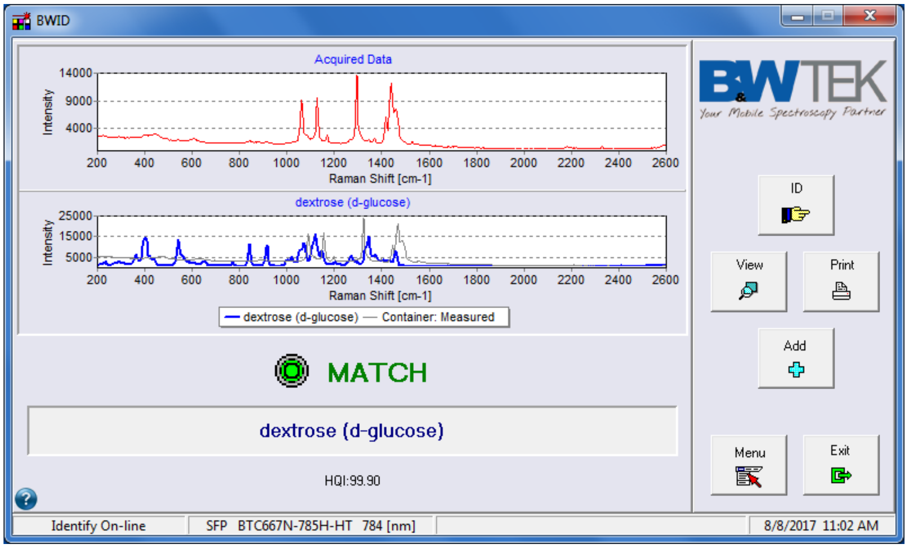


MATCH

dextrose (d-glucose)

HQI:99.90

Identify On-line | SFP BTC667N-785H-HT 784 [nm] | 8/8/2017 11:02 AM

BWID® V2.04 User Manual

290020113-J (2024/11/22)

Table of Contents

1. Introduction

BWID® is a Raman spectrometer identification program. It allows a user to identify or verify materials based on user-built and/or ready-to use licensed spectra libraries (BWTek and ST Japan libraries).
Starting from BWID® version 2.02.10, the software includes a STID (See Through ID) identification module, allowing for direct creation of libraries with STRam® instrument, and material identification through opaque packaging using the STRaman® technology, or with direct sample identification, taking advantage of the system adaptability with sampling adaptors for sample measurement.
The program supports a USB spectrometer interface only.

There are two versions of the BWID® software – the Standard Edition and the Pharma Edition. The Pharma Edition is an enhanced version of the Standard Edition. It supports the FDA CFR21 Part 11 regulation for electronic records and electronic signatures and provides system access control, electronic signatures and audit trail of data activities.

2. Program Features

The list below is a comparison of the program features available in the Standard and Pharma editions of BWID® software.

Program Features		*Program Edition*	
		Standard	*Pharma*
User Access Control			√
	User login		√
	Password change		√
	User accounts management		√
Audit Trail			√
	Audit trail generation		√
	Audit trail viewing		√
Electronic Records		√	√
Electronic Signatures			√
Operation Preset Configuration		√	√
Data Library Generation		√	√
Sample Identification		√	√

Diagnostic Tests	√	√
Reports	√	√
Program Configuration	√	√

3. Installation

Operating Systems Supported

Windows 7
Windows 8
Windows 10

Minimum Hardware Requirement

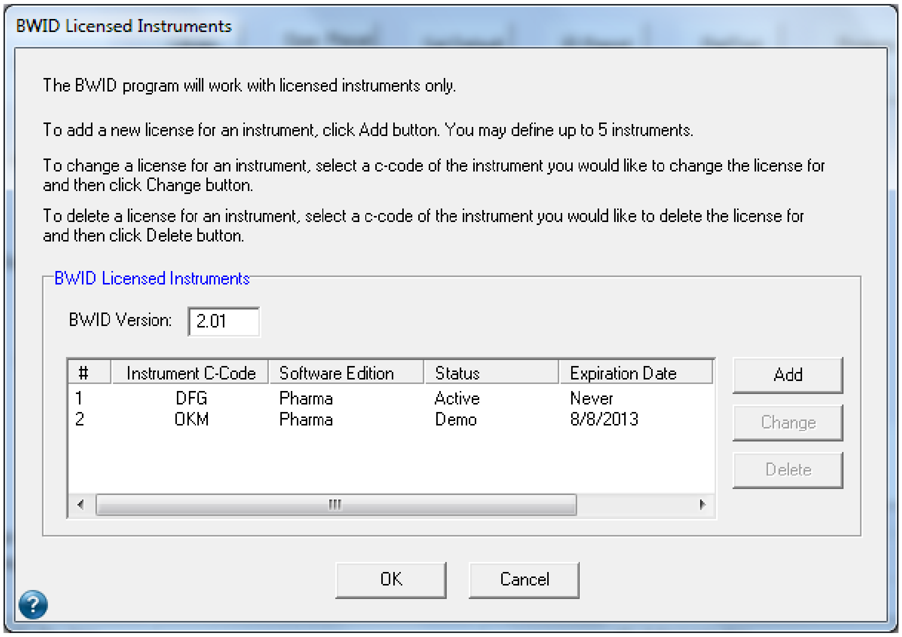
Your PC’s operating system must meet or exceed the following hardware specifications:

- Processor: 2GHz or faster
- RAM: 2GB or more
- Hard disk space: 5GB available or more

Installation

Run the Setup.exe file and follow the on-screen instructions. Make sure that you have administrative privileges on your computer when running the installation.

Once the installation is finished, start the BWID® software and add a BWID® license key for an instrument
that will be used with the software (via Menu->Setup->Instruments option), if the license key had not been set yet.
A BWID® license key is a 32-alphanumeric character string generated by BWTek for a given instrument (identified by a c-code), program version and edition (Standard or Pharma).
Please note that there may be up to 5 license keys for different instruments installed on a single computer at one time.



BWID Licensed Instruments

The BWID program will work with licensed instruments only.

To add a new license for an instrument, click Add button. You may define up to 5 instruments.

To change a license for an instrument, select a c-code of the instrument you would like to change the license for and then click Change button.

To delete a license for an instrument, select a c-code of the instrument you would like to delete the license for and then click Delete button.

BWID Licensed Instruments

BWID Version: 2.01

#	Instrument C-Code	Software Edition	Status	Expiration Date
1	DFG	Pharma	Active	Never
2	OKM	Pharma	Demo	8/8/2013

When working with the STRam instrument, the BWID® (ver. 2.02.10 and higher) can operate on the STRam tablet computer or on an external PC. If the program will be run on the tablet, the instrument computer switch (on the back) should be set to “INT”. If the program will be run on the external computer, the instrument computer switch (on the back) should be set to “EXT”. Additionally, the laser interlock plug should be connected and the interlock loop should be closed for normal operation. See the STRam user manual for more information about the STRam operation.

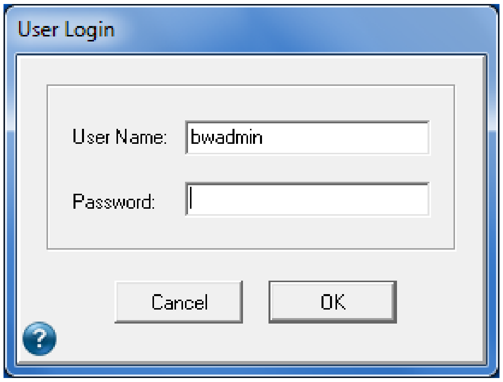
Known Issue:

When starting a BWID® on Windows 8 or 10, the program may fail with an error saying that bwtekusb.dll or bwid.dll is missing. This is due to a missing Microsoft Visual C++ 2008 redistributes on the PC. To solve the issue: Install Microsoft Visual C++ 2008 Redistributable Package (x86) - use vcredist_x86.exe in \ISSetupPrerequisites\{0BE9572E-8558-404f-B0A5-8C347D145655} under the Installation folder.

4. Starting the BWID® Program

Upon starting the BWID® program, the system prompts the user to enter a *User Name* and *Password* to have access to the application according to the access level assigned by the *Administrator* (Pharma Edition only).

User Login



User Login

User Name: bwadmin

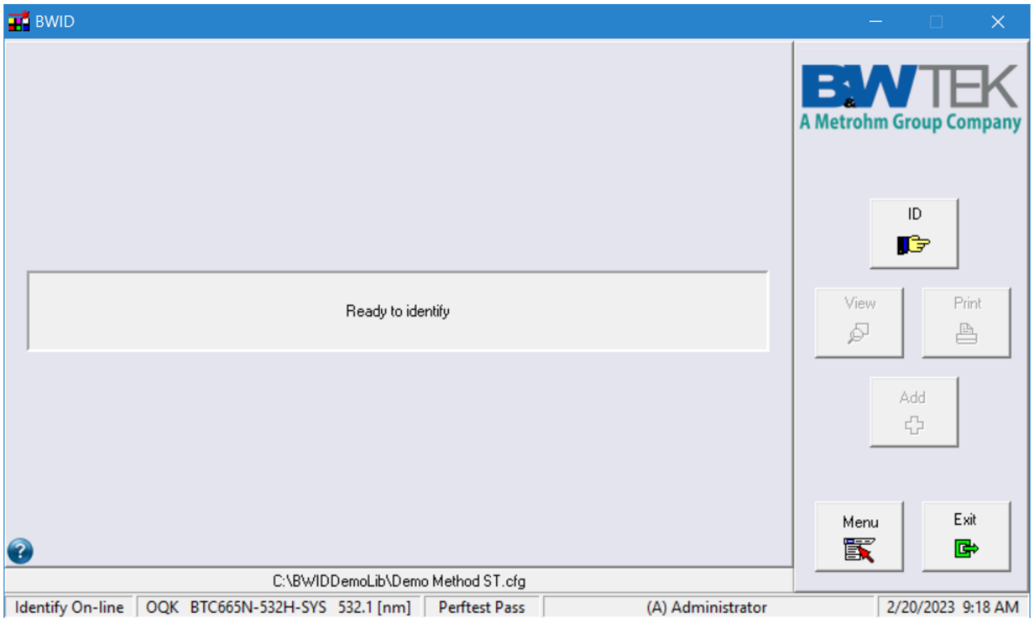
Password:

Upon program's first installation on a PC there is one user with *Administrator* privileges that can grant access to all features within the module. The user ID is *bwadmin* and the password is *bwtek*. Both the user ID and the password are case sensitive.

The *bwadmin* user is a default user and should be used only to define other *Administrator* users with a meaningful *user name* assigned for a particular person who is going to perform administrative tasks within the program. Once the second *Administrator* user is defined, the *bwadmin* user should be disabled. For more information regarding the user access control, see the User Access Control paragraph.

Program Main Window

Below is the main window of the BWID® program.



Ready to identify

C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line	OQK BTC665N-532H-SYS 532.1 [nm]	Perftest Pass		(A) Administrator	2/20/2023 9:18 AM

If working with an STRam, i-Raman Pro, or i-Raman Prime instrument, there is an instrument warm up time that will be displayed the first time of connection after program start. Data can be collected during this time, though it is better to wait until the detector has cooled to the defined level.

The *ID* button allows the user to start an identification analysis.

The *View* button allows the user to view details of a recently performed ID analysis. The button works like a toggle switch between the ID analysis result window and the ID analysis details window.

The *Print* button allows the user to print out a report for a recently performed ID analysis.

The *Add* button allows the user to add a spectrum, acquired in ID analysis, to a data library.

The *Menu* button allows the user to display program menu options.

The program also supports a pop-up menu. Right clicking with your mouse anywhere on the background ofthe main window will display the pop-up menu with program menu options with the four most frequently used program functions at the top of the menu: *View ID Results*, *Setup Library*, *Setup Operation Preset*, and *Configure Program*.

The *Exit* button allows the user to close the program.

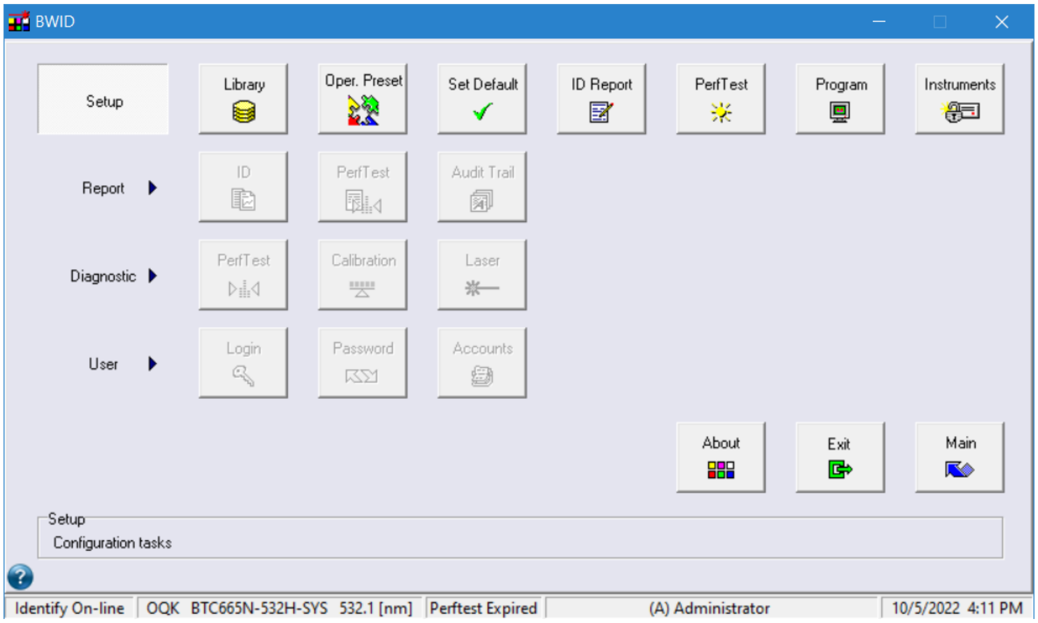
The top status bar displays current operation preset selected for ID analysis.

The bottom status bar consists of four boxes. The box on the far left is used to display the current identification mode which is one of four options: *Identify On-line* or *Identify Off-line* for identification of an unknown sample and *Verify On-line* or *Verify Off-line* for identity verification of a known sample, on-line and off-line respectively. The second box shows connected instrument information (c-code, model and laser wavelength).
The third box displays current status of a performance test for the connected instrument which is one of four options: *Perftest Pass*, *Perftest Fail*, *Perftest Expired*, *Perftest N/A* (or empty field in case instrument is not connected).
The fourth box displays the first and last name of the user who is currently logged in and the category: (A) for *Administrator*, (D) for *Developer* or (O) for *Operator*. The box on the far right displays the current date and time.

The user can access program help at any time by clicking the question icon located in the bottom left-hand corner of the main window and in all other dialogs within the program.

5. Program Menu

Upon clicking the *Menu* button in the main window, the Menu dialog will be displayed, as shown below.



Setup
Configuration tasks

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Expired | (A) Administrator | 10/5/2022 4:11 PM

The menu options are divided into four categories: Setup, Report, Diagnostic and User, and are represented by the corresponding buttons. Clicking on a category button will activate the menu options for each given category.

The *Setup* button allows the user to perform various configuration tasks, including a measurement method setup, a new data library creation, or modification of an existing library.

The *Report* button allows the user to view and/or print sample identification or performance test results.

The *Diagnostic* button allows the user to run diagnostic tests.

The *User* button allows the user to perform various access control tasks (login, password changing, user accounts management). This button is available in the Pharma Edition only.

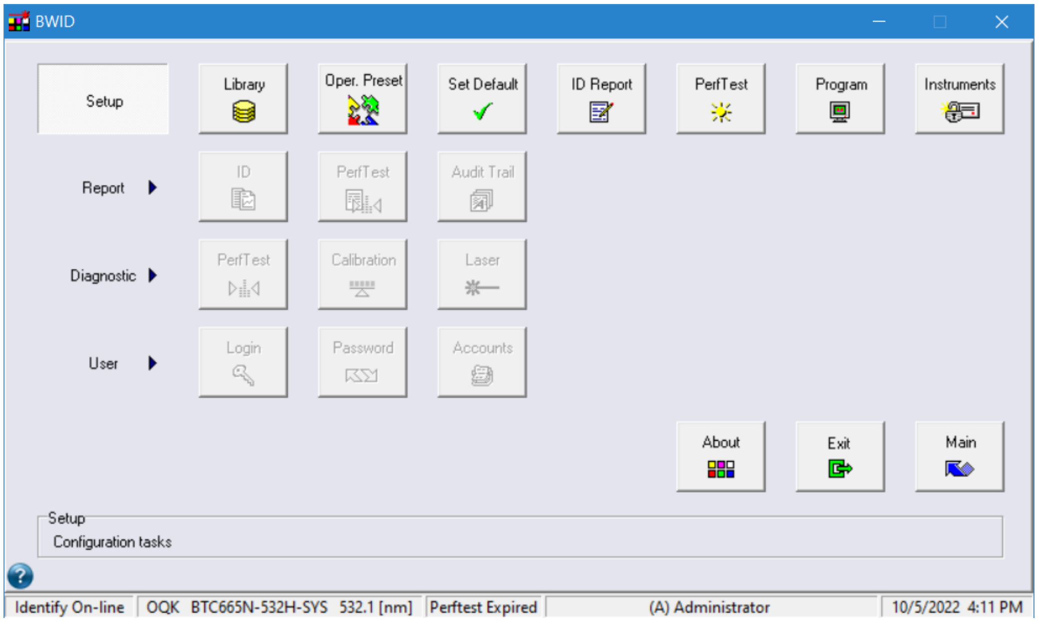
The *About* button displays information about the BWID® program.

The *Exit* button allows the user to close the program.

The *Main* button allows the user to close the Menu dialog and go back to the program main window.

Setup Menu

Upon clicking the *Setup* button in the Menu window, the Setup menu options will be enabled as follows:



Setup
Configuration tasks

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Expired | (A) Administrator | 10/5/2022 4:11 PM

The *Library* button allows the user to create a new data library or view/modify an existing one. It also allows the user to manage BWTek protected libraries licenses stored on the PC or provided on a BWID® dongle.

The *Oper. Preset* button allows the user to configure an operation preset.

The *Set Default* button allows the user to select an operation preset that will be used for sample identification.

The *ID Report* button allows the user to configure parameters for ID analysis report.

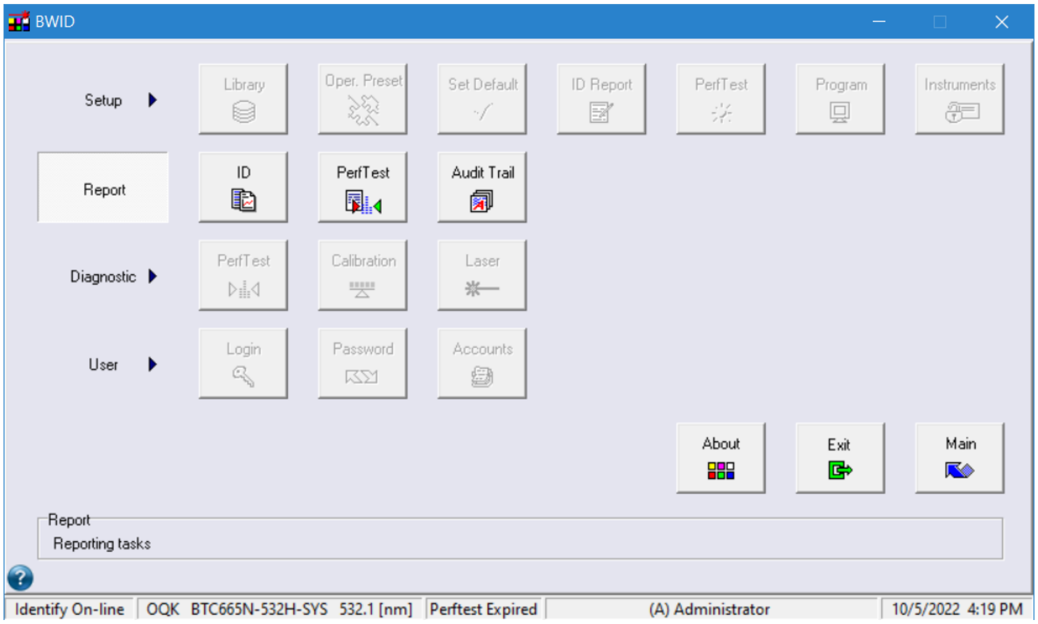
The *Perf Test* button allows the user to configure parameters for the instrument performance test.

The *Program* button allows the user to configure program general options, for example graphical user interface.

The *Instruments* button allows the user to enter the license information for up to five instruments.

Report Menu

Upon clicking the *Report* button in the Menu window, the Report menu options will be enabled as follows:



Report
Reporting tasks

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Expired | (A) Administrator | 10/5/2022 4:19 PM

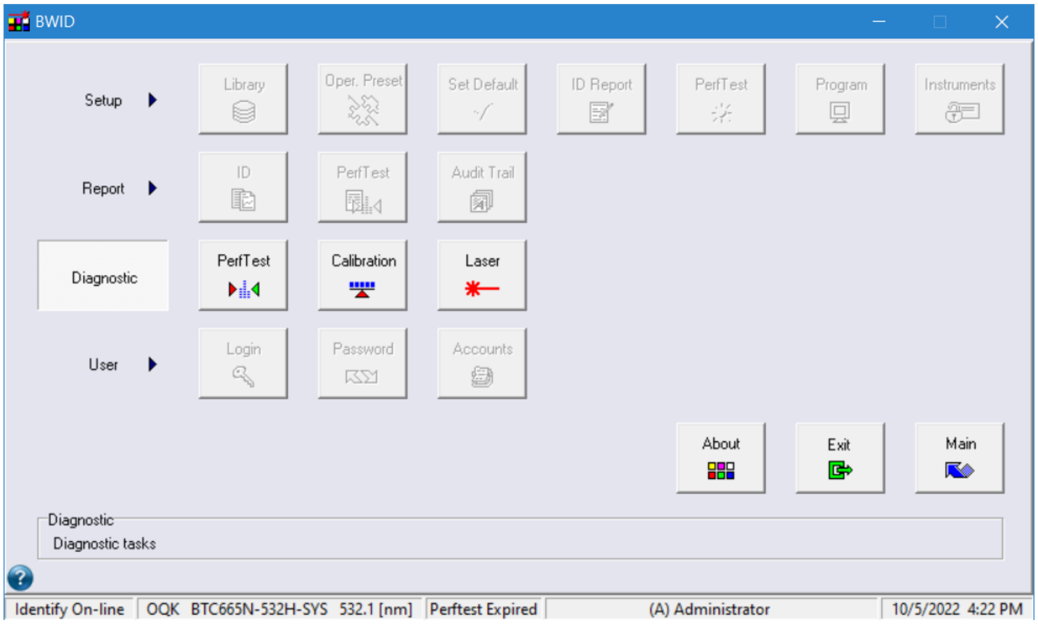
The *ID* button allows the user to view and print results from sample identification measurements.

The *Perf Test* button allows the user to view and print results from a performance test.

The *Audit Trail* button allows the user to view the audit trail of all activities within the program. This button is available in the Pharma Edition only.

Diagnostic Menu

Upon clicking the *Diagnostic* button in the Menu window, the Diagnostic menu options will be enabled as follows:



Diagnostic
Diagnostic tasks

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Expired | (A) Administrator | 10/5/2022 4:22 PM

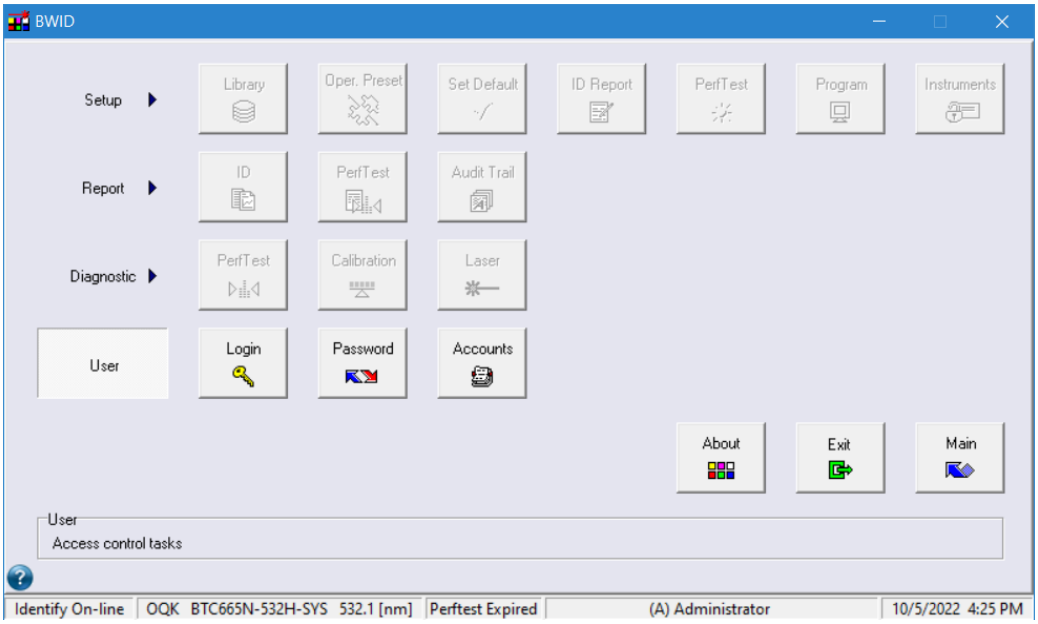
The *Perf Test* button allows the user to start a performance test of the instrument.

The *Calibration* button allows the user to start instrument calibration.

The *Laser* button allows the user to turn the laser ON and OFF.

User Menu

Upon clicking the *User* button in the Menu window, the User menu options will be enabled as follows:



User
Access control tasks

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Expired | (A) Administrator | 10/5/2022 4:25 PM

The *Login* button allows the user to re-login to the program with a different account name without having to close the program and start it again.

The *Password* button allows the user to change his (or her) own password.

The *Accounts* button enables the *Administrator* user to view and modify existing user accounts as well as add new user accounts.

6. Operation Preset Configuration

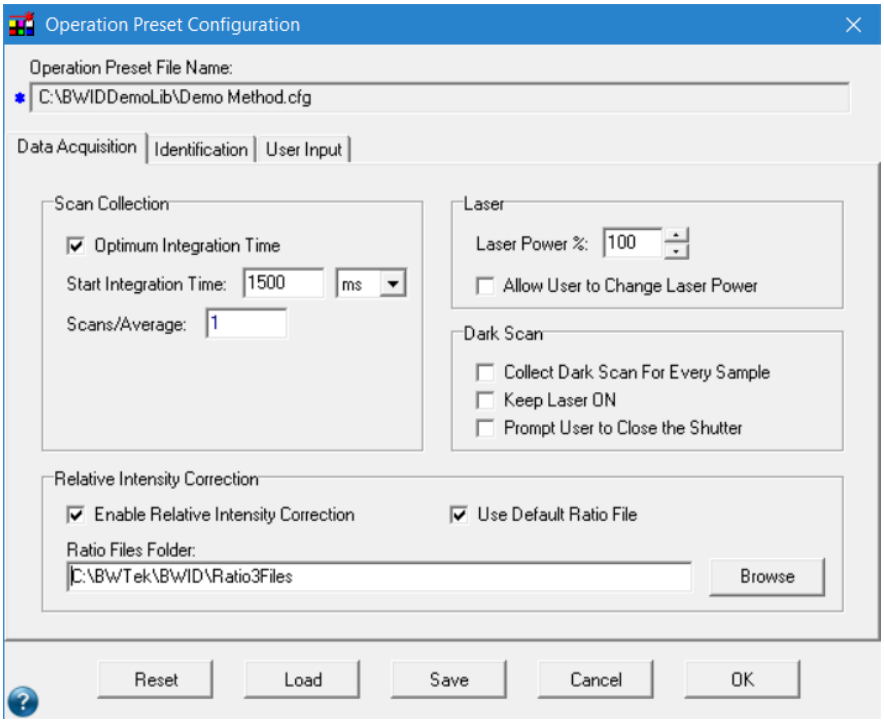
Starting Operation Preset Configuration

In order to identify a sample or generate a new data library, an operation preset (later referred to as a preset) must be configured.

To start a preset configuration, click the *Setup* button in the Menu window and then the *Oper.Preset* button in the Setup menu.
The Operation Preset Configuration dialog will appear as shown below. It will hold current preset parameters.

Current preset is an operation preset, which parameters have been currently loaded into the program, and is selected as follows:

- default preset for sample identification at the program startup and also each time a sample identification is performed
- a preset accepted by the user by clicking the *OK* button in the Operation Preset Configuration dialog, if the recently performed task was the preset setup.


Operation Preset Configuration

Operation Preset File Name:
* C:\BWIDDemoLib\Demo Method.cfg

Scan Collection
☑ Optimum Integration Time
Start Integration Time: 1500 ms
Scans/Average: 1

Laser
Laser Power %: 100
☐ Allow User to Change Laser Power

Dark Scan
☐ Collect Dark Scan For Every Sample
☐ Keep Laser ON
☐ Prompt User to Close the Shutter

Relative Intensity Correction
☑ Enable Relative Intensity Correction
☑ Use Default Ratio File
Ratio Files Folder:
C:\BWTek\BWID\Ratio3Files

If the current preset is stored in a file, the preset file name is displayed in the *Operation Preset File Name* field. Otherwise, the field is empty.
If the current preset is the default preset for sample identification, the blue asterisk character (*) will be displayed to the left of the preset file name.

The preset parameters are grouped into three categories: *Data Acquisition, Identification and User Input*, with tabs assigned accordingly.

Click the *Reset* button to reset the preset parameters to default settings.

Click the *Load* button to load preset settings from an operation preset file (*.cfg).

Click the *Save* button to save preset settings in an operation preset file. The preset is stored in a binary format file with default file extension “.cfg”.

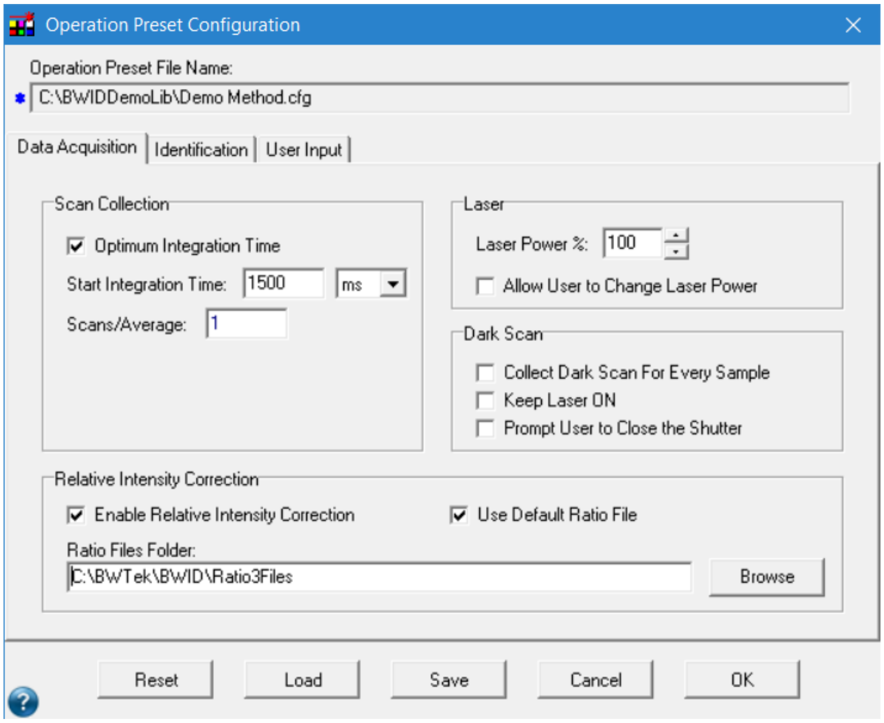
Note: When configuring a preset for sample identification, the preset has to be saved in a file and then set as a default preset (see Setting Default Operation Preset for Sample Identification below).

Click the *OK* button to accept settings as the current preset, close the dialog and return to the Menu window.

Click the *Cancel* button to cancel the preset configuration, close the dialog and return to the Menu window.

Data Acquisition Parameters

The *Data Acquisition* tab holds parameters related to the data collection from an instrument.



Operation Preset Configuration

Operation Preset File Name: C:\BWIDDemoLib\Demo Method.cfg

Data Acquisition | Identification | User Input

Scan Collection
☑ Optimum Integration Time
Start Integration Time: 1500 ms
Scans/Average: 1

Laser
Laser Power %: 100
☐ Allow User to Change Laser Power

Dark Scan
☐ Collect Dark Scan For Every Sample
☐ Keep Laser ON
☐ Prompt User to Close the Shutter

Relative Intensity Correction
☑ Enable Relative Intensity Correction
☑ Use Default Ratio File
Ratio Files Folder: C:\BWTek\BWID\Ratio3Files

Optimum Integration Time - check this box if the program should automatically determine an integration time at which an optimum Raman signal can be collected for each sample. Uncheck the box if a fixed integration time should be used for data

collection.
Select appropriate time units for integration time – ms for milliseconds or us for microseconds.

Start Integration Time (available if *Optimum Integration Time* box is checked) – set the initial value of the integration time for automatic detection of the optimum integration time. The program will use this value for every first scan of a sample and then increase the value accordingly to get enough information to determine optimum integration time.

Integration Time (available if *Optimum Integration Time* box is unchecked) – set a fixed integration time that will be used to collect scans.

Scans/Average – set number of scans per average.

Laser Power – set the laser power (percentage) that will be used for laser excitation. This option is enabled for a Raman system with adjustable laser power only.

Allow User to Change Laser Power – check this box if the user should be able to change the laser power prior to data collection.

Collect Dark Scan For Every Sample – check this box if the dark scan should be taken for each scanned sample. If the box is unchecked, the dark scan will be taken only if there is no dark scan collected for a given integration time.

Keep Laser ON – check this box if the laser should be kept ON at all times, including during dark scan collection. If the box is unchecked, the laser will be turned OFF each time the dark scan is being collected or a sample scanning is done.
If the box is checked, the *Prompt User to Close the Shutter* box should be also checked in order to collect a correct dark scan.

Prompt User to Close the Shutter – check this box if the user should be reminded to close the shutter before a dark scan collection.

Enable Relative Intensity Correction - check this box if a relative intensity correction should be performed on a collected sample scan. Relative intensity correction corrects the intensity response of a spectrometer thus allows the user to acquire instrument independent spectra. A ratio file is required for relative intensity correction, and it is provided on a USB stick for each B&W Tek Raman instrument. The file name is Ratio3_XXX.txt, Ratio3_XXX_L.txt, or Ratio3_XXX_yyyyyyyyy.txt, where XXX is the c-code of the instrument, and yyyyyyyyy is the serial number of a probe. The ratio file reflects the optical property of the system, which include the spectrometer and the probe. If multiple probes are used on the same instrument, each probe should have its own ratio file.

NOTE: *Relative Intensity Correction* must be enabled to acquire library spectra or spectra for ID.

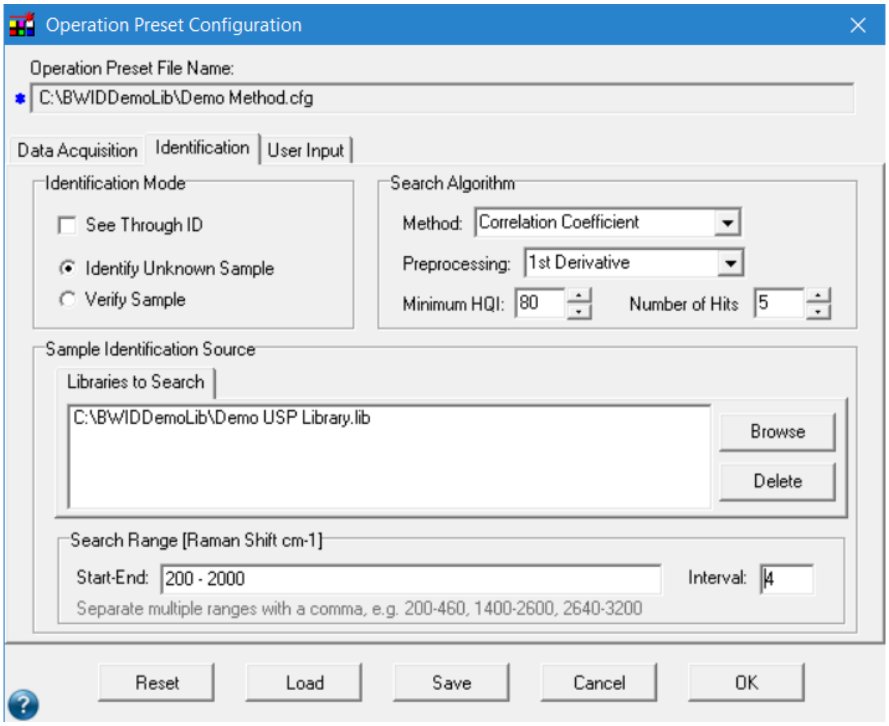
Use Default Ratio File –If this box is checked, the program will look for a ratio file that matches the c-code of the connected instrument, under the *Ratio Files Folder*. This only works if the file name is in the format of Ratio3_XXX.txt or Ratio3_XXX_L.txt. To be certain which ratio file is being used, it recommended to leave this box unchecked.

Ratio Files Folder – if *Use Default Ratio File* is checked, use *Browse* to select a folder where the ratio file for relative intensity correction is located; otherwise, use *Browse* to select the ratio file itself. It is recommended the ratio files be placed in the BWID program folder.

Identification Parameters

The *Identification* tab holds parameters related to sample identification.

If the preset being configured will be used for a data library creation/modification, the Identification parameters are irrelevant and they do not need to be set.



Operation Preset File Name: C:\BWIDDemoLib\Demo Method.cfg

☐ See Through ID
● Identify Unknown Sample
○ Verify Sample

Method: Correlation Coefficient
Preprocessing: 1st Derivative
Minimum HQI: 80
Number of Hits: 5

C:\BWIDDemoLib\Demo USP Library.lib

Start-End: 200 - 2000
Interval: 4
Separate multiple ranges with a comma, e.g. 200-460, 1400-2600, 2640-3200

See Through ID – check this box if you want to run see through ID measurements (STID) using an ST probe with an STRam instrument. Uncheck the box if you want to run conventional ID measurements with a Raman instrument.

Identify Unknown Sample – select this radio button if you want to identify an unknown sample against data in the search libraries (selected in the *Libraries to Search*).

Verify Sample – select this radio button if you want to verify the identity of a known sample against data in the search libraries (selected in the *Libraries to Search*).

The first difference between these two identification modes is that the user will have to enter/select a sample name at the beginning of the identification process in *Verify Sample* mode. The other difference is that the *Verify Sample* analysis will return a *Pass*/*Fail* result, while the *Identify Unknown Sample* analysis will return a *Match*/*No Match* result.

Conventional ID parameters (*See Through ID* box unchecked):

Method – select a search algorithm that will be used to compare a collected spectrum of the measured sample against the spectral data in the libraries and to generate a hit quality index (HQI) as a result of the data comparison.
There are seven available methods for computing the HQI: scalar product algorithm, derivative algorithm, squared derivative algorithm, difference algorithm, squared difference algorithm, correlation coefficient algorithm and derivative correlation coefficient algorithm. The default setting is the correlation coefficient algorithm.
See Appendix A – Spectrum Search Algorithms for details.

Preprocessing – select preprocessing that will be applied to spectral data.
The following four preprocessing options are available: none (if no processing should be applied), Savitzky-Golay smoothing, Savitzky-Golay first derivative and Savitzky-Golay second derivative. The default setting is Savitzky-Golay first derivative.

Minimum HQI – set minimum Hit Quality Index to define an outlier threshold.
A sample below the minimum HQI will be treated as an outlier. The default value is 80.
Hit quality index is a numeric rank obtained as the result of a spectral library search. Spectral library search results are ranked from an HQI of 100 (best match) to an HQI of 0 (worst match).

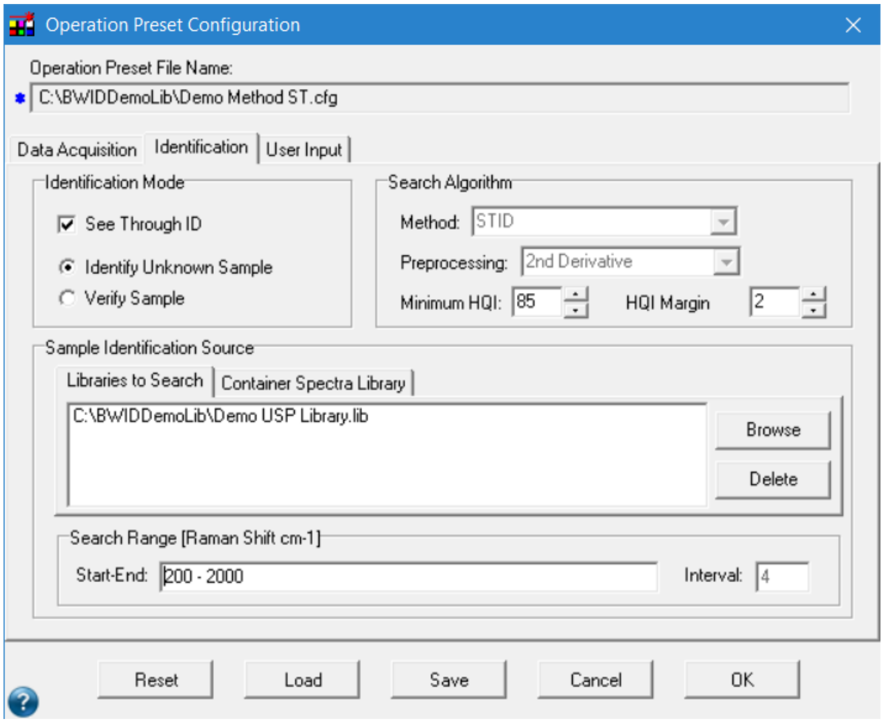
Number of Hits – set number of hit results returned to the user. The default value is 5.

Libraries to Search – select data libraries (*.lib files) that will be used in sample identification.
Click the *Browse* button to browse for a library file and add it to the list. At least one library must be specified. The user can select up to ten compatible user-defined and/or BWTek/ST Japan licensed libraries.

Click the *Delete* button to delete a selected library from the list.

Search Range (Start-End, Interval) – set a search range to limit library search to particular spectral region(s). The specified range should be within data range of libraries selected in the *Libraries to Search* list and can consist of one consecutive range or multiple ranges separated with a comma. The default range is 200 -2000 with a 4 cm^{-1} resolution.

See Through ID parameters (*See Through ID* box checked):



Operation Preset Configuration

Operation Preset File Name: C:\BWIDDemoLib\Demo Method ST.cfg

Identification Mode
☑ See Through ID
● Identify Unknown Sample
○ Verify Sample

Search Algorithm
Method: STID
Preprocessing: 2nd Derivative
Minimum HQI: 85
HQI Margin 2

Sample Identification Source
Libraries to Search: C:\BWIDDemoLib\Demo USP Library.lib

Search Range [Raman Shift cm-1]
Start-End: 200 - 2000
Interval: 4

Method – a STID search algorithm is used to compare a collected spectrum of the measured sample against the spectral data in the libraries and to generate a hit quality index (HQI) as a result of the data comparison. The method selection is disabled for see through ID measurements.

Preprocessing – a Savitzky-Golay second derivative preprocessing will be applied to spectral data. The preprocessing selection is disabled for See Through ID measurements.

Minimum HQI – set minimum Hit Quality Index to define an outlier threshold.
A sample below the minimum HQI will be treated as an outlier. The default value is 85. You may increase this value for a more discriminating analysis, but it is recommended to not set this value above 95 or below 85.

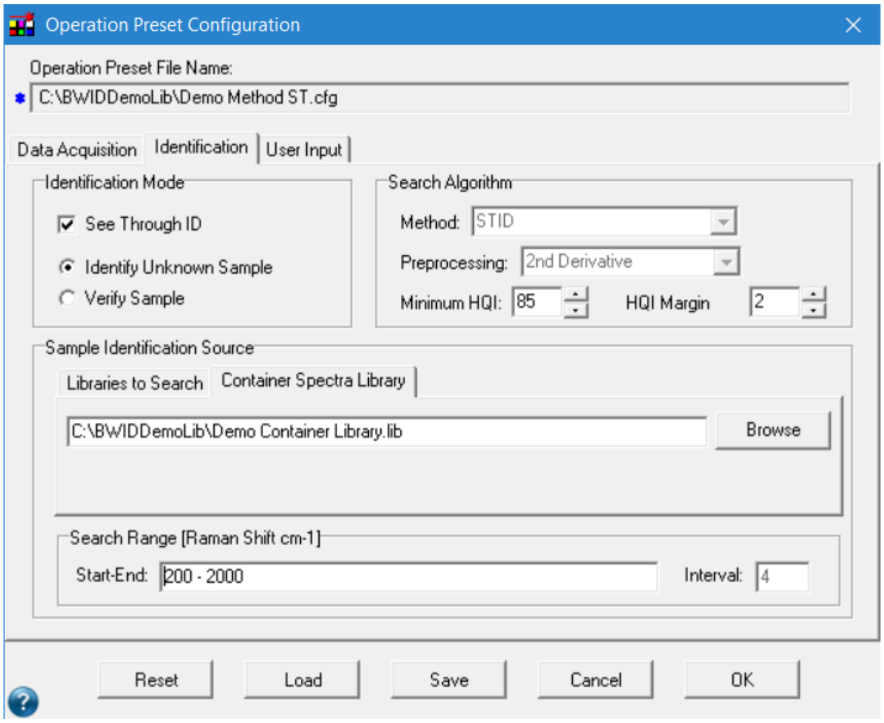
Hit quality index is a numeric rank obtained as the result of a spectral library search. Spectral library search results are ranked from an HQI of 100 (best match) to an HQI of 0 (worst match).

HQI Margin – set Hit Quality Index margin to define an outlier threshold margin. The default value is 2. It is not recommended to change this value.
The M*inimum HQI* and *HQI Margin* will be used together to determine the outliers for see through ID measurements.

Libraries to Search – lists data libraries (*.lib files) that will be used in sample identification.
Click the *Browse* button to browse for a library file and add it to the list. At least one library must be specified. The user can select up to ten compatible user-defined and/or BWTek/ST Japan licensed libraries. All selected libraries must have the same resolution.

Search Range (Start, End, Interval) – set a search range to limit library search to a particular spectral region. The specified range should be consecutive and within data range of libraries selected in the *Libraries to Search* list. The default range is 200 - 2000 cm^{-1}. The search interval (*Interval*) with be automatically set with the resolution of the first library in the *Libraries to Search* list. The default interval is 4 cm^{-1}.

Container Spectra Library – a container library is required for the See Through ID option. Click the tab to switch to the container spectra library selection (shown below). Select a library with container spectral data (*.lib file) that will be used in sample identification. The container library must have the same resolution as the libraries selected in the *Libraries to Search* list.



Operation Preset File Name: C:\BWIDDemoLib\Demo Method ST.cfg

☑ See Through ID

● Identify Unknown Sample

○ Verify Sample

Method: STID

Preprocessing: 2nd Derivative

Minimum HQI: 85

HQI Margin: 2

C:\BWIDDemoLib\Demo Container Library.lib

Start-End: 200 - 2000

Interval: 4

Click the *Browse* button to browse for a library file. Only one library can be specified. The library range must be compatible with selected search libraries and has to contain spectra with a 4 cm^{-1} resolution.

A default library (ContainerSpectra.lib) is provided with the BWID® (ver. 2.02.10 and higher) installation package, but due to the variability of packaging materials (LDPE, HDPE, PVC, different levels of fillers, and container thicknesses) it is recommended that the user collects and adds the spectra of containers (to be used with measured samples) to the library to get the most accurate results. The container spectra should only have signatures of the container. On STRam, container spectra can be acquired on an empty container (or an area on the container surface that has no content material underneath) using the ST probe. If this is not available, an alternative is to focus the beam on the container surface using the Focus Adaptor and Surface Regulator attached as shown in Figure 1 below.

The container spectra library may be edited in the Library option (Setup menu). Container spectra can also be added when a new container spectrum is collected during the ID steps and a match result is returned.

Figure 1: Focus Adaptor + Surface Regulator to Measure Package Material

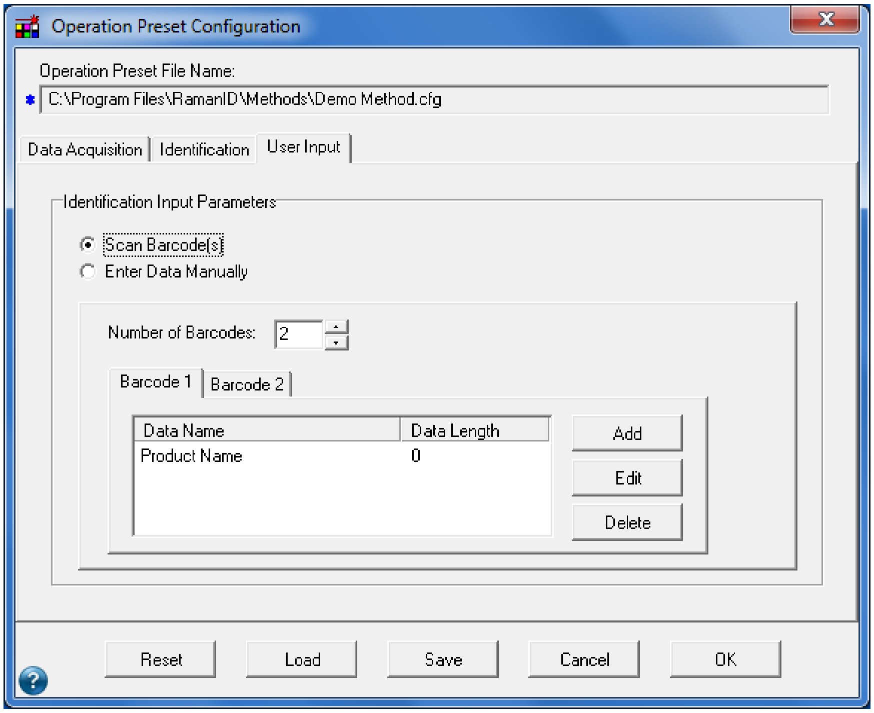
Recommended settings are:

- HQI: 85
- HQI Margin: 2
- Libraries to search: DEFINE YOUR LIBRARY
- Container spectra library: Demo Container Library.lib
- Search Range: 200-2000

User Input Parameters

The *User Input* tab holds parameters related to the user input for ID analysis.

If the preset being configured will be used for a data library creation or modification, the User Input parameters are irrelevant and they do not need to be set.


Operation Preset Configuration

Operation Preset File Name: C:\Program Files\RamanID\Methods\Demo Method.cfg

Identification Input Parameters

● Scan Barcode(s)
○ Enter Data Manually

Number of Barcodes: 2

Data Name	Data Length
Product Name	0

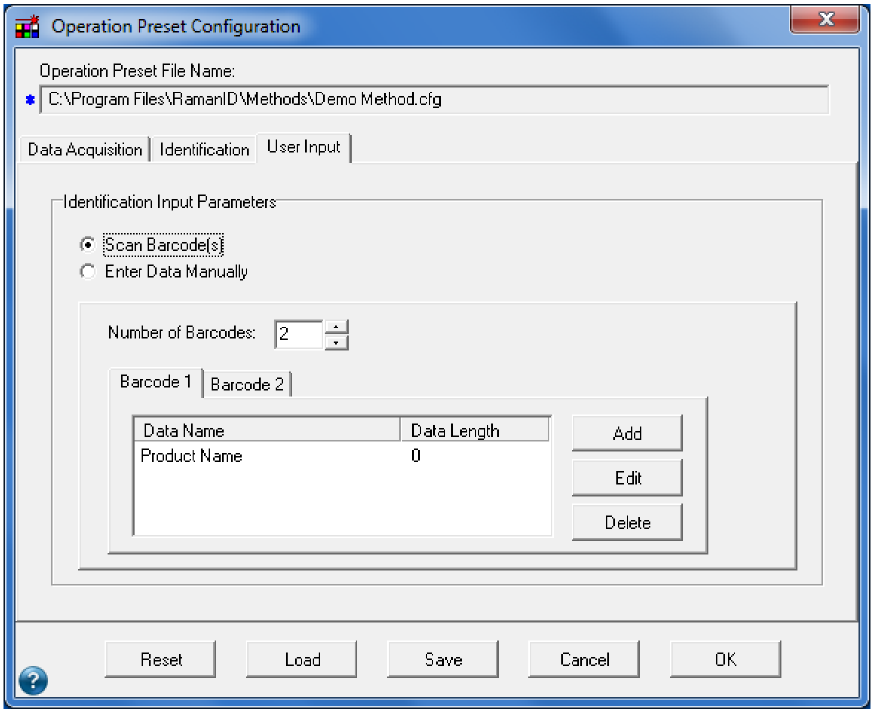
The user can input ID analysis parameters either using a barcode scanner or entering the data manually. All selected input parameters will be mandatory and will have to be provided by the user at the beginning of the ID analysis.

Scan Barcode(s) – select this radio button if the user should use a barcode scanner to enter ID analysis parameters at the beginning of a measurement.

Enter Data Manually – select this radio button if the user should use a keyboard to enter ID analysis parameters at the beginning of a measurement.

Barcode Input Mode

In the barcode mode (*Scan Barcode(s)* is checked) up to three barcodes can be used to scan input parameters. Each barcode can consist of a single data (e.g. product name) or multi data (e.g. a batch number followed by a lot number).



Operation Preset File Name: C:\Program Files\RamanID\Methods\Demo Method.cfg

Identification Input Parameters

● Scan Barcode(s)

○ Enter Data Manually

Number of Barcodes: 2

Data Name	Data Length
Product Name	0

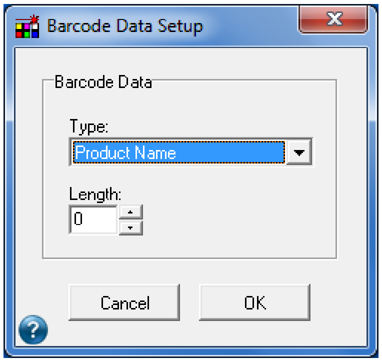
Number of Barcodes - set number of barcodes that the user should scan to collect complete input data.

Click the *Add* button to define new data for a given barcode.

Click the *Edit* button to modify selected barcode data for a given barcode.

Click the *Delete* button to delete selected barcode data for a given barcode.

Upon clicking the *Add* or *Edit* button, the Barcode Data Setup dialog will pop up as shown below.



Barcode Data

Type: Product Name

Length: 0

Type – select the barcode data type. The following data types are available: product name, product number, batch number, lot number, container number, supplier number.

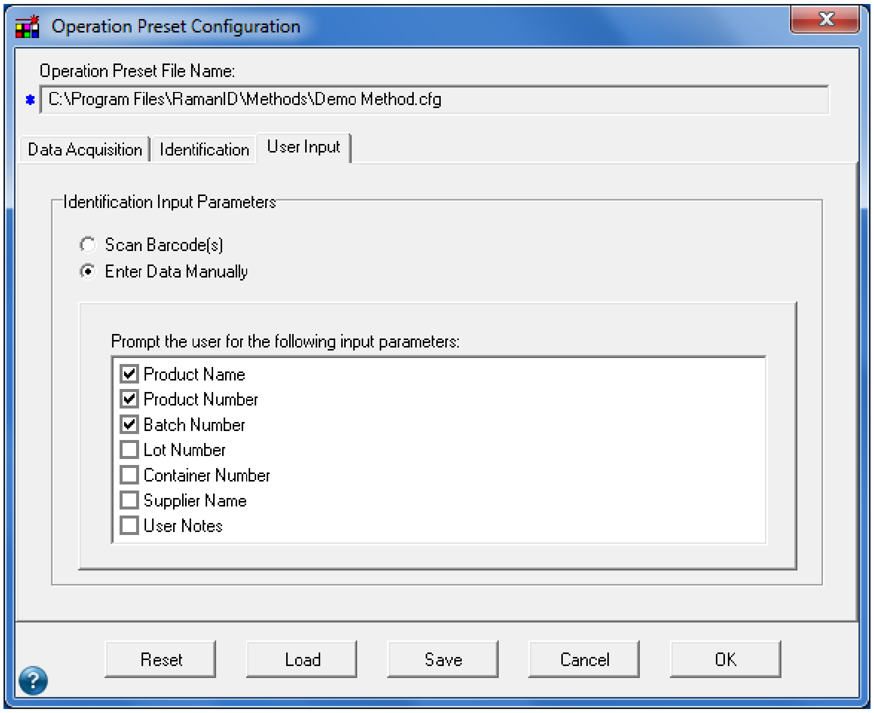
Length – set the barcode data length (number of characters representing the data in the barcode). For a single data barcode, the data length is optional (set to 0). For a multi data barcode, the data length for each data component is mandatory (e.g. 4 characters for a batch number followed by 6 characters for a lot number).

Click *OK* to accept the barcode data settings and close the dialog.

Click *Cancel* to abort the setup.

Manual Input Mode

In the manual mode (*Enter Data Manually* is checked) the following parameters can be selected for the user input, as shown below.



