HORIBAJOBIN YVON

LabSpec5 User's Manual

HORIBA JOBIN YVON

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1 - LabSpec5 general overview

LabSpec 5 is a general data acquisition and data analysis software, based on open NexGen module architecture. LabSpec 5 controls all the HORIBA Jobin-Yvon Raman instruments, enables different data acquisition modes(eg. single spectrum, multidimensional data set, video image etc.)

The data analysis routines include many commonly used Raman and FTIR tools, such as baseline correction, linear and non-linear filters, peaks fitting Kramers-Kronig transform etc. The mapping technique enables to generate and visualize map by using different spectral features : band intensity, peak position and so on.

The module architecture allows to customize software to support specific operation, for example read foreign data file format, implement data acquisition trigger etc.

The Visual Basic script language of Microsoft is supported, that yield possibility to create macro commands or include specific data analysis function. The LabSpec 5 can be used also as Active X control in third part application.

2 - LabSpec5 installation

3 - LabSpec5 main window

The main menu bar

The main icons bar

Graphics tools associated to the active object.

Window of the active objects

The control panel

The status bar

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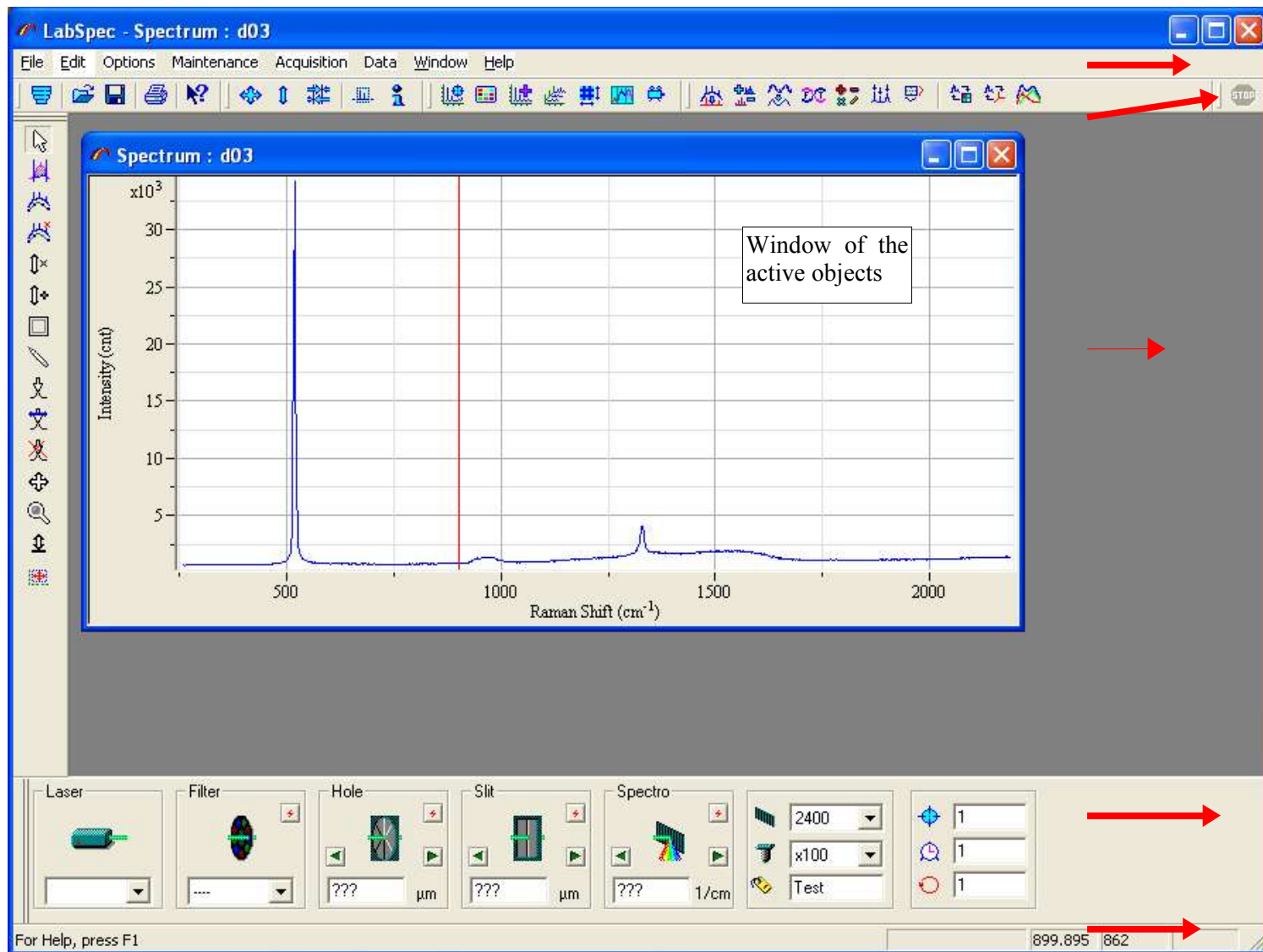
4 - The main menu bar

The main menu bar is located on top of the **LabSpec5** main window.
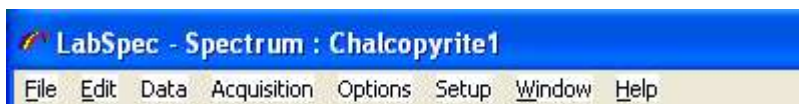
4.1 - File menu
The **File** commands menu permits to manage the data files and the data printout.

To access the **File** menu click on the File button of the main menu bar or type Alt+f or Alt+F keys.

Data file management functions

Data printout management functions

Last loaded files
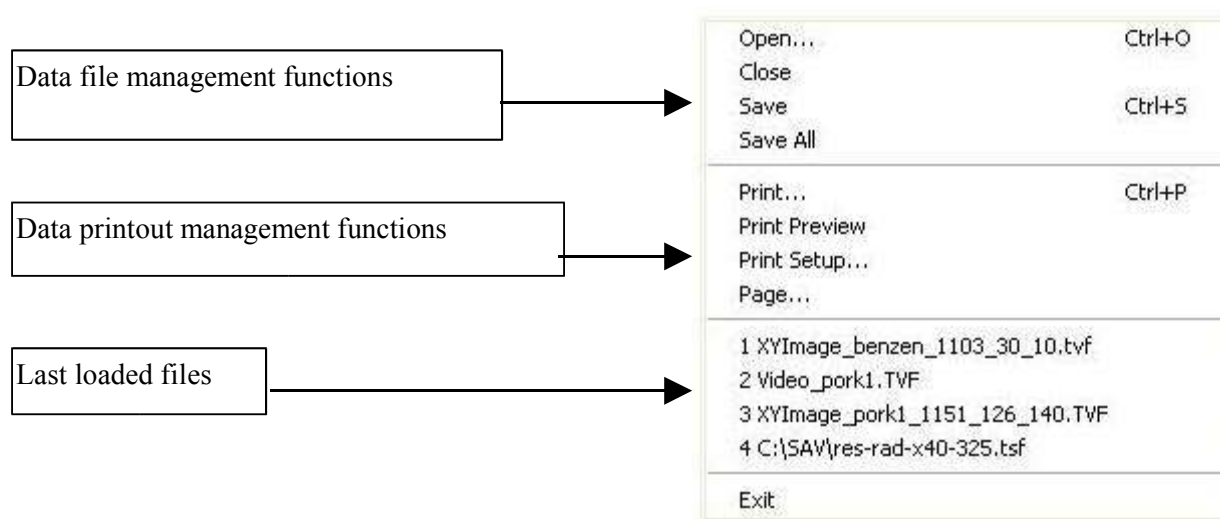
> **Data file management functions**

Open....................................To open a previously saved object for display.
Close....................................To close and to remove the current object
Save .... To save the current object in a file for later retrieval
Save All.............................. To save all the objects of the current window.

> **Data printout management functions**

Print…................................. Output to the default printer.
Print Preview..................... To preview the page before printing.
Print Setup….......................To setup the printer parameters
Page….................................To define the layout of the page.

Exit...................................... To close and quit the **LabSpec5** application.

4.1.1 - Open... function

The ***Open…*** command permits to select a previously saved file to load it.
To access this command select ***Open…*** from the File commands menu in the Main menu bar or use the keyboard shortcut Ctrl + O or click directly on the following open icon ⬛ in the main icons bar.

Select here the folder in which the file has been saved.

Select in the list of files the one you wish to load.

Click on the Open button to open the selected file.

Click on the Cancel button to abort the operation and to close the window.

Select here the type of the researched file.
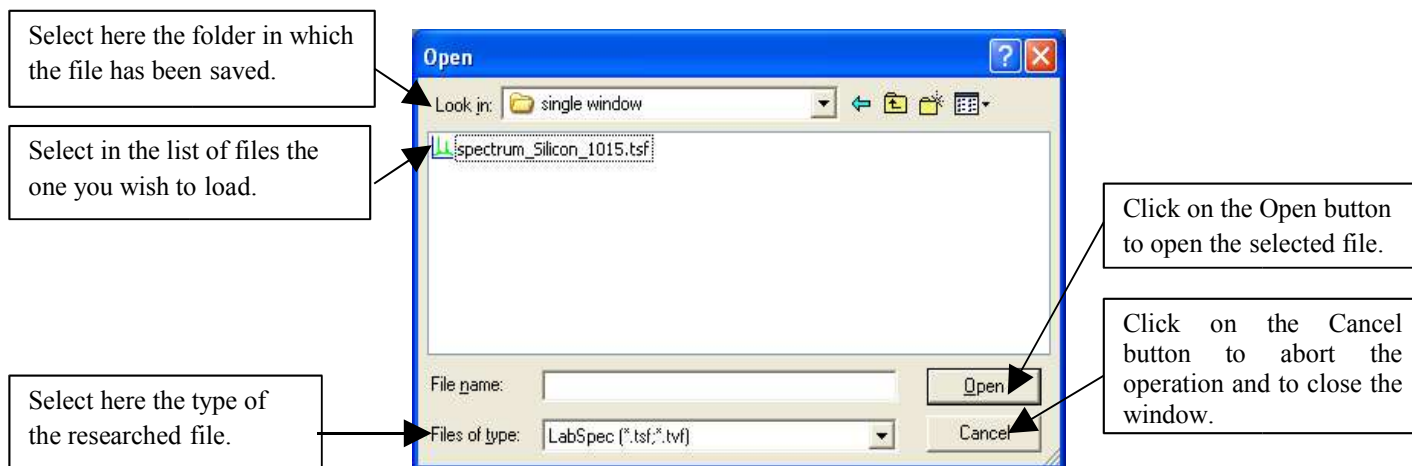
4.1.2 - Close function

The ***Close*** command removes the current object of the active window without saving the changes.

To access this command select ***Close*** from the File commands menu in the Main menu bar.

4.1.3 - Save function

The ***Save*** command permits to record the active object in a file for future retrieving.

To access this command select ***Save*** from the **File** commands menu in the Main menu bar or use the keyboard shortcut Ctrl + S or click directly on the following save icon ⬛ in the main icons bar.

Select here the folder in which you want the file to be recorded.

List of the files already existing in the chosen folder.

Click on the Save button to save the selected object.file.

Enter here the name you wish to assign to the file.

Click on the Cancel button to abort the operation and to close the window.

Select here the file format.

4.1.4 - Save All function

The **Save All** command permits to record all the objects of the active window in a file for future retrieving.

To access this command select **Save All** from the **File** commands menu in the Main menu bar.

Select here the folder in which you want the file to be recorded.

List of the files already existing in the chosen folder.

Enter here the name you wish to assign to the file.

Select here the file format.

Click on the Save button to save the selected object.file.

Click on the Cancel button to abort the operation and to close the window.

4.1.5 - Print function

The **Print…** command prints out to the default printer the objects of the active window. The layout page is the one defined with the **Page…** command.

To access this command select **Print…** from the **File** commands menu in the Main menu bar or use the keyboard shortcut Ctrl + P or click directly on the following print icon in the main icons bar.
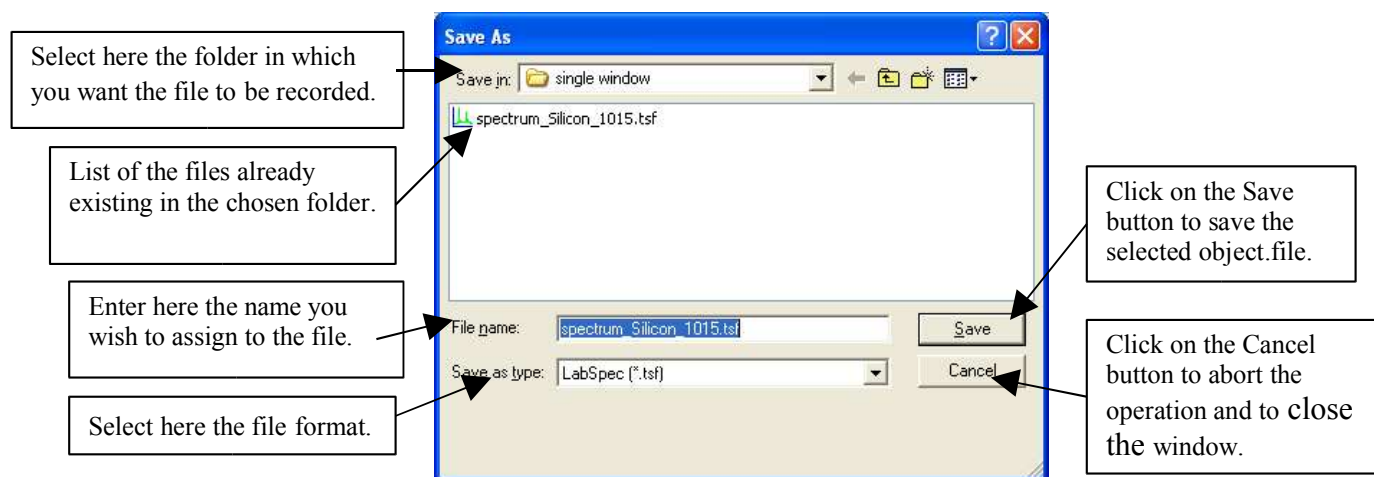
Print icon

File menu

Print…

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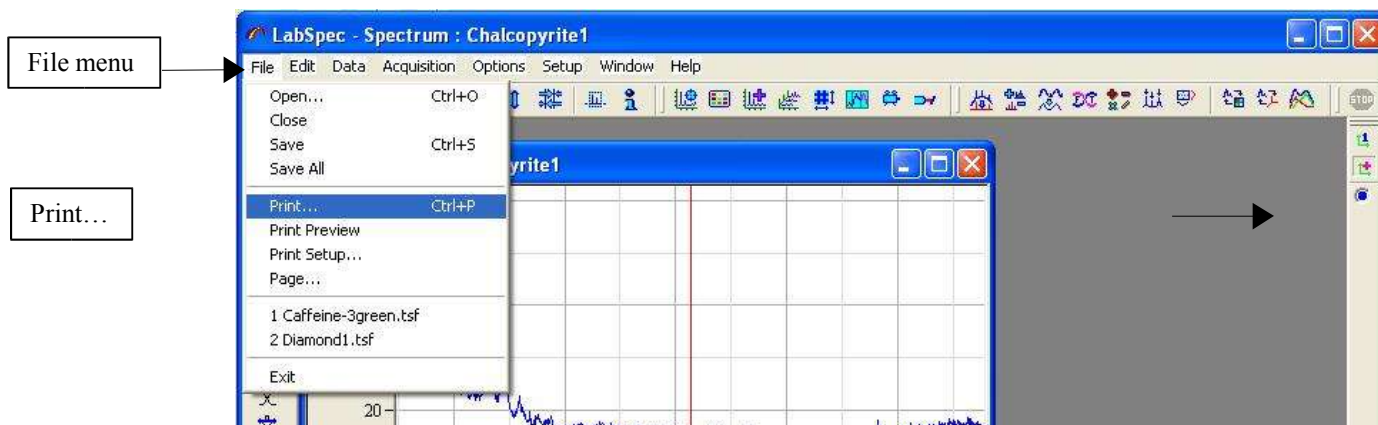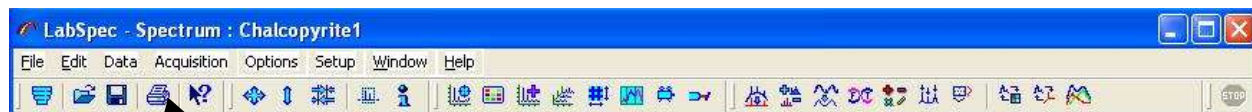
4.1.6 - Print Preview function

The *Print Preview* command allows to display the to-print page before printing.
To access this command select *Print preview* from the **File** commands menu in the Main menu bar.

➢ **The Print Preview window**

The to-print page is displayed in the *print preview* window as it will appeared at print out so you can check the page layout before starting the printing operation.

To modify the page layout , use the *Page…* function of the **File** menu.
On top of the print preview window some specific buttons commands are available.

