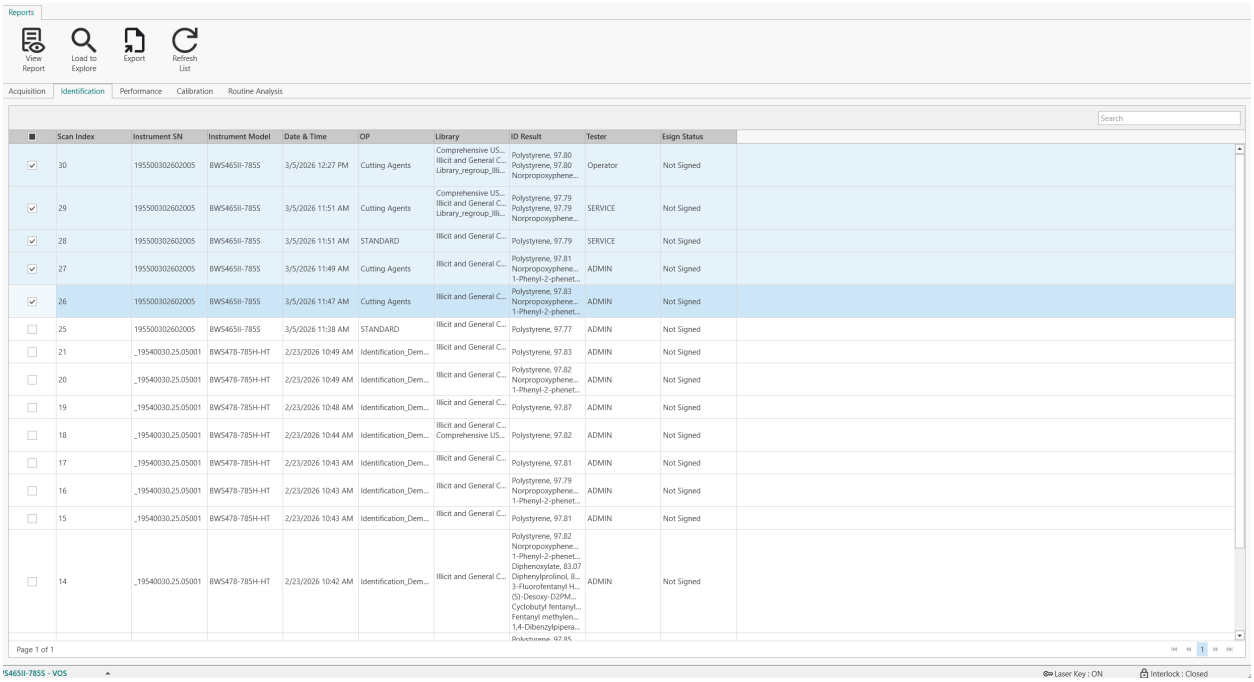
Sunday, December 7, 2025

3/3

11.7 Bulk Export

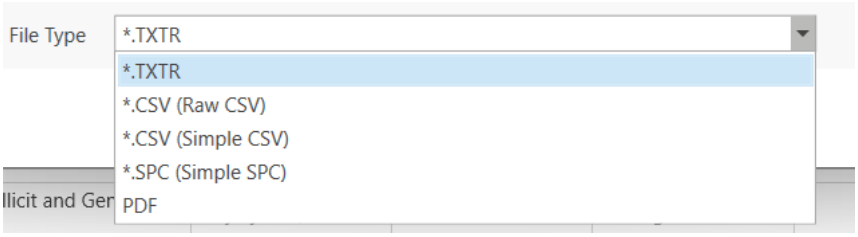
In all report tabs, users can select 1 or multiple records and then export the spectra file in a different format.

Selecting the record by checking the checkboxes on the left



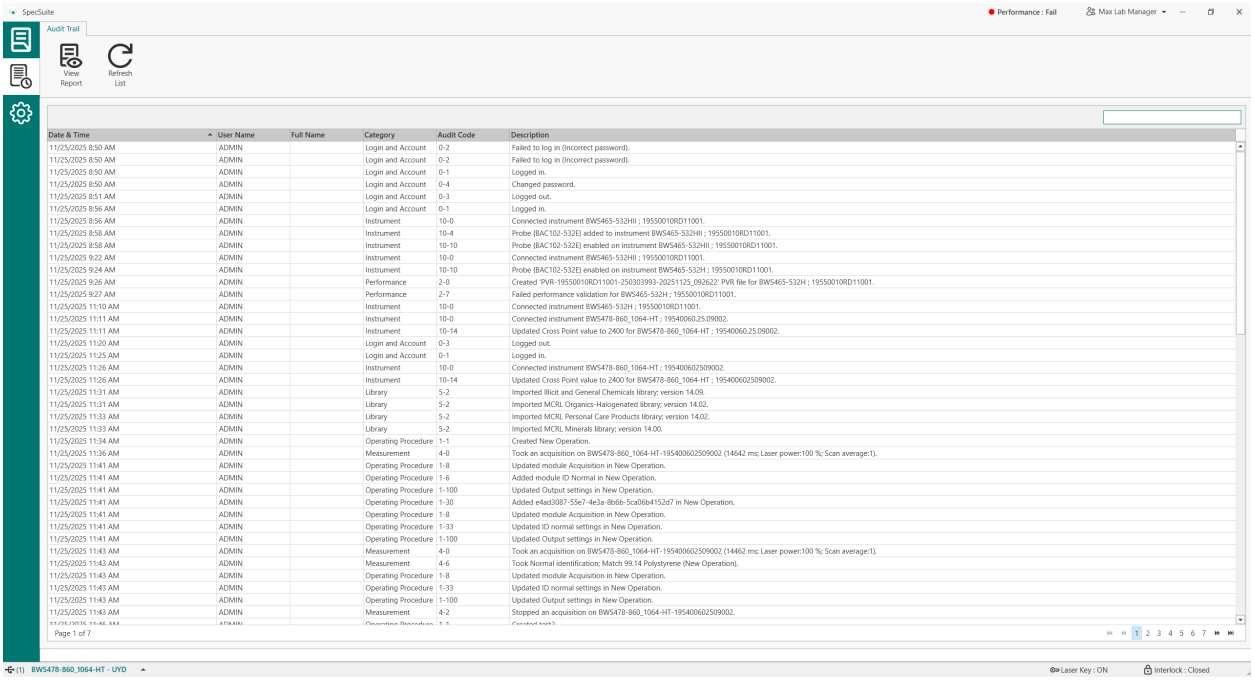
Then click Export 

A new dialog will appear, and the user can select the file type of the spectra to export:



In the Identification, Performance, and Routine analysis report tabs, users can also export the PDF report directly by clicking Export. There is no PDF report for export in the Acquisition or Calibration Tab.

12. Audit Trail



The Audit Trail contains records of all users and system actions. Audit Trail records include date and time, Username, category, description, notes, and device serial number.

- **View Report:** Loads offline file(s) to perform a routine on.

Category is a number associated with a function or module:

0: Login and Account

1: Setup

2: Operating Procedure

3: Library

4: Method

5: Performance

6: Measurement (application)

7: Initialization

8: General

9: Calibration

Description is a summary of the action. Device SN will be included in the Description for actions like Measurement and Calibrations.

Audit Code is a numerical code which can be provided to support to add context in the event an error occurs. The first number refers to the category; the second number refers to the action.

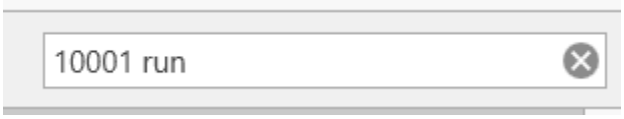
Username is the name of the user logged in at the time of the action. In the case that no user is involved with an occurrence, the associated username is 'SYSTEM'.

NOTICE: The Audit Trail module will be visible only when a 21CFR compliance license is loaded to SpecSuite. Regardless of license status, all the audit trail actions will be recorded and saved. After a compliant license is added to SpecSuite, all audited actions will be seen in the Audit Trail module.

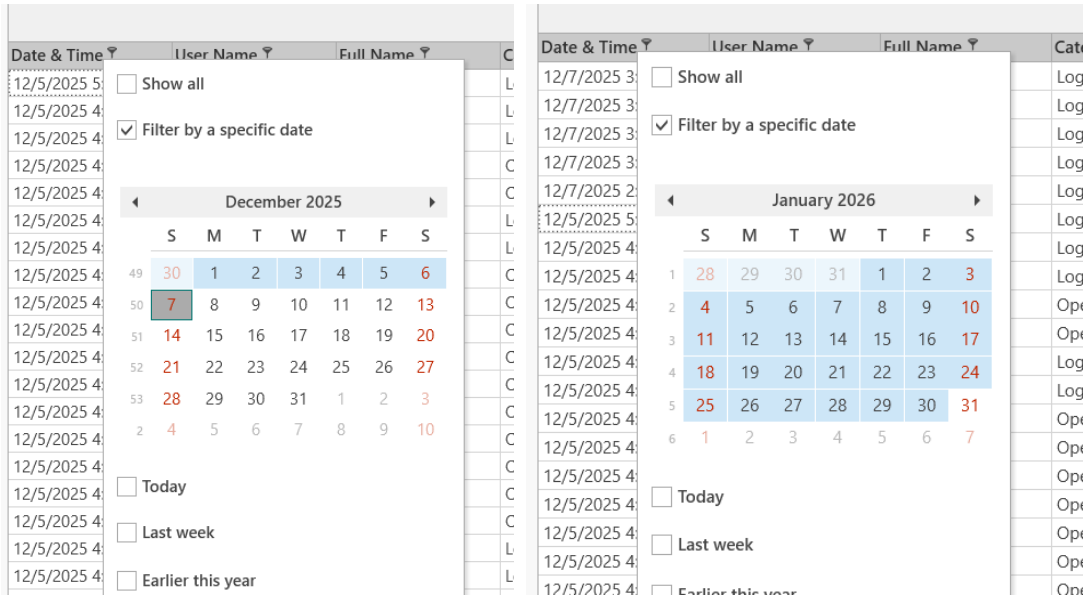
12.1 Audit Trail Filtering

SpecSuite provides users with the capability to search and filter audit trail content.

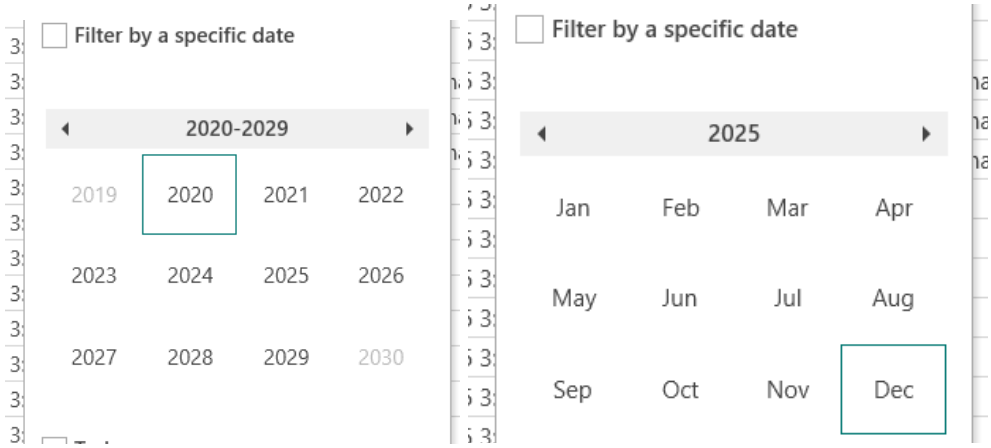
Search Filter: Users can type in any string in the search bar and search through the entire Audit Trail content. For example, if a user would like to know all the information of a routine analysis with Run ID 10001, users can type in "10001 run" in the search bar.



