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NIRS Vision 4.1

NIRS Vision
Manual Reference
4.1
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1 General Information

1.1 Visit us on the internet

Metrohm web page contains updated information about Vision solutions and patches. It also includes information about new hardware products, applications, validation, and technical support. Plus, a schedule of upcoming spectroscopy events and in-house training classes is available, to keep you abreast of current NIR and Raman developments.

Our web address is:

https://www.metrohm.com/en/products/spectroscopy/.

On this page you will find lots of information about Metrohm spectroscopy solutions.

1.2 Help in Vision

Vision offers online help.

Online help

Click on **[Help]** and choose from:

Index – provides the following files in PDF format:

- Manual – Reference
- Manual – Theory
- Tutorial – Instrument Operation
- Tutorial – Diagnostics
- Tutorial – Instrument Calibration

[About Vision]: displays the version of Vision and Service Pack currently installed.

1.3 Documentation

The release notes are separate documents. The release notes are located on the Metrohm website under **Support and Service ▶ Software Center ▶ Vision**. You find the complete set of release notes under the following link:

https://www.metrohm.com/en/support-and-service/software-center/vision/

2 Structure of Vision

2.1 Modes

Vision is based on the concept of a mode. Mode is a part of the program that groups related software functions. There are 4 modes in Vision.

2.1.1 Data Acquisition Mode

Data Acquisition mode combines all functions related to instrument and spectral management. Major functions of this mode include:

- Instrument configuration and diagnostics
- Spectral acquisition
- Spectra viewing and management
- Export and import of data, projects, and libraries
- Security

2.1.2 Qualitative Analysis Mode

Qualitative Analysis mode includes all functions related to the creation, development and validation of pattern recognition libraries. Major functions of this mode include:

- Sample selection
- Identification method development
- Qualification method development
- Library validation

2.1.3 Quantitative Analysis Mode

Quantitative Analysis mode involves all functions associated with calibration development and maintenance. Major functions of this mode include:

- Sample selection
- Equation development (regression)
- Equation development (leverage)
- Equation validation (predict)
- Unscrambler predict
- Pre- or Post-processing equations

2.1.4 Routine Analysis Mode

Routine Analysis mode includes functions related to the routine acquisition and storage of data, and qualitative or quantitative predictions, such as:

- Operations Method configuration
- Real time analysis
- Stored data analysis
- Report generation
- Results storage and management

2.2 Major Concepts

2.2.1 Databases

Vision software keeps all operational and configuration data in databases. There are several types of databases involved in the software.

Security Database

The security database contains all the information necessary to recognize multiple users and assigns to each of them the proper access to the software. In specific, this database contains user IDs, passwords, security access levels, and user preferences information.

Project Database

The project database is password protected and contains all spectral and constituent information needed for qualitative or quantitative model development.

Library Database

The library database contains qualitative models and pointers to spectra in the appropriate project databases.

Diagnostics Database

The database stores the results of instrument diagnostics.

2.2.2 Data Collection Method

Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans or acquisition time) and selected performance test parameters (like pass/fail limits). A project must have at least one DCM. However, DCMs are not shared between projects. The user is prompted to define a DCM every time a new project is created.

A single project can have many DCMs, and a project database can store spectra acquired from different types of instruments and modules. During sample selection the user specifies filter settings (amplifier type and spectral region) which allows Vision to search the project for samples satisfying these criteria.

2.2.3 Sample Selection

Sample selection is a necessary step in model development. In qualitative model development, all spectra transferred to the library product form a temporary set and have to go through the sample selection procedure. Sample selection divides them into a training set (good data), an acceptance set (redundant samples) if desired, and a rejection set (outliers). Only when the sample selection results are saved, can the model be developed from the training set. The same applies to quantitative model development, where the analogous sets are called the calibration set, the validation set, and the outlier set.

2.3 Data, Methods, and Results Storage

Understanding how Vision stores information will help in proper software operation.

Spectral data, constituent data, DCMs, and all parameters related to spectral acquisition and manipulation (e.g., dates and times of acquisition, audit trails) are kept in the Project Database.

All qualitative methods (identification and qualification method) and their parameters, as well as the validation results are kept in the Library Database.

Calibration equations are kept in the Project Database.

Operations Methods are stored in the Project Database.

Results and spectra from Routine Analysis are stored in an output project database (created during the Routine Analysis set-up) and/or in other file formats. ASCII files for example, are not associated with any database and can be stored in any location, including network drives.

2.4 User Preferences

The security database contains preferences for each registered Vision user. User preferences are a set of default parameters applied every time a given user is logged into Vision. In general, these parameters include math pretreatments and methods used in the last method development session. These preferences are updated every time the user edits a method and saves it. User preferences are local, i.e., each part of Vision software may have its own set.

User preferences for qualitative and quantitative sample selection, identification method development, qualification method development, and regression can be viewed and modified before method development starts.

2.4.1 Intelligent Default System

Intelligent default system facilitates fast new methods development and edition of existing methods. Methods that are being redeveloped have old parameters as defaults. New methods take default values from user preferences. When user preferences do not exist (a method of this kind has never been developed in the past), the system defaults are applied.

3 Data Acquisition Mode

3.1 Introduction

Data acquisition mode controls instrument configuration and diagnostics, spectral acquisition, spectra viewing and management, export and import of data, and security. When the user logs into Vision, the Data Acquisition mode is entered by default. The last active project is opened, and if the instrument was connected during the last session, Vision tries to connect it.

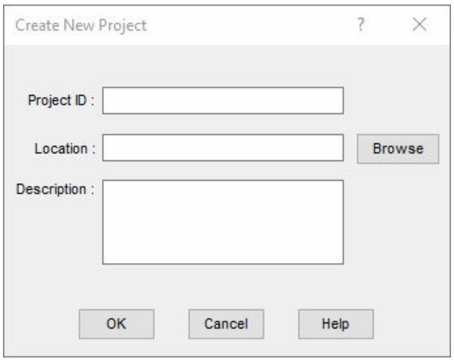
3.2 Creating and Configuring a New Project

The Project is a basic unit of data storage in Vision. Each Project represents a separate database, which includes spectra, constituent values, and instrument configuration. Before any data (instrument diagnostics or spectral data) can be collected, a Project must be setup.

3.2.1 Creating a New Project

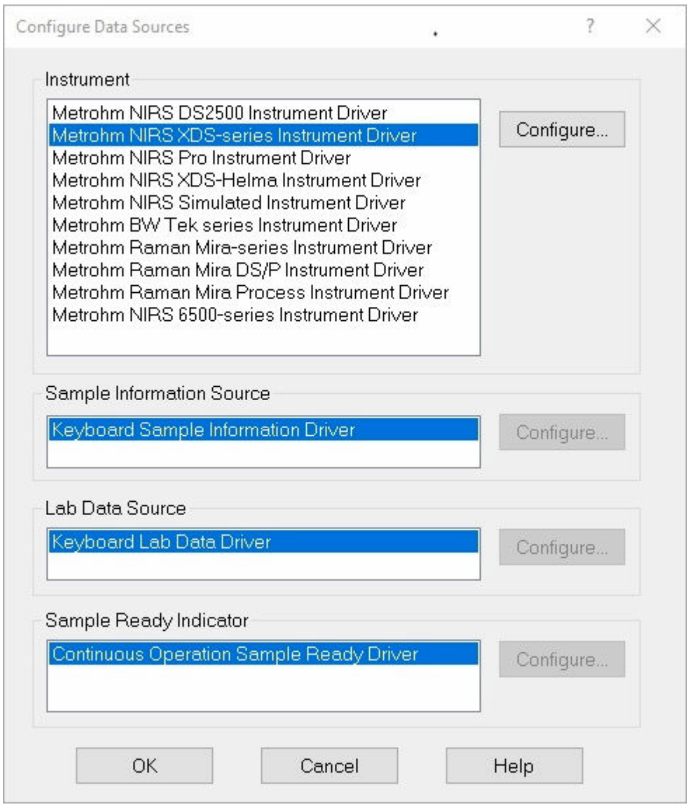
1 Click on **File ▶ Project ▶ New** on the main menu. If an existing Project is currently open, you will be prompted to close it.

A **Create New Project** dialog box opens.



2 Enter a Project name and location for the Project. The default location is C:\Vision unless specified; a **[Browse]** button is available for easy access to other locations.

The **Configure Data Sources** window displays.



Instrument

Metrohm NIRS DS2500 Instrument Driver
Metrohm NIRS XDS-series Instrument Driver
Metrohm NIRS Pro Instrument Driver
Metrohm NIRS XDS-Helma Instrument Driver
Metrohm NIRS Simulated Instrument Driver
Metrohm BW Tek series Instrument Driver
Metrohm Raman Mira-series Instrument Driver
Metrohm Raman Mira DS/P Instrument Driver
Metrohm Raman Mira Process Instrument Driver
Metrohm NIRS 6500-series Instrument Driver

Sample Information Source: Keyboard Sample Information Driver

Lab Data Source: Keyboard Lab Data Driver

Sample Ready Indicator: Continuous Operation Sample Ready Driver

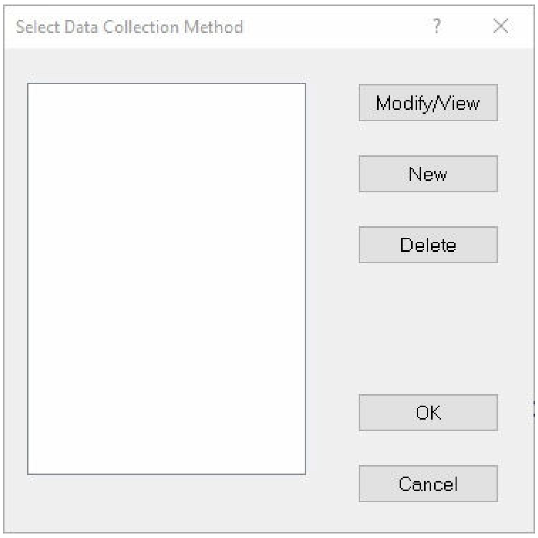
3 Choose the proper instrument driver and click on **[Configure]**.

Refer to corresponding analyzer User Manual for configuring the connection.

4 From the **Connect to Instrument** dialog box, choose to **[Acquire data]** or **[Use Existing data]**.

If you choose to Use Existing data, Vision will open the new Project, without connecting to the instrument.

If you choose to Acquire new data, Vision will try to connect the instrument. The **Select Data Collection Method** dialog box appears.



Click on **[New]** if you do not have any DCMs in the Project. Follow the instructions below on how to create a DCM.

Highlight the name of the DCM and click on **[OK]**.

3.2.2 Creating Data Collection Method (DCM)

1 From the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** window, enter the data acquisition parameters according to the type of the analyzer.

3 Click on **[OK]** when done.

3.2.3 Opening a Project

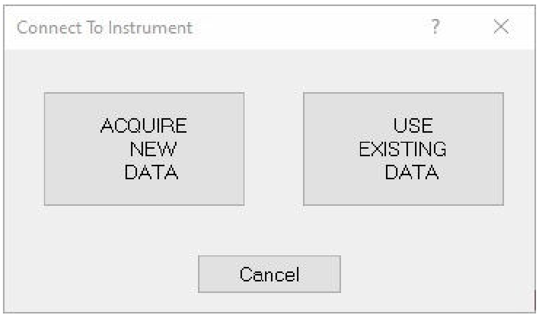
1 Click on **File** ► **Project** ► **Open** or on the **Open Project icon**:

2 Click on **[OK]** if prompted to close the active Project.

3 The **Open Project** window lists regular and output projects in separate areas.

From the **Open Project** window select the Project you want to open and click on **[Open]**.

4 From the **Connect to Instrument** dialog box, choose either **[Acquire Data]** or **[Use Existing Data]** .



If you choose to use existing data, Vision will open the selected Project without connecting to the instrument.

If you choose to acquire new data, Vision will try to connect the instrument. The **Select Data Collection Method** dialog box appears. Highlight the name of the DCM and click on **[OK]**. If you do not have a DCM, you can create one by clicking on **[New]**.

3.3 Data Acquisition

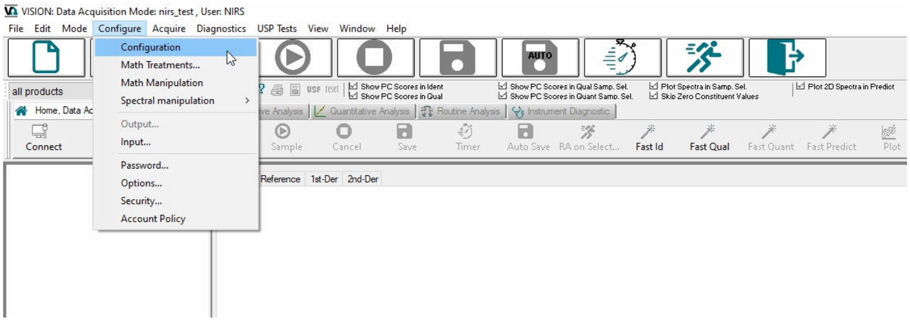
Spectra in Vision can be acquired manually, or this process can be automated using the data acquisition timer and the autosave feature.

Vision saves acquired spectra in the database of the active project. The spectra of the same substance are usually saved in one product.

3.3.1 Acquiring Data

1. If you do not have a Project open, click on **File ▶ Project ▶ Open** to select and open a Project.

2. If necessary, connect to the instrument by clicking on **Acquire ▶ Connect**.



(If under Acquire you can see the Disconnect option instead of Connect, you are already connected).

Select the DCM and click on **[OK]**.

3 Click on **Acquire** ▶ **Reference** to scan the reference. Alternatively, you may click on the **Reference icon**: Ref

The red progress bar at the bottom of the screen shows the status. After the scan is complete, click on the **Reference** tab at the top of the screen to view the reference spectrum.

4 Click on **Acquire** ▶ **Sample** to scan the sample spectrum. Alternatively, you may click on the **Sample icon**: ▶

The blue progress bar at the bottom of the screen shows the status. After the scan is over, click on the **Sample** tab at the top of the screen to view the sample spectrum. The last spectrum acquired is displayed in black.

NOTICE

You can also scan reference and sample using the cuvette icons located below the main menu. Place the cursor on the icon to see its function.

3.3.2 Saving Spectra

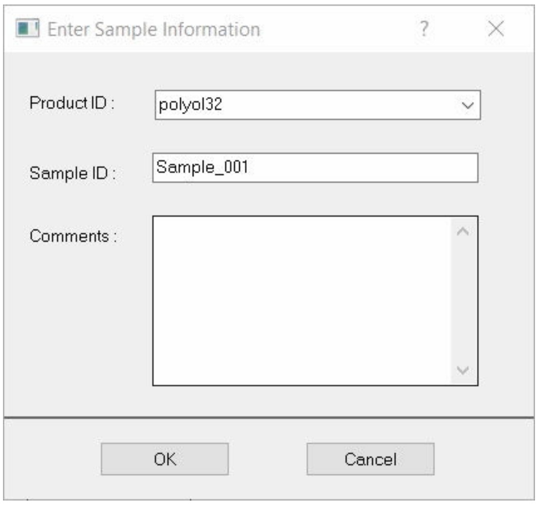
You can save the last acquired spectrum as follows:

1 Click on **Acquire** ▶ **Save** or on the **Save icon**: 💾

The **Enter Sample Information** dialog box will be displayed:

2 In the **Enter Sample Information** dialog box, type in the Product ID (or choose it from the dropdown list) and the Sample ID. Enter the optional comment and click on **[OK]**.

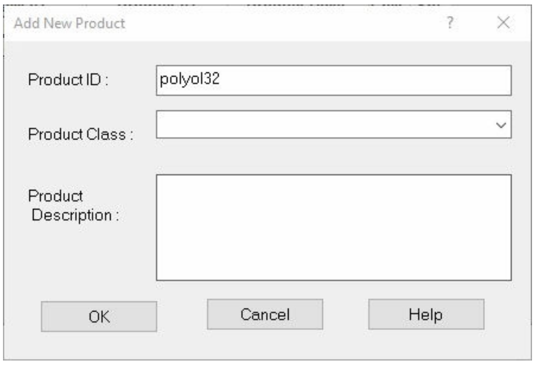
An example is given below:



Product ID : polyol32

Sample ID : Sample_001

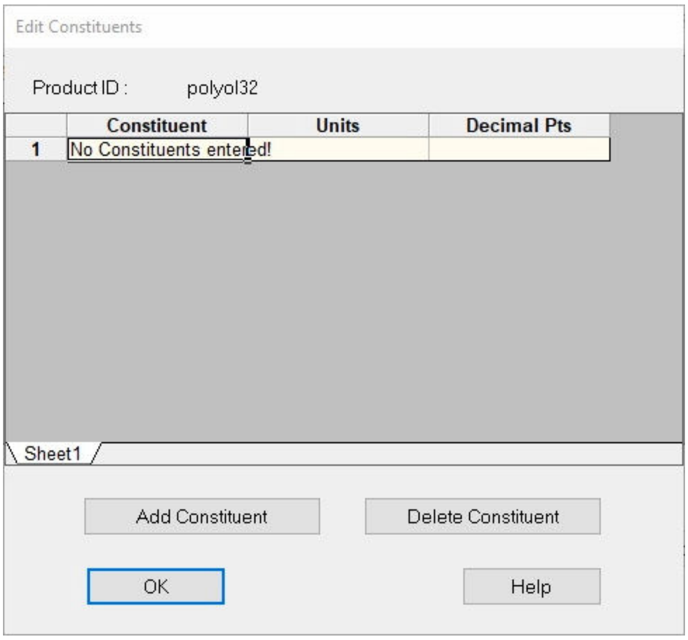
3 Vision will ask if you wish to create a new product:



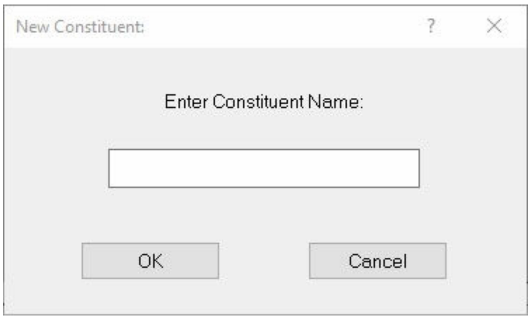
Product ID : polyol32

4 In the **Add New Product** window enter the optional product class and description. Click on **[OK]** when done.

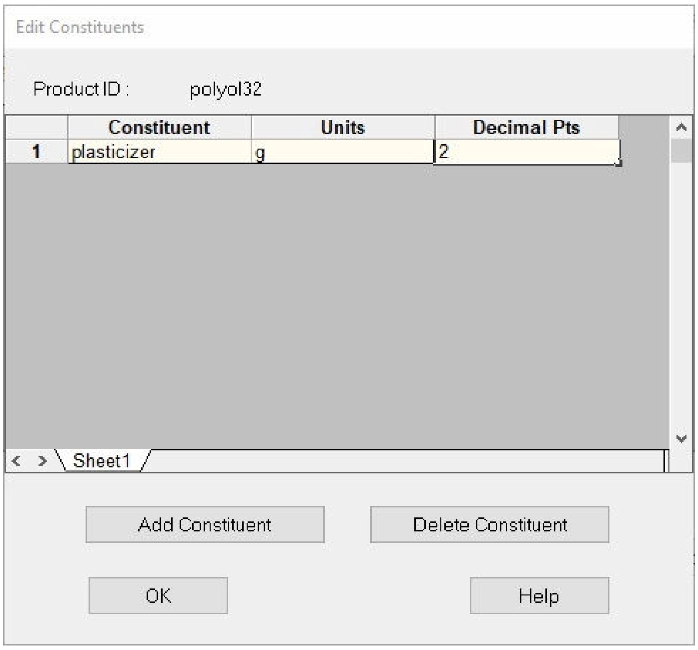
The **Edit Constituents** window will be displayed:



5 In the **Edit Constituents** window, click **[Add]** to enter a constituent.



6 Enter the constituent name, and click on **[OK]**. Constituents may be added to the product at a later time, if that is more convenient.



Product ID : polyol32

	Constituent	Units	Decimal Pts
1	plasticizer	g	2

7 The constituent name “plasticizer” was added. Next, enter the units, and decimal points to be displayed. In this case, “2” is entered, to display 2 digits after the decimal point. Click on **[OK]**.

This procedure holds for the first sample saved in a product. When next samples are saved, Vision assumes the same product, class, and constituent configuration as for the previous sample. Alternatively, the user may enter new information, to create a new product during the session.

3.3.3 Using the Stored Reference

Vision allows a reference scan to be saved and retrieved later. This is not the normal procedure, as the stored reference can contribute to spectral inaccuracy, under some conditions. Consult Metrohm NIRS representative before implementation of a Stored Reference.

1 Click on **Acquire ▶ Store Reference** to save the last taken reference spectrum.

2 In the **Store Reference** window, enter the reference name and click on **[OK]**.

3 To retrieve a stored reference, click on **Acquire ▶ Select Reference**. In the **Select Reference** window, highlight the name of the reference you want to use and click on **[Load]**. The loaded reference will be the active reference until you acquire or load a new one.

3.3.4 Using the External Reference

The **External Reference** feature in Vision allows for correction for the fiber length or fiber characteristics on a **6500-Series Process** instrument. It is highly recommended for use in all 6500-Series process instruments. XDS Process Instruments use Reference Standardization instead.

In normal data acquisition, the reference spectrum (in the log(1/R) form) is subtracted from the analogous form of the sample spectrum, resulting in the absorbance spectrum. This standard approach works very well for instruments for which the reference light path (channel) is identical to the sample light path (channel), most often laboratory systems.

On the other hand, on most process instruments the reference and the sample fibers are separate. The reference fiber (channel) is identical on all instruments. However, the sample fiber (channel) is most often much longer than the reference fiber; its length depends on the actual instrument configuration. The qualitative or quantitative models created on such an instrument depend on the difference of the lengths of reference and sample channels. These models work well on the instrument they have been created for, but method transfer is often complicated.

The use of External Reference allows the user to get rid of the fiber characteristics from the acquired spectra, and consequently from the analytical methods.

The recommended way of using the External Reference feature is as follows:

1 Acquire a spectrum of the empty sample channel (no sample present, e.g., empty process line).

2 Save the spectrum in a chosen product. This spectrum contains the fiber characteristics.

3 When ready to take real spectra, click on **Acquire ▶ Use External Reference**.

Vision will subtract the whole External Reference spectrum (empty channel minus reference) from each acquired spectrum (filled channel minus reference). The reference channel is almost identical, so the reference spectra will cancel out. The final result is that each acquired spectrum is corrected for the empty channel.

This feature has been developed mainly for the process instruments, but it is also possible to use it on laboratory systems. Consult a Metrohm representative before using External Reference on an XDS system.

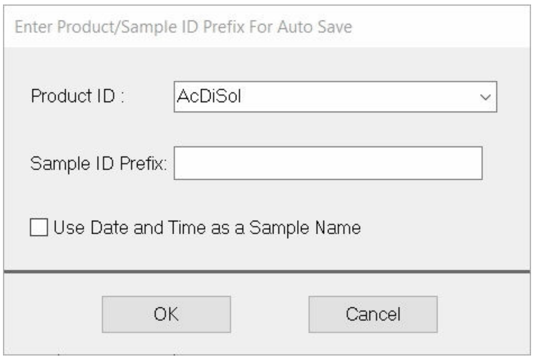
Please note that the External Reference feature is different from Stored Reference, where the data acquisition proceeds in a normal way using a reference spectrum saved previously in the Project.

3.3.5 Using the Autosave Function

The Autosave function allows saving of an acquired spectrum in a specified product with a predefined name. To configure the Autosave:

1 Click on **Acquire ▶ Autosave** or the Autosave icon: AUTO

2 In the dialog box select the product ID from the drop-down list. You can also enter a new product name. In this case you will have to define class and constituent parameters for this new product.



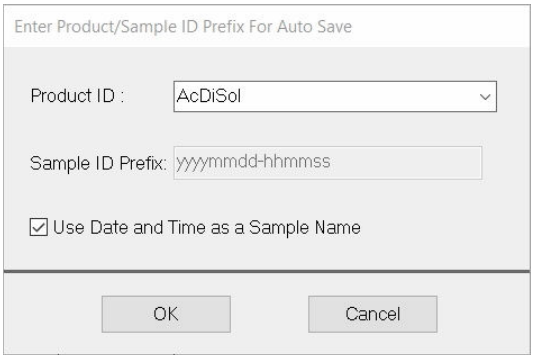
Enter Product/Sample ID Prefix For Auto Save

Product ID : AcDiSol

Sample ID Prefix:

☐ Use Date and Time as a Sample Name

3 Enter the sample name prefix or enable the use of Date and Time as sample name. Samples will be saved with names created from the prefix with a 4-digit consecutive number appended.



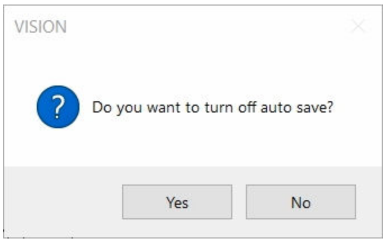
Enter Product/Sample ID Prefix For Auto Save

Product ID : AcDiSol

Sample ID Prefix: yyyymmdd-hhmmss

☑ Use Date and Time as a Sample Name

4 To stop Autosave function, click on **Acquire ▶ Autosave** to disable it.



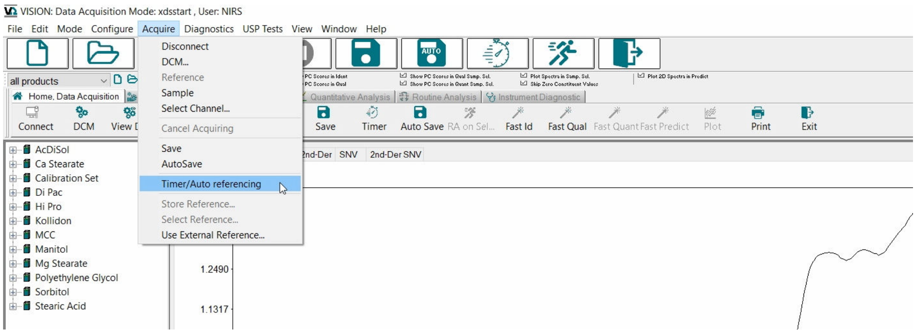
VISION

Do you want to turn off auto save?

3.3.6 Using the Data Acquisition Timer

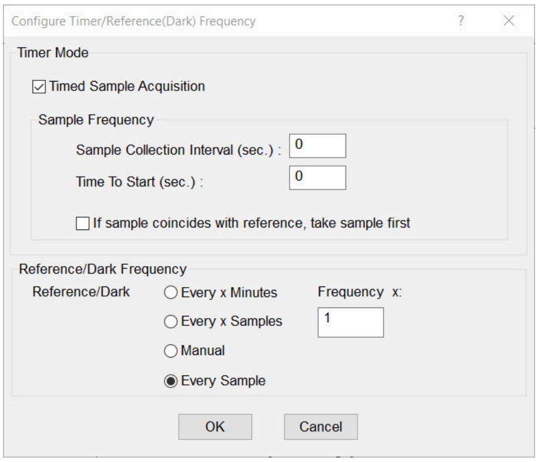
The data acquisition timer allows data acquisition to run automatically and to scan the reference and samples in predefined time intervals. The acquired spectra are saved by the Autosave function. This function is used most often with process instruments. To program the timer:

1 Click on **Acquire ► Timer/Auto referencing**:



VISION: Data Acquisition Mode: xdsstart , User: NIRS

2 The **Configure Timer/Reference(Dark) Frequency** window opens:



Configure Timer/Reference(Dark) Frequency

Timer Mode

☑ Timed Sample Acquisition

Sample Frequency

Sample Collection Interval (sec.) : 0

Time To Start (sec.) : 0

☐ If sample coincides with reference, take sample first

Reference/Dark Frequency

Reference/Dark

○ Every x Minutes

○ Every x Samples

○ Manual

● Every Sample

Frequency x: 1

3 In the **Sample Frequency** field:

- Enter the sample collection interval in seconds. Please note that the additional time interval should be added to the duration of one full measurement. For example, if the duration of the measurement is 65 seconds with 15 seconds interval, the sample collection interval should be set at 80 seconds.
- Enter the delay time for start of the timer

In the **Reference Frequency** field select the reference acquisition interval.

- When sample and reference scans are coincident, Vision will scan reference first, unless the check box is marked.

4 Click on **[OK]** when done.

5 Configure the **Autosave** function as described above.

6 Vision will start timed data acquisition according to the timer settings. In order to stop the data acquisition timer click again on **Acquire ▶ Timer**.

3.3.7 Changing the Data Collection Method

1 In order to change the DCM, click on **Acquire ▶ DCM** and select the DCM.

You can also create a new DCM at this point.

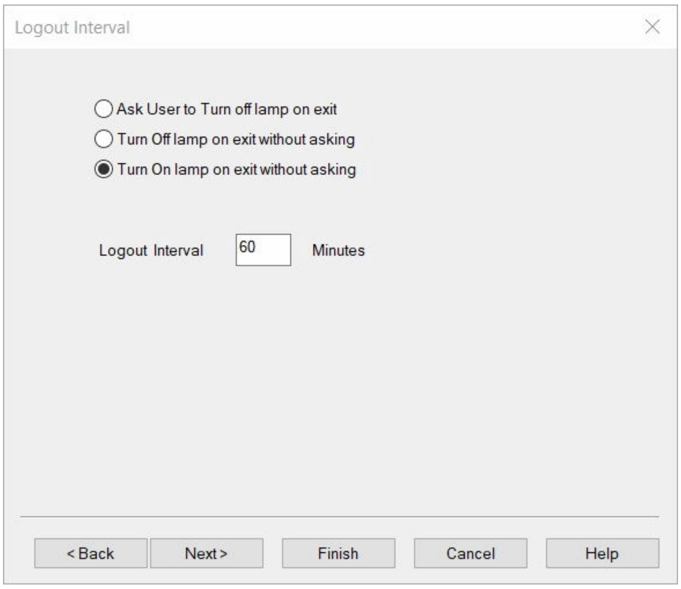
NOTICE

Once a spectrum has been saved using an existing DCM, the DCM cannot be changed.

3.3.8 Lamp Status Management

When closing a Project or exiting Vision when connected to the analyzer, the program can turn the instrument lamp off, leave it on, or ask the user.

1 To configure this option, click on **Configure ▶ Configuration** from Data Acquisition mode.


Logout Interval

○ Ask User to Turn off lamp on exit

○ Turn Off lamp on exit without asking

● Turn On lamp on exit without asking

Logout Interval 60 Minutes

2 Select the **Logout Interval/Lamp Life** tab on the dialog.

3 Select desired option, either **Ask**, **Off** or **On**. The default is **Ask**, which means that Vision will ask whether the lamp is to be turn off upon each exit.

This is the Vision dialog box:

If the instrument will be used again within a few hours, click on **[No]** to leave the lamp on. If the instrument will not be used for some time, such as overnight or over a weekend, click on **[Yes]** to turn the lamp off.

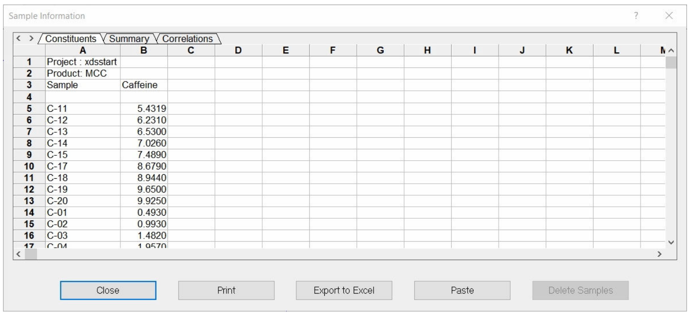
NOTICE

The **Lamp Status Management** differs based on the configuration and applies only if the Lamp Status jumper is used. Please bare in mind that the jumper is used by default unless indicated otherwise.

3.4 Viewing Constituent Data

1 In order to view constituent data, click on a product or sample spectrum to highlight it.

2 Click on **Edit ► Constituent Values**. A spreadsheet with constituent data will be displayed.



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Project : xdsstart												
2	Product: MCC												
3	Sample	Caffeine											
4													
5	C-11	5.4319											
6	C-12	6.2310											
7	C-13	6.5300											
8	C-14	7.0260											
9	C-15	7.4890											
10	C-17	8.6790											
11	C-18	8.9440											
12	C-19	9.6500											
13	C-20	9.9250											
14	C-01	0.4930											
15	C-02	0.9930											
16	C-03	1.4820											
17	C-04	1.9570											

The data can be printed or the whole spreadsheet exported to Excel.

Click on tab **Constituents** to display the constituent values for all constituents.

Click on tab **Summary** to display the statistics for all constituents: maximum value, minimum value, mean, and standard deviation.

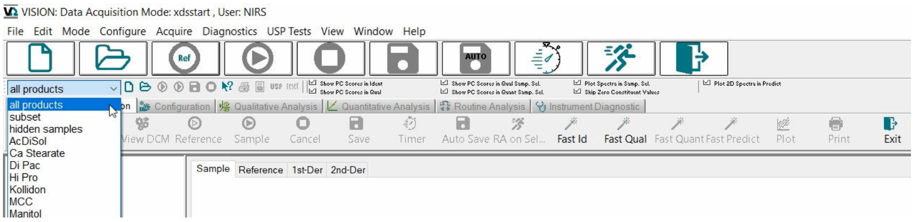
Click on the **Correlations** tab to display intercorrelations between constituents.

3.4.1 Viewing and Hiding Spectra

As each sample is scanned it is displayed in black, and if it is not saved it is replaced with the next sample scan. If the sample is saved, the spectrum can be displayed in color, but stays in black until selected. The color of the spectrum and the check symbol at the sample name are the same, and as a sample is selected and deselected a predetermined series of colors are used to identify the sample name and spectrum. Specific products or groups of products can be viewed, and spectra can be “hidden” or removed from the sample list.

To view a sample spectrum, expand the product it belongs to, and click on the sample name. Click on the sample again to deselect it. You can display multiple samples from various products by simply clicking on them in turn. To display a range of sample spectra from a product, click on the first spectrum in the range, and then holding down the Shift key click on the last spectrum. To clear the spectral display, click on **Edit ► Unselect All**.

At the top of the sample list column, on the left side of the tool bar, is a combo-box with a drop-down menu from which a display option can be selected. The default setting for spectral display is to List All Products. To view spectra of a particular product, click on the combo box arrow and select the desired product.



All samples of the selected Product are listed, and the samples which you wish to view must be individually clicked on from the list.

View spectra from a subset of products by selecting that item from the List Box. Select the products to display from the **Define Subset** list box which appears. You must individually select which samples to plot by clicking on the sample name.

The **hidden** samples remain in the project database, but they are neither displayed nor used for the model development. There are 2 ways to **hide samples**. The quickest is to click on and drag the sample name you wish to hide down to the highlighted **Hide Samples** bar at bottom of the sample list column. A sample can also be hidden by right-clicking on the sample name and selecting Properties from the menu to bring up the **Sample Information** dialog box, and clicking **[Hide This Sample]**. With either hiding method a popup box asks for confirmation.

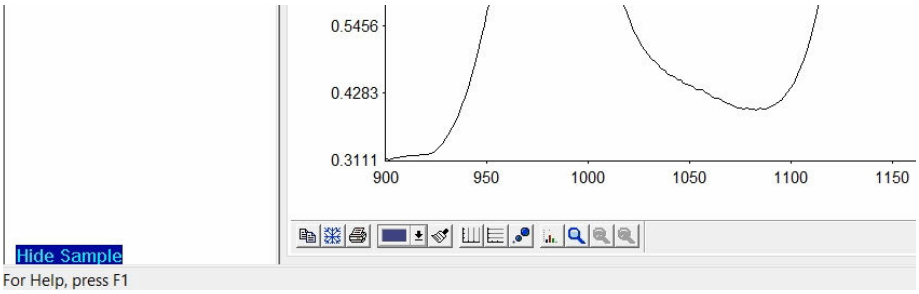
List hidden samples by double clicking on the **Hidden Samples** bar, or by selecting Hidden Samples from the combo box. To **retrieve hidden samples** either click and drag them to the **Shown Samples** bar at the bottom of the list column, or by deselecting the **Sample Information** check box, **[Hide This Sample]**. Double click on **Shown Samples** to return to the shown samples list. You will not be asked to confirm retrieved samples.

The button bar shown here is at the bottom of the display. Right-click on a button to display the definition of its function.

The chart tool bar floats. Pick it up by clicking and holding the mouse button in the blank portion to the right of the buttons and drag it to the desired location. Moving it may be necessary when displaying and changing background colors. To return the tool bar to its original position, double click on the tool bar's title bar. If the tool bar disappears, click on a sample name to turn it back on.

To **display absorbance and wavelength values**, position the cursor near a spectrum and hold down the left mouse button. A crosshair replaces the mouse arrow and attaches to the spectrum. As the mouse moves, the crosshair will follow the coordinates of the spectrum. At the top of the display the wavelength and absorbance values for the crosshair position is displayed beneath a color band indicating the spectrum which has been selected. In case multiple spectra are displayed, the crosshair will follow the spectrum closest to the arrow tip when left-clicked.

At the bottom of the spectral display window there is a number of icons.



Copy spectra to the Windows clipboard by clicking the **copy icon**. Select either a Bitmap or Windows Meta File (WMF) format. The WMF format is preferable because it is fully scalable. Only if your word processor cannot handle WMF should you select Bitmap format. After copying the spectrum to the clipboard, change to your processing software, click the mouse pointer at the place in the document where you want the spectrum and select Edit and Paste to put it there.

Directly print a spectrum by clicking the **printer icon**. To change print parameters, open the **File** menu and choose **Print Setup**. You will probably want to set the orientation to Landscape. After changing the orientation and exiting the **Print Setup** dialog, click on the **print icon** to reprint the spectra. If adding a new printer, the Windows driver disks may be required.

Change the display background color by clicking the color list arrow. Click on the desired color to change the color in the box to the left of the list arrow, then place the mouse button over the color box and hold down the left arrow to drag a paint can to the desired area of the display and release the mouse button. It is often helpful to change the background color to white when taking a spectral plot to a word processor document. In this case, color both the frame around the spectrum and the spectrum background.

To **annotate spectra**, click on the **paintbrush icon**. The annotator allows for drawing arrows and writing text descriptions. To draw an arrow, position cursor at the end of the arrow, press the left mouse button, and move the pointer to the front of the arrow. Release the mouse button. To add text to the arrow, left-click it and choose **Draw Text** from the popup menu. To delete the arrow, left-click it and choose **Delete Arrow**. This action also deletes accompanying text, if it exists. The spectral window should not be resized after arrows are drawn. The spectral view can be copied to the clipboard with arrows and text as a bitmap.

Copying as Windows Metafile will not include arrows. Deselect the icon when done.

Add **vertical or horizontal grids** to the spectrum view by clicking the **grid icons**.

Change the **size of the data points** with the **bubble icon**. There are 4 size levels ranging from none to large. Keep toggling this icon to return data points to their original size.

The **properties of the plot** can be changed by clicking on the **chart properties icon**. It is recommended to use the default properties.

Add a title to the spectra by selecting the chart properties icon the Titles tab. The title appears in the top border of the display window.

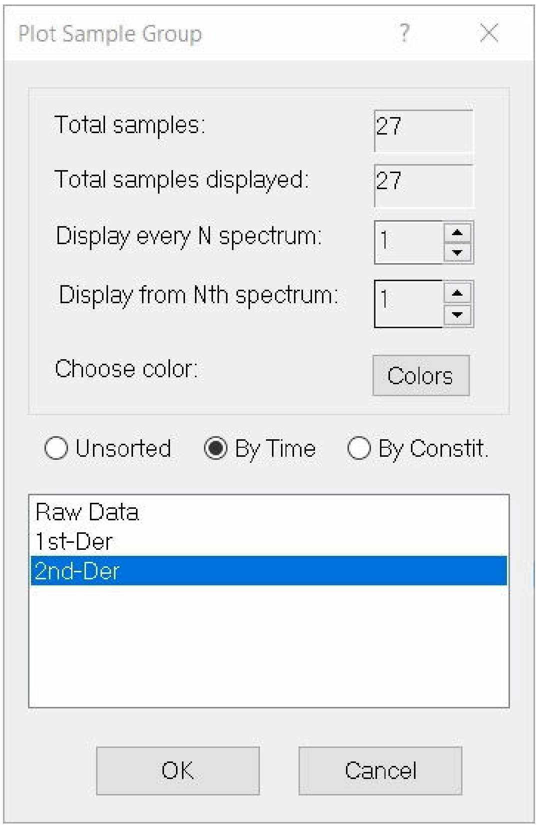
To **expand regions of the spectrum**, click on **[zoom]** and the cursor changes to a magnifying glass. Select an area to zoom by holding down the left mouse button, dragging the cursor to the desired point and then releasing it. A double click in the colored portion at the top of the new spectrum display box or the maximize icon expands it to full screen size. Double click again to return the box to its previous size. The zoomed in area can be dynamically changed by dragging the zoom box in the original display.

3.4.2 Using the Plot Sample Group Function

The Plot Sample Group Function is designed for displaying a large number of spectra. It provides means of displaying only a representative subset of selected spectra and also has color control for the spectra as a group.

1. Select the range of spectra or entire product.

2. Right click the selection and choose **Plot Sample Group**. The box below is displayed. This dialog is self-explanatory. In this example, out of the total of 9 spectra selected, 3 will be displayed, starting from the second spectrum and displaying every third spectrum. Before displaying, spectra will be sorted according to time. 2nd derivative spectra will be shown.



Plot Sample Group

Total samples: 27

Total samples displayed: 27

Display every N spectrum: 1

Display from Nth spectrum: 1

Choose color:

○ Unsorted ● By Time ○ By Constit.

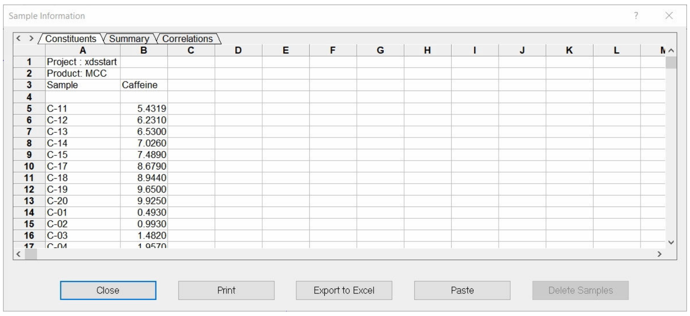
Raw Data
1st-Der
2nd-Der

3 Click **[Colors]** to choose the color for the group. The window with spectra stays on top, and the user can select another group and display it in the same window with different parameters.

3.4.3 Viewing Constituent Data

1 In order to view constituent data, click on a product or sample spectrum to highlight it.

2 Click on **Edit ▶ Constituent Values**. A spreadsheet with constituent data will be displayed.



Sample Information

Constituents / Summary / Correlations

	A	B
1	Project : xdsstart	
2	Product: MCC	
3	Sample	Caffeine
4		
5	C-11	5.4319
6	C-12	6.2310
7	C-13	6.5300
8	C-14	7.0260
9	C-15	7.4890
10	C-17	8.6790
11	C-18	8.9440
12	C-19	9.6500
13	C-20	9.9250
14	C-01	0.4930
15	C-02	0.9930
16	C-03	1.4820
17	C-04	1.9570

The data can be printed or the whole spreadsheet exported to Excel.

Click on tab **Constituents** to display the constituent values for all constituents.

Click on tab **Summary** to display the statistics for all constituents: maximum value, minimum value, mean, and standard deviation.

Click on the **Correlations** tab to display intercorrelations between constituents.

3.4.4 Constituent Data Display Precision

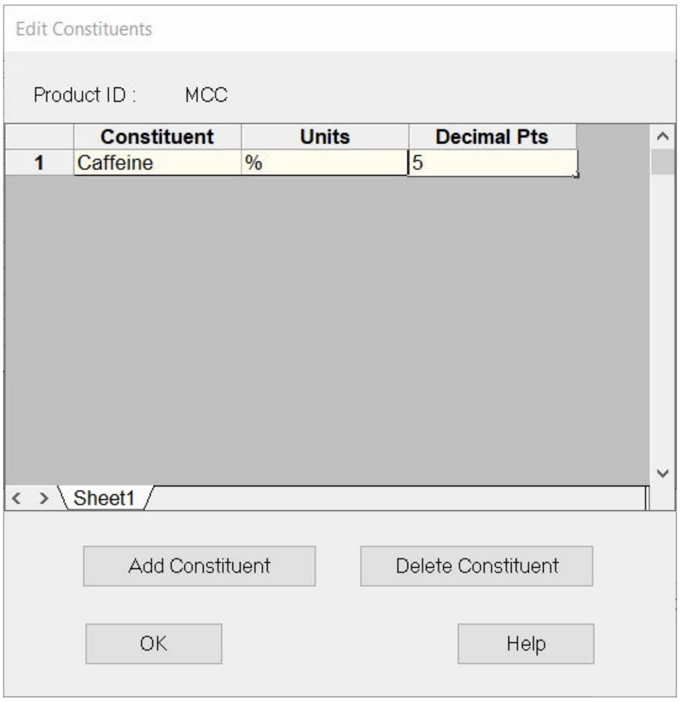
The number of digits after the decimal point can be changed. The change will affect all spreadsheets where constituent data or predicted values are listed, including Routine Analysis Report.

To change the constituent data display precision:

1 In **Data Acquisition** mode click on **Edit ▶ Products**.

2 Select **Constituents** radio button and click on **[Edit]**.

3 Enter the number of digits in the Decimal Points field and press **[Enter]** key. The precision is defined for each constituent separately.



Edit Constituents

Product ID : MCC

	Constituent	Units	Decimal Pts
1	Caffeine	%	5

NOTICE

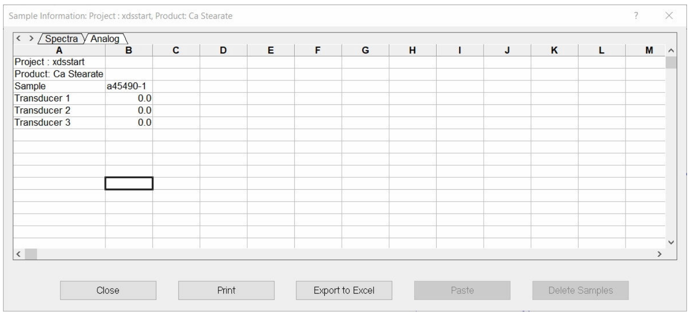
The default precision is 4 digits.

3.4.5 Viewing Transducer (Analog) Values

Transducer Values are used in process applications.

1 Connect Transducer Values to a temperature sensor to collect quant data for each sample in routine analysis.

2 To view transducer values, select a sample or product in **Data Acquisition** mode, choose Spectra from **Edit** menu, and click on the **Analog** tab in the spreadsheet.



Sample Information: Project : xdsstart, Product: Ca Stearate

A	B	C	D	E	F	G	H	I	J	K	L	M
Project : xdsstart												
Product: Ca Stearate												
Sample	a45490-1											
Transducer 1	0.0											
Transducer 2	0.0											
Transducer 3	0.0											

3.4.6 Viewing Math Treated Spectra

Vision performs math conversions, but it does not save converted spectra to the database.

The math treatments can be chained in the desired order and the results displayed and inspected.

To view math treated spectra:

1 Click on **Configure ▶ Math Treatments**, to display the **Select Math Treatments** dialog box.

Combinations Of Math Treatments

- 1st-Der
- 2nd-Der
- SNV

Math Treatments

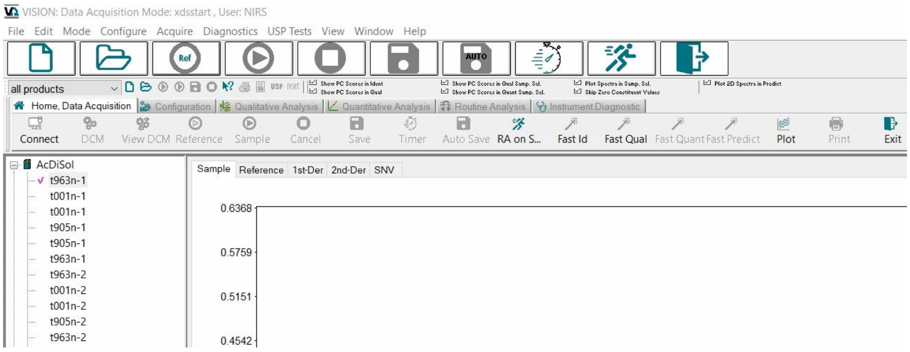
- N-Point Smooth
- 1st derivative
- 2nd derivative
- 3rd derivative
- 4th derivative
- Standard Normal Variate
- Baseline Correction
- Detrend
- Savitzky-Golay
- Thickness Correction

2 Select the desired treatments in the proper order from the menu that is displayed. Click on **[Add]** when done.

3 From the **Math Treatment Properties** window, select the math treatment parameters and click on **[OK]** when done.

4 When you are finished, click on **[Close]** to exit the math treatments dialog box.

5 The spectral view page will now have tabs at the top denoting the selected math treatments and their combinations. Click on a tab to view the spectra with treatments applied.



6 Initially, the math treated spectra display is empty. Deselect all spectra and select them again.

NOTICE

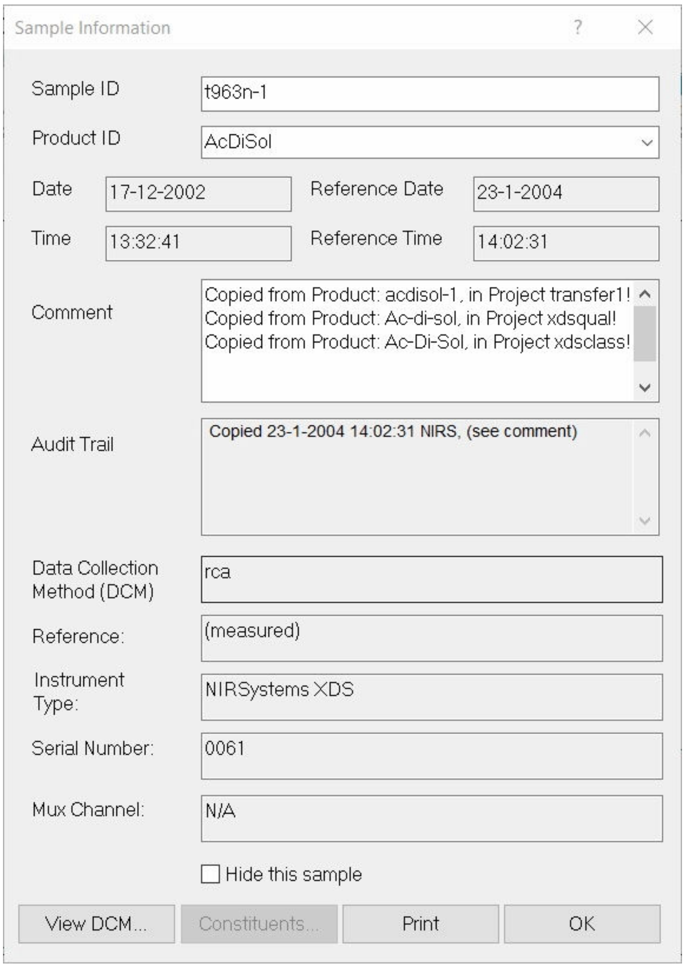
If you want to create 2 or more tabs with the same math treatment type, Vision will prompt you to type new names for multiple tabs.

3.5 Data Management

3.5.1 Sample Information

1 You can review sample information by right-clicking on the sample name in the project tree window, and selecting Properties from the displayed menu.

The sample information includes the sample and product ID, date and time of collecting the spectrum, comment and audit trail, and the DCM name.



Sample Information

Sample ID t963n-1

Product ID AcDiSol

Date 17-12-2002

Reference Date 23-1-2004

Time 13:32:41

Reference Time 14:02:31

Comment Copied from Product: acdisol-1, in Project transfer1! Copied from Product: Ac-di-sol, in Project xdsqual! Copied from Product: Ac-Di-Sol, in Project xdsclass!

Audit Trail Copied 23-1-2004 14:02:31 NIRS, (see comment)

Data Collection Method (DCM) rca

Reference: (measured)

Instrument Type: NIRSystems XDS

Serial Number: 0061

Mux Channel: N/A

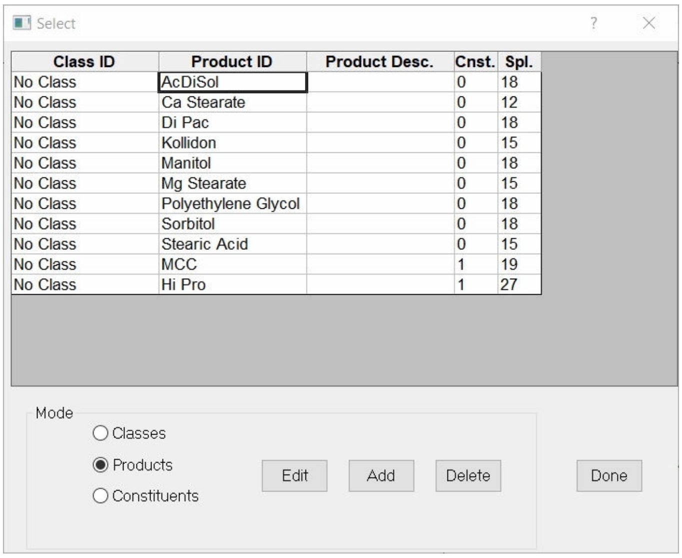
☐ Hide this sample

2 You can view the Data Collection Method, constituent values, or print the sample information by clicking on the appropriate button.

3.5.2 Editing Product Information

1 You can view and edit product information by clicking on **Edit ▶ Products** from the main menu.

This will display a spreadsheet with all products in the active Project.



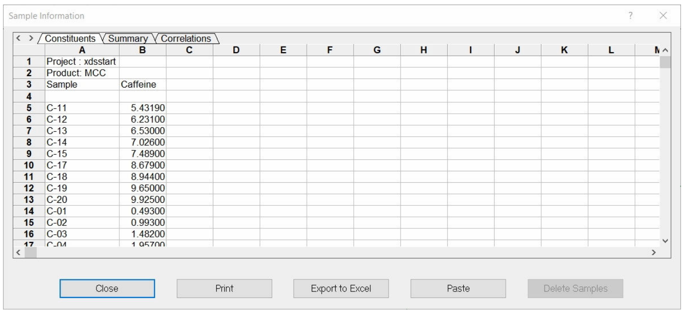
Class ID	Product ID	Product Desc.	Cnst.	Spl.
No Class	AcDiSol		0	18
No Class	Ca Stearate		0	12
No Class	Di Pac		0	18
No Class	Kollidon		0	15
No Class	Manitol		0	18
No Class	Mg Stearate		0	15
No Class	Polyethylene Glycol		0	18
No Class	Sorbitol		0	18
No Class	Stearic Acid		0	15
No Class	MCC		1	19
No Class	Hi Pro		1	27

2 You can add, edit, or delete products, classes, or constituents. Click on **[Done]** to close the window.

3.5.3 Editing or Adding Constituent Values

Constituent values can be added or edited in the spreadsheet that displays them in the following way:

1 In **Data Acquisition** mode select a spectrum or product and click on **Edit ▶ Constituent** Values.



	A	B	C	D	E	F	G	H	I	J	K	L
1	Project : xdsstart											
2	Product: MCC											
3	Sample	Caffeine										
4												
5	C-11	5.43190										
6	C-12	6.23100										
7	C-13	6.53000										
8	C-14	7.02600										
9	C-15	7.48900										
10	C-17	8.67900										
11	C-18	8.94400										
12	C-19	9.65000										
13	C-20	9.92500										
14	C-01	0.49300										
15	C-02	0.99300										
16	C-03	1.48200										
17	C-04	1.95700										

2 Enter the constituent value into the proper cell and press **[Enter]** key.

NOTICE

It is possible to copy and paste columns of data from other Windows applications and ASCII files.

If the column of data is pasted, make sure that the destination column is of the same length as selected in Vision.

3.5.4 Averaging Spectra

Spectra in Vision can be averaged in 2 ways. In manual averaging selected spectra are averaged and the single result placed in the selected product. In automatic averaging all spectra in the selected product are divided into groups and spectra within groups averaged. The user has to define the number of spectra in a group.

If selected spectra have constituent values, they are also averaged.

Manual Averaging of Spectra

To average spectra manually:

1. Select spectra to be averaged. Selected spectra will have check marks next to them.
2. Click on **Edit** ▶ **Average Samples**.

Product ID : AcDiSol

Sample ID : average

Comments : average of 4 spectra

3 From the **Save Averaged Sample** dialog box, choose the product where you want to save the averaged spectrum. You can also create a new product by typing its name in the Product ID field. In this case Vision will guide you through the product setup process.

4 Type in the sample ID and optional comment.

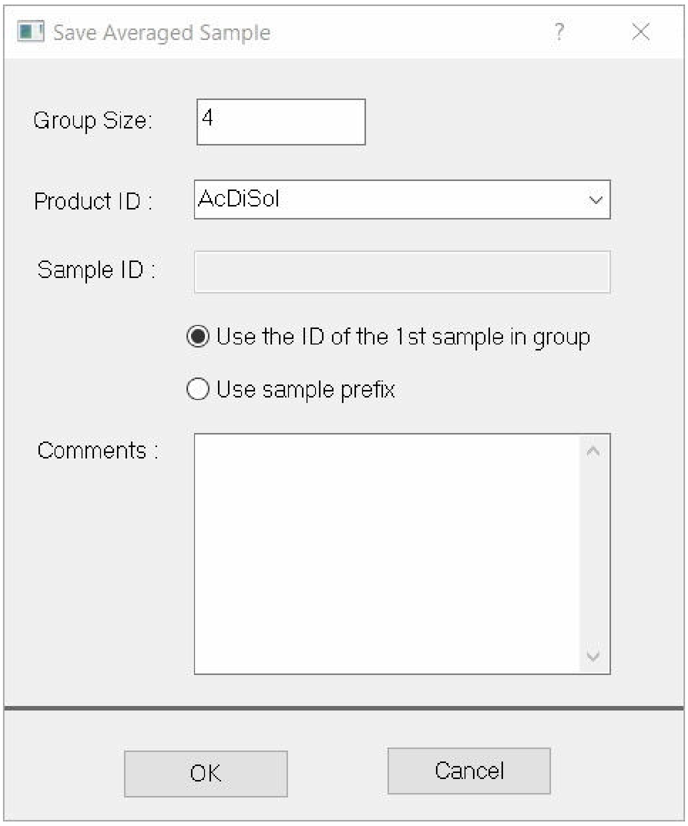
5 Click on **[OK]**.

Automatic Averaging of Spectra

To average spectra automatically:

1 Select the product to be averaged by clicking on it.

2 Click on **Edit ▶ Average Samples**.



Save Averaged Sample

Group Size: 4

Product ID : AcDiSol

Sample ID :

● Use the ID of the 1st sample in group

○ Use sample prefix

Comments :

3 In the **Save Averaged Sample** dialog box, type in the group size. Vision will split spectra into groups in the order they appear on the tree and calculate the average within each group.

4 Choose the product to save the averaged spectra. You can also create a new product by typing its name in the Product ID field. In this case Vision will guide you through the product setup process.

5 Define spectra ID. You can use the name of the first spectrum in each group, or define a prefix, which Vision will append with four digits consecutive number.

6 Type in an optional comment and click on **[OK]**.

NOTICE

Spectra for averaging have to be selected from the same product. Constituent records of the averaged spectra and destination product have to match. If they do not match, Vision issues an error message and aborts averaging. Automatic averaging will average spectra in the order they have been saved in the project. Re-sorting spectra before averaging does not affect the order and results of averaging.

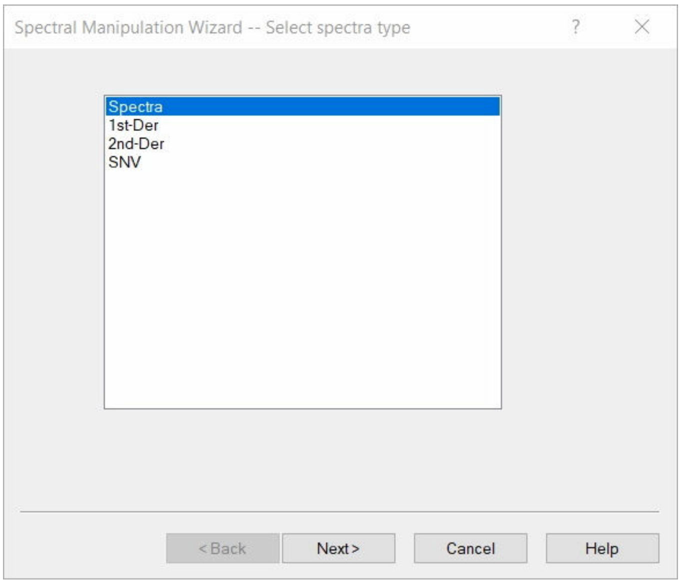
3.5.5 Spectral Manipulation

Spectral manipulation allows users to do addition or subtraction of spectra, multiplication of a spectrum by a constant, and division by a constant.

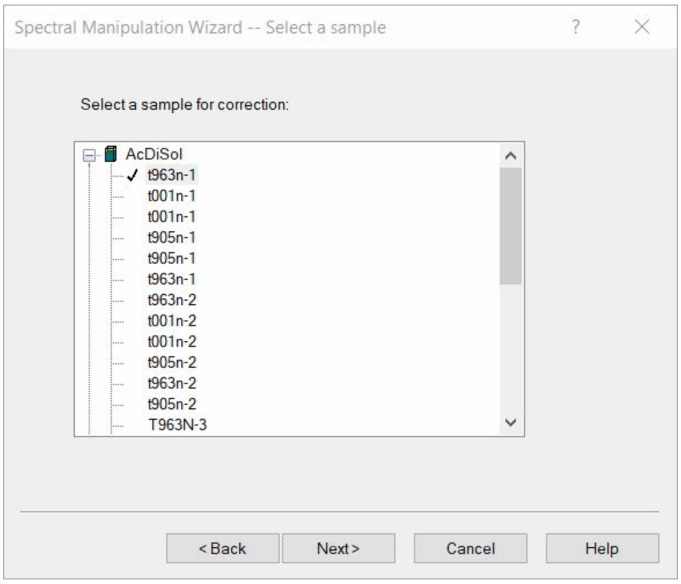
To use the function:

1 Click **Configure ▶ Spectral Manipulation** from the Data Acquisition mode.

2 Select the desired operation. You can process raw or math treated spectra.



3 From the next window select first spectrum and click **[Next]**. Select the second spectrum (or the numerical factor for the division and multiplication) and click **[Finish]**. The result is displayed in black color.



4 The resulting spectrum can be saved by clicking the **Save icon** and typing a new name. In order to delete the result of the operation, click **Configure ▶ Spectral Manipulation ▶ Clear**.

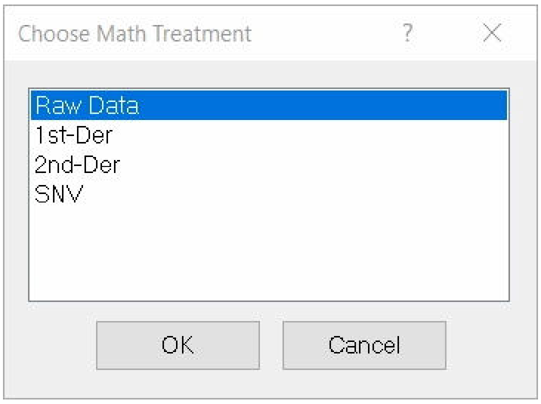
3.5.6 Computing Standard Deviation Spectra

The standard deviation spectrum of a group of spectra can be computed and saved.

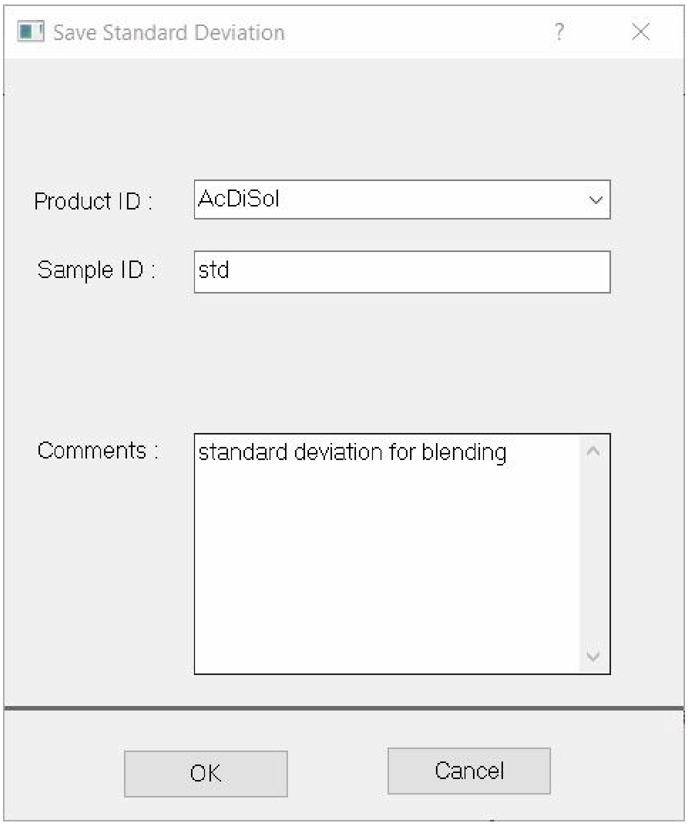
In order to compute the standard deviation:

1 Select the group of spectra in Data Acquisition. The selected spectra are displayed. When computing the standard deviation of a whole product, select the product name.

2 Click on **Edit ▶ Compute Standard Deviation**. The window that opens shows available pretreatments (all pretreatments for which tabs in spectral display window are created are available).



3 Select pretreatment and click on **[OK]**.



Product ID : AcDiSol

Sample ID : std

Comments : standard deviation for blending

4 Select the product and new sample name in order to save it.

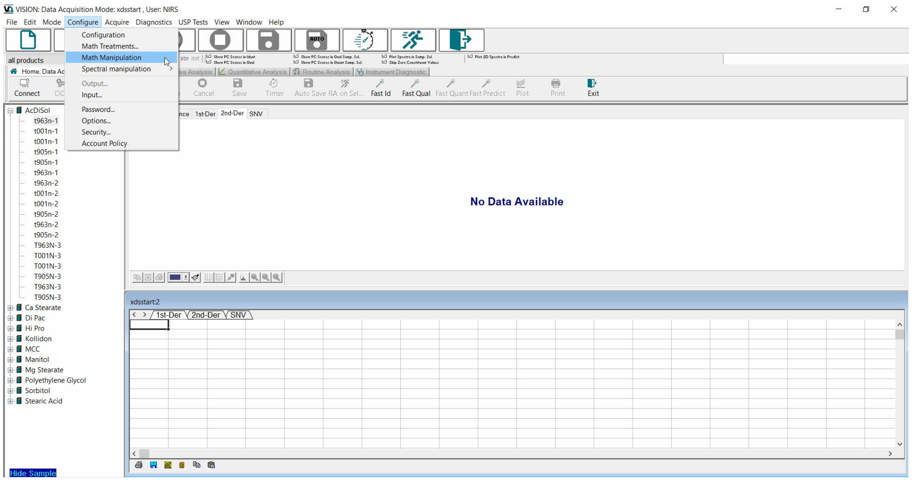
NOTICE

Important: Only spectra from a single product can be used. The minimum number of spectra for calculation is 3.