Print Preview specific commands

The to-print page
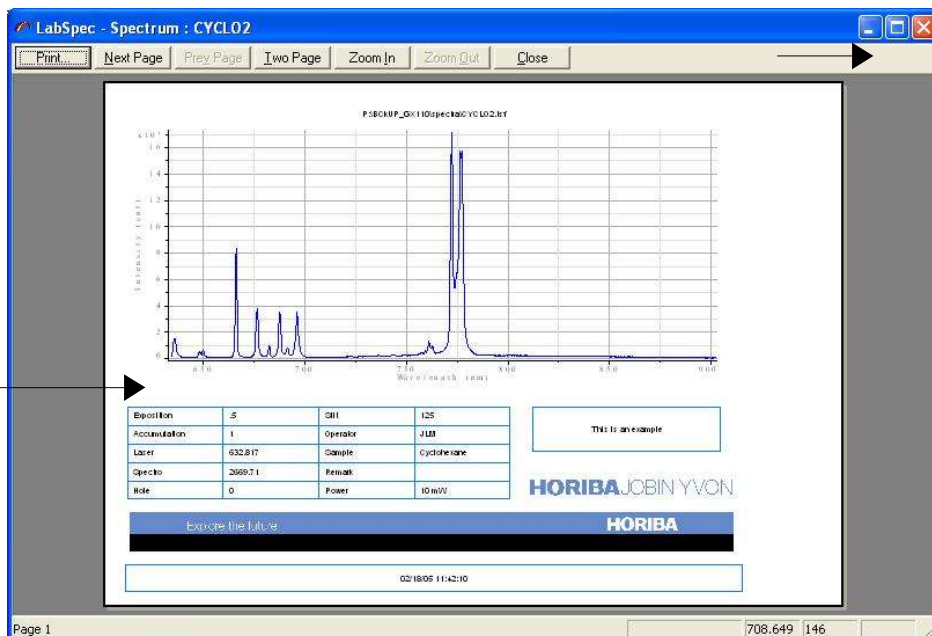
The Print Preview commands

Print... Click on this button or press P-key or p-key to start the print out.

Next Page Click on this button or press N-key or n-key to display the second page in case of a to-print document on 2 pages. For the moment the layout of a to-print document is only on one page.

Prev Page Not available. (Future expansion)

Two Page Click on this button or press T-key or t-key to display the 2 pages of the document. Useful for to-print document on 2 pages (future expansion)

Zoom In Click on this button or press I-key or i-key to zoom the previewed page.

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![Zoom Out] Click on this button or press O-key or o-key to zoom-back the previewed page. This button is available only if the Zoom function has been activated .

![Close] Click on this button or press C-key or c-key to quit the *Print preview* function and to return to the **LabSpec5** application.

4.1.7 - Print Setup function

The *Print Setup…* command permits to select the printer and to define its properties.

To access this command select *Print Setup…* from the **File** commands menu in the Main menu bar.

➢ **The Print Setup window**

Select here the printer to use.

Click on this button to check or set the parameters specific to the model of the printer used. Report to the manual of your printer for detailed information.

Select here the format of the sheet of paper to use and its location in the printer.

The orientation parameter is linked to the one set with the Page… function.

Click on this button to choose a printer on your network.

Click on the OK button to validate the settings and to close the window.

Click on the Cancel button to abort the changes and to close the window.

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4.1.8 - Page function

The *Page*... command permits to define the layout of the to-print document.

To access this command select *Page*... from the File commands menu in the Main menu bar.

> **The Page window**

Page tools bar

Components of the to-print page

Each icon allows to define the size and the position of each different predefined component type of the to-print page

Header page
Associated toole:

Data object
Associated tool:

Text object
Associated tool:

graphic object
Associated tool:

Image object
Associated tool:

Information parameters
Associated tool:

Bottom of page
Associated tool:

> **The page buttons**

Load — To load an already recorded template.

Save — To save the current template into a file.

OK — To validate the settings and to close the Page window.

Cancel — To close the Page window without validating the current Page settings.

➢ **Using the Page tools icons**

To insert a component in the to-print page click on the corresponding tool. Then move the mouse on the page so a cross appears. Then move the cross at the wished location, press on the left mouse button and move the mouse to define the size of the corresponding component.

➢ **How to select a component of the to-print page**

Move the mouse on the chosen component and click on the left mouse button. Then a dotted rectangle is displayed around the selected component.
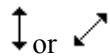
➢ **Moving a component of the to-print page**

Select the component. Then when the following mouse cursor ⬍ appears, click on left mouse button and drag the mouse.

➢ **Re-sizing a component of the to-print page**

First, click on the object to select it. Selection handles appear around the selected object.
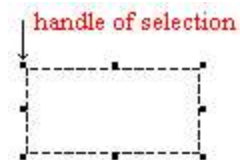
Move the mouse pointer on one of the selection handles until to have the size pointer: ↕ or ↗ .Keep the mouse button pressed and move the selection handle and modify the size of the object.

➢ **Modifying or creating the contents of a to-print page component**

Except the data object, the contents of all the other objects could be modified by double-clicking on the wished component.

Then a dedicated window appears with the tools to modify the corresponding component:

- The **options** window for the header page, the bottom of page and the Text object.

-The **parameters** window for the array of experiment information parameters.

-The **Open** window for the Image object.

➢ **Modifying the general page presentation or display**

Click anywhere on the to-print page on the right button of the mouse to display the following menu
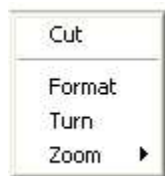
 Cut   To remove the selected component

Format To define the parameters of the sheet of paper. (See Page Setup)

Turn   To define the page orientation Portrait or Landscape

Zoom   To define the display of the to-print page inside the **Page** window.

➢ **The Parameters function**

On the printed document the selected parameters are laid out in an array. The **Parameters** function permits to select the data parameters you wish to be printed and to define the style of the array.

To access this command double click with the left mouse button on the *information parameters* object when defining the layout of the to-print document with the **Page…** command

➢ **The Parameters window**

List of the non printed data parameters.

NSParameters tools to manage the list of the data parameters to print.

Print list: List of the data parameters selected to be printed.

Click on the Style button to open the **NSOptions** window to define the design of the array.

Enter in the **Title** field the printed name of the parameter selected in the print list

Click on the OK button to validate the settings and to close the window.

Enter here the number of columns of the printed data parameters array.

Click on the Cancel button to abort the changes and to close the window.

➢ **Example of a printed data parameters array**

You will find below the data parameters array corresponding to the settings of the **parameters** screen copy as it appears on the printed document.

Operator	nf	Laser	784.87	Exposure	40
Sample	acetylsalicylic acid	Power	11.2mw @ sample	Grating	950
Date	6-05-2003 18:55	Detector	CCD4	Remark	
Spectro	312.20	Accumulation	2		

Exposure is the printed label for the exposition

Column 1   Column 2   Column 3

Remark:
A column contains 2 fields: the data parameter label and the data parameter value.

➢ **The Parameters tools**

Add the selected data parameter to the print list.
Remove the selected data parameter from the print list.

⬆ In the print list move the selected parameter to the previous line.

⬇ In the print list move the selected parameter to the next line.

4.1.9 - Exit

The *Exit* command permits to close all the opened objects and quit the application.
To access this command select **Exit** from the File commands menu in the Main menu bar or click on the

Close icon ❌ in the upper right corner of the **LabSpec5** main window.
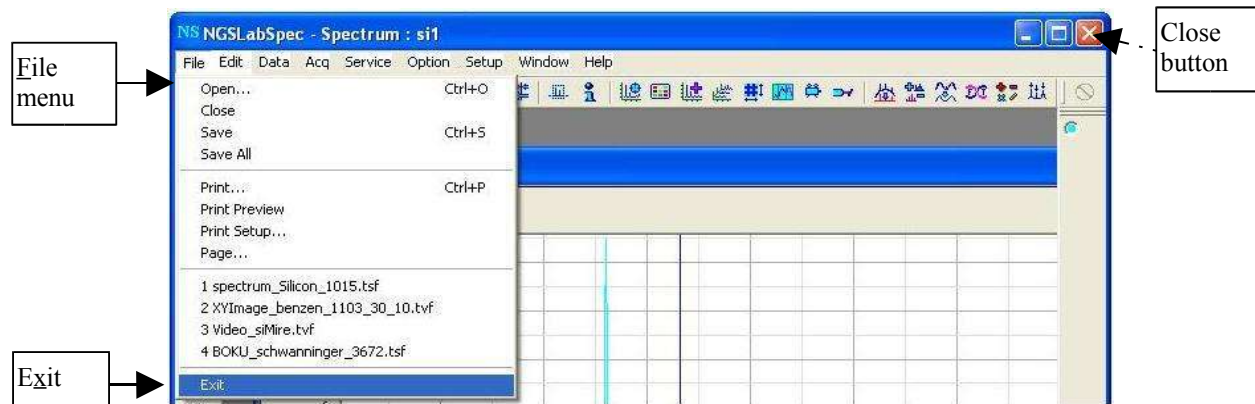
4.2 - Edit menu

The **Edit** commands menu enables to exchange data between different applications and facilitates the data analysis process.

To access the **Edit** menu click on the Edit button of the main menu bar.
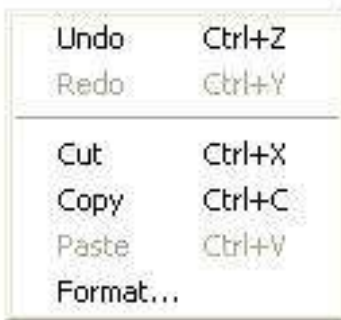
Undo *(CTRL+Z)*....... To undo the last operation.

Redo *(CTRL+Y)*....... To redo the last operation.

Cut *(CTRL+X)*.......To cut the active data object in clipboard.

Copy *(CTRL+X)*....... To copy the active data in clipboard. You can select the data format with the **Format…** command.

Paste *(CTRL+V)*....... To insert the clipboard contents. You can select the clipboard format with the **Format…** command.

Format….................. To select the **Copy** and **Paste** clipboard data formats.

4.2.1 - Format function

This command permits to define the format of the data you export to the clipboard or and the one of the data you import from the clipboard.
To access this command select Format… from the Edit commands menu in the Main menu bar.

➢ **The Copy/Paste data formats selection**

In the Copy format column select the format of the data exported to the clipboard.

In the Paste format column select the format of the data imported from the clipboard.

Copy/Paste Properties

Copy format
- ○ Data
- ○ Text
- ● Picture

Paste format
- ● Data
- ○ Text

OK
Help
Cancel

Click on the OK button to validate the settings and close the window

Click on the Cancel button to abort the changes and close the window.

- **Data**Native NextGen format. Can be used to create the exact copy of the data object.

- **Text**Create the text spreadsheet of the active data object.

- **Picture**Create the screen copy picture of the active window.

4.3 - Data menu

The **Data** menu commands permit to activate a data object and to see the list of object of the active window. This list is shown as a set of color radio buttons on the right pan of the screen.

To access the **Data** menu click on the Data button of the main menu bar.
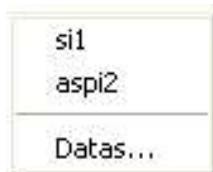
You can activate one of the data object of the active window by clicking directly in the list of the **Data** menu **.**

Datas… Select this command to show the full objects list of the active window.
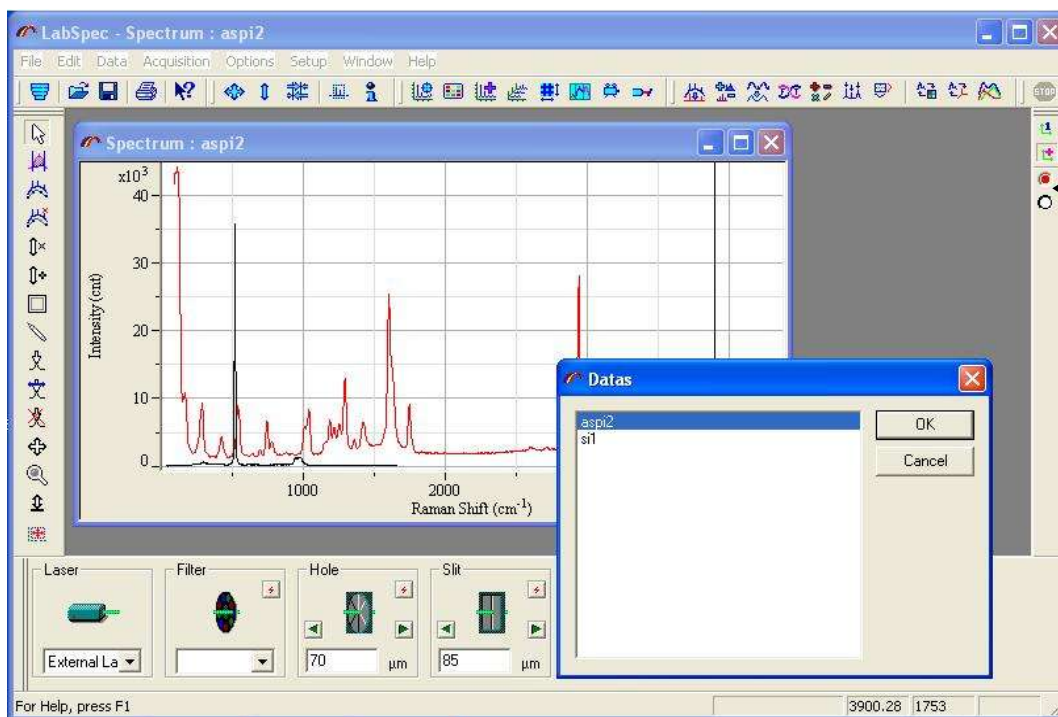
On the following screen copy the active window contains 2 objects. (2 spectra) .
You can activate one object also by clicking on the colored radio button.

4.4 - Acquisition menu

The **Acquisition** menu commands permit to setup the data acquisition parameters.

To access the **Acquisition** menu click on the *Acquisition* button of the main menu bar.
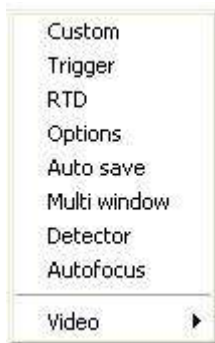
Custom .... To customize the data properties.

Trigger...................... To set the properties of the manual trigger

RTD........................... To set the properties of the **R**eal **T**ime **D**isplay acquisition mode.

Options...................... To set the parameters of the data acquisition, such as exposure time, binning, acquisition mode and so on….

Auto save................... To set the 'Save' parameters to save automatically the data at end of acquisition.

Multi window............ To set the parameters to define the acquisition spectral regions.

Detector.................... To set the detector properties such as readout zone, gain etc.

Autofocus.................. To set the autofocus properties.

Video......................... To set the video acquisition properties.

4.4.1 - Custom function

The *Custom* function allows to modify the data properties table during the data acquisition.

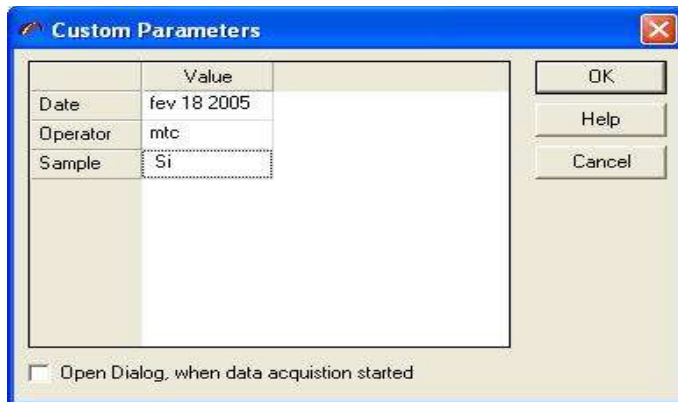To access this command select *Custom* in the **Acquisition** menu.

To insert or remove properties click on the right mouse button and select **Insert Row** or **Remove Row** menu item.
Check **Open** Dialog box to display this dialog automatically when the data acquisition process starts.

4.4.2 - Trigger function

The *Trigger* function allows you to set and customize the properties of the manual trigger. These parameters are common for any acquisition procedure, except in RTD mode.

To access this function select *Trigger* item in the **Acq** menu.

In the Start or in the Sample field you have the possibility to customize the message which will appear.
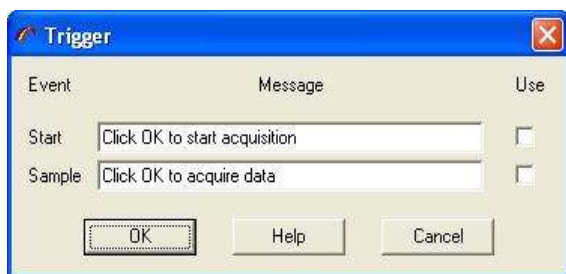
You can select at which level of the acquisition procedure you need to trig manually the data readout.

This could be just before each data readout or for exemple in case of mapping when positionning at a new sample point.

Start ....Select the corresponding **Use** box to see the associated message each time the acquisition starts. You can customize the message text.

Sample ....Select the **Use** box to see the associated message each time when a new sample point is selected for measurement. You can customize the message text.

4.4.3 - Real Time Display function

The *Real Time Display Properties* Dialog window allows to modify the data acquisition properties for the Real time CCD-image readout (⊞ Detector image RTD function) or the spectra readout in adjustment mode (.📈 RTD function Spectrum)

To access this function select *RTD* item in the **Acquisition** menu.
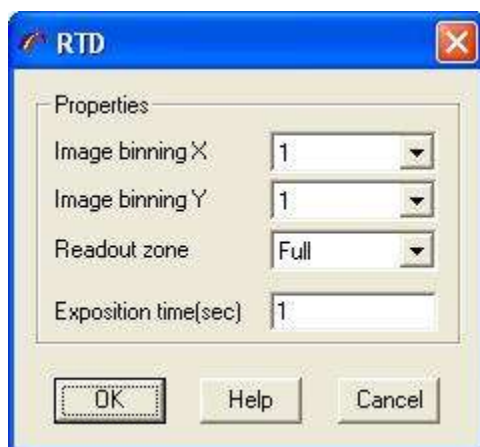
Image binning X ......Set the binning factor in the X direction for the CCD-image readout . This allows to increase the acquisition speed and the signal intensity level.

Image binning Y ......Set the binning factor in the Y direction for the CCD-image readout. This allows to increase the acquisition speed and the signal intensity level.

Image zone................Define here the chip area you wish to load for the RTD CCD-image. You can choice to read the full chip matrix (select Full) or only the chip area corresponding to the spectrum readout area (select Spectrum).

