



SOFTWARE MANUAL

BioLight Studio Software UV
Version 1.03.01

BL Studio Software Manual

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Description

BL Studio software allows complete instrument control with data acquisition and storage. Furthermore it offers various result calculators and a report generator. Data acquisition, calculations and report generation can be fully automated in process methods.

In the ES version the Software package offers full security features including electronic signature, password protected login, user rights and audit trail.

BL Studio Software is a modular package to cover the demands of modern analytical Laboratories for both highly flexible research environments and regulated environments (ES version). The software features a structured and controlled flow, but is nevertheless easy to use.

Due to its modular structure it is possible to add new applications without changing the existing system, making it easy to validate.

Research environments

In research environments the BL Studio Basic software package offers full access to all methods and data. Methods and data can easily be imported, exported, reloaded and modified at any location of the pc. Methods and data are saved as files, allowing simplified maintenance.

The user can carry out the simplest of measurements, involving only data collection and real-time display, through to highly sophisticated data treatment and programmed calculations with built-in report.

This is made possible by the work flow structure, which offers a series of steps describing a typical experiment. These are, in logical order:

Sample definition (including selection of reference samples)

Data acquisition parameters

Calculations, either free calculation or concentration calculation. For the latter, pre-treatment of raw data is also possible, for example calculation of spectral peak area and feeding the area result into the concentration calibration.

Presentations, this is the user-definable report.

Administration, e.g. exporting results or informing a client, whenever a measurement finished.

Manual control, used for aligning and calibration accessories, checking sample location etc.

For **Calculations**, **Presentations** and **Administrations** the user can select 'None' as option, meaning that the method consists only of sample definition and data acquisition & display.

The Basic version already supports a basic user management, electronic signatures for data/method creation and an event-protocol to allow for traceability of the results. All files are checksum protected, ensuring that corrupted data can be detected immediately. Together these features make it possible to seamlessly update the system to the ES version.

Installation

Requirements

The following items are required for operation of BL Studio:

- PerkinElmer Lambda Spectrometer 2-45 with RS232 serial interface
- PC Pentium 500 MHz with CD-ROM drive and one free RS232 serial com port.
- At least 64 MB Ram
- Operating System: Windows 8, Windows 7, Windows Vista, Windows XP

Installation Procedure

Start the installation by double clicking on SetupBLStudio.exe. Please note that you need Windows administration rights to run the installation.

If BLStudio has already been installed you will be asked if you want to uninstall the existing version. To update the version first uninstall it, then re-start SetupBLStudio.exe.

Now follow the instructions. During the installation you can change the program and data directory. **Please ensure that all analysts will have read/write access to the data directory.**

Installed Programs

The BL Studio software package for UV consists of 4 programs:

BLDevelopment	Flexible tool for method development and measurements
BLCalculator	Free form calculator.
BLAdministration	Administration tool
BLRoutine	Tool for routine measurements

Setting up a new System

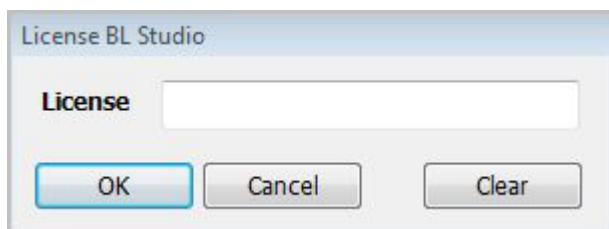
After the installation has finished you can start BL Studio either from the icon on the bench-top or via the start menu. Please note that BL Studio is installed in Demo mode by default (Data and Methods cannot be saved). To enable full access to BL Studio you need to enter your license key now:

Entering the License Key

From the applications menu select Help/About. Click on the first line in the license table, then on the Enter License button:



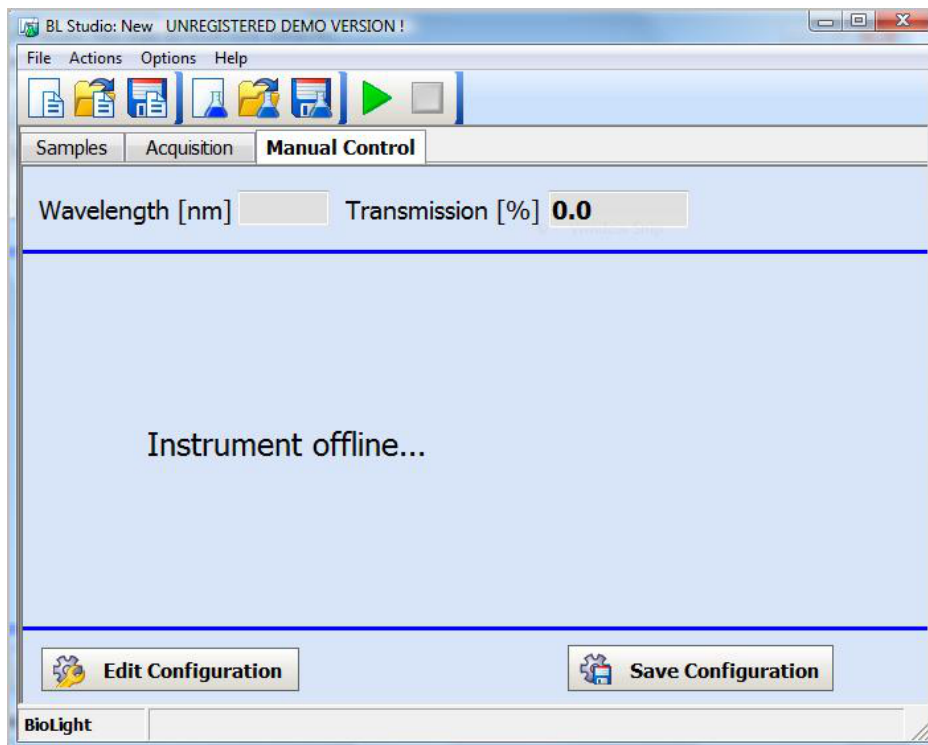
Now enter or paste your license key:



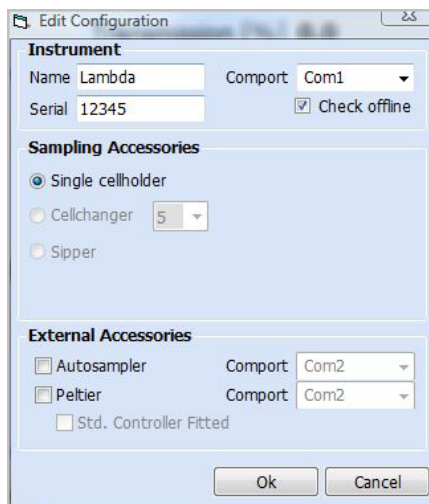
and press the “Ok” button. If the License key is invalid the dialogue will stay open and an error message is displayed.

Changing the Configuration

By default BL Studio uses Com1 as interface for the Spectrometer. External accessories are disabled. To change the configuration select the Manual Control tab.



Now click on the “Edit Configuration” button and select the comport in the configuration dialogue:

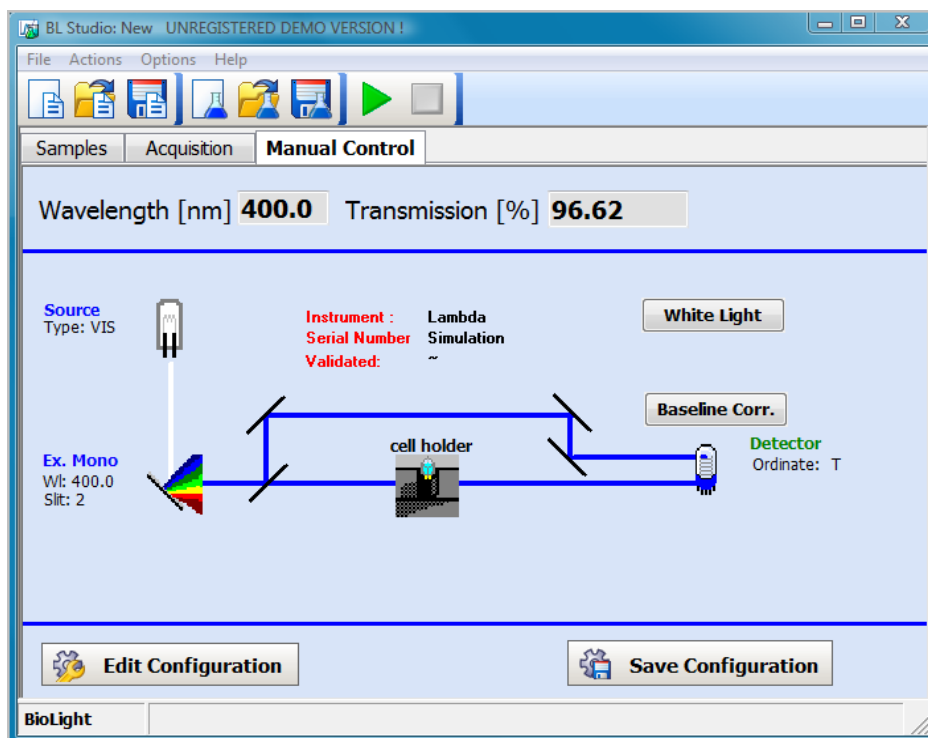


Please note that if the comport is above com3 it cannot be selected from the list but must be entered manually.

At this point you can also define a user friendly name for the instrument. This name will be used in reports and the validation. Furthermore you can select a S10 auto-sampler or P1 peltier module as external accessory: Select the corresponding option and define the desired comport.

All other accessories can be selected in simulation mode only, otherwise they are determined by the configuration of the currently connected instrument.

After pressing Ok the software re-connects to the instrument.



To save the new configuration the “Save Configuration” button.

Measurement Control

Description

To achieve flexible yet easy control of an experiment or routine data acquisition BLStudio utilizes application frames. These frames define the work flow of an experiment and the data management.

To avoid large, monolithic and hard to validate programs BL Studio offers specific frames for different user groups and requirements (e.g. routine measurements, method development and trending in both, ES and Non ES environments).

The frame houses modules for sample preparation, data acquisition, online-calculations, presentation, data handling and direct instrument control. It has the following design paradigms:

- It controls the work flow of an experiment
- It parses information and data between the steps within the work flow
- It manages all input and output of data, whether this is to a file-based system, or a database.
- The frame has no intelligence with respect to the contents of the steps
- The frame does not communicate with hardware

Typically all modules in the frame are updated, whenever the data acquisition for each sample is completed, (data is save, calculations are performed, the report is updated), thus allowing for a comfortable overview of the status and validity of the measurement process.

BL Studio is installed with a set of standard modules. However, it is easily possible to remove (or only hide) modules to simplify validation or to add new add-on applications without having to re-install the Studio.

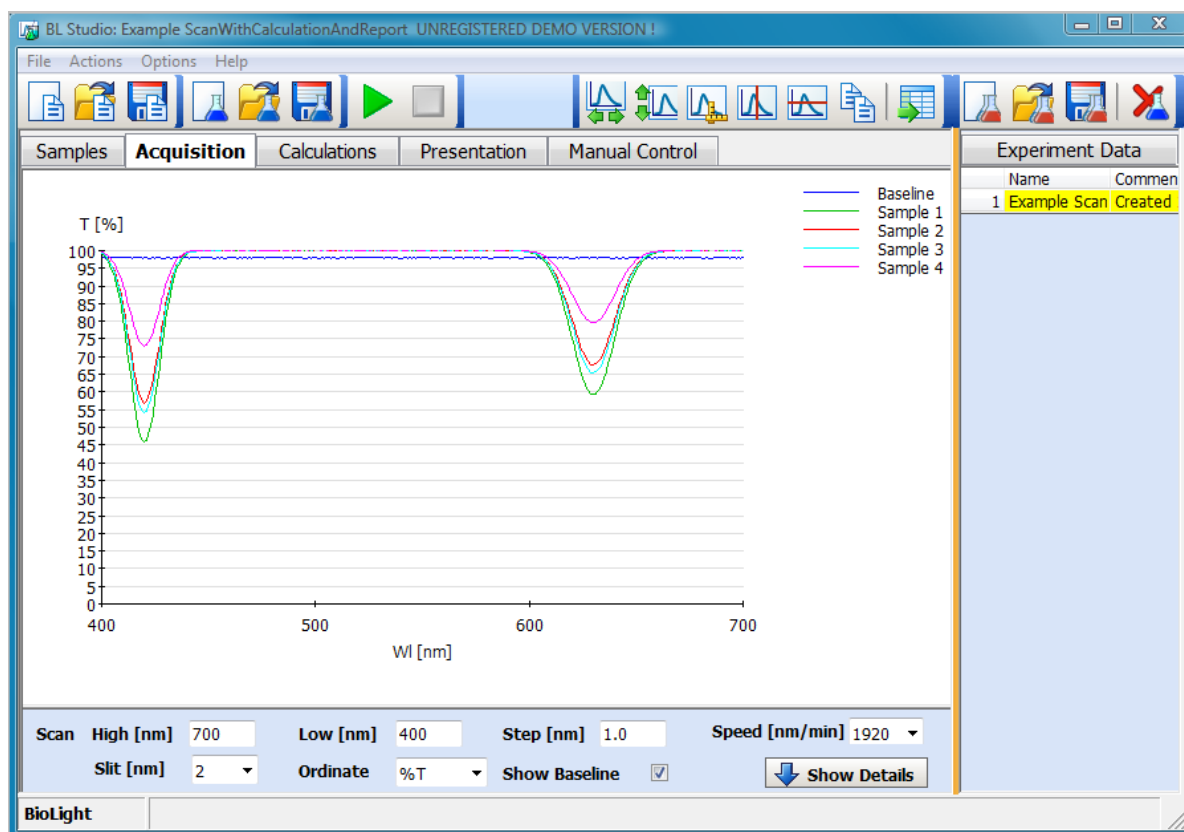
These add-on applications can be built to your specific requirements (e.g. controlling a specific sample preparation system, to generate specific reports or to import/export data from/to your LIMS system. Since the add ons can be installed completely independently of the BL Studio frame work only the new module must be validated.

For a list of already available add-on applications check our homepage www.biolight.com.

The Development Frame

This, highly flexible, frame is specialized for method development. The work flow consists of a logical series of steps. These steps are represented by tabs on the main page. The basic steps are “Samples” representing the sample preparation and “Acquisition” containing all parameters for the data acquisition. They are supplemented by “Manual Control” to control the instrument directly.

Optionally three further steps can be added: “Calculations”, containing online-data processing, “Presentation” to automatically generate reports and “Administration” to perform administrative tasks.



The main page consists of a menu, a toolbar, the tab pages, the application detail area, the experiment data section and a status bar.

The left part of the toolbar is populated with a set of generic icons, while the right part contains a set of icons which are modified according to the currently selected step to display graphics icons etc. The tab pages define the work flow. Application-specific details are displayed in the application detail area.

Main Menu

The following items are available in the menu:

File:

- New Method: Starts the New Method dialogue, to define all steps of a new method
- Load Method: Starts a File Open dialogue to load a method from hard disk
- Save Method: Starts a File Save dialogue to save the current method to hard disk
- Load Sample Info: Opens the Import Sample info file dialogue. (see also Importing Sample Info)
- Save Sample Info: Opens the Export Sample info file dialogue. (see also Exporting Sample Info)
- Clear Data: Clears the data in all steps
- Load Data: Starts a File Open dialogue to load data from hard disk and displays it

Save Data:	Starts a File Save dialogue to save the currently displayed data to hard disk
Clear Experiment:	Removes all results from the experiment data list
Load Experiment:	Starts a File Open dialogue to load an experiment data set
Save Experiment:	Starts a File Save dialogue to save the complete experiment
Exit:	Exit BL Studio

Actions:

Start freeform calculator:	Starts the BL Calculator program
Send results to calculator:	Starts the BL Calculator program and loads currently selected curves

Options:









Function Keys:	Starts the Define Function Keys dialogue
Data Options:	Opens the Data Options dialogue
Display Options:	Opens the Display Options dialogue
New Calculator:	Allows the user to define a new calculator without clearing current data
New Presentation:	Allows the user to define a new report without clearing current data

Help:

About:	Displays the about dialogue
--------	-----------------------------

Main Toolbar

The following items are available in the main toolbar:





	New Method:	Starts the New Method dialogue, to define all steps of a new method
	Load Method:	Starts a File Open dialogue to load a method from hard disk
	Save Method:	Starts a File Save dialogue to save the current method to hard disk
	Clear Result:	Clears the results in all pages
	Load Result:	Starts a File Open dialogue to load a result from hard disk and displays it
	Save Result:	Starts a File Save dialogue to save the currently displayed result to hard disk
	Start Measurement:	Starts a Measurement
	Stop Measurement:	“Gracefully” stops the current measurement

Experiment Data

This list displays all results collected or loaded during an experiment. While result datasets are limited to be collected with one method, experiment data can contain several results, each measured with a different method. Each result can be viewed by just clicking on the corresponding result name in the list.

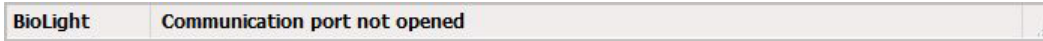
It is possible to add or delete results and to save the complete experiment into a single dataset. Reloading the experiment allows the user to view all results belonging to the experiment. Moreover all used methods can easily be restored.

The experiment data toolbar consists of the following icons:

	Clear Experiment:	Removes all results from the experiment data list
	Load Experiment:	Starts a File Open dialogue to load an experiment data set
	Save Experiment:	Starts a File Save dialogue to save the complete experiment
	Remove Result:	Removes the selected result from the experiment data list

Status bar

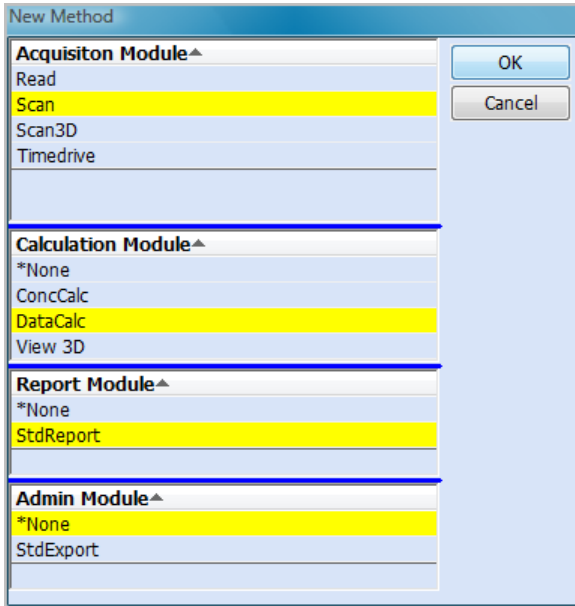
In the first field of the status bar the full name of the user currently logged on is displayed.



The second field is used to display status and error messages.

Creating a new Method

Select this function from the file menu or the toolbar. The New Method dialogue opens



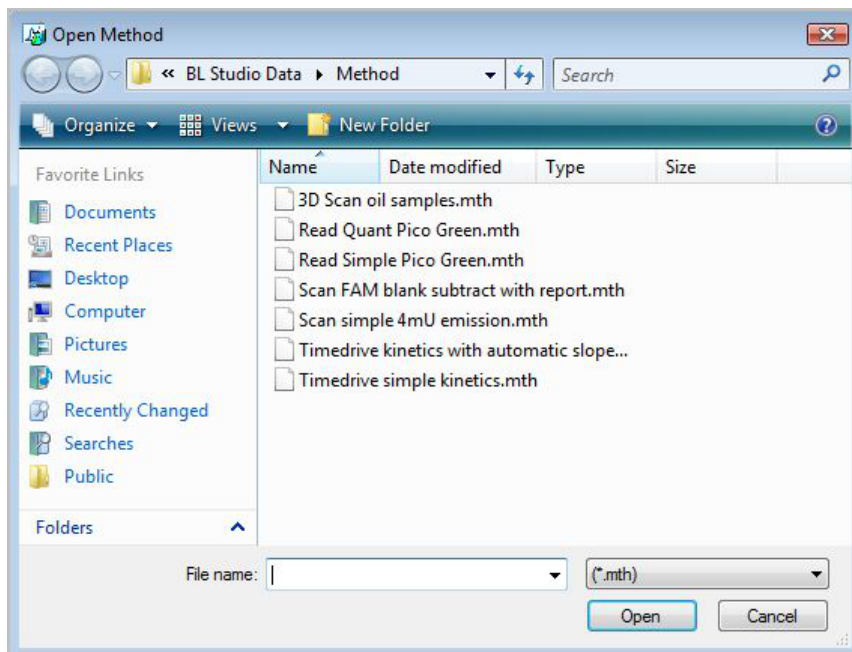
Now you can select a module from each category: Data-Acquisition, Online-Calculations, Reports and Administration. Together these modules will define the measurement method. Please note that you can select None for the calculation, presentation or administration module respectively, skipping these steps. After pressing Ok the selected modules are loaded into the Application frame.

New modules can easily be installed/loaded via the Registry program without modifying the existing installation. Likewise it is also possible to uninstall/unload modules.

Creating a new method will automatically clear all currently loaded data. If you wish to re-evaluate data using a new calculator or present them using a new report module use the functions "New Calculator", "New Presentation", "New Administration" from the Options menu instead.

Loading a Method

Select this function from the file menu or the toolbar. A standard windows file open dialogue opens

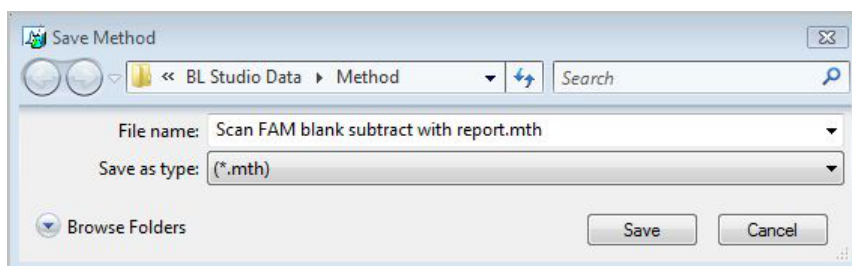


By default the dialogue displays all methods in the standard method directory (see also Defining the standard directories). However, it is possible to load methods from any other location by changing the directory. The next time the load method dialogue is called the new directory will be remembered.

After the method was selected, all required modules are loaded into the application frame automatically and the method parameters are displayed. In case a required module is not available the corresponding error message is displayed. Please note that all currently loaded result data are cleared before the new method is loaded. Leaving the dialogue with cancel will neither clear the current data, nor will it load the new method.

Saving a Method

Select this function from the file menu or the toolbar. Firstly all method parameters are validated. If one or more parameters are invalid an error message is displayed, otherwise the file save dialogue opens

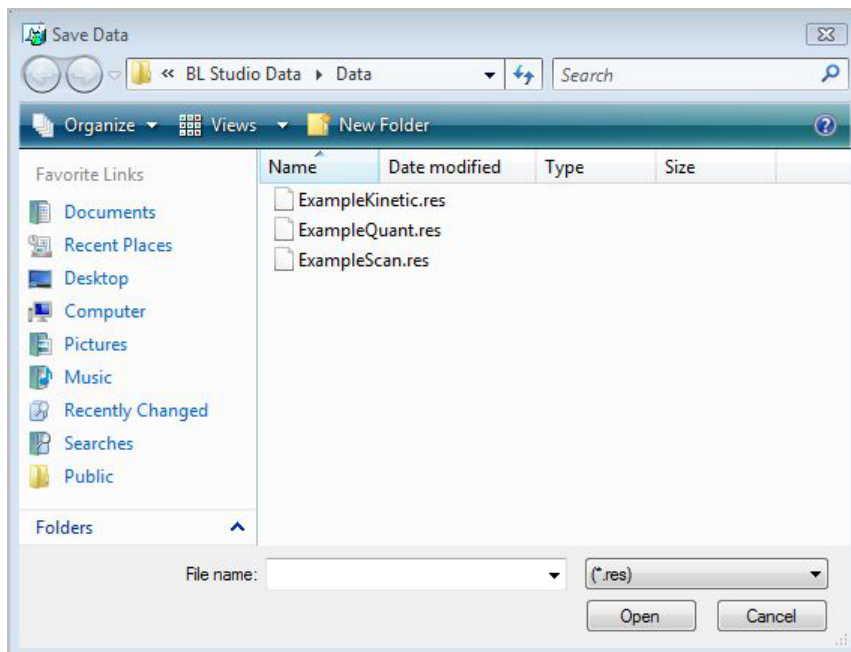


By default the standard method directory is selected in the dialogue (see also Defining the standard directories). However, it is possible to save methods to any other location by changing the directory (e.g. via the browse folders option). The next time the method save dialogue is called the new directory will be remembered. Leaving the dialogue with Save saves the method to the selected directory. If the method already exists an overwrite warning is issued. Clearing Data

Select this function from the file menu or the toolbar. All currently measured data is cleared in all modules, the current result in the experiment data list is unselected.

Loading existing Data

Select this function from the file menu or the toolbar. A standard windows file open dialogue opens:

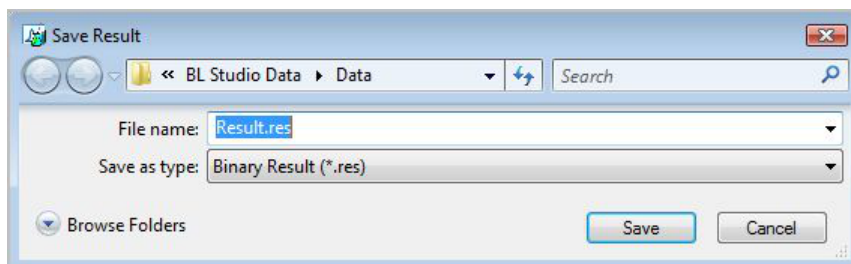


By default the dialogue displays all data in the standard data directory (see also Defining the standard directories). However, it is possible to load data from any other location by changing the directory. The next time the load data dialogue is called the new directory will be remembered.

After the data was selected, the data is loaded into the Experiment Data List and selected. Then the complete method is extracted from the data, all required modules are loaded into the application frame and the method parameters are displayed. If the result contains background correction data, the correction is sent to the instrument. Finally the results are displayed, online-calculations are performed if applicable and a new report is generated. In case a required module is not available the corresponding error message is displayed.

Saving Data

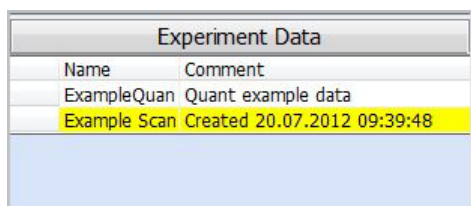
Select this function from the file menu or the toolbar. A standard windows file save dialogue opens



By default the standard data directory is selected in the dialogue (see also Defining the standard directories). However, it is possible to save data to any other location by changing the directory (e.g. via the browse folders option). The next time the save data dialogue is called the new directory will be remembered. Leaving the dialogue with Save saves the data to the selected directory. If the data already exists an overwrite warning is issued.