3.5.7 Math Manipulation

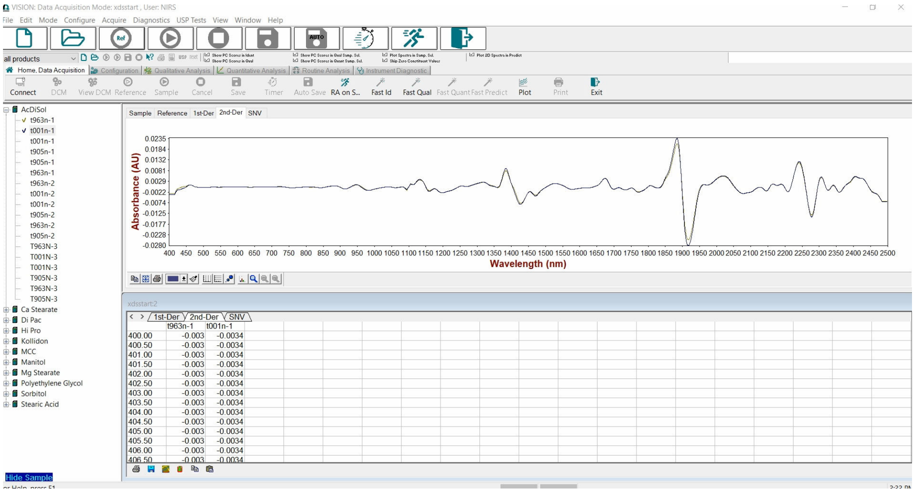
Math manipulation function allows operations on raw and math-treated spectra in the numerical form. Please note that in order to use the function, you have to select and configure appropriate math treatments on the main Data Acquisition page.

1 Click on **Configure ▶ Math Manipulation** to open a blank spreadsheet window. Please note that the top of the window contains tabs that correspond to your selected math pretreatments.



No Data Available

2 Click on the proper tab and the selected spectrum or spectra on the left panel to import the numerical values. The example below shows 2 spectra imported into the spreadsheet as thickness corrected spectra.

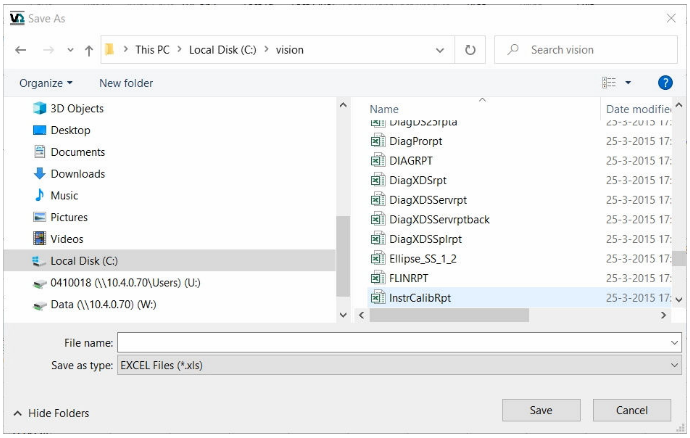


	t963n-1	t001n-1
400.00	-0.003	-0.0034
400.50	-0.003	-0.0034
401.00	-0.003	-0.0034
401.50	-0.003	-0.0034
402.00	-0.003	-0.0034
402.50	-0.003	-0.0034
403.00	-0.003	-0.0034
403.50	-0.003	-0.0034
404.00	-0.003	-0.0034
404.50	-0.003	-0.0034
405.00	-0.003	-0.0034
405.50	-0.003	-0.0034
406.00	-0.003	-0.0034
406.50	-0.003	-0.0034

3 Spectral processing is done by means of icons at the bottom of the page.

To print the spreadsheet, click on the **printer icon**.

To save the spreadsheet in the Excel format, click on the **diskette icon**.



File name:

Save as type: EXCEL Files (*.xls)

Click on **Designer mode icon** (or double right-click the spreadsheet) to open the Tidestone Formula One Workbook Designer. The designer mode allows you to process spectral data using standard Excel-compatible formulas.

Clicking on the **Copy icon** allows you to place selected part of the spreadsheet in the Clipboard.

The **Import Sample icon** allows importing processed or external data back to Vision as normal spectra. In order to import spectra to Vision follow these steps:

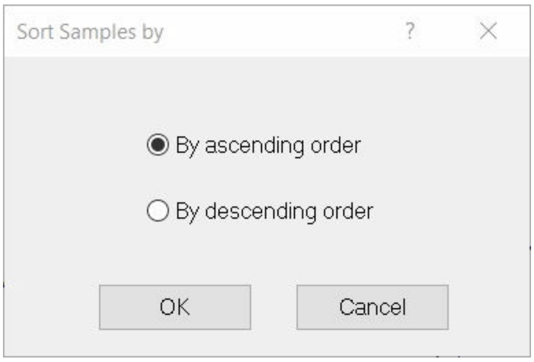
- Open **Math Manipulation** window. Import data and perform desired processing. Alternatively, paste into the spreadsheet spectral data as a column of numbers. To paste data copied from other application (such as Excel), select the cell at the top of the page, and use **Paste icon**.
- Highlight the spectral values intended for import. For multiple spectra highlight the range of values, for a single spectrum double click the top value.
- Click on the **Import icon**. Vision will ask you to select the DCM, product name, and sample name (in case of importing multiple samples you will have to enter a name for each spectrum).

3.5.8 Sorting Spectra

Product spectra displayed on the tree can be sorted by constituent values, sample ID, chronological order, or stored order.

To sort product spectra:

1. Select a product to be sorted by clicking on it.
2. Click on **Edit ▶ Sort Product Samples**. Choose the sorting criteria.
3. From the dialog box, choose the sorting order.



4 Click on **[OK]** when done.

NOTICE

Sorting does not permanently change the order of spectra in a product. Sorting by constituent values is possible only when the product to be sorted has at least one constituent.

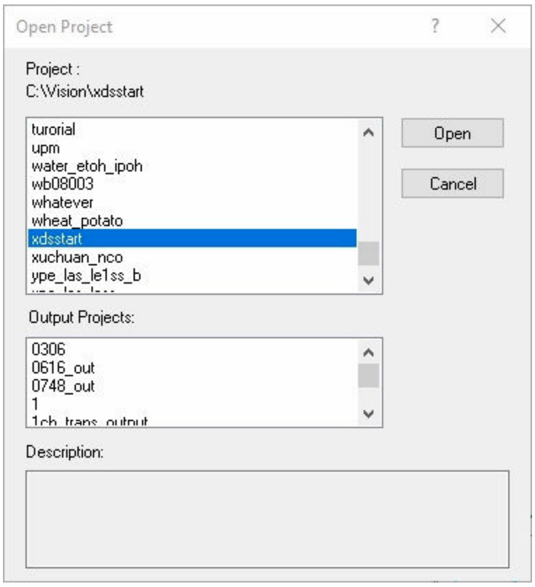
3.5.9 Copying Spectra between Projects and Products

You can copy spectra from one product or project to another. The copied spectra are not removed from the original product.

In order to copy spectra:

1 Select spectra you want to copy by clicking on them. The selected spectra will have a check mark next to them.

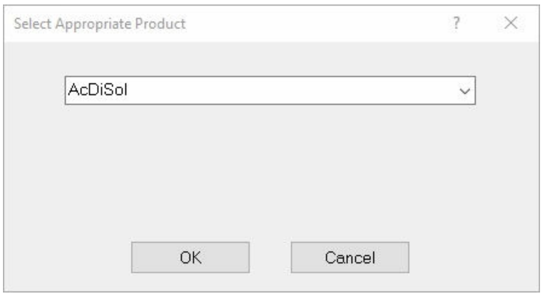
2 Click on **Edit ▶ Copy** (Paste).



Project :
C:\Vision\xdsstart

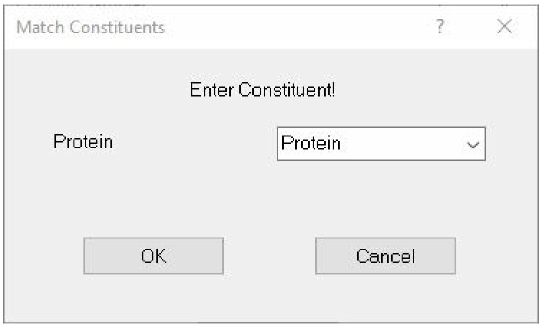
3 In the **Open Project** window, highlight the destination project. You can copy spectra to the active project. Click on **[Open]** when done.

4 In the next window select the destination product and click on **[OK]**.



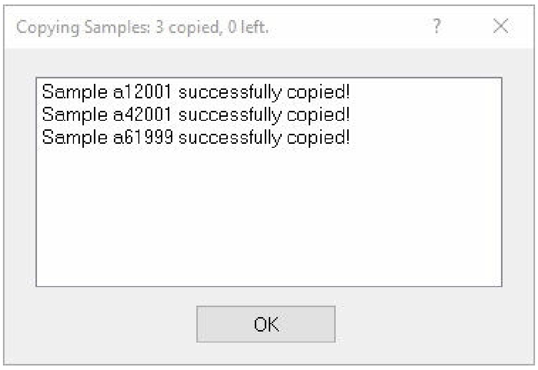
AcDiSol

5 If the copied spectra have constituents, the **Match Constituents** window shows up. You can transfer constituent values to an existing constituent, or create new name.



Protein Protein

6 The next window displays the results of the operation.



Sample a12001 successfully copied!
Sample a42001 successfully copied!
Sample a61999 successfully copied!

3.5.10 Moving Spectra between Projects and Products

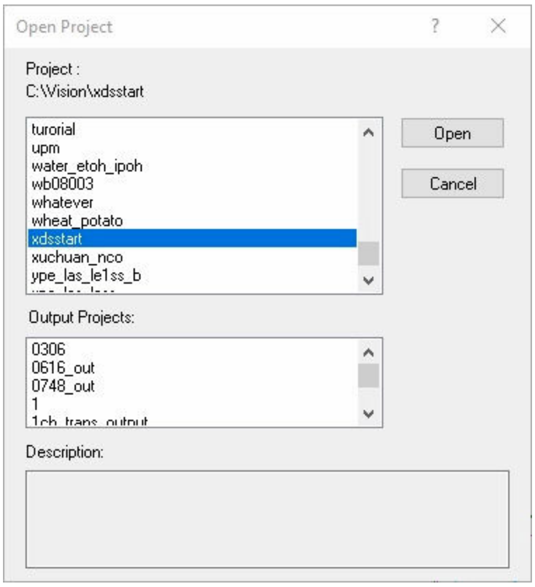
You can move spectra from one product to another. The spectra selected for moving are deleted from the original location and copied to the new one. If 21 CFR Part 11 compliance is on, you will have to give reasons for deleting and copying.

In order to move spectra:

1 Select spectra you want to move by clicking on them. The selected spectra will have a check mark next to them.

2 Click on **Edit** ▶ **Move**. If in the Part 11 compliant mode, enter the reason for deletion of spectra from the original location such as "moving"

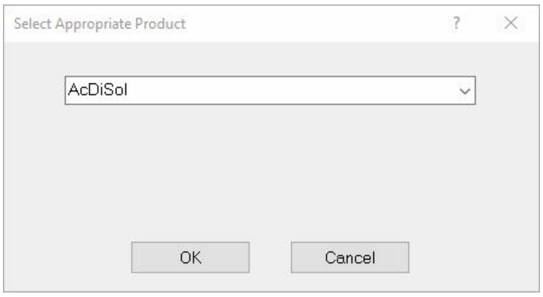
3 In the **Open Project** window highlight the destination Project. You can move spectra to the active Project. Click on **[Open]** when done.



Project :
C:\Vision\xdsstart

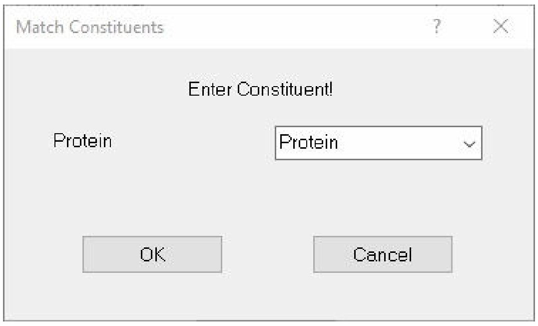
4 If in the Part 11 compliant mode, enter the reason for copying spectra to the new location:

5 In the next window select the destination product and click on **[OK]**.


Select Appropriate Product

AcDiSol

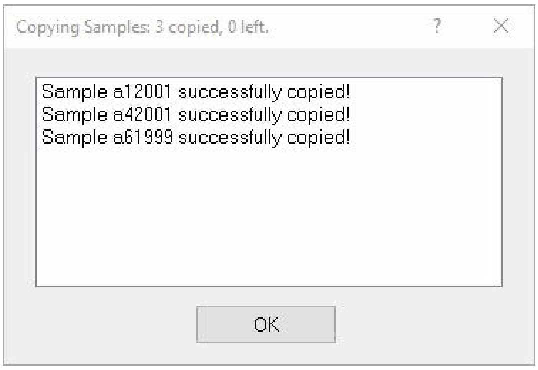
6 If the moved spectra have constituents, the Match Constituents window shows up. You can transfer constituent values to an existing constituent, or create new name.


Match Constituents

Enter Constituent!

Protein Protein

7 The next window displays the results of the operation.


Copying Samples: 3 copied, 0 left.

```
Sample a12001 successfully copied!
Sample a42001 successfully copied!
Sample a61999 successfully copied!
```

3.5.11 Printing Spectra with Associated Information

A selected spectrum can be printed with its properties on a single sheet of paper. The properties include Project ID, product ID, sample ID, date and time of acquisition, user ID, comment, and instrument serial number.

1 To print spectrum with properties select a spectrum and click on **Edit ▶ Print Sample Info**.

3.5.12 Removing Spectra from Products

Although it is possible to delete spectra from products permanently, it is strongly recommended to hide spectra. This will allow to add them back to the sample set when necessary. Although hidden spectra formally still belong to their products, they are ignored when a qualitative or quantitative method is developed.

1 To hide a spectrum, highlight it and drag and drop it to the **Hide Sample** area at the bottom of the **Sample** window.

You can also hide a sample from the **Edit** menu or from the **Sample Information** window.

2

3.5.13 Expanding and Converting Vision Data

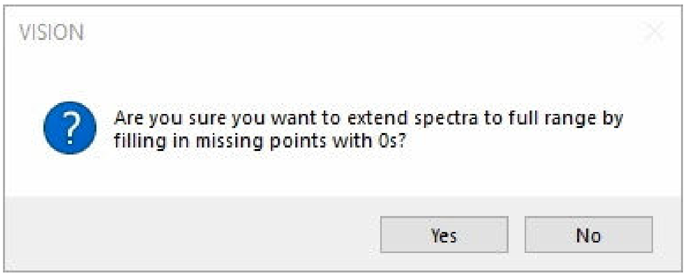
Expand and Convert functions bring older NSAS and Vision data to the most recent format with spectral range 400 to 2500nm and 0.5nm data resolution.

Expanding Project Data

Expand Project Data function increases the wavelength coverage of all spectra in the project to the full range (400 to 2500nm). Missing parts of spectra are filled with data points with value of 0.

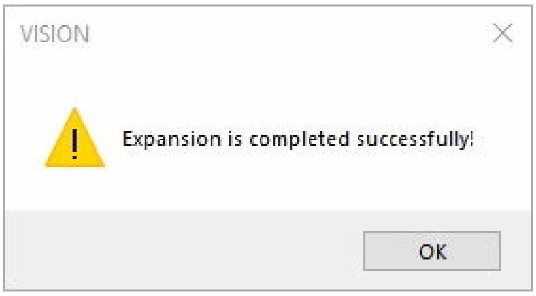
In order to expand project data:

1 Click on **File ▶ Project ▶ Expand Data**. Vision will ask for confirmation:



Are you sure you want to extend spectra to full range by filling in missing points with 0s?

2 Click on **[Yes]** to confirm. After successful expansion Vision will display the confirmation message:



Expansion is completed successfully!

Converting Project Data

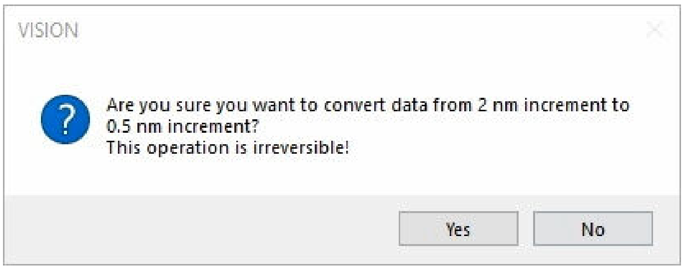
Vision provides utility to convert spectra from SystemII format (2nm spacing) to XDS data format (0.5nm spacing). The conversion is done on all spectra in an active project. During the conversion Vision gives an option to reset the existing quant equations. If this option is chosen, all calibration constants are deleted, but the sample selection results remain intact.

In order to convert the spectra follow these steps:

1 Enter **Data Acquisition** mode and open the project to be converted.

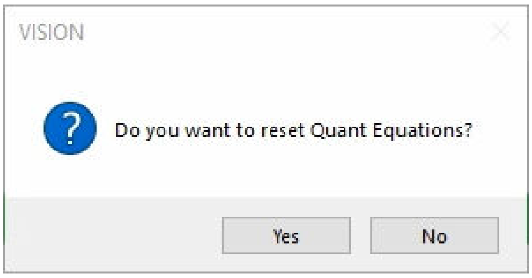
2 Click on **File ▶ Project ▶ Convert Data**.

3 Confirm the operation:



Are you sure you want to convert data from 2 nm increment to 0.5 nm increment?
This operation is irreversible!

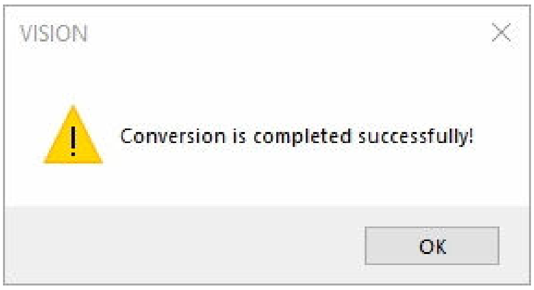
4 If the project contains calibrations, you will have an option to reset the equations:



Do you want to reset Quant Equations?

It is recommended to do so and redevelop calibrations; however in some cases user may want to retain the old equation. In particular, equations developed on 2nm (SystemII) data can be used to prediction on XDS analyzers. In this case Vision will skip extra points and apply SystemII calibration on XDS data correctly.

5 After successful conversion Vision displays the confirmation message:



Conversion is completed successfully!

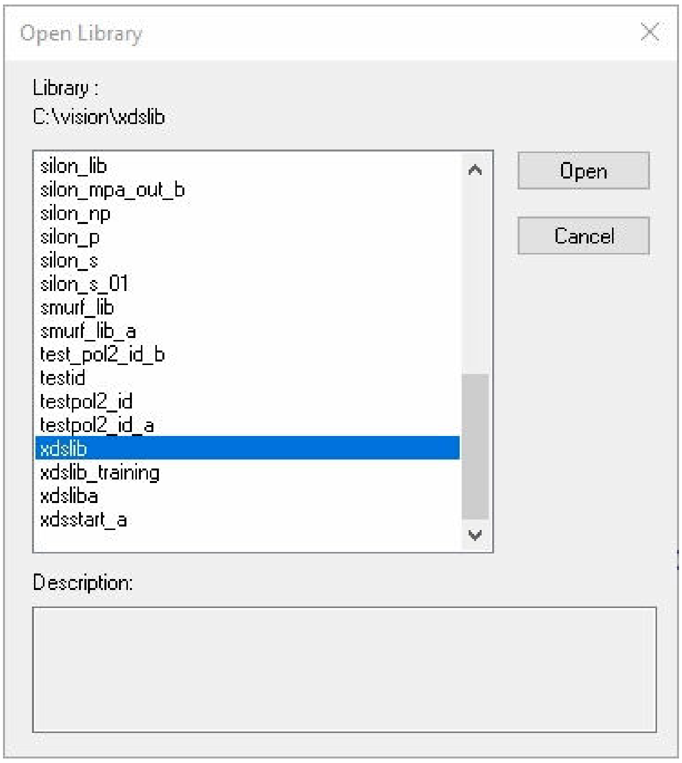
Converting Library Data

Vision provides utility to convert libraries from SystemII format (2nm spacing) to XDS data format (0.5nm spacing). The conversion is done on the library and all spectra in projects linked to the library. During the conversion Vision deletes all library methods (ID method and qualification methods). However, the sample selection results and library structure remain intact.

In order to convert library follow these steps:

1 Enter **Data Acquisition** mode.

2 Click on **File** ▶ **Library** ▶ **Convert Data**. The **Open Library** window opens:


Open Library

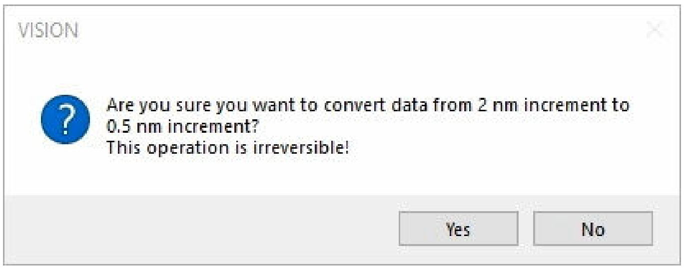
Library :
C:\vision\xdslib

silon_lib
silon_mpa_out_b
silon_np
silon_p
silon_s
silon_s_01
smurf_lib
smurf_lib_a
test_pol2_id_b
testid
testpol2_id
testpol2_id_a
xdslib
xdslib_training
xdsliba
xdsstart_a

Description:

3 Select the library to be converted from the list and click on **[Open]**.

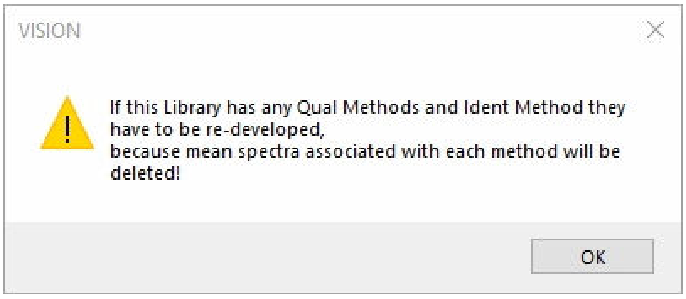
4 Confirm the operation from the next window:


VISION

Are you sure you want to convert data from 2 nm increment to 0.5 nm increment?
This operation is irreversible!

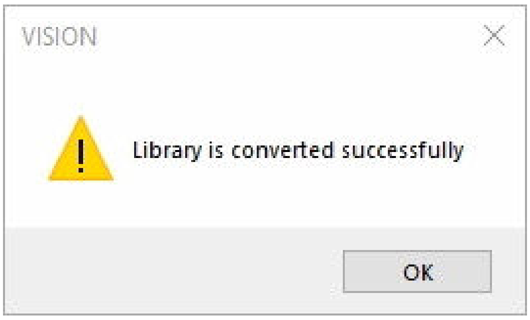
5 If operating under 21CFR Part 11 compliance, you will have to give a reason for methods deletion:

6 And confirm:



If this Library has any Qual Methods and Ident Method they have to be re-developed,
because mean spectra associated with each method will be deleted!

7 After successful conversion Vision displays the confirmation message:



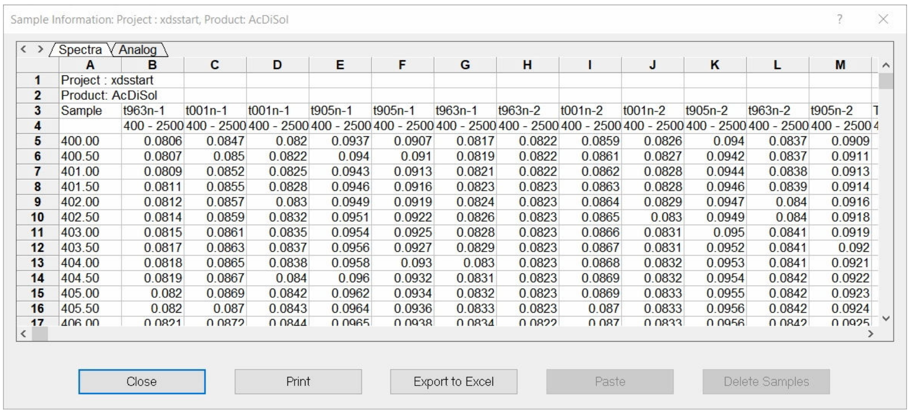
Library is converted successfully

3.6 Spreadsheet Representation of Spectra

3.6.1 Absorbance Spectra

1 Click on the product name to highlight it.

2 Click on **Edit ▶ Spectra** (or right-click on the product name and click on Spectra). This will display a window with a spreadsheet. The spreadsheet contains columns with all spectra in the product.



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Project : xdsstart												
2	Product: AcDiSol												
3	Sample	t963n-1	t001n-1	t001n-1	t905n-1	t905n-1	t963n-1	t963n-2	t001n-2	t001n-2	t905n-2	t963n-2	t905n-2
4		400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500	400 - 2500
5	400.00	0.0806	0.0847	0.082	0.0937	0.0907	0.0817	0.0822	0.0859	0.0826	0.094	0.0837	0.0909
6	400.50	0.0807	0.085	0.0822	0.094	0.091	0.0819	0.0822	0.0861	0.0827	0.0942	0.0837	0.0911
7	401.00	0.0809	0.0852	0.0825	0.0943	0.0913	0.0821	0.0822	0.0862	0.0828	0.0944	0.0838	0.0913
8	401.50	0.0811	0.0855	0.0828	0.0946	0.0916	0.0823	0.0823	0.0863	0.0828	0.0946	0.0839	0.0914
9	402.00	0.0812	0.0857	0.083	0.0949	0.0919	0.0824	0.0823	0.0864	0.0829	0.0947	0.084	0.0916
10	402.50	0.0814	0.0859	0.0832	0.0951	0.0922	0.0826	0.0823	0.0865	0.083	0.0949	0.084	0.0918
11	403.00	0.0815	0.0861	0.0835	0.0954	0.0925	0.0828	0.0823	0.0866	0.0831	0.095	0.0841	0.0919
12	403.50	0.0817	0.0863	0.0837	0.0956	0.0927	0.0829	0.0823	0.0867	0.0831	0.0952	0.0841	0.092
13	404.00	0.0818	0.0865	0.0838	0.0958	0.093	0.083	0.0823	0.0868	0.0832	0.0953	0.0841	0.0921
14	404.50	0.0819	0.0867	0.084	0.096	0.0932	0.0831	0.0823	0.0869	0.0832	0.0954	0.0842	0.0922
15	405.00	0.082	0.0869	0.0842	0.0962	0.0934	0.0832	0.0823	0.0869	0.0833	0.0955	0.0842	0.0923
16	405.50	0.082	0.087	0.0843	0.0964	0.0936	0.0833	0.0823	0.087	0.0833	0.0956	0.0842	0.0924
17	406.00	0.0821	0.0872	0.0844	0.0965	0.0938	0.0834	0.0822	0.087	0.0833	0.0956	0.0842	0.0925

The spreadsheet can be printed or saved in Excel format by clicking on the appropriate button.

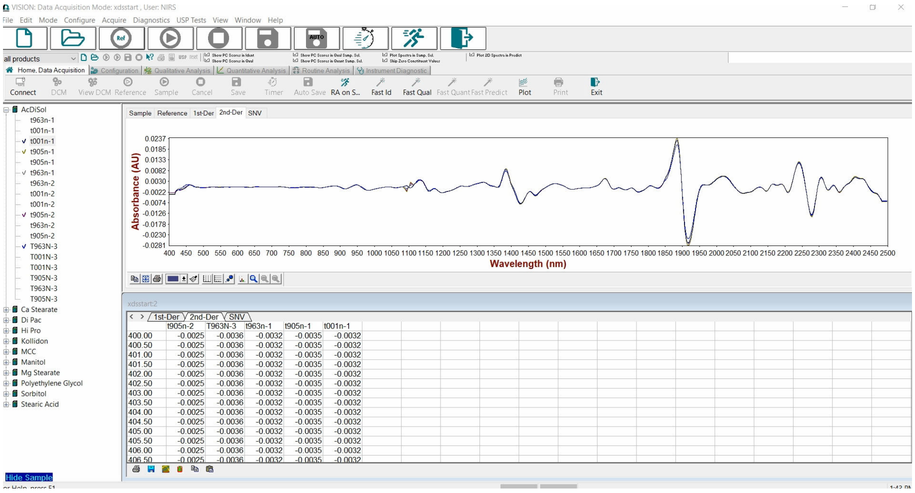
NOTICE

Be aware that printing even a single spectrum will use a lot of paper.

3.6.2 Math-treated Spectra

1 Click on **Configure ▶ Math Manipulation** to open a spreadsheet window. The window contains tabs that correspond to your selected math pretreatments.

2 Click on the proper tab and the selected spectrum to import the numerical values.



	t905n-2	T963N-3	t963n-1	t905n-1	t001n-1
400.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
400.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
401.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
401.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
402.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
402.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
403.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
403.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
404.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
404.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
405.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
405.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
406.00	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032
406.50	-0.0025	-0.0036	-0.0032	-0.0035	-0.0032

To print the spreadsheet, click on the **printer icon**. Please see the note above.

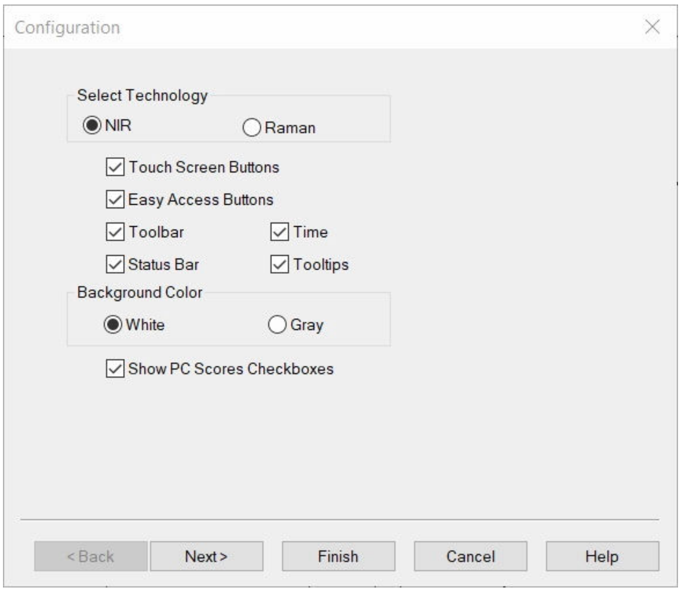
To save the spreadsheet in the Excel format, click on the **diskette icon**.

Clicking on the **page icon** allows you to cut and paste, enter your own formulas, or do spreadsheet manipulation.

3.7 Editing Vision Configuration

Edit Configuration window allows to select visible elements of Vision interface, lamp status for XDS instruments, logout interval and print and save options. Additionally, the user is prompt to select the correct Technology used as Vision currently accommodates both NIR and Raman technologies within the same version.

1 Select **Configure ▶ Configuration** from the main menu. The Configuration edit window will open:



Select Technology
● NIR ○ Raman
☑ Touch Screen Buttons
☑ Easy Access Buttons
☑ Toolbar ☑ Time
☑ Status Bar ☑ Tooltips
Background Color
● White ○ Gray
☑ Show PC Scores Checkboxes

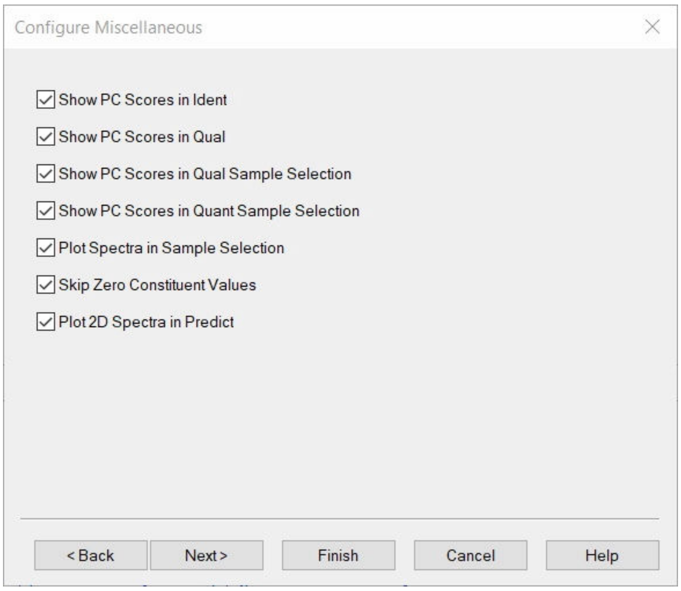
NOTICE

Make sure to select the correct Technology used. For each Technology, NIR or Raman, the Project options as well as the Diagnostics are predefianed in Vision.

2 Select desired interface elements: Touch Screen Buttons, Easy Access Buttons, Status Bar, Tooltips, and Time. All elements are active after Vision installation by default.

The default **White** color scheme gives Vision appearance consistent with most Windows applications. It can be changed to **Grey** to improve contrast of spectra for visualization.

3 Vision allows the user for Miscellaneous configuration:

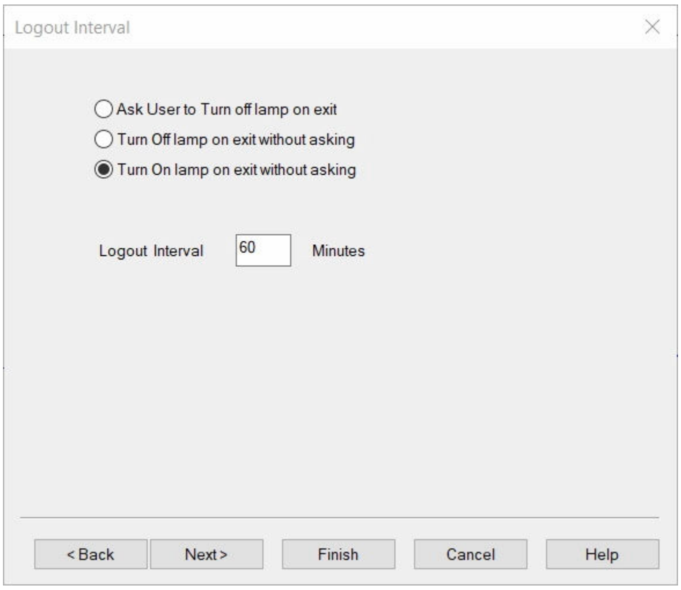


Configure Miscellaneous

☑ Show PC Scores in Ident
☑ Show PC Scores in Qual
☑ Show PC Scores in Qual Sample Selection
☑ Show PC Scores in Quant Sample Selection
☑ Plot Spectra in Sample Selection
☑ Skip Zero Constituent Values
☑ Plot 2D Spectra in Predict

Enable the preferred plot and special visualization options relevant to chemometric model development.

4 For logout configuration and lamp management continue to **Logout Interval** tab:



Logout Interval

○ Ask User to Turn off lamp on exit
○ Turn Off lamp on exit without asking
● Turn On lamp on exit without asking

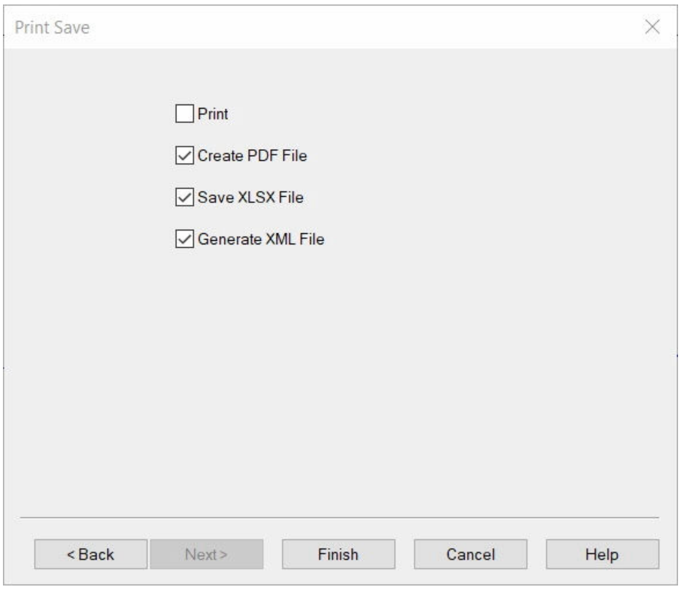
Logout Interval 60 Minutes

The **Turn off lamp** option permits the user to either turn the lamp automatically, leave it on, or asks for action upon logout or when exiting Vision. Most users stay with the default **Turn on lamp without asking** setting, unless directed to set it otherwise. For more information, please visit the Lamp Status Management (section 3.3.8).

Logout Interval may be set as needed, up to 60 minutes as is shown here. After the set time, Vision locks the screen and the user must enter his password to continue.

When set to “0”, Vision never logs out. This setting is not applicable to regulated environments, as it is not compliant with 21 CFR Part 11 rules.

5 For print and save options, click on **Print Save** tab:



☐ Print
☑ Create PDF File
☑ Save XLSX File
☑ Generate XML File

Select whether you want to print your results or save them as PDF file, as XLSX file or as XML file.

3.8 Configuring the Data Acquisition Options

Each Project has a number of specific options, which define the conditions in which data can be acquired, and the general data acquisition defaults.

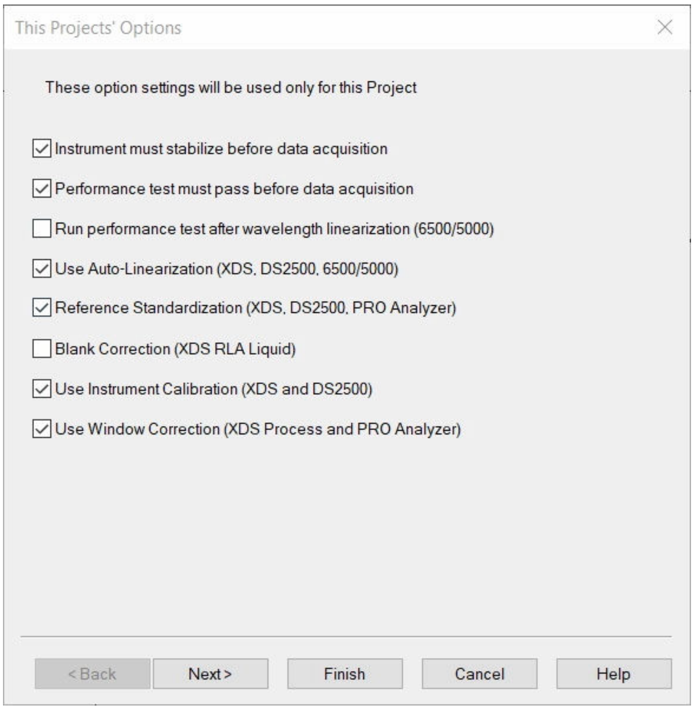
3.8.1 Changing the Options for the NIR Technology

1 Click on **Configure ▶ Options** to open the **Edit Options** window.

2 Click on the proper tab at the top of the window.

If **System Project Defaults** is selected, the defined options will apply to all new Projects.

If the **Project selection** tab is selected, the defined options will apply only to the current Project.


This Projects' Options

These option settings will be used only for this Project

☑ Instrument must stabilize before data acquisition

☑ Performance test must pass before data acquisition

☐ Run performance test after wavelength linearization (6500/5000)

☑ Use Auto-Linearization (XDS, DS2500, 6500/5000)

☑ Reference Standardization (XDS, DS2500, PRO Analyzer)

☐ Blank Correction (XDS RLA Liquid)

☑ Use Instrument Calibration (XDS and DS2500)

☑ Use Window Correction (XDS Process and PRO Analyzer)

3 Check the selected set of options.

- **Instrument must stabilize before data acquisition**. When this option is checked, Vision will not acquire any data before the instrument reaches the proper operating temperature.
- **Performance Test must pass before data acquisition**. When this option is checked, Vision will not acquire any data before the Performance Test passes.
- **Run Performance Test after wavelength linearization**. When this option is checked, Vision will automatically run the Performance Test every time the instrument is relinearized. This is not necessary with the XDS and the DS2500 Solid Analyzer.
- **Use autolinearization (XDS, DS2500 Solid Analyzer, PRO Analyzer)**. When this option is checked, Vision will calculate fine tuning corrections to the linearization constants every time a reference spectrum is collected. These corrections are not stored in the instrument but applied only to the next spectrum collected. It is recommended to have this option on at all times.
- **Reference Standardization (XDS, DS2500 Solid Analyzer, PRO Analyzer)**. Use this option to standardize the instrument and acquire standardized spectra on reflectance measurements. This option must be chosen before creating a DCM. If this option is selected after creation of a DCM, it does not apply the change to existing DCMs. You must create a new DCM to use Reference Standardization.

- **Blank Correction**. This option is used to create a correct transmission reference on the XDS Rapid Liquid Analyzer.
- **Use Instrument Calibration (XDS and DS2500 Solid Analyzer)**. This is a method used to adjust the instrument wavelength profile to an external, traceable wavelength standard. This feature must be used to assure method transferability.
- **Use Window Correction (XDS Process and PRO Analyzer)**. This is selected when using the XDS Process instrument with either Transmission Pair or Interactance Immersion Probes. This option should not be used with Interactance Reflectance.

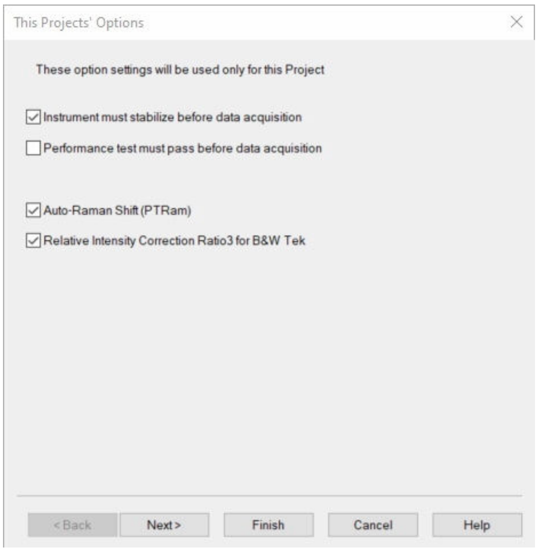
3.8.2 Changing the Options for the Raman Technology

1 Click on **Configure ► Options** to open the **Edit Options** window.

2 Click on the proper tab at the top of the window.

If **System Project Defaults** is selected, the defined options will apply to all new Projects.

If the **Project selection** tab is selected, the defined options will apply only to the current Project.



This Projects' Options

These option settings will be used only for this Project

☑ Instrument must stabilize before data acquisition

☐ Performance test must pass before data acquisition

☑ Auto-Raman Shift (PTRam)

☑ Relative Intensity Correction Ratio3 for B&W Tek

3 Check the relevant set of options:

- **Instrument must stabilize before data acquisition**. When this option is checked, Vision will not acquire any data before the instrument reaches the proper operating temperature.
- **Performance Test must pass before data acquisition**. When this option is checked, Vision will not acquire any data before the Performance Test passes.

- **Use Auto-Raman Shift (PTRam)**. This is an option used to adjust the Raman shift for the PTRam instrument. This feature must be used to assure method transferability.
- **Use Relative Intensity Correction Ratio 3 for B&W Tek**. This option allows to correct the spectral response against a known reference. An instrument unit specific correction file is used for this correction to function. This feature must be used to assure method transferability.

3.9 Programmed Instrument Warm Up

This function of Vision allows the user to program the time when the instrument lamp will turn on automatically, software will let the instrument to warm up and stabilize, and then complete the performance test.

In order to use the Programmed Instrument Warm Up function, both the computer and the instrument have to be on. However, the computer monitor and the instrument lamp can both be turned off.

3.10 Export of Vision Data

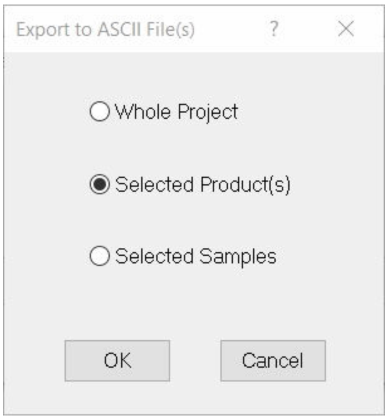
Vision data from the active project can be exported and transferred to other applications as either MVACDF files, NSAS, SPC or in the ASCII proprietary format.

Vision also can export whole projects and libraries to be transferred to other computers.

3.10.1 Export to ASCII, NSAS or SPC Format

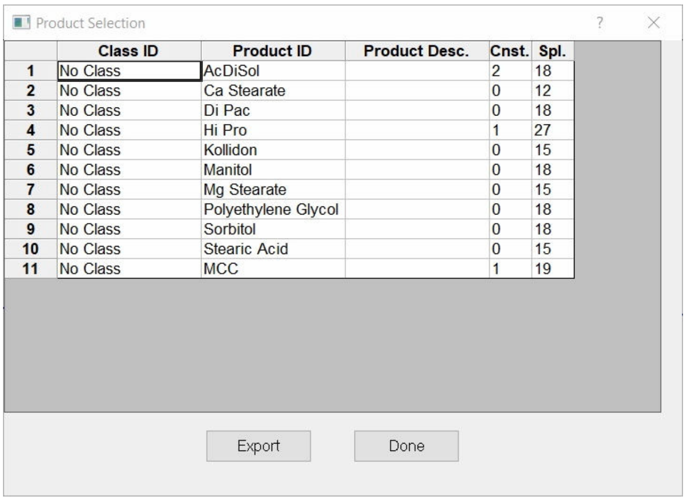
A whole project, selected products, or selected spectra can be exported to ASCII, NSAS or SPC formats. If you export whole products, each product is saved as a separate file. For example, in order to export to ASCII format:

1 Click on **File ▶ Export ▶ ASCII**.



2 From the **Export to ASCII** window, select **Whole Project**, **Selected Product**, or **Selected Samples**. Click on **[OK]** when done.

3 If you are exporting products or samples, choose them from the selection window. Click on **[Export]**.



	Class ID	Product ID	Product Desc.	Cnst.	Spl.
1	No Class	AcDiSol		2	18
2	No Class	Ca Stearate		0	12
3	No Class	Di Pac		0	18
4	No Class	Hi Pro		1	27
5	No Class	Kollidon		0	15
6	No Class	Manitol		0	18
7	No Class	Mg Stearate		0	15
8	No Class	Polyethylene Glycol		0	18
9	No Class	Sorbitol		0	18
10	No Class	Stearic Acid		0	15
11	No Class	MCC		1	19

4 In the **Save As** window, enter the location and the name of the saved file.

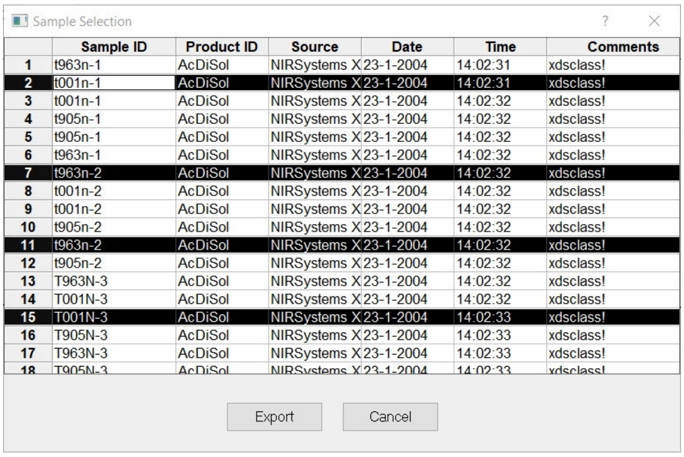
3.10.2 Export to MVACDF format

The export to MVACDF format is applicable for Vision 4.0 and older versions.

In order to export spectra to MVACDF format follow these steps:

1 Open project with samples to be exported in **Data Acquisition**.

2 From the menu select **File ▶ Export ▶ MVACDF**. The following window opens:



	Sample ID	Product ID	Source	Date	Time	Comments
1	t963n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:31	xdsclass!
2	t001n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:31	xdsclass!
3	t001n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
4	t905n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
5	t905n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
6	t963n-1	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
7	t963n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
8	t001n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
9	t001n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
10	t905n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
11	t963n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
12	t905n-2	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
13	T963N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
14	T001N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:32	xdsclass!
15	T001N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:33	xdsclass!
16	T905N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:33	xdsclass!
17	T963N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:33	xdsclass!
18	T905N-3	AcDiSol	NIRSystems X	23-1-2004	14:02:33	xdsclass!

3 The window lists all spectra in the project, with product name they belong to. Select a spectrum by clicking on it. A range of spectra can be selected by Shift+click, and multiple spectra by Control+click

4 Click on **[Export]** when all desired spectra are selected.

The spectra are saved in the project folder.

3.10.3 Exporting (Backing Up) Libraries

Vision has built-in an export libraries function. A library is compressed before saving, so it occupies much less space than original data. There are 2 ways in which a library can be exported:

- A library can be exported together with all linked projects (i.e., projects from which spectra are used in the library development). A library exported this way can be further developed when it is imported to another computer. In particular, new products can be added, or library methods modified.
- A library can also be exported without the linked projects. A library exported this way cannot be further developed or modified when imported to another computer. It has to be used in Routine Analysis as is.

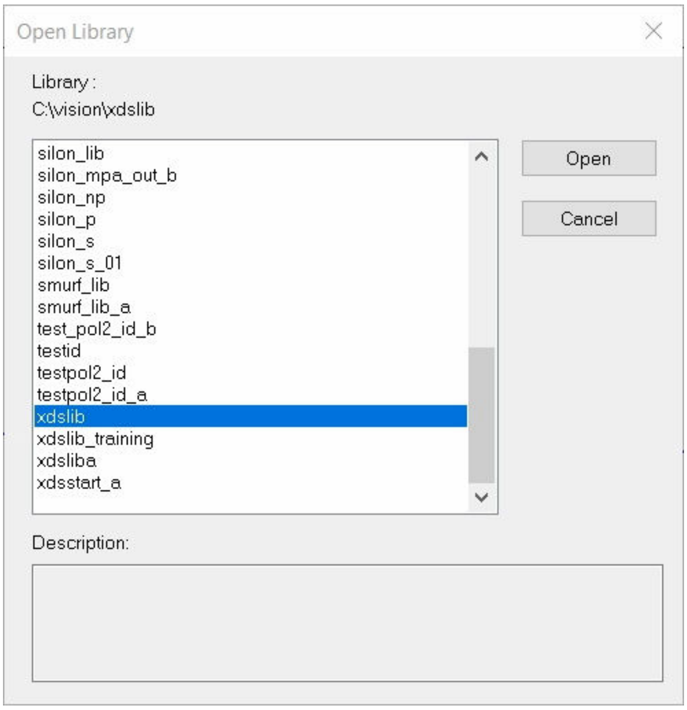
Libraries can be exported to a hard disk, network drive or external drive. Exporting libraries provides an easy way to transfer data and developed qualitative methods between computers, as well as backing up the models.

A library is exported together with all qualitative methods (identification and qualifications methods) developed for the library.

In order to export a library follow these steps:

1 Make sure you are in the **Data Acquisition** mode.

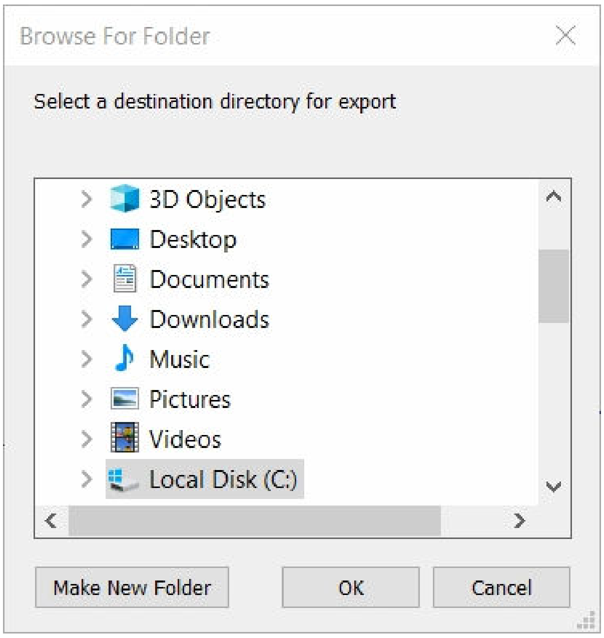
2 Click on **File ▶ Backup ▶ Backup Library**.



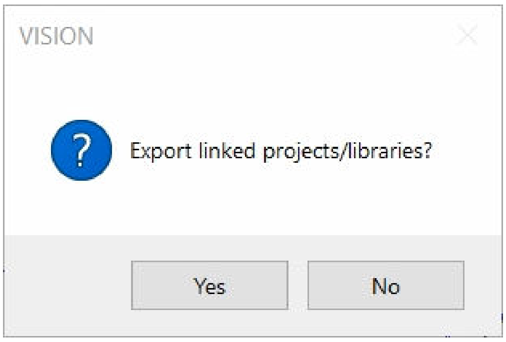
Library :
C:\vision\xdslib

3 From the **Open Library** dialog box, select the library to be exported and click on **[Open]**. If in Part 11 compliance mode, you will be asked for a reason.

4 From the next window, select the destination for the compressed library. If necessary, click on the plus next to the drive or directory name to expand it.



5 If necessary, create a new directory by clicking on **[Create Dir]**. If you do not want to create a new directory, click on **[OK]**.



Export linked projects/libraries?

6 The next window prompts the user to select a way of export (export linked projects/libraries). If you click on **[Yes]**, the linked projects will be exported together with the library. If you click on **[No]**, the links will be broken and the library will be exported alone. A library exported this way cannot be further developed or modified when imported to another computer. It has to be used in Routine Analysis “as is”.

Vision will save a single file in a ZIP format in the selected drive. It can then be restored on another computer from the Vision software.

3.10.4 Exporting (Backing Up) Projects

Vision has an export project function built-in. The projects are compressed before saving, so they occupy much less space than original data. There are 2 ways in which a project can be exported:

- A project can be exported together with a library linked to an Operations Method (if the Operations Method exists). A linked library exported with a project cannot be further developed or modified when imported to another computer, unless it uses only spectra from the exported project. It has to be used in Routine Analysis as is.
- A project can also be exported without the linked library or output projects.

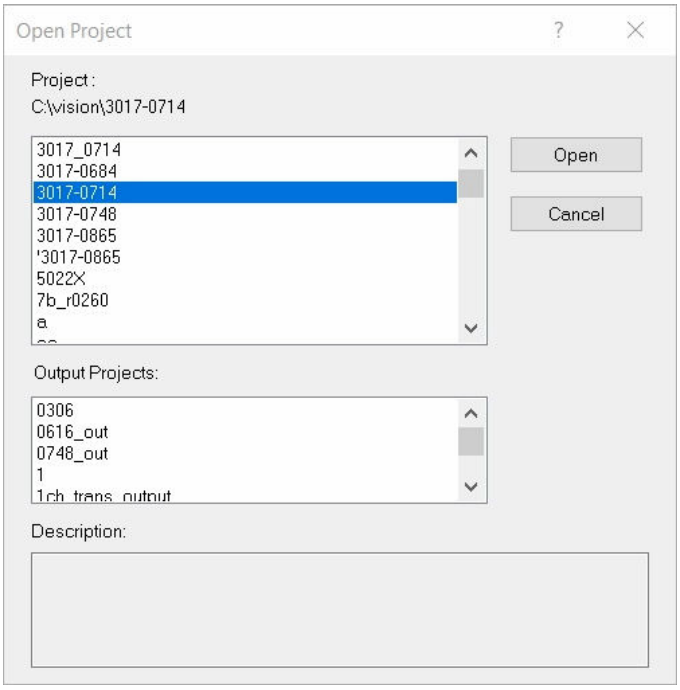
Calibration equations and Operations Methods that were created in a project are always exported with the project. The Operations Method output project is exported only when a linked library or project is exported.

If you want to export a project and be able to modify a library used by the project Operations Method, make sure that all library spectra come from the exported project. Export the project with links.

Projects can be exported to a hard disk, network drive or external drive. Exporting projects provides an easy way to exchange data and develop quantitative methods between computers.

In order to export a project, follow these steps:

1. Make sure you are in Data Acquisition mode.
2. Click on **File ► Backup ► Backup Project**.
3. From the **Open Project** dialog box select the project to be exported and click on **[Open]**.



Project :
C:\vision\3017-0714

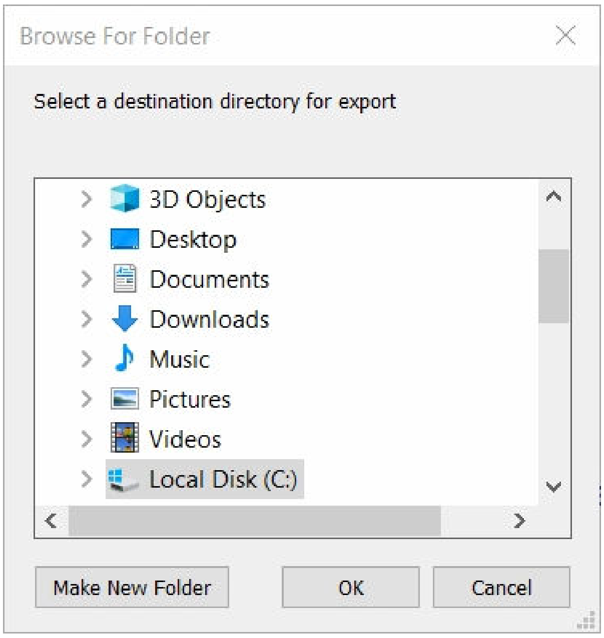
3017_0714
3017-0684
3017-0714
3017-0748
3017-0865
'3017-0865
5022X
7b_r0260
a

Output Projects:

0306
0616_out
0748_out
1
1ch_trans_output

Description:

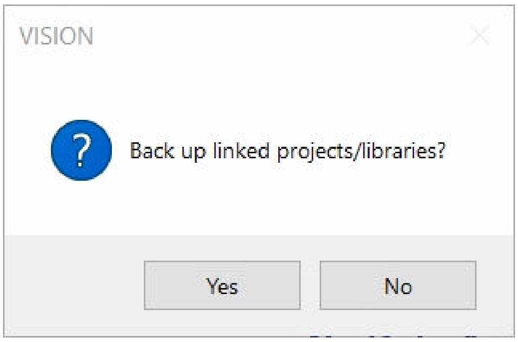
4 From the next window, select the destination for the compressed library. If necessary, click on the plus next to the drive or directory name to expand it.



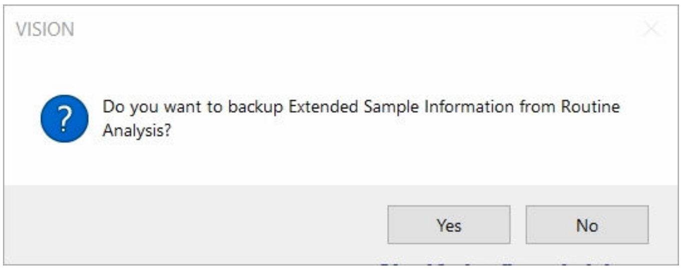
Select a destination directory for export

5 If necessary, create a new directory by clicking on **[Make New Folder]**. If you do not want to create a new directory, click on **[OK]**.

6 The next window prompts you to select a way of export (Export linked projects?).


VISION

Back up linked projects/libraries?


VISION

Do you want to backup Extended Sample Information from Routine Analysis?

If you Click on **[Yes]**, the linked library and output project (if exist) will be exported together with the project Operations Method. If you click on **[No]**, the links will be broken and the project will be exported alone. A linked library exported with the project cannot be further developed or modified when imported to another computer. It has to be used in Routine Analysis as is.

Vision will save a single file in a ZIP format in the selected drive.

3.11 Importing Data

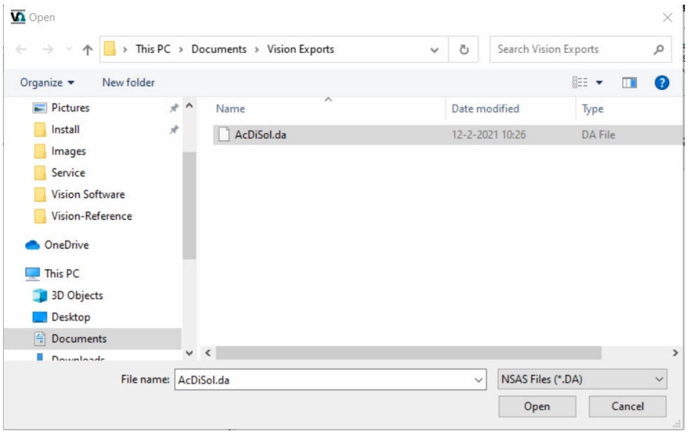
Vision can accept NSAS spectral and constituent files and import all the information from these files into an active project database. In addition, Vision can accept more file formats as ISI, JCamp, Vision Air, CSV or SPC. All spectra from a single data file are imported as a separate product. The product name is identical with the name of the spectral file.

Vision can also import previously exported projects and libraries.

3.11.1 Importing NSAS Data Files

1 Log into the desired project.

2 Click on **File ▶ Import ▶ NSAS.**



AcDiSol.da 12-2-2021 10:26 DA File

File name: AcDiSol.da

NSAS Files (*.DA)

3 In the **Open** dialog box enter the directory with the NSAS files.

4 Click on a file to highlight and select it.

You can select multiple files by holding down Control key while clicking on the files.

You can select a range of files by clicking on the first file in the range, and then holding down the Shift key and clicking on the last file.

5 Click on **[Open]** when all the files you want to import are selected.

NOTICE

Vision creates a separate DCM for each imported file. Do not be surprised by the number of DCMs in your project after the files import. The DCM may not truly reflect how the original data was collected as this information was not part of the original file.

NOTICE

Vision allocates a buffer to hold the names of spectral files to import. The size of the buffer is sufficient to import approximately 100 files with typical name length. If the buffer gets overfilled, import of data is not successful. In this case import your files in several smaller groups.

3.11.2 Import of Vision Air Data Files

Vision allows for import of data files created and saved in Vision Air software. The files have an extension *.NIR, *CAL or *.XML and have to match the Vision supported data points spacing to be successfully imported.

*.NIR and *.CAL files are imported by using the ISI data import. *.XML files are imported by using the Vision Air import function.

1 In order to import a data file click on **File ▶ Import ▶ ISI** or **File ▶ Import ▶ Vision Air** in the **Data Acquisition** Mode. The following window opens:

2 Browse to the file location, select it, and click on **[Open]**.

Within the current project Vision creates a new product with name matching the name of the selected file, and transfers all the spectra contained in the file to the product.

3 Some ISI data do not have the amplifier type attached. In this case Vision will ask to choose Reflectance or Transmission amplifier:

Click on the proper amplifier type.

4 XML files do not include information about the used data collection method (DCM). Vision will ask to define the correct DCM.

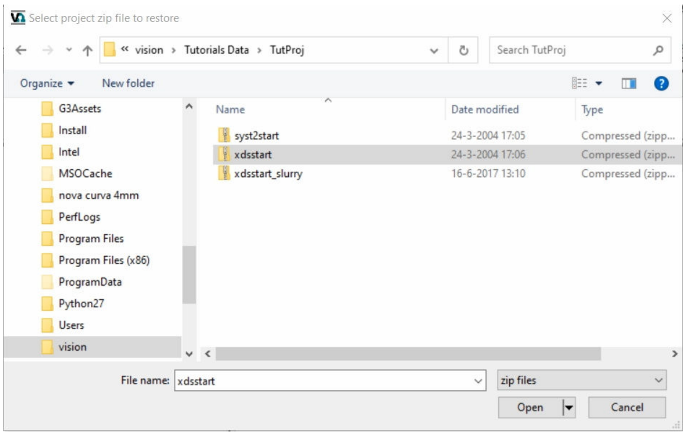
3.11.3 Importing (Restoring) Vision Projects

Previously exported Vision projects can be imported back to Vision and restored. Vision will decompress the zipped projects file and create a new project name in the security database.

If the project, was exported together with linked library and output project, all databases will be added to the security database.

In order to import a project, follow these steps:

1 In the **Data Acquisition** mode click on **File ▶ Restore ▶ Restore Project**.



Select project zip file to restore

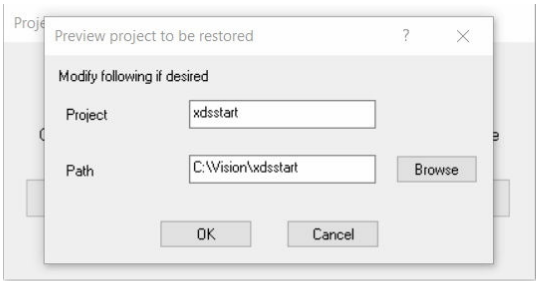
« vision › Tutorials Data › TutProj

Name	Date modified	Type
syst2start	24-3-2004 17:05	Compressed (zipp...
xdsstart	24-3-2004 17:06	Compressed (zipp...
xdsstart_slurry	16-6-2017 13:10	Compressed (zipp...

File name: xdsstart

zip files

2 In the above window find the location of the zipped project file. Highlight the file and click on **[Open]**.



Preview project to be restored

Modify following if desired

Project: xdsstart

Path: C:\Vision\xdsstart

3 In the next window, select the project name and destination directory. Vision by default tries to restore the project with its original name and location. If a project already exists, Vision will give you an option to overwrite.

NOTICE

If the Project with the same name as the imported Project already exists, you will be prompted to overwrite. The Project can be renamed while being imported.