Exposition time......... Set here the exposure time value in seconds.. This value appears also in the bottom control panel.
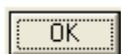
OK ....Click on the OK button to validate the settings and to close the window
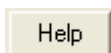
Help ....Click on the Help button to retrieve the informations concerning the parameters of this window.
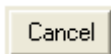
Cancel ....Click on the Cancel button to close the window without validating the changes.setting

4.4.4 - Options function

The *Acquisition Options* window allows to define the data acquisition common properties.

To access to this window select the **Options** item in the **Acquisition** menu.
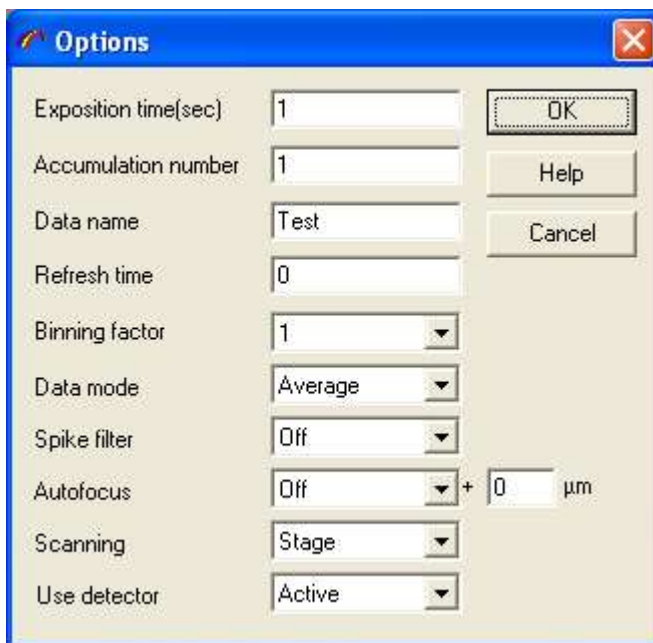
Exposition time...................Set here the exposure time value in seconds. This value appears also in the bottom control panel.

Accumulation number ......Set here the number of times you wish to repeat the detector exposure.This is useful in case of signal overflow. This value appears also in the bottom control panel.

Data name...........................Set here the data label and the default file name

Refresh time........................This parameter is usefull in case of fast acquisition process or big data sizes. The data display is not refreshed on the screen until this time is elapsed.

Binning factor.....................Define the number of data points per spectrum.The signal intensity is proportional to this value, but the number of data point (and spectral resolution) will be reduced in the same way.

Data mode...........................This parameter is used in case of data accumulation (Accumulation number >1.)
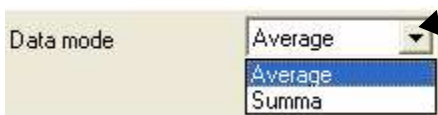
Click on the down arrow icon to display the Data mode list

Then select how should be defined the final spectrum

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* **Average**...Final spectrum = (Spectrum1+Spectrum2+....+Spectrumn) / n

* **Summa** ...Final spectrum = (Spectrum1+Spectrum2+....+Spectrumn)
where n is the value of the accumulation number

Spike filter...........................Allows to remove or not the spike cosmic noise of the CCD detector.

Spike filter   Off
Off
Double expo
Single pass

Click on the down arrow icon to display the Spike filter option list

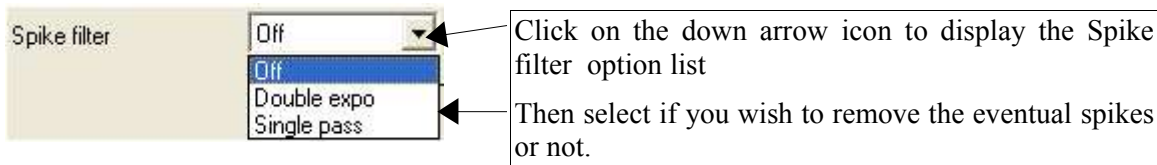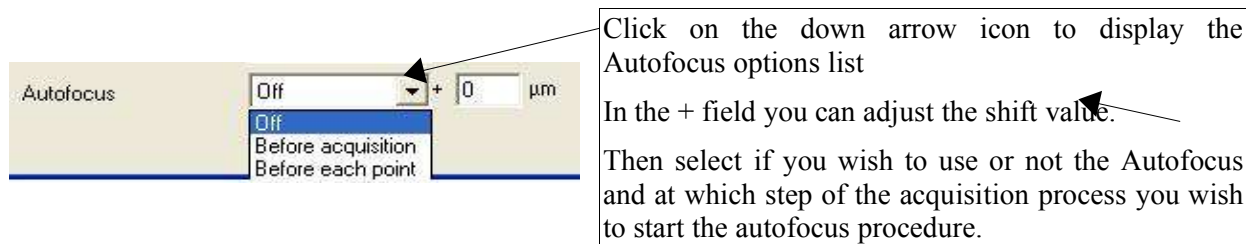Then select if you wish to remove the eventual spikes or not.

* **Off**........... No spike removal
* **Double expo**........... The cosmic spikes are removed by comparison of the signal values of the different accumulation. So the accumulation number will be increased on the one time in this case.
* **Single pass**...............This method allows to remove spike in a single accumulation acquisition by analysing bans for sharpness and intensity. This algorithm has to used with care . Very sharp Raman bands could be modified. Nevertheless this method works fine and save time when looking broad bands as it is the case for Raman analysis of amorphous materials or photoluminescence applications....

Autofocus............................ Allows to adapt or not automatically the Z position to obtain a maximal signal level. The process is based on the detection of the laser beam reflection.
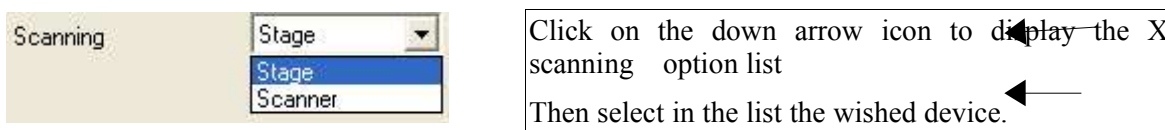
Autofocus   Off   + 0   µm
Off
Before acquisition
Before each point

Click on the down arrow icon to display the Autofocus options list

In the + field you can adjust the shift value.

Then select if you wish to use or not the Autofocus and at which step of the acquisition process you wish to start the autofocus procedure.

* **Off**........... The autofocus procedure is not used in the data acquisition process.
* **Before acquisition.** The autofocus procedure is applied before each data readout
* **Before each point..** The autofocus procedure is applied at each new measurement point positionning
* **Shift value**.............. The shift value allows to adjust the difference between the position where the laser reflection is at maximum level and the one where the spectroscopic signal is at maximum level .

Scanning..............................Allows you to define which scanning device has to be used to   record a spectral image the XY stage or the Scanner.

Scanning   Stage
Stage
Scanner

Click on the down arrow icon to display the X scanning   option list

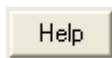Then select in the list the wished device.

Use detector .... On systems with 2 detectors this option allows you to acquire data either from only the current active detector or from the 2 installed detectors.

Use detector	Active ▼
	Active
	Both

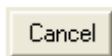Click on the down arrow icon to display the Use detector list.

Then select the wished option.
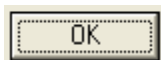
OK .... Click on the OK button to validate the settings and to close the window

Help .... Click on the Help button to retrieve the informations concerning the parameters of this window.

Cancel .... Click on the Cancel button to close the window without validating the changes.setting

4.4.5 - Autosave function

The *Auto Save* window allows to modify the properties of the acquisition auto save option.
To access this window select *Auto Save* item in the **Acquisition** menu.

Save acquired data............. Select this box to save automatically the data when the acquisition process is finished.

Format................................ Select here the file format. The list of the different format supported is the same one as for **Open/Save** functions.

Folder .... Edit here the path where to save the files. Click on the [...] button to select the folder in the tree structure.

Year................................... Select this box to add the year number to the folder name.

Month................................. Select this box to add the month number to the folder name.

Day.................................... Select this box to add the day number to the folder name.

File.................................... Edit here the file prefix name.

Hour .... Select this box to add the hour to the file name.

Min .... Select this box to add the minute to the file name.

Count .... Select this box to add the counter value to the file name. The counter is modified each time the auto save function is called. But you can edit the start value of the counter sequence.

4.4.6 - Multi window function

The **_Multi Window_** function allows to set the properties of the acquisition in multi window mode. This mode enables to record data automatically over an extended range with a defined integration time and averaging. The extended range is covered by taking a number of individual single shot windows and 'gluing' these together..

To acces this Dialog select **_Multi Window_** item in the **Acquisition** menu.
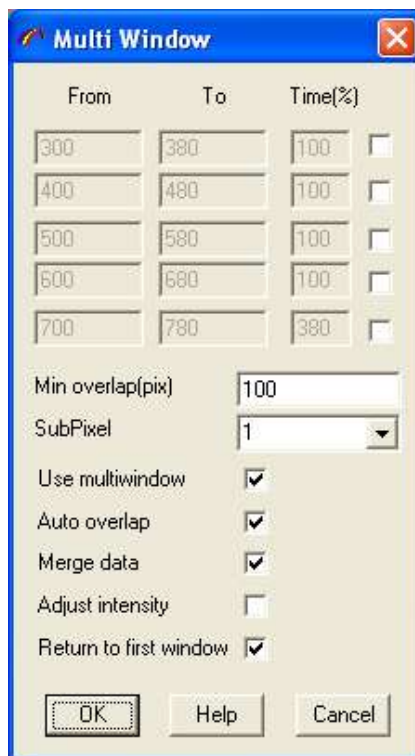
From.......... Edit here the value of the first limit of the spectral window in the current spectral unit. Select the following ☐ to activate the associated spectral window.

To............... Edit here the value of the end limit of the spectral window in the current spectral unit. Select the following ☐ to activate the associated spectral window.

Time........... Edit the relative exposure time(in %) of this window. This value is used to compensate the differences of signal level.

Min overlap (pix)..... Define here the overlap between the individual windows in pixels. A value of 50 gives generally good results.

SubPixel..... Selecting a value >1 allows to restore the fine shape features. The method is based on the shifting of the spectrograph position on a distance less than the detector pixel size.

Use multi window.....Select this box to activate the multi window acquisition mode

Auto overlap............. Select this box to automatically define the overlapping size.

Merge data................ Select this box to create one data object for each active spectral window. In the other case a data object is generated for each spectral range corresponding to the spectrograph position.
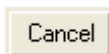
Adjust intensity........ Select this box to adapt the intensity to the same values on the overlapping parts. This adaptation is based on the linear shift of the data.
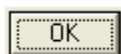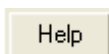
| OK |...................Click on the OK button to validate the settings and to close the window

| Help |...................Click on the Help button to retrieve the informations concerning the parameters of this window.

| Cancel |...................Click on the Cancel button to close the window without validating the changes.setting

4.4.7 - Detector function

The *Detector function* allows to set the detector parameters. These parameters are common for any acquisition process.
To access to this window select *Detector* item in the **Acquisition** menu.

In this part select the active detector and the readout mode (Spectrum or CCD image)

In the *Sizes* part enter the readout limits of the detector chip for the *mode* selected in the *Type* part.

Set here the parameters options attached to the detector.
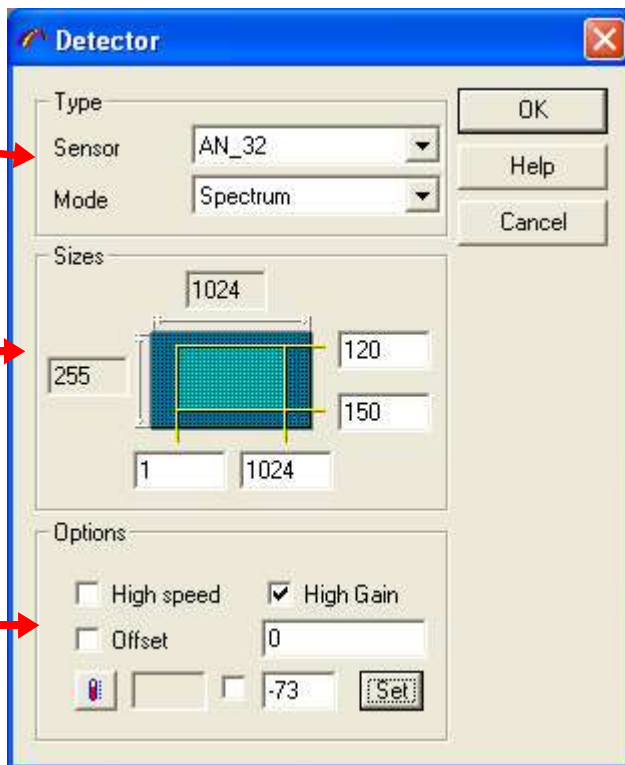
➢ **Type**

Sensor........................Select the active detector.

Mode..........................Select the readout mode. Single spectrum readout or CCD image mode.

➢ **Sizes**

Sizes...........................Edit the readout limits of the detector chip. To check the readout zone run the detector image Real Time Display, by clicking on the ⊞ icon.

➢ **Options**

This section groups together parameters specific to the detector model. So this section appears differently following the model of the installed detector. The most commonly used parameters will be described hereafter. It is possible that some parameters does not appear if the correponding option is not available on the on your current detector.

High speed................. Check this box to enable high speed data transfer.

High gain...................Check this box to enable high gain level of the detector amplifier.

Offset ....Check this box to subtract the dark current offset from the intensity values. Edit the offset value to subtract in the associated field.

Temperature

Click on the ![button] button to capture the current detector temperature.
The current temperature read is displayed in this field.

To set the temperature edit the value to reach in this field and then click on the Set button.
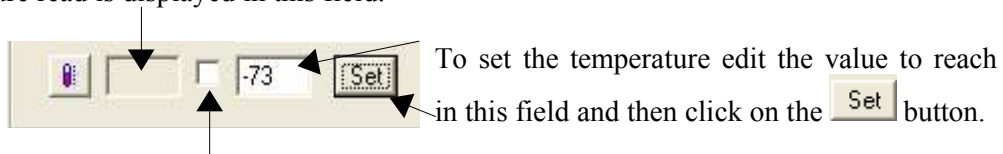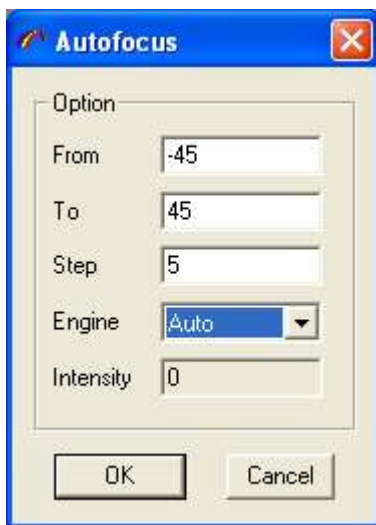
Check this box to have a continuous refresh of the temperature value.

4.4.8 - Autofocus function

The **Autofocus** ensures an optimal focus is reached before an acquisition.

This function allows you to define the properties of the *Autofocus* function.To acces to this window select **Autofocus** item in the **Acquisition** menu.

From.......... Set the start position (in μm) for the autofocus movement.

To............... Set the stop position (in μm) for the autofocus movement.

Step .... Set the step size (in μm) for the autofocus movement.

Engine........ Allows you to select the device used for the autofocusing

- ◆ **Auto**: The software select automatically between the Z-motor and the piezo following the size of the movement defined by the From and To parameters.
- ◆ **Z-motor**: Force the software to use the Z-motor for autofocussing
- ◆ **Piezo**: Force the software to use the piezo for autofocussing.

- ◆ **Z-motor & piezo**. The software uses the both devices for autofocusing. A first approach is done with the Z-motor. The research of the final position is then refined by using the piezo.

Intensity.....Display the autofocus diode intensity.
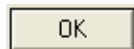
[OK]..Validate the settings and close the Autofocus window.
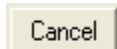
[Cancel]..... Close the Autofocus window without validating the setting.

4.4.9 - Video functions

➢ **Laser Position**

The **Laser Position** window allows you to modify the position of the laser beam on the video image. These parameters are used when the XY scanning is used during the acquisition process. To access this window run the video preview and then select **Laser** item in the **Acquisition/Video** menu. Then you can click and drug the laser position indicator with the mouse and the current position is refreshed in the CenterX and Center Y field . It is also possible to enter the position directly in the CenterX / Center Y through the keyboard.

Click the OK button to validate the settings and Close the Laser Position window.

Click on the Cancel button to close the Laser position window without validating the settings.

➢ **Image Scale**

The **Image scale** window allows you to adjust the scale of the video image. These parameters are used when using an XY scanning device (Stage or Scanner) during the acquisition process. To access this window run the video preview and then select **Scale** item in the **Acquisition/Video** menu.
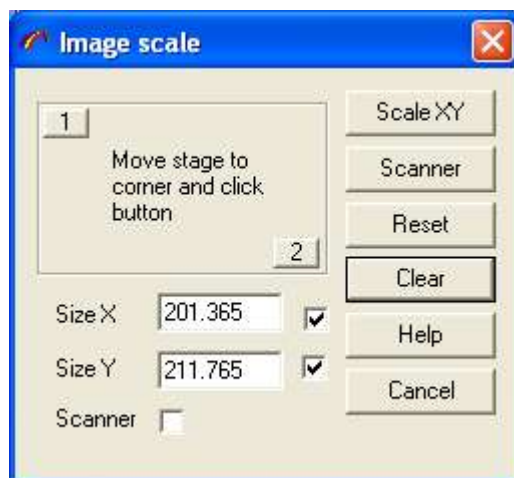
Corner points Move the XY stage to left-up rectangle corner and click on the point #1. Then move stage to right-bottom corner and click on the point #2. Program will read the stage position and use this values as rectangle sizes.

SizeX   X size of the rectangle.