Selecting Data

Selecting data from the Experiment Data List is a very convenient way to display and compare previously measured data. Simply click on the row displaying the name of the desired data.



Experiment Data	
Name	Comment
ExampleQuan	Quant example data
Example Scan	Created 20.07.2012 09:39:48

The row becomes yellow to indicate the result is selected. Then the complete method is extracted from the data, all required modules are loaded into the application frame and the method parameters are displayed. Finally the results are displayed, online-calculations are performed if applicable and a new report is generated. In case a required module is not available the corresponding error message is displayed.


Starting a Measurement

Select this function from the toolbar . The following procedure starts:

- 1.) Firstly the menu, all icons from the toolbar that would bring up a dialogue or change the method/data and all data acquisition parameter are locked. The stop button is enabled, the start button is disabled.
- 2.) If a result is selected in the experiment list and the method has not been modified new data are appended to the existing results. If no result is selected or the method has been modified a new result is generated and added to the experiment list.
- 3.) The software performs a new Baseline Correction if necessary.
- 4.) Then the sample preparation for the first sample is performed (see Sample Preparation modules). If the sample preparation is not automated the user is prompted to update the sample information and insert the sample.
- 5.) Afterwards the actual data-acquisition is started for the first sample. The collected data is displayed online in the acquisition module. After the acquisition is completed for the sample, the data is sent to the data calculation module and all calculations are performed. Then the results are sent to the presentation module, which updates the report from the raw and calculated data.
- 6.) Step 2 and 3 are performed for all samples.
- 7.) If selected in the data options the raw data is saved automatically, the stop button is disabled, the menu and the toolbar are unlocked.

After the measurement has been finished the data can be saved at any time via the save data icon. Furthermore it is possible to modify any calculation or presentation parameters to re-evaluate the data.

Stopping a Measurement

Select this function from the toolbar . The function performs a “graceful” stop. This means that data-acquisition runs to completion for the current sample and all data are automatically saved (if selected in the data options). (see also emergency stop)

Continuing a Measurement

To append data to an existing result select the result from the experiment data list and press the start button. This includes the possibility to stop a measurement, save the data, reload the data at a later time and then continue the measurement. Thus the user can interrupt current measurements for high priority samples, or generate trend data for a long time period.

Performing a Background Correction

A background correction can be started in two different ways:

Manually

By pressing the corresponding function key (typically F2). The correction will be started using the current method parameters. The resulting data are stored in the currently selected result. If no result has been selected, a new result is created. All subsequent measurements are automatically corrected with the background spectrum. If the current result already contains a correction spectrum it is overwritten with the new correction, measurements corrected with the old background spectrum stay unchanged.

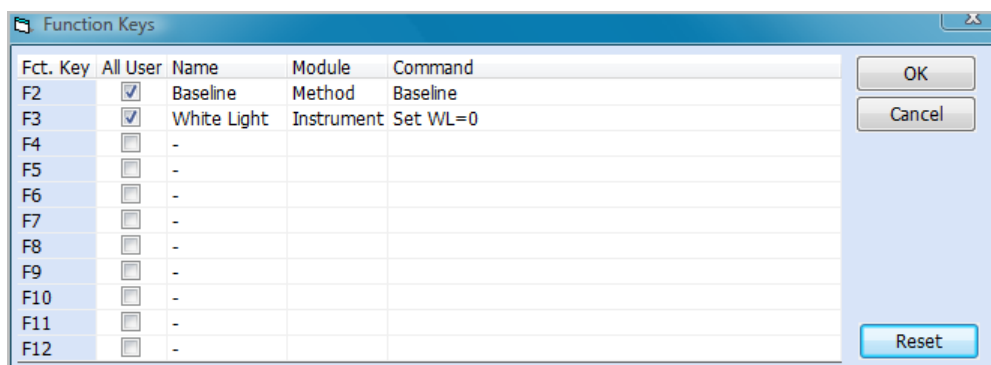
Automatically

Whenever a new measurement is started a background is performed automatically, using the current method parameters. The resulting correction is stored in the result. All subsequent measurements are corrected automatically until the method parameters are changed or a new result is created. In these cases a new correction spectrum is measured.

Please note, that loading a result also loads the corresponding background correction and sends it to the instrument. Appended measurements use the loaded correction. However, if the loaded correction is older than one day, the user is prompted to perform a new background correction.

Function Keys

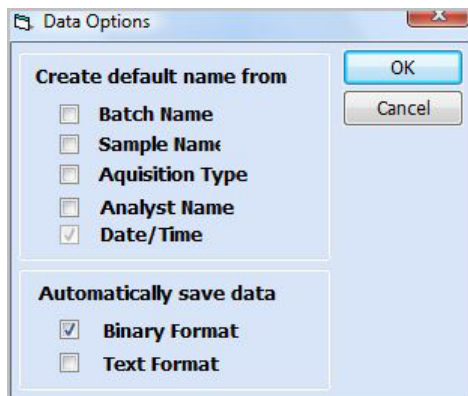
Select this function from the options menu. The Define Function Keys dialogue is started:



Via this dialogue commands can be assigned to the function keys F2 – F12. The functions can be either available for all users or for the current user only. The module defines to which module the command is sent. (Currently only the Instrument module is available). The command column contains the command to be sent. In the example pressing the F2 key will start a baseline measurement, while pressing F3 will set the monochromator to white light. Please note, that the function keys will also be available in the Routine and Validation applications.

Data Options

Select this function from the options menu. The Data Options dialogue is displayed:






The default name options can be combined to obtain a default result name. (The data/time option cannot be unselected to ensure an unique name).

If the Automatically save data option is selected, raw data are always stored in binary format. This occurs when a measurement has finished or was stopped.

Display Options

Select this function from the options menu. The Flow Options dialogue is displayed:

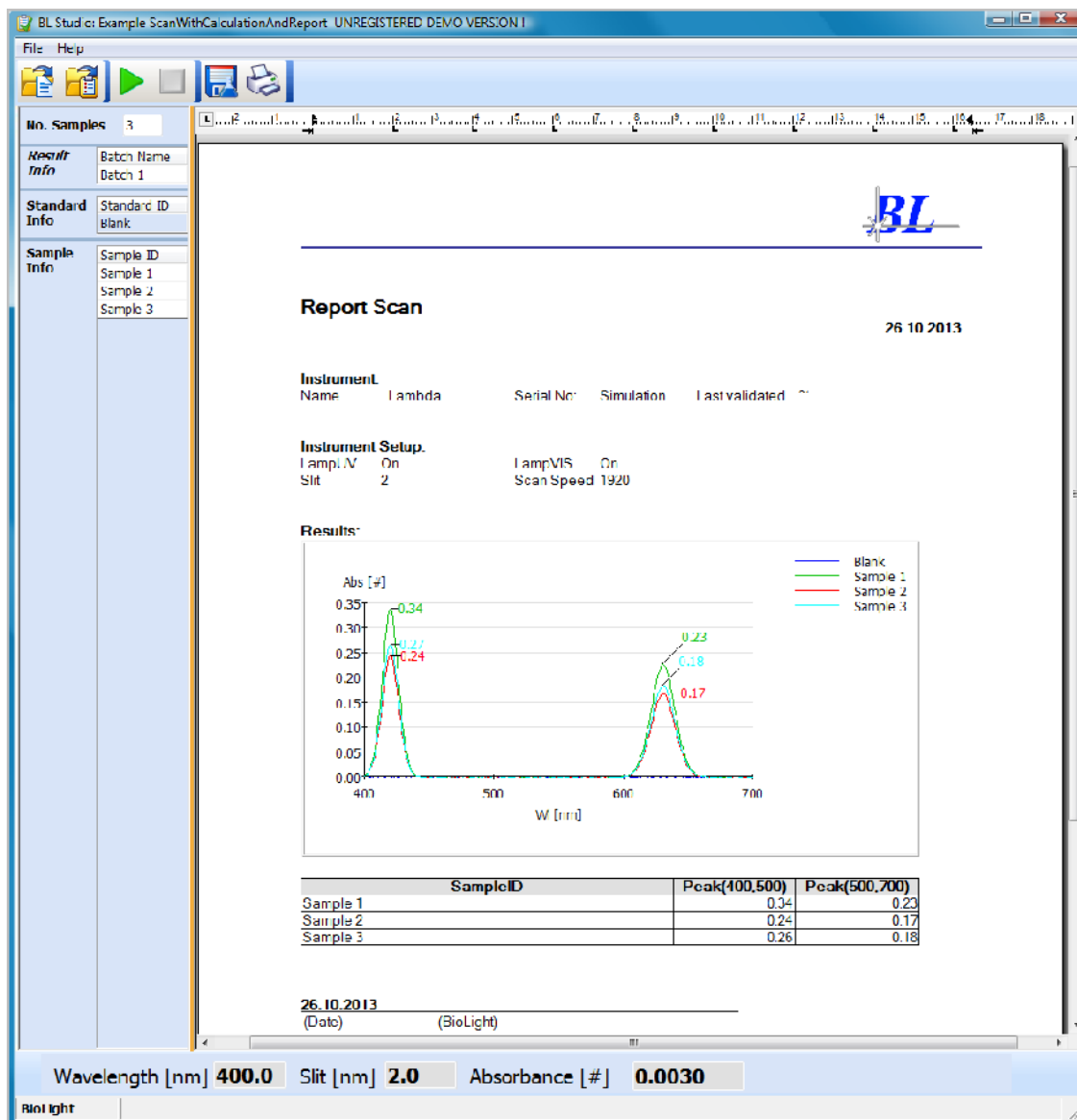


If the clear results option is selected, previously collected data is cleared automatically before a new measurement is started. In this case the data acquisition parameters can optionally be changed between measurements. If the option is unselected old data are not cleared automatically. This allows either the continuation of a measurement that has been stopped or the loading of previous data and appending a new measurement. If data is loaded the Start icon  is replaced by the Continue icon . Please note that the data acquisition parameters are locked to ensure that all data is collected using the same parameters. To unlock the acquisition parameters the data must be cleared manually via the clear data icon  in the toolbar.

If the Send Curves to Calculator option is selected all collected curves are sent to the free-form Calculator program automatically after data acquisition has finished. This is especially useful if data collected with different acquisition parameters is to be compared. (In BL Studio the data must be cleared before changing the parameters).

The Routine Frame

The routine frame is specialized for routine daily use and result measurements with pre-defined methods. It supports the same modules as the development frame. Thus any method, developed with the development frame can be loaded and executed. The simplified user interface guides the user safely through the measurement. The routine frame displays all information on a single page:



The routine frame consists of a menu, a toolbar, on the left hand the sample information area, the result/report area and at the bottom, the live display and the status bar.

Main Menu

The following items are available in the menu:

File:







Load Method:	Starts the select method dialogue to load a method
Load Sample Info:	Opens the Load Sample info file dialogue. (see also Importing Sample Info)
Clear Result:	Clears the currently measured result
Save Result:	Saves the current result
Print Result:	Prints the current result
Exit:	Exit BL Studio

Help:

About:	Displays the about dialogue
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Main Toolbar

The following items are available in the main toolbar:

 Load Method:	Starts the select method dialogue to load a method
 Load Sample Info:	Opens the Load Sample info file dialogue. (see also Importing Sample Info)
 Start Measurement:	Starts a Measurement
 Stop Measurement:	“Gracefully” stops the current measurement
 Save Result:	Starts the File Save dialogue to save the current result to hard disk
 Print Result:	Starts the print dialogue to send the current result to the printer

Sample Information Toolbar

The sample information toolbar becomes visible, when the standard or sample info table is selected:

 Fill down:	The contents of the current cell are copied to all successive cells in the column
 Fill down increment:	The contents of the current cell are incremented and copied to all successive cells in the column.

Live Display

The Live Display provides live system and instrument readings. These are the current wavelengths, the current reading and the current temperature (if a temperature sensor is fitted)

Wavelength [nm] **0,0** Slit [nm] **2,0** Transmission [%] **97,91**

If the instrument is initializing, offline or in an error state a corresponding message is displayed.

Status bar

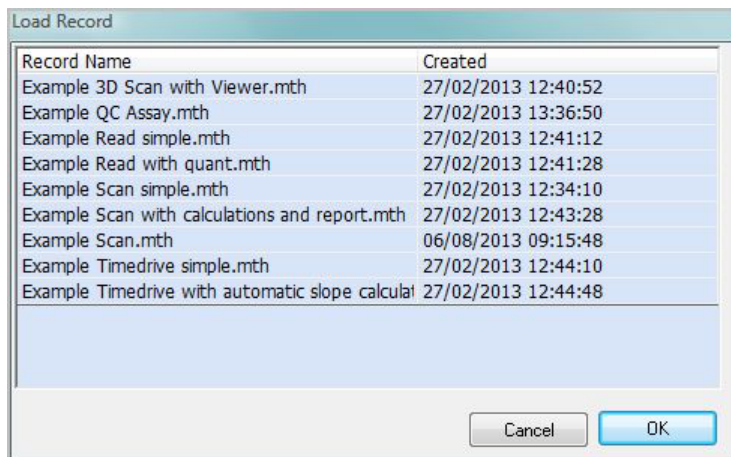
In the first field of the status bar the full name of the user currently logged on is displayed.

BioLight Communication port not opened

The second field is used to display status and error messages.

Loading a Method


Select this function from the file menu or the toolbar. The Load Method dialogue opens:



The dialogue displays all methods available for the current user. In difference to the Development program it is not possible to load methods from any other location.

After the method was selected, all required modules are loaded into the application frame automatically. Please note In case a required module is not available the corresponding error message is displayed. Please note that all currently loaded result data are cleared before the new method is loaded. Leaving the dialogue with cancel will neither clear the current data, nor will it load the new method.


Starting a Measurement

Select this function from the from the file menu or the toolbar . The following procedure starts:

- 1.) Firstly the menu, all icons from the toolbar that would bring up a dialogue or change the method/data and all data acquisition parameter are locked. The stop button is enabled, the start button is disabled.
- 2.) The software performs a new Baseline Correction if necessary.
- 3.) Then the sample preparation for the first sample is performed (see Sample Preparation modules). If the sample preparation is not automated the user is prompted to update the sample information and insert the sample.
- 4.) Afterwards the actual data-acquisition is started for the first sample. The collected data is displayed online in the acquisition module. After the acquisition is completed for the sample, the data is sent to the data calculation module and all calculations are preformed. Then the results are send to the presentation module, which updates the report from the raw and calculated data.
- 5.) Step 2 and 3 are performed for all samples.
- 6.) If selected in the data options the raw data is saved automatically, the stop button is disabled, the menu and the toolbar are unlocked.

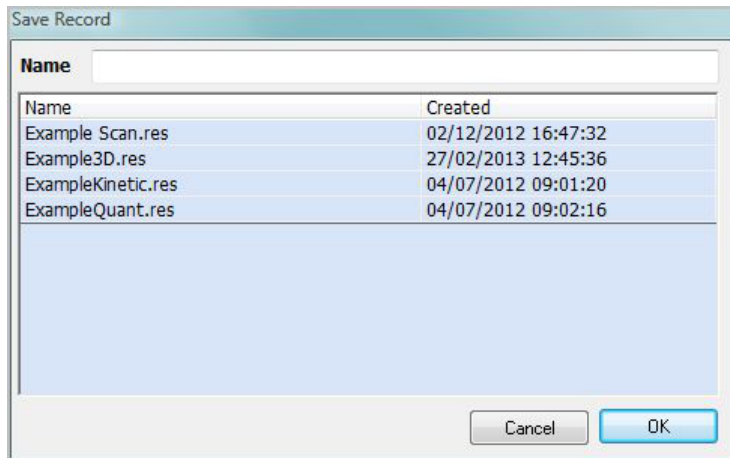
After the measurement has been finished the data can be saved at any time via the save data icon.

Stopping a Measurement

Select this function from the from the file menu or the toolbar . The function performs a “graceful” stop. This means that data-acquisition runs to completion for the current sample and all data are automatically saved (if selected in the data options). (see also emergency stop)

Saving Data


Select this function from the file menu or the toolbar. The Save Data dialogue opens:

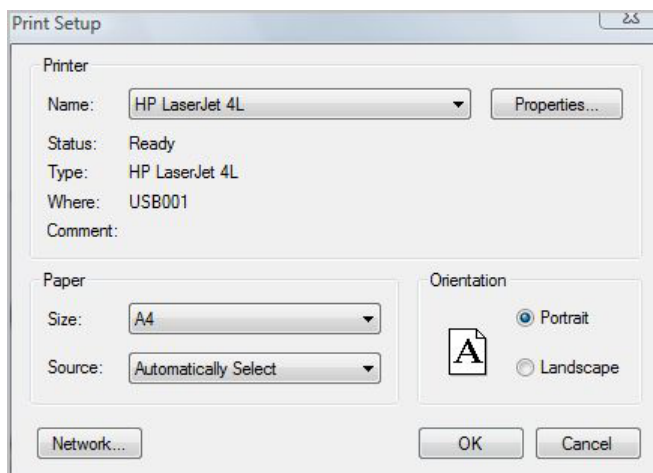


The dialogue displays the contents of the result directory assigned to the user. To save the result enter the new result name into the “Name” textbox and press ok.

In difference to the Development program it is not possible to save data to any other location. If the user tries to overwrite an existing result an error message is issued.

Printing a Result

After clicking the print button  the standard print setup dialogue is opened:



Select the printer and press ok to print the result, using the report template defined in the method.

If no result has been measured or no report template is defined in the method an error message is issued.

Sample Preparation

Description

The sample preparation module contains the management of sample information as well as the control of sample preparation. It additionally allows the user to exclude samples from offline processing. The sample preparation module is dedicated to a specific sample preparation system. It is possible to install a module for any sample preparation after measurement.

It is good documentation practice to store all sample information together with the measured data. Furthermore, some measurements require sample-dependent and sample-independent data for the calculation of results.

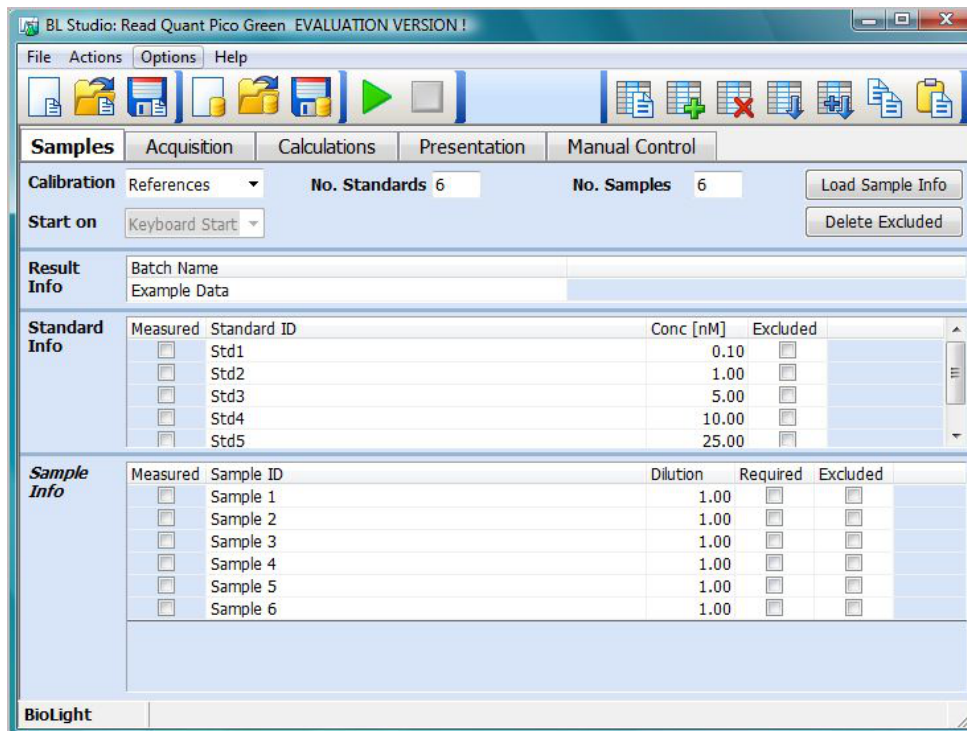
BL Studio therefore provides the possibility to define a set of 'required' information within each method. During data acquisition this information *must* be provided by the analyst, either by typing the data in manually or by loading it from a LIMS system. To improve the correctness of typed data it is possible to define the type and the permitted range for each sample information item.

It is also possible to lock certain information from input. In this case the analyst must load the corresponding information from the LIMS system and cannot enter the data manually. Thus the integrity of this sample information data is guaranteed. It is possible to define the output format of the sample information.

The Standard Sample Module

The standard sample module supports all internal sample accessories of the LS45/50/55 as well as the external accessories: S10-Autosampler and P1-Peltier of PerkinElmer. The current fitted accessory is interrogated from the connected instrument. The upper part of the window shows the sample preparation parameters, depending on the accessory. The lower part is accessory independent. Here the batch/sample information is managed.

The following picture shows a set of parameters for the **single cell holder** accessory:

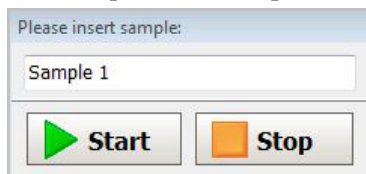


Generic Entries

Start On

This list box offers different methods to trigger the start of sample measurement:

- **Keyboard Start:** A message box is displayed before the measurement of each sample, allowing the user to update the sample information.



Pressing the Start-Button starts the measurement. If necessary a new sample information row is added to the sample information table. Pressing the Stop-Button terminates the measurement.

- **External trigger:** The run starts on closure of the external trigger input of the LS, or on pressing the button of the biokinetics accessory.
- **File:** The run starts when the file "SampleInfo.txt" is created in the Sample directory. The information of the current sample is updated from the file and the corresponding entry in the file is deleted. If no entry remains, the complete file is deleted. The format of the text file is the same as for loading/saving sample info. To generate a template press the Save Sample info button.

Calibration

Here, the type of data calibration can be selected:

- None: Data is not calibrated. Run starts immediately with sample measurements.
- Blank: The standard table becomes visible, allowing one blank. The blank sample is measured at the beginning of the run. It can be used e.g. in the calculation module to subtract the blank result from all successive measurements.
- References: The standard table becomes visible, allowing any number of reference measurements. The results can be used in the calculation module (e.g. in the concentration module) to generate a calibration curve for successive measurements.

Delete Excluded Button

Pressing this button immediately deletes the data (i.e. all samples/references marked as “exclude”) from the raw data. Note that this action is not reversible. This button is only visible if result data were measured or loaded and the user has the right to delete data.

Single Cell Holder

No. References

The number of references to be measured must be entered in this text box. After exiting the text box (e.g. by pressing the return key) the number of rows in the Standard Info table is updated. If the calibration type None/Blank was selected the number of references is set to 0/1 respectively. Please note that it is NOT possible to add references during the measurement. The text box is not visible if an automated sample accessory (such as WPR) is fitted.

No. Samples

The number of samples to be measured can be entered in this text box. After exiting the text box (e.g. by pressing the return key) the number of rows in the Sample Info table is updated. Please note that it is possible to automatically add samples later on during the measurement. The text box is not visible if an automated sample accessory (such as the WPR) is fitted.

Sipper Accessory

Not implemented in the current version

Peltier Accessory

The biokinetics accessory allows the user to measure actively tempered samples. The peltier element sets the sample temperature to the desired value, a temperature sensor allows the monitoring the temperature of the sample.

The screenshot shows a control panel with the following settings: Calibration is set to 'Blank' (dropdown), No. Standards is '1' (text box), No. Samples is '0' (text box), Start on is 'Keyboard Start' (dropdown), Stirrer Speed is 'Off' (dropdown), and Temperature [°C] is '~' (text box). A 'Delete Excluded' button is visible on the right side of the panel.

Stirrer Speed Use the stirrer to avoid temperature gradients. The speed can be set in three steps: off, low and high.

Temperature Defines the start temperature of the sample. Before the actual measurement begins the peltier is set to this temperature. The system then waits, until the temperature is reached. To avoid the system waiting for a temperature enter ~ in the text box. The measurement will then start immediately.

Please note that the temperature monitored is acquired from the block temperature of the biokinetics accessory rather than from the sample itself. To compensate for lags use the temperature calibration defined in the manual control module.

Cell Changer Accessory

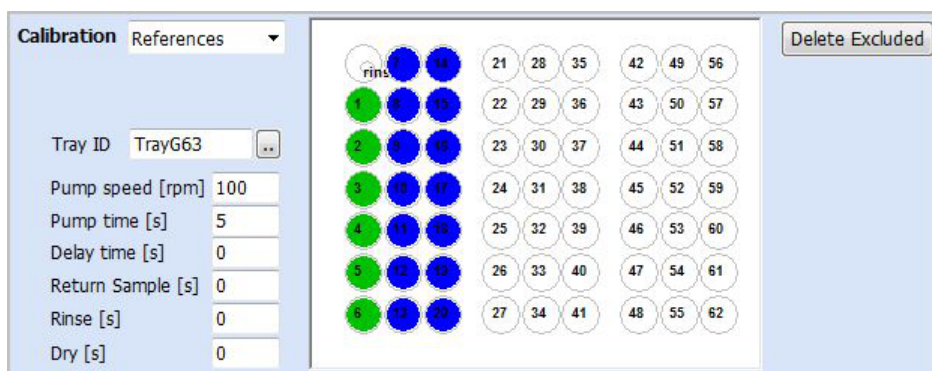
Not implemented in the current version

Auto Sampler Accessory

The auto sampler accessory allows the user to automatically measure a complete tray during one run.

A new tray definition plate can be loaded from file by clicking on the .. button besides the Tray ID text box. After selecting the file from the standard file selector dialogue an image of the tray is displayed. (Please note, that the tray definition files are located in BL Studio Data/System).

To define samples left click on the desired position on the tray image. The position will become blue and a new row will be added to the sample list. To add more than one sample press the left mouse button and drag the mouse over all desired sample positions. Right clicking on a position (dragging the mouse over several positions with right mouse button pressed) removes the corresponding samples.



If calibration-type is set to blank the blank tube is indicated by a black cycle. To change the blank position simply left click on the new position keeping the shift-key pressed.

If calibration-type is set to standards it is possible to add a standard by left clicking on a position, keeping the shift-key pressed (or drag the mouse over the range pressing the left mouse-button and the shift key simultaneously). The position(s) will become green and the standards(s) are added to the standard list. To remove the standards press the right mouse-button and the shift key, while dragging over the positions to be deleted.

It is possible to add an unknown sample and a standard at the same position. The start on list-box is not available for the plate reader.

Pump Speed The same pump speed is applied for sipping, purging, rinsing and drying

Pump Time Defines the time that the system pumps to fill the flow-cell with the sample.

Delay Time The delay time is the time the systems waits after sipping to allow for de-bubbling.

Return Sample Enter a value greater than zero to return precious sample after the measurement.

Rinse Enter the rinse-time in this text-box: The auto-sampler is sent to the rinse-position and the sipper pumps the rinse solution for the given time.