4 Click on **[OK]**.

5 Repeat this for all linked projects and libraries.

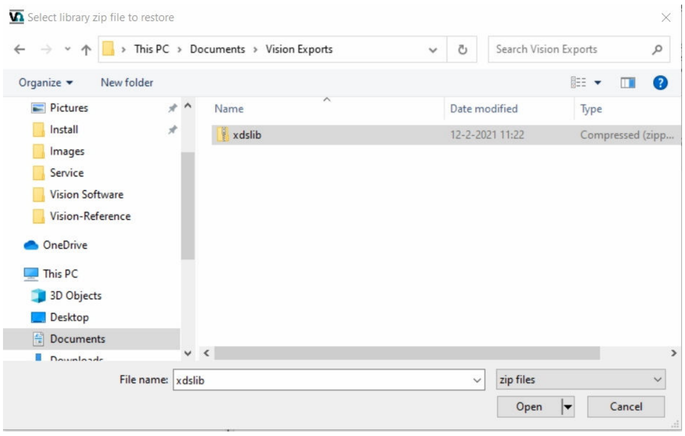
3.11.4 Importing (Restoring) Vision Libraries

Previously exported Vision libraries can be imported back to Vision. Vision will decompress the zipped library file and create a new library name in the security database.

If the library was exported together with linked projects, all projects will be added to the Security Database.

In order to import a library, follow these steps:

1 In the Data Acquisition mode click on **File ▶ Restore ▶ Restore Library**.



Select library zip file to restore

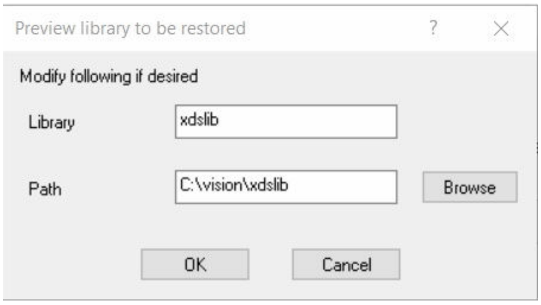
This PC › Documents › Vision Exports

Name	Date modified	Type
xdslib	12-2-2021 11:22	Compressed (zipp...

File name: xdslib

zip files

2 In the next window, find the location of the zipped library file, highlight the file and click on **[Open]**.



Preview library to be restored

Modify following if desired

Library: xdslib

Path: C:\vision\xdslib

3 In the next window, select the library name and destination directory. Vision, by default, tries to restore the library with its original name and location. If a library already exists, Vision will give you an option to overwrite.

NOTICE

If the library name is already in use, you will be prompted to overwrite. The file can be renamed on importing.

4 Click on **[OK]**.

5 Repeat this for all linked libraries.

3.11.5 Adopting Vision Projects

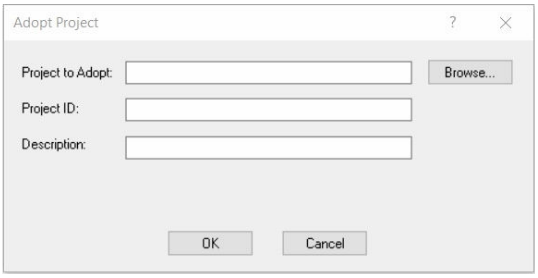
Vision project can be opened by Vision if it is complete (all project database files are present in the project folder) and if the location of the project is in Vision security database. Projects backed up and restored in Vision automatically create a record in the security database. However, if a project is moved from one computer to another without backing up (as a collection of project database files, whether compressed or not) restoring it requires special tools.

Vision provides a function to adopt (restore) such databases. In order to adopt Vision project follow these steps:

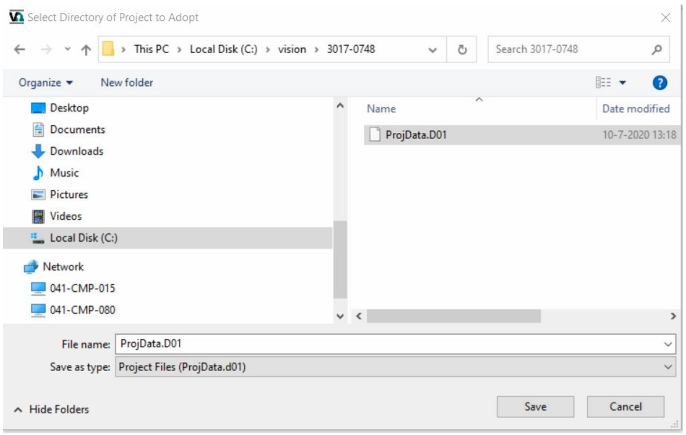
1 If the project is in a removable media (such as CD or memory stick) insert the media into the drive or connect it into the USB port. Open Windows Explorer and make sure Windows recognizes the media.

2 Inspect the project file. If it is in a compressed form (e.g., a ZIP file) use appropriate program (such as WinZip) to unzip it. It is highly recommended to copy the project files from removable media to the hard drive.

3 Open Vision. Click on **File** ▶ **Project** ▶ **Adopt**. The following window opens:



4 Click on **[Browse]** and in the new window find the project location.



File name: ProjData.D01

Save as type: Project Files (ProjData.d01)

5 Select the ProjData.D01 file and click on **[Save]**. Vision defaults the Project ID to the name of folder with project files. Modify it if necessary. Enter optional description and click on **[OK]**.

3.12 Transfer Data from System II to XDS

3.12.1 Transfer of Calibration Data on the same computer

A calibration equation developed on a System II instrument cannot be used to predict on an XDS instrument. The spectra from the System II can be used (after conversion) to create a new calibration for XDS predictions.

Before leaving the System II instrument, while in the project you want to convert for use on the XDS instrument:

1 Go to **Configure ▶ Options** and select the option for **Reference Standardization** followed by **Acquire ▶ Connect**.

2 At the **Select Data Collection Method** dialogue box, create a new DCM for your instrument. The box for **Reference Standardize** should be active. Select that DCM followed by **[OK]**.

3 Move to **Diagnostics ▶ Reference Standard ▶ Create Reference Standard**.

4 Vision prompts for the ceramic reference. Position the ceramic reference and click on **[OK]** for scanning to begin.

5 Vision requests positioning of the 80% Reflectance Reference. Position the correct reference standard for your instrument and click **[OK]** to scan the Certified Reference.

6 Vision then requests the Standard File for the Certified Reference. This file is provided with the accompanying the Standard(s) and may be copied to the Vision directory for ease of use. The file is contained in RSSxxxx.da Click on the file, then click **[Open]**.

7 Vision will plot the spectrum of the ceramic reference, click **[OK]**; plot the Reflectance Reference spectrum, click **[OK]**; and plot the correction spectrum, click **[OK]**. Correction downloaded successfully is now displayed.

8 Click **[Close Report]**.

9 Choose **Diagnostics ▶ Reference Standardization ▶ Reference Standardize Project** to Reference Standardize the current project.

10 Move to **File ▶ Project ▶ Convert**. The software will ask if you are sure. Answer **[YES]**. Remember this is not reversible. Click **[OK]**.

11 If your project data was collected from 1100-2500nm it must be expanded to full range of 400-2500nm as all XDS instruments scan full range. Go to **File ▶ Project ▶ Expand** to expand to full range. If the original data was collected from 400 to 2500nm, this is not necessary.

12 Now you can proceed to go through Sample Selection and Regression to develop a new calibration equation using the standardized, converted, expanded data. Frequently the same math treatments and regression techniques can be used.

13 Create a new Operations Method using the Reference Standardized DCM and the new Calibration Equation.

3.12.2 Transfer of Library on the same computer

Before leaving the System II instrument, open the project from which you developed the Library that you want to convert for use on the XDS instrument:

1 Go to **Configure ▶ Options** and select the option for **Reference Standardization** followed by **Acquire ▶ Connect**.

2 At the **Select Data Collection Method** dialogue box, create a new DCM for your instrument. The box for **Reference Standardize** should be active. Select that DCM followed by **[OK]**.

3 Move to **Diagnostics ▶ Reference Standard ▶ Create Reference Standard**.

4 Vision prompts for the ceramic reference. Position the ceramic reference and click on **[OK]** for scanning to begin.

5 Vision requests positioning of the 80% Reflectance Reference. Position the correct reference standard for your instrument and click **[OK]** to scan the Certified Reference.

6 Vision then requests the Standard File for the Certified Reference. This file is provided accompanying with the Standard(s) and may be copied to the Vision directory for ease of use. The file is contained in RSSxxxx.da Click on the file, then click **[Open]**.

7 Vision will plot the spectrum of the ceramic reference, click **[OK]**; plot the Reflectance Reference spectrum, click **[OK]**; and plot the correction spectrum, click **[OK]**. Correction downloaded successfully is now displayed. Click **[Close Report]**.

8 Choose **Diagnostics ▶ Reference Standardization ▶ Reference Standardize Project** to Reference Standardize the current project.

9 Move to **File ▶ Project ▶ Convert**. The software will ask if you are sure. Answer **[YES]**. Remember this is not reversible. Click **[OK]**

10 If your project data was collected from 1100-2500nm it must be expanded to full range of 400-2500nm as all XDS instruments scan full range. Go to **File ▶ Project ▶ Expand** to expand to full range. If the original data was collected from 400 to 2500nm, this is not necessary.

11 Go to **File ▶ Library ▶ Convert** to prepare the Library structure to accept 0.5nm data. Library Products and their Sample Selection Results will remain intact.

12 The ID and Qual methods developed for System II are automatically deleted when you do a Library Convert. Recreate the ID and Qual methods for your Library.

NOTICE

NOTE: When you recreate these methods the previously used parameters - wavelength regions, math pretreatments, etc., will appear as User Preferences and can be used for redeveloping the models. Even if the red “Q” remains after Library Convert. The previous models cannot be used in Routine Analysis.

13 Create a new Operations Method using the Reference Standardized DCM and the new Library.

3.12.3 Transfer to another computer

When moving from a System II instrument to an XDS instrument and you also want to move your data from a previous computer (A) to a new computer (B), follow this approach:

1 Follow the “same computer” steps to prepare your Calibration Equations and Libraries on computer A.

2 If you only have (or care about) Calibration Equations, go to **File ▶ Backup ▶ Backup Project**. When asked about “with linked projects and Libraries” answer **[NO]**. Do the Backup to a network drive or separate storage device such as flash memory or CD.

3 Move to the new computer (B) and Restore the Project.

4 If you have only a Library, go to **File ▶ Backup ▶ Backup Library**. When asked about “with linked projects” answer **[YES]**. Do the Backup to a network drive or separate storage device such as flash memory, or CD.

5 Move to the new computer (B) and Restore the Library with links.

6 If you have both a Calibration Equation and a Library, go to **File ▶ Backup ▶ Backup Project**. When asked about “linked projects and Libraries” answer **[YES]**. Do the Backup to a network drive or separate storage device such as flash memory, or CD.

7 Move to the new computer (B) and Restore the Project with Links.

3.13 Archiving in Vision

Vision software provides a tool for data archiving in many format types supported by different Data Management Systems.

For example, an archive in XML format consists of two files. The first file is the Vision backup file with extension ZIP. The second file is called metadata file. It contains information about contents of the archive.

Names of archives are composed of the name of the archived unit and dates and times of the first and the last piece of data in the unit.

For example, the archive of a unit named:

"MyProject" storing data created between June 4, 2021 at 9:02:23 and July 9, 2021 at 15:45:21

will be named:

"MyProject_20210604090223_20210709154521.ZIP".

The associated metadata file will be named:

"MyProject_20210604090223_20210709154521.ZIP.NGA".

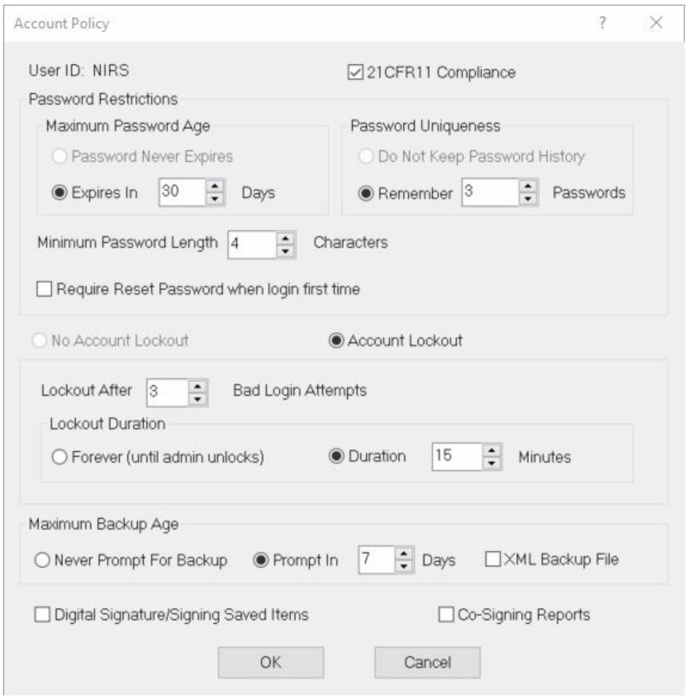
The 24hour clock is used to define names.

The archival of main projects or libraries is done manually, and archival of output projects is done automatically using the scheduler in Routine Analysis. Raw data from output projects will be removed during the archiving by the scheduler or manual archiving through the function in Routine Analysis. Data from main projects and libraries will not be removed during manual archiving.

3.13.1 Manual Archiving

The manual archival can be set it in the Account Policy window. This requires the system to be CFR 21 part 11 compliant.

1. Enter the **Data Acquisition** mode and click on **Configure ▶ Account Policy**.


Account Policy

User ID: NIRS
☑ 21CFR11 Compliance

Password Restrictions
Maximum Password Age
○ Password Never Expires
● Expires In 30 Days
Password Uniqueness
○ Do Not Keep Password History
● Remember 3 Passwords
Minimum Password Length 4 Characters
☐ Require Reset Password when login first time

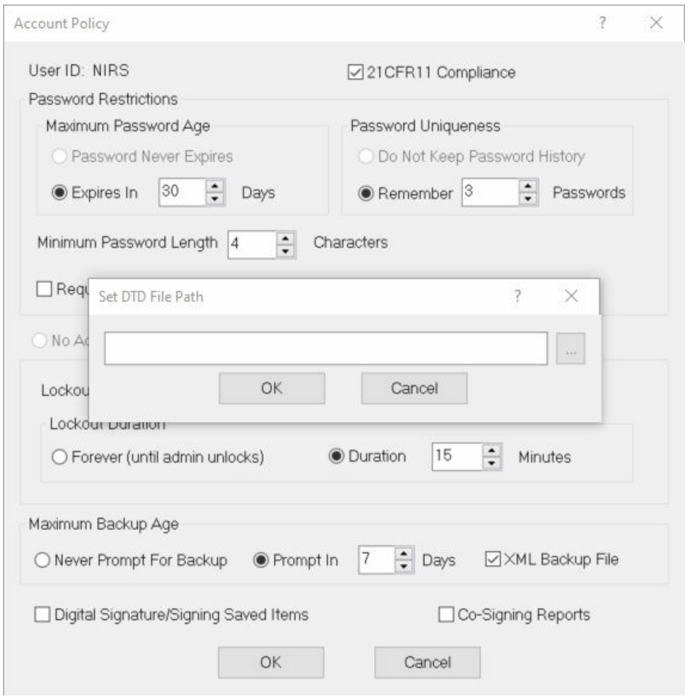
○ No Account Lockout
● Account Lockout
Lockout After 3 Bad Login Attempts
Lockout Duration
○ Forever (until admin unlocks)
● Duration 15 Minutes

Maximum Backup Age
○ Never Prompt For Backup
● Prompt In 7 Days
☐ XML Backup File

☐ Digital Signature/Signing Saved Items
☐ Co-Signing Reports

2 The **Account Policy** window will appear and you must select **CFR 21 Compliance** and then **XML Backup File**.

3 When you select XML Backup File, this window is displayed.


Account Policy

User ID: NIRS
☑ 21CFR11 Compliance

Password Restrictions
Maximum Password Age
○ Password Never Expires
● Expires In 30 Days
Password Uniqueness
○ Do Not Keep Password History
● Remember 3 Passwords
Minimum Password Length 4 Characters

Set DTD File Path

Lockout Duration
○ Forever (until admin unlocks)
● Duration 15 Minutes

Maximum Backup Age
○ Never Prompt For Backup
● Prompt In 7 Days
☑ XML Backup File

☐ Digital Signature/Signing Saved Items
☐ Co-Signing Reports

Using the browse button at the right **[...]**, find the location of the DTD file which comes with NuGenesis and defines the metadata file format (pftemplate.DTD).

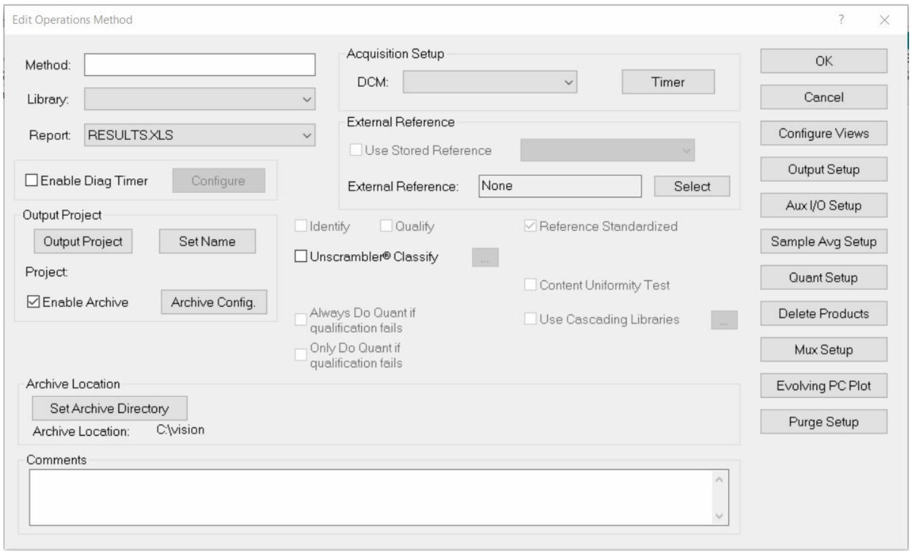
4 One can also set the frequency with which the system will prompt the user for the backup as the Maximum Backup Age (default is 7 days).

3.13.2 Automatic Archiving

The setup of automatic archival of an Output Project is done in the Operations Method.

1 From the **Data Acquisition** mode, click on **Mode ▶ Routine Analysis ▶ Define Operations Method**.

2 Select an existing Operations Method or create a new one. The **Edit Operations Method** window appears.



Method:

Library:

Report: RESULTS.XLS

☐ Enable Diag Timer

External Reference: None

☑ Enable Archive

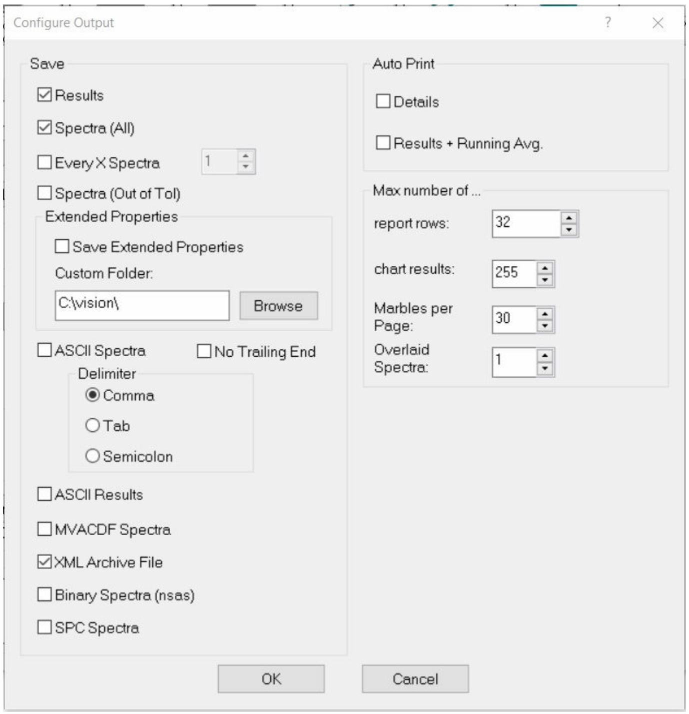
☐ Unscrambler® Classify

☑ Reference Standardized

Archive Location: C:\vision

Comments

3 Click on **[Output Setup]**. This will display the following dialog:



☑ Results

☑ Spectra (All)

☐ Every X Spectra 1

☐ Spectra (Out of Tol)

☐ Save Extended Properties

Custom Folder: C:\vision\

☐ ASCII Spectra ☐ No Trailing End

● Comma

○ Tab

○ Semicolon

☐ ASCII Results

☐ MVACDF Spectra

☑ XML Archive File

☐ Binary Spectra (nsas)

☐ SPC Spectra

☐ Details

☐ Results + Running Avg.

report rows: 32

chart results: 255

Marbles per Page: 30

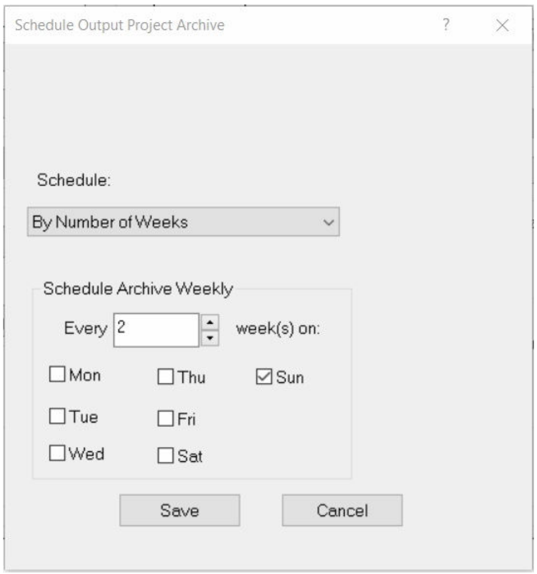
Overlaid Spectra: 1

4 Select **XML Archive File** to enable archiving of the output projects (if the path to the DTD file has not been defined yet, Vision will prompt you to find it).

5 Click on **[OK]**.

6 Back in the **Edit Operations Method** dialog, click on **[Enable Archive]** to setup the scheduler for automatic archiving.

7 Click **[Archive Configuration]** to setup the archiving scheduler:



Schedule: By Number of Weeks

Schedule Archive Weekly

Every 2 week(s) on:

☐ Mon ☐ Thu ☑ Sun

☐ Tue ☐ Fri

☐ Wed ☐ Sat

3.14 Communicating with Metrohm Raman Instruments

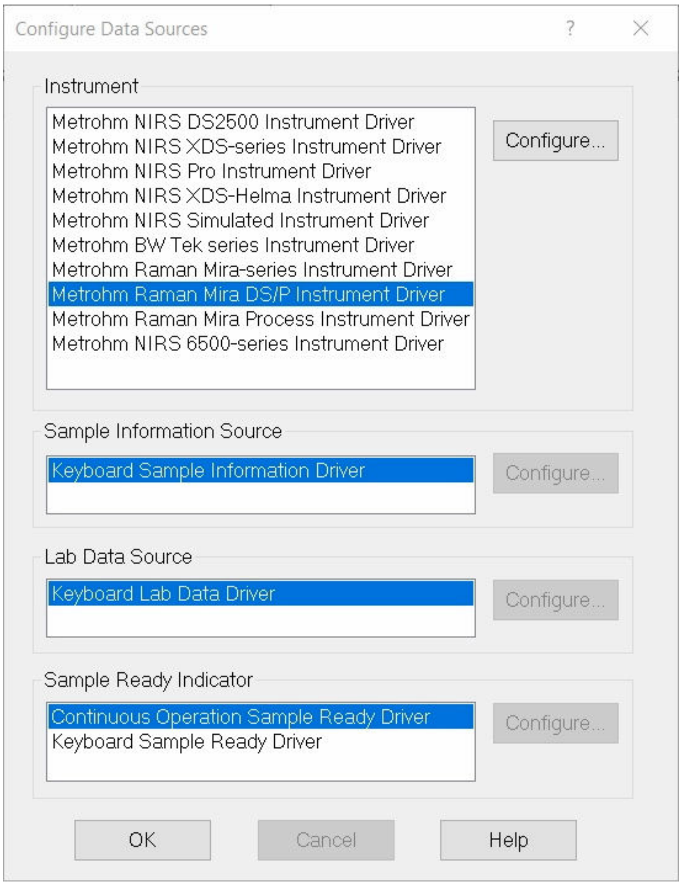
To communicate with a Metrohm Raman instrument, the user must connect the instrument directly at the same computer with a compatible Vision version (versions higher than 4.1.1.156).

3.14.1 Mira DS/P Instrument Driver

1 Click on **File** ▶ **Project** ▶ **New** on the main menu. If an existing Project is currently open, you will be prompted to close it.

Enter a Project name and click OK

2 The Configure Data Sources window displays. Choose the Metrohm Mira DS/P Instrument Driver as you can see below:



Instrument

Metrohm NIRS DS2500 Instrument Driver
Metrohm NIRS XDS-series Instrument Driver
Metrohm NIRS Pro Instrument Driver
Metrohm NIRS XDS-Helma Instrument Driver
Metrohm NIRS Simulated Instrument Driver
Metrohm BW Tek series Instrument Driver
Metrohm Raman Mira-series Instrument Driver
Metrohm Raman Mira DS/P Instrument Driver
Metrohm Raman Mira Process Instrument Driver
Metrohm NIRS 6500-series Instrument Driver

Sample Information Source

Keyboard Sample Information Driver

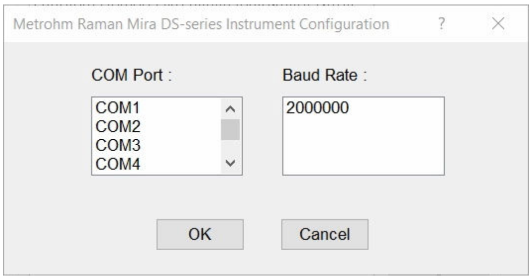
Lab Data Source

Keyboard Lab Data Driver

Sample Ready Indicator

Continuous Operation Sample Ready Driver
Keyboard Sample Ready Driver

3 Click on **[Configure]**:



COM Port :

COM1
COM2
COM3
COM4

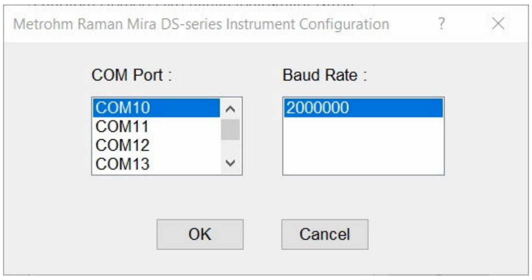
Baud Rate :

2000000

NOTICE

Please refer to the corresponding User Manual for configuring the connection properly

4 Click on the correct COM Port and on the single option for the Baud Rate:

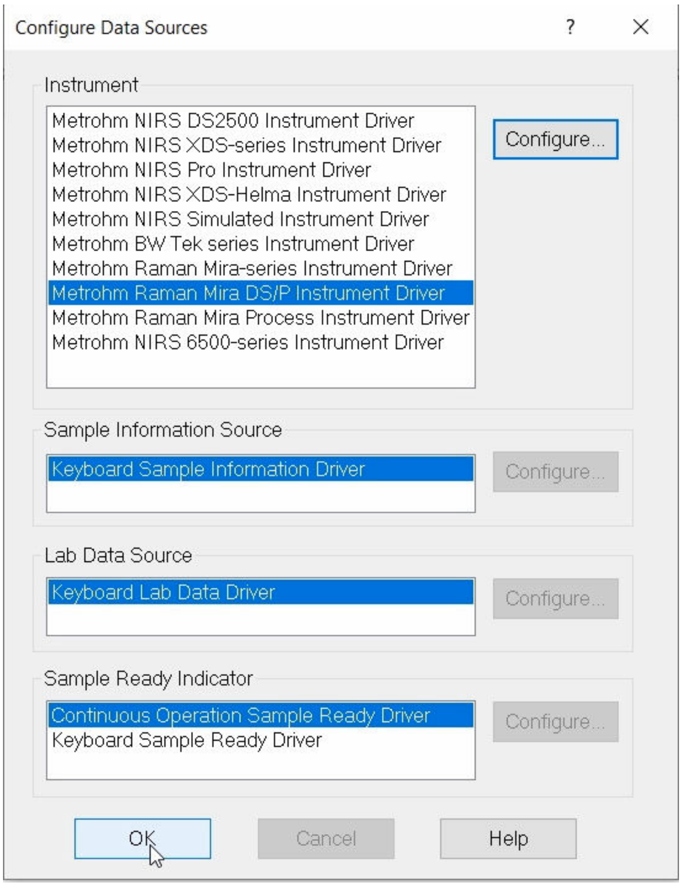


Metrohm Raman Mira DS-series Instrument Configuration

COM Port :
COM10
COM11
COM12
COM13

Baud Rate :
2000000

Click **[OK]** to the above and the following window:



Configure Data Sources

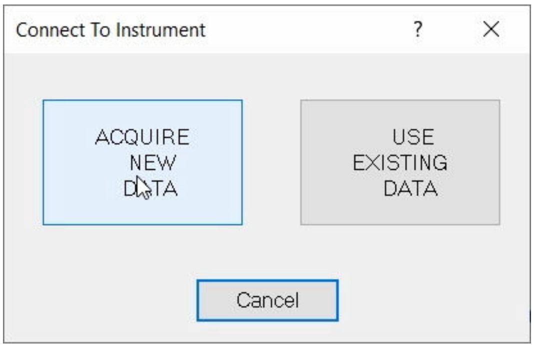
Instrument
Metrohm NIRS DS2500 Instrument Driver
Metrohm NIRS XDS-series Instrument Driver
Metrohm NIRS Pro Instrument Driver
Metrohm NIRS XDS-Helma Instrument Driver
Metrohm NIRS Simulated Instrument Driver
Metrohm BW Tek series Instrument Driver
Metrohm Raman Mira-series Instrument Driver
Metrohm Raman Mira DS/P Instrument Driver
Metrohm Raman Mira Process Instrument Driver
Metrohm NIRS 6500-series Instrument Driver

Sample Information Source
Keyboard Sample Information Driver

Lab Data Source
Keyboard Lab Data Driver

Sample Ready Indicator
Continuous Operation Sample Ready Driver
Keyboard Sample Ready Driver

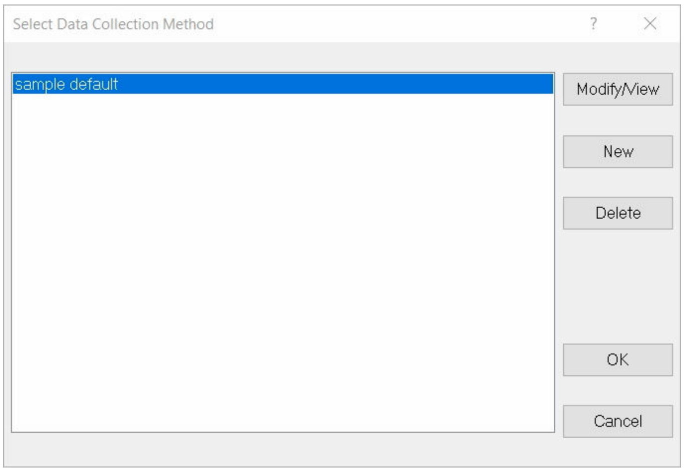
5 From the **Connect To Instrument** dialog box, choose to **[Acquire New Data]** or **[Use Existing Data]**.



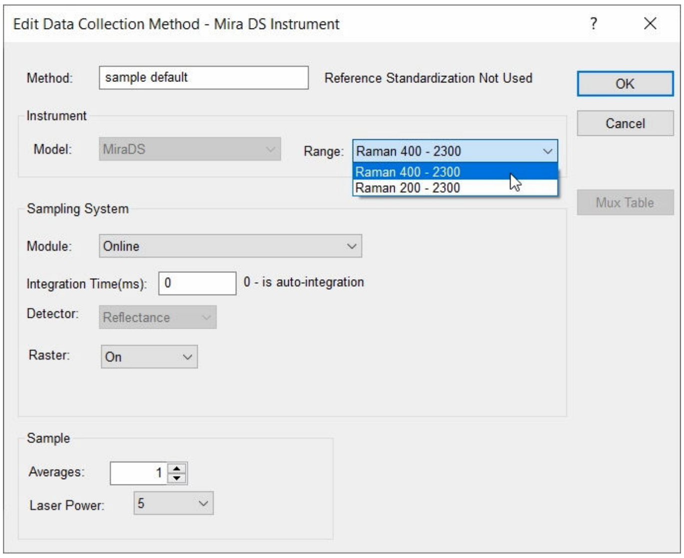
If you choose to Use Existing Data, Vision will open the new Project, without connecting to the instrument.

If you choose to Acquire New Data, Vision will try to connect the instrument.

6 The **Select Data Collection Method** dialog box appears:



The **[Sample default]** is the default DCM method. Click on **[Modify/View]** to select the correct Raman Range based on the type of the instrument from the drop-down down menu:



Edit Data Collection Method - Mira DS Instrument

Method: sample default

Reference Standardization Not Used

Instrument

Model: MiraDS

Range: Raman 400 - 2300

Sampling System

Module: Online

Integration Time(ms): 0

0 - is auto-integration

Detector: Reflectance

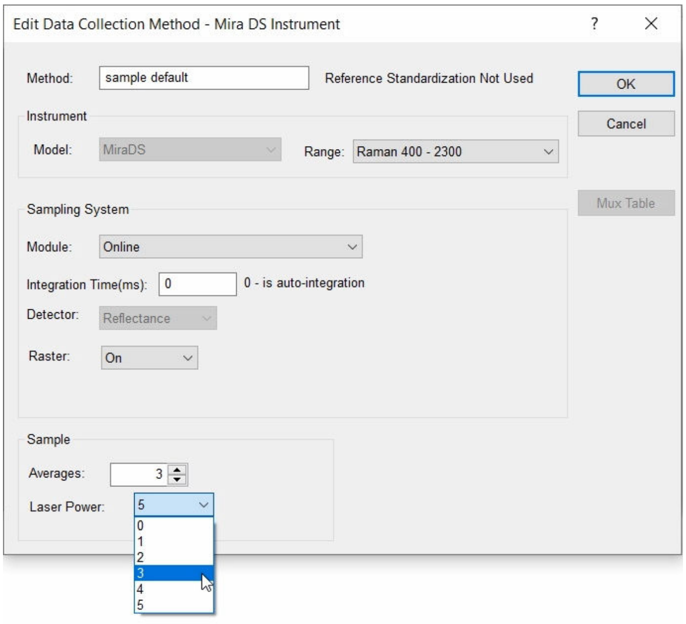
Raster: On

Sample

Averages: 1

Laser Power: 5

At this point, the user can set the integration time in ms or keep the default auto-integration option set at **[0]**, the number of averages per sample measurement, and the Laser Power using the drop-down menu:



Edit Data Collection Method - Mira DS Instrument

Method: sample default

Reference Standardization Not Used

Instrument

Model: MiraDS

Range: Raman 400 - 2300

Sampling System

Module: Online

Integration Time(ms): 0

0 - is auto-integration

Detector: Reflectance

Raster: On

Sample

Averages: 3

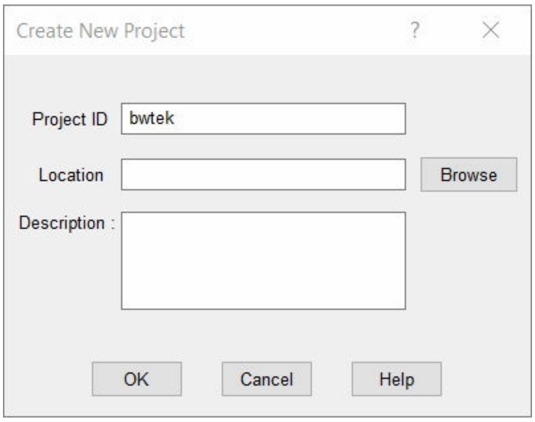
Laser Power: 5

Modify the default name of the DCM, if desired, and click on **[OK]**.

3.15 Communicating with B&W Tek Instruments

To communicate with a B&W Tek series instrument driver, the user should connect the instrument directly at the same computer with a compatible Vision version (versions higher than 4.1.1.156).

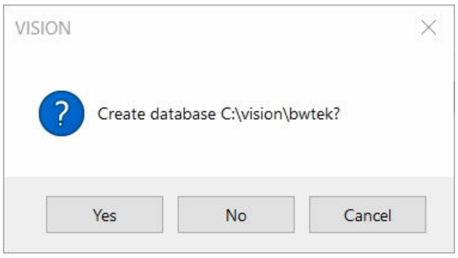
1 Click on **File ▶ Project ▶ New** on the main menu.



Project ID: bwtek

Location:

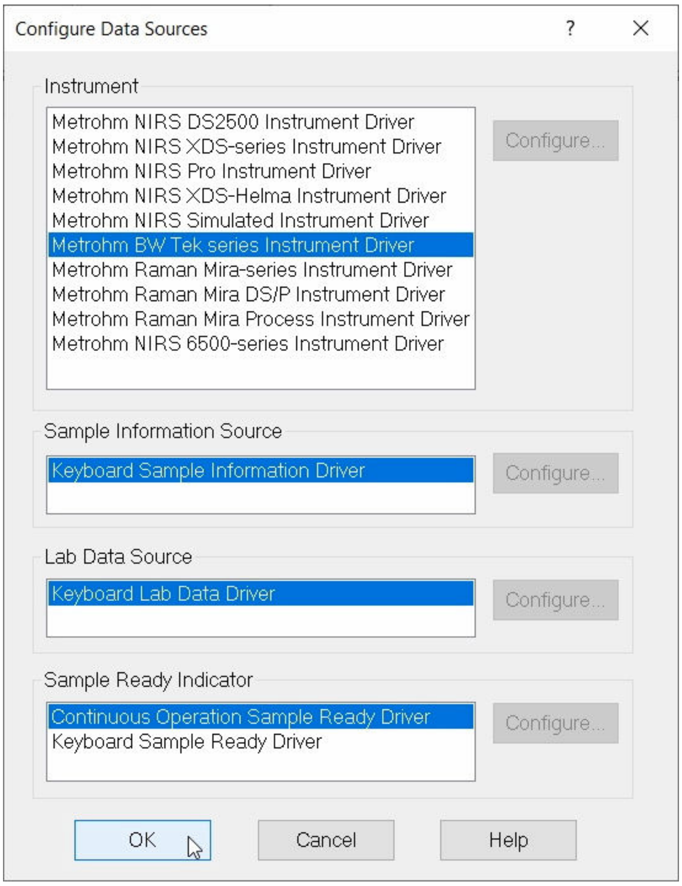
Description :



Create database C:\vision\bwtek?

If an existing Project is currently open, you will be prompted to close it.

2 The Configure Data Sources window displays. Choose the B&W Tek series Instrument Driver as you can see below:



Configure Data Sources

Instrument

- Metrohm NIRS DS2500 Instrument Driver
- Metrohm NIRS XDS-series Instrument Driver
- Metrohm NIRS Pro Instrument Driver
- Metrohm NIRS XDS-Helma Instrument Driver
- Metrohm NIRS Simulated Instrument Driver
- Metrohm BW Tek series Instrument Driver
- Metrohm Raman Mira-series Instrument Driver
- Metrohm Raman Mira DS/P Instrument Driver
- Metrohm Raman Mira Process Instrument Driver
- Metrohm NIRS 6500-series Instrument Driver

Sample Information Source

- Keyboard Sample Information Driver

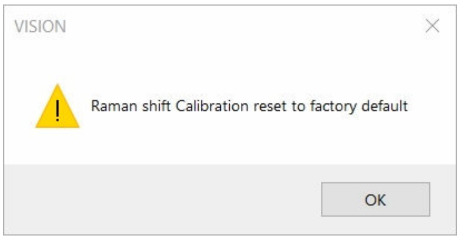
Lab Data Source

- Keyboard Lab Data Driver

Sample Ready Indicator

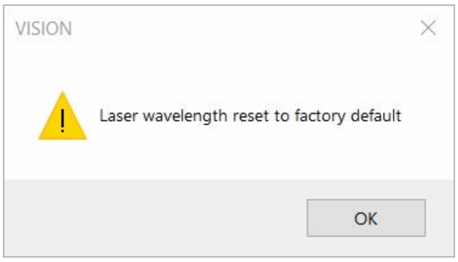
- Continuous Operation Sample Ready Driver
- Keyboard Sample Ready Driver

Vision will prompt the user to click **[OK]** to the information below:



VISION

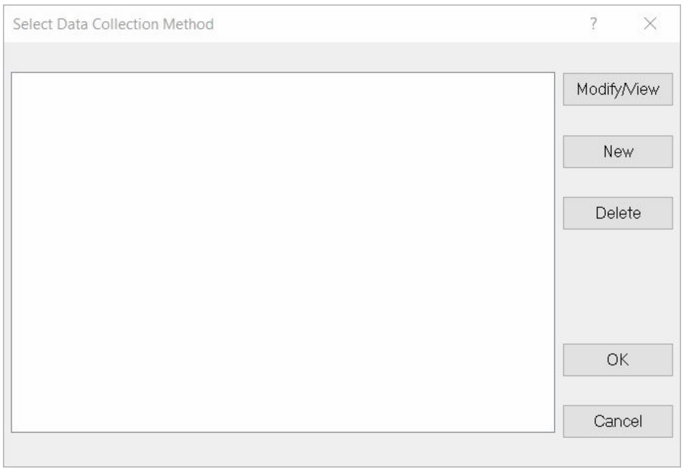
Raman shift Calibration reset to factory default



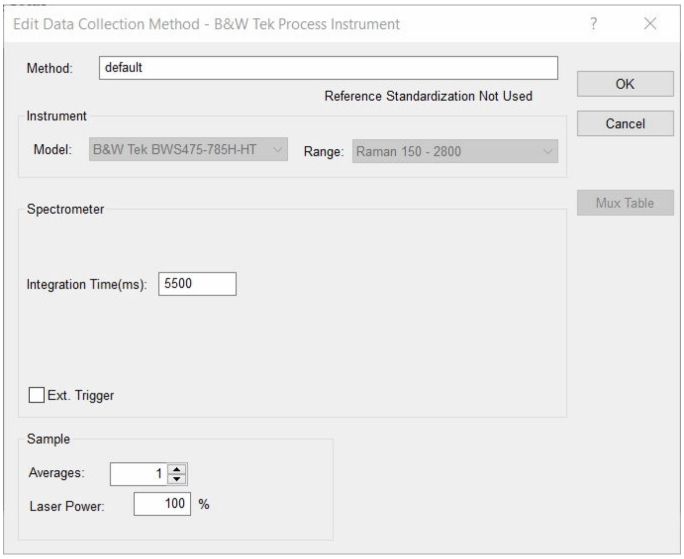
VISION

Laser wavelength reset to factory default

3 The **Select Data Collection Method** dialog box appears:



Click on the **[New]** to create a DCM:



Method: default

Reference Standardization Not Used

Model: B&W Tek BWS475-785H-HT

Range: Raman 150 - 2800

Integration Time(ms): 5500

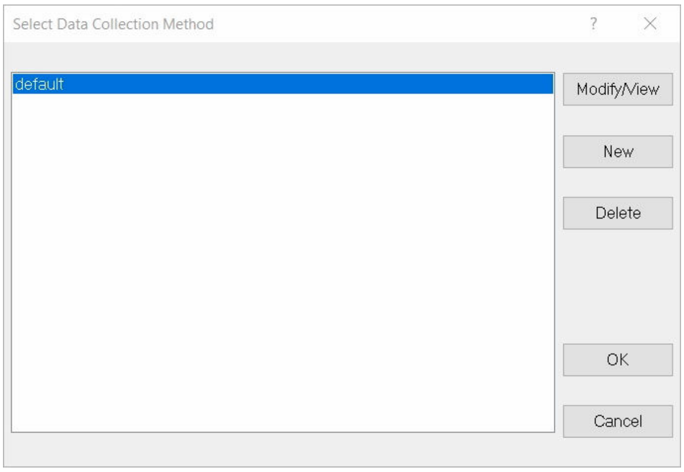
☐ Ext. Trigger

Averages: 1

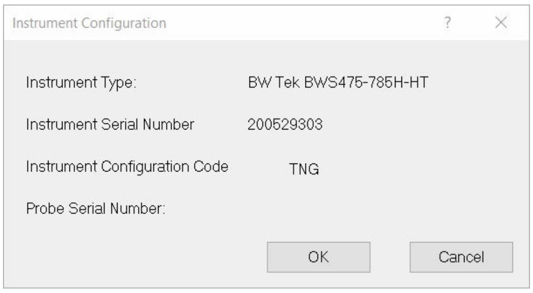
Laser Power: 100 %

The instrument information is displayed automatically. At this point, the user can set the integration time in ms, enable or disable the use of an external trigger to acquire a measurement, use sample averaging or modify the Laser Power, and click on **[OK]**.

4 Select the previously created DCM and click **[OK]**



5 The Instrument Configuration window appears with relevant information. Simply click **[OK]**and continue.


Instrument Configuration

Instrument Type: BW Tek BWS475-785H-HT

Instrument Serial Number 200529303

Instrument Configuration Code TNG

Probe Serial Number:

3.16 Communicating with Metrohm NIRSystems XDS Instruments

To communicate with a Metrohm NIRSystems XDS instrument, the user must have Vision software on a computer capable of supporting it.

3.16.1 Static IP Address (or direct connection)

If the instrument is connected to a network with a standard Ethernet cable and no DHCP Server is available, the user is responsible to make sure the IP address of the computer where Vision resides is compatible with the IP address of the instrument. (169.254.0.2). If not, Metrohm Support can help you to change the IP address within the instrument for compatibility or the user can change the IP address in the computer.

If the instrument is not connected to a network, use a crossover cable to connect between the computer and the instrument and the static IP address will be assigned. This will work most of the time; however, a crossover cable is not the most reliable approach to communication.

3.16.2 Cable Connections

Network Connections – one standard Ethernet cable from the instrument to a network connection, and one standard Ethernet cable from the computer to a network connection.

Direct Connect or Crossover connection – one crossover cable (gray) from computer to instrument.

Hub Connection – one standard Ethernet cable (blue) from the computer to the hub, and one standard Ethernet cable (blue) from the hub to the instrument.

3.16.3 Troubleshooting

If Vision “doesn’t see instrument” it may be caused by incompatible IP Address and/or Subnet Mask.

- Change IP Address as explained later in this section.
- Change the Subnet Mask as explained later in this section. The Subnet Mask is listed in the 4th line of the Notepad entry (ex. Subnet=255.255.255.0).
- If 2 network cards are used (not recommended mode of operation!), and Subnet masks and IP addresses are compatible and you still can’t see the instrument, type in ”XXX.XXX.XXX.XXX, port=2083” in Configure/Input Menu, inside IP Address box in NIRSystems XDS-series Instrument Configuration, and try to connect.

Figure here

3.16.4 Windows or third party firewall configuration

Windows Firewall

1 In Windows, go to **Programs ► Windows Firewall.**

2 Select the **Exception** tab.

3 Click on **[Add Program]**.

4 Select **Vision.exe** or use **[Browse]** to locate the Vision directory followed by the Vision.exe file.

VPN-1

VPN-1 (usually installed on laptops), Citrix through Metrohm, or any other software which provides secure channel communication.

- For VPN-1, older versions, locate the **VPN-1 icon** on the lower tool bar, right click on it and choose the option to Close.

- For VPN-1 newer versions, close it as above and then turn it off by going to **Windows ▶ Network Connections ▶ Properties**. Deselect VPN-1 from the list.
- For Citrix, treat like older version of VPN-1 and right click on the icon located on the bottom toolbar and choose close.
- For other software packages that provide similar secure channel communication you will have to look. There should be a screen similar to the one for Windows Firewall.
- Network cards: Metrohm does not recommend the use of 2 network cards. If multiple communication channels are required, use a hub.

3.16.5 Changing the IP Address

Changing the IP Address of the computer:

1 Use the IPConfig Utility in Windows.

Changing the IP Address of the XDS instrument:

1 Go to **Windows ▶ Accessories ▶ Notepad**.

2 Enter the following exactly as shown:

- [Set IP]
- Do Update=1
- IP=XXX.XXX.XXX.XXX
- Subnet=XXX.XXX.XXX.XXX

Optionally add the line

- Gateway=63.121.141.1

This is usually done by IT people who know if this line is required.

3 Fill in IP address you need to replace XXX. The same for Subnet mask.

4 Save the file as “xds_set_ip.ini” in the Vision directory.

5 Open Vision and go to Status on the tool bar.

6 When the Status dialogue is displayed, click on **[Update]**. A message “The IP address has been changed successfully” will be displayed.

7 Close Vision, recycle power to the instrument and reopen Vision. You are ready to go!

3.17 Communicating with Metrohm DS2500 Solid Analyzer

To communicate with a Metrohm DS2500 Solid Analyzer, the user must have Vision software on a computer capable of supporting it.

3.17.1 Dynamic IP Address

If the instrument is connected to a network using standard Ethernet cable where DHCP server resides, a compatible IP address will be assigned.

Use a standard Ethernet cable.

4 Migration to Vision Air

NOTICE

Warning: In certain cases, the DeTrend pretreatment might deviate between Vision and Vision Air. If you use DeTrend on a small segment, ensure that the model works correctly in Vision Air.

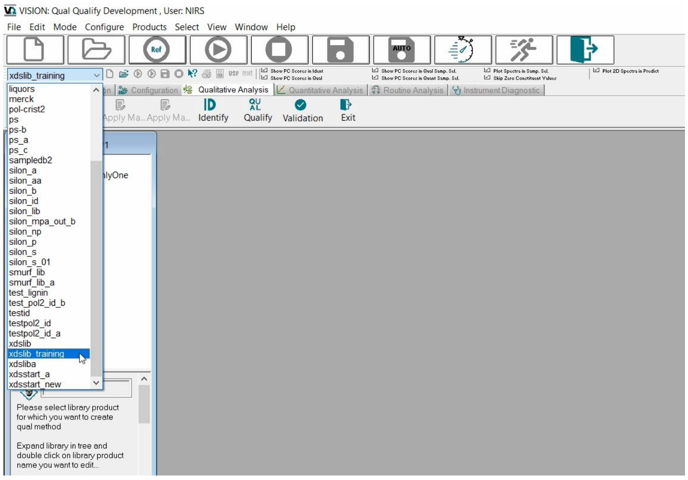
4.1 Export Library Models

1 Open an appropriate Project.

2 Perform the following Menu operations:

Mode ▶ Qualitative Analysis ▶ Qualify Method Development

3 Select a library to work on from the drop down list.

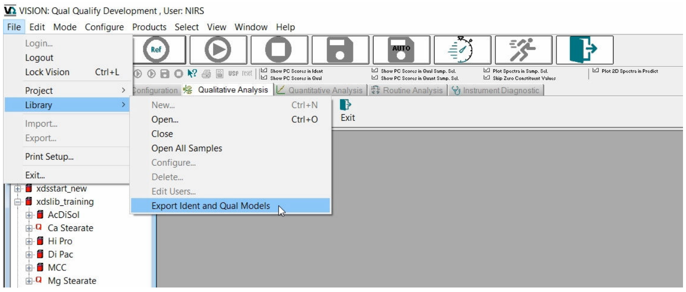


Please select library product for which you want to create qual method

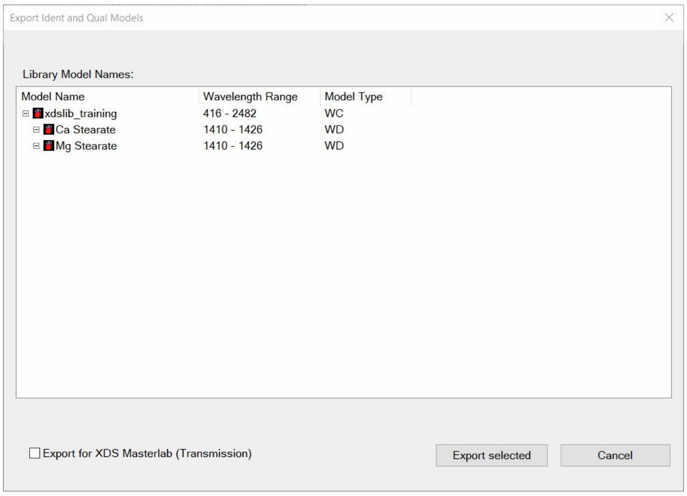
Expand library in tree and double click on library product name you want to edit...

4 Perform the following Menu operations:

File ► Library ► Export Qual and Indent Models



The following dialog is presented which shows the available **Library Model Names** in an expanded treelist format.



Model Name	Wavelength Range	Model Type
⊟ xdslib_training	416 - 2482	WC
⊟ Ca Stearate	1410 - 1426	WD
⊟ Mg Stearate	1410 - 1426	WD

☐ Export for XDS Masterlab (Transmission)

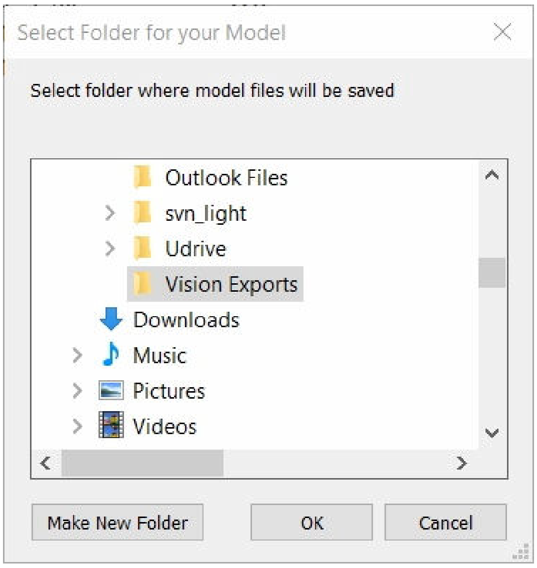
5 Select one or more **Library Model Names** for Export and click on **[Export selected]**.

6 In the following Dialog create a new folder.

NOTICE

Note: Creating a new folder is needed.

7 Rename the new folder and press **[Enter]**.



Select folder where model files will be saved

8 Press **[OK]** to start the Export progress.

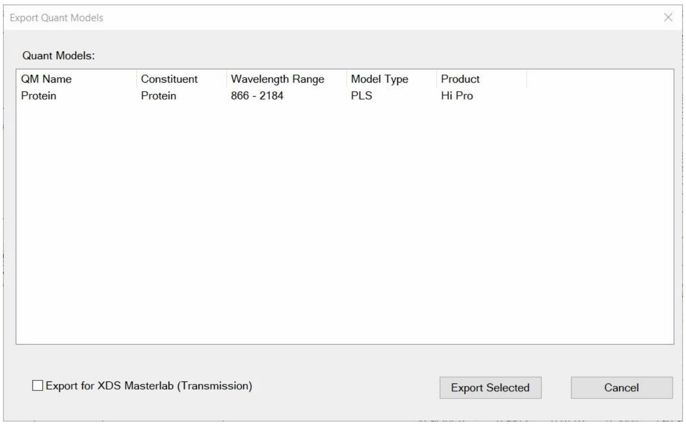
4.2 Export Quant Models

1 Open an appropriate Project.

2 Perform the following Menu operations:

File ▶ Project ▶ Export Quant Models

The following dialog is displayed which shows the **Quant Models** that are available for Exporting:



Quant Models:

QM Name	Constituent	Wavelength Range	Model Type	Product
Protein	Protein	866 - 2184	PLS	Hi Pro

☐ Export for XDS Masterlab (Transmission)

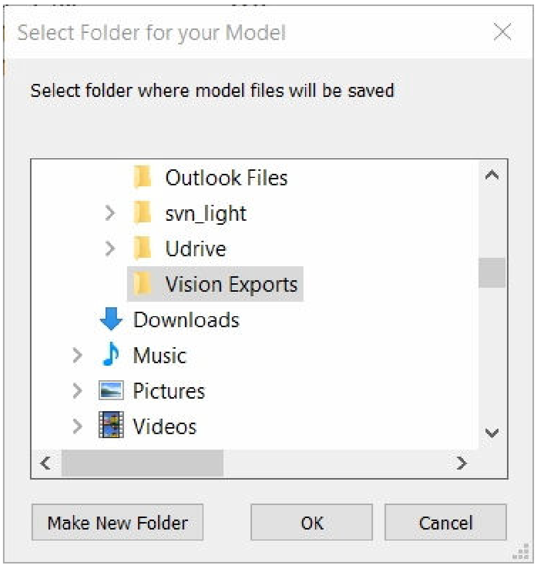
3 Select one or more **Quant Model Names** for Export and press **[Export Selected]**.

4 In the following Dialog create a new folder.

NOTICE

Note: Creating a new folder is needed.

5 Rename the new folder and press **[Enter]**.


Select Folder for your Model

Select folder where model files will be saved

6 Press **[OK]** to start the Export progress.

The option Export for XDS Masterlab (Transmission) is available if one of the following units is used for the calibration.

Table 1 Units for Export for XDS Masterlab

%	#	#-%	µg/L
µm	1000/mL	Absorbance Units	g/L
g/mL	mg/dL	mg/L	mK
mL/100g	mM	mmol/10kg	mmol/L
°Brix	°C	°TH	°SH
Volume-%	Weight-%	"mm	kg/hL
lb/Bu	mm^3	cm^3	mmol/kg
Mcal/lb	Mcal/kg	ppm	ppb
g/lb	mg/lb	meq	mL
mg/100g	mgN/dL	kg	g
lb	rpm	J	mg/g

in	kJ/kg

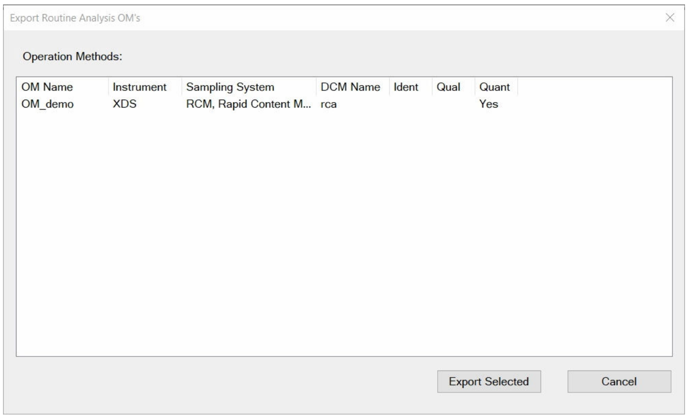
4.3 Export Operation Method

1 Open an appropriate Project.

2 Perform the following Menu operations:

File ▶ Project ▶ Export Operation Method

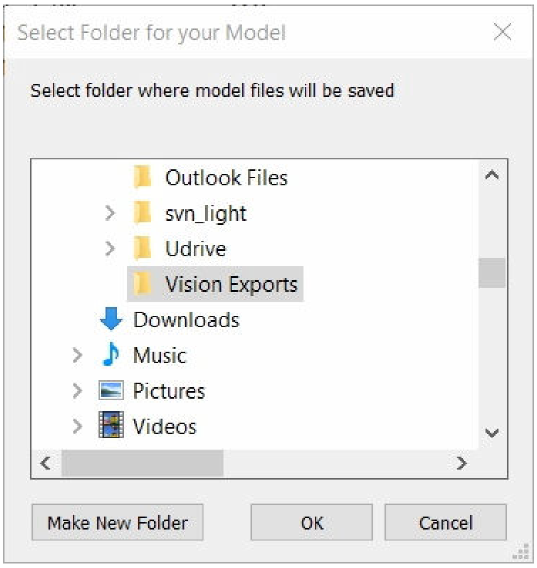
The **Export Routine Analysis OM's** dialog is displayed which shows all **Operation Methods**.



OM Name	Instrument	Sampling System	DCM Name	Ident	Qual	Quant
OM_demo	XDS	RCM, Rapid Content M...	rca			Yes

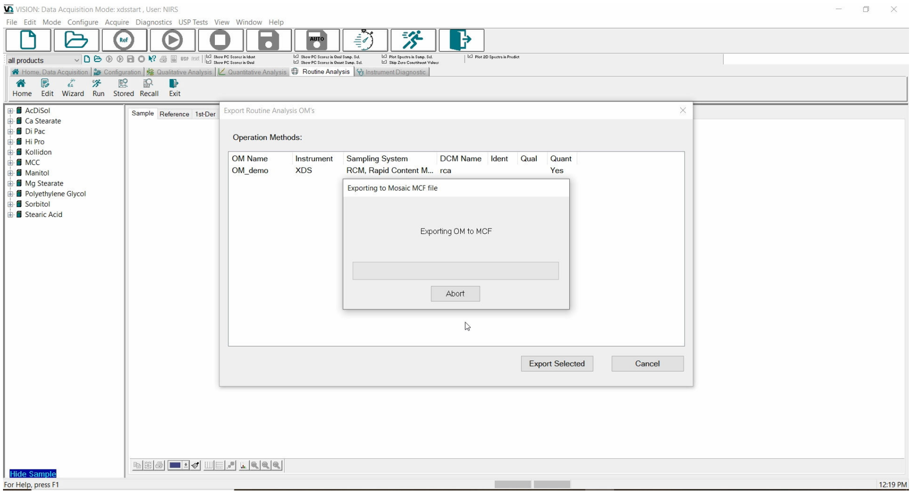
3 Select one or more **Operation Methods** for Export and press **[Export Selected]**.

4 In the following dialog choose a folder for the exported OM file and press **[OK]**.



Select folder where model files will be saved

The **Exporting to Mosaic MCF file** dialog shows the **Export Operation Model** progress.



Export Routine Analysis OM's

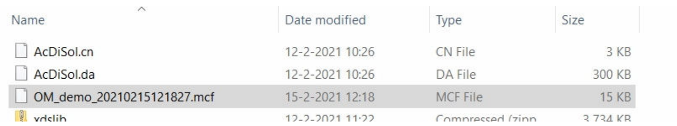
Operation Methods:

OM Name	Instrument	Sampling System	DCM Name	Ident	Qual	Quant
OM_demo	XDS	RCM, Rapid Content M...	rca			Yes

Exporting to Mosaic MCF file

Exporting OM to MCF

This dialog shows the result of the Export.



Name	Date modified	Type	Size
AcDiSol.cn	12-2-2021 10:26	CN File	3 KB
AcDiSol.da	12-2-2021 10:26	DA File	300 KB
OM_demo_20210215121827.mcf	15-2-2021 12:18	MCF File	15 KB
xdslib	12-2-2021 11:22	Compressed (zipp	3 734 KB

4.4 Export Data Collection Method

NOTICE

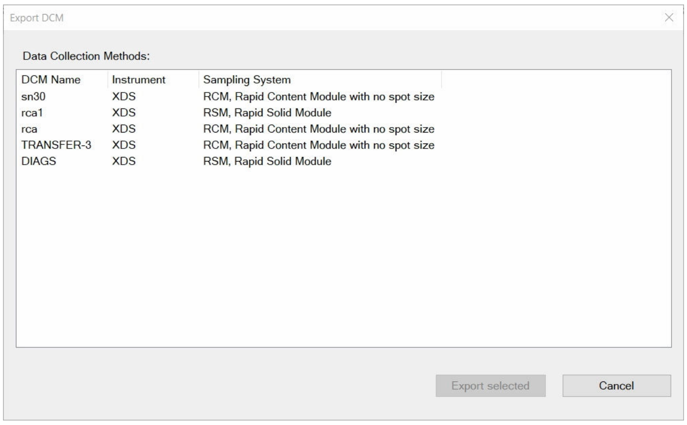
Warning: Keep in mind that the maximum number of subscans differs between Vision and Vision Air. During migration a higher number defined in Vision (1-9999) will automatically be cut to fit Vision Air requirements (1-99).

1 Open an appropriate Project.

2 Perform the following Menu operations:

File ▶ Project ▶ Export DCM

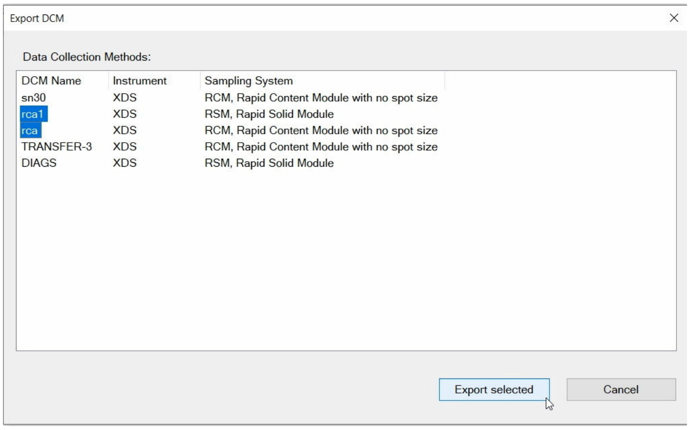
The dialog **Export DCM** is displayed and shows all DCMs.



Data Collection Methods:

DCM Name	Instrument	Sampling System
sn30	XDS	RCM, Rapid Content Module with no spot size
rca1	XDS	RSM, Rapid Solid Module
rca	XDS	RCM, Rapid Content Module with no spot size
TRANSFER-3	XDS	RCM, Rapid Content Module with no spot size
DIAGS	XDS	RSM, Rapid Solid Module

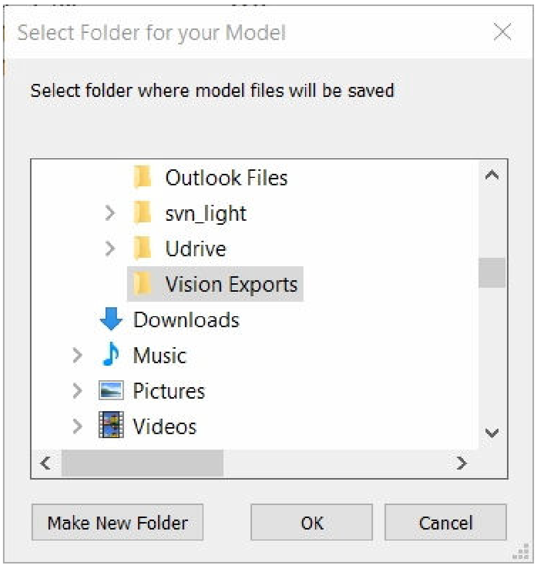
3 Select one or more DCMs for Export and press **[Export Selected]**.



