User Manual

YL-Clarity

Chromatograph Data System

YL INSTRUMENT CO., LTD.

YL-Clarity

HPLC

Easy Manual

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

YL INSTRUMENT CO., LTD.

Chapter 1. Installation

1-1. Hardware Installation

1-1-1. Standard packing kit

1) Body of Instrument
2) Power cable
3) LAN cable or RS 232 cable
4) Hub

1-1-2. Connection of LAN cable

1) Connect LAN cable from rear side of instrument to the hub one by one.

<9111 Binary pump>

<9160 PDA detector>

2) Connect LAN cable from the hub to the PC.

3) If you have RID, ELSD, ECD or Autosampler, connect from the Serial port on rear side of instrument to the PC with the RS232 Cable directly.

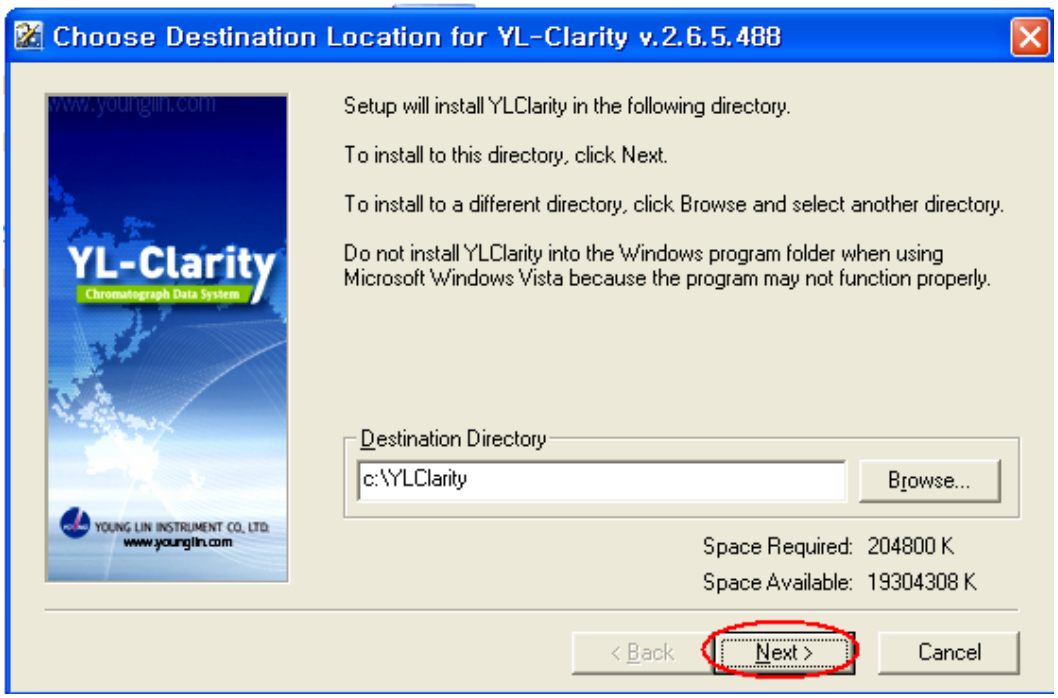
1-2. Software Installation

1-2-1. Installation of YL-Clarity

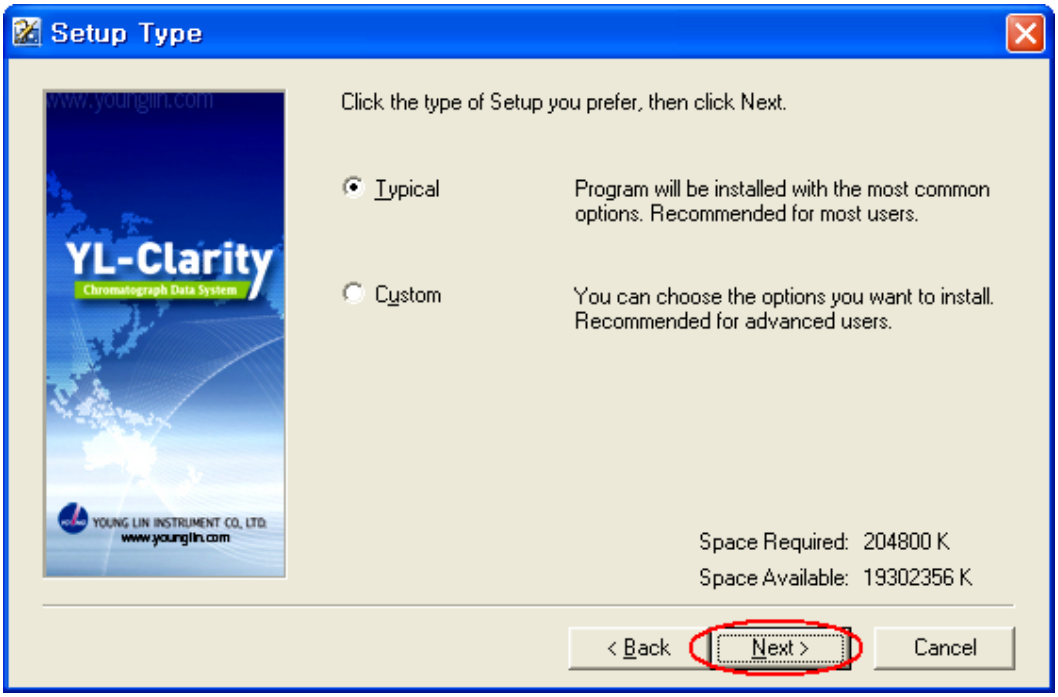
1) Run **YLClarity \ Install.exe** () in the folder of CD-ROM.

2) Install YL-Clarity by following the installation wizard.

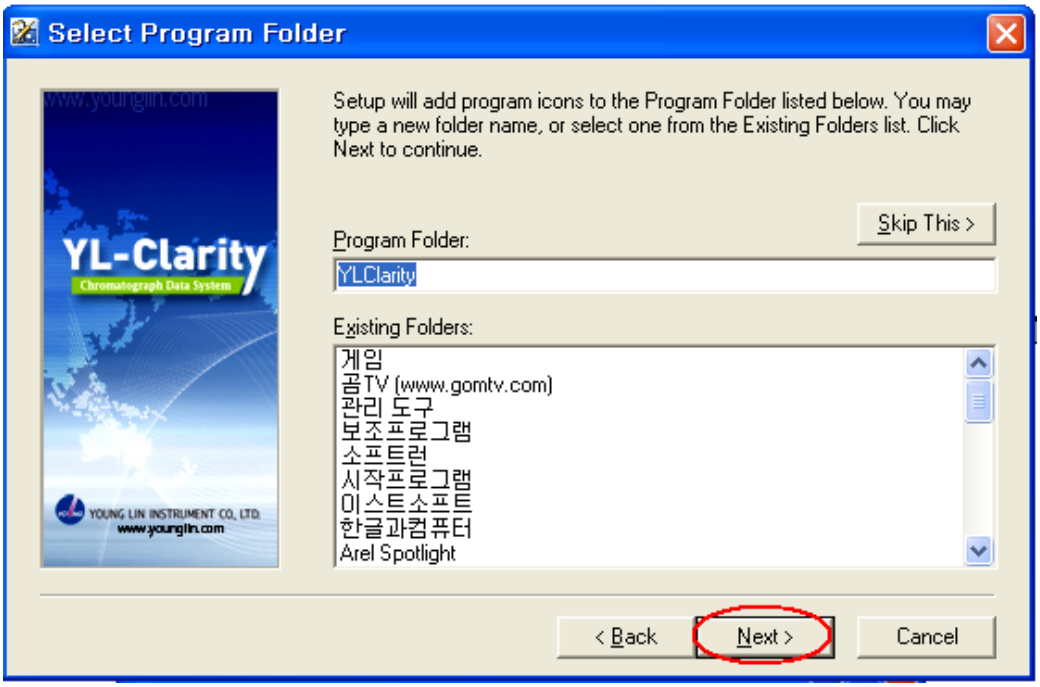
1-2-2. Choose destination location of YL-Clarity



1-2-3. Set up type



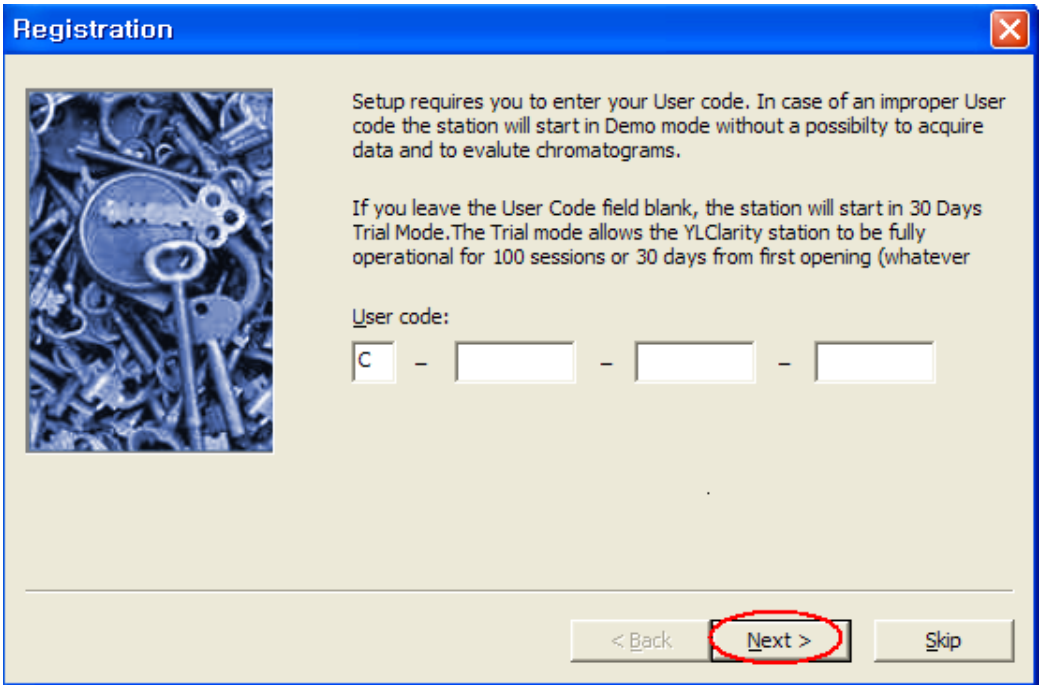
1-2-4. Select program folder



1-2-5. Registration

1) Input the **User code** which you have

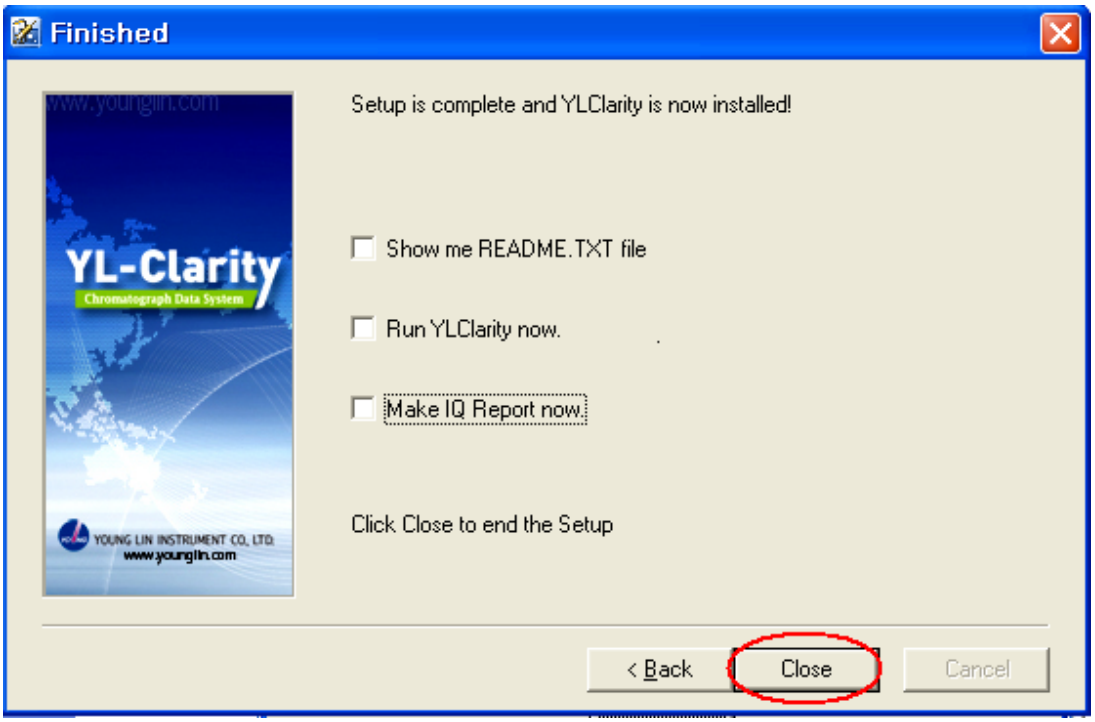
2) Click the **Skip** if you want to input the user code later.