Operation Preset Configuration

Operation Preset File Name: C:\Program Files\RamanID\Methods\Demo Method.cfg

Identification Input Parameters

○ Scan Barcode(s)
● Enter Data Manually

Prompt the user for the following input parameters:

☑ Product Name
☑ Product Number
☑ Batch Number
☐ Lot Number
☐ Container Number
☐ Supplier Name
☐ User Notes

Product Name – check this box if the user should enter a product name for a sample that is about to be measured. This parameter is mandatory for the *Verify* mode.

Product Number – select this box if the user should enter a product number for a sample that is about to be measured.

Batch Number – select this box if the user should enter a batch number for a sample that is about to be measured.

Lot Number – select this box if the user should enter a lot number for a sample that is about to be measured.

Container Number – select this box if the user should enter a container number for a sample that is about to be measured.

Supplier Name – select this box if the user should enter a supplier (manufacturer) name for a sample that is about to be measured.

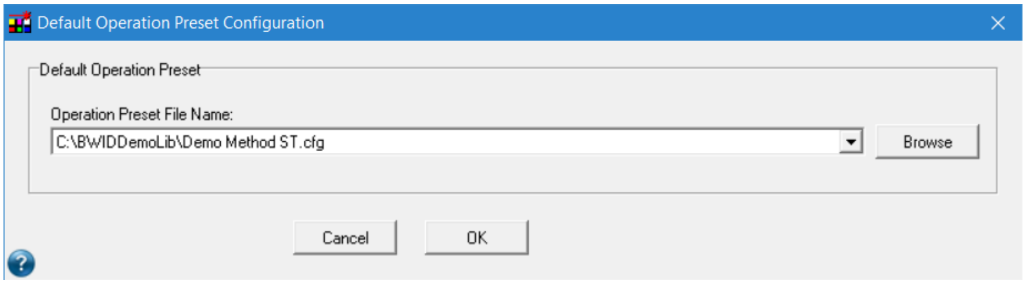
User Notes – select this box if the user should enter notes for a sample that is about to be measured.

7. Setting Default Operation Preset for Sample Identification

In order to have the ability to run sample identification, a default operation preset has to be selected.

Click the *Setup* button in the Menu window and then the *Set Default* button in the Setup menu.

The Default Operation Preset Configuration dialog will be displayed as shown below.



Operation Preset File Name: C:\BWIDDemoLib\Demo Method ST.cfg

Click the *Browse* button to browse for a preset file (*cfg).

The drop-down list contains all operation presets from a predefined operation presets folder (see *Data Storage Configuration* and *Default Data Storage* in *Program Configuration* paragraph) as well as currently selected default operation preset if saved somewhere else. This allows the user to quickly select a preset from the operation presets folder.

For operator user (Pharma edition only), a Browse button is disabled, so the user can select only from the drop-down list.
For developer and higher privilege user (Pharma edition only) as well as in Standard edition, the Browse button is enabled, so the user can select the preset from any location. If newly selected preset is from other location (i.e. not from predefined operation presets folder) then the preset is added to the drop-down list.
If the user selects a new preset and previous default preset was not from the predefined operation presets folder, then the previous default preset is removed from the drop-down list.

Once the preset file has been selected, click *OK* to accept the settings and close the dialog. The selected preset file will be used for sample identification.

Click the *Cancel* button to cancel default preset selection and close the dialog.

8. Data Library

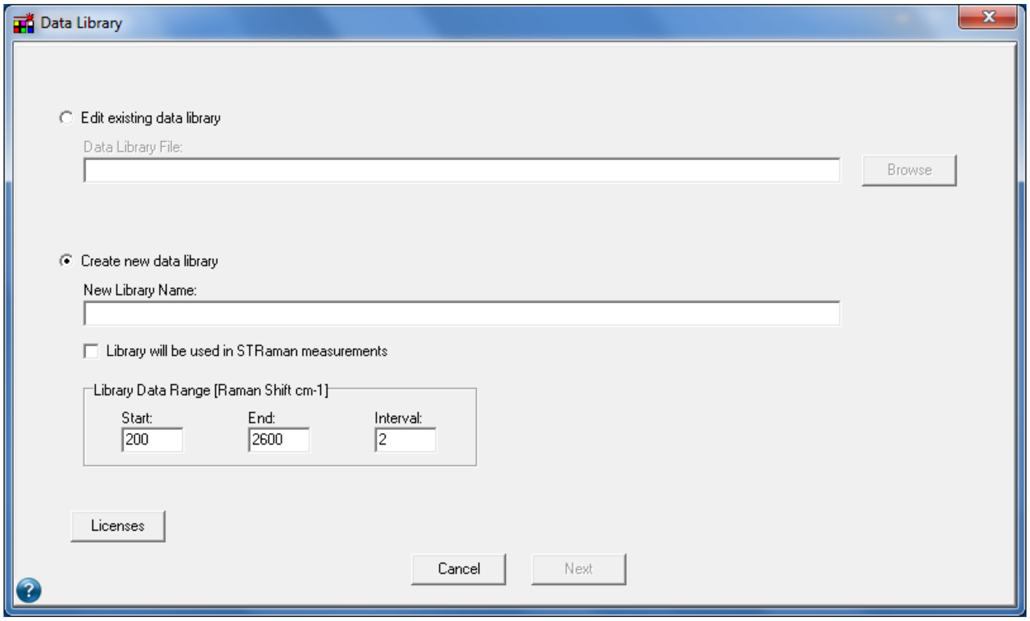
The program allows the user to create a new data library and modify an existing user-defined library. It also allows the user to view a library, including a licensed library (BWTek library or ST Japan library saved in the BWID® format).
Additionally, it allows the user to view and update a library license (stored on the PC or on a BWID® dongle) provided for a BWTek protected library.

A single library consists of six files, all with the same name, but different extensions: ".lib", ".ifm", ".ist", ".stm", ".pik" and ".sdp", where the ".lib" file is the main file of the library. The file with ".sdp" extension is optional and may not be present for the libraries created with a BWID® ver. 2.02.05 or older but it will be created automatically if needed.

Library Selection

To create a new data library or view and modify an existing one, click the *Setup* button in the Menu window and then the *Library* button in the Setup menu.

The Data Library dialog will appear as shown below.



○ Edit existing data library
Data Library File:

● Create new data library
New Library Name:

☐ Library will be used in STRaman measurements

Library Data Range [Raman Shift cm-1]
Start: 200
End: 2600
Interval: 2

To view or modify an existing library, click the *Edit existing data library* button and then specify the library file name in the *Data Library File* field. Click *Browse* to browse for a library file (*.lib).

To create a new data library, click the *Create new data library* button and then enter the library name (description) in the *New Library Name* field.
Next, you may check the *Library will be used in STRaman measurements* box. Checking the box, will set a default library range from 172 to 2600 with 4 cm^{-1} resolution for see through ID measurements. Unchecking the box, will set default library range from 200 to 2600 with 2 cm^{-1} resolution for conventional ID measurements.
Finally, set the *Start*, *End* and *Interval* fields with the desired Raman Shift data range for the library.

To view or update a BWTek library license click the *Licenses* button.

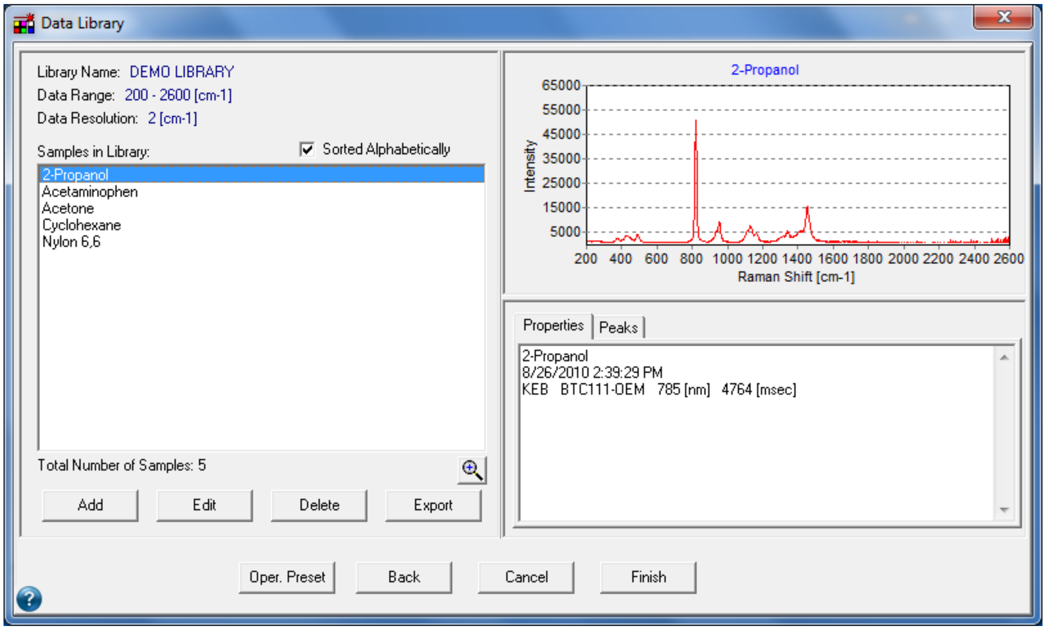
Click *Next* to proceed with the next step. The *Next* button becomes available when all required parameters are provided: library file name for an existing library selection or library name and data range for a new library creation.

Click the *Cancel* button to cancel library generation, modification or viewing and return to the Menu window.

Note: The library generation is based on the current operation preset settings (see Operation Preset Configuration paragraph).

Library Contents

Upon clicking the *Next* button in the library selection dialog, the dialog with library contents will be displayed as shown below.



Library Name: DEMO LIBRARY
Data Range: 200 - 2600 [cm-1]
Data Resolution: 2 [cm-1]

Samples in Library: ☑ Sorted Alphabetically

- 2-Propanol
- Acetaminophen
- Acetone
- Cyclohexane
- Nylon 6,6

Total Number of Samples: 5

2-Propanol
8/26/2010 2:39:29 PM
KEB BTC111-OEM 785 [nm] 4764 [msec]

The graph in the right pane displays a spectrum of a sample selected from the list in the left pane. Double clicking on the graph will maximize the dialog. Double clicking on the graph in the maximized dialog will restore the original dialog size.
The properties panel shows all parameters of the selected sample.
The peaks panel lists up to 7 highest peaks in the spectrum, starting from highest one.
Click on the *Peaks* tab to switch to peaks panel, click on the *Properties* tab to switch back to the properties panel.

To add a new sample to the library, click the *Add* button.

To modify properties of a library sample, select the sample from the list and then click the *Edit* button.

To delete a sample from the library, select the sample from the list and then click the *Delete* button. The option to delete the sample is disabled if there is only one sample in the library.

To export samples from the library, select the samples you wish to export and then click the *Export* button.

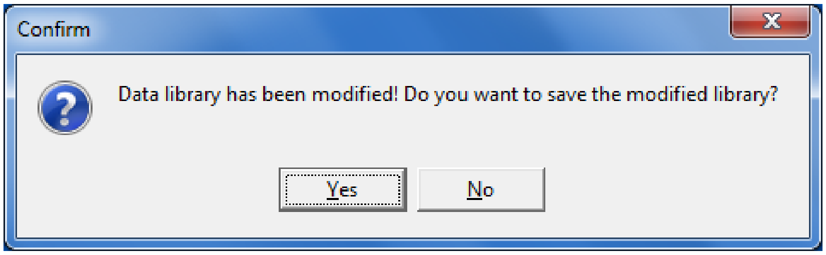
To search for a sample in the library, click the *Search* button with a magnifying glass icon. The button is only available when the library contains more than one sample.

Please note that for a licensed library (protected BWTek or ST Japan library), the *Add*, *Edit*, *Delete*, *Export* and *Finish* buttons will be disabled. If the license for a protected library is provided on a dongle, the dongle has to be present on the PC all the time while viewing the library. If the license for the protected library is provided for a given PC, the license has to be added to the PC only once (see BWID® Library Licenses paragraph).

To view or change spectral data acquisition parameters for the library modifications, click the *Oper. Preset* button.

To finish library generation and save library data in a file, click the *Finish* button. The *Finish* button becomes available upon the library modification (by adding a new sample, editing or deleting the existing sample).

To quit library creation or viewing, click the *Cancel* button. In case modifications were made to the library, the confirmation message will be displayed as follows:



Data library has been modified! Do you want to save the modified library?

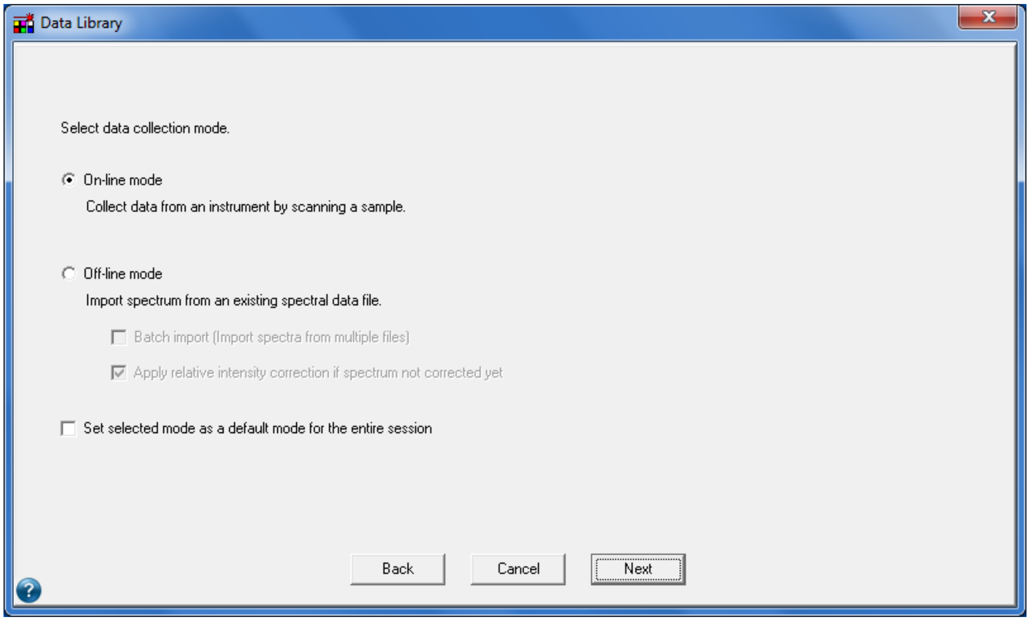
Click *Yes* to save the library.
Click *No* to abort changes to the library.

To select another library, click the *Back* button.

Adding a New Sample

The program will guide the user step by step through the process of adding a new sample to the library. The user can cancel the library modification at any time by clicking the *Cancel* button.

Upon clicking the *Add* button, the following dialog will appear:



Select data collection mode.

● On-line mode
Collect data from an instrument by scanning a sample.

○ Off-line mode
Import spectrum from an existing spectral data file.

☐ Batch import (Import spectra from multiple files)

☑ Apply relative intensity correction if spectrum not corrected yet

☐ Set selected mode as a default mode for the entire session

On-line mode – select this button to acquire a spectrum from an instrument.

Off-line mode – select this button to import a spectrum from a file.

Batch import (import spectra from multiple files) – select this button to import spectral data in a batch.

Apply relative intensity correction if spectrum not corrected yet – select this button to apply relative intensity correction to imported spectrum, if it has not been already corrected. This option is available only for the spectrum imported from a BWSpec Spectrum Text file (*.txt). The setting will be ignored if the spectrum is imported from files of other format: Grams SPC file (*.spc) or Spectrum Text file (*.txt).

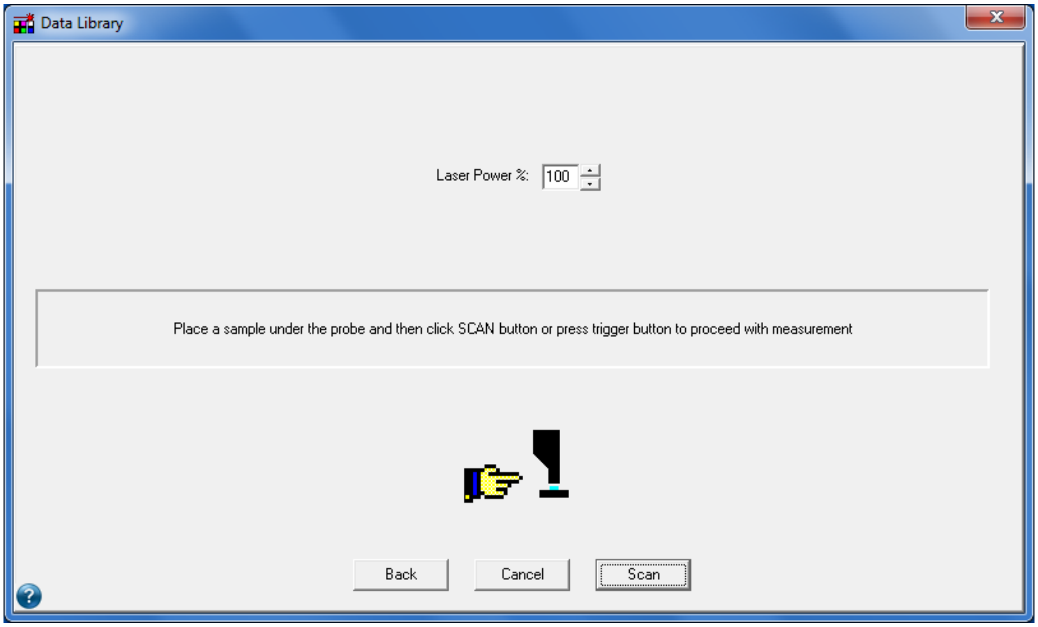
Set selected mode as a default mode for the entire session – check this box to skip the Data Collection Mode dialog the next time the *Add* button is clicked for the entire session, (i.e. until closing the Data Library dialog, or selecting another library).

Upon clicking the *Next* button while the *On-line mode* box is checked, the Data Library dialog will appear as in the next section.

Upon clicking the *Next* button while the *Off-line mode* box is checked, the Spectral Data File Selection dialog will appear (see Off-line Data Import paragraph below).

On-line Data Collection

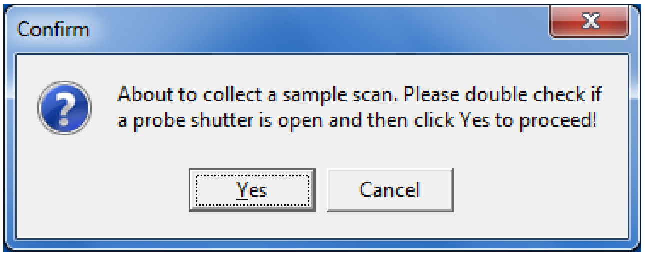
For the on-line data collection mode, the following dialog will appear as shown below.



Place a sample under the probe and then click SCAN button or press trigger button to proceed with measurement

Once a sample is in place for a measurement, click the *Scan* button to collect spectrum from the sample.

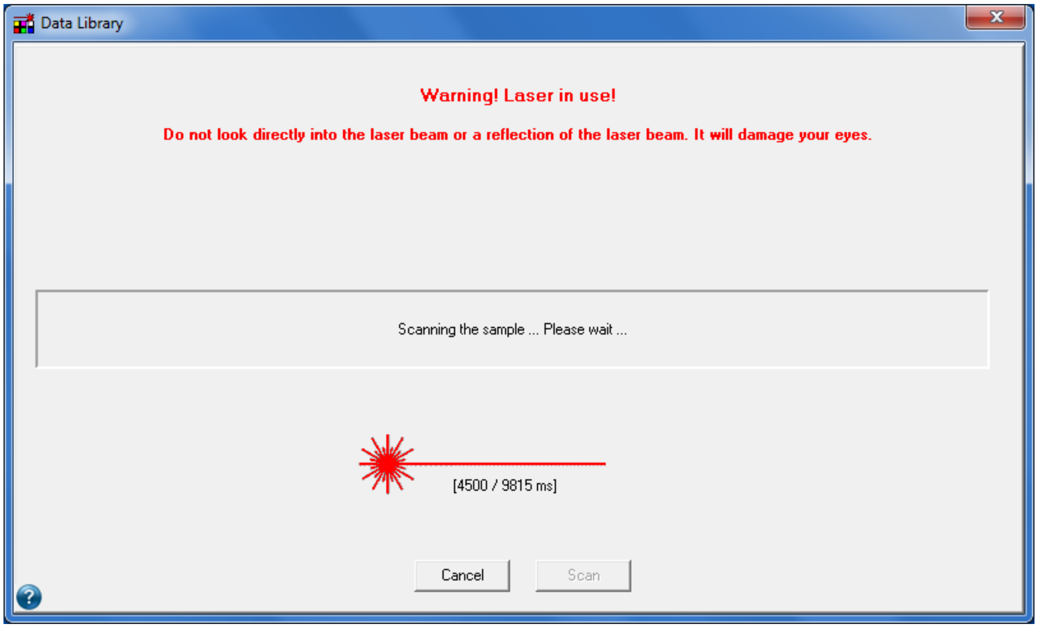
First, a raw spectrum of the sample will be collected.
If the user should be reminded to open/close the shutter before a scan collection, a reminder message to open the shutter will pop up first.



About to collect a sample scan. Please double check if a probe shutter is open and then click Yes to proceed!

Click *Yes* when ready to collect data.
Clicking the *Cancel* button will abort adding the new sample to the library. In this case, the program will return to the library contents dialog.

Upon clicking *Yes*, the next dialog will appear.



Warning! Laser in use!

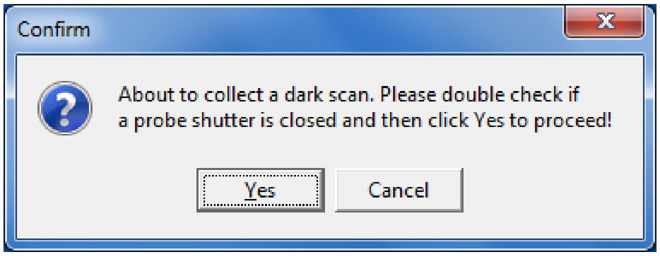
Do not look directly into the laser beam or a reflection of the laser beam. It will damage your eyes.

Scanning the sample ... Please wait ...

[4500 / 9815 ms]

At this time the sample is being scanned once or more depending on the *Optimum Integration Time* selection in the current operation preset.
If the *Optimum Integration Time* is enabled, the program will scan the sample several times (at least 2 but no more than 5 times) with different integration times to determine the optimum integration time for the best Raman shift signal.
If the *Optimum Integration Time* is disabled, the program will use the fixed integration time to collect a sample scan.

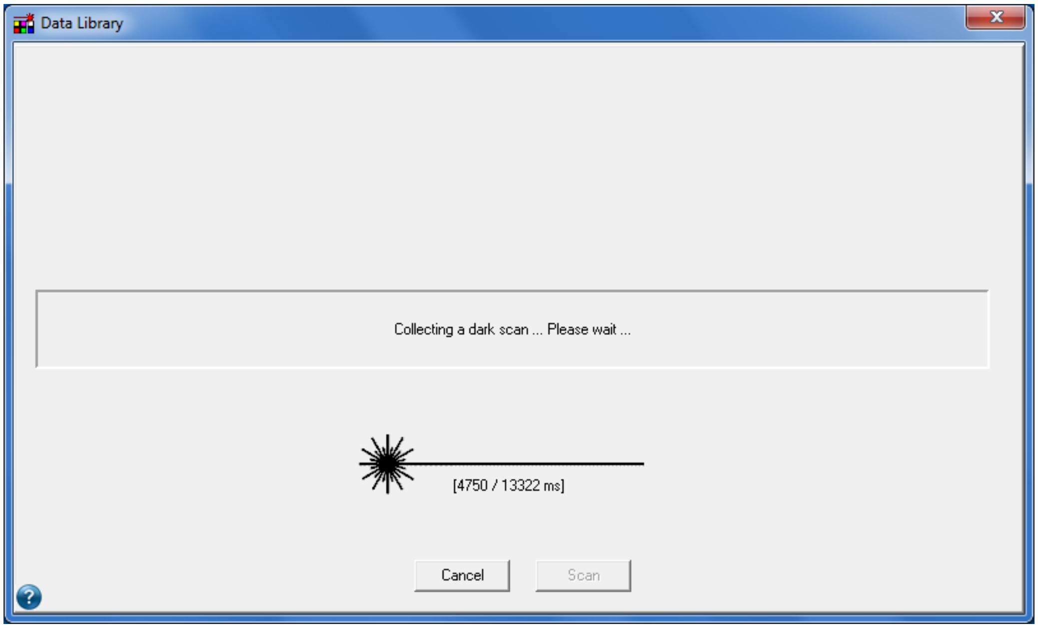
Next, a dark scan will be acquired (if not collected yet for that given integration time).
If the user should be reminded to close the shutter before a dark scan collection, a reminder message will pop up first.



About to collect a dark scan. Please double check if a probe shutter is closed and then click Yes to proceed!

Click *Yes* when ready to collect a dark scan.
Clicking the *Cancel* button will abort the scan. In this case the collected sample spectrum will be automatically discarded and the program will return to the library contents dialog.

Upon clicking *Yes*, the next dialog will appear.

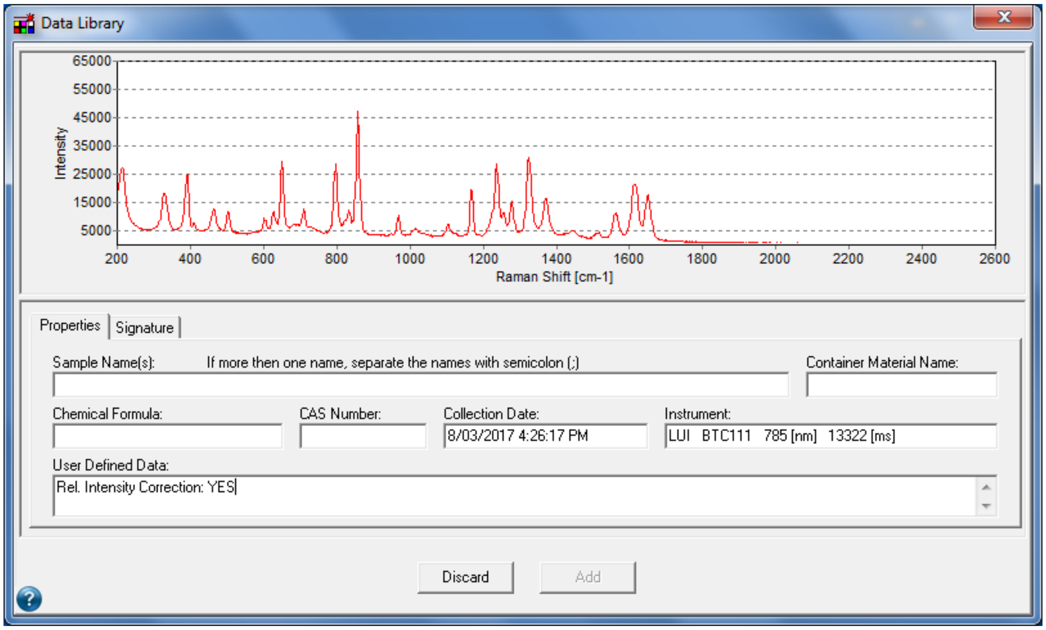


Collecting a dark scan ... Please wait ...

[4750 / 13322 ms]

At this point the user can see the value of the integration time with which the spectrum of the sample was collected. In this example it is 13322 ms.

When a spectrum and a dark scan have been successfully acquired, the next dialog is displayed as shown below:



Sample Name(s): If more then one name, separate the names with semicolon (;)

Container Material Name:

Chemical Formula:

CAS Number:

Collection Date: 8/03/2017 4:26:17 PM

Instrument: LUI BTC111 785 [nm] 13322 [ms]

User Defined Data: Rel. Intensity Correction: YES

The dialog shows the collected spectrum of the sample. The spectrum is dark subtracted and relative intensity corrected if so specified in the method parameters. Double clicking on the graph will maximize the dialog. Double clicking on the maximized dialog will restore original dialog size.

At this point, the user can decide to either accept the collected spectrum and add it to the library, or reject the spectrum.

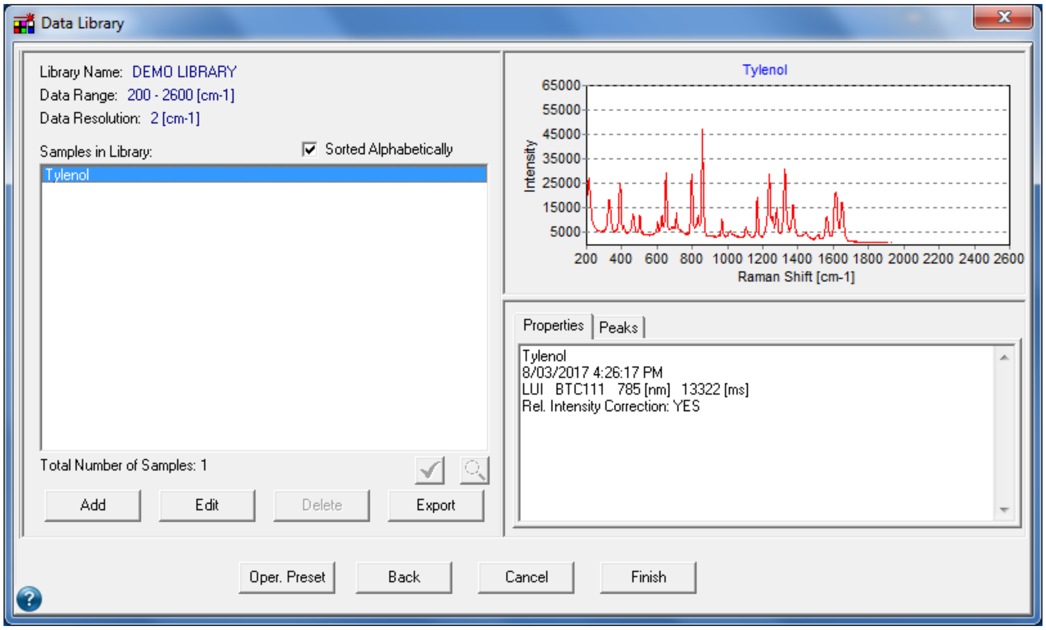
If it is decided to add the spectrum to the library, the user must enter the name of the scanned sample.
Type the sample name(s) into the *Sample Name(s)* box. If more than one name is entered, the names must be separated with a semicolon character (";").
All other parameters are optional.

In this example, a new sample of Tylenol will be added to the library.

To accept collected spectrum and add samples to the library, click the *Add* button. The *Add* button becomes available when the sample name is provided.

To ignore collected spectrum and abort adding sample to the library, click the *Discard* button.

Upon clicking the *Add* or *Discard* button, the program will return to the library contents dialog. If a new sample has been added to the library, the library contents dialog will reflect the modifications as shown below.



Library Name: DEMO LIBRARY
Data Range: 200 - 2600 [cm-1]
Data Resolution: 2 [cm-1]

Samples in Library: ☑ Sorted Alphabetically
Tylenol

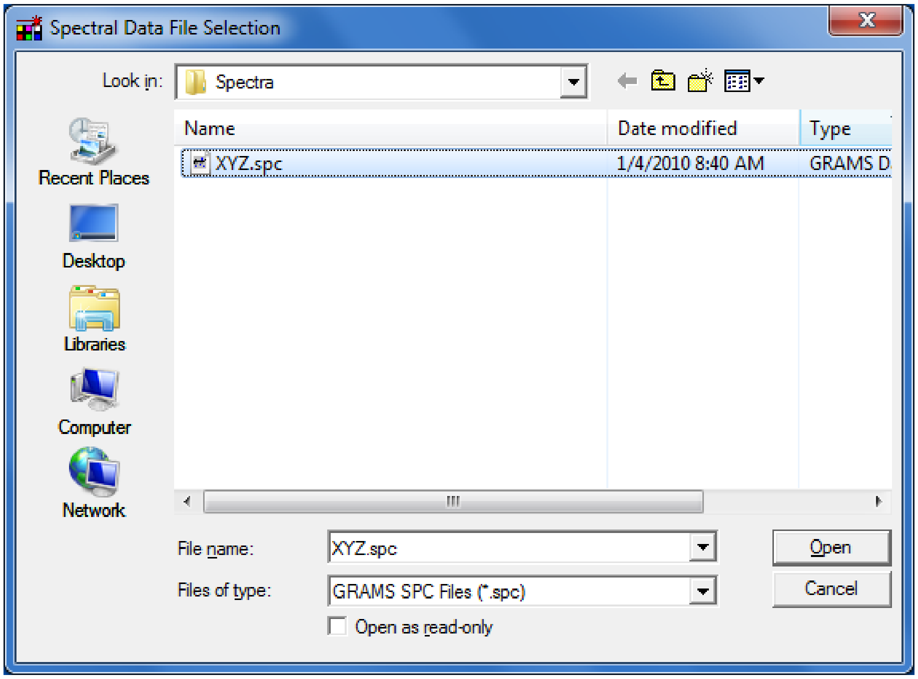
Total Number of Samples: 1

Tylenol
8/03/2017 4:26:17 PM
LUI BTC111 785 [nm] 13322 [ms]
Rel. Intensity Correction: YES

Once all modifications to the library are completed, click *Finish* to save the library.

Off-line Data Import

For the off-line data collection mode, the following dialog will appear as shown below.



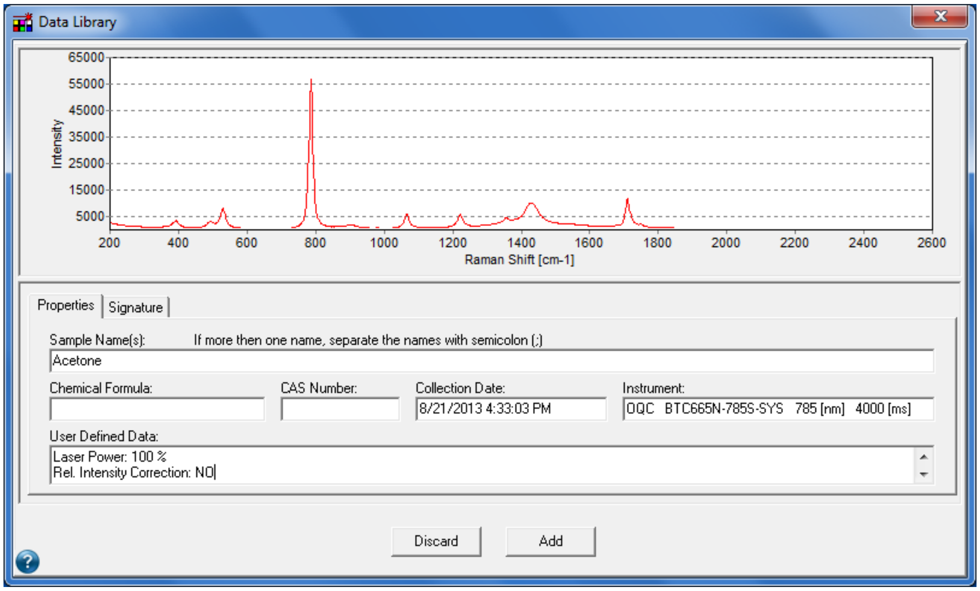
The user can select a Grams SPC file or BWSpec text file with a spectrum to be imported into the library.

In order to successfully import the spectrum into the library:

- the spectrum must be compatible with the library data range
- the Grams SPC file must have a spectrum in evenly spaced Raman Shift units
- the BWSpec file must be in pixel format

If the spectrum is being imported from the BWSpec text file and *Apply relative intensity correction if spectrum not corrected yet* box was checked, then the program will attempt to find a corresponding ratio coefficients file in a folder specified in a current operation preset. If the file cannot be found then the user will be prompted to select the ratio coefficients file manually.

When the spectrum has been successfully imported, the next dialog with imported spectrum is displayed as shown below:



Sample Name(s): If more then one name, separate the names with semicolon (;)
Acetone

Chemical Formula:

CAS Number:

Collection Date: 8/21/2013 4:33:03 PM

Instrument: OQC BTC665N-785S-SYS 785 [nm] 4000 [ms]

User Defined Data:
Laser Power: 100 %
Rel. Intensity Correction: NO

Double clicking on the graph will maximize the dialog. Double clicking on the maximized dialog will restore the original dialog size.

At this point, the user can decide either to accept the imported spectrum and add it to the library, or discard the spectrum.

If it is decided to add the spectrum to the library, the user must enter the name of the imported sample.
Type the sample name(s) into the *Sample Name(s)* box. If more than one name is entered, the names must be separated with a semicolon character (“;”).
All other parameters are optional.

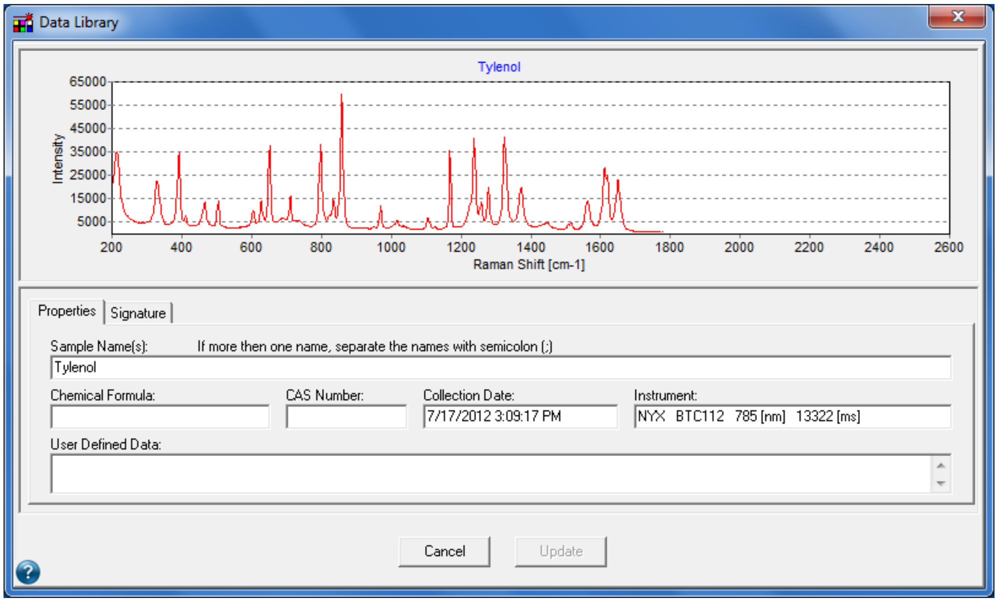
To accept imported spectrum and add the sample to the library, click the *Add* button. The *Add* button becomes available when the sample name is provided.

To ignore the imported spectrum and abort adding the sample to the library, click the *Discard* button.

Upon clicking the *Add* or *Discard* button, the program returns to the library contents dialog. If a new sample has been added to the library, the library contents dialog will reflect the modifications.

Editing Sample

To edit properties of an existing sample, select the sample in the list and then click the *Edit* button. The following dialog will appear:



Sample Name(s): If more then one name, separate the names with semicolon (;)
Tylenol

Chemical Formula:

CAS Number:

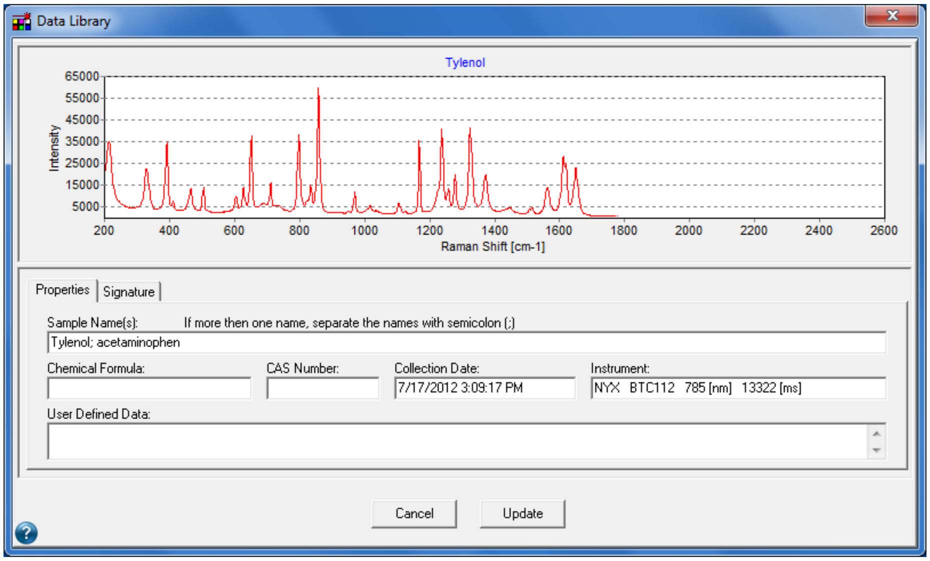
Collection Date: 7/17/2012 3:09:17 PM

Instrument: NYX BTC112 785 [nm] 13322 [ms]

User Defined Data:

Update properties of the sample and click the *Update* button to accept the changes.

Click *Cancel* to close the dialog without changing the sample properties.



Sample Name(s): If more then one name, separate the names with semicolon (;)
Tylenol; acetaminophen

Chemical Formula:

CAS Number:

Collection Date: 7/17/2012 3:09:17 PM

Instrument: NYX BTC112 785 [nm] 13322 [ms]

User Defined Data:

The changes are reflected in the Properties panel in the library contents dialog.

Once all modifications are done to the library, click *Finish* to save the library.

Deleting Samples

To delete a sample from the library, select the sample you wish to delete in the list and then click the *Delete* button. A confirmation message will be displayed before the sample is deleted.

Once all modifications are done to the library, click *Finish* button in the library contents dialog to save the library.

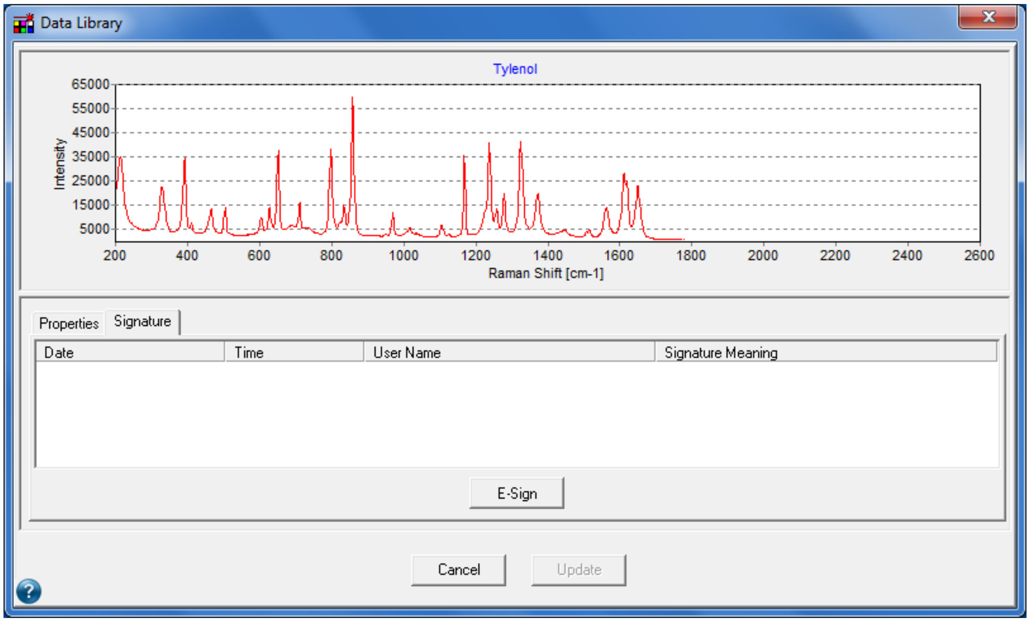
E-Signing the Sample Spectrum

The program (Pharma edition only) supports two-level electronic signatures for library spectra to protect data from being purposely or inadvertently altered by an individual.
To be able to sign the spectra, the option has to be configured in the *Library Spectra Signature* tab in the *Program Configuration* dialog.

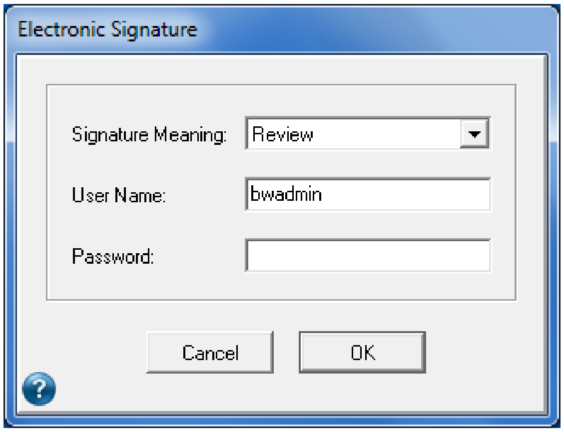
On the first level, the user (Developer or Administrator only) can review or reject the spectrum. If the spectrum is rejected, this is a final rejection and the spectrum cannot be signed on the second level.

On the second level, the user (Developer or Administrator only) can approve or reject the spectrum that was reviewed on the first level. This will be a final signature.

To e-sign the spectrum of an existing sample, select the sample in the list, click the *Edit* button then select a *Signature* tab. The following dialog will appear:



Click the *E-Sign* button. The Electronic Signature dialog will pop up, as shown below.



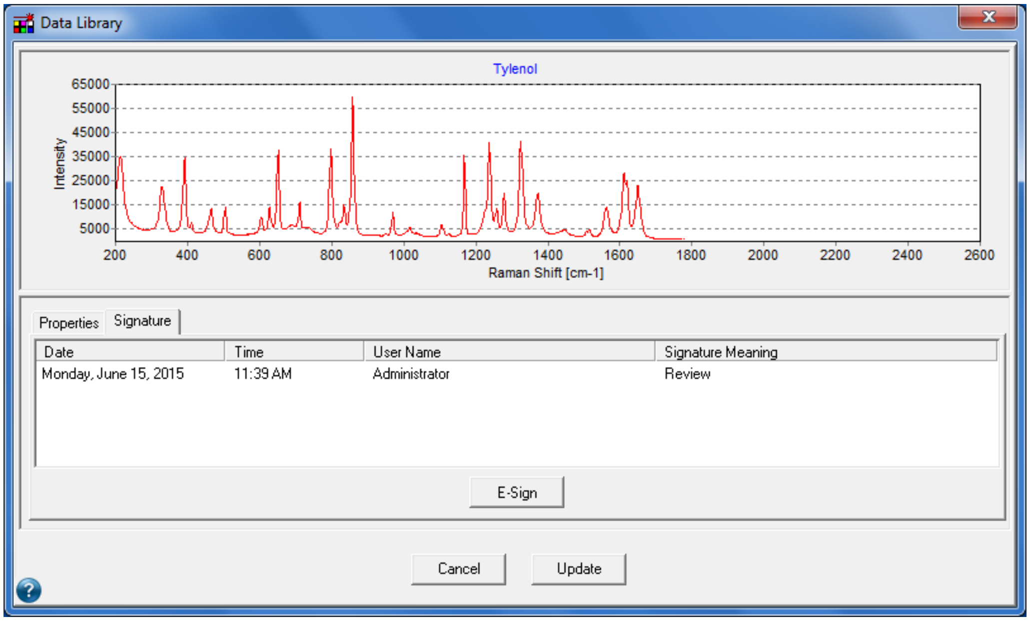
Signature Meaning: Review
User Name: bwadmin
Password:

Select the signature meaning (review, approve, reject) then enter the password. The E-signature requires the password entry, even if the user is already logged in to the program.

Click *Cancel* to close the dialog without signing the spectrum.

Click *OK* to sign the spectrum.

Once the spectrum is signed, the information associated with the signature is displayed in the Signature tab in the Data Library dialog as shown below:

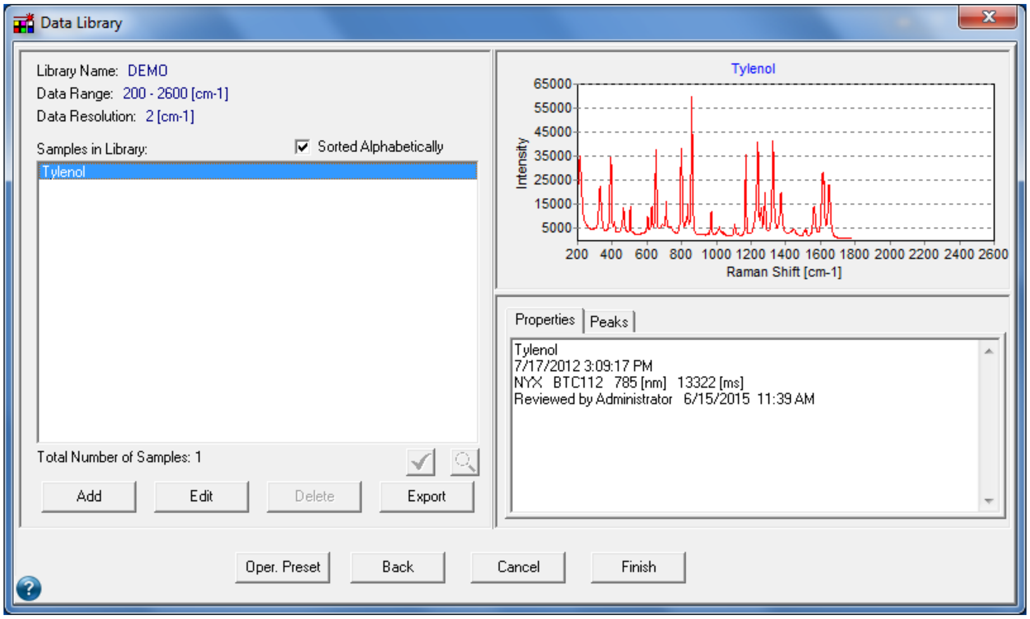


Date	Time	User Name	Signature Meaning
Monday, June 15, 2015	11:39 AM	Administrator	Review

The signed spectrum contains the full name of the signer, the date and time when the signature was executed and the meaning associated with the signature.

The *E-Sign* button will become disabled if the record is finally signed (approved or rejected).

The e-signature is also displayed in the spectrum properties panel in the Data Library dialog as shown below:



Library Name: DEMO
Data Range: 200 - 2600 [cm-1]
Data Resolution: 2 [cm-1]
Samples in Library:
☑ Sorted Alphabetically
Tylenol
Total Number of Samples: 1

Tylenol
7/17/2012 3:09:17 PM
NYX BTC112 785 [nm] 13322 [ms]
Reviewed by Administrator 6/15/2015 11:39 AM

Changing Properties of Signed Spectrum

Once the spectrum is e-signed (any level), the user will not be able to change date/time of the spectrum.

Depending on the Library Spectra Signature configuration settings, the user (developer or administrator) may change the properties of the signed spectrum excluding date/time (e.g. correct misspelled spectrum name, add new name, add user-defined properties, etc.) if the signature is not final (1st level review signature applied).
If spectrum properties have changed, the program will force the user to re-sign the spectrum on the 1st level (review signature) upon accepting the changes.
Any changes to properties of partially signed spectrum will be audit trailed.

Once the spectrum is finally signed (2nd level approve signature), the user will not be able to change the properties.

Deleting Signed Spectrum

Depending on the Library Spectra Signature configuration settings, the program may allow the user to delete signed spectra as follows:

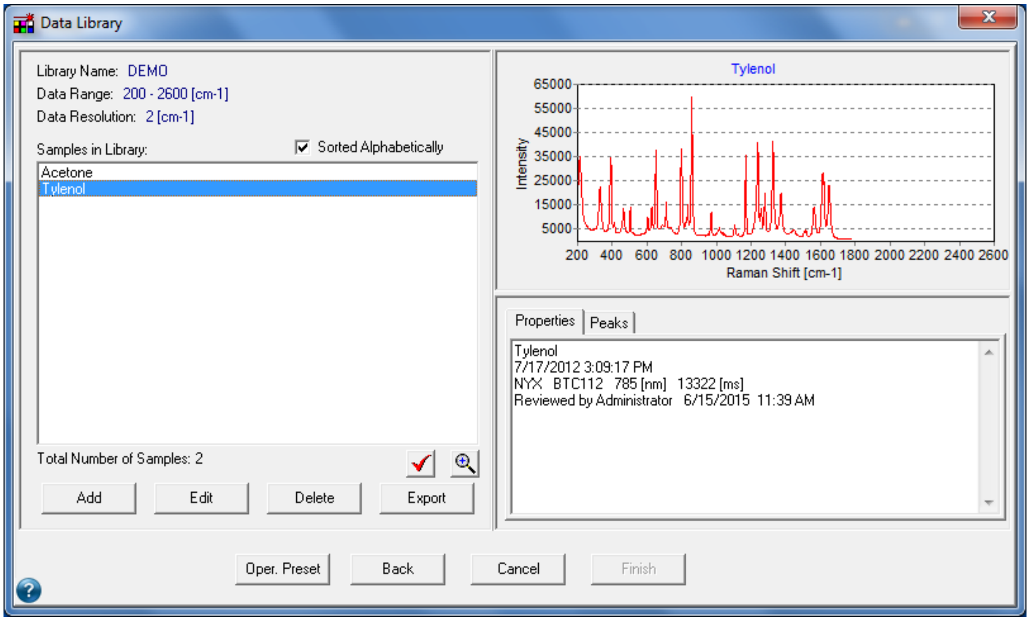
- The developer may be able to delete rejected spectra only.
- The administrator may be able to delete any signed spectrum (rejected, reviewed or approved).

Each deleted spectrum will be listed in the audit trail (spectrum identified by spectrum name and date/time from spectrum properties).

Checking Spectra Approve Signature

While in the Library dialog, the program allows the user to check if all spectra in the library are approved.

To start the signature checking procedure, click the red check mark icon ✓.



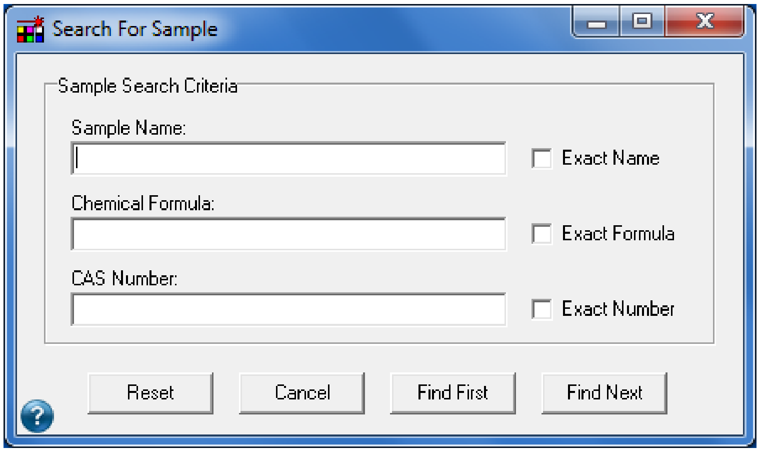
Library Name: DEMO
Data Range: 200 - 2600 [cm-1]
Data Resolution: 2 [cm-1]
Samples in Library: ☑ Sorted Alphabetically
Acetone
Tylenol
Total Number of Samples: 2

Tylenol
7/17/2012 3:09:17 PM
NYX BTC112 785 [nm] 13322 [ms]
Reviewed by Administrator 6/15/2015 11:39 AM

The program will stop the checking procedure at the first not approved spectrum and it will report its name to the user.

Searching for a Sample

To search for a sample in the library, click the *Search* icon 🔍. The following dialog will appear:



The search is based on the conjunction of the selected criteria, and is not case sensitive. The found sample is selected in the library contents list.

Sample Name – enter a full or partial name of a sample you are looking for.

Exact Name - check this box to find a sample with the exact name specified in the *Sample Name* field.

Chemical Formula – enter a full or partial chemical formula of a sample you are looking for.

Exact Formula - check this box to find a sample with the exact formula specified in the *Chemical Formula* field.

CAS Number – enter a full or partial CAS number of a sample you are looking for.

Exact Number - check this box to find a sample with the exact CAS number specified in the *CAS Number* field.

Click the *Find First* button to search for a sample from the beginning of the library contents list.

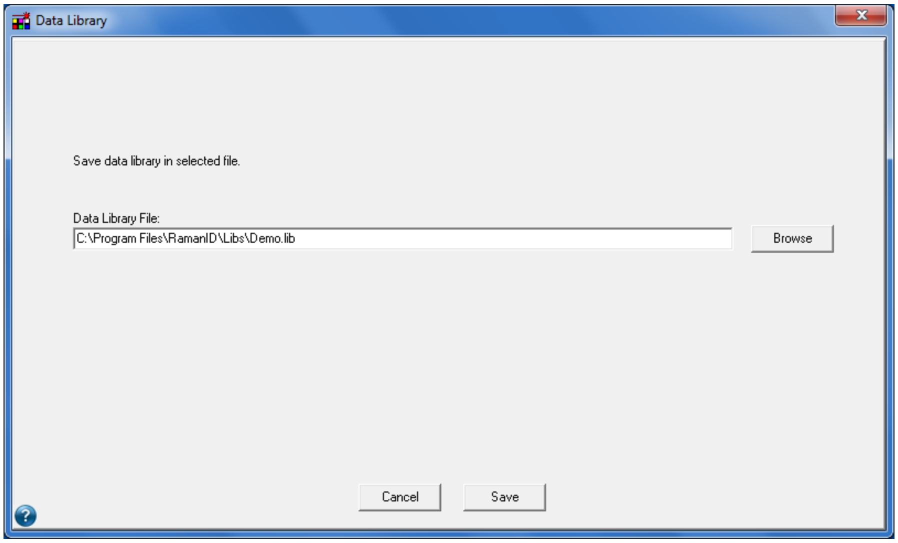
Click the *Find Next* button to search for a sample from the position of the currently selected sample in the library contents list.