Dry Enter a value greater than zero to dry the tubes after rinsing. The auto-sampler head is moved to the upper position and air is pumped through the tubes for the given time.

The Result Info Table

This table contains all sample independent information. All information is stored in the method. Besides the mandatory columns, new columns can be easily added. (Add new Sample Information)

Mandatory Columns:

Batch name: contains a description of the measurement, e.g. the batch name. Please note that the caption of the column can be changed easily, if you wish to store a different information. This field is used to generate a default result name in the Data Options dialogue.

The Standard Info Table

This table contains all standard information. All of this information is stored in the method. Besides the mandatory columns new columns can be easily added. (Add new Sample Information)

Mandatory Columns:

Measured: Indicates if data for this standard is available.

StandardID: Contains a unique identifier for the standard that is used in other modules to identify the standard.

Conc: Contains the expected result for a standard. Please note that the caption and unit for the expected result can be easily changed.

Exclude: Select this option to exclude samples (see Excluding samples from evaluation)

The Sample Info Table

This table contains all sample information. Basically only the structure of the table is stored in the method and not the sample information itself. Besides the mandatory columns new columns can easily be added. (Add new Sample Information)

Mandatory Columns:


Measured: Indicates if data for this standard is available.

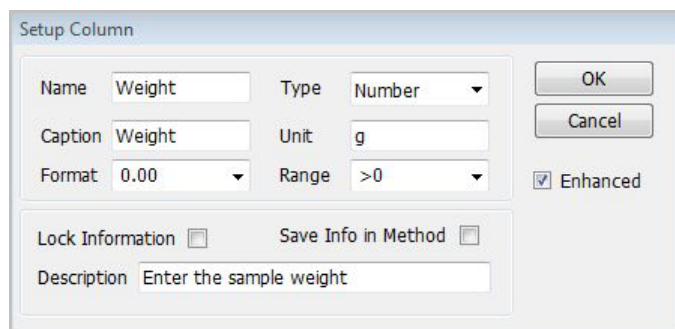
SampleID: Contains a unique name for the sample that is used in other modules to identify the sample.

Required: Indicates that this sample must be measured during data acquisition. Information for required samples is stored in the method. Furthermore required samples can be used in calculations.

Exclude: Select this option to exclude samples (see Excluding samples from evaluation)

Adding a new Information Column

Select the column before which the new information column is to be inserted by clicking on the columns caption. If no column is selected the new column is appended after the last user defined column. Now select  from the toolbar. The Add Sample Information dialogue is displayed:



Name

Contains a unique name identifying the sample information. The name is used in other modules e.g. in the calculations and report module and therefore cannot be modified once the information variable has been defined.

Type

Contains the type of the sample information (see also variable types). The name is used in other modules e.g. in the calculations and report module and therefore cannot be modified once the information variable has been defined.

Caption

Contains the caption of the information column to be displayed on the sample info table. Changing the caption allows e.g. for localized methods.

Unit

Contains the unit of the information column to be displayed on the sample info table. This entry field is visible for numeric types only.

Format

Defines how the information is formatted in the sample info table. This function allows the user, to for example, define the number of decimals of a value. This entry field is visible for numeric or date types only. (see also variable formats)

Range

Defines the valid range for an information variable. This function can stop the entry of invalid values for data acquisition parameters. This entry field is visible for numeric types only. (see also variable ranges)

Force Input

If this option is selected the user is forced to enter a text. This entry field is visible for the text type only.

Enhanced

Selecting this option displays the following entries:

Lock Information

Select this option to prevent the user from changing this sample information during the data acquisition.


Do not save Info in Method

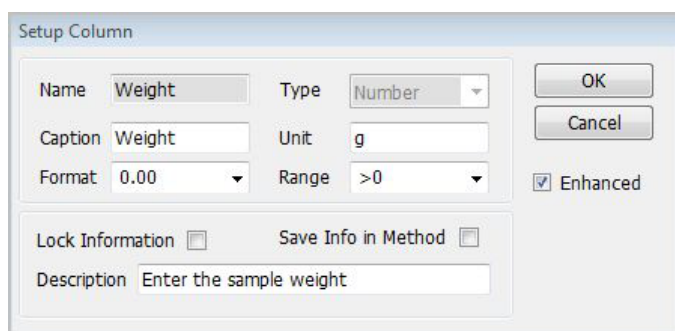
If this option is selected the specific information is not saved in the method: Result information, standard information and sample information for “required” samples is stored in the method. However, some of this information may be updated during measurement. This would result in a modified (and therefore unapproved) method. To avoid this scenario select this option for these fields.

Description

The text entered in this entry field is displayed as tool tip in the insert sample dialogue that appears during the data acquisition.


Editing an Information Column

In the desired table select the information column to be edited by clicking on the columns caption. Now select  from the toolbar. The Edit Sample Information dialogue is displayed:




For the description of the fields please refer to Adding a New Sample Information. Please note that the name and the type of the Information column cannot be modified in this dialogue.


Removing an Information Column

In the desired table select the information column to be deleted by clicking on the columns caption. Now select  from the toolbar to delete the column.

Fill Down Sample Information


In the desired table select the cell from where the fill down process should start. After pressing the  icon on the toolbar, the contents of the current cell are copied to all successive cells in the column.

Fill Down Sample Information with Increment


In the desired table select the cell from where the fill down process should start. After pressing the  icon on the toolbar the contents of the cell are incremented and copied to all successive cells in the column.

The following rules apply to the increment: If the cell above the selected cell ends with a number and the selected cell ends with a number the increment step is set to the difference. If one of the cells does not end with a number or the selected cell is the first cell of the column the increment step is set to 1.

Copy Sample Information

Select the desired table and press  on the toolbar. The content of the table is copied as tab-delimited text to the clipboard. The first line contains the captions of the table.

Paste Sample Information

Select the desired table and press  on the toolbar. The content of the clipboard is pasted into the selected table. The content of the clipboard must be tab-delimited text. The first line must contain the column captions. The function first checks if a matching column exists on the table and then copies the corresponding information.

Importing Sample Information from a File

Selecting Load Sample Info from the file menu a standard Windows file selector. Select the desired file and leave the dialogue with ok. BL Studio compares the column captions defined in the method against the captions defined in the file and copies the corresponding sample information into the result/standard and sample info tables. The sample information file must be a tab delimited ASCII file with the following structure:

[Generic]

<ColCaption1>Tab<ColCaption1>...

<InfoCol1>Tab<InfoCol2>...

[Standards]

<ColCaption1>Tab<ColCaption1>...

<InfoStd1Col1>Tab<InfoStd1Col2>...

<InfoStd2Col1>Tab<InfoStd2Col2>...

...

[Samples]

<ColCaption1>Tab<ColCaption1>...

<InfoSmp1Col1>Tab<InfoSmp1Col2>...

<InfoSmp2Col1>Tab<InfoSmp2Col2>...

...

To generate a template press the Save Sample Info Button.

Exporting Sample Information to a File

Selecting Save Sample Info from the file menu opens a standard Windows file selector. Select the desired file name and leave the dialogue with ok. The contents of the result info table, the standard info table and the sample info table is stored in ASCII format to the selected file. The information can be re-loaded via the Import Sample Info button.

Excluding Samples from Evaluation

Selecting the exclude option on the standard table or sample table hides the sample in all modules. That is, the respective sample is no longer shown on the online graph/table of the data acquisition module, it is not evaluated in the calculation module and it is hidden in a report.

However, the sample is not deleted from the raw data set. Thus it is possible, to re-include the sample at any time by deselecting the exclude option. The status of the delete options is stored in the raw data. When data is re-loaded previously excluded samples will stay excluded.

To permanently delete standard data click on the “Delete Excluded” button. Please note, that this step is irreversible: The data for this sample is lost.

Deleting Sample-Data from Results

Select the exclude option for the standards/samples to be deleted and click on the “Delete Excluded” button. This will permanently delete the corresponding data. Please note, that this step is irreversible: The data for this sample is lost.

Data Acquisition

Description

The data acquisition modules handle the complete data acquisition from one or more instruments. Beside the manual module only these modules contain any information about the connected instruments.

These modules are dedicated to a specific instrument and to a specific type of measurement. Currently BL Studio offers 4 standard data acquisition modules for the PerkinElmer Lambda series: Read, Timedrive, Scan and 3DScan.

In the base version BL Studio offers four data acquisition modules:

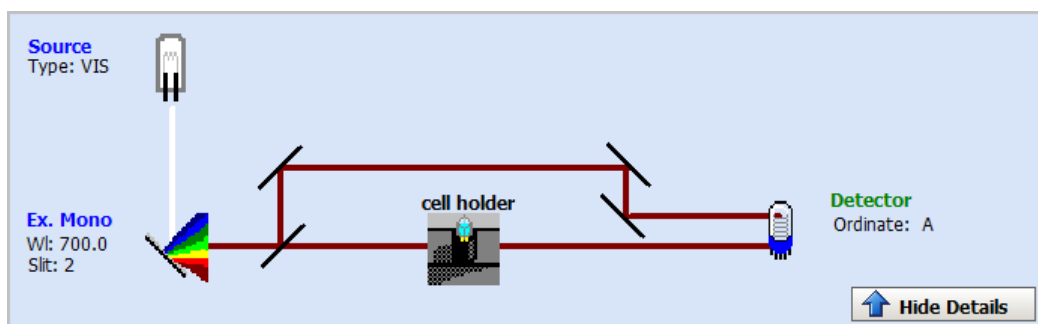
- Read: Collects single data points
- Time drive: Offers acquisition of kinetic data
- Scan: Collects spectral data
- 3D Scan: Collects spectral data vs. time

If required specific acquisition modules can be added.

The Instrument Setup Panel

Typically the modules are separated in two parts: the specific data acquisition section and the generic instrument setup section. Before any data acquisition starts, the instrument is automatically updated with the setup parameters, ensuring reproducible results.

The instrument setup is displayed on a schematic of the Lambda optical system with icons representing the individual components. The setup of the instrument is described by the text next to the icons. The colours of the beams between each icon in the optical schematic are an approximate indication of the wavelength:



It is possible to change the setting of instrument parameters by clicking on the icon relating to that part of the optical system. This accesses a series of specific instrument configuration dialogues (Detailed descriptions of the dialogues can be found in the Manual Control Chapter).

Please note, that changes are recorded in the application method only and are not sent to the instrument immediately.

The Read Module

The Read application enables measurements (transmission, absorbance) to be made at fixed wavelengths.

The screenshot shows the Read Module interface. At the top, there is a header bar with 'Sample ID' and 'T(700) [%]'. Below this is a large, empty light blue area representing the data table. At the bottom, there is a control panel with several elements: 'Insert WL' and 'Remove WL' buttons on the left; a 'WL [nm]' input field with '700' entered; 'Int. Time [s]' set to '1.0'; 'Slit [nm]' set to '2'; 'Ordinate' set to '%T'; and a 'Show Details' button with a downward arrow.

Result Table

The result table displays the measured data online. The following information is displayed:

- SampleID displays the sample identifier
- %T(WL) displays the measured transmission(absorbance respectively) for each defined wl,

Wavelength(s)

Displays all wavelengths to me measured,

Insert WL

Press this button to insert a new row into the wavelength table. Then enter the desire wavelength.

Remove WL

Select a row in the wavelength table and press this button to remove the wavelength.

Integration Time

Enter the required integration time in seconds. The optimal signal-to-noise ratio is obtained by selecting a long integration time. However for fast kinetics a short integration time should be used.

Ordinate

Use to select the ordinate units: %T for transmission, A for absorbance.

Slit

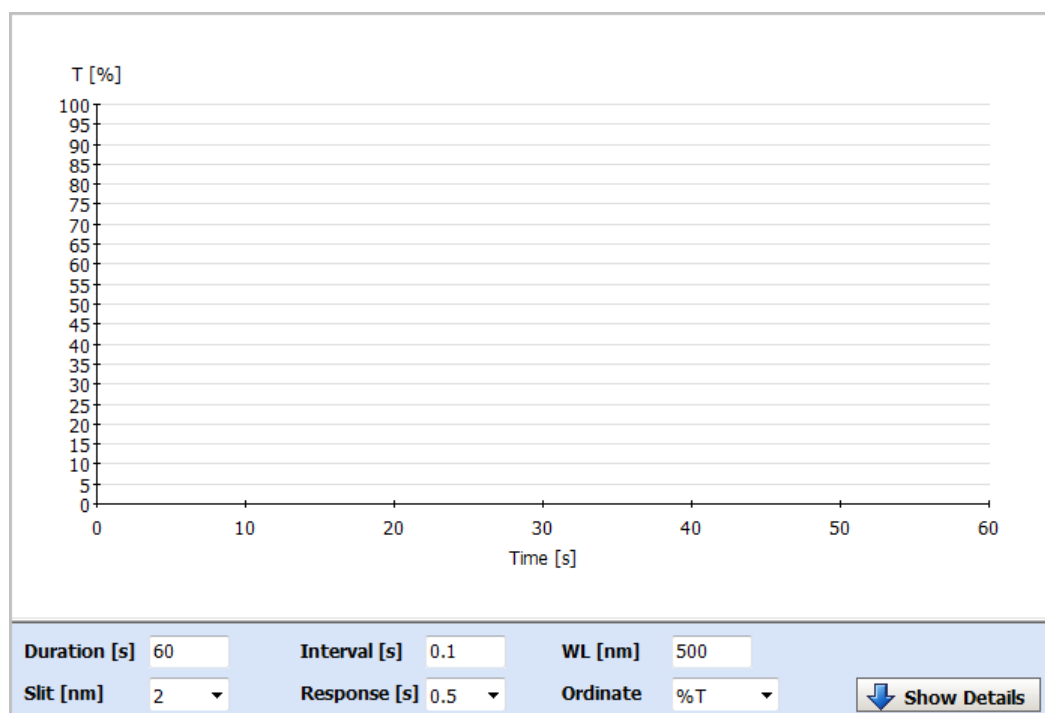
The slit width is the spectral band width of the monochromator. In order to obtain the best spectral resolution, select a narrow slit width, e.g. 1 nm. The best signal-to-noise ratio is obtained by selecting a large slit width. Please note that changing the value in this text-box automatically updates the value in the instrument panel.

Show Details

Pressing this button displays the Instrument Setup panel.

The Time Drive Module

The Time Drive application enables time-dependent measurements (transmission, absorbance) to be made at fixed wavelengths, with defined intervals over a specified period of time.



Result Graph

The result table displays one curve per measured sample online. The following graph functions are supported: Zoom, auto scale x, auto scale y, scale axis, x-cursor, y-cursor, copy graph, display as table. (For a detailed description of these functions refer to the chapter Graph Functions). Furthermore it is possible to select curves and send them to the free-form calculator (see Sending curves to the free form Calculator)

Result Table

The result table displays the scan parameter and data of all measured samples online. For each sample a new column is added. The following table functions are supported: Copy table, display as graph. (For a detailed description of these functions refer to the chapter Table Functions)

Duration

This text-box contains the duration (total time for data collection) for the Time Drive in seconds.

Interval

Enter the required data interval (interval between two measuring points) in seconds. Note that in time drive mode the data interval is equivalent to the integration time.

Wavelength

Contains the wavelength in nm. Please note that changing the value in this text-box automatically updates the value in the instrument panel.

Slit

The slit width is the spectral band width of the monochromator. Please note that changing the value in this text-box automatically updates the value in the instrument panel.

Response

This text-box contains the response time. The longer the response time the smoother the curve appears.

Ordinate

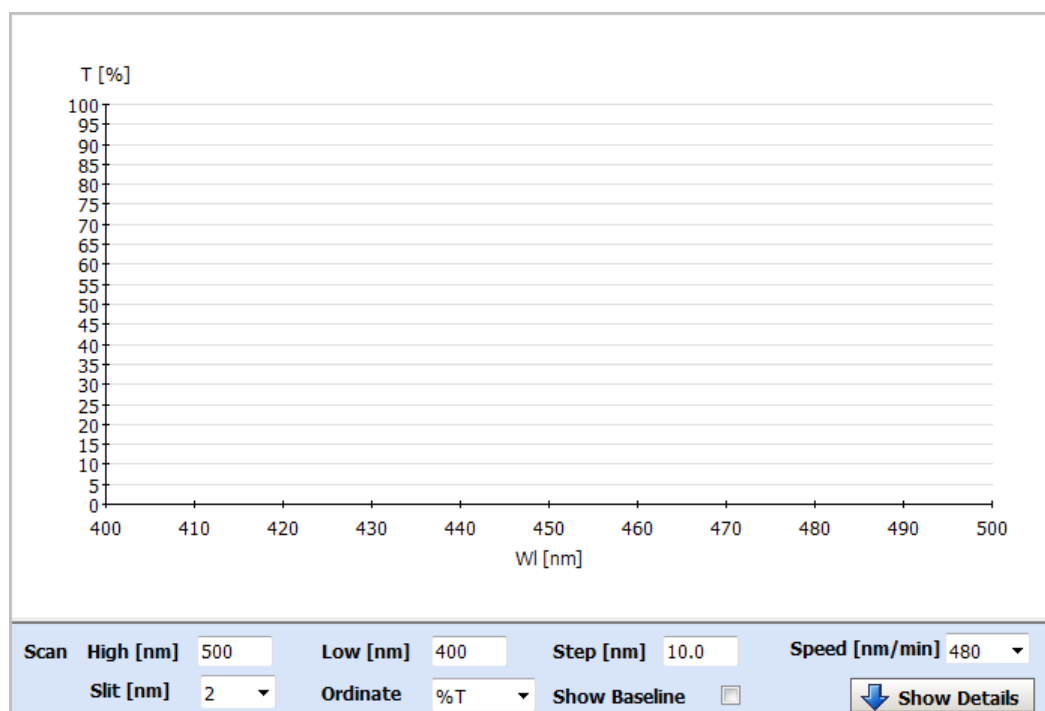
Use to select the ordinate units: %T for transmission, A for absorbance.

Show Details

Pressing this button displays the Instrument Setup panel.

The Scan Module

The scan application enables measurements (transmission, absorbance) scanning the wavelengths.



Result Graph

The result table displays one curve per measured sample online. The following graph functions are supported: Zoom, auto scale x, auto scale y, scale axis, x-cursor, y-cursor, copy graph, display as table. (For a detailed description of these functions refer to the chapter Graph Functions). Furthermore it is possible to select curves and send them to the free-form calculator (see Sending curves to the free form Calculator)

Result Table

The result table displays the scan parameter and data of all measured samples online. For each sample a new column is added. The following table functions are supported: Copy table, display as graph. (For a detailed description of these functions refer to the chapter Table Functions)

Scan High

Defines the start wavelength for the scan. Please note that changing the value in this text-box automatically updates the setting of the monochromator in the instrument panel.

Scan Low

Defines the end wavelength for the scan. The end wavelength must be higher than the start wavelength.

Scan Step

Defines the data interval for the scan in nm.

Scan Speed

Defines the required scan speed. The scan speed determines the integration time of the data acquisition. The optimal signal-to-noise ratio is obtained by selecting a slow scanning speed.

Slit

The slit width is the spectral band width of the excitation monochromator. Please note that changing the value in this text-box automatically updates the value in the instrument panel.

Ordinate

Use to select the ordinate units: %T for transmission, A for absorbance.

Show Baseline

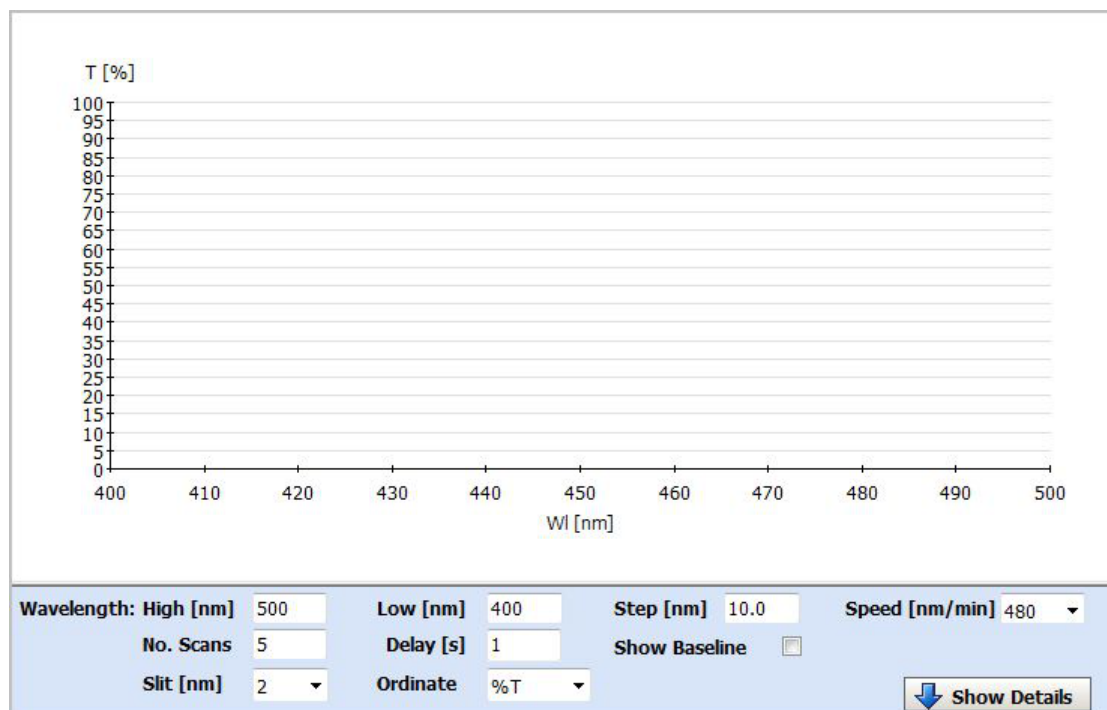
If this option is selected, the baseline curve is displayed on the graph when a baseline correction is performed. Since the baseline is saved with the raw data, it is possible to use this option to view the baseline offline, even for loaded data. (For more information please refer to Performing a Baseline Correction).

Show Details

Pressing this button displays the Instrument Setup panel.

The Kinetic Scan Module

The Kinetic Scan application enables wavelength scans (transmission, absorbance) over a period of time at user definable intervals. The results can be displayed in the 3D Viewer module.



Result Graph

The result table displays one curve per y-axis scan value online. The following graph functions are supported: Zoom, auto scale x, auto scale y, scale axis, x-cursor, y-cursor, copy graph, display as table. (For a detailed description of these functions refer to the chapter Graph Functions). Furthermore it is possible to select curves and send them to the free-form calculator (see Sending curves to the free form Calculator)

Result Table

The result table displays the scan parameter and data of all measured scans online. For each y-axis scan value a new column is added. The following table functions are supported: Copy table, display as graph. (For a detailed description of these functions refer to the chapter Table Functions)

Scan High

Defines the start wavelength for the scan. Please note that changing the value in this text-box automatically updates the setting of the monochromator in the instrument panel.

Scan Low

Defines the end wavelength for the scan. The end wavelength must be higher than the start wavelength.

Scan Step

Defines the data interval for the scan in nm.

Scan Speed

Defines the required scan speed. The scan speed determines the integration time of the data acquisition. The optimal signal-to-noise ratio is obtained by selecting a slow scanning speed.

No. Scan

Defines the number of times the scan is repeated.

Delay

Defines the delay between repeated scans in seconds. The first scan always starts at 0 seconds.

Show Baseline

Select this option to display the baseline,

Slit

The slit width is the spectral band width of the excitation monochromator. Please note that changing the value in this text-box automatically updates the value in the instrument panel.

Show Baseline

If this option is selected, the baseline curve is displayed on the graph when a baseline correction is performed. Since the baseline is saved with the raw data, it is possible to use this option to view the baseline offline, even for loaded data. (For more information please refer to Performing a Baseline Correction).

Show Details

Pressing this button displays the Instrument Setup panel.

Calculations

Description

One purpose of calculation modules is to visualize calculated data during the data acquisition process, to comfortably control the validity of the measurement. To achieve this whenever the measurement of a sample is completed the collected data is sent to these modules, it is re-calculated and the results are displayed.

On the other hand all data calculated in these modules can be displayed in the reports.

In the base version BL Studio offers 3 data calculation modules:

- The Standard Calculator: A flexible programmable calculator for scalar and curve calculations

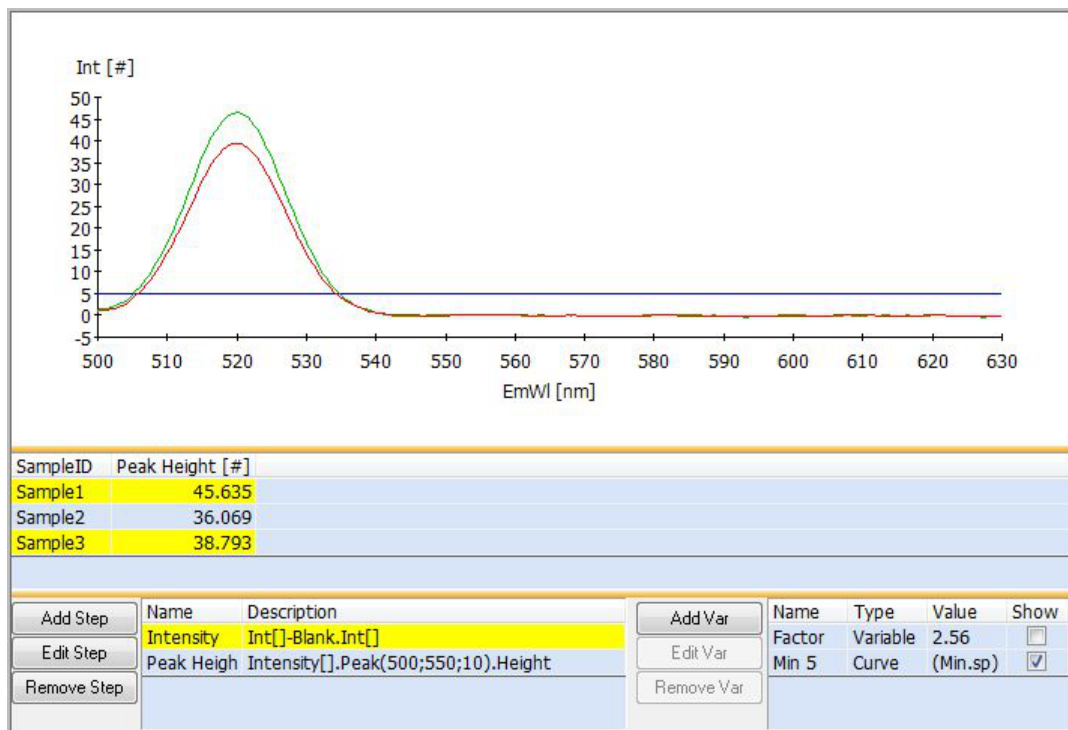
- The Concentration Calculator: A module for quantitation

- The 3D Viewer: Displays 3D data

If required specific calculation modules can be added.

The Online Data Calculation

The online data collection module consists of four areas: The curve results area, the scalar results area, the calculation steps area and the global variables area.