1-2-6. Finished

1) Click the check box, if you want the those.

2) After the installation is completed, click on ***Close*** to exit.



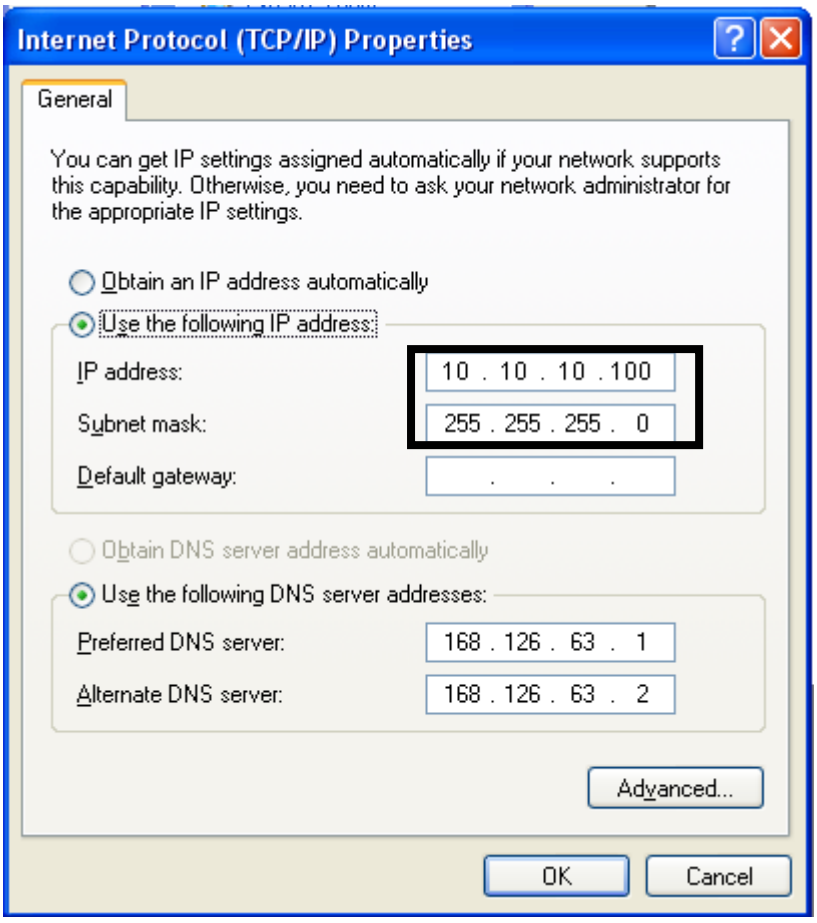
Chapter 2. Software Control

2-1. Adding TCP/IP address

1. Go to **Control Panel- Network Connection** – **Local Network Connection** - **Properties**
   - Select the **Internet Protocol (TCP/IP)** and click on **Properties**. The screen is shown as below.
2. Set the IP address as below.

IP Address(I) **: 10 . 10 . 10 . 100**

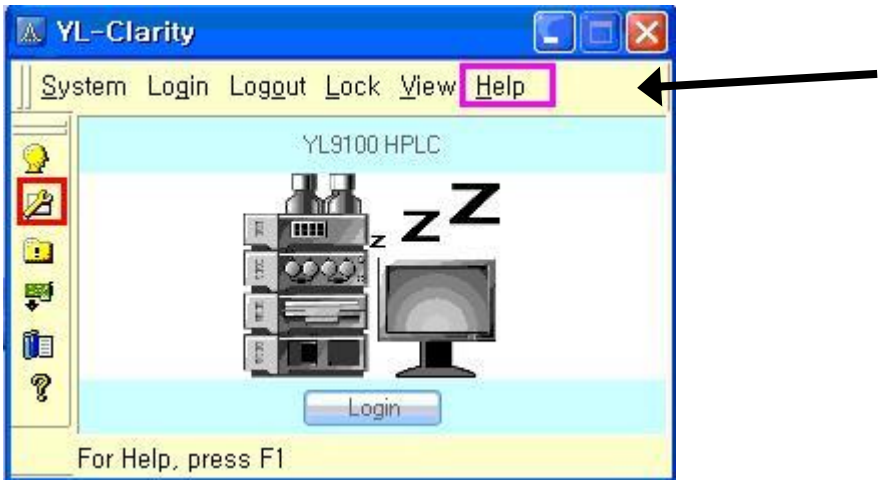
Subnet mask(U) **: 255 . 255 . 255 . 128**



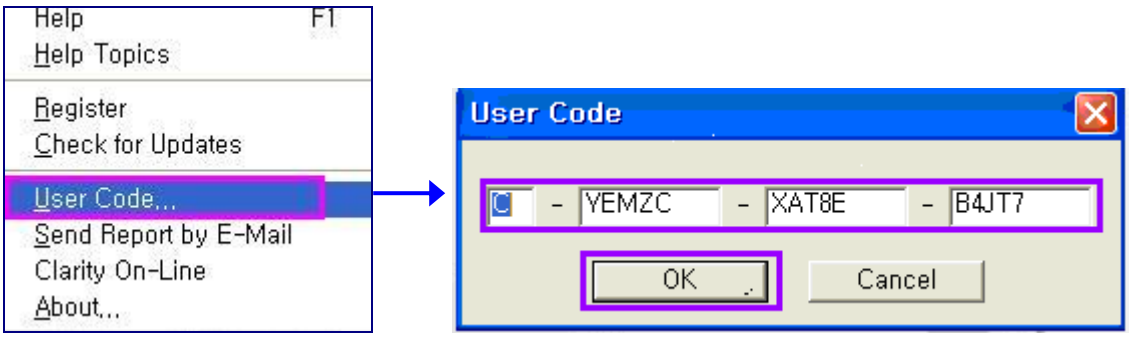
2-2. Entering User Code

1. Install the Clarity Serial Key on PC, and click the icon 

on the desktop. The screen is shown as below.



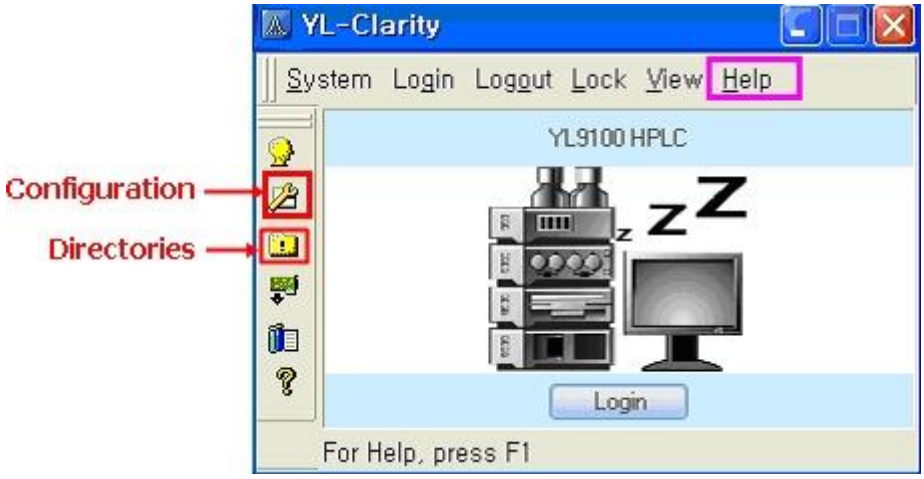
2. Click on **Help** – **User code** on the menu bar.
3. Enter the user code and click on **OK**.



* When you are installing the Clarity software, you could input the **User code**

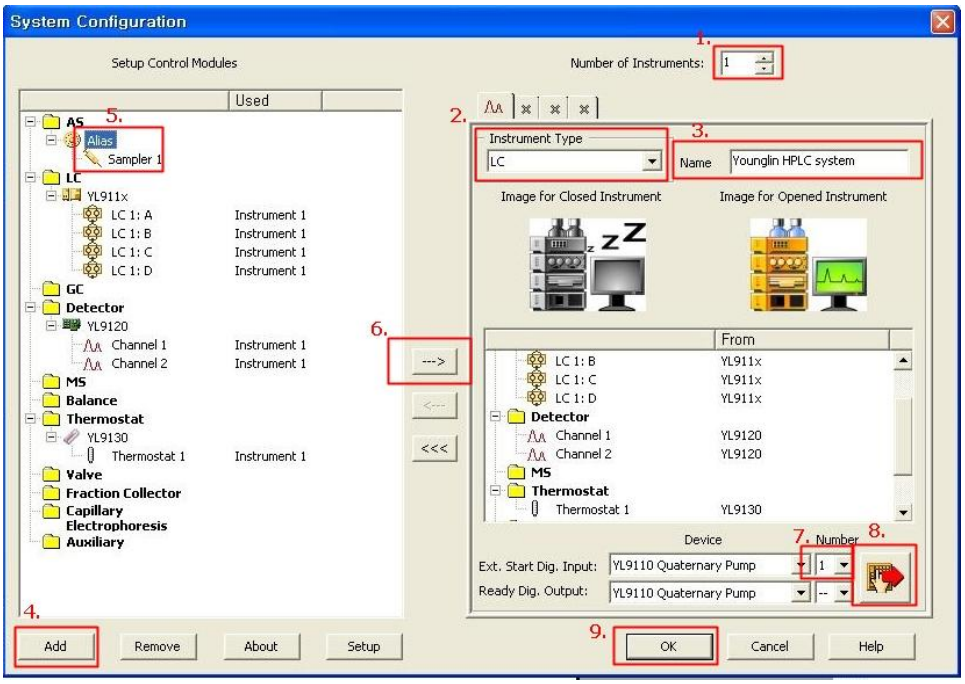
2-3. Instrument setting

1. Click  on the left side of initial screen, the below is shown to set the instruments.



- To select the polder for project file, click the **Directories**

<Selecting folder for Project file>



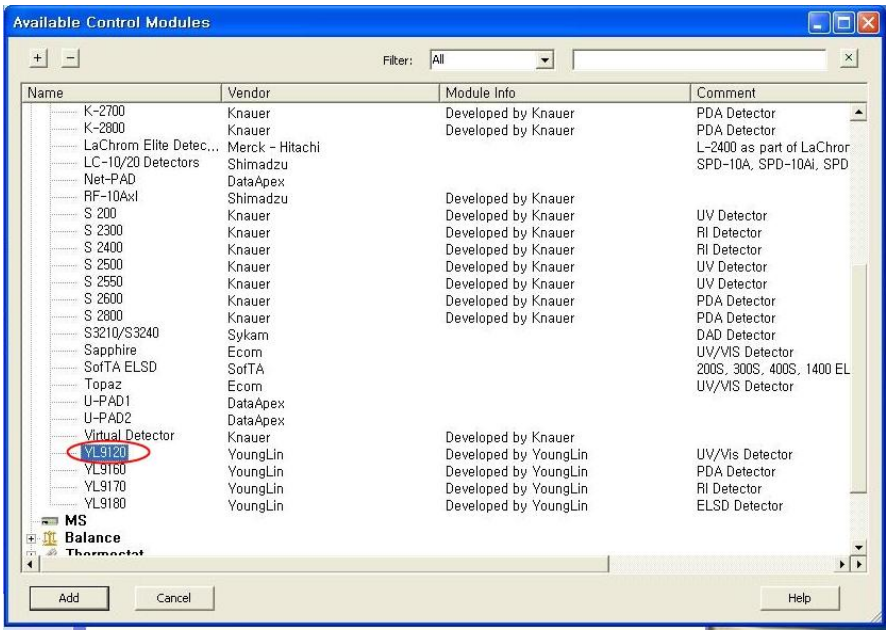
<System configuration window>

2. Select the **number of system(1)** → Select Instrument **Type(2)** as LC, LC-PDA or GPC → Input the **name of instrument(3)**

3. Click on **ADD(4)** to add the instrument.

- On the setup control window, select the module (AS, LC, Detector, etc.) and input the IP and Port Number.