Data Collection Methods:

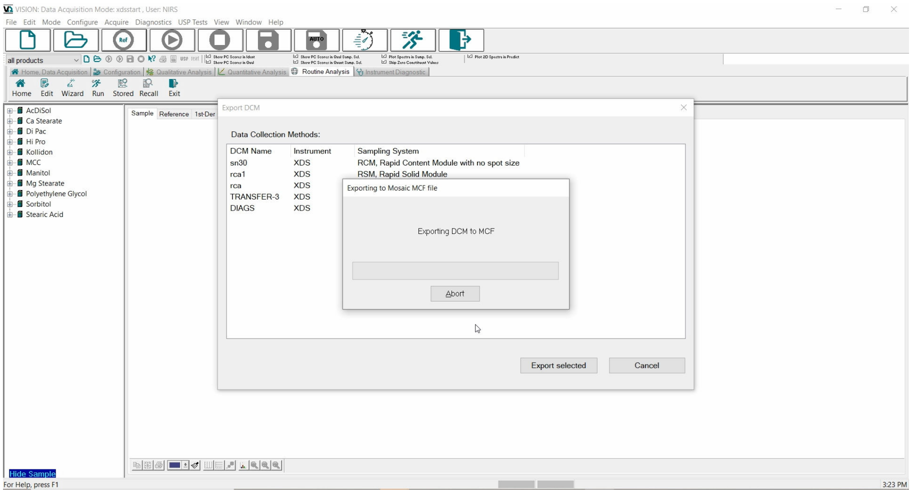
DCM Name	Instrument	Sampling System
sn30	XDS	RCM, Rapid Content Module with no spot size
rca1	XDS	RSM, Rapid Solid Module
rca	XDS	RCM, Rapid Content Module with no spot size
TRANSFER-3	XDS	RCM, Rapid Content Module with no spot size
DIAGS	XDS	RSM, Rapid Solid Module

4 In the following dialog choose a folder for the exported DCM files and press **[OK]**.



Select folder where model files will be saved

The **Exporting to Mosaic MCF file** dialog shows the Export Method progress.



Export DCM

Data Collection Methods:

DCM Name	Instrument	Sampling System
sn30	XDS	RCM, Rapid Content Module with no spot size
rca1	XDS	RSM, Rapid Solid Module
rca	XDS	
TRANSFER-3	XDS	
DIAGS	XDS	

Exporting to Mosaic MCF file

Exporting DCM to MCF

4.5 Versioning of Vision Air Models

If the user exports a model for the first time, it gets version 1.0.0.0 and a unique ID. If the user exports the model again to the same folder, the version number is increased to 2.0.0.0. The ID is maintained. This enables the possibility to upgrade the model when importing it in Vision Air. If the user does not want to upgrade the model, then the user has to remove or rename the old version before exporting the new version.

5 Qualitative Analysis Mode

5.1 Introduction

A library is composed of products, each product being represented by a set of spectra. The two major purposes of the library are to identify and to qualify incoming spectra. In identification, the whole or part of a library is searched to find a library product or products that match an unknown spectrum according to the criteria of the identification method. The list of possible matches (which may contain one or more products) may be passed to a qualification step, where even more rigorous methods confirm the identity of an unknown spectrum and establish its quality.

In Qualitative Analysis mode, the library model is developed and validated. The library model is made up of at least one method, but the fully developed library may include a number of identification methods and a qualification method for each product.

Before sample spectra can be used for method development, they must be processed through the sample selection routine and the results are saved. Only then can a method or a series of methods be developed and validated.

5.2 Sample Selection

The purpose of sample selection is to identify outliers as well as redundant samples. Dragging and dropping samples from the project product to the library product creates a temporary set (denoted by question marks to the left of the sample spectra names). A library product with the temporary set may be created from a single project product, or it can contain spectra from many different products.

Since spectra from various products may not be compatible in terms of spectral ranges or detector used, spectra from the temporary set are filtered prior to sample selection, according to the criteria specified in the Edit Sample Selection Parameters dialog box. Only the spectra fitting these criteria (detector cell type and wavelength range) will be let through sample selection.

Sample selection can be performed on raw spectra. In order to get rid of scattering effects or to emphasize spectral features, one can use any combination and order of available math treatments.

During sample selection, suspected outliers and redundant spectra are identified according to the threshold that the user can modify. Outliers are placed in the rejection set and redundant samples into the acceptance set. Good samples carrying unique spectral information are selected and placed into the training set.

5.2.1 Methods of Sample Selection

3 methods are available: random selection, selection by Principal Component Analysis (PCA), and selection by wavelength distance. Optionally, each of these methods can be followed by manual sample selection.

Random Selection

The Random Selection method selects samples at random for training and acceptance sets.

No rejection set is created when this method is used.

If all product spectra are to be included in the training set choose Random Selection and declare 100% of the spectra to be in the training set. The Math Treatment option is not available when Random Selection is chosen.

Selection by Mahalanobis Distance

Selection by PCA first calculates a principal component model for a product. All samples with Mahalanobis distances from the center of the distribution greater than a user defined threshold (default 3.0) are flagged as outliers. Samples located in high density regions of the population (nearest neighbors) are identified as redundant, so that the Euclidean distances between sample PCA scores in the training set is greater than the threshold (default 0.6).

Selection by Wavelength Distance

Selection by wavelength uses a maximum distance concept (maximum conformity index) to identify outliers. Samples with the maximum distance from the mean product spectrum greater than the threshold (default value 3.0) are placed in the rejection set. Selection of redundant samples uses a method similar to selection by Mahalanobis Distance, except that the Euclidean distance in wavelength space is used.

5.2.2 Sample Selection Procedure

Preparation

1 Enter Sample Selection by choosing **Mode ▶ Qualitative Analysis ▶ Sample Selection** from the main menu. In the left window of the **Sample Selection** screen, project folder(s) are displayed in green and red library folder(s) are displayed in red.

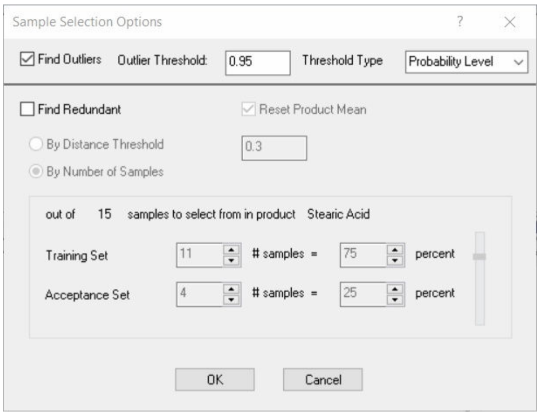
2 Optionally, create a new library by selecting **File ▶ Library ▶ New** from the menu.

5.2.3 Automated Library Development

Vision allows pre-configuring sample selection methods (method's algorithm, outlier and redundant sample detection) and performing sample selection unsupervised on a range of selected products. To perform automated library development:

1 Enter **Qual Sample Selection** mode. Make sure only one library (the one to be developed) is opened.

2 Click on **Configure** and from the proper menu configure outlier and redundant sample selection, select method, and configure its parameters:



☑ Find Outliers Outlier Threshold: 0.95 Threshold Type Probability Level

☐ Find Redundant ☑ Reset Product Mean

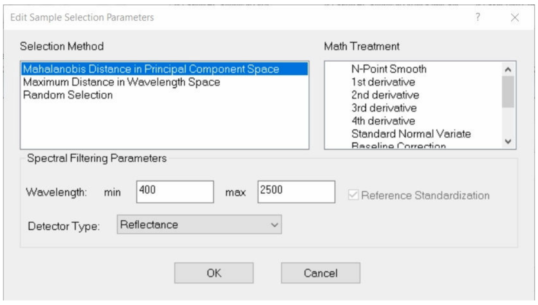
○ By Distance Threshold 0.3

● By Number of Samples

out of 15 samples to select from in product Stearic Acid

Training Set 11 # samples = 75 percent

Acceptance Set 4 # samples = 25 percent



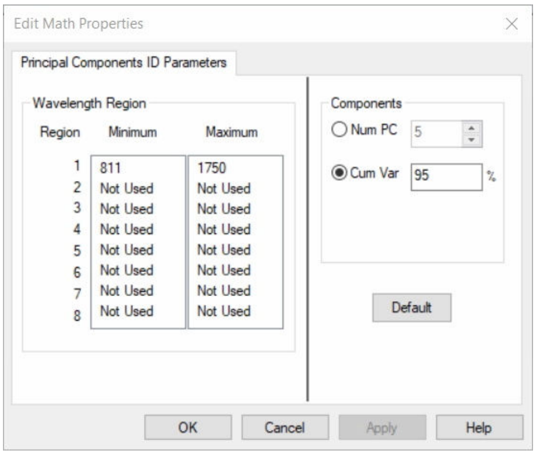
Selection Method
- Mahalanobis Distance in Principal Component Space
- Maximum Distance in Wavelength Space
- Random Selection

Math Treatment
- N-Point Smooth
- 1st derivative
- 2nd derivative
- 3rd derivative
- 4th derivative
- Standard Normal Variate
- Baseline Correction

Wavelength: min 400 max 2500

☑ Reference Standardization

Detector Type: Reflectance



Wavelength Region

Region	Minimum	Maximum
1	811	1750
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

Components

○ Num PC 5

● Cum Var 95 %

3 Select products to be processed from project by clicking on them. You can also Shift+click to select a range of products. Selected products acquire a check mark.

4 Click on **Edit ▶ Add Selected Products To Library** to start.

NOTICE

Note: If a selected product already exists in the library, Vision will skip it.

5.3 Library and Library Project Management

Sample Selection program includes options for library and library products editing and management.

Sorting products

To be able to manage big projects and libraries, both project and library products can be sorted by name, time, or storing order.

1 To sort, right-click on project or library and select **Sort Products** from the menu.

Deleting library products

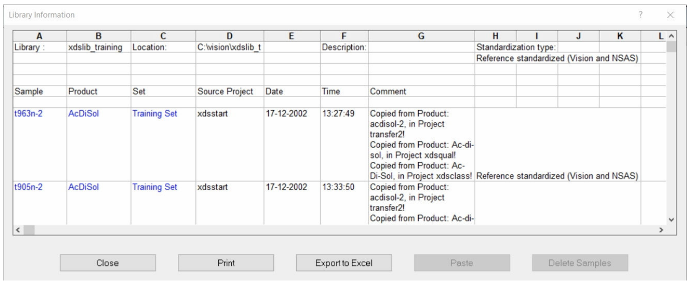
1 To delete a library product, highlight it and choose **Products ▶ Delete** from the main menu.

Deleting a library

1 A library can be deleted only from the **Data Acquisition** mode. Click on **File ▶ Library ▶ Delete**, select a library from the list and click on **[Delete]**.

Displaying library information

1 To display all samples in the library, right-click on the library name and choose Info from the menu that opens:



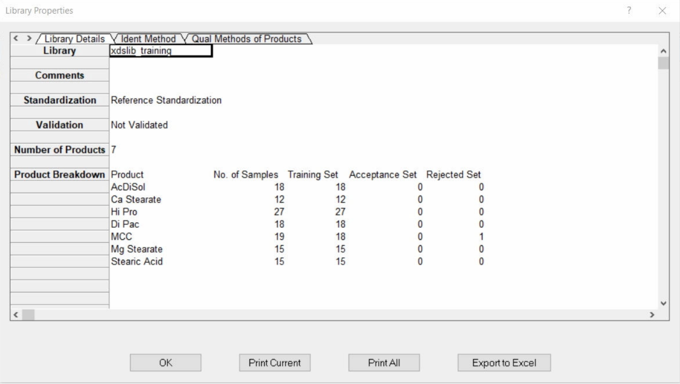
A	B	C	D	E	F	G	H	I	J	K	L
Library :	xdslib_training	Location:	C:\vision\xdslib_t		Description:		Standardization type:				
							Reference standardized (Vision and NSAS)				
Sample	Product	Set	Source Project	Date	Time	Comment					
t963n-2	AcDiSol	Training Set	xdsstart	17-12-2002	13:27:49	Copied from Product: acdisol-2, in Project transfer2! Copied from Product: Ac-di-sol, in Project xdsqual! Copied from Product: Ac-Di-Sol, in Project xdsclass!	Reference standardized (Vision and NSAS)				
t905n-2	AcDiSol	Training Set	xdsstart	17-12-2002	13:33:50	Copied from Product: acdisol-2, in Project transfer2! Copied from Product: Ac-di-					

2 To display all samples in a given product, right-click on the product name and choose Properties from the menu that opens.

Displaying summary of library methods

1 To display the summary of all methods created for a library, right-click on the library name and choose **Properties** from the menu that opens.

The summary window displays information about global ID method, qualification methods for all library products, validation information and status, and library compositions.



Library xdslib_training

Comments

Standardization Reference Standardization

Validation Not Validated

Number of Products 7

Product Breakdown

Product	No. of Samples	Training Set	Acceptance Set	Rejected Set
AcDiSol	18	18	0	0
Ca Stearate	12	12	0	0
Hi Pro	27	27	0	0
Di Pac	18	18	0	0
MCC	19	18	0	1
Mg Stearate	15	15	0	0
Stearic Acid	15	15	0	0

5.4 Identification Method Development

5.4.1 Introduction

Identification is a very important step in qualitative analysis.

A single identification method can be developed. This method is global for the library in the sense that it applies to all the products in the library with a single identification threshold. On the other hand, if a Principal Component based identification method is used (Mahalanobis distance or Residual Variance), a local PC model for each product is calculated.

Since the PC models are local, it is strongly recommended that each library product contain at least 30 sample spectra when identification by Mahalanobis distance or Residual Variance is attempted.

5.4.2 Cross-checking of Library Samples

The identification method development program checks for misidentified samples and conflicting products when the method parameters are calculated. This in fact is a full validation of the method. The results are displayed in the form of a 3D histogram and in numerical format.

5.4.3 Identification Methods and Types of Thresholds

There are 4 identification methods available: **Mahalanobis Distance** in Principal Component space, **Residual Variance** in Principal Component space, **Maximum Distance** in Wavelength space, and **Correlation** in Wavelength space.

For Mahalanobis distance and Residual Variance methods it is possible to calculate the probability that a given spectrum belongs to the distribution represented by the product spectra. Therefore, for those methods, Vision offers 2 kinds of thresholds: match value (the actual number representing distance or residual variance), and the probability level. For the 2 remaining methods, only the match value type of threshold is possible.

Any combination of available math pretreatments can be applied to the spectra with each of the methods.

Mahalanobis Distance in Principal Component Space

In this method, the local Principal Component model is calculated for each product in the library. During the analysis, the unknown spectrum PC scores are calculated for each product model and Mahalanobis distance is calculated. The unknown is identified as a product when the Mahalanobis distance for this product is within the threshold value. The default threshold is 0.6 for match value and 0.84 for probability level.

Residual Variance in Principal Component Space

In this method, the local Principal Component model is calculated for each product in the library. Each product Principal Component model is used to reconstruct the unknown spectrum. The difference between original and reconstructed spectrum is used to calculate the residual variance. The unknown is identified as a product when the residual variance for this product's Principal Component model is within the threshold value. The default threshold is 3 for match value and 0.84 for probability level.

Maximum Distance in Wavelength Space

Maximum distance belongs to the group of wavelength methods. For each product, the training set of spectra is used to calculate the mean product spectrum and the inflated standard deviation spectrum. During the analysis, the unknown spectrum is subtracted from the mean product spectrum and divided by the standard deviation at each wavelength. The unknown is identified as a product when the maximum value is within threshold limits. The default threshold is 3.

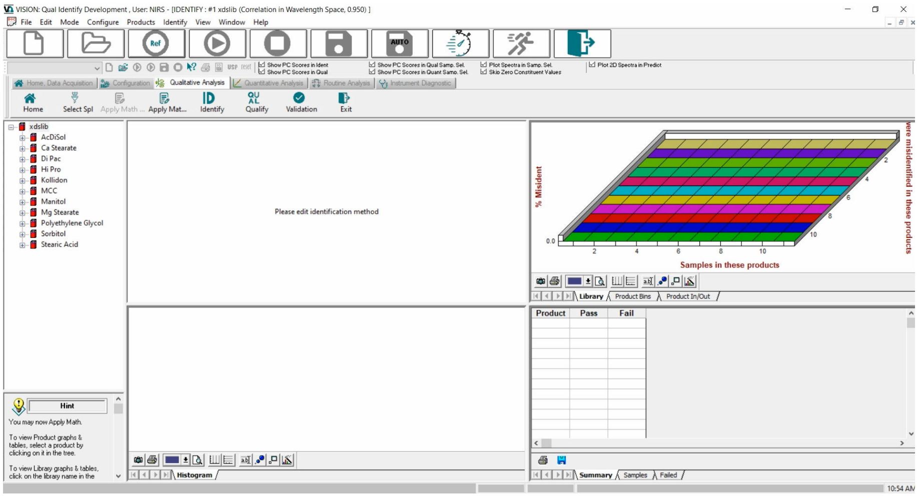
Correlation in Wavelength Space

Wavelength correlation is an example of another wavelength method. During the analysis, the dot product is calculated between the unknown spectrum and the mean spectrum of each library product. The unknown is identified as a product when the value is higher than the threshold. The default value of the threshold is 0.85.

5.4.4 Identification Method Development Procedure

Preparation

1 From the main menu, select **Mode ▶ Qualitative Analysis ▶ Identify Method Development** to enter the **Identification Development** program.



VISION: Qual Identify Development , User: NIRS - [IDENTIFY : #1 xdslib (Correlation in Wavelength Space, 0.950)]

Please edit identification method

Hint

You may now Apply Math.

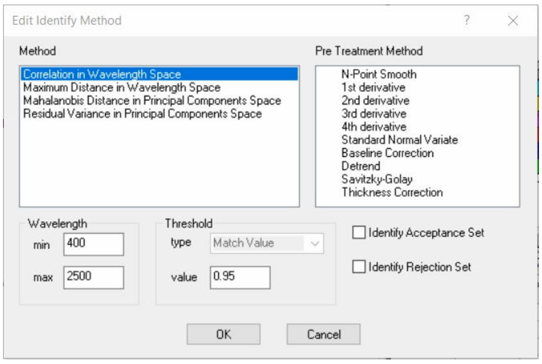
To view Product graphs & tables, select a product by clicking on it in the tree.

To view Library graphs & tables, click on the library name in the

2 Open the **combo** box and double click the library name for which you want to create the method.

Define the identification parameters

1 From the menu select **Identify ▶ Apply Math**.



Edit Identify Method

Method
- Correlation in Wavelength Space
- Maximum Distance in Wavelength Space
- Mahalanobis Distance in Principal Components Space
- Residual Variance in Principal Components Space

Pre Treatment Method
- N-Point Smooth
- 1st derivative
- 2nd derivative
- 3rd derivative
- 4th derivative
- Standard Normal Variate
- Baseline Correction
- Detrend
- Savitzky-Golay
- Thickness Correction

Wavelength
min 400
max 2500

Threshold
type Match Value
value 0.95

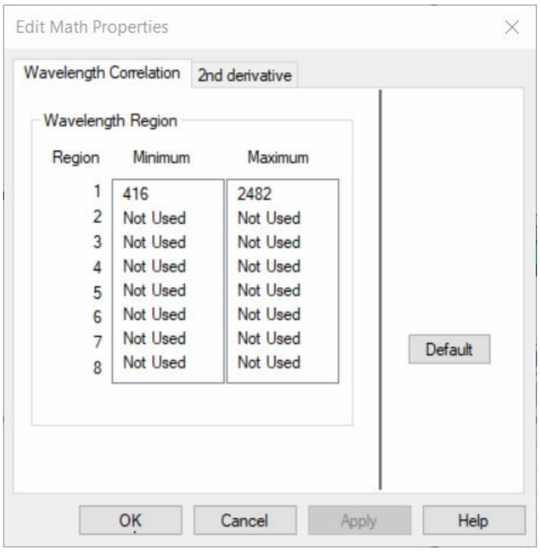
☐ Identify Acceptance Set

☐ Identify Rejection Set

2 In the **Edit Identify Method** dialog box configure the following parameters:

- From the **Identification Method** list choose the method.
- From the **Pretreatment Method** list choose the desired math pretreatment methods. You can choose multiple methods; they will be applied in the order of choice.
- In the **Wavelength** box specify the overall wavelength range.
- In the **Threshold** box declare the preferred type of threshold (match value or probability, when appropriate). Optionally edit the threshold value.
- Check the **Identify Acceptance Set** box if you want Vision to identify samples in the **Acceptance Set**.
- Check the **Identify Rejection Set** box if you want Vision to identify samples from the **Rejection Set**.
- When wavelength maximum distance is chosen as the identification method, the **Library Stabilization** box appears. You can change the default value (0nm) of the stabilization constant to remove false negative results caused by zerocrossovers.

3 Click on **[OK]** when done.



Region	Minimum	Maximum
1	416	2482
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

4 In the **Edit Math Properties** dialog box configure the following parameters:

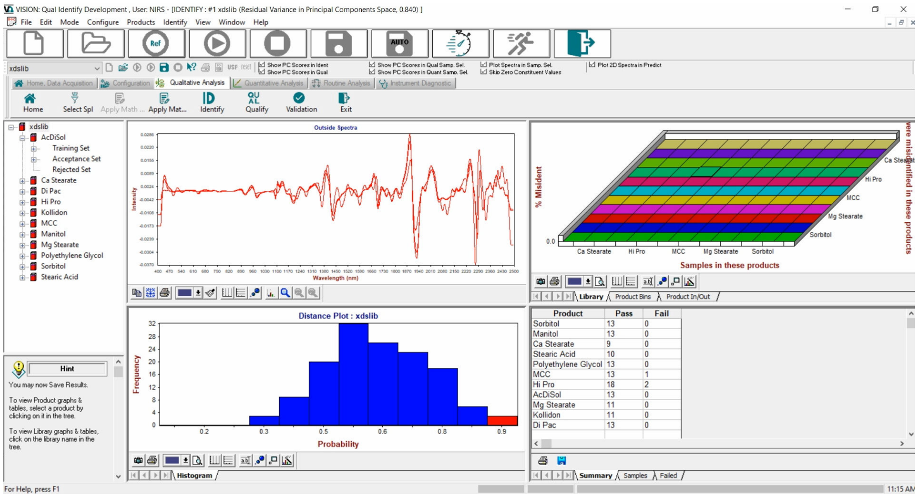
- In the **Wavelength Region** box, declare up to 8 wavelength regions.
- If the **Mahalanobis Distance** or **Residual Variance** method is used, in the **Components** box define how many PCs Vision should use. Specify either the number of PCs or the percent of cumulative variance to calculate this number.
- If **Wavelength Distance** is used, you can declare a **Minimum Variance** value. The calculated standard deviation spectrum will not have values lower than this parameter.

- If a math pretreatment was chosen, you can change defaults by clicking on the proper tab.

5 Click on **[OK]** when done.

Visual Display of Results

The right side of the results screen contains a series of graphs.



VISION: Qual Identify Development , User: NIRS - [IDENTIFY : #1 xdslib (Residual Variance in Principal Components Space, 0.840)]

☑ Show PC Scores in Ident
☑ Show PC Scores in Qual
☑ Show PC Scores in Qual Samp. Sel.
☑ Show PC Scores in Quant Samp. Sel.
☑ Plot Spectra in Samp. Sel.
☑ Skip Zero Constituent Values
☑ Plot 2D Spectra in Predict

Product	Pass	Fail
Sorbitol	13	0
Manitol	13	0
Ca Stearate	9	0
Stearic Acid	10	0
Polyethylene Glycol	13	0
MCC	13	1
Hi Pro	18	2
AcDiSol	13	0
Mg Stearate	11	0
Kollidon	11	0
Di Pac	13	0

Hint

You may now Save Results.

To view Product graphs & tables, select a product by clicking on it in the tree.

To view Library graphs & tables, click on the library name in the tree.

For Help, press F1

The results utilize a uniform color code to denote spectra. The red color designates outsiders, the spectra that failed identification to their own products. The dark blue spectra (insiders) are the spectra that were identified correctly. The left hand side of the screen shows the library tree.

The first graph shows outsiders. If there are no outsiders in the library, it is blank. Initially the display shows the overall library information. In order to obtain the specific information about the given product, click on this product on the library tree.

The second graph contains 3 pages that can be displayed by clicking on the proper tab. The Library screen shows the 3D histogram with bars representing misidentified samples and conflicting products. The Product Bins page shows the percent outsiders in all library products. The Product In/Out page shows individual products, after the product name is clicked on in the library tree.

The third graph is the histogram of the samples distribution. Initially the display shows the overall library information. In order to obtain the specific information about the given product, click on this product on the library tree.

If the maximum distance is the identification method, the third graph includes a page displaying mean product spectra with a standard deviation envelope around them. The number of standard deviations corresponds to that parameter chosen for the identification method.

The fourth graph contains 2 pages that can be displayed by clicking on the proper tab. The Summary page shows the overall library information. The Samples screen shows the details of the method validation. Asterisks below the sample name mean that this sample was identified as more than one product.

The graphs can be easily rescaled by dragging the division lines to the desired position.

Saving the identification method

1 Click on **Identify ▶ Save Results** to save the created identification method in the library.

5.5 Qualification Method Development

5.5.1 Introduction

Qualification is the final step in the analysis. Qualification method helps to confirm the identity of the unknown, and to establish if the quality of the sample fits the method’s criteria.

Each product in the library may have its own qualification method with a different threshold. Methods have to be created separately for each product.

It is strongly recommended that each library product contain at least 30 sample spectra when qualification by Mahalanobis Distance or Residual Variance is attempted.

5.5.2 Qualification Methods and Types of Thresholds

There are 4 qualification methods available: **Mahalanobis Distance** in Principal Component space, **Residual Variance** in Principal Component space, **Maximum Distance** in Wavelength space, and **Correlation** in Wavelength space.

For Mahalanobis Distance and Residual Variance methods it is possible to calculate the probability that a given spectrum belongs to the distribution represented by the product spectra. Therefore, for those methods, Vision offers 2 kinds of thresholds: **match value** (the actual number representing distance or residual variance), and the **probability level**. For the 2 remaining methods, only the match value type of threshold is possible.

Any combination of available math pretreatments can be applied to the spectra with each of the methods.

Mahalanobis Distance in Principal Component Space

In this method, the local Principal Component model is calculated for the product. During the analysis, the unknown spectrum PC scores are calculated from the identified product model and Mahalanobis distance is calculated. The unknown is qualified as the product when the Mahalanobis distance is within the threshold value. The default threshold is 0.5 for match value and 0.95 for probability level.

Residual Variance in Principal Component Space

In this method, the local Principal Component model is calculated for the product. The product's Principal Component model is used to reconstruct the unknown spectrum. The difference between original and reconstructed spectrum is used to calculate the residual variance. The unknown is qualified as the product when the residual variance for the product's Principal Component model is within the threshold value. The default threshold is 2.5 for match value and 0.95 for probability level.

Maximum Distance in Wavelength Space

Maximum Distance belongs to the group of wavelength methods. For each product, the training set of spectra is used to calculate the mean product spectrum and the inflated standard deviation spectrum. During the analysis, the identified spectrum is subtracted from the mean product spectrum and divided by the standard deviation spectrum at each wavelength. The sample is qualified when the maximum value is within threshold limits for the product. The default threshold is 3.

Correlation in Wavelength Space

Wavelength Correlation is an example of another wavelength method. During the analysis, the dot product is calculated between the identified spectrum and the mean spectrum of the library product. The sample is qualified when the value is higher than the threshold for the product. The default value of the threshold is 0.9.

5.5.3 Qualification Method Development Procedure

Preparation

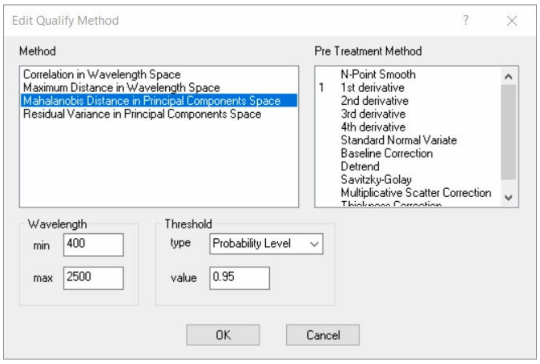
1 From the main menu, select **Mode ▶ Qualitative Analysis ▶ Qualify Method Development** to enter the **Qualification Development** program.

2 Open the **Combo** box and select the library for which you want to create methods.

Define the qualification parameters

1. Expand the library tree by clicking on the plus next to the library name. Double click the product for which you want to develop a qualification method. When selected, the product icon will turn gray.

2. From the menu choose **Select ► Apply Math**.



Edit Qualify Method

Method: Mahalanobis Distance in Principal Components Space

Pre Treatment Method: 1 1st derivative

Wavelength min: 400

Wavelength max: 2500

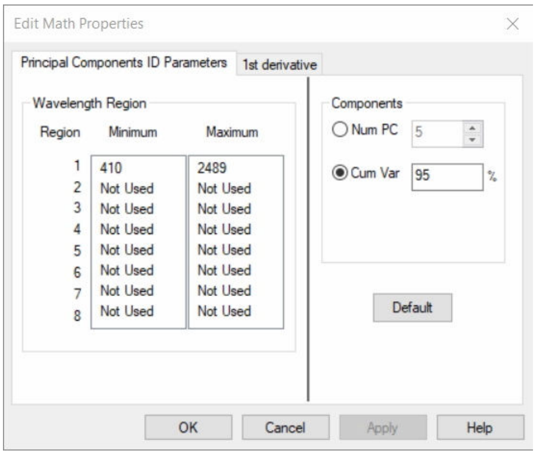
Threshold type: Probability Level

Threshold value: 0.95

In the **Edit Qualify Method** dialog box, configure the following parameters:

- From the **Method** list, choose the method.
- From the **Pretreatment Method** list, choose the desired math pretreatment methods. You can choose multiple methods; they will be applied in the order of choice.
- In the **Wavelength** box, specify the overall wavelength range.
- In the **Threshold** box, declare the preferred type of threshold (match value or probability, when appropriate). Optionally edit the threshold value.
- When wavelength maximum distance is chosen as the qualification method, the **Library Stabilization** box appears. You can change the default value (0nm) of the stabilization constant to remove false negative results caused by zerocrossovers.

3. Click on **[OK]** when done.



Wavelength Region

Region	Minimum	Maximum
1	410	2489
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

Components

○ Num PC 5

● Cum Var 95 %

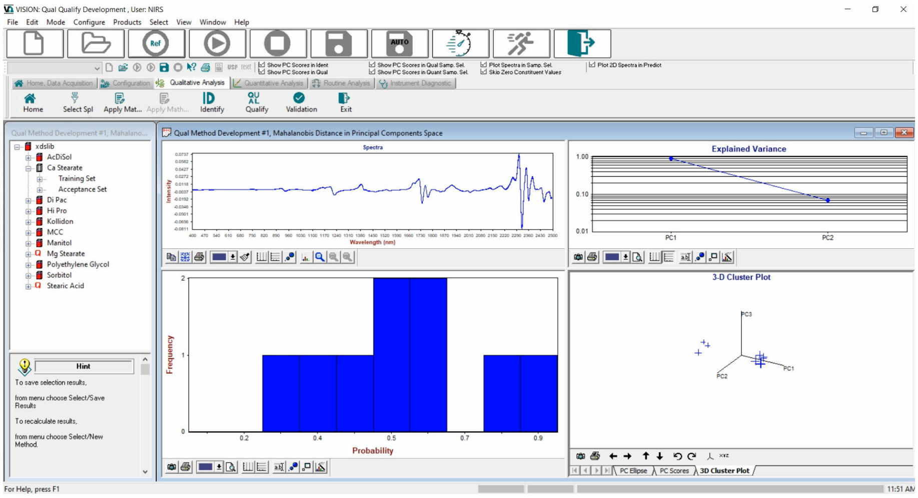
4 In the **Edit Math Properties** dialog box configure the following parameters:

- In the **Wavelength Region** box define up to 8 wavelength regions.
- If the **Mahalanobis** distance or residual variance method is used, in the **Components** box define how many PCs Vision should use. Specify either the number of PCs or the percent of cumulative variance to calculate this number.
- If maximum distance is used, you can declare a **Minimum Variance** value. The calculated standard deviation spectrum will not have values lower than this parameter.
- If a math pretreatment was chosen, you can change defaults by clicking on the proper tab.

5 Click on **[OK]** when done.

Visual Display of Results

The right side of the results screen contains a series of graphs, the number and kind of graph depends on your choice of qualification method.



Hint

To save selection results,

from menu choose Select/Save Results

To recalculate results,

from menu choose Select/New Method.

For Help, press F1

The results utilize a uniform color code to denote spectra. The red color designates spectra that failed qualification to their own products. The dark blue spectra are the spectra that were qualified correctly.

The left hand side of the screen shows the library tree. When the product for which the method has just been created is expanded, the names of spectra are also color coded.

If a **Principal Component** method is used for qualification, you can identify samples on the 3D cluster plot by doubleclicking on the cross representing a sample. A yellow check mark will appear next to the sample name.

Creating a new Qualification method

It is possible to try a new qualification method without losing the result of the previous trial. In order to do it:

1. Click on **Select ▶ New Method**.
2. Click on **Select ▶ Apply Math** and follow the standard procedure.
3. The results of previous qualification methods can be viewed by choosing the proper method screen from the Window submenu.

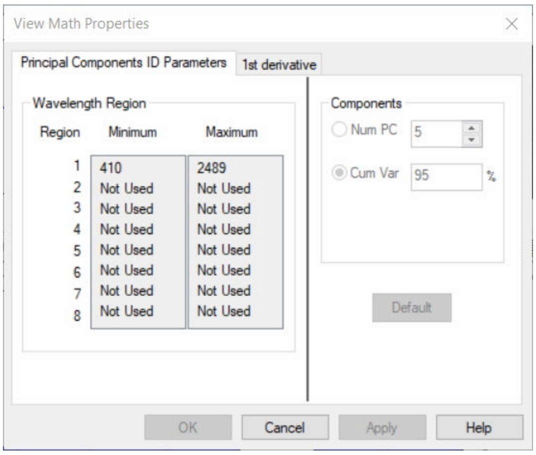
Saving the Qualification method

1. If multiple qualification methods were attempted, make sure that the method you want to save is in the active window. If necessary, switch to the proper method.

2 To save the results in the library, choose **Select ▶ Save Results**. A red "Q" will appear next to the product name to designate that the product has been qualified and saved.

Displaying the method properties

1 Information about math treatment, wavelength ranges, and Principal Component's details can be displayed by selecting a library product and clicking on **Edit ▶ Qual Method** on the main menu.



Region	Minimum	Maximum
1	410	2489
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

○ Num PC 5
● Cum Var 95 %

Displaying summary of library methods

Information about the qualification method choice and threshold can be found in the library summary window.

1 To display it, select a library and click on **Edit ▶ Properties** on the main menu.

5.6 Library Validation

5.6.1 Introduction

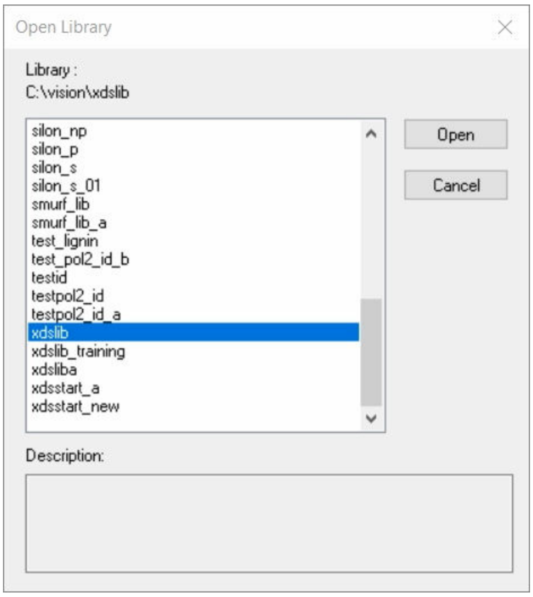
Library validation is an important step in the process of qualitative method development. It evaluates the suitability of a library for use in Routine Analysis. The test determines whether all samples were correctly assigned to their corresponding products, detects conflicting products, and helps to establish correct thresholds. This test is essential in identification and is important for qualification as well.

During the validation process, Vision processes all library spectra. Each spectrum is run through all existing library methods, identification, and qualification. If any of the methods does not exist, Vision will bypass the test and the N/A (not applicable) statement will appear in the proper place on the validation report.

5.6.2 Library Validation Procedure

Preparation

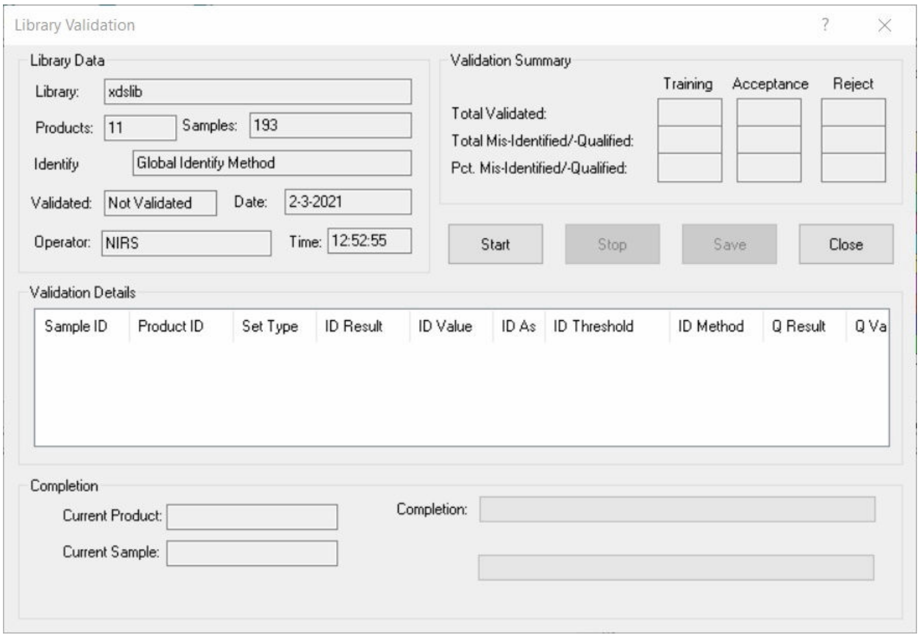
1 From the main menu, select **Mode ▶ Qualitative Library Validation** to enter the library validation program.



2 In the **Open Library** dialog box, highlight the library which you want to validate and click on **[Open]**.

Run Validation

1 Choose **Run Validation** from the Library menu.



Library: xdslib

Products: 11 Samples: 193

Identify: Global Identify Method

Validated: Not Validated Date: 2-3-2021

Operator: NIRS Time: 12:52:55

Total Validated:

Total Mis-Identified/-Qualified:

Pct. Mis-Identified/-Qualified:

Validation Details

Sample ID	Product ID	Set Type	ID Result	ID Value	ID As	ID Threshold	ID Method	Q Result	Q Va

Current Product:

Current Sample:

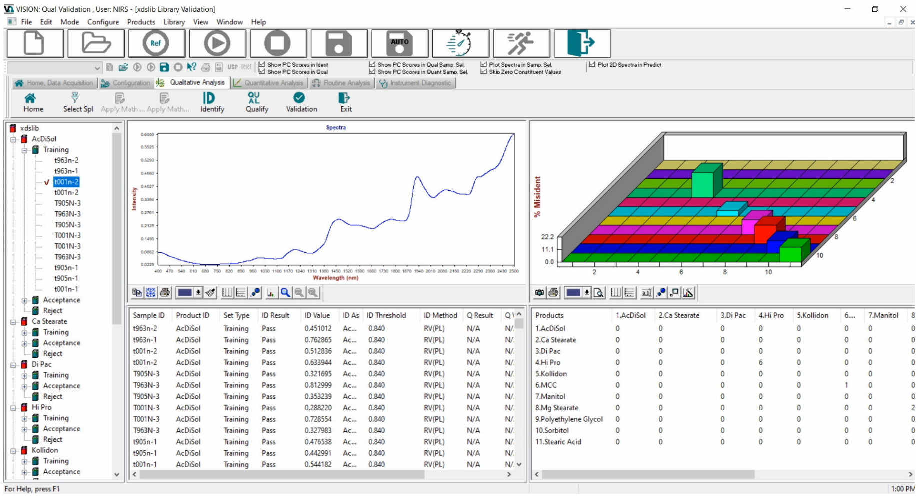
Completion:

2 Click on **[Start]** to begin validation. Progress bars show the status of the validation. After the operation is completed, you can save the results by clicking on **[Save]**.

3 Click on **[Close]** to return to the main validation screen.

Viewing the Results

1 The results screen contains 2 graph displays and 2 result displays.



VISION: Qual Validation , User: NIRS - [xdslib Library Validation]

Sample ID	Product ID	Set Type	ID Result	ID Value	ID As	ID Threshold	ID Method	Q Result	Q V
t963n-2	AcDiSol	Training	Pass	0.451012	Ac...	0.840	RV(PL)	N/A	N/.
t963n-1	AcDiSol	Training	Pass	0.762865	Ac...	0.840	RV(PL)	N/A	N/.
t001n-2	AcDiSol	Training	Pass	0.512836	Ac...	0.840	RV(PL)	N/A	N/.
t001n-2	AcDiSol	Training	Pass	0.633944	Ac...	0.840	RV(PL)	N/A	N/.
T905N-3	AcDiSol	Training	Pass	0.321695	Ac...	0.840	RV(PL)	N/A	N/.
T963N-3	AcDiSol	Training	Pass	0.812999	Ac...	0.840	RV(PL)	N/A	N/.
T905N-3	AcDiSol	Training	Pass	0.353239	Ac...	0.840	RV(PL)	N/A	N/.
T001N-3	AcDiSol	Training	Pass	0.288220	Ac...	0.840	RV(PL)	N/A	N/.
T001N-3	AcDiSol	Training	Pass	0.728554	Ac...	0.840	RV(PL)	N/A	N/.
T963N-3	AcDiSol	Training	Pass	0.327983	Ac...	0.840	RV(PL)	N/A	N/.
t905n-1	AcDiSol	Training	Pass	0.476538	Ac...	0.840	RV(PL)	N/A	N/.
t905n-1	AcDiSol	Training	Pass	0.442991	Ac...	0.840	RV(PL)	N/A	N/.
t001n-1	AcDiSol	Training	Pass	0.544182	Ac...	0.840	RV(PL)	N/A	N/.

Products	1.AcDiSol	2.Ca Stearate	3.Di Pac	4.Hi Pro	5.Kollidon	6....	7.Manitol	8
1.AcDiSol	0	0	0	0	0	0	0	0
2.Ca Stearate	0	0	0	0	0	0	0	0
3.Di Pac	0	0	0	0	0	0	0	0
4.Hi Pro	0	0	0	6	0	0	0	0
5.Kollidon	0	0	0	0	0	0	0	0
6.MCC	0	0	0	0	0	1	0	0
7.Manitol	0	0	0	0	0	0	0	0
8.Mg Stearate	0	0	0	0	0	0	0	2
9.Polyethylene Glycol	0	0	0	0	0	0	0	0
10.Sorbitol	0	0	0	0	0	0	0	0
11.Stearic Acid	0	0	0	0	0	0	0	0

2 The spectral display graph displays a spectrum after it is clicked on the library tree. The 3D bar graph shows the percent of misidentified spectra in each product.

3 The 2 result displays show the validation results at the product and sample level.

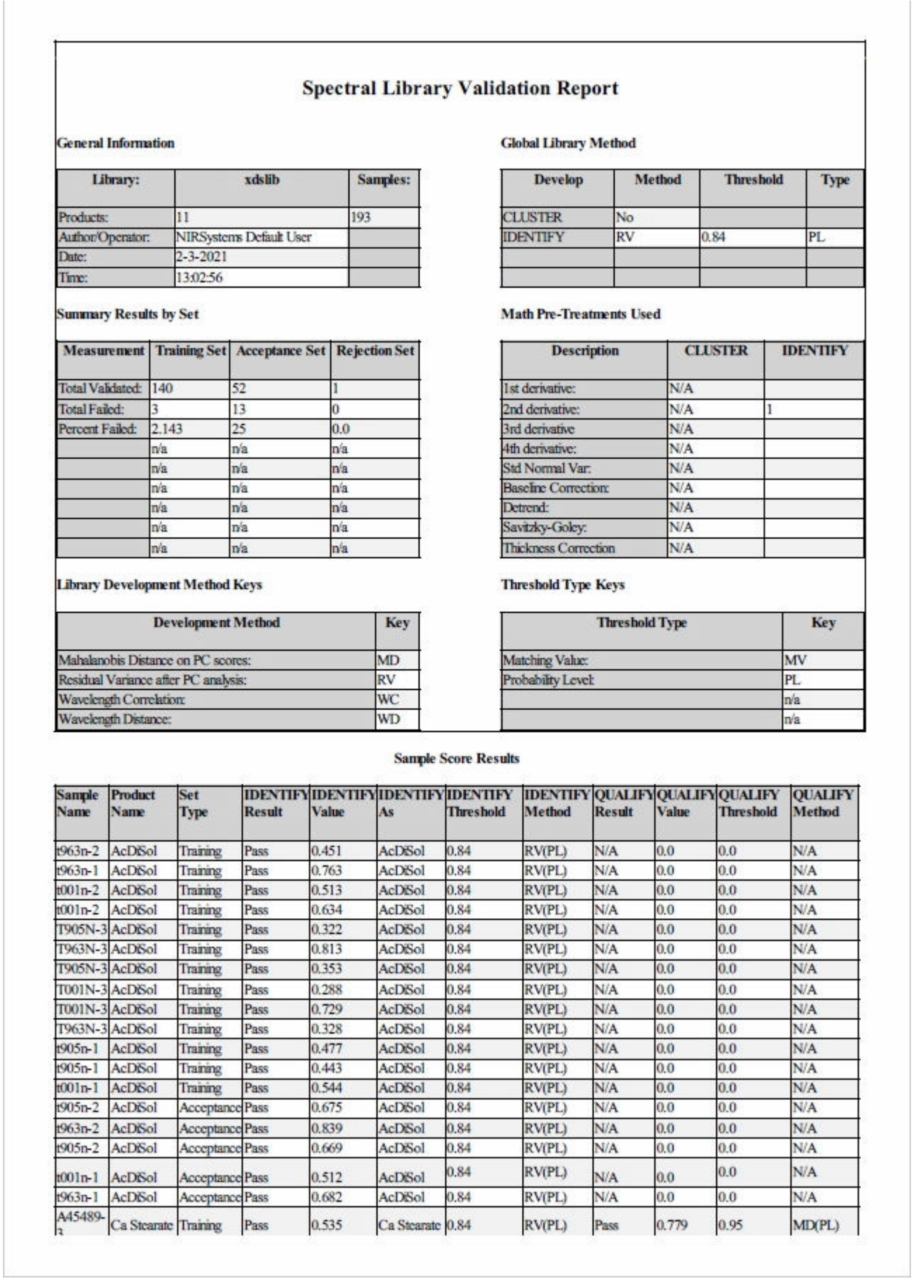
Printing and Saving the Validation Results

1 To print the validation report, choose **Print Report** from the library menu.

2 Click on **Library ▶ Save Results** to save the validation report. Type in optional comments and click on **[OK]**.

5.6.3 Library Validation Report Viewer

The viewer opens the validation report in a separate window, and allows users to save the report as Excel Report, HTML Report or PDF Report. To save a report with more than 30,000 samples, the user can choose between HTML Report and PDF Report. To open the viewer click on **Library ▶ View Report** after the validation is completed.



Spectral Library Validation Report

General Information

Library:	xdslib	Samples:
Products:	11	193
Author/Operator:	NIRSystems Default User	
Date:	2-3-2021	
Time:	13:02:56	

Global Library Method

Develop	Method	Threshold	Type
CLUSTER	No		
IDENTIFY	RV	0.84	PL

Summary Results by Set

Measurement	Training Set	Acceptance Set	Rejection Set
Total Validated:	140	52	1
Total Failed:	3	13	0
Percent Failed:	2.143	25	0.0
	n/a	n/a	n/a
	n/a	n/a	n/a
	n/a	n/a	n/a
	n/a	n/a	n/a
	n/a	n/a	n/a
	n/a	n/a	n/a

Math Pre-Treatments Used

Description	CLUSTER	IDENTIFY
1st derivative:	N/A	
2nd derivative:	N/A	1
3rd derivative	N/A	
4th derivative:	N/A	
Std Normal Var:	N/A	
Baseline Correction:	N/A	
Detrend:	N/A	
Savitzky-Goley:	N/A	
Thickness Correction	N/A	

Library Development Method Keys

Development Method	Key
Mahalanobis Distance on PC scores:	MD
Residual Variance after PC analysis:	RV
Wavelength Correlation:	WC
Wavelength Distance:	WD

Threshold Type Keys

Threshold Type	Key
Matching Value:	MV
Probability Level:	PL
	n/a
	n/a

Sample Score Results

Sample Name	Product Name	Set Type	IDENTIFY Result	IDENTIFY Value	IDENTIFY As	IDENTIFY Threshold	IDENTIFY Method	QUALIFY Result	QUALIFY Value	QUALIFY Threshold	QUALIFY Method
t963n-2	AcDiSol	Training	Pass	0.451	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t963n-1	AcDiSol	Training	Pass	0.763	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t001n-2	AcDiSol	Training	Pass	0.513	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t001n-2	AcDiSol	Training	Pass	0.634	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T905N-3	AcDiSol	Training	Pass	0.322	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T963N-3	AcDiSol	Training	Pass	0.813	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T905N-3	AcDiSol	Training	Pass	0.353	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T001N-3	AcDiSol	Training	Pass	0.288	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T001N-3	AcDiSol	Training	Pass	0.729	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
T963N-3	AcDiSol	Training	Pass	0.328	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t905n-1	AcDiSol	Training	Pass	0.477	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t905n-1	AcDiSol	Training	Pass	0.443	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t001n-1	AcDiSol	Training	Pass	0.544	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t905n-2	AcDiSol	Acceptance	Pass	0.675	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t963n-2	AcDiSol	Acceptance	Pass	0.839	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t905n-2	AcDiSol	Acceptance	Pass	0.669	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t001n-1	AcDiSol	Acceptance	Pass	0.512	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
t963n-1	AcDiSol	Acceptance	Pass	0.682	AcDiSol	0.84	RV(PL)	N/A	0.0	0.0	N/A
A45489-3	Ca Stearate	Training	Pass	0.535	Ca Stearate	0.84	RV(PL)	Pass	0.779	0.95	MD(PL)

5.6.4 The Library Validation Report

The library validation report contains a lot of information. This section will describe the report layout and its information content in detail.

The first page of the validation report contains the general library information, like the library name, number of products and spectra, operator ID, time of validation, library methods and pretreatments used.

Following this information is a table which details how each spectrum was analyzed by the library methods. The table is made up of 12 columns. The columns contain the following information:

1. Sample name.
2. Name of the product the sample belongs to.
3. Type of set (training, acceptance, or rejection).
4. Identification result (pass or fail).
5. Identification value (correlation, maximum distance, Mahalanobis distance, or residual value).
6. Product to which a spectrum was identified as (based on the closest match).
7. Identification method threshold.
8. Identification method symbol and the threshold type symbol (symbols are explained in the report header).
9. Qualification result (pass or fail).
10. Qualification values (correlation, maximum distance, Mahalanobis distance, or residual value).
11. Qualification method threshold.
12. Qualification method symbol and the threshold type symbol. The following symbols are used:
    a. WD - maximum wavelength distance
    b. WC - wavelength correlation
    c. MD - Mahalanobis distance
    d. RV - Residual Variance
    e. PL - probability level
    f. MV - match value

Each sample is passed through the following sequence: clustering, identification, and qualification. If a given stage of this sequence does not have a method created, Vision bypasses this step (N/A appears on the report). If a sample fails at any stage, the consecutive steps are not executed (N/A appears on the report).

The nomenclature used in the validation is complicated and needs closer description:

1. Samples that did not pass clustering method show FAIL CLUSTERING result.
2. Sample that can be uniquely identified and/or qualified, show PASS in the result column.
3. Samples that cannot be identified and/or qualified to the proper product show FAIL result.
4. Multiple lines with asterisks designate an ambiguous sample, i.e., a sample that was identified to more than one product. In this case Vision will try to qualify the sample using qual methods of all identified products. If the sample qualifies as the correct product, it is flagged as PASS. If the library does not have qualification methods, or is qualified to more than one product, the sample remains flagged as AMBIGUOUS.
5. MISMATCH means that the sample was identified or qualified to a wrong product.

6. NO MATCH means that the sample was not identified or qualified to any product in the library.

6 Quantitative Analysis Mode

6.1 Introduction

Quantitative Analysis mode is the part of Vision where calibration equations are developed and tested. The created calibration equations can be used in Routine Analysis to predict unknown sample composition in real time.

In order to develop a calibration equation, a set of spectra with corresponding constituent data from reference analysis is needed. These data have to be processed through the sample selection program to detect outliers and redundant samples (in some cases the sample selection can be performed before the reference analysis, as described in the sample selection part.)

Once the calibration set of spectra has been selected, it is used to develop a calibration equation. The calibration equation relates spectral and constituent data, and can be developed using various methods.

It is also possible to import calibration equations saved in the NSAS format. This can be done in the Sample Selection program.

6.2 Sample Selection

6.2.1 Types of Sample Selection

Vision offers 2 basic types of quantitative sample selection. The first type is based on spectral data only and allows to detect spectral outliers and redundant samples. The second type looks at the constituent data and allows to manipulate the data set to obtain optimum boxcar distribution. Those methods can be used independently and their results saved and passed to the regression program.

The purpose of sample selection in quantitative analysis is somehow different from the qualitative approach. In qualitative analysis sample selection is a way to detect outliers and redundant samples from spectral data only.

In quantitative analysis, the situation is more complicated. Sample selection should be able to detect spectral outliers, indicate a possible typing error in constituent values, and make it possible to inspect and correct the distribution of constituent values for a product. Since the reference analysis is expensive and time consuming, another purpose of quantitative sample selection is to pick from many collected sample spectra the optimal subset. This subset is then analyzed and used to develop the calibration equation.

Vision fulfills all these requirements by an optional twostep sample selection. In the first step, the initial set of spectra (without constituent values) undergoes the sample selection based on spectral information. Once the spectral outliers and redundant samples have been detected and set aside in validation and outlier sets, the spectra forming the calibration set are analyzed. At the second step of sample selection, some spectra can be removed from the calibration set to improve the distribution.

Additional possibility of outlier detection exists in the regression program. During regression possible outliers can be removed from the training set without having to return to the sample selection stage.

6.2.2 Spectral Data Sample Selection Methods

3 methods are available for sample selection based on spectral information: random selection, selection by PCA, and selection by wavelength distance.

Random Selection

The Random Selection method selects samples at random for calibration and validation sets. No outlier set is created when this method is used.

The Math Treatment option is not available when Random Selection is chosen.

Selection by Mahalanobis Distance

Selection by PCA first calculates a principal component model for a product. All samples with Mahalanobis distances from the center of the distribution greater than a user defined threshold (default 0.6 for match value or 0.95 for probability) are flagged as outliers. Samples located in high density regions of the population (nearest neighbors) are identified as redundant, so that the Euclidean distances between samples in the training set is greater than the threshold.

Selection by Wavelength Distance

Selection by wavelength distance uses a maximum distance concept (maximum conformity index) to identify outliers. Samples with the maximum distance from the mean product spectrum greater than the threshold (default value 3.0) are placed in the outlier set. Selection of redundant samples uses a method similar to selection by PCA, except that the Euclidean distance in the wavelength space is used.

Lab Data Sample Selection Method

This sample selection method is based on the results from the reference analysis. The program displays the histogram of the reference values distribution, and allows user to correct this distribution by moving samples between calibration, validation, and outlier sets. Also, the errors from entering incorrect concentration values can be corrected.

Combined Sample Selection Method

In this method, the user can create a temporary set of samples without knowing the corresponding reference values. The temporary set is processed by spectral sample selection, and the calibration, validation, and outlier sets are saved. The samples belonging to the calibration set are then analyzed.

The saved set undergoes the Lab Data Direct Sample Selection. This sample selection method does not start from the temporary set, but uses the previously saved sets. The reference values are entered into Vision, and the sample distribution corrected as necessary.

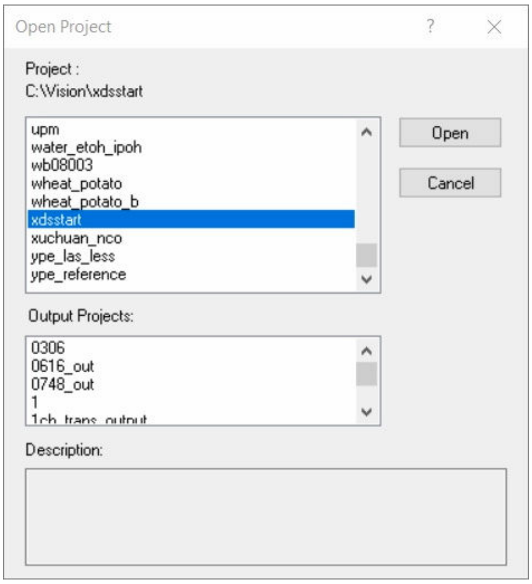
This type of sample selection is useful when dealing with large sample set, and/or limited access to the reference analysis.

6.2.3 Sample Selection Procedure

Preparation

1 Enter Sample Selection by choosing **Mode ▶ Quantitative Analysis ▶ Sample Selection** from the main menu. The last active project is opened and displayed in the left window of the **Sample Selection** screen.

2 If you want to work with a different project, click on **File ▶ Project ▶ Open** from the main menu (make sure that the left window is in focus).



Project :
C:\Vision\xdsstart

upm
water_etoh_ipoh
wb08003
wheat_potato
wheat_potato_b
xdsstart
xuchuan_nco
ype_las_less
ype_reference

Output Projects:

0306
0616_out
0748_out
1
1ch_trans_output

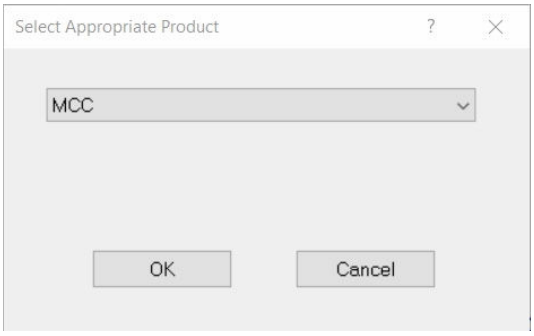
Description:

The **Open Project** window opens.

3 You can preview spectra from a product by expending the product and selecting spectra for display. To view a sample spectrum, click on the sample name. Click on the sample again to deselect it. You can display multiple samples from various products by simply clicking on them in turn. To display a range of sample spectra from a product, click on the first spectrum in the range, and then holding down the Shift key click on the last spectrum. To clear the spectral display, click on **Edit ► Unselect All**.

Creating Equations and Temporary Sets

1 Select product from the project folder by clicking on **Select ► Select Product** from the menu and choosing the product from the dropdown list.



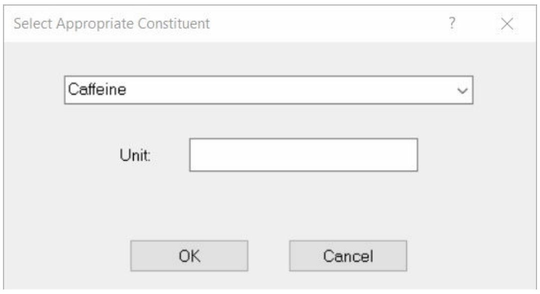
The selected product icon turns gray.

2 You can also select a product by double-clicking it, selecting it from the combo box, or right-clicking on it.

3 Drag and drop the chosen product spectra to the **Equation icon**.

4 You can drag and drop the whole product or selected spectra. You can also select spectra, click on **Edit ► Copy**, highlight the **Calibration Equation** field, and click on **Edit ► Paste**.

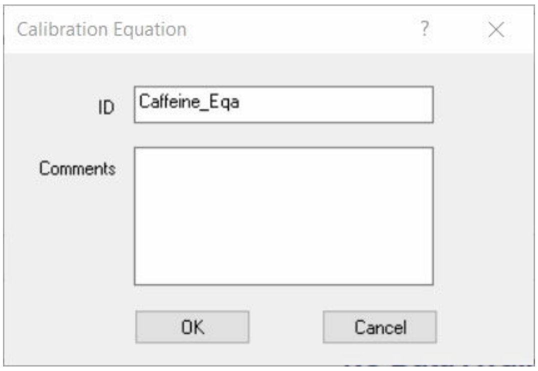
5 When the product is dragged to the equation, you will be prompted to select the constituent:



Caffeine

Unit:

and the equation name:

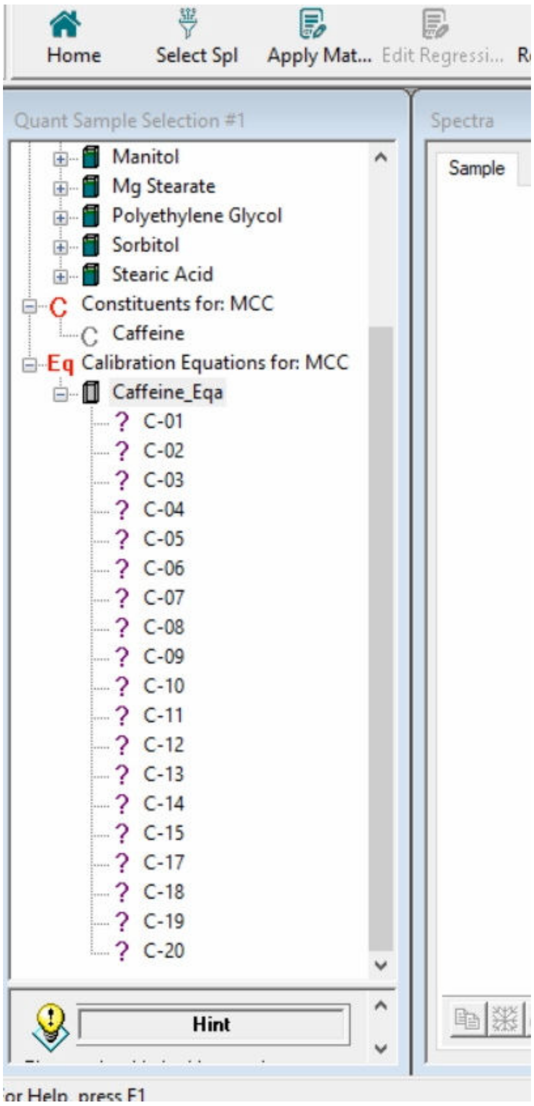


ID Caffeine_Eqa

Comments

The default equation name is the name of the constituent.

6 Question marks next to the sample names in newly created equation indicate that the samples form the temporary set:



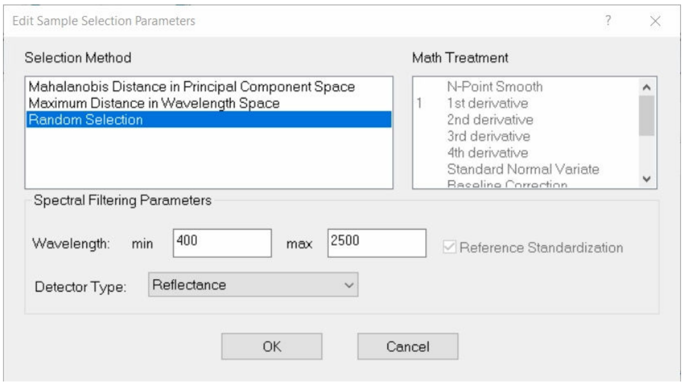
Dragging spectra to the saved equation will destroy its structure and place all existing product spectra together with new spectra back in the temporary set. When this is done by mistake, it can be reversed by exiting the Sample Selection program and re-entering it.

You can create a new constituent by entering a new name in the **Select Constituent** box. The initial constituent values will be all zeroes.

Performing Spectral Data Type of Sample Selection

1 Click on the equation containing the temporary set.

2 Choose **Select** ▶ **Apply Math** to start sample selection.


Edit Sample Selection Parameters

Selection Method

Mahalanobis Distance in Principal Component Space
Maximum Distance in Wavelength Space
Random Selection

Math Treatment

N-Point Smooth
1 1st derivative
2nd derivative
3rd derivative
4th derivative
Standard Normal Variate
Baseline Correction

Spectral Filtering Parameters

Wavelength: min 400 max 2500

☑ Reference Standardization

Detector Type: Reflectance

3 From the upper part of the **Edit Sample Selection Parameters** dialog box choose the selection method and math treatment.

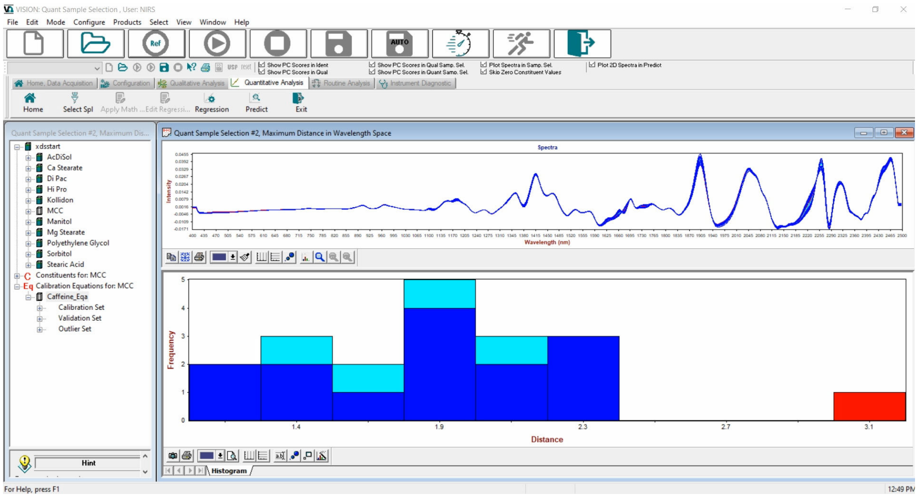
4 From the lower part of the **Edit Sample Selection Parameters** dialog box choose the filter options. Only the spectra fitting these criteria (detector cell type and wavelength range) will be let through sample selection. Click on **[OK]**.

5 If **Random Selection** method was chosen, define the distribution of spectra between sets and click **[OK]**. Continue with step 8.

6 If selection by **PCA** or **Wavelength** was chosen, from the **Edit Math Properties** box choose appropriate parameters for the selection method and math treatment, then click **[OK]**.

7 In the **Sample Selection Options** dialog box optionally check the **Redundant** and **Outliers** boxes, configure the appropriate parameters of outlier and redundant sample detection, and click **[OK]**.

8 The **Sample Selection** algorithm will proceed with calculations and display results.



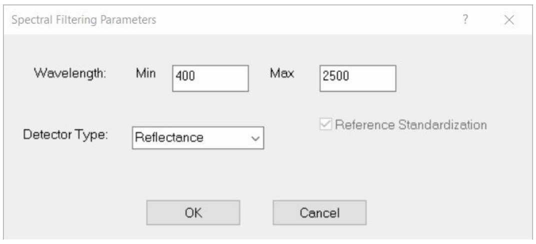
The right side of the screen contains a series of graphs, the number and kind depending on your choice of sample selection method. The results utilize a uniform color code to denote spectra. The red color designates outliers, and light blue redundant samples. The dark blue samples are the calibration set spectra. The left hand side of the screen shows the product tree and the distribution of samples between the calibration, validation, and outliers sets.

9 Choose **Select ▶ Save Results** to save the results of the sample selection. If the Validation or Outliers set contained any spectra, you will have an option to save them for validation purposes.