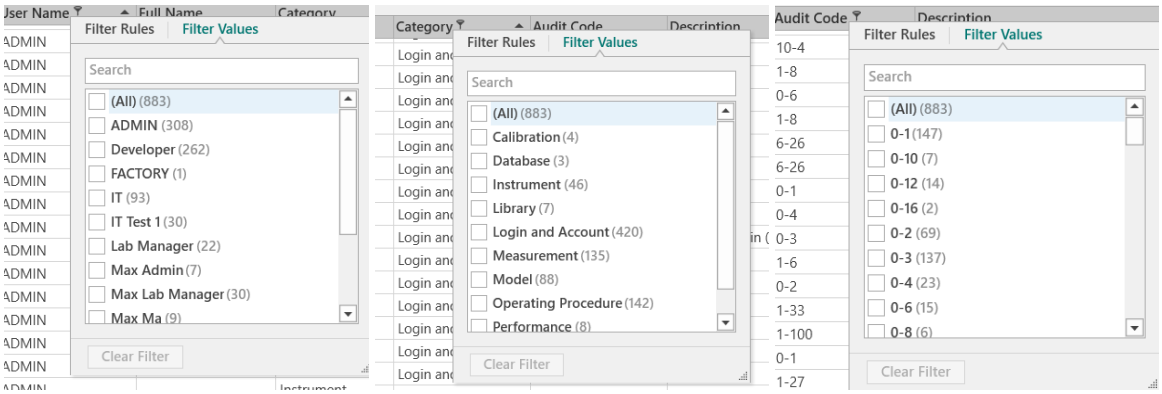
Date and time filter: Users can click the funnel icon in the table headers to filter data by specific time ranges. Users can choose a specific date range by first selecting the start date, then drag the date range across the entire month. If dates across multiple months need to be selected, users can navigate to the next month, then drag the date range while holding down “SHIFT” key on the keyboard.



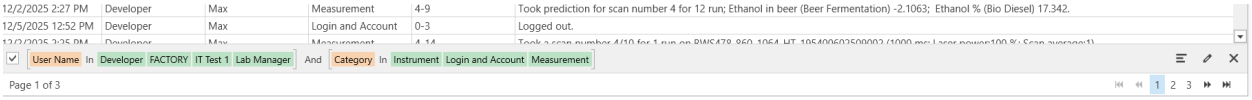
Users can also click on the Month name and the Year name to select dates for a specific month or year.



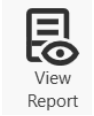
User Name filter, Full Name filter, Category filter, Audit Code filter can all be configured through the  icon in the table headers. Click the table icon, then a list of available filters can be selected:



Once the filter is selected, the summary of all filter conditions will show up at the bottom of the screen:



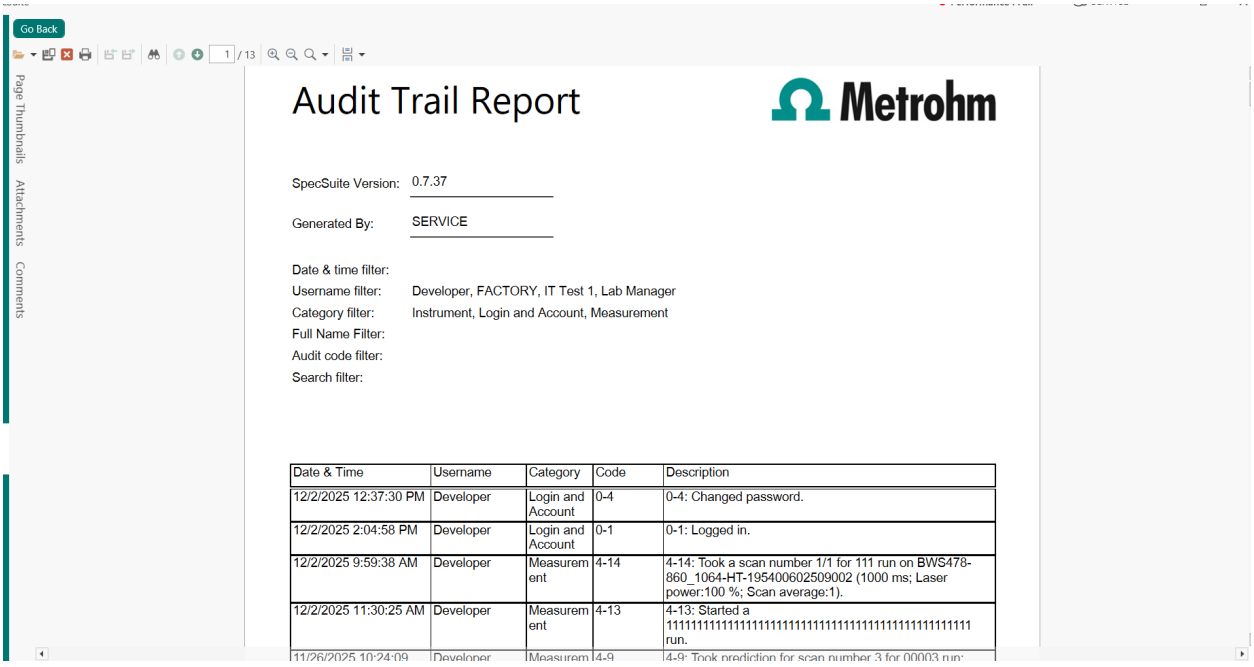
12.2 Audit Trail Reporting

Audit Trail Reports can be generated by clicking the View Report icon. 

An Audit Trail Report will include all the audit trail data that is currently filtered, including:

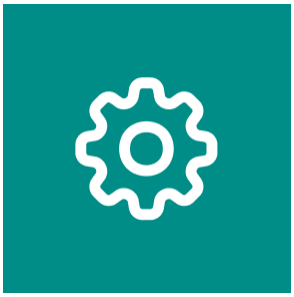
- Date and Time
- User Name
- Full name
- Category
- Audit Code
- Descriptions of the actions.

All filter conditions (except for description filter) will be listed at the top of the audit trail report, along with the software version, and the user who generated the Audit trail PDF.



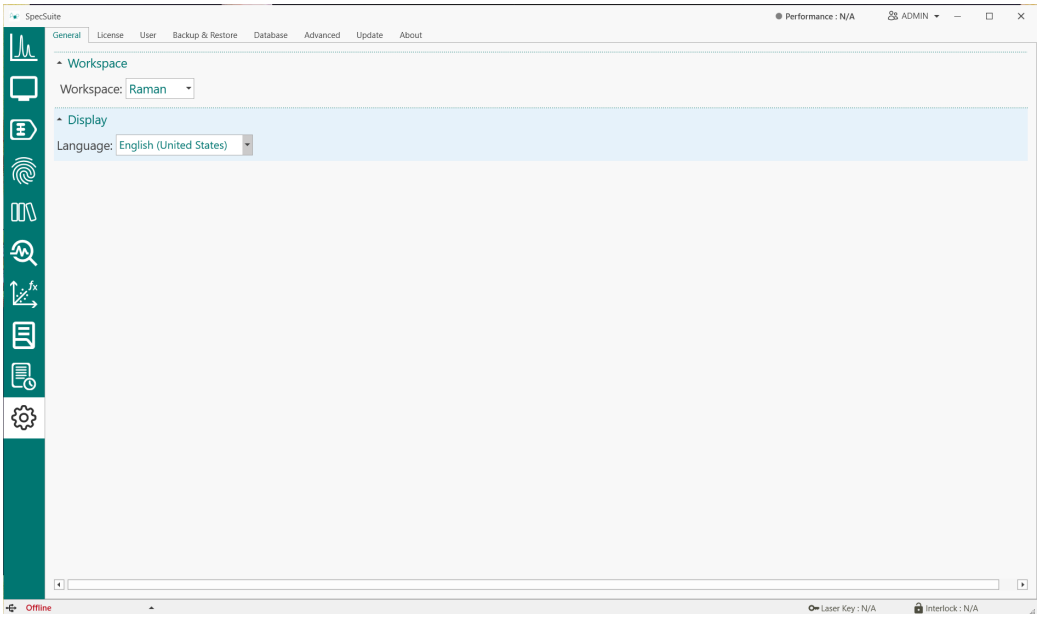
Audit Trail reports can be exported to PDF and printed through the PDF printing/viewing tool.

13. Settings



13.1 General

General settings show options for Workspace and Display.



Workspace

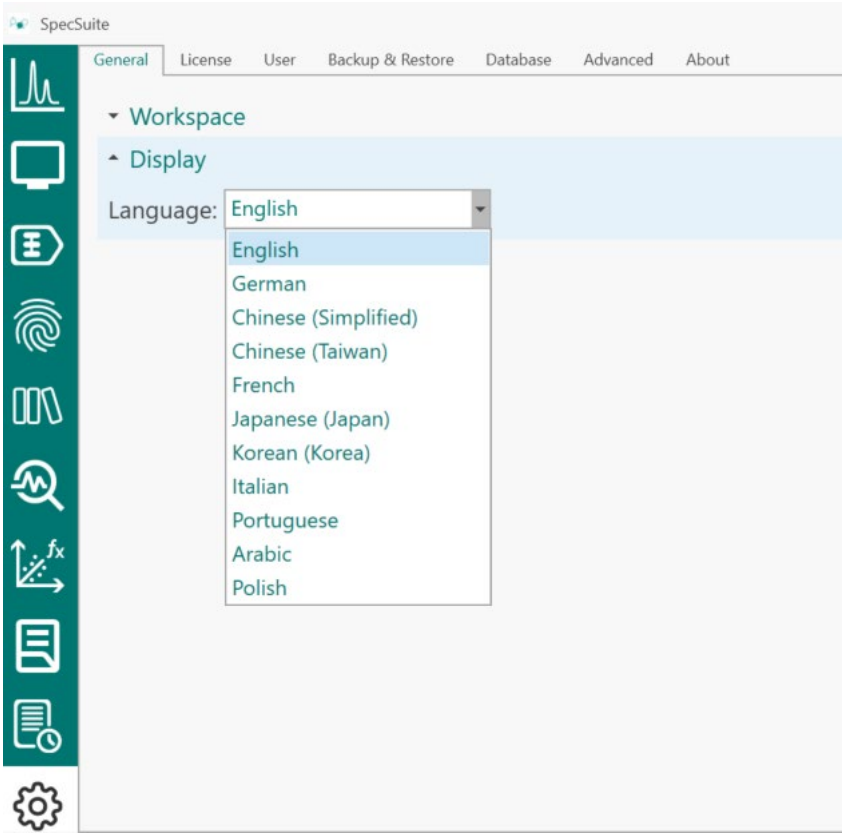
Raman workspace is available. Future workspace options will be released based on specific spectroscopy techniques.

Users can switch between different workspaces to change the default UI display in the software.

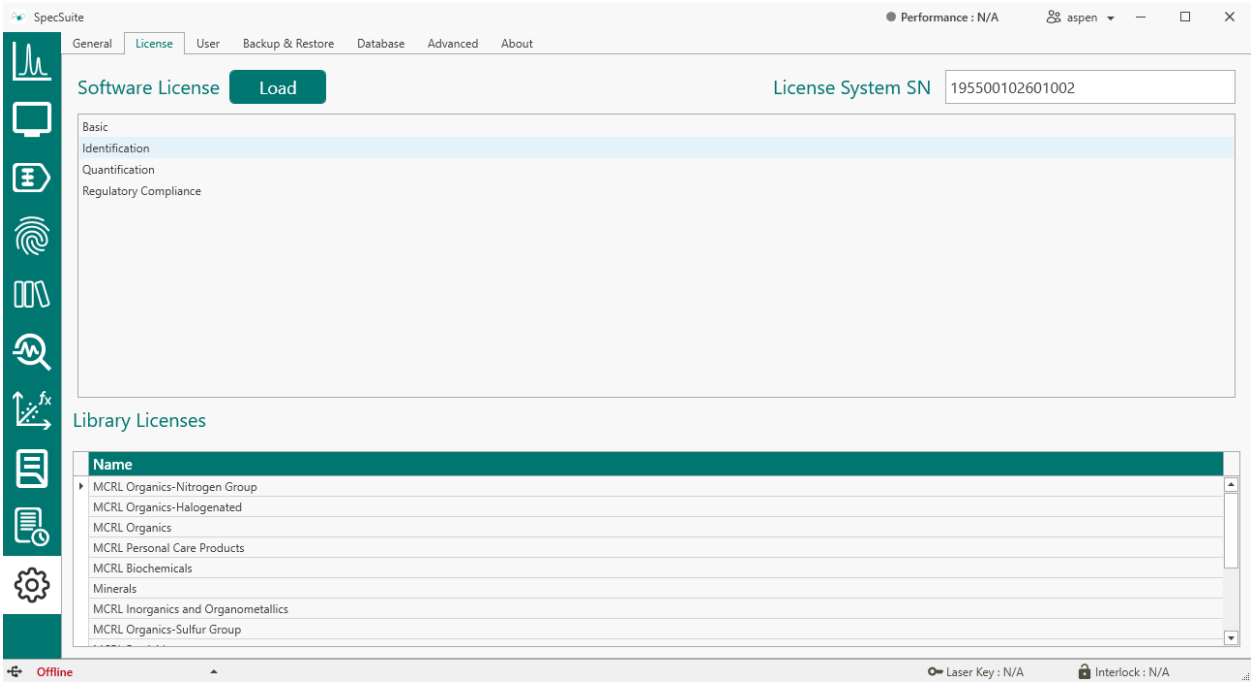
Display

During software launch, SpecSuite will recognize user's Windows language choice and default to use the Windows's language as the display language.