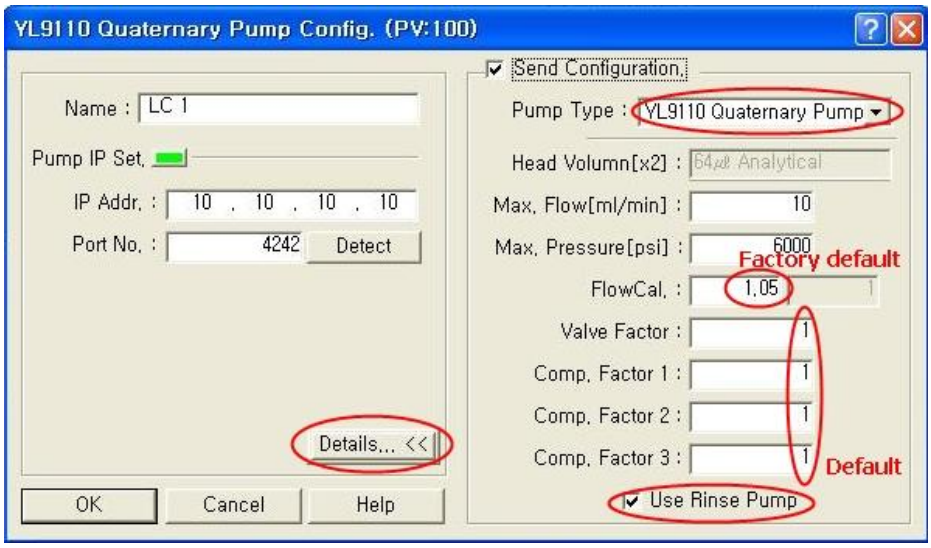
(The IP address and Port for each module of YL9100 are set automatically)



<Add window>

- RID, ELSD, ECD and Auto sampler have to use the serial port on computer.

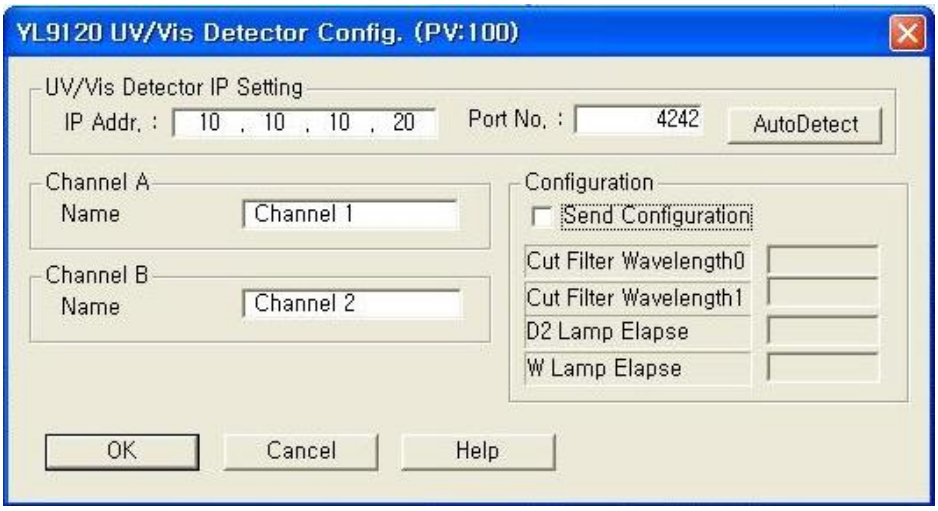
Add => LC => Select Pump 9110(Quaternary)=> IP 10.10.10.10, Port 4242



<Pump configuration>

- In detail window, select the type of pump and check up using rinse pump.

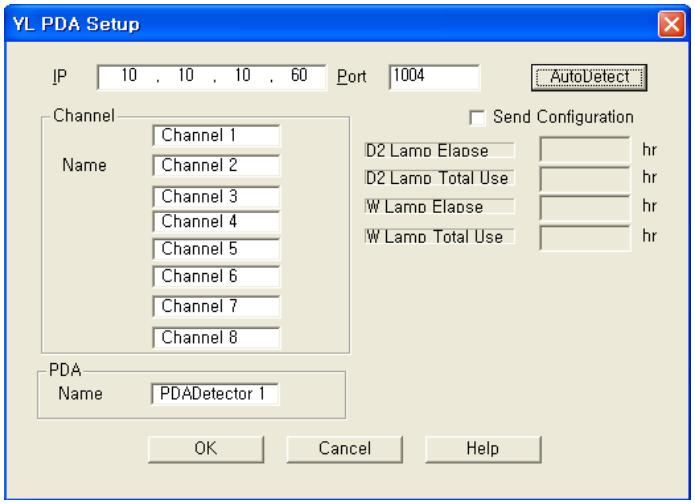
Add => Detector => Select 9120(UV/Vis)=> IP 10.10.10.20, Port 4242



<UVD configuration>

- If you change the lamps, make zero of the lamps's elapse in this window.

Select 9160(PDA)=> IP 10.10.10.60, Port 1004



<PDA configuration>

- If you change the lamps, make zero of the lamps's elapse in this window.

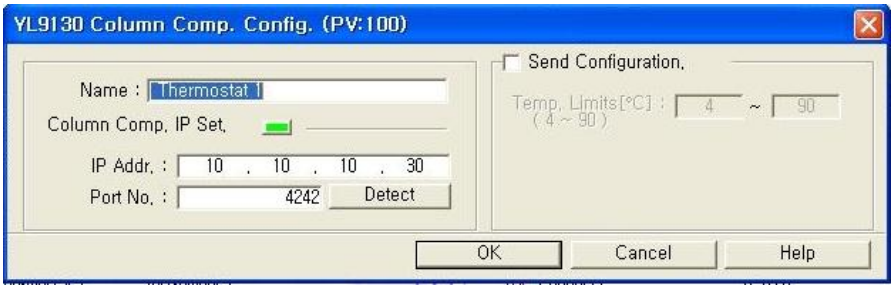
Select 9170(RID)=> Select the COM No.

<RID configuration>

Select 9180(ELSD)=> Select the COM No.

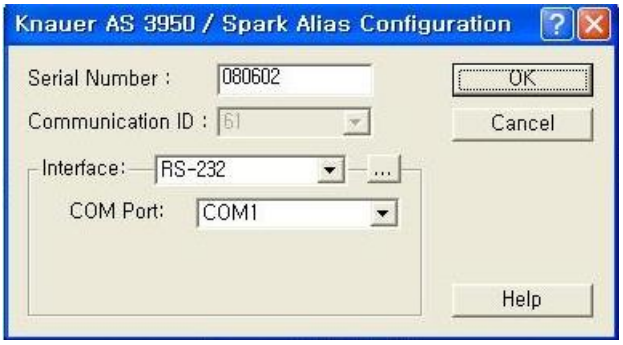
<ELSD configuration>

Add => Thermosat => Select 9130 => IP 10.10.10.30, Port 4242



<Column compartment configuration>

Add => Autosampler => Select Spark Alias => ID 61, Select the COM No.



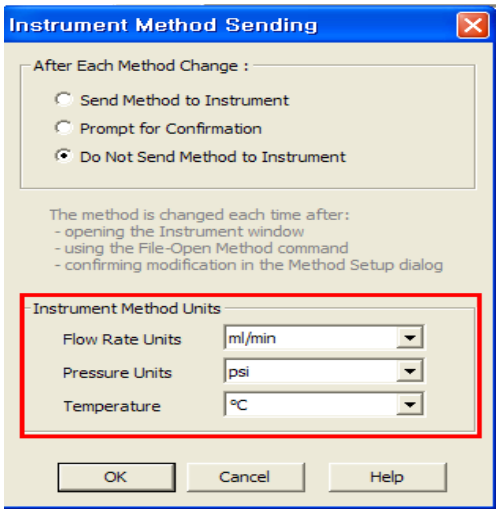
<Auto sampler configuration>

Select Spark Midas => ID 60, Select the COM No.

4. Select each **modules(5)** located at left side, and then using the **arrow button(6),** insert each module to the right window to activate the system.

5. Select the module connected with remote cable and choose No. 1**.(7)**

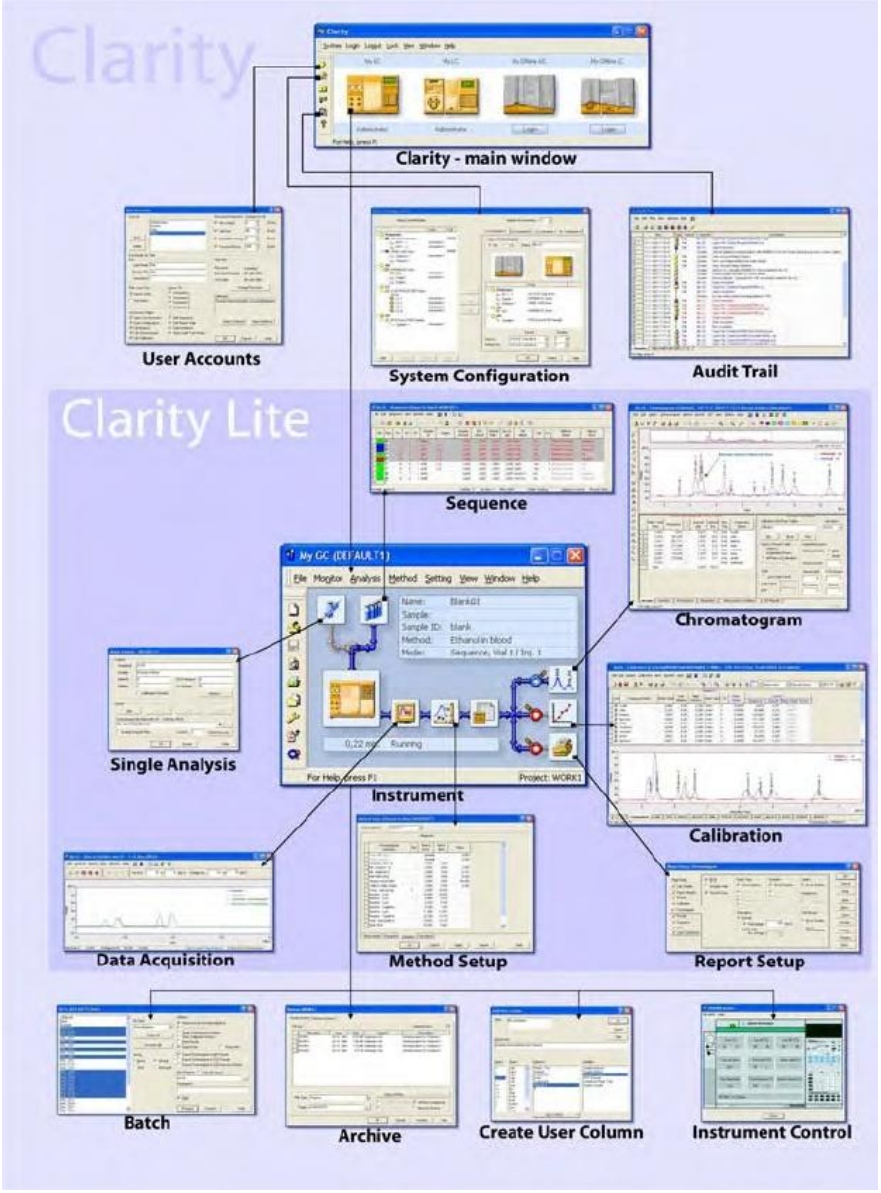
→ Press the icon  **(8),** and select the unit, and then click OK**(9)** button.