Curve Results

The curve results area displays all **selected** curve results. To display a curve result select the sample(s) to be displayed and click on the step(s) to be shown (see also selecting table rows). You can display any combination of samples and steps. Please note that if either no sample or no step is selected the curve results graph will stay empty.

Please note that only steps resulting in a curve will be displayed in this area. All scalar results are automatically shown for every sample on the scalar results table

Scalar Results

On this table all scalar (single number) step results are shown for all samples. The first column always contains the Sample ID, followed by a column for each scalar step. The caption of the column, the variable type and the format can be defined in the Add/Edit Step dialogues.

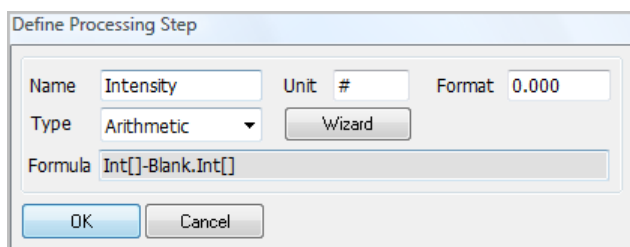
Calculation Steps

In this area all calculation steps can be defined. The first column of the step table contains the name of the step, the second column displays the formula, describing the step.

Whenever new data is loaded or measured for all samples the results of all steps are calculated and displayed automatically.

Add Step

Press this button to open the Define Step Dialogue:



The 'Define Processing Step' dialog box contains the following fields and controls:

- Name:** Intensity
- Unit:** #
- Format:** 0.000
- Type:** Arithmetic (dropdown menu)
- Wizard:** Wizard button
- Formula:** Int[]-Blank.Int[]
- Buttons:** OK, Cancel

Name, unit and format define either the caption and format of the corresponding column on the Scalar results table or the curve name in the Curve Results graph, formula displays the description of the formula used to calculate the result.

To enter a new formula select the calculation type from the type list-box and click on the wizard button. Depending on the type different dialogues open. Enter the desired parameters in these dialogues and leave with ok.

The following calculation types are available: Arithmetic, Curve Point, Peak, Area Normalize, Filter, Derivative, Slope.

Leaving the dialogue with ok adds the new steps and automatically calculates and displays the result automatically. The result type (curve/scalar) is automatically determined from the formula.

Edit Step

After selecting a step from, the step table this button becomes available. Clicking on the edit step button opens the Define Step Dialogue with the parameters of the selected step. The parameters can now be changed. Leaving the dialogue with ok applies the changes. All results are re-calculated automatically.

Remove Step

After selecting a step from, the step table this button becomes available. Clicking on the remove step button deletes the selected step. All other steps are re-calculated. Please note that it is NOT checked if any other step depends on the selected step. Deleting a step may result in Invalid results ~.

Global Variables

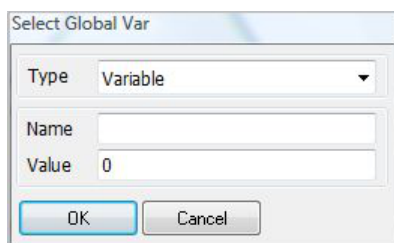
This area allows the user to define or load global variables. These variables can be used in the calculation steps.

The first column of the global variables step table contains the name of the variable, followed by the style, the current value and an option to show global curves.

BLStudio supports two types of variables: Scalars (single numbers) and curves. The current value of a variable is displayed for scalars only (for curves ### is shown). To display a global curve select the Show option, the curve is then displayed in the Results graph. (This is especially useful to compare a current result against previous results or to define limits).

Add Variable

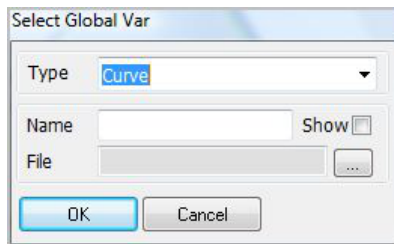
Click on this button to open the Define Global Variable dialogue:



The 'Select Global Var' dialog box contains the following fields and controls:

- Type:** Variable (dropdown menu)
- Name:** (empty text field)
- Value:** 0
- Buttons:** OK, Cancel

Select the desired Name and value for the new variable. To load a curve select curve from the type list box. The dialogue will change to



Define the name in the Name text-box. Click on the ... button to open a Windows File Open dialogue. Select the desired file and press ok. The loaded file name is displayed in the file text-box. Selecting show displays the loaded curve in the results graph.

Edit Variable

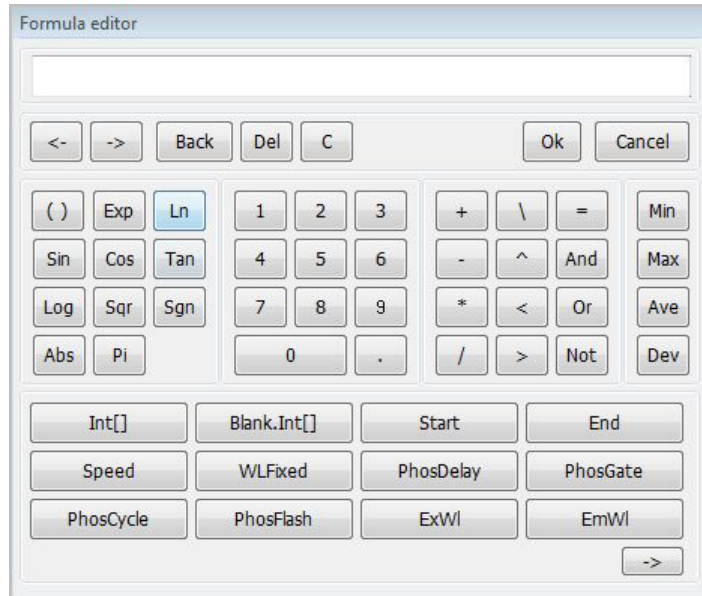
Select a global variable from the table and press this button to modify the value of the variable. The Define step dialogue is opened. After changing the value leave the dialogue with ok. All steps depending on the global variable are re-calculated automatically.

Remove Variable

Select a global variable from the table and press this button to remove the variable. Please note that it is NOT checked if any calculation step depends on the variable. Removing a global variable may cause invalid results ~.

The Arithmetic Dialogue

Use the Arithmetic Dialogue to perform mathematical operations on single values or curves. To generate a formula simply click on the appropriate buttons on the editor or enter the formula via the keyboard. To implement the formula click on the 'OK' button. The formula is then checked for syntax errors. If errors are detected an error message is displayed and the formula can be corrected:



Formula Area

The formula text-box displays the current formula. It can be edited directly via the keyboard. However, to avoid misspelling it is recommended to use the buttons in the function and variable area. To navigate in the text-box the following buttons are available:

- Arrow left** Moves the current insertion point one step to the left.
- Arrow right** Moves the current insertion point one step to the right.
- Backspace** Moves the current insertion point one step to the left and deletes the character under the cursor.
- Delete** Deletes the character under the cursor.
- Clear** Clears the text-box.

Function Area

The function area contains buttons to add functions and operators to your formula. Please note that the functions work on both numbers and curves as argument. If the argument is a curve the function is calculated for each value of the curve and the result is a curve again.

Operators can also take numbers and curves as arguments. Operations on two numbers result in a number. For two curves each value of the first curve is operated with each value of the second curve, the result is a curve. If the first argument is a curve and the second is a number each value of the curve is operated with the number, the result is a curve. The following buttons are available:

- Brackets** Click on this button to add two brackets () at the current insertion point in the formula. The insertion point is automatically set behind the first bracket.
- Number block** Click on a button to insert the corresponding number into the formula. Please note that the decimal delimiter is always independent of the local setting.
- + operator** Returns the sum of two numbers or curves.
- operator** Returns the difference of two numbers or curves
- * operator** Returns the product of two numbers or curves
- / operator** Divides two numbers or curves.

\ operator	Divides two numbers or curves and returns an integer result(s)
^ operator	Used to raise a number to the power of an exponential.
= comparison	Returns 'true' if the value of the expression left of the = is equal to the value of the right expression. Otherwise 'false' is returned.
< comparison	Returns 'true' if the value of the expression left of the '<' is smaller than the value of the right expression. Otherwise 'false' is returned.
> comparison	Returns 'true' if the value of the expression left of the '>' is less greater than the value of the right expression. Otherwise 'false' is returned.
And operator	Used to perform a logical concatenation of two expressions. The results are as follows: TRUE And TRUE = TRUE TRUE And FALSE = FALSE FALSE And TRUE = FALSE FALSE And FALSE=FALSE
Or operator	Used to perform a logical disjunction on two expressions. The results are as follows: TRUE Or TRUE = TRUE TRUE Or FALSE = TRUE FALSE Or TRUE = TRUE FALSE Or FALSE=FALSE
Not operator	Used to perform logical negation on an expression: Not TRUE=FALSE Not FALSE=TRUE
Exp	Returns e (natural logarithm) raised to a power.
Ln	Returns the natural logarithm of a number.
Sin	Returns the sine of an angle.
Log	Returns logarithm (base 10) of a number.
Sqr	Returns the square root of a number
Cos	Returns the cosine of an angle
Sgn	Returns an Integer indicating the sign of a number: Number is Sgn returns > 0 1 0 0 < 0 -1
Tan	Returns the tangent of an angle
Abs	Returns the absolute value of a number.
Min	Returns the minimum y-value of a curve
Max	Returns the maximum y-value of a curve
Ave	Returns the average of the y-values of a curve
Dev	Returns standard deviation of the y-values of a curve
[x]	Returns the x's element of a vector (e.g. Int[3] returns the 3 rd element of Int[])

Variable Area

The lower part of the dialogue displays all available variables. The contents depends on the sample preparation, the acquisition and the calculation method, Variables with an trailing [] represent curves, all other variables contain numbers. Please note that all curves are linear interpolated to the acquisition scan parameters where applicable.

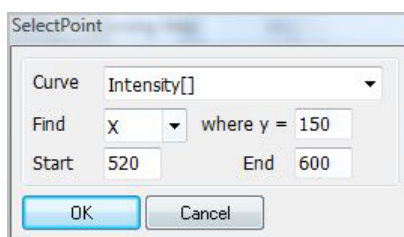
The dialogue displays 12 variables at a time. To access more variables press the → button. Pressing a button adds the variable name at the current cursor position in the formula text-box. The following variables are available:

Raw Results All collected raw data. Data applying to all samples are displayed with their name only e.g. Int[] for scan data. Data applying to one sample/standard only are displayed with a qualified name e.g. Standard1.Int[]. Qualified data occurs for all samples pre-defined in the method: all standards and samples with the required flag.

- Sample Info** All numeric variables defined on sample prep page as columns of the batch info, sample info and standard info tables.
- Acquis. Setup** All numeric parameters defined on the acquisition page, including the scan parameters
- Global Vars** All global variables and curves.
- Step Results** All results from calculation steps.

The Curve Point Dialogue

Use this dialogue to calculate a coordinate of a curve point. First select the curve to be used from the Curve list-box.



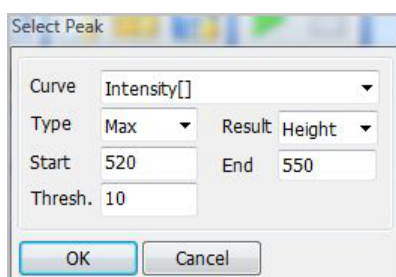
Then select one of the following functions from the find list-box:

- Y:** returns the y-value of a given x-value of the curve.
- X:** returns the first x-value for a given y-value in the given range (start, end text boxes).
- Max:** returns the maximum y-value of the curve in the given range (start, end text boxes).
- Min:** returns the minimum y-value of the curve in the given range (start, end text boxes).

If the start,end value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

The Peak Dialogue

Use this dialogue to calculate a information about a peak/base of a curve. First select the curve to be used from the Curve list-box:



The define in the type list-box if the result are to be calculated for a peak or a base. The start, end text-boxes define the range in which the peak is searched. The threshold defines the minimum height a peak must have to be valid.

The following properties of a the first valid peak in the range can be determined:

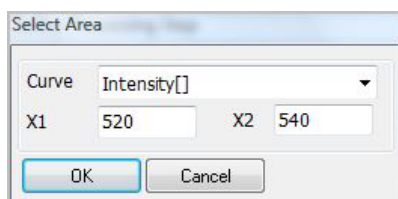
- Y:** returns the absolute maximum y-value of the peak
- X:** returns corresponding x-value of the peak
- Height:** returns the baseline corrected maximum y-value. The baseline is determined using the given Start, End values
- Area:** returns the baseline corrected area under the peak/base. The borders of the area and the baseline are determined using the given Start, End values

If no valid peak is detected in the given area all properties are set to the invalid value ~.

If the start,end value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

The Area Dialogue

Use this dialogue to calculate the absolute area under a given range of a curve. First select the curve to be used from the Curve list-box:

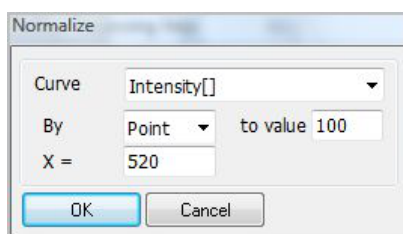


The enter the desired x-range in the x1, x2 text-boxes. The absolute area for this range is calculated. To obtain a baseline corrected area use the Peak function.

If the x1, x2 value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

The Normalize Dialogue

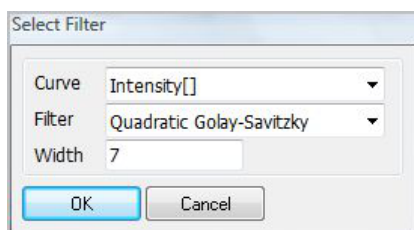
Use this dialogue to normalize a given a curve. First select the curve to be used from the Curve list-box:



The function first determines either the maximum y-value or the y-value for the given x-value of the curve. Then the factor is calculated by $f=100/y$. Finally each y-value of curve is multiplied with the factor.

The Filter Dialogue

Use this dialogue to apply a filter on a given a curve. First select the curve to be used from the Curve list-box:

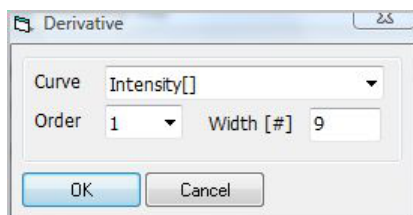


Now select one of the four available filters form the filter list-box: Moving Average, Triangular, Quadratic Golay-Savitzky, Cubic Golay-Savitzky

For a detailed description of these filters refer to Smoothing Filter. Finally enter the number of points to be used to calculate the filtered data (the more points used the smoother the filtered curve appears).

The Derivative Dialogue

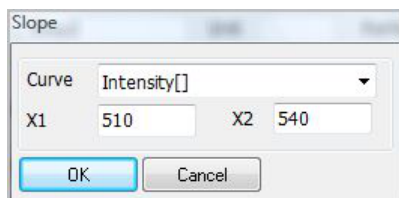
Use this dialogue to calculate a derivative of a given a curve. First select the curve to be used from the Curve list-box:



Then enter the desired order of the derivative and the number of points to be used to calculate the derivative. (the more points used the smoother the derivative appears).

The Slope Dialogue

Use this dialogue to calculate the slope between two points of a given a curve. First select the curve to be used from the Curve list-box, then determine the two points by their x-values.



The Concentration Module

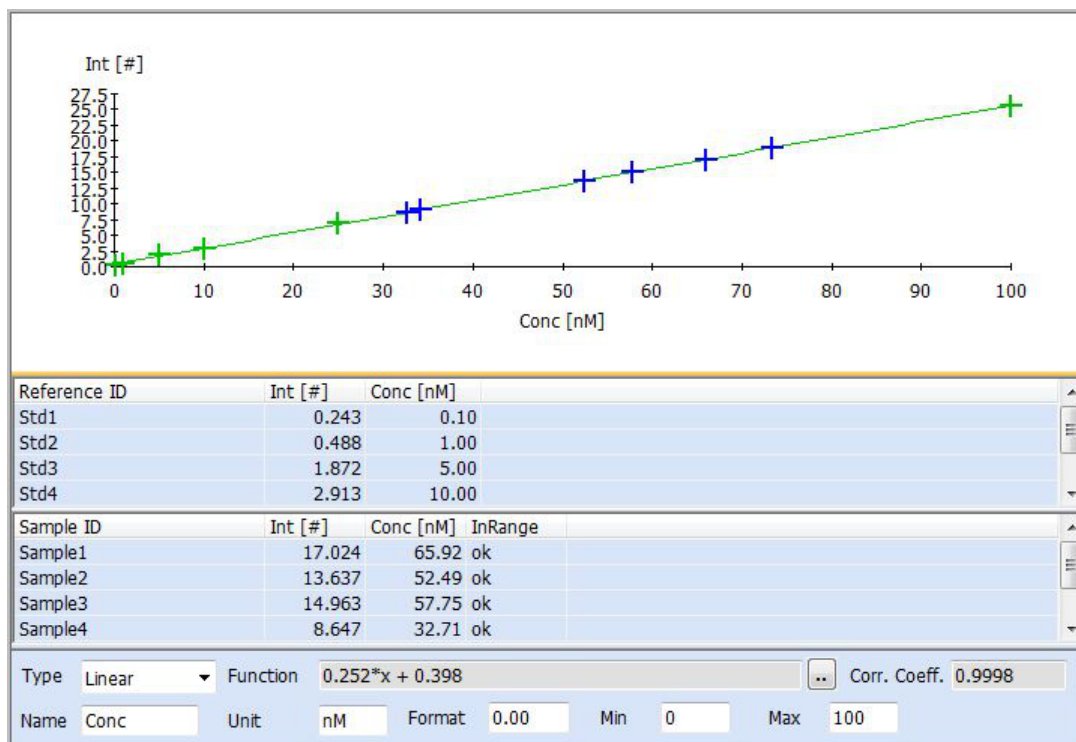
In combination with the read, scan or timedrive acquisition module the Concentration module allows the user to carry out routine quantitation of unknown samples, providing ease-of-use and flexibility.

Basically It is possible to enter a calibration function manually (in this case it is not necessary to measure standards).

Alternatively the calibration function can be recalculated each time new samples are to be measured. In this case a set of standards must be defined in the sample preparation module. As the data for these standards is collected the calibration curve is constructed and updated.

Whenever a sample is measured, its concentration is automatically calculated and displayed on the calibration graph and the results table.

The concentration module page consists of up to four regions: The calibration graph, the result tables, the data reduction panel and the calculation parameter panel:



The Calibration Graph

The calibration graph visualizes the calibration function (green line) . Additionally it displays the position of the standards used to calculate the calibration (green crosses) to allow the user to quickly recognize outliers and to judge the quality of the calibration fit.

The Y-axis of the graph displays the measured (calculated values if data reduction is necessary) values while the on the X-axis the defined (for standards) and calculated (for samples) concentrations are shown. The caption and the unit of the X-axis can be modified on the Parameter Panel. The range of the X-axis is basically set to the valid calibration range, defined on the Parameter Panel. If a sample/standard lies outside this range the range is expanded. However the calibration function curve is only drawn within the valid calibration range.

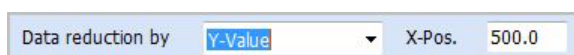
The following graph functions are enabled: zoom, copy to clipboard, auto-expand X-axis, auto-expand Y-axis, set axis range, x-cursor, y-cursor.

The Result Tables

The results for standards and unknown samples are displayed on two separate tables (note, that if no standards are defined the standard result table becomes invisible). On the standard results table the standard ID, the measured (calculated) value and the known concentration is displayed. The sample results table the sample ID, the measured (calculated) value and the calculated concentration is displayed. The last column displays a field indicating if the calculated concentration lies within the valid concentration range.

Data Reduction Panel

If the concentration module is combined with a data-acquisition module that produces curves rather than single numbers as result (e.g. Scan, Timedrive) the data reduction panel becomes visible automatically. On this panel the user can define how to calculate a single number as result from the curve:



The following functions are currently available:

- Y-Value** returns the y-value of the curve at the given x value. If necessary a linear interpolation is performed.
- Area** returns the area under the curve within the range given by x-start and x-end.
- Slope** returns the slope of the line, defined by x- and y-values given by x-start and x-end.
- Peak Height** returns baseline corrected height of the first peak found in the range given by x-start and x-end. Threshold defines the minimum size of a peak to be detected. The x-start and x-end values are also used to define the base line.
- Peak Area** returns baseline corrected area under the first peak found in the range given by x-start and x-end. Threshold defines the minimum size of a peak to be detected. The x-start and x-end values are also used to define the base line.
- Base Depth** as peak height, but for bases
- Base Area** as peak area, but for bases

Please note that selecting a function automatically changes the caption of the y-axis of the calibration graph and the captions of the standard and sample results tables. Furthermore all data is re-calculated, the calibration graph and result tables are updated.

The Calculation Parameter Panel

On this panel the parameters for the actual concentration fit can be defined. First select the desired fit function type from the type list-box. The following fit-types are available:

- Linear** Fits a line, requires at least two standards
- Quadratic** Fits a quadratic curve, requires at least three standards
- Cubic** Fits a cubic curve, requires at least three standards
- Rodbard** Fits a S-curve, requires at least four standards
- Exponential** Fits an exponential curve, requires at least three standards
- Logarithmic** Fits a logarithmic curve, requires at least three standards

After the type is selected the corresponding function description is displayed in the function text box. If sufficient results for standards have been measured or loaded the fit is automatically carried out, the calculated parameters are inserted in the functional description and the correlation coefficient is displayed. Furthermore the calibration graph and the result tables are updated. Clicking on the .. button allows the user to customize the calibration function including to completely define the function manually.

It is further possible to define the caption, unit and format of the concentration value. Changing these values automatically updates the calibration graph and the result tables.

Finally a valid range for the calibration can be defined via the Min and Max text-boxes. All samples outside this range are marked as <Min or Y>Max.

Customizing the Calibration Function

Clicking on the .. button on the calculation parameter panel opens the following dialogue (in this example for a quadratic fit function):

Function Parameter	Format	Hold
A0	0.294	0.000 <input type="checkbox"/>
A1	0.269	0.000 <input type="checkbox"/>
A2	0.300	0.000 <input type="checkbox"/>

The caption displays a description of the function parameters. In the parameter column the calculated parameters for the current fit are displayed (set to 1 if no fit has been calculated). You can modify these values to define start values for the next fit. The format field allows the user to define with how many decimals each parameter is displayed on the calibration parameter panel and finally in the report. (please note that all calculations always use the full precision).

The hold option can be used to exclude parameters from fitting. This is useful if you already know a parameter (e.g. setting a0 to zero and selecting hold forces the fitted curve to go through (0;0)). Furthermore each held parameter reduces the number of required samples by one: If all parameters are marked as hold no standard measurement is required, the calibration function can be defined manually.

Excluding a Standard/Sample

To exclude standards from the calibration calculation or samples from reporting they must be excluded on the sample preparation page (please refer to Excluding Samples from Evaluation)

Remeasure a Standard/Sample

To re-measure a standard or a sample the auto clear results option in the Data Options dialogue must be disabled. Exclude AND delete the respective sample on the sample preparation page. When the measurement is continued the standard is remeasured.

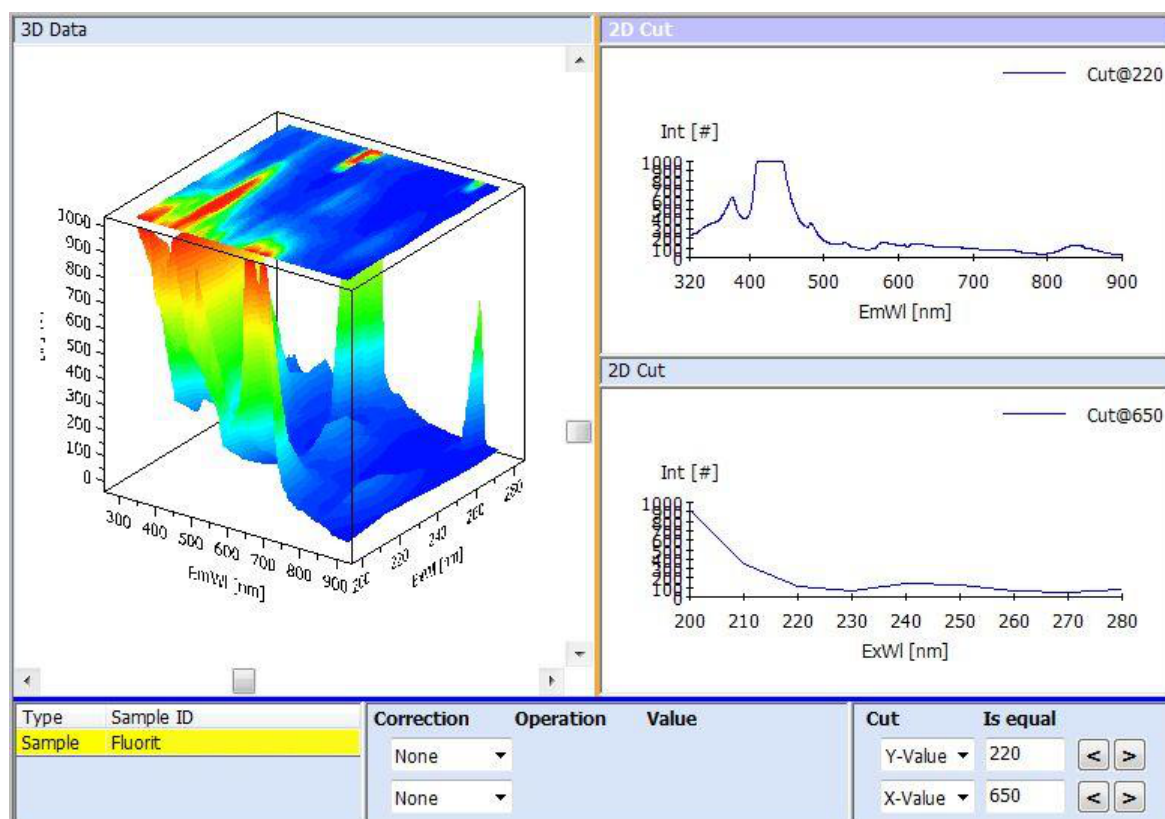
Calculation of diluted Samples

If the sample info table on the sample preparation page contains a column with the ID "Dilution" and the type Number the concentration module automatically adds the columns "Dilution" and "Calc. Conc." to the sample result table. Dilution contains the dilution value defined in the sample preparation table for each sample. Calc. Conc. Display the calculated concentration = Conc. * Dilution.

The 3D Viewer Module

The 3D Viewer module allows the user to visualize 3D scans (e.g. collected with the 3D Scan acquisition module) or 2D data (e.g. collected with the Scan or time drive acquisition module) for all samples.





Besides the possibility to display the data in tabular the application offers a graphical views:



The graph updates whenever new set of 2D data is collected (either when the next wavelength has been measured in 3D scan or when 2D data for the next sample has been collected in scan or time drive).

The 3D data can be displayed as surface projection, as contour map or as combination of both. Additionally vertical and horizontal cuts of the 3D data can be generated and viewed.