Users can change the display language using the drop-down menu. Once the language is changed, the software will remember to use the selected language for display during startup.



13.2 License



Some SpecSuite features and settings are controlled with a license that can be purchased from Metrohm. SpecSuite Licenses are bound to an instrument serial number. Users must connect the software to the instrument with the same serial number to activate and load the license.

To load your license, press the Load button and select the license file sent by Metrohm. If the license is valid for the requested computer, the License's settings will appear on this page. A prompt will appear asking the user to confirm that this license is correct, and if so, SpecSuite will be automatically restarted. Pressing cancel will clear the license information, and nothing will be changed.

Once uploaded, the License file can be found in this location on PC:
C:\ProgramData\Metrohm\SpecSuite

In case an unwanted license is loaded to SpecSuite, go to this location and delete the license, then put the correct license at this location named 'license.lic'

There are 4 different license configurations that can be purchased by customers:

- Basic
- ID
- Quant
- 21CFR.

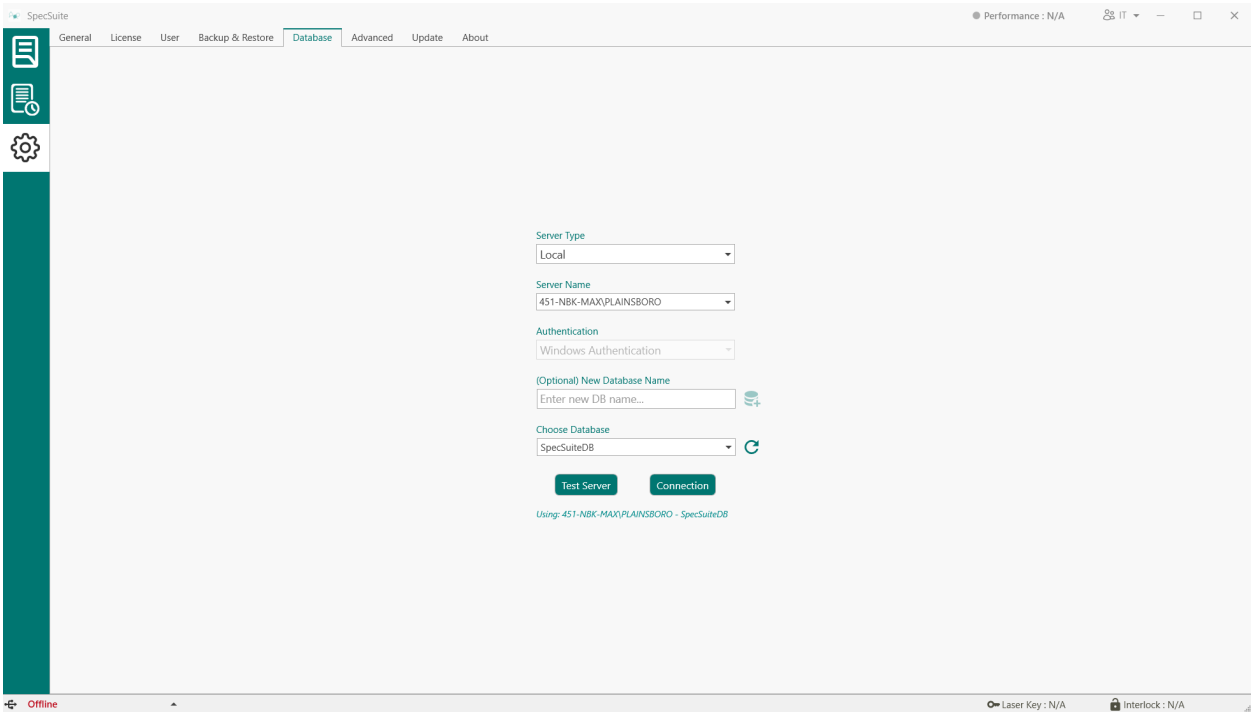
Default configurations are shown below:

Modules	Basic License	Identification License	Quantification License	Regulatory Compliance License
Explore	on	-	-	-
Identification	off	on	-	-
Routine Analysis	off	-	on	-
Compliance (including Audit Trail)	off	-	-	on
Performance	on	-	-	-
Instrument	on	-	-	-
Operating Procedure	on	-	-	-
Library	off	on	-	-
Settings	on	-	-	-
Report	on	-	-	-

A trial license is included with SpecSuite and enables all features. The trial license expires after 30 days. The license will then revert to a Basic license.

All licenses include the current Illicit and General Chemicals library. Additional library packages and licenses must be purchased from Metrohm.

13.3 Database



The database tab is reserved for IT users only. Users can:

1. Switch between local and remote databases.

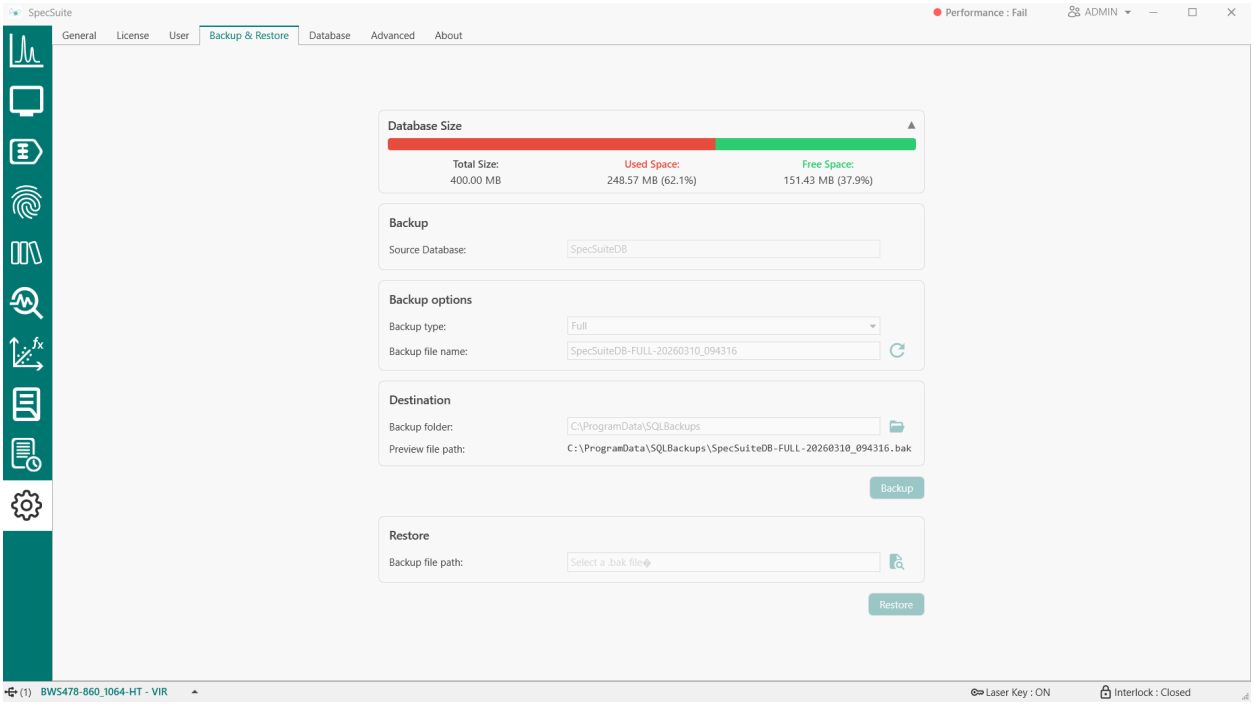
2. Connect to the Server with Server Name or IP address.

3. Create a new database in the connected server instance.

4. Select the database to connect.

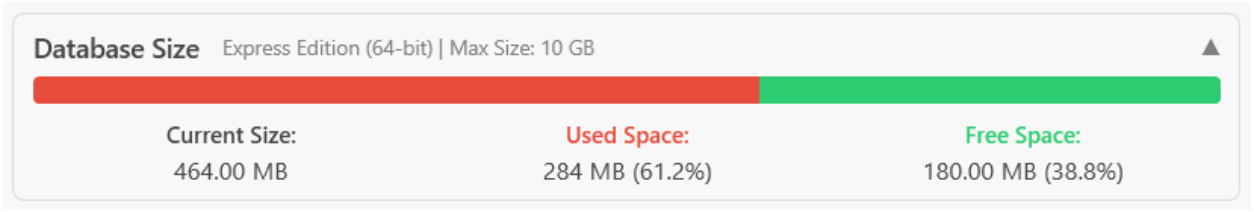
Detailed instructions for setting up server/database connections are described in chapter 1.3 and chapter 1.4.

13.4 Backup and Restore

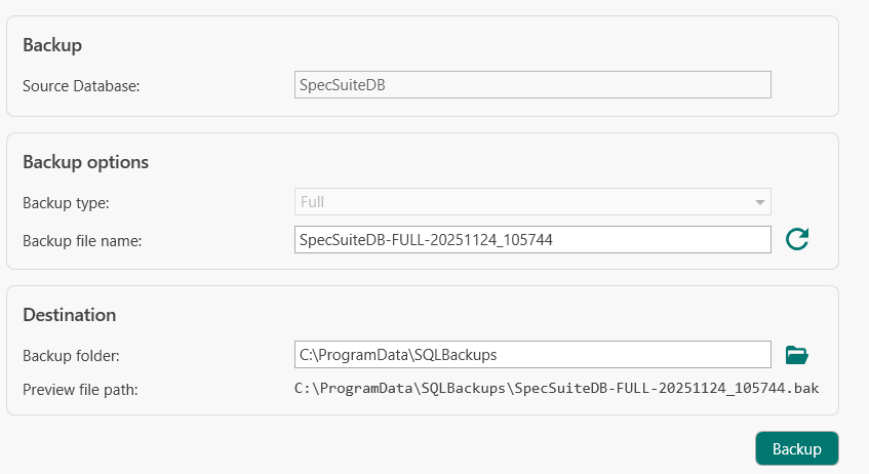


Database Size

SpecSuite will display the Current Size, Used Space and Free Space of the connected database. The database total size is dynamic and will grow automatically as data is added over time. For SQL Server Express, 10GB is the maximum size your database is allowed to grow.



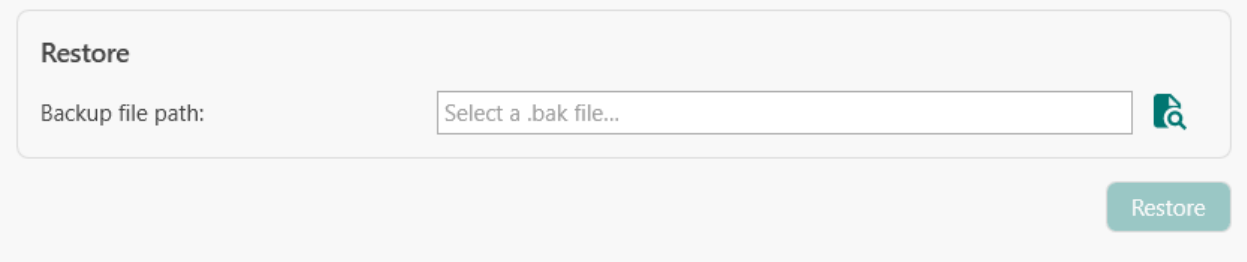
Backup Database



Backup Database can be used to manually back up the database. Use the default location or select a new location to store the backup data. The backup file name can be left as the default or be renamed. The backup file name will refresh based on the local timestamp by clicking the refresh button

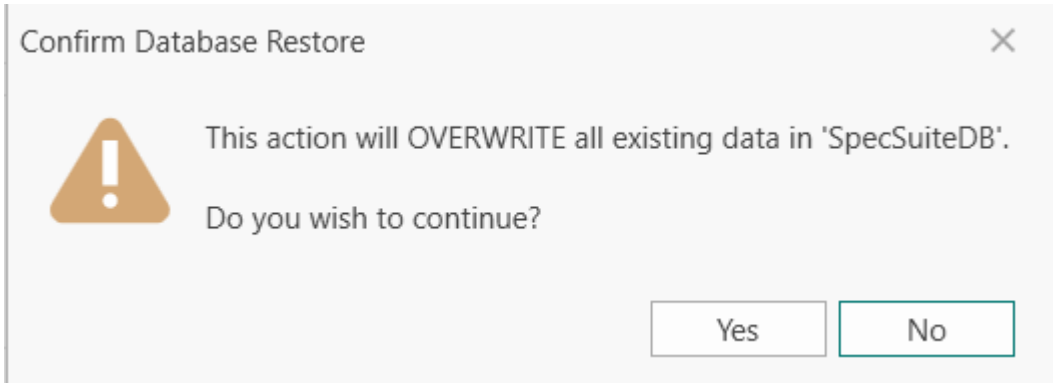
Backup Now will start to back up all data in the database for the name and location specified above. Users can back up to a remote PC as long as Windows permissions allow it.