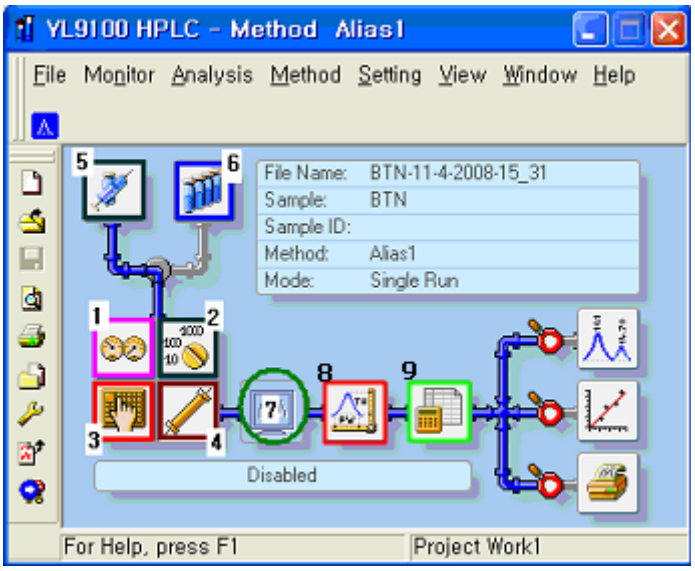
6. When you click Login button on the initial window, the method window is displayed.

※ If you already configured the system, it is not necessary to open the **System config**.( ) menu.

2-4. System Method setup



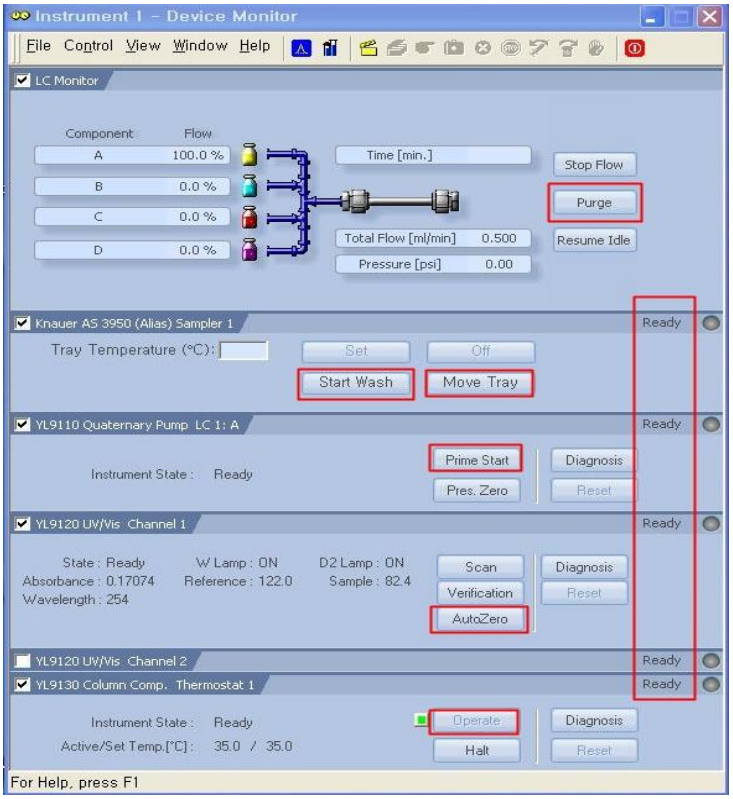
<Fundamental structure of YL clarity>



<Method window>

(1) Device Monitor(1)  **Icon**

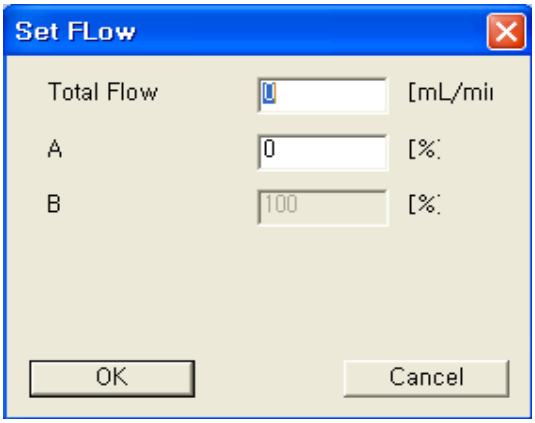
: On this window, you can control simple operation menu as like **Prime Start, Purge**. **Auto zero of Detector, Turn on & off lamps** and can monitor the system status.



<Device window>

1) Prime/Purge of Pump

- Click Purge button and set the solvent ratio and flow rate(set A solvent to 100% at first).
- This window is different depending on the pump configuration (isocratic/binary/quaternary)



<Binary Pump window>

- Open the Prime/Purge valve(Turn this valve to open way).
- Click "**Prime Start"** button and check it on the waste tubing.
- Do the same procedure for the other solvents(solvent B, C, D).

2) Wash / Move tray

- When you change the washing solvent or replace the syringe, try to "**Wash"** three times.
- When you insert or take out the tray, use "**Move tray"**.

3) Ready of each modules.

- Click the "**Send method**" in method setup window then you can make ready status of each modules.

Acquisition(2)  **, Control(3)**  **, Measurement(4)**  **, Integration(8)**  **, Calculation(9)**

 Button.

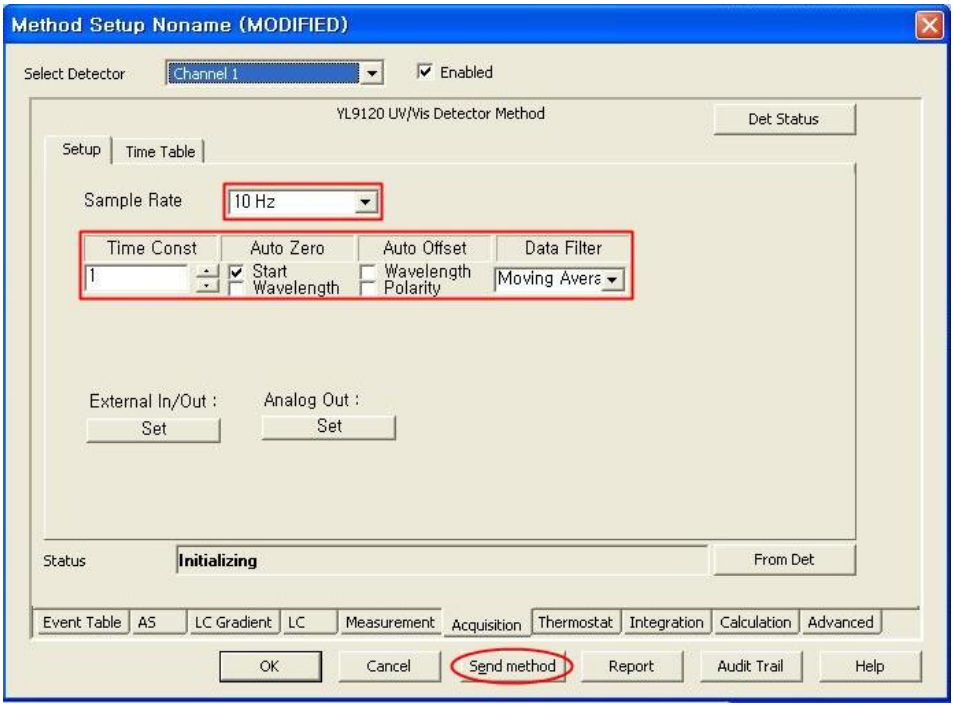
If you click one of these icon, the Method setup window is displayed to set the instrument control. You can set all of conditions concern with system control, data acquisition, and data process in one window.

(2) Acquisition

- Set the detector control parameters.

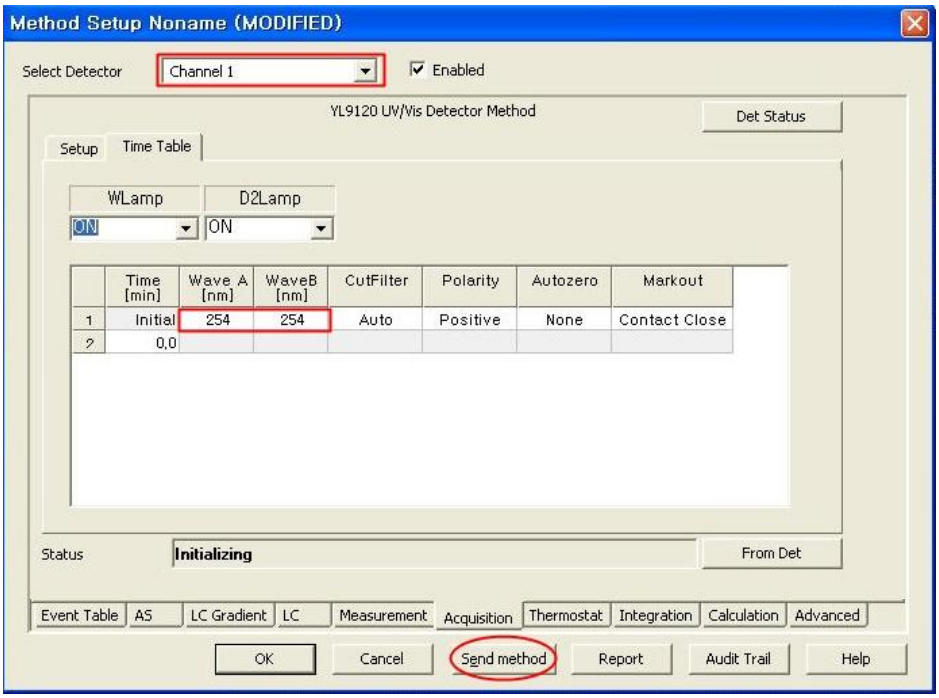
a) Setup

- Sample Rate → Dual wavelength(1 Hz) / Single wavelength(10 Hz) are Default value.



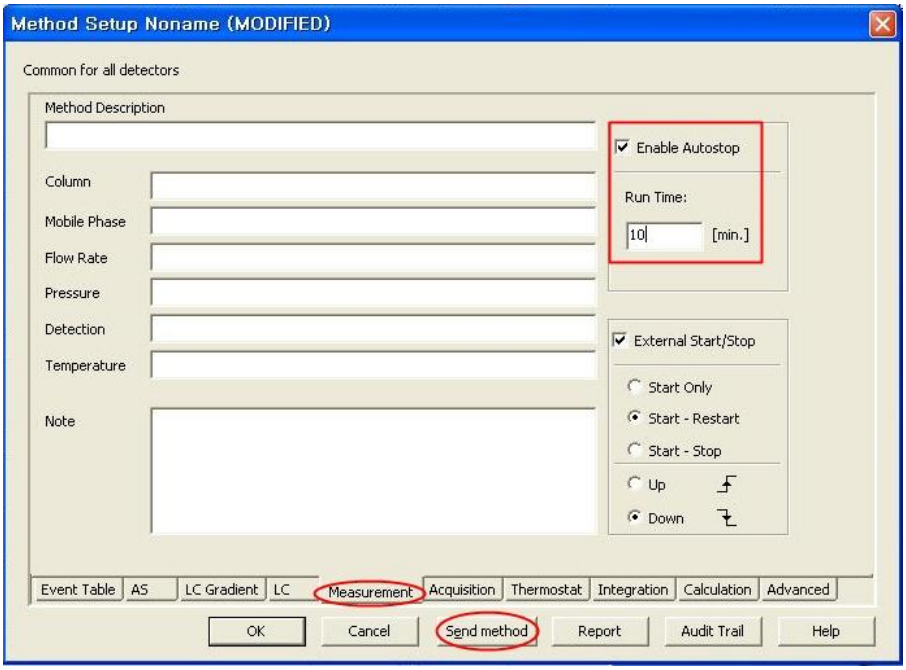
b) Time Table

: In case of single wavelength, Wavelength A, B has to be set same wavelength.