Click the *Reset* button to reset all fields to default: (i.e. empty edit fields and uncheck boxes).

Click the *Cancel* button to close the search dialog.

Saving Libraries

Click the *Finish* button to finish library generation and save the library data to a file. The following dialog will appear:



C:\Program Files\RamanID\Libs\Demo.lib

Click the *Browse* button to browse for a file name. The ".lib" file extension is mandatory for the BWID® library.

Click *Cancel* to quit library saving. All modifications in the library will be aborted.

Click *Save* to save the library in the selected file.
At this point, the library is being saved in the selected file. This step may take up to few seconds depending on the number of spectra added to the library as well as library data range.

A single library consists of six files, all with the same name, but different extensions: ".lib", ".ifm", ".ist", ".stm", ".pik" and ".sdp".

When finished, the program will return to the Menu window.

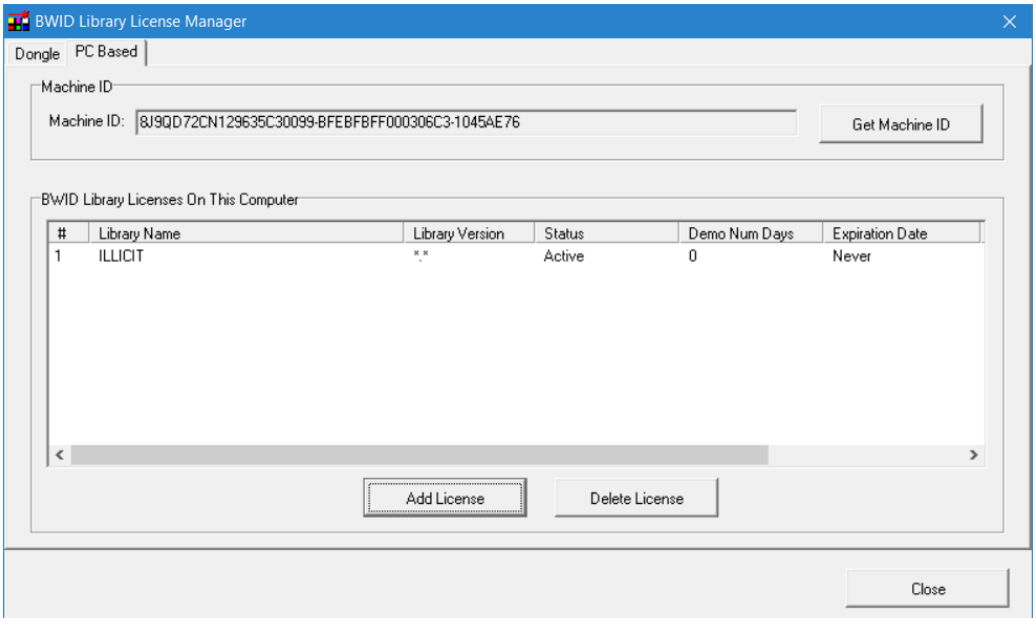
In case of any error, an appropriate message will be displayed.

BWID® Library Licenses

In order to use a BWID® protected library in the program (the ID analysis and the Library options) a valid license for the library is required. The library license can be issued for a given PC (PC based license) to be used with the library on that PC only or can be issued on a BWID® dongle to be used on any PC.

Upon accessing the BWID® protected library, the program will first check the licenses stored on the PC. If there is no valid license on the PC then it will check the dongle. If there is no valid license present on the PC and on the dongle (inserted into a USB port on the PC), an appropriate message will be displayed to the user and the program will not continue with the execution.

To view available BWID® library licenses click the *Licenses* button in the library selection dialog. A *BWID® Library License Manager* dialog will open displaying the licenses stored on the PC as shown below.



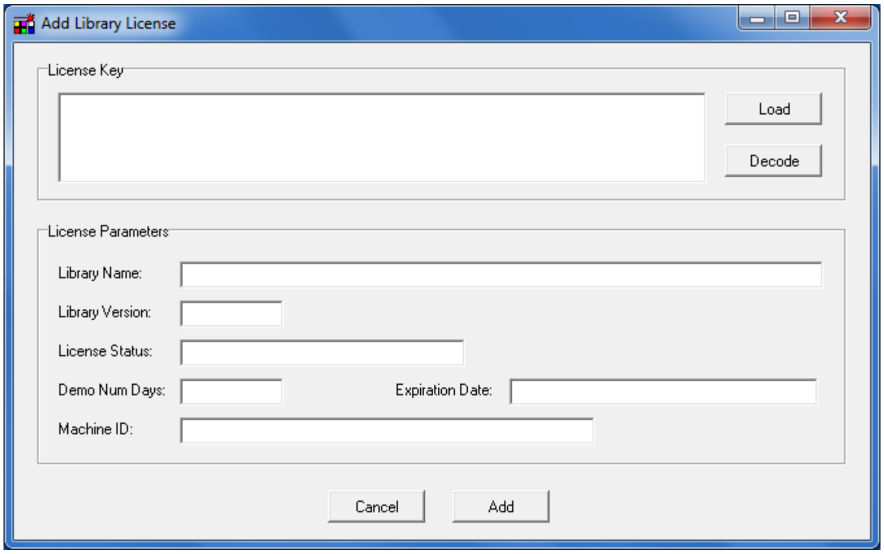
Machine ID: 8J9QD72CN129635C30099-BFEBFBFF000306C3-1045AE76

#	Library Name	Library Version	Status	Demo Num Days	Expiration Date
1	ILLICIT	*.*	Active	0	Never

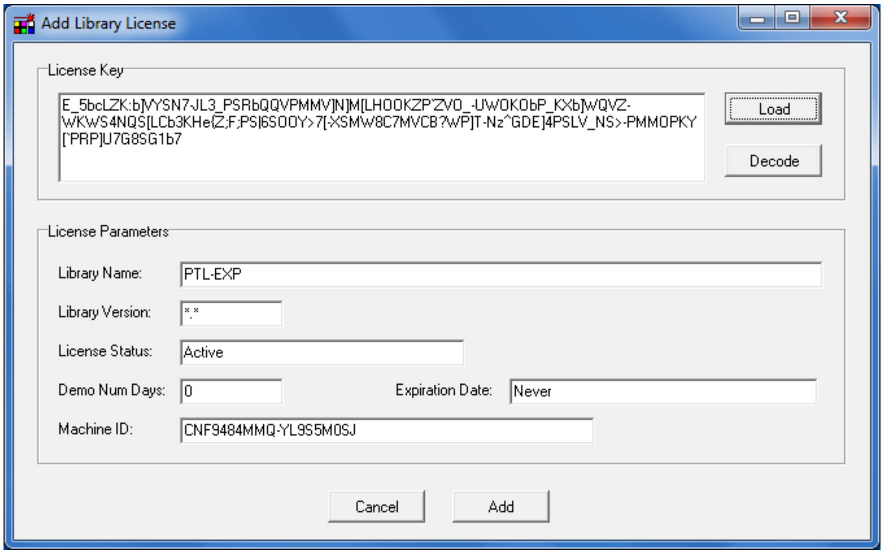
In order to get the PC-based library license, a machine ID code needs to be sent to B&W Tek (custsupport@bwtek.com). Just copy the machine ID code from a *Machine ID* box and paste to an email with a request for the library license. B&W Tek will generate the library license for the given machine ID and send it back in a license text file. Once the user receives the license file, it may be added in the BWID library license manager on the PC.

To add a new license on the PC, click the *Add License* button. The *Add Library License* dialog will be displayed as shown below.

To delete an existing license on the PC (e.g. when it expires), click the *Delete License* button. A confirmation message will be displayed before proceeding with the license deletion.



Click the *Load* button to load the license from a license file. Upon successful reading from the file, the license will be automatically decoded and displayed in the *Add Library License* dialog as shown below.
Or, open the license file (e.g. in a Notepad), copy a license string from a "License Key = " line (copy all text after = character) and paste it to a *License Key* box then click the *Decode* button to decode it. The license information will be displayed in the dialog.

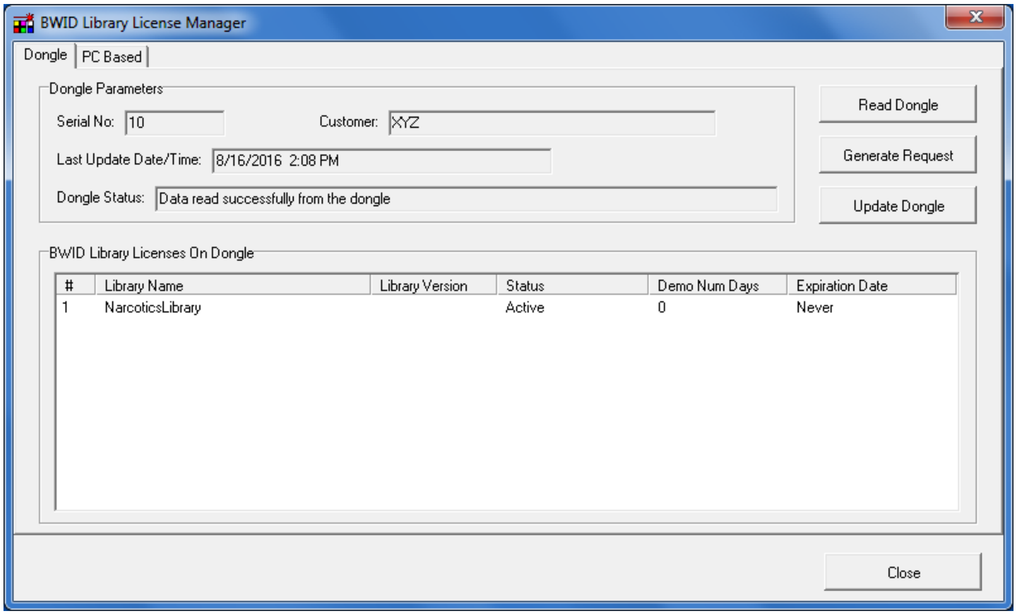


```
E_5bcLZK:b]VYSN7-JL3_PSRbQQVPMMV]N]M[LHOOKZP'ZVO_-UWOKObP_KXb]WQVZ-
WKWS4NQS[LCb3KHe{Z;F;PS|6SOOY>7[-XSMW8C7MVCB?WP]T-Nz^GDE]4PSLV_NS>-PMMOPKY
[`PRP]U7G8SG1b7
```

Library Name: PTL-EXP
Library Version: *.*
License Status: Active
Demo Num Days: 0
Expiration Date: Never
Machine ID: CNF9484MMQ-YL9S5M0SJ

Click the *Add* button to add the license to the PC. If the license already exists on the PC or for some reason cannot be stored on the PC (e.g. already expired or it is not for this PC) an appropriate message will be displayed.

To view licenses stored on the BWID® dongle, first insert the BWID® dongle into a USB port then click the *Dongle* tab in the *BWID® Library License Manager* dialog. The program will automatically read the dongle (only once, when switching for the first time to the Dongle tab) and then display its contents as shown below.



Serial No: 10
Customer: XYZ
Last Update Date/Time: 8/16/2016 2:08 PM
Dongle Status: Data read successfully from the dongle

#	Library Name	Library Version	Status	Demo Num Days	Expiration Date
1	NarcoticsLibrary		Active	0	Never

Click *Read Dongle* button to read the dongle again or to read another dongle.

Changes to the dongle can be only done by sending a request file to B&W Tek and then getting an update file in return.

Click *Generate Request* button to generate a request file. The user will be asked to select a folder and file name of the request file (default name: BWIDDongleRequest.dat). The file should be sent to B&W Tek when requesting changes to the dongle, e.g. to update the library license, add a new license or delete an existing license.

Click *Update Dongle* button to update the dongle contents with an update file received from B&W Tek. The user will be asked to select a folder and file name of the update file (default name: BWIDDongleUpdate.dat).

Click *Close* button to close the dialog and return to the library selection dialog.

9. Sample Identification

Starting Sample Identification

Click the *ID* button in the main window to start sample identification.

The program will guide the user step by step. The user can cancel sample identification at any time by clicking the *Cancel* button.

Spectra Signature Checking

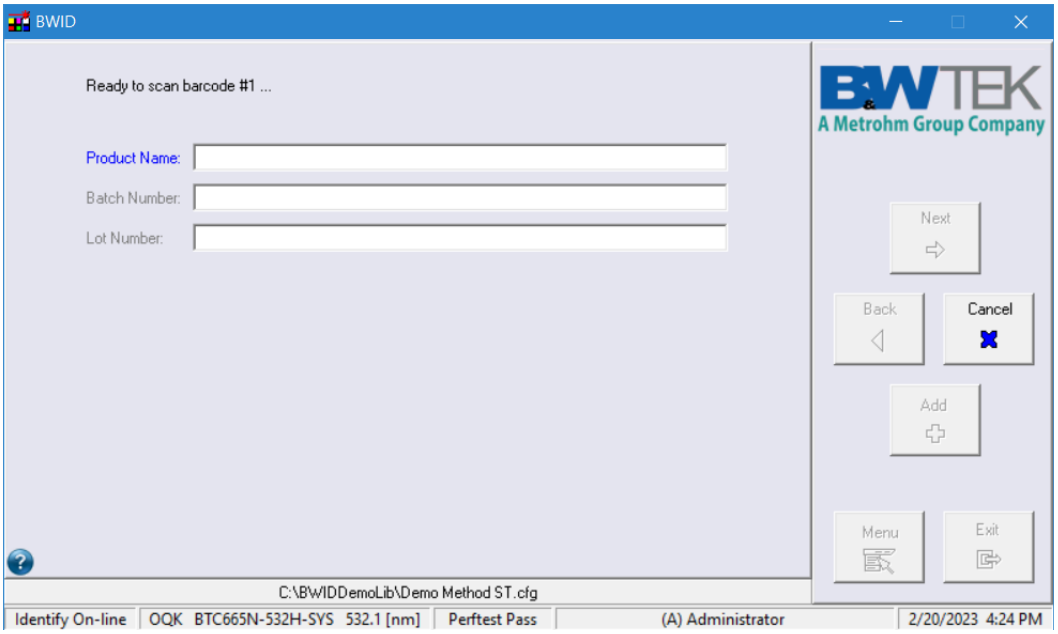
Upon starting the ID analysis (Pharma edition only) the program may check if all spectra in the search libraries are approved. If all spectra in the search libraries should have approve signature, upon finding a first not approved spectrum (unsigned, reviewed or rejected spectrum) the program will display an appropriate error message and quit the ID analysis.

User Input

At the beginning of sample identification, the user will be prompted to enter all mandatory input parameters using a barcode scanner or keyboard.
If there are no mandatory input parameters, this step will be omitted.

Barcode Scanning

In the barcode scanner mode, the user will be asked to scan one or more barcodes depending on the method configuration. Data titles displayed in blue represent the barcode to be scanned (e.g. Product Name in the example below). Data titles for additional scans (if any) are grayed out (e.g. Batch Number and Lot Number in the example below).


Ready to scan barcode #1 ...

Product Name:

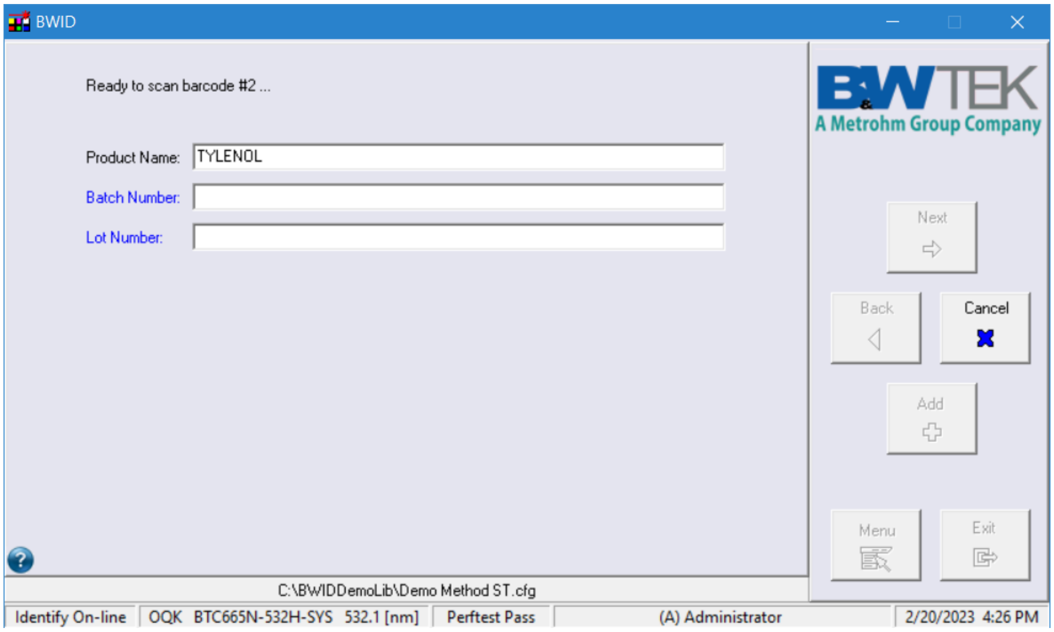
Batch Number:

Lot Number:

C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:24 PM

Once the barcode is successfully scanned, the data will be displayed in the barcode data fields (with titles now in black). If there is more than one barcode is specified the next required filed title will be displayed in blue, as shown in the dialog below.



Ready to scan barcode #2 ...

Product Name: TYLENOL

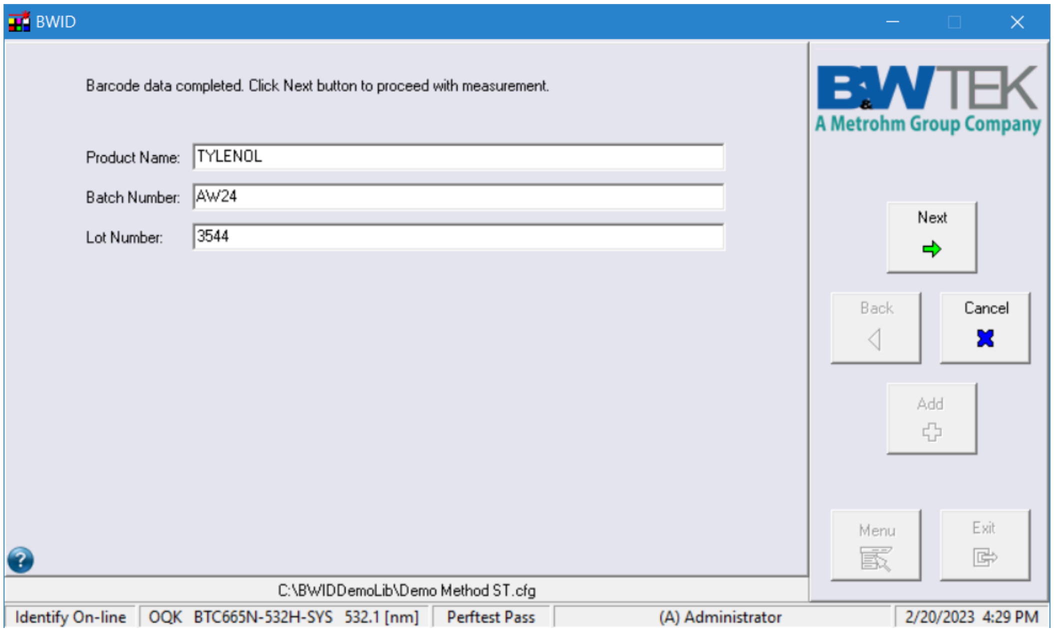
Batch Number:

Lot Number:

C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:26 PM

Once all barcodes are scanned, the *Next* button will become available.



Barcode data completed. Click Next button to proceed with measurement.

Product Name: TYLENOL

Batch Number: AW24

Lot Number: 3544

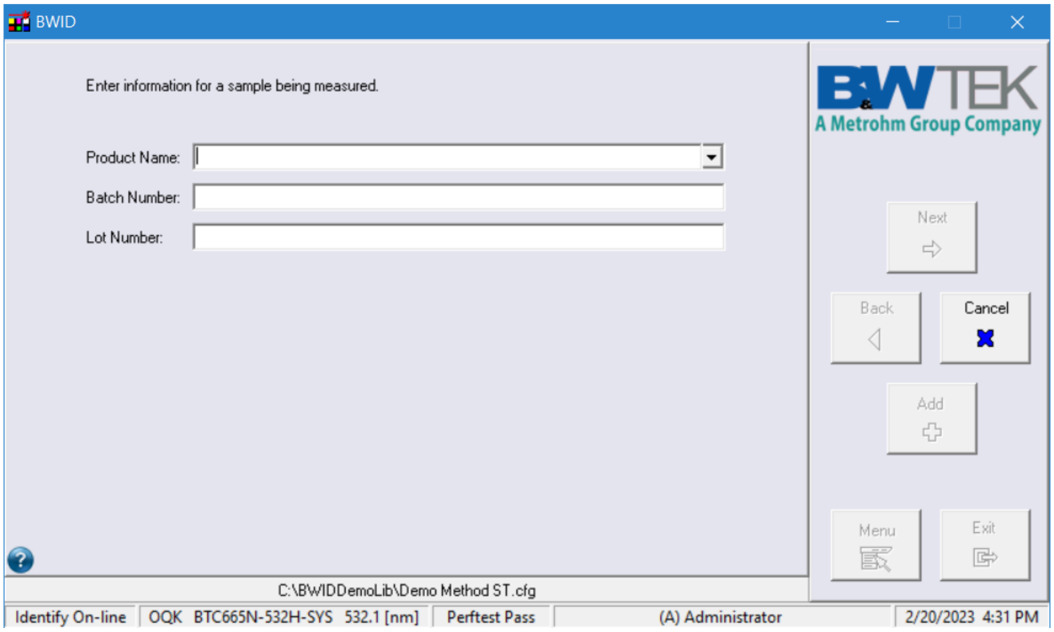
C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:29 PM

Click the *Next* button to proceed with the measurement.

Entering Data Manually

In the manual mode, the user will be asked to enter data using the keyboard.



Enter information for a sample being measured.

Product Name:
Batch Number:
Lot Number:

C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:31 PM

In this case, the user must enter a product name, product number and batch number for a sample being measured. Other possible input parameters are: lot number, container number, supplier (manufacturer) name, and user notes. The product name field can hold up to 256 characters while all other input parameter fields hold up to 50 characters each.

Once all input parameters are provided, click the *Next* button to proceed with the measurement.

ID Measurement

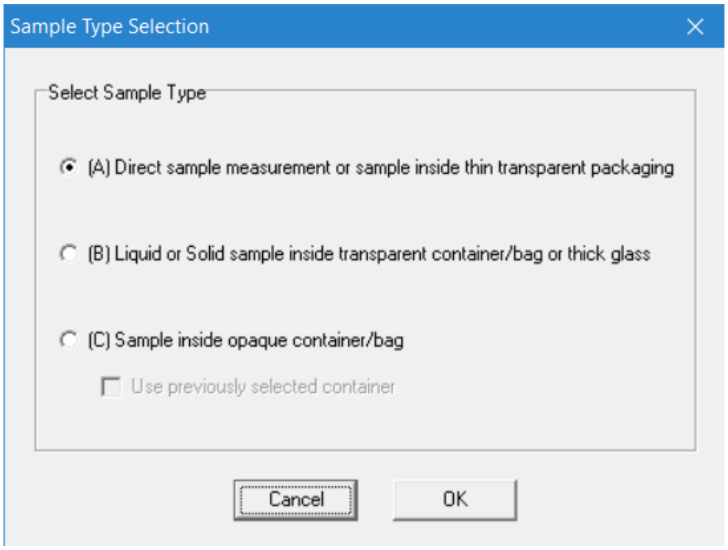
There are two types of ID measurements in the BWID® software: see through ID and conventional ID.
The see-through ID measurement should be run using an ST probe with STRam instrument, while the conventional ID measurement can be run with any Raman instrument.

Additionally, depending on the program setting, the ID measurement can be run in on-line or off-line mode (see Program Configuration paragraph for details).

See Through ID Measurement

There are two basic See Through ID operation modes that are applied based on the selection of sample type made when beginning the measurements. The See Through algorithm is used for both modes. The first mode, direct mode, operates with the conventional library identification based on the collected sample spectrum alone (options A and B in *Sample Type Selection* dialog). The second mode, ST mode, works for samples (option C in *Sample Type Selection* dialog) that are covered by a container material that generates significant Raman signal of itself, and requires a spectrum of the container material (either selected from container library, or collected just before sample spectrum collected which is recommended as there is large variation in the formulations of plastic packaging materials).

Upon starting the measurement, the user will be prompted to select a sample type as shown in the following dialog:



Sample Type Selection

Select Sample Type

● (A) Direct sample measurement or sample inside thin transparent packaging

○ (B) Liquid or Solid sample inside transparent container/bag or thick glass

○ (C) Sample inside opaque container/bag

☐ Use previously selected container

If the user selects sample type (A) or (B) at the prompt, the system operates like a regular Raman ID analyzer and acquires the spectrum of the sample directly and ID is based on this spectrum alone with identification done using the STID identification algorithm. This works well for uncovered samples (liquid or solid material in the direct contact), as well as samples in transparent containers where the container itself does not produce significant Raman signature (for example samples in glass containers or thin clear plastic bags, some coated tablets). In this mode, the ST probe can be used alone which gives a larger sampling area so is also good for heterogeneous solids (option A), or with the Focus Adaptor, option B, which has a longer focal distance. Figure 2 shows measurement using the ST Probe with the Focus Adaptor to measure a liquid in a glass container. The BWID® software prompts the user for the type of adaptor to use based on the selected sample type and container.

Figure 2: Focus Adaptor in place on the ST Probe

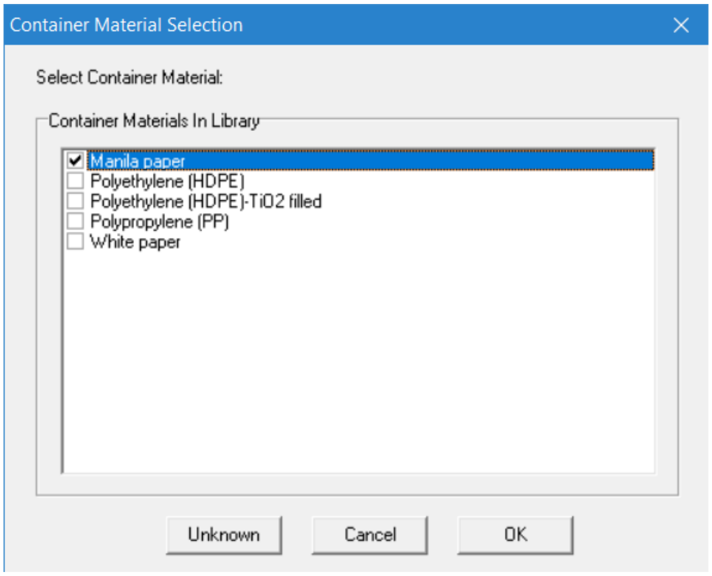
Optimal probe configuration depends on the sample type:

- Uncovered solid, or solid sample in thin plastic bag (< 1 mm thick) or thinly coated tablets: use the ST Probe alone. Glass tends to generate strong fluorescence. Using the ST probe avoids focusing the laser on the glass and helps minimize the fluorescence.
- Liquid in a glass container (clear or amber): use the ST Probe with the Focus Adaptor so that the laser can be focused inside on the sample. The signal may be too weak if the ST probe is used alone.
- Solid in a thick (> 1 mm thick) or double layer glass container: use the ST Probe with the Focus Adaptor.

If the user selects sample type (C), the program will run a ST measurement designed for samples that are covered by a container material that generates significant Raman signal of itself, such as polymer, paper, and fabric. This signature will contaminate the Raman signal of the sample, making it difficult to identify the sample directly by a correlation comparison of the collected spectrum to library spectra. The ST mode works by obtaining two spectra, including a 1st spectrum of the package material alone (this may be a spectrum selected from the "Container Spectra Library"), and a 2nd spectrum of the sample with the package material. The analysis then identifies the sample by removing the contribution of the 1st spectrum from the 2nd spectrum.

The ST measurement will be able to make the sample identification when there is sufficient sample signal within the collected spectrum of samples and container. The increased spot size and penetration depth of the ST probe are effective in such measurements through a variety of materials with opacity that allows light to pass through the container wall, and the Raman backscattering to also pass back. Dark plastics which are a few mm thick, as well as brown kraft paper are challenging for such measurement, especially when the sample inside the container is a weak Raman scatterer.

Upon accepting sample type (C), the following dialog will pop up prompting the user to choose an existing container material from a container library, or measure it if he/she is uncertain of its composition or if it is not in the container library.



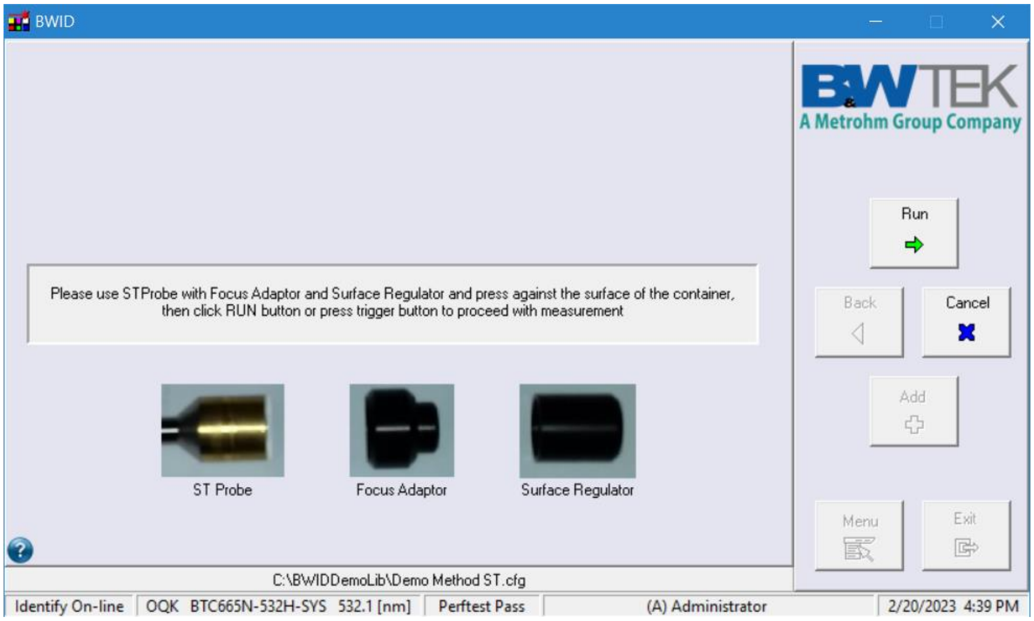
Click on a container material in the container materials list, if selecting an existing container material from a container library.
Click *Unknown* button to measure it if you are uncertain of container material composition or if it is not in the container library.

Use previously selected container check box in the Sample Type Selection dialog allows the user to use previously selected container in the subsequent analysis. When the box is checked, the Container Material Selection dialog will not be shown, thus only one OK click to proceed with the next scan.
The *Use previously selected container* box is only available if there is a previous container type already chosen by the user. Previously selected container name will be displayed in the Sample Type Selection dialog below the checkbox for user info.

On-line Measurement

If the user had selected sample type (C) and had chosen the container material as Unknown, the following dialog will be displayed prompting the user to use the ST probe with the Focus Adaptor and the Surface Regulator so that the focus can be conveniently placed on the container surface to collect the container spectrum.

NOTE: The above suggested configuration assumes the container material is not damaged by the focused laser. In case the container material, such as kraft paper, is susceptible to damage, use the ST probe without the Focus Adaptor or the Surface Regulator instead.

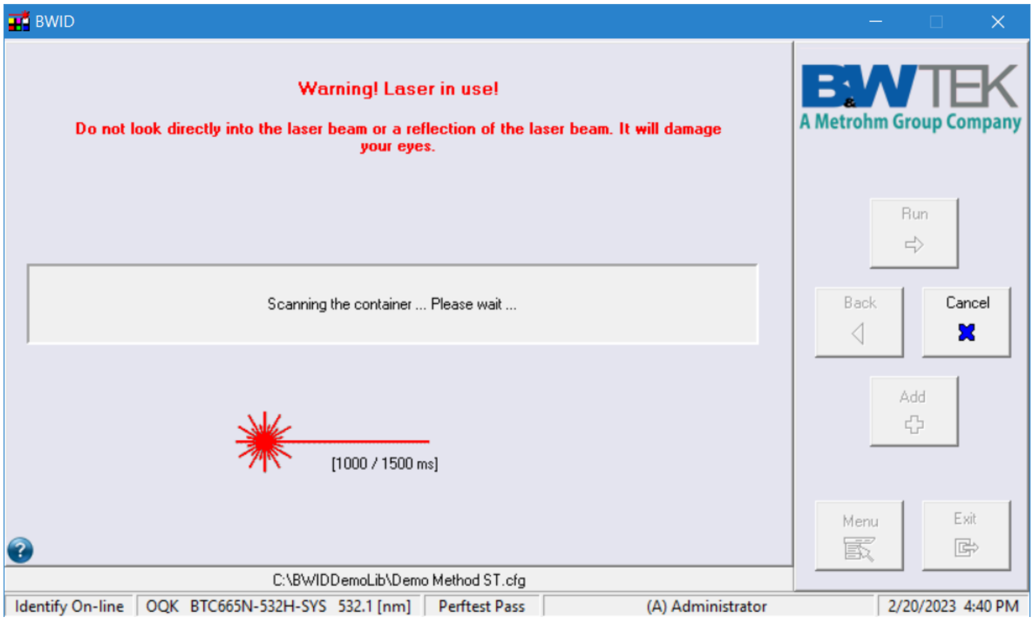


Please use STProbe with Focus Adaptor and Surface Regulator and press against the surface of the container, then click RUN button or press trigger button to proceed with measurement

C:\BWIDDemoLib\Demo Method ST.cfg

The user should try to acquire a container spectrum with as little as possible signature from the content material, by placing the probe on a part of the container that does not have the content underneath.

When ready to scan the container, click the *Run* button or press a trigger button on the probe (if enabled) to start the acquisition. The dialog will be displayed as shown below.



Warning! Laser in use!

Do not look directly into the laser beam or a reflection of the laser beam. It will damage your eyes.

Scanning the container ... Please wait ...

[1000 / 1500 ms]

C:\BWIDDemoLib\Demo Method ST.cfg

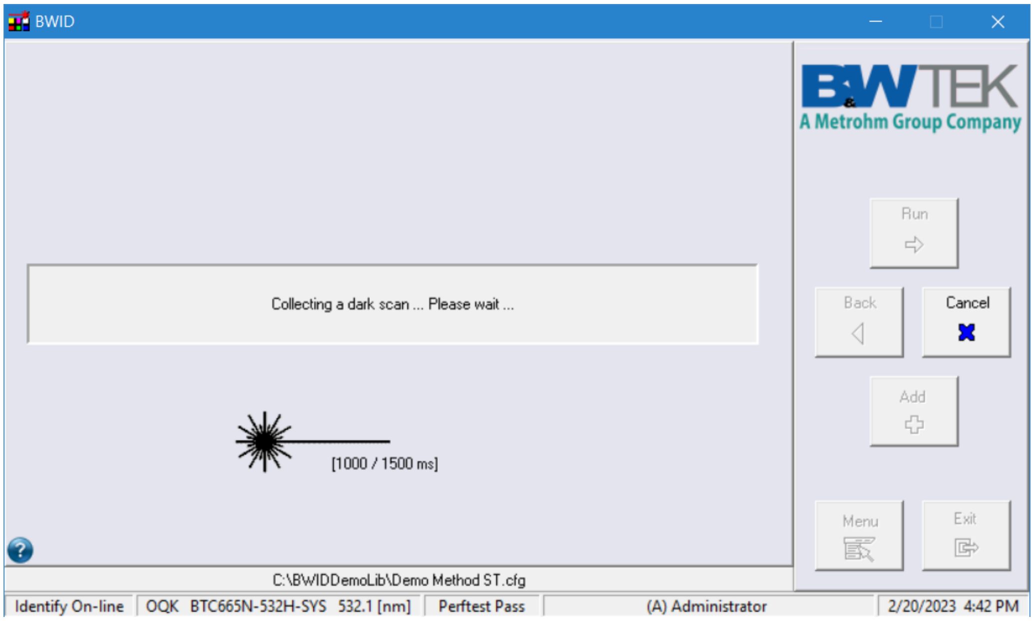
Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:40 PM

First, a raw spectrum of the container is collected.

If the user should be reminded to open the shutter before a raw data scan collection, a reminder message will appear first.

At this point, the sample is being scanned one or more times depending on the *Optimum Integration Time* setting in the default preset.
If the *Optimum Integration Time* is enabled, the program will scan the sample several times (at least 2 but no more than 5 times) with different integration times to determine the optimum integration time for the best Raman shift signal.
If the *Optimum Integration Time* is disabled, the program will use fixed integration times to collect a sample scan.

Next, a dark scan is acquired if not yet collected for that given integration time.
If the user should be reminded to close the shutter before a dark scan collection, a reminder message will pop up first.



Collecting a dark scan ... Please wait ...

[1000 / 1500 ms]

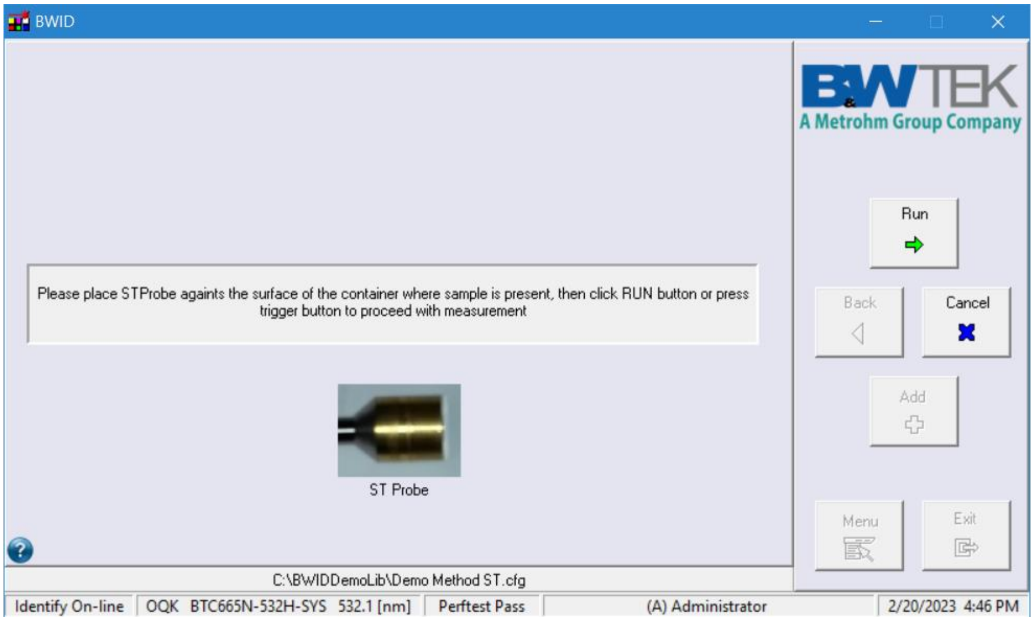
C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:42 PM

Once the container spectrum acquisition is finished the following dialog will be displayed prompting the user to place the ST Probe against the container at a place where there is sample to collect the sample and container spectrum.

If sample type (A) or (B) was selected, the dialog will prompt the user to place the ST Probe against the sample to collect the sample spectrum.

Depending on the sample type selection, the user will be asked to use the ST probe alone or the ST probe with the Focus Adaptor.



Please place STProbe againts the surface of the container where sample is present, then click RUN button or press trigger button to proceed with measurement

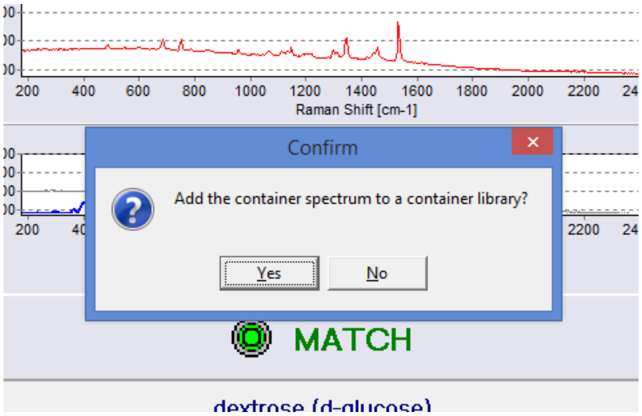
C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:46 PM

When ready to scan the sample, click the *Run* button or press a trigger button on the probe (if enabled) to start the acquisition. The sample spectrum will be collected the same way the container spectrum was collected - sample scan followed by the dark scan.

Once the sample scan is finished, the data library is searched for a match.

When a Match is found and the container spectrum was measured before the sample (not selected from the library), the user will be asked if the container spectrum should be added to the container library.



Add the container spectrum to a container library?

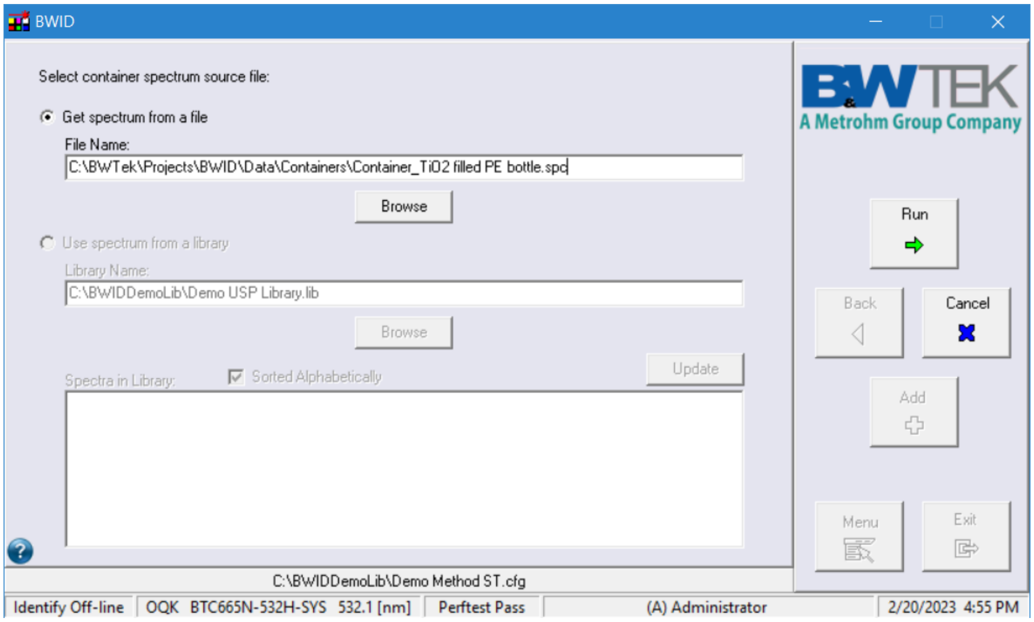
dextrose (d-glucose)

If answer Yes, then the user will be prompted to enter a container name, and the container spectrum will be added to the

Container library, and available for future use.

Off-line Measurement

In the off-line mode, if the user had chosen the container material as Unknown, the following dialog will be displayed prompting the user to select a file with a container material spectrum.



BWID

Select container spectrum source file:

● Get spectrum from a file

File Name: C:\BWTek\Projects\BWID\Data\Containers\Container_Ti02 filled PE bottle.spc

○ Use spectrum from a library

Library Name: C:\BWIDDemoLib\Demo USP Library.lib

☑ Sorted Alphabetically

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:55 PM

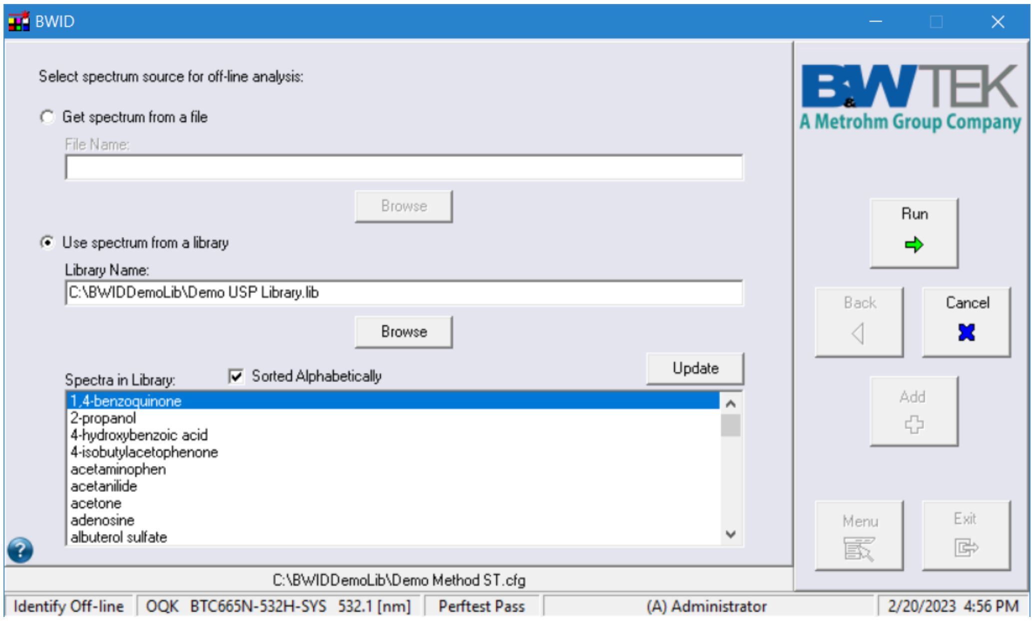
Click *Browse* to browse for the file. The user can select a Grams SPC file or BWSpec text file.

In order to successfully load the spectrum for ID analysis:

- the spectrum must be compatible with the library search data range
- the Grams SPC file must be generated with the BWID® program and must have a spectrum in evenly spaced Raman Shift units
- the BWSpec file must be in pixel format

Click *Run* to load the container spectrum.

Once the container spectrum is successfully loaded from the selected file or if “direct” measurement was selected (sample type A, B, C, D) the following dialog will be displayed prompting the user to select a file with a sample spectrum.



Select spectrum source for off-line analysis:

○ Get spectrum from a file

File Name:

● Use spectrum from a library

Library Name: C:\BWIDDemoLib\Demo USP Library.lib

Spectra in Library: ☑ Sorted Alphabetically

- 1,4-benzoquinone
- 2-propanol
- 4-hydroxybenzoic acid
- 4-isobutylacetophenone
- acetaminophen
- acetanilide
- acetone
- adenosine
- albuterol sulfate

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:56 PM

Click the *Get spectrum from a file* button to allow spectral data file selection.
Click *Browse* to browse for the file. The user can select a Grams SPC file or BWSpec text file.

Click the *Use spectrum from a library* button to allow spectrum selection from a data library. Click the *Browse* button to select the library and to upload available samples into the Spectra in Library list. Then select the name of the spectrum that will be used in ID analysis.

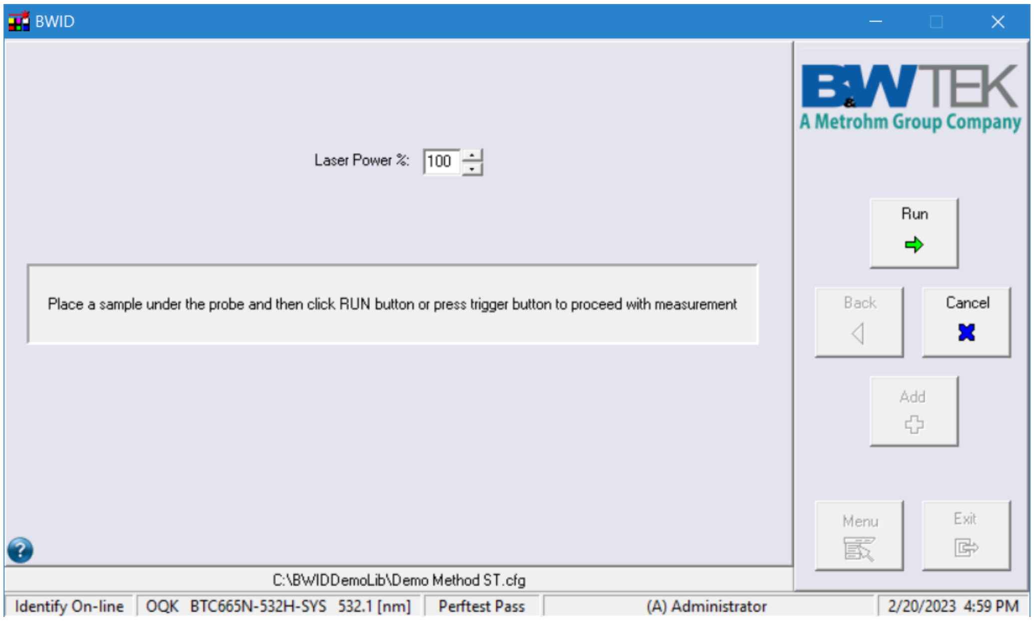
Click *Run* to load the spectrum and search data libraries for a match.

In case of an error, an appropriate message will be displayed to the user.

Conventional ID Measurement

On-line Measurement

Upon starting the measurement in the on-line mode, the following dialog will appear:



Laser Power %: 100

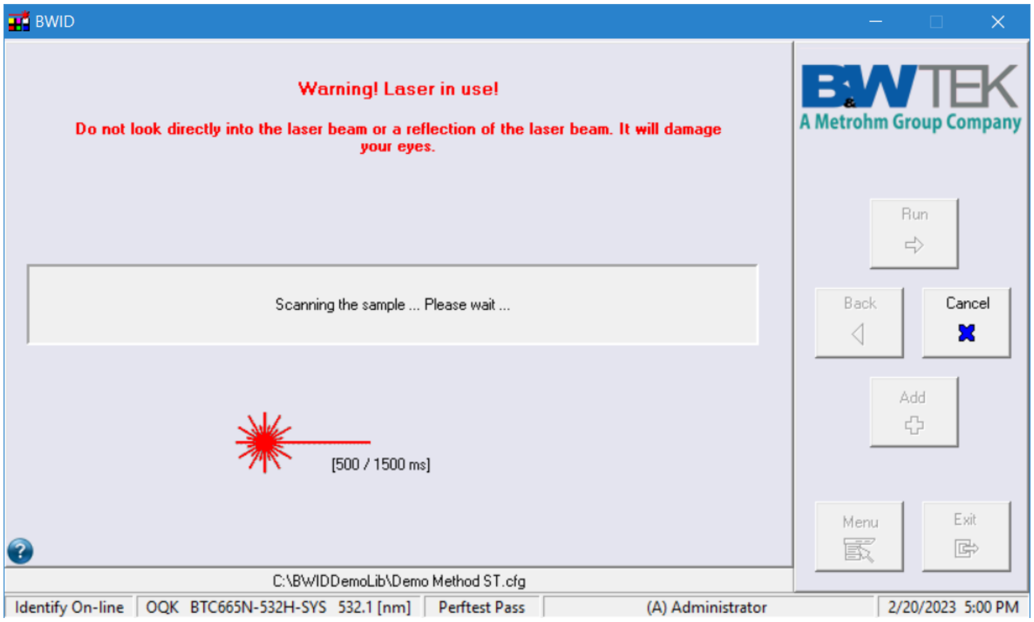
Place a sample under the probe and then click RUN button or press trigger button to proceed with measurement

C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 4:59 PM

Click the *Back* button to go back to the previous dialog to change information for a product being measured (only changes for data entered manually are permitted).

Once a sample is in place for a measurement, click the *Run* button to scan the sample. The dialog will be displayed as shown below.



Warning! Laser in use!

Do not look directly into the laser beam or a reflection of the laser beam. It will damage your eyes.

Scanning the sample ... Please wait ...

[500 / 1500 ms]

C:\BWIDDemoLib\Demo Method ST.cfg

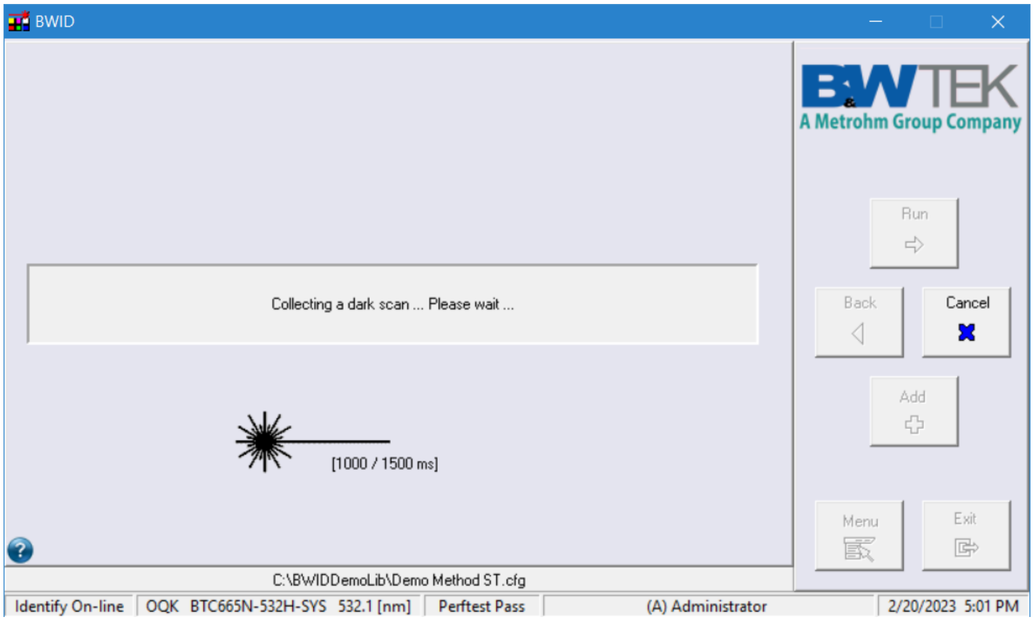
Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:00 PM

First, a raw spectrum of the sample is collected.

If the user should be reminded to open the shutter before a raw data scan collection, a reminder message will appear first.

At this point, the sample is being scanned one or more times depending on the *Optimum Integration Time* setting in the default preset.
If the *Optimum Integration Time* is enabled, the program will scan the sample several times (at least 2 but no more than 5 times) with different integration times to determine the optimum integration time for the best Raman shift signal.
If the *Optimum Integration Time* is disabled, the program will use fixed integration times to collect a sample scan.

Next, a dark scan is acquired if not yet collected for that given integration time.
If the user should be reminded to close the shutter before a dark scan collection, a reminder message will pop up first.



Collecting a dark scan ... Please wait ...

[1000 / 1500 ms]

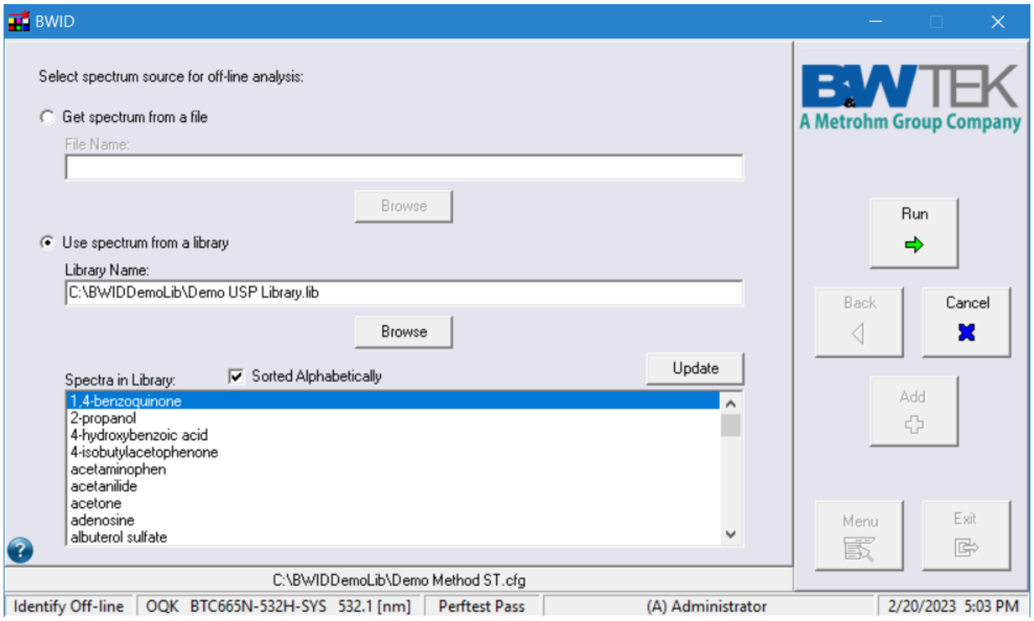
C:\BWIDDemoLib\Demo Method ST.cfg

Identify On-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:01 PM

Once a sample scan and a dark scan are collected, the data library is searched for a match.