Restore Database

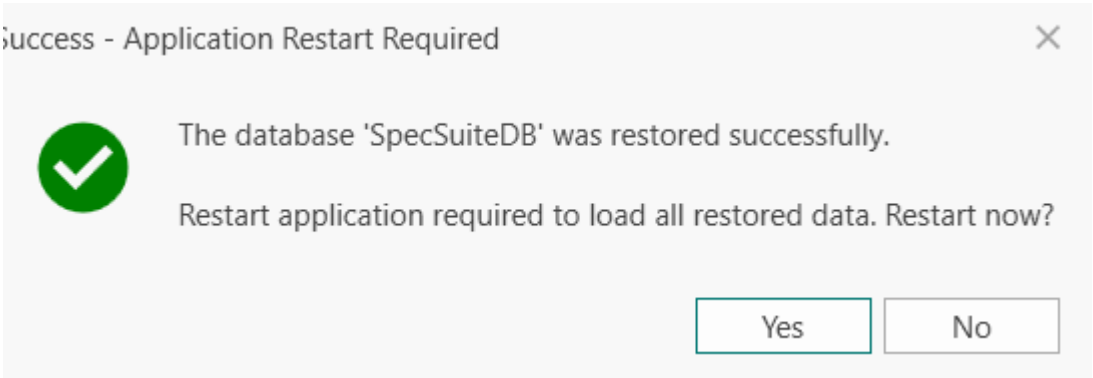


A database may be restored to a previous backup file. Restoring the database performs a full restore, replacing the current database content with the contents of the backup file.

Users can select the .bak file by clicking , then clicking the Restore button. A warning message will appear to warn the user before restoring. Choose “Yes” to continue or “No” to cancel.



Once the restore is successful, a message will appear, and the user must restart the application before the restore takes effect. Click “Yes” to continue.



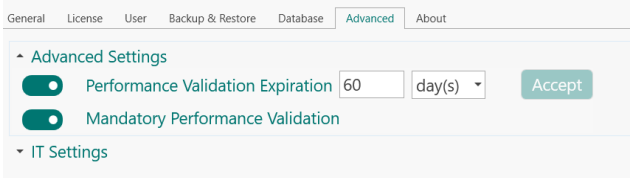
13.5 Advanced

The IT user can adjust these advanced settings:

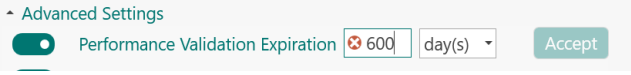
- Performance Validation Expiration
- Mandatory Performance Validation
- Log out after inactivity
- Password Expiration

Advanced Settings

In Advanced Settings, users can toggle performance validation expiration, adjust the duration, and enable or disable enforcement. The drop-down menu can be used to switch between days and hours, and to enter a number to define the duration.



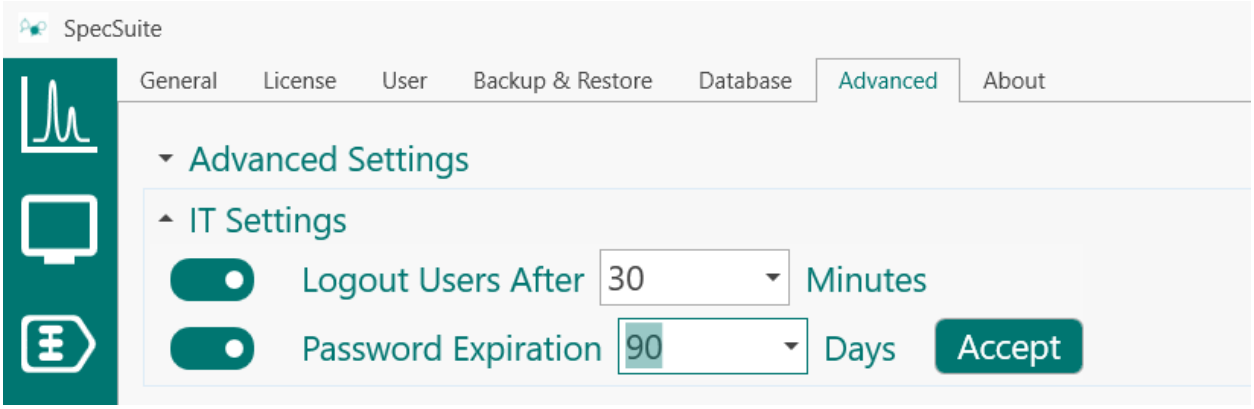
The user can enter a value between 1 and 365 days and 2 and 999 hours; any invalid entry will be rejected. Changes to this setting will be logged in the Audit Trail.



When performance validation expires, the performance status on the top right corner of the software will change to fail with a red indicator.

Users can also toggle Mandatory Performance Validation on or off. When enabled, the user is not allowed to acquire data in Identification and Routine Analysis unless the current performance validation status is Pass.

IT Settings

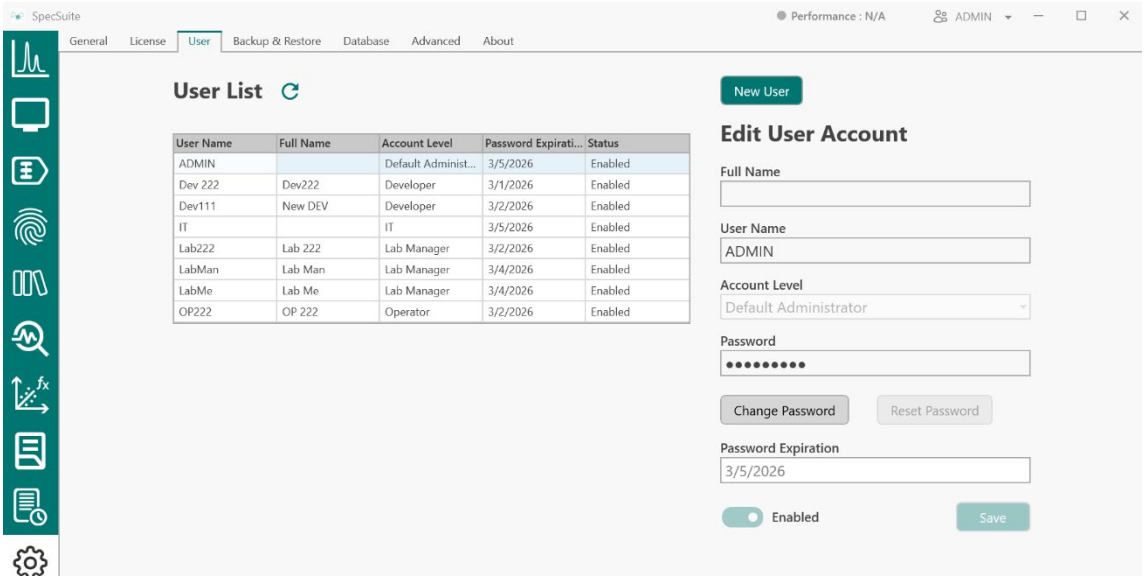


The IT user can enable/disable automatic user logout after inactivity. The auto-logout period can be set to 5, 10, 15, 30, 60, or 120 minutes. Auto-logout will apply to ALL users. Auto-logout will not be triggered during the period when an operating procedure is running with an active timeline acquisition.

IT users can also adjust the default number of days before a password expires. Password expiration days can be set to 7, 30, 60, 90, or 120 days, or manually entered. The password expiration date can also be disabled or enabled. This setting will apply to ALL newly created users and will not affect the current users' password expiration date. IT users can change the current user's password expiration date through the User tab. By default, password expiration is set to 90 days for all new users.

13.6 User

The User page lists the users in the SpecSuite database. Administrator and Developer-level users can see all other users and levels, and reset passwords as needed. Operator-level users can only see their own account's details.



User Name, Full Name, and Level are displayed in the Current Users list. When a User is selected from the table, the row is highlighted, and the user's information is populated in the fields on the right side of the screen.

In the Edit User Account panel, enter Full Name, User Name, Account Level, Password Expiration, and status to create a new account. Once a user account is created, only Level, Password, and Status may be changed. Password expiration cannot currently be changed; by default, it is set to 90 days from account creation. After any change, the account must be saved for the changes to take place. The changed password must be different than the last-used password.

Usernames and passwords may only use ASCII characters and the following special characters: !@#$%^&*?. The username length is limited to 4 - 20 characters. Username cannot contain space. Username cannot start with a special character. Usernames are unique.

Default Accounts

Default Account (User level): For these accounts ONLY default passwords are 999999.

- ADMIN (Administrator)
- IT (IT)

New Accounts

Only an Administrator or IT user can create a new user. Only IT users can create other IT users. The 'New user' button is not available to Operator or Developer-level users.

When the New User button is pressed, the Edit User Account panel will become blank and editable.

User Name: A username must be unique. User Name will be used for e-signature signing.

Full Name: Full name must be unique. It will display, in addition to the User Name on Reports, and at the top of the window to indicate the signed-in user.

User Level Permissions

Level: There are 5 different user levels:

- IT
- Administrator
- Developer
- Operator
- Lab Manager

IT level users will have full IT function access, such as database creation, backup and restore, user management, etc. IT-level users can also create additional IT-level users and reset other users' passwords. IT-level users do not have access to any instrument control or data collection/measurement functions.

Administrator-level users will have full instrument setup, control, measurement capabilities, and partial IT function access, such as user management, changing display language, and updating software license. Administrator users will not have access to sign reports or advanced functions such as backup/restore or database creation.

Developer-level users have access to full instrument setup, control, and measurement capabilities, creating qualitative and quantitative libraries/methods and setting up operating procedures for operators.

Operator-level users have view-only access to instrument setup and operating procedure details and can select/use operating procedures for material identification and Routine analysis.

Lab Manager-level users have access to view and sign reports and view audit trails.