3D Viewer Toolbar

-  Set-up Graphical View
-  Copy to Clipboard
-  Switch to Tabular Data View
-  Switch to Graphical Data View

Correcting 3D Data

The 3D Viewer allows the user to correct 3D data before they are displayed. The user can apply up to two corrections in any combination:

Correction	Operation	Value
X-Curve	Multiply	Sample1
Point	Subtract	10

The following correction types are available:

- Point: Each point of the 3D curve is corrected with a constant value
- X-Curve: Each column of the 3D Curve is corrected with a 2D Curve
- Y-Curve: Each row of the 3D Curve is corrected with the a 2D Curve

2D Cuts

The 3D Viewer allows the user to generate horizontal or vertical cuts which are displayed in separate 2D graph windows. It is possible to define two cuts:

Cut	Is equal
Y-Value	440
X-Value	480

If both cuts have the same type (horizontal, vertical) the resulting spectra are displayed in the same graph. If the cuts have different types they are displayed in two graphs. Clicking on the move left, move right buttons move the cut position one data step to the left or right.

In tabular view it is possible to copy the cut spectra to the clipboard or to save them directly to file by right clicking on the table.

3D View Setup Dialogue

Click on the 3D setup button to open the first page of the setup dialogue.

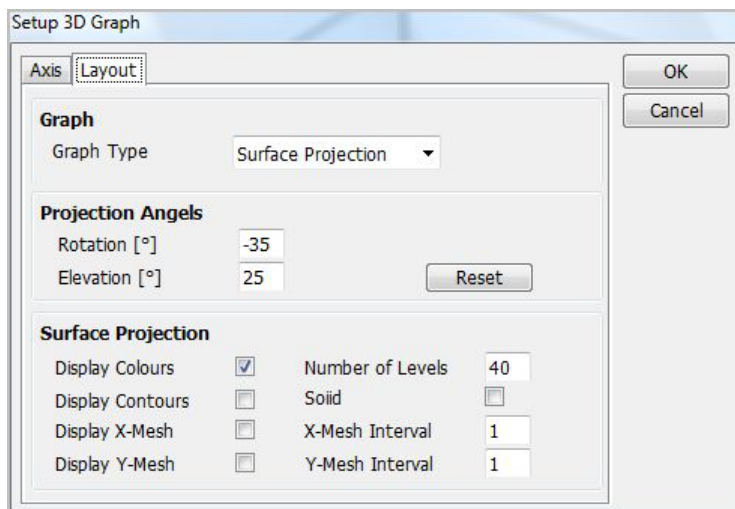
The dialog box titled "Setup 3D Graph" has two tabs: "Axis" and "Layout". The "Axis" tab is active. It contains three sections for configuring axes:

- X-Axis:** Caption: EmWl, Unit: nm, Axis Min: 300, Axis Max: 500
- Y-Axis:** Caption: ExWl, Unit: nm, Axis Min: 200, Axis Max: 360
- Ordinate:** Caption: Int, Unit: #, Axis Min: 0, Axis Max: 1000

Buttons for "OK" and "Cancel" are located in the top right corner.

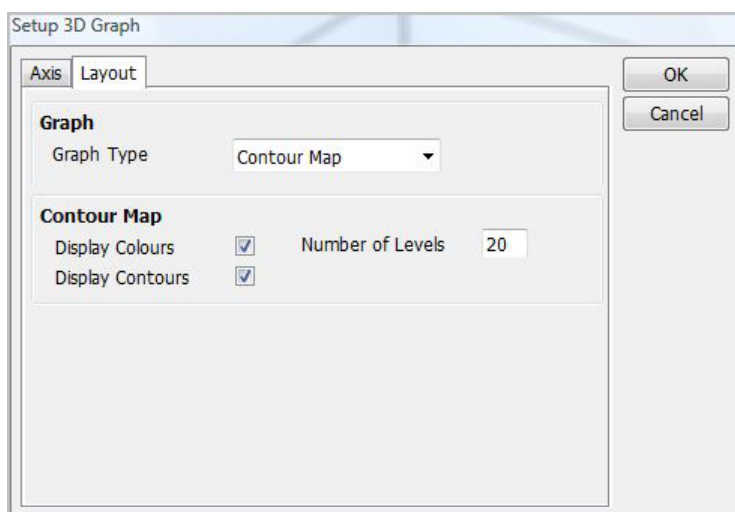
On this page the caption, the unit and the ranges for each axis can be defined. Please note that for the 3D View it is not possible to auto-expand data.

On the second page of the dialogue the layout of the 3D view can be defined. Depending on the selected graph type either the surface projection parameters:



- Rotation:** Defines the elevation angle
- Elevation:** Defines the elevation angle
- Solid:** If this option is selected the graph displays a solid skirt around the data
- Display Colours:** Different ordinate values are depicted by different colours. Can be combined with colours
- Display Contours:** Points at equal intensity are joined, resulting in a series of contour lines. Can be combined with colours.
- Number of levels:** Specifies the number contours/colour transitions on the contour map
- Display X-Mesh:** Draws the x-lines of a mesh over the data. The distance between lines is determined by the X-Mesh Interval.
- X-Mesh Interval:** Defines the distance between mesh x-lines in multiples of the x-interval. When set to 0 the chart automatically determines the best interval.
- Display Y-Mesh:** Draws the y-lines of a mesh over the data. The distance between lines is determined by the Y-Mesh Interval.
- Y-Mesh Interval:** Defines the distance between mesh y-lines in multiples of the y-interval. When set to 0 the chart automatically determines the best interval.

or the contour map parameters are displayed:



- Display Colours:** Different ordinate values are depicted by different colours. Can be combined with colours

Display Contours: Points at equal intensity are joined, resulting in a series of contour lines. Can be combined with colours.

Number of levels: Specifies the number contours/colour transitions on the contour map

Modifying the projection Angles

In the 3D Viewer module the rotation and elevation projection angles can be modified to change the appearance of a surface projection.

You can change the projection angles of a surface projection without displaying the Format 3D View dialogue, using the scroll bars; the vertical scroll bar changes the elevation angle, and the horizontal scroll bar changes the rotation angle.

Presentation

Description



Reports are the formatted representation of data. Reports are the result of a merge of the acquired raw data with a report template, containing fields, tables and graphs to evaluate and visualize the data.

If a method contains a presentation module a report is created online during the data collection. That is, after the measurement of each sample all fields, tables and graphs of the template are updated and displayed.

Please note, that the report template is stored in the raw data, rather than the report itself (Whenever the raw data are loaded the report is re-generated). Thus it is possible to modify the report of already measured data at any time.

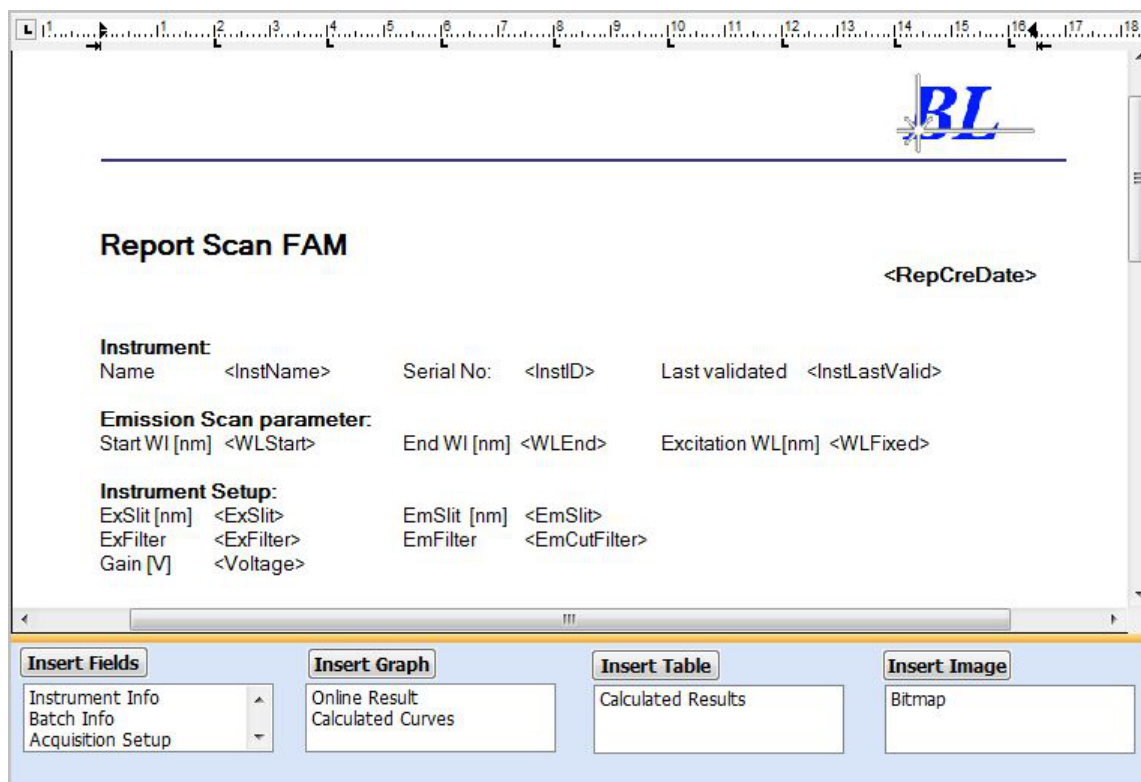
Finally a report can be exported to different formats (e.g. pdf).

The Standard Presentation Module

The standard presentation module offers two pages: The template view to modify the presentation template and the report view to display the final report. The “Show template”  and the “Show report”  buttons of the report menu can be used to switch between these pages.

Template View Page





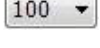





The upper part of the page displays the report template of the current method, while the lower part shows all available fields, tables and graphs that can be inserted in the template:



The report template consists of the main document, a header and a footer section.

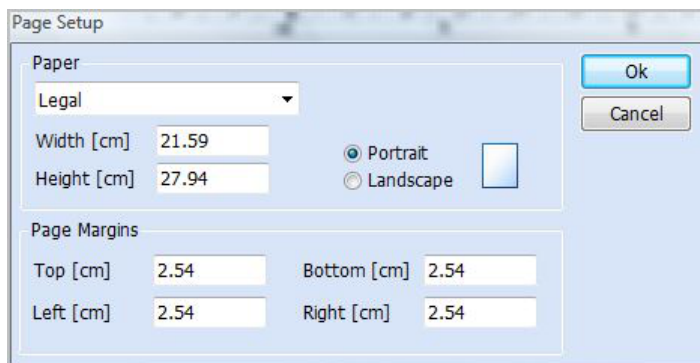
Template Tool Bar

The template tool bar is located at the upper left corner of the main window. It appears only when a report template is displayed.

- | | | |
|---|------------------|--|
|  | Font Name: | Select the desired font type from this list-box. T |
|  | Font Size: | Select the desired font size from this list-box. |
|  | Font Bold: | Click on this button to set the letters of the selected text to bold. |
|  | Font Italic: | Click on this button to set the letters of the the selected text to italic. |
|  | Zoom Factor | Select the desired zoom factor of the report template from this list-box. |
|  | Toggle Header | Click on this button to toggle between main section, header section and footer section of the document |
|  | Format Page | Click on this button to start the Format Page dialogue |
|  | Format Paragraph | Click on this button to start the Format Paragraph dialogue |
|  | Format Character | Click on this button to start the Format Character dialogue |
|  | View Report | Click on this button to generate the report and display it in the Report View. |

Format Page Dialogue

This dialogue offers several parameters change the page format of the document.



Selecting the paper type from the list-box automatically sets the corresponding width and height. Alternatively it is possible to set the height and/or width manually, in this case the paper type is set to custom.

Furthermore you can select if the page is displayed as portrait or landscape and all margins for the page.

Format Paragraph Dialogue

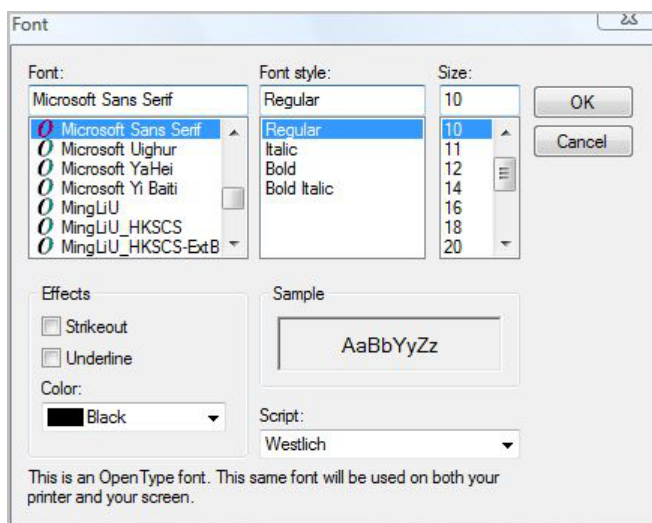
This dialogue is used to format a paragraph. Firstly the alignment and line spacing of the paragraph can



be set as well as the left and right indents. The special list box allows the user to set indents for the first line. Finally the distances before and after the paragraph can be defined. All values must be given in cm.

Format Character Dialogue

This dialogue is the standard Windows Font dialogue. It allows the user to change the font type, the font size,



the style and the colour, Leaving the dialogue with ok updates the selected text.

Editing the Template Document

The standard presentation module is based on a word processing system rather than a desktop publishing module. That is, basically all text can e.g. be inserted , deleted, formatted, copied and pasted like in MS Word. (for additional information see also Template Menu Bar).

Fields, table and graphs must be inserted and modified using specific functions (refer to Insert/Modify Fields, Insert /Modify Tables, Insert/Modify Graphs. To delete one of these objects select it by left clicking on the object and then press delete. **Please do not copy and paste** tables, graphs or fields.

Please note, that the undo function is not implemented yet. (Currently undo would significantly reduce the speed reports are generated)

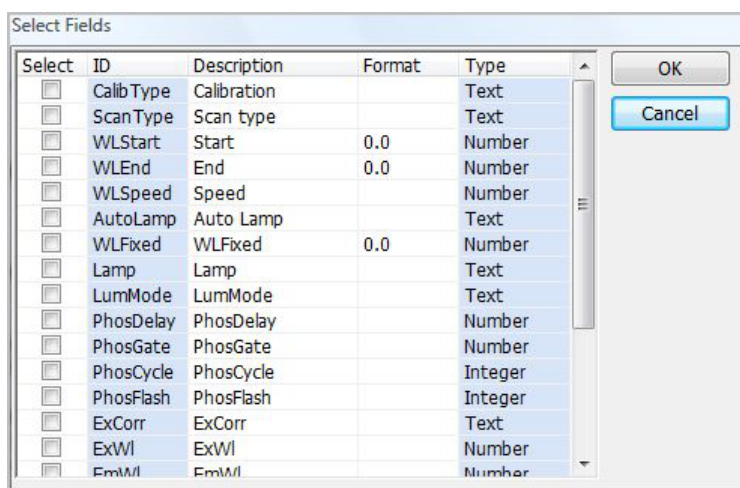
Inserting Fields

To insert new field(s) first left click on the location in the template where the field is to be inserted. Now click on the insert field button and select the desired fields from the Insert Field dialogue. All selected fields and their captions are automatically inserted in the report template. Depending on the selected field type, the instrument used, the acquisition and calculation module the The Insert Field dialogue offers different variables.

The **Instrument info** group contains all variables describing the instrument like type, name and last validation date. **Batch Info** contains all variable defined in the Result Info table of the sample preparation module. In the **Acquisition** group all acquisition parameters like instrument set-up and scan parameters can be found. **Calculation** contains parameters defined in the calculation module. **Method Info, Data Info** and **Report Info** contain information like name, creation date and electronic signatures for the corresponding object.

Insert Field dialogue

To allow for a comfortable insertion the insert field dialogue allows the user to select several fields at one time.



Click on a option-box in the select column to select/deselect the corresponding field. The ID column displays the unique ID of the field. The description field contains a short text, that is inserted before the actual field in the report template. In the format column the output format for each field can be defined (see Variable Formats). The type column shows the type of the field (see Variable Types).

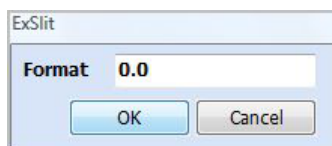
After leaving the dialogue with ok all selected fields are inserted at the current position in the report template, e.g.:

```
Start    <WLStart>
End      <WLEnd>
Speed    <WLSpeed>
```

The description and the field are separated by a tab, each field starts in a new line.

Modifying Fields

It is possible to modify the output format of any existing field: Right click on the field to open the format field dialogue:



and enter the desired format (see also Variable Formats). The font and paragraph can be formatted by using the corresponding toolbar items.

Deleting Fields

Left click on the field to select it. The background of the field will change to grey. Now press the delete key on the keyboard to remove the field.

Inserting Graphs

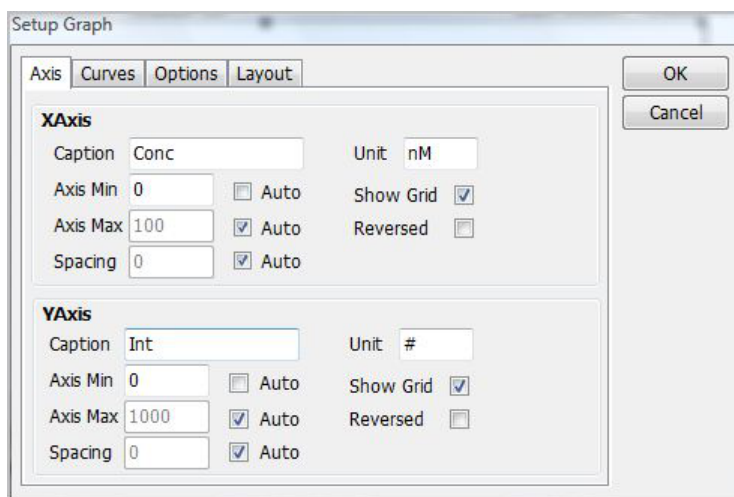
To insert a new graph first left click on the location in the template where the graph is to be inserted. Then select one of the available graphs templates from the list-box and click on the Insert Graph button. An empty graph is then inserted into the report template.

Modifying Graphs

The standard presentation module allows the user to change the layout of an existing graph template. Right click on the graph to open the Setup Graph dialogue. The dialogue consists of four pages:

Axis Page

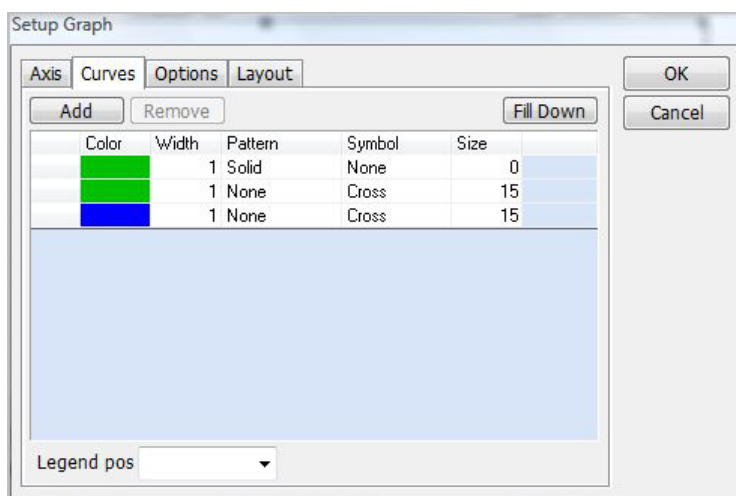
On the axis page all parameters for the x- and y-axis can be defined. The axis minimum, maximum and space values can either be set to fixed values or to auto. If auto is selected optimized values are calculated from the loaded data.



Show grid displays grid lines for the corresponding axis. The distance of the grid lines is define by the value of spacing. Last not least the axis can be reversed by selecting the reverse option.

Curve Page

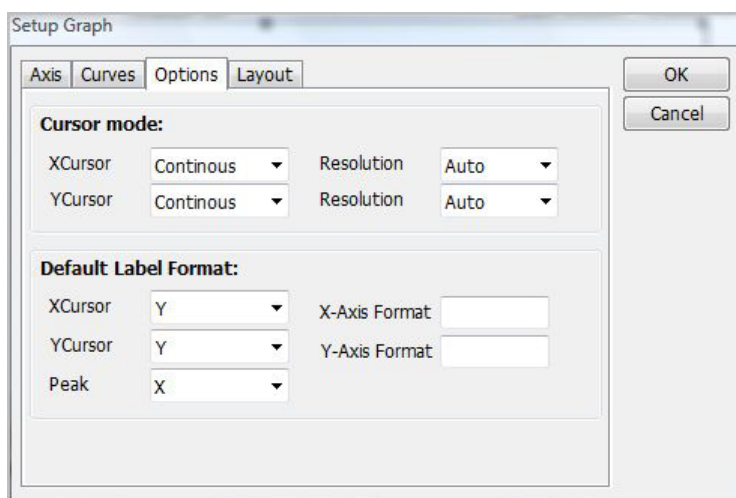
On the curves page the line colour, line width and line pattern for each curve can be defined. Furthermore it is possible to add symbols to each curve line.



The first row applies to the first curve in the graph, the second line to the second etc. If there are more curves than description rows default values are applied. Furthermore it is possible to define the position of the legend in the graph.

Options Page

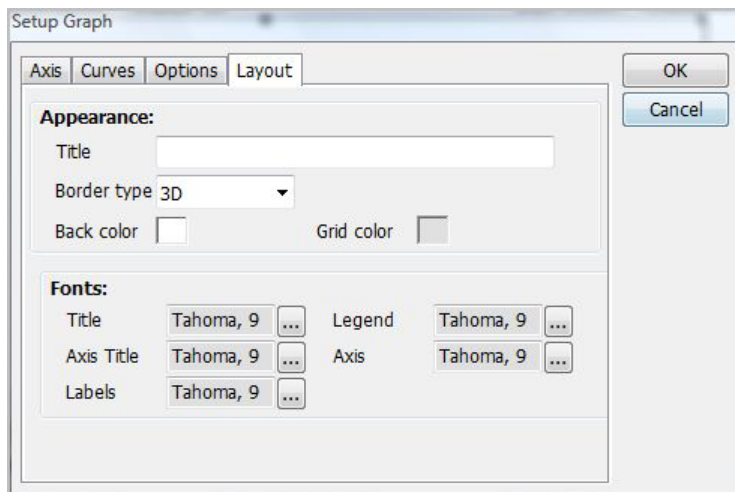
On this page the behaviour of the cursors can be defined. If continuous mode is selected the cursor can be moved in equidistant steps along the axis. In the resolution combo-box the steps size can either be set to a fixed value or to auto. In auto mode the optimal step size is calculated from the current axis range (especially useful when the axis range is changed dynamically e.g. by zooming). In point mode the cursor only jumps to actually measured values (this option is available for the x-axis only)



Additionally the format of labels can be defined for x-cursor, y-cursor and peak labels. If Y is selected only the y-axis value is displayed. X display the x-axis value only. Y/X, X/Y display both values one on top of the other, (X:Y), X:Y display the values side by side (in the first case in brackets). The Axis format text-boxes define the format for the x,y values (see also Variable Formats).

Layout Page

The layout page allows the user to change the appearance of the graph. Title defines a title to be displayed on top of the graph. Via the border type list-box a border can be selected that is drawn around the graph. To change the background or grid colour left click on the colour-box and select the desired colour from the colour dialogue.



Finally it is possible to change the font of the title, the axis captions, all labels, the legend and the axis marking by clicking on the corresponding ... button and selecting the desired font from the font dialogue.

Sizing and Positioning Graphs

It is always possible to change the size and position of the graph: Firstly select the graph by left clicking on it. Now you can resize the appearing frame to the desired size or drag it to a new position.

Deleting Graphs

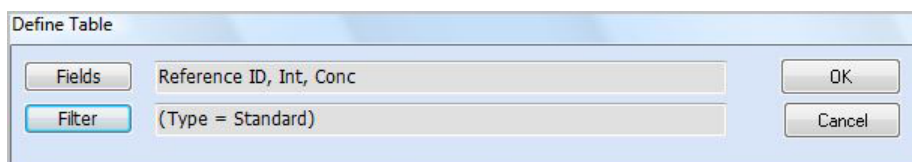
Left click on the graph to select it. The selection will be indicated by a black frame. Now press the delete key on the keyboard to remove the graph.

Inserting Tables

To insert a new table first left click on the location in the template where the table is to be inserted. Then select one of the available table templates from the list-box and click on the Insert Table button. Then the table header with one empty row is inserted into the report template. Please not that it is possible to modify the table (e.g. add/remove columns ore change the size of the columns) at any time.

Modifying Tables

The standard presentation module allows the user to add/remove and resize columns of an existing table template. Furthermore it is possible to filter the displayed data. Right click on a table to open the Define Table dialogue.



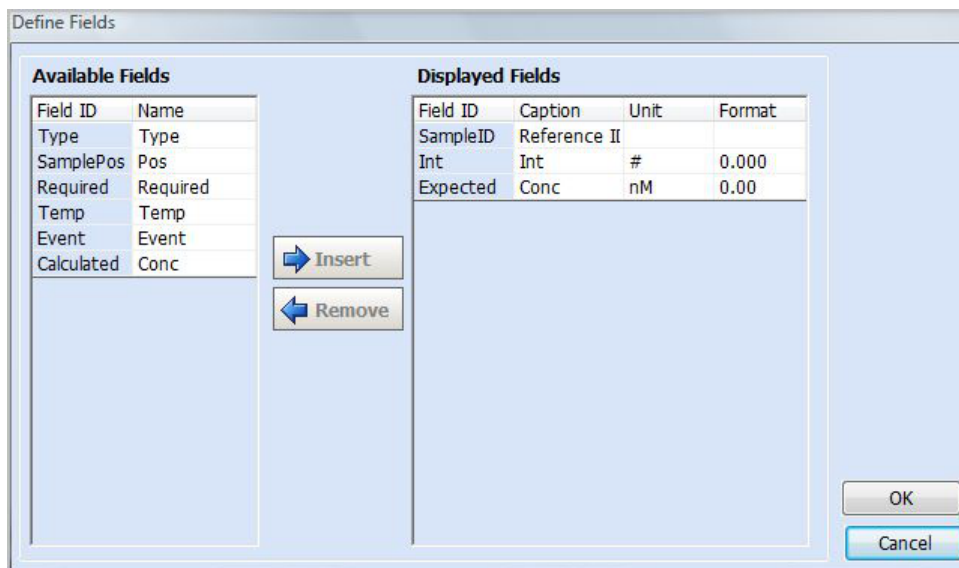
Fields: click on this button on this button to start the Table Fields dialogue.

Filters: click on this button on this button to start the Table Filter dialogue.

Leaving the dialogue with ok, applies the fields and filters to the selected table. The font can be formatted by using the corresponding toolbar items.