Performing Lab Data Type of Sample Selection

1 Click on the equation containing the temporary set.

2 Choose **Select ▶ Lab Data** to start sample selection.


Spectral Filtering Parameters

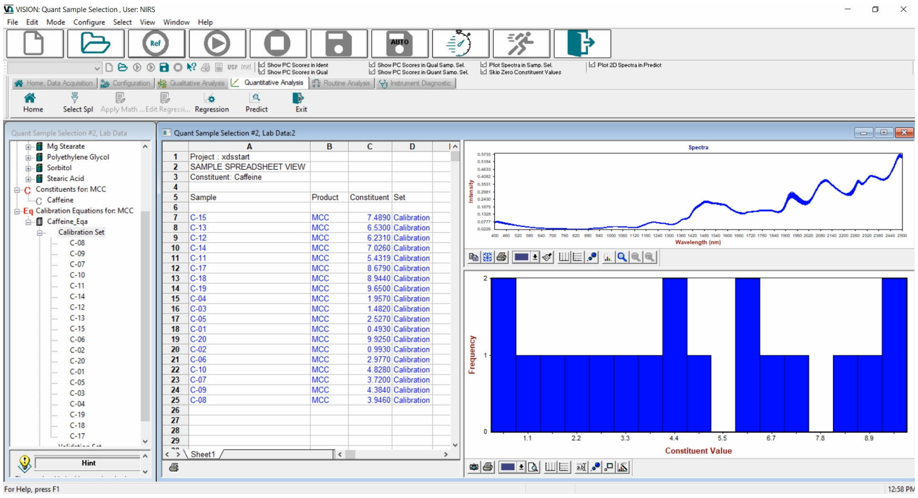
Wavelength: Min 400 Max 2500

Detector Type: Reflectance

☑ Reference Standardization

3 From the **Spectral Filtering Parameters** choose the filter options. Only the spectra fitting these criteria (detector cell type and wavelength range) will be let through sample selection. Click on **[OK]**.

4 The sample selection algorithm will proceed with calculations and display results.



	A	B	C	D
1	Project : xdsstart			
2	SAMPLE SPREADSHEET VIEW			
3	Constituent: Caffeine			
4				
5	Sample	Product	Constituent	Set
6				
7	C-15	MCC	7.4890	Calibration
8	C-13	MCC	6.5300	Calibration
9	C-12	MCC	6.2310	Calibration
10	C-14	MCC	7.0260	Calibration
11	C-11	MCC	5.4319	Calibration
12	C-17	MCC	8.6790	Calibration
13	C-18	MCC	8.9440	Calibration
14	C-19	MCC	9.6500	Calibration
15	C-04	MCC	1.9570	Calibration
16	C-03	MCC	1.4820	Calibration
17	C-05	MCC	2.5270	Calibration
18	C-01	MCC	0.4930	Calibration
19	C-20	MCC	9.9250	Calibration
20	C-02	MCC	0.9930	Calibration
21	C-06	MCC	2.9770	Calibration
22	C-10	MCC	4.8280	Calibration
23	C-07	MCC	3.7200	Calibration
24	C-09	MCC	4.3840	Calibration
25	C-08	MCC	3.9460	Calibration
26				
27				
28				
29				

The right side of the screen contains complete information about the data set: a spreadsheet with sample names and constituent values, a plot with spectra, and a histogram showing the distribution of the constituent values. The results utilize a uniform color code to denote spectra. The red color designates outliers, and light blue redundant samples. The dark blue samples are the calibration set spectra. The left hand side of the screen shows the product tree and the distribution of samples between the calibration, validation, and outliers sets.

Initially, all samples from the temporary set are placed in the calibration set. Double-clicking on any histogram bar will change the color of the corresponding spectra to yellow. It will also highlight the corresponding spectra in the spreadsheet and on the product tree. The selected spectra can be dragged from a given set and dropped into another. Also, the reference values can be corrected in the spreadsheet.

5 Choose **Select ▶ Save Results** to save the results of the sample selection. If the Validation or Outlier set contained any spectra, you will have an option to save them for validation purposes.

Performing Combined Sample Selection

1 Follow the procedure for spectral data type sample selection.

2 After saving the results, choose **Select ▶ Lab Data Direct**.

You will enter the **Lab Data** sample selection with the spectra already distributed between sets. You can type in the constituent values, and move samples between sets as described above.

3 Choose **Select ▶ Save Results** to save the results of the sample selection. If the Validation or Outlier set contained any spectra, you will have an option to save them for validation purposes.

Creating Multiple Sample Selection Methods

A newly created **Sample Selection** method may be tested, without losing the result of the previous trial. In order to do this:

1 Click on **Select ▶ New Method**. All graphs will reset.

2 Follow the standard sample selection procedure.

3 The results of previous sample selection methods can be viewed by choosing the proper method screen from the Window submenu.

4 If multiple sample selection methods were attempted, make sure that the method you want to save is in the active window before saving. If necessary, switch to the proper method.

If the user attempts to create a new product before the created temporary set undergoes sample selection, a multiple choice window will be displayed. The user can select to proceed with previous product sample selection, save all samples from the temporary set to the training set, or empty the temporary set.

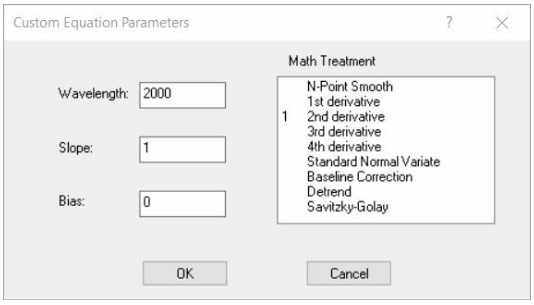
After saving the sample selection results, the equation icon changes from a gray cuvette symbol to a question mark. This signifies that the calibration set is ready for equation development.

6.3 Creating Custom Equations

Vision allows creation of a one term MLR equation with manually entered bias and slope. Custom equations can be created in Quantitative Sample Selection. To create a custom equation:

1 Follow sample selection procedure to a temporary set stage.

2 Click on **Select ▶ Create Custom Equation**.



Custom Equation Parameters

Wavelength: 2000

Slope: 1

Bias: 0

Math Treatment

- N-Point Smooth
- 1st derivative
- 1 2nd derivative
- 3rd derivative
- 4th derivative
- Standard Normal Variate
- Baseline Correction
- Detrend
- Savitzky-Golay

3 From the **Custom Equation Parameters** dialog box, select wavelength, slope, bias, and math pretreatment.

4 Click on **[OK]**.

6.4 Regression

Regression program allows users to develop a calibration equation from the calibration set. Vision offers 2 types of calibration development: Multilinear Regression and Partial Least Squares.

6.4.1 Multilinear Regression

Multilinear Regression (MLR) is a least squares method that uses spectral information at one or several wavelengths. In the simplest case (one wavelength), the method reduces to simple Linear Regression.

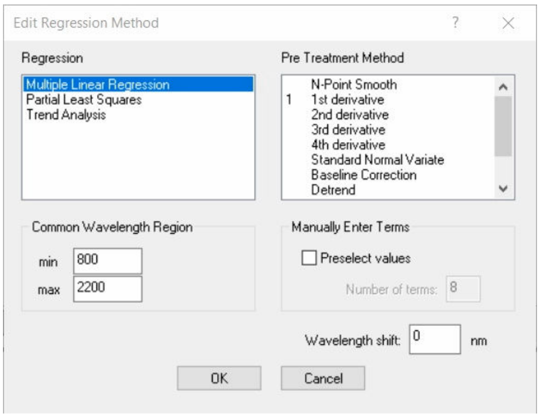
Preparation

1 Click on **Mode ▶ Quantitative Analysis ▶ Regression** to enter the calibration development program. The last active project will be opened. Expand the product for which you want to create the equation. The product should have the calibration set saved from the sample selection program.

2 Select the proper equation by doubleclicking on it. The equation icon will turn in color.

Configuring the Method

1 Click on **Regression** ▶ **Edit Regression Method**.



Pre Treatment Method: 1 1st derivative

min 800

max 2200

☐ Preselect values

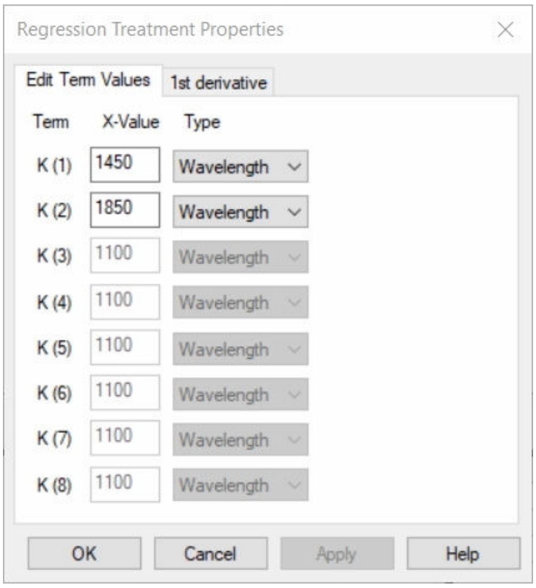
Number of terms: 8

Wavelength shift: 0 nm

2 From the **Edit Regression Method** dialog box select **Multiple Linear Regression**, **proper math pretreatments**, and the **wavelength region**.

Optionally enter the value for **Wavelength Shift parameter** (in nanometers). If the parameter is different from 0, Vision will use its value to shift every spectrum in the calibration set left and right along the wavelength axis. The resulting set of spectra, 3 times larger than the original set, is used for calibration. Constituent values of the shifted spectra are identical with these of the original spectrum.

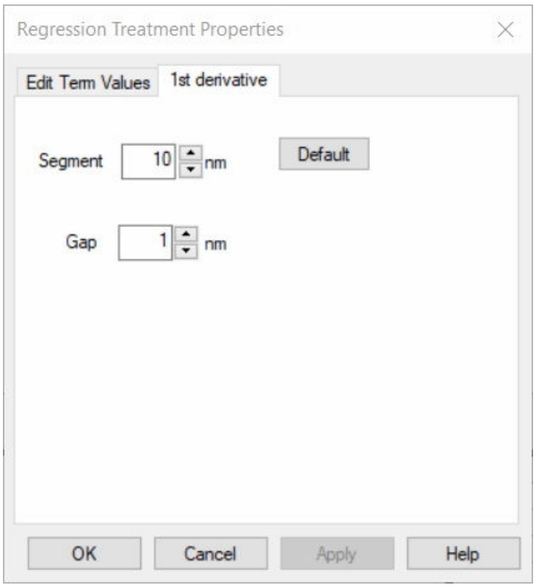
If you know what wavelengths you want to use, or if you want to use analog (transducer) values in the equation, click on Preselect Values in the **Manually Enter Terms** field.



Term	X-Value	Type
K (1)	1450	Wavelength
K (2)	1850	Wavelength
K (3)	1100	Wavelength
K (4)	1100	Wavelength
K (5)	1100	Wavelength
K (6)	1100	Wavelength
K (7)	1100	Wavelength
K (8)	1100	Wavelength

Specify the number of terms to be used in the equation. Click on **[OK]** when done.

3 In the **Regression Treatment Properties** dialog box, define the math treatment parameters and the wavelengths or transducers values (if you selected **Manually Enter Terms** in the above step)

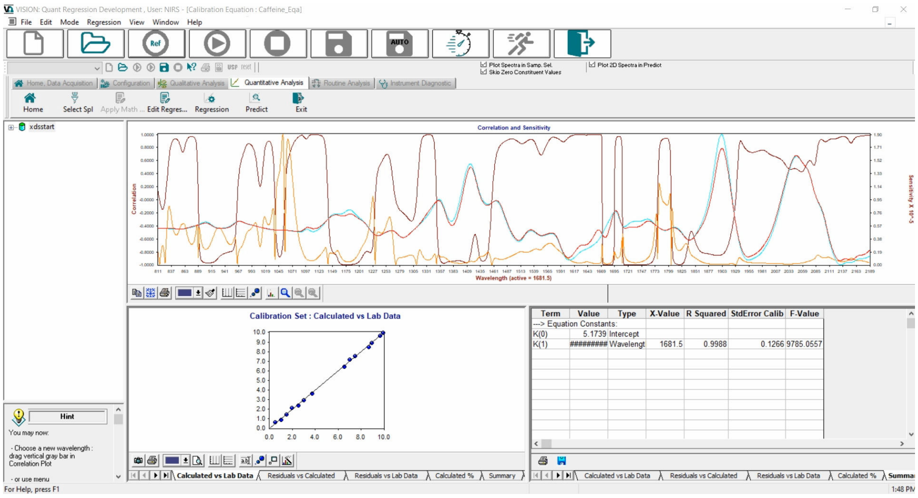


Segment 10 nm

Gap 1 nm

4 Click on **[OK]** when done. Vision will perform calculations and display results.

Displaying the Results



VISION: Quant Regression Development , User: NIRS - [Calibration Equation : Caffeine_Eqa]

You may now:

- Choose a new wavelength : drag vertical gray bar in Correlation Plot

- or use menu

For Help, press F1

Term	Value	Type	X-Value	R Squared	StdError Calib	F-Value
---> Equation Constants:						
K(0)	5.1739	Intercept				
K(1)	#########	Wavelengt	1681.5	0.9988	0.1266	9785.0557

The upper part of the results screen shows a correlation plot (green), sensitivity plot (magenta), and the spectra that correspond to the lowest and the highest constituent values (red and blue). The lower part of the screen contains a series of graphs that can be displayed by clicking on the appropriate tab:

- 45 degree plot (calculated vs. lab data)
- residuals vs. calculated values
- residuals vs. lab values
- calculated % (prediction of the calibration set)
- summary of results showing the wavelengths, calibration constants, correlation, standard error of calibration and F statistics
- average differences control chart X with confidence limits
- range of differences control chart R with confidence limit
- term intercorrelation table

The graphs can be displayed by clicking on the proper tab at the bottom of the display. If the validation set or outlier set was saved, they can be displayed by clicking on View and selecting the proper set to be shown.

Equation Editing

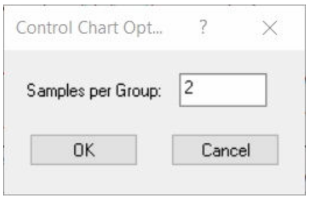
Vision selects the wavelength or wavelengths so that the maximum correlation is obtained. The last active wavelength is shown by the gray bar on the upper display. This wavelength can be changed by dragging the bar to the desired wavelength position, or by clicking on **Regression ▶ Edit Wavelength** and typing in the value.

To add a new wavelength to the equation by clicking on **Regression ▶ Add Term**. The equation parameters, statistics, and graphs are recalculated and views updated.

The last wavelength can be removed from the MLR equation by clicking on **Regression** ▶ **Rollback Term**. The equation parameters, statistics, and graphs are recalculated and views updated.

To move spectra between calibration, validation, and outlier sets, right click on a dot representing a spectrum in any plot or the spectrum name in the equation tree. Vision will reset the MLR equation to the first term. The equation parameters, statistics, and graphs are recalculated and views updated.

To change the control chart options, click on **View** ▶ **Control Chart Parameters**.



Samples per Group: 2

To save the equation, click on **Regression** ▶ **Save Equation**. To save the equation under a different name, click on **Regression** ▶ **Save Equation As**.

6.4.2 Partial Least Squares

Partial Least Squares (PLS) regression allows a user to use the spectral information of a whole range of wavelengths, even the full spectrum. This method eliminates colinearity (high correlation between wavelength terms) that are difficult to overcome with classical methods.

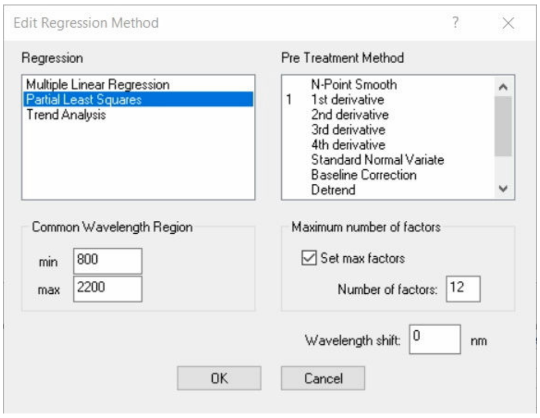
Preparation

1 Click on **Mode** ▶ **Quantitative Analysis** ▶ **Regression** to enter the calibration development program. The last active project will be opened. Expand the product for which you want to create the equation. The product should have the calibration set saved in the sample selection program.

2 Select the proper equation by doubleclicking on it. The equation icon will turn color.

Configuring the Method

1 Click on **Regression** ▶ **Edit Regression Method**.



Edit Regression Method

Regression

- Multiple Linear Regression
- Partial Least Squares
- Trend Analysis

Pre Treatment Method

- N-Point Smooth
- 1 1st derivative
- 2nd derivative
- 3rd derivative
- 4th derivative
- Standard Normal Variate
- Baseline Correction
- Detrend

Common Wavelength Region

min 800

max 2200

Maximum number of factors

☑ Set max factors

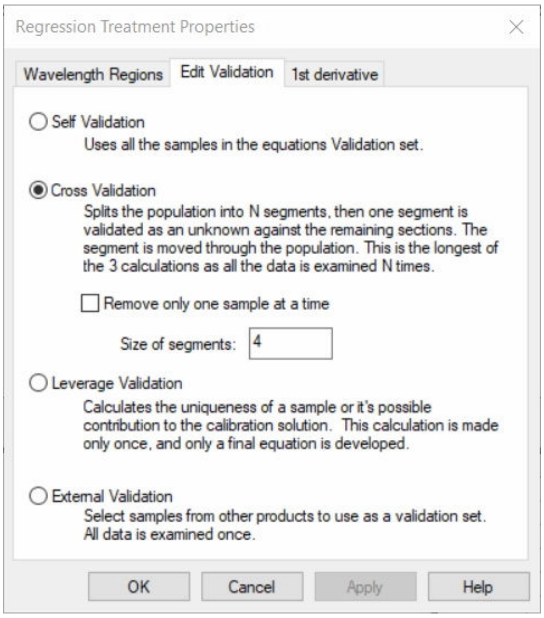
Number of factors: 12

Wavelength shift: 0 nm

2 From the **Edit Regression Method** dialog box, select **Partial Least Squares**, desired **Math Pretreatments**, and the **Wavelength Region**. In the **Maximum Number of Factors** field you can specify the number of factors to be calculated. Click on **[OK]** when done.

Optionally enter the value for **Wavelength Shift** parameter (in nanometers). If the parameter is different from 0, Vision will use its value to shift every spectrum in the calibration set left and right along the wavelength axis. The resulting set of spectra, 3 times larger than the original set, is used for calibration. Constituent values of the shifted spectra are identical with these of the original spectrum.

3 In the **Regression Treatment Properties** dialog box define the **Wavelength Regions**, **Math Treatment parameters**, and the **Validation method**.



Regression Treatment Properties

○ Self Validation

Uses all the samples in the equations Validation set.

● Cross Validation

Splits the population into N segments, then one segment is validated as an unknown against the remaining sections. The segment is moved through the population. This is the longest of the 3 calculations as all the data is examined N times.

☐ Remove only one sample at a time

Size of segments: 4

○ Leverage Validation

Calculates the uniqueness of a sample or it's possible contribution to the calibration solution. This calculation is made only once, and only a final equation is developed.

○ External Validation

Select samples from other products to use as a validation set. All data is examined once.

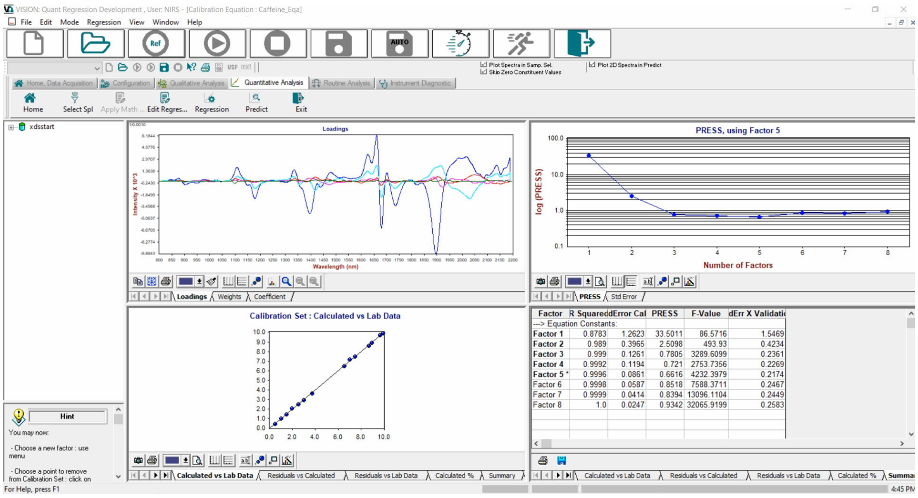
PLS equation validation is a procedure that helps to establish the optimum number of factors for the equation. This is done by finding a minimum of the PRESS value.

Vision offers 4 validation methods:

- Self Validation - the equation is developed from the training set of spectra, and the validation set is predicted. The PRESS value is calculated as the sum of squared residuals.
- Cross Validation - a moving segment is removed from the training set and predicted by the equation developed from the remaining samples. In full cross validation only one sample is removed at a time. The PRESS value is calculated as the sum of squared residuals.
- Leverage Validation - the training set itself is predicted. The residuals are then corrected by the leverage factor. The PRESS value is calculated as the sum of squared residuals.
- External Validation - allows the use of selected samples from another product as a prediction set. The PRESS value is calculated as the sum of squared residuals.

4 Click on **[OK]** when done to proceed with PLS calculations.

Displaying the Results



Factor	R Squared	dError Cal	PRESS	F-Value	dErr X Validati
---> Equation Constants:					
Factor 1	0.8783	1.2623	33.5011	86.5716	1.5469
Factor 2	0.989	0.3965	2.5098	493.93	0.4234
Factor 3	0.999	0.1261	0.7805	3289.6099	0.2361
Factor 4	0.9992	0.1194	0.721	2753.7356	0.2269
Factor 5 *	0.9996	0.0861	0.6616	4232.3979	0.2174
Factor 6	0.9998	0.0587	0.8518	7588.3711	0.2467
Factor 7	0.9999	0.0414	0.8394	13096.1104	0.2449
Factor 8	1.0	0.0247	0.9342	32065.9199	0.2583

You may now:

- Choose a new factor : use menu
- Choose a point to remove from Calibration Set : click on

The upper part of the results screen shows PLS loadings and weights, and the PRESS or standard error as a function of the number of factors. The lower part of the screen contains a series of graphs:

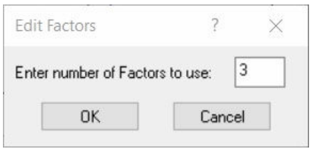
- 45 degree plot (calculated vs. lab data)
- residuals vs. calculated values
- residuals vs. lab values
- calculated %

- summary of results showing for each factor the correlation, standard error of calibration, PRESS and F statistics
- average differences control chart X with confidence limits
- range of differences control chart R with confidence limit

The graphs can be displayed by clicking on the proper tab at the bottom of the display. If the validation set or outlier set was saved, they can be displayed by clicking on View and selecting the proper set to be shown.

Equation Editing

Initially, the displayed results are based on the number of factors recommended by Vision, i.e., corresponding to the minimum on the PRESS plot. You can change the number of factors in the equation by clicking on **Regression ▶ Edit Factors**.



Enter number of Factors to use: 3

The equation parameters, statistics, and graphs are recalculated and views updated.

To move spectra between calibration, validation, and outlier sets, right click on a dot representing a spectrum in any plot or the spectrum name in the equation tree. The equation parameters, statistics, and graphs are recalculated and views updated.

To display a different number of loadings and weights, click on the factor number on the spreadsheet with equation parameters (i.e., summary tab).

To save the equation, click on **Regression ▶ Save Equation**. To save the equation under a different name, click on **Regression ▶ Save Equation As**.

6.4.3 Trend Analysis

Trend Analysis is located in the Regression part of Vision. However, no lab data are necessary to perform trend analysis. Trend analysis has been designed to look at the trend of spectral values at selected parts of spectra, and judge the progress of a reaction based on the trend direction and magnitude.

The trend function is calculated over a defined wavelength range and can be defined in several ways:

- As an average spectral value over the range
- As the highest or lowest spectral value within the range
- As an integral of spectral values within the range
- As standard deviation of spectral values within the range

The spectral values can be simply absorbance, or any combination of available math pretreatments can be used. The chosen pretreatment type is global to all selected ranges.

Up to 8 wavelength ranges can be used, and each can have a uniquely calculated trend magnitude. Trend magnitudes from multiple regions can be combined in the final expression, using basic mathematical operations.

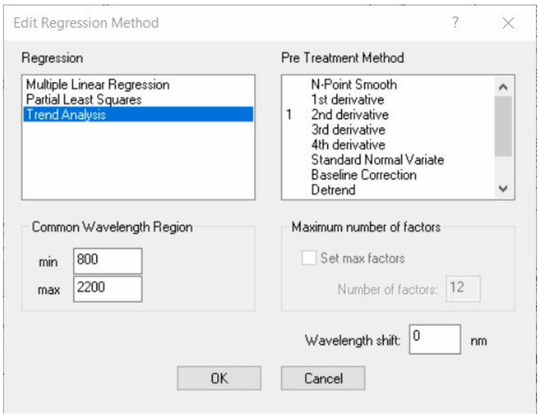
A range can contain only one data point. In this particular case, trend analysis allows the user to create a custom equation with up to 8 wavelengths, with manually entered constants.

To create an equation for trend analysis:

1 Perform the standard quantitative sample selection.

2 Click on **Mode** ▶ **Quantitative Analysis** ▶ **Regression**.

3 Select the equation and click on **Regression** ▶ **Edit Regression Method**.



Edit Regression Method

Regression: Trend Analysis

Pre Treatment Method: 1 2nd derivative

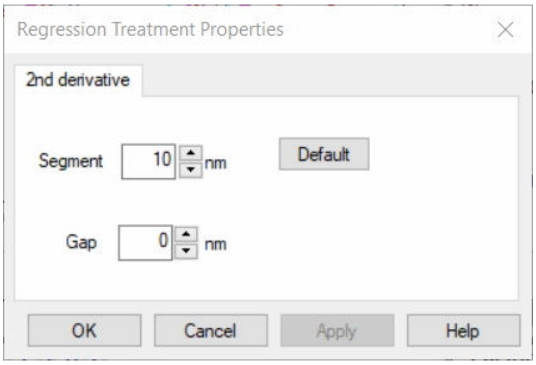
Common Wavelength Region: min 800, max 2200

Maximum number of factors: ☐ Set max factors, Number of factors: 12

Wavelength shift: 0 nm

4 From the dialog box that opens select **Trend Analysis** and the appropriate combination of pretreatments. Click on **[OK]**.

5 Configure pretreatment properties (if used) and click on **[OK]**.



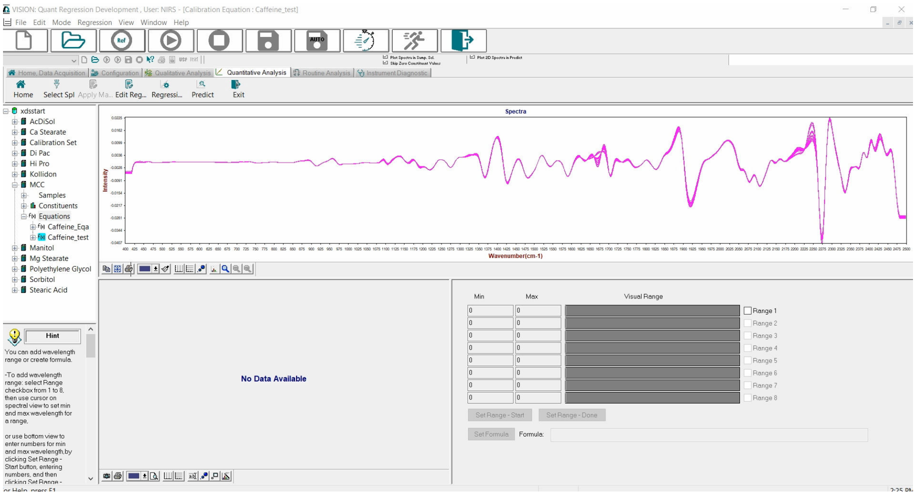
Regression Treatment Properties

2nd derivative

Segment 10 nm

Gap 0 nm

6 The screen that opens is made of 4 panels:



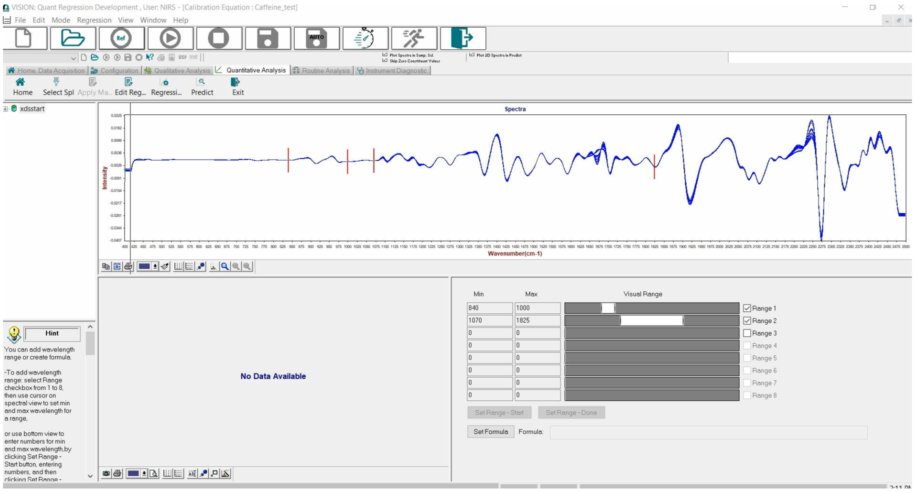
You can add wavelength range or create formula.

-To add wavelength range: select Range checkbox from 1 to 8, then use cursor on spectral view to set min and max wavelength for a range.

or use bottom view to enter numbers for min and max wavelength,by clicking Set Range - Start button, entering numbers, and then clicking Set Range -

The left panel shows the project tree and hints. The top right panel shows calibration set spectra with pretreatment(s) applied. The bottom right panel shows ranges and allows creating formulas. The remaining panel shows results of the trending equation.

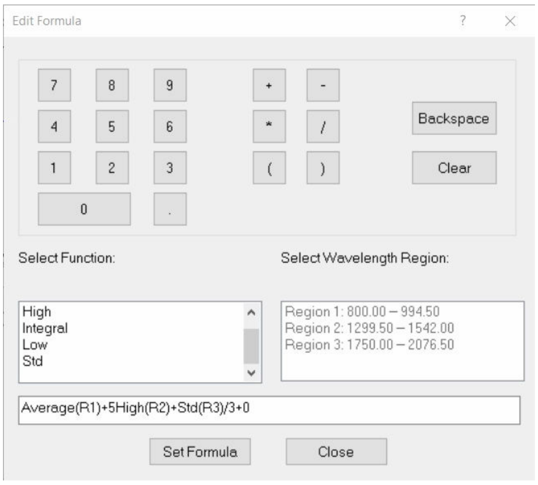
7 To select the first range click on the **Range1** check box. Click on **Set Range – Start** and enter the minimum and maximum wavelengths of the range. Click on **Set Range – Done** when finished.



Min	Max	
840	1000	☑ Range 1
1070	1825	☑ Range 2
0	0	☐ Range 3
0	0	☐ Range 4
0	0	☐ Range 5
0	0	☐ Range 6
0	0	☐ Range 7
0	0	☐ Range 8

Repeat the previous step for the rest of the ranges.

8 When all ranges are selected, click on **Set Formula**. The following dialog is displayed:



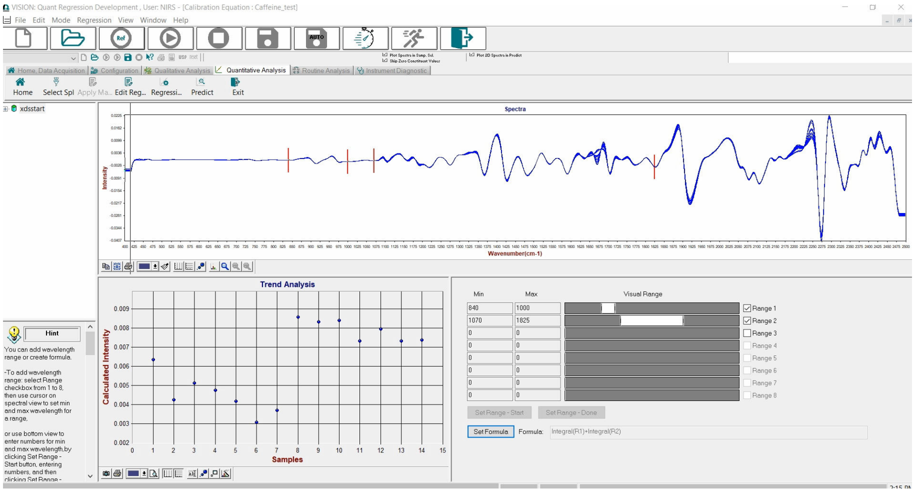
Region 1: 800.00 – 994.50
Region 2: 1299.50 – 1542.00
Region 3: 1750.00 – 2076.50

Average(R1)+5High(R2)+Std(R3)/3+0

This dialog defines functions used on each range, and the overall formula combining the functions. To create a formula, click on the function, then on the desired region. Add another segment to the formula using provided operands and constants. The created formula is listed below functions and ranges.

To apply the formula on the calibration spectra:

1 Click on **[Set Formula]** and then on **[Close]**. The plot shows the trend resulting from the created formula applied on the calibration spectra:



You can add wavelength range or create formula.

-To add wavelength range: select Range checkbox from 1 to 8, then use cursor on spectral view to set min and max wavelength for a range,

or use bottom view to enter numbers for min and max wavelength,by clicking Set Range - Start button, entering numbers, and then clicking Set Range -

Min	Max	
840	1000	☑ Range 1
1070	1825	☑ Range 2
0	0	☐ Range 3
0	0	☐ Range 4
0	0	☐ Range 5
0	0	☐ Range 6
0	0	☐ Range 7
0	0	☐ Range 8

Formula: Integral(R1)+Integral(R2)

2 Click on the **Save icon** to save the formula. The created formula can be used in Routine Analysis and the results displayed on a Trend Chart.

6.5 Leverage Calculation Equation

The **[Leverage]** value is in simple words a measure to evaluate the influence of a sample in a PCA model. Usually a sample with high leverage, is a sample with high influence on the model. In a dataset, the samples with high leverage need to be evaluated carefully as they indicate unusual variation of a constituent and as a result, they can bias the model significantly.

During Routine Analysis, a PLS model is used to predict values for a particular constituent and application. Vision allows the calculation of the leverage value, strongly connected to a specific PLS model, for every new sample tested. The leverage calculation in combination with the PLS model used for quantification, increase the confidence in the quantitative predictions as possible outliers are detected on the go.

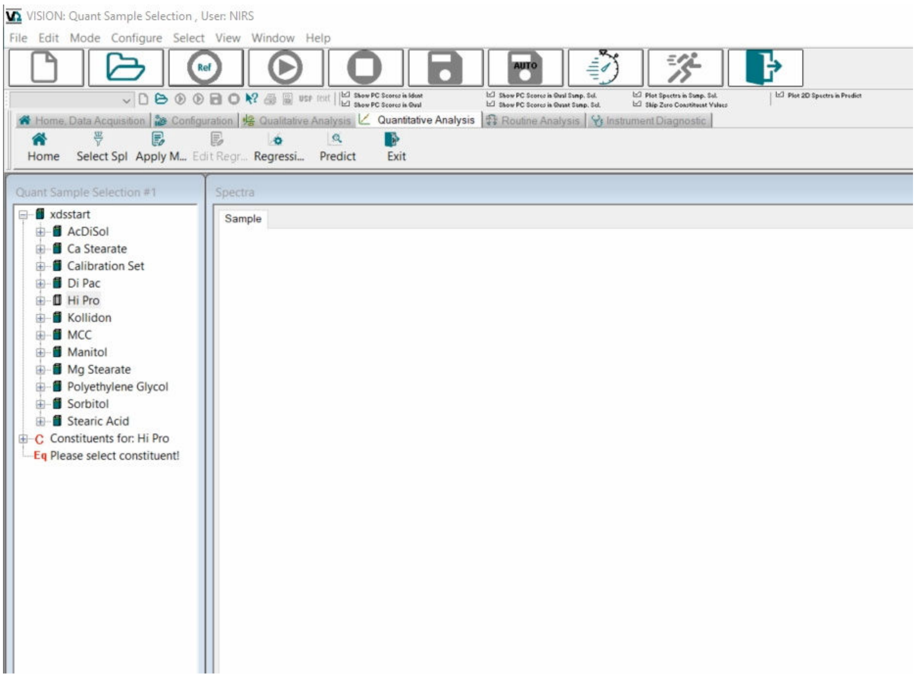
NOTICE

Only Vision version 4.1.1.156 or higher should be used for the leverage calculation functionality to work.

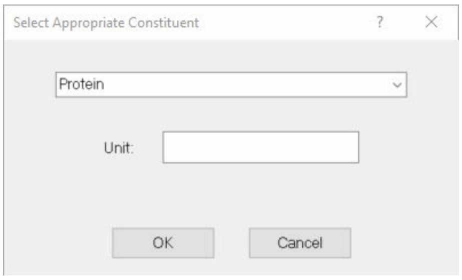
Preparation

Create a PLS model

1 Click on **Mode ▶ Quantitative Analysis ▶ Sample Selection** to enter the sample selection program. The last active project will be opened. Expand the product for which you want to create the equation as you can see below:



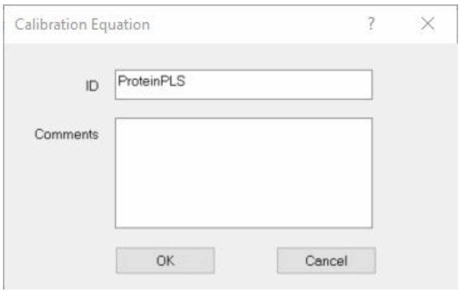
2 Drag and drop the product **[Hi Pro]** to **[Eq]**. Select the constituent of interest and click **[OK]**.



Protein

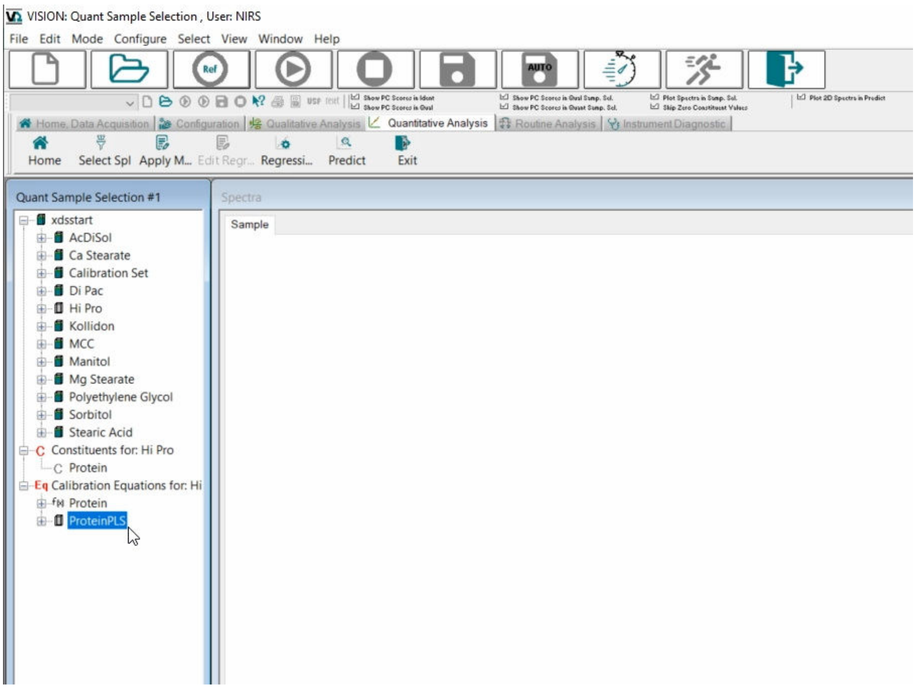
Unit:

3 Give a unique name for this new equation:

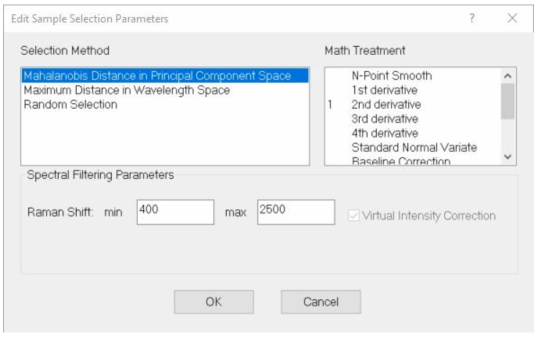


ID ProteinPLS

4 Make sure that the newly created equation is highlighted and continue by clicking on **[Apply Math]**:



5 Choose the **[Selection Method]**and **[Math Treatment]**:



Edit Sample Selection Parameters

Selection Method

Mahalanobis Distance in Principal Component Space
Maximum Distance in Wavelength Space
Random Selection

Math Treatment

N-Point Smooth
1st derivative
1 2nd derivative
3rd derivative
4th derivative
Standard Normal Variate
Baseline Correction

Spectral Filtering Parameters

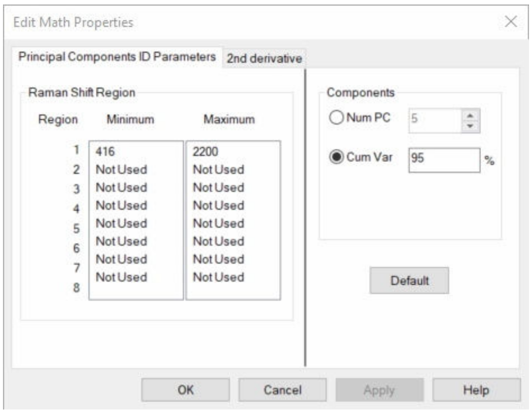
Raman Shift: min 400 max 2500

☑ Virtual Intensity Correction

NOTICE

The **[Spectral Filtering Parameters]**are relevant to the operational spectral range of the instrument which generated the data and not to the wavelength regions used for model development.

6 The user can setup the **[Edit Math Properties]** following all the steps as described in the **Regression ▶ Partial Least Squares** section of this manual:



Edit Math Properties

Principal Components ID Parameters | 2nd derivative

Raman Shift Region

Region	Minimum	Maximum
1	416	2200
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

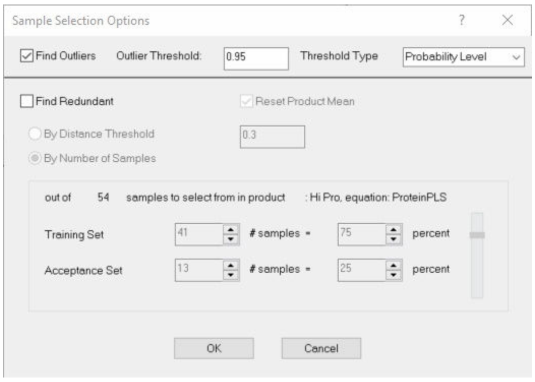
Components

○ Num PC 5

● Cum Var 95 %

After finishing configuration, click **[OK]**:

7 Parametrize the **[Sample Selection Options]**:



Sample Selection Options

☑ Find Outliers Outlier Threshold: 0.95 Threshold Type Probability Level

☐ Find Redundant ☑ Reset Product Mean

○ By Distance Threshold 0.3

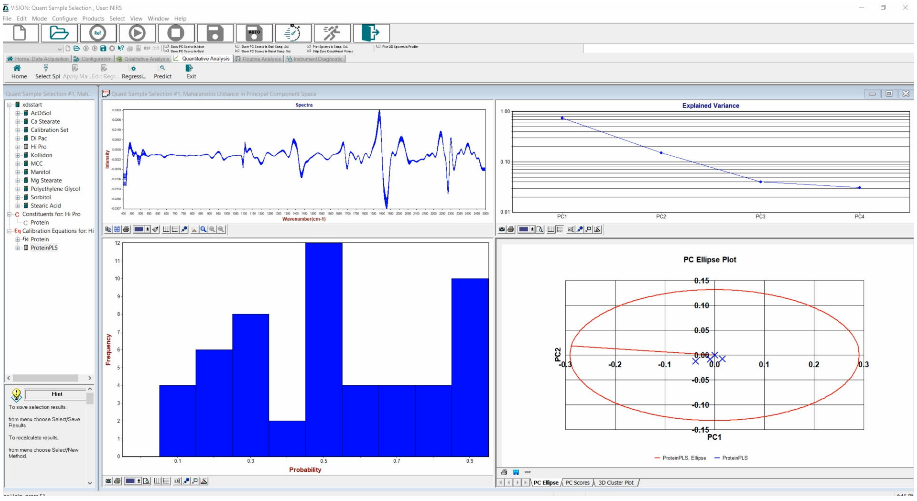
● By Number of Samples

out of 54 samples to select from in product : Hi Pro, equation: ProteinPLS

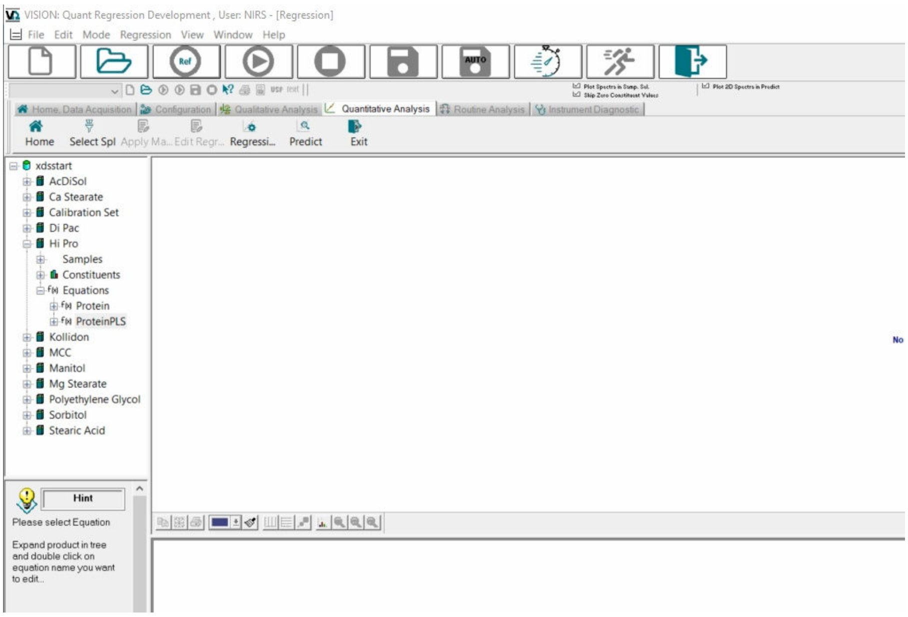
Training Set 41 # samples = 75 percent

Acceptance Set 13 # samples = 25 percent

Click on the **[Save]** icon on the upper left side of the **[Quant Sample Selection]** screen and continue to **[Regression]**.



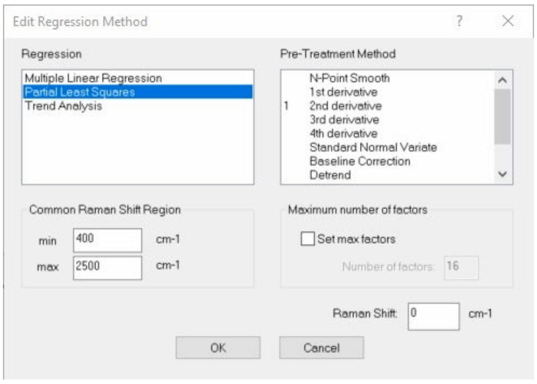
8 Click on **[Regression]** and navigate to the equation that was created previously **Xdsstart ▶ Hi Pro ▶ f(x) Equations**. Click on the **[ProteinPLS]** equation:



Please select Equation

Expand product in tree and double click on equation name you want to edit...

9 Click on **[Edit Regression]** and select the **[Regression]** and the **[Pre-Treatment Method]**:



1 2nd derivative

min 400 cm-1

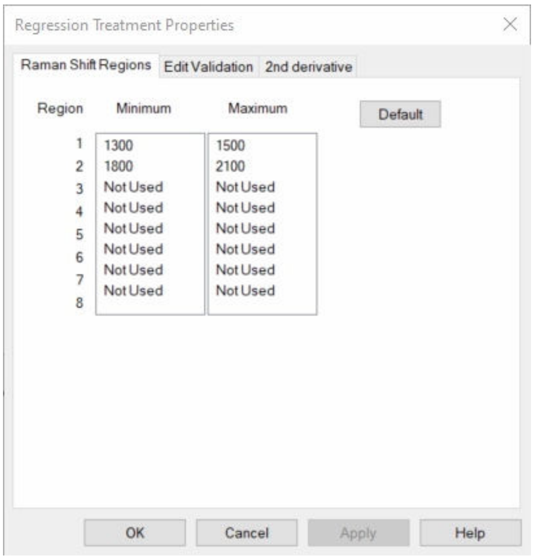
max 2500 cm-1

☐ Set max factors

Number of factors: 16

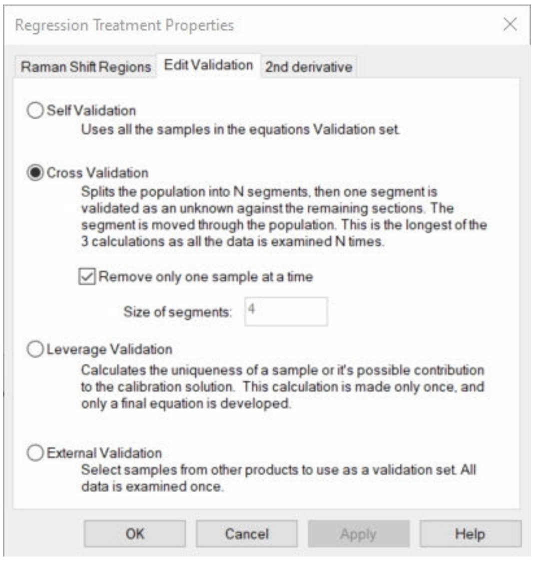
Raman Shift 0 cm-1

10 Enter the **[Wavelength Region(s)]**:



Region	Minimum	Maximum
1	1300	1500
2	1800	2100
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

11 Continue to the **[Edit Validation]**:



○ Self Validation
Uses all the samples in the equations Validation set.

● Cross Validation
Splits the population into N segments, then one segment is validated as an unknown against the remaining sections. The segment is moved through the population. This is the longest of the 3 calculations as all the data is examined N times.

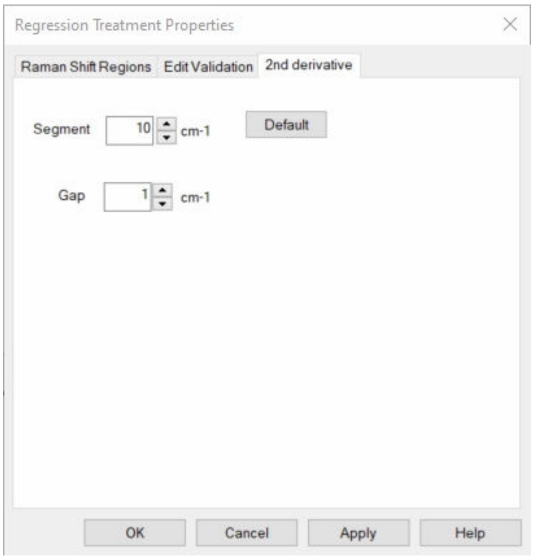
☑ Remove only one sample at a time

Size of segments: 4

○ Leverage Validation
Calculates the uniqueness of a sample or it's possible contribution to the calibration solution. This calculation is made only once, and only a final equation is developed.

○ External Validation
Select samples from other products to use as a validation set. All data is examined once.

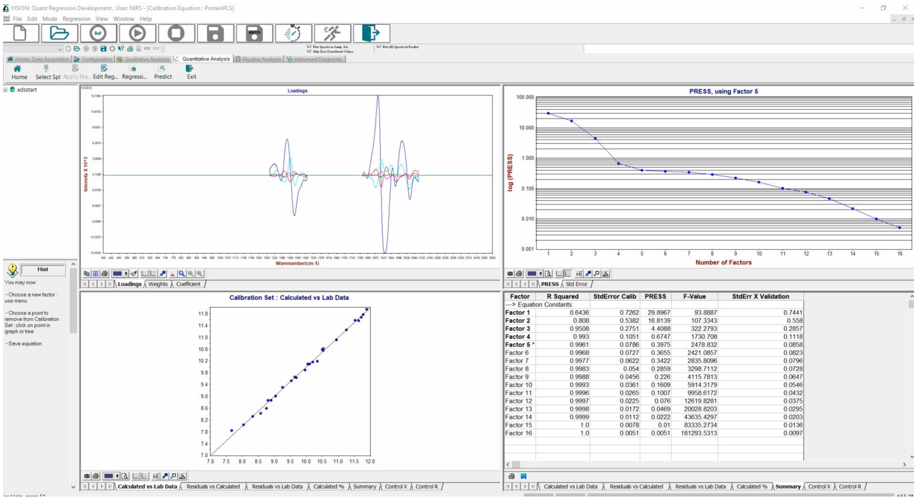
And finish by configuring the **[2nd derivative]**:



Segment 10 cm-1

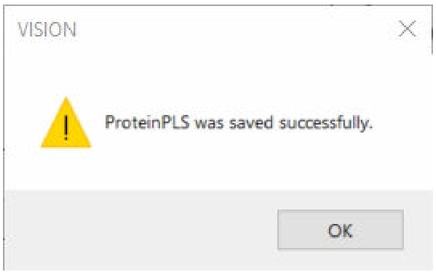
Gap 1 cm-1

12 Evaluate the performance of the PLS model and modify accordingly.



Factor	R Squared	StdError Calib	PRESS	F-Value	StdErr X Validation
---> Equation Constants:					
Factor 1	0.6436	0.7262	29.8967	93.8887	0.7441
Factor 2	0.808	0.5382	16.8139	107.3343	0.558
Factor 3	0.9508	0.2751	4.4088	322.2793	0.2857
Factor 4	0.993	0.1051	0.6747	1730.708	0.1118
Factor 5 *	0.9961	0.0786	0.3975	2478.832	0.0858
Factor 6	0.9968	0.0727	0.3655	2421.0857	0.0823
Factor 7	0.9977	0.0622	0.3422	2835.8096	0.0796
Factor 8	0.9983	0.054	0.2859	3298.7112	0.0728
Factor 9	0.9988	0.0456	0.226	4115.7813	0.0647
Factor 10	0.9993	0.0361	0.1609	5914.3179	0.0546
Factor 11	0.9996	0.0265	0.1007	9958.6172	0.0432
Factor 12	0.9997	0.0225	0.076	12619.8281	0.0375
Factor 13	0.9998	0.0172	0.0469	20028.8203	0.0295
Factor 14	0.9999	0.0112	0.0222	43635.4297	0.0203
Factor 15	1.0	0.0078	0.01	83335.2734	0.0136
Factor 16	1.0	0.0051	0.0051	181293.5313	0.0097

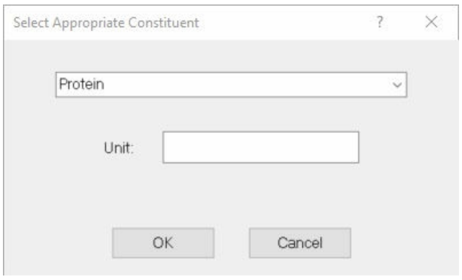
13 Click on the **[Save]** icon. Vision confirms that the **[ProteinPLS]** equation is saved:



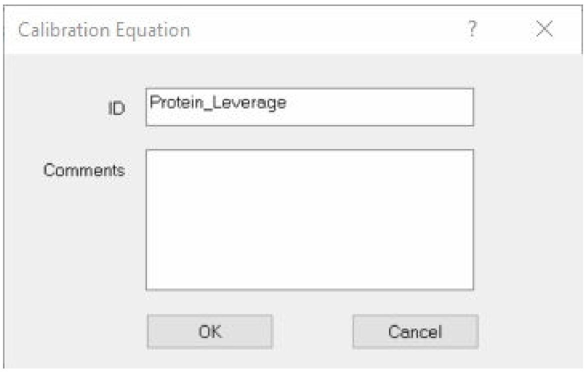
ProteinPLS was saved successfully.

Create Leverage Equation

1 Go to **Quantitative Analysis ▶ Sample Selection**. Drag and drop the product containing the PLS equation, **[Hi Pro]**to **[Eq]** and select the same constituent for which you want to create the leverage equation:

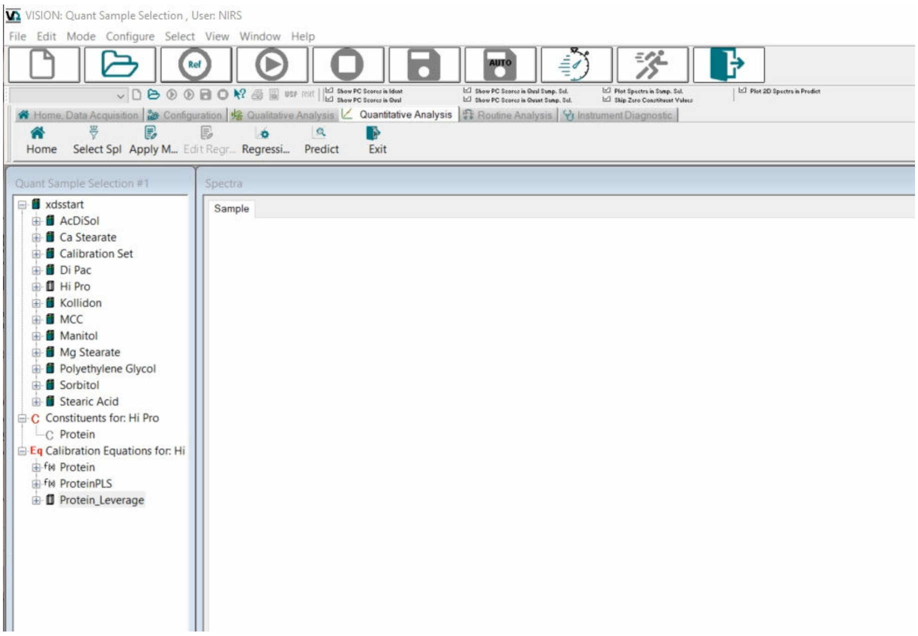


2 Provide a unique name for the leverage equation:

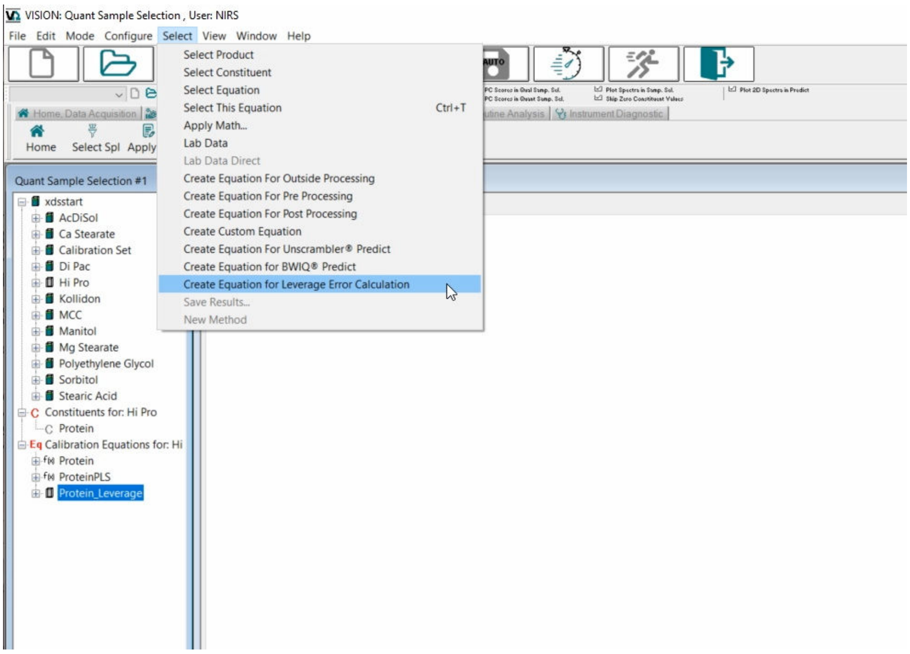


ID: Protein_Leverage

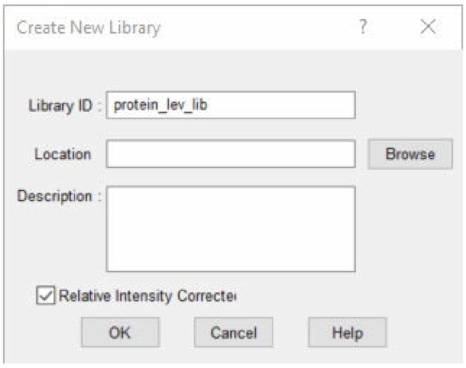
Click **[OK]** and make sure that the equation was created successfully:



3 Go to **Select ▶ Create Equation for Leverage Error Calculation**:



4 Enter the name of the library you want to create and provide a relevant name:



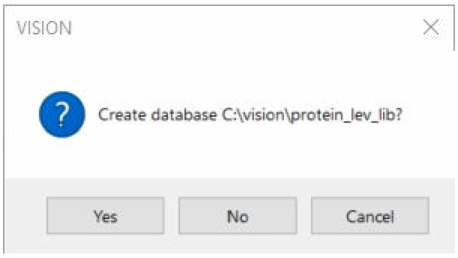
Library ID : protein_lev_lib

Location

Description :

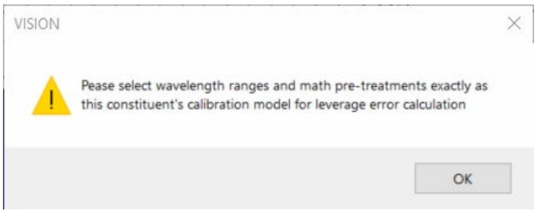
☑ Relative Intensity Correcte

Click on **[OK]** and **[Yes]** to create the database:



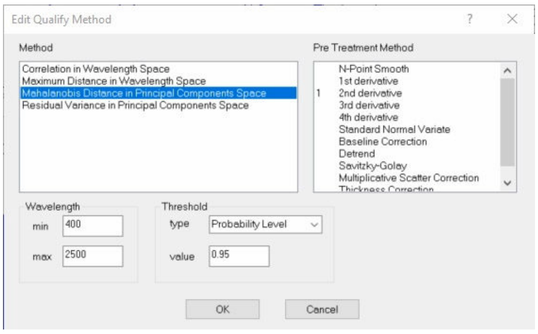
Create database C:\vision\protein_lev_lib?

5 Vision will immediately inform the user to use the same configuration used for the creation of the PLS model, for the subsequent successful creation of the leverage equation:



Pease select wavelength ranges and math pre-treatments exactly as this constituent's calibration model for leverage error calculation

6 Select the Method **[Mahalanobis Distance in Principal Component Space]** and the Pre-Treatment Method as in the **[ProteinPLS]** as well as for the rest of the settings:

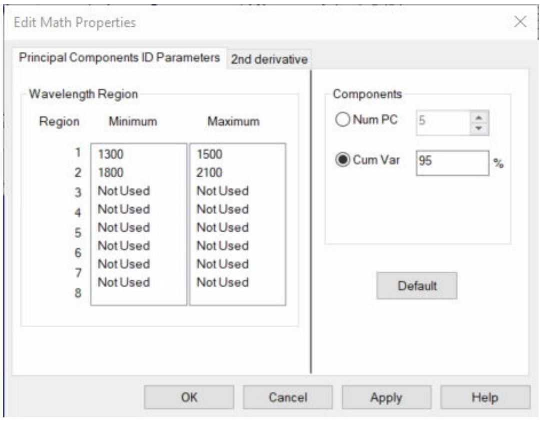


Method: Mahalanobis Distance in Principal Components Space

Pre Treatment Method: 1 2nd derivative

Wavelength
min 400
max 2500

Threshold
type Probability Level
value 0.95



Edit Math Properties

Principal Components ID Parameters | 2nd derivative

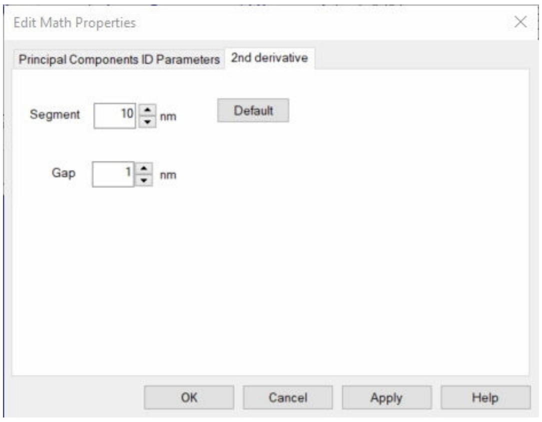
Wavelength Region

Region	Minimum	Maximum
1	1300	1500
2	1800	2100
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

Components

○ Num PC 5

● Cum Var 95 %



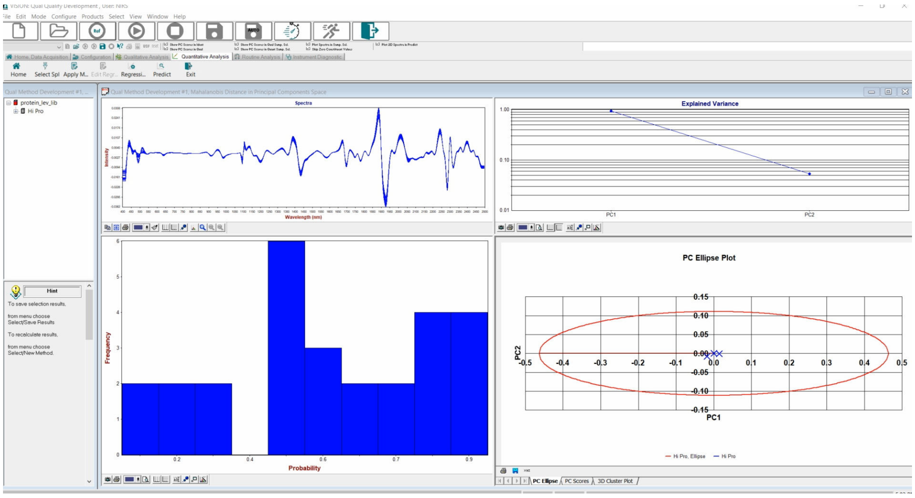
Edit Math Properties

Principal Components ID Parameters | 2nd derivative

Segment 10 nm

Gap 1 nm

7 Vision develops a qualification method, save, and click on **[Yes]**.



Vision: Qual Method Development #1, Mahalanobis Distance in Principal ...