The detailed user privilege table is shown here:

Module	Sub – module	IT	Administrator	Developer	Operator	Lab Manager
Instrument	Instrument Module – Menu Tab	Not Visible or Editable				Not Visible or Editable
	Device Info Tab	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Device Info - Show Details	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Device Info - Read Flash	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Hardware Setup Tab	Not Visible or Editable	Full Access	Full Access	Visible Only	Not Visible or Editable
	Hardware Setup - Detector Settings	Not Visible or Editable	Full Access	Full Access	Visible Only	Not Visible or Editable
	Hardware Setup - Accessory	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Laser Setup Tab	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Laser Setup - Laser Settings	Not Visible or Editable	Full Access	Full Access	Visible Only	Not Visible or Editable
	Laser Setup - Laser info	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Laser Setup - Add Laser/Remove Laser	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Performance Tab	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Performance - Select Reference File	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Performance - Export	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Performance - Import	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Performance - Create PVR	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Performance - Select Probe	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Performance - Run	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Performance - Stop	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Calibration Tab	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Calibration - Raman Shift Calibration	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable

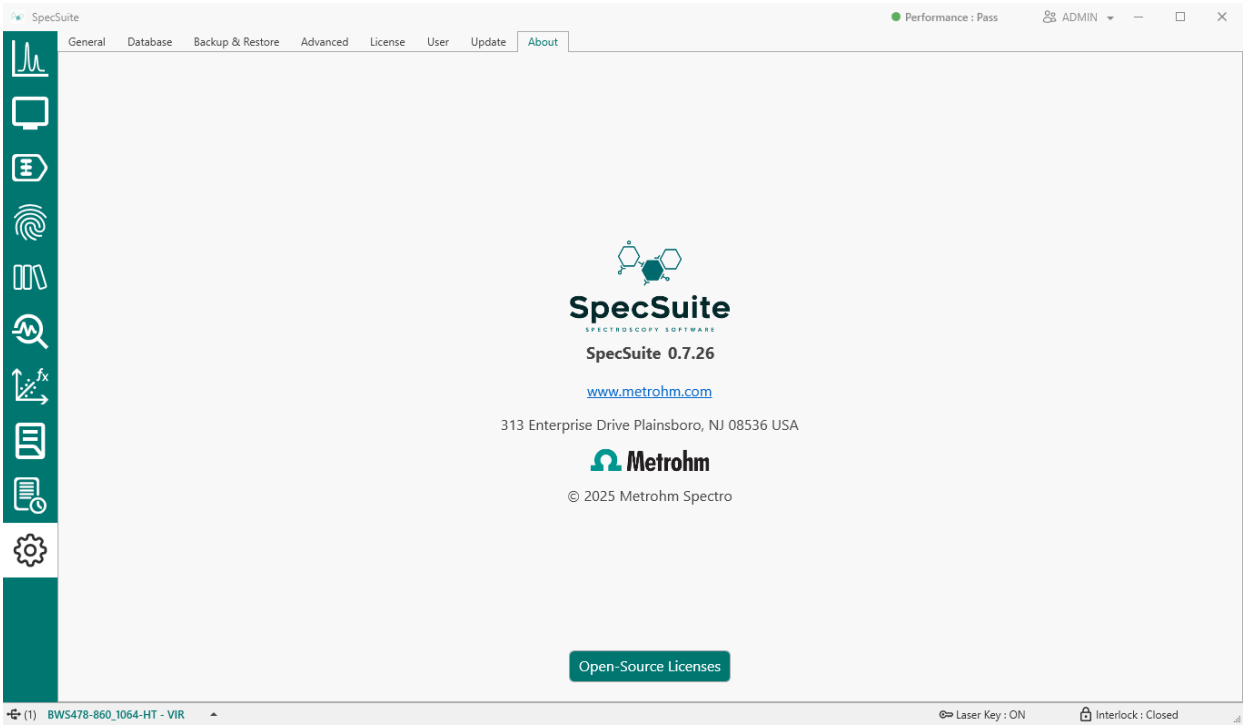
	Calibration - Laser Wavelength Calibration	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Calibration - Relative Intensity Correction	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Connection Tab – Virtual Devices	Not Visible or Editable	Full Access	Visible Only	Visible Only	Not Visible or Editable
Module	**Sub – module**	**IT**	**Administrator**	**Developer**	**Operator**	**Lab Manager**
Operating Procedure	Operating Procedure Module – Menu Tab	Not Visible or Editable				Not Visible or Editable
	OP/Method/Variables - View	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	OP - New	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	OP - Archive	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	OP - Edit	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	OP - Save OP	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Variables - Save	Visible Only	Visible Only	Visible Only	Visible Only	Visible Only
	Method - New	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Method - Edit	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Method - Save	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
Identification	ID Module	Not Visible or Editable				
	ID - Select OP	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	ID - Change OP Settings	Not Visible or Editable	Full Access	Full Access	Visible Only On	Not Visible or Editable
	ID - Run (online ID)	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	ID - Run Offline (offline ID)	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	ID - Rerun	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	ID - Stop	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable

Module	Sub – module	IT	Administrator	Developer	Operator	Lab Manager
Library	Library Module	Not Visible or Editable			Not Visible or Editable	
	Library - New	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Edit	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Validate	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Invalidate	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Archive	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Export	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Import	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Withdraw	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Library - Sample (Sample Info section)	Not Visible or Editable	Full Access	Full Access	Visible Only On	Not Visible or Editable
	Library - Sample (Edit, Import, Load, Save, etc.)	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
Routine Analysis	Routine Analysis Module	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Select Method	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
	Select OP	Not Visible or Editable	Full Access	Full Access	Full Access	Not Visible or Editable
Module	Model Module – Menu Tab	Not Visible or Editable	Full Access	Full Access	Visible Only	Not Visible or Editable
	Model - New	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
	Model - Edit/Save/Withdraw	Not Visible or Editable	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable
Reports and Audit Trail	Reports and Audit Trail Module – Menu Tab	Visible	Visible	Visible	Visible	Visible
	Report - View Report	Full Access	Full Access	Full Access	Full Access	Full Access

	Report - Load to Explore	Full Access	Full Access	Full Access	Not Visible or Editable	
	Report - Print	Full Access	Full Access	Full Access	Full Access	Full Access
	Report - Export	Full Access	Full Access	Full Access	Full Access	Full Access
	Report: E-signature	Not Visible or Editable	Not Visible or Editable	Full Access	Full Access	Full Access
	Report: E-signature – approval/reject	Not Visible or Editable	Not Visible or Editable	Full Access	Not available	Full Access
	Audit Trail: View	Full Access	Full Access	Full Access	Full Access	Full Access
	Audit Trail: Export	Full Access	Full Access	Full Access	Full Access	Full Access
Module	**Sub – module**	**IT**	**Administrator**	**Developer**	**Operator**	**Lab Manager**
Account	Account Module					
	New	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Archive	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Batch creation	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	View Account info (self)	Full Access	Full Access	Full Access	Full Access	Full Access
	View Account info (others)	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Enable/Disable Account	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Reset Password (self)	Full Access	Full Access	Full Access	Full Access	Full Access
	Reset Password (others)	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Set Password Expiration Date	Full Access	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable	Not Visible or Editable
	Password Expire	Yes	Yes	Yes	Yes	Yes
	Create IT Accounts, Disable/Enable IT Accounts, Reset IT Account Passwords	Yes	No	No	No	No
Settings	Settings Module					
	General Tab	Full Access	Full Access	Full Access	Full Access	Full Access
	General - Workspace (Default Defined in License)	Full Access	Full Access	Full Access	Full Access	Full Access
	General - Display: Language	Full Access	Full Access	Full Access	Full Access	Full Access

	Database Tab (Entire Tab)	Full Access	Visible Only	Visible Only	Visible Only	Visible Only
	Advanced Tab	Full Access	Full Access	Visible Only	Visible Only	Full Access
	Advanced – IT Settings	Full Access	Full Access	Visible Only	Visible Only	Visible Only
	License Tab	Full Access	Full Access	Visible Only	Visible Only	Visible Only
	License: view	Full Access	Full Access	Full Access	Full Access	Visible Only
	License: Import/add	Full Access	Full Access	Not Visible or Editable	Not Visible or Editable	Visible Only
	About	Full Access	Full Access	Full Access	Full Access	Full Access

13.7 About



About shows the installed version of SpecSuite along with contact information for Metrohm and Metrohm Service.

A list of open-source licenses used to create SpecSuite can be viewed here.

14. Terminologies

Scan – Any time the detector is recording information. Scan will usually refer to the collection of data while an external light source is firing.

Dark Scan – A scan collected while the light source is not firing.

"Complete" Scan – Data scan + Dark scan

Check Signal – This is known as "Continuous Scan" in BWSpec4. The laser is on and collecting scans consecutively at the set integration time until the Stop command is given.

Integration Time – The duration of time that the detector is collecting data.

Auto-Time – The optimal integration time is automatically calculated by the software to achieve a maximum signal of 40,000 to 60,000 counts .

Average – Used to describe the averaging of 2 or more spectra. The average is done for each y-value.

Laser Power – Refers to the percentage of total laser power being used.

External Trigger – When the trigger function is enabled, the instrument will wait for a trigger signal to be received at the External Trigger port. As an example, some i-Raman probes have a small trigger button on them which can trigger the scan start.

Auto Dark – When enabled, a dark scan of the same integration time as the data scan will be collected immediately after the data scan without the user having to take any additional action.

cCode – A 3–6-digit long string of letters used to name a spectrometer. This is a legacy term and will be depreciated for utilizing a Metrohm defined Serial Number instead.

Ratio3 – Refers to the output file generated by Relative Intensity Correction. It is a means of regulating data between spectrometers. Ratio3 is a .TXT file which includes information like cCode and coefficients. The data is two columns, one of Pixel and one for the multiplication factor of that pixel. The y-value of each pixel is multiplied by the Ratio value

PVR – Performance Validation Reference. This refers to the file generated in Hardware setup > Performance > Create PVR.

PV – Performance Validation. This refers to the test run by the performance module.

SERS – Surface Enhanced Raman Spectroscopy

See-Through – This term may also be referred to as ST. See-Through is a proprietary means of collecting data from a sample behind an opaque barrier using both physical means and calculations.

CAS – A Chemical Abstracts Service (CAS) Number is a unique numeric identifier assigned to a chemical.

Classification – Classifications are used within libraries to broadly describe a chemical.

Formula – Refers to the chemical formula for a sample in a library

Molecular Weight - The molar mass is defined as the mass of a given substance divided by the amount of a substance, is expressed in grams per mol (g/mol).

Workspace – Defines which modules and features are available across SpecSuite based on the intended application

Compliance – This refers to the 21CFR specifications for the pharmaceutical industry.

Model – Chemometric Model that takes multiple spectra and output a prediction value.

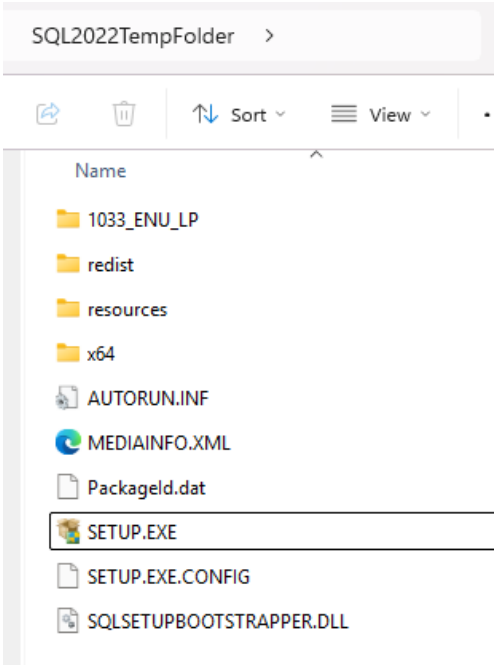
Online – An instrument that is powered on and connected to SpecSuite is online. Online data is collected live by the instrument.

Offline – When there is not an instrument connected to SpecSuite, the instrument is considered to be Offline. When data is loaded to SpecSuite which was not actively collected by a connected instrument, this is considered offline data. Some analyses can be completed without an instrument online; these are considered offline.