Off-line Measurement

In the off-line mode, the following dialog will appear:



Select spectrum source for off-line analysis:

○ Get spectrum from a file

File Name:

Browse

● Use spectrum from a library

Library Name: C:\BWIDDemoLib\Demo USP Library.lib

Browse

Spectra in Library: ☑ Sorted Alphabetically

Update

1,4-benzoquinone
2-propanol
4-hydroxybenzoic acid
4-isobutylacetophenone
acetaminophen
acetanilide
acetone
adenosine
albuterol sulfate

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:03 PM

Click the *Get spectrum from a file* button to allow spectral data file selection.
Click *Browse* to browse for the file. The user can select a Grams SPC file or BWSpec text file.

In order to successfully load the spectrum for ID analysis:

- the spectrum must be compatible with the library search data range
- the Grams SPC file must be generated with the BWID® program and must have a spectrum in evenly spaced Raman Shift units
- the BWSpec file must be in pixel format

Click the *Use spectrum from a library* button to allow spectrum selection from a data library. Click the *Browse* button to select the library and to upload available samples into the Spectra in Library list. Then select the name of the spectrum that will be used in ID analysis.

Click *Run* to load the spectrum and search data libraries for a match.

In case of an error, an appropriate message will be displayed to the user.

ID Analysis Files

When the sample identification is completed, the collected spectrum and analysis results are saved in the files.
The spectrum is stored in a Grams SPC data file format (*.spc), while the ID analysis results are saved in a BWTek proprietary binary file format (*.bwl).

The output file names are created automatically by a date pattern: ID_*yyyymmddhhmmss.ext*, where *yyyy* stands for a year, *mm* is the month, *dd* is the day, *hh* is the hour (24 hour format), *mm* is minutes and *ss* is seconds of date and time when the sample identification was performed, and *ext* is the “spc” and “bwl” for the spectra and results file respectively.

The files, by default, are stored in the LogData\ID*Year* subfolder of the BWID® application main folder, where *Year* is the year when the analysis was performed. See Data Storage Configurations in Program Configuration paragraph for user defined data storage option.

ID Analysis Result

See Through ID Measurement

There are 3 possible results for an Identify Unknown Sample run:

- If only one chemical in the library matches the sample signature, then the result is a Match.
- If more than one chemical in the library matches the sample signature above the threshold HQI, and within the margin to the highest HQI value then they are listed as “Likely Match”.
- If no chemical in the library matches the sample signature, then the result is “No Match”.

For a Verify Sample run the possible results are based on the HQI value of the sample spectrum vs. the selected product. In this mode the software at first makes the comparison of the collected spectrum to the user-designated product. If there is no match with the user-designated product then the software does search the full library.

- Pass – sample is identified with HQI >= threshold HQI and there is a match with the user-designated product (product name must match).
- Fail- sample HQI< threshold HQI or HQI >= threshold HQI but the user-designated product name does not match with identified sample name.

Conventional ID Measurement

There are 2 possible results for an Identify Unknown Sample run:

- If at least one chemical in the library matches the sample signature, then the result is a Match.

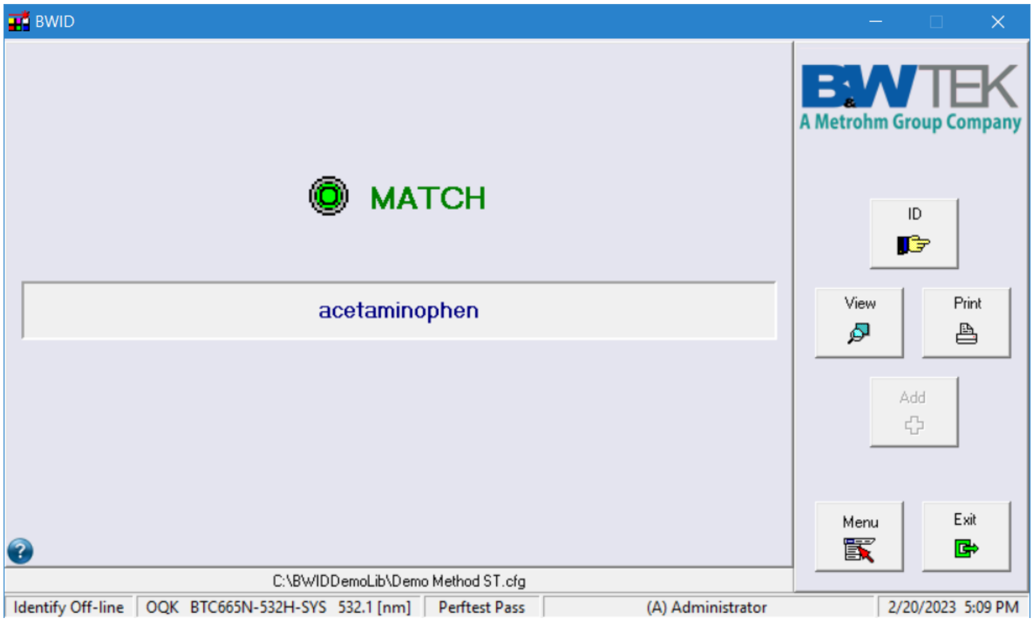
- If no chemical in the library matches the sample signature, then the result is “No Match”.

For a Verify Sample run the possible results are based on the HQI value of the sample spectrum vs. the selected product.

- Pass – sample is identified with HQI >= threshold HQI and there is a match with the user-designated product (product name must match).
- Fail- sample HQI< threshold HQI or HQI >= threshold HQI but the user-designated product name does not match with identified sample name.

If there is a match, the result dialog will appear (as shown below) indicating identification status (Match, Likely Match or Pass, depending on the ID mode) and the identified sample name.

ID result dialog with Simple ID Result option selected (see Program Configuration):



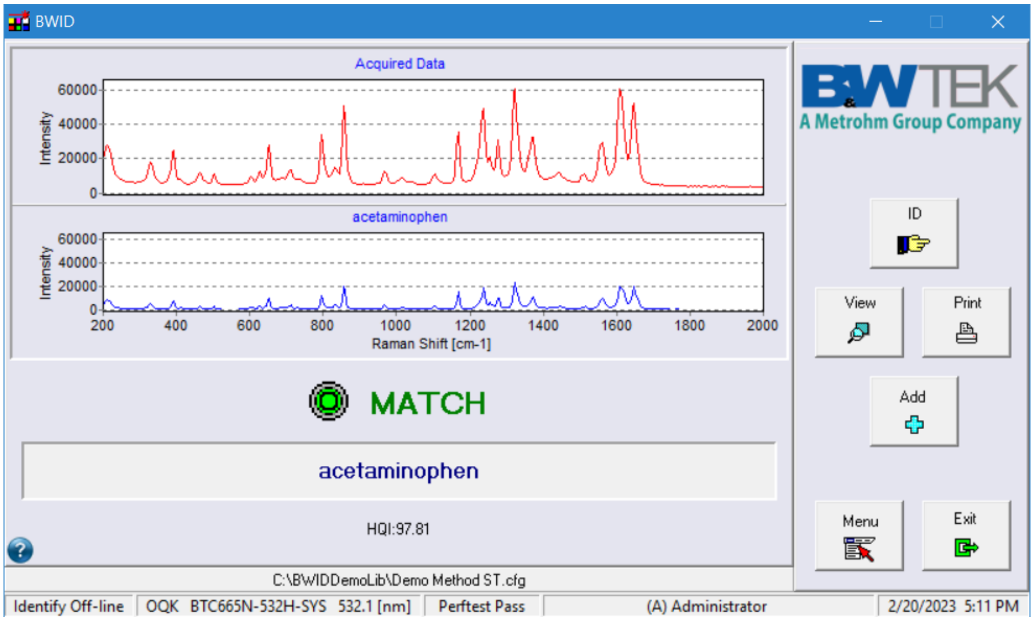
MATCH

acetaminophen

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:09 PM

ID result dialog with Simple ID Result option disabled (see Program Configuration):



MATCH

acetaminophen

HQI:97.81

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:11 PM

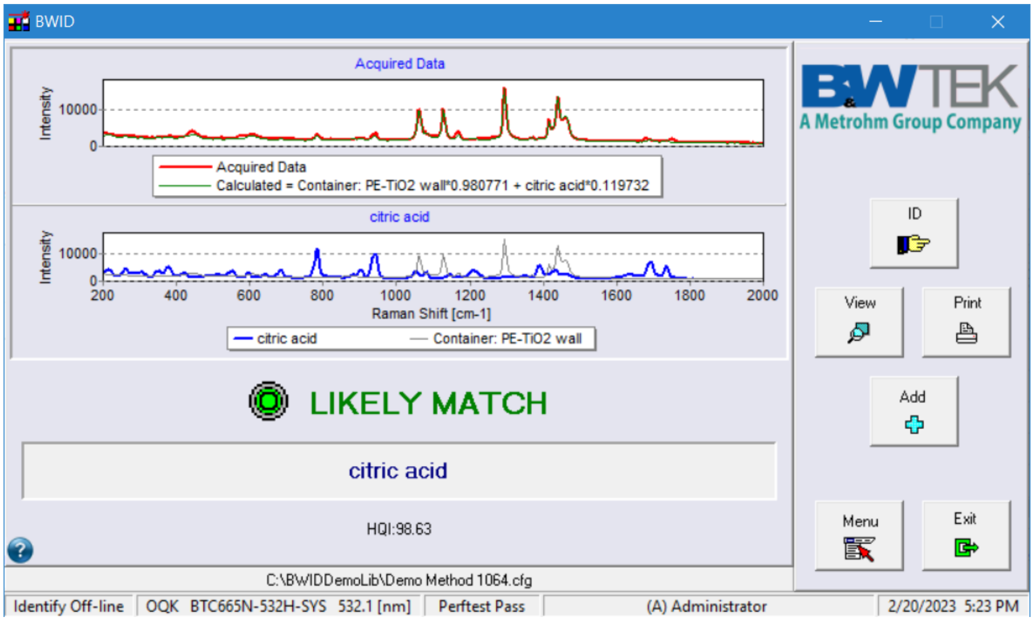
The upper graph shows the collected spectrum of the sample being analyzed while the lower graph displays the spectrum of a matched sample from the search library as well as the container material spectrum (if container spectrum was used in the see-through ID analysis).

For see through ID using a container spectrum, the upper graph will also include a Calculated Spectrum, with is a sum of the matched spectrum and the container spectrum with their weights also displayed. The displayed HQI is the matching index between the acquired spectrum and the Calculated Spectrum.

The HQI value of the match is displayed under the name of the matching spectrum.

Double clicking on a graph will maximize the dialog. Double clicking on a graph in the maximized dialog will restore original dialog size.

If there is likely match (see through ID only), the result dialog will appear as shown:



LIKELY MATCH

citric acid

HQI:98.63

C:\BWIDDemoLib\Demo Method 1064.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:23 PM

Click *View* to see analysis results details as shown under ID Analysis Results.

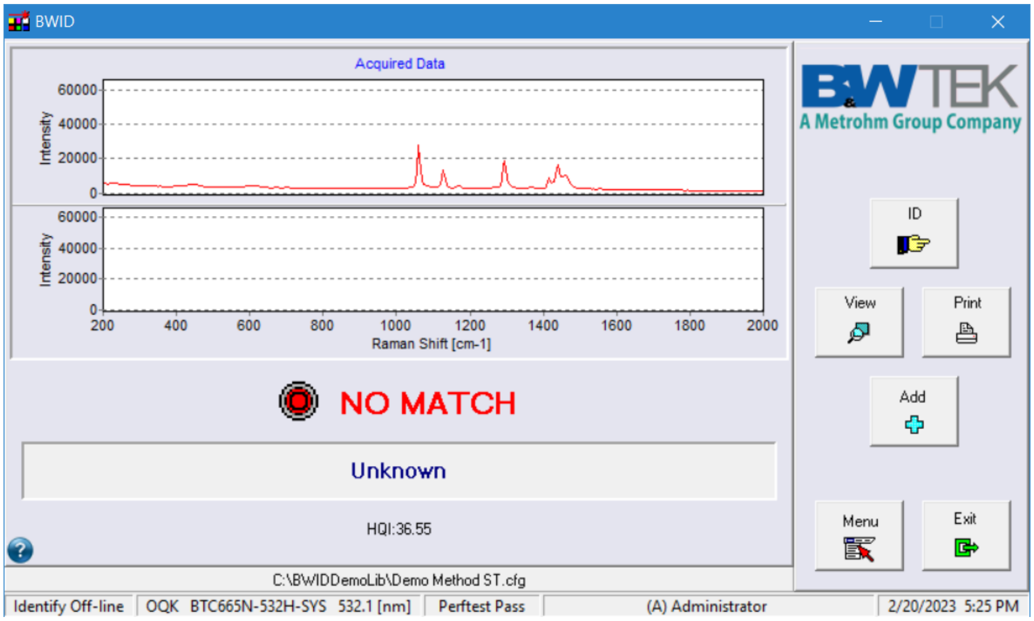
Click the *Print* button to print out the sample identification report.

Click *Add* to add collected spectrum to a library. This button is disabled when the spectrum for ID analysis is acquired from a library.

Click the *ID* button to start a new sample identification.

If the identification mode is set to Verify Sample and the identified sample name is the same as the sample name selected for the verification, the displayed status will be PASS (instead of MATCH).

If there is no match, the result dialog will appear as shown:



NO MATCH

Unknown

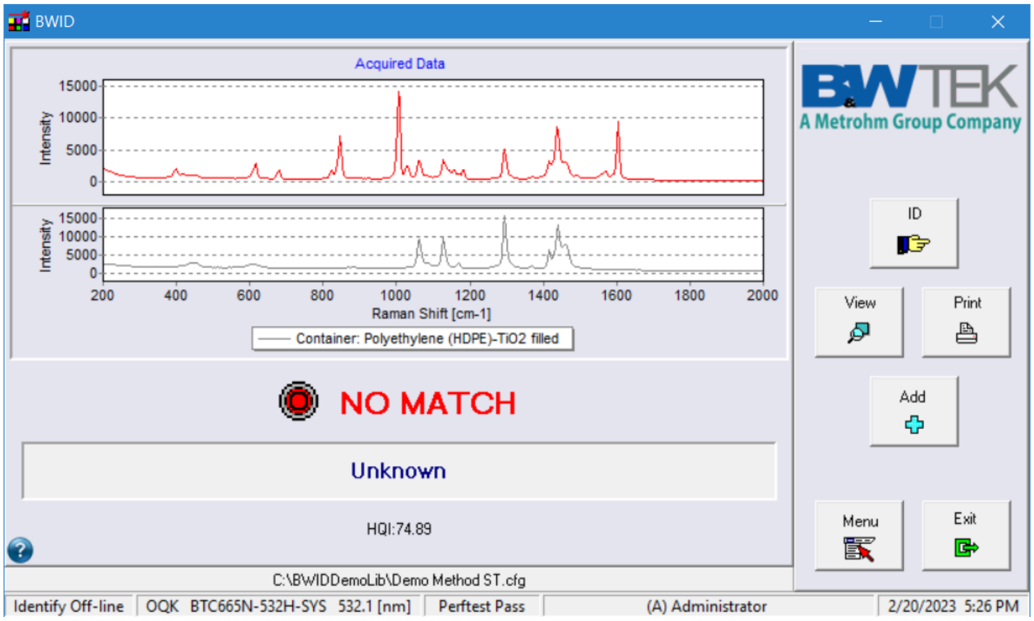
HQI:36.55

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:25 PM

If the identification mode is set to *Identify Unknown Sample*, the status is *No Match* and the sample name is *Unknown*.

If container spectrum was used in the see-through ID analysis, the lower graph will display the container material spectrum as shown below.



NO MATCH

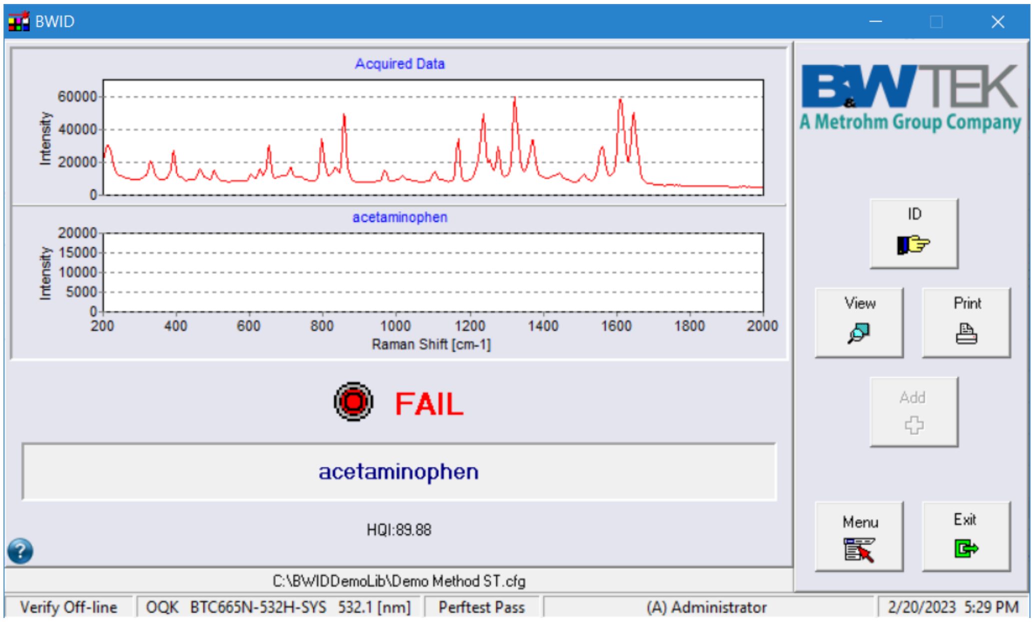
Unknown

HQI:74.89

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:26 PM

For the *Verify Sample* mode, the status is *Fail* and the sample name can be either an identified sample name found within the data library or UNKNOWN, if not found in the library.



FAIL

acetaminophen

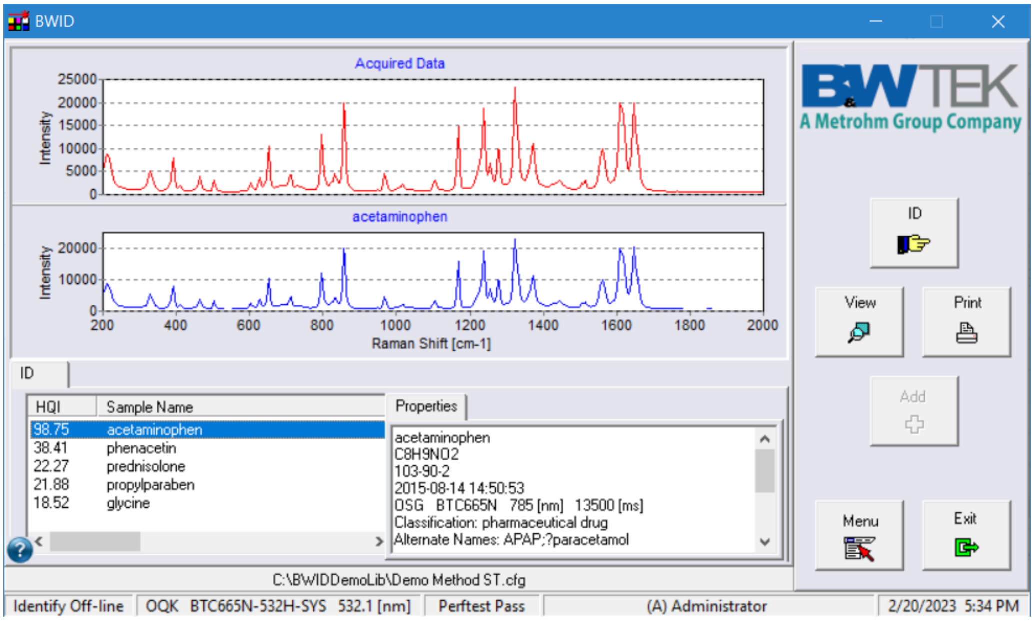
HQI:89.88

C:\BWIDDemoLib\Demo Method ST.cfg

Verify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:29 PM

ID Analysis Details

Upon clicking the *View* button, the following dialog will appear:



HQI	Sample Name
98.75	acetaminophen
38.41	phenacetin
22.27	prednisolone
21.88	propylparaben
18.52	glycine

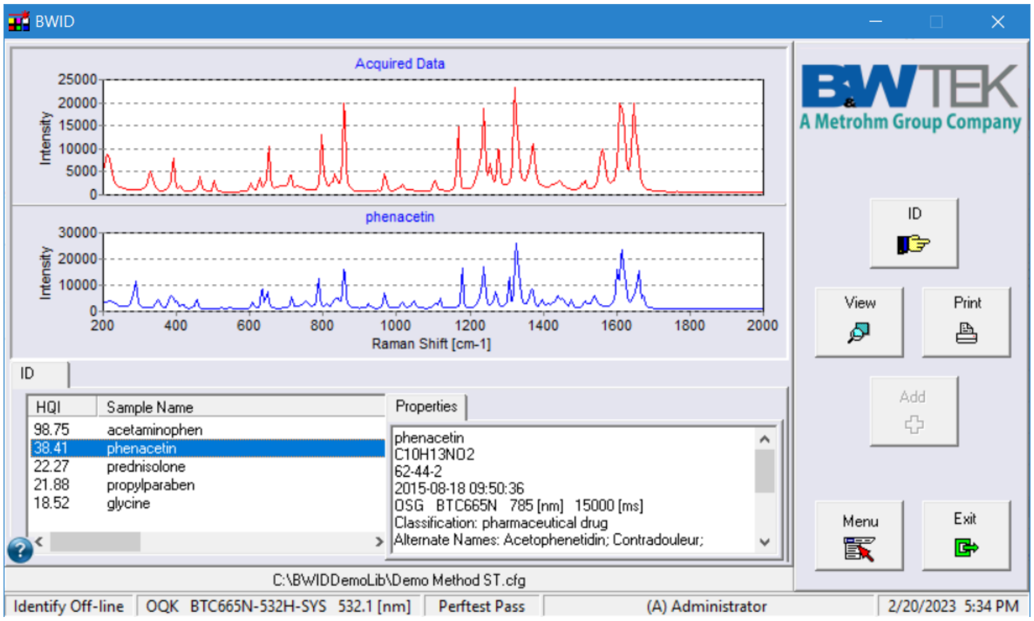
acetaminophen
C8H9NO2
103-90-2
2015-08-14 14:50:53
OSG BTC665N 785 [nm] 13500 [ms]
Classification: pharmaceutical drug
Alternate Names: APAP;?paracetamol

C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:34 PM

The left panel displays a list of *N* best hits of the ID search, where *N* is the number of hits specified by the user in the default method.

The Properties panel shows parameters of a sample selected in the hit list while the lower graph displays a spectrum of that sample.



HQI	Sample Name
98.75	acetaminophen
38.41	phenacetin
22.27	prednisolone
21.88	propylparaben
18.52	glycine

phenacetin
C10H13NO2
62-44-2
2015-08-18 09:50:36
OSG BTC665N 785 [nm] 15000 [ms]
Classification: pharmaceutical drug
Alternate Names: Acetophenetidin; Contradouleur;

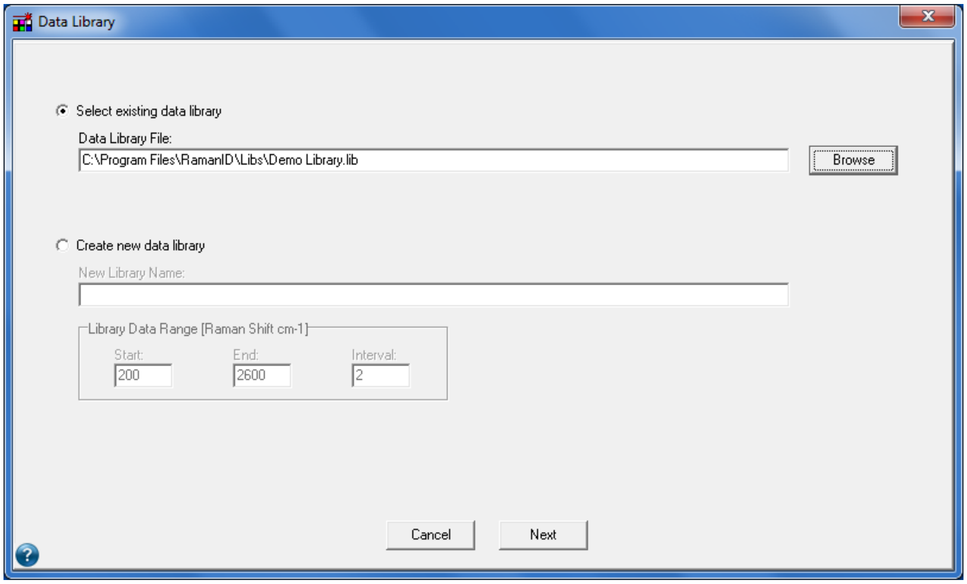
C:\BWIDDemoLib\Demo Method ST.cfg

Identify Off-line | OQK BTC665N-532H-SYS 532.1 [nm] | Perftest Pass | (A) Administrator | 2/20/2023 5:34 PM

Click the *View* button to go back to the ID analysis result dialog.

Add ID Spectrum to Library

Upon clicking the *Add* button, the following dialog will appear:



● Select existing data library

Data Library File: C:\Program Files\RamanID\Libs\Demo Library.lib

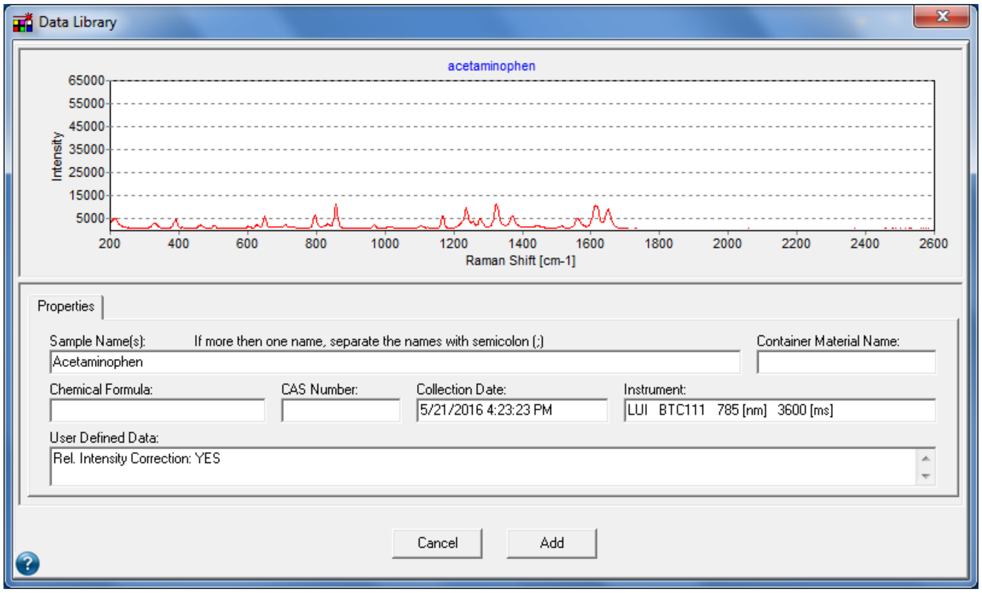
○ Create new data library

New Library Name:

Library Data Range [Raman Shift cm-1]

Start: 200
End: 2600
Interval: 2

Select a library (existing or new) to which you want to add the spectrum and then click the *Next* button. The following dialog will appear:



Sample Name(s): If more then one name, separate the names with semicolon (;)

Acetaminophen

Container Material Name:

Chemical Formula:

CAS Number:

Collection Date: 5/21/2016 4:23:23 PM

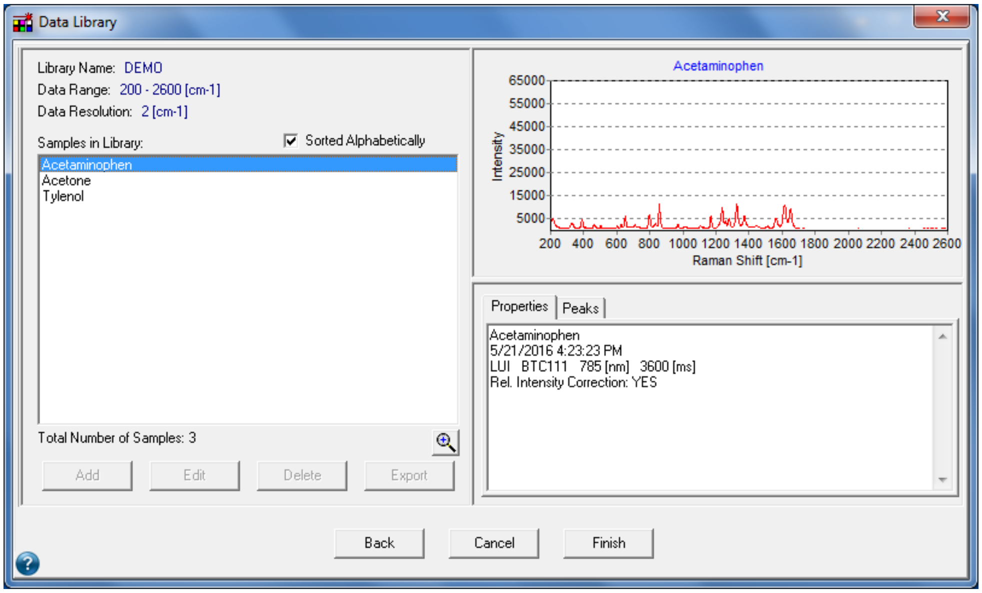
Instrument: LUI BTC111 785 [nm] 3600 [ms]

User Defined Data: Rel. Intensity Correction: YES

To cancel adding spectrum to the library, click the *Cancel* button.

To add the sample to the library, enter the sample name (mandatory) and other information (optional) related to the sample, then click the *Add* button.

Upon clicking the *Add* button, the following dialog will be displayed showing the contents of the library with the new sample added to it:



Library Name: DEMO
Data Range: 200 - 2600 [cm-1]
Data Resolution: 2 [cm-1]

Samples in Library: ☑ Sorted Alphabetically

- Acetaminophen
- Acetone
- Tylenol

Total Number of Samples: 3

Acetaminophen
5/21/2016 4:23:23 PM
LUI BTC111 785 [nm] 3600 [ms]
Rel. Intensity Correction: YES

Click the *Finish* button to finish library generation and save the library data in the file.

Click the *Cancel* button to quit library modifications.

Click the *Back* button to select another library to which you want to add the spectrum.

10. Diagnostic Tests

Performance Test

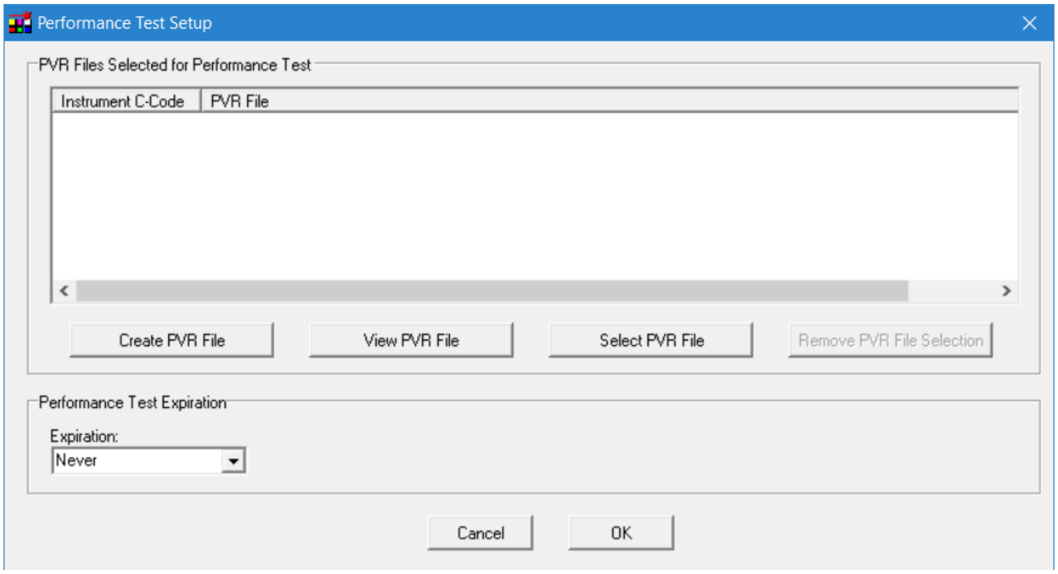
The performance test is a procedure that evaluates electronical and optical performance of a device.
It consists of several items which cover from hardware stability to spectral performance. These items include:
electronic bias, readout noise, dark current, spectral range, Raman shift accuracy, photometric accuracy and precision, HQI for shape check.

The test settings are saved in a Performance Validation Reference (PVR) file. The user has to pre-select a PVR file to be used for performance validation with given instrument.

The performance test should be executed on a regular basis to ensure the consistency and quality of performance output from the instrument.

Test Configuration

Click the *Setup* button in the Menu window and then *PerfTest* in the Setup menu to configure the performance test.
The Performance Test Setup dialog will appear:



PVR Files Selected for Performance Test list holds pre-selected PVR files that will be used when running instrument performance validation. There can be one PVR file selected for a given instrument.

Click *Create PVR File* to generate a PVR file. For more details, see the PVR File Creation paragraph below.

Click *View PVR File* to see the test settings of a PVR file. For more details, see the PVR File Viewing paragraph below.

Click *Select PVR File* to select a PVR file to be used in instrument performance validation. For more details, see the PVR File Selection paragraph below.

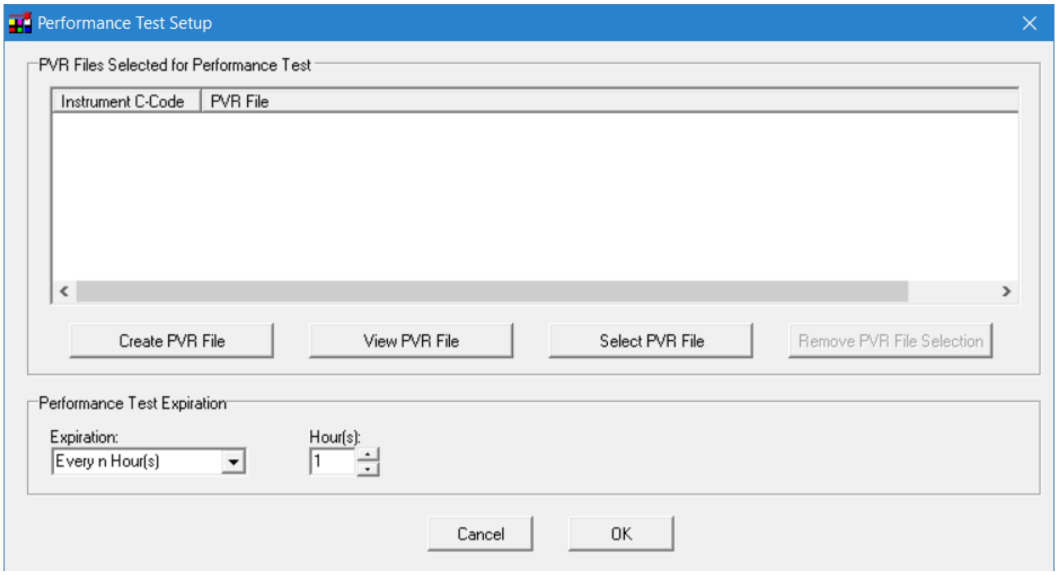
Click *Remove PVR File Selection* to delete selection from the list. A confirmation message will be displayed before the PVR file selection will be deleted from the list.

Performance test expiration allows to define how long a last passed performance test will remain valid.
Expiration – set the schedule for a performance test to be expired. Select one from the following options: never, every n

hours, every n days, every n weeks, every n months.

If *never* option is selected, no mandatory performance test is required and the test will be run at the discretion of the user.
For all other expiration options, the user will be asked to run a new performance test if the last performed test is out of date or has failed.
If the user is of Operator status, the user will not be able to use the instrument to run ID analysis (or create a data library) until the performance test passes.
If the user is of Developer or Administrator status, the user will be notified that a new performance test should be run, but will be able to run ID analysis or generate a data library.

If *Every n Hours(s)* is selected, the test will expire every *N* hours from time the test was executed, where *N* is specified in the *Hour(s)* field, as shown below:



Performance Test Setup

PVR Files Selected for Performance Test

Instrument C-Code	PVR File

Performance Test Expiration

Expiration: Every n Hour(s)

Hour(s): 1

The maximum hourly expiration is 24 hours.

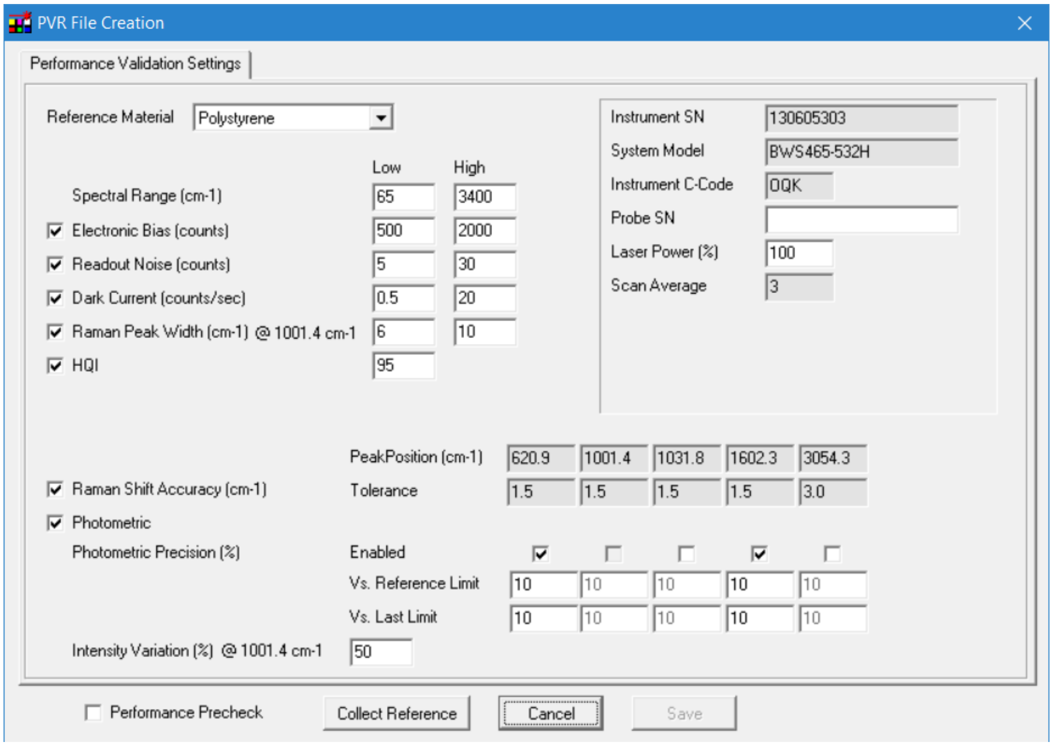
For all other expiration options, the corresponding field will allow the user to set number of days, weeks or months with maximum value of 356 days, 56 weeks and 12 months respectively.

Click the *OK* button to accept performance test settings and return to the Menu window.

Click the *Cancel* button to abort performance test settings and return to the Menu window.

PVR File Creation

Upon clicking the *Create PVR File* button in the Performance Test Setup dialog, the PVR File Creation dialog will appear:



☐ Performance Precheck

Reference Material: Polystyrene

	Low	High
Spectral Range (cm-1)	65	3400
☑ Electronic Bias (counts)	500	2000
☑ Readout Noise (counts)	5	30
☑ Dark Current (counts/sec)	0.5	20
☑ Raman Peak Width (cm-1) @ 1001.4 cm-1	6	10
☑ HQI	95	

Instrument SN: 130605303
System Model: BWS465-532H
Instrument C-Code: 0QK
Probe SN:
Laser Power (%): 100
Scan Average: 3

	PeakPosition (cm-1)	620.9	1001.4	1031.8	1602.3	3054.3
☑ Raman Shift Accuracy (cm-1)	Tolerance	1.5	1.5	1.5	1.5	3.0
☑ Photometric						
Photometric Precision (%)	Enabled	☑	☐	☐	☑	☐
	Vs. Reference Limit	10	10	10	10	10
	Vs. Last Limit	10	10	10	10	10

Intensity Variation (%) @ 1001.4 cm-1: 50

Reference material – select one of the following standard materials to be used for performance validation: Polystyrene (default), Cyclohexane, Acetaminophen (Paracetamol).

Spectral Range – set spectral data range (Raman shift) to be used in the test. For default spectral range of a given instrument type see “Test Limits for Hardware Stability” table below.

Note, that selection of the reference material type along with spectral range will determine how many peaks will be available for the peak related tests.

Electronic Bias (counts) – check the box and set the low and high limits to run electronic bias test. This test checks electronic bias of the detector, measured as the average intensity of all pixels acquired in dark with minimum integration time. Refer to “Test Limits for Hardware Stability” table below for default range values.

Readout Noise (counts) – check the box and set the low and high limits to run readout noise test. Refer to “Test Limits for

Hardware Stability" table below for default range values.

Dark current (counts/sec) – check the box and set the low and high limits to run dark current test. Dark current is proportional to integration time and is measured on a dark spectrum acquired with a long integration time of 60 seconds. Refer to "Test Limits for Hardware Stability" table below for default range values.

Raman Peak Width (cm-1) @ 1001.4 cm-1– check the box and set the low and high limits to test main peak's Raman shift width (also called Raman peak FWHM). Refer to "Test Limits for Hardware Stability" table below for default range values. Main peak (and its Raman shift position) dependents on selected reference material. For the polystyrene, it is at 1001.4 cm-1. Refer to "Reference Standard Peaks Parameters" table below for the details. Refer to "Reference Standard Peaks Parameters" table below for the details. If the main peak is not within selected spectral range, the test is disabled.

HQI – check the box and set a threshold to run relative correlation HQI test, which is to check the entire spectrum in selected spectral range for the shape and to make sure there is no significant offset such as hot pixel, stray light and etc. Default threshold is 95.

Raman Shift Accuracy (cm-1) – check the box to test Raman shift accuracy (also called wavelength accuracy) for all predefined standard peaks within selected spectral range. Refer to "Reference Standard Peaks Parameters" table below for predefined peaks positions and accuracy limits (fixed settings). If there is no peak within spectral range, the test is disabled.

Photometric – check the box to test photometric precision (also called intensity precision) on selected peaks (main peak excluded) and intensity variation (also called intensity accuracy) on the main peak. If there is no peak within selected spectral range, the whole photometric test is disabled. If the main peak is not within spectral range, the intensity variation test is disabled. If the main peak is the only standard peak within spectral range, the photometric precision test is disabled. Refer to "Reference Standard Peaks Parameters" table below for predefined peaks positions and the main peak definition.

Photometric precision (%) will check two variations on normalized spectra: measured vs. reference spectrum and measured vs. last validation spectrum. All spectra (measured, reference and from last validation) are normalized to their heights at the same main peak. Variation of measured vs. reference is the percentage ratio of difference between peak height from measured scan and from reference scan divided by peak height from reference scan at the same peak position. Variation of measured vs. last is the percentage ratio of difference between peak height from measured scan and from last validation scan divided by peak height from last validation scan at the same peak position.

For photometric precision test select peaks that should be tested by checking *Enabled* check boxes for corresponding peak. Peaks NOT highlighted in green in the "Reference Standard Peaks Parameters" table below are selected by default. Then specify the limits for all selected peaks (default limit is 10%).

Intensity variation (%) @ 1001.4 cm-1 is the height deviation from measured validation data to reference spectrum at the same main peak of the same kind of reference material. Default limit is 50 %.

Laser Power (%) – set laser power to collect reference spectrum with (default 100).

Probe SN – serial number of a probe to be used to collect reference spectrum (optional).

All other fields are set automatically and they are read only: *Instrument SN* – instrument serial number, *System Model* – instrument system model, *Instrument C-Code* – instrument c-code, *Scan Average* – number of average scans to collect reference spectrum.

Performance Precheck – check the box to validate instrument performance upon creating a PVR file (on Save button click).

Click *Collect Reference* button to acquire spectral data for a PVR file creation.

Table: Test Limits for Hardware Stability

Product Name	Model	Electronic Bias	Readout Noise	Dark current	Raman Peak FWHM*	Spectral Range (cm-1)
QTRam, STRam-785	BWS475-785H-HT(ST, CU)	(100,500)	(2,7)	(0.5,10)	(7.5,10)	(150,2800)
STRam-1064	BWS475-1064-ST	(1000,4000)	(5,30)	(20,200)	(12,18)	(100,2500)
i-Raman Pro	BWS475-785S	(100,500)	(2,7)	(0.5,10)	(6,8)	(65,3350)
	BWS475-785H	(100,500)	(2,7)	(0.5,10)	(5.5,7.5)	(65,2800)
	BWS475-532S	(100,500)	(2,7)	(0.5,10)	(8.5,12.5)	(65,4200)
	BWS475-532H	(100,500)	(2,7)	(0.5,10)	(7.5,11.5)	(65,3400)
i-Raman Prime	BWS475-785H-HT	(100,500)	(2,7)	(0.5,10)	(7.5,10)	(150,2800)
	BWS475-785S-HT	(100,500)	(2,7)	(0.5,10)	(8.5,12.5)	(150,3350)
	BWS475-532H-HT	(100,500)	(2,7)	(0.5,10)	(9.5,13.5)	(150,3400)
	BWS475-1064-HT	(1000,4000)	(5,30)	(20,200)	(12,18)	(100,2500)
i-Raman Plus	BWS465-785S	(500,2000)	(5,30)	(0.5,20)	(5,9)	(65,3350)
	BWS465-785H	(500,2000)	(5,30)	(0.5,20)	(4,8)	(65,2800)
	BWS465-532S	(500,2000)	(5,30)	(0.5,20)	(7,11)	(65,4200)
	BWS465-532H	(500,2000)	(5,30)	(0.5,20)	(6,10)	(65,3400)
i-Raman EX	BWS485II	(1000,4000)	(5,30)	(20,200)	(12,18)	(100,2500)

*** Use peak position defined in the table below.**

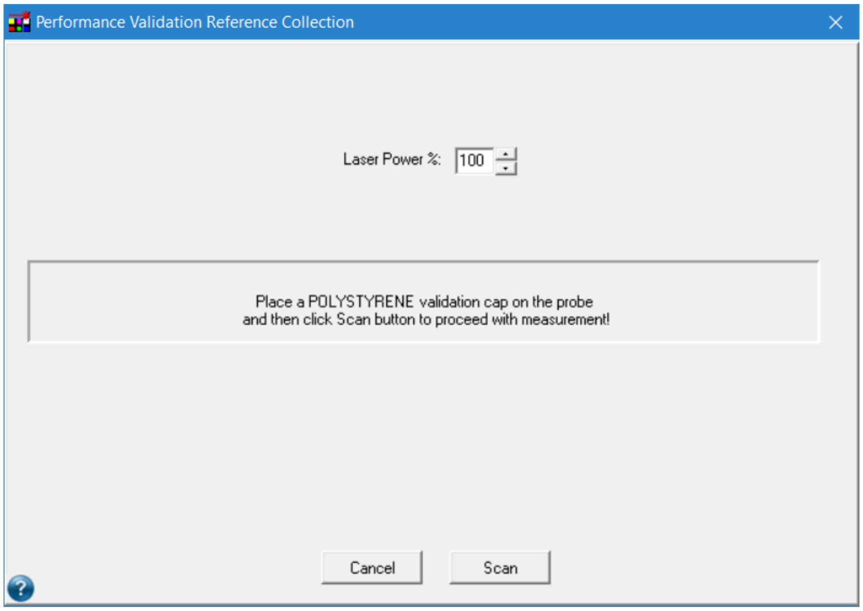
Table: Reference Standard Peaks Parameters

Reference Material	Wavenumber shifts (cm-1)	Tolerance(cm-1) benchtop
Polystyrene	620.9	1.5
	1001.4*	1.5
	1031.8	1.5
	1602.3	1.5
	3054.3	3.0
Acetaminophen	797.2	1.5
	857.9*	1.5

	1168.5	1.5
	1236.8	1.5
	1323.9	1.5
	1648.4	1.5
	2931.1	2.0
Cyclohexane	801.3*	1.5
	1028.3	1.0
	1266.4	1.0
	1444.4	1.0
	2852.9	2.0

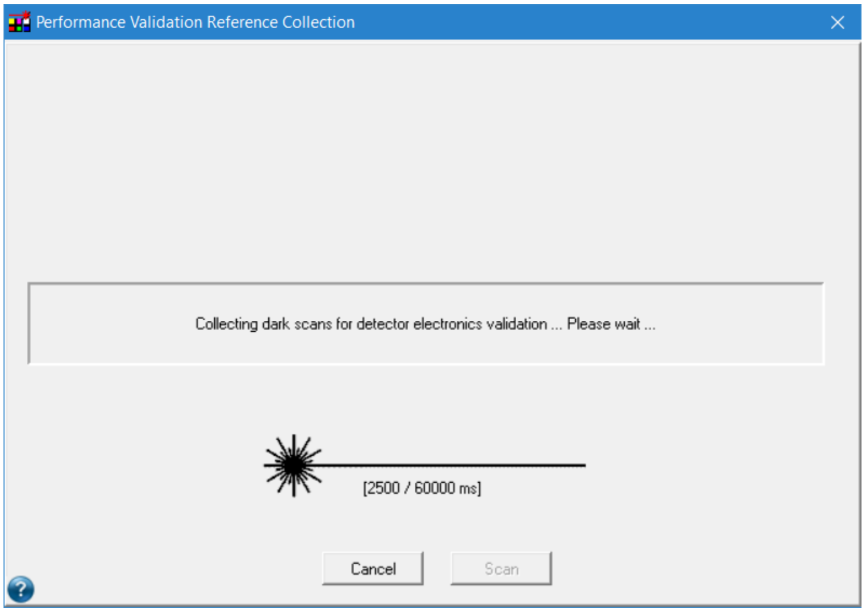
*** Main peak for given reference standard material**

Upon clicking the *Collect Reference* button, the following dialog will appear.



Place a POLYSTYRENE validation cap on the probe
and then click Scan button to proceed with measurement!

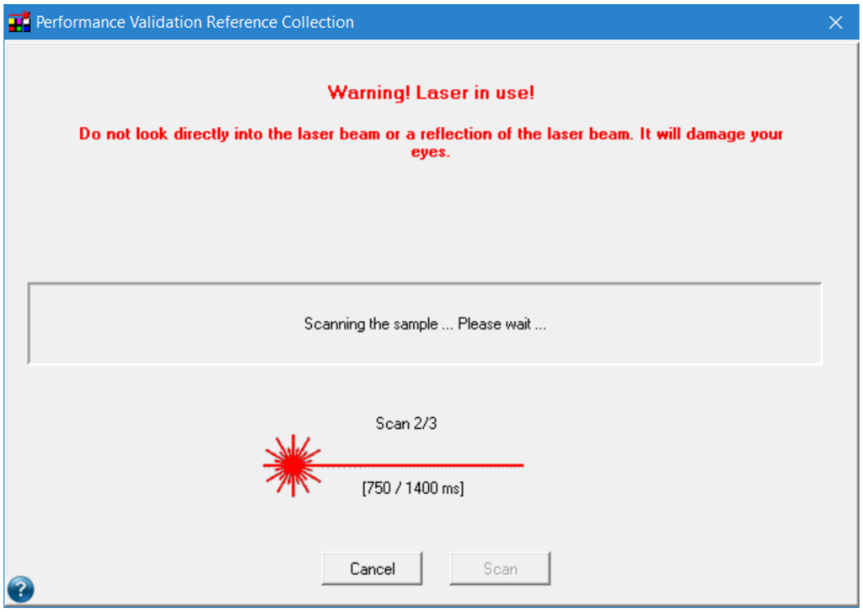
Once a reference standard sample is in place for a measurement, click the *Scan* button. First, the program will collect three dark spectra for detector electronics validation (2 spectra with instrument’s minimum integration time and the 3rd one with 60 seconds integration time).



Collecting dark scans for detector electronics validation ... Please wait ...

[2500 / 60000 ms]

Next the program will scan the reference sample (raw and dark spectra with 3 average scans for each) with auto integration.



Warning! Laser in use!

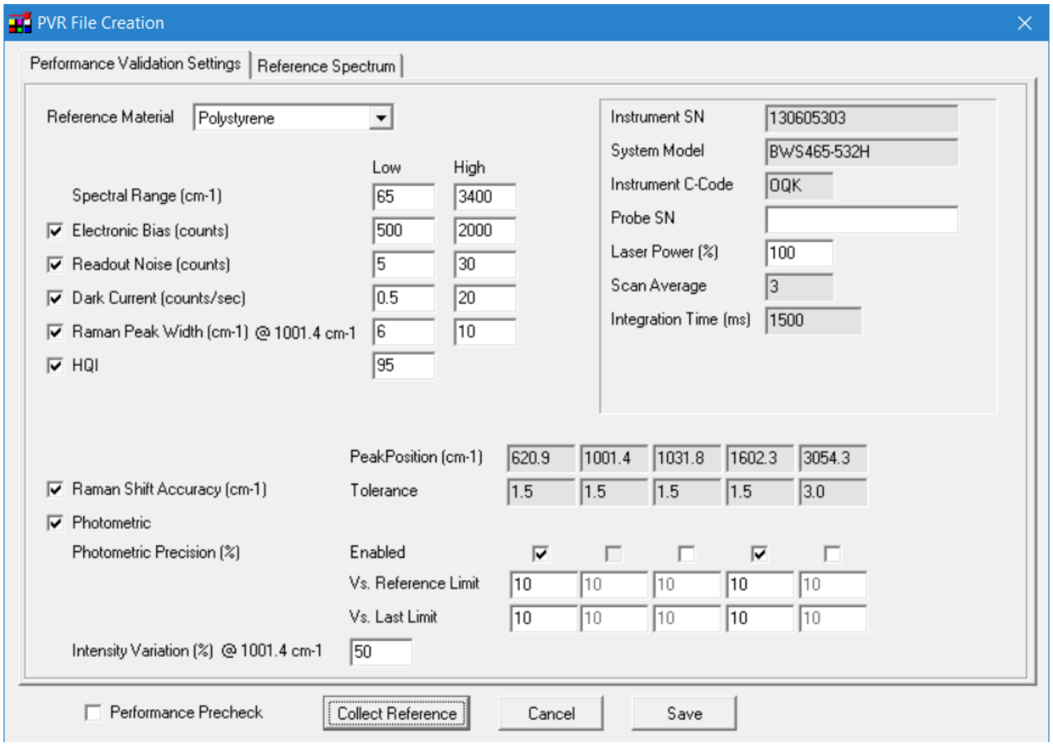
Do not look directly into the laser beam or a reflection of the laser beam. It will damage your eyes.

Scanning the sample ... Please wait ...

Scan 2/3

[750 / 1400 ms]

Once the spectra are collected, the PVR File Creation dialog will contain additional data: collected reference spectrum (dark subtracted) in the Reference Spectrum tab and the integration time used to collect reference spectrum in the *Integration Time* field in Performance Validation Reference tab as shown below.



Reference Material: Polystyrene

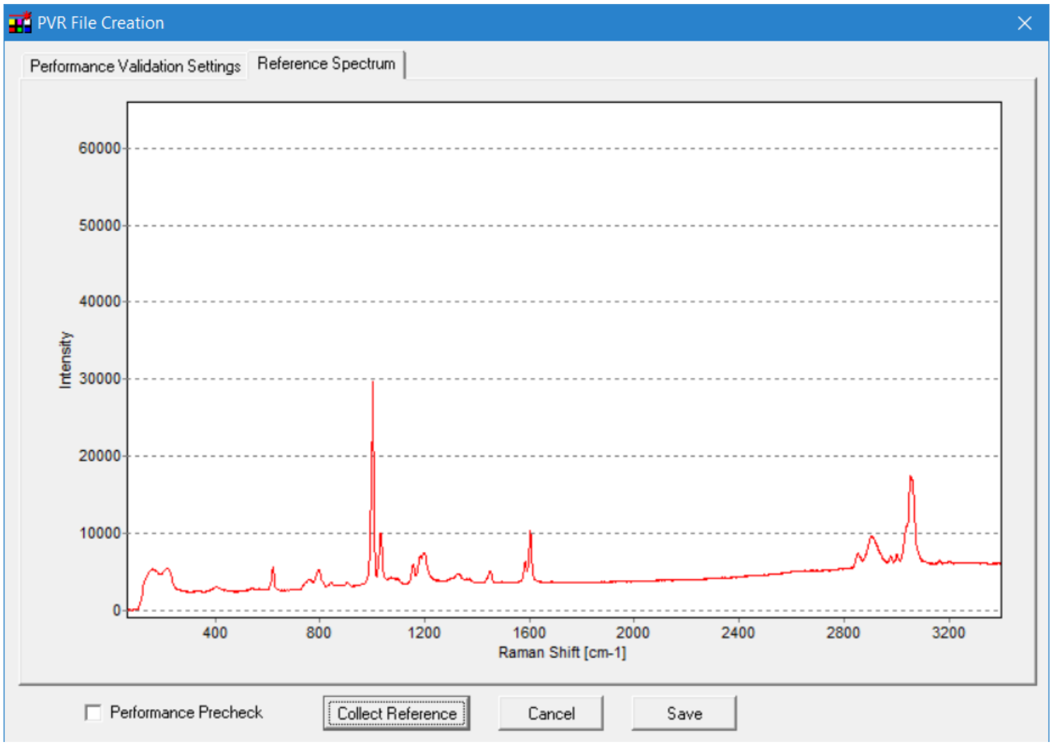
	Low	High
Spectral Range (cm-1)	65	3400
☑ Electronic Bias (counts)	500	2000
☑ Readout Noise (counts)	5	30
☑ Dark Current (counts/sec)	0.5	20
☑ Raman Peak Width (cm-1) @ 1001.4 cm-1	6	10
☑ HQI	95	

Instrument SN: 130605303
System Model: BWS465-532H
Instrument C-Code: 0QK
Probe SN:
Laser Power (%): 100
Scan Average: 3
Integration Time (ms): 1500

	PeakPosition (cm-1)	620.9	1001.4	1031.8	1602.3	3054.3
☑ Raman Shift Accuracy (cm-1)	Tolerance	1.5	1.5	1.5	1.5	3.0
☑ Photometric						
Photometric Precision (%)	Enabled	☑	☐	☐	☑	☐
	Vs. Reference Limit	10	10	10	10	10
	Vs. Last Limit	10	10	10	10	10

Intensity Variation (%) @ 1001.4 cm-1: 50

☐ Performance Precheck



Click *Save* button to generate a PVR file. The standard Save As dialog will apear to allow the user to select an output file name and its location.