SizeY   Y size of the rectangle

Stage   Click on the button to modify video scale, used by XY stage. This operation should be done for each microscope objective.
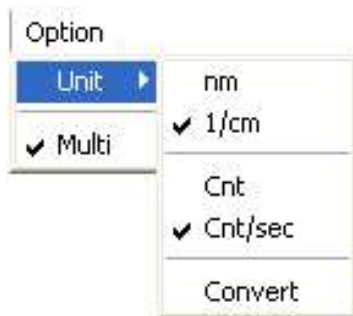
Scanner   Click on the button to modify scanner scale.

Clear   Clears **SizeX** and **SizeY** fields for stage joystick operation.

4.5 - Option menu

The **Option** menu commands allows to select the default working unit and to convert the active data object to the selected units when necessary.

To access the **Option** menu click on the **Option** button of the main menu bar.

Unit........ Select this command to modify the default spectral and intensity units.

    Nm............. To give the frequencies in nanometer (Wavelength spectral unit)
    1/cm........... To give the frequencies in cm-1 (Raman shift (relative wavenumber) spectral unit)
    Cnt............. To give the intensity in Counts.
    Cnt/sec...... To give the intensity in Counts per second.
    Convert..... To give the active data object in the selected units.

Multi...... Select this option to apply any data treatment operation to all the data of the active window.
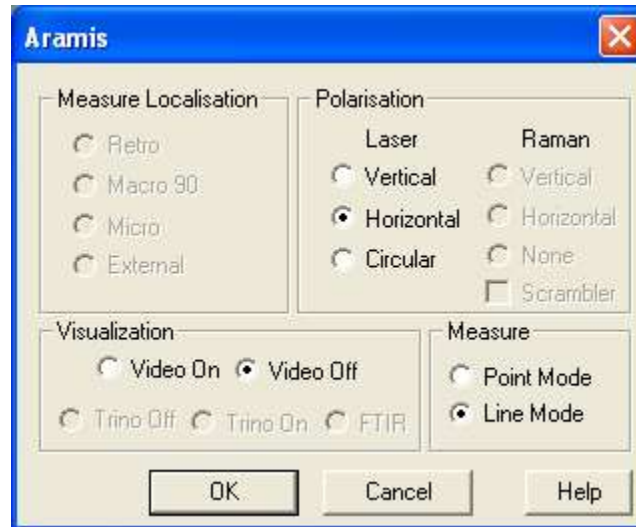
4.6 - Setup menu

4.6.1 - Instrument

This function allows you to setup the instrument following the needs of the measurement and the configuration of the instrument.

Actually this function is available only for the Aramis system.

To access this function select *Instrument* item in the **Setup** menu.

The *Aramis* window is organized by functions: Measure localisation, Polarization, Visualization, Measure. The software checks the presence of the different motors and their position. So if a motor is not present the corresponding commutation appears in gray and could not be selected.

➢ **Measure Localization**

Retro .... Select this oprion to set the appropriate mirror to capture the Retro-Raman signal

Macro 90....Select this option to set the appropiate mirror to capture the raman signal from the macro plate.

Micro..........Select this option to set the appropiate mirror to capture the raman signal from the microscope.

External..... Select this option to set the appropiate mirror to capture the raman signal from the fiber input.

➢ **Polarization**

* Laser
Vertical...... Setup the λ/2 slide to obtain a vertical polarization of the laser.
Horizontal. Set in place the optical to retrieve the natural polarization of the laser.
Circular..... Set in place the λ/4 slide to obtain a circular polarization of the laser.

* Raman

Vertical...... Set in place the analyser on the raman path to polarize it vertically.
Horizontal. Set in place the analyser on the raman path to polarize it horizontally.
None........... Remove the analyser to have no polarization of the raman signal.

Scrambler option.
This option is available only if Retro or Macro90 or Micro option is selected.
Select the scrambler option to cancel any polarization effect on the raman signal.

➢ **Visualization**

Video on ....Set in place the camera beamsplitter.
Video off ... Remove the camera beamsplitter

Trino off.... Set in place the trino for the selected option.
Trino on
Trino FTIR

➢ **Measure**

Point mode Set in place the pinhole and the lenses assembly following the selected measure mode.
Line mode

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4.7 - Window menu

The **Window** menu commands permit to arrange automatically the data windows inside the main **LabSpec5** window.

To access the **Window** menu click on the **Window** button of the main menu bar.

Functions of the **Window** menu

List of the different opened windows.
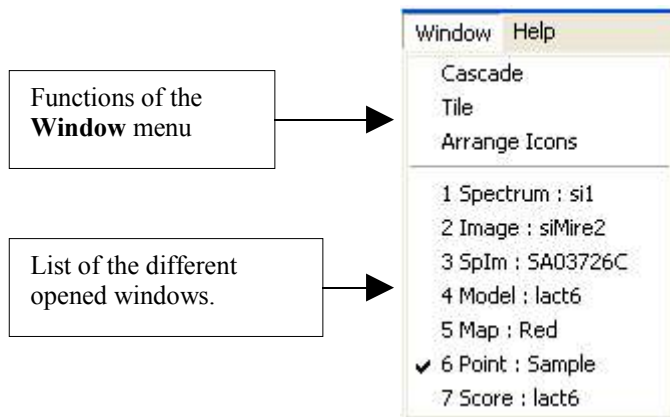
Cascade..........................Cascade the windows so they overlap.
Tile................................. Tile the windows.
Arrange Icons.............. Arrange the icons at the bottom of a main window.

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5 - The control panel

The Control Panel located on the bottom of the screen contains divisions which are directly related to the System configuration. This panel will show <u>only</u> the devices which are installed on the System. The description below details all of the available sub-units.

5.1 - Laser
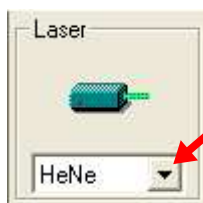
Click here to open the list of the installed laser.

Then select in the list the working laser.

If your instrument is full automated (Aramis instrument) the set of the necessary optical pieces will be automatically set in place so the chosen excitation light reaches the sample.

In case this part is not automated on your instrument a warning message similar to the following on will be displayed.
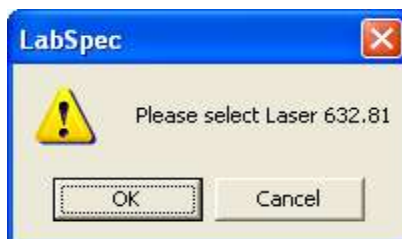
When everything is in place, click then on the OK button.

5.2 - Filter
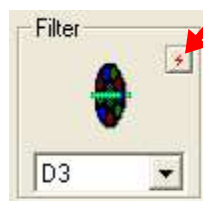
Click here to reset the filter wheel and to set in place the filter displayed in the filter field.

Click here to open the list of the 6 neutral filters installed.

Then select the one you wish to be in place.

Note: The reset function of the filter wheel is usefull when for any reason the selected filter is not well in place or does not match the selected one.

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There are 6 neutral filters installed with the optical densities 0.3, 0.6, 1, 2,3 or 4.

[...] = no attenuation (P_0)
[**D0.3**] = $P_0/2$
[**D0.6**] = $P_0/4$
[**D1**] = $P_0/10$
[**D2**] = $P_0/100$
[**D3**] = $P_0/1000$
[**D4**] = $P_0/10000$

5.3 - Confocal hole

Initialize the confocal hole by closing the hole and opening it to the previous value.

Close the confocal hole aperture.

Set here the value of the aperture of the confocal hole

Open the confocal hole to the maximum value of aperture.

5.4 - Slit.

Initialize the slit by closing the slit and opening it to the previous value.

Close the slit.aperture.

Set here the value of the aperture of the slit.

Open the slit to the maximum value of aperture.

5.5 - Spectro

Initialize the spectrograph grating position. Move to the zero order position and then move to the position value previously set.
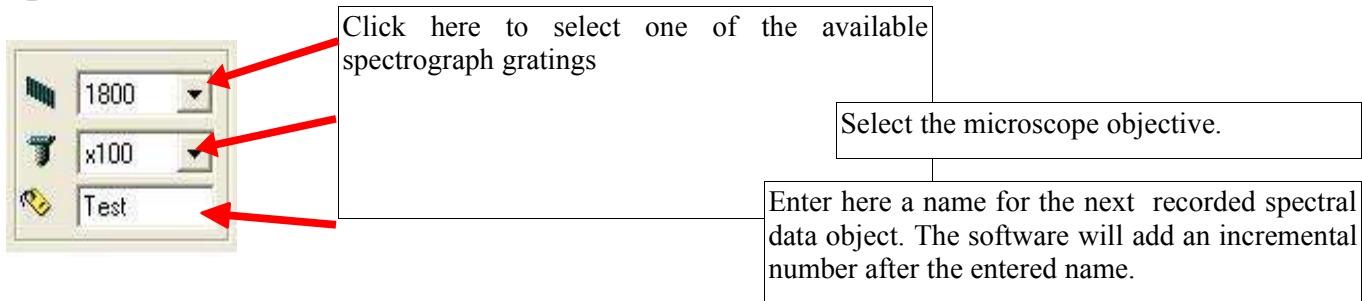
Move the spectrograph grating to the zero order position. (0nm)

Enter here the spectrograph grating position value in the active spectral unit.

Move the spectrograph grating to the highest value of position.
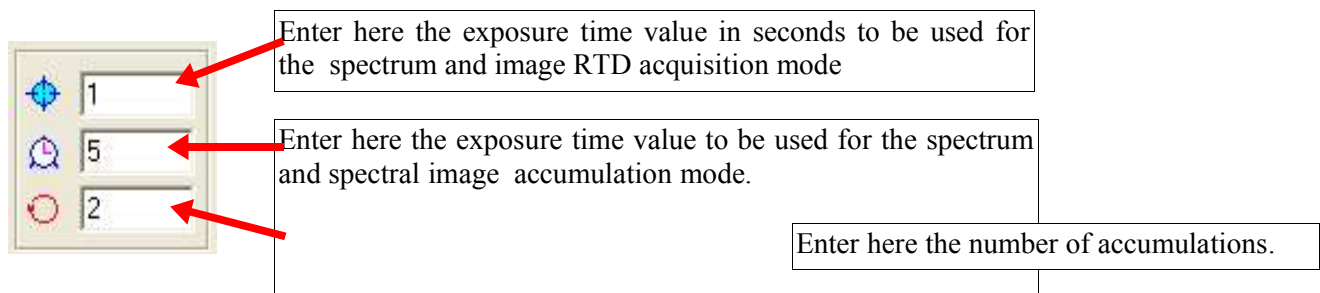
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5.6 - Options

Click here to select one of the available spectrograph gratings

Select the microscope objective.

Enter here a name for the next recorded spectral data object. The software will add an incremental number after the entered name.

5.7 - Exposure times

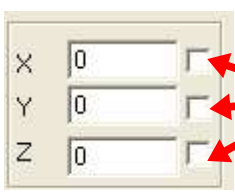Enter here the exposure time value in seconds to be used for the spectrum and image RTD acquisition mode

Enter here the exposure time value to be used for the spectrum and spectral image accumulation mode.

Enter here the number of accumulations.

5.8 - Motorized XY/Z Table

Position of the different axis of the motorized XY/Z table.

Enter here also the position you want the table to be moved.

Select the small blank box attached to each table moving axis to have the corresponding position value refreshed in real time even when moving with the joystick.

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6 - The main icons bar

In this bar you will find all the icons correponding to the LabSpec5 main functions for the spectral data acquisition, managing and treatment. These icons are grouped together by interest center.

* Tools for data management
* Data object display and information.
* Data acquisition
* Basic data treatment
* High-level data treatment

Data management tools	Display and information	Data acquisition	Basic data treatment	High level data treatment
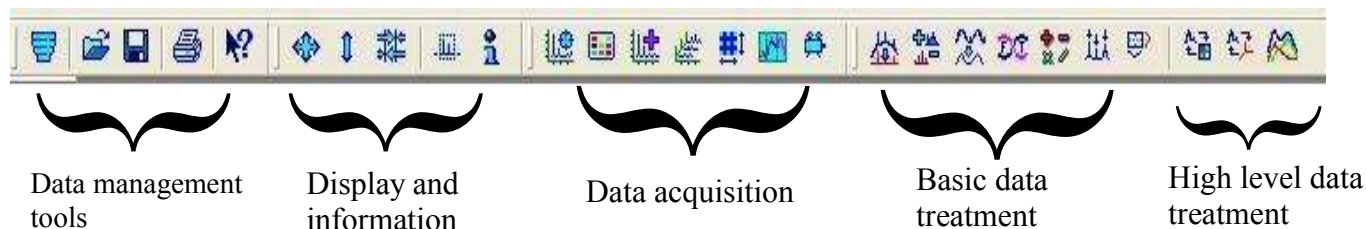
6.1 - Data management tools

6.1.1 - CUT

Delete the active objects.

6.1.2 - OPEN

Open a data file.

6.1.3 - SAVE

Save the active objects into a file.

6.1.4 - PRINT

Print to the current printer the active to-print page. For more details please report to the description of the *print* , *print preview*, *print setup* and *page* function in the **File** menu chapter.

6.1.5 - HELP

Open the LabSpec5 Help index.

6.2 - Objects display and information

6.2.1 - Scale normalization

Automatic scaling optimization of the active data objects.

6.2.2 - Intensity normalization

Normalize the current object in intensity.

6.2.3 - Pointers centering

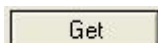Brings the pointers to the center of the active window.
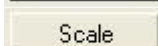
6.2.4 - Data sizes

This function reports the limits for each dimension of the active object in the following window.and allows you to re-define it if necessary.

The **Size** field reports the number of the spectral points for the correponding axis.

..............Click on the Get button to update the limits of the current active displayed object.

..............Use the Scale button to apply the limits to the active displayed object.

..............Extract the data included in the limits defined in the corresponding fields to build a new object..

6.2.5 - Data parameters

Clicking on this icon displays the array of the acquisition parameters attached to the active object.

6.3 - Data acquisition

6.3.1 - Spectrum Real Time Display

The main purpose of this function is to offer a tool to allow you to adjust quickly the focus and the other experimental conditions to maximize the Raman signal. Clicking on this icon starts in continuous the following cycle:

- Acquisition in single shot window of a spectrum.
- Display of the acquired spectrum.

Each spectrum displayed replaces the previously displayed spectrum. There is no averaging or spectra accumulation and no extended coverage possible. For this use the dedicated accumulation functions described below.

The exposure time used is the one set in the **RTD exposure time** field in the control panel (Report to the exposure time section in the control panel chapter).

The CCD pixels read are the one set in the **Acquisition / RTD** function.

To stop the continuous readout click on the STOP icon located at right end of the main icons bar.

6.3.2 - Detector image Real Time Display

The purpose of this function is the same as the one described in the pevious section applied to the CCD image.

The CCD image is a 2D image of the intensity of each pixel of the CCD chip. Following the parameters set in the **Acquisition / RTD** function this could be the full chip but also a part of the chip.

6.3.3 - Spectra accumulation

Clicking on this icon allows spectra to be acquired with multiple accumulations and averaging and/or with coverage over extended spectral ranges following the parameters setting of the **Acquisition / Detector** function , the one of the **Acquisition / Multi window** function.

6.3.4 - Spectral Images accumulation

With some suitable optional accessories installed on your instrument it is possible to acquire spectra in function of one or a combination of some specific variable parameters to obtain for example XYZ volume, XY mapped images, line (X/Y), depth (Z) , time and temperature profiles.

So the main purpose of this function is to acquire an array (3D for volume, 2D for map or 1D for profile) of spectra, with each spectrum acquired with specific variable parameters like for example position, time, temperature...

In all cases the result spectral array is saved in one single file for fast and easy data analysis.

The array below shows some examples of general possible applications following the different additional optional dveices innstalled.

➢ **Main examples of applications**

Variable parameter	Results	Optional device used
X or Y position	Line profile	Motorized XY table / Scanner
Z position	Depth or Z profile	Motorized Z motor / Piezo

Variable parameter	Results	Optional device used
Time	Time profile	No additional device
Temperature	Temperature profile	Heating/cooling stage
X and Y position	Map	Motorized XY table
X,Y and Z positions	Volume	Motorized XY/Z stage or Motorized XY stage and piezo

6.3.5 - Spectral Image properties

6.3.6 - Multi window

Clicking on this icon allows you to define the properties of the spectra acquisition over extended spectral ranges. You can also acces to this function from the main menu bar . *Acquisition / Multiwindow.* So please report to this section for detailed explanations.

6.3.7 - Video

Clicking on this icon starts the continuous video image grabbing. To freeze the image press on the STOP icon located at the right end of the main icons bar.

6.4 - Basic data treatment

6.4.1 - Baseline correction

Clicking on this icon allows you to access the baseline correction functions.
The Baseline correction performs baseline correction of data by using a manual or automatic approach and converts baseline profile to data array.

➢ **Manual Baseline Correction**

The *Manual Baseline Correction* method is based on polynomial or line-segmented correction using referenced points selected by the user.

To perform a manual base line correction :

1. In the Baseline window options select the baseline **Type** : **Line Segmented** or **Polynomial**.
2. In the Baseline window options select the Degree for the **Polynomial** baseline.
3. Then in the left object associated graphics tools panel select the Baseline tool [icon] Moving the mouse inside the window of the active objet moves a cross pointer.
   This enables you to add or move the points by clicking at the desired place.
   By setting the **Attach** parameter in the options of the Baseline window to Yes the selected baseline points are attached to the spectrum data.Setting this Attach parameter to No allows you to freely place the points anywhere in the window.
4. In the Baseline window options use the **Style** list to select the style to display the baseline calculated from the selected points.
5. Click on **Sub** button to subtract the baseline from the data.