15. Appendix

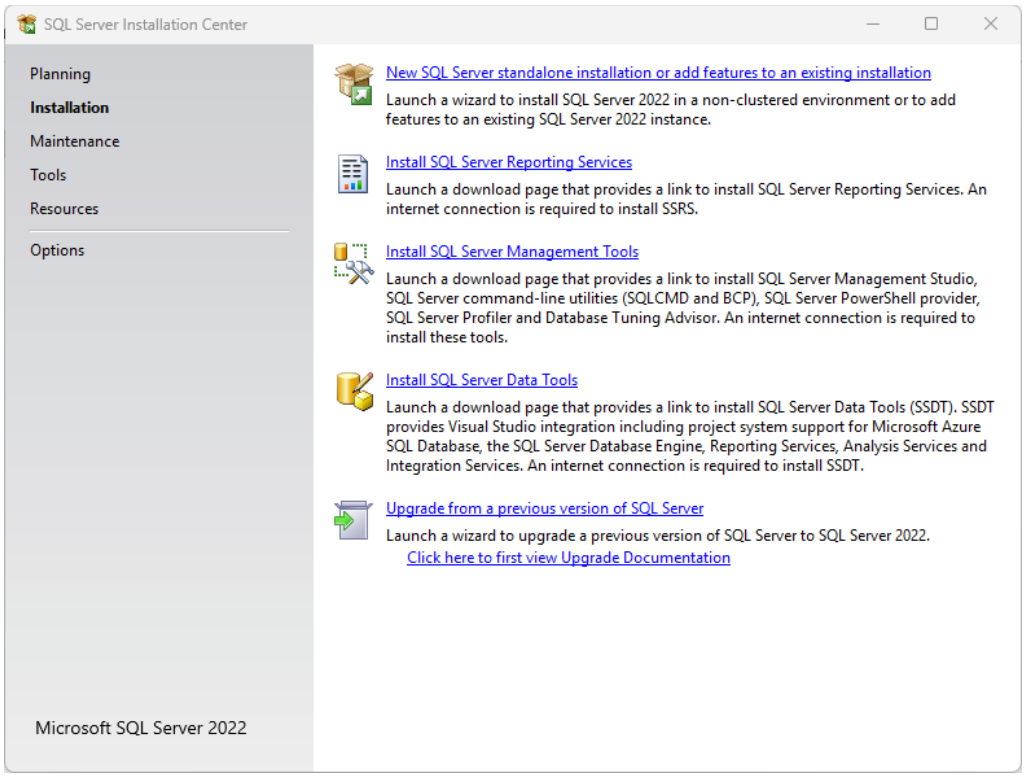
A. Manually creating a server instance (Optional, for IT only)

Only perform this procedure after SpecSuite has been installed and working properly with the default database. To create a new server, go to C:\SQL2022TempFolder. Locate the SETUP application, then right-click and select Run as Administrator to launch it

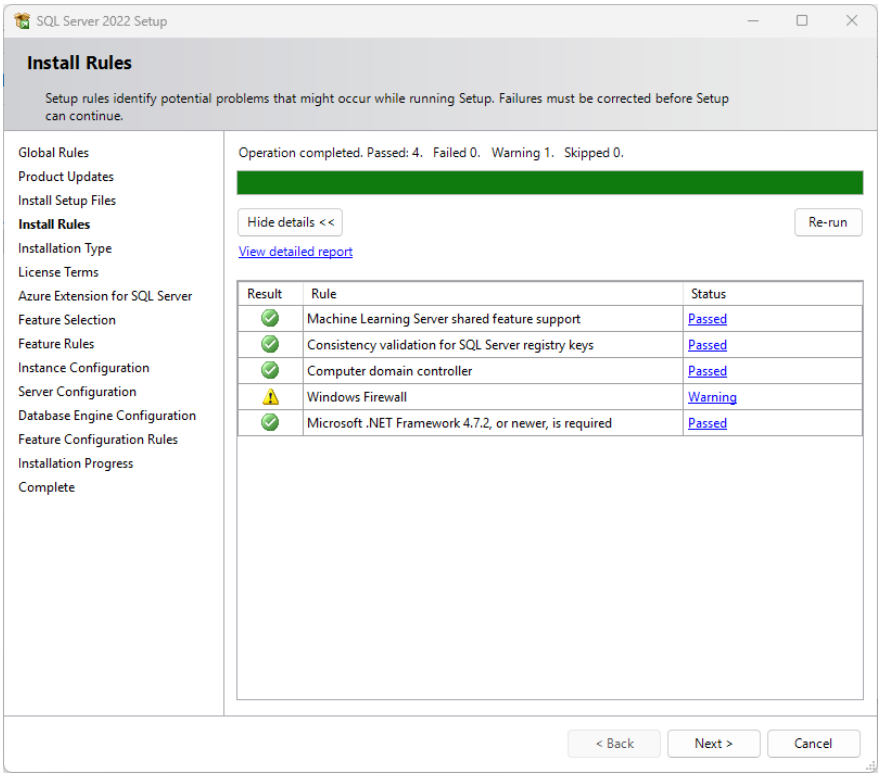


Advanced: If the SpecSuite installer has not been run yet, or the SQL Express installation has failed for some reason, a new local server can be created using the SQLEXPR_x64_ENU.exe application in the installation folder, located here: SpecSuite_[*version*]\ISSetupPrerequisites\{92E7C888-3945-4A13-B74C-8C05CFE2BDF0}. Double click the application; SQL Express files will need to be extracted. The length of the file path to the installation media cannot be too long, so we recommend copying it directly to the C: drive before running.

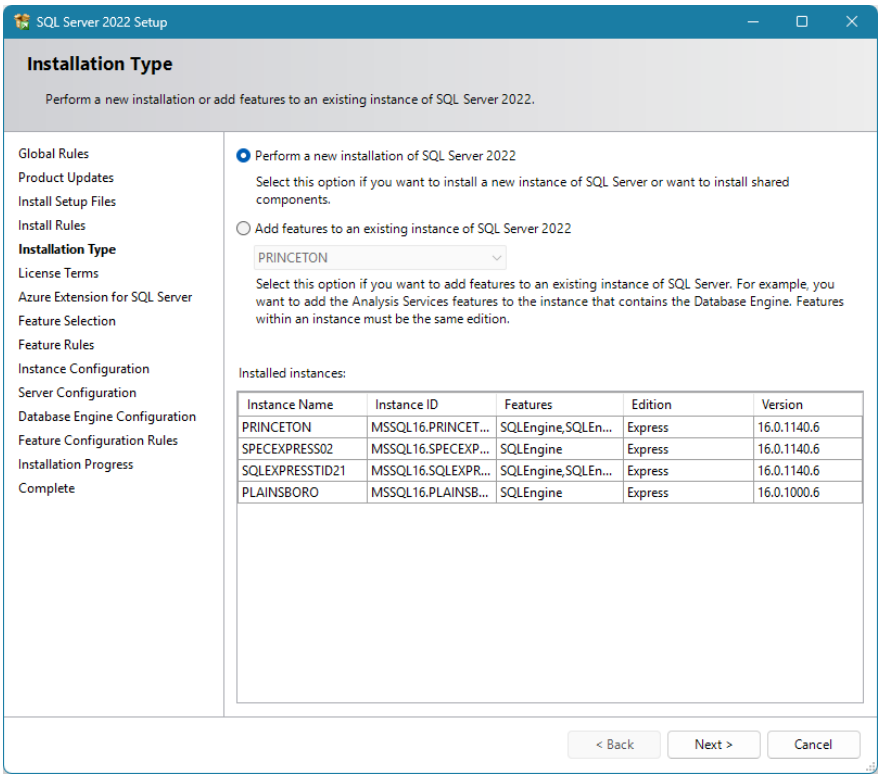
After launching, the SQL Server Installation window will appear. Choose 'New SQL Server standalone installation…'



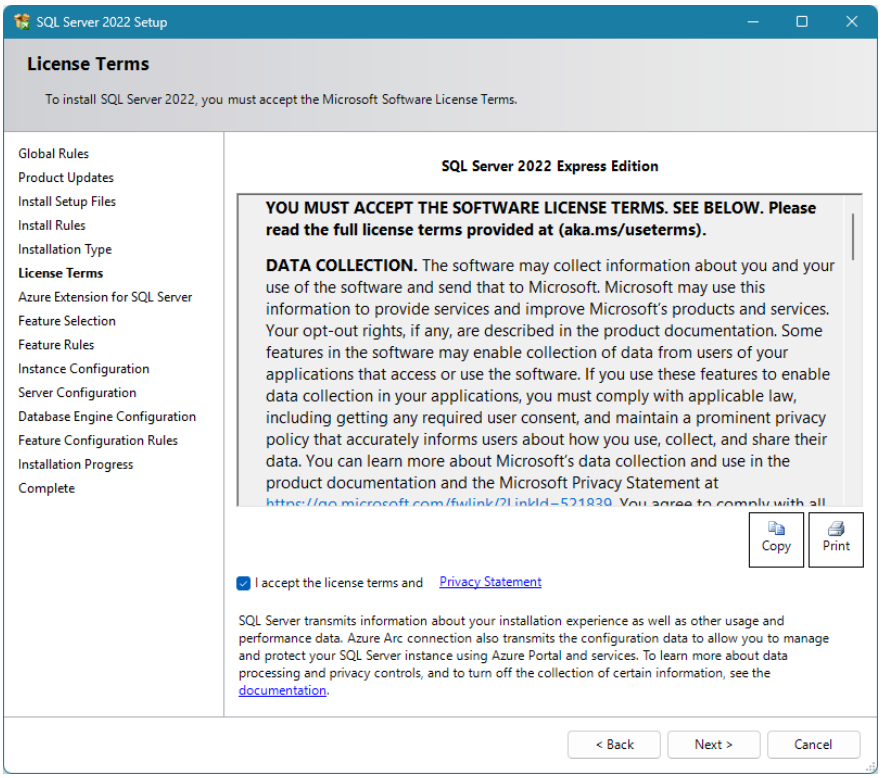
Next the Install Rules appear. If these are all successful, press Next. Windows Firewall may show a warning, but this does not cause any issues.



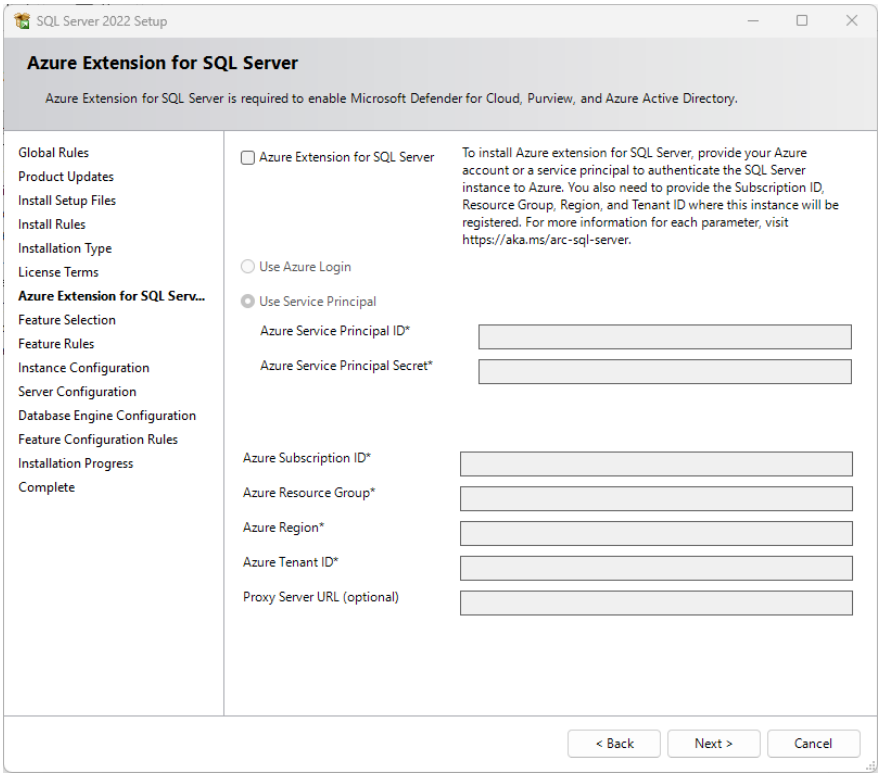
Select ‘Perform a new installation of SQL Server 2022’ then press next.



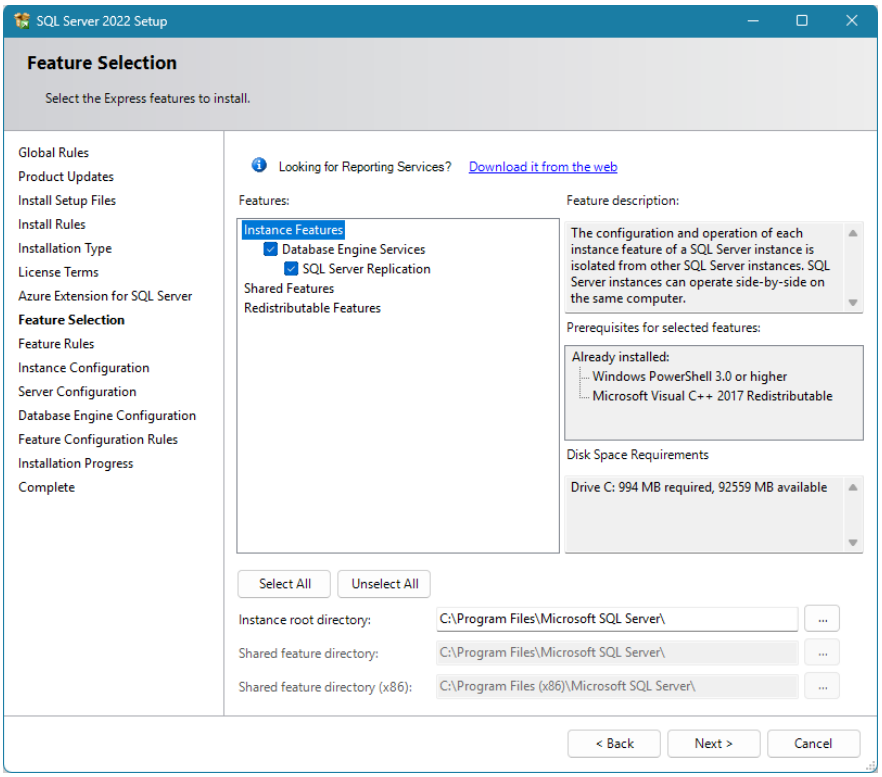
Accept the license terms and privacy statement for SQL Server 2022 Express and press Next.