Do you need to save Developed Qualify Method?

8 The Leverage equation has been created successfully and it is ready to be used for Routine Analysis.

6.6 Viewing Equation Properties

The calibration equation sample sets and equation properties can be displayed and inspected.

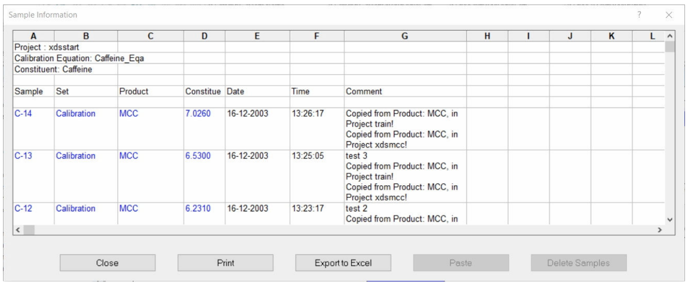
6.6.1 Calibration Equation Sets

1 In order to view sample sets used for calibration equation development, enter the **Quant Sample Selection** program.

2 Select the product and constituent.

All calibration equations for the selected product and constituent will be displayed.

3 Highlight the chosen equation and click on **Edit ▶ Properties**.



A	B	C	D	E	F	G	H	I	J	K	L
Project : xdsstart											
Calibration Equation: Caffeine_Eqa											
Constituent: Caffeine											
Sample	Set	Product	Constitue	Date	Time	Comment					
C-14	Calibration	MCC	7.0260	16-12-2003	13:26:17	Copied from Product: MCC, in Project train! Copied from Product: MCC, in Project xdsmcc!					
C-13	Calibration	MCC	6.5300	16-12-2003	13:25:05	test 3 Copied from Product: MCC, in Project train! Copied from Product: MCC, in Project xdsmcc!					
C-12	Calibration	MCC	6.2310	16-12-2003	13:23:17	test 2 Copied from Product: MCC, in					

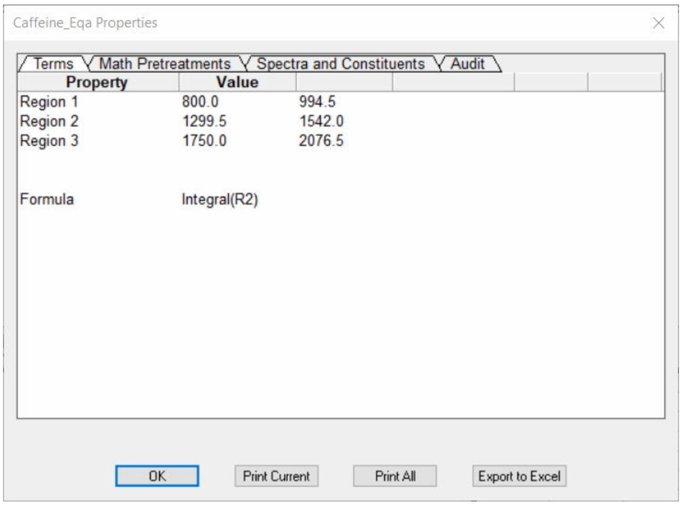
This will display a spreadsheet with sample sets.

6.6.2 Calibration Equation Parameters

1 In order to view parameters of a calibration equation, enter the **Quant Regression** program.

2 Expand the chosen product and right click on the equation name.

3 Select Properties from the menu.



Property	Value	
Region 1	800.0	994.5
Region 2	1299.5	1542.0
Region 3	1750.0	2076.5
Formula	Integral(R2)	

The **Properties** window displays calibration constants, math treatments, corrections, Standard Error of Calibration, and squared correlation.

The **Properties** window is empty if no calibration equation has been developed.

6.7 Import of NSAS Calibration Equations

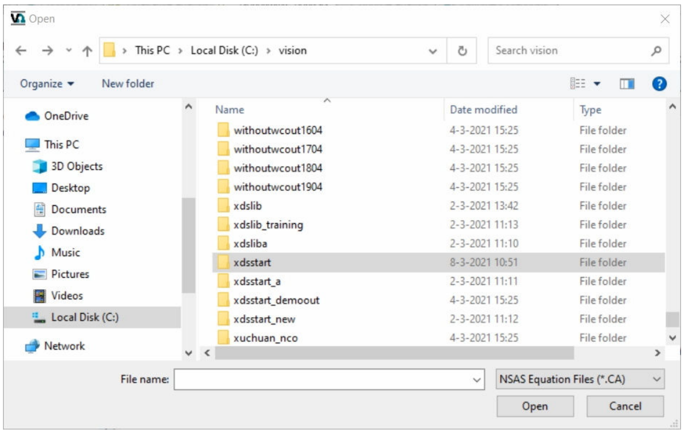
Vision supports the NSAS calibration equation format. The NSAS equations can be imported to Vision in the **Quantitative Sample Selection**. An equation is linked to a particular product and its particular constituent. The imported equation cannot be modified.

Calibration Equation Import Procedure

1 Enter **Sample Selection** by choosing **Mode ▶ Quantitative Analysis ▶ Sample Selection** from the main menu. In the left window of the **Sample Selection** screen, the project recently worked on is displayed in green.

2 If you want to work with a different project, click on **File ▶ Project ▶ Open** from the main menu.

3 Click on **File ▶ Import** from the main menu.



Name	Date modified	Type
withoutwcout1604	4-3-2021 15:25	File folder
withoutwcout1704	4-3-2021 15:25	File folder
withoutwcout1804	4-3-2021 15:25	File folder
withoutwcout1904	4-3-2021 15:25	File folder
xdslib	2-3-2021 13:42	File folder
xdslib_training	2-3-2021 11:13	File folder
xdsliba	2-3-2021 11:10	File folder
xdsstart	8-3-2021 10:51	File folder
xdsstart_a	2-3-2021 11:11	File folder
xdsstart_demoout	4-3-2021 15:25	File folder
xdsstart_new	2-3-2021 11:12	File folder
xuchuan_nco	4-3-2021 15:25	File folder

File name:

NSAS Equation Files (*.CA)

4 In the **Open** dialog box enter the directory with the NSAS files. Click on a file to highlight and select it. Click on **[Open]**.

5 From the **Select Product** dialog box choose the product to which you want to link the calibration equation. Click on **[OK]**.

6 From the **Select Constituent** dialog box choose the constituent to which you want to link the equation. You can also create a new constituent by typing the name. Optionally enter the units. Click on **[OK]** when done.

NOTICE

NOTE: If you want to export your data to Vision Air, additional rules have to be fulfilled. Only a list of predefined units are supported.

7 In the **Calibration Equation** dialog box optionally edit the calibration equation name and enter a comment. Click on **[OK]**.

6.8 Prediction and Equation Adjustment

Vision allows you to use either a validation set or an external prediction set in order to check the performance of the calibration, and, if necessary, to correct bias and/or slope.

The **[Prediction]** functionality accommodates regular chemometric models developed within Vision and furthermore, **[Unscrambler Predict]** allows the direct use of models, previously developed by **[Unscrambler]** software (Camo Analytics).

6.8.1 Prediction Procedure

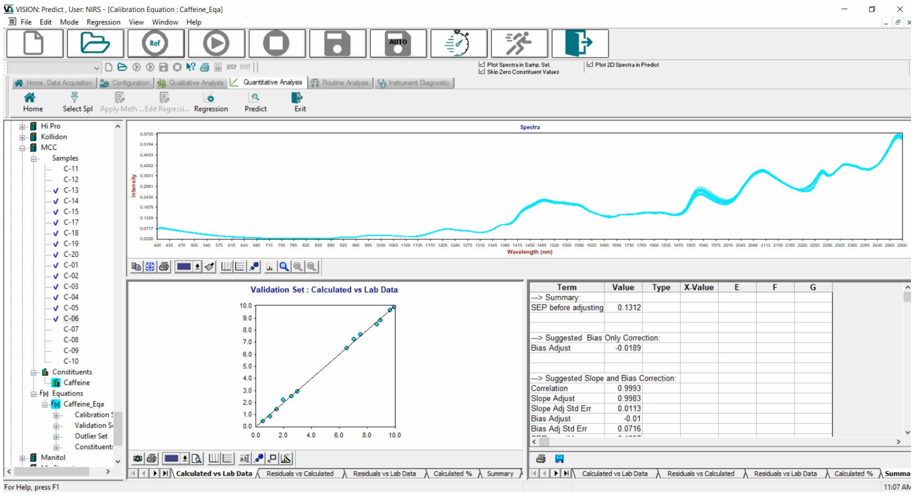
1. Click on **Mode ▶ Quantitative Analysis ▶ Predict** to enter the prediction program. All your projects will be displayed. Expand the project and product with the equation.

2. Select the equation by double-clicking on it. The **equation icon** will turn in color.

3. Select the constituent of the product to be predicted by double-clicking on it. Select the product spectra for prediction by clicking on each spectrum. You can also select a range of spectra by clicking on the first spectrum in the range and Shiftclicking on the last one.

   Make sure that the constituent and spectra come from the same product.

4. Click on **Regression ▶ Evaluate Samples** to predict the selected samples.



Term	Value	Type	X-Value	E	F	G
---> Summary:						
SEP before adjusting	0.1312					
---> Suggested Bias Only Correction:						
Bias Adjust	-0.0189					
---> Suggested Slope and Bias Correction:						
Correlation	0.9993					
Slope Adjust	0.9983					
Slope Adj Std Err	0.0113					
Bias Adjust	-0.01					
Bias Adj Std Err	0.0716					

5 The upper part of the results screen shows the predicted spectra. The lower part of the screen contains a series of graphs that can be displayed in 2 panes:

- 45 degree plot (calculated vs. lab data)
- residuals vs. calculated values
- residuals vs. lab values
- calculated % (prediction results)
- summary of results
- average differences control chart X with confidence limits
- range of differences control chart R with confidence limit

The graphs can be displayed by clicking on the proper tab at the bottom of the display.

The spreadsheet with summary of results displays the SEP before adjustment, correlation and SEP after adjustment, and correction factors together with their confidence limits.

To adjust the equation, click on **Regression ▶ Adjust Equation** and choose **Bias Adjustment** or **Bias and Slope Adjustment** from the dialog box.

● Adjust Bias only
○ Adjust Slope and Bias

To save the adjusted equation, click on **Regression ▶ Save Adjusted Equation**. If you do not want to save the adjusted equation, simply exit the prediction program.

The spreadsheet can be displayed in **Designer Mode** by a double right-click. Designer Mode allows copying results or saving the spreadsheet in Excel format.

6.8.2 Unscrambler Prediction Procedure

This feature requires the following prerequisites to function:

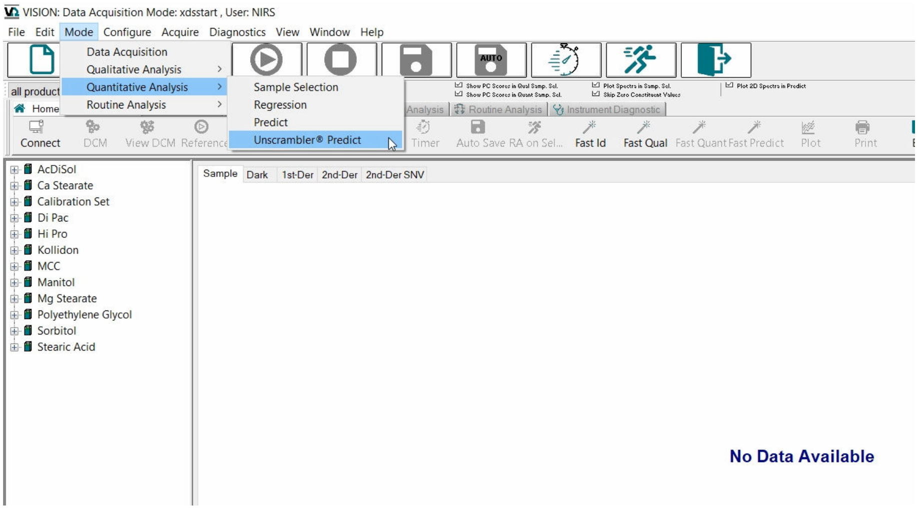
- **Unscrambler X Prediction Engine:** this is a necessary piece of software designed to interface with Vision software and our NIRS analyzers.
- **Unscrambler X model:** offline model developed using Unscrambler X software.
- **Vision:** a version of 4.1.1.156 or higher needs to be used.

NOTICE

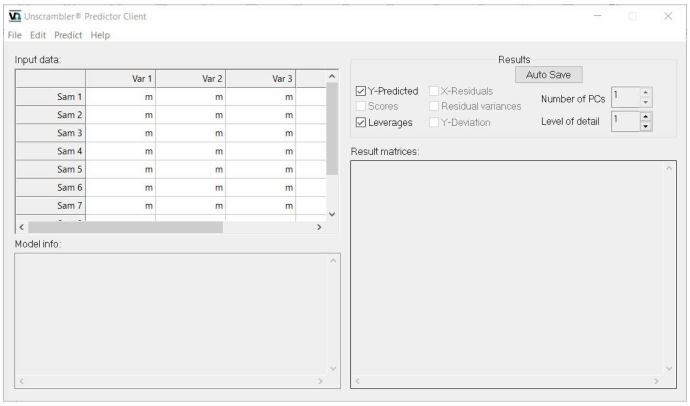
The Unscrambler X software for model development does not form part of the Unscrambler X Prediction Engine package

1 Initiate Vision and open the project that contains the samples to be used for Unscrambler Prediction.

2 Go to **Mode ▶ Quantitative Analysis ▶ Unscrambler Predict**:

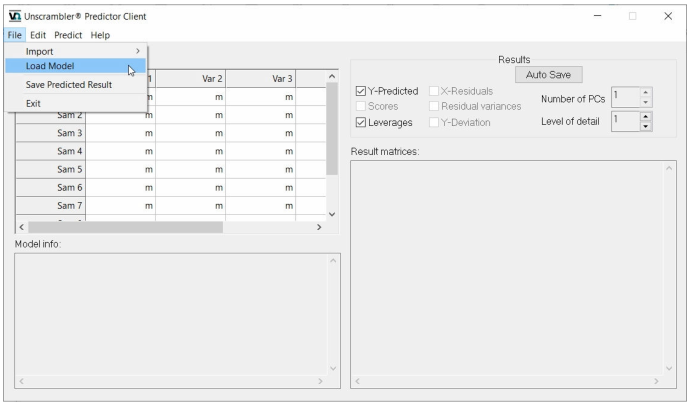


3 The predictor client opens:



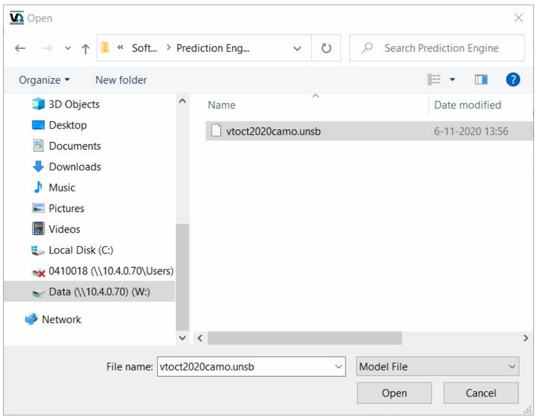
	Var 1	Var 2	Var 3
Sam 1	m	m	m
Sam 2	m	m	m
Sam 3	m	m	m
Sam 4	m	m	m
Sam 5	m	m	m
Sam 6	m	m	m
Sam 7	m	m	m

Click on **File ▶ Load Model**:



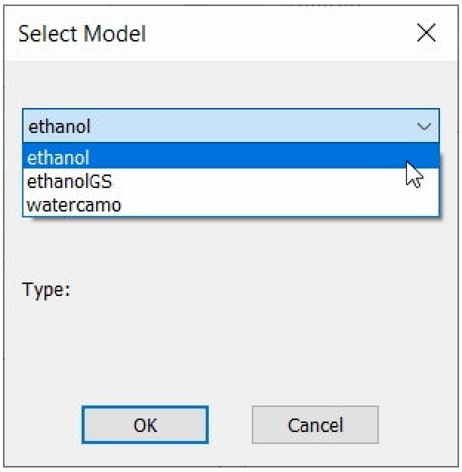
☑ Y-Predicted
☑ Leverages
Number of PCs 1
Level of detail 1

4 Select the Unscrambler equation by choosing the correct unsb file:



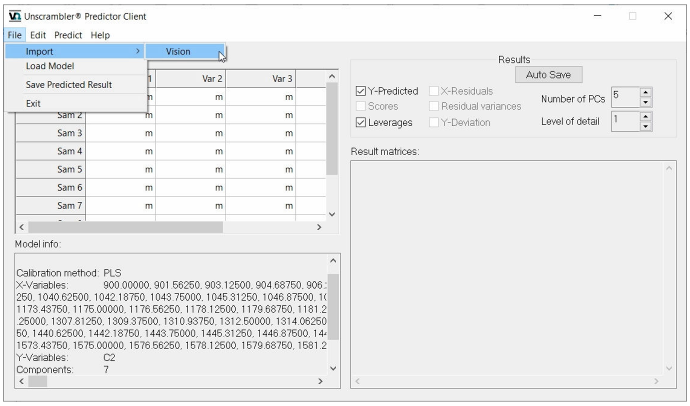
File name: vtoct2020camo.unsb
Model File

Make sure you choose the appropriate model:



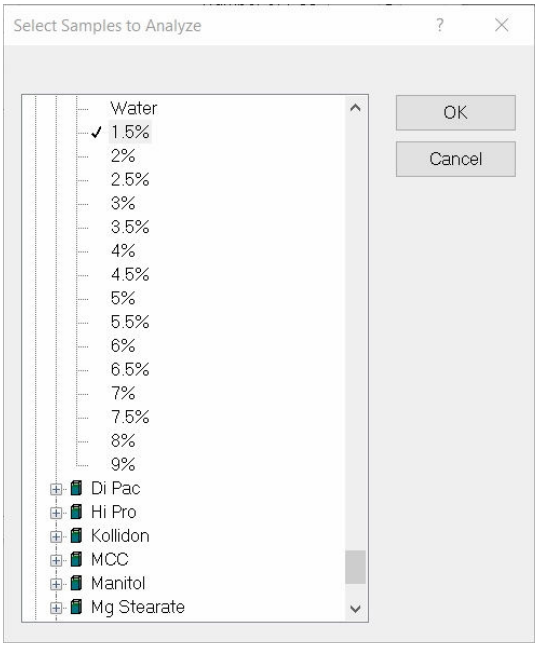
ethanol

5 Click on **File ▶ Import ▶ Vision**:

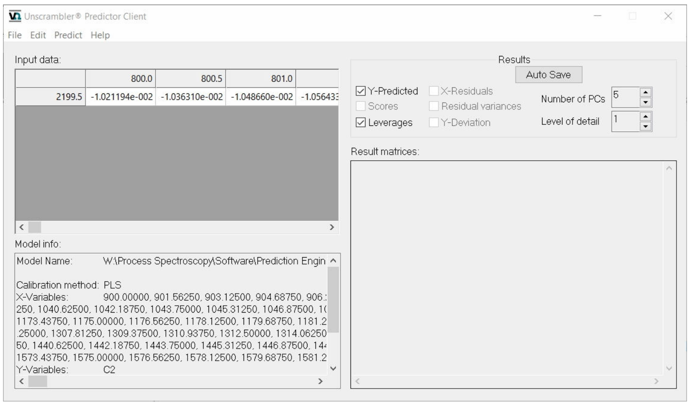


```
Calibration method:  PLS
X-Variables:         900.00000, 901.56250, 903.12500, 904.68750, 906.:
250, 1040.62500, 1042.18750, 1043.75000, 1045.31250, 1046.87500, 1(
1173.43750, 1175.00000, 1176.56250, 1178.12500, 1179.68750, 1181.2
.25000, 1307.81250, 1309.37500, 1310.93750, 1312.50000, 1314.06250
50, 1440.62500, 1442.18750, 1443.75000, 1445.31250, 1446.87500, 14
1573.43750, 1575.00000, 1576.56250, 1578.12500, 1579.68750, 1581.2
Y-Variables:         C2
Components:          7
```

6 Select the spectrum for prediction by expanding the navigation tree:



Note the **[Input data]** is filled in:

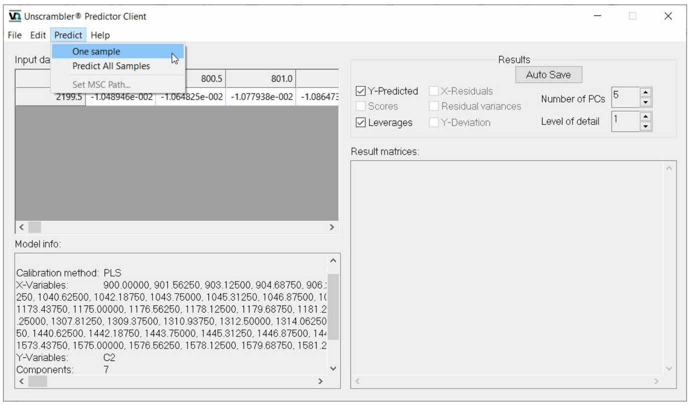


	800.0	800.5	801.0	
2199.5	-1.021194e-002	-1.036310e-002	-1.048660e-002	-1.05643:

```
Model Name:          W:\Process Spectroscopy\Software\Prediction Engin

Calibration method:  PLS
X-Variables:         900.00000, 901.56250, 903.12500, 904.68750, 906.:
250, 1040.62500, 1042.18750, 1043.75000, 1045.31250, 1046.87500, 1(
1173.43750, 1175.00000, 1176.56250, 1178.12500, 1179.68750, 1181.2
.25000, 1307.81250, 1309.37500, 1310.93750, 1312.50000, 1314.06250
50, 1440.62500, 1442.18750, 1443.75000, 1445.31250, 1446.87500, 14
1573.43750, 1575.00000, 1576.56250, 1578.12500, 1579.68750, 1581.2
Y-Variables:         C2
```

7 Click on **Predict ► One sample**:

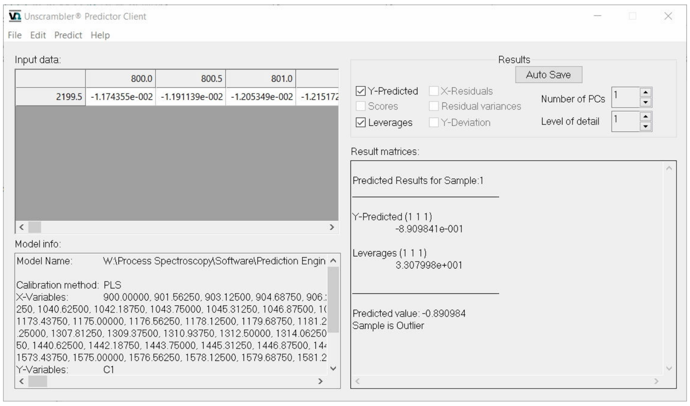


	800.5	801.0	
2199.5 -1.048946e-002	-1.064825e-002	-1.077938e-002	-1.08647

☑ Y-Predicted ☐ X-Residuals Number of PCs 5
☐ Scores ☐ Residual variances
☑ Leverages ☐ Y-Deviation Level of detail 1

```
Calibration method:  PLS
X-Variables:         900.00000, 901.56250, 903.12500, 904.68750, 906.:
250, 1040.62500, 1042.18750, 1043.75000, 1045.31250, 1046.87500, 1(
1173.43750, 1175.00000, 1176.56250, 1178.12500, 1179.68750, 1181.2
.25000, 1307.81250, 1309.37500, 1310.93750, 1312.50000, 1314.06250
50, 1440.62500, 1442.18750, 1443.75000, 1445.31250, 1446.87500, 14
1573.43750, 1575.00000, 1576.56250, 1578.12500, 1579.68750, 1581.2
Y-Variables:         C2
Components:          7
```

8 The outcome, whether the sample is an outlier or not, is displayed at the bottom right:



	800.0	800.5	801.0	
2199.5	-1.174355e-002	-1.191139e-002	-1.205349e-002	-1.215172

☑ Y-Predicted ☐ X-Residuals Number of PCs 1
☐ Scores ☐ Residual variances
☑ Leverages ☐ Y-Deviation Level of detail 1

```
Model Name:          W:\Process Spectroscopy\Software\Prediction Engin

Calibration method:  PLS
X-Variables:         900.00000, 901.56250, 903.12500, 904.68750, 906.:
250, 1040.62500, 1042.18750, 1043.75000, 1045.31250, 1046.87500, 1(
1173.43750, 1175.00000, 1176.56250, 1178.12500, 1179.68750, 1181.2
.25000, 1307.81250, 1309.37500, 1310.93750, 1312.50000, 1314.06250
50, 1440.62500, 1442.18750, 1443.75000, 1445.31250, 1446.87500, 14
1573.43750, 1575.00000, 1576.56250, 1578.12500, 1579.68750, 1581.2
Y-Variables:         C1
```

```
Predicted Results for Sample:1
________________________________

Y-Predicted (1 1 1)
        -8.909841e-001

Leverages (1 1 1)
        3.307998e+001

________________________________

Predicted value: -0.890984
Sample is Outlier
```

NOTICE

Note that batch prediction of multiple samples is not supported at the moment

6.9 Pre- and Post-Processing

Pre- and post-processing allows users to setup a parametric calibration equation. Parametric calibration predicts results from NIR spectra and a number of parameters, different for each sample.

For example, a standard equation applied to a sample spectrum will calculate the concentration of the component of interest. If the user is interested in the amount of the component, the result needs to be multiplied by the mass of the analyzed sample. Parametric equation will allow the operator to enter the independently measured sample mass during Routine Analysis, and will do the multiplication (post-processing) automatically.

It may be expected that the above example input data for calibration will consist of reference method results in the form of the amount of the component in each calibration sample, and the corresponding sample mass. Vision can calculate the concentration values in the step called pre processing (by dividing the amount by mass), and then proceed with calibration based on concentration.

More than one parameter can be used for pre- and post-processing. For example, calculation of the tablet adjusted potency involves tablet weight and thickness. The mathematical operation is not limited to multiplication and division. Subtraction and addition can also be used.

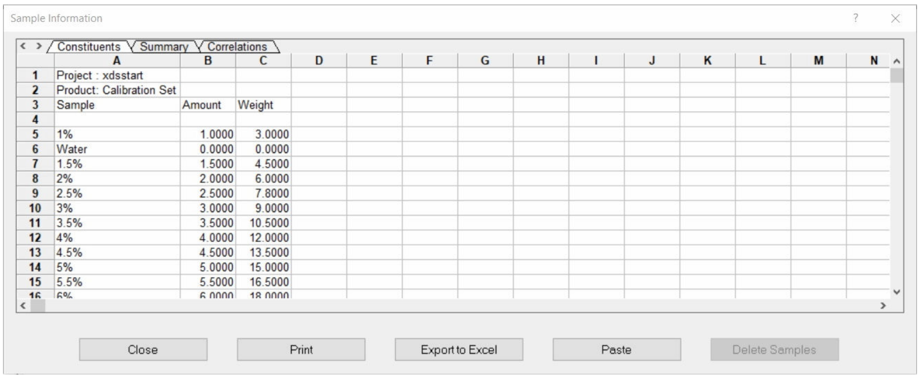
One can easily notice that pre and post processing steps are exactly opposite. Pre- and post-processing should be used in cases when a calibration cannot be developed directly, but the reference values can be transformed to a form directly related to the NIR spectrum.

Procedure for developing Pre-Processing equations:

(The following procedure lists steps for the above described example of predicting amount of the component in a sample by indirect measurement of concentration.)

1 The calibration development should start with collecting spectra of the calibration samples. For each sample the amount of the component and sample weight should be known. These should be entered into Vision as regular constituents.

After checking product constituent values, they should be displayed as shown below:

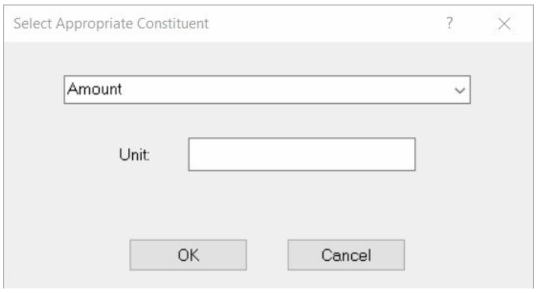


	A	B	C
1	Project : xdsstart		
2	Product: Calibration Set		
3	Sample	Amount	Weight
4			
5	1%	1.0000	3.0000
6	Water	0.0000	0.0000
7	1.5%	1.5000	4.5000
8	2%	2.0000	6.0000
9	2.5%	2.5000	7.8000
10	3%	3.0000	9.0000
11	3.5%	3.5000	10.5000
12	4%	4.0000	12.0000
13	4.5%	4.5000	13.5000
14	5%	5.0000	15.0000
15	5.5%	5.5000	16.5000
16	6%	6.0000	18.0000

2 The next step (pre-processing), will create a new constituent by combining the values of the Amount and Weight into Concentration.

Click on **Mode** ▶ **Quantitative Analysis** ▶ **Sample Selection**.

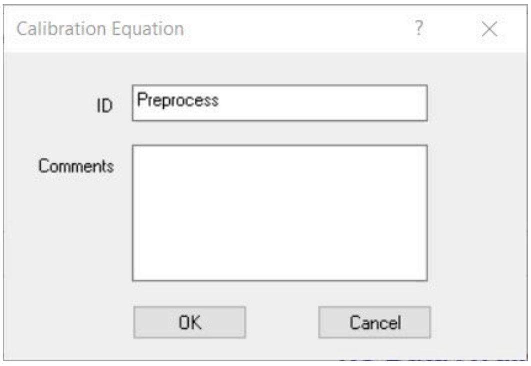
Drag and drop the product with calibration spectra to the **Equation** field. Select the constituent as shown:



Amount

Unit:

And the equation name:



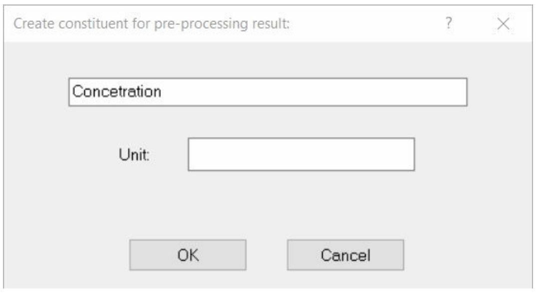
ID Preprocess

Comments

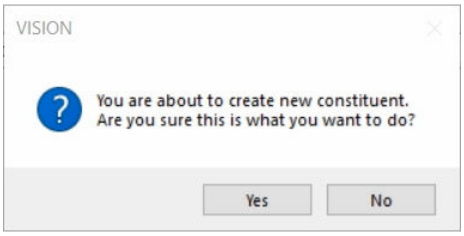
NOTICE

It is not important at this point to select any particular constituent

Click on **Select ▶ Create Equation for Pre-Processing**. If the menu item is not active, make sure the newly created equation is selected and highlighted. Vision displays a window. Type in the pre-processing constituent name, in our case Concentration.



Click on **[OK]** and confirm the creation of the new constituent.



VISION

You are about to create new constituent.
Are you sure this is what you want to do?

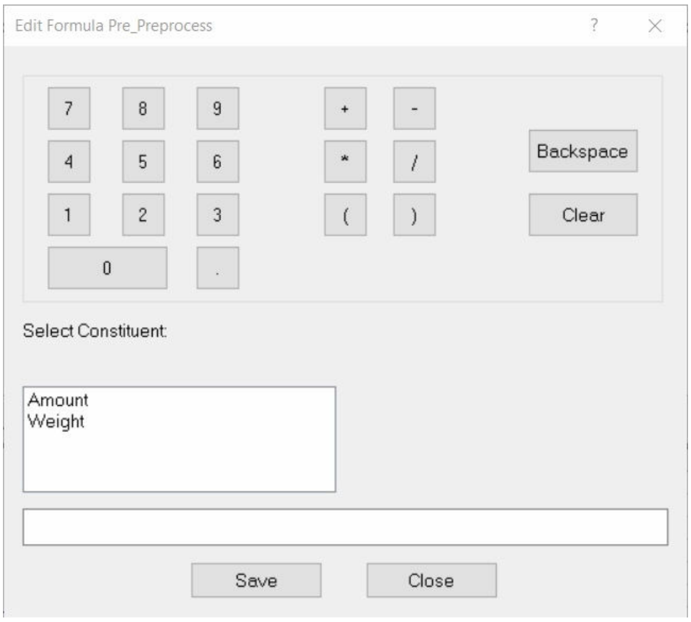
This will automatically save the equation. You will also notice that the equation name has been changed. A prefix Pre_ has been added, so now the equation name is Pre_PREPROCESS.

3 The next step is to define the pre-processing formula.

Click on **Mode ▶ Quantitative Analysis ▶ Regression**.

Select the equation and click on **Regression ▶ Adjust Constituent** (Pre-processing).

Vision will display the following window:

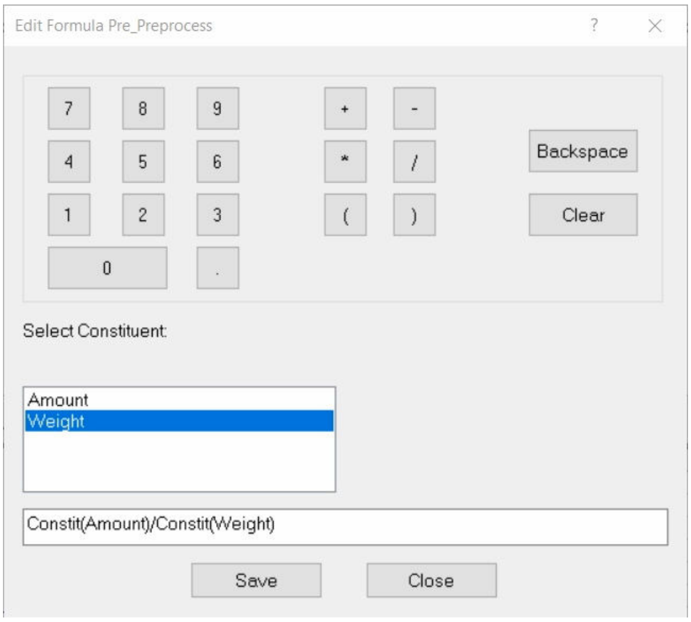


This window works as a calculator and can create formulas combining various constituents.

In our example dividing amount by weight creates the formula for concentration.

It can be entered by clicking on the **AMOUNT** constituent, then the **division symbol**, and finally the **WEIGHT** constituent.

The formula below will be shown:



Constit(Amount)/Constit(Weight)

Click on **[Save]** to save the formula and close the window.

4 Vision will display the spreadsheet with the new calculated constituent values.

Procedure for developing Post-Processing equations:

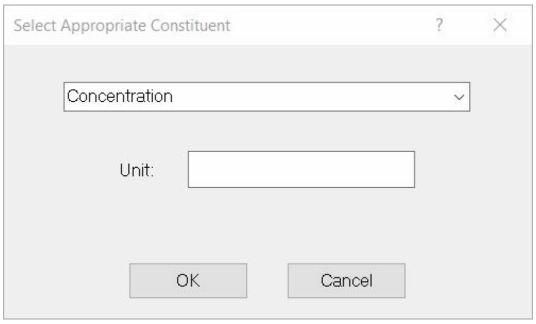
1 The next step consists of creating and developing a standard calibration based on spectral data and the new constituent **[Concentration]** created as the result of pre-processing.

In our example, the regression will be performed on spectra from product Calibration Set and constituent Concentration.

The regression can be done using either the MLR or PLS method. This step is discussed in other parts of the manual and will not be described here in detail.

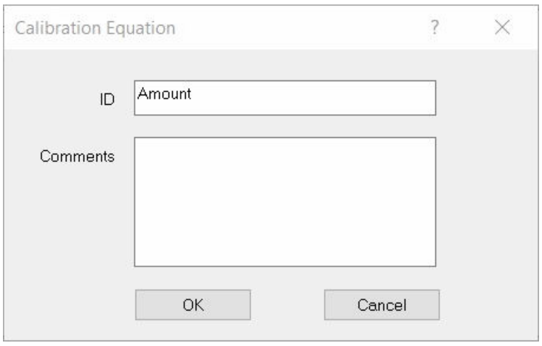
2 The post-processing equation needs to be created and configured.

Enter the **Quantitative Sample Selection** and drag product with calibration samples into the **Equation** field. Select the constituent Concentration and enter Amount as the equation name:



Concentration

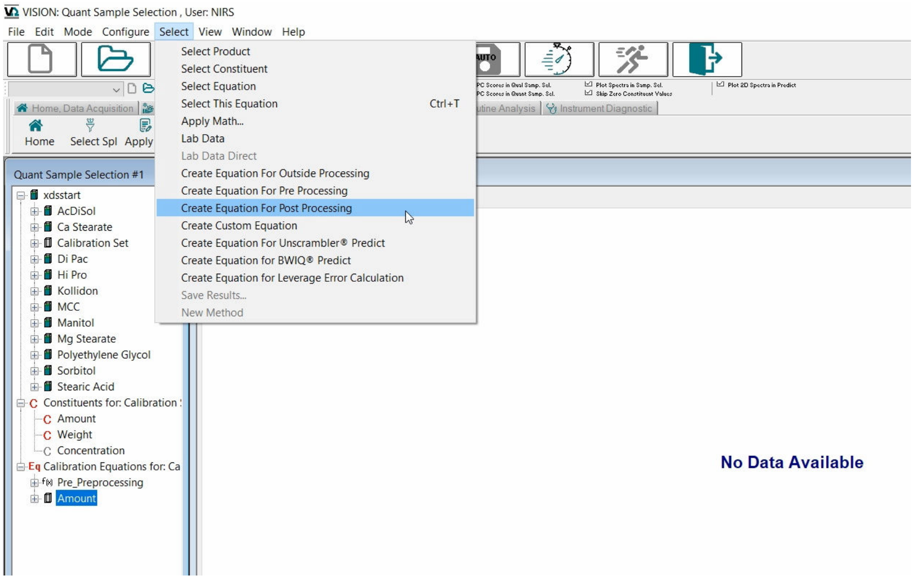
Unit:



ID: Amount

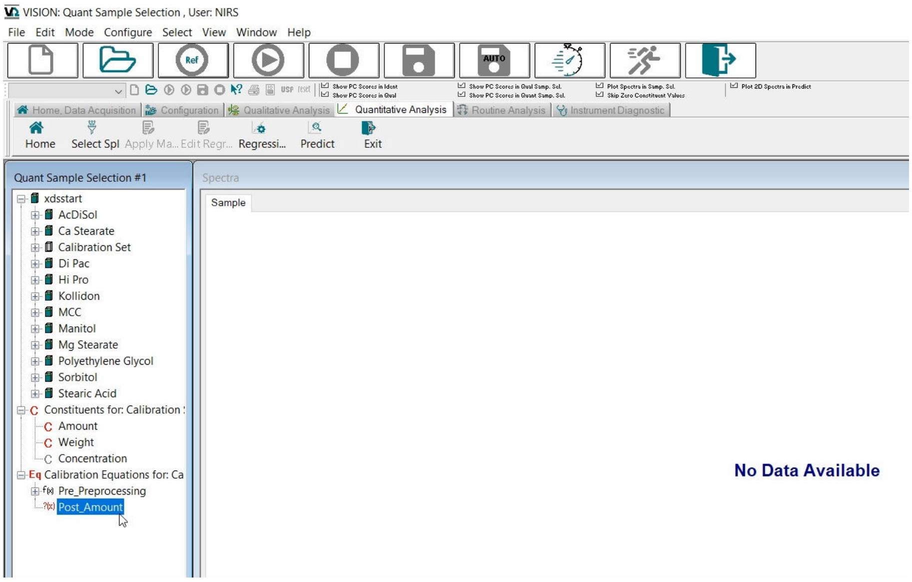
Comments:

Make sure the new equation is highlighted, and click on **Select ▶ Create Equation** for Post-Processing:



NOTICE

Note that Vision adds the prefix Post_ in front of the equation name



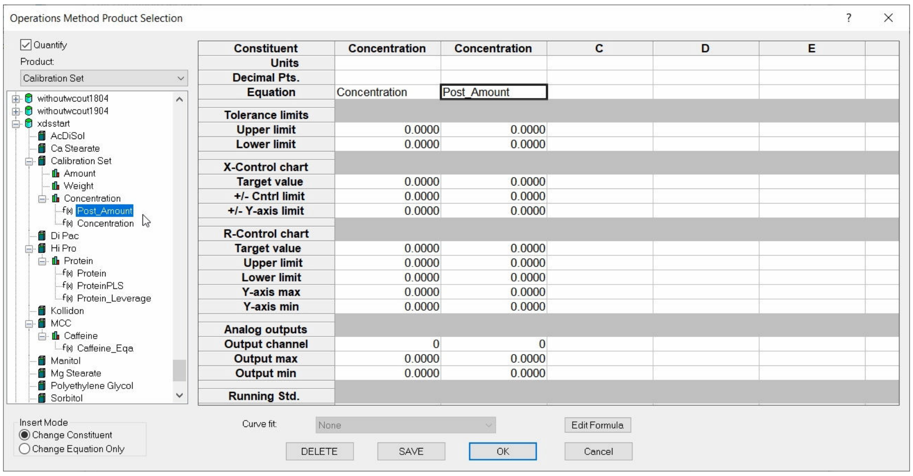
3 Proceed to **Operations Method** setup.

Configure the **Operations Method** as described in the appropriate part of the manual.

Click on **[Quant Setup]**. Select the product and expand the tree to find the equations created for product with calibration samples (please note that pre-processing equation is not listed).

Double-click first the standard equation (called CALIBRATION in this example), and then the post-processing equation. Click on **[Save]**.

The screen should look like this:



☑ Quantify

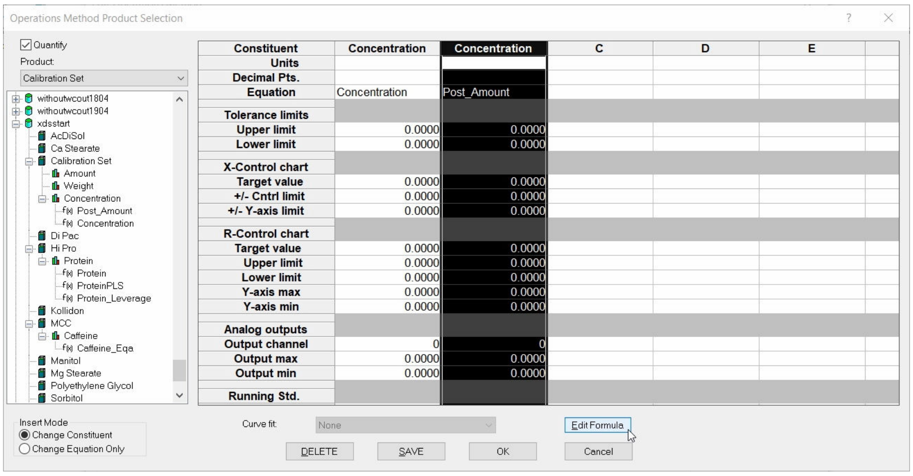
Product: Calibration Set

Constituent	Concentration	Concentration	C	D	E
Units					
Decimal Pts.					
Equation	Concentration	Post_Amount			
Tolerance limits					
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
X-Control chart					
Target value	0.0000	0.0000			
+/- Cntrl limit	0.0000	0.0000			
+/- Y-axis limit	0.0000	0.0000			
R-Control chart					
Target value	0.0000	0.0000			
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
Y-axis max	0.0000	0.0000			
Y-axis min	0.0000	0.0000			
Analog outputs					
Output channel	0	0			
Output max	0.0000	0.0000			
Output min	0.0000	0.0000			
Running Std.					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

4 Click on the spreadsheet header to highlight the column with the post-processing equation.



☑ Quantify

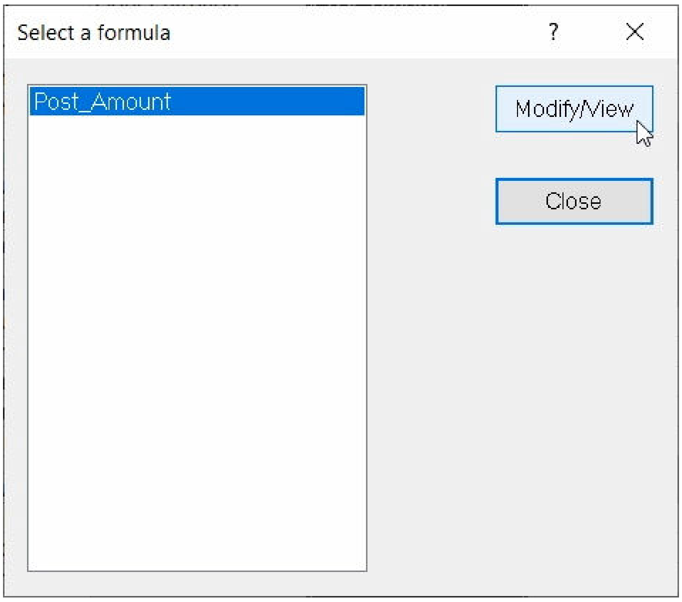
Product: Calibration Set

Constituent	Concentration	Concentration	C	D	E
Units					
Decimal Pts.					
Equation	Concentration	Post_Amount			
Tolerance limits					
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
X-Control chart					
Target value	0.0000	0.0000			
+/- Cntrl limit	0.0000	0.0000			
+/- Y-axis limit	0.0000	0.0000			
R-Control chart					
Target value	0.0000	0.0000			
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
Y-axis max	0.0000	0.0000			
Y-axis min	0.0000	0.0000			
Analog outputs					
Output channel	0	0			
Output max	0.0000	0.0000			
Output min	0.0000	0.0000			
Running Std.					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

Click on **[Edit Formula]**. Select the post-processing equation and click on **Modify ▶ View**.

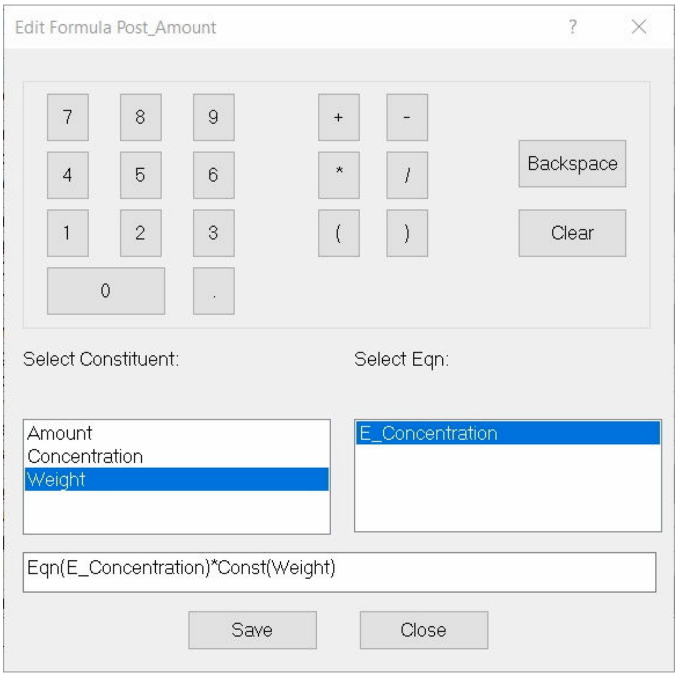


The windows that opens allows one to combine equations and constituents into a formula for post-processing.

In our example, the Amount will be calculated as a product of Concentration and Weight.

Click on E_Concentration (E_ denotes equation), multiplication operator, and the constituent Weight.

This is shown below:

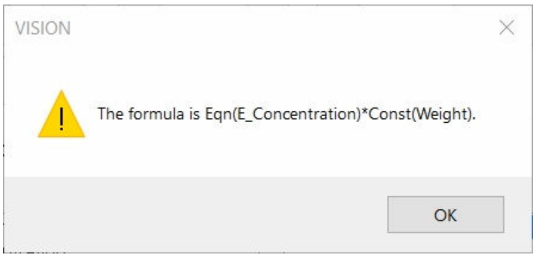


Select Constituent: Weight

Select Eqn: E_Concentration

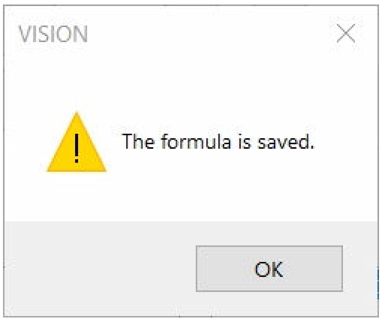
Eqn(E_Concentration)*Const(Weight)

5 Click on **[Save]** and close all windows.



VISION

The formula is Eqn(E_Concentration)*Const(Weight).



VISION

The formula is saved.

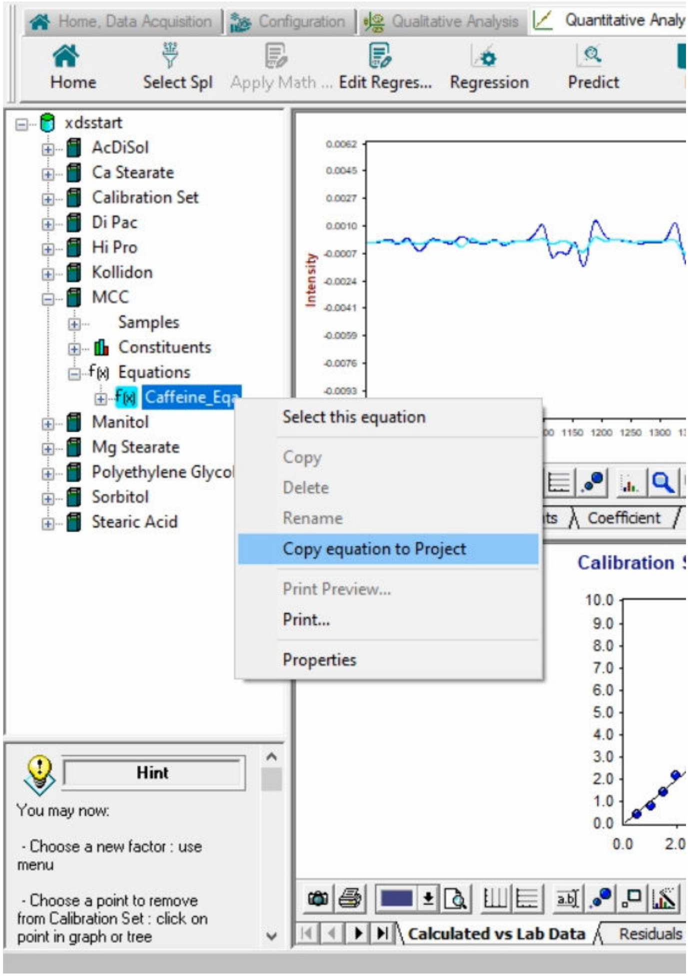
When the Routine Analysis is performed, Vision will display the box where the value of Weight needs to be entered. Amount calculation is based on this value, and the Concentration is calculated from a spectrum.

6.10 Copying Calibrations Between Projects

Calibrations can be copied between projects.

1. To copy a calibration, enter the **Quant Regression development** mode.

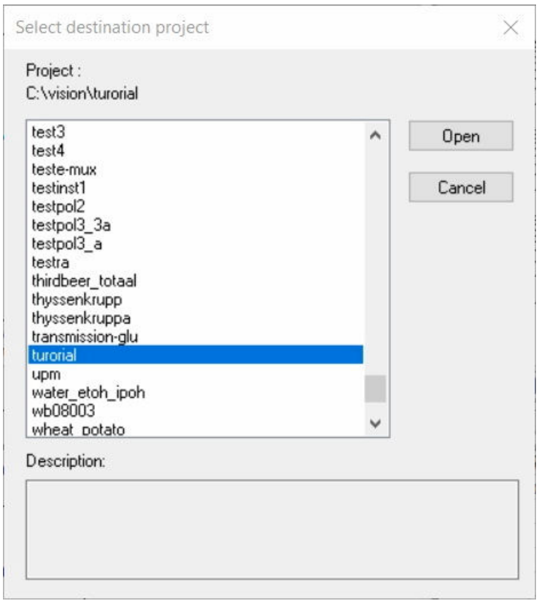
2. Select the equation to be copied, right-click on it, and click on **Copy Equation to Project**.



You may now:

- Choose a new factor : use menu

- Choose a point to remove from Calibration Set : click on point in graph or tree



Project :
C:\vision\turorial

test3
test4
teste-mux
testinst1
testpol2
testpol3_3a
testpol3_a
testra
thirdbeer_totaal
thyssenkrupp
thyssenkruppa
transmission-glu
turorial
upm
water_etoh_ipoh
wb08003
wheat_potato

Description:

3 Select the destination project. A calibration in the destination project will be overwritten if it exists. An empty product will be created in the destination project if necessary.

7 Routine Analysis Mode

7.1 Introduction

Routine Analysis combines data acquisition parameters with the library model and calibration equations for use in real time analysis or analysis of stored data.

All Routine Analysis parameters are brought together in the Operations Method. If those parameters come from both project database and library database, the library used within the Operation Method is linked permanently to the project database and can not be changed. In order to use a different library, the user has to create a new Operations Method. This is the case of calibration equation and multiplexer set up.

An Operations Method is used for qualitative and/or quantitative analysis of unknowns in real time or from stored data. Routine Analysis mode also allows the user to recall the results of all analyses done within a specific period of time.

A sample can be analyzed as an unknown or as a known product.

If a sample is analyzed as an unknown, it has to first be identified and qualified by the qualitative library. In the next step the sample spectrum can be optionally quantified by a calibration equation linked to the identified product.

If a sample is analyzed as a known product, it can be qualified by the library and then optionally quantified. In this mode of analysis the qualitative step can be skipped completely, and the known product just quantified by a calibration equation developed for this product.

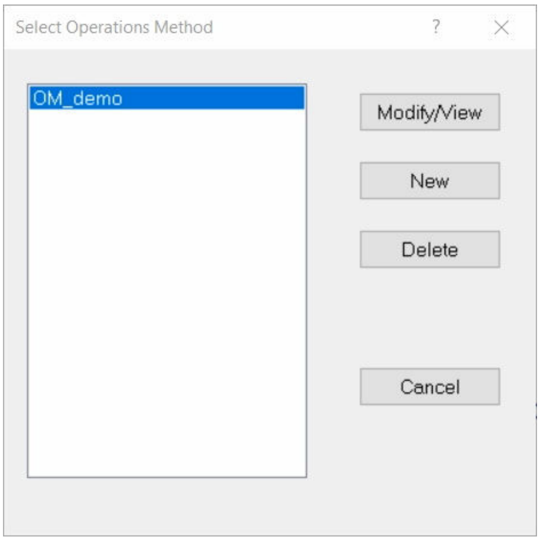
7.2 Operation Method Set-up

Since the Operations Method includes data acquisition parameters, it can be set up only from the Data Acquisition mode. There is a wizard available for creating an operations method, described later in this chapter.

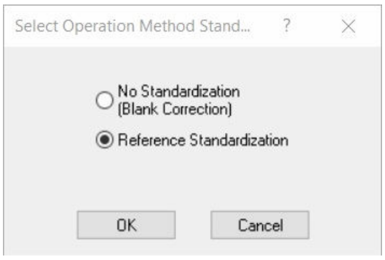
7.2.1 Preparation

1 If necessary, enter the **Data Acquisition** mode by clicking on **Mode ▶ Data Acquisition**.

2 Click on **Mode ▶ Routine Analysis ▶ Define Operations Method** to start the set up.



3 In the **Select Operations Method** dialog box click on **[New]** to configure a new method. You can also retrieve an existing method by highlighting its name on the list and clicking on **Modify ▶ View**.

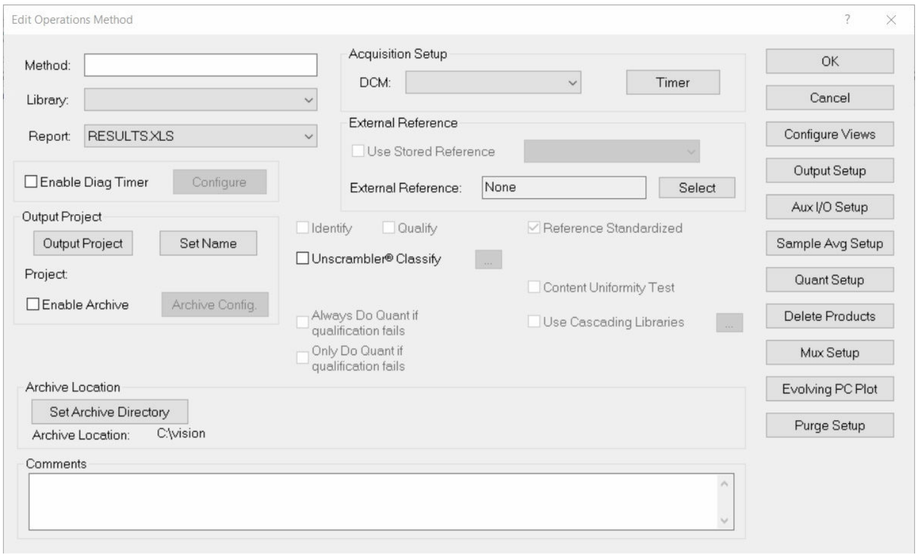


○ No Standardization (Blank Correction)
● Reference Standardization

Choose Standardization Method and click **[OK]**.

7.2.2 Operations Method Configuration

The blank **Edit Operations Method** dialog box appears.



Edit Operations Method

Method:

Library:

Report: RESULTS.XLS

External Reference: None

☑ Reference Standardized

Archive Location: C:\vision

The window contains a number of fields and buttons, which are outlined below.

Right before opening the **Edit Operations Method** dialog, Vision may display one or more error messages. This occurs when some Projects and/or Libraries have been deleted through Windows Explorer, and Vision cannot find them in locations specified in the Security Database. Never delete Vision Projects or Libraries using Windows Explorer.

Method Field

Enter the name of the Operations Method in this field.

Library Field

Select the library with qualitative methods from the drop-down list. Select **None** if only the quantitative analysis is to be performed.

Only libraries consistent with the standardization type chosen for the Operations Method are displayed.

Report Field

Select the report format from the drop-down list. The default format is RESULTS.XLS. It is used for single constituent quantification. Apart from this format, additional options exist:

- BATCHRXM.XLS – used for ReactSys (Batch Reaction Monitor)
- CUTEST.XLS – used with Multitab for Context Uniformity Test
- MUXRSLT.XLS – used with multiplexer for a single constituent
- MUXRSLTL.XLS - used with multiplexer for a single constituent and a Leverage or Unscrambler equation

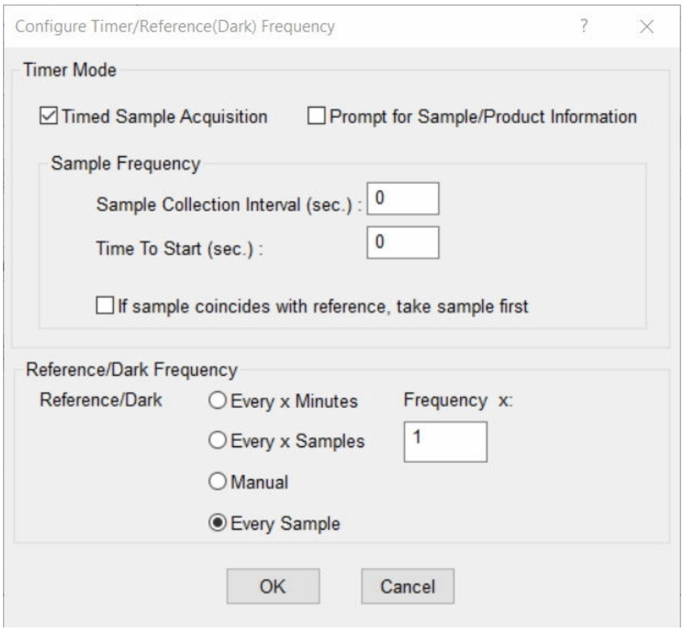
- MUXRSLT2.XLS - used with multiplexer for 2 constituents
- RESULTSL.XLS – used for 1 constituent with a Leverage or Unscrambler equation (single point system)
- RESULTS2.XLS – used for 2 constituents (single point system)
- RESULTSBWIQ.XLS– used for BWIQ equation (single point system)
- RESCOMM.XLS – displays sample comment in the prediction table
- RESHORT – does not include Details page

For number of constituents not listed above, use a report with the number of constituent higher than required. The list box displays also templates used for reporting diagnostics results.

Acquisition Setup Field

Acquisition Setup field configures the acquisition parameters:

1 Click on **[Timer]** to program the data acquisition timer for continuous or non-continuous data collection.



Configure Timer/Reference(Dark) Frequency

Timer Mode

☑ Timed Sample Acquisition
☐ Prompt for Sample/Product Information

Sample Frequency

Sample Collection Interval (sec.) : 0
Time To Start (sec.) : 0
☐ If sample coincides with reference, take sample first

Reference/Dark Frequency

Reference/Dark
○ Every x Minutes
○ Every x Samples
○ Manual
● Every Sample
Frequency x: 1

The timer option allows configuration of Vision for the Sample Frequency, Timer Mode and Reference Frequency.

[Timer Mode]: check the Timed Sample Acquisition box for continuous sample analysis. If this box is not checked, Vision will analyze only a single sample at a time.

[Sample Frequency]: enter interval between samples in seconds, or “0” for no delay **[Sample Collection Interval (sec)]**. Do not check the “If coincident, take sample first” box.

[Time to Start (sec)]: enter a time in this box to set a delay prior to sample analysis.

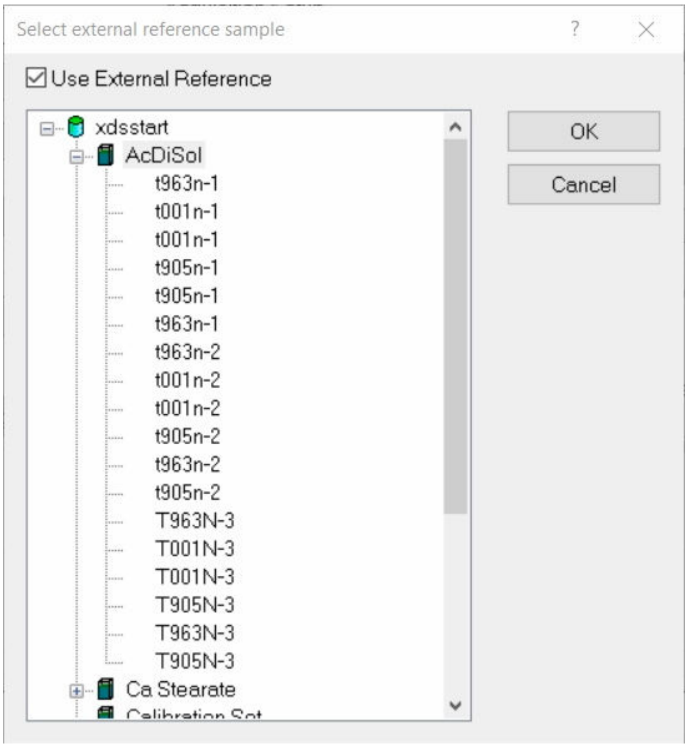
[Reference Frequency]: in this field, the method in which the reference spectrum is acquired can be configured. Typically, “Every Sample” is collected, however the reference can be acquired “Manually” or by “Every X Minutes” or “Every X Samples”, where X is specified in the “Frequency X” box.

2 Choose **Data Collection Method** from the drop-down list in the **DCM** field. Only DCMs consistent with the standardization type are displayed.

External Reference Field

1 If a stored reference exists in the project, you can select it after checking the **Use Stored Reference** check box.

2 Optionally select an external reference:



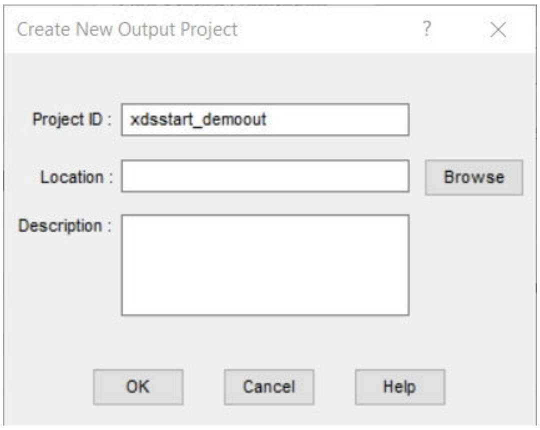
Select external reference sample

☑ Use External Reference

- xdsstart
  - AcDiSol
    - t963n-1
    - t001n-1
    - t001n-1
    - t905n-1
    - t905n-1
    - t963n-1
    - t963n-2
    - t001n-2
    - t001n-2
    - t905n-2
    - t963n-2
    - t905n-2
    - T963N-3
    - T001N-3
    - T001N-3
    - T905N-3
    - T963N-3
    - T905N-3
  - Ca Stearate

Output Project Field

1 Click on **Output Project** to create an output project. Output projects store saved spectra and results from Routine Analysis. You can create a new output project or use an existing one.



Project ID : xdsstart_demoout

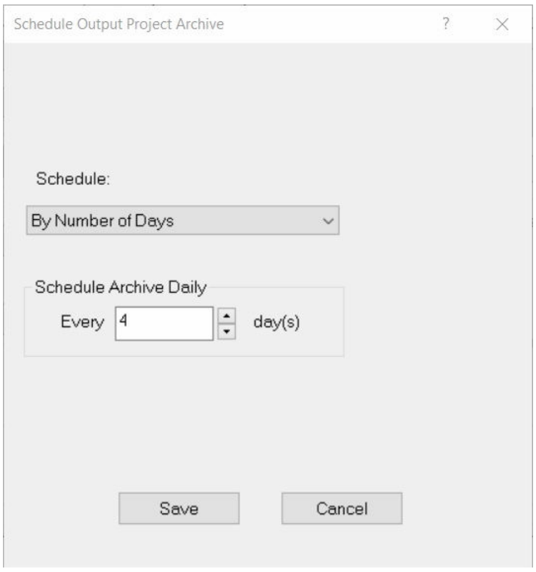
Location :

Description :

2 Select **Enable Archive** to configure the archiving scheduler.

The scheduler makes it possible to automatically archive the output project on a timely basis without interrupting Routine Analysis. During scheduled archiving the existing output project is emptied, and the archive ZIP file is saved into the Vision installation folder. The name of the archive file includes the name of the output Project, and date and time of archiving.

3 Clicking on **Archive Configuration** displays the scheduler.



Schedule: By Number of Days

Schedule Archive Daily

Every 4 day(s)

4 Select the appropriate frequency, and click on **[Save]** and then on **[Close]**.

NOTICE

If automatic archiving is to be used, the spectra in Routine Analysis cannot be acquired continuously. There must be a delay between spectra. The archiving scheduler does not work when analyzing stored data.