This operation could be applied to multidimensional data set, visualized in one-dimensional curve mode (1D)
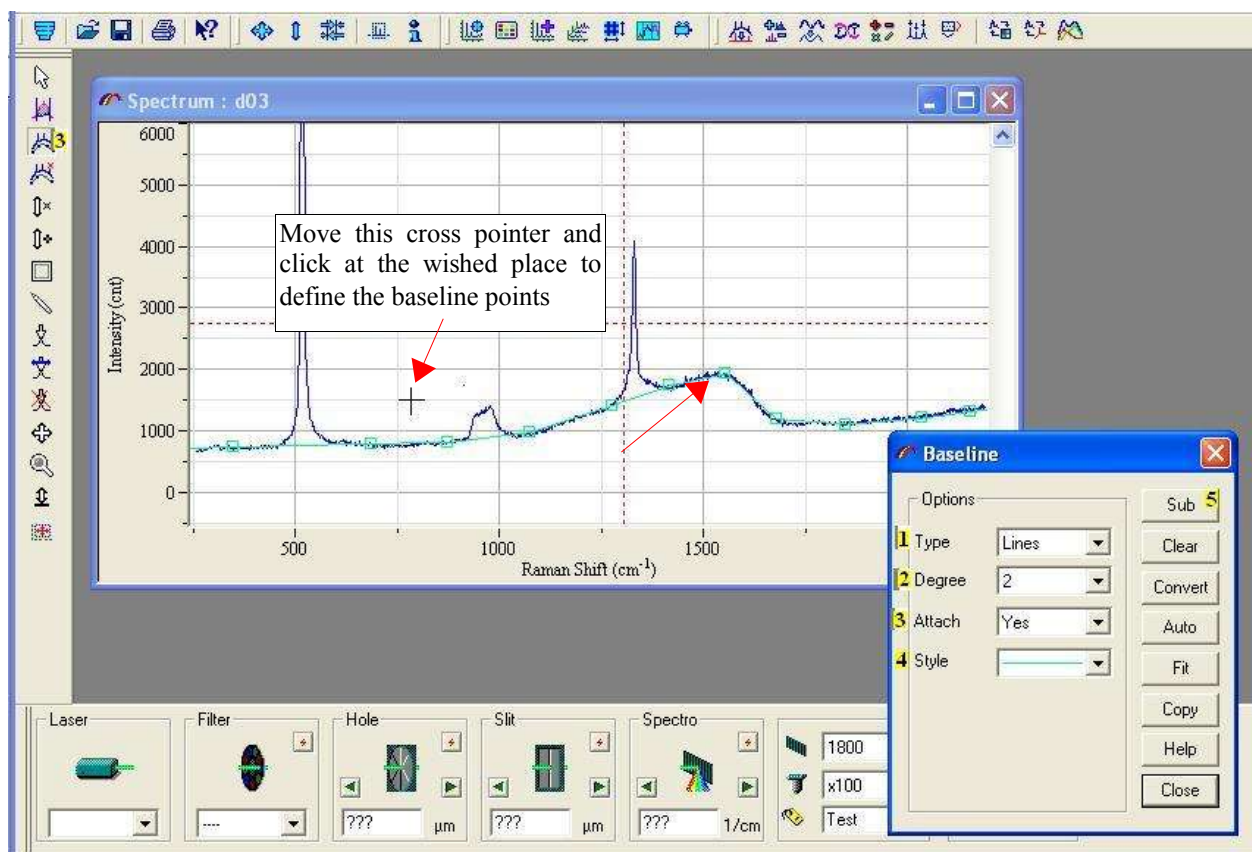
> **Automatic Baseline Correction**.

The *Automatic Baseline Correction* iteratively fits a polynomial to the baseline (non-peak) of the data. The algorithm starts with a full set of data points. The points above the baseline are removed and the fitting procedure continues until the fitting errors are less than the predefined value or the number of points is not changed. Click on **Auto** button to start the procedure. The baseline is then automatically subtracted from the data and the finalresult is displayed.
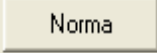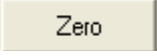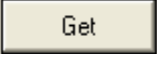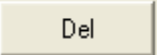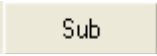
To calculate the baseline without subtraction, click on the **Fit** button.

> **Baseline Conversion**.

The *Baseline Correction* operation replaces the data by the baseline trace. This operation allows the baseline trace to be saved as a data file for future retrieving. Click on the **Convert** button to start this function.

> **Baseline Clear**.

Click on the **Clear** button to remove the baseline points.

The baseline is displayed in the selected style.

6.4.2 - Data correction

The **Data correction** function allows you to modify all the traces of a multidimensional data matrix. Some of these operations require an additional spectrum as a second parameter of the operation.
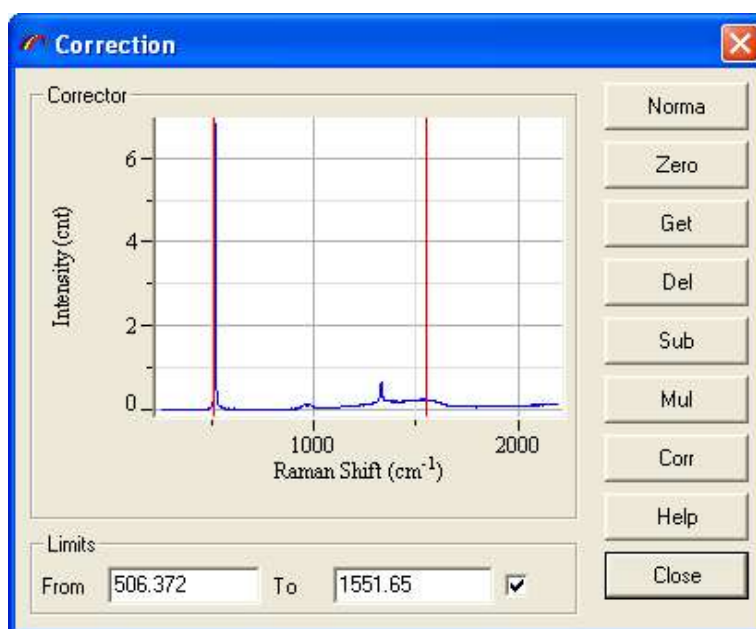
Norma	.... The **Norma** button normalizes all the traces to same area value (100).
Zero	.... The **Zero** button moves all the traces to the minimum intensity level.
Get	.... The **Get** button takes the activated spectrum and put it in **Corrector** frame. This data object will be used as parameter.
Del	.... The **Del** button removes the **Corrector** spectrum.
Sub	............The **Sub** button subtracts the **Corrector** spectrum from all the traces.
Mul	............The **Mul** button multiplies all the traces by the **Corrector** spectrum.
Corr	............The **Corr** button subtracts the **Corrector** spectrum from all the traces. The intensity of the **Corrector** is multiplied to fit the intensity of the trace

Limits Select the small blank box if you want that only a part of the trace is used for operation. This parameter is used for **Norma** and **Corr** operation.
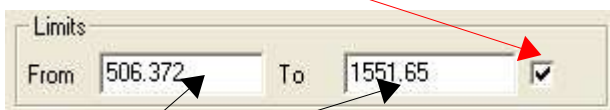
From and **To** Edit these fields   to modify the limits of the selected region.

6.4.3 - Filtration

This function allows linear and non-linear smoothing and calculates the derivatives of first and second degrees. The Linear Savitsky-Golay smoothing and derivative computing are based on the convolution approach which performs a least squares fit of polynomial.
The larger is the **Size** value and the lower is the **Degree value** result in a higher smoothing effect.
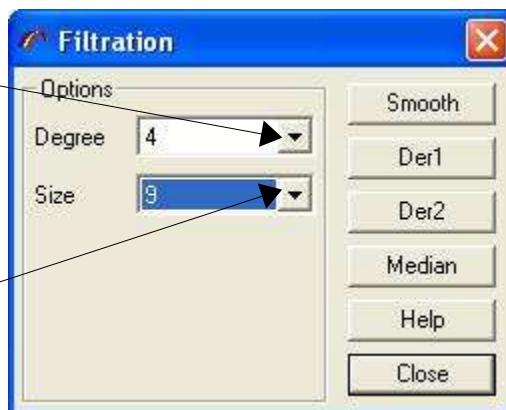
> **Degree**

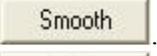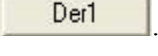Set in this field the degree of the polynomial.

The lower is the degree the more intense is the smoothing effect .

> **Size**

Set in this field the number of the adjacent data points to be used for the calculation.

The larger is the **Size** value the more intense is the smoothing effect

|	
Smooth	.... Click on the **Smooth** button to perform the Savitsky-Golay smoothing.
Der1	.... Click on the **Der 1** button to calculate the first degree derivate.

| Der2 | .... Click on the **Der 2** button to calculate the second degree derivate. |
| Median | .... Click on the **Median** button to apply the median smoothing. The Median smoothing is a non-linear data filter method. |

6.4.4 - Fourier transformation

The **Fourier Smoothing** is based on the direct Fourier data transformation, applying filter and apodization function and inverse the Fourier transformation. The dialog window shows the real and imaginary Fourier functions and allows you then to select the smoothing property.
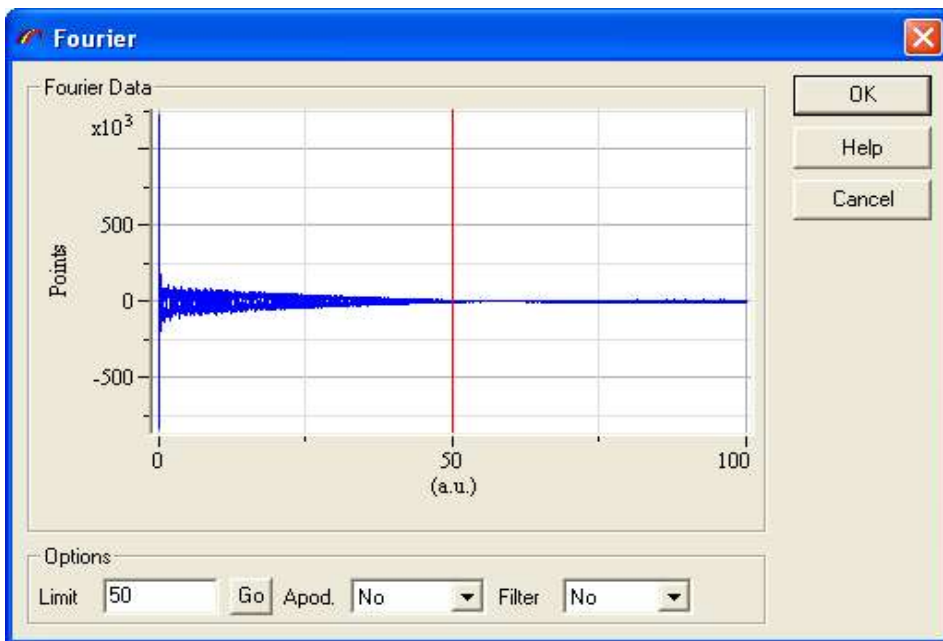
> **Limit** – Enter in this field the position of the cutoff point in %. This parameter defines the smoothing factor 0 – full smoothed, 100 – no smoothing. Click on the **GO** button to apply the value or drag the pointer to select the **Limit** visually.

> **Apod** – Select here the type of the apodization function with apodization value reaching zero at a **Limit** point.

None..........................	**No apodization function**
Line...........................	**Linear function**
Sqr	**Parabolic function**
Cos............................	**Cosinus function**

> **Filter** –Select here the type of the filter function.

None	**No filter function**

Traffic ....Traffic function

6.4.5 - Arithmetical operation

The **Math Operation** can be used to apply commonly used mathematical formulas to a data object.
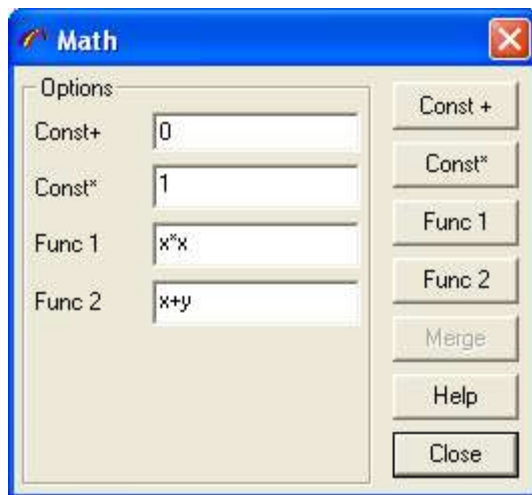
> ➢ **Addition of a constant value**

Enter the value in the **Const+** field and click on the **Const**+ button to add the constant value to the data object.

> ➢ **Multiplication by a constant value**

Enter the value in the **Const*** field and click on the **Const*** button to multiply the data object by the constant value.

> ➢ **Application of a complex mathematical function**

Enter the mathematical function in the **Func1** or **Func2** fields and click on the **Func1** or **Func2** button to apply the correponding function to the data object.
The mathematical formula can include basic mathematical function (+, -, *, /, ^), negating, pow, log, exp, sin, cos, asin, acos, atan, abs, sqrt, step.

For example the "sin(a)" formula replaces the data intensities by sinus function.
The "1000*log(abs(x)+1)" converts intensity to logarithm scale.

The following rules are applied for the variables names:

– the variables **a**, **b**, **c**, … correspond to the values of 1,2, … data axis
– the **x** and **y** value are consider as intensity of data objects.

> ➢ **Merge function**

Click on the MERGE button to multiply data objects into a single.
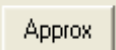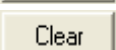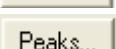

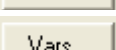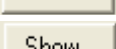### 6.4.6 - Peaks and Bands operations
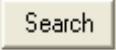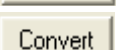
➢ **General presentation**

The **Peak Fitting** operation performs a peak search and curve fitting for a single data trace or a multidimensional data set. The following list of capabilities is offered by the program:

- **Manual** or **Auto** peak selection routine.
- Gaussian, Lorentzian, Polynomial and other mathematical formulas for peak.
- **Fixing** peak parameters during curve fitting operation.
- **Mapping** peak parameters for multidimensional data matrices.
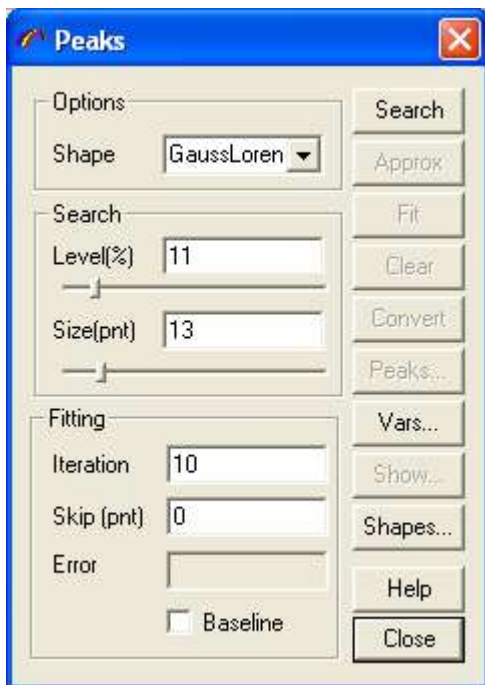
Click on button on the right side of the **Peaks** window to call one of the following functions:

| Search | .... Calls the peak auto finder procedure. |
Approx	.................Approximates the height and width of peaks without fitting.
Fit	...................Calls the peak fitting procedure.
Clear	.................Removes all peaks and baselines of the data.
Convert	...................Converts the sum shape of peaks and baselines to data trace.
Peaks...	...................Opens tables showing the parameters of peaks.
Vars...	.................Opens the tables of variables, used in curve formulas.
Show...	.................Opens the display properties dialog.
Shapes...	.................Opens the display properties dialog.

➢ **Peaks selection**

The **Peak Edit Properties** control the automatic and manual peak correction.

Select or edit P**eak Shape** control to modify the peak curve shape. This value will be used, when you insert a peak manually or call the peak **Search** procedure.

Edit the **Search Min** L**evel** box to modify the parameters level for the peak **Search** algorithm.

Edit the **Search Size** box to modify the number of points for the peak **Search** algorithm.
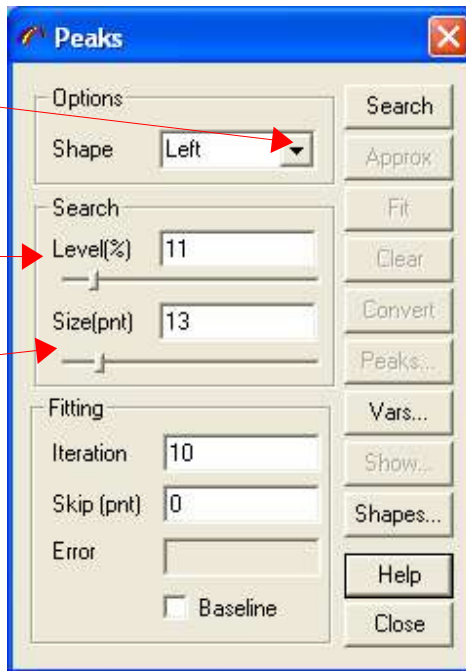
To select and define peaks manually use the following icons on the left graphics tool panel.

.... To add or move a peak

.... To adjust the height and width of a peak.

.... To remove a peak.

• **Adding or moving a peak**.

Click on this icon.