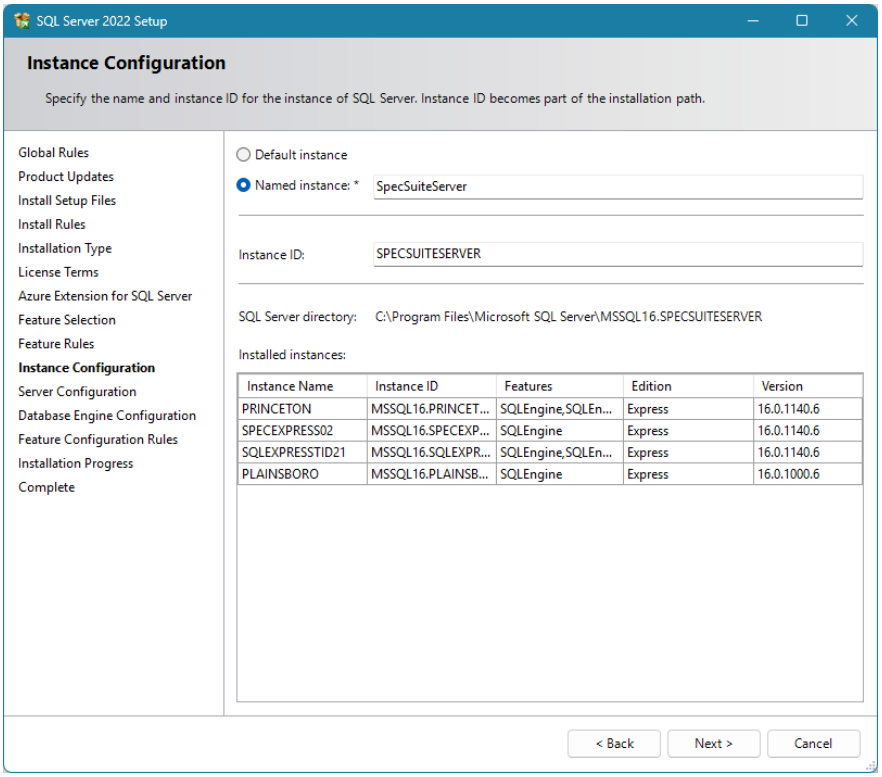
Uncheck the Azure Extension for SQL Server option, then press next.



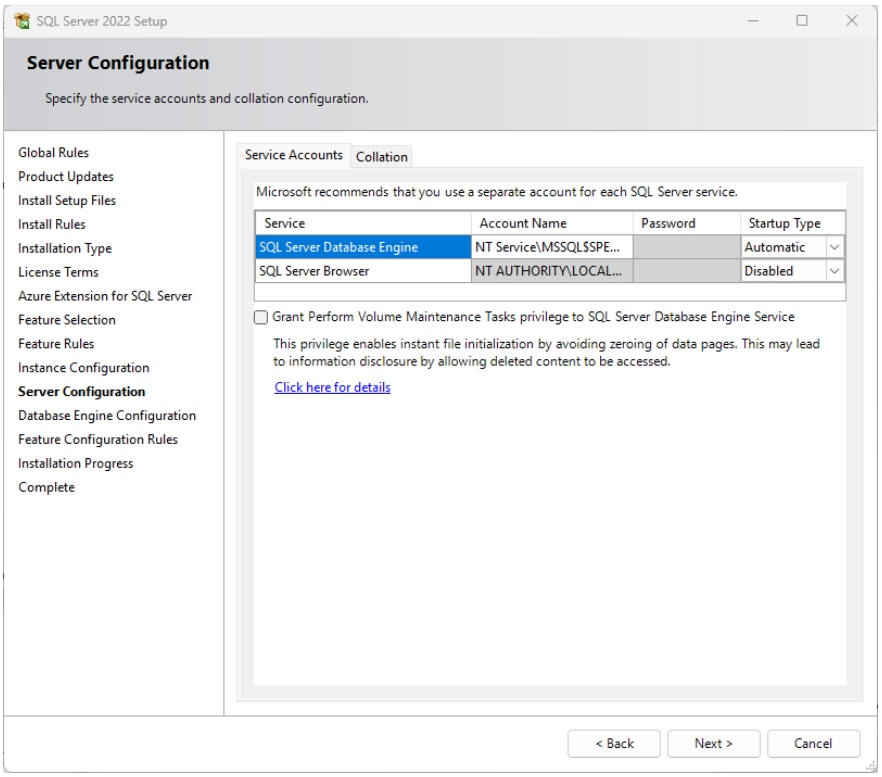
In Feature Selection, make sure both Database Engine Services and SQL Server Replication are both checked. The Instance Root Directory can be changed to a different location if desired. Press Next to continue.



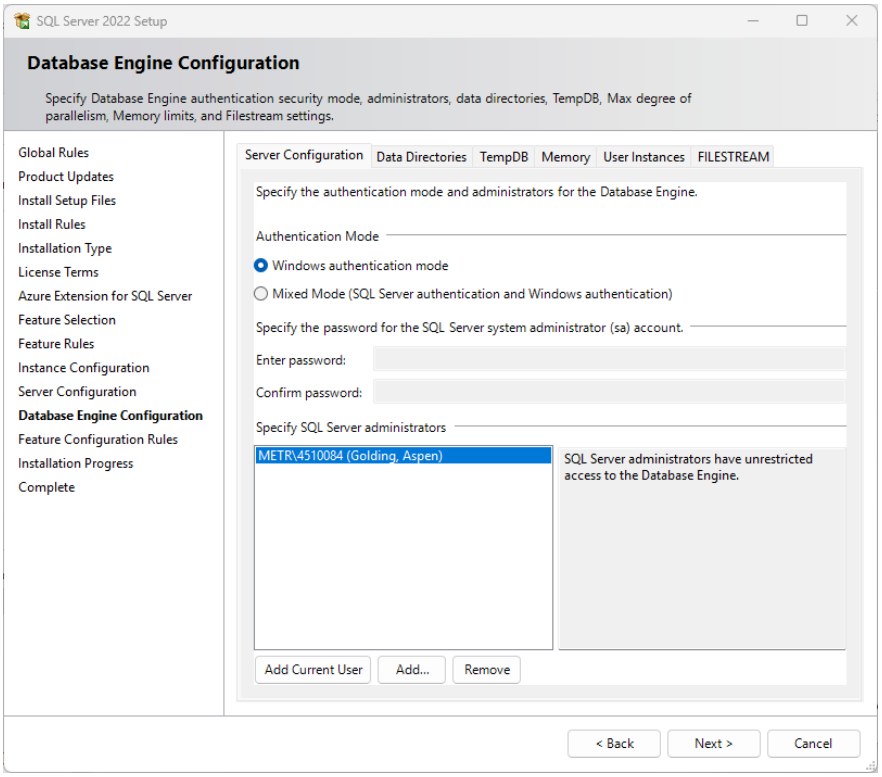
Name the instance something unique, then press Next.



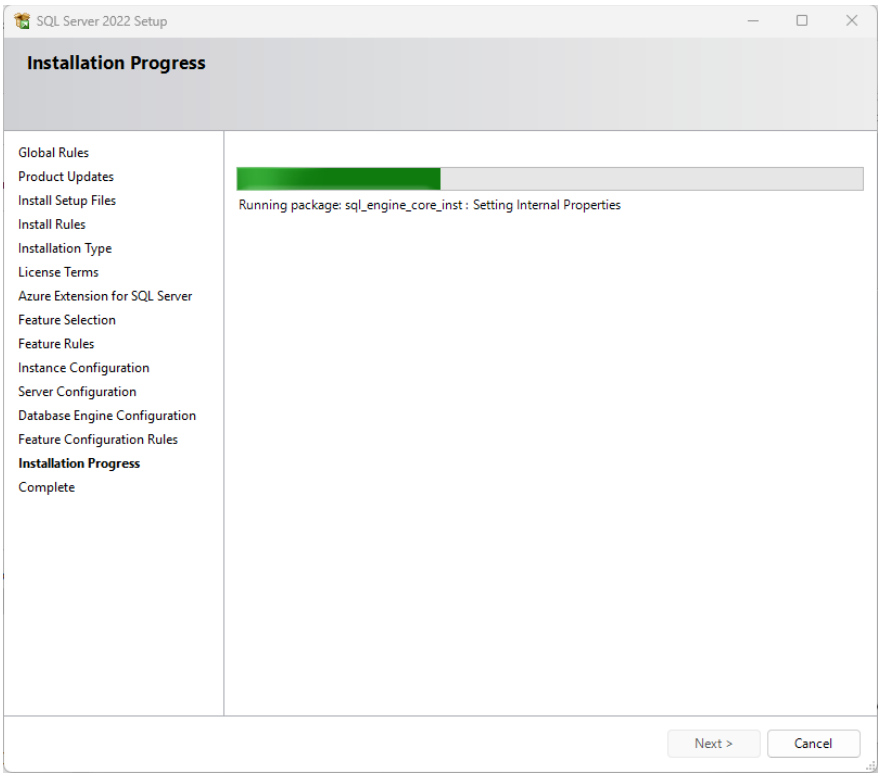
There are no necessary changes to make at this step, press Next.



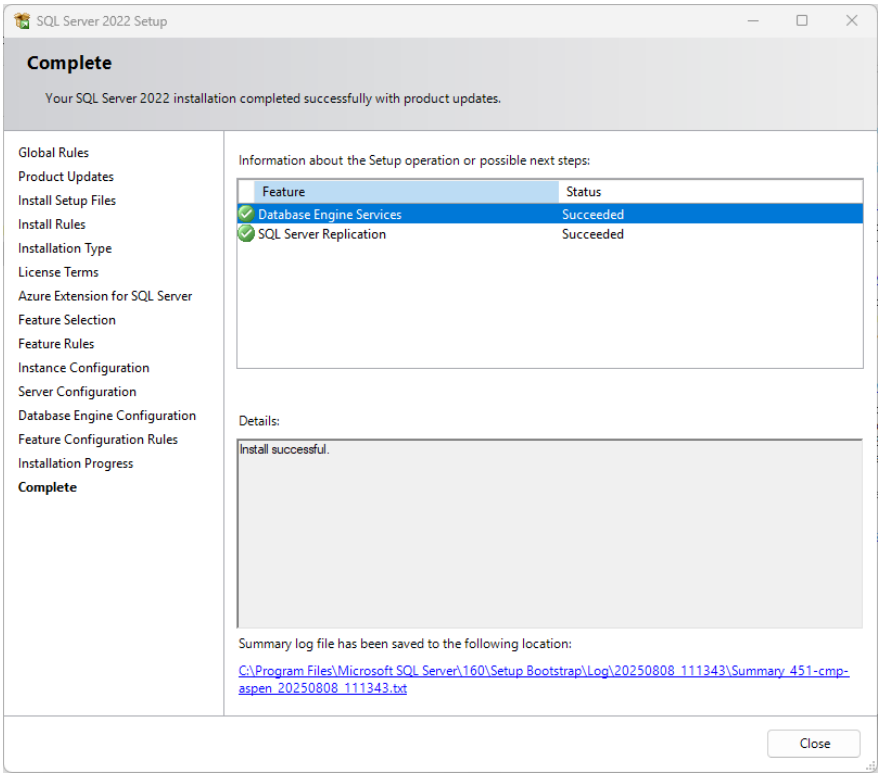
Select Windows Authentication Mode then press Next.



Press Next to begin installation. This may take several minutes.



The installation should be completed successfully.



If it fails, try again, making sure to run the SETUP application as Administrator. See the Troubleshooting section or contact Metrohm Support & Service from metrohm.com for assistance.

Finally, follow the instructions in section 2.3.1. to connect to a different local server.

B. Peak Analysis Definition

B.1 Peak Terminology

SpecSuite uses the following peak terminology. The figure below illustrates each term on a representative peak shape.