Table Fields Dialogue

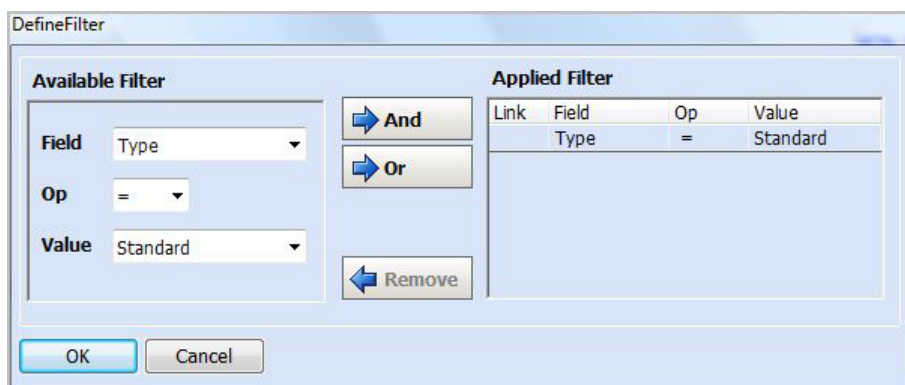
Use this dialogue to (re)define the fields displayed on a table. On the left hand of the dialogue all available fields are listed with their ID and (for better readability) their name. The right hand side shows the currently used fields. To add a field left click on the corresponding Field ID in the available fields list. Then click on the insert button. You can now update the caption, the unit and the format for the field.



To remove a field, click on the corresponding field id in the display fields list and press the Remove button. Leaving the dialogue with ok, applies the fields to the selected table.

Table Filter Dialogue

Use this dialogue to (re)define filters for the data displayed on a table. On the left hand available filters are listed.



Select the field for the filter from the field list-box. Then select the comparison operator and the comparison value. Finally click on the and/or button to add the filter.

To remove a filter, select the corresponding row in the applied filter list and press the Remove button. Leaving the dialogue with ok, applies the filters to the selected table.

Deleting Tables

To delete a table left click anywhere on the table and press the delete key on the keyboard.

Inserting Bitmaps

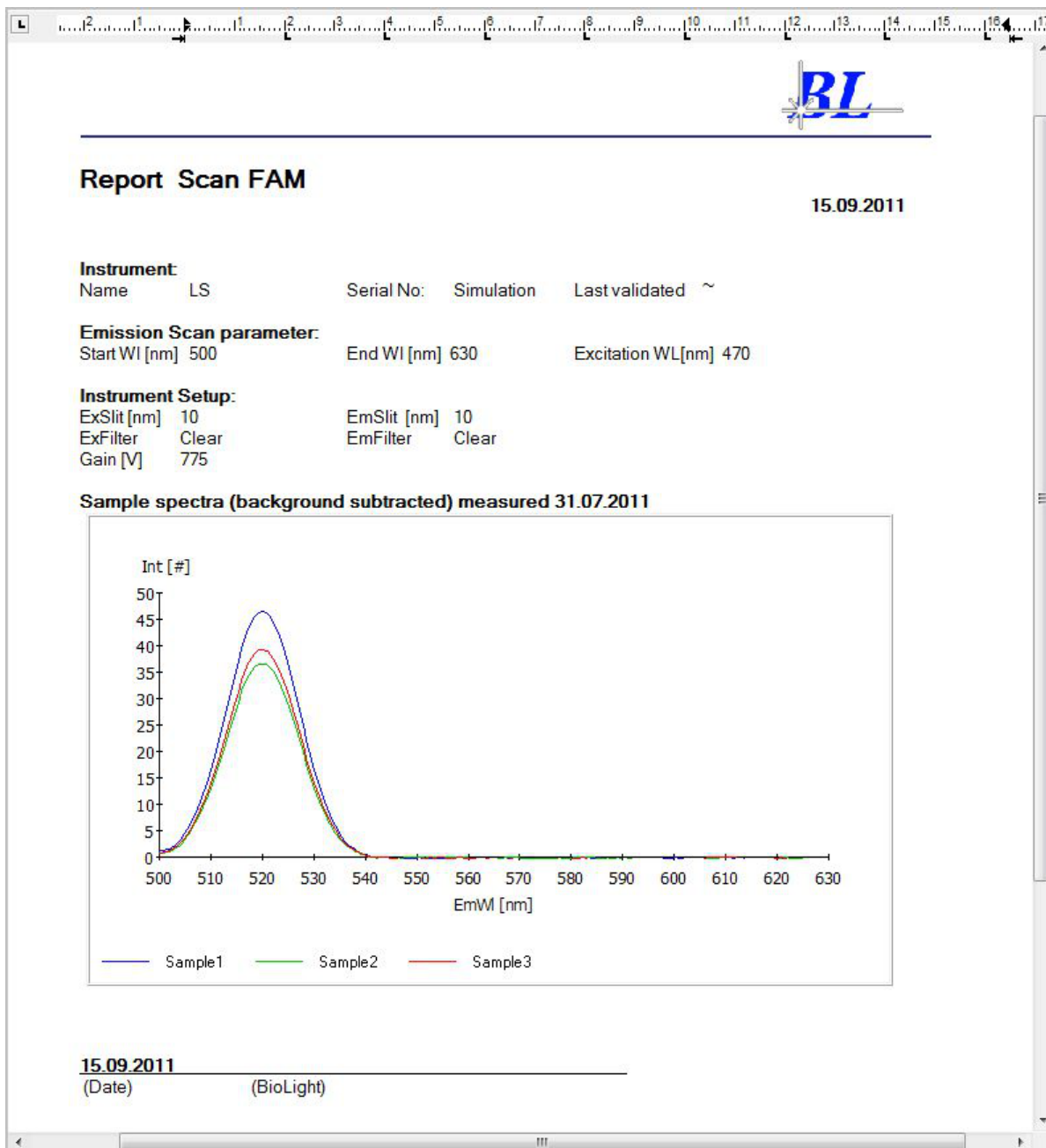
The standard presentation module allows the user to insert bitmaps at any point of the text. First left click on the location in the template where the bitmap is to be inserted. After selecting the entry Bitmap and clicking on the Insert Image button a standard Windows File dialogue comes up. Select the desired bitmap and leave the dialogue with Ok. The bitmap is then inserted in the template document with the full size. To reduce the size of the bitmap select it via left click, then drag a corner until the desired size is obtained.

Deleting Bitmaps

To delete a bitmap left click anywhere on the bitmap and press the delete key on the keyboard.

Report View Page

Clicking on the report view icon merges loaded result data with the current report template. In no data is loaded all fields display an invalid value ~.







After a report has been generated it is no longer possible to modify any text or values. The only allowed modification is to add labels to graphs.

However, it is possible at any time to go back to the template view, perform the desired modifications and re-create the report. Especially the zoom factor that applies for both views can be set in the template view only.

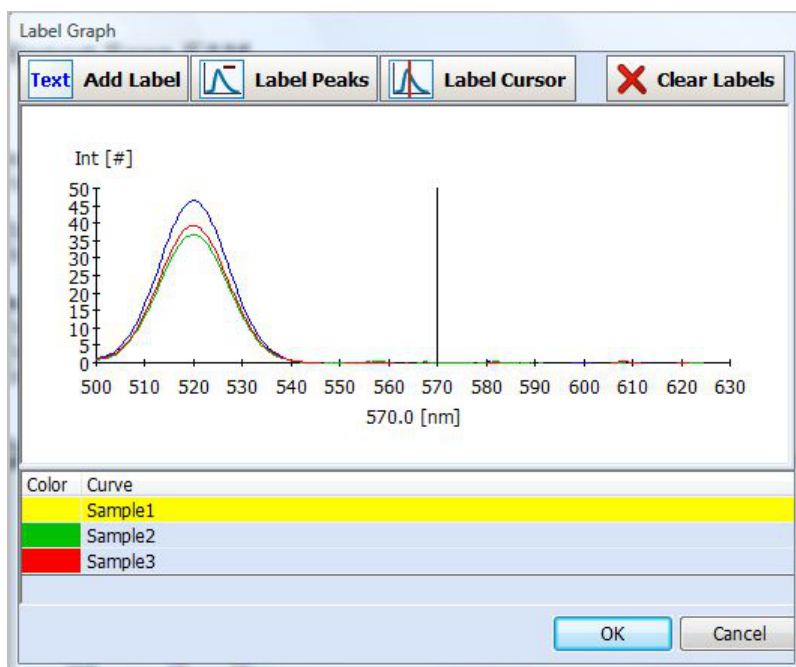
Report Toolbar

The report tool bar is located at the upper left corner of the main window. It appears only when a report is displayed.

- | | | |
|---|---------------|---|
|  | Copy | Copies the report to the clipboard (see also Copying a Report). |
|  | Print | Prints the report to a selectable printer (see also Printing a Report). |
|  | Export | Exports the report (see also Exporting a Report). |
|  | View Template | Click on this button to go to the Template View |

Adding Labels to a Graph

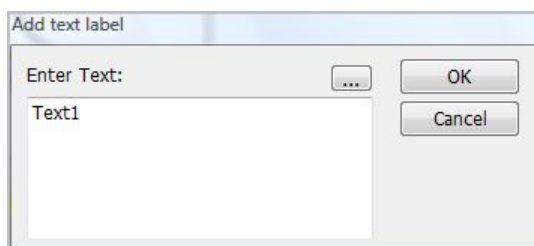
To label a graph right click on the desired graph. The Label Graph dialogue comes up:



Firstly select the desired curve(s) from the sample list. (If no curve is selected the peaks are applied to all curves).

Add Label

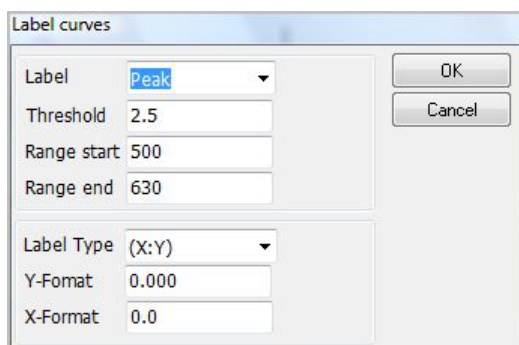
The add label button allows the user to enter a freely movable text. First enter the desired text and format (press the ... button) in the add text label dialogue:



After leaving the dialogue with ok the text appears on the graph and can be dragged to the desired position. It is possible to add several text labels.

Label Peaks

You can label the peaks/bases of the selected curve via the Label Peak button. In the label peak dialogue

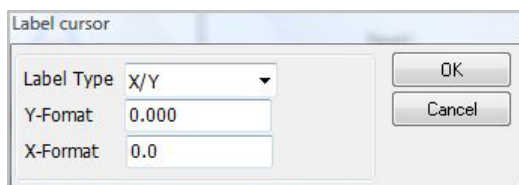


select if you want to label the peaks/bases or both. The threshold defines the minimum height for a peak to be labelled (the higher this value the less peaks/bases are detected). Range start and end define the x-axis range in which peaks are searched.

Finally the format of the labels can be defined. If Y is selected only the y-axis value is displayed. X display the x-axis value only. Y/X, X/Y display both values one on top of the other, (X:Y), X:Y display the values side by side (in the first case in brackets). The Axis format text-boxes define the format for the x,y values (see also Variable Formats).

Label Cursor

Press this button to add label(s) for all selected curves at the current cursor position




Like in the Label Peak dialogue the format of the label can be defined.

Clear Labels


To delete all labels of the selected curve(s) press the clear labels button.

After the dialogue is left with ok all defined labels are displayed on the graph in the report.

Copying a Report

After clicking the copy button  the selected text of the report is copied to the clipboard. If no text is selected the complete document is copied. The text is formatted in Rich Text Format (RTF) to allow to easily paste it into a word processing program for further processing. Please note, that exporting a report does not copy any digital signatures, therefore these documents may need to be re-approved.

Exporting a Report


After clicking the export button  a standard file save dialogue is opened. Select the desired location and format for the report and click ok.

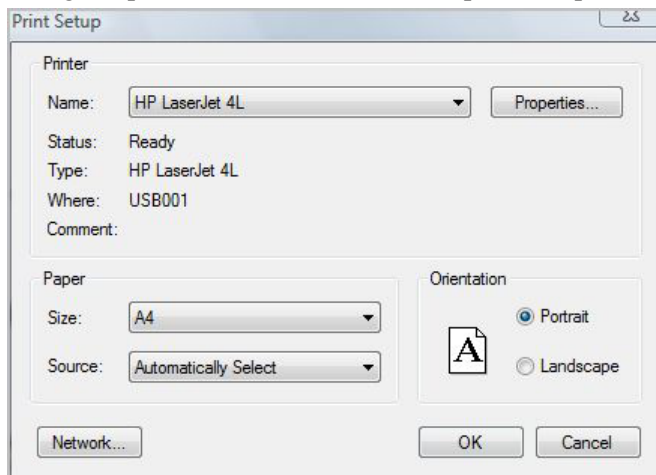
The following export format are supported:

- pdf: exports the report as PDF document
- rtf: exports the report as generic Rich Text document
- html: exports the report as html document
- text: exports the report as plain ASCII text (all formatting is lost)

To save an report in doc(docx) format it is possible to use the copy/paste function.

Printing a Report

After clicking the print button  the standard print setup dialogue is opened:



Select the printer and press ok to print the report.

Transactions

Description

Transaction modules are used to perform administrative actions at the end of measurements.

The Standard Export Module

The standard export module offers functions to automatically export results into different file formats and to start end-of-run applications:

The screenshot displays two panels from a software interface. The top panel, titled 'Actions', contains two sections: 'On Sample Measured' and 'On Batch Measured'. Under 'On Sample Measured', there are two checked checkboxes: 'Export to File' and 'Execute Application'. The 'Execute Application' checkbox is followed by a text box containing the word 'Notepad'. Under 'On Batch Measured', there is one unchecked checkbox labeled 'Execute Application'. At the bottom of this panel is a button labeled 'Export all Samples'. The bottom panel, titled 'Export File Definition', contains several fields and tables. It starts with a dropdown menu for 'Export Result' set to 'T'. Below it is a dropdown for 'File Type' set to 'Perkin Elmer Spectrum(.sp)'. The 'Directory' field is 'C:\Data' with a browse button (...). The 'Sub Directory' section contains a table with columns 'Name' and 'Format', and buttons 'Insert' and 'Remove'. The table has four rows: 'Method' (empty), 'Fixed' (backslash), and 'Date' (yyyymmdd). The 'File Name' section contains another table with columns 'Name' and 'Format', and buttons 'Insert' and 'Remove'. This table has four rows: 'SampleID' (empty), 'Fixed' (hyphen), and 'Time' (hhnnss). At the bottom, the 'Name Example' field shows the path 'C:\Data\MethodName\20131012\SampleID_122423.sp'.

Actions Panel

Execute Application: Enter the name of the program to be started in the textbox. If the program is not located in the windows directory the full path must be entered, the extension can be omitted. The program is executed automatically after the sample (all samples of the batch respectively) is measured. The name of the exported file (if selected) is automatically passed to the program via the command line. Please note, that BLStudio immediately continues and does NOT wait until the program terminates.

Export to file: Select this option to automatically export the result of a sample to a file, after the sample has been measured. The location of the file, the file name and the format of the file is defined on the Export File Definition panel.

Export all Samples: Press this button to export the results of all samples of the currently loaded batch result to file. The location of the file, the file name and the format of the file is defined on the Export File Definition panel.

Export File Definition Panel

Export Result: Select which value is to be exported

File Type: Select the file type from 4 available formats:

- Perkin Elmer Spectrum: sp Ascii format, few instrument, method information
- Perkin Elmer Kinetic: td Ascii format, few instrument, method information
- Biolight Ascii: Ascii format, most instrument, method information
- Tab delimited ascii: Ascii format, no instrument, method information

Directory: Defines the root directory, where the results are to be saved. Press the ... button to select the directory from a dialogue or enter the directory manually into the textbox.

Sub Directory: Allows to define a specific subdirectory for each sample result. If the directory does not exist it will be created on run time. Press the insert button to add a new section to the subdirectory name. Then click on the cell containing the Name and select the desired information from the list box. If desired modify the format of the information in the format cell. To remove a section select the corresponding row in the table and press the remove button.

File Name: Allows to define a specific file name for each sample result. If the file does not exist it will be created on run time otherwise it will be overwritten without further message. (To ensure files are not overwritten add the Time information to the file name). Press the insert button to add a new section to the file name. Then click on the cell containing the Name and select the desired information from the list box. If desired modify the format of the information in the format cell. To remove a section select the corresponding row in the table and press the remove button.

Available Directory/Filename Information: The following standard entries are available

- Fixed: The string defined in the format column. (Use “\” to start a new subdirectory)
- Time: The creation time of the result dataset using the format defined in the format column
- Date: The creation date of the result dataset using the format defined in the format column
- Method: The name of the method used to measure the result dataset
- Inst: The name of the instrument used to measure the result dataset
- User: The name of the user who created the result dataset.
- BatchID: The batch id defined in the result dataset

Additionally all information defined in the sample info of the result data set can be added.

Name Example: Displays an example for an export file name, using the current definitions.

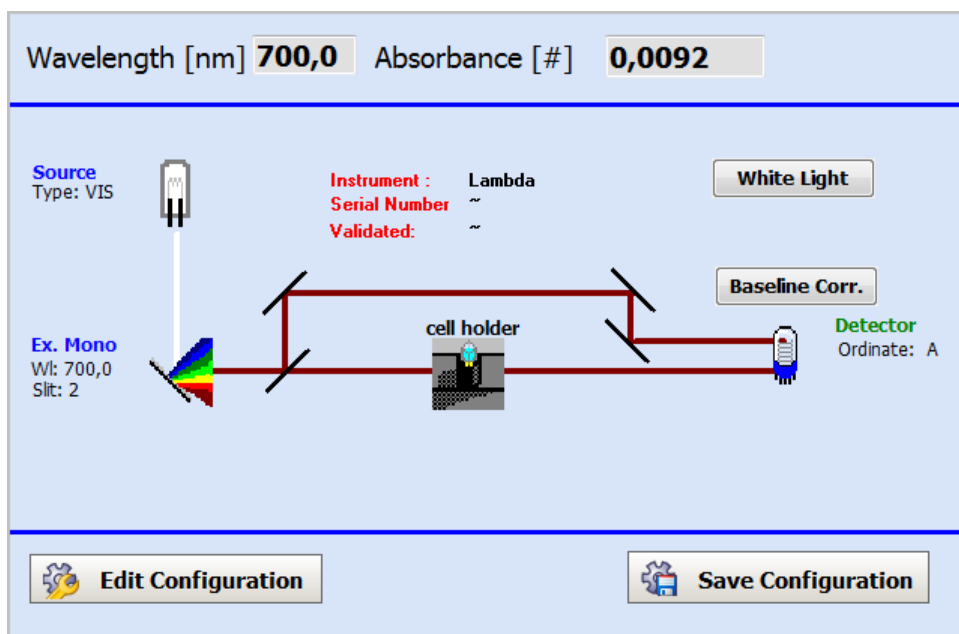
Manual Control Modules

Description

The manual control module allows the user to directly set-up the instrument. Together with the “live display” which online displays the currently measured values it can be used to perform quick measurements.

Manual Control Lambda

The status page displays a schematic of the Lambda's optical system with icons representing the individual components. The current status of the instrument is described by the text next to the icons. Furthermore the instrument type, the firmware revision and the serial number of the instrument are displayed. The colours of the beams between each icon in the optical schematic are an approximate indication of the wavelength.



On top of the Lambda-Module the current wavelength and measured value is displayed.

It is possible to change the instrument parameters by left clicking on the icon relating to that part of the optical system. This accesses a series of specific instrument parameter dialogues.

Right clicking on an icon opens a dialogue to setup the configuration or calibration of an optical system. Please note that it is necessary to save changes made via the configuration setup dialogues with the save configuration button, otherwise the changes are lost the next time BL Studio is started.

White Light Button

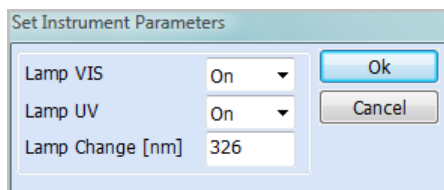
Sets the monochromator to white light (0 nm).

Baseline Corr. Button

Performs a baseline correction at the current wavelength. The correction is applied as long as neither the wavelength nor the slit width is changed.

Source Parameter Dialogue

Left clicking on the source symbol opens the source parameter dialogue.



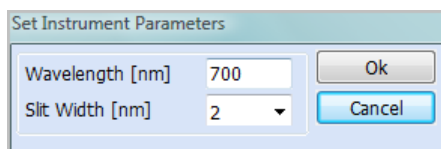
Lamp VIS Switches the VIS lamp on and off

Lamp UV Switches the VIS lamp on and off

Lamp Change Below this wavelength the UV Lamp is used as source, above the wavelength the VIS lamp is used.

Excitation Parameter Dialogue

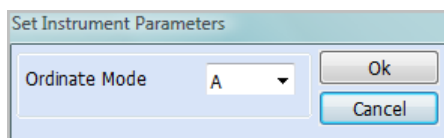
Left clicking on the monochromator symbol opens the excitation parameter dialogue.



After clicking OK the values for the wavelength and the slit width are validated and sent to the instrument. In case of an invalid value the corresponding text box is marked with a red background, the dialogue stays open and an error message is displayed.

Detector Parameter Dialogue

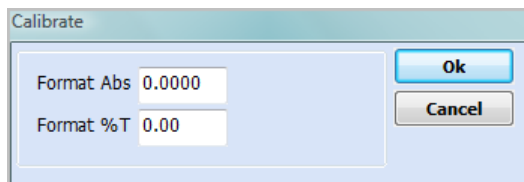
Left clicking on the detector symbol opens the detector parameter dialogue.



The ordinate mode can be selected from the listbox. The following modes are available: A measures the absorbance, T the transmission, E1 returns the intensity of the sample beam, E2 the intensity of the reference beam. After clicking ok the ordinate mode is sent to the instrument and the live display is updated.

Detector Setup Dialogue

Right clicking on the detector symbol opens the detector setup dialogue.

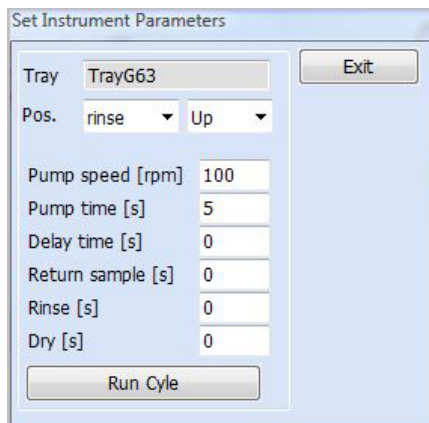


Format Abs: Defines the format of the result value in Absorbance mode. The format is used in the life-display and in all tables.

Format %T: Defines the format of the result value in %T mode. The format is used in the life-display and in all tables.

Auto-Sampler Control Dialogue

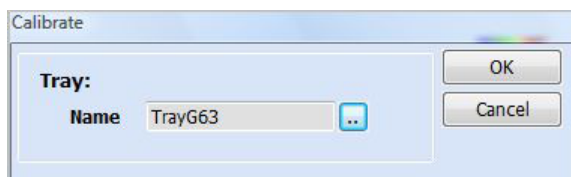
This dialogue allows the user to manually control a connected auto-sampler (AS90,AS93,S10). To send the auto sampler to a position just select the desired position from the Pos. list-boxes. To access the pumps enter the desired pump times in the corresponding text boxes and press the Run Cycle button.



Please note that the tray description can be selected from the Auto Sampler Setup Dialogue (right click on the Auto Sampler icon).

Auto Sampler Setup Dialogue

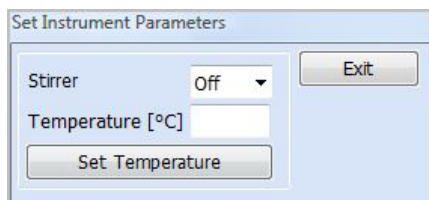
Right clicking on the Auto Sampler symbol opens this dialogue. Via this dialogue the user can load a tray definition from file.



To load a plate definition click on the ... button. Then select the definition file from the standard file dialogue. Please note, that the tray definition files are located in the BL Studio Data/System folder. Click on the OK button to use the tray definition in the control dialogue. Press the save configuration button to keep the definition when BL Studio is started the next time. Please note that the tray definition is used for the Control dialogue only, all methods contain their specific tray definitions

Peltier Control Dialogue

This dialogue allows the user to manually control a connected peltier controller (PTP1). Selecting the desired stirrer speed from the list-box immediately sets the speed. To set a temperature enter the desired temperature in the text box and press the set temperature button.



Please note that the function returns immediately and does not wait until the new temperature is actually reached.

Peltier Setup Dialogue

If a P1 peltier accessory is connected right clicking on the BioKinetics symbol opens this dialogue. It allows the user to enter a calibration curve for the sample temperature and to define the temperature accuracy of the P1.

The 'Calibrate' dialog box contains the following elements:

- Use Calibration
- Buttons: Add Point, Remove Point, OK, Cancel
- Table with columns: Temperature Peltier [°C], Temperature Sample [°C]
- Temperature Accuracy [°C] dropdown menu set to 0.1

Temperature Peltier [°C]	Temperature Sample [°C]
10.0	12.0
20.0	19.0
30.0	29.0
50.0	47.5
100.0	96.0

To determine the calibration curve use the peltier control dialogue to set a peltier temperature. Wait until the sample has equilibrated and measure the temperature in the sample with an external temperature sensor. Then insert the temperature pair in the table. The number of points used can be modified via the Add and Remove buttons. For the calibration a linear interpolation is used where necessary.

Select the Use Calibration option to apply the temperature calibration curve.

The temperature accuracy value can be used in conjunction with the temperature scan add ons. When the the reported peltier temperature is within the desired temperature +/- the accuracy the desired temperature is considered reached: A lower accuracy leads to shorter scan times.

Changing the Configuration

Clicking on the edit configuration button opens this dialogue. This dialogue can be used to define the name of the instrument, the comports and external sampling accessories of the spectrometer. If the instrument is set to simulation it is also possible to define internal accessories:

The 'Edit Configuration' dialog box contains the following sections:

- Instrument**
 - Name: Lambda
 - Comport: Com1
 - Serial: 12345
 - Check offline
- Sampling Accessories**
 - Single cellholder
 - Cellchanger (5)
 - Sipper
- External Accessories**
 - Autosampler (Comport: Com2)
 - Peltier (Comport: Com2)
 - Std. Controller Fitted

Name Enter a user friendly name for the instrument. This name will be used in all reports and the validation.

Serial Number	Enter a serial number for the instrument. This number will be used in all reports and the validation.
Comport	Determines the serial comport for the spectrometer. If the comport above com3 is required it cannot be selected from the list but must be entered manually. Selecting simulation sets the instrument to the simulation mode. In this case internal accessories can be configured.
Check Offline.	If this option is selected the software checks if the instrument is connected and switched on, otherwise the instrument is marked offline. Unselect this option if your RS232 cable or your UDS-RS232 converter does not support the DSR line.
Sampling Accs.	If simulation mode is selected the configuration for the internal sampling accessories can be defined here. Otherwise the configuration is determined from the connected instrument.
External Accs.	If a S10 auto sampler or P1 peltier module is connected to the PC it can be registered here by selecting the corresponding option and defining the comport. It is possible to set the accessories to simulation mode. Please note, that only one sampling accessory (internal or external) can be used at a time..