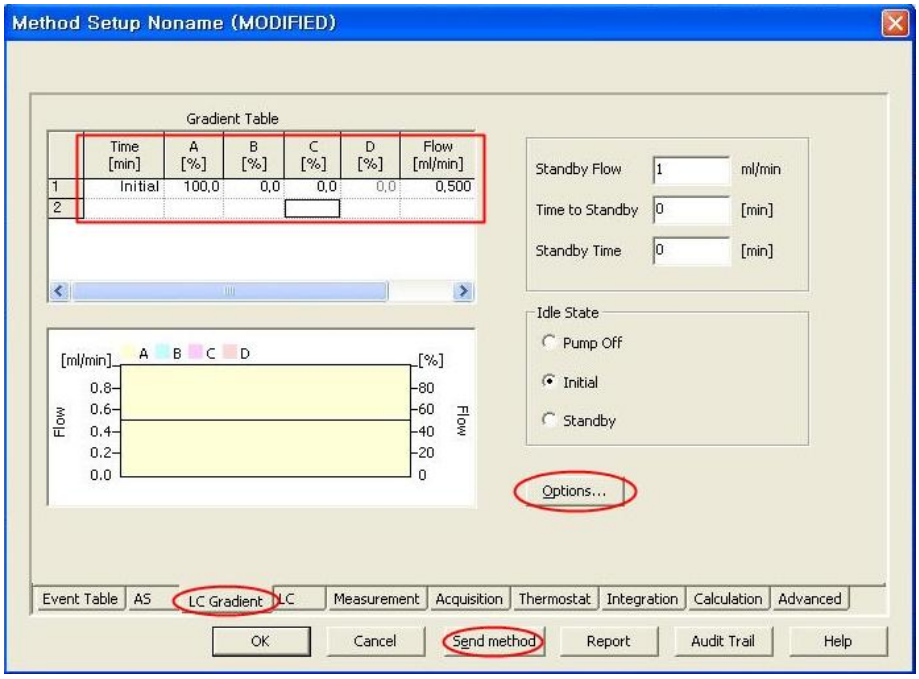
(3) Measurement

- Input the information of analysis conditions such as column, mobile phase, flow rate, etc., and input note.
- In this window, you have to check the “Enable Autostop” and set the Run time.
- The Run Time should be higher than analysis time of autosampler.



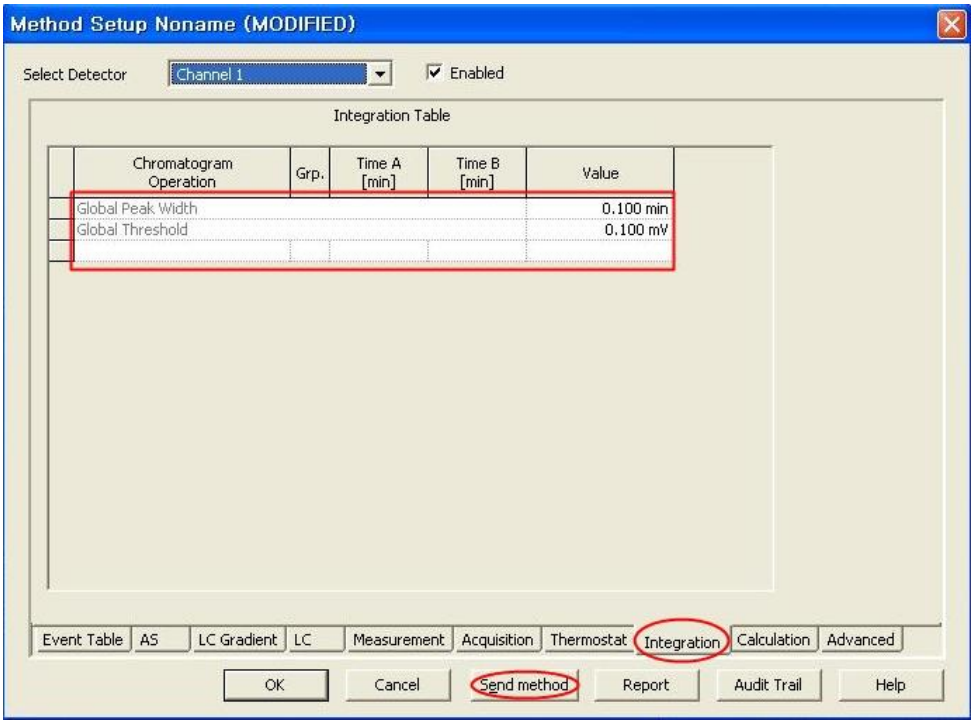
(4) LC Gradient

- Input the flow rate and solvent ratio of pump.
- If you want to use the gradient condition, make a gradient program on this window.
- You can make the name of solvent in “Options” window



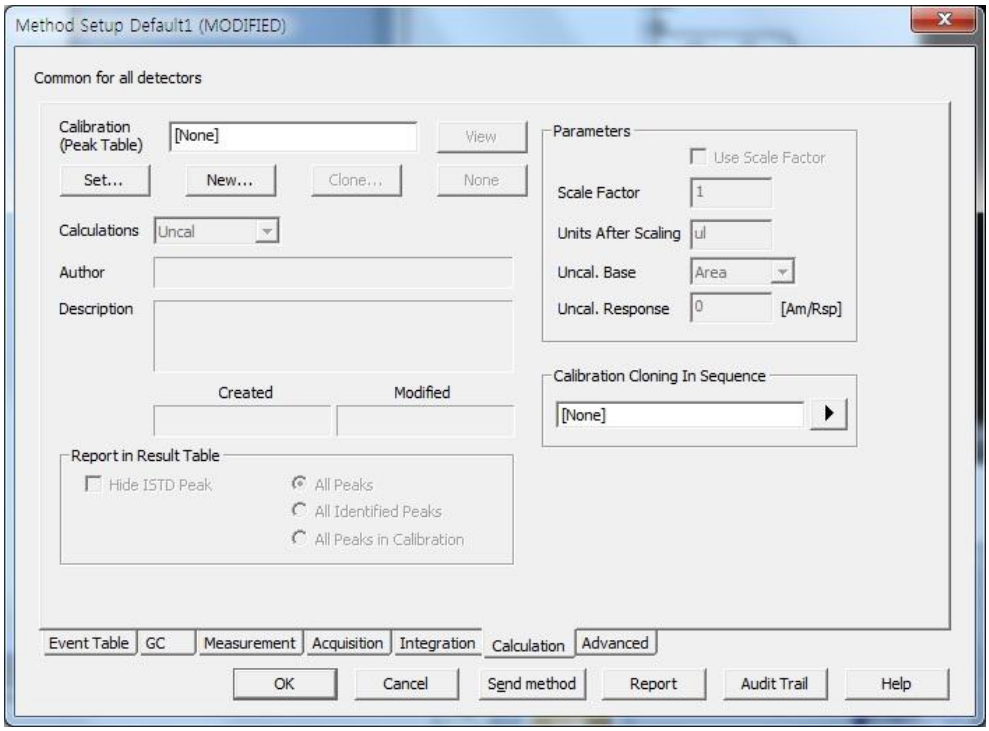
(5) Integration

- Input the global setting values and integration events.



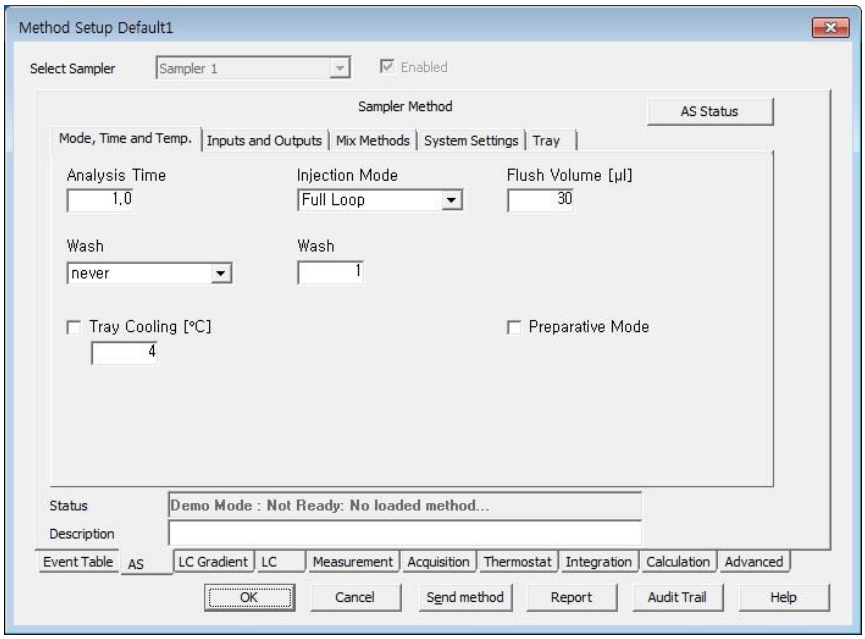
(6) Calculation

- Apply a calibration file in calculation window

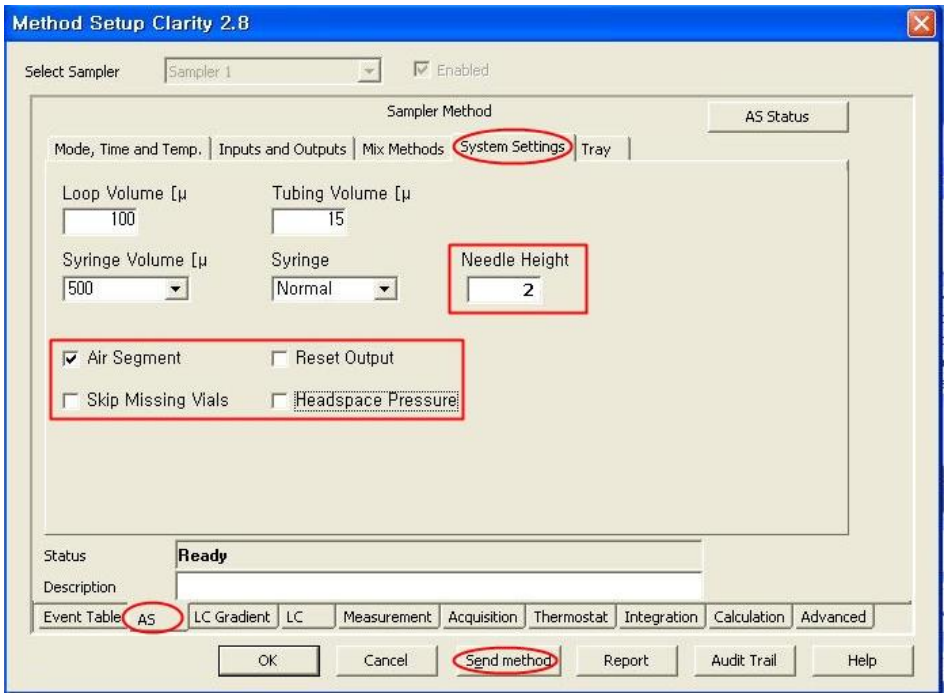


(7) AS

- If you use an autosampler, set the operation condition of autosampler.
- Set Analysis Time, Injection mode and washing method.

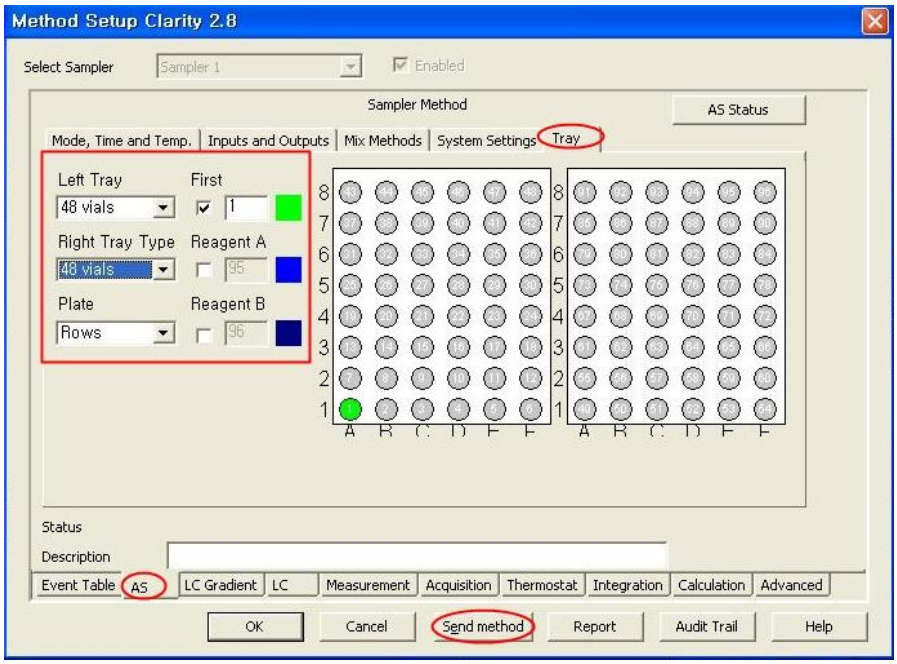


- Check up the parameters in System Setting window.