Then move the cross at the desired position. A peak will appear in function of the settings of the SHOW properties.
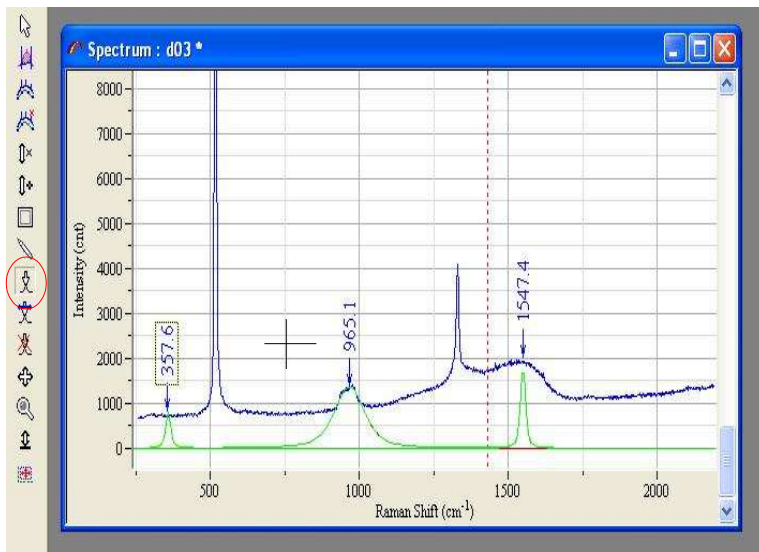
- **Adjusting peak height and width**

Click on this icon to define or modify the height and width of the selected peak.

Peak height modification
Move the mouse on the height of the peak to modify. When the following symbol appears click and drag the mouse to the wished height.

Peak width modification.
Move the mouse on one of the sides of the peak to modify. When the following symbol or appears click and drag the mouse to obtain the wished width.

- **Removing a peak**

Click on this icon to remove peaks.

Move the mouse pointer on the peak you wish to remove. When the following symbol appears click on the left mouse button. The correponding peakk is removed.
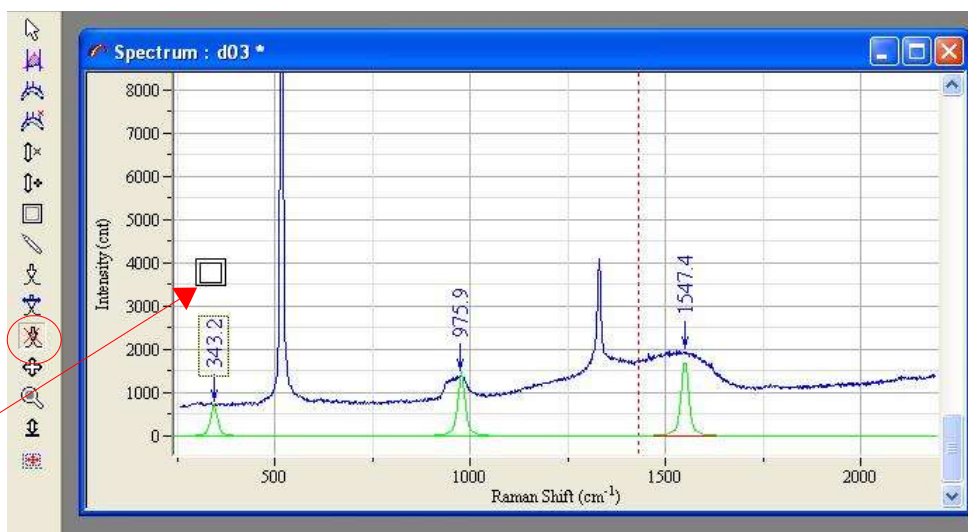
- **SEARCH function**

The **Peak Search** operation performs a search for peaks. It iterates all the points of the data trace to localize the local maxima.

In the Search **Size** field define the number of points in the maximum locality.

The Search **Level** parameter controls the minimum intensity value of local maximum.

- **APPROX function**
The **Peak Approximation** procedure can be used to estimate the initial values of the peak parameters. The height and width of the peaks are modified by this method; the other parameters are not changed. The height of the peak is replaced by the intensity value at the peak position point. The width is replaced by the difference in position of the peak and the intensity value of the nearest point, less then half of height.

> **FIT function**

The **Peak Fit** algorithm uses the Levenberg-Marquart method of non-linear peak fitting. It is based on the iteratively adjustment of every peak parameter to attempt the minimal value of χ^2. The basic problem of such an approach is that it can be the multitude of possible solutions and depending on the starting values of peak parameters. To avoid such a situation you should select the position and shape of the peak as much to presumed solution as possible.

The **Approx** procedure allows the initial values to be adapted to the intensity of data points around the peak. The other way is to **fix** the parameters which are known. You can select the maximum number of iteration to limit the treatment time. Increasing the number of skip data point allows to check quickly the convergence of the algorithm and the quality of the initial value selection.

Edit the **Iteration** field to modify the maximum iteration.

Edit the **Skip point** field to modify the number of data points skipped from the fitting procedure.

The **Error** box displays the error value, as distance between original data and curve sum of all peaks and baselines. This value is named usually as $\chi2$.

Check **Baseline** box to fit baseline together with the peaks.
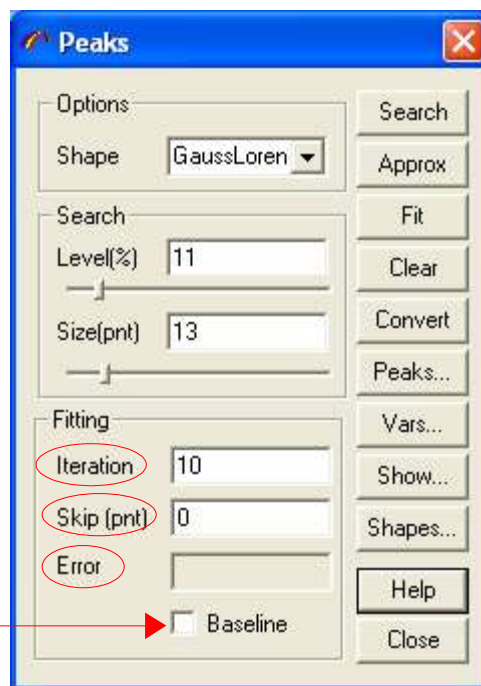
> **PEAKS**... **function**

The **Peak Table** dialog shows the peaks parameters. You can edit each of these parameters, add new peaks and remove existing ones.

	p	Fix	Map	a	Fix	Map	w	Fix	Map	g	Fix	Map	Formula
1	517.331	□	□	57585.5	□	□	20	□	□	0.5	□	□	GaussLoren()
2	971.647	□	□	5705.61	□	□	20	□	□	0.5	□	□	GaussLoren()
3	1321.59	□	□	11827.9	□	□	20	□	□	0.5	□	□	GaussLoren()

p, a, w… columns show the values of the peak parameters. The number of the parameter depends from the peak shape formula.

p	peak position (cm-1)
a	amplitude (max. Intensity)
w	full width half max (cm-1)
g	gaussian contribution (1= max)
s	integrated area of band

Fix .... Check this box to fix the parameters during the fitting operation

Map .... Check this box to display the map of the parameters. This option is available for multidimensional data set.

Formula .... Shows the peak shape formula.

Click on the right mouse button and select **Insert row** or **Remove row** menu items to add or remove peaks.
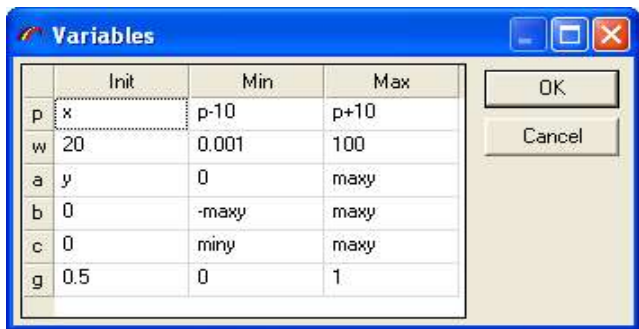
➢ **CLEAR function**

Remove all peaks and baselines of the data.

➢ **CONVERT function**

Convert the sum shape of peaks and baselines to data trace.

➢ **VAR**... **function**

The **Peak parameters Initialization** dialog enables you to select the initial value for the peak parameters. The parameters are displayed in a spreadsheet. To move inside the spreadsheet use the arrow-keys.

Edit **Name** column to select the peak parameter variable name. This name must be the same as in the peak shape formula. To edit the name double click on the variable name.

Edit **Init** column to select the initial value of the parameters. You can use number or mathematical formulae with the the following predefined variables:

x	x coordinate of the peak insertion point
y	y coordinate of the peak insertion point
minx	low limit of x data axis.
maxx	high limit of x data axis.
miny	low limit of y data axis.
maxy	high limit of y data axis.
dx	maxx-minx
dy	maxy-miny

Edit **Min** and **Max** columns to select the parameter limits. These limits will be used during the fit. You can use number or mathematical formulae in the same way as for **Init**.

➢ **SHOW... function**

The **Peak Fitting Show Properties** allows you to customize the display of the fitting results in the data object current window.

Check **Show** box to display the following items.
Click on the **Style control** to modify and select the style of the selected item.

Text .... shows peak label.
Arrow ....shows the peak arrow stick.
Shape ....shows the band shape.
Sum .... shows the result shapes of the all bands.
Res ....shows the residual between the original data and band sum.

Check **Use data style** to control the use data color when drawing the peak tick and label. In other cases the **Arrow** and **Text** styles will be used.
Check **Shape multicolor** box to personalize the color for each peak.
Check **Attach arrow** box to show the peak label tick immediately above data shape.
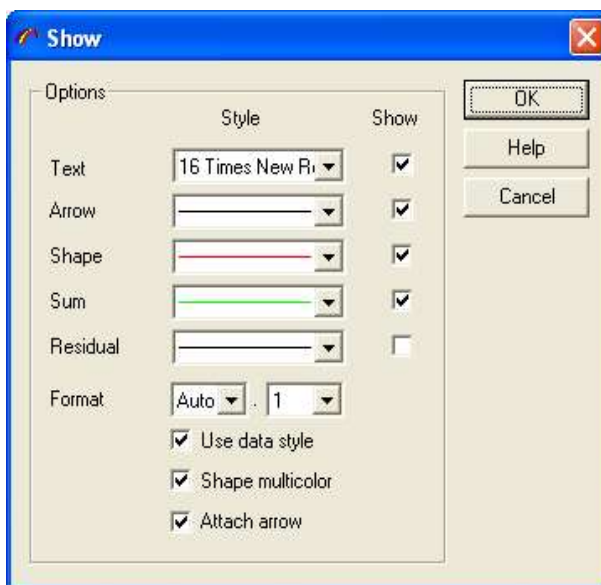
➢ **SHAPES... function**

The **Peak Shapes** allows to customize the shape of the peak.

Edit the shape **Name** in the left column. This name will then appear in the list of the available peak shapes of the Shape item in the Peaks window.
Edit then the corresponding mathematical **Formula** in the Formula column. Some of the formula parameters have a predefined meaning :
• **a** peak amplitude
• **w** peak width
• **p** peak position
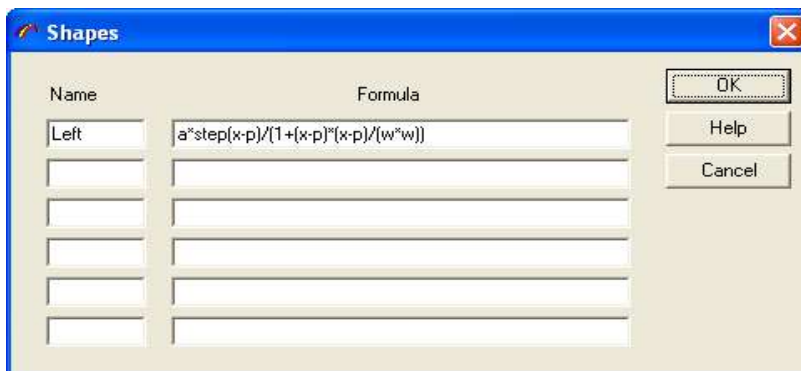
Then use the peak parameters initialization function (VAR... button) dialog to set or modify the initial value of these parameters.

6.4.7 - Profile

The **Profile** operation performs a visualization of the vertical or horizontal profile of an image.
To start a **Profile** operation :

- Load an image and activate image display window.
- Select cross line pointer by using window menu **Pointer** item.
- Click on the following icon   to open the profile window.
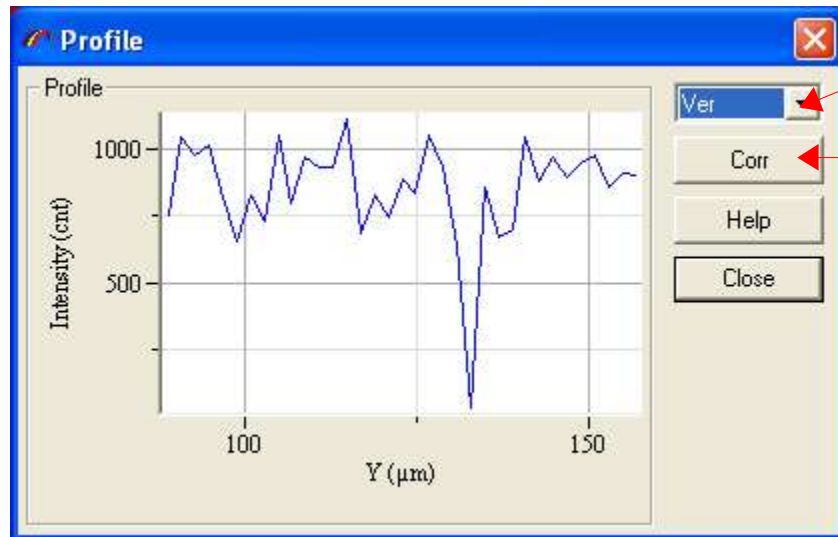
Choose **Hor** or **Ver** control to select between horizontal and vertical profiles.
Click on the **Corr** button to replace the image profile. This operation can be useful when you apply some operations to the profile (for example smoothing) and then you want to set data back to the image.

6.5 - High level data treatment.

6.5.1 - Mapping

The **Mapping** procedure generates a map by using the signal intensity in the selected spectral regions. Up to 4 maps can be displayed when you load or acquire the spectral image: the first three are the average signal intensity and the last is the signal ratio.
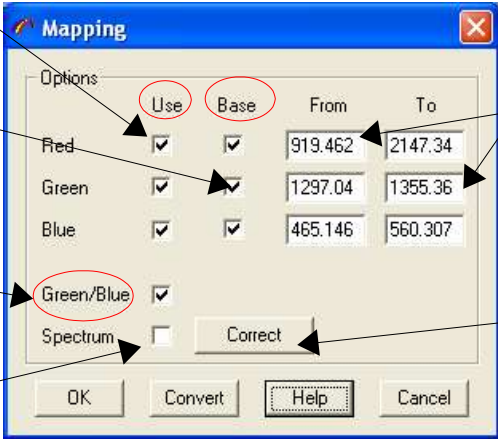The selection of the spectral region is done with the **Red**, **Green** or **Blue** pointer in the spectral image window.

Check **Use** box to generate the corresponding map.

Check **Base** box to subtract baseline.

You can edit **From** and **To** fields to adjust the limits of the spectral regions.

Check Green/blue box to generate the map of the corresponding ratio.

Check **Spectrum** box to see the spectrum of the selected data point(s) .

Click on the **Correct** button to modify data on the selected data point(s).

OK ....Click on the OK button to generate the map following the settings and close the mapping window.

Convert ....Click on the Convert button to convert the current map into spectral image and close the mapping window.

Help ....Click on the Help button to retrieve the informations concerning the parameters of this window.
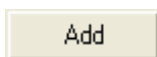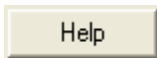
Cancel ....Click on the Cancel button to close the Mapping window without without validating the changes.setting

6.5.2 - New spectral profile

The **Spectral Profile** operation allows you to create and modify the all traces of spectral profile data matrix.

.... Click on the **NEW** button to take the activated spectrum and create a new spectral profile . Edit the **Name** box to define the spectral profile.

.... Click on the Add button to take the activated spectrum and add it to the end of spectral profile.

.... Click on the Insert button to take the activated spectrum and insert it to the spectral profile, selected by cursor pointer.

.... To removes the trace selected by cursor pointer from the spectral profile.

.... Click on the Help button to retrieve the informations concerning the parameters of this window.

.... Click on the Cancel button to close the window without validating the changes setting.

6.5.3 - Modeling

Click on **Modeling** icon to open *DCLS* Dialog.

The *Direct Classical Least Squares* finds the linear combination of data from pure components making up the combination that most closely matches the original data. This operation, applied to all traces of the original data sets, yields the maps of each component. The multiplicative constants used on the pure spectra are proportional to the concentrations of respective components. The difference between the sample and the linear combination is the residual spectrum, which could be useful for diagnostic purposes. *DCLS* requires the spectra of all components presented in the sample, and assumes that this spectra are not the changed when the component are mixed together. To apply *DCLS* mapping :

- Activate the multidimensional Data Matrix

- Click on the   icon to open *DCLS* Dialog.

- Activate the Spectrum window
- Enter Model **Name**.
- Click on **New** button to use the spectrum as **Model.**
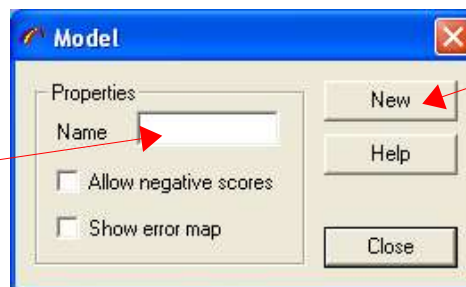
If you choose **Allow negative scores** check box, the program will use any type of combination, even if this combination includes negative values. Such a combination corresponds to negative concentrations that do not have a physical sense. This case often happens when the set of component are not completed or a contribution of some components is near to zero.

Select **Show** error map to see the distribution of the error.

7 - The graphics tools panel

The **graphics Tool Panel** on the left part of the screen allows you to modify the data appearance and run visual edit operations. Following the type of the current data object the tool panel is updated.
You will find hereafter a description of all the tools available.