Saving the Configuration

Click on the save configuration button to save the current configuration. If the configuration is not saved all changes will be lost the next time BL Studio is opened.

Transmission Mode:

In this mode the spectrometer measures the transmission:

$$T = \frac{I}{I_0}$$

where T is the transmission, I is the intensity of the light that has passed through the sample beam path and I_0 is the intensity of the light that passed through the reference beam path.

Absorbance Mode:

In this mode the spectrometer measures the absorbance:

$$A = -\log_{10} \left(\frac{I}{I_0} \right),$$

where A is the absorbance, I is the intensity of the light that has passed through the sample beam path and I_0 is the intensity of the light that passed through the reference beam path.

Sample Beam Energy Mode (E1):

In this mode the instrument measures the intensity of the light that passes through the sample beam path. This mode is useful instrument validation and service purposes mainly.

Reference Beam Energy Mode (E2):

In this mode the instrument measures the intensity of the light that passes through the reference beam path. This mode is useful instrument validation and service purposes mainly.

The Free-Form Calculator

Description

The Free-Form Calculator allows the user to perform calculations on single numbers and curves. As complement to the calculators used in the BL Studio data acquisition process it offers to handle data with a very high flexibility. Besides loading and saving of text- and Biolight binary formats the import of most PE data formats and export to PE text format is supported.

To allow other people to view results, generated with BL Studio, the free form calculator is available as license free stand-alone version.

The main page consists of a menu, a toolbar, the data view area and the calculations area.

Menu

Toolbar

Data View Area

Calculation Area

Main Menu

The following items are available in the menu:

File:

- New: Starts a validation run
- Load Curve: Exits the Validation
- Save Curve: Exits the Validation
- Add Curve: Exits the Validation

View:

Auto scale X:	Automatically expands the X-axis
Auto scale Y:	Automatically expands the Y-axis
Scale Axis:	Opens a dialogue to scale the X and Y axis
Show X-Cursor:	Enables the vertical cursor
Show Y-Cursor:	Enables the horizontal cursor
Add Text Label:	Opens a dialogue to define a text-label to be displayed on the graph
Label Cursor:	Add a label at the current position of the X-Cursor (Y-Cursor respectively)
Label Peaks:	Opens the label peaks dialogue
Delete Labels:	Deletes all selected labels
Copy Graph:	Copies the picture of the graph as emf to the clipboard
Setup Graph:	Opens the set-up graph dialogue.

Options:

Graph Options:	Opens the Graph Options dialogue
PE Unit conversions:	Opens the Unit Conversion dialogue

Main Toolbar

The following items are available in the main toolbar:



Clear Result: Clears the results in all pages



Load Result: Starts a File Open dialogue to load a result from hard disk and displays it



Save Result: Starts a File Save dialogue to save the currently selected result to hard disk

Graph Toolbar

The following items are available in the graph toolbar (please refer also to generic graph functions):



Auto expand X: Automatically expands the X-axis



Auto expand Y: Automatically expands the Y-axis



Vertical Cursor: Enables the vertical cursor



Horizontal Cursor: Enables the horizontal cursor



Scale Graph: Opens a dialogue to scale the X and Y axis



Add Text Label: Opens a dialogue to define a text-label to be displayed on the graph



Label Peaks: Opens the label peaks dialogue



Copy Graph: Copies the picture of the graph as emf to the clipboard



Setup Graph: Opens the set-up graph dialogue.

Calculations

Arithmetik

Performs mathematical operations on single values or curves: Click on the formula button to start the Arithmetic dialogue. To generate a formula simply click on the appropriate buttons on the editor or enter the formula via the keyboard. To implement the formula click on the 'OK' button. The formula is then checked for syntax errors. If errors are detected an error message is displayed and the formula can be corrected.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The result is added to the results table.

Curve Point

Calculates a coordinate of a curve point: Select the curve to be used from the Curve list-box. Then select one of the following functions from the find list-box:

- Y:** returns the y-value of a given x-value of the curve.
- X:** returns the first x-value for a given y-value in the given range (start, end text boxes).
- Max:** returns the maximum y-value of the curve in the given range (start, end text boxes).
- Min:** returns the minimum y-value of the curve in the given range (start, end text boxes).

If the start,end value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The result is added to the results table.

Peak

Calculates information about a peak/base of a curve. Select the curve to be used from the Curve list-box. Then define in the type list-box if the result are to be calculated for a peak or a base. The start, end text-boxes define the range in which the peak is searched. The threshold defines the minimum height a peak must have to be valid.

The following properties of a the first valid peak in the range can be determined:

- Y:** returns the absolute maximum y-value of the peak
- X:** returns corresponding x-value of the peak
- Height:** returns the baseline corrected maximum y-value. The baseline is determined using the given Start, End values
- Area:** returns the baseline corrected area under the peak/base. The borders of the area and the baseline are determined using the given Start, End values

If no valid peak is detected in the given area all properties are set to the invalid value ~. If the start,end value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The result is added to the results table.

Area

Calculates the absolute area under a given range of a curve. Select the curve to be used from the Curve list-box Then enter the desired x-range in the x1, x2 text-boxes. The absolute area for this range is calculated. To obtain a baseline corrected area use the Peak function.

If the x1, x2 value of the range is invalid it is replace by the minimum x-value (the maximum x-value respectively) of the curve.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The result is added to the results table.

Normalize

Normalizes a given a curve. Select the curve to be used from the Curve list-box. The function first determines either the maximum y-value or the y-value for the given x-value of the curve. Then the factor is calculated by $f=100/y$. Finally each y-value of curve is multiplied with the factor.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The normalized curve is added to the results table and displayed on the graph.

The Filter Dialogue

Applies a filter on a given a curve. Select the curve to be used from the Curve list-box. Now select one of the four available filters form the filter list-box: Moving Average, Triangular, Quadratic Golay-Savitzky, Cubic Golay-Savitzky

For a detailed description of these filters refer to Smoothing Filter. Finally enter the number of points to be used to calculate the filtered data (the more points used the smoother the filtered curve appears).

Now enter the desired result name into the test box below the calculate button and press the calculate button. The filtered curve is added to the results table and displayed on the graph.

Derivative

Calculates a derivative of a given a curve. Select the curve to be used from the Curve list-box. Then enter the desired order of the derivative and the number of points to be used to calculate the derivative. (the more points used the smoother the derivative appears). Now enter the desired result name into the test box below the calculate button and press the calculate button. The result curve is added to the results table and displayed on the graph.

Slope

Calculate the slope between two points of a given a curve. Select the curve to be used from the Curve list-box, then determine the two points by their x-values. Now enter the desired result name into the test box below the calculate button and press the calculate button. The result is added to the results table.

Merge

Merges two curves: Select the first curve curve from the Curve list. Then select the second curve to be merged and x-value, at which the curves are to be merged.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The merged curve is added to the results table and displayed on the graph.

Generate Curve

Generates a user-defined curve: Click on the formula button and enter the desired formula in the arithmetic dialogue. Then select the start, end and step for the x-axis. Finally enter the ID, unit and format for the x- and y-axis.

Now enter the desired result name into the test box below the calculate button and press the calculate button. The user defined curve is added to the results table and displayed on the graph.

The Administration(Basic Version)

Description

In the basic version the administration offers three features: A protocol function, the user management and the maintenance of BL Studio components and licenses.

Logging Events

The BL Studio protocol is designed as a system log rather than an assembly of record histories. This has the advantage, that the user gets an overview what happened before and during his measurements to the whole system.

For ease of maintenance the events are bundled in one record for each day. To view all events that occurred during a day simply select the corresponding date from the leftmost column.

Select the Protocol Events option to start the event log.

Date	#	Time	Analyst	Application	Description
21.01.2013	104	13:31:46	BioLight	BLAcquisition	Logged out
20.01.2013	103	13:31:33	BioLight	BLAcquisition	Stopped acquisition: User stop requested
19.01.2013	102	13:31:30	BioLight	BLAcquisition	Saved result Result(13.31.30_21.01.2013) ({D00BA97
	101	13:31:30	BioLight	BLAcquisition	Measured sample Sample2
	100	13:31:26	BioLight	BLAcquisition	Measured sample Sample1
	99	13:31:20	BioLight	BLAcquisition	Measured standard Std6
	98	13:31:17	BioLight	BLAcquisition	Measured standard Std5
	97	13:31:15	BioLight	BLAcquisition	Measured standard Std4
	96	13:31:12	BioLight	BLAcquisition	Measured standard Std3
	95	13:31:09	BioLight	BLAcquisition	Measured standard Std2
	94	13:31:06	BioLight	BLAcquisition	Measured standard Std1
	93	13:31:03	BioLight	BLAcquisition	Started acquisition Concentration
	92	13:30:29	BioLight	BLAcquisition	Changed instrument configuration: PELS#Simulation
	91	13:30:22	BioLight	BLAcquisition	Loaded method Concentration ({14F07FD3-853B-42C5
	90	13:30:18	BioLight	BLAcquisition	Started application
	89	13:30:13	BioLight	BLAdministration	Enabled audit trail

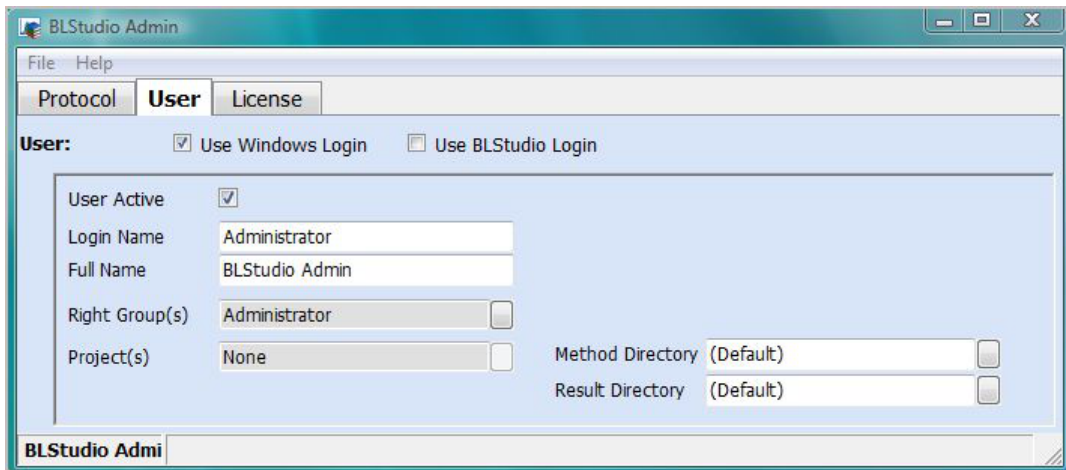
To view all events that occurred during a day simply select the corresponding date from the leftmost column. Each event contains an electronic signature describing who caused the event together with a date/time stamp. Furthermore the application and the description of the event are recorded.

All log-records are checksum protected. In the basic version the user is responsible to ensure that the records are not deleted.

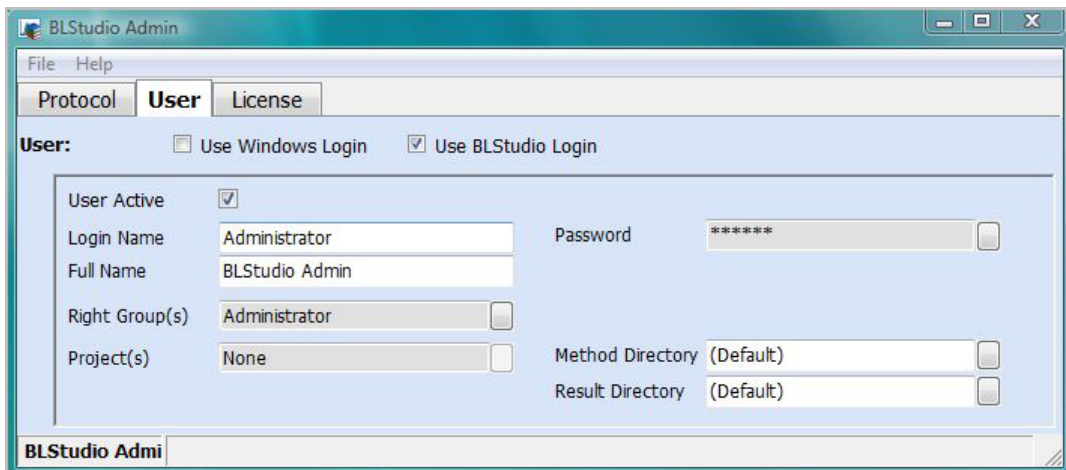
Managing User Accounts

Login Systems

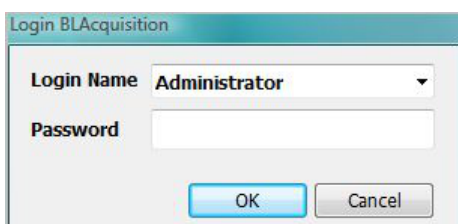
BL Studio offer two different login systems: The Windows login is based on the current Windows user. The Windows login name is compared against the login name defined on the user dialogue. **Please note that the login names must match exactly, the comparison is case sensitive.** This system has the advantage, that the user has to login only once and has to remember only one password. Furthermore for each user specific access rights to methods and data can be defined at operating system level.



Alternatively the BLStudio login system can be enabled. Using this system the user must login whenever a BLStudio component is started. Therefore a password must be defined for each user. In this system BLStudio users are completely independent from the Windows user accounts. It is not necessary to create a Windows account for each BLStudio user. Furthermore the BLStudio user can change without having to logout and re-login to Windows.



Whenever a BLStudio component is started (except the free form calculator) the user must identify via a login dialogue:



User Data

The following information can be defined for BLStudio users:

Active	Login Name	Full Name	Right Group	Project	GUID
<input checked="" type="checkbox"/>	Administrator	BLStudio Admin	Administrator	None	{F0CF0A8B-4BD8-4F83-9730-1C1FB861CCE3}
<input checked="" type="checkbox"/>	Senne	New	Analyst	None	{59C3DA99-D7A8-4E57-BCA5-168C1BA49C14}

- User Active** If this option is unchecked the corresponding user is de-activated and cannot login to BL Studio. The user can be re-activated, keeping his GUID.
- Login Name** If the Windows login is activated the login name is used to determine the BLStudio user from the Windows login. Otherwise the login name is used in the BLStudio login dialogue.
- Password** This text box is only visible if the BLStudio login is enabled. It is used in the BLStudio login dialogue to verify the login name. To change the password click on the button and enter the password in the dialogue.
- Full Name** The full name is used for documentation purposes, e.g. in all reports.
- Right Group** Click on the button to assign the user to a right group. Depending on this group the user is granted read, write, modify, delete and signature rights on various records. Please note that in the basic version only three pre-defined right groups are available.
- Project** Via this field the user can be assigned to projects. In the basic version the project management is disabled. Instead user dependent method- and result directories can be defined.
- Method Dir.** The method directory defines the directory from which methods can be loaded for each user. If “(default)” is selected the BLStudio default method directory is used (typically C:\BL Studio Data\Data\Methods). To change the directory click on the button and select a directory from the Select Directory dialogue or enter the directory directly into the text box. If the directory does not exist the text box is set to (default).
- Result Dir.** The result directory defines the directory to which results are stored for each user. If “(default)” is selected the BLStudio default result directory is used (typically C:\BL Studio Data\Data\Results). To change the directory click on the button and select a directory from the Select Directory dialogue or enter the directory directly into the text box. If the directory does not exist the text box is set to (default).
- User Table.** Displays an overview of all BLStudio user accounts.

Creating a new User

To create a new user click on the “New User” button. The new user is appended to the User Table, a new GUID is assigned, the user account is selected and can be edited.

Editing User Data

Select the desired user account from the User Table by clicking on the corresponding row. The row becomes yellow and the user data are displayed on the User Data window. Now the user information can be modified. After a text box is left with <enter> or a dialogue is ended with ok the corresponding information is updated in the user table. Please note that the user information must be saved via the “Save Config” button, before the changes become effective.

Deleting a User

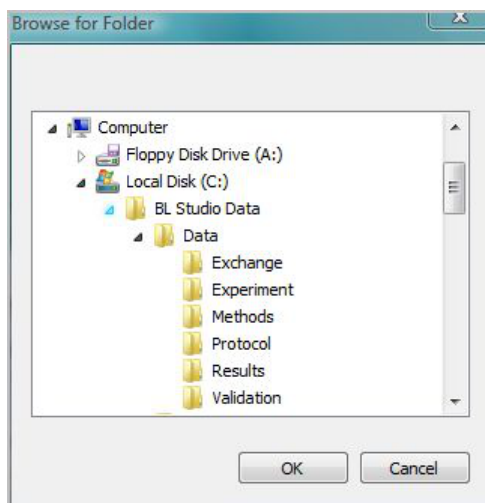
Select the desired user account from the User Table by clicking on the corresponding row. Then press the “Delete User” button to remove the account from the user table. Please note that the user information must be saved via the “Save Config” button, before the changes become effective.

Saving the User Configuration

Save the user information by pressing the “Save Config” button. If the information was saved successfully a corresponding message is displayed, otherwise an error message is issued.

Selecting a Directory

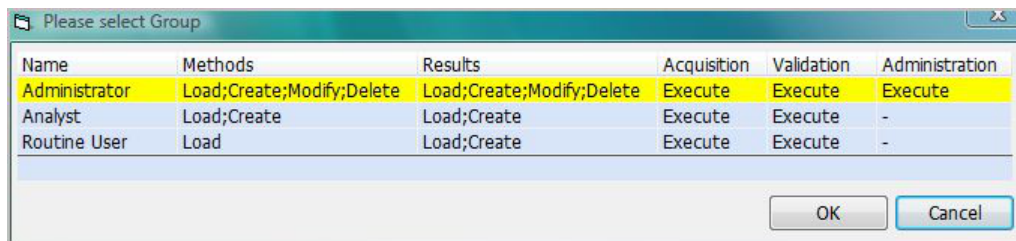
Clicking on one of the two directory buttons starts the Browse for Folder dialogue:



After leaving the dialogue with ok the full path of the selected folder is displayed in the corresponding text box. Please note that the user information must be saved via the “Save Config” button, before the new folder is used.

Selecting a Right Group

To select a right group click on the corresponding button. The following dialogue will come up:



Click on the desired right group and leave the dialogue via the OK button. The name of the right group is displayed in the corresponding text-box. Please note that the user information must be saved via the "Save Config" button, before the new right group is actually assigned.

Pre-defined Right Groups

In the basic version BLStudio offers the following three right groups:

Routine User Assign this group to users, performing day to day routine measurements. Members of this group can load methods (but not modify parameters) and execute the Acquisition and Validation modules, creating new results. Furthermore routine users can load and view old data.

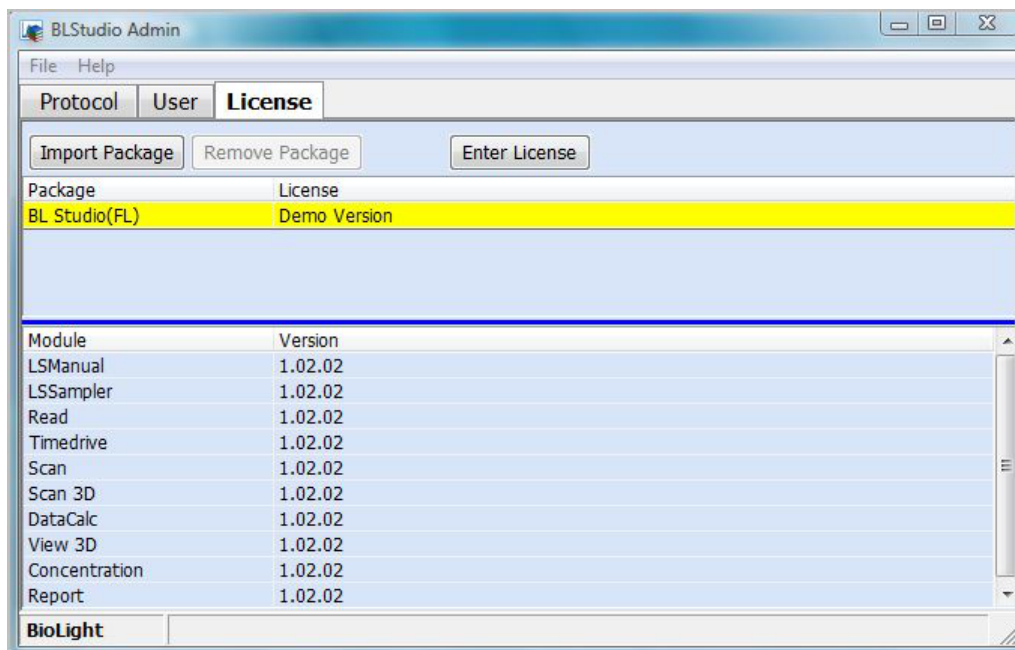
Analyst Members of this group can additionally modify method parameters and save modified methods under a new name. Old data can be loaded, calculation parameters can be modified and the result can be saved in a new record. Analysts cannot overwrite or delete existing methods or data.

Administrator Members of this group have full rights to manage results and methods. Only Administrators can execute the Administration module.

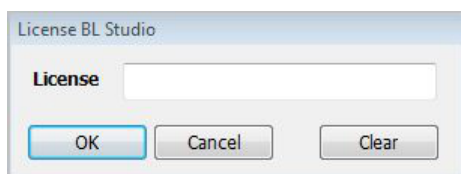
Managing BL Studio Components

BL Studio allows an administrator to add/remove modules e.g. to control a new sample preparation, to perform specific data acquisition or data processing or to add customized reports. Thus BL Studio supports a wide range of applications still offering a lean user interface rather.

To import modules click on the Import Add On button. A standard file dialogue comes up. Simply select the .inf file delivered with the add on package and click ok. The add on modules of the package will then be installed automatically and available the next time BL Studio is started. Please note that you will need windows administrator rights to install add on modules, otherwise an error message will be issued.



After installation of an add on module you can select the corresponding row of the module table and click on the Enter License button to enter the license key to enable the add on (otherwise it will run in demo mode, not allowing to save methods or data).



Pressing the ok button will verify the entered license key. If no valid key has been entered the dialogue will not close. Please note that it is also possible to enter the license in the help/about dialogue of the data acquisition program

To delete an add on click on the corresponding row of the module table. If the module is an add on the delete add on button becomes enabled. Clicking on the button removes all components of the add on from your computer. Base modules cannot be removed.

Miscellaneous

Background Correction

UV/VIS spectroscopy is based on the measurement of the transmission or absorbance of a sample. The transmission is the ratio between the light falling upon the sample and the light transmitted through the sample. The Absorbance (Abs) = $-\log_{10}(\text{transmission})$.

Using a dual beam spectrometer, the transmission is measured by ratioing the intensity of the sample beam against the intensity of the reference beam. Ideally, the transmission with sample and reference beams both empty (i.e. no sample) should be 100%T or 0A. In reality, however, the optical elements and detection electronics in the sample and reference beams are not identical, resulting in small, wavelength-dependent deviations from 100%T (0A).

To correct for these instrument-dependent deviations, a background correction is performed. A transmission (or absorbance) spectrum is measured with the sample and reference positions both empty. All subsequent measurements are corrected using this spectrum.

Since the correction depends on the slit width, scan speed and the wavelength, the correction spectrum must be re-measured whenever one of these parameters is changed. Furthermore the correction should be repeated at least every day, to compensate for time-dependent changes in the optical system.

A second approach is to determine the transmission of a diluted analyte directly, by placing a cuvette containing only the solvent in the reference beam. However, the transmission of the solvent might change un-noticed during the measurement, eg. due to evaporation or the formation of bubbles.

For this reason it is recommended not to place the “blank” sample in the reference compartment, but to measure a blank sample before the analytical sample and then perform the a blank subtraction using the data calculator.

Message and Error Display

BL Studio displays status and error messages in the status bar rather than bringing up message boxes. This has the advantage that the user does not have to respond to every message.

If e.g. a method contains more than one invalid parameter BL Studio will display the corresponding input fields with a red background. After such a field is selected the corresponding error message is displayed in the status bar.

Input/Display of variables

Types

The following variable types are available:

- Text: The column can contain any text. Non-empty fields can be forced via the column range.
- Number: The column can contain any number. The format of the number (e.g. number of decimals) is determined via the column format: valid acceptable range can be defined via column range.
- Time: The column can contain times. The format of the time is determined via the column format.
- Boolean: The column can contain ‘true’ or ‘false’. The actual string displayed can be altered via the column format.

Undefined/Invalid Values

Under some circumstances it is possible, that values are not defined or invalid. For example on a validation report always the results for all samples and for all validation wavelengths are displayed. If a user has stopped the validation some of the results may be undefined. It is also possible that an equation produces an invalid result (e.g. division by 0). In these cases the result is displayed as an “~”.

Formats

Depending on the variable type the following formats are available:

Number:*

None: Display the number with no formatting.

(0): Digit place-holder. Display a digit or a zero. If the expression has a digit in the position where the 0 appears in the format string, display it; otherwise, display a zero in that position.

If the number has fewer digits than there are zeros (on either side of the decimal) in the format expression, display leading or trailing zeros.

If the number has more digits to the right of the decimal separator than there are zeros to the right of the decimal separator in the format expression, round the number to as many decimal places as there are zeros.

If the number has more digits to the left of the decimal separator than there are zeros to the left of the decimal separator in the format expression, display the extra digits without modification.

- (#): Digit place-holder Display a digit or nothing. If the expression has a digit in the position where the # appears in the format string, display it; otherwise, display nothing in that position. This symbol works like the 0 digit place-holder, except that leading and trailing zeros aren't displayed if the number has the same or fewer digits than there are # characters on either side of the decimal separator in the format expression.
- (.): Decimal place-holder The decimal place-holder determines how many digits are displayed to the left and right of the decimal separator.
If the format expression contains only number signs to the left of this symbol, numbers smaller than 1 begin with a decimal separator. To display a leading zero displayed with fractional numbers, use 0 as the first digit place-holder to the left of the decimal separator. The actual character used as a decimal place-holder in the formatted output depends on the Number Format recognised by your system.
- (%): Percentage place-holder The expression is multiplied by 100. The percent character (%) is inserted in the position where it appears in the format string.
- (E- E+ e- e+): Scientific format. If the format expression contains at least one digit place-holder (0 or #) to the right of E-, E+, e-, or e+, the number is displayed in scientific format and E or e is inserted between the number and its exponent.
The number of digit place-holders to the right determines the number of digits in the exponent. Use E- or e- to place a minus sign next to negative exponents.
Use E+ or e+ to place a minus sign next to negative exponents and a plus sign next to positive exponents.
- + \$ (): Display a literal character. To display a character other than one of those listed, precede it with a backslash (\) or enclose it in double quotation marks (" ").
- (SF): Significant figures. If the format string starts with SF the following number is interpreted as number of significant figures.