- Peak Center (Position) – The x-axis location of the peak maximum.
- Peak Height (Intensity) – The y-axis value at the peak maximum.
- Peak Width and FWHM – The full width at half maximum of the peak.
- Peak Area – The integrated area under the peak curve.
- Selected Range – Defined by RangeStart and RangeEnd, specifying the spectral region to analyze.

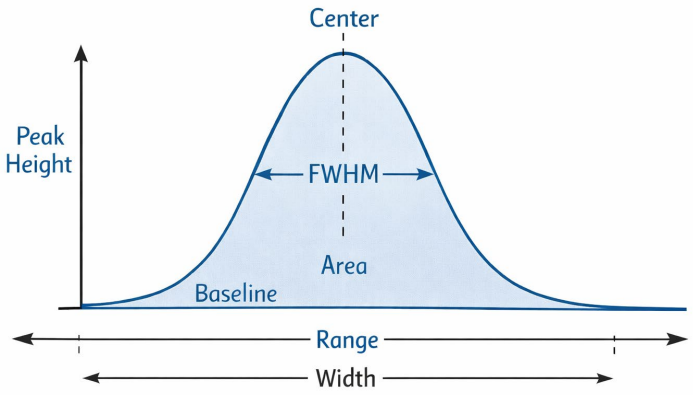


Figure 1: Peak terms illustrated on a representative peak shape.

B.2 Peak Analysis Algorithms

SpecSuite provides three algorithms for peak analysis, each suited to different use cases:

- Data Points – A local peak value-based method that identifies peaks directly from the measured data points.
- Parabolic – A parabolic fitting method that uses minimum height and width thresholds to identify and characterize peaks.
- CurveFit – A nonlinear curve fitting method supporting Gaussian, Lorentzian, or Voigt peak shapes.

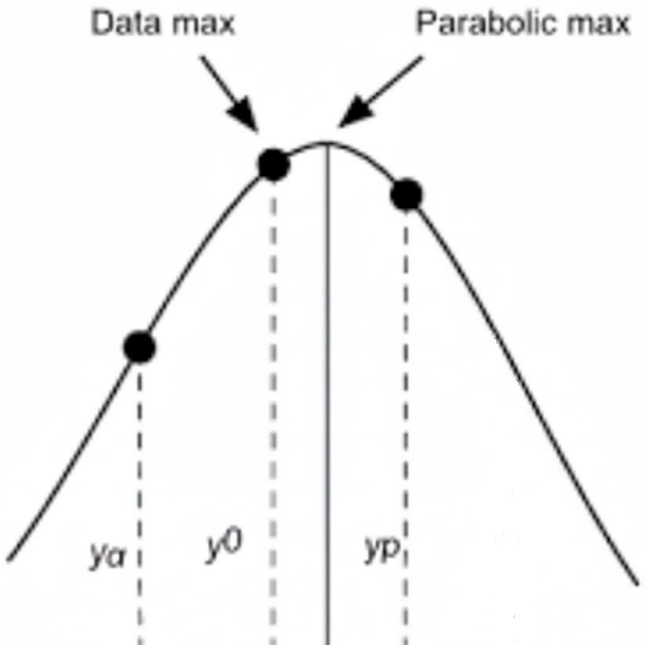


Figure 2: Data Points vs. Parabolic peak detection.

B.3 Parabolic – FWHM

When using the Parabolic algorithm, the Full Width at Half Maximum (FWHM) is calculated as the difference between the right mid-height point and the left mid-height point of the peak.

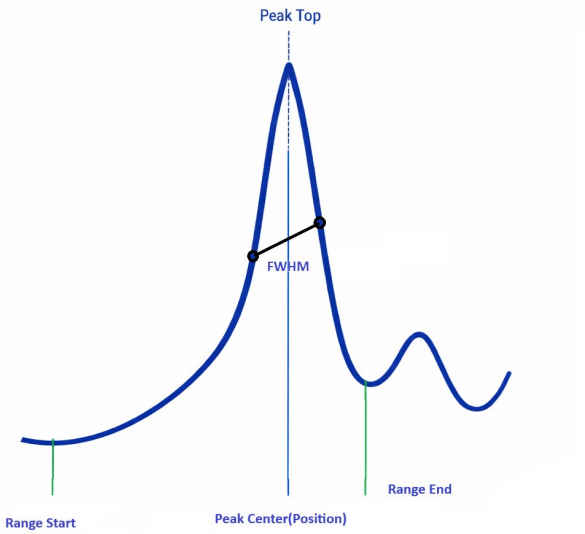


Figure 3: FWHM calculation using the Parabolic method.

B.4 Curve Fit – Gaussian Distribution

The Gaussian model is often called normal distribution, which is assuming the peak shape follows Gaussian distribution.

$$y = offset + Ae^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Where:

- A: The maximum amplitude (peak height) of the curve
- μ: The center position of the peak
- σ : The standard deviation, which determines the width or "spread" of the bell curve

In this distribution,

Gaussian $FWHM = 2\sqrt{2ln2} \cdot \sigma \approx 2.35482\,\sigma$

This model is commonly applicable for atomic emission spectroscopy (e.g., low-pressure Hg) and NIR molecular spectroscopy.

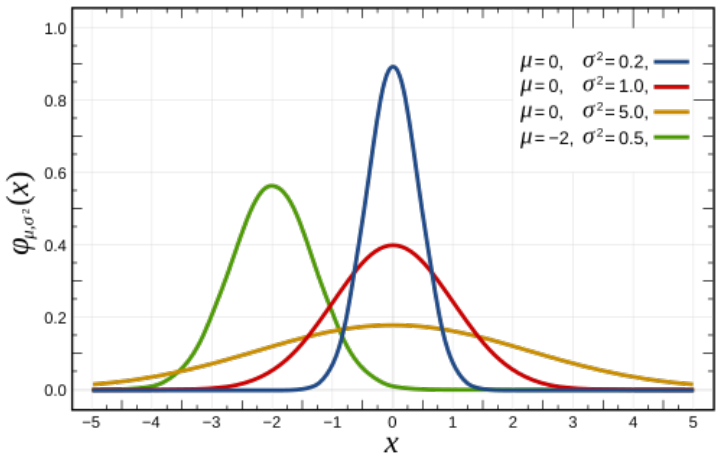


Figure 4: Gaussian distribution – equation parameters (left) and probability density curves (right).

B.5 Curve Fit – Lorentzian Distribution

The Lorentzian model is also called Cauchy distribution:

$$y = offset + \frac{A}{1 + (\frac{x-\mu}{\gamma})^2}$$

Where:

- A: The maximum amplitude (peak height) of the curve
- μ: The center position of the peak
- γ: Half-width at half-maximum (HWHM)

In this distribution,

Lorentzian $FWHM = 2\gamma$

This model is commonly applicable for atomic absorption spectroscopy and Raman spectroscopy.

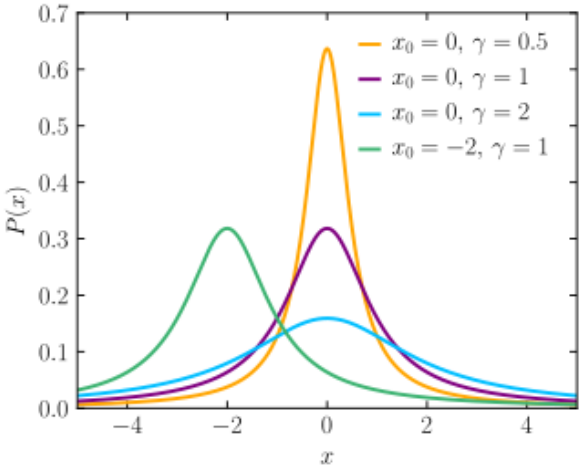


Figure 5: Lorentzian distribution – equation parameters (left) and probability density curves (right).

B.6 Curve Fit – Voigt Distribution

The Voigt model uses a pseudo-Voigt blend (not a full convolution). It combines a Gaussian component and a Lorentzian component using a mixing ratio η ∈ (0,1).

$$\eta = \frac{1}{1+e^{-p^4}} \; where \; \eta \in (0,1)$$

Where:

- Gaussian component: $g = e^{-\frac{(x-\mu)^2}{2\sigma_G{}^2}}$, with $\sigma_G = \frac{shared\ FWHM}{2\sqrt{2ln2}}$
- Lorentzian component: $l = \frac{1}{1+(\frac{x-\mu}{\gamma_L})^2}$, with $\gamma_L = \frac{shared\ FWHM}{2}$
- Final peak model: $y = A \cdot (\eta \cdot l + (1-\eta) \cdot g)$

Both components share a common FWHM. This model is suitable for mixed environments such as high-pressure Hg and Raman mixture analysis.

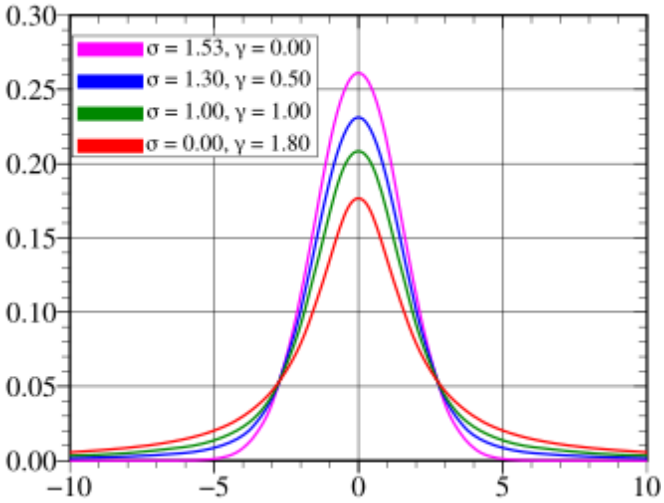


Figure 6: Voigt distribution – equation parameters (left) and probability density curves (right).

B.7 Key Points for Good Curve Fitting

Curve fitting uses initial peak parameters to reconstruct the measured curve by modelling it as a combination of fitted peak shapes. The quality of the fit depends on:

- Initial peak parameters: the number of peaks and the starting values for each peak (position, intensity, width). It defines how peaks are expected in the fitting which will eventually contribute to final fitted curve. Incorrect initial parameters include:

1. Peak exists in original data but not included in initial list

2. Peak does not exist in original data but defined in initial list
3. Peak parameter, especially peak position(center) is far away from the theoretical position

- Data range: the spectral range of the measured data being fitted.

Please keep in mind that curve fitting is trying to optimize all peak parameters then reconstruct the curve which is the closest to the original curve. The larger data points are involved, the more calculation is made and the more compromise to regions out of interest.

- Noise: noise-caused artifacts can create false multi-peak detections.
- Baseline: proper baseline correction before curve fitting significantly improves results.

Curve fitting formula includes offset which is calculated baseline to satisfy the optimization of curve fit. However, it will significantly impact the parameters of peaks. Please remove baseline before peak analysis to achieve the best performance.

C. SPC data definition

fxtype		X Axis Title in SpecSuite	fytype		Y Axis Title in SpecSuite
0	Arbitrary		0	Arbitrary intensity	
1	Wavenumber (cm^{-1})	Wavenumber	1	Interferogram	
2	Micrometers (μm)		2	Absorbance	Absorbance
3	Nanometers (nm)	Wavelength	3	Kubelka–Munk	
4	Seconds		4	Counts	
5	Minutes		5	Volts	
6	Hertz (Hz)		6	Degrees	
7	Kilohertz (kHz)		7	Milliamps	
8	Megahertz (MHz)		8	Millimeters	

9	Mass (m/z)		9	Millivolts	
10	Parts per million (ppm)		10	Log(1/R)	
11	Days		11	Percent	
12	Years		12	Intensity	Processed
13	Raman shift (cm^{-1})	RamanShift	13	Relative intensity	
14	eV		14	Energy	
16	Diode number		16	Decibel	
17	Channel		19	Temperature (°F)	
18	Degrees		20	Temperature (°C)	
19	Temperature (°F)		21	Temperature (K)	
20	Temperature (°C)		22	Index of refraction (N)	
21	Temperature (K)		23	Extinction coefficient (K)	
22	Data points	Pixel	24	Real	
23	Milliseconds		25	Imaginary	
24	Microseconds		26	Complex	
25	Nanoseconds		128	Transmission	Transmission/Reflection
26	Gigahertz (GHz)		129	Reflectance	
27	Centimeters (cm)		130	Arbitrary	
28	Meters (m)		131	Emission	
29	Millimeters (mm)				

30	Hours				
255	Double interferogram				

*Y axis option Absorbance and Transmission are to be implemented.