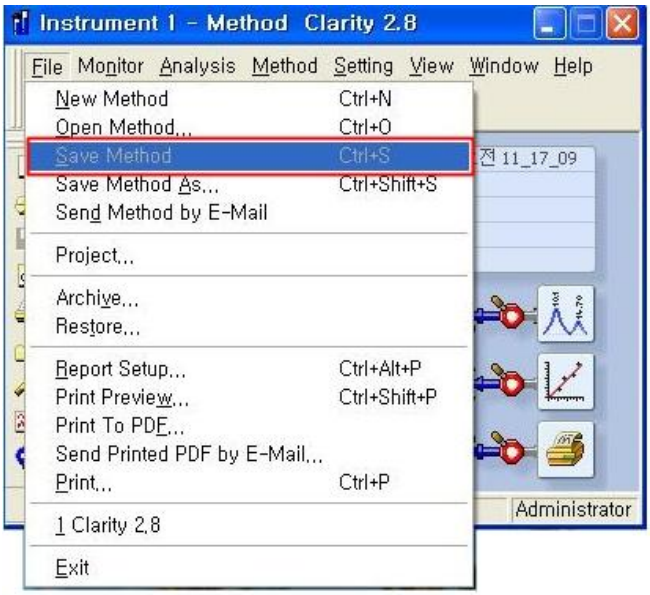
<Recommended setting for auto sampler>

- Finally, set a kind of Tray and First vial in Tray window.



(8) Save Method

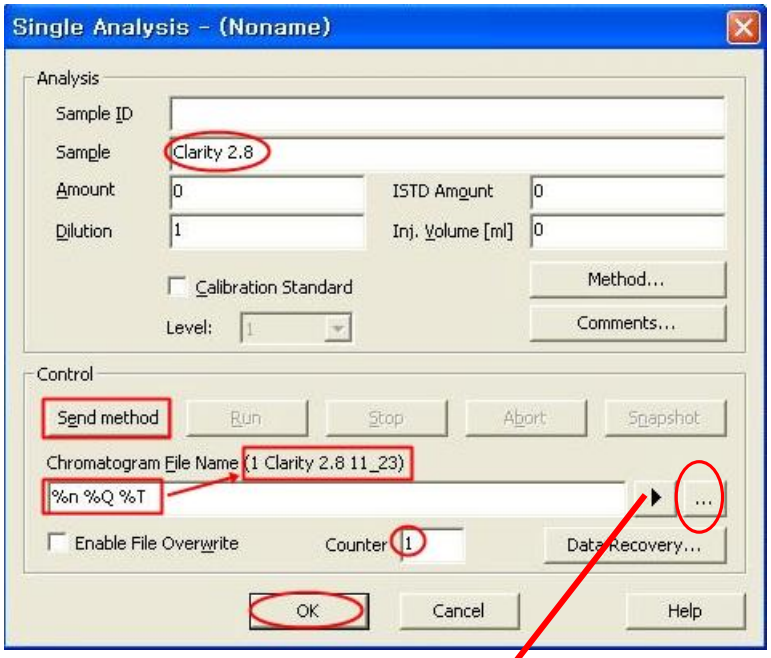
- After input the parameters, click "**Send method"** button and **OK**.
- On the File menu, select Save as Method or Save the Method file as a *.met.

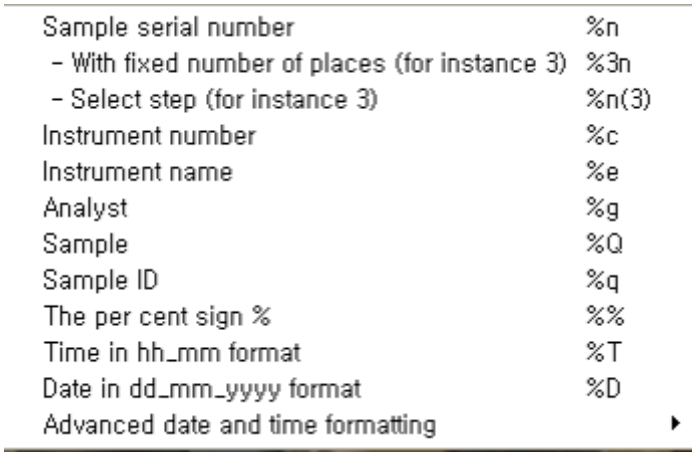


2-5. Sample Analysis

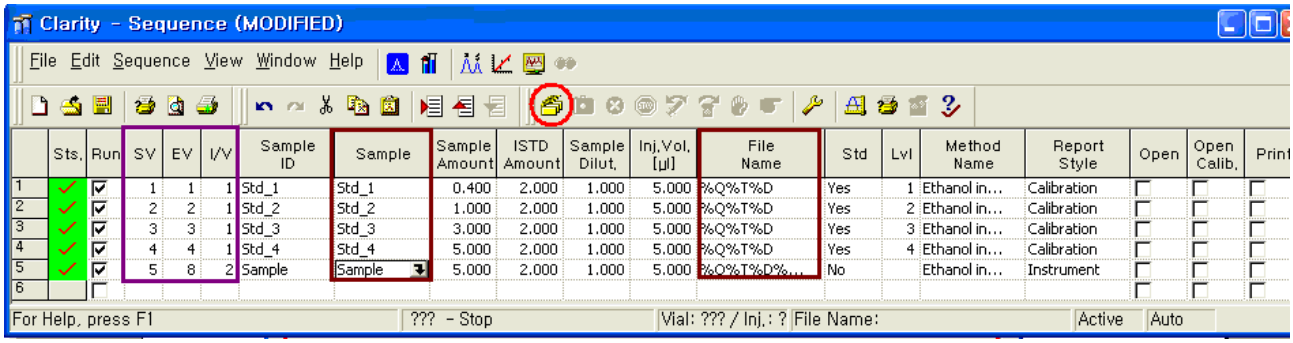
1) Single Analysis

- On the main window, click  icon, and input the sample name and file name, after that click OK button.
- If the Remote Start Line is connected from the injector, the data will be collected when you inject the sample.
- If you want to set the directory to save data, click arrow button under the Chromatogram File name. And then directory selection window is opened.





2) Sequence : When you use an Autosampler, you can make a sequence table. Click  icon on the main window.



- Input Start Vial(SV) number, End Vial(EV) number, and the number of injection per each vial(I/V).
- Setup Sample name, File name, and Injection volume.
- If you want to use different Method file for each vial, you can set different Method file for each line.
- After setup the sequence, click Run Sequence  icon, and then the sample injection starts.

2-6. Data acquisition

1) If you click  icon on the main window, the data acquisition window is displayed.

2) You can set the time range on the Time from 00 to 00 min.

3) Icons

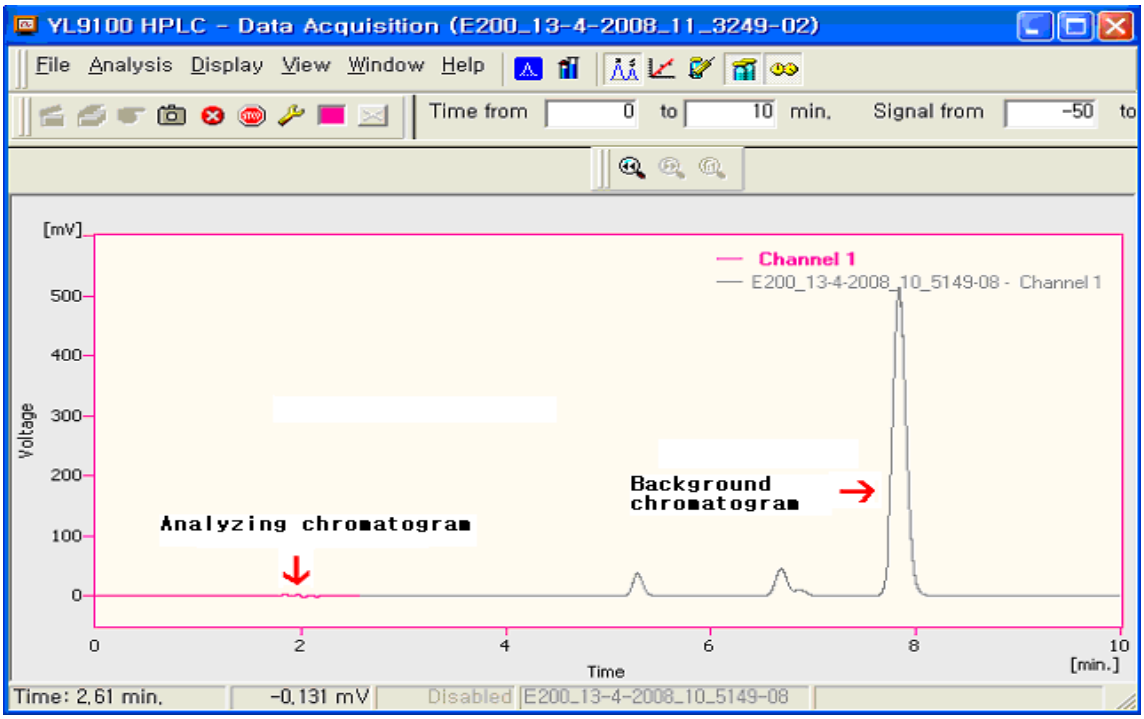
 Snapshot : If you click this icon, you can get integration result during data acquisition.

 Abort : If you click this icon, stop the data acquisition and the data is not saved.

 Stop :. If you click this icon, stop the data acquisition and the data is saved.

4) Background chromatogram

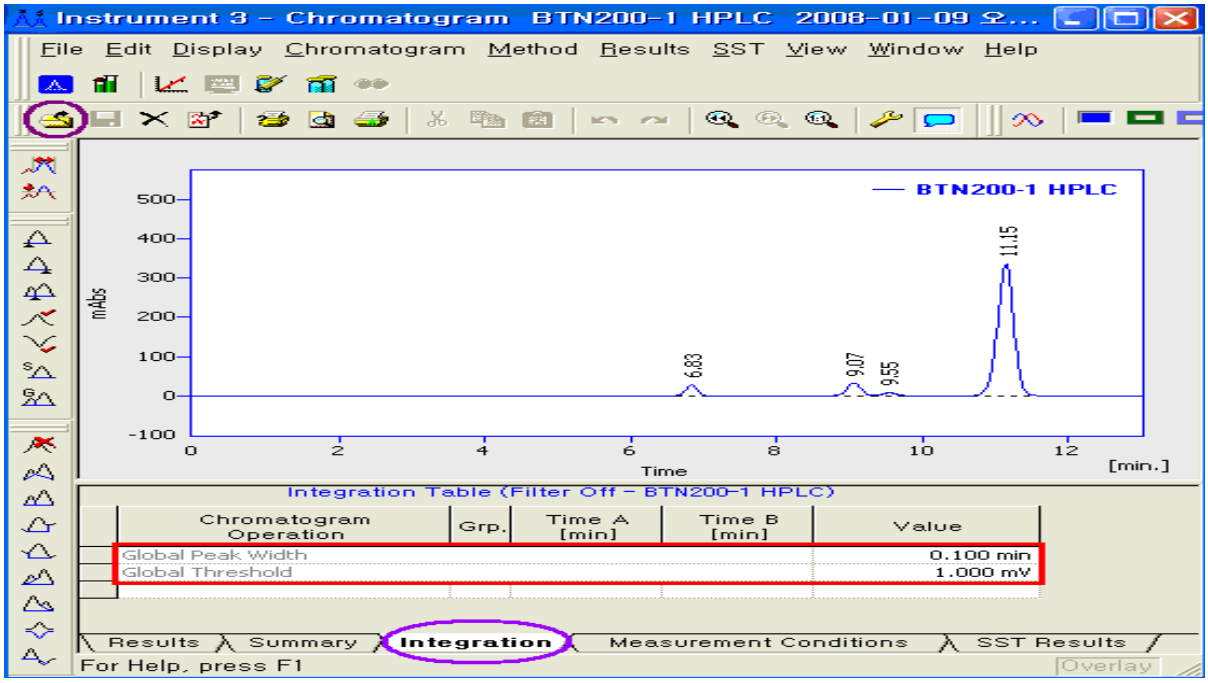
Click "**File**" menu on the top → Click "**Set Background Chromatogram**" → Select chromatogram file you want to use as a background → Background chromatogram is displayed on the data acquisition window