The following table contains some example format expressions for numbers. (These examples all assume that your system's local setting is English-U.S.) The first column contains the format strings; the other columns contain the resulting output if the formatted data has the value given in the column headings.

Format string	5	0.5	0.051
	5	0.5	0.05
0	5	1	1
0.00	5.00	0.50	0.05
0.0#	5.0	0.5	0.05
0.0%	500.0%	50.0%	5.1%
0.00E-00	5.00E00	5.00E-01	5.10E-02
SF3	5.00	0.500	0.0510

Boolean:

None: Display 'true' or 'false'

{text1,text2}: Display text1 if 'true', text2 if 'false'

The following table contains some sample format expressions:

Format string	TRUE	FALSE
	true	false
{passed,failed}	passed	failed
{ok,}	ok	

Time:

None: Display the time using your system's short time format; includes hours, minutes, seconds

(:): Time separator. The time separator separates hours, minutes, and seconds when time values are formatted. The actual character used as the time separator in formatted output is determined by your system settings.

h: Display the hour as a number without leading zeros (0 – 23).

hh: Display the hour as a number with leading zeros (00 – 23).

m: Display the minute as a number without leading zeros (0 – 59).

mm: Display the minute as a number with leading zeros (00 – 59).

s: Display the second as a number without leading zeros (0 – 59).

ss: Display the second as a number with leading zeros (00 – 59).

Ranges

In order to avoid the input of invalid numbers, the valid acceptable range for numbers can be defined. The following range definitions are available (a,b,c.. represent any numbers):

None: Number is not checked for range

<>a: Number must not be equal to a. Otherwise a range error is issued.

>a: Number must be greater than a. Otherwise a range error is issued.

>=a: Number must be greater than or equal to a. Otherwise a range error is issued.

<a: Number must be lower than a. Otherwise a range error is issued.

<=a: Number must be lower than or equal to a. Otherwise a range error is issued.

{a,b,c}: Number must be equal to either a or b or c. Otherwise a range error is issued.

[a,b]: Number must be greater than or equal to a and lower than or equal to b. Otherwise a range error is issued.

{a,[b,c]}: Number must be either equal to a, or be between b and c. Otherwise a range error is issued.

Generic Table Functions

Customising the Column Width of a Table

It is possible to customise the width of the columns of tables. Move the mouse over the left or right border of the header of the column to be modified. The mouse pointer will change to indicate the border can be selected. Now drag the border to the desired position. The column width will be resized accordingly.


Selecting a Row

To select a row either click on any locked cell of the row or, when existing, on the row header (first column). The row background colour will change to yellow to indicate it has been selected. To deselect the row click on a locked cell (the header) again. The row background will turn back to its original colour. Depending on the table it is possible to select more than one row at a time. To select more than one row click on the row while keeping the ctrl-key (to add a row) or shift-key (to add a range) pressed.

Selecting a Column

To select a column click on the corresponding header. The column background colour will change to yellow to indicate it has been selected. To deselect the column click on the header again. The column background will turn back to its original colour. Note that only one column can be selected at a time. An already selected column becomes automatically deselected when a new column is selected.

Copying to the Clipboard

In most cases the contents of tables can easily be copied to the clipboard either via the toolbar  or by right clicking on the table and selecting the “copy” option from the pop up menu. The contents of the table is copied as a tab-delimited text file, containing the column caption in the first line.


Display Data on Graph

Clicking this button  changes the display from a tabular to a graphical view.


Generic Graph Functions

The following functions are available via the generic graph menu (please note that not all functions are available on every graph) :


Auto-expansion of the X-axis

Click on this button  to show the entire abscissa range of all selected data files. If e.g. you have selected two Time Drives of 5 and 10 minutes duration respectively and then click the button for auto-expansion of the X-axis, the abscissa will be set to 0 to 10 minutes.


Auto-expansion of the Y-axis

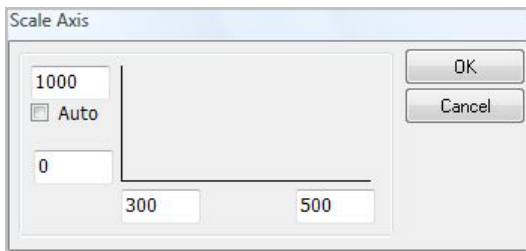
Click on this button  to show the entire ordinate range of all selected data files. If e.g. you have selected two Time Drives of 0-50 and 20-200 ordinate ranges and then click the button for auto-expansion of the Y-axis, the ordinate range will be set to 0 to 200.

Copying the Graph to the Clipboard

In most cases a picture of a graph can easily be copied to the clipboard either via the toolbar  or by right clicking on the graph and selecting the “copy” option from the pop up menu. A picture of the graph is copied in the windows vector format wmf, allowing to resize the picture.


Formatting of the Graph Ranges

Click on the format graph button  to open a window for the manual formatting of abscissa and ordinate ranges:




Enter the required abscissa and ordinate values. Click on OK to confirm and to close the dialogue. Click the on the Cancel button if you wish to proceed without altering the graph ranges.

Vertical Cursor


Click on this button  to activate the vertical cursor. The cursor can be continuously moved to the right and the left to show the appropriate abscissa value. To move the cursor, move the mouse indicator onto the cursor until it takes the form of a double arrow, click with the left hand mouse key and drag the cursor to the desired spot. To deactivate the cursor, click on the button again.

Horizontal Cursor

Click on this button  to activate the vertical cursor. The cursor can be continuously moved to the right and the left to show the appropriate ordinate value. To move the cursor, move the mouse indicator onto the cursor until it takes the form of a double arrow, click with the left hand mouse key and drag the cursor to the desired spot.

To deactivate the cursor, click on the button again.

Adding a Text Label

Click on this button  to start the Add Label dialogue:




After leaving the dialogue with ok, the text label is inserted into the graph and can be move to the desired position with drag and drop.

Display Data on Table

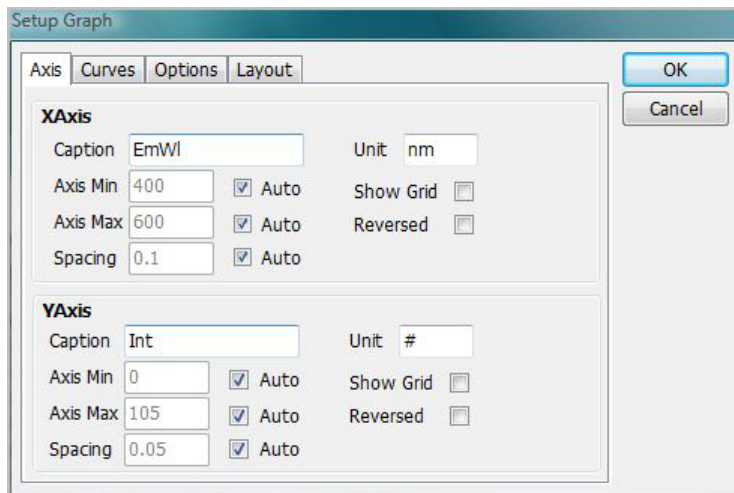
Clicking this button  changes the display from a tabular to a graphical view.

Setting up the Graph

Clicking on the setup button  starts the setup graph dialogue. The dialogue consists of 4 tabs:

Axis Tab

On this tab the properties for the X and Y axis can be entered:

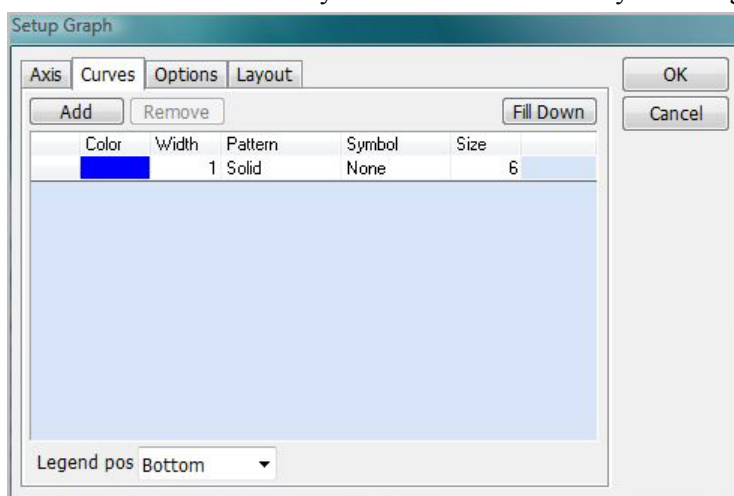


The Axis minimum and maximum can be set to a fixed value. Alternatively the minimum and/or maximum can be determined automatically from the loaded data. Please note, that this function does NOT perform an auto-scale: The axis will only re-scale if the actual maximum is larger than the pre-set fixed value (actual minimum smaller than fixed value respectively). To ensure the graph is always re-scaled to fit the actual data enter “~” into the min/max values.

Accordingly the spacing can be either set to a fixed value, or it can be calculated from the actual axis minimum/maximum during run-time. Please note, that the spacing will only be re-calculated while zooming, if the spacing mode is set to auto. The grid spacing is always set to the axis spacing.

Curves Tab

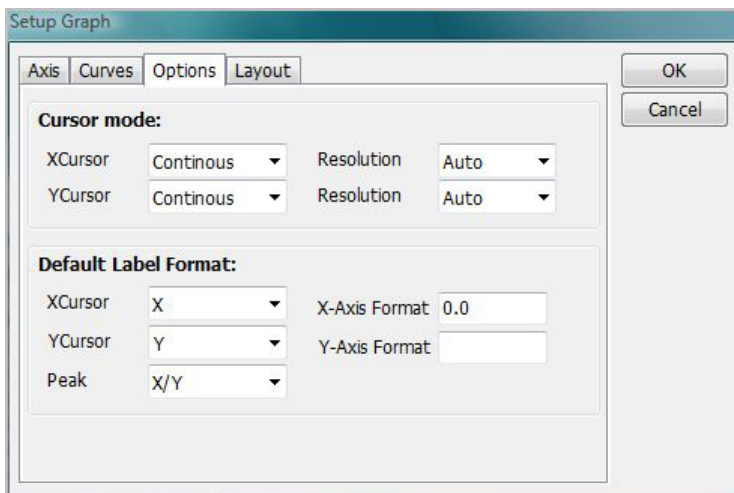
Use this tab to define the colour, width, pattern and symbols for curves. The first curve style is assigned to the first curve etc. If no curve style is defined a default style is assigned.



Additionally the position of the curve legend can be defined in this tab.

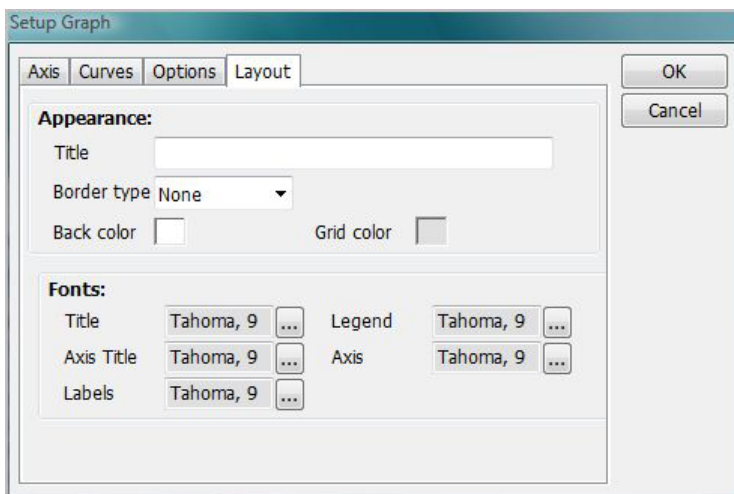
Options Tab

On this tab options for cursors and labels can be defined:



Layout Tab

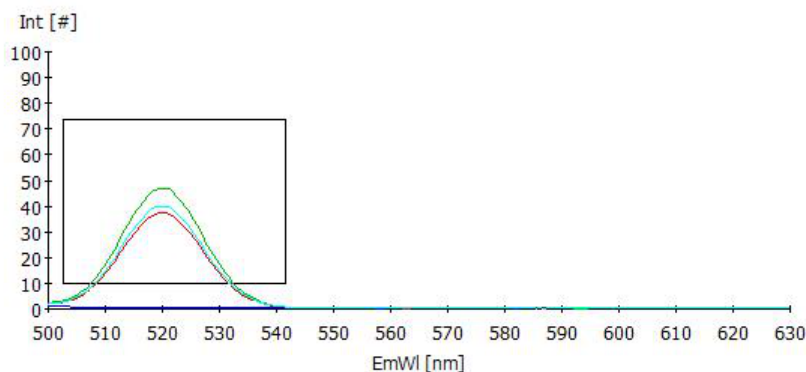
From this tab the title of the graph can be defined. The title is displayed as caption within the graph. Furthermore it is possible to define a border style, the background colour of the graph and the colour of the grid.



Finally, clicking on a font button starts the standard Windows font dialogue, allowing the user to change the corresponding font.

Zooming into the Graph

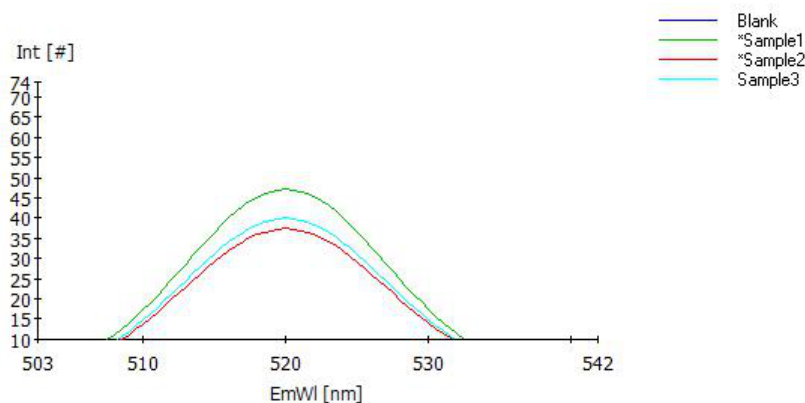
To select the desired area left click with the mouse on the upper left point and move the mouse to the lower right point, keeping the left mouse button pressed. A black rectangle appears,



Releasing the mouse button will set then actually perform the zoom. To undo a zoom just right click into the graph. It is possible to zoom into a graph in several steps. The undo zoom will then undo the zooms step by step

Selecting a curve

Select a curve (e.g. to send it to the free form calculator) by clicking on an unselected curve.



To select more than one curve either hold down the Ctrl key and click on each unselected curve you want to select, or hold down the shift key and click on the first and the last curve of a range of curves to be selected. To unselect a curve click on a selected curve. Please note that the names of selected curves appear with an asterisk, while the names of unselected curves stay normal.

By default curves are already selected when they are loaded into a graphic window.

Emergency Stop

Stopping a run via the stop button on any prompt will cause a “graceful” termination of the measurement: The data collection for the current sample is finished, if defined a sample release procedure is executed. All data is saved. This way the correctness and completeness of the results is ensured.

However it may be desirable to interrupt a measurement immediately. To stop a measurement immediately, press the Esc-button. Note that in this case no results are saved

Command Line Parameter

BLStudio supports loading a method or a result from the command line. Thus it is possible to start BLStudio by double clicking on a method/result in the file explorer, after assigning the .mth, .res extensions to BLStudio.

Alternatively shortcuts can be created on the desktop which immediately load a method or result.

Smoothing Filter

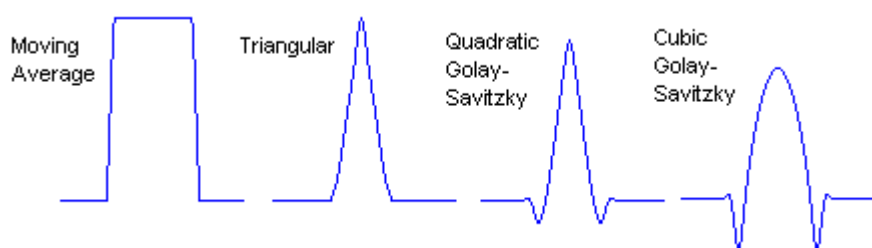
Smoothing filters are used to reduce the noise on collected curves. The premise of smoothing is that the noise varies quicker than the signal. Smoothing filters replace each data point by some kind of local average of surrounding data points.

The filter width determines how many surrounding data points are used for averaging (e.g. a filter width of 33 corresponds to 16 points before the current data point and 16 points behind it are being used). The larger the width of the filter, the more points are used for averaging, the poorer is the resolution of the filter. (Please note that during the averaging process the number of data points is reduced by the filter width. To compensate for this loss the left filterwidth/2 points and the right filterwidth/2 points are interpolated. This may lead to artefacts in this regions.)

The type of the filter determines, how the surrounding points are weighted during the average procedure. BL Studio offers four smoothing filter for offline smoothing:

Moving Average, Triangular, Quadratic Golay-Savitzky, Cubic Golay-Savitzky.

The following scheme shows the principle shape of the weighting factors for the averaging process:

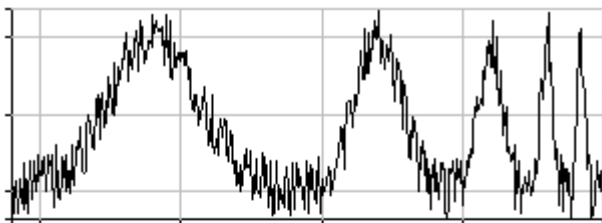


The type of the filter influences the shape of the signal which is smoothed. In general the moving average and the triangular filter are better suited for step signals, while the Golay-Savitzky filters give better results for peaks.

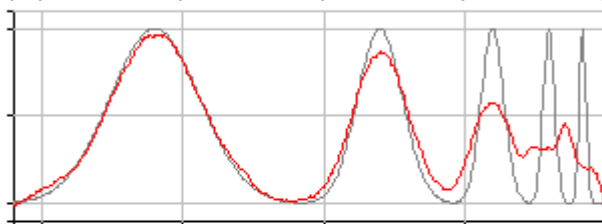
As a rough guideline, for peaks best results are obtained with the quadratic Golay-Savitzky, with the width of the filter between 1 and 2 times the expected FWHM of the peaks. For step shaped signals the triangular filter is recommended with a filter width of about the length of the step.

Smoothing peaks

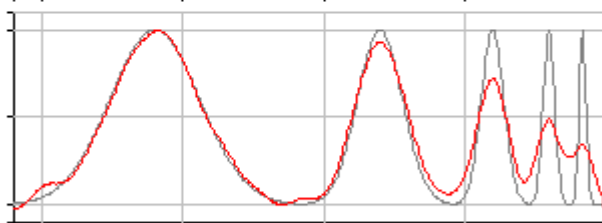
The following graphic shows the influence of different smoothing filters on gaussian shaped peaks, typical for spectral scans. (All filters have the same filter width of 33 points, the gray curves represent the peaks without noise):



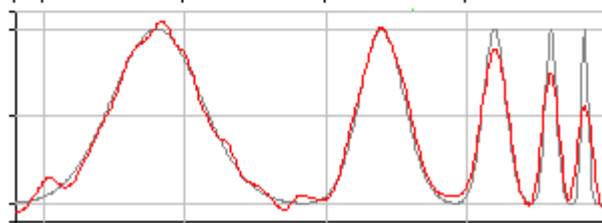
Synthetic noisy data consisting of a sequence of progressively narrower peaks with additive white noise. (heights = 100 units, full widths at half maximum (FWHM)= 90, 45, 22, 11, 5 points)



Result of smoothing the data by a 33 point wide "moving average" filter. Note that narrow features are broadened and suffer corresponding loss of amplitude



Result of smoothing the data by a triangular filter.



Result of smoothing the data by a quadratic Savitzky-Golay filter using the same 33 points. While there is less smoothing of the broadest peak, the heights and widths of the narrower peaks are better preserved.

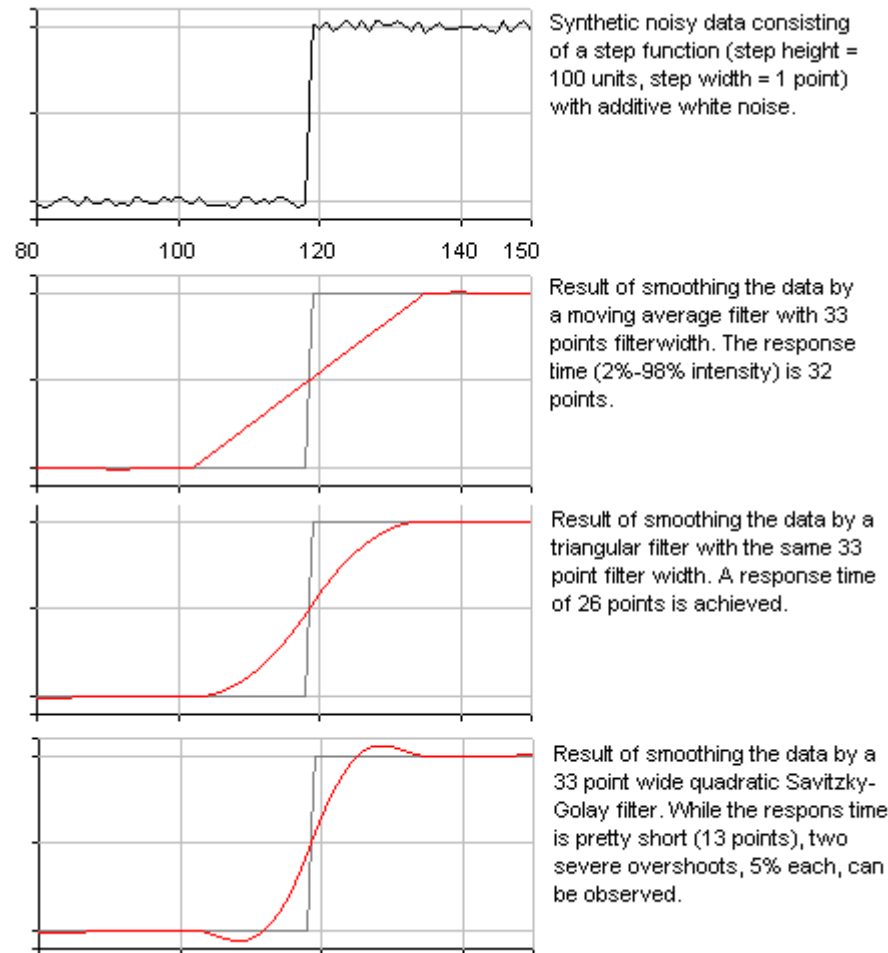
The **moving average** filter always reduces the height and increases the width of a peak, while preserving the area under the peak. The amount of the height reduction depends on the ratio between peak width and filter width. The example shows that the broadest peak is represented well, while the narrower peaks suffer considerable loss of height and increase of width. Peaks with a distance of about the filter width are not resolved. This filter is better suited for smoothing step signals.

The **triangular** filter preserves the heights and widths of the peaks better than the simple moving average but still worse than the Golay-Savitzky filter.

The **quadratic Golay-Savitzky** filter preserves the heights and widths of the peaks best. A trade-off is that the broadest peak is less smoothed. As a rough guideline, best results are obtained when the width of the filter is between 1 and 2 times the expected FWHM of the peaks.

Smoothing steps

The following graphic shows the influence of different smoothing filters on step signals, typical for kinetic time drives. (All filters have the same filter width of 33 points, the gray curves represent the signal without noise):



The **moving average** filter preserves the height of the signal before and after the step well. The response time (time between 2% and 98% of the step intensity) is about equivalent to the width of the filter.

The **triangular** filter preserves the height of the signal well. The response time is better as with the moving average filter. This makes this filter type the first choice for kinetic time drives.

The **quadratic Golay-Savitzky** filter gives the best response time. But the filter generates an artificial base and an artificial peak, both larger than 5% of the step size.

Security

Login

BLStudio offers two different login system: Within the BLStudio login system, users can be defined freely. For each user a password must be defined. Whenever an application is started the user must login again. This login system can be used, if several users have the same Windows user account.

Alternatively the login system can be based on the Windows login. In this case the BLStudio user is determined from the current Windows user. when a module is started, the login name of the current user is checked against the login names of the user accounts, defined within BL Studio. If a user account is found, the user obtains the relevant project group and user rights from this account. Otherwise the login is rejected. Using this login system, the user has to login only once, when starting Windows. Furthermore each user can have specific Windows rights for accessing data.

If the login system of BL Studio is disabled (no user accounts are installed), each user will have access to all functions of BL Studio. Nevertheless the user name from the operating system will be used for signature.

At certain times when using BL Studio, the user has to re-enter his password. This happens when signing off data, methods and reports, in order to store this data with his e-signature.

Electronic Signature

Each time data are produced or changed, or when data are “reviewed” or “approved”, the system stores an electronic signature together with the data. Each data set contains the electronic signature of the last modification and when applicable, the signature of the last “approval”. This allows an auditor to follow exactly who created, changed or approved the data.

In addition the electronic signature is stored in the audit trail with each event. This creates the entire history of a data set.

The electronic signature includes the following information:

Login Name	Login name of the user in the operating System
Full Name	Full user-name for documentation purposes
User GUID	Unique user id
Local Time	System-time including date and time
Universal Time	GMT
Purpose	Description of the purpose of the signature

Generally the full name is used as user-name in a signature (e.g. on reports). When there is no entry for “Full Name”, the system will use the login name.

Data Integrity

A critical part of BL Studio’s security system is data integrity. This is achieved via the following principles:

All sensitive information (i.e. information which can be altered by the user) is stored as binary (BLOB) format and checked using a 32-bit checksum function. If data has been altered by error during transfer or by unauthorised modification, then the checksum fails and this is reported when the data is next loaded.

During authorised modifications or during approval, both data and electronic signature of the user will be stored in the binary data-block. Then the checksum for the entire block will be re-calculated. This ensures that electronic signatures are protected against unauthorised modification.

All raw measurement data is stored in the result data sets. A result data set contains a copy of the method parameters, a copy of the sample information and all raw data including exact time and an electronic

signature of the user. With this information it will be possible at any time to reproduce any result from the raw data, the original method or sample information is not required.

Data Storage

In the base version BL Studio saves all methods, configurations and result data in a folder structure.

The following sub-folders are created automatically when BL Studio is installed:

System

\Config	Configuration files for users and applications, plate and tray definitions
\Documentation	The installer/user can copy all documentation into this directory
\Instrument	Instrument information, e.g. validation date, accessories etc
\Projects	Project configuration files (not used in basic version)
\Resoure	Resource files
\Rights	Right-group configuration files (not used in basic version)
\Setup	Module configuration, Licences, add-on modules
\Temp	Temporary files, e.g. report pictures
\User	User definition files

Data

\Exchange	Used to import/export data
\Methods	Default directory for methods
\Protocol	Contains the audit trail
\Results	Default directory for results
\Validation	Contains validation raw data and the validation overview

Please ensure that all BL Studio users have read/write access to all directories