7.1 - Activate the pointer

The **Pointers** permit you to check the coordinates of the data matrix axis at the desired location.
To activate a pointer click on the **pointer** icon in the graphics tools bar (left bar).
To change a pointer position click with the left mouse button and drag to the wished position. The current pointer coordinates are displayed in the status bar at the bottom of the main window.

If the current active data object is a 2D spectral image click on the SpImRed, or SpImGreen or SpImBlue icon to activate the corresponding pointer.

In any case to initialize the pointer position (move to the window center) click on the pointers centering icon in the main icons bar.

LabSpec**5** offers also the possibility to customize the pointers display by using the *pointer* function of the **Window context menu**.

7.2 - Integral

The **Integral Operation** can be used to calculate the area of a spectrum peak. Click on the **Integral** icon in the graphics tool panel to open the **Integral Operation** dialog.
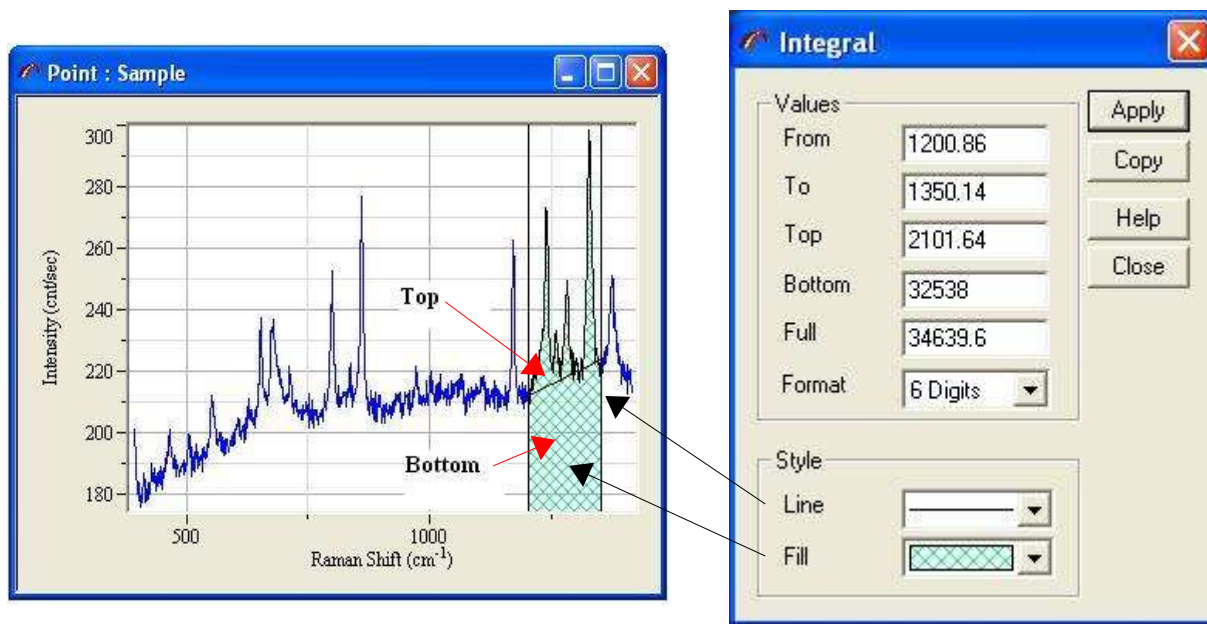
From..........................Edit here the the low integral limit. You can also drag the pointer to select the limit interactively

To..............................Edit here the high integral limit. You can also drag the pointer to select the limit interactively

Top............................Shows the integral result without baseline.

Base...........................Shows the baseline value

Full............................Shows the **Top** + **Base** value.

Format.....................Select here the number of digits to display the result numbers

Line ....Click on the control to modify the color and line style.

Fill.............................Click on the control to modify the color and style of the background.
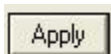
Apply   Click on the **Apply** button to apply the **From**, **To**, **Line** and **Fill** settings.
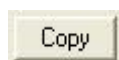
Copy   Click on the **Copy** button to copy the values to the clipboard. This is usefull to retrieve these values by using Copy/Paste functions from other softwares.

7.3 - Baseline

Use this tool to define the points to build the baseline to perform a manual baseline correction. Moving the mouse inside the window of the active objet moves a cross pointer. This enables you to add or move the points by clicking at the desired place.

Use this tool to remove some points of the baseline. Move the mouse inside the window of the active object on the point you wish to be removed. When the square cursor appears click on the left mouse button to remove the wished point.

7.4 - Manual contant multiplication to data

Use this tool to multiply by a constant the active spectrum. This a manual method using the mouse. Press the **Mul const** icon and move the spectrum up or down to the wished position.

7.5 - Manual constant addition to data

Use this tool to add a constant to the active spectrum. This a manual method using the mouse. Press the **Add const** icon and move the spectrum up or down to the wished position.

7.6 - Remove 'spike'

Use this tool to remove no desired points like spikes , cosmics rays,...

7.7 - Correct data shape

This tool allows you to modify a spectrum by correcting each point of the spectrum.

7.8 - Peak tools

This tool allows you to display the wavelength or the wavenumber of the selected peaks. The label is displayed following the style parameters set in the *show* function of the **Peaks and Bands operations** function. This tool is also used to define manually peaks for the fitting operation.

Use this tool to define or modify the height and width of the selected peak for band fitting operation. Report to the **Peaks and Bands operations** chapter for details concerning the use of this tool.

Use this tool to remove displayed peaks label or to remove bands selected for bands fitting. For details concerning this tool report to the **Peaks and Bands operations** chapter.
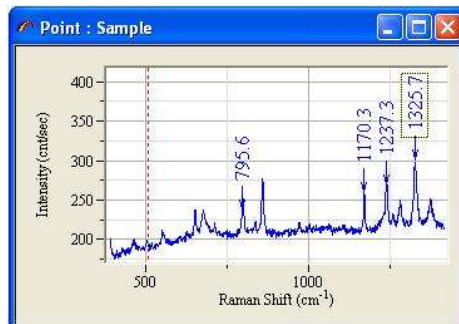
7.9 - Linear shift of the scale limits

Use this tool to move the vertical or/and horizontal of the active object.

7.10 - Zoom scale

This tool allows you to select the part of the active object you want to zoom. Press the left mouse button and draw a rectangle to define the wished part.
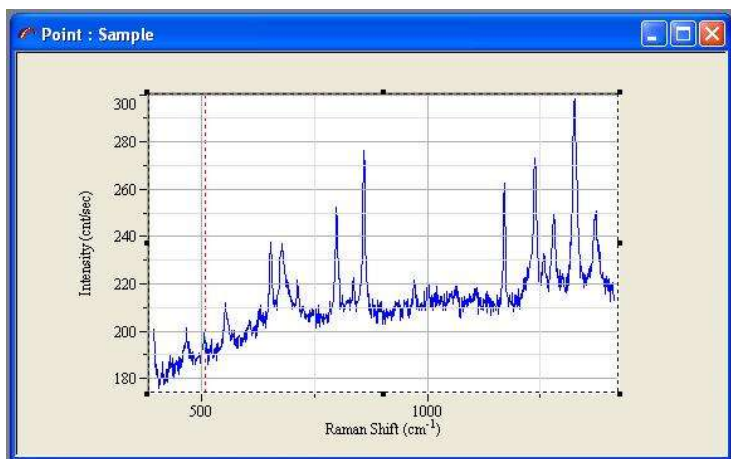
7.11 - Intensity shift

Use this tool to adjust the intensity scale of the active data object.

7.12 - Axes

Use this tool to position and dimension the axes rectangle inside the active window.

When clicking on this tool icon a dotted rectangle is displayed.

To re-dimension the rectangle:

Move the mouse pointer on one of the selection handles until to have the size

pointer: ↕ or ↗ .Keep the mouse button pressed and move the selection handle to modify the size of the axes rectangle.

To move the rectangle:

Move the mouse pointer anywhere inside the rectangle . When the moving pointer
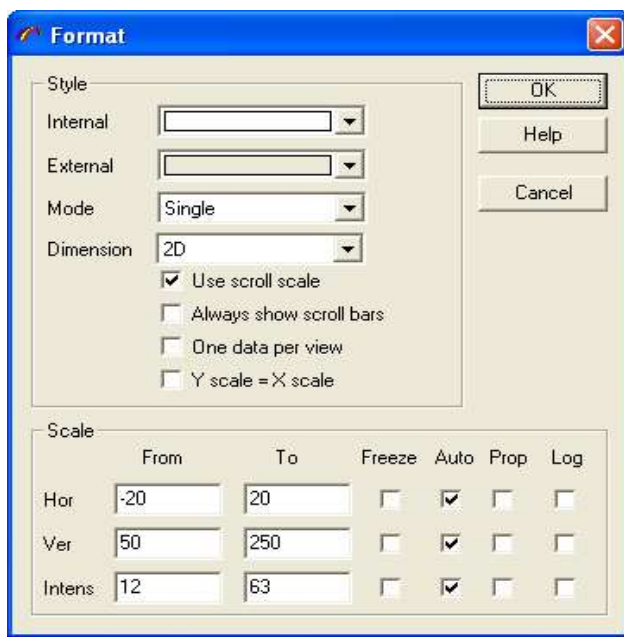
appears press the left mouse button and drag to move the rectangle inside the active window.

7.13 - Change 3D axes.

8 - Window context menu

8.1 - Format

You can open **Vizualization Format** dialog by selecting **Format** menu item

- ➢ **Internal** Click on this control to modify the color and style of the data field background

- ➢ **External C**lick on this control to modify the color and style of the window border. Usually it is where the axes are painted.

- ➢ **Mode**   Select one of the following data display modes

> **Single..........**only activated data object is displayed
> **Overlay......** all data objects are displayed on the same place
> **Tile..............**data objects will be shown in the separated rectangles
> **Projection..** trace of the activated data object will be shown in the separated rectangles
> **Trace..........** single trace of the activated object will be shown.
> Use the right scroll bar to change the trace.

- ➢ **Dimension**
1D / 2D 3D

- ➢ **Use scroll scale** check this box to use the window bottom and right scroll bar

- ➢ **Always show scroll bar** check this box to always show the scroll bars, when the visual zone is large then the data limits.
- ➢ **One data per view** if you check this box, the next time data is displayed a new window will be created.

➢ **Y scale** = **X scale** uses the same scale for both axes; useful for 2D image presentation.
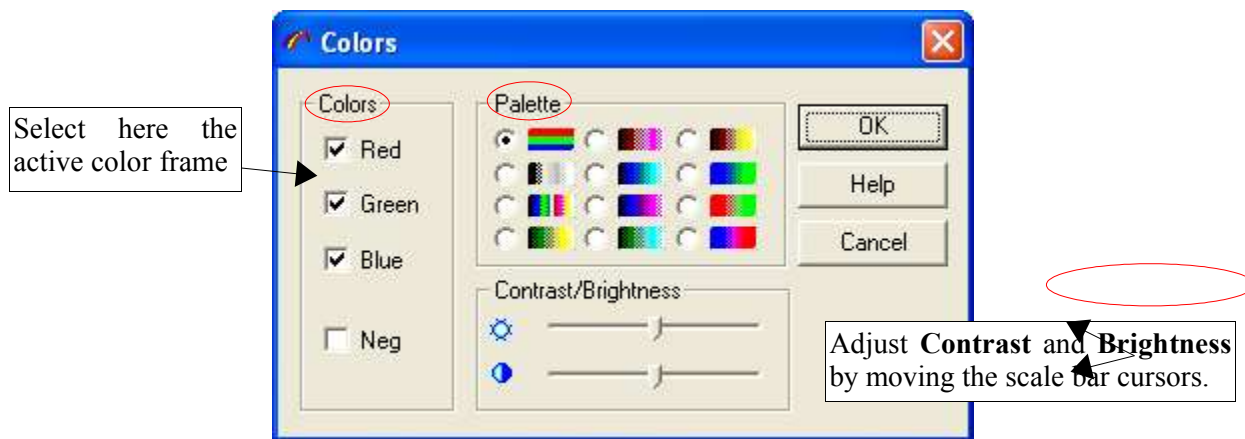
> **Scale ....** shows the scale properties for each of the window axes.
> **From ....** value of low axis limit
> **To ....** value of high axis limit
> **Freeze ....** fixes axis limits.
> The scale will be skipped when normalization function is applied.
> **Auto ....** enables auto scaling when data object axis is changed
> **Prop ....** enables proper scale limits for each data object.
> **Log ....** enables logarithm scale for the axis

8.2 - Norma
8.3 - Colors

The Colors Dialog enables the image color properties to be modified. Such properties are used when displaying images.
To access this function click on the right mouse button and select **Colors** menu items.

Select here the active color frame

Adjust **Contrast** and **Brightness** by moving the scale bar cursors.

In the **Colors** frame you can turn on/off **Red**, **Green** or **Blue** color.
To make image negative choose **Neg** check box.

In the **Palette** frame select one of the following styles:

> True color................... All colors are displayed without modification
> Black and White.
> False color.
> Green .... Yellow scale.
> Red .... Magenta scale.
> Blue .... Cyan scale.
> Blue .... Magenta scale.
> Green .... Cyan scale.
> Red .... Yellow scale.
> Blue .... Green scale
> Red .... Green scale.
> Blue .... Red scale.

8.4 - Axes

The **Axes dialog** allows you to customize the appearance of the graph axes.
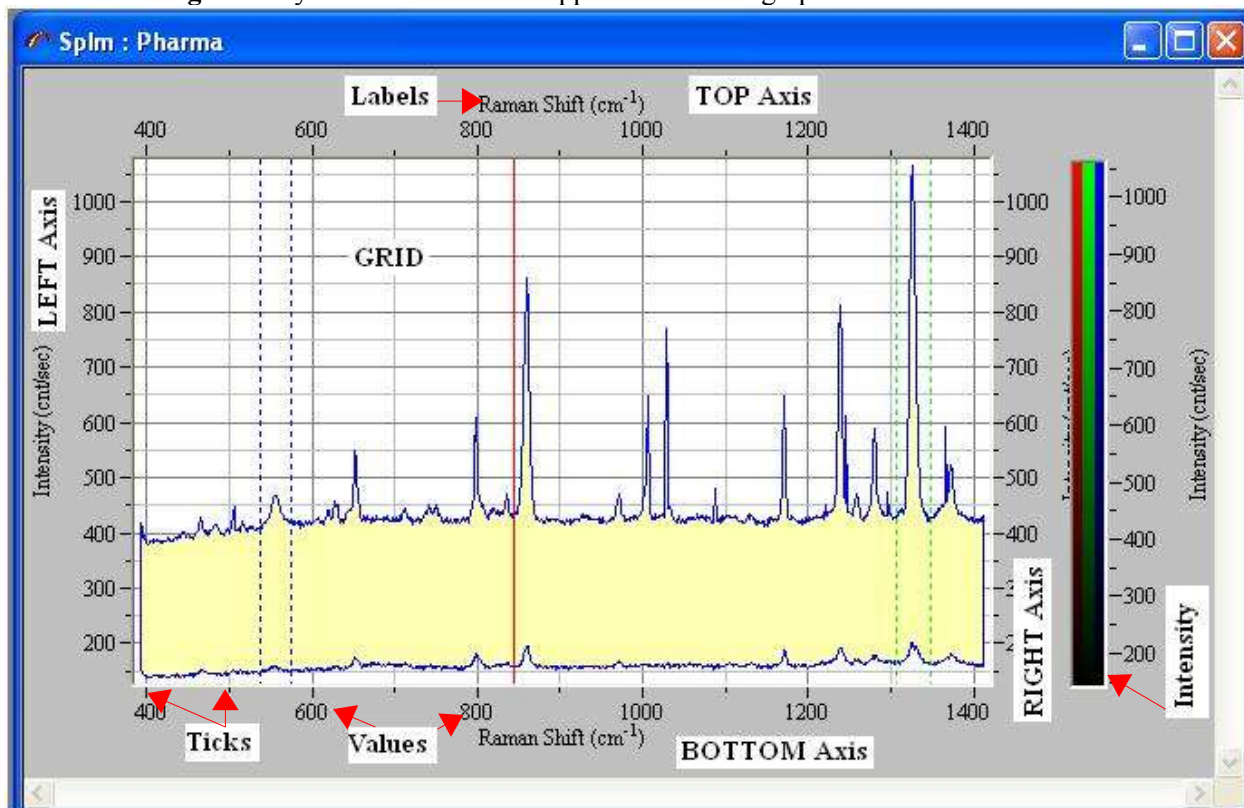
As shown on the picture above there are 4 axis. The Axes Dialog allows you to define independently each component of each axis. You access to the Axes Dialog by selecting the **Axes** item of the window context menu.

> **Options**

Tick ...... Check the box to enable the painting of ticks.

Grid....... Check the box to create a grid for tick levels.

Values .. Check the box to enable the painting of number values associated to ticks.

Labels .. Check the box to create an axis label and enable customization of the axis label.In the Labels blank field enter the text you wish to be appeared for the corresponding axis.
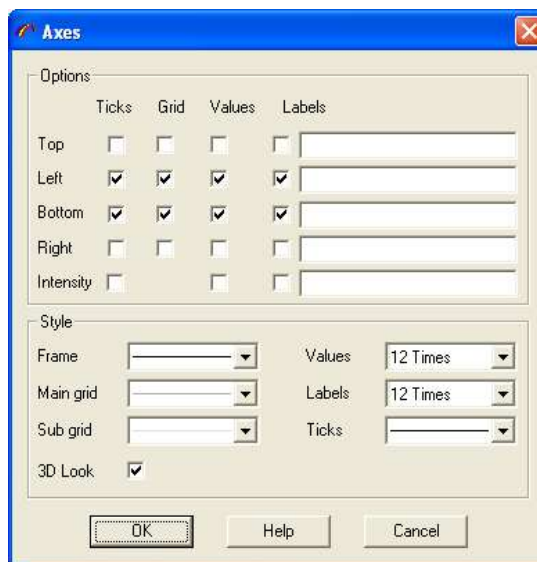
> **Style**

> Frame ....click on the control to modify the color and style of axis edge.
> This parameter is used for a non 3D look.
> **Main Grid .**click on the control to modify the color and style of the main grid
> **Sub Grid ...** click on the control to modify the color and style of the sub grid
> **Values ....**click on the control to modify the values font.
> **Labels ....**click on the control to modify the labels font
> **Ticks ....**click on the control to modify the color and style of the ticks.
> **3D Look ....** Check this box to enable a 3D outlook for the edge

8.5 - Graph

This function allows you to customize the appearance of 1D dimension displayed data objects.(Spectrum or Spectral Image)

8.5.1 - Spectrum

If the active object is a spectrum selecting **Graph** item of the window context menu opens the **spectrum Properties** dialog which allows you to modify the display properties of the spectrum.