If you are using the acquisition timer, you must allow a delay between samples, for archiving to occur. Use Timer dialog to set delay.

Identify, Qualify, Always do Quant, Only do Quant, Reference Standardized, Master Standardized, Content Uniformity check boxes

- Select the desired combination of qualitative analysis options including Identification, and/or Qualification.

☑ Identify ☑ Qualify

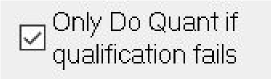
Leave all boxes blank if only quantitative analysis is to be performed.

- If the **Always Do Quant if Qualification Fails** option is selected, Vision will perform quantitative predictions even if qualification fails.

☑ Always Do Quant if qualification fails

The **Always Do Quant** option becomes active only after a calibration is connected to a product.

- If the **Only Do Quant if Qualification Fails** option is selected, Vision will perform quantitative predictions only when qualification fails.



☑ Only Do Quant if qualification fails

- Check **Reference Standardized** box if your methods are reference standardized. All elements of the Operation Method (DCM, qualitative, and quantitative methods) should have the same standardization type.


☑ Reference Standardized

- If the **Use Cascading Libraries** box is checked, the selected Cascading libraries are activated. To select the libraries, click on the icon with the 3 dots on the right side of the check box.


☑ Use Cascading Libraries

- If **Content Uniformity Test** is checked, Vision will perform the test automatically. This option requires a Multi-Tab Data Collection Method, and use of the Multi-Tab Analyzer.

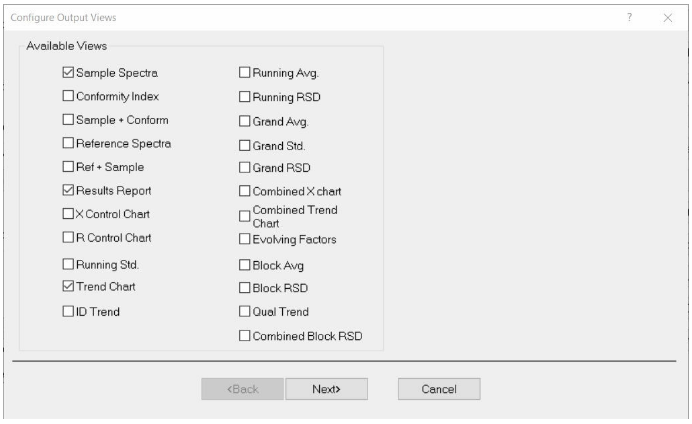

☐ Content Uniformity Test

Comments Field

Comments field allows to enter a comment or description of the Operations Method:

Configure Views Button

1 Click on **[Configure Views]** to select the **Routine Analysis** output screen and report:


Configure Output Views

Available Views

☑ Sample Spectra
☐ Conformity Index
☐ Sample + Conform
☐ Reference Spectra
☐ Ref + Sample
☑ Results Report
☐ X Control Chart
☐ R Control Chart
☐ Running Std.
☑ Trend Chart
☐ ID Trend
☐ Running Avg.
☐ Running RSD
☐ Grand Avg.
☐ Grand Std.
☐ Grand RSD
☐ Combined X chart
☐ Combined Trend Chart
☐ Evolving Factors
☐ Block Avg
☐ Block RSD
☐ Qual Trend
☐ Combined Block RSD

2 Select up to 8 views from the list and click on **[Next]**.

- ☑ Sample Spectra
- ☐ Conformity Index
- ☐ Sample + Conform
- ☐ Reference Spectra
- ☐ Ref + Sample
- ☑ Results Report
- ☐ X Control Chart
- ☐ R Control Chart
- ☐ Running Std.
- ☑ Trend Chart
- ☐ ID Trend
- ☐ Running Avg.
- ☐ Running RSD
- ☐ Grand Avg.
- ☐ Grand Std.
- ☐ Grand RSD
- ☐ Combined X chart
- ☐ Combined Trend Chart
- ☐ Evolving Factors
- ☐ Block Avg
- ☐ Block RSD
- ☐ Qual Trend
- ☐ Combined Block RSD

Pick Layout: ○ ●

3 Choose the layout of the views by clicking on the view in the list, and then on the proper rectangle representing the view location.

4 Click on **[Next]** and **[Finish]** buttons to return to the wizard.

The following views are available for display:

- **Sample Spectra** – displays last acquired sample spectra.
- **Conformity Index** – displays conformity index spectrum from the qualification step if maximum distance is used as a qualification method. If Mahalanobis distance or Residual Variance is used as a qualification method, the view displays residual spectrum (the part not modeled by PC method). If correlation or no qualification method is used, or sample spectrum does not pass identification, the display is empty.
- **Sample + Conformity Index** – displays last acquired sample spectrum and conformity index spectrum on one plot.
- **Reference Spectra** – displays last acquired reference spectrum.
- **Reference + Sample Spectra** – displays last acquired reference and sample spectra on one plot.
- **Results Report** – displays the report with Routine Analysis results.
- **X Control Chart** – displays the average differences control chart. The chart has to be configured in Quant Setup.
- **R Control Chart** – displays the range of differences control chart. The chart has to be configured in Quant Setup.
- **Running Standard Deviation** – displays the control chart with running standard deviation. The chart has to be configured in Quant Setup.
- **Trend Chart** – displays predicted results vs. time chart. The chart has to be configured in Quant Setup.
- **ID Trend** – displays the trend chart of predicted ID values.
- **Running Average** – displays the control chart with running average. The chart has to be configured in Quant Setup.

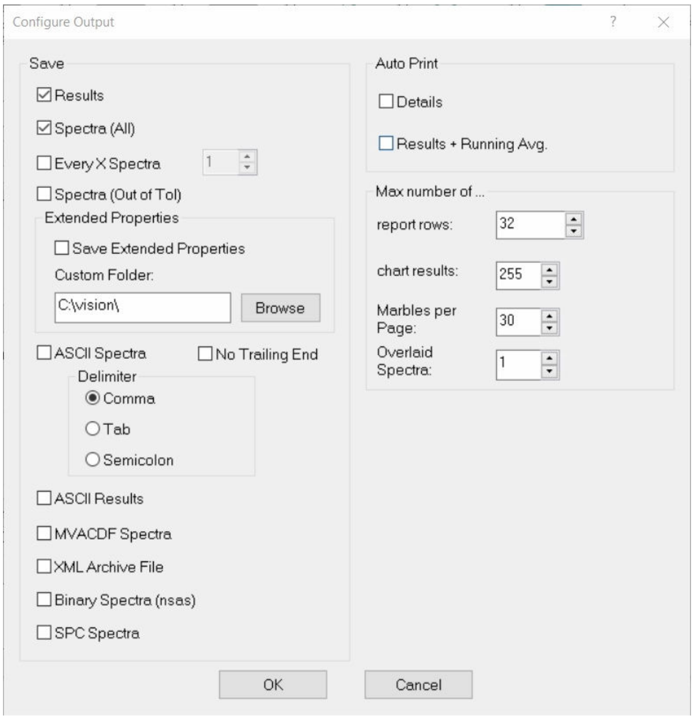
- **Running Residual Standard Deviation** – displays the control chart with residual standard deviation. The chart has to be configured in Quant Setup.
- **Grand Average** – displays the control chart with grand average. The chart has to be configured in Quant Setup.
- **Grand Standard Deviation** – displays the control chart with grand standard deviation. The chart has to be configured in Quant Setup.
- **Grand Residual Standard Deviation** - displays the control chart with grand residual standard deviation. The chart has to be configured in Quant Setup.
- **Combined X Chart** – displays single average differences control chart for all constituents in the selected product. The chart has to be configured in Quant Setup.
- **Combined Trend Chart** - displays single results vs. time chart for all constituents in the selected product. The chart has to be configured in Quant Setup.
- **Evolving Factors** – displays Evolving Factors plot. The plot has to be configured from Operations Method setup window.
- **Block Average** - displays the control chart with averages calculated on blocks of results. The chart has to be configured in Quant Setup.
- **Block RSD** - displays the control chart with Residual Standard Deviation calculated on blocks of results. The chart has to be configured in Quant Setup.
- **Qual Trend** - displays the trend chart of predicted Qual values.
- **Combined Block RSD** - displays the control chart with Residual Standard Deviation calculated on blocks of results for all constituents in the selected product. The chart has to be configured in Quant Setup.

Trend Chart with End Point Estimation

Trend chart can be used to estimate the end point of a batch reaction. When the trend chart is used for this purpose, Vision fits a pre-defined curve (straight line, exponent, or parabola) to the block of last acquired analytical results (the size of the block is configured by the user). Then Vision extrapolates the curve and calculates the time left to reach the end point (target value). The calculated time is displayed on the trend chart.

To configure Vision for end point estimation:

1 Click on **[Output Setup]** button to configure items to be saved, displayed, and printed during routine analysis.


Configure Output

Save

☑ Results

☑ Spectra (All)

☐ Every X Spectra 1

☐ Spectra (Out of Tol)

Extended Properties

☐ Save Extended Properties

Custom Folder: C:\vision\

☐ ASCII Spectra ☐ No Trailing End

Delimiter

● Comma

○ Tab

○ Semicolon

☐ ASCII Results

☐ MVACDF Spectra

☐ XML Archive File

☐ Binary Spectra (nsas)

☐ SPC Spectra

Auto Print

☐ Details

☐ Results + Running Avg.

Max number of ...

report rows: 32

chart results: 255

Marbles per Page: 30

Overlaid Spectra: 1

2 In the **Save** field, click on the appropriate boxes for desired information such as results, all spectra, spectra out of tolerance, ASCII spectra, ASCII results, and others. Results and spectra are saved in the output project. MVACDF spectra, binary (NSAS) spectra, ASCII results, ASCII spectra, and SPC spectra are saved in the output project folder (one per analysis). Archiving in the XML format requires the DTD file (definition of the XML file format) to reside on the computer and the path to this file to be defined in Account Policy window.

In the **Auto Print** field, check the appropriate options. You can automatically print a general results report with running average and/or details report.

Maximum number of report rows defines the number of samples analyzed before the Results page prints. When the report reaches this number, the results table maintains a constant size.

Maximum number of chart results defines the maximum number of result points displayed on trend chart and control charts. After reaching this number, the chart starts to scroll.

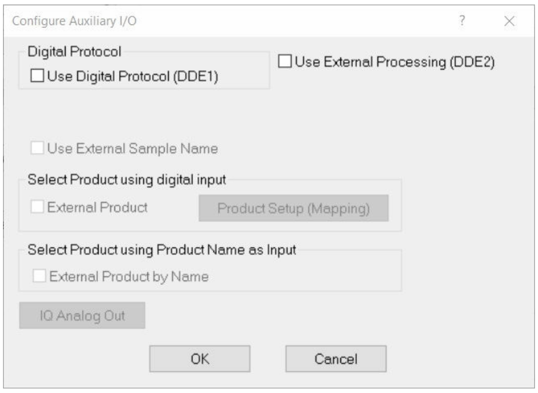
Maximum number of marbles defines the maximum number of result points displayed on standard deviation, RSD, and average charts. After reaching this number, the chart starts to scroll.

Aux I/O Setup Button

Configure Auxiliary I/O dialog define data exchange protocol with process control or data archiving systems in order to establish one- or two-way communication with device such as Distributed Control System (DCS) or Programmable Logical Controller (PLC).

Through Auxiliary I/O Vision supports analog protocols such as 4 - 20 mA, or multiple digital protocols such as OPC, Modbus, or Profibus. For complete list of supported protocols please contact Metrohm representative. Auxiliary I/O also can provide communication through Vision ActiveX control with third party software capable of supporting ActiveX. Please contact Metrohm representative for details.

Please note that external communication is not included in the basic Vision package and requires purchase of additional software or hardware. Please contact Metrohm representative for details.

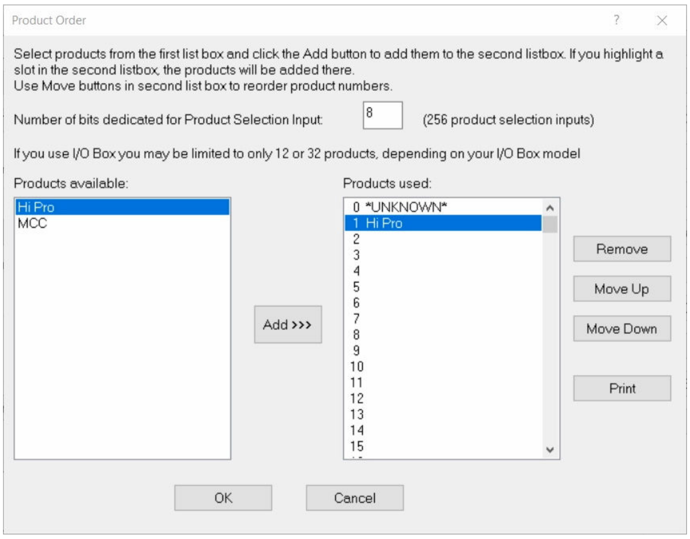


Use **Digital Protocol (DDE1.1)** box must be checked in order to use external communication with any digital or analog protocol.

Use **Digital Protocol (DDE1.2)** and **Use External Processing (DDE2)** boxes should not be checked in most situations. This communication channel is used for custom software development, where acquired spectrum needs to be moved outside Vision for processing by external software, and the calculated result passed back to Vision to be displayed and saved in Vision database. Please contact Metrohm representative for more details.

Use External Sample Name box becomes active when one of the protocols is selected. This option allows passing the sample name from external software or process control system to Vision through digital protocol or ActiveX (not available for analog 4 - 20 mA communication).

External Product box becomes active when one of the protocols is selected. This option allows external software or process control system to define product to be analyzed by a specific calibration equation attached to this product in Vision Routine Analysis. In order to link the product name to a specific number, click on **[Product Setup]** Button. The following Window opens:


Product Order

Select products from the first list box and click the Add button to add them to the second listbox. If you highlight a slot in the second listbox, the products will be added there.
Use Move buttons in second list box to reorder product numbers.

Number of bits dedicated for Product Selection Input: 8 (256 product selection inputs)

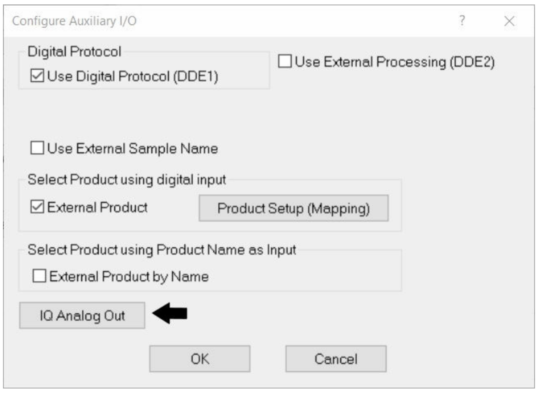
If you use I/O Box you may be limited to only 12 or 32 products, depending on your I/O Box model

Products available:
- Hi Pro
- MCC

Products used:
- 0 *UNKNOWN*
- 1 Hi Pro
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15

The list of Products Available displays all products with calibration attached. Select a product and click **[Add]** to link the product with the next available number. Click on **[OK]** when done. This option can be used with both digital protocols and analog communication.

IQ Analog Out is used to configure identification and qualification results for analog 4 - 20 mA communication. After clicking the button the following window opens:


Configure Auxiliary I/O

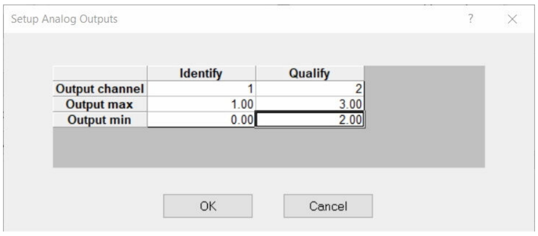
Digital Protocol
☑ Use Digital Protocol (DDE1)

☐ Use External Processing (DDE2)

☐ Use External Sample Name

Select Product using digital input
☑ External Product

Select Product using Product Name as Input
☐ External Product by Name


Setup Analog Outputs

	Identify	Qualify
Output channel	1	2
Output max	1.00	3.00
Output min	0.00	2.00

Select the output channel for Identification or/and Qualification and enter scaling factors. In the example above, the Identification result is passed out on Channel 1, and it is scaled so the match value of 0.0 corresponds to 4 mA, and the match value of 1.0 corresponds to 20 mA.

Configuring Auxiliary I/O is described in more detail in Vision I/O Module manual and in Digital Protocols manuals.

Sample Avg Setup Button

Click on this button to display **Configure Sample Averaging** dialog. This dialog allows you to define how many spectra will be averaged for further processing.

N Samples In Average field defines the number of spectra that will be averaged before qualitative and/or quantitative results are calculated.

If the **Average N good samples** or **Average good samples out of N taken** option is chosen, Vision applies the identification method first. Only the samples that pass identification are averaged, samples that fail are rejected.

In the **Group** field define the number of results to be averaged before displayed on the control chart.

Moving Average defines the number of results used to calculate moving average and moving standard deviations.

Block Avg/RSD defines the number of results used to calculate block average and block Residual Standard Deviations.

Vision also offers the calculation of grand average and grand standard deviation. Those parameters do not reset by stopping Routine Analysis or exiting Vision. To reset them, click on **Mode ▶ Routine Analysis ▶ Reset**.

Quant Setup Button

If a library has been selected in the Library field of the Edit Operations Method dialog box, you can attach calibration equations from all projects to any product from this library. If no library has been selected, you can attach calibration equations from any project to any product from the active project.

NOTICE

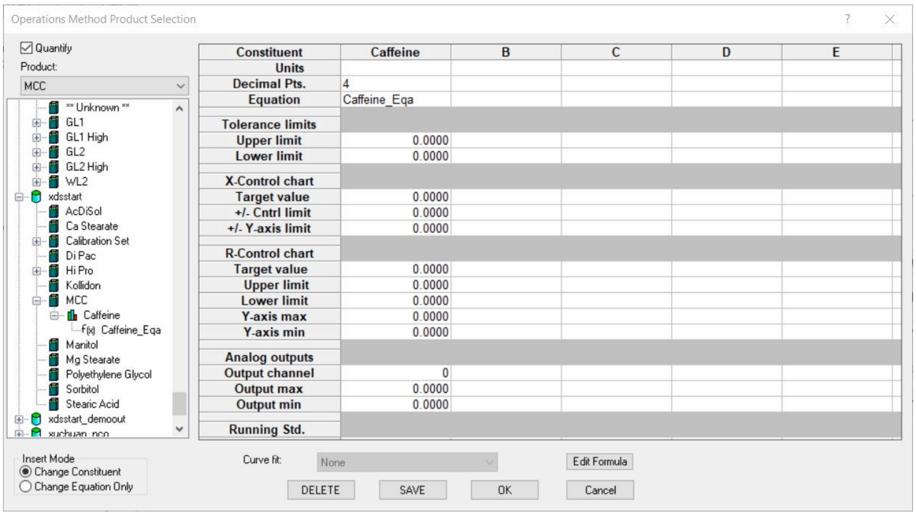
Once a calibration equation is connected to a library in the Operations Method, you will not be able to change the library specified for this method

NOTICE

Leverage or Unscrambler equations require extra setup steps. Make sure to read the respective procedures carefully

Vision Quant Equations

1 Click on **[Quant Setup]** to attach calibration equations to library or project database products. The **Operations Method Product Selection** window appears.



Constituent	Caffeine	B	C	D	E
Units					
Decimal Pts.	4				
Equation	Caffeine_Eqa				
Tolerance limits					
Upper limit	0.0000				
Lower limit	0.0000				
X-Control chart					
Target value	0.0000				
+/- Cntrl limit	0.0000				
+/- Y-axis limit	0.0000				
R-Control chart					
Target value	0.0000				
Upper limit	0.0000				
Lower limit	0.0000				
Y-axis max	0.0000				
Y-axis min	0.0000				
Analog outputs					
Output channel	0				
Output max	0.0000				
Output min	0.0000				
Running Std.					

2 From the Product drop-down list select a product from the selected library or the active project.

3 Expand the tree with projects below and double-click on the equation you want to link to the product.

4 Click on the letter designating the empty column to highlight the whole column and then double-click on the new equation in the project tree, if you want to add more equations.

5 To enter the tolerance limits and control chart parameters, click on the proper cell of the spreadsheet and typing in the numbers.

6 To replace the existing equation, click on the constituent name to highlight the whole column and then double-click on the new equation in the project tree. Select the **Insert Mode** from the field below the tree. If you are in the **Change Constituent** mode, the whole equation is replaced. If you are in the **Change Equation Only** mode, the constituent name is not replaced.

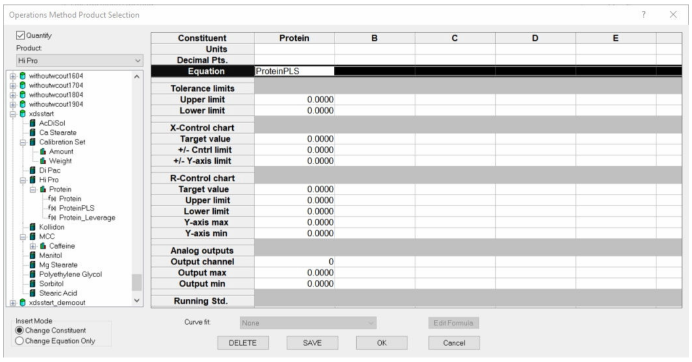
7 To delete an equation from a product, click on the constituent name to highlight the whole column and then click on **[Delete]**.

8 Click on **[Save]** to complete the links and on **[Done]** to close the window.

Only the equations consistent with the selected DCM and standardization type are displayed and can be connected to a product.

Vision Leverage Equations

1 In the **[Quant Setup]**, double-click on the PLS equation **[ProteinPLS]** for which the Leverage equation was created at a posterior step:



☑ Quantify

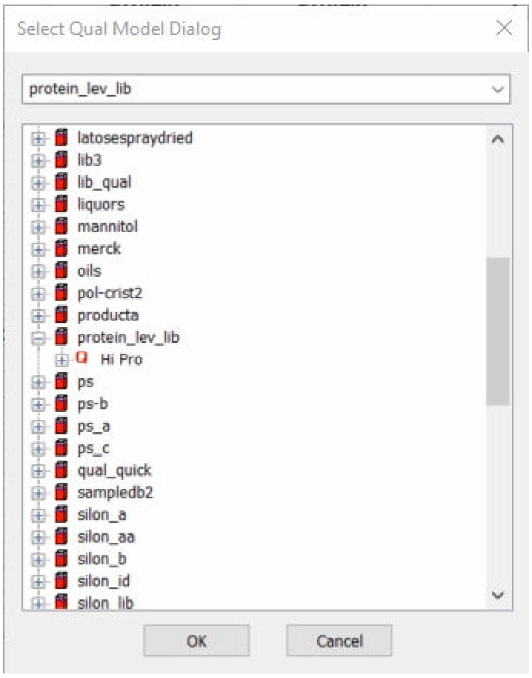
Product: Hi Pro

Constituent	Protein	B	C	D	E
Units					
Decimal Pts.					
Equation	ProteinPLS				
Tolerance limits					
Upper limit	0.0000				
Lower limit	0.0000				
X-Control chart					
Target value	0.0000				
+/- Cntrl limit	0.0000				
+/- Y-axis limit	0.0000				
R-Control chart					
Target value	0.0000				
Upper limit	0.0000				
Lower limit	0.0000				
Y-axis max	0.0000				
Y-axis min	0.0000				
Analog outputs					
Output channel	0				
Output max	0.0000				
Output min	0.0000				
Running Std.					

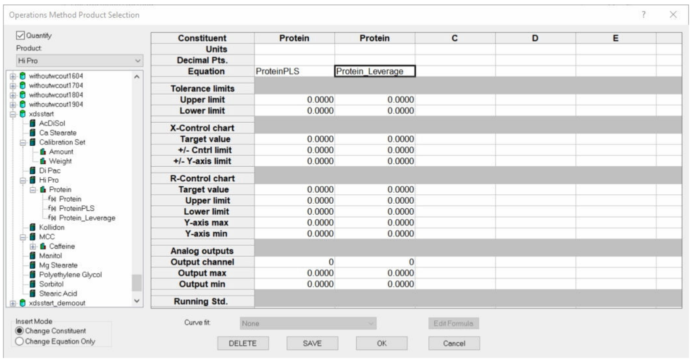
Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

2 Next, double-click on the Protein_Leverage equation. Select the correct library **[protein_lev_lib]** and click on the correct equation. Make sure the **[Q]** is displayed:



3 The Leverage equation is now in the second column. The user can configure tolerance limits, control charts limits as well as analog output, if desired.



☑ Quantify

Product: Hi Pro

Constituent	Protein	Protein	C	D	E
Units					
Decimal Pts.					
Equation	ProteinPLS	Protein_Leverage			
Tolerance limits					
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
X-Control chart					
Target value	0.0000	0.0000			
+/- Cntrl limit	0.0000	0.0000			
+/- Y-axis limit	0.0000	0.0000			
R-Control chart					
Target value	0.0000	0.0000			
Upper limit	0.0000	0.0000			
Lower limit	0.0000	0.0000			
Y-axis max	0.0000	0.0000			
Y-axis min	0.0000	0.0000			
Analog outputs					
Output channel	0	0			
Output max	0.0000	0.0000			
Output min	0.0000	0.0000			
Running Std.					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

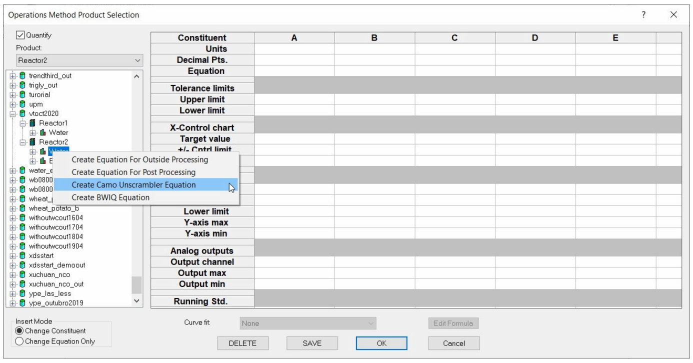
Click **[OK]** and Save.

NOTICE

Make sure to use the correct report to be able to visualise properly the leverage results during Routine Analysis mode

Unscrambler X Equations

1 Click on **[Quant Setup]**. Navigate in the project of interest, to the constituent to be used for prediction. Right-click on the constituent node and click on **[Create Unscrambler Equation]**:



☑ Quantify

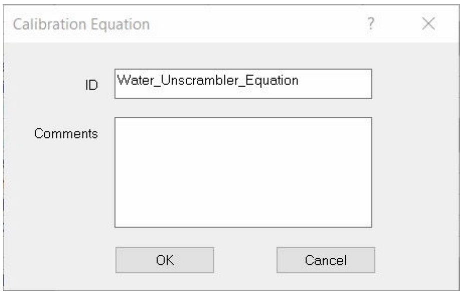
Product: Reactor2

trendthird_out
trigly_out
turorial
upm
vtoct2020
Reactor1
Water
Reactor2
withoutwcout1604
withoutwcout1704
withoutwcout1804
withoutwcout1904
xdsstart
xdsstart_demoout
xuchuan_nco
xuchuan_nco_out
ype_las_less
ype_outubro2019

Insert Mode
● Change Constituent
○ Change Equation Only

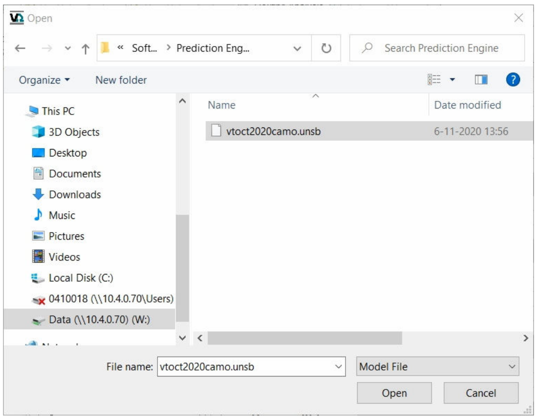
Curve fit: None

2 Provide a name for the equation and click **[OK]**:



ID: Water_Unscrambler_Equation

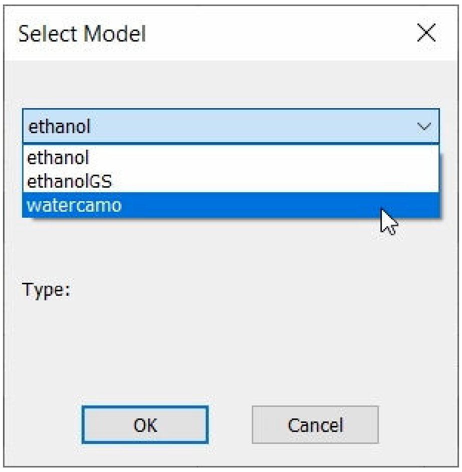
3 Select the unsb file you created with the Unscrambler software, click **[Open]**, and select the model from the drop-down list:



Name	Date modified
vtoct2020camo.unsb	6-11-2020 13:56

File name: vtoct2020camo.unsb

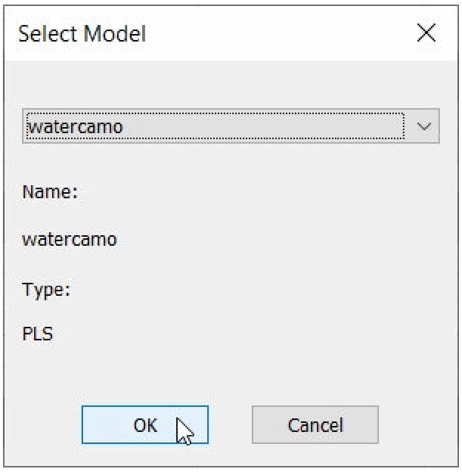
Model File



Select Model

ethanol

Type:



watercamo

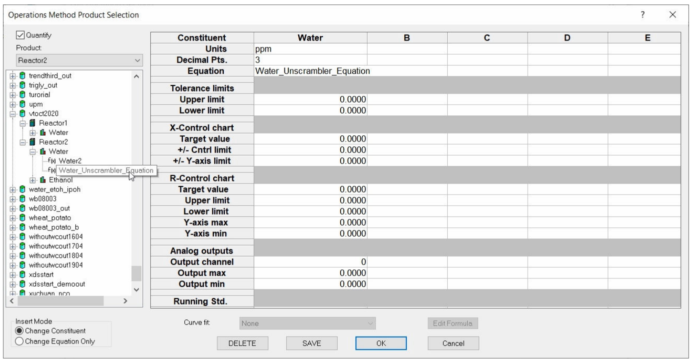
Name:

watercamo

Type:

PLS

4 The equation appears in the first column on the right:



☑ Quantify

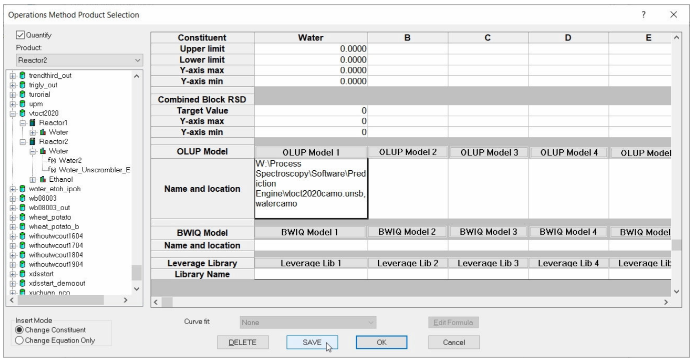
Product: Reactor2

Constituent	Water	B	C	D	E
Units	ppm				
Decimal Pts.	3				
Equation	Water_Unscrambler_Equation				
Tolerance limits					
Upper limit	0.0000				
Lower limit	0.0000				
X-Control chart					
Target value	0.0000				
+/- Cntrl limit	0.0000				
+/- Y-axis limit	0.0000				
R-Control chart					
Target value	0.0000				
Upper limit	0.0000				
Lower limit	0.0000				
Y-axis max	0.0000				
Y-axis min	0.0000				
Analog outputs					
Output channel	0				
Output max	0.0000				
Output min	0.0000				
Running Std.					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

Scroll down until you can see **[OLUP Model]** and verify that the correct model is selected:



Operations Method Product Selection

☑ Quantify

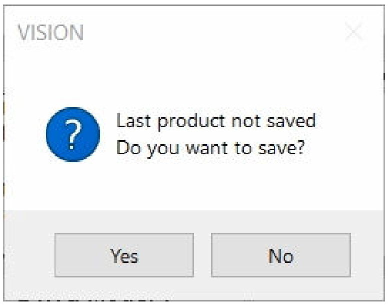
Product: Reactor2

Constituent	Water	B	C	D	E
Upper limit	0.0000				
Lower limit	0.0000				
Y-axis max	0.0000				
Y-axis min	0.0000				
Combined Block RSD					
Target Value	0				
Y-axis max	0				
Y-axis min	0				
OLUP Model	OLUP Model 1	OLUP Model 2	OLUP Model 3	OLUP Model 4	OLUP Model
Name and location	W:\Process Spectroscopy\Software\Prediction Engine\vtoct2020camo.unsb, watercamo				
BWIQ Model	BWIQ Model 1	BWIQ Model 2	BWIQ Model 3	BWIQ Model 4	BWIQ Model
Name and location					
Leverage Library	Leverage Lib 1	Leverage Lib 2	Leverage Lib 3	Leverage Lib 4	Leverage Lib
Library Name					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

5 Click on **[OK]** and confirm the changes:



Last product not saved
Do you want to save?

NOTICE

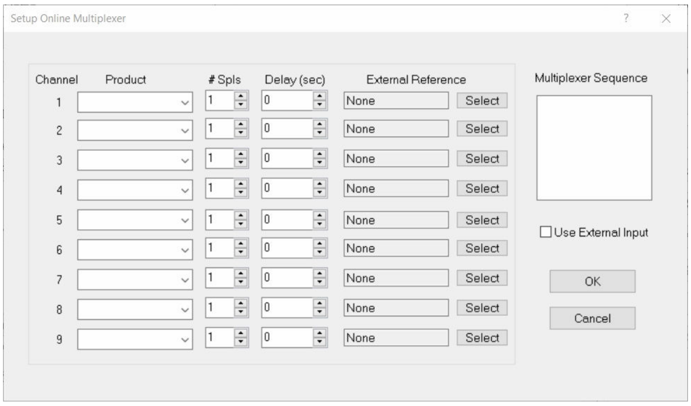
Make sure you use the correct report type: **ResultswwL**, where ww is the number of constituents used

Delete Products Button

The user can create a product by entering a new product name while operating routine analysis. These products appear in the output project. Click on **[Delete Products]** to remove these products from the list of available products.

Mux Setup Button

1 Click on **[Mux Setup]** to configure the online multiplexer. A typical screen is shown:



Channel	Product	# Spls	Delay (sec)	External Reference	
1		1	0	None	Select
2		1	0	None	Select
3		1	0	None	Select
4		1	0	None	Select
5		1	0	None	Select
6		1	0	None	Select
7		1	0	None	Select
8		1	0	None	Select
9		1	0	None	Select

2 For each channel choose the product name. If you have a library with an identification method declared in the Operations Method, you can also analyze Unknown product. Only products with equations connected are displayed.

3 In the **# Samples field** enter the number of spectra acquired for a given channel.

4 In the Delay field enter the time delay before sampling a given channel.

5 In the **Multiplexer Sequence** box define the sampling sequence for the channels (up to 32 entries). The channel numbers should be separated by spaces. This sequence will be repeated in a loop.

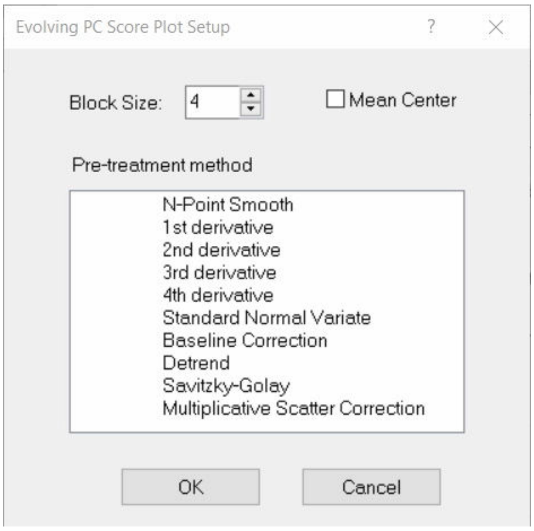
6 Click on **[OK]** when done.

Evolving PC Plot Button

Evolving PC plot displays Principal Component scores calculated on a moving block of spectra. A predefined number of last acquired spectra in Routine Analysis (block size) are used to calculate a Principal Components model. Principal Component scores of all spectra scanned since the start of Routine Analysis are calculated based on this model and displayed.

In order to configure the evolving PC plot follow these steps:

1 Click on **[Evolving PC Plot]**.

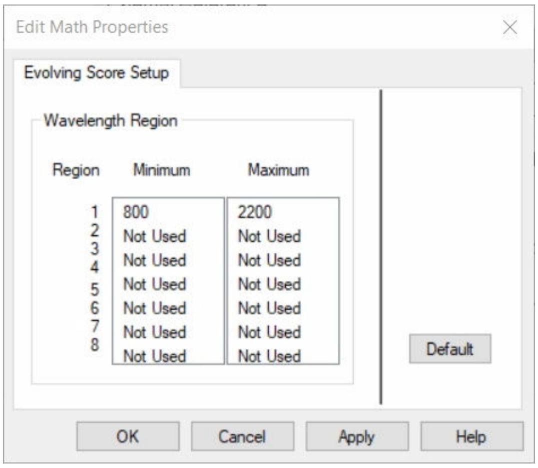

Evolving PC Score Plot Setup

Block Size: 4

☐ Mean Center

Pre-treatment method

2 Select the block size and spectral pretreatment. Select the **Mean Center** check box if the spectra need to be mean-centered before PC calculation. Click on **[OK]**.


Edit Math Properties

Evolving Score Setup

Wavelength Region

Region	Minimum	Maximum
1	800	2200
2	Not Used	Not Used
3	Not Used	Not Used
4	Not Used	Not Used
5	Not Used	Not Used
6	Not Used	Not Used
7	Not Used	Not Used
8	Not Used	Not Used

3 Select wavelength ranges, configure pretreatment, and click on **[OK]**.

4 From **Configure Views** options, select **Evolving Factors** view.

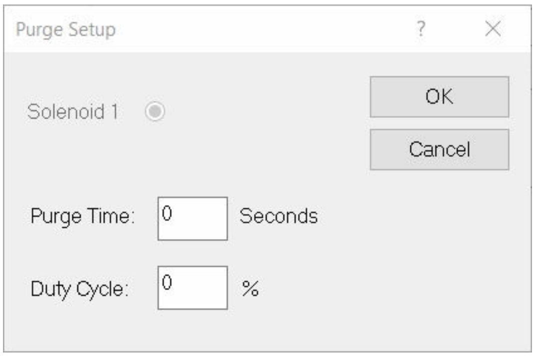
5 Run **Routine Analysis**.

Purge Setup Button

This option is to be used only in combination with **Spoon Probes** which require a solenoid valve which in turn is controlled by Vision.

1 Click on **[Purge Setup]**

2 This dialog box is displayed:



Purge Setup

Solenoid 1 ●

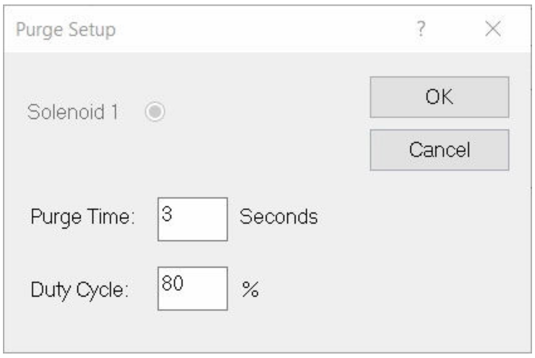
Purge Time: 0 Seconds

Duty Cycle: 0 %

The values for “Purge Time” and “Duty Cycle” are default values, which remain until changed and saved.

Please proceed.

3 Enter a value of 1 to 3 seconds for the “Purge Time” (3 is the maximum allowed). The time entered will depend upon your application considerations. Enter “80” for the “Duty Cycle”. This is an optimum value for the solenoid under these conditions.



Purge Setup

Solenoid 1 ●

Purge Time: 3 Seconds

Duty Cycle: 80 %

Click “OK” to save these values and close.

NOTICE

Please set appropriate “Sample Collection Interval” at the "Timer" section.

If the purge is 3 seconds, an entry of 5 seconds in this field allows time for the sample to settle before another sample is acquired. This time example varies with the application. If this timer setting is too short, the data may be meaningless.

Click **[OK]**.

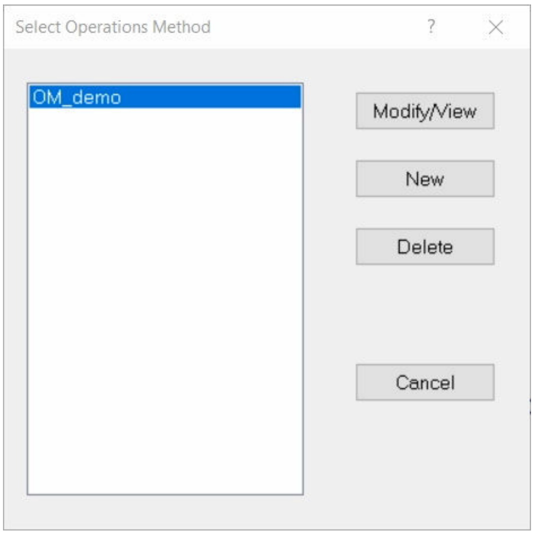
7.2.3 Operations Method Wizard

An alternative method of configuring an Operation Method is to use the Operation Method Wizard. The wizard leads the user through a series of setup screens. All options available in standard setup are accessible through the wizard. For simple Operation Methods most wizard screens can be skipped by just clicking on **[Next]** button and advancing to the next screen.

Please refer to the Operation Method Setup section for detailed description of individual options.

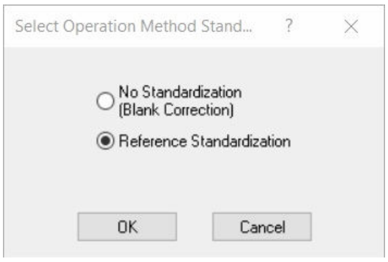
In order to configure an Operation Method using the wizard follow these steps:

1 Click on **Mode ▶ Routine Analysis ▶ OM Wizard**.



2 From the **Select Operations Method** window select an existing Operation Method and click on **[Modify/View]** if it needs editing. If creating a new method, click on **[New]**.

If a new method is chosen, Vision will display the following window:



Select Operation Method Stand...

○ No Standardization (Blank Correction)

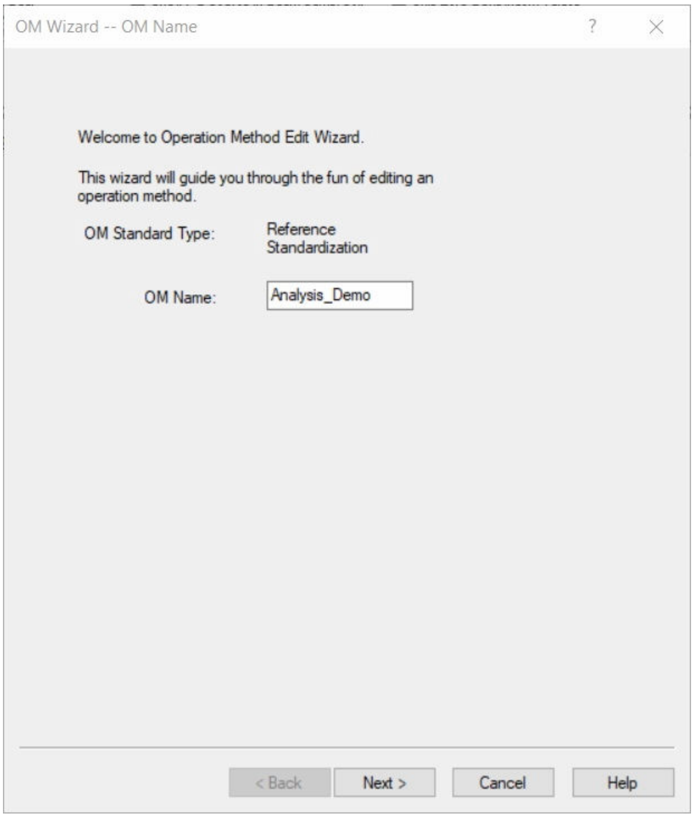
● Reference Standardization

Please note that this window is not displayed if an existing method is edited.

3 Select the standardization type compatible with your data and models. During the Operations Method setup Vision will display only items (DCMs and models) consistent with chosen standardization. Other items will be filtered out.

Click on **[OK]**.

4 On the next screen, type in the Operation Method name (if the new method is being created). Click on **[Next]**.



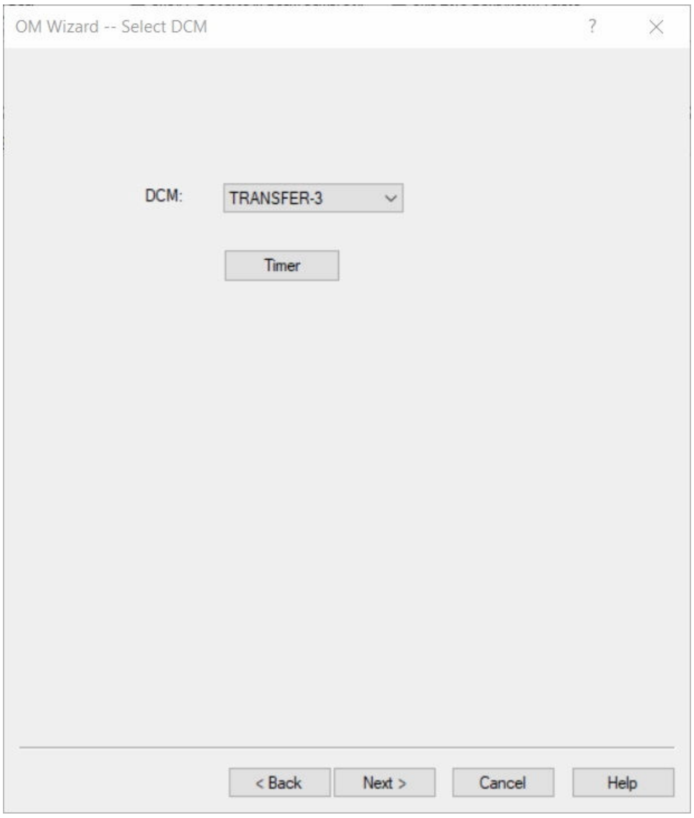
Welcome to Operation Method Edit Wizard.

This wizard will guide you through the fun of editing an operation method.

OM Standard Type: Reference Standardization

OM Name: Analysis_Demo

5 From the next screen select the Data Collection Method from the list:

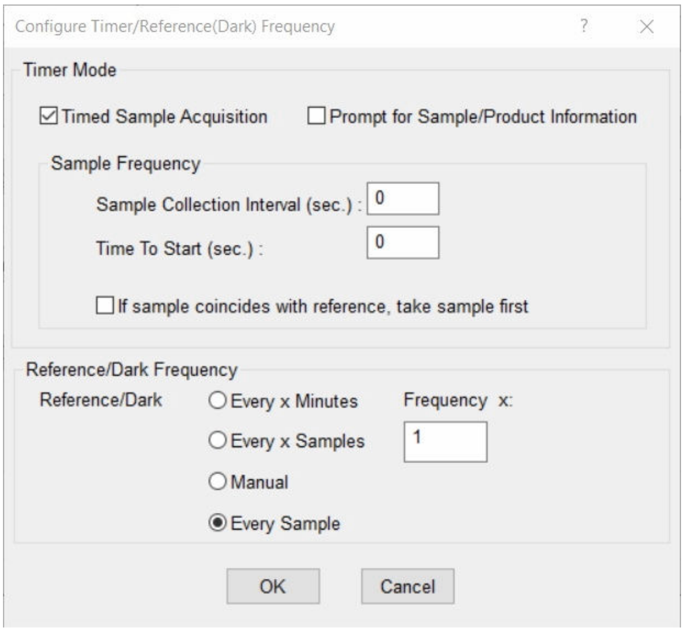


OM Wizard -- Select DCM

DCM: TRANSFER-3

By clicking on **[Timer]** you can define the reference and sample acquisition frequency. This configuration is optional and recommended only for process analyzers.

If automatic archiving is to be used, the spectra in Routine Analysis cannot be acquired continuously. There must be a delay between spectra. The archiving scheduler does not work when analyzing stored data.



Configure Timer/Reference(Dark) Frequency

Timer Mode

☑ Timed Sample Acquisition
☐ Prompt for Sample/Product Information

Sample Frequency

Sample Collection Interval (sec.) : 0
Time To Start (sec.) : 0
☐ If sample coincides with reference, take sample first

Reference/Dark Frequency

Reference/Dark
○ Every x Minutes
○ Every x Samples
○ Manual
● Every Sample

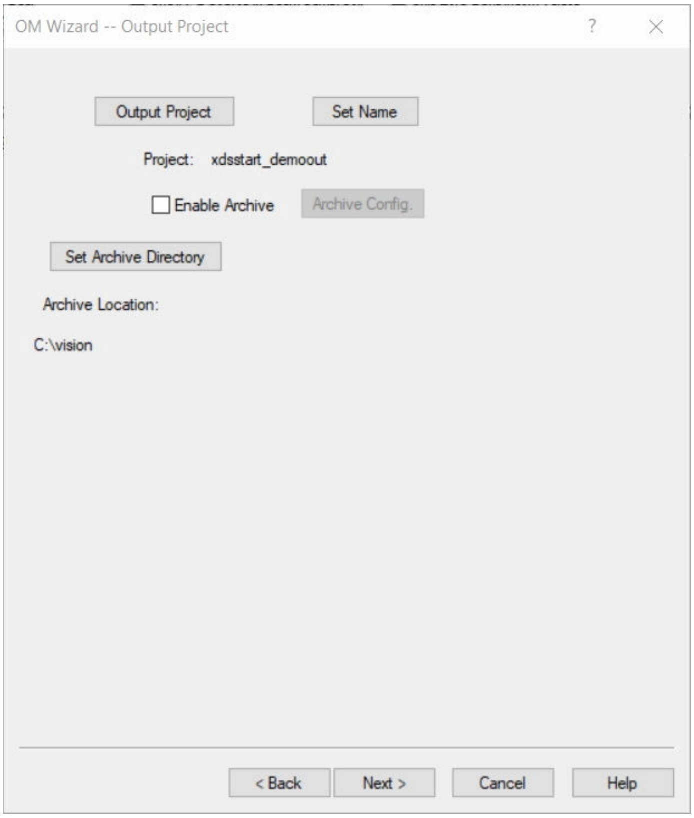
Frequency x: 1

NOTICE

For a detailed information, please refer to the Operations Method Configuration section

6 After configuration, click on **[OK]** to return to the previous screen. Click on **[Next]**.

The next screen defines output project which stores are Routing Analysis results. It also configures the results archiving.



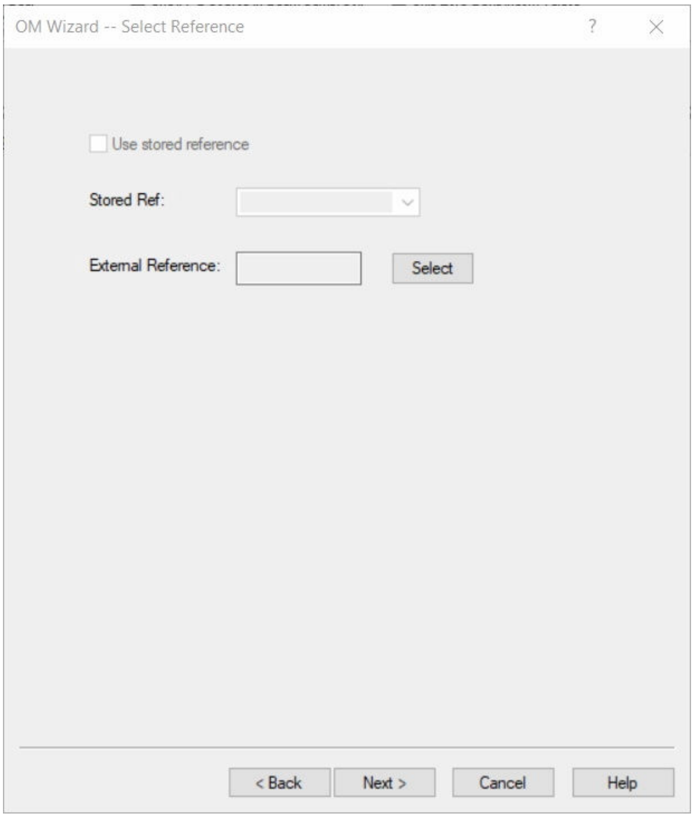
7 Click on **[Output Project]** to create a new output project or attach an existing one to the Operation Method.

If the analysis results are to be archived, check the **Enable Archive** box. The **[Archive Configuration]** button becomes active. Click on it to configure the archiving frequency.

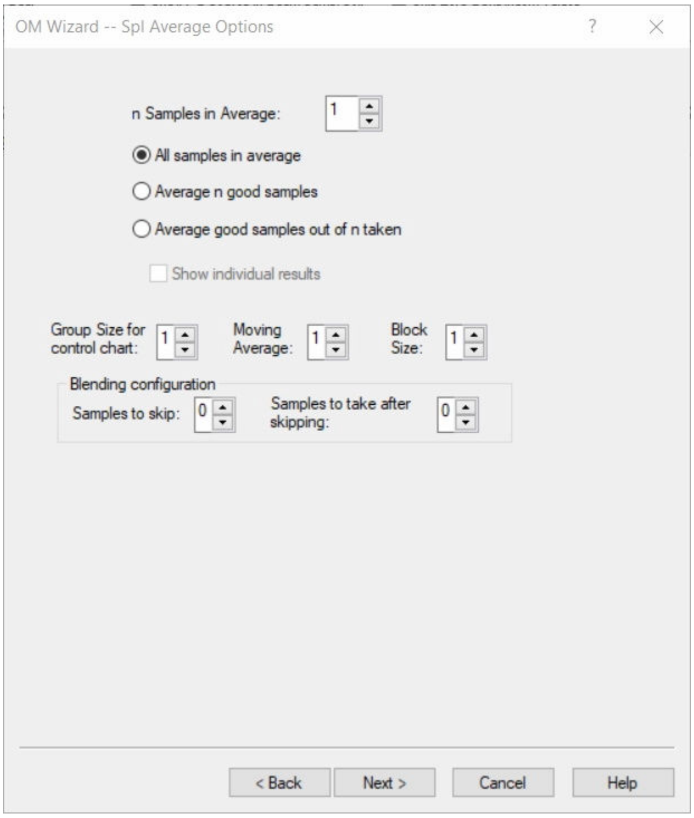
By default the results are archived to C:\Vision. You can change this location by clicking on **[Set Archive Directory]** button.

8 Click on **[Next]** to advance to the next screen.

The **Select Reference** Screen opens. This screen allows selecting stored or external reference to be used in Routine Analysis. Please note that **[Use Stored Reference]** button is inactive when no stored reference is saved.



9 Click on **[Next]** to advance to the next screen.


OM Wizard -- Spl Average Options

n Samples in Average: 1

● All samples in average

○ Average n good samples

○ Average good samples out of n taken

☐ Show individual results

Group Size for control chart: 1

Moving Average: 1

Block Size: 1

Blending configuration

Samples to skip: 0

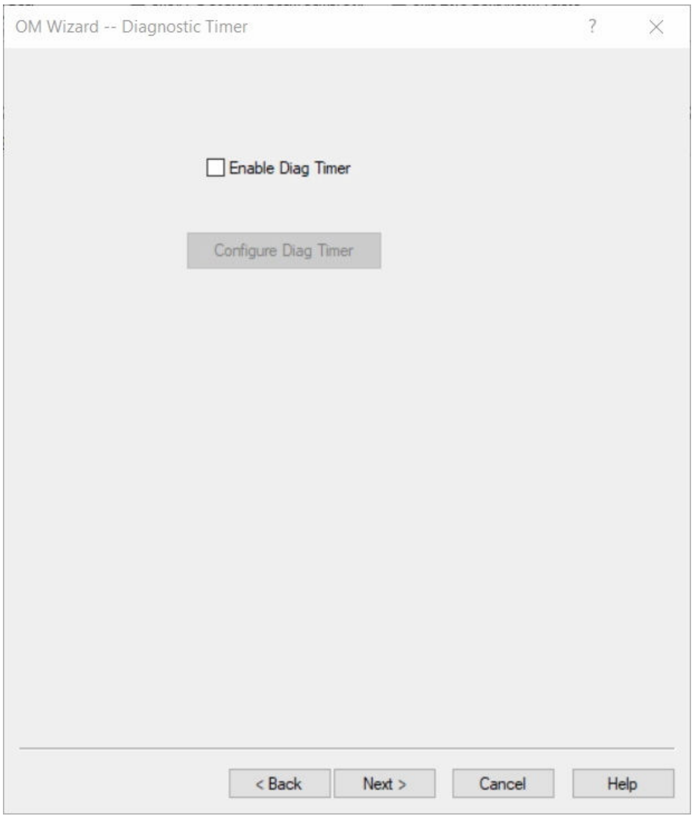
Samples to take after skipping: 0

The **Sample Averaging Options** screen defines the number of spectra to be averaged for further processing defines sample groups for charts, and parameters for blending analysis.

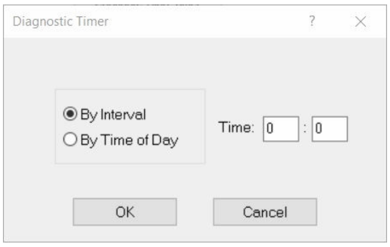
- **N Samples in Average** defines the number of spectra that will be averaged before qualitative and/or quantitative results are calculated.
- If the **Average N good samples** or **Average good samples out of N taken** option is selected, Vision applies the identification method first. Only the samples that pass identification are averaged and passed to the quantification step. Samples that fail ID are rejected.
- In the **Group Size for Control Chart** field, define the number of results to be averaged before display on the control chart.
- **Moving Average** defines the number of results used to calculate moving average and moving standard deviations.
- **Block Size** defines the number of results used to calculate block average and block Residual Standard Deviation.
- **Blending Configuration** defines the number of spectra to skip after the identification starts to pass and the number of spectra to analyze after skipping.

10 Click on **[Next]** to advance to the next screen.

The next screen configures the diagnostic timer.



11 Check the **Enable Diagnostic Timer** box to activate the **[Configure Diagnostic Timer]** button. Click on the button to configure the timer:

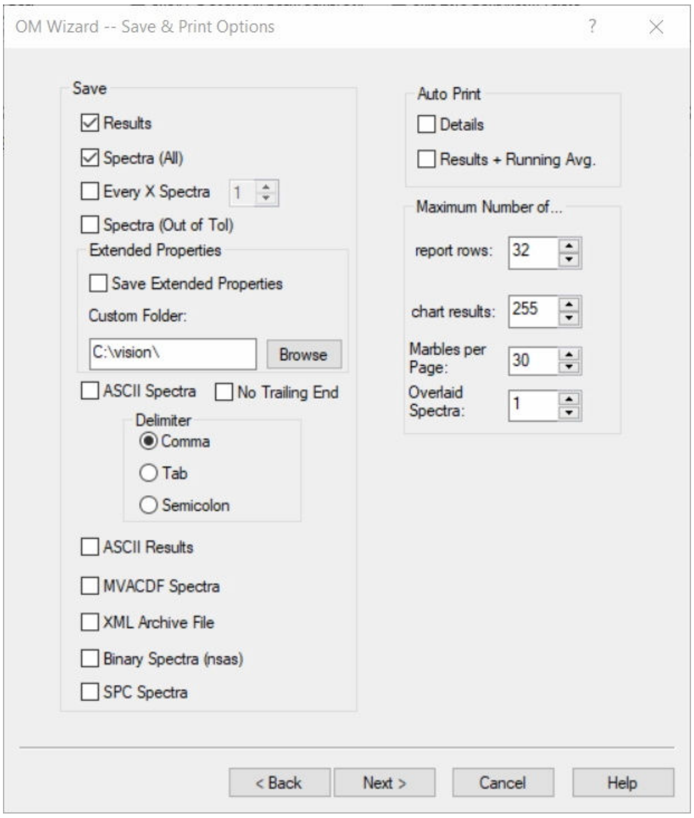


Time: 0 : 0

12 Select appropriate value and click on **[OK]** to return to the previous screen.

13 Click on **[Next]** to advance to the next screen.

The **Save and Print Options** screen configures items to be saved, displayed, and printed during routine analysis.



OM Wizard -- Save & Print Options

Save

☑ Results

☑ Spectra (All)

☐ Every X Spectra 1

☐ Spectra (Out of Tol)

Extended Properties

☐ Save Extended Properties

Custom Folder: C:\vision\

☐ ASCII Spectra ☐ No Trailing End

Delimiter

● Comma

○ Tab

○ Semicolon

☐ ASCII Results

☐ MVACDF Spectra

☐ XML Archive File

☐ Binary Spectra (nsas)

☐ SPC Spectra

Auto Print

☐ Details

☐ Results + Running Avg.

Maximum Number of...

report rows: 32

chart results: 255

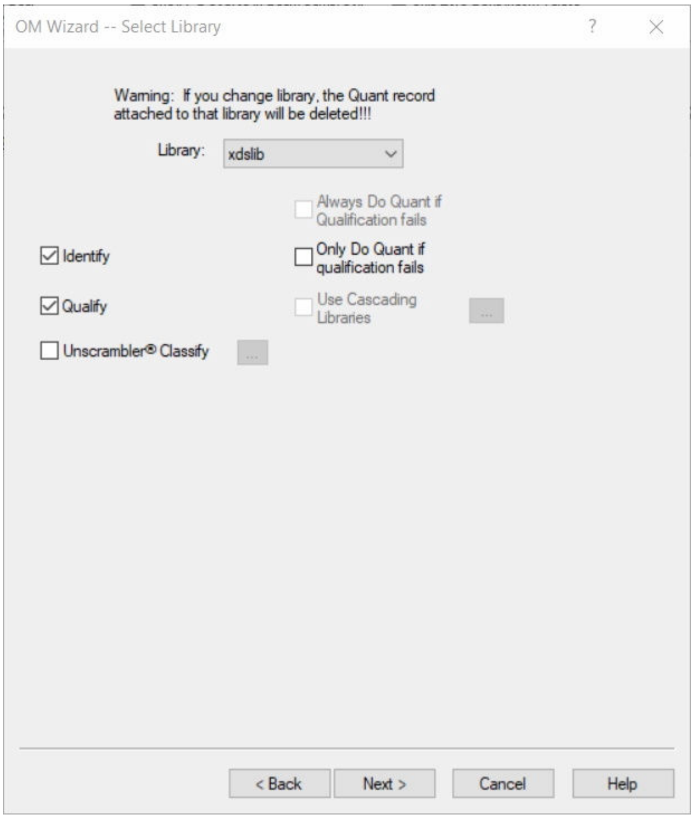
Marbles per Page: 30

Overlaid Spectra: 1

- In the **Save** field, click on the appropriate boxes for desired information such as results, all spectra, spectra out of tolerance, ASCII spectra, ASCII results, and others. Results and spectra are saved in the output project. MVACDF spectra, binary (NSAS) spectra, ASCII results, ASCII spectra, and SPC spectra are saved in the output project folder (one per analysis). Archiving in the XML format requires the DTD file (definition of the XML file format) to reside on the computer and the path to this file to be defined in Account Policy window.
- In the **Auto Print** field, check the appropriate options. You can automatically print a general results report with running average and/or details report.
- **Maximum number of report rows** defines the number of samples analyzed before the Results page prints. When the report reaches this number, the results table maintains a constant size.
- **Maximum number of chart results** defines the maximum number of result points displayed on trend chart and control charts. After reaching this number, the chart starts to scroll.
- **Maximum number of marbles** defines the maximum number of result points displayed on standard deviation, RSD, and average charts. After reaching this number, the chart starts to scroll.

14 Click on **[Next]** to advance to the next screen.

The **Select Library** screen allows choosing the desired combination of qualitative analysis options.



OM Wizard -- Select Library

Warning: If you change library, the Quant record attached to that library will be deleted!!!

Library: xdslib

☐ Always Do Quant if Qualification fails

☑ Identify

☐ Only Do Quant if qualification fails

☑ Qualify

☐ Use Cascading Libraries

☐ Unscrambler® Classify

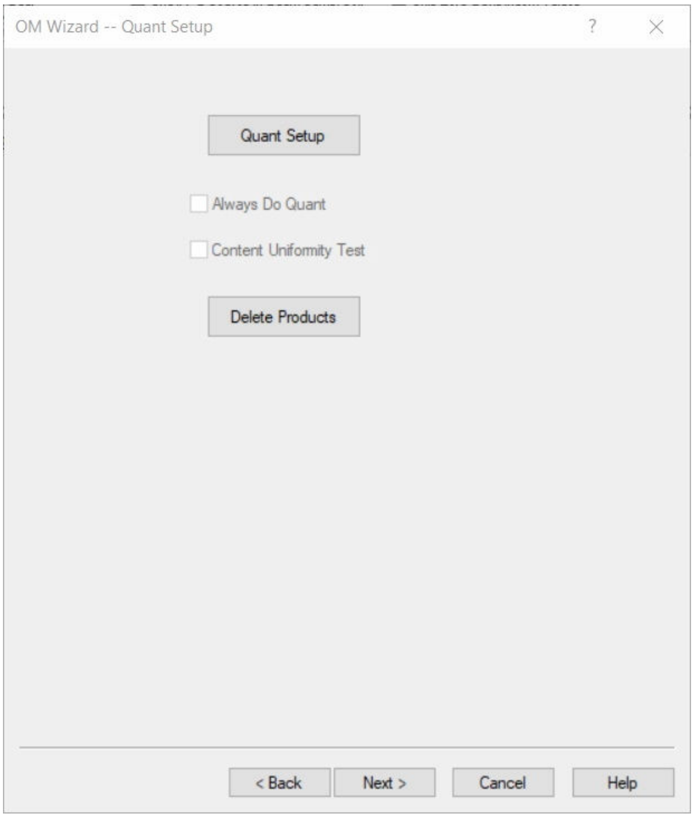
Select library to be used and options for which methods were developed in the defined library. Leave all boxes blank if only quantitative analysis is to be performed.

NOTICE

For a detailed information, please refer to the Operations Method Configuration section

15 Click on **[Next]** to advance to the next screen.

In the **Quant Setup** window user can link calibrations to products and define parameters of control and trend charts.