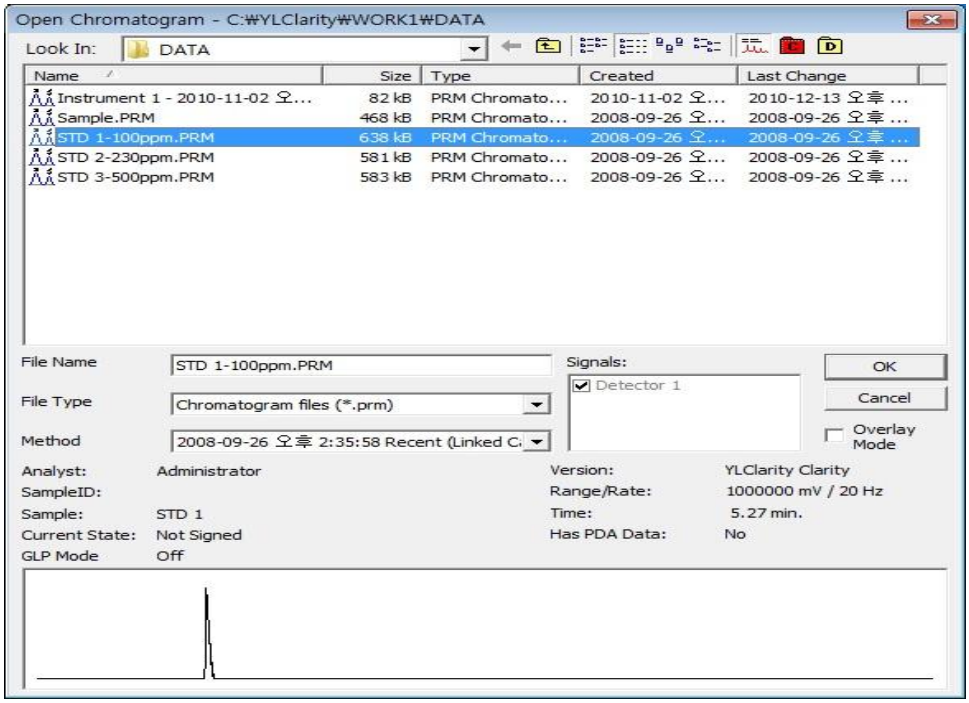
- The monitoring signal can be displayed if there is no sample injection.
- After finished data acquisition, chromatogram is saved in the Data folder, this data can be checked on the chromatogram window  .

2-7. Integration

If you click chromatogram window  icon on the main window, the following is displayed.



1) Click  icon and select a data file want to integrate.



2) The chromatogram is displayed on the Open chromatogram window. If you want to load this data, click OK button.

3) Setup Integration Factor

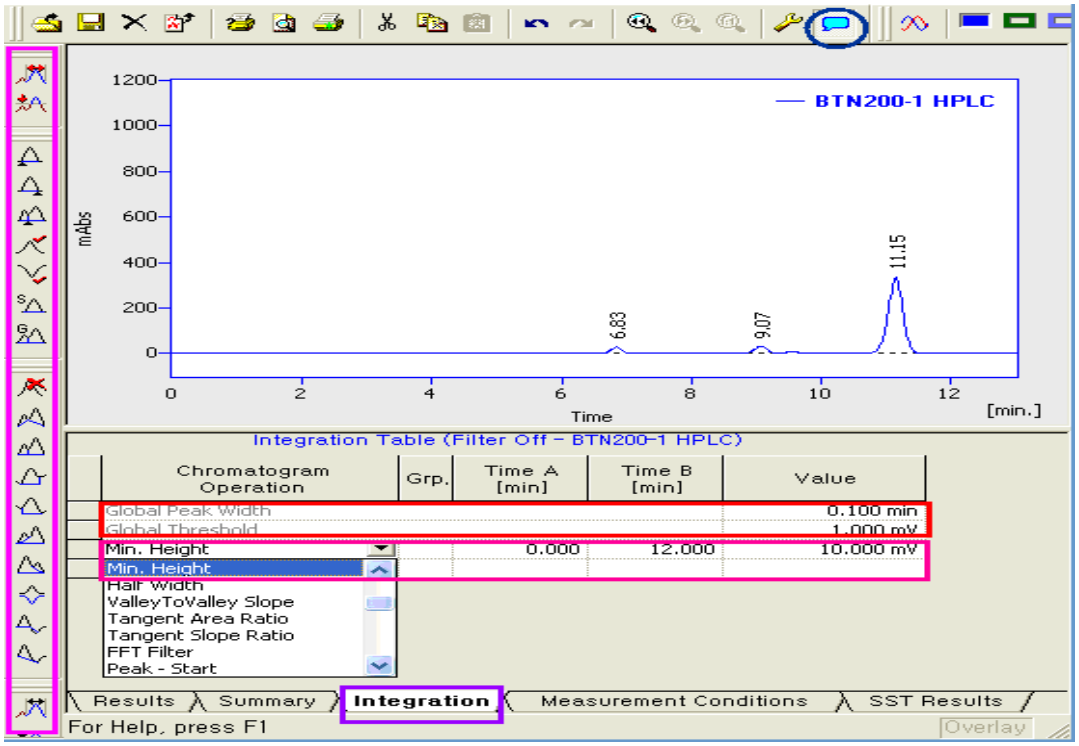
Click Integration menu on the chromatogram window,

a. Set Basic integration Factor (Peak width, Threshold) Value and Enter.

b. Additional integration Factor setup

- Click integration event table and select event want to use, and input the time range and value. Press Enter.

- Using integration event icons on the left side, input the integration event. At first, select the event icon want to use and then click start /stop point to apply the event on the chromatogram.

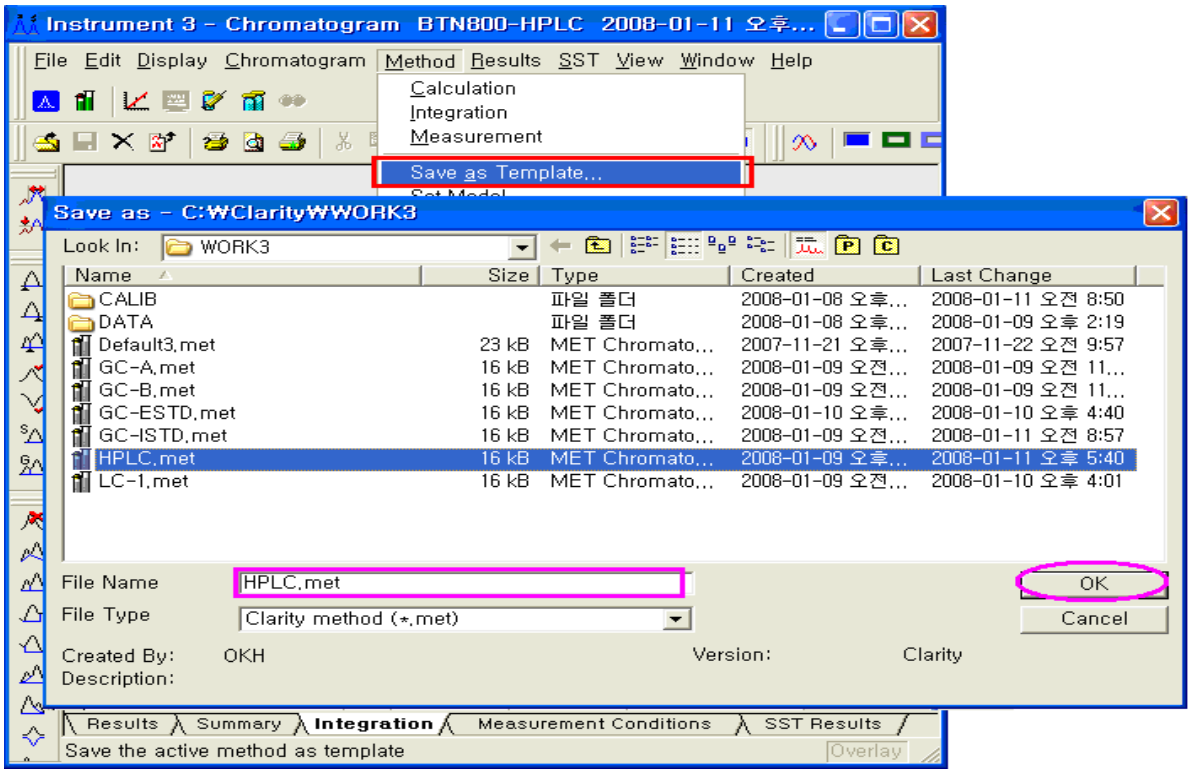


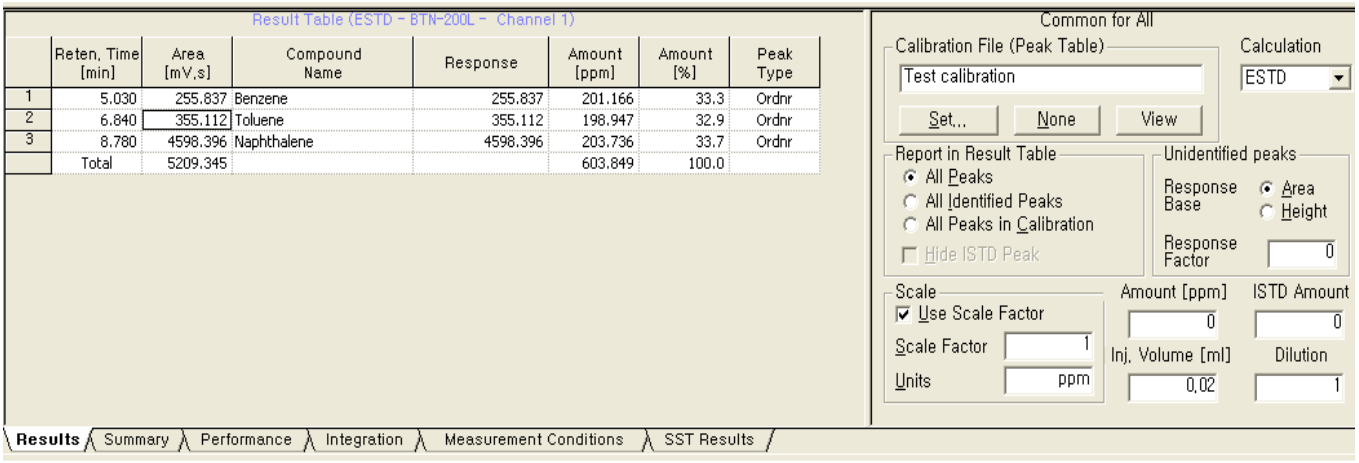
4) Using  (next, previous)buttons, you can apply integration events on the other chromatogram data.

5) Save Factor Method(Batch operation)

- Click Method menu on the top, select Save as Template.

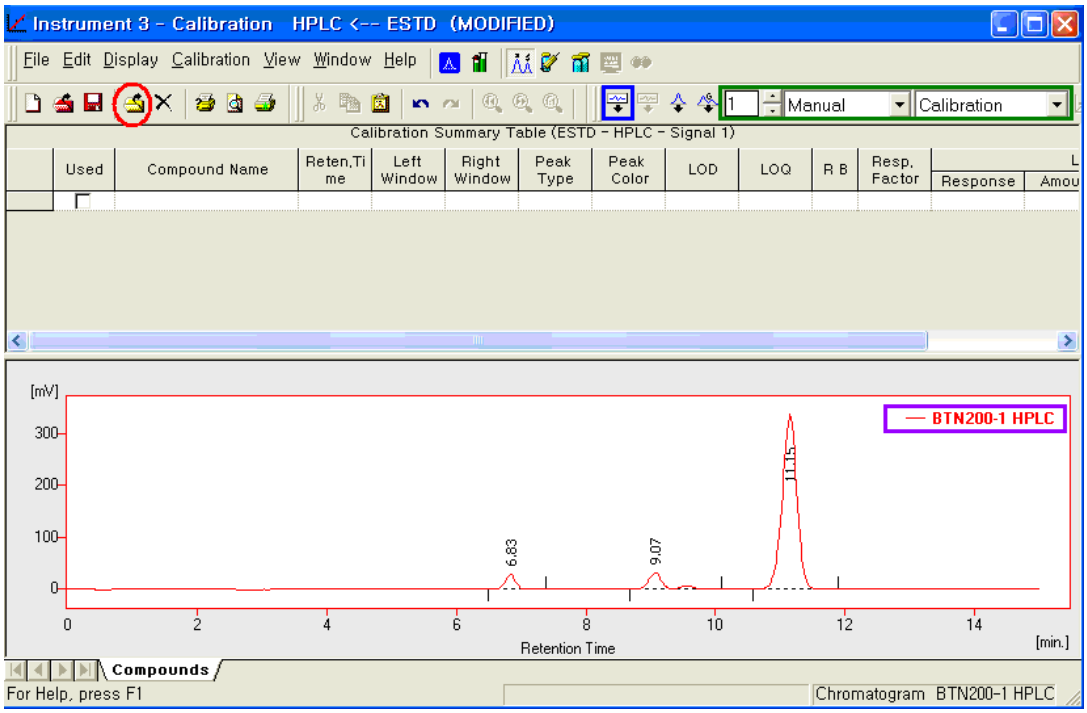
- Input Method file name and click OK to save.