Prior to the file creation, depending on the *Performance Precheck* box status, the performance validation settings and collected reference spectral data will be validated.

If the *Performance Precheck* box is unchecked (default), the program checks if collected reference spectrum matches with selected reference material.

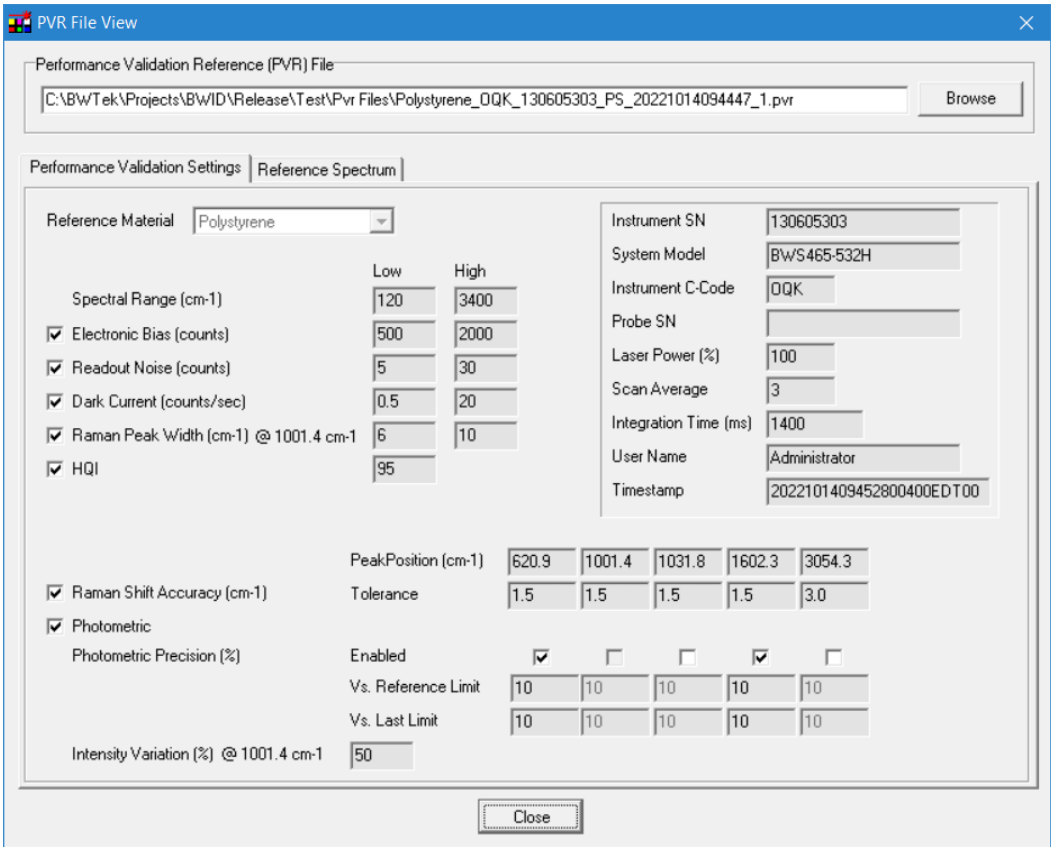
If the *Performance Precheck* box is checked, the program first checks if collected reference spectrum matches with selected reference material. Then upon success, it validates all other PVR file settings, collected reference spectrum (with regards to selected peaks in spectral range, Raman shift accuracy and Raman peak width, if selected) as well as detector electronics (if selected).

If validation fails due to mismatching scanned reference spectrum with selected reference material type, the PVR file will not be cretaed. Otherwise, even if the performance precheck fails (e.g. detector electronics test failed), the PVR file will be created but a correspodning warning message will be displayed.

Click *Cancel* to abort PVR file creation and return to the Performance Test Setup dialog.

PVR File Viewing

Upon clicking the *View PVR File* button in the Performance Test Setup dialog, the following dialog will appear.



Performance Validation Reference (PVR) File: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

Reference Material: Polystyrene

	Low	High
Spectral Range (cm-1)	120	3400
☑ Electronic Bias (counts)	500	2000
☑ Readout Noise (counts)	5	30
☑ Dark Current (counts/sec)	0.5	20
☑ Raman Peak Width (cm-1) @ 1001.4 cm-1	6	10
☑ HQI	95	

Instrument SN: 130605303
System Model: BWS465-532H
Instrument C-Code: OQK
Probe SN:
Laser Power (%): 100
Scan Average: 3
Integration Time (ms): 1400
User Name: Administrator
Timestamp: 2022101409452800400EDT00

	PeakPosition (cm-1)	620.9	1001.4	1031.8	1602.3	3054.3
☑ Raman Shift Accuracy (cm-1)	Tolerance	1.5	1.5	1.5	1.5	3.0
☑ Photometric						
Photometric Precision (%)	Enabled	☑	☐	☐	☑	☐
	Vs. Reference Limit	10	10	10	10	10
	Vs. Last Limit	10	10	10	10	10

Intensity Variation (%) @ 1001.4 cm-1: 50

If there is a PVR selected in the PVR files list in the Performance Test Setup dialog, the PVR File View dialog will show selected PVR file data.

Click *Browse* button to select a PVR file to be loaded for viewing.

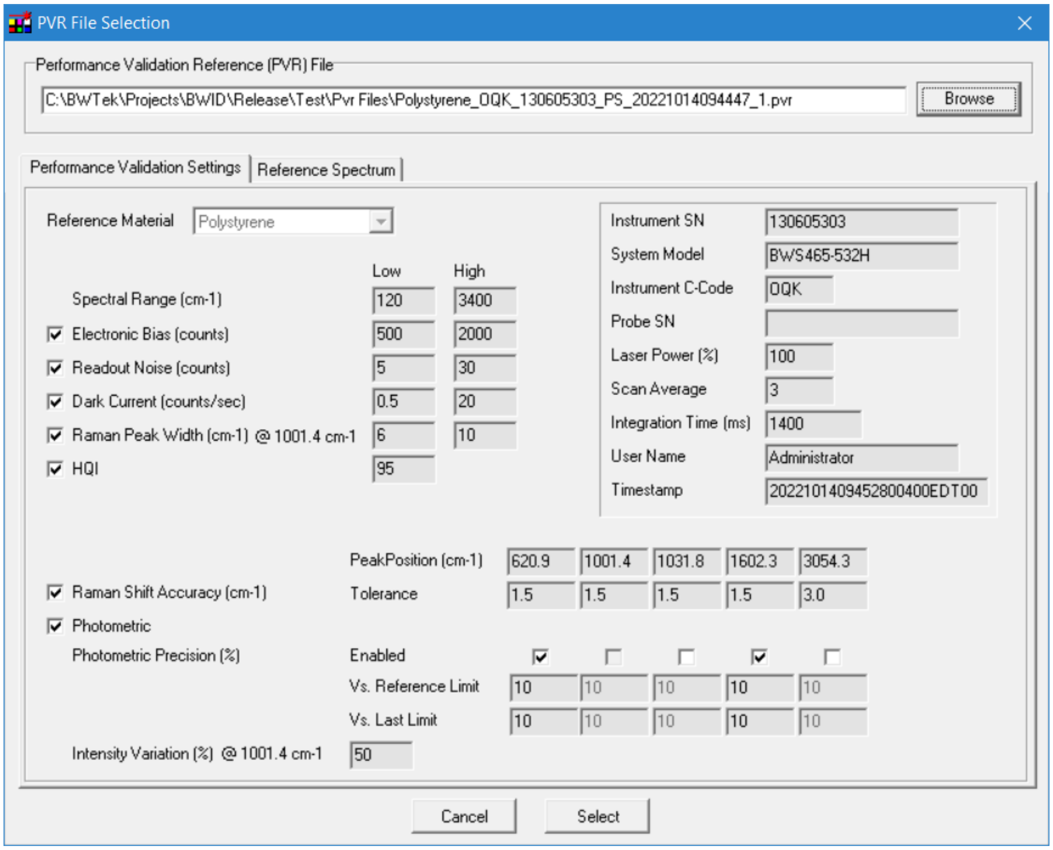
Timestamp – shows date and time of PVR file creation in the YYYYMMDDHHMMSSTimeZoneInfo format, where:
YYYY, MM and DD are year, month, and day respectively,
HH, MM and SS are hours, minutes and seconds respectively,
TimeZoneInfo is the UTC time offset (five digits, the first digit 0 for negative time offset and 1 for positive time offset, next 2 digits for hours and last 2 digits for minutes) followed by five characters representing the time zone abbreviation (if abbreviation length is less than 5, it is filled with trailing number 0). Example of time zone info: 00500EST00 which is decoded as UTC-05:00 Eastern Standard Time (US and Canada).

See Appendix B for list of time zone abbreviations used in the timestamp.

PVR File Selection

Upon clicking the *Select PVR File* button in the Performance Test Setup dialog, a standard open file dialog will be displayed to allow the user to pre-select a PVR file that will be used for an instrument validation. The c-code of the instrument stored in the selected PVR file will determine for which instrument the PVR file will be used.

Once the PVR file is selected the following dialog will appear showing the settings of selected PVR file.



Performance Validation Reference (PVR) File: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

Reference Material: Polystyrene

	Low	High
Spectral Range (cm-1)	120	3400
☑ Electronic Bias (counts)	500	2000
☑ Readout Noise (counts)	5	30
☑ Dark Current (counts/sec)	0.5	20
☑ Raman Peak Width (cm-1) @ 1001.4 cm-1	6	10
☑ HQI	95	

Instrument SN: 130605303
System Model: BWS465-532H
Instrument C-Code: OQK
Probe SN:
Laser Power (%): 100
Scan Average: 3
Integration Time (ms): 1400
User Name: Administrator
Timestamp: 20221014094528000400EDT00

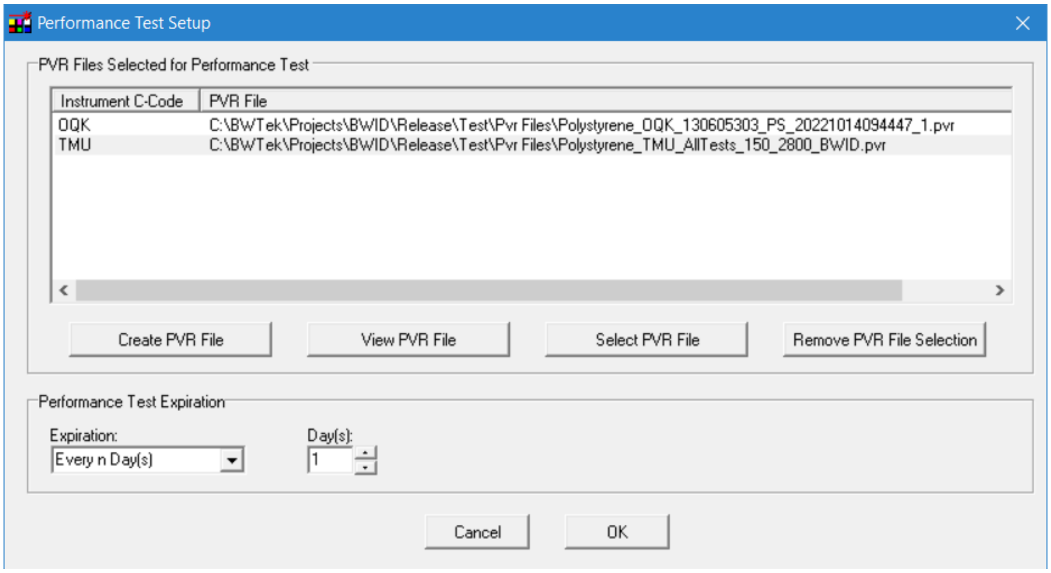
	PeakPosition (cm-1)	620.9	1001.4	1031.8	1602.3	3054.3
☑ Raman Shift Accuracy (cm-1)	Tolerance	1.5	1.5	1.5	1.5	3.0
☑ Photometric						
Photometric Precision (%)	Enabled	☑	☐	☐	☑	☐
	Vs. Reference Limit	10	10	10	10	10
	Vs. Last Limit	10	10	10	10	10
Intensity Variation (%) @ 1001.4 cm-1	50					

Click *Browse* button to select another PVR file.

Click *Cancel* to abort PVR file selection and return to the Performance Test Setup dialog.

Click *Select* button to pre-select the PVR file to be used in performance validation for the instrument with given instrument c-code.

The list with PVR files selected for performance test in the Performance Test Setup dialog will be updated accordingly.



Instrument C-Code	PVR File
OQK	C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr
TMU	C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_TMU_AllTests_150_2800_BWID.pvr

Expiration: Every n Day(s)

Day(s): 1

Click *OK* button to accept all settings.

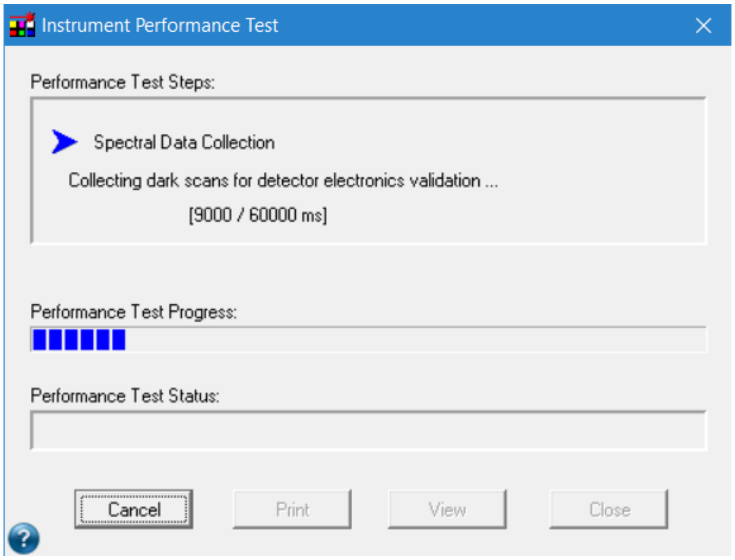
Click *Cancel* button to abort the performance test setup.

Test Running

Click the *Diagnostic* button in the Menu window and then *PerfTest* in the Diagnostic menu to run a performance test. First, the user will be asked to place a polystyrene validation cap on the probe and click *OK* button to proceed with the test (or *Cancel* button to abort the test).

Upon clicking the *OK* button, the performance test will begin. The current step and progress of the performance validation will be displayed. The user may abort the test any time by clicking the *Cancel* button.

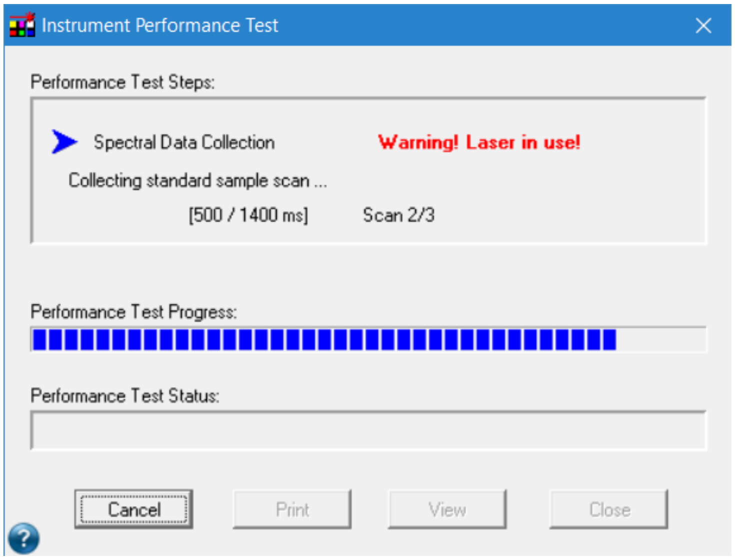
If there is at least one test of detector electronics selected in the PVR file, the dark spectra (2 scans with instrument's minimum integration time and 3rd scan with 60 seconds integration time) for detector electronics validation will be collected first as shown below.



Collecting dark scans for detector electronics validation ...

[9000 / 60000 ms]

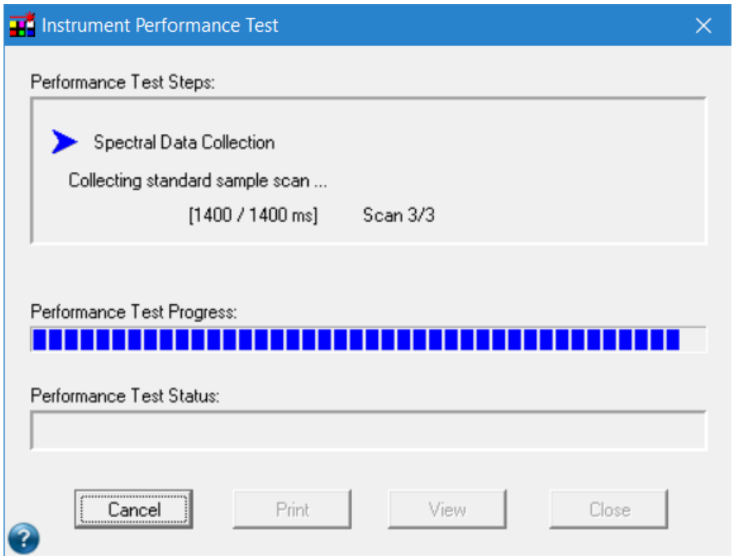
Next the program will scan the reference sample (raw and dark spectra with 3 average scans for each) with the same integration time the reference spectrum in the PVR file was collected.



Warning! Laser in use!

Collecting standard sample scan ...

[500 / 1400 ms] Scan 2/3



Instrument Performance Test

Performance Test Steps:

Spectral Data Collection

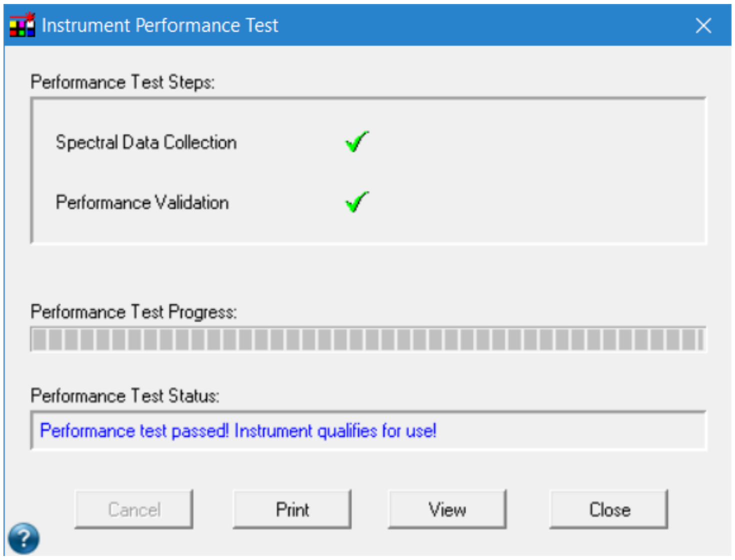
Collecting standard sample scan ...

[1400 / 1400 ms] Scan 3/3

Performance Test Progress:

Performance Test Status:

Once the test is completed, the collected spectra and results are saved, and the user can view the results or print a test report.



Instrument Performance Test

Performance Test Steps:

Spectral Data Collection ✓

Performance Validation ✓

Performance Test Progress:

Performance Test Status:

Performance test passed! Instrument qualifies for use!

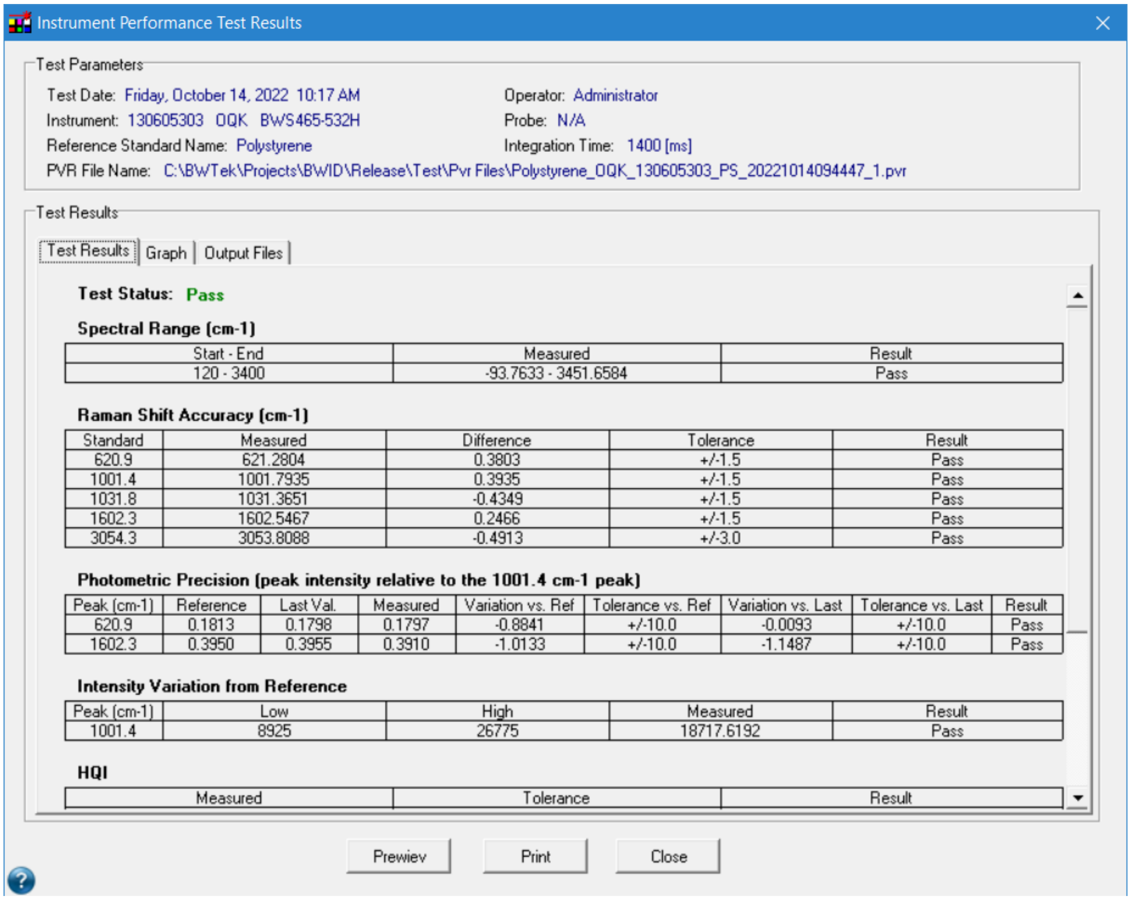
Click the *View* button to view detailed test results (see Test Results below).

Click *Print* to print test results report.

Click *Close* to close the performance test dialog and go back to the Menu window.

Test Results

Upon clicking the *View* button, the Instrument Performance Test Results dialog will appear as shown below.



Test Date: Friday, October 14, 2022 10:17 AM
Operator: Administrator
Instrument: 130605303 OQK BWS465-532H
Probe: N/A
Reference Standard Name: Polystyrene
Integration Time: 1400 [ms]
PVR File Name: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

Test Status: Pass

Spectral Range (cm-1)

Start - End	Measured	Result
120 - 3400	-93.7633 - 3451.6584	Pass

Raman Shift Accuracy (cm-1)

Standard	Measured	Difference	Tolerance	Result
620.9	621.2804	0.3803	+/-1.5	Pass
1001.4	1001.7935	0.3935	+/-1.5	Pass
1031.8	1031.3651	-0.4349	+/-1.5	Pass
1602.3	1602.5467	0.2466	+/-1.5	Pass
3054.3	3053.8088	-0.4913	+/-3.0	Pass

Photometric Precision (peak intensity relative to the 1001.4 cm-1 peak)

Peak (cm-1)	Reference	Last Val.	Measured	Variation vs. Ref	Tolerance vs. Ref	Variation vs. Last	Tolerance vs. Last	Result
620.9	0.1813	0.1798	0.1797	-0.8841	+/-10.0	-0.0093	+/-10.0	Pass
1602.3	0.3950	0.3955	0.3910	-1.0133	+/-10.0	-1.1487	+/-10.0	Pass

Intensity Variation from Reference

Peak (cm-1)	Low	High	Measured	Result
1001.4	8925	26775	18717.6192	Pass

HQI

Measured	Tolerance	Result

Test Parameters box displays performance validation parameters.

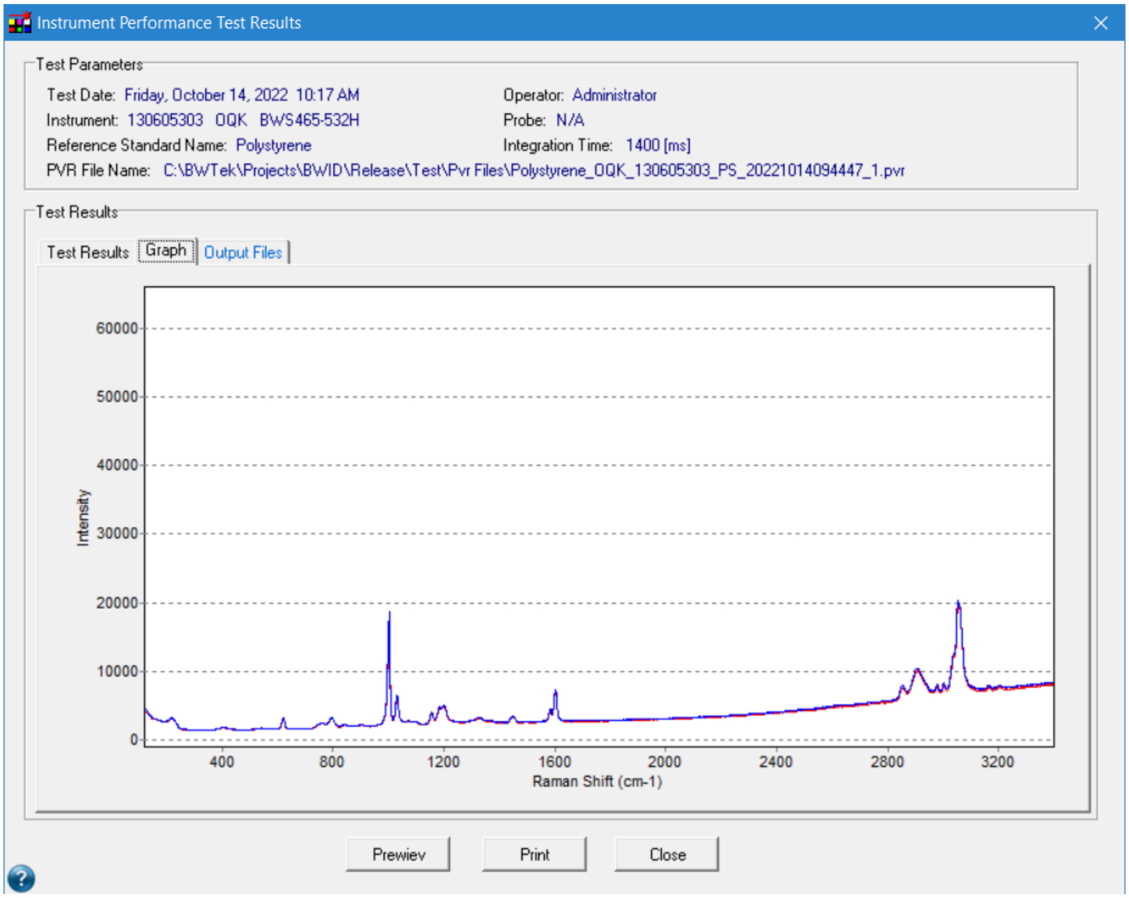
Test Date – date and time when the performance test was executed
Instrument – serial number, c-code and system model of the instrument on which the test was performed
Reference Standard Name – name of a reference standard used in the test
PVR File Name – name of a PVR file used in the test
Operator – name of the user who performed the test
Probe – serial number of a probe used to collect the spectrum

Integration Time – integration time of collected spectrum

The *Test Results* tab shows the limits and results of a performance test.

Test Status – overall status of the performance test: Pass (in green) or Fail (in red). All selected tests have to pass to get Pass for overall status.
Spectral Range – selected and measured range of spectral data, test status (Pass/Fail)
All other limits and results sections vary and are displayed when a given test is selected in the PVR file.
Raman Shift Accuracy – for each standard peak within selected spectral range: standard peak position, peak measured position, difference between measured peak position and the standard peak position, limit, test status (Pass/Fail)
Photometric Precision – for each enabled standard peak within selected spectral range: standard peak position, normalized height of peak in reference spectrum, normalized height of peak in last validation measured spectrum, normalized height of peak in measured spectrum, intensity variation of peak in measured vs. reference spectrum, intensity variation limit of peak in measured vs. reference spectrum, intensity variation of peak in measured vs. last validation spectrum, intensity variation limit of peak in measured vs. last validation spectrum, test status (Pass/Fail).
Last validation measured spectrum and peaks are from last performance validation test with Pass result. If the last validation data are not available, the reference peaks are used instead for measured vs. last calculations.
Intensity Variation from Reference – main peak position of reference standard, low and high limits calculated from intensity of the main peak in the reference spectrum and intensity variation limit in the PVR file, main peak intensity in the measured spectrum, test status (Pass/Fail)
HQI – HQI calculated on measured spectrum, HQI threshold, test status (Pass/Fail)
Raman Peak Width FWHM – main peak position of reference standard, low and high limits, main peak width in the measured spectrum, test status (Pass/Fail)
Detector Electronics – name of measured parameter, low and high limits, measured value, status (Pass/Fail)

The *Graph* tab displays standard reference spectrum from the PVR file (red) and measured spectrum (blue).



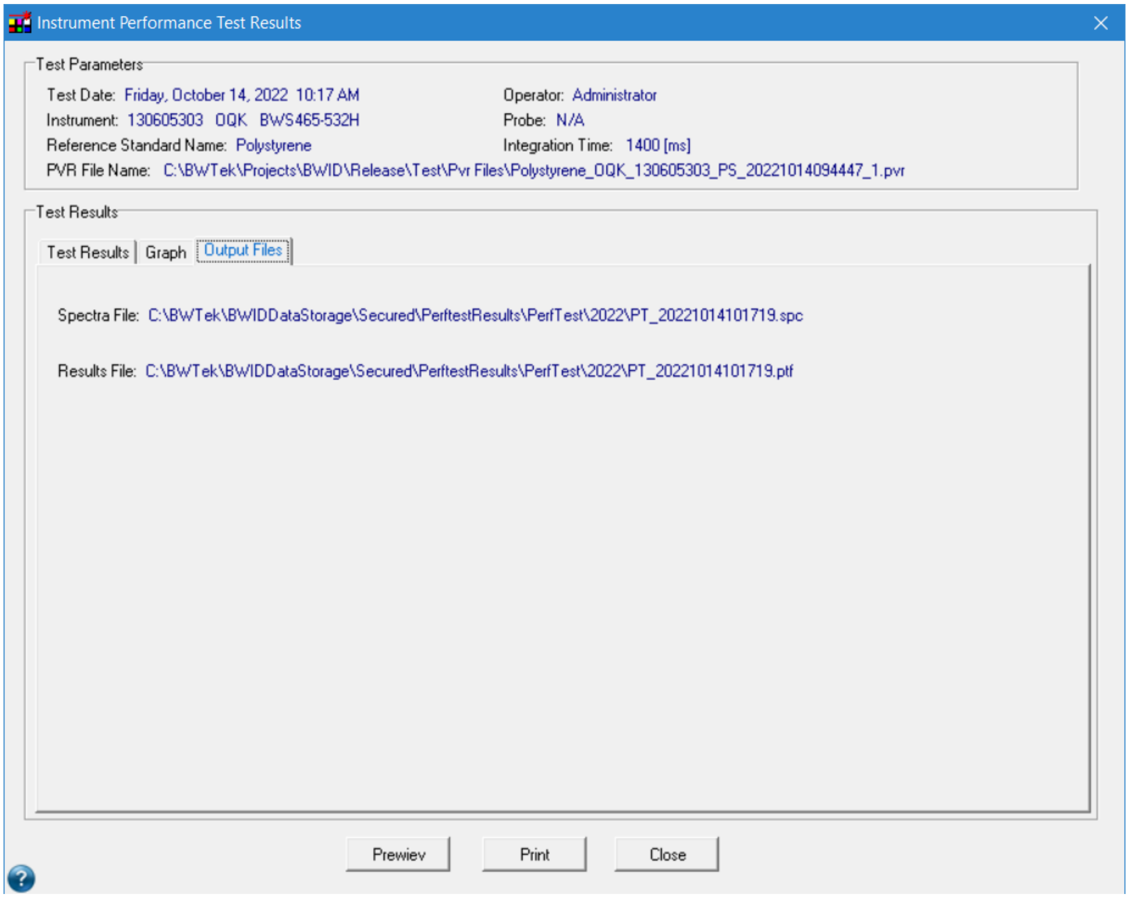
Test Date: Friday, October 14, 2022 10:17 AM
Operator: Administrator
Instrument: 130605303 OQK BWS465-532H
Probe: N/A
Reference Standard Name: Polystyrene
Integration Time: 1400 [ms]
PVR File Name: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

The *Output Files* tab shows spectra and results file names and location.

The spectra are stored in a Grams SPC data file format (*.spc), while the test results are saved in a BWTek proprietary binary file format (*.ptf).

The output file names are created automatically by a date pattern: ID_yyyy*mmddhhmmss.ext*, where *yyyy* stands for the year, *mm* is the month, *dd* is the day, *hh* is the hour (24 hours format), *mm* is minutes and *ss* is seconds of the date and time when the performance test was executed; *ext* is the “spc” and “ptf” for the spectra and results files respectively.

By default, the files are stored in the LogData\PerfTest*Year* subfolder of the BWID® application main folder, where *Year* is the year of the test execution. See Data Storage Configurations in Program Configuration paragraph for user defined data storage option.



Test Date: Friday, October 14, 2022 10:17 AM

Operator: Administrator

Instrument: 130605303 OQK BWS465-532H

Probe: N/A

Reference Standard Name: Polystyrene

Integration Time: 1400 [ms]

PVR File Name: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

Spectra File: C:\BWTek\BWIDDataStorage\Secured\PerftestResults\PerfTest\2022\PT_20221014101719.spc

Results File: C:\BWTek\BWIDDataStorage\Secured\PerftestResults\PerfTest\2022\PT_20221014101719.ptf

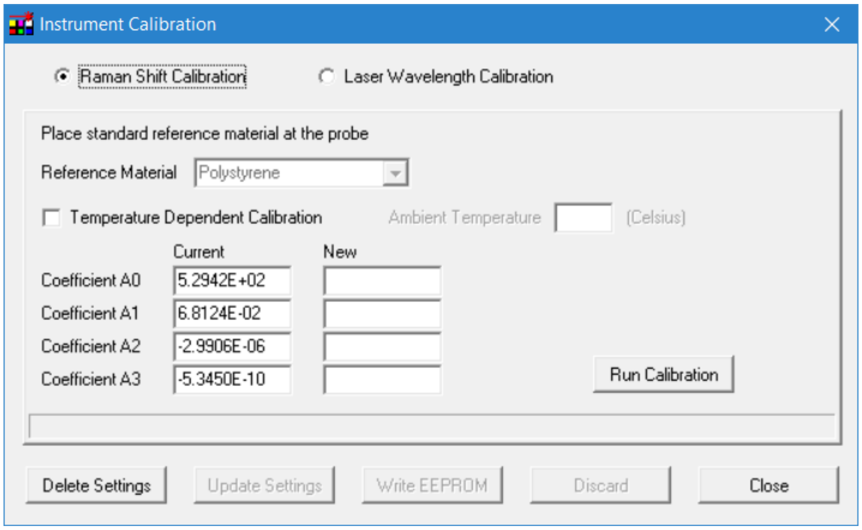
Click *Preview* to view a test results report.

Click *Print* to print the test results report.

Click *Close* to close the performance test results dialog and go back to the Menu window.

Instrument Calibration

Upon clicking the *Calibration* button in the Diagnostic menu, the *Instrument Calibration* dialog will appear as follows:



Place standard reference material at the probe

Reference Material: Polystyrene

☐ Temperature Dependent Calibration Ambient Temperature ____ (Celsius)

	Current	New
Coefficient A0	5.2942E+02	
Coefficient A1	6.8124E-02	
Coefficient A2	-2.9906E-06	
Coefficient A3	-5.3450E-10	

Select *Raman Shift Calibration* radio button to switch to Raman shift calibration dialog.

Select *Laser Wavelength Calibration* radio button to switch to laser wavelength calibration dialog.

Raman Shift Calibration

Raman shift calibration allows to compute new A-coefficients that are used to convert data from pixels to wavelength, wave number or Raman shift. The Raman shift calibration can be run in case there is too much shift in Raman shift peaks positions.

Reference Material – standard material used in the calibration. BWID allows the user to use polystyrene only, with peaks at 620.9, 1001.4 and 1602.3 cm-1.

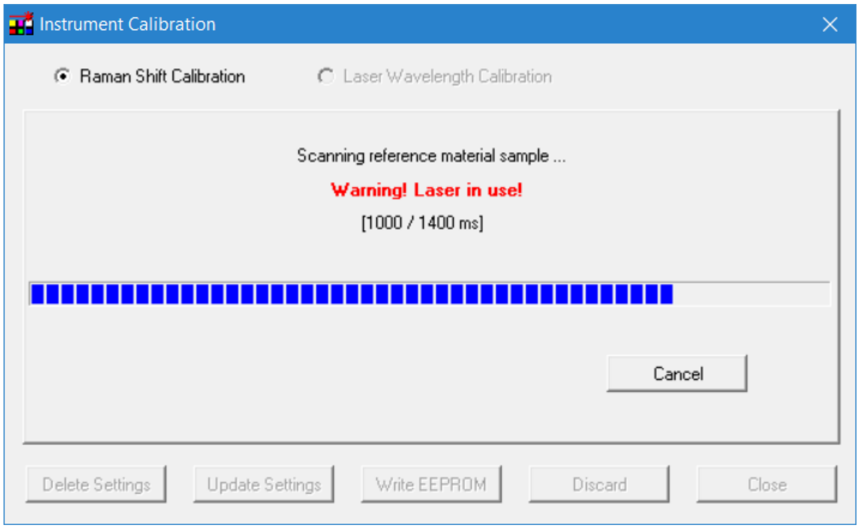
Temperature Dependent Calibration – check this box to take ambient temperature into consideration when running the calibration.

Ambient Temperature – set ambient temperature (in Celsius).

Coefficient A0, …, A3 – instrument's A-coefficients: currently used coefficients in the *Current* column and newly calculated from calibration in the *New* column.

Click *Run Calibration* button to start Raman shift calibration.

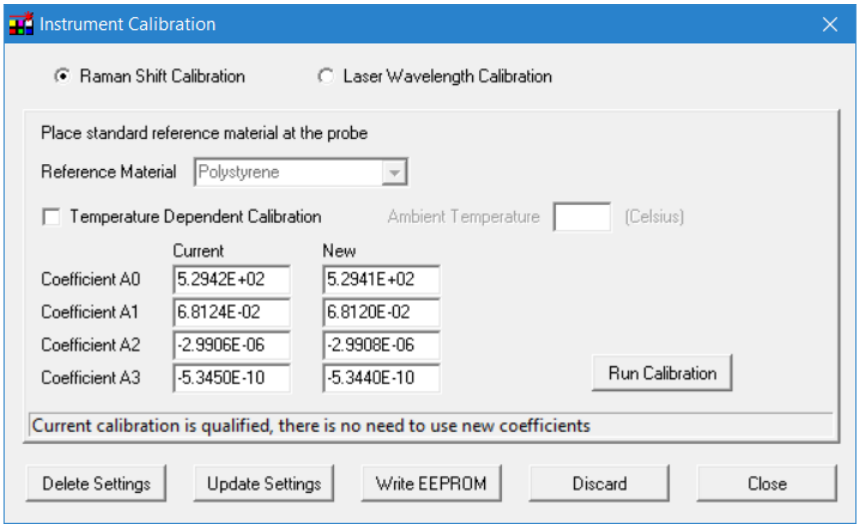
The program will collect raw and dark spectra of the reference sample using auto integration time and then will calculate new A-coefficients, as shown in the dialogs below.



Scanning reference material sample ...

Warning! Laser in use!

[1000 / 1400 ms]



Place standard reference material at the probe

Reference Material: Polystyrene

☐ Temperature Dependent Calibration   Ambient Temperature ☐ (Celsius)

	Current	New
Coefficient A0	5.2942E+02	5.2941E+02
Coefficient A1	6.8124E-02	6.8120E-02
Coefficient A2	-2.9906E-06	-2.9908E-06
Coefficient A3	-5.3450E-10	-5.3440E-10

Current calibration is qualified, there is no need to use new coefficients

Click *Delete Settings* to delete Raman shift calibration data (A-coefficients) locally saved on a PC. Doing so will result in the software using A-coefficients loaded from instrument's EEPROM on the program startup.

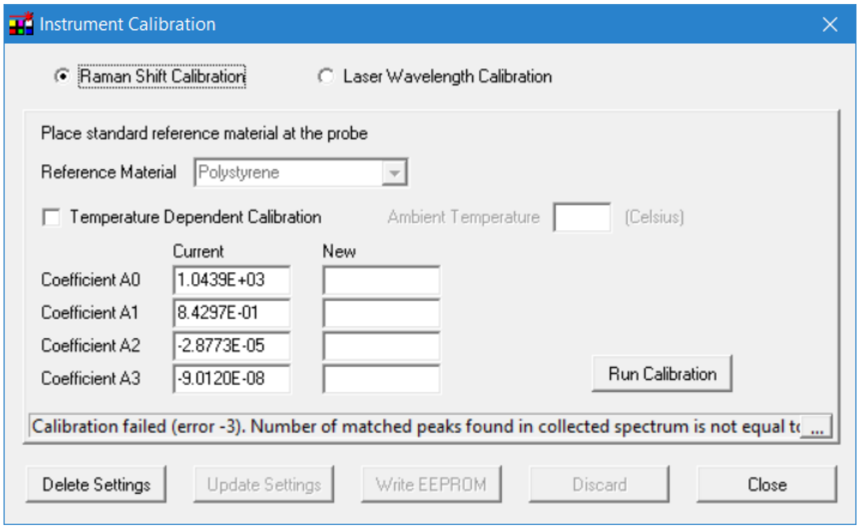
Click *Update Settings* to save Raman shift calibration data (new A-coefficients) locally on a PC, so they will be used for data collection from now on instead of the settings from EEPROM. Upon starting the program, it will load the A-coefficients from a local file on a PC.

Click *Write EEPROM* to save Raman shift calibration data (new A-coefficients) in instrument's EEPROM.

Click *Discard* to discard calculated Raman shift calibration data (new A-coefficients).

Click *Close* to close the Instrument Calibration dialog.

In case of a calibration error, the error message will be displayed in the status bar in the Instrument Calibration dialog as shown below.



Instrument Calibration

● Raman Shift Calibration ○ Laser Wavelength Calibration

Place standard reference material at the probe

Reference Material: Polystyrene

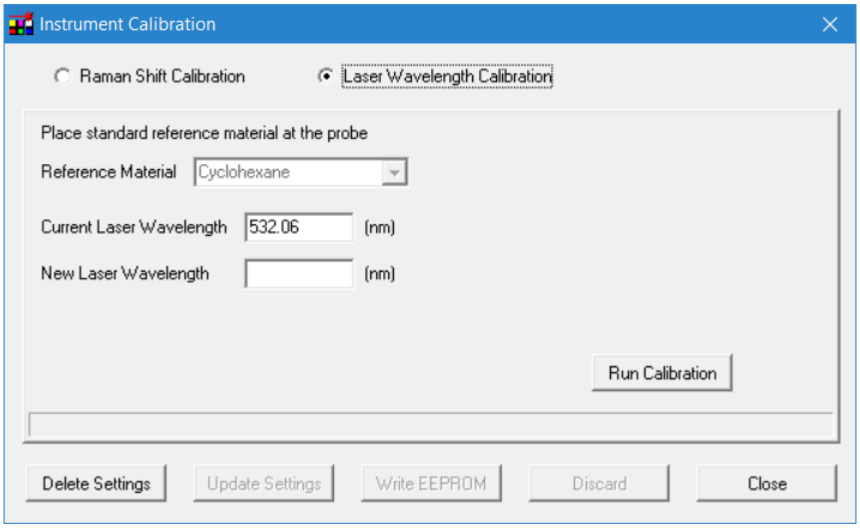
☐ Temperature Dependent Calibration Ambient Temperature (Celsius)

	Current	New
Coefficient A0	1.0439E+03	
Coefficient A1	8.4297E-01	
Coefficient A2	-2.8773E-05	
Coefficient A3	-9.0120E-08	

Calibration failed (error -3). Number of matched peaks found in collected spectrum is not equal t

Laser Wavelength Calibration

Laser wavelength calibration allows to compute new laser excitation wavelength that is used to convert data from pixels to wavelength, wave number or Raman shift. The laser wavelength calibration can be run in case there is too much shift in Raman shift peaks positions.



Place standard reference material at the probe

Reference Material: Cyclohexane

Current Laser Wavelength: 532.06 (nm)

New Laser Wavelength: (nm)

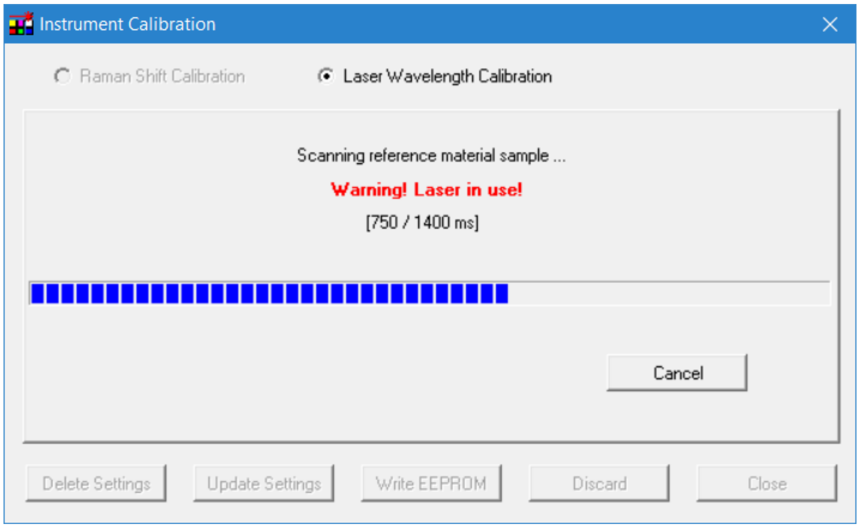
Reference Material – standard material used in the calibration. BWID allows the user to use a cyclohexane only, with peaks at 801.3, 1028.3 and 1444.4 cm-1.

Current Laser Wavelength – currently used laser excitation wavelength

New Laser Wavelength – newly calculated laser excitation wavelength from calibration

Click *Run Calibration* button to start the laser wavelength calibration.

The program will collect raw and dark spectra of the reference sample using auto integration time and then will calculate new laser excitation wavelength, as shown in the dialogs below.

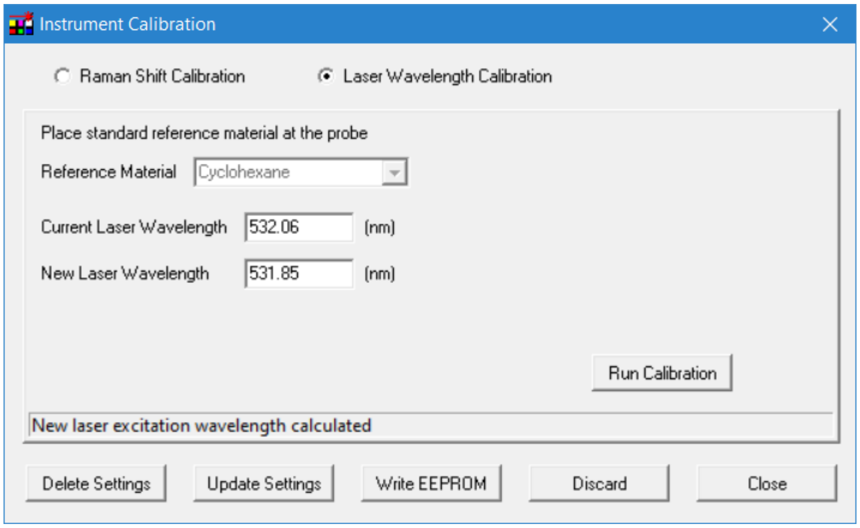

Instrument Calibration

○ Raman Shift Calibration ● Laser Wavelength Calibration

Scanning reference material sample ...

Warning! Laser in use!

[750 / 1400 ms]


Instrument Calibration

○ Raman Shift Calibration ● Laser Wavelength Calibration

Place standard reference material at the probe

Reference Material: Cyclohexane

Current Laser Wavelength: 532.06 (nm)

New Laser Wavelength: 531.85 (nm)

New laser excitation wavelength calculated

Click *Delete Settings* to delete laser wavelength calibration data (laser wavelength) locally saved on a PC. Doing so will result in the software using the laser wavelength loaded from instrument’s EEPROM on the program startup.

Click *Update Settings* to save laser wavelength calibration data (new laser wavelength) locally on a PC, so it will be used for data collection from now on instead of the setting from EEPROM. Upon starting the program, it will load the laser wavelength from a local file on a PC.

Click *Write EEPROM* to save calibration data (new laser wavelength) in instrument’s EEPROM.

Click *Discard* to discard calculated laser wavelength calibration data (new laser wavelength).

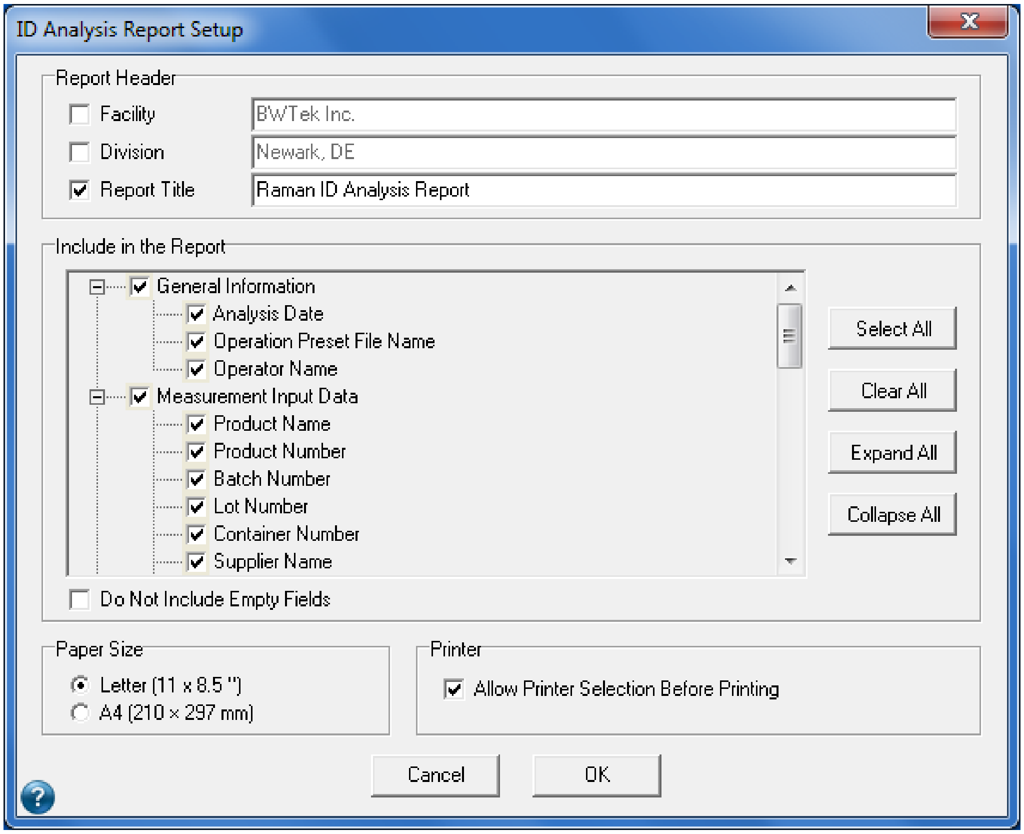
Click *Close* to close the Instrument Calibration dialog.

11. Reports

ID Analysis Report

ID Analysis Report Configuration

To start the ID analysis report configuration, click the *Setup* button in the Menu window and then the *ID Report* button in the Setup menu.
The ID Analysis Report Setup dialog will appear as shown below.



ID Analysis Report Setup

Report Header
☐ Facility: BWTek Inc.
☐ Division: Newark, DE
☑ Report Title: Raman ID Analysis Report

Include in the Report
- ☑ General Information
  - ☑ Analysis Date
  - ☑ Operation Preset File Name
  - ☑ Operator Name
- ☑ Measurement Input Data
  - ☑ Product Name
  - ☑ Product Number
  - ☑ Batch Number
  - ☑ Lot Number
  - ☑ Container Number
  - ☑ Supplier Name

☐ Do Not Include Empty Fields

Paper Size
● Letter (11 x 8.5 ")
○ A4 (210 x 297 mm)

Printer
☑ Allow Printer Selection Before Printing

Facility – select this box to print out a facility name in the header of a report and then specify the facility name. By default, the facility name is not printed out on the report.

Division – select this box to print out a division name in the header of a report and then specify the division name. By default, the division name is not printed out on the report.

Report Title – select this box to print out a report title in the header of the report and then specify the report title. The default title is "Raman ID Analysis Report".

In the Include in the Report list, check all report items you want to include on the report and uncheck those you do not want to include. By default, all items are printed out on the report.

Do Not Include Empty Fields – select this box to remove all empty items (values not provided) that have been selected for inclusion in the report. Checking this option will optimize the report printout.

In the *Paper Size* box, select an appropriate paper size (Letter or A4) for the report printout.

Allow Printer Selection Before Printing – check this box to select the printer on which the report will be printed out. If this box is unchecked, the report will print on the default printer configured for the PC.

Click the *OK* button to accept ID report settings and return to the Menu window.

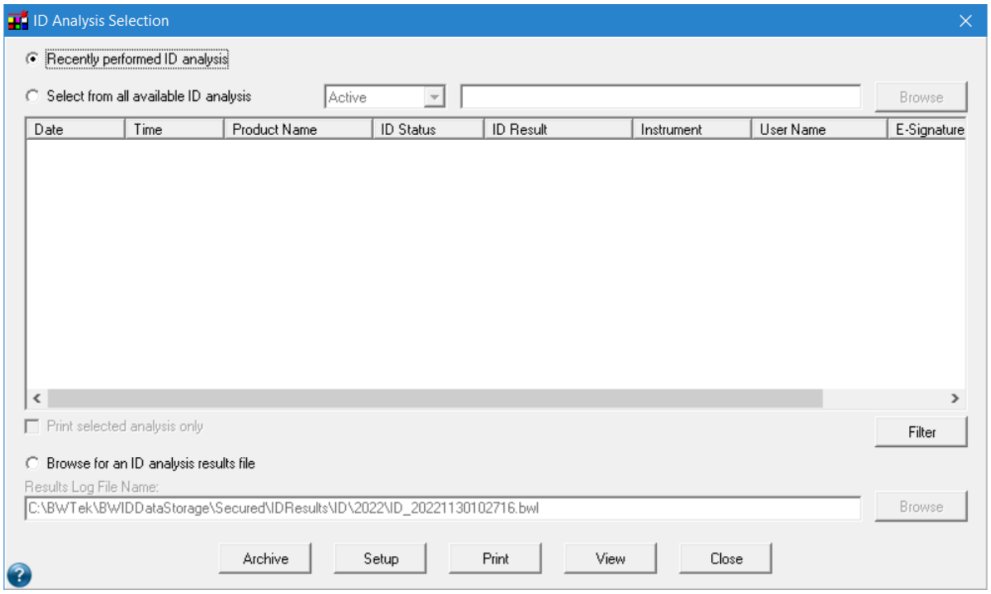
Click the *Cancel* button to abort ID report settings and return to the Menu window.