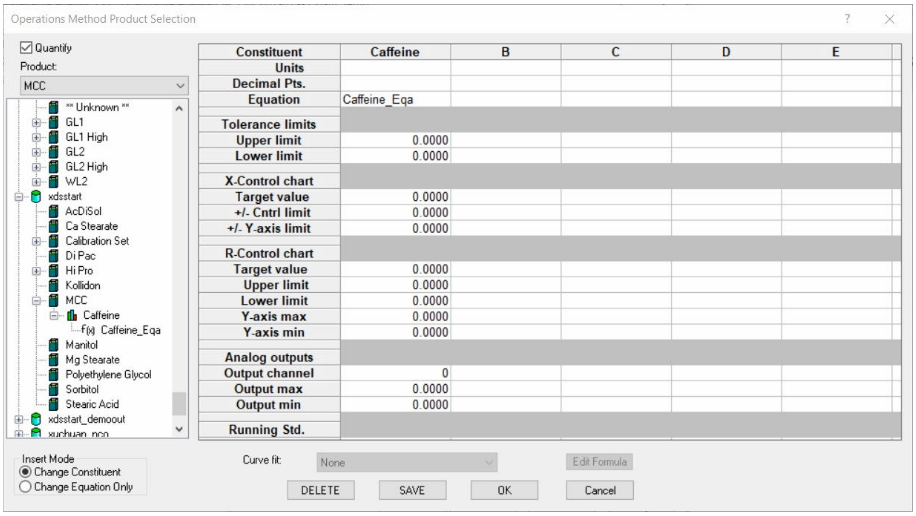


If a library has been selected in the previous wizard screen, you can attach calibration equations from all Projects to any product from this library. If no library has been selected, you can attach calibration equations from any project to any product from the active project.

Once a calibration equation is connected to a library in the Operations Method, you will not be able to change the library specified in this operations method.

In order to link calibrations to library or project products follow these steps:

16 Click on **[Quant Setup]** to attach calibration equations to Library or Project database products. The **Operations Method Product Selection** window appears.



☑ Quantify

Product: MCC

Constituent	Caffeine	B	C	D	E
Units					
Decimal Pts.					
Equation	Caffeine_Eqa				
Tolerance limits					
Upper limit	0.0000				
Lower limit	0.0000				
X-Control chart					
Target value	0.0000				
+/- Cntrl limit	0.0000				
+/- Y-axis limit	0.0000				
R-Control chart					
Target value	0.0000				
Upper limit	0.0000				
Lower limit	0.0000				
Y-axis max	0.0000				
Y-axis min	0.0000				
Analog outputs					
Output channel	0				
Output max	0.0000				
Output min	0.0000				
Running Std.					

Insert Mode
● Change Constituent
○ Change Equation Only

Curve fit: None

From the Product drop-down list, select a product from the Library or the active Project.

Expand the tree with Projects below, and double-click on the equation to be linked to the product. Only the equations consistent with the selected DCM and standardization type are displayed and can be connected to a product.

To add more equations click on the letter designating the next empty column to highlight the whole column, and double-click on the new equation in the Project tree.

To enter tolerance limits and control chart parameters, click on the proper cell of the spreadsheet and type in the numbers.

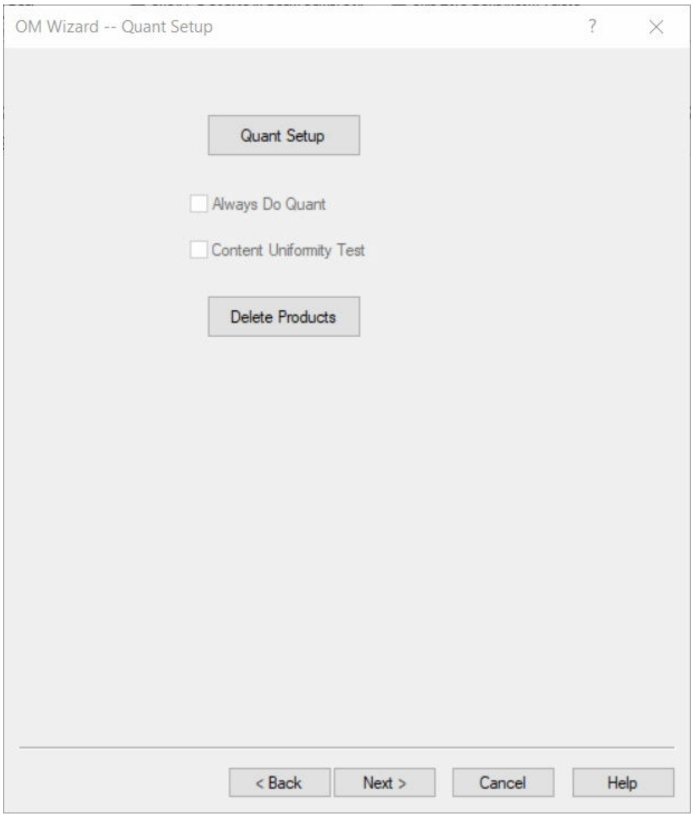
To replace the existing equation, click on the constituent name to highlight the whole column, and then double-click on the new equation in the Project tree. Select the **Insert Mode** from the field below the tree. If you are in the **Change Constituent** mode, the whole equation is replaced. If you are in the **Change Equation Only** mode, the constituent name is not replaced.

To delete an equation from a product, click on the constituent name to highlight the whole column and then click on **[Delete]**.

NOTICE

For Leverage or Unscrambler equations, please refer to the Quant Setup at Operations Method Configuration

17 Click on **[Save]** to complete the links, and on **[OK]** to close the window and return to the wizard.



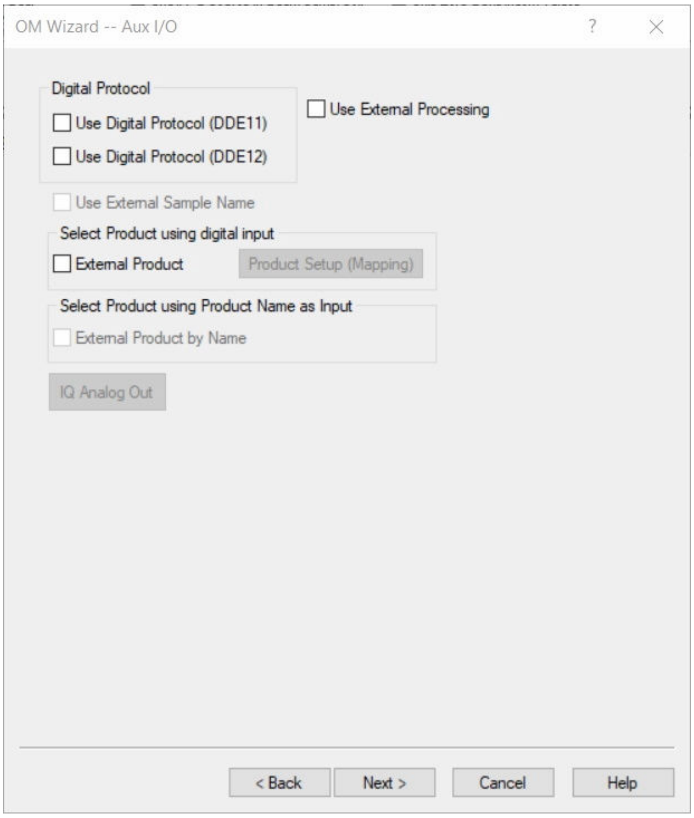
If the **Always Do Quant** option is selected, Vision will perform quantitative predictions even if qualification fails.

If **Content Uniformity Test** is checked, Vision will perform the test automatically. (This option requires a MultiTab Data Collection Method, and use of the MultiTab Analyzer.)

The **Always Do Quant** option becomes active only after a calibration is connected to a product.

18 Click on **[Next]** to advance to the next screen.

The **Auxiliary I/O** screen allows connection to **Vision I/O** module (used for analog 4 - 20 mA process communication) and process digital protocols.



19 **Checking Use Digital Protocol (DDE11)** box connects routine analysis output to external process control system through 4 - 20 mA link or through digital protocols such as OPC, Modbus, or Profibus. For list of available protocols please contact Metrohm representative.

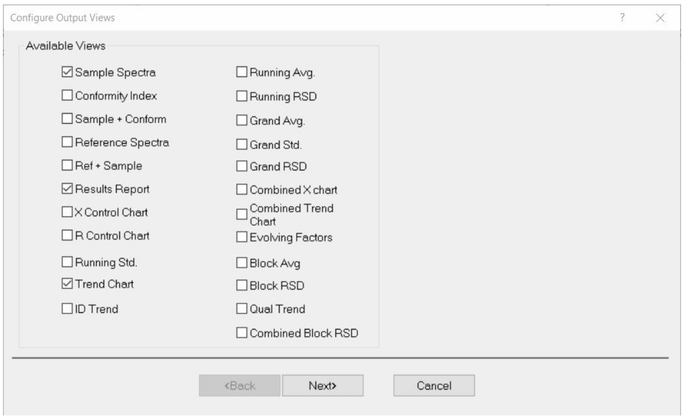
Configuration of other options can be found in digital protocols or Vision I/O Module manuals.

20 Click on **[Next]** to advance to the next screen.

The **Configure Output** screen allows choosing views available during routine analysis.

Report: RESULTS.XLS

21 Click on **[Configure Views]** to select the **Routine Analysis output** screen and report:



Available Views

- ☑ Sample Spectra
- ☐ Conformity Index
- ☐ Sample + Conform
- ☐ Reference Spectra
- ☐ Ref + Sample
- ☑ Results Report
- ☐ X Control Chart
- ☐ R Control Chart
- ☐ Running Std.
- ☑ Trend Chart
- ☐ ID Trend
- ☐ Running Avg.
- ☐ Running RSD
- ☐ Grand Avg.
- ☐ Grand Std.
- ☐ Grand RSD
- ☐ Combined X chart
- ☐ Combined Trend Chart
- ☐ Evolving Factors
- ☐ Block Avg
- ☐ Block RSD
- ☐ Qual Trend
- ☐ Combined Block RSD

22 Select up to 8 views from the list and click on **[Next]**.

Available Views

- ☑ Sample Spectra
- ☐ Conformity Index
- ☐ Sample + Conform
- ☐ Reference Spectra
- ☐ Ref + Sample
- ☑ Results Report
- ☐ X Control Chart
- ☐ R Control Chart
- ☐ Running Std.
- ☑ Trend Chart
- ☐ ID Trend
- ☐ Running Avg.
- ☐ Running RSD
- ☐ Grand Avg.
- ☐ Grand Std.
- ☐ Grand RSD
- ☐ Combined X chart
- ☐ Combined Trend Chart
- ☐ Evolving Factors
- ☐ Block Avg
- ☐ Block RSD
- ☐ Qual Trend
- ☐ Combined Block RSD

Pick Layout

○
●

Choose the layout of the views by clicking on the view in the list, and then on the proper rectangle representing the view location.

23 Click on **[Next]** and **[Finish]** to return to the wizard.

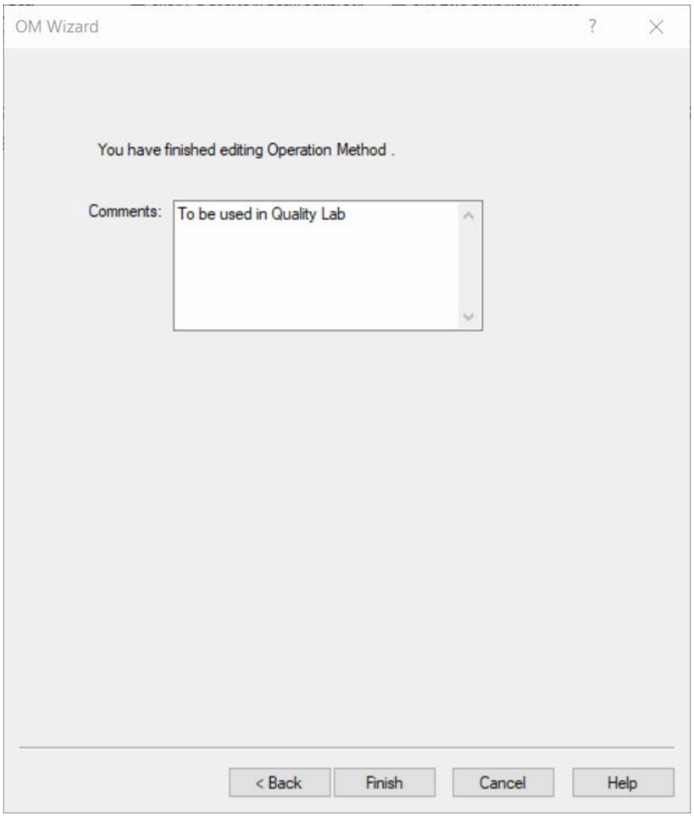
The following views are available for display:

- **Sample Spectra** – displays last acquired sample spectra.
- **Conformity Index** – displays conformity index spectrum from the qualification step if maximum distance is used as a qualification method. If Mahalanobis distance or Residual Variance is used as a qualification method, the view displays residual spectrum (the part not modeled by PC method). If correlation or no qualification method is used, or sample spectrum does not pass identification, the display is empty.
- **Sample + Conformity Index** – displays last acquired sample spectrum and conformity index spectrum on one plot.
- **Reference Spectra** – displays last acquired reference spectrum.
- **Reference + Sample Spectra** – displays last acquired reference and sample spectra on one plot.
- **Results Report** – displays the report with Routine Analysis results.
- **X Control Chart** – displays the average differences control chart. The chart has to be configured in Quant Setup.
- **R Control Chart** – displays the range of differences control chart. The chart has to be configured in Quant Setup.
- **Running Standard Deviation** – displays the control chart with running standard deviation. The chart has to be configured in Quant Setup.
- **Trend Chart** – displays predicted results vs. time chart. The chart has to be configured in Quant Setup.
- **ID Trend** – displays the trend chart of predicted ID values.
- **Running Average** – displays the control chart with running average. The chart has to be configured in Quant Setup.

- **Running Residual Standard Deviation** – displays the control chart with residual standard deviation. The chart has to be configured in Quant Setup.
- **Grand Average** – displays the control chart with grand average. The chart has to be configured in Quant Setup.
- **Grand Standard Deviation** – displays the control chart with grand standard deviation. The chart has to be configured in Quant Setup.
- **Grand Residual Standard Deviation** - displays the control chart with grand residual standard deviation. The chart has to be configured in Quant Setup.
- **Combined X Chart** – displays single average differences control chart for all constituents in the selected product. The chart has to be configured in Quant Setup.
- **Combined Trend Chart** - displays single results vs. time chart for all constituents in the selected product. The chart has to be configured in Quant Setup.
- **Evolving Factors** – displays Evolving Factors plot. The plot has to be configured from Operations Method setup window.
- **Block Average** - displays the control chart with averages calculated on blocks of results. The chart has to be configured in Quant Setup.
- **Block RSD** - displays the control chart with Residual Standard Deviation calculated on blocks of results. The chart has to be configured in Quant Setup.
- **Qual Trend** - displays the trend chart of predicted Qual values.
- **Combined Block RSD** - displays the control chart with Residual Standard Deviation calculated on blocks of results for all constituents in the selected product. The chart has to be configured in Quant Setup.

24 Click on **[Next]** to advance to the next screen.

25 This is the last wizard screen. Enter optional comment.



You have finished editing Operation Method .

Comments: To be used in Quality Lab

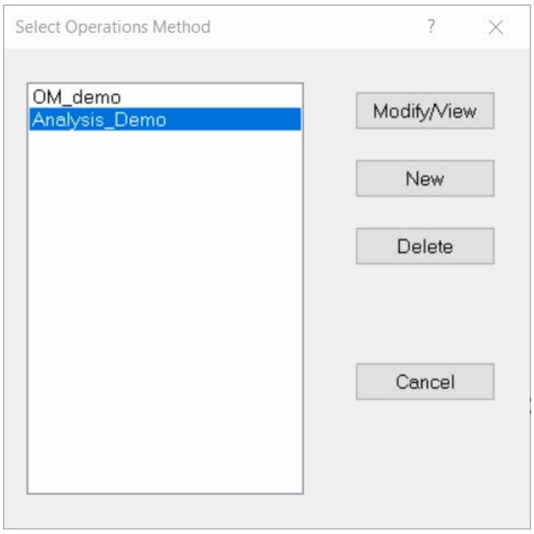
26 Click on **[Finish]** to complete the Operation Method setup.

7.3 Running Routine Analysis

Once the Operations Method is configured properly, you can run Routine Analysis to analyze samples in real time. Vision will automatically open the Routine Analysis output project. If data acquisition timer has been configured, Vision will start to acquire sample spectra automatically.

7.3.1 Routine Analysis Procedure

1 Click on **Mode ▶ Routine Analysis ▶ Run Routine Analysis** to start the program.



2 From the **Select Operations Method** dialog box choose the Operations Method.

3 If the data acquisition timer is not set up, click on the **reference icon** to collect the reference spectrum, and then on the **spectrum icon**.

4 The **Enter Sample Information** dialog box shows up. Enter the necessary information into the box:

From the Product ID dropdown list choose the Unknown or the product name.

Click on **[OK]** when done.

5 The X and Y axes can be manually configured on trend charts and control charts. To configure axes click on the **configuration icon** next to the appropriate graph.

6 Vision will start the data collection. After the spectrum is acquired, Vision will perform the analysis and display the results.

7 Click on **Mode ▶ Routine Analysis ▶ Run Routine Analysis** and unselect it to quit Routine Analysis. During spectral acquisition click on the **Stop icon** first.

You can print the results of Routine Analysis at any time by clicking on **File ▶ Print**. Make sure that the results view is the active window.

Comments entered into **Sample Information** window are transferred to the report spreadsheet and displayed in Details sheet. If a number is entered instead of comment, it can be used in the report spreadsheet for results postprocessing. This requires report modification.

7.3.2 Viewing Best Matches

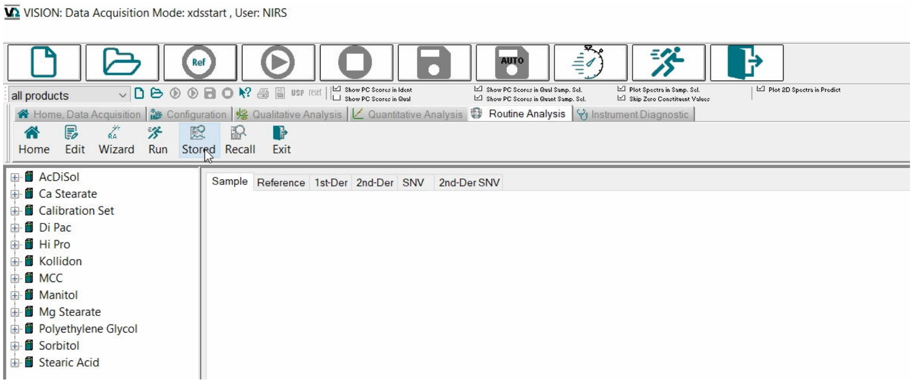
Up to 10 best qualitative matches can be displayed in Routine Analysis. To view best matches, click on the **10 best matches icon** (leftmost icon on the toolbar). When clicked, Vision displays a window with up to 10 library products arranged according to decreasing similarity to analyzed sample, together with match values. This feature uses library identification function to create the list of best matches.

7.4 Analyzing Stored Data

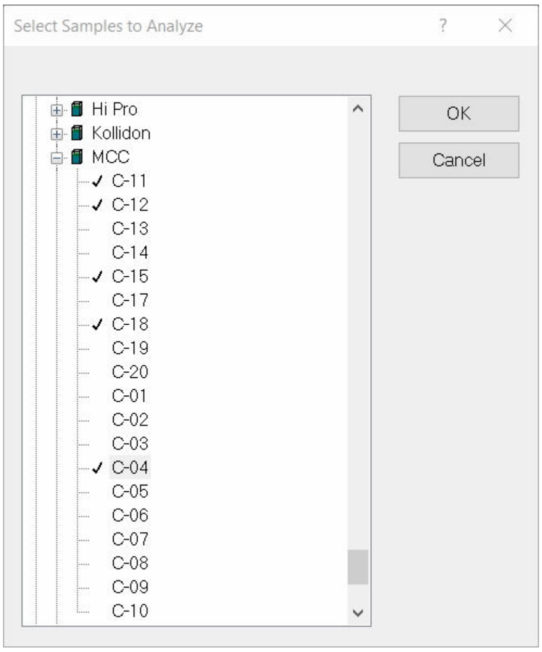
Vision allows for analysis of spectra stored in a project using an appropriate Operations Method.

Stored Spectra Analysis Procedure:

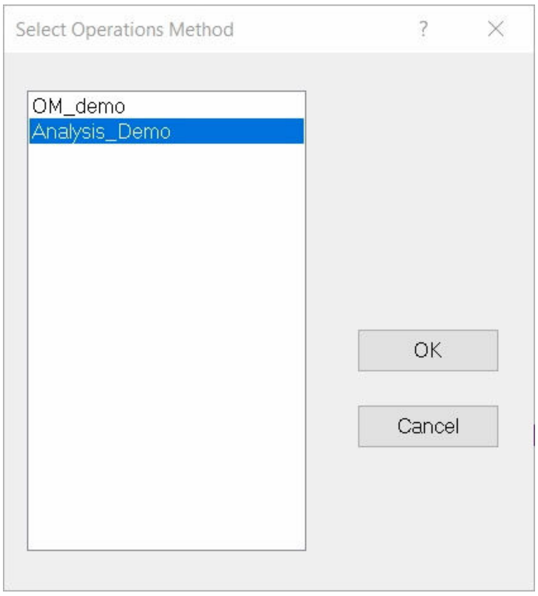
1 Click on **Mode ▶ Routine Analysis ▶ Analyze Stored Data** to start the program.



2 From the **Select Samples to Analyze** dialog box expand the project and product from which you want to analyze spectra. Select spectra by clicking on them. Click on **[OK]** when done.



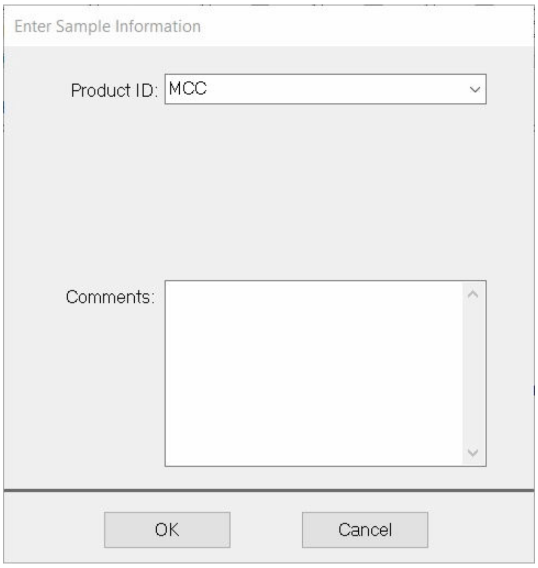
3 From the **Select Operations Method** dialog box choose the Operations Method and click on **[OK]**.



4 The **Enter Sample Information** dialog box shows up. Enter the necessary information into the box:

From the Product ID dropdown list choose the Unknown or the product name.

Click on **[OK]** when done.



Product ID: MCC

5 Vision will perform the analysis of the first selected spectrum and display the results.

The displayed window allows you to analyze samples one by one or continuously.

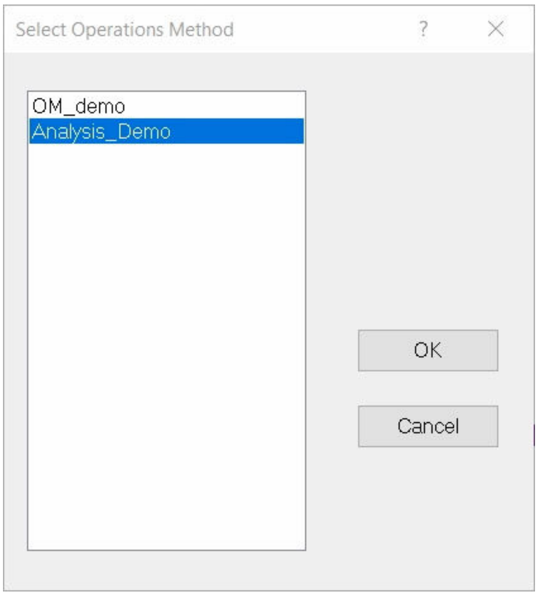
6 Click on **Mode ▶ Routine Analysis ▶ Analyze Stored Data** and deselect it to quit the program.

You can print the results of Stored Data Analysis at any time by clicking on **File ▶ Print**. Make sure that the results view is the active window.

7.4.1 One-click Analysis of Stored Data

Stored data can be easily and quickly analyzed from the Data Acquisition window.

1 Open project with spectra to be analyzed and select desired spectra or the entire product. From the main menu select **Edit ▶ Run Routine Analysis**. The following window opens:



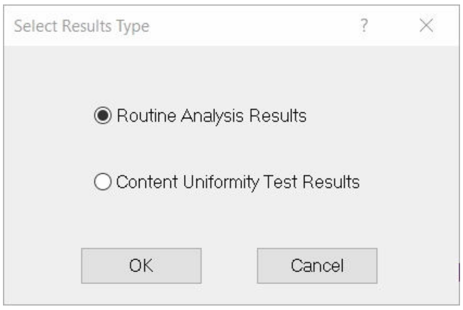
2 Select the Operations Method to use for the analysis.

3 Click on **Mode ▶ Data Acquisition** to return to Data Acquisition mode.

7.5 Recalling Results

Vision allows you to recall results stored in the output project even if the spectra were not saved.

1 Click on **Mode ▶ Routine Analysis ▶ Recall Results** to start the program.

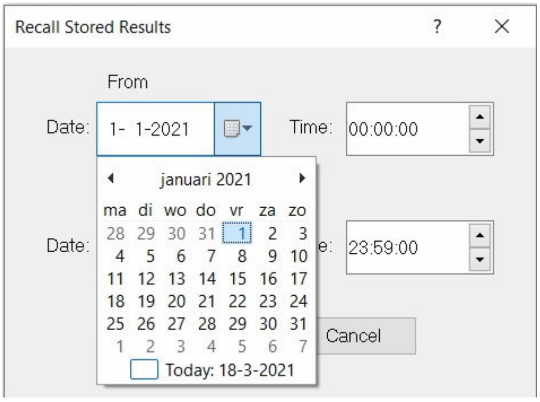


● Routine Analysis Results

○ Content Uniformity Test Results

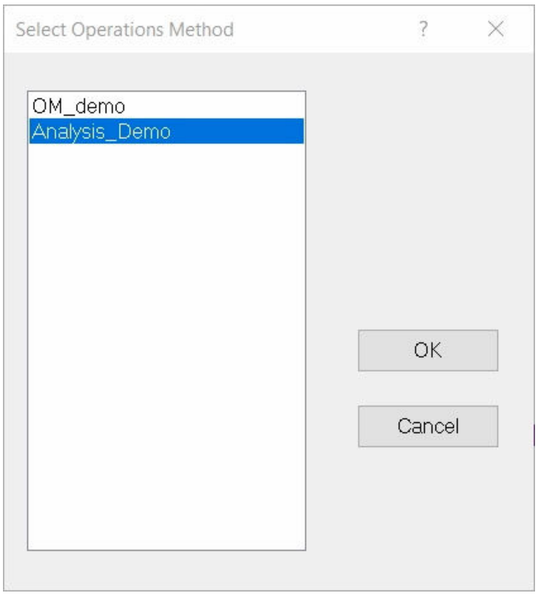
Select the Routine Analysis results or Content Uniformity Test results.

2 In the **Recall Stored Results** dialog box select the time period for recalling results. Click on **[OK]** when done.



Date: 1- 1-2021
Time: 00:00:00
Date:
e: 23:59:00

3 From the **Select Operations Method** dialog box, choose the Operations Method and click on **[OK]**.



4 The results will be displayed.

5 Click on **Mode** ▶ **Routine Analysis** ▶ **Recall Results** and unselect it to quit the program.

You can print the results of Stored Data Analysis at any time by clicking on **File** ▶ **Print**. Make sure that the results view is the active window.

7.6 Unattended Routine Analysis

Vision, when started in the unattended mode, enters Routine Analysis directly, without logging in. It opens selected Operations Method and initiates scanning. The unattended mode also constitutes the lowest level of access – the user's functions are limited to running Routine Analysis and exiting Vision. The user does not have access to other parts of Vision.

After entering Routine Analysis, Vision may display Sample Information window which requires entry from the operator. However, under certain circumstances, the window is suppressed and Vision starts data acquisition without operator's intervention. Apart from the Timer being enabled in the Operations Method, one of the following conditions has to be fulfilled for Vision to start Routine Analysis data acquisition:

- The Operations Method uses identification that precedes quantification step, with calibrations linked to library products, or
- The project with Operations Method linked to it has only one product, and the calibration is attached to that product in the Operations Method.

This configuration allows Vision to recognize which product should be analyzed with proper calibration equation.

To enter the unattended mode, Vision has to be run with inline parameters, which are the name of the Operations Method and the name of the project where the method has been created. For example, if the name of the Operations Method is OpMet, and the name of the project is MyProj, executing the following command will start Vision in the unattended mode:

C:\Vision\Vision.exe_ /*MyProj_/OpMet (where the symbol "_" stands for space).

This assumes that executable program Vision.exe is located in folder C:\Vision\.

To run Vision Routine Analysis in the unattended mode:

1 In a project called MyProj create and configure an Operations Method. In this example we will use the name OpMet.

2 Close Vision.

3 Run Vision with inline parameter: C:\Vision\Vision.exe_/* MyProj_/OpMet.

To start analysis automatically, make sure that:

1. Vision is closed with instrument connected.
2. The Operations Method Timer is enabled and configured.
3. The Operations Method uses identification, or
4. When the library is not used, the project has only one product with calibration attached.

Vision can be started with inline parameter from Run window (click on **Start ▶ Run**) or you can create a shortcut with the inline parameter. Optionally, the shortcut can be added to Windows Startup folder. In this case Vision automatically will resume Routine Analysis after power is cut off and restored.

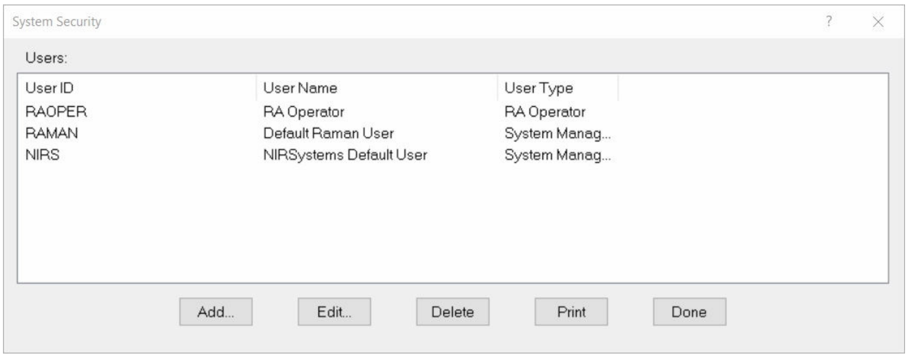
7.7 Setting up the Routine Analysis (RA) Operator

The RA Operator can perform only limited set of functions:

- Run Routine Analysis with preconfigured Operations Method
- Change own password
- Exit Vision
- Archive output project

The Operations Method for RA Operator has to be configured by the System Manager. To setup the RA Operator follows these steps:

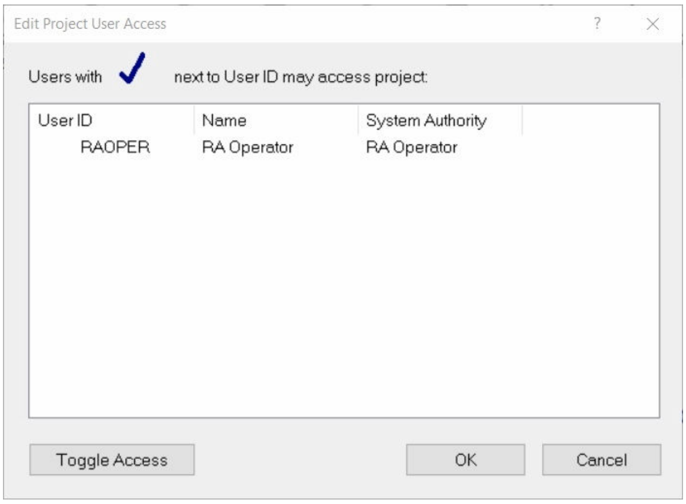
1. Make sure you are logged into Vision as a System Manager.
2. Create and configure Operations Method so it is ready to use.
3. Create and configure the RA Operator user.



User ID	User Name	User Type
RAOPER	RA Operator	RA Operator
RAMAN	Default Raman User	System Manag...
NIRS	NIRSystems Default User	System Manag...

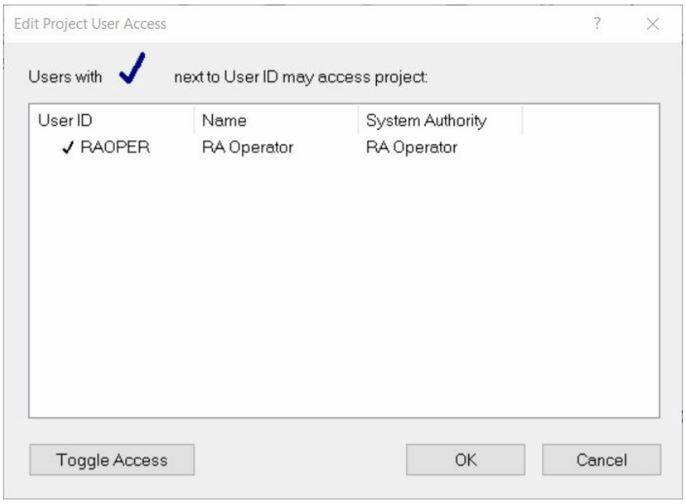
4. Give the user ID and password to the Routine Analysis Operator.

5 Give the RA Operator user access to the project with Operations Method. Make sure the proper project is opened. Click on **File ▶ Project ▶ Edit Users** from Data Acquisition menu. The following window opens:



User ID	Name	System Authority
RAOPER	RA Operator	RA Operator

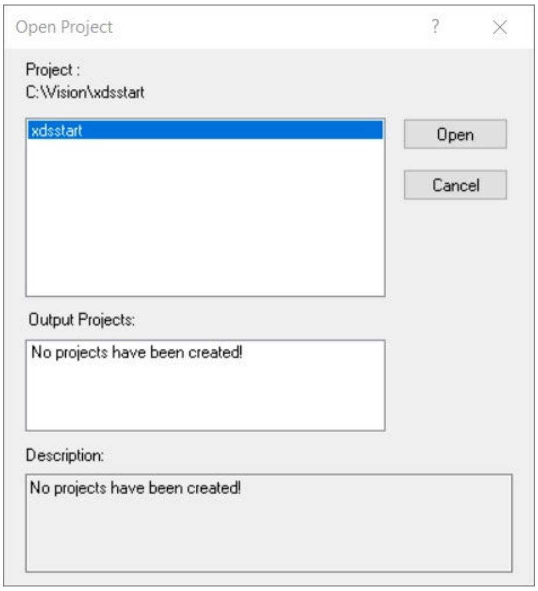
6 Click on the User ID (in this case RAOPER) to highlight it and then click on **[Toggle Access]** button. The user acquire a check mark next to the User ID:



User ID	Name	System Authority
✓ RAOPER	RA Operator	RA Operator

Click on **[OK]** when done.

7 Log out of Vision (DO NOT EXIT) and log in as the RA Operator. Click on **Open Project icon** and open the project with the Operations Method (only one project should show in the Open Project dialog).



Project :
C:\Vision\xdsstart

xdsstart

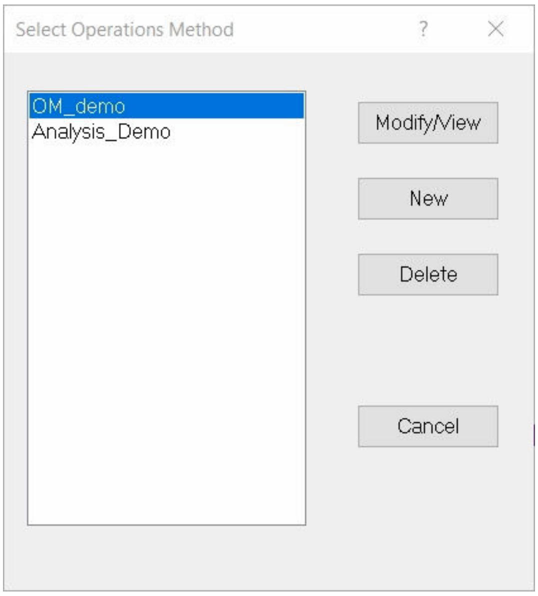
Output Projects:
No projects have been created!

Description:
No projects have been created!

Close Vision.

When the Routine Analysis Operator starts Vision and logs in with RA Operator credentials, the **Connect To Instrument** window opens.

8 The **Select Operations Method** dialog will open and direct the RA Operator to the Routine Analysis.



OM_demo
Analysis_Demo

It is recommended that in the regulated environment the RA Operator change the password immediately after the first login to Vision.

7.8 Using Bar Code Reader for Product Qualification

Vision includes a method to use a bar code reader and read coded sample name directly from the container label without operating keyboard or mouse. The bar code reader has to be of the “wedge” type, plugged between keyboard and the computer. It has to be programmable, i.e., it has to be able to automatically send preamble and postamble (string of ASCII characters added before and after the scanned bar code) information to Vision.

To use this option:

1. Program the bar code reader so that preamble is made of one horizontal tab (ASCII symbol HT, decimal code 009) and the postamble is made of 2 tabs and an enter (ASCII symbol CR, decimal code 013. Please note that the bar code reader may insert Enter after each transmission by itself. If you want to see and check what you did, open Word and scan any bar code. If you click on **Show/Hide icon** (kind of funny double letter P with the belly backwards) you will see the symbols on the screen.

2. Create an Operations Method. Configure the method in a standard way and click on **[Timer]**. In the timer window select Timed Acquisition and Prompt for Sample/Product Information. Make sure that **No Delay Between** option is selected. Choose the reference frequency and click on **[OK]**.

3. Now you can start Routine Analysis. After the reference is taken, the Sample Information window is displayed. Vision attempts to analyze as Unknown when Identify is selected in Operations Method, and as a product when only Qualify is checked. If you change to a different product, it will become a default analyzed product.

4. Scanning a bar code (with the reader properly programmed) will enter the code into the **Sample ID** field, and close the **Sample Information** window. Pulling the Smart Probe trigger will start spectral acquisition.

5. As soon as the acquisition is complete and results calculated, the new **Sample Information** window is displayed waiting for the new bar code.

Bar code reader feature is intended to be used with Smart Probe, but can be used with other sampling modules as well. In this case it is recommended to select **Keyboard Sample Ready Driver**. When **Continuous**

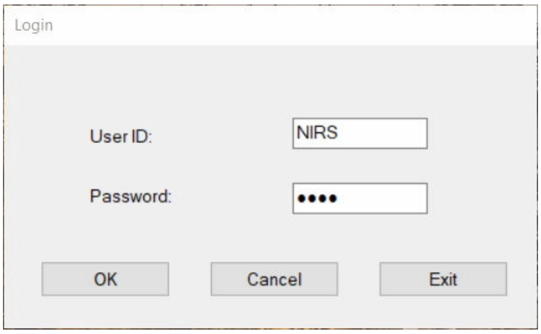
Sample Ready driver is selected, Vision will start data acquisition immediately after the bar code is scanned.

8 Security in Vision

8.1 Default User

When Vision software is installed, a default user NIRS with the password NIRS is created.

This user ID and password should be used for login into Vision the first time.



User ID: NIRS

Password: ●●●●

The default NIRS user is a System Manager. It has access to all software functions, including security setup.

8.2 Security Access Levels

Vision allows you to create 4 types of users: System Manager, Developer, Operator, and Routine Analysis Operator. These types of users differ by the level of access to software functions.

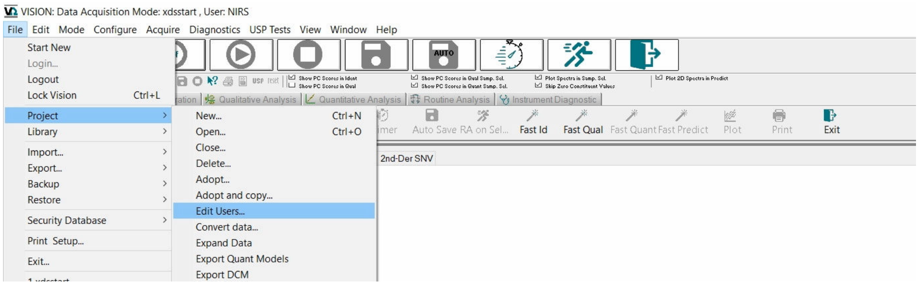
8.2.1 System Manager

The System Manger has access to all software functions, including security and 21 CFR Part 11 functions. In particular, the System Manager can create new users, including other System Managers.

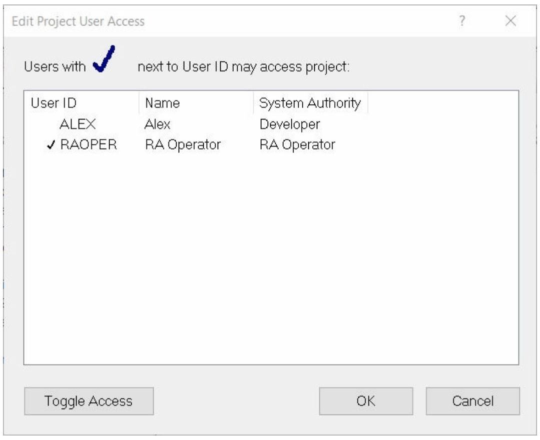
The System Manager has access to all projects that exist and also access to all libraries.

System Managers can grant access to their projects to other users at the Developer or Operator level. In order to grant access to a project:

1. If necessary, switch to **Data Acquisition** mode.
2. Open the project to which you want to grant access.
3. Click on **File** ▶ **Project** ▶ **Edit Users**.



4 The **Edit Project User Access** window lists all developers and operators.



Users with ✓ next to User ID may access project:

User ID	Name	System Authority
ALEX	Alex	Developer
✓ RAOPER	RA Operator	RA Operator

The users with a check mark next to the User ID have access to this particular project.

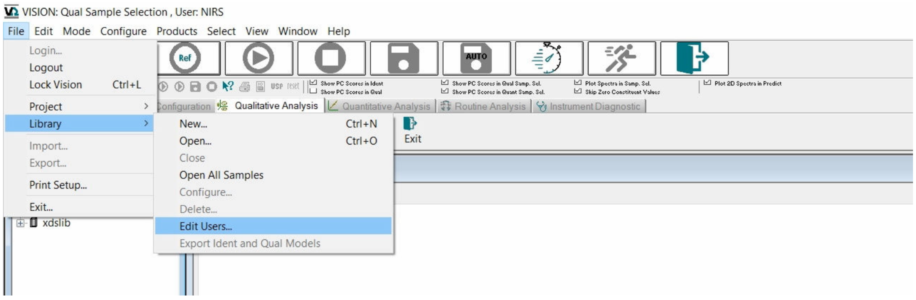
5 You can grant or deny access to the project by highlighting the user ID and clicking on **[Toggle Access]**.

System Managers can grant access to libraries to other users at the developer level. In order to grant access to a library:

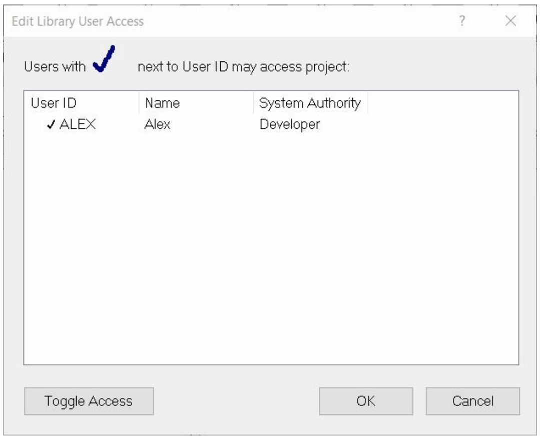
1 Enter **Qualitative Sample Selection** mode.

2 Open the library to which you want to grant access.

3 Click on **File ▶ Project ▶ Edit Users**.



4 The **Edit Project User Access** window lists all users. The users with a check mark next to the User ID will have access to the opened library.



Users with ✓ next to User ID may access project:

User ID	Name	System Authority
✓ ALEX	Alex	Developer

5 You can grant or deny access to the project by highlighting the user ID and clicking on **[Toggle Access]**.

8.2.2 Developer

The Developer has access to all software functions, excluding security.

Developers have access to projects and libraries that they created or were granted access to by the System Manager.

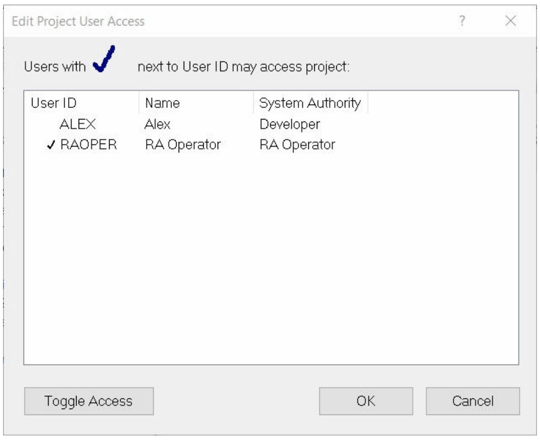
Developers can grant access to their projects to other users at the operator level. In order to grant access to a project:

1 If necessary, switch to **Data Acquisition** mode.

2 If necessary, switch to **Data Acquisition** mode.

3 Click on **File ▶ Project ▶ Edit Users**.

4 The **Edit Project User Access** window lists all operators. The users with a check mark next to the User ID have access to the opened project.



Users with ✓ next to User ID may access project:

User ID	Name	System Authority
ALEX	Alex	Developer
✓ RAOPER	RA Operator	RA Operator

5 You can grant or deny access to the project by highlighting the user ID and clicking on **[Toggle Access]**.

Developers can grant access to their libraries to other users at the developer level. In order to grant access to a library:

1 Enter **Qualitative Sample Selection** mode.

2 Open the library to which you want to grant access.

3 Click on **File ▶ Library ▶ Edit Users**.

4 The **Edit Project User Access** window lists all users. The users with a check mark next to the User ID will have access to the opened library.

5 You can grant or deny access to the project by highlighting the user ID and clicking on **[Toggle Access]**.

8.2.3 Operator

The Operator has limited access to Vision functions, including:

- creating a new project
- opening and closing accessible projects
- running Performance Test
- acquiring and saving spectra
- changing own password
- running Routine Analysis when an Operations Method is configured by a higher security access user

8.2.4 Routine Analysis (RA) Operator

The RA Operator can perform only the following functions:

- running Routine Analysis with preconfigured Operations Method
- changing own password

8.3 Setting Up Security

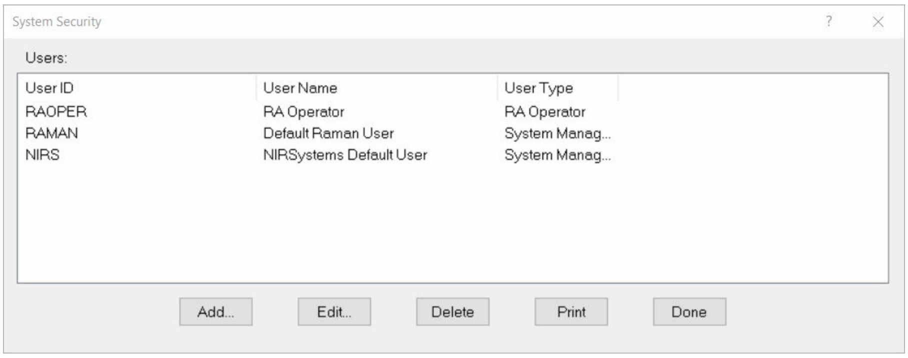
8.3.1 Adding a New User

Only a System Manager can add a new user. To add a new user follows these steps:

1 Make sure you are logged into Vision as a System Manager.

2 If necessary, enter the DA mode.

3 Click on **Configure** ► **Security**. The **System Security** window shows up.



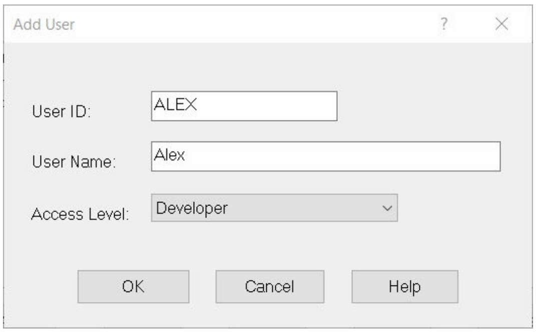
System Security

Users:

User ID	User Name	User Type
RAOPER	RA Operator	RA Operator
RAMAN	Default Raman User	System Manag...
NIRS	NIRSystems Default User	System Manag...

4 Click on **[Add]**.

5 In the **Add User** window type in the user ID and user name. Choose the access level from the dropdown list. Click on **[OK]** when done.



Add User

User ID: ALEX

User Name: Alex

Access Level: Developer

6 Note the user’s password (it can be changed later).

The password for user ALEX is:

FFBHGPG

7 Close the **System Security** window.

8.3.2 Deleting a User

Only a System Manager can delete an existing user. To delete a user follow these steps:

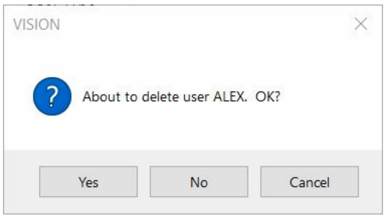
1 Make sure you are logged into Vision as a System Manager.

2 If necessary, enter the DA mode.

3 Click on **Configure ▶ Security**. The **System Security** window shows up.

4 Highlight the User ID to be deleted by clicking on it.

5 Click on **[Delete]**.



About to delete user ALEX. OK?

6 Confirm the deletion.

7 Close the **System Security** window.

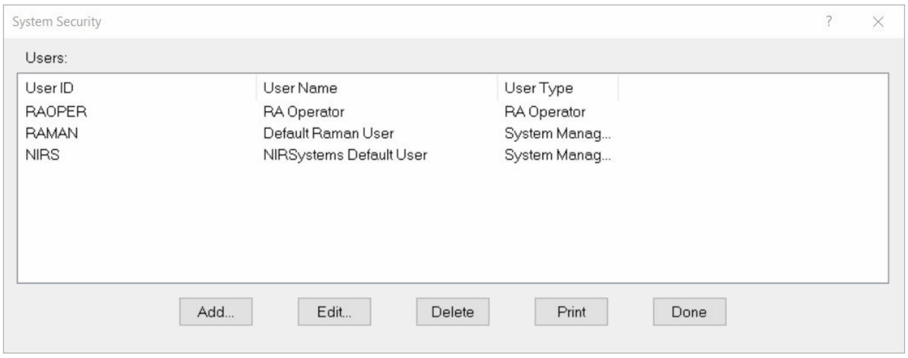
8.3.3 Editing a User

Only a System Manager can edit an existing user. To edit a user follow these steps:

1 Make sure you are logged into Vision as a System Manager.

2 If necessary, enter the DA mode.

3 Click on **Configure** ► **Security**. The **System Security** window shows up.



Users:

User ID	User Name	User Type
RAOPER	RA Operator	RA Operator
RAMAN	Default Raman User	System Manag...
NIRS	NIRSystems Default User	System Manag...

4 Highlight the User ID to be edited by clicking on it.

5 Click on **[Edit]**.

6 Edit the User ID, name, or access level.

7 Click on **[Password]** to change it.

8 Close the **System Security** window.

NOTICE

The System Manager does not have to know the old user password in order to change it.

8.3.4 Printing the List of Users

Only a System Manager can print a list of existing users. To print a list of users follow these steps:

1 Make sure you are logged into Vision as a System Manager.

2 If necessary, enter the DA mode.

3 If necessary, enter the DA mode.

4 Click on **[Print]**.

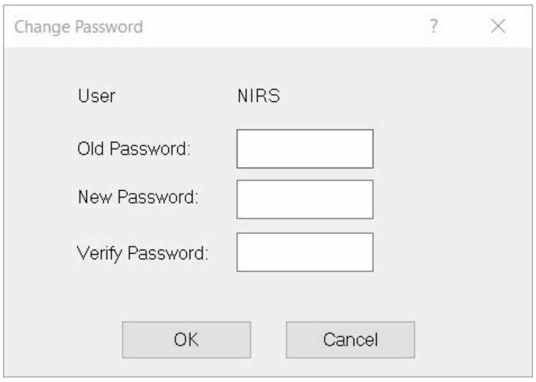
5 Close the **System Security** window.

8.3.5 Changing a Password

Each Vision user can change his/her own password regardless of the security access level. The knowledge of the old password is required to change it. To change a password follow these steps:

1 If necessary, enter the DA mode.

2 Click on **Configure ▶ Password**.



User NIRS

Old Password:

New Password:

Verify Password:

3 In the **Change Password** dialog box type in the old password, the new password, and the confirmation.

4 Click on **[OK]** when done.

8.4 Log-out Interval

If Vision is not operated for a given period of time, you will have to reenter the password to continue operation. If instead of entering a password, a **[Cancel]** button is clicked on, Vision will close all active projects and libraries and logout from the current user.

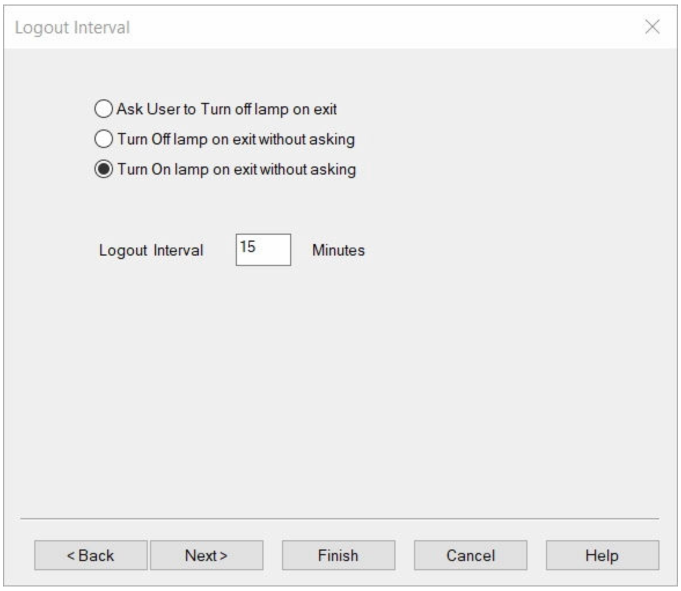
The default logout interval is 15 minutes. This time can be changed to any value. If you want to disable this function, define the logout interval value of 0.

To change the logout interval value follow these steps:

1 Enter the **Data Acquisition** mode.

2 Click on **Configure ▶ Configuration**.

3 In the **Edit Configuration** window, click on the **Logout Interval** tab.



Logout Interval

○ Ask User to Turn off lamp on exit
○ Turn Off lamp on exit without asking
● Turn On lamp on exit without asking

Logout Interval 15 Minutes

4 Type in the desired value and click on **[OK]**.

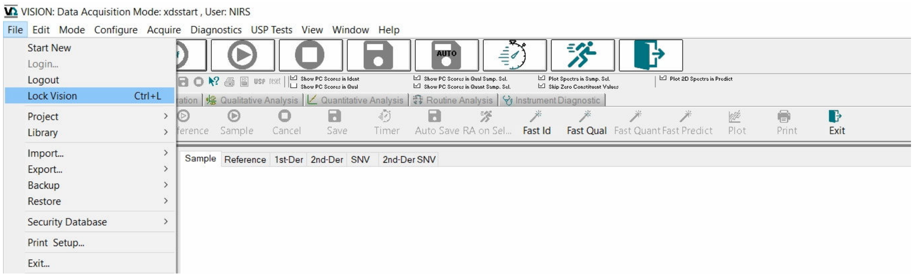
Only a System Manager can configure logout interval.

If the logout time expires when data acquisition timer is running, Vision will continue spectral acquisition. The acquired spectra will be saved in the normal way, although a window prompting you to reenter the password will show up.

8.5 Lock Function

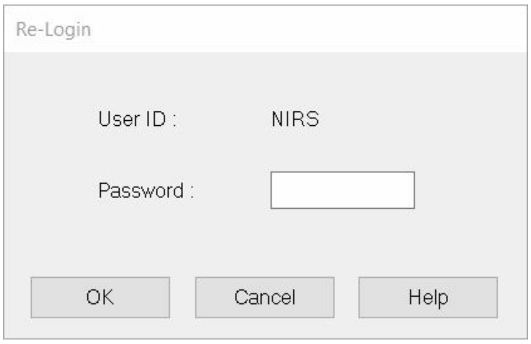
Lock function temporarily disables Vision and could be used instead of logout when the operator leaves workstation for short time. The program can not be accessed until a password is reentered.

1 To use, click on **File ▶ Lock Vision** or press **[CTRL]+[ALT]+[L]** from any place in Vision.



VISION: Data Acquisition Mode: xdsstart , User: NIRS

2 The screen below will be displayed. Enter valid password to resume operation.



NIRS

NOTICE

Note: Locking Vision will not stop Performance Test, Data Acquisition, or Routine Analysis in progress.

9 21 CFR Part 11 Compliance Features

Important:

This version of Vision software is compliant with 21 CFR Part 11 (electronic records). The new features that make Vision compliant may make software operation too cumbersome for users who do not need to be compliant. During software installation a user has to decide whether Vision needs to be compliant with 21 CFR Part 11 regulations. Choosing non-compliant installation will disable some of features described later in this chapter.

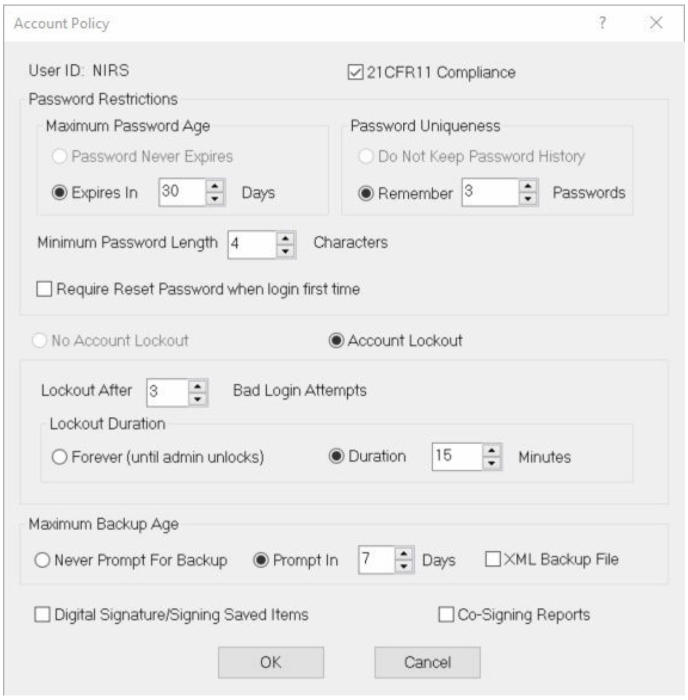
Those features can be disabled or enabled by the System Manager after Vision is installed. The way to do it is described later in this chapter.

Please note that the 21 CFR Part 11 compliance are not available in the standard version of Vision.

9.1 Configuration screen for 21 CFR Part 11 Enhancements

Only the System Manager has authority to configure 21 CFR Part 11 features.

1 In Data Acquisition mode, click on **Configure ▶ Account Policy**. This opens the **Account Policy configuration** window. This window (shown below) contains a number of check boxes and fields.



User ID: NIRS

☑ 21CFR11 Compliance

Password Restrictions

Maximum Password Age

○ Password Never Expires

● Expires In 30 Days

Password Uniqueness

○ Do Not Keep Password History

● Remember 3 Passwords

Minimum Password Length 4 Characters

☐ Require Reset Password when login first time

○ No Account Lockout

● Account Lockout

Lockout After 3 Bad Login Attempts

Lockout Duration

○ Forever (until admin unlocks)

● Duration 15 Minutes

Maximum Backup Age

○ Never Prompt For Backup

● Prompt In 7 Days

☐ XML Backup File

☐ Digital Signature/Signing Saved Items

☐ Co-Signing Reports

9.1.1 CFR11 Compliance Check Box

This box toggles the compliance on and off. When the compliance is disabled, the System Manager has to confirm and sign the change. All changes in the compliance status are logged into Audit Trail.

9.1.2 Maximum Password Age

This configurable list box defines the number of days after which Vision will request password change.

9.1.3 Password Uniqueness

This configurable list box defines the number of unique passwords that have to be created for a particular user before an old password can be reused.

9.1.4 Minimum Password Length

This configurable list box defines the minimum number of characters in a password.

9.1.5 Require Reset Password When Login First Time

When this option is selected, the system requires a password reset at the first login.

9.1.6 Lockout After X Bad Login Attempts

This configurable list box defines how many times Vision allows users to try to login. When this number is exceeded, Vision locks out.

9.1.7 Lockout Duration Forever

This option will cause lockout to last until System Manager logs in with his user ID and password.

9.1.8 Lockout Duration X Minutes

This option will unlock Vision and allow for another login attempt after specified number of minutes.

9.1.9 Maximum Backup Age

When the number of days from the last library or project backup exceeds the number defined in this list box, Vision issues a backup reminder when a project or a library is opened.

9.1.10 Digital Signature/Signing Saved Items

When this option is selected, the user has to sign each spectrum or result with his password. This option is available only in 21 CFR Part 11 compliant mode.

Before raw data or a method can be changed, the user has to enter the reason for change when compliant with 21 CFR Part 11. In many cases Vision will provide a list of standard reasons to choose from, or the user can type in a reason as a comment.

If the reason for change is not given, the change will not be implemented.

All changes are logged into the Audit Trail.

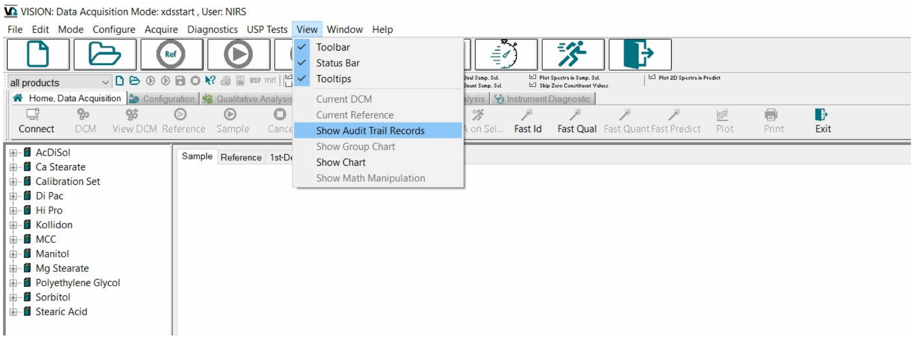
9.1.11 Co-Signing Reports

When this option is selected, Vision will prompt for report signing. All reports printed or saved to Excel format have to be signed by reviewer or approver. This includes Routine Analysis reports, Library Validation reports, and Performance Test reports. The person signing reports has to have a user ID and password different from the user logged in during the task.

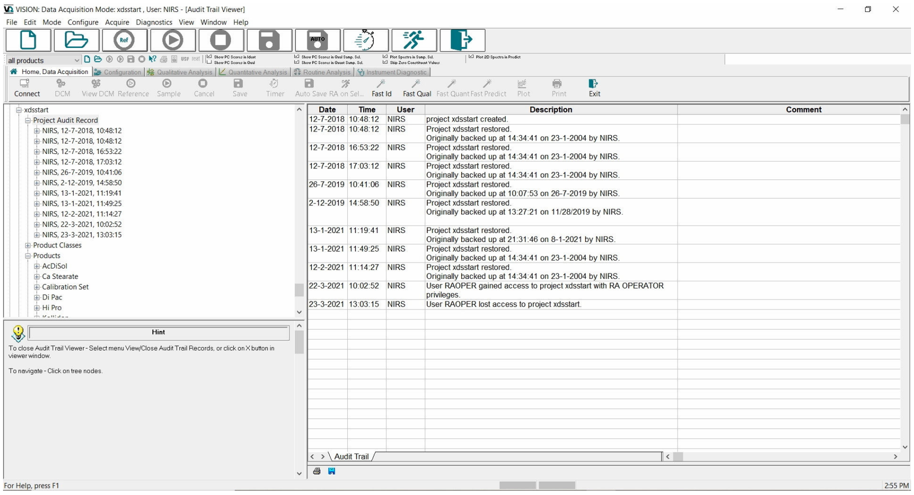
9.2 Audit Trail

Vision has built-in an Audit Trail, which stores all activities and changes done on projects, calibrations, libraries, operations methods, and security.

To view the Audit Trail, click on **View ▶ Show Audit Trail Records**. Vision displays a window composed of a tree view and a spreadsheet.



The tree view includes 3 major branches – Security, Projects, and Libraries. The branches and their sub-branches can be expanded or collapsed by clicking on + or – before the branch name.


VISION: Data Acquisition Mode: xdsstart , User: NIRS - [Audit Trail Viewer]

To close Audit Trail Viewer - Select menu View/Close Audit Trail Records, or click on X button in viewer window.

To navigate - Click on tree nodes.

Date	Time	User	Description	Comment
12-7-2018	10:48:12	NIRS	project xdsstart created.	
12-7-2018	10:48:12	NIRS	Project xdsstart restored. Originally backed up at 14:34:41 on 23-1-2004 by NIRS.	
12-7-2018	16:53:22	NIRS	Project xdsstart restored. Originally backed up at 14:34:41 on 23-1-2004 by NIRS.	
12-7-2018	17:03:12	NIRS	Project xdsstart restored. Originally backed up at 14:34:41 on 23-1-2004 by NIRS.	
26-7-2019	10:41:06	NIRS	Project xdsstart restored. Originally backed up at 10:07:53 on 26-7-2019 by NIRS.	
2-12-2019	14:58:50	NIRS	Project xdsstart restored. Originally backed up at 13:27:21 on 11/28/2019 by NIRS.	
13-1-2021	11:19:41	NIRS	Project xdsstart restored. Originally backed up at 21:31:46 on 8-1-2021 by NIRS.	
13-1-2021	11:49:25	NIRS	Project xdsstart restored. Originally backed up at 14:34:41 on 23-1-2004 by NIRS.	
12-2-2021	11:14:27	NIRS	Project xdsstart restored. Originally backed up at 14:34:41 on 23-1-2004 by NIRS.	
22-3-2021	10:02:52	NIRS	User RAOPER gained access to project xdsstart with RA OPERATOR privileges.	
23-3-2021	13:03:15	NIRS	User RAOPER lost access to project xdsstart.	

The spreadsheet includes fields with date, time, user, change or activity description, and optional reason (comment).

In order to close the Audit Trail viewer, click on **View ▶ Close Audit Trail Records**.