Instrument 3 - Chromatogram BTN800-HPLC 2008-01-11 오후...
File Edit Display Chromatogram Method Results SST View Window Help
Calculation
Integration
Measurement
Save as Template...
Save as - C:₩Clarity₩WORK3
Look In: WORK3
Name Size Type Created Last Change
CALIB 파일 폴더 2008-01-08 오후... 2008-01-11 오전 8:50
DATA 파일 폴더 2008-01-08 오후... 2008-01-09 오후 2:19
Default3.met 23 kB MET Chromato... 2007-11-21 오후... 2007-11-22 오전 9:57
GC-A.met 16 kB MET Chromato... 2008-01-09 오전... 2008-01-09 오전 11...
GC-B.met 16 kB MET Chromato... 2008-01-09 오전... 2008-01-09 오전 11...
GC-ESTD.met 16 kB MET Chromato... 2008-01-10 오후... 2008-01-10 오후 4:40
GC-ISTD.met 16 kB MET Chromato... 2008-01-09 오전... 2008-01-11 오전 8:57
HPLC.met 16 kB MET Chromato... 2008-01-09 오후... 2008-01-11 오후 5:40
LC-1.met 16 kB MET Chromato... 2008-01-09 오전... 2008-01-10 오후 4:01
File Name HPLC.met
File Type Clarity method (*.met)
OK
Cancel
Created By: OKH
Version: Clarity
Description:
Results Summary Integration Measurement Conditions SST Results
Save the active method as template
Overlay


Result Table (ESTD - BTN-200L - Channel 1)
Reten. Time [min] Area [mV.s] Compound Name Response Amount [ppm] Amount [%] Peak Type
1 5.030 255.837 Benzene 255.837 201.166 33.3 Ordnr
2 6.840 355.112 Toluene 355.112 198.947 32.9 Ordnr
3 8.780 4598.396 Naphthalene 4598.396 203.736 33.7 Ordnr
Total 5209.345 603.849 100.0
Common for All
Calibration File (Peak Table)
Test calibration
Set... None View
Calculation
ESTD
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peak
Unidentified peaks
Response Base Area Height
Response Factor 0
Scale
Use Scale Factor
Scale Factor 1
Units ppm
Amount [ppm] 0
ISTD Amount 0
Inj. Volume [ml] 0.02
Dilution 1
Results Summary Performance Integration Measurement Conditions SST Results

2-8. Calibration

If you click calibration window  icon on the main window, the following is displayed.



1) Open Data for calibration 

Click  icon => select Data file => OK!

- The selected data is displayed on the Calibration Window.

2) Calibration table 

Input calibration Level (concentration level of standard) and select [Calibration].

Click “Add All(insert component)” icon  (Confirm present Level and click OK)

=> The following window is displayed as much as the number of compounds.

After input conditions, the following calibration table is displayed.

Calibration Summary Table (ESTD - HPLC - Signal 1)

	Used	Compound Name	Reten,Time	Left Window	Right Window	Peak Type	Peak Color	LOD	LOQ	R B	Resp. Factor	Level 1			
												Response	Amount	Resp. Fac	Rec No.
1	☑	Benzene	6.833	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	304.4057	200.000	0.6570	1
2	☑	Toluene	9.067	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	529.4299	200.000	0.3778	1
3	☑	Naphthalene	11.150	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	5279.8061	200.000	0.0379	1
	☐														

Used : Check on the compound want to calibrate

Compound Name : Input the name of compound

Peak Type : When you use ESTD, check Level and Response, and input Amount(concentration) of standard sample.

=> Level 1 STD inputting is finished.

For the Level 2, Level 3, etc., repeat above 1), 2) procedure

Add Level and concentration.

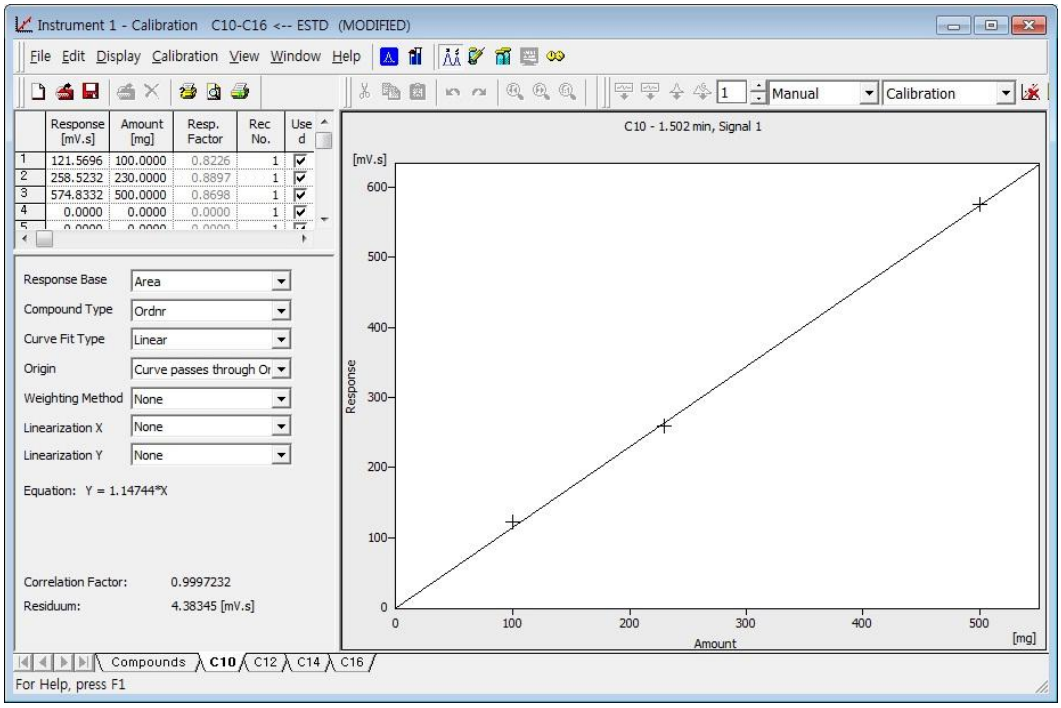
3) Calibration curve

If you click the name of compound on the calibration window, the calibration curve and the other information is displayed.

Response Base : Select Area or Height

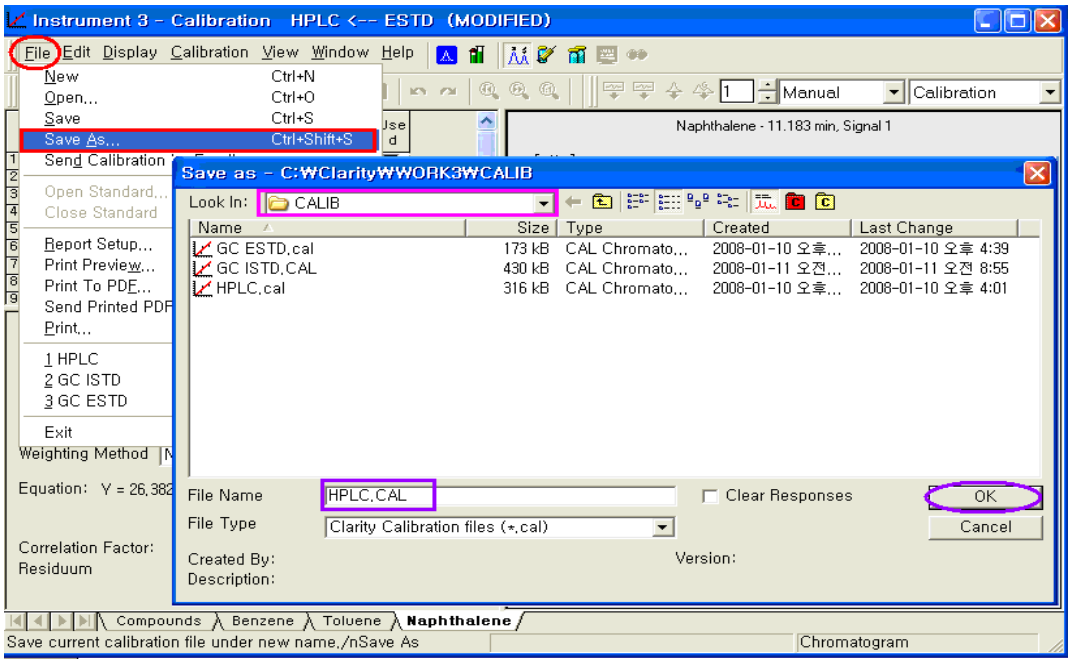
Origin : Select **Ignore origin**, **Compute with origin** or **Curve passes through origin**

Correlation Factor : R^2 value



4) Save Calibration file

Select File => Save As => Input the name of Calibration file, folder => OK

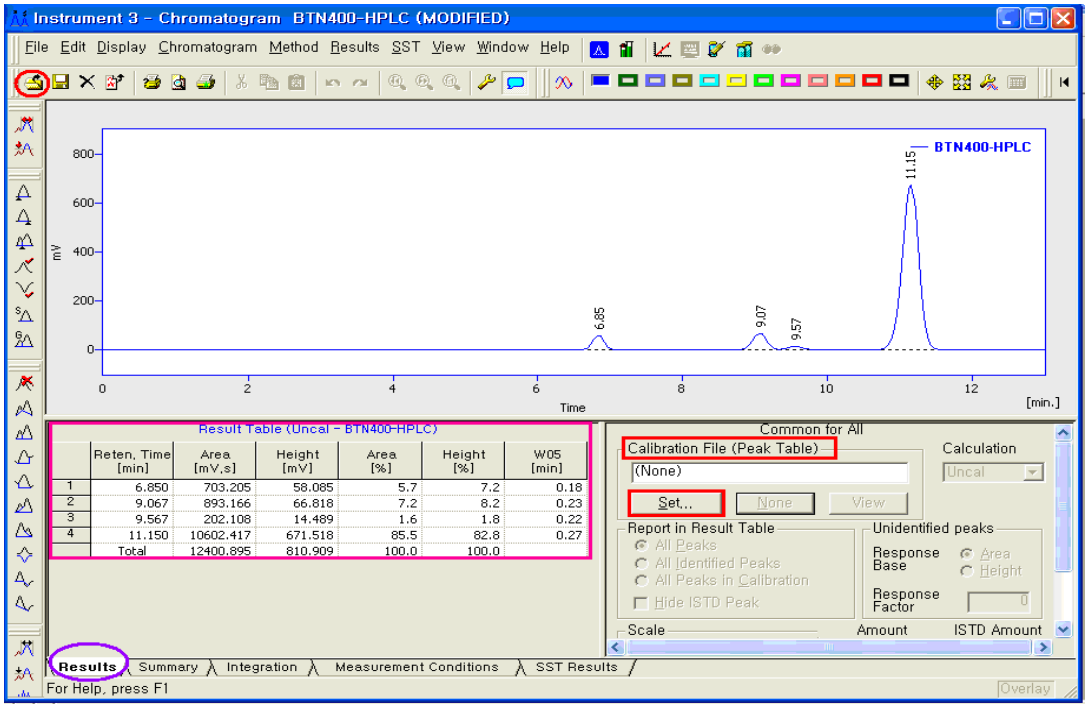


2-9. Quantification

1) Open Data