Starting ID Analysis Report

Click the *Report* button in the Menu window and then the *ID* button in the Reports menu to start the ID analysis report feature. This feature allows the user to view, sign (Pharma Edition only) and print out a report for any available ID analysis. Clicking the *ID Report* button will open the ID Analysis Selection dialog as shown below.

ID Analysis Selection

The dialog allows the user to select an ID analysis, for which a report will be generated. Additionally, it allows the user to filter ID analysis for batch printing.



● Recently performed ID analysis

○ Select from all available ID analysis — Active

☐ Print selected analysis only

○ Browse for an ID analysis results file

Results Log File Name: C:\BWTek\BWIDDataStorage\Secured\IDResults\ID\2022\ID_20221130102716.bwl

Select the *Recently performed ID analysis* button if you wish to generate a report for recently performed sample identification.

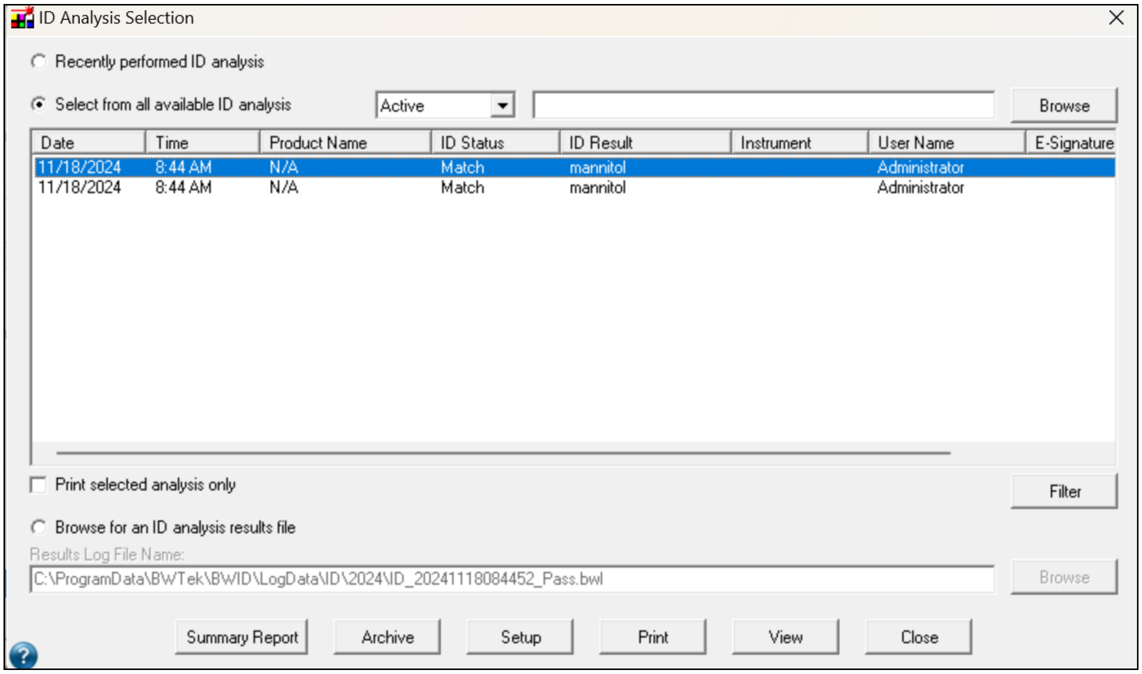
Check the *Select from all available ID analysis* button to choose an ID analysis for which a report will be generated from one of three views: *Active*, *Archived* and *In Folder*.

The *Active* view lists all ID analysis results that have not been archived yet.
The *Archived* view displays all available archived ID analysis results.
The *In Folder* view allows the user to view all results stored in a selected folder. Click the *Browse* button to select the folder with results.

Upon clicking the button, the list is set with all available ID analysis in current view, as shown below. This step may take some time depending on how many ID analysis results are present.

Click the *Filter* button to configure and apply a filter for ID analysis displayed in the list.

Select the *Browse for an ID analysis results file* button if you know an ID analysis results file (*.bwl), from which you wish to generate a report.
Then click the *Browse* button to select the results file.
By default, the *Results Log File Name* is set with a file name of a recently performed ID analysis.



ID Analysis Selection

○ Recently performed ID analysis

● Select from all available ID analysis — Active

Date	Time	Product Name	ID Status	ID Result	Instrument	User Name	E-Signature
11/18/2024	8:44 AM	N/A	Match	mannitol		Administrator	
11/18/2024	8:44 AM	N/A	Match	mannitol		Administrator	

☐ Print selected analysis only

○ Browse for an ID analysis results file

Results Log File Name: C:\ProgramData\BWTek\BWID\LogData\ID\2024\ID_20241118084452_Pass.bwl

Once the ID analysis is selected, click the *View* button to view the ID analysis results.

Click *Print* to perform batch printing for filtered or selected ID analyses. See the Batch Printing paragraph for details.

Click *Summary Report* to view and/or print the Summary Report of the selected measurements.

Click *Archive* to archive or copy the ID analysis results. See ID Analysis Archive paragraph for details.

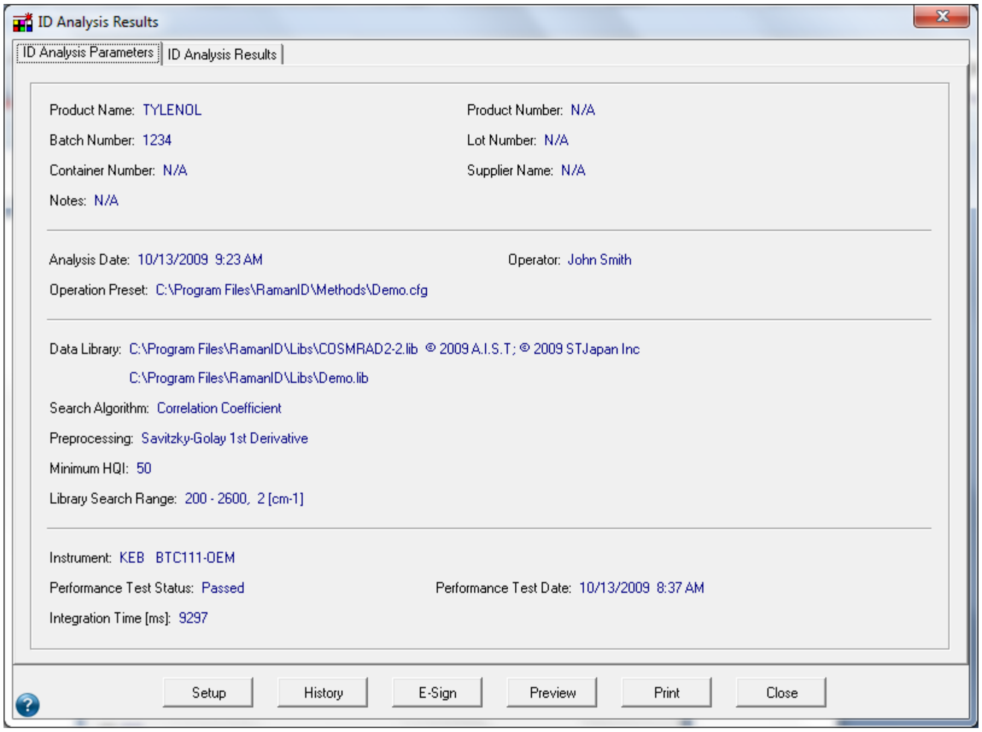
Click *Setup* to view or modify the ID analysis report configuration settings. See ID Analysis report Configuration for details.

Click *Close* to close the ID Analysis Selection dialog and go back to the Menu window.

ID Analysis Results

Upon clicking the *View* button, the ID Analysis Results dialog will appear as shown below. The dialog shows all parameters and results of the ID analysis regardless of the ID Analysis Report Configuration settings.

The *ID Analysis Parameters* tab holds details of the sample identification parameters.



Product Name: TYLENOL
Product Number: N/A
Batch Number: 1234
Lot Number: N/A
Container Number: N/A
Supplier Name: N/A
Notes: N/A

Analysis Date: 10/13/2009 9:23 AM
Operator: John Smith
Operation Preset: C:\Program Files\RamanID\Methods\Demo.cfg

Data Library: C:\Program Files\RamanID\Libs\COSMRAD2-2.lib © 2009 A.I.S.T; © 2009 STJapan Inc
C:\Program Files\RamanID\Libs\Demo.lib
Search Algorithm: Correlation Coefficient
Preprocessing: Savitzky-Golay 1st Derivative
Minimum HQI: 50
Library Search Range: 200 - 2600, 2 [cm-1]

Instrument: KEB BTC111-OEM
Performance Test Status: Passed
Performance Test Date: 10/13/2009 8:37 AM
Integration Time [ms]: 9297

Product Name – name of the measured sample
Product Number – product number of the measured sample
Batch Number – batch number of the measured sample
Lot Number – lot number of the measured sample
Container Number – container number of the measured sample
Supplier Name – name of the supplier (manufacturer) of the measured sample
Notes – user notes about the measured sample

Analysis Date – date and time when the sample identification was performed
Operation Preset – name of an operation preset file used in ID analysis
Operator – name of the user who performed the sample identification (Pharma edition only)

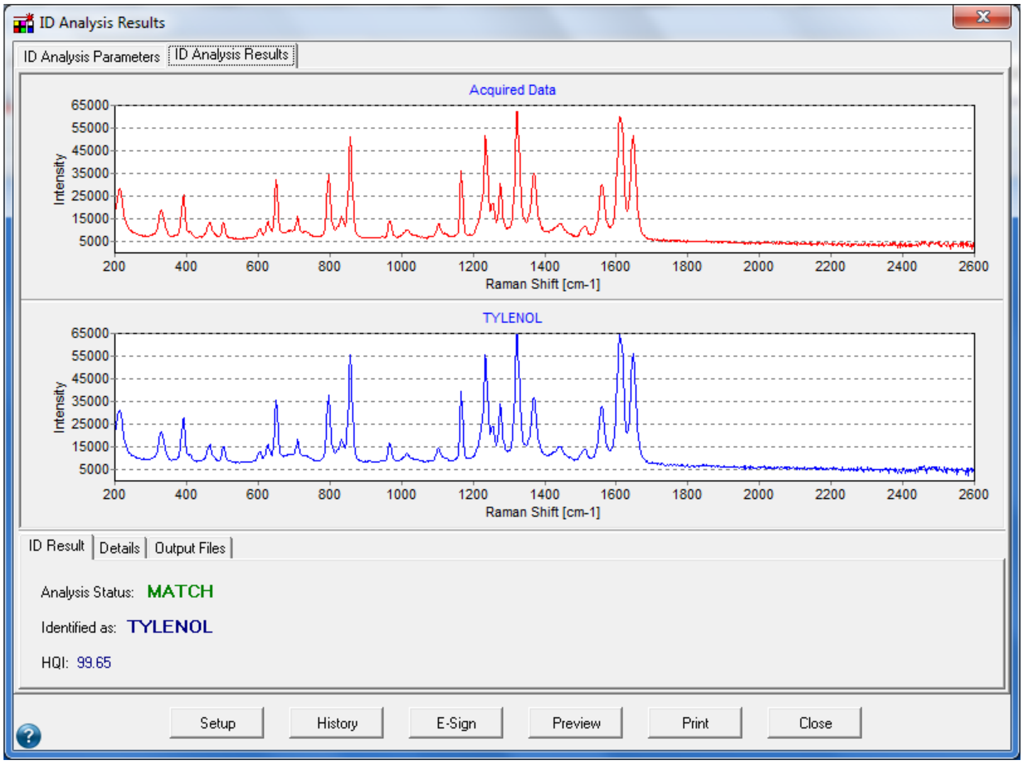
Data Library – names of data library files used in ID analysis
Search Algorithm – name of a search algorithm used to identify the sample
Preprocessing – name of the preprocessing algorithm applied to the spectral data in ID analysis
Minimum HQI –threshold value of the Hit Quality Index to detect an outlier
Library Search Range – library data search range and resolution

Instrument parameters displayed for on-line analysis only:
Instrument – c-code and name of instrument on which the ID analysis was performed
Performance Test Status – status of the last performance test executed on the instrument (Pass/Fail if a test was performed or N/A if a test was not performed)
Performance Test Date – date and time of the last performance test executed on the instrument (N/A if a test was not performed)

Spectrum parameters displayed for off-line analysis only:
Off-line Spectrum Source – name of spectrum file
Spectrum Name – name of spectral data

Integration Time – integration time of the spectrum collected for the ID analysis

The *ID Analysis Results* tab contains details of the sample identification results.



Analysis Status: MATCH
Identified as: TYLENOL
HQI: 99.65

Graphs panel – the upper graph displays the spectrum collected in the ID analysis, while the lower graph shows a matching spectrum, if any.

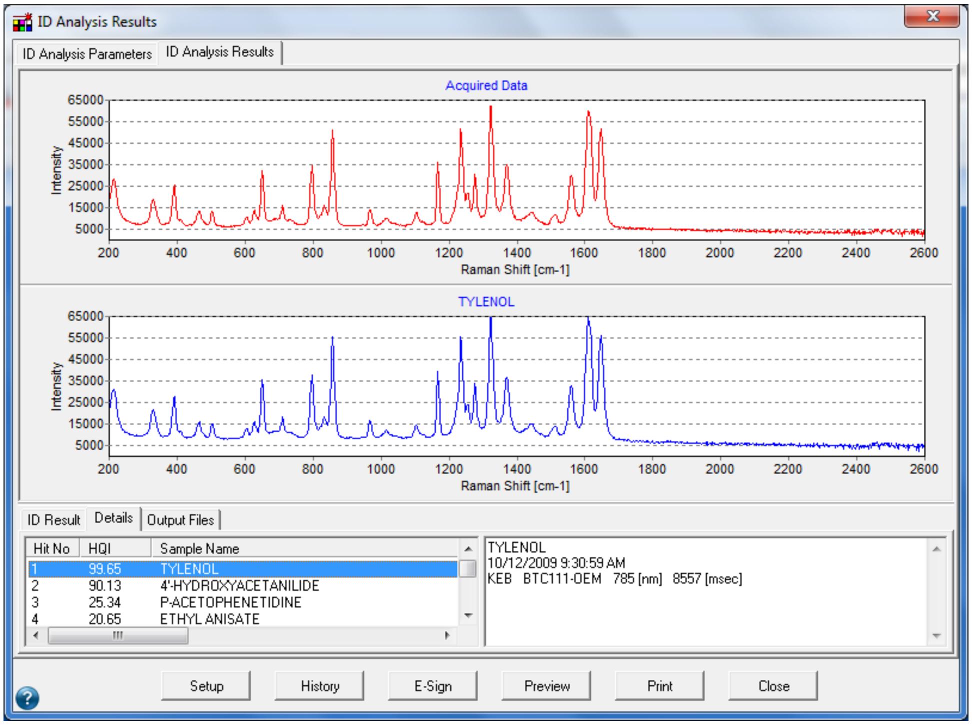
In the *ID Result* tab:

Analysis Status – status of the sample identification: MATCH (in green) or NO MATCH (in red) for Identify sample mode, or PASS (in green) or FAIL (in red) for Verify sample mode

Identified as – in Identify sample mode, the name of a matching sample (if there is a match) or UNKNOWN *Verified as* – in Verify sample mode, the name of a matching sample or UNKNOWN

HQI – Hit quality index computed for the matching sample (the higher the value, the better the match)

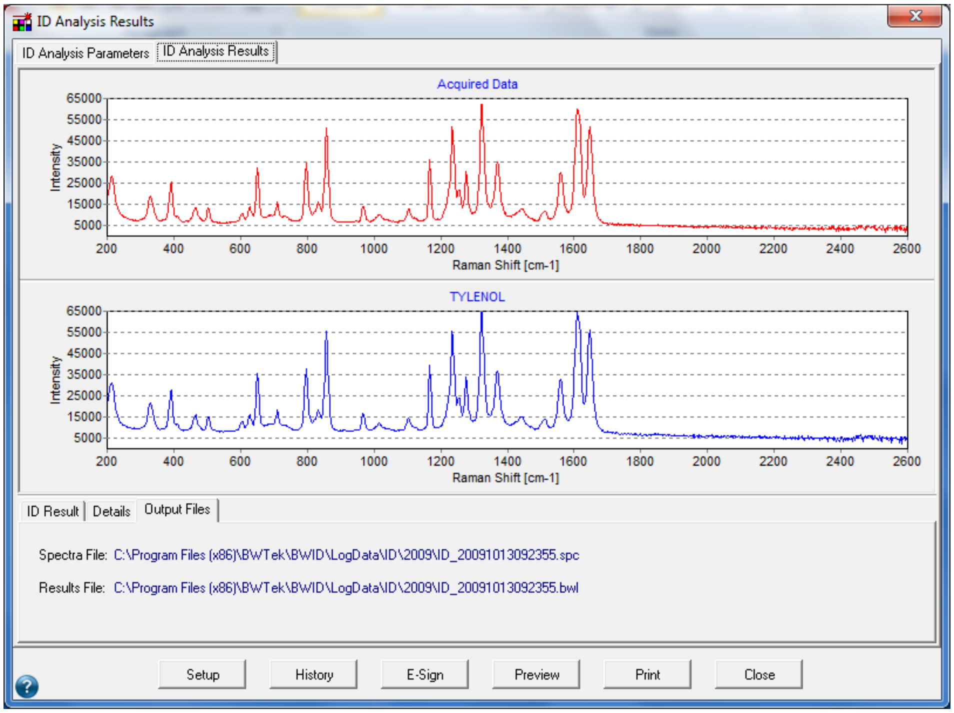
E-Signature – electronic signature (signer name, date of signing off the record, signature meaning); visible if the record is signed



Hit No	HQI	Sample Name
1	99.65	TYLENOL
2	90.13	4'-HYDROXYACETANILIDE
3	25.34	P-ACETOPHENETIDINE
4	20.65	ETHYL ANISATE

TYLENOL
10/12/2009 9:30:59 AM
KEB BTC111-OEM 785 [nm] 8557 [msec]

In the *Details* tab, the left panel displays a list of the best results of the ID search, while the right panel shows parameters of a sample selected in the hit list and the lower graph displays a spectrum of that sample.



Spectra File: C:\Program Files (x86)\BWTek\BWID\LogData\ID\2009\ID_20091013092355.spc

Results File: C:\Program Files (x86)\BWTek\BWID\LogData\ID\2009\ID_20091013092355.bwl

In the *Output Files* tab:
Spectra File – name of the file that contains a spectrum collected during ID analysis (*.spc)
Results File – name of the file that contains ID analysis results (*.bwl)

Click the *Setup* button to view or modify the ID analysis report configuration settings. See ID Analysis Report Configuration for details.

Click the *History* button to view history information for the ID analysis.

Click *E-Sign* to electronically sign the ID analysis record (Pharma edition only). The button is enabled if the record has not been signed (up to three levels depending on the signature on the first level). Once the record has been signed, it cannot be re-signed.

Click the *Preview* button to view the ID analysis report printout on the screen.

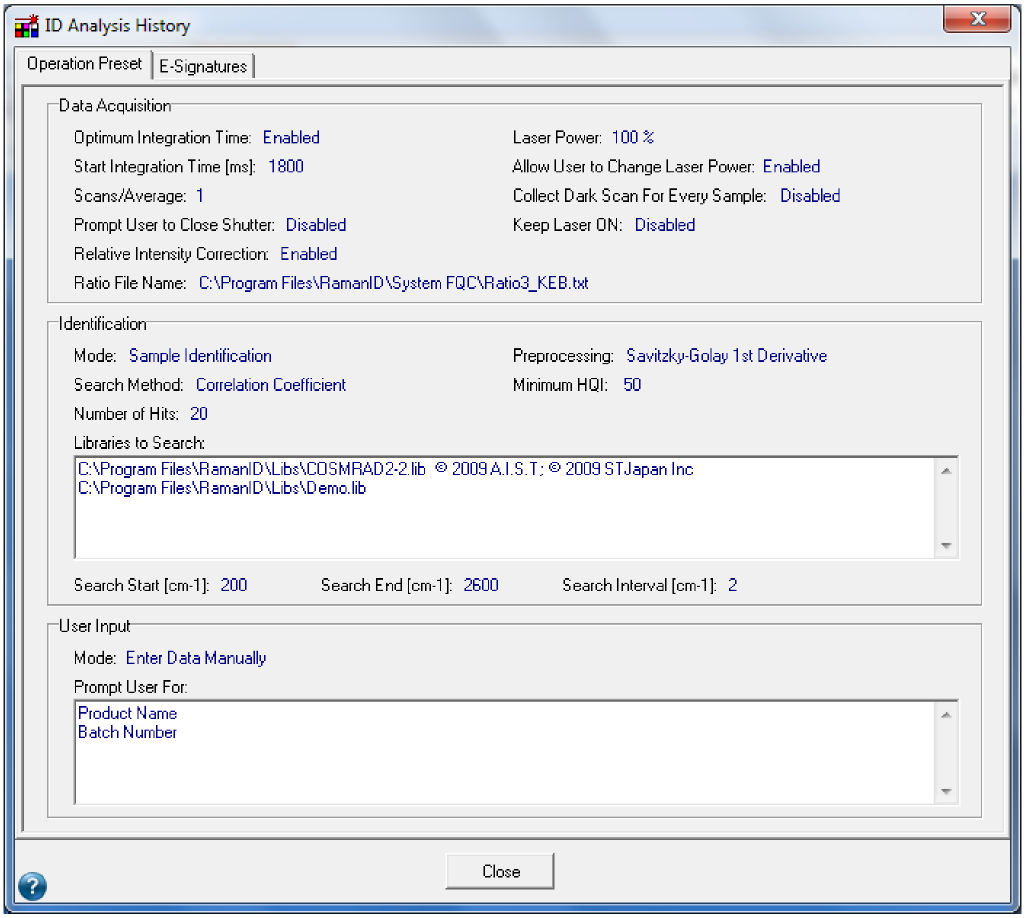
Click the *Print* button to print the ID analysis report.

Click *Close* to close the ID Analysis Results dialog and go back to the ID Analysis Selection dialog.

ID Analysis History

While in the ID Analysis Results dialog, click *History* to view data history of the ID analysis. The ID Analysis History dialog will pop up:

The *Operation Preset* tab dialog displays all parameters of the operation preset used to perform the ID analysis.



Data Acquisition

Optimum Integration Time: Enabled
Start Integration Time [ms]: 1800
Scans/Average: 1
Prompt User to Close Shutter: Disabled
Relative Intensity Correction: Enabled
Ratio File Name: C:\Program Files\RamanID\System FQC\Ratio3_KEB.txt
Laser Power: 100 %
Allow User to Change Laser Power: Enabled
Collect Dark Scan For Every Sample: Disabled
Keep Laser ON: Disabled

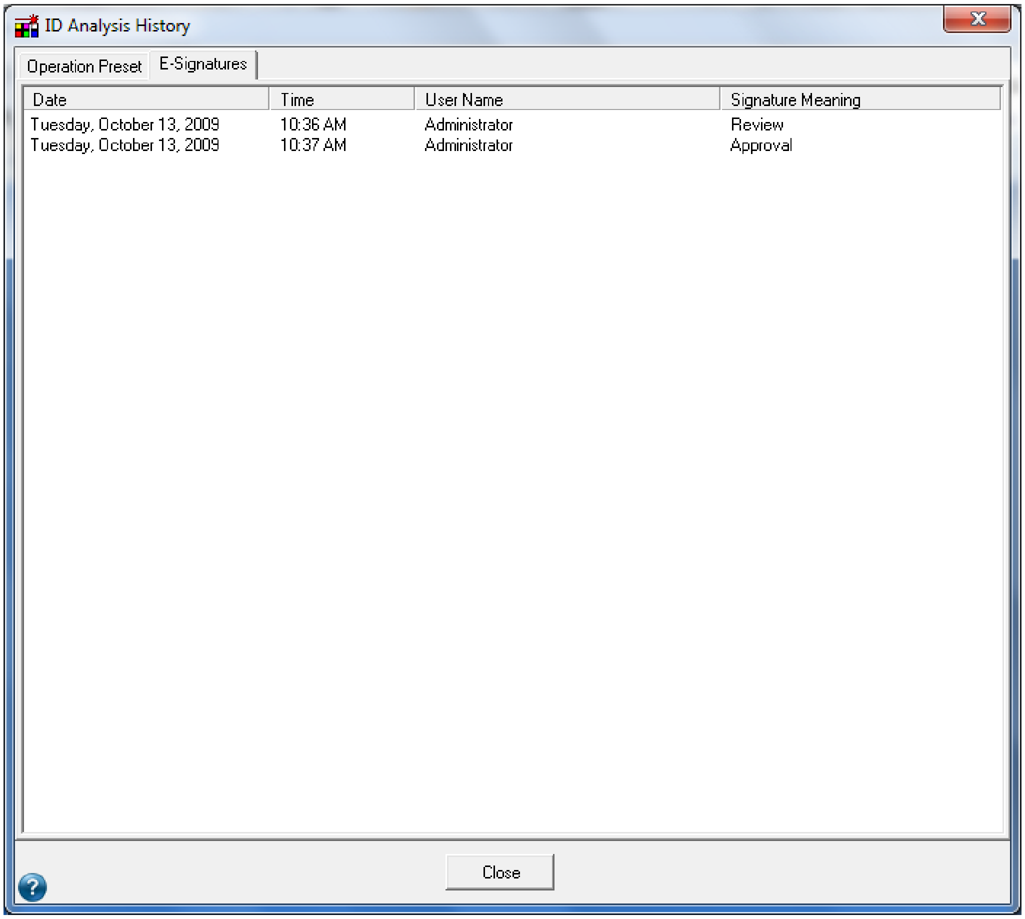
Identification

Mode: Sample Identification
Search Method: Correlation Coefficient
Number of Hits: 20
Preprocessing: Savitzky-Golay 1st Derivative
Minimum HQI: 50
Libraries to Search:
C:\Program Files\RamanID\Libs\COSMRAD2-2.lib © 2009 A.I.S.T; © 2009 STJapan Inc
C:\Program Files\RamanID\Libs\Demo.lib
Search Start [cm-1]: 200
Search End [cm-1]: 2600
Search Interval [cm-1]: 2

User Input

Mode: Enter Data Manually
Prompt User For:
Product Name
Batch Number

The *E-Signatures* tab dialog (Pharma Edition only) displays electronic signatures information:



Date	Time	User Name	Signature Meaning
Tuesday, October 13, 2009	10:36 AM	Administrator	Review
Tuesday, October 13, 2009	10:37 AM	Administrator	Approval

In this example, the ID analysis record has already been signed on all available levels: first reviewed and then approved. See Signing the ID Analysis Record for more details.

Signing the ID Analysis Record

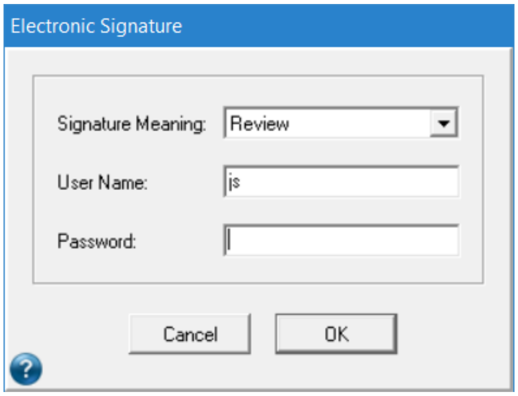
The program supports up to three-level electronic signatures.

On the first level, the user (of any category) can review or reject an ID analysis record. If the record is rejected by the user of Developer or Administrator status, this is a final rejection and the record cannot be signed on the second level.

On the second level, depending on the first level signature, the user (Developer or Administrator only) can do the following:
- approve or reject the record if a user of any category reviewed it on the first level
- reject, review or approve the record if it was rejected by a user with operator status on the first level.

The third level is only available if the record is rejected by the operator on the first level and then reviewed on the second level. Only a eDveloper or Administrator can ultimately approve or reject the record.

While in the ID Analysis Results dialog, click *E-Sign* to electronically sign the ID analysis record (Pharma edition only). The Electronic Signature dialog will pop up, as shown below.

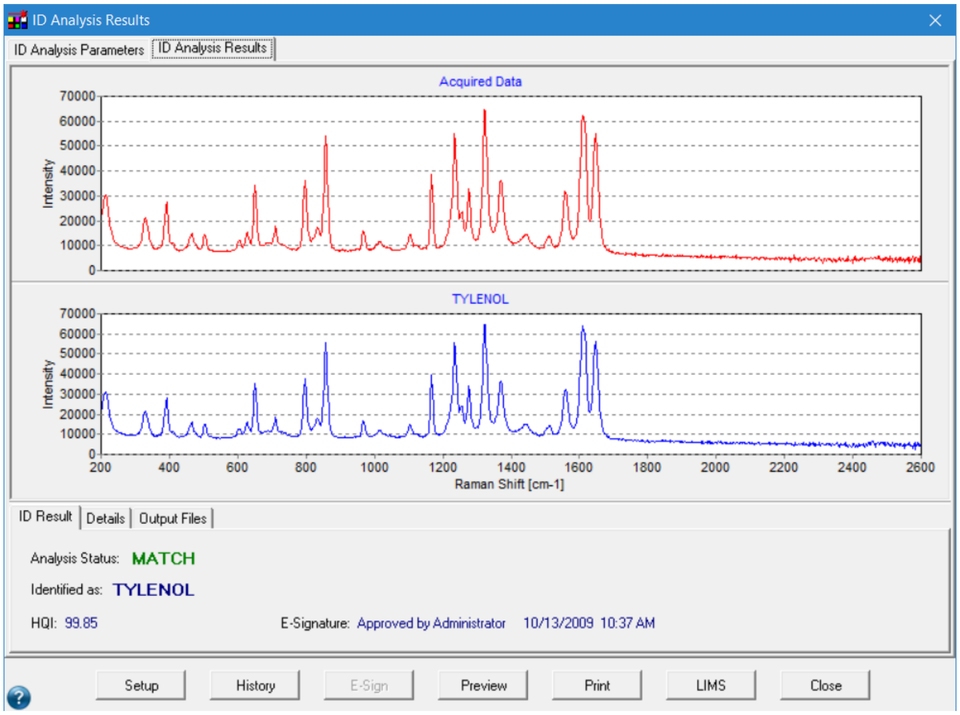


Signature Meaning: Review
User Name: js
Password:

The E-signature requires a password entry, even if the user is already logged in to the program.

Click *Cancel* to close the dialog without signing the ID analysis record.

Click *OK* to sign the ID analysis record. Once the record is signed, the information associated with the signature will be displayed in the E-Signature field in the ID Analysis Results dialog as shown below:



Analysis Status: MATCH

Identified as: TYLENOL

HQI: 99.85

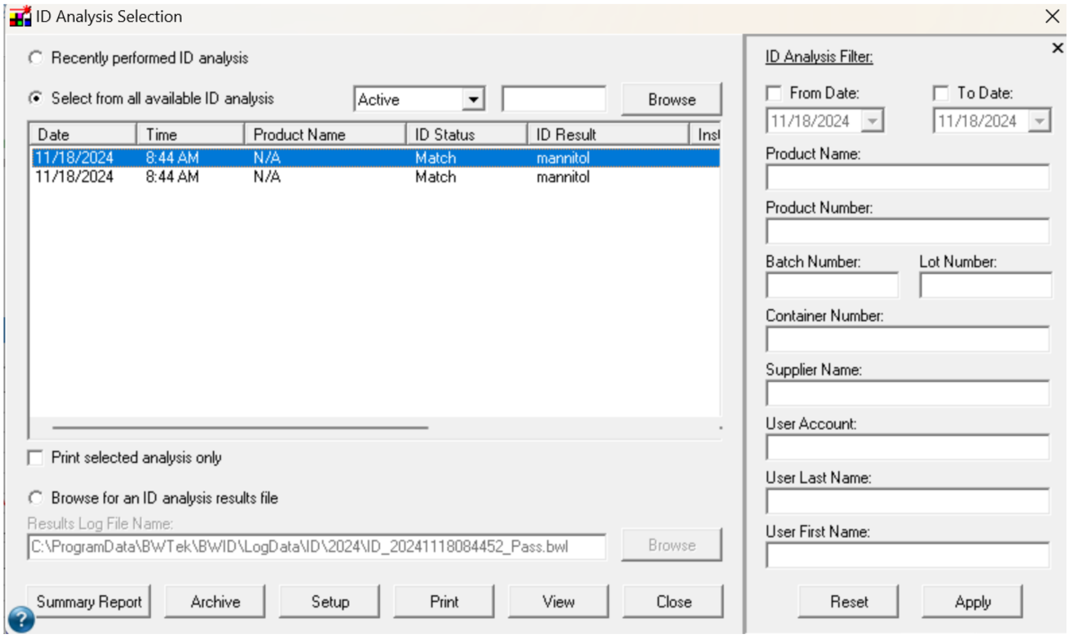
E-Signature: Approved by Administrator 10/13/2009 10:37 AM

The signed ID analysis record contains the full name of the signer, the date and time when the signature was executed and the meaning associated with the signature.

The *E-Sign* button will become disabled if the record is already signed.

ID Analysis Filter

The ID analysis filter allows the user to view and print selected ID analysis records.
To filter ID analysis entries displayed in the list, click the *Filter* button. The ID Analysis Filter panel will appear in the main window:



ID Analysis Selection

○ Recently performed ID analysis

● Select from all available ID analysis — Active

Date	Time	Product Name	ID Status	ID Result	Inst
11/18/2024	8:44 AM	N/A	Match	mannitol	
11/18/2024	8:44 AM	N/A	Match	mannitol	

☐ Print selected analysis only

○ Browse for an ID analysis results file

Results Log File Name: C:\ProgramData\BWTek\BWID\LogData\ID\2024\ID_20241118084452_Pass.bwl

ID Analysis Filter:

☐ From Date: 11/18/2024
☐ To Date: 11/18/2024
Product Name:
Product Number:
Batch Number:
Lot Number:
Container Number:
Supplier Name:
User Account:
User Last Name:
User First Name:

The ID analysis records can be selected using the following filter criteria:

- Date range (between specified dates)
- Product name
- Product number
- Batch number
- Lot number
- Container number
- Supplier name
- User account
- User name (first and last name)

All criteria excluding date range are searched based on the text string within the appropriate field of the record. The text search is not case sensitive.

Once the filter is configured, click the *Apply* button to filter records. The ID Analysis list will be updated according to the filter settings.

To reset the filter settings in the filter panel, click the *Reset* button.

To turn the filter off, reset the filter settings first (by clicking the *Reset* button) and then click *Apply* in the filter panel.

To hide the filter panel, click the *x* button in the top right corner of the filter panel.

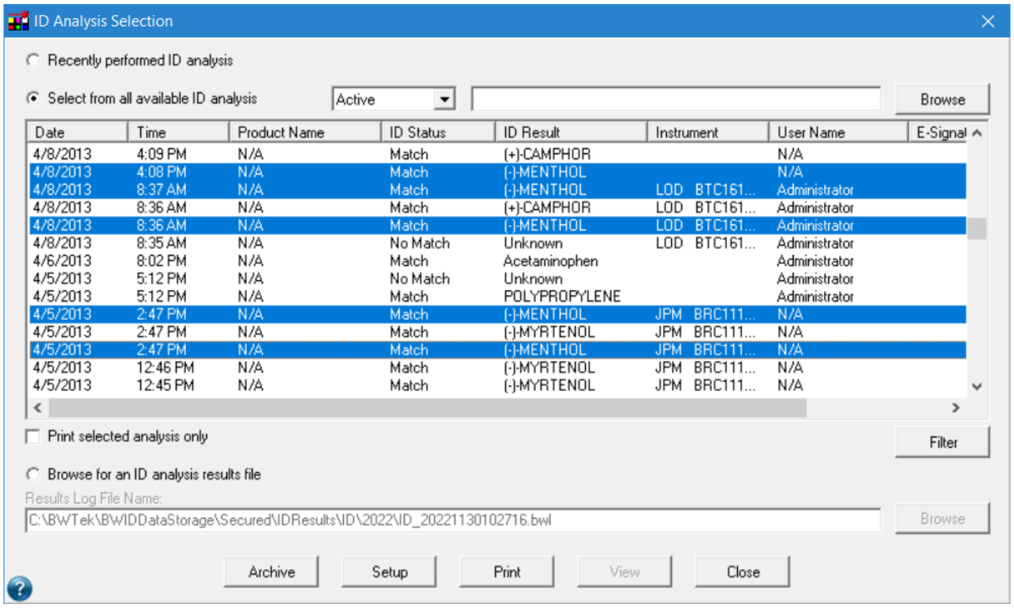
Batch Printing

Batch printing allows the user to print out multiple ID analysis reports for ID analyses of particular interest.

To select ID analyses for batch printing use the Filter function to display the list of ID analyses that are of particular interest.

To print reports for all ID analyses shown in the list, uncheck the *Print selected analysis only* box and click the *Print* button.

To print reports for only a few ID analyses in the list (as shown below), select those ID analyses (by holding down the Ctrl key on your keyboard while selecting the items in the list), check the *Print selected analysis only* box and then click the *Print* button.



○ Recently performed ID analysis

● Select from all available ID analysis: Active

Date	Time	Product Name	ID Status	ID Result	Instrument	User Name	E-Signat
4/8/2013	4:09 PM	N/A	Match	(+)-CAMPHOR		N/A	
4/8/2013	4:08 PM	N/A	Match	(-)-MENTHOL		N/A	
4/8/2013	8:37 AM	N/A	Match	(-)-MENTHOL	LOD BTC161...	Administrator	
4/8/2013	8:36 AM	N/A	Match	(+)-CAMPHOR	LOD BTC161...	Administrator	
4/8/2013	8:36 AM	N/A	Match	(-)-MENTHOL	LOD BTC161...	Administrator	
4/8/2013	8:35 AM	N/A	No Match	Unknown	LOD BTC161...	Administrator	
4/6/2013	8:02 PM	N/A	Match	Acetaminophen		Administrator	
4/5/2013	5:12 PM	N/A	No Match	Unknown		Administrator	
4/5/2013	5:12 PM	N/A	Match	POLYPROPYLENE		Administrator	
4/5/2013	2:47 PM	N/A	Match	(-)-MENTHOL	JPM BRC111...	N/A	
4/5/2013	2:47 PM	N/A	Match	(-)-MYRTENOL	JPM BRC111...	N/A	
4/5/2013	2:47 PM	N/A	Match	(-)-MENTHOL	JPM BRC111...	N/A	
4/5/2013	12:46 PM	N/A	Match	(-)-MYRTENOL	JPM BRC111...	N/A	
4/5/2013	12:45 PM	N/A	Match	(-)-MYRTENOL	JPM BRC111...	N/A	

☐ Print selected analysis only

○ Browse for an ID analysis results file

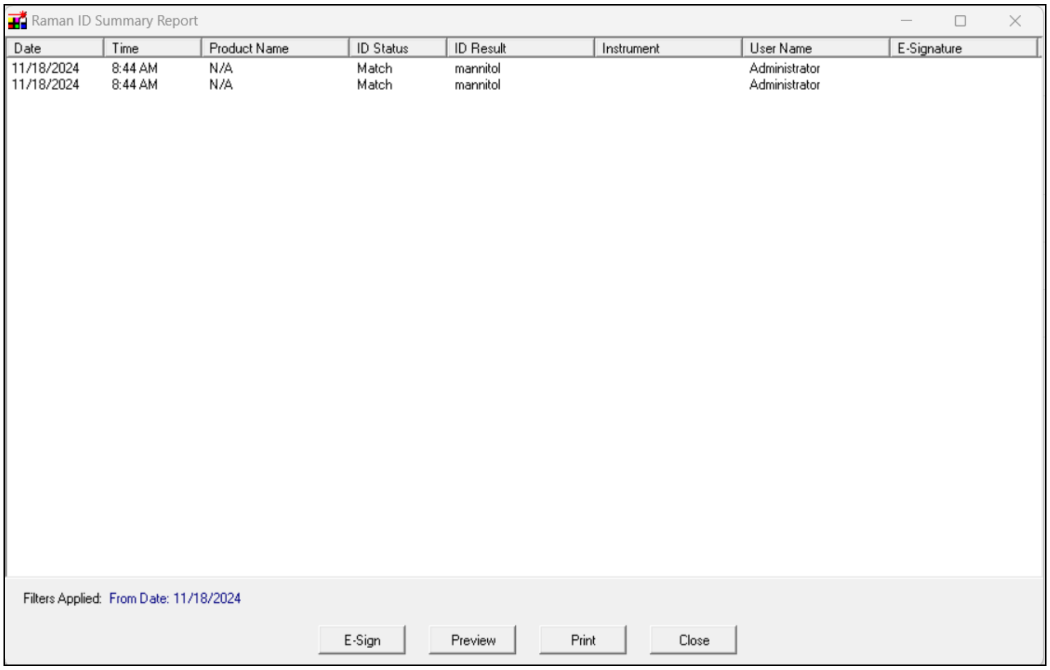
Results Log File Name: C:\BWTek\BWIDDataStorage\Secured\IDResults\ID\2022\ID_20221130102716.bwl

Once you are finished with the batch printing, undo the multiple selection by clicking on any ID analysis in the list.

Summary Report

The *Summary Report* function allows the user to select multiple ID analysis reports to be compiled in a single summary report.

To create a summary report, select the ID analyses of a particular interest. This can be done either by manual selection, or by the filter function. Click *Summary Report* and the view of the summary report will appear.



Date	Time	Product Name	ID Status	ID Result	Instrument	User Name	E-Signature
11/18/2024	8:44 AM	N/A	Match	mannitol		Administrator	
11/18/2024	8:44 AM	N/A	Match	mannitol		Administrator	

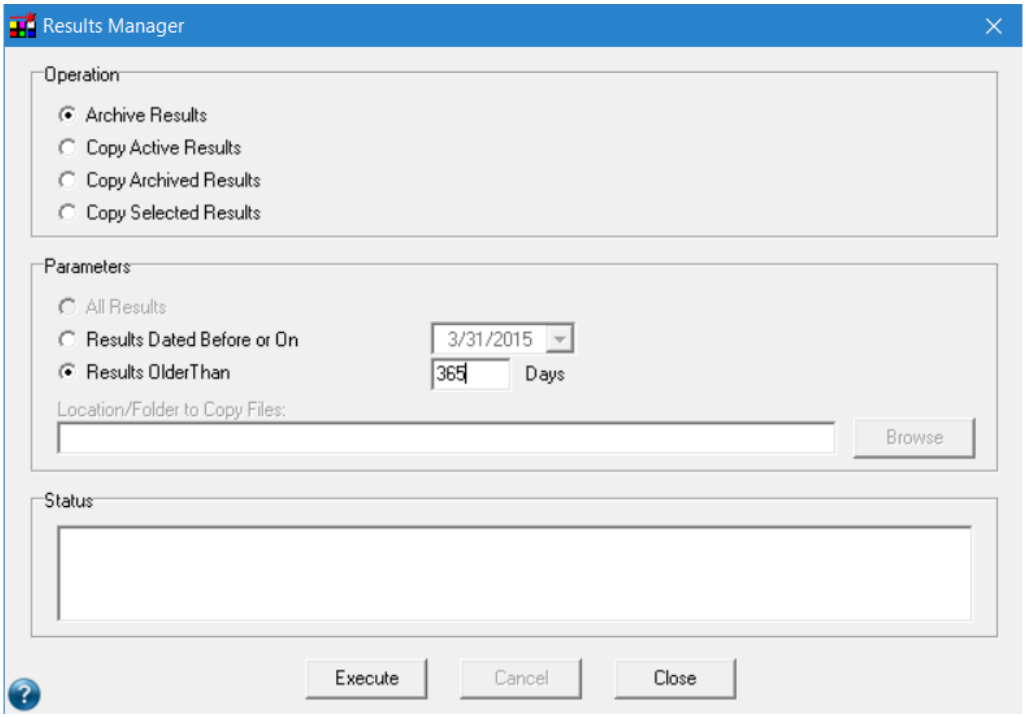
Filters Applied: From Date: 11/18/2024

Sign the summary report by clicking *E-Sign*.

To view a preview of the report, click *Preview*. To print a copy of the report, click *Print.*

ID Analysis Archive

Upon clicking the *Archive* button in the ID Analysis Selection dialog, the Results Manager dialog will appear:


Results Manager

Operation
● Archive Results
○ Copy Active Results
○ Copy Archived Results
○ Copy Selected Results

Parameters
○ All Results
○ Results Dated Before or On 3/31/2015
● Results OlderThan 365 Days
Location/Folder to Copy Files:

Status

The Results Manager dialog allows the user to perform the following actions:

- Archive ID analysis results (by moving the results files from the Active view to the Archived view)
- Copy active or archived results to a location selected by the user
- Copy results, selected in the current view in the ID Analysis Selection dialog, to a location of the user's choice

In the *Operation* box, select the action to be performed.

In the *Parameters* box, select:

- *All Results* – to copy all results (from Active, Archived or selected in current view) to a location of the user's choice (option disabled for *Archive* operation)
- *Results Dated Before or On* – to archive or copy the results collected on or before given date (option disabled for *Copy Selected Results* operation)
- *Results Older Than* – to archive or copy the results older than a given number of days (option disabled for *Copy Selected Results* operation)

In the *Location/Folder to Copy Files*, enter the folder to which the files will be copied. Click the *Browse* button to select the folder (selection is disabled for the *Archive* operation).

Click the *Execute* button to perform the selected operation. The operation status will be displayed in the *Status* box.

NOTE: For software running on Windows 7 or newer, the program must be run in elevated mode (run as administrator from Windows system) in order to successfully perform the Archive Results operation. This is due to restricted privileges to the *Program Files* folder.

Click the *Cancel* button to abort operation execution.

Click the *Close* button to close the dialog and return to the ID Analysis Selection dialog.

Performance Test Report

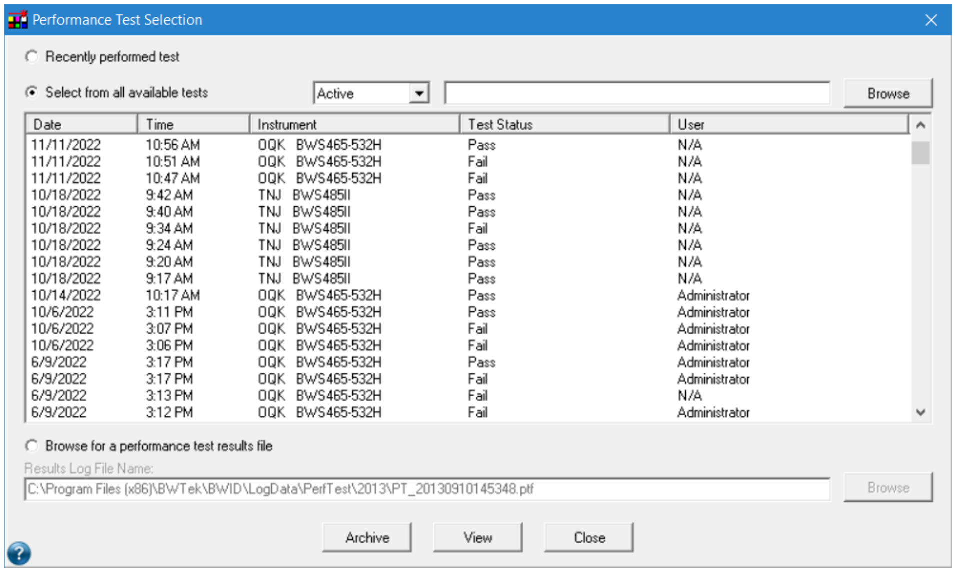
Starting the Performance Test Report

Click the *Report* button in the Menu window and then the *PerfTest* button in the Reports menu to start the performance test report feature. This option allows the user to view and print out a report for any available performance test.

Clicking the *Performance Test Report* button will open the Performance Test Selection dialog.

Performance Test Selection

This dialog allows the user to select a performance test, for which a report will be generated.



○ Recently performed test

● Select from all available tests — Active

Date	Time	Instrument	Test Status	User
11/11/2022	10:56 AM	OQK BWS465-532H	Pass	N/A
11/11/2022	10:51 AM	OQK BWS465-532H	Fail	N/A
11/11/2022	10:47 AM	OQK BWS465-532H	Fail	N/A
10/18/2022	9:42 AM	TNJ BWS485II	Pass	N/A
10/18/2022	9:40 AM	TNJ BWS485II	Pass	N/A
10/18/2022	9:34 AM	TNJ BWS485II	Fail	N/A
10/18/2022	9:24 AM	TNJ BWS485II	Pass	N/A
10/18/2022	9:20 AM	TNJ BWS485II	Pass	N/A
10/18/2022	9:17 AM	TNJ BWS485II	Pass	N/A
10/14/2022	10:17 AM	OQK BWS465-532H	Pass	Administrator
10/6/2022	3:11 PM	OQK BWS465-532H	Pass	Administrator
10/6/2022	3:07 PM	OQK BWS465-532H	Fail	Administrator
10/6/2022	3:06 PM	OQK BWS465-532H	Fail	Administrator
6/9/2022	3:17 PM	OQK BWS465-532H	Pass	Administrator
6/9/2022	3:17 PM	OQK BWS465-532H	Fail	Administrator
6/9/2022	3:13 PM	OQK BWS465-532H	Fail	N/A
6/9/2022	3:12 PM	OQK BWS465-532H	Fail	Administrator

○ Browse for a performance test results file

Results Log File Name: C:\Program Files (x86)\BWTek\BWID\LogData\PerfTest\2013\PT_20130910145348.ptf

Select the *Recently performed test* button if you wish to generate a report for a recently executed performance test.

Check the *Select from all available tests* button to choose a performance test, for which a report will be generated, from one of three views: Active, Archived and In Folder.

The Active view lists all performance test results that have been not archived yet.
The Archived view displays all archived performance tests results.
The In Folder view allows the user to view all results stored in a selected folder. Click the *Browse* button to select the folder with results.

Upon clicking this button, a list of all available performance tests will be displayed, as shown above. This step may take some time depending on how many performance test results are present in selected view.

Select the *Browse for a performance test results file* button, if you know a performance test results file (*.ptf), from which you wish to generate a report.
Click the *Browse* button to select the results file.
By default, the *Results Log File Name* is set with a file name of a recently performed test.

Once the performance test is selected, click the *View* button to view the test results.

Click *Archive* to archive or copy performance tests results. See the Performance Test Archive paragraph for details.

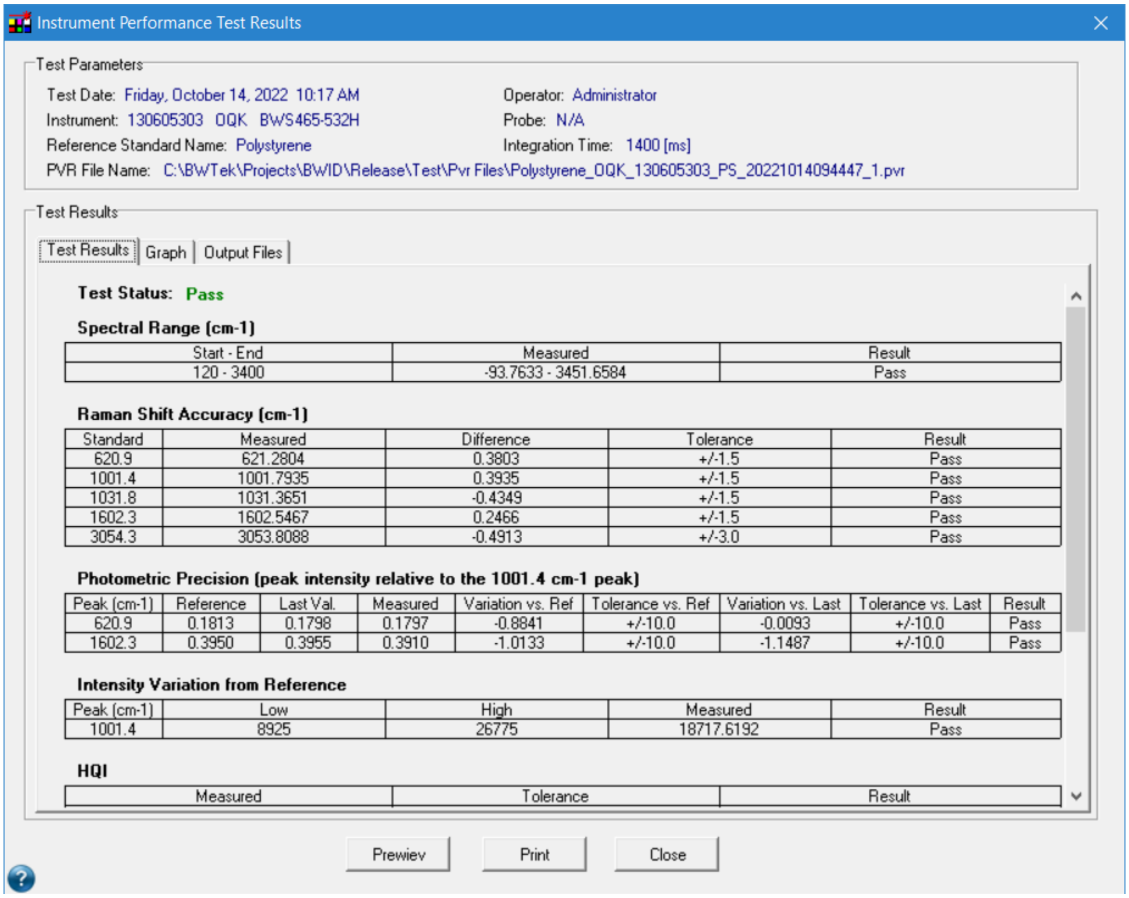
Click *Close* to close the Performance Test Selection dialog and go back to the Menu window.

Performance Test Results

Starting from the BWID version 2.04.06 there is a new performance test with a PVR file. The program supports test results for the new performance test as well as for the old one (any test performed with the BWID ver. 2.04.05 or older).

For the new performance test, upon clicking the *View* button, the Instrument Performance Test Results dialog will appear as shown below.

This dialog shows the parameters and results of the performance test.



Test Date: Friday, October 14, 2022 10:17 AM
Operator: Administrator
Instrument: 130605303 OQK BWS465-532H
Probe: N/A
Reference Standard Name: Polystyrene
Integration Time: 1400 [ms]
PVR File Name: C:\BWTek\Projects\BWID\Release\Test\Pvr Files\Polystyrene_OQK_130605303_PS_20221014094447_1.pvr

Test Status: Pass

Spectral Range (cm-1)

Start - End	Measured	Result
120 - 3400	-93.7633 - 3451.6584	Pass

Raman Shift Accuracy (cm-1)

Standard	Measured	Difference	Tolerance	Result
620.9	621.2804	0.3803	+/-1.5	Pass
1001.4	1001.7935	0.3935	+/-1.5	Pass
1031.8	1031.3651	-0.4349	+/-1.5	Pass
1602.3	1602.5467	0.2466	+/-1.5	Pass
3054.3	3053.8088	-0.4913	+/-3.0	Pass

Photometric Precision (peak intensity relative to the 1001.4 cm-1 peak)

Peak (cm-1)	Reference	Last Val.	Measured	Variation vs. Ref	Tolerance vs. Ref	Variation vs. Last	Tolerance vs. Last	Result
620.9	0.1813	0.1798	0.1797	-0.8841	+/-10.0	-0.0093	+/-10.0	Pass
1602.3	0.3950	0.3955	0.3910	-1.0133	+/-10.0	-1.1487	+/-10.0	Pass

Intensity Variation from Reference

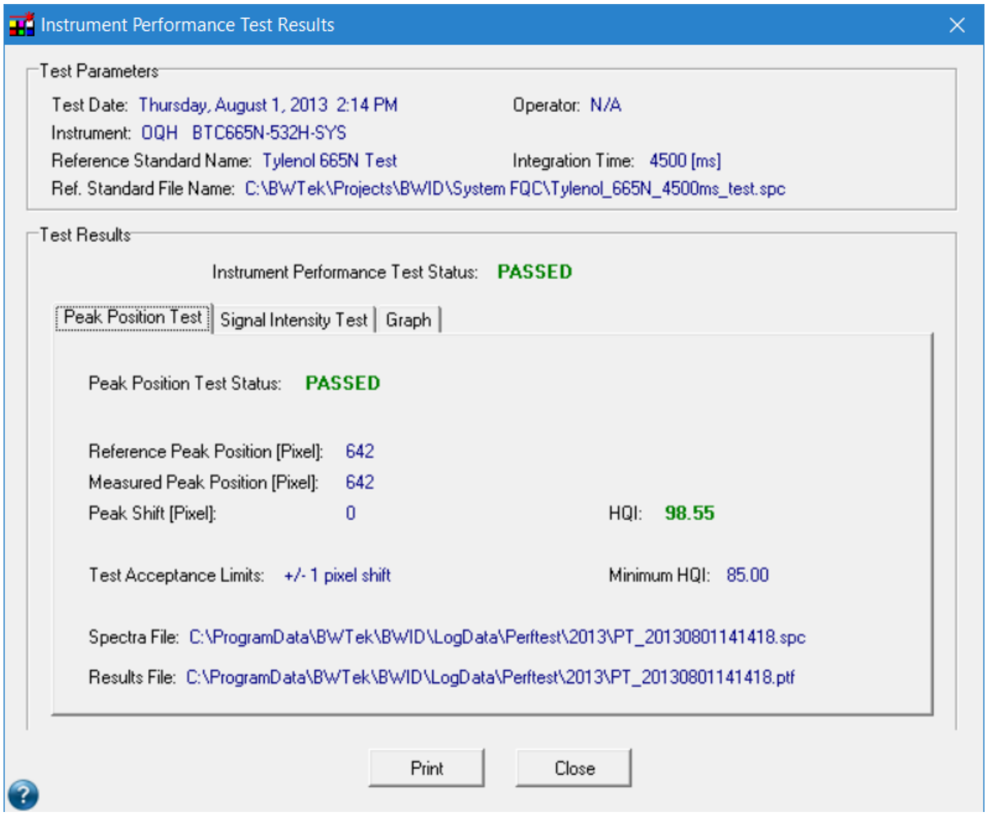
Peak (cm-1)	Low	High	Measured	Result
1001.4	8925	26775	18717.6192	Pass

HQI

Measured	Tolerance	Result

For more details see the Test Results in the Performance Test of the Diagnostic Tests paragraph.