> Select one of the **Style** controls to display spectrum as a set of **Lines, Points** or **Bars**.

> Click **Line** control to modify the color, thickness and line type.

Lines

Points

Bar
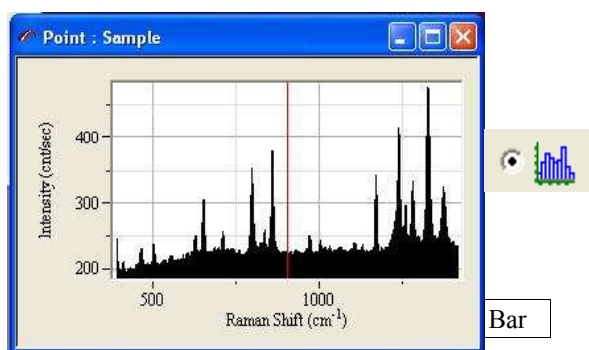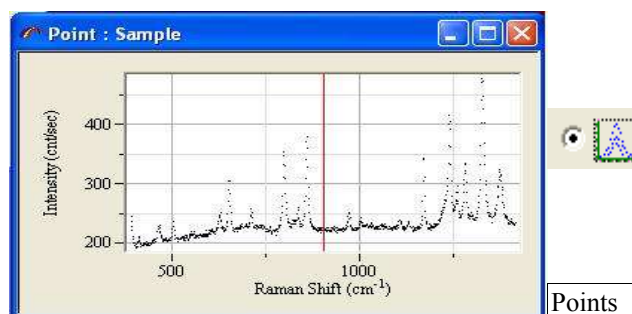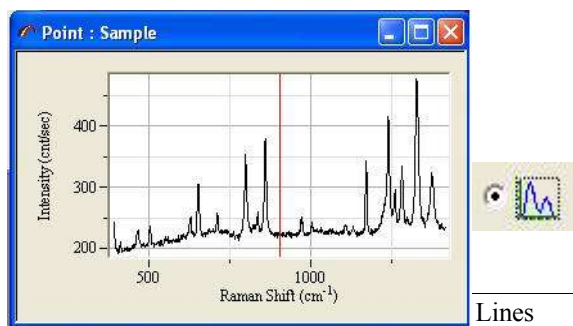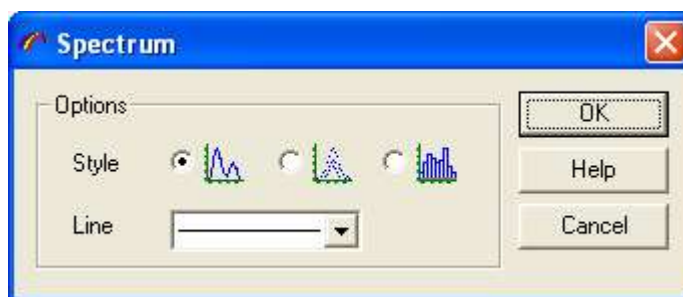
8.5.2 - Spectra

If the active object is a spectral image selecting **Graph** item of the window context menu opens the **spectra Properties** dialog which allows you to modify the display properties of the SpIm object.
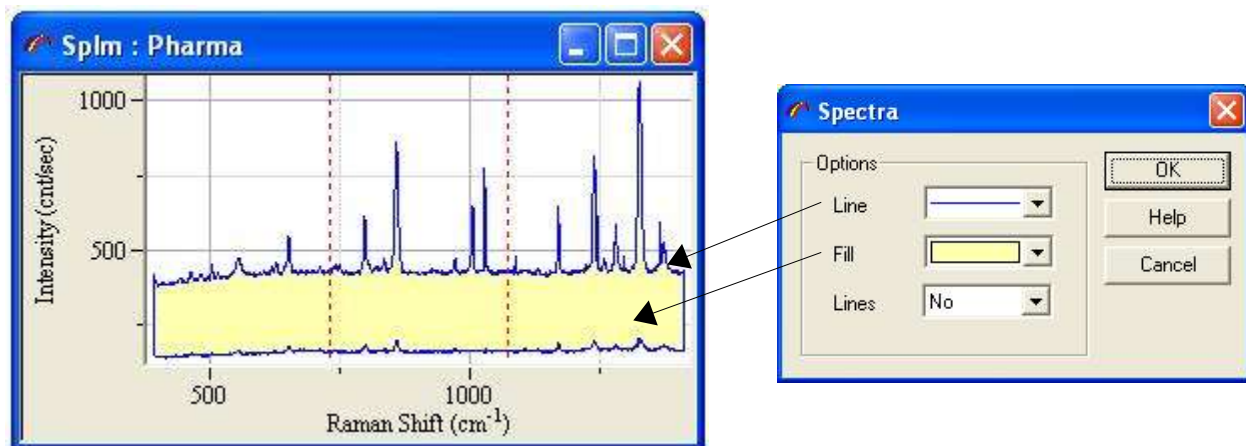

➢ Click **Line** control to modify the color, thickness and line type.
➢ Click **Fill** control to modify the color and fill style of the filled zone.
➢ Click **Lines** control to select the representation mode of all the spectra. You can select to display **All** the spectra , leave the software to display **auto**matically the necessary spectra so it is readable, or as shown on the picture above not to display all the spectra.

8.6 - Pointers

The **Pointers dialog** allows you to customize the appearance of the pointers.You access it by selecting the **Pointers** item of the window context menu.

➢ Click on the **Style** control to choose one of the following pointer types:

Line ...... single vertical line.
Cross .... vertical and horizontal lines.
Level .....vertical and horizontal lines.
The position of horizontal line corresponds to the data intensity value.
**Double**...two vertical lines.
Rect....... rectangle.
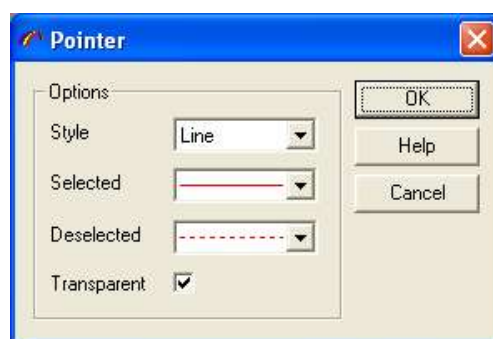
➢ Click on the **Active** control to choose the line style, when the pointer is selected (you can drag pointer with the mouse).

➢ Click on the **Hidden** control to choose the line style, when the pointer is deactivated.

➢ Check **Transparent** box to draw a pointer in transparent style. In such cases the image of the pointer is superposed with the window background.

8.7 - Image

The **Image Properties** Dialog enables to modify the appearance of the images data objects. To access this dialog, select **Image** item from the window context menu.

➢ Select **Style** mode, to make or not a linear interpolation of image intensity along X and/or Y axes.

Smoothed along column

Unsmoothed

Smoothed along line

Smoothed along diagonal
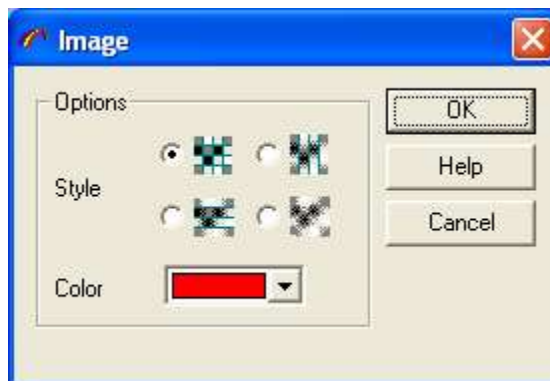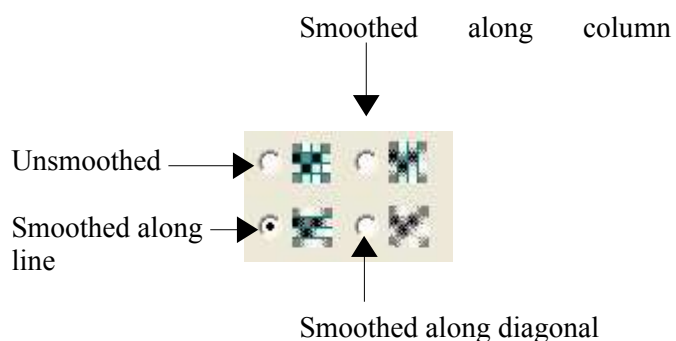
➢ Click **Color** to modify the image color. This color will be used, when you select overlay mode for the data display.

8.8 - Scale bar

The **Scale Bar Properties** dialog allows you to modify the display properties of the scale bar and its associated legend of the 2D presentations. To access this dialog, select **Scale Bar** item from the window context menu.

➢ Click on **Line** control to select the bar border style and color of the scale bar.
➢ Click on **Fill** control to select the sacle bar filling style and color.

➢ Click on **Font** control to select they the scale bar legend font properties
➢ Click on **Color** control to select scale bar legend text color.

Scale bar legend

Scale bar
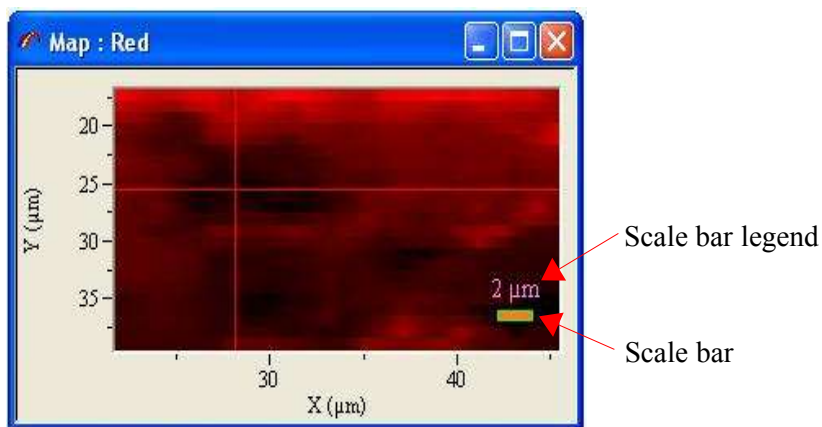
8.9 - Image3D

The **Image3D Properties** Dialog enables the modification of the appearance of a 3D representation of the data object. To open this dialog, select the Image3D item from the window context menu.

- ➢ **Type** Select between polygon and gradation display mode.

- ➢ **Gradation** Select the axis which defines the direction of the the color gradation

- ➢ Click on the **Color** control to modify the polygon border style and color.

- ➢ Click on the **Fill** control to modify the internal polygon fill-style.
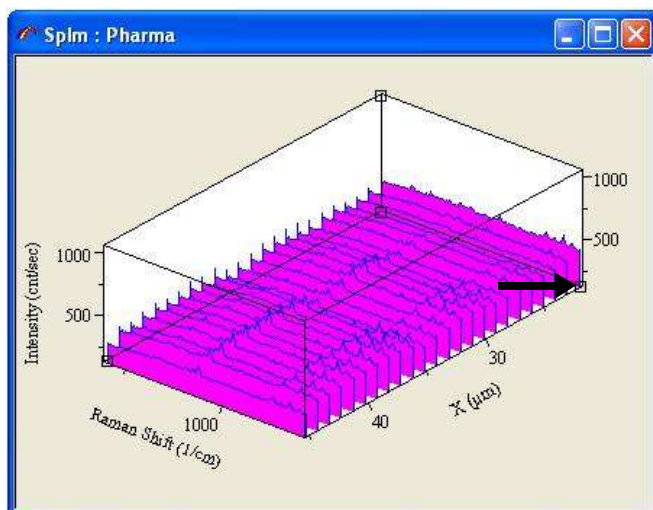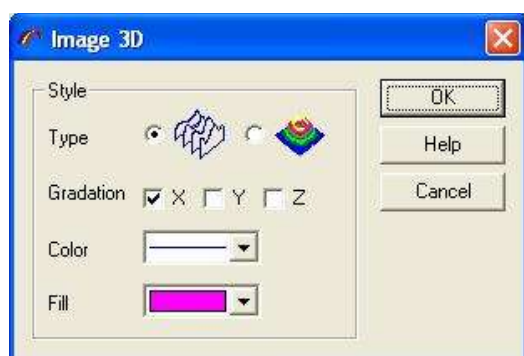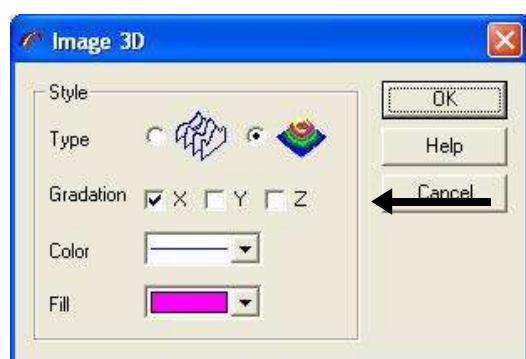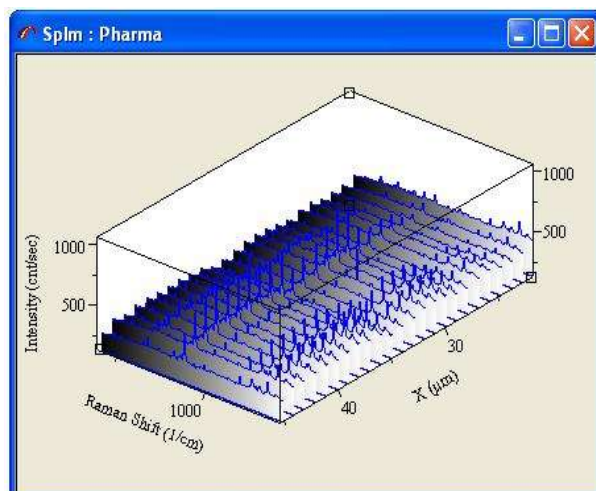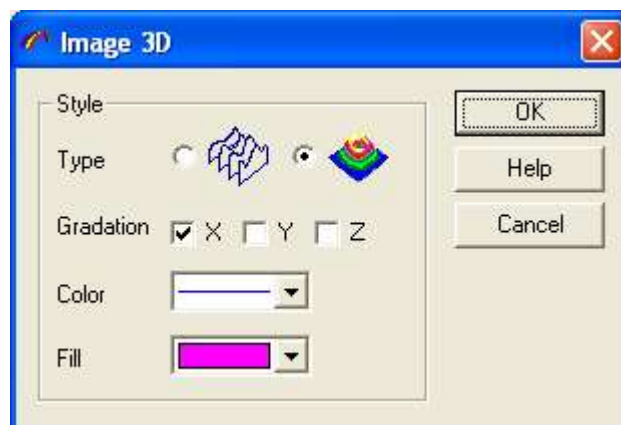
8.10 - 3DAxes

The **3D Axes Dialog** allows you to modify the appearance of the axes for 3D representation of data objects. You access to this Axes dialog by selecting the **Axes** item from the window context menu.

➢ **Options**

First select the axis you wish to customize.

Ticks .... Check this box to enable the drawing of ticks.

Values .. Check this box to enable the display of the number values for ticks.

Label..... Check this box to create the axis output label and edit the label field to customize the axis.

X<>Y..... Click on this button to switch between the X and Y axis.

Center... Click on this button to re-center the 3D object in the active window.
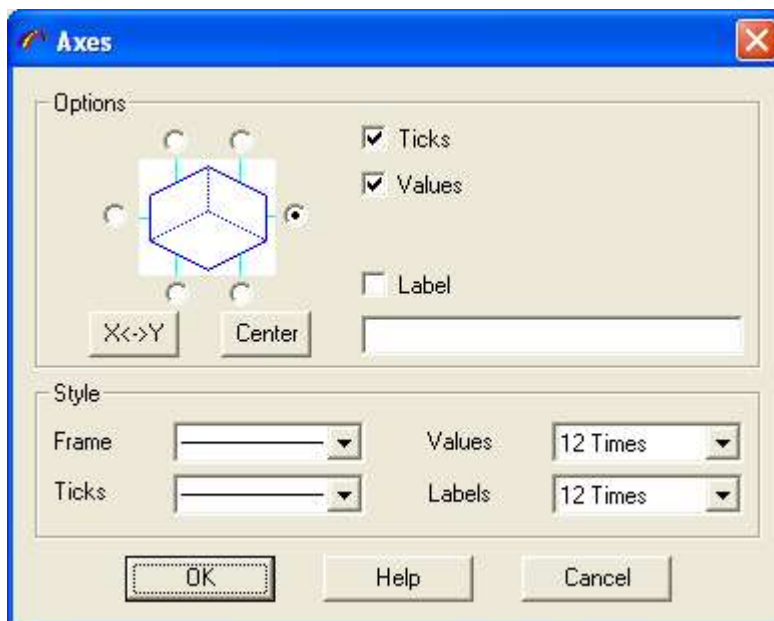
➢ **Style**

    Frame.... Click on the control to modify the color and style of axis edge.
    Values... Click on thes control to modify the font values
    Ticks...... Click on the control to modify the color and style of the ticks
    Labels.... Click on the control to modify the labels font

9 - Service