For the old performance test, upon clicking the *View* button, the Instrument Performance Test Results dialog will appear as shown below.



Instrument Performance Test Results

Test Parameters

Test Date: Thursday, August 1, 2013 2:14 PM
Operator: N/A
Instrument: 0QH BTC665N-532H-SYS
Reference Standard Name: Tylenol 665N Test
Integration Time: 4500 [ms]
Ref. Standard File Name: C:\BWTek\Projects\BWID\System FQC\Tylenol_665N_4500ms_test.spc

Test Results

Instrument Performance Test Status: PASSED

Peak Position Test Status: PASSED

Reference Peak Position [Pixel]: 642
Measured Peak Position [Pixel]: 642
Peak Shift [Pixel]: 0
HQI: 98.55

Test Acceptance Limits: +/- 1 pixel shift
Minimum HQI: 85.00

Spectra File: C:\ProgramData\BWTek\BWID\LogData\Perftest\2013\PT_20130801141418.spc

Results File: C:\ProgramData\BWTek\BWID\LogData\Perftest\2013\PT_20130801141418.ptf

The dialog shows the parameters and results of a performance test.

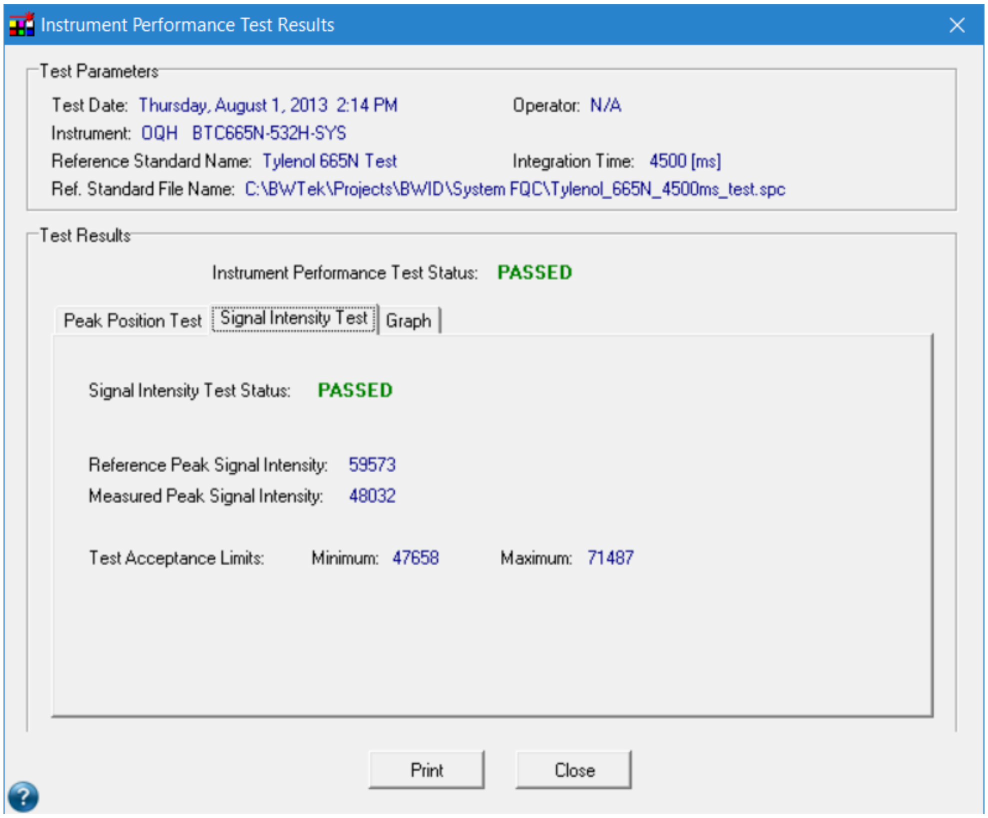
In the *Test Parameters* box:
Test Date – date and time when the performance test was executed
Instrument – name of the instrument on which the test was performed
Reference Standard Name – name of a reference standard used in the test
Reference Standard File Name – name of a reference standard file used in the test
Integration Time – integration time of collected spectrum
Operator – name of the user who performed the test

In the *Test Results* box:
Instrument Performance Test Status –status of the performance test: PASSED (in green) or FAILED (in red)

Peak Position Test tab – holds details of the peak position test
Signal Intensity Test tab – holds details of the peak's signal intensity test
Graph tab – displays collected spectrum and reference standard spectrum

In the *Peak Position Test* tab:
Peak Position Test Status – status of the peak position test: PASSED (in green) or FAILED (in red)
Reference Peak Position – position (in pixels) of the reference peak in the reference standard spectrum
Measured Peak Position – position (in pixels) of the measured peak in the collected spectrum
Peak Shift – a shift (in pixels) between the measured and the reference peak
Test Acceptance Limits – condition to pass the peak position test

In the *Signal Intensity Test* tab:



Test Date: Thursday, August 1, 2013 2:14 PM
Operator: N/A
Instrument: 0QH BTC665N-532H-SYS
Reference Standard Name: Tylenol 665N Test
Integration Time: 4500 [ms]
Ref. Standard File Name: C:\BWTek\Projects\BWID\System FQC\Tylenol_665N_4500ms_test.spc

Instrument Performance Test Status: PASSED

Signal Intensity Test Status: PASSED

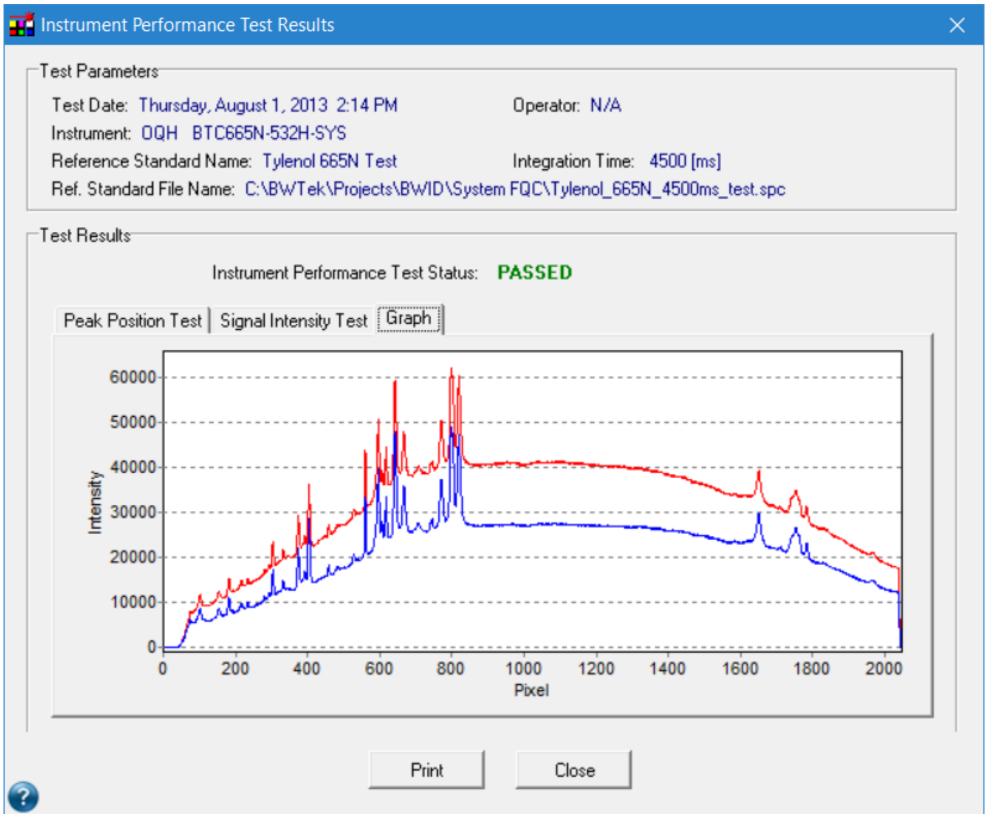
Reference Peak Signal Intensity: 59573
Measured Peak Signal Intensity: 48032

Test Acceptance Limits: Minimum: 47658 Maximum: 71487

Signal Intensity Test Status – status of the peak's signal intensity test: PASSED (in green) or FAILED (in red)
Reference Peak Signal Intensity – signal intensity of the reference peak in the reference standard spectrum
Measured Peak Signal Intensity – signal intensity of the measured peak in the collected spectrum
Test Acceptance Limits – condition to pass the signal intensity test

Minimum – minimum value of the signal intensity to pass the test
Maximum – maximum value of the signal intensity to pass the test

In the *Graph* tab:



Instrument Performance Test Results

Test Parameters

Test Date: Thursday, August 1, 2013 2:14 PM
Operator: N/A
Instrument: 0QH BTC665N-532H-SYS
Reference Standard Name: Tylenol 665N Test
Integration Time: 4500 [ms]
Ref. Standard File Name: C:\BWTek\Projects\BWID\System FQC\Tylenol_665N_4500ms_test.spc

Test Results

Instrument Performance Test Status: PASSED

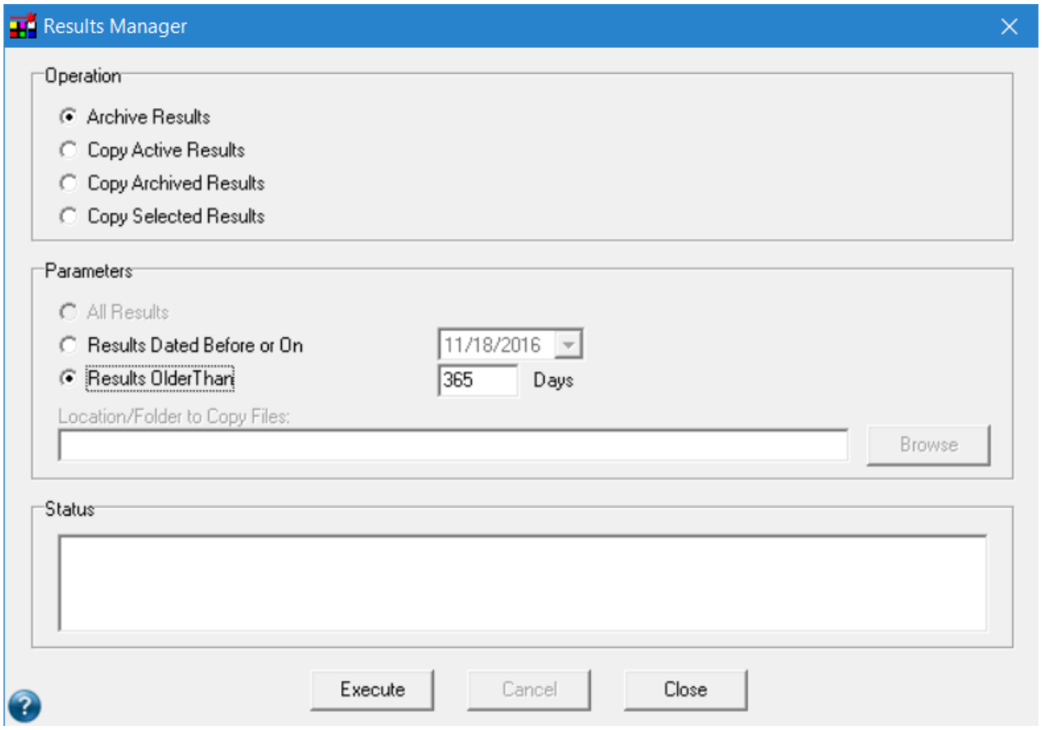
In red – reference standard spectrum (in pixels)
In blue – collected spectrum (in pixels)

Click *Print* to print the test results report.

Click *Close* to close the performance test results dialog and go back to the Performance Test Selection dialog.

Performance Test Archive

Upon clicking the *Archive* button, the Results Manager dialog will appear:



Results Manager

Operation
- ● Archive Results
- ○ Copy Active Results
- ○ Copy Archived Results
- ○ Copy Selected Results

Parameters
- ○ All Results
- ○ Results Dated Before or On: 11/18/2016
- ● Results Older Than: 365 Days

Location/Folder to Copy Files:

Status

The Results Manager dialog allows the user to perform the following actions:

- Archive performance tests results (by moving the results files from the Active view to the Archived view)
- Copy active or archived results to a location selected by the user
- Copy results, selected in the current view in the Performance Test Selection dialog, to a location of the user's choice

In the *Operation* box, select the action to be performed.

In the *Parameters* box, select:

- *All Results* – to copy all results (from Active, Archived or selected in current view) to a location of the user's choice (option disabled for Archive operation)
- *Results Dated Before or On* – to archive or copy the results collected on or before given date (option disabled for *Copy Selected Results* operation)
- *Results Older Than* – to archive or copy the results older than given number of days (option disabled for *Copy Selected Results* operation)

In the *Location/Folder to Copy Files*, enter the folder to which the files will be copied. Click the *Browse* button to select the folder (selection is disabled for the *Archive* operation).

Click the *Execute* button to perform the selected operation. The operation status will be displayed in the *Status* box.

NOTE: For software running on Windows 7 or newer, the program must be run in elevated mode (run as administrator from Windows system) in order to successfully perform the Archive Results operation. This is due to restricted privileges to the *Program Files* folder.

Click the *Cancel* button to abort operation execution.

Click the *Close* button to close the dialog and return to the Performance Test Selection dialog.

12. User Access Control

User Types

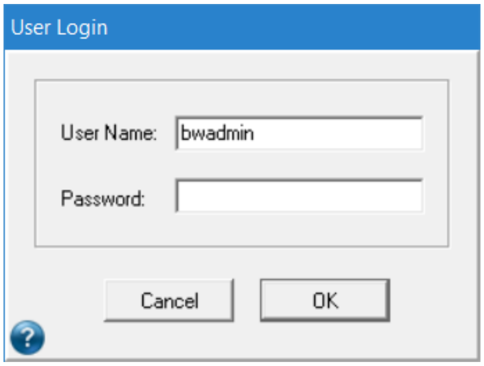
There are three different user types which determine the level of access to the BWID® program and its functions: *Operator, Developer* and *Administrator*. These categories differ by the set of the functions available to each type.

User Type	*User Privileges*
Operator	Run a sample identification Perform diagnostic tests Print results for recently performed ID analysis and performance test Electronically sign an ID analysis record Change his/her own password
Developer	All Operator Privileges Create/modify a data library Setup an operation preset Configure performance test parameters Configure ID analysis report Select, view, and print a report for any ID analysis and performance test Electronically sign and approve an ID analysis record Configure graphical user interface (GUI) settings Configure licensed instruments

Administrator	All Operator and Developer Privileges Manage user accounts: • View user accounts • Add/lock/unlock/reset/disable a user account • Modify user account properties • Backup/restore user accounts file • Configure access policy

Login

Clicking on the *Login* button in the User menu dialog (see User Menu) displays the Login dialog. The program will prompt the user to enter his/her user name and password.



User Name: bwadmin

Password:

Once the user name and password are entered, click the *OK* button to login to the program.

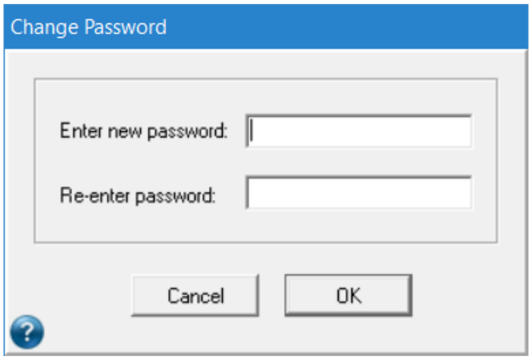
Click the *Cancel* button to abort login.

Please note that the user name and password are case sensitive.

Please also note that after a predefined number (default of three) of consecutive failed attempts to login (wrong user name and/or password), the program will lock the user account that was used to login. In this case, the administrator must unlock the locked account in order to enable login next time.

Change Password

Click the *Change Password* button in the User menu dialog (see User Menu) to change your own password.
The Change Password dialog will appear as shown:



Enter a new password, then enter it again in the appropriate input fields of the Change Password dialog. Click the *OK* button to accept the new password.

Click the *Cancel* button to abort password changing.

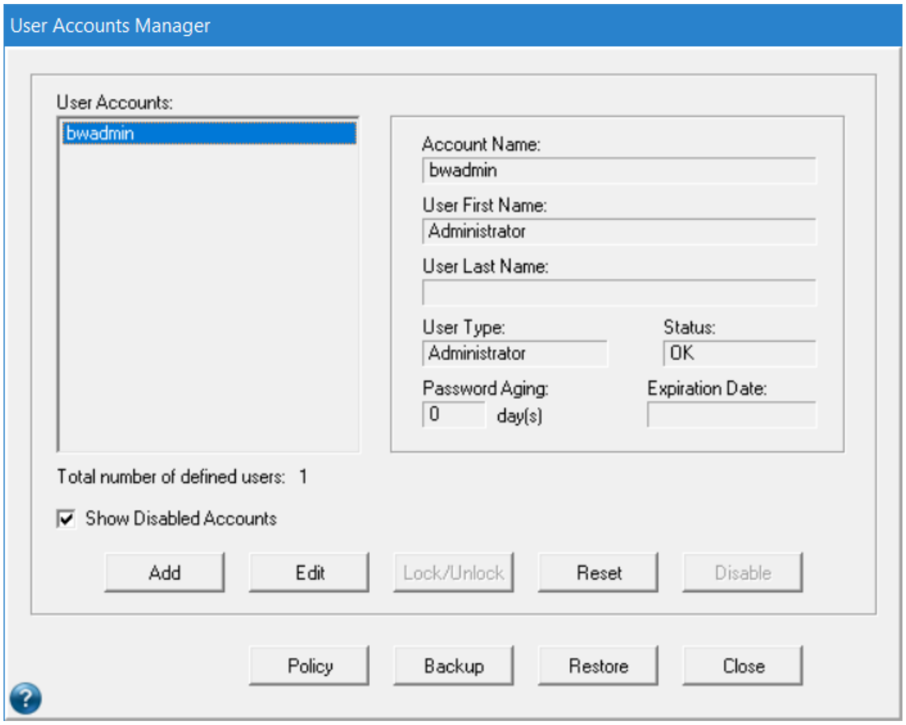
Please note that the password is case sensitive.

Accounts Management

Only an Administrator user has access to the User Accounts Manager through the *Manage Accounts* button in the User menu dialog (see User Menu).

The *Manage Accounts* function enables the *Administrator* user to perform various administrative tasks such view and modify existing user accounts, add new account, lock, unlock, reset or disable an account, customize the access policy as well as backup and restore user accounts.

Below is the User Accounts Manager dialog:



User Accounts:
bwadmin

Account Name: bwadmin
User First Name: Administrator
User Last Name:
User Type: Administrator
Status: OK
Password Aging: 0 day(s)
Expiration Date:

Total number of defined users: 1

☑ Show Disabled Accounts

The *User Accounts* box on the left displays all existing accounts (account names only) in the system. If the *Show Disabled Accounts* box is unchecked, the list will contain all accounts except disabled ones.

The box on the right shows properties of currently selected accounts in the *User Accounts* box.
The *Account Name* uniquely defines a user within the system. The next two properties (first and last name) are self-explanatory. *User type* can be one of the following: *Operator*, *Developer* or *Administrator*. The *Status* shows current status of the account and can be one of the following: *OK*, *Expired*, *Reset*, *Locked* or *Disabled*. The *Password Aging* shows how many days the password is valid, while the *Expiration Date* shows the actual date that the password will expire.

The *Add* button allows the user to add a new user account.

The *Edit* button enables the user to modify selected account properties: user type or/and password expiration.

The *Lock/Unlock* button allows the user to lock a selected account if the account is not locked and unlock a locked account.
The *Reset* button enables the user to reset a password for selected account.

The *Disable* button allows the user to disable a selected account.

The *Policy* button allows the user to view or customize the Access Policy. See Access Policy section below.

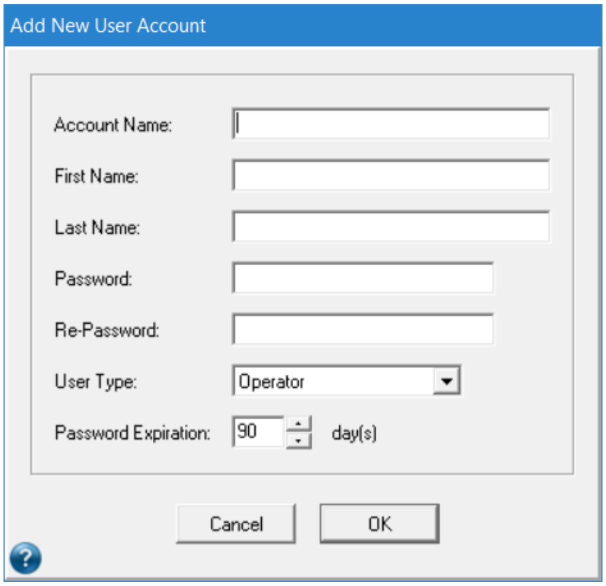
The *Backup* button allows the user to make a backup of the user accounts.

The *Restore* button enables the user to restore the user accounts from a backup of the user accounts.

The *Close* button allows the user to close the User Accounts Manager and go back to the Menu window.

Adding a New Account

To add a new user account, click the *Add* button in the User Accounts Manager dialog. The Add New User Account dialog will appear:



User Type: Operator

Password Expiration: 90 day(s)

Account Name, *User First Name and User Last Name* are strings of alphanumeric characters (default min. 2, max. 30; see Access Policy for customized settings).
In the *Account Name* field, enter a name that will uniquely define the new user within the system. Next, enter the new user's first and last name in the *First Name* and *Last Name* fields respectively.

The *Password* is a string of alphanumeric characters (default min. 5, max. 30; see Access Policy for customized settings).

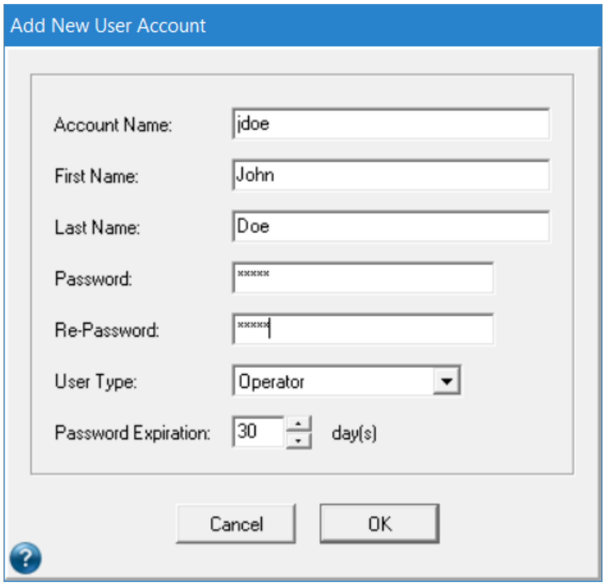
Enter an initial password for the new user in the *Password* field and then enter it again in the *Re-Password* field.

Please note that all names and password are case sensitive!

From the dropdown list, select the user type of the new user being added to the system: *Operator*, *Supervisor* or *Administrator*.

The *Password Expiration* defines the number of days after the password is created/changed that it will expire.
In the *Password Expiration* field, set the value within range of 1 to 720 for the *Operator* user and in the range of 0 to 720 for the *Developer* or *Administrator* user. Zero (0) days indicates that the password will never expire.

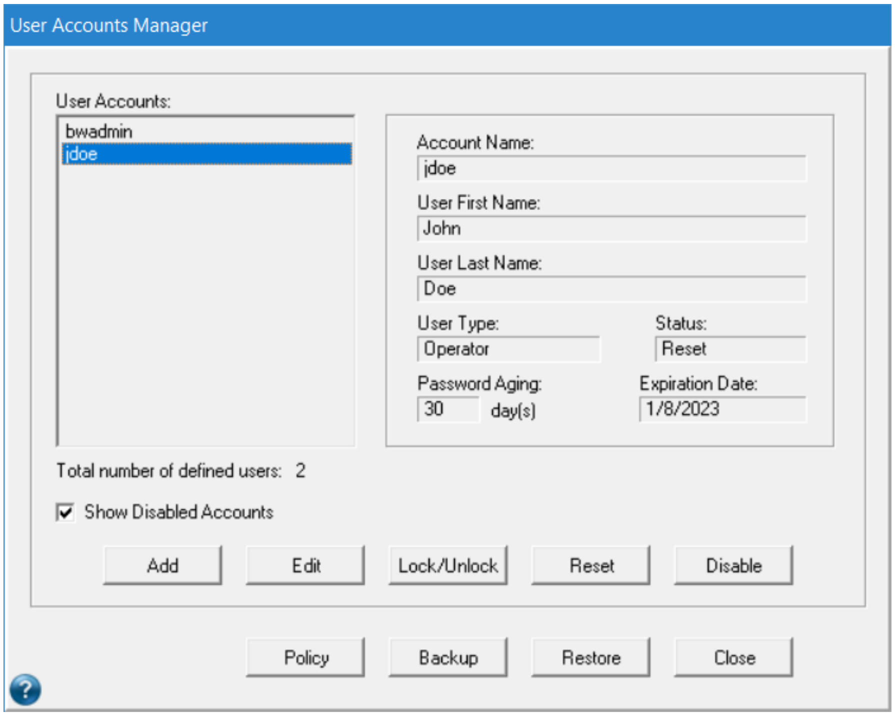
Below is an example showing the Add New User Account dialog filled out for a new user:



Account Name: jdoe
First Name: John
Last Name: Doe
Password: *****
Re-Password: *****
User Type: Operator
Password Expiration: 30 day(s)

Click the *OK* button to accept the settings of a new account.
After clicking the *OK* button, the new user account is added to the system and the changes are reflected in the User Accounts Manager dialog, as shown below.

Click the *Cancel* button to abort adding a new user account.



User Accounts Manager

User Accounts:
bwadmin
jdoe

Account Name: jdoe
User First Name: John
User Last Name: Doe
User Type: Operator
Status: Reset
Password Aging: 30 day(s)
Expiration Date: 1/8/2023

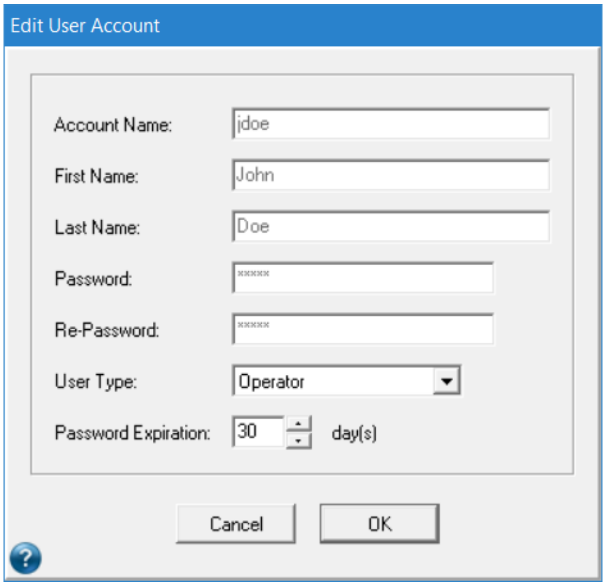
Total number of defined users: 2

☑ Show Disabled Accounts

When a new account is added to the system, the account status is always set to *Reset*. The new user will be forced to change the password the first time he logs in to the program using the password set by the *Administrator* (see Resetting Password below).

Editing an Account

To modify an existing account, select the account in the *User Accounts* box and then click the *Edit* button in the User Accounts Manager dialog. The Edit User Account dialog will appear:



Edit User Account

Account Name: jdoe

First Name: John

Last Name: Doe

Password: *****

Re-Password: *****

User Type: Operator

Password Expiration: 30 day(s)

The dialog allows the *Administrator* to modify *User Type* and/or *Password Expiration* properties only.

Click the *OK* button to accept changes.

Click the *Cancel* button to abort account changes.

Locking/Unlocking an Account

The *Lock/Unlock* button is a toggle switch that can be used for locking or unlocking a selected account.

After a predefined number (default of three) of consecutive unsuccessful user attempts to login to the program, the user account will automatically be locked. Only the *Administrator* is able to unlock the user account. **It is strongly recommended to create at least two *Administrator* accounts so that if one account becomes locked or an Administrator has lost his/her access to the application, there is an additional user with the ability to unlock the second one.**

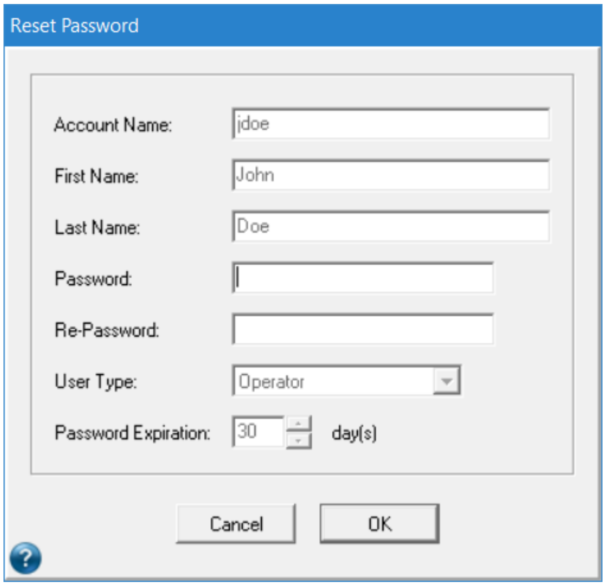
To lock an account, select the account in the *User Accounts* box and then click the *Lock/Unlock* button. Please note that a disabled account cannot be locked.

To unlock a locked account, select the account with the *Locked* status in the *User Accounts* box and then click the *Lock/Unlock* button. Unlocking the account will restore the account status.

Resetting a Password

Resetting a password is useful when a user forgets his/her password or when a disabled account needs to be activated again. Using this function, the *Administrator* can set a temporary password for the user.

To reset a password for an existing account, select the account in the *User Accounts* box and then click the *Reset* button in the User Accounts Manager dialog. The Reset Password dialog will appear:



Account Name: jdoe
First Name: John
Last Name: Doe
Password:
Re-Password:
User Type: Operator
Password Expiration: 30 day(s)

Type a new password in the *Password* field and then type the same password into the *Re-Password* field.

Click the *OK* button to accept the new password.

Click the *Cancel* button to abort resetting the password.

Once the user password is reset, the next successful login to the system will force the user to change the password to a new one. "Password has been reset by the administrator! Please define a new one." message will appear, followed by the Change Password dialog (see Changing Password section above).

Disabling an Account

The User Accounts Manager does not allow an Administrator user to delete an existing account (due to CFR21 Part 11 compliance). When an account is no longer needed, it can be disabled.

To disable an existing account, select the account in the *User Accounts* box and then click the *Disable* button in the User Accounts Manager dialog.

Once the account is disabled it can only be enabled again by pressing the *Reset* button and creating a new password.

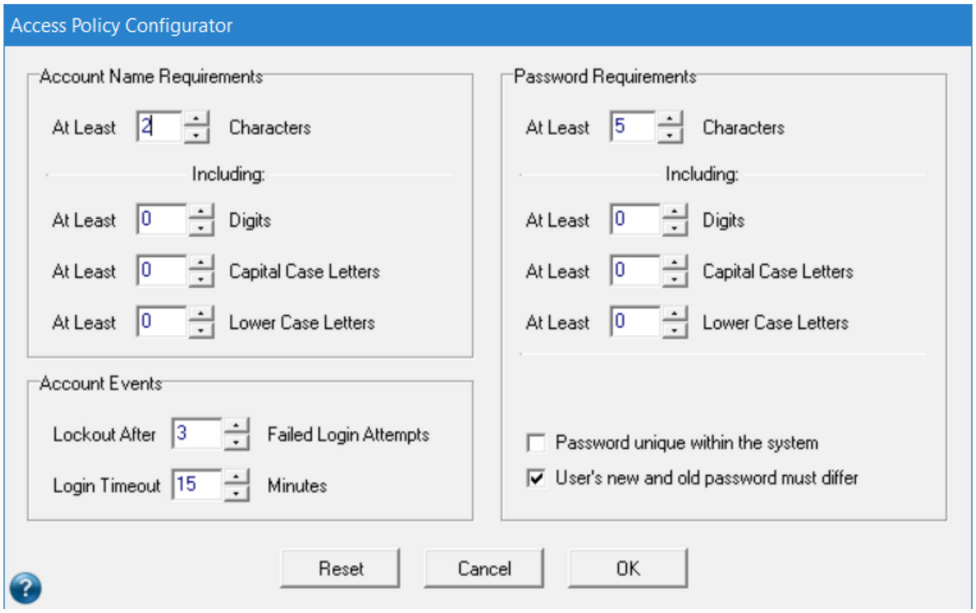
Access Policy

Access Policy is a set of rules defining the requirements for a user password, user account name and account events.

By default, the Access Policy consists of the following rules:

- Account
    - Must contain at least 2 alphanumeric characters (excluding leading and trailing spaces)
    - Is case sensitive
    - Is unique within the system, (i.e. two or more users cannot have the same account name)
    - Is locked after 3 failed login attempts
    - User will be automatically logged out after 15 minutes of the user’s inactivity within the program
- Password
    - Must contain at least 5 alphanumeric characters (excluding leading and trailing spaces)
    - Is case sensitive
    - Is not unique within the system, (i.e. two or more users may have the same password)
    - The old and newly defined password must differ, (i.e. user cannot change his/her password to the same password)

To view or customize the current Access Policy, click the *Policy* button in the User Accounts Manager dialog. The Access Policy Configurator dialog will appear, as shown below.



Account Name Requirements
At Least 2 Characters
Including:
At Least 0 Digits
At Least 0 Capital Case Letters
At Least 0 Lower Case Letters

Account Events
Lockout After 3 Failed Login Attempts
Login Timeout 15 Minutes

Password Requirements
At Least 5 Characters
Including:
At Least 0 Digits
At Least 0 Capital Case Letters
At Least 0 Lower Case Letters
☐ Password unique within the system
☑ User's new and old password must differ

The Access Policy Configurator allows the *Administrator* user to define:

- minimum length of an account name (accepted range from 2 to 30 characters), including minimum number of digits, capital and/or lower-case letters (accepted range from 0 to 30 characters)
- maximum number of failed login attempts before the account lockout (accepted range from 0, i.e. no lockout at all, to 10)
- login timeout for inactive user (accepted range from 0, i.e. no login timeout, to 120 minutes)
- minimum password length (accepted range from 2 to 30 characters), including minimum number of digits, capital and/or lower-case letters (accepted range from 0 to 30 characters)
- password uniqueness

Click the *Reset* button to reset settings to the default Access Policy.

Click the *OK* button to accept the current settings in the dialog and close the window.

Click the *Cancel* button to close the dialog without accepting the settings.

Accounts Backup

The *Backup* button allows the *Administrator* user to make a backup of the all user accounts defined within the system.
It is recommended to do the backup on a regular basis to keep a copy of the latest settings.
When the backup is completed, a message with status confirmation will appear. In the case of an error, an appropriate

message will appear.

Accounts Restoring

The *Restore* button allows the *Administrator* user to restore user accounts from the last backup (performed using the *Backup* button). Note that all account modifications completed after the last backup will be lost upon restoring the accounts from the backup.

Upon clicking the *Restore* button, the user will be warned of losing all accounts added after the last backup and will have an option to proceed with the backup, or cancel it.

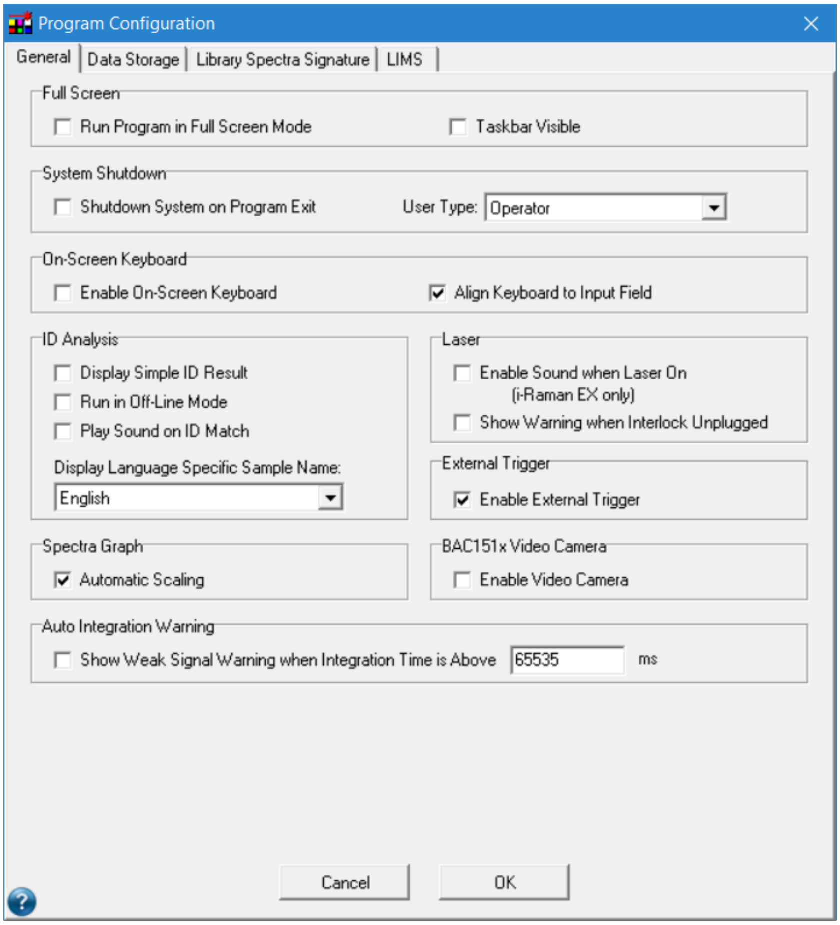
When the accounts restoration is completed, a message with status confirmation will appear. In the case of an error, an appropriate message will be shown.

13. Program Configuration

To configure program parameters (such as GUI or default paths) click the *Setup* button in the Menu window and then the *Program* button from the Setup menu. The Program Configuration contains four pages: General, Data Storage, Library Spectra Signature (Pharma edition only), and LIMS.

General Configurations

On the General page, the following dialog will be displayed:



Program Configuration

Full Screen
☐ Run Program in Full Screen Mode
☐ Taskbar Visible

System Shutdown
☐ Shutdown System on Program Exit
User Type: Operator

On-Screen Keyboard
☐ Enable On-Screen Keyboard
☑ Align Keyboard to Input Field

ID Analysis
☐ Display Simple ID Result
☐ Run in Off-Line Mode
☐ Play Sound on ID Match
Display Language Specific Sample Name: English

Laser
☐ Enable Sound when Laser On (i-Raman EX only)
☐ Show Warning when Interlock Unplugged

External Trigger
☑ Enable External Trigger

Spectra Graph
☑ Automatic Scaling

BAC151x Video Camera
☐ Enable Video Camera

Auto Integration Warning
☐ Show Weak Signal Warning when Integration Time is Above 65535 ms

Run Program in Full Screen Mode - check this box to maximize the main window of the program. This feature allows the program to lock out user access to the desktop and computer's hard disk while the program is running.

Taskbar Visible – check this box to have the taskbar visible when the program's main window is maximized. This will allow the user to open a Windows touch keyboard on a tablet as the program's on-screen keyboard may not work correctly on the tablet.

Shutdown System on Program Exit - check this box to shut down the Windows system upon closing the program.

User Type – select the maximum user level for which the Windows system will shut down upon closing the program (Pharma Edition only).

Example: For *Operator* level the program will shut down the Windows system if the logged-in user is of *Operator* status; if the *Developer* level is selected, the program will shut down the Windows system if the logged-in user is of *Operator* or *Developer* status.

The system shutdown feature combined with running the program in full screen mode provides full protection from unauthorized access to the desktop and computer's hard disk whether the program is running or not.

Enable On-Screen Keyboard – check this box to display a soft keyboard on the screen whenever the user clicks in an edit type field in any dialog of the program. For more details, see the Using On-Screen Keyboard paragraph.

Align Keyboard to Input Field – check this box to align the soft keyboard to an input field being clicked.

Display Simple ID Result - check this box to display match/no match and identified sample name only in the ID Result window. If not checked, the ID Result window will additionally display spectra graphs and HQI value.

Run in Off-line Mode - check this box to allow the user to run off-line ID analysis, where the input spectra for ID analysis will be selected from a file. If not checked, the on-line ID analysis will be enforced, where a connection with the instrument is required.

Play Sound on ID Match - check this box to play a sound when there is a match in ID analysis.

Display Language Specific Sample Name – select the language (English or Chinese) in which sample name will be displayed in ID analysis. By default, the sample name is in English. To display Chinese name of the sample, the Chinese name entry ("Chinese Name: ") must be present in the sample's properties in a data library. If the Chinese language is selected but there is no corresponding Chinese name in the library or the Chinese name cannot be displayed properly (e.g. due to non-Chinese locale setting on a PC), the English name will be displayed instead.

Enable Sound when Laser On (i-Raman EX only) - check this box to play a beep sound when the laser is in emission state. This option is available on i-Raman EX instruments only.

Show Warning when Interlock Unplugged - check this box to display a warning message when the program detects that interlock is not plugged in. The interlock status is checked on program startup and before a scan. Please note that on the older systems, the interlock status may be read incorrectly thus showing interlock unplugged message when actually the interlock is plugged in, and vice versa. In such case this option should be unchecked.

Enable External Trigger - check this box to allow the user use of an external trigger to start spectrum acquisition. If this box is checked, the program will start scanning upon pressing a Scan button in a program window or external trigger button on a measurement probe. If this box is unchecked, pressing the external trigger button will not start the acquisition.

Automatic Scaling - check this box to automatically scale a spectra graph to fit all spectra displayed in the graph. If the box is unchecked, the fixed range from 0 to 65000 is used.

Enable Video Camera - check this box to enable the video camera when the video microscope sampling system BAC151 (ver. A, B or C) is coupled with the Raman system. If this box is check, the video camera image will be displayed on the screen.

Show Weak Signal Warning when Integration Time is Above - check this box to enable a warning message if auto integration time is enabled and the integration time determined exceeds a value specified in the box. In case it does, the user has the choice to proceed with the measurement, or cancel it (for example this may be caused by a closed shutter, a low laser power setting, etc.).

Click *OK* to accept these settings and close the dialog.

Click *Cancel* to cancel the program configuration and close the dialog.

Data Storage Configurations

On the Data Storage page, the data storage locations for various types of data can be set.

Windows Account Name: AdminTest

Password: *****

Re-Password: *****

Operation Presets Folder – set path for saving operation presets.

Spectral Libraries Folder – set path for saving user-defined data libraries.

Performance Validation Reference Files Folder – set path for saving PVR files.

Program Configurations Folder – set path for saving program configurations.

ID Results Folder – set main path for saving identification results. The program will automatically create ID\YYYY subdirectories (where YYYY is a year number) to store there the results from analyses performed in YYYY year.

Test Results Folder – set main path for saving tests results. The program will automatically create PerfTest\YYYY subdirectories (where YYYY is a year number) to store there the results from tests performed in YYYY year.

Audit Trail Folder – set path for saving audit trail files (Pharma edition only).

Secured Folders - check this box if the specified data folders are secured (limited user access) within the Windows system (Pharma edition only). If this box is checked, the user has to also set up the *Secured Folders Access* fields.

Store Data in Secured Folders Only – check this box, if the software should force the user to save an operation preset or a spectra library file in the secured folder only (Pharma edition only).

Secured Folders Access – enter the name and password of a special Windows account that has full access to the data folders (Pharma edition only). The user account will be used within the BWID® program whenever the software needs to write into a secured folder. See a *Secured Folders Setup* paragraph for details.

Backup Folder – set path for program data backup or restoration. See *Data Backup* section below for details.

Click *OK* to accept these settings and close the dialog.

Click *Cancel* to cancel the program configuration and close the dialog.

Default Data Storage

If a field is not set, a default data storage location will be used as follows:

Data Folder Type	*Default Location*
Operation Presets Folder	Program main folder
Spectra Libraries Folder	Folder of last saved library; if none saved yet then the program main folder
Performance Validation Reference Files Folder	Folder of last saved PVR file; if none saved yet then the program main folder
Program Configurations Folder	*CommonAppData*\BWTek\BWID\Config
ID Results Folder	*CommonAppData*\BWTek\BWID\LogData\ID
Test Results Folder	*CommonAppData*\BWTek\BWID\LogData\PerfTest
Audit Trail Folder	*CommonAppData*\BWTek\BWID\LogData\ATFiles

where *CommonAppData* depends on Windows version:

- Windows 10, 8, 7, and Vista - *C:\ProgramData* folder

- Windows XP and 2000 **-** *C:\Documents and Settings\All Users\Application Data* folder.

The folder may be hidden so in order to access it, the user will have to check “Show hidden files, folders, or drivers” in Windows Explorer view settings.

Secured Folders Setup

By default, the data folders are not secured and they should have full read/write/delete/modify access for all Windows users. To configure secured folders for BWID® data (Pharma edition only), the following steps should be performed:

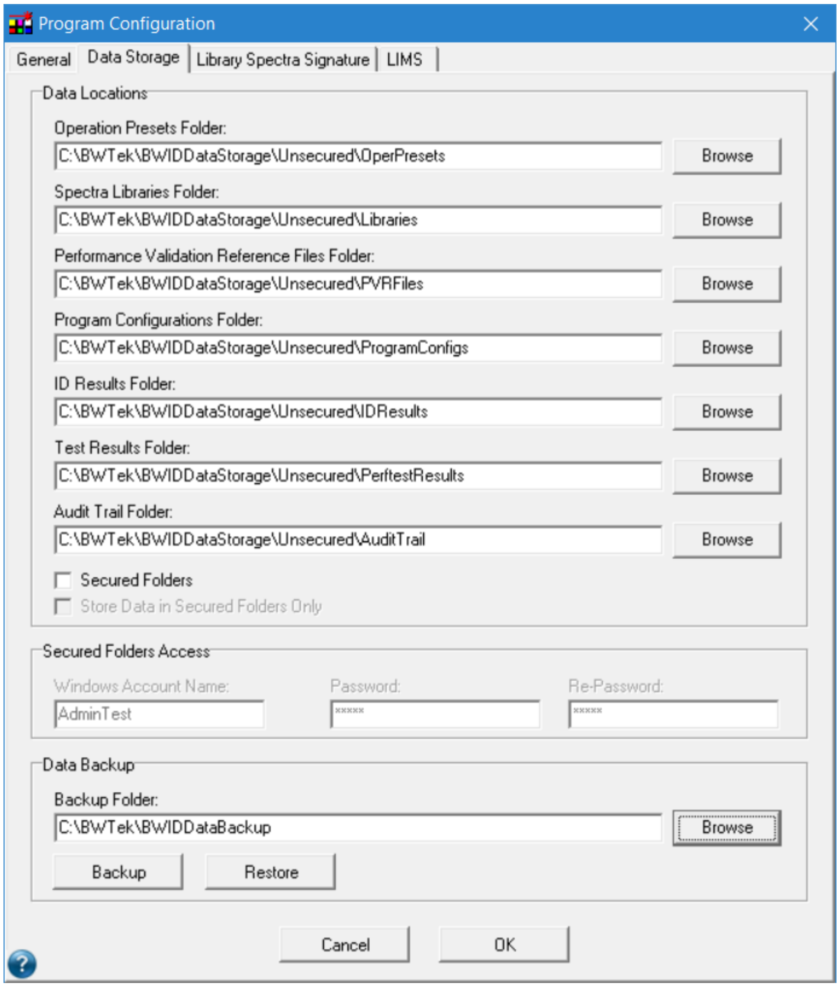
In Windows explorer (done by IT professional)**:**

- create folders that will be used for secure storage in the BWID®
- assign appropriate user access levels to the folders:
    - there has to be a special Windows user (or a group of users) who will have full access to the secured folders; a new Windows account can be created solely for that purpose or an existing account for a real user can be used
    - all other Windows users should have limited access (ALLOW: read and execute, list folder contents, read; DENY: create files/write data, create folders/append data, write attributes, delete subfolders and files, delete, change permissions, take ownership)
    - apply the above settings to the folders, subfolders and files

In the BWID® program (log in as a BWID® administrator)**:**

- select data folders (if you leave empty field for a given data type, the default storage folder will be used)
- check "Secured Folders" box, if the folders you specified are secured for limited user access
- if "Secured Folders" is checked, enter name and password for special Windows user account with full access to the secured folders

Data Backup



Operation Presets Folder: C:\BWTek\BWIDDataStorage\Unsecured\OperPresets

Spectra Libraries Folder: C:\BWTek\BWIDDataStorage\Unsecured\Libraries

Performance Validation Reference Files Folder: C:\BWTek\BWIDDataStorage\Unsecured\PVRFiles

Program Configurations Folder: C:\BWTek\BWIDDataStorage\Unsecured\ProgramConfigs

ID Results Folder: C:\BWTek\BWIDDataStorage\Unsecured\IDResults

Test Results Folder: C:\BWTek\BWIDDataStorage\Unsecured\PerftestResults

Audit Trail Folder: C:\BWTek\BWIDDataStorage\Unsecured\AuditTrail

☐ Secured Folders

☐ Store Data in Secured Folders Only

Windows Account Name: AdminTest

Password: *****

Re-Password: *****

Backup Folder: C:\BWTek\BWIDDataBackup

The backup folder should be selected before clicking *Backup* or *Restore* button.

Backup

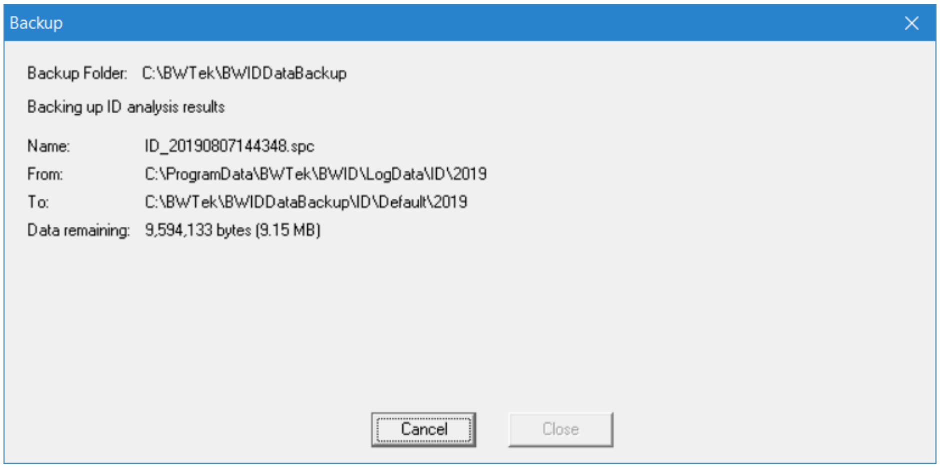
Upon clicking the *Backup* button, the program will check if there is enough space on the disk to back up the program data. Then it will ask the user if he wants to proceed with the backup operation.

The program will back up data from the default data storage and from user data storage locations, if there is any selected folder as shown in the dialog above.

The following data will be backed up from the default data storage: program configurations, ID analysis results, performance test results, audit trail.

The backup folder will contain several predefined subfolders with backed up data. Do not change any subfolder name as the program will use the predefined subfolders to restore data to correct folders in Restore option.

The program will display the backup status and progress as shown in the dialog below.

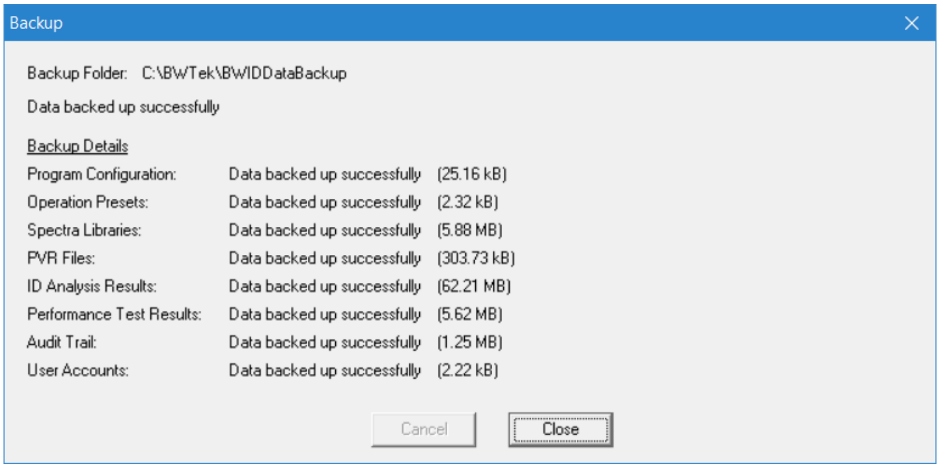


Backup Folder: C:\BWTek\BWIDDataBackup

Backing up ID analysis results

Name: ID_20190807144348.spc
From: C:\ProgramData\BWTek\BWID\LogData\ID\2019
To: C:\BWTek\BWIDDataBackup\ID\Default\2019
Data remaining: 9,594,133 bytes (9.15 MB)

Once the backup is finished, the program will display the final status as shown below.



Backup Folder: C:\BWTek\BWIDDataBackup

Data backed up successfully

Backup Details

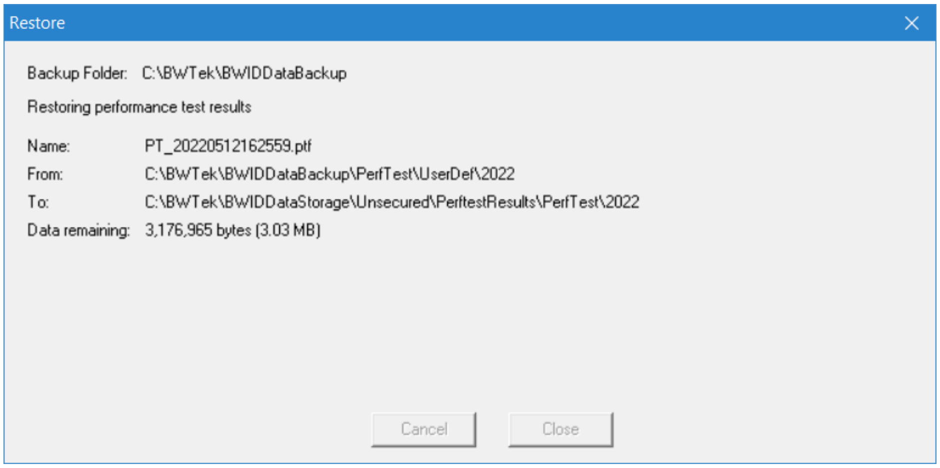
Program Configuration:	Data backed up successfully	(25.16 kB)
Operation Presets:	Data backed up successfully	(2.32 kB)
Spectra Libraries:	Data backed up successfully	(5.88 MB)
PVR Files:	Data backed up successfully	(303.73 kB)
ID Analysis Results:	Data backed up successfully	(62.21 MB)
Performance Test Results:	Data backed up successfully	(5.62 MB)
Audit Trail:	Data backed up successfully	(1.25 MB)
User Accounts:	Data backed up successfully	(2.22 kB)

Restore

Upon clicking the *Restore* button, the program will check if there is enough space on the disk to restore the data from the backup. Next it will warn the user that all current data will be deleted and then it will ask the user if he wants to proceed with the operation.

The program will restore the data into the default data storage and to user data storage locations, if such data exist in the backup.

The program will display the data restoration status and progress as shown in the dialog below.

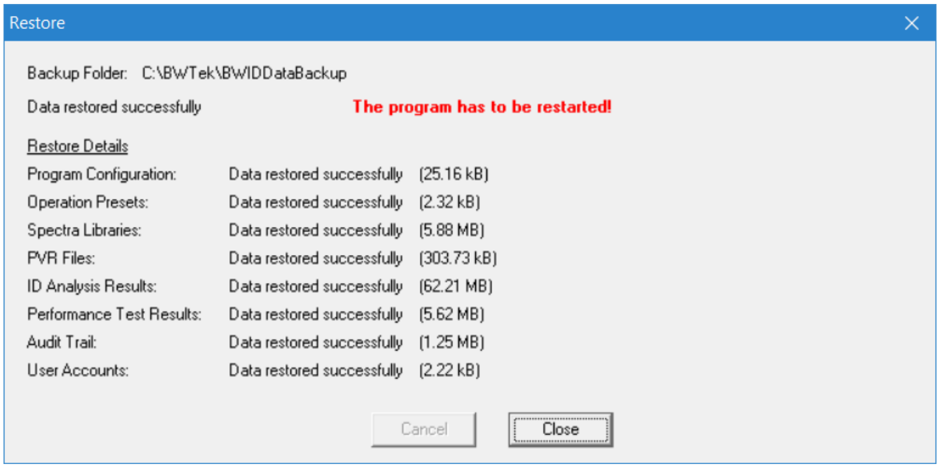


Backup Folder: C:\BWTek\BWIDDataBackup

Restoring performance test results

Name: PT_20220512162559.ptf
From: C:\BWTek\BWIDDataBackup\PerfTest\UserDef\2022
To: C:\BWTek\BWIDDataStorage\Unsecured\PerftestResults\PerfTest\2022
Data remaining: 3,176,965 bytes (3.03 MB)

Once the data restoration is finished, the program will display the final status as shown below.



Backup Folder: C:\BWTek\BWIDDataBackup

Data restored successfully

The program has to be restarted!

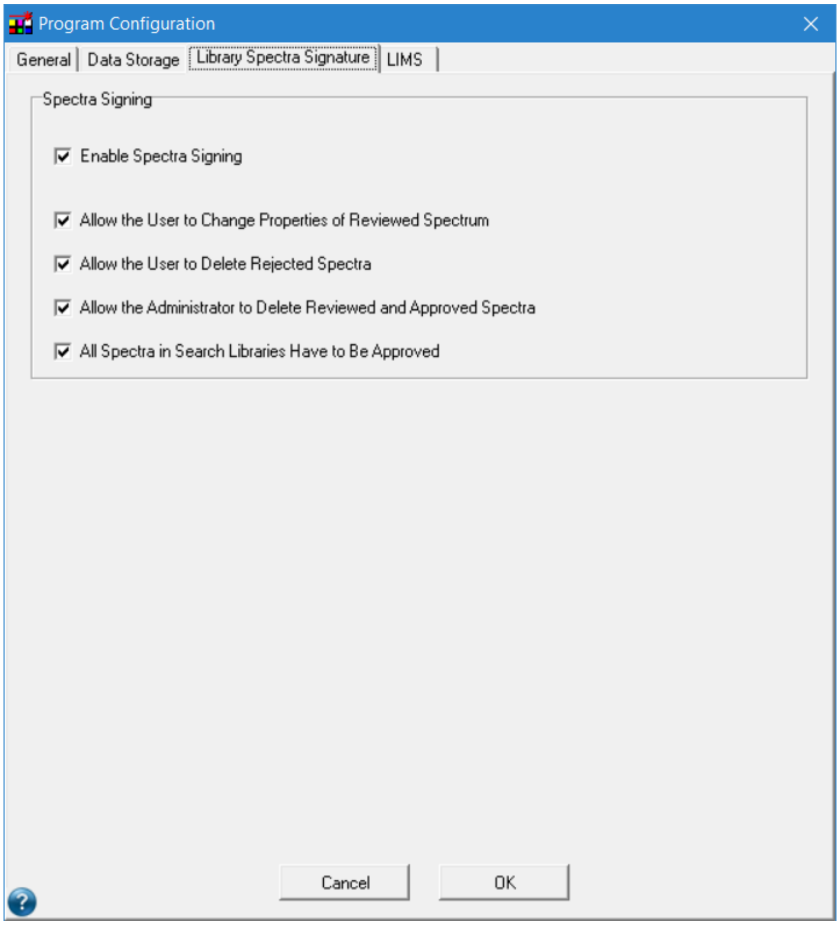
Restore Details

Program Configuration:	Data restored successfully	(25.16 kB)
Operation Presets:	Data restored successfully	(2.32 kB)
Spectra Libraries:	Data restored successfully	(5.88 MB)
PVR Files:	Data restored successfully	(303.73 kB)
ID Analysis Results:	Data restored successfully	(62.21 MB)
Performance Test Results:	Data restored successfully	(5.62 MB)
Audit Trail:	Data restored successfully	(1.25 MB)
User Accounts:	Data restored successfully	(2.22 kB)

Upon clicking the *Close* button the program will inform the user that the BWID software will be closed after restoring the data to finish the operation.

Library Spectra Signature Configurations

On the Library Spectra Signature page (Pharma edition only), the following dialog will be displayed:



Spectra Signing

☑ Enable Spectra Signing

☑ Allow the User to Change Properties of Reviewed Spectrum

☑ Allow the User to Delete Rejected Spectra

☑ Allow the Administrator to Delete Reviewed and Approved Spectra

☑ All Spectra in Search Libraries Have to Be Approved

Enable Spectra Signing - check this box to allow the user to electronically sign spectra in a user-defined library. If enabled, the user can review, approve or reject the spectra in the library. By default, the setting is disabled and all other settings listed below are irrelevant.

Allow the User to Change the Properties of Reviewed Spectrum - check this box to allow the user to change properties of the spectrum that has been reviewed. By default, the setting is disabled and the program will prohibit from making any changes to the reviewed spectrum.

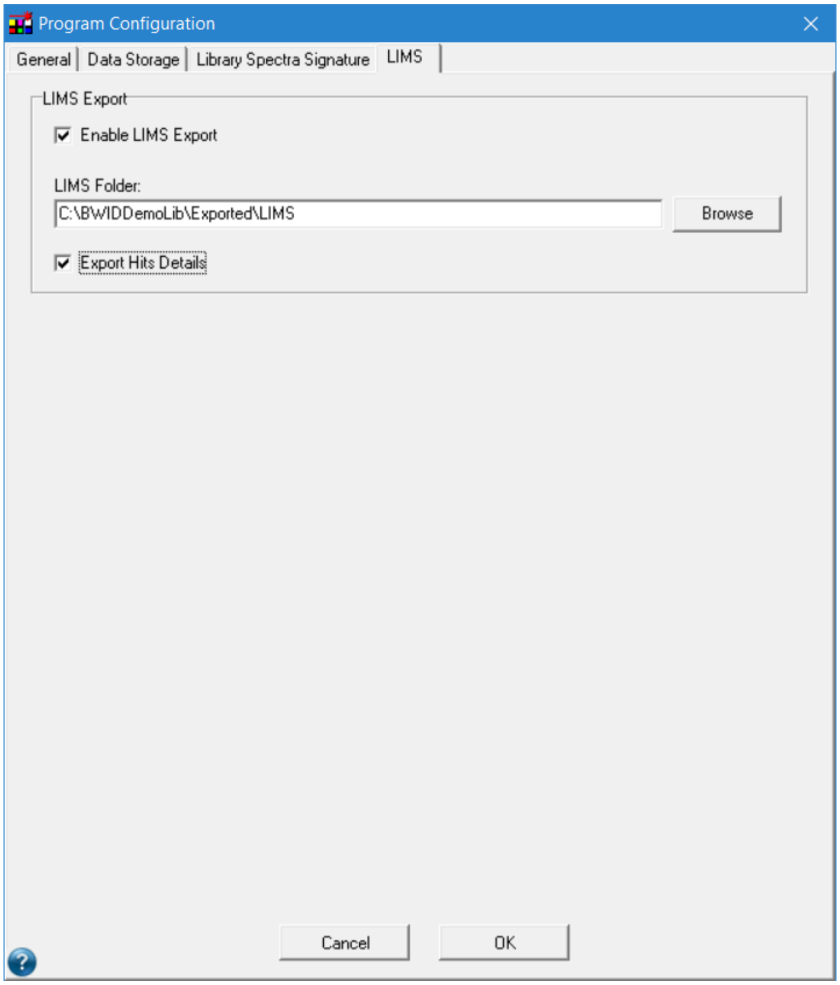
Allow the User to Delete Rejected Spectra - check this box to allow the user to delete a rejected spectrum. By default, the setting is disabled and the program will prohibit from deleting any rejected spectrum.

Allow the Administrator to Delete Reviewed and Approved Spectra - check this box to allow the administrator user to delete spectra that are either approved or rejected. By default, the setting is disabled and the program will prohibit from deleting any reviewed or approved spectrum.

All Spectra in Search Libraries Have to Be Approved - check this box to make sure that all spectra in the search libraries have been reviewed and then approved. If the setting is enabled, upon starting ID analysis the program will validate spectra signatures in the search libraries and will proceed with the measurement only if all spectra are approved. By default the setting is disabled.

LIMS

The BWID® program supports Laboratory Information Management System (LIMS) export.
On the LIMS page, the user can configure LIMS export parameters.



☑ Enable LIMS Export

LIMS Folder: C:\BWIDDemoLib\Exported\LIMS

☑ Export Hits Details

Enable LIMS Export - check this box to enable LIMS export. If the LIMS export is enabled, the BWID® program will export analysis results into a LIMS data format file (aka LIMS file) once the identification is completed and the results are displayed to the user.
The LIMS file is a comma separated values (CSV) file (see Appendix B for LIMS file format details).
The following file name convention is used for the LIMS file: LIMS_XXX_YYYYMMDDHHNNSS.csv where:

- XXX is instrument's c-code (up to 6 characters); in case of no c-code (off-line analysis) a "XXX999" c-code will be used;
- YYYYMMDDHHNNSS is analysis date and time: year (YYYY), month (MM), day (DD), hour (HH) in 24-hour format, minutes (NN), seconds (SS).

LIMS Folder – select a folder to store LIMS files. Once the BWID® program saves LIMS data in the folder it is LIMS responsibility to check the folder for the files presence and move them to the LIMS system. The BWID® program will not delete any data from the LIMS folder.

Export Hits Details - check this box to enable export of optional hit details (hit HQIs, hit spectra names, hit libraries and hit spectra).

Please see Appendix C for LIMS file format.

Click *OK* to accept these settings and close the dialog.

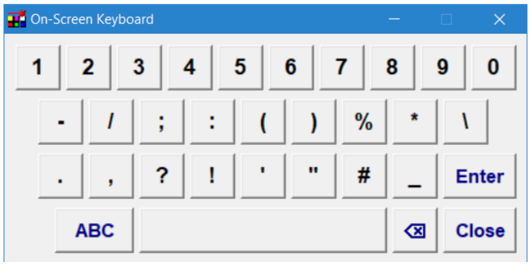
Click *Cancel* to cancel the program configuration and close the dialog.

14. Using an On-Screen Keyboard

If the on-screen keyboard is enabled (see Program Configuration paragraph), the soft keyboard will pop up whenever the user clicks on an editable field in any dialog of the program:

The *abc* button in the alphabetical keyboard is a toggle button to switch the caps lock on and off. It has the *abc* caption when the caps lock is off, indicating that all alphabetical key buttons are lower case, or the *ABC* caption when the caps lock is on, indicating that all alphabetical key buttons are upper case.

Click the *123* button in the alphabetical keyboard to switch to a numerical keyboard:



Click the *ABC* button in the numerical keyboard to switch to the alphabetical keyboard.

The soft keyboard enlarges a non-control key when pressed down, so that the user receives visual feedback as he/she types.

The soft keyboard can be moved to any position on the screen by simply dragging the keyboard window.

Click the *Enter* button to close the soft keyboard window if the input field is a single line field, or to move cursor to a new line if the input field is a multi-lines field.

Click the backspace button to delete character(s) to the left of the cursor in the input field.

Click the *Close* button to close the soft keyboard window.

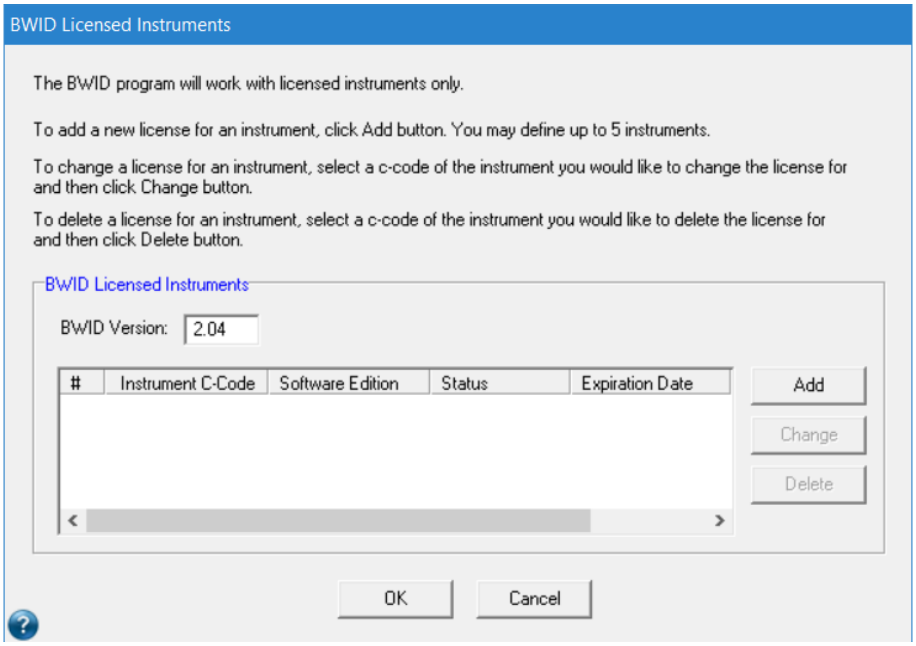
15. Setting Licensed Instruments

In order to use the program with an instrument, a valid license key for the instrument must be provided in the licensed instruments table. The license key can be obtained from B&W Tek.

If there is no valid license key installed on the PC on which the program is run, an appropriate message will be displayed upon starting the program.
In this case, the program will disable all features except the instrument’s configuration.

To configure the licensed instruments table, click the *Setup* button in the Menu window and then the *Instruments* button from the Setup menu.

The BWID® Licensed Instruments dialog will be displayed:



The BWID program will work with licensed instruments only.

To add a new license for an instrument, click Add button. You may define up to 5 instruments.

To change a license for an instrument, select a c-code of the instrument you would like to change the license for and then click Change button.

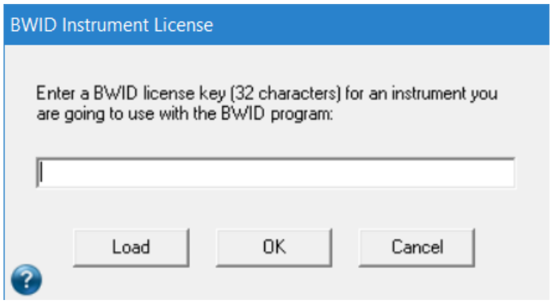
To delete a license for an instrument, select a c-code of the instrument you would like to delete the license for and then click Delete button.

BWID Licensed Instruments

BWID Version: 2.04

#	Instrument C-Code	Software Edition	Status	Expiration Date

Click *Add* to add a new license key to the table. The BWID® Instrument License dialog will appear, as shown below.

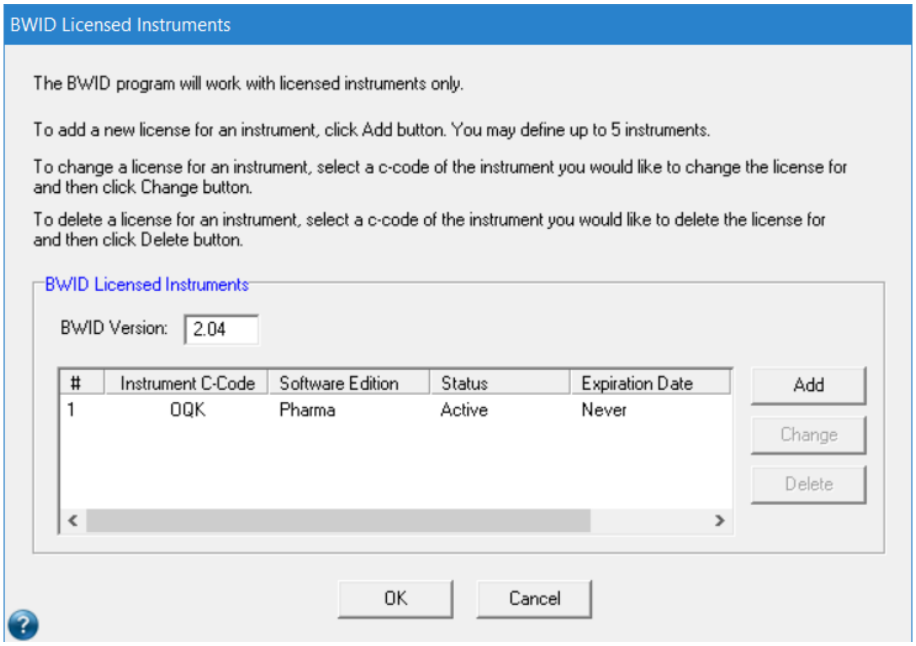


Enter a BWID license key (32 characters) for an instrument you are going to use with the BWID program:

Click the Load button to browse for a BWID® instrument license key file (*.txt) (obtained from B&W Tek) and retrieve a license key from the file, or enter a license key manually.

Once an instrument license key is entered, click OK to add the license key to the table. The new license key will be displayed in the table as shown in the dialog below.

Click *Cancel* to abort adding a license key to the table.



BWID Licensed Instruments

The BWID program will work with licensed instruments only.

To add a new license for an instrument, click Add button. You may define up to 5 instruments.

To change a license for an instrument, select a c-code of the instrument you would like to change the license for and then click Change button.

To delete a license for an instrument, select a c-code of the instrument you would like to delete the license for and then click Delete button.

BWID Licensed Instruments

BWID Version: 2.04

#	Instrument C-Code	Software Edition	Status	Expiration Date
1	0QK	Pharma	Active	Never

Click *Change* to update the license for a selected instrument in the table, e.g. from Standard Edition to Pharma.

Click *Delete* to delete selected license key from the table.

Once all modifications are complete, click OK to accept the settings and close the dialog.

Click Cancel to abort modifications and close the dialog.

16. Audit Trail

The Audit Trail keeps track of all sensible/critical operations performed within the BWID® program. It is implemented to meet the US FDA 21 CFR Part 11 “Electronic Records; Electronic Signatures” requirements regarding the audit trail.

Each time a sensible or critical operation is performed, the appropriate information (later referred to as “entry”) is stored in a predefined Audit Trail Log file (later referred to as “AT file”). The default name for the AT file is BWID.ATF and the file is stored in the application’s working directory.

The Audit Trail Log file is a binary file that stores the date and time of operator entries and actions that create, modify, or delete electronic records, as well as any actions that are sensible or critical for the application performance.

AT Logging

The audit trail generation is transparent and secure from unauthorized alteration. Each entry contains a binary check sum that allows detection of any data alteration.

The audit trail has the ability to record the following information (as a single entry):

- Date and time of performed operation
- User ID
- User full name (if provided)
- System/application name
- Performed operation category
- Operation description
- Reason for the performed operation (if provided)

The local time is taken from the system clock and is recorded to determine the sequence of steps. It shows hour, minutes and seconds of performed operation.

The data logged into the Audit Trail Log file falls into the following categories:

Category:	***Operation:***
Security	Login to /logout from a program
	Unsuccessful login attempts
	Adding a new user account
	Locking/unlocking a user account
	Resetting a user account/password
	Disabling a user account
	Changing a user type or password expiration
	Changing a user password
Measurement	Sample identification execution
	Performance test execution
	Dark scan test execution

Configuration	New operation preset setup Existing operation preset modifications Default operation preset selection Data library generation and modifications Performance test parameters setup

AT Backup

The audit trail is automatically backed up when the file reaches 2 MB size. Then a new audit trail file is created and the first entry is added containing back-up info (date, time and name of backup file).

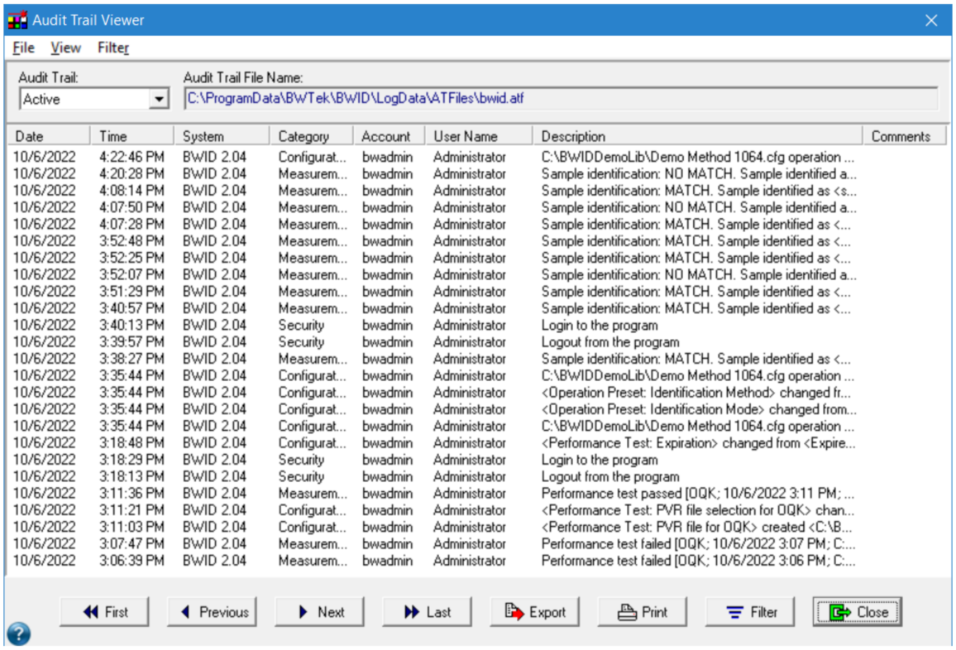
The backup file name is automatically created by the date pattern: *yymmdd.atf*, where *yy* stands for the last two digits of the current year, *mm* is the number of the current month and *dd* is the date.
The backup file is stored in the same location as the original AT file.

For each additional backup performed on the same day (if any occur), the backup file name is created by the following pattern: yy*mmdd_n.atf*, where *n* is the next consecutive number.
If a backup file already exists, the consecutive backup file name will be used in the backup operation.

If for any reason the backup operation cannot be performed, the backup will be postponed until the next login to the Audit Trail Log file occurs.

AT Viewing

Click the *Report* button in the Menu window and then *Audit Trail* button in the Report menu to view the audit trail (AT). The Audit Trail Viewer dialog will be displayed:



Audit Trail: Active

Audit Trail File Name: C:\ProgramData\BWTek\BWID\LogData\ATFiles\bwid.atf

Date	Time	System	Category	Account	User Name	Description	Comments
10/6/2022	4:22:46 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Demo Method 1064.cfg operation ...	
10/6/2022	4:20:28 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: NO MATCH. Sample identified a...	
10/6/2022	4:08:14 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <s...	
10/6/2022	4:07:50 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: NO MATCH. Sample identified a...	
10/6/2022	4:07:28 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:52:48 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:52:25 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:52:07 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: NO MATCH. Sample identified a...	
10/6/2022	3:51:29 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:40:57 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:40:13 PM	BWID 2.04	Security	bwadmin	Administrator	Login to the program	
10/6/2022	3:39:57 PM	BWID 2.04	Security	bwadmin	Administrator	Logout from the program	
10/6/2022	3:38:27 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MATCH. Sample identified as <...	
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Demo Method 1064.cfg operation ...	
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Operation Preset: Identification Method> changed fr...	
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Operation Preset: Identification Mode> changed from...	
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Demo Method 1064.cfg operation ...	
10/6/2022	3:18:48 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: Expiration> changed from <Expire...	
10/6/2022	3:18:29 PM	BWID 2.04	Security	bwadmin	Administrator	Login to the program	
10/6/2022	3:18:13 PM	BWID 2.04	Security	bwadmin	Administrator	Logout from the program	
10/6/2022	3:11:36 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Performance test passed [OQK; 10/6/2022 3:11 PM; ...	
10/6/2022	3:11:21 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: PVR file selection for OQK> chan...	
10/6/2022	3:11:03 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: PVR file for OQK> created <C:\B...	
10/6/2022	3:07:47 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Performance test failed [OQK; 10/6/2022 3:07 PM; C:...	
10/6/2022	3:06:39 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Performance test failed [OQK; 10/6/2022 3:06 PM; C:...	

The Audit Trail Viewer allows the user to:

- select an Audit Trail Log view (active or from a file)
- view entries stored within an Audit Trail Log
- filter entries stored within an Audit Trail Log
- print out entries stored within an Audit Trail Log
- export entries stored within an Audit Trail Log into a ASCII text file

To view the active Audit Trail Log, select the *Active* option in the *Audit Trail* box (default selection). The *Audit Trail File Name* field will hold the file name with active Audit Trail Log.

To view an Audit Trail Log stored in a given file, select the *From File* option in the *Audit Trail* box. The Audit Trail File Selection dialog will be open to allow the user to select an AT file. Upon AT file selection, the list will be set with AT entries loaded from the file. The *Audit Trail File Name* field will hold the name of selected AT file.

The entries in the list are displayed in chronological order with a newest AT entry on the top of the list.

The list can be set to one of the following formats:

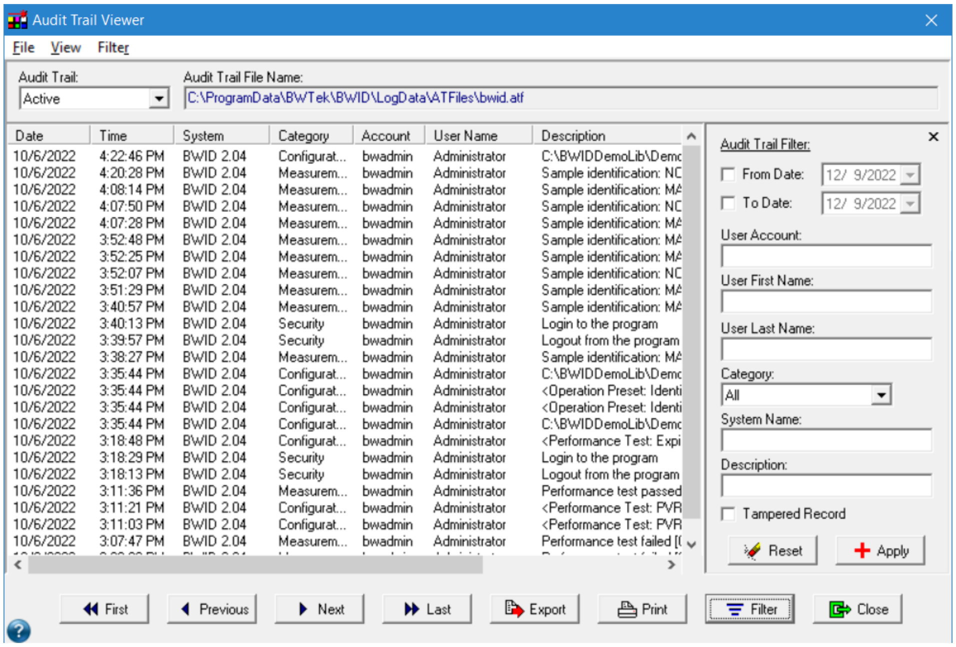
- Multi pages - 25 entries per page
- Full page - all entries in one page

By default, the list is set to multi pages with 25 entries per page.

To change the list format from one to another, click the *View->Full List* menu item.

If the list format is set to multi pages, the *First*, *Previous*, *Next* and *Last* buttons can be used to move between the pages.
The *First* button or *View->First Page* will display the first page with the 25 newest records (filtered if applicable) from the AT file.
The *Last* button or *View->Last Page* will display the last page with the 25 oldest records (filtered if applicable) from the AT file.
The *Previous* button or *View->Previous Page* menu item will display a page with newer entries than the current page information.
The *Next* button or *View->Next Page* menu item will display a page with older entries than the current page information.

To filter AT entries, click the *Filter* button or *Filter->Setup* menu item. The Audit Trail Filter panel will appear in the main window:



Audit Trail: Active

Audit Trail File Name: C:\ProgramData\BWTek\BWID\LogData\ATFiles\bwid.atf

Date	Time	System	Category	Account	User Name	Description
10/6/2022	4:22:46 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Dem
10/6/2022	4:20:28 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: N
10/6/2022	4:08:14 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	4:07:50 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: N
10/6/2022	4:07:28 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:52:48 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:52:25 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:52:07 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: N
10/6/2022	3:51:29 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:40:57 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:40:13 PM	BWID 2.04	Security	bwadmin	Administrator	Login to the program
10/6/2022	3:39:57 PM	BWID 2.04	Security	bwadmin	Administrator	Logout from the program
10/6/2022	3:38:27 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Sample identification: MA
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Dem
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Operation Preset: Identi
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Operation Preset: Identi
10/6/2022	3:35:44 PM	BWID 2.04	Configurat...	bwadmin	Administrator	C:\BWIDDemoLib\Dem
10/6/2022	3:18:48 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: Expi
10/6/2022	3:18:29 PM	BWID 2.04	Security	bwadmin	Administrator	Login to the program
10/6/2022	3:18:13 PM	BWID 2.04	Security	bwadmin	Administrator	Logout from the program
10/6/2022	3:11:36 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Performance test passed
10/6/2022	3:11:21 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: PVR
10/6/2022	3:11:03 PM	BWID 2.04	Configurat...	bwadmin	Administrator	<Performance Test: PVR
10/6/2022	3:07:47 PM	BWID 2.04	Measurem...	bwadmin	Administrator	Performance test failed [

Audit Trail Filter:

☐ From Date: 12/ 9/2022

☐ To Date: 12/ 9/2022

User Account:

User First Name:

User Last Name:

Category: All

System Name:

Description:

☐ Tampered Record

The filter feature allows the user to view, print or export the AT records of particular interest.
The records can be selected using the following criteria:

- Date range (between specified dates)
- Application name
- Category (all, security, measurement, configuration)

- User account
- User name (first and last name)
- Entry description
- Tampered entry

All criteria (excluding date range) perform searching based on the text string within the appropriate field of the record. The text search is not case sensitive. For each of the text search criteria there can be more than one string defined (text strings separated by space characters). In this case, the record meets the criteria if any of the specified strings found within the record's field.

Once the filter is configured, click the *Apply* button to filter entries. The AT entries list will be updated according to the filter settings.

To reset the filter settings in the filter panel, click the *Reset* button.

To turn the filter off, click the *Filter->Reset* menu item or reset the filter settings first (*Reset* button) and then click the *Apply* button in the filter panel.

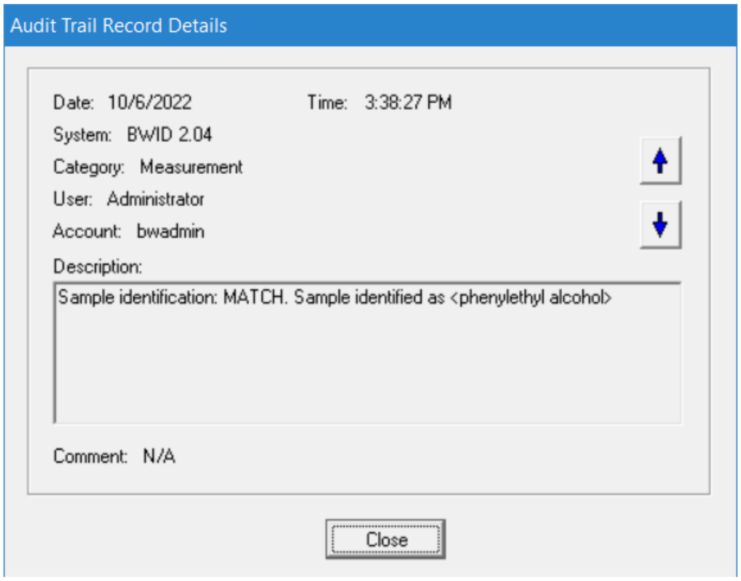
To hide the filter panel, click the x button in the top right-hand corner of the filter panel.

To print AT entries (filtered if applicable), click the Print button or File->Print menu item.

To export AT entries (filtered if applicable) into a text file, click the *Export* button or *File->Export* menu item. The output file selection dialog will be open.

The AT entries list is not updated automatically with new records logged in while viewing the AT file.
To refresh the list, click the *View->Refresh* menu item.

To see Audit Trail entry details in a more convenient format, double click on the entry you wish to view. The Audit Trail Record Details dialog will appear:



Date: 10/6/2022 Time: 3:38:27 PM

System: BWID 2.04

Category: Measurement

User: Administrator

Account: bwadmin

Description:

Sample identification: MATCH. Sample identified as <phenylethyl alcohol>

Comment: N/A

To see the previous AT entry from the list, click the “arrow up” icon.

To see the next AT entry from the list, click the “arrow down” icon.

17. Appendix A. Spectrum Search Algorithms

For all search algorithms, the best match is 100 and the worst is 0.

Scalar Product Algorithm

The Scalar Product algorithm calculates the angle between the unknown spectrum and the library spectrum vectors using the scalar product of the two intensity vectors:

$$HQI = \arccos\left(\frac{Unk \bullet Lib}{|Unk| \bullet |Lib|}\right)$$

Where *Lib* is the library entry being searched and *Unk* is the unknown spectrum.

Difference Algorithm

The Difference (a.k.a. Absolute Value) HQI of the unknown spectrum from a library entry is calculated as the sum of the absolute difference vector:

$$HQI = \frac{\sum_{i=1}^{n} |Lib_i - Unk_i|}{n}$$

Where *Lib* is the library entry being searched, *Unk* is the unknown spectrum, and *n* is the number of data points in the library entry and unknown spectrum.

This algorithm does not enhance the spectral differences and therefore is suitable for cases where there are additional large spikes in the unknown. Note that this algorithm provides poor discrimination among hits. It will typically return many library entries with identical or similar HQI values.

Squared Difference Algorithm

The Squared Difference (a.k.a. Least Squares) HQI between the unknown spectrum and the library entry is calculated as the sum of the squares of the vector difference:

$$HQI = \frac{\sum_{i=1}^{n} (Lib_i - Unk_i)^2}{n}$$

Where *Lib* is the library entry being searched, *Unk* is the unknown spectrum, and *n* is the number of data points in the library entry and unknown spectrum.

Derivative Algorithm

Squared Derivative Algorithm

These two Full spectrum search algorithms are identical to their non-derivative counterparts with one exception: before the Difference or Squared Difference HQI is calculated, the derivatives of the unknown and library entry are calculated. This derivative is simply the difference between each set of points in the spectrum:

For the Derivative: $$HQI = \frac{\sum_{i=1}^{n} \left| (Lib_i - Lib_{i-1}) - (Unk_i - Unk_{i-1}) \right|}{n}$$

For the Squared Derivative: $$HQI = \frac{\sum_{i=1}^{n} \left((Lib_i - Lib_{i-1}) - (Unk_i - Unk_{i-1}) \right)^2}{n}$$

Where *Lib* is the library entry being searched, *Unk* is the unknown spectrum, and *n* is the number of data points in the library entry and unknown spectrum. The values of Lib_0 and Unk_0 are defined to be the same as Lib_1 and Unk_1, respectively.

The two derivative searches have the advantage of removing most of the error from a slowly varying baseline error in the unknown from the search results. They are especially useful when the baseline error is not linear and therefore cannot be removed by the standard GIFTS algorithm.

Correlation Coefficient Algorithm

The Correlation Coefficient HQI of an unknown to a library entry is a least squares dot product of mean centered unknown spectrum and library data:

$$HQI = 1 - \frac{(Lib_m \bullet Unk_m)^2}{(Lib_m \bullet Lib_m)(Unk_m \bullet Unk_m)}$$

Where the vectors are defined as:

$$Lib_m = Lib - \frac{\sum_{i=1}^{n} Lib_i}{n} \qquad Unk_m = Unk - \frac{\sum_{i=1}^{n} Unk_i}{n}$$

Where *Lib* is the library entry being searched and *Unk* is the unknown spectrum. In the case where the signal to noise ratio and baseline in the library and unknown spectra are very similar, the mean values will be effectively the same. Note that if the mean centering step is removed, the equation reduces to the square of the Euclidean Distance. However, the mean centering step has one very important effect: the Hit Quality Index is independent of the normalization of the spectra. In Euclidean distance, the spectra must be normalized between 0 and 1 before the calculation. If the spectrum is noisy, or if there are sharp negative dips in the spectrum (i.e. water vapor, CO_2, etc.), they will be normalized to 0. This causes the baseline in the unknown to be normalized to a value significantly greater than 0. Therefore, the library spectrum and unknown spectrum will not match very well, and incorrect hits will be given. By centering each spectrum about its mean, this problem is avoided.

In almost all cases, correlation searching will provide better or equal hit quality information when compared to Euclidean Distance searching. However, due to the extra mean centering step, expect the correlation search to be slightly slower.

Derivative Correlation Algorithm

This is the same as the correlation algorithm, with one exception; the first derivative of both the unknown and library spectra are taken before calculating the HQI. Even though the correlation algorithm can compensate for noise and negative dips, it cannot correct for bad baselines. Normally, baseline correction pre-processing is used in an attempt to "flatten" the unknown before applying the search algorithm. Sometimes, however, it is not good enough. Like the other first derivative-based search algorithms, this attempts to remove the non-linear effects of the baseline that cannot be compensated for by the baseline preprocessing.

The algorithm is the same as the correlation search except that the first derivatives of both the library and the unknown are calculated. First the mean centering (described in the "Correlation Algorithm" section) is applied to the library and unknown spectra. Then their first derivatives are taken by subtracting previous points.

$$Lib_i = Lib_i - Lib_{i-1} \qquad Unk_i = Unk_i - Unk_{i-1}$$

Where Lib_0 and Unk_0 are defined to be equal to Lib_1 and Unk_1, respectively.

18. Appendix B. Timestamp Time Zone Abbreviations

Standard Time TZ Abbreviation	Daylight Time TZ Abbreviation	Standard Time Zone Name	Standard Time UTC Offset and Location
ACST	ACDT	AUS Central Standard Time	(UTC+09:30) Darwin
ACST	ACDT	Cen. Australia Standard Time	(UTC+09:30) Adelaide
ACWST	ACWST	Aus Central W. Standard Time	(UTC+08:45) Eucla
AEST	AEDT	AUS Eastern Standard Time	(UTC+10:00) Canberra, Melbourne, Sydney
AEST	AEDT	E. Australia Standard Time	(UTC+10:00) Brisbane
AEST	AEDT	Tasmania Standard Time	(UTC+10:00) Hobart
AFT	AFT	Afghanistan Standard Time	(UTC+04:30) Kabul
AKST	AKDT	Alaskan Standard Time	(UTC-09:00) Alaska
AMT	AMT	Caucasus Standard Time	(UTC+04:00) Yerevan
AMT	AMST	Central Brazilian Standard Time	(UTC-04:00) Cuiaba
AMT	AMST	SA Western Standard Time	(UTC-04:00) Georgetown, La Paz, Manaus, San Juan
ART	ART	Argentina Standard Time	(UTC-03:00) City of Buenos Aires
AST	ADT	Arab Standard Time	(UTC+03:00) Kuwait, Riyadh
AST	ADT	Arabic Standard Time	(UTC+03:00) Baghdad
AST	ADT	Atlantic Standard Time	(UTC-04:00) Atlantic Time (Canada)
AWST	AWST	W. Australia Standard Time	(UTC+08:00) Perth
AZOT	AZOST	Azores Standard Time	(UTC-01:00) Azores
AZT	AZT	Azerbaijan Standard Time	(UTC+04:00) Baku
BRT	BRST	Bahia Standard Time	(UTC-03:00) Salvador
BRT	BRST	E. South America Standard Time	(UTC-03:00) Brasilia
BRT	BRST	SA Eastern Standard Time	(UTC-03:00) Cayenne, Fortaleza
BRT	BRST	Tocantins Standard Time	(UTC-03:00) Araguaina
BST	BST	Bangladesh Standard Time	(UTC+06:00) Dhaka
BST	BST	Bougainville Standard Time	(UTC+11:00) Bougainville Island
CAT	CAT	Namibia Standard Time	(UTC+02:00) Windhoek
CAT	CAT	South Sudan Standard Time	(UTC+02:00) Juba
CAT	CAT	Sudan Standard Time	(UTC+02:00) Khartoum
CET	CEST	Central Europe Standard Time	(UTC+01:00) Belgrade, Bratislava, Budapest, Ljubljana, Prague
CET	CEST	Central European Standard Time	(UTC+01:00) Sarajevo, Skopje, Warsaw, Zagreb
CET	CEST	Romance Standard Time	(UTC+01:00) Brussels, Copenhagen, Madrid, Paris
CET	CEST	W. Europe Standard Time	(UTC+01:00) Amsterdam, Berlin, Bern, Rome, Stockholm, Vienna
CHAST	CHADT	Chatham Islands Standard Time	(UTC+12:45) Chatham Islands
CLST	CLST	Magallanes Standard Time	(UTC-03:00) Punta Arenas, Chile

CLT	CLST	Pacific SA Standard Time	(UTC-04:00) Santiago
COT	COT	SA Pacific Standard Time	(UTC-05:00) Bogota, Lima, Quito, Rio Branco
CST	CDT	Canada Central Standard Time	(UTC-06:00) Saskatchewan
CST	CDT	Central America Standard Time	(UTC-06:00) Central America
CST	CDT	Central Standard Time	(UTC-06:00) Central Time (US & Canada)
CST	CDT	Central Standard Time (Mexico)	(UTC-06:00) Guadalajara, Mexico City, Monterrey
CST	CST	China Standard Time	(UTC+08:00) Beijing, Chongqing, Hong Kong, Urumqi
CST	CDT	Cuba Standard Time	(UTC-05:00) Havana
CST	CST	Taipei Standard Time	(UTC+08:00) Taipei
CVT	CVT	Cape Verde Standard Time	(UTC-01:00) Cabo Verde Is.
EAST	EASST	Easter Island Standard Time	(UTC-06:00) Easter Island
EAT	EAT	E. Africa Standard Time	(UTC+03:00) Nairobi
EET	EEST	E. Europe Standard Time	(UTC+02:00) Chisinau, Moldova
EET	EEST	Egypt Standard Time	(UTC+02:00) Cairo
EET	EEST	FLE Standard Time	(UTC+02:00) Helsinki, Kyiv, Riga, Sofia, Tallinn, Vilnius
EET	EEST	GTB Standard Time	(UTC+02:00) Athens, Bucharest
EET	EEST	Jordan Standard Time	(UTC+02:00) Amman
EET	EEST	Libya Standard Time	(UTC+02:00) Tripoli
EET	EEST	Middle East Standard Time	(UTC+02:00) Beirut
EET	EEST	Syria Standard Time	(UTC+02:00) Damascus
EET	EEST	West Bank Standard Time	(UTC+02:00) Gaza, Hebron
EST	EDT	Eastern Standard Time	(UTC-05:00) Eastern Time (US & Canada)
EST	EDT	Eastern Standard Time (Mexico)	(UTC-05:00) Chetumal
EST	EDT	Haiti Standard Time	(UTC-05:00) Haiti
EST	EDT	Turks And Caicos Standard Time	(UTC-05:00) Turks and Caicos
EST	EDT	US Eastern Standard Time	(UTC-05:00) Indiana (East)
FJT	PHOT	Fiji Standard Time	(UTC+12:00) Fiji
GET	GET	Georgian Standard Time	(UTC+04:00) Tbilisi
GMT	BST	GMT Standard Time	(UTC+00:00) Dublin, Edinburgh, Lisbon, London
GMT	GMT	Greenwich Standard Time	(UTC+00:00) Monrovia, Reykjavik
GST	GST	Arabian Standard Time	(UTC+04:00) Abu Dhabi, Muscat
HAST	HADT	Aleutian Standard Time	(UTC-10:00) Aleutian Islands
HOVT	HOVDT	Altai Standard Time	(UTC+07:00) Barnaul, Gorno-Altaysk; Altai, Mongolia
HOVT	HOVT	W. Mongolia Standard Time	(UTC+07:00) Hovd
HST	HDT	Hawaiian Standard Time	(UTC-10:00) Hawaii
ICT	ICT	SE Asia Standard Time	(UTC+07:00) Bangkok, Hanoi, Jakarta
IDL	IDL	Dateline Standard Time	(UTC-12:00) International Date Line West
IRKT	IRKT	North Asia East Standard Time	(UTC+08:00) Irkutsk
IRST	IRDT	Iran Standard Time	(UTC+03:30) Tehran

IST	IST	India Standard Time	(UTC+05:30) Chennai, Kolkata, Mumbai, New Delhi
IST	IDT	Israel Standard Time	(UTC+02:00) Jerusalem
JST	JST	Tokyo Standard Time	(UTC+09:00) Osaka, Sapporo, Tokyo
KGT	KGT	Central Asia Standard Time	(UTC+06:00) Astana
KRAT	KRAT	N. Central Asia Standard Time	(UTC+07:00) Novosibirsk
KRAT	KRAT	North Asia Standard Time	(UTC+07:00) Krasnoyarsk
KRAT	KRAT	Tomsk Standard Time	(UTC+07:00) Tomsk
KST	KST	Korea Standard Time	(UTC+09:00) Seoul
KST	KST	North Korea Standard Time	(UTC+09:00) Pyongyang
LHST	LHDT	Lord Howe Standard Time	(UTC+10:30) Lord Howe Island
LINT	LINT	Line Islands Standard Time	(UTC+14:00) Kiritimati Island
MAGT	MAGT	Magadan Standard Time	(UTC+11:00) Magadan
MART	MART	Marquesas Standard Time	(UTC-09:30) Marquesas Islands
MAST	MADT	Mid-Atlantic Standard Time	(UTC-02:00) Mid-Atlantic - Old
MMT	MMT	Myanmar Standard Time	(UTC+06:30) Yangon (Rangoon)
MSK	MSD	Belarus Standard Time	(UTC+03:00) Minsk
MSK	MSK	Russian Standard Time	(UTC+03:00) Moscow, St. Petersburg
MSK	MSK	Volgograd Standard Time	(UTC+03:00) Volgograd
MST	MDT	Mountain Standard Time	(UTC-07:00) Mountain Time (US & Canada)
MST	MDT	Mountain Standard Time (Mexico)	(UTC-07:00) Chihuahua, La Paz, Mazatlan
MST	MDT	US Mountain Standard Time	(UTC-07:00) Arizona
MST	MST	Yukon Standard Time	(UTC-07:00) Yukon
MUT	MUT	Mauritius Standard Time	(UTC+04:00) Port Louis
NFT	NFDT	Norfolk Standard Time	(UTC+11:00) Norfolk Island
NPT	NPT	Nepal Standard Time	(UTC+05:45) Kathmandu
NST	NDT	Newfoundland Standard Time	(UTC-03:30) Newfoundland
NZST	NZDT	New Zealand Standard Time	(UTC+12:00) Auckland, Wellington
OMST	OMST	Omsk Standard Time	(UTC+06:00) Omsk
PETT	PETT	Kamchatka Standard Time	(UTC+12:00) Petropavlovsk-Kamchatsky - Old
PETT	PETT	Russia Time Zone 11	(UTC+12:00) Anadyr, Petropavlovsk-Kamchatsky
PGT	PGT	West Pacific Standard Time	(UTC+10:00) Guam, Port Moresby
PKT	PKT	Pakistan Standard Time	(UTC+05:00) Islamabad, Karachi
PMST	PMDT	Saint Pierre Standard Time	(UTC-03:00) Saint Pierre and Miquelon
PST	PDT	Pacific Standard Time	(UTC-08:00) Pacific Time (US & Canada)
PST	PDT	Pacific Standard Time (Mexico)	(UTC-08:00) Baja California
PYT	PYST	Paraguay Standard Time	(UTC-04:00) Asuncion
QYZT	QYZT	Qyzylorda Standard Time	(UTC+05:00) Qyzylorda
SAKT	SAKT	Sakhalin Standard Time	(UTC+11:00) Sakhalin
SAMT	SAMT	Astrakhan Standard Time	(UTC+04:00) Astrakhan, Ulyanovsk
SAMT	SAMT	Russia Time Zone 3	(UTC+04:00) Izhevsk, Samara
SAMT	SAMT	Saratov Standard Time	(UTC+04:00) Saratov

SAST	SAST	South Africa Standard Time	(UTC+02:00) Harare, Pretoria
SBT	SBT	Central Pacific Standard Time	(UTC+11:00) Solomon Is., New Caledonia
SGT	SGT	Singapore Standard Time	(UTC+08:00) Kuala Lumpur, Singapore
SLST	SLST	Sri Lanka Standard Time	(UTC+05:30) Sri Jayawardenepura
SRET	SRET	Russia Time Zone 10	(UTC+11:00) Chokurdakh
STP	STP	Sao Tome Standard Time	(UTC+00:00) Sao Tome
TMT	TMT	West Asia Standard Time	(UTC+05:00) Ashgabat, Tashkent
TOT	TOT	Tonga Standard Time	(UTC+13:00) Nukualofa
TRT	TRT	Turkey Standard Time	(UTC+03:00) Istanbul
ULAT	ULAST	Ulaanbaatar Standard Time	(UTC+08:00) Ulaanbaatar
USZ1	USZ1	Kaliningrad Standard Time	(UTC+02:00) Kaliningrad
UTC	UTC	UTC	(UTC) Coordinated Universal Time
UTC02	UTC02	UTC-02	(UTC-02:00) Coordinated Universal Time-02
UTC08	UTC08	UTC-08	(UTC-08:00) Coordinated Universal Time-08
UTC09	UTC09	UTC-09	(UTC-09:00) Coordinated Universal Time-09
UTC11	UTC11	UTC-11	(UTC-11:00) Coordinated Universal Time-11
UTC12	UTC12	UTC+12	(UTC+12:00) Coordinated Universal Time+12
UTC13	UTC13	UTC+13	(UTC+13:00) Coordinated Universal Time+13
UYT	UYT	Montevideo Standard Time	(UTC-03:00) Montevideo
VET	VET	Venezuela Standard Time	(UTC-04:00) Caracas
VLAT	VLAT	Vladivostok Standard Time	(UTC+10:00) Vladivostok
WAT	WAST	W. Central Africa Standard Time	(UTC+01:00) West Central Africa
WET	WEST	Morocco Standard Time	(UTC+01:00) Casablanca
WGT	WGST	Greenland Standard Time	(UTC-03:00) Greenland
WST	WST	Samoa Standard Time	(UTC+13:00) Samoa
YAKT	YAKT	Transbaikal Standard Time	(UTC+09:00) Chita
YAKT	YAKT	Yakutsk Standard Time	(UTC+09:00) Yakutsk
YEKT	YEKST	Ekaterinburg Standard Time	(UTC+05:00) Ekaterinburg

19. Appendix C. LIMS File Format

The LIMS file is a comma separated values (CSV) file as follows:

- single row – single entry data
- first column – entry name
- second column - entry value
- in case of multiple values for a single entry, the values will be stored in the third, fourth and so on columns

While parsing the file to retrieve exported data, there should be no assumption that data entries are in exact order as listed below (except for spectral data, they should be in continuous blocks: rows 31-36, 37-42 and 47-52).

Row #	*Entry Name*	*Entry Value*	*Comments*
1.	Report Type	Identification Report	Fixed string
2.	BWID Version	XX.YY.ZZ	XX, YY, ZZ are major, minor and release number respectively
3.	Analysis Date	MM/DD/YYYY HH:NN	MM = month, DD = day, YYYY = year, HH = hour (24-hours format), NN = minutes
4.	Operation Preset	Operation preset file name	
5.	User Name	User Full Name	N/A if not provided
6.	Device CCode	Device c-code	N/A if off-line analysis
7.	Product Name	Product name	N/A if not provided
8.	Product Number	Product number	N/A if not provided
9.	Batch Number	Batch number	N/A if not provided
10.	Lot Number	Lot number	N/A if not provided
11.	Container Number	Container number	N/A if not provided
12.	Supplier Name	Supplier name	N/A if not provided
13.	Notes	User notes	N/A if not provided

14.	Analysis Mode	One of the following strings: • Sample Identification • Sample Verification • See-Through Sample Identification • See-Through Sample Verification	
15.	Data Library	Search library file name	Up to 10 libraries can be listed (separated with comma). If the library is protected, a copyright string in parenthesis will follow the library name.
16.	Container Library	Container library file name	N/A if Analysis Mode = Sample Identification or Sample Verification
17.	Container Spectrum	One of the following strings: • Measured • From Container Library • N/A	N/A if Analysis Mode = Sample Identification or Sample Verification
18.	Container Name	Container name from container library	N/A if Container Spectrum = Measured or N/A
19.	Search Algorithm	One of the following strings: • Scalar Product • Derivative • Squared Derivative • Difference • Squared Difference • Correlation Coefficient • Derivative Correlation • STID	
20.	Preprocessing	One of the following strings: • None • FFT Smoothing • Savitzky-Golay Smoothing • Savitzky-Golay 1st Derivative • Savitzky-Golay 2nd Derivative	
21.	Minimum HQI	Minimum HQI (integer)	
22.	HQI Margin	HQI margin (integer)	N/A if Analysis Mode = Sample Identification or Sample Verification
23.	Search Range	R1 [cm-1] – R2 [cm-1]	Library search range in Raman Shift units: R1 = start

			search end, R2 = end search range; multiple non-consecutive ranges will be separated with comma
24.	PerfTest Status	One of the following: • Pass • Fail • N/A	N/A if performance test status is not available for given instrument or it is off-line analysis
25.	PerfTest Date	One of the following: • MM/DD/YYYY HH:NN • N/A	MM = month, DD = day, YYYY = year, HH = hour (24-hours format), NN = minutes
26.	Offline Spectrum	Offline spectrum file name	N/A if on-line analysis
27.	Integration Time	One of the following: • N [U] • N/A	N = Integration time (integer), U = integration time units (ms for milliseconds, us for microseconds); N/A if unknown integration time for off-line analysis
28.	Analysis Status	One of the following: • Match • No Match • Likely Match • Pass • Fail	
29.	Matched Sample Name	One of the following: • Sample name • Unknown	There will be more than one sample name if Analysis Status = Likely Match
30.	HQI	HQI (floating point value) for matching sample	There will be more than one HQI value if Analysis Status = Likely Match
31.	Sample Data	Number of spectral data points in acquired sample spectrum	
32.	Raman Shift	Intensity	Fixed string
33.	RS1	I1	RS1 = Raman Shift (integer) of the first point in the acquired sample spectrum (e.g. 176) I1 = intensity (floating point value) of the first point in the sample spectrum (e.g. 2544.57)
34.	RS2	I2	RS2 = Raman Shift (integer) of the second point in the sample spectrum (e.g. 180) I2 = intensity (floating point value) of the second point in the sample spectrum (e.g. 2044.23)
35.	…		
36.	RSn	In	Raman Shift and intensity value of the last point in

			the sample spectrum (from Sample Data entry)
37.	Container Data	Number of spectral data points in container spectrum	Data defined in the rows 37-42 are optional and will be present in the file only if Container Spectrum = Measured or From Container Library (see row 17)
38.	Raman Shift	Intensity	Fixed string
39.	RS1	I1	RS1 = Raman Shift (integer value) of the first point in the container spectrum (e.g. 176) I1 = intensity (floating point value) of the first point in the container spectrum (e.g. 18274.56)
40.	RS2	I2	RS2 = Raman Shift (integer value) of the second point in the container spectrum (e.g. 180) I2 = intensity (floating point value) of the second point in the container spectrum (e.g. 18609.42)
41.	…		
42.	RSn	In	Raman Shift and intensity value of the last point in the container spectrum (from Container Data entry)
43.	Hit Number	Number of hits (integer)	Data defined in the rows 43-52 are optional and will be present in the file only if hits details export is enabled
44.	Hit HQIs	Hit HQI (floating point) values	Number of hits values separated with comma
45.	Hit Names	Hit spectra names	Number of hits spectra names separated with comma
46.	Hit Library Names	Hit spectra library names	Number of hits library names separated with comma. If the library is protected a copyright string in parentis will follow the library name.
47.	Hit Data	Number of spectral data points in hit spectra	
48.	Raman Shift	Intensity	Fixed string
49.	RS1	I1	RS1 = Raman Shift (integer value) of the first point in the hit spectra I1 = intensity (floating point value) of the first point in the hit spectra There will be number of hits I1 values separated with comma.

			If spectrum is from a protected library, the value will be scrambled in 0-1 range.
50.	RS2	I2	RS2 = Raman Shift (integer value) of the second point in the hit spectra I2 = intensity (floating point value) of the second point in the hit spectra There will be number of hits I2 values separated with comma. If spectrum is from a protected library, the value will be scrambled in 0-1 range.
51.	…		
52.	RSn	In	Raman Shift and intensity values of the last point in the hit spectra (from Container Data entry) There will be number of hits intensity values separated with comma. If spectrum is from a protected library, the value will be scrambled in 0-1 range.
53.	END	N/A	End of data file indicator. LIMS may check for the END entry in the file to ensure that the file is ready for LIMS. Or it should try to open the file in write mode (operation will fail if the BWID has not finished saving data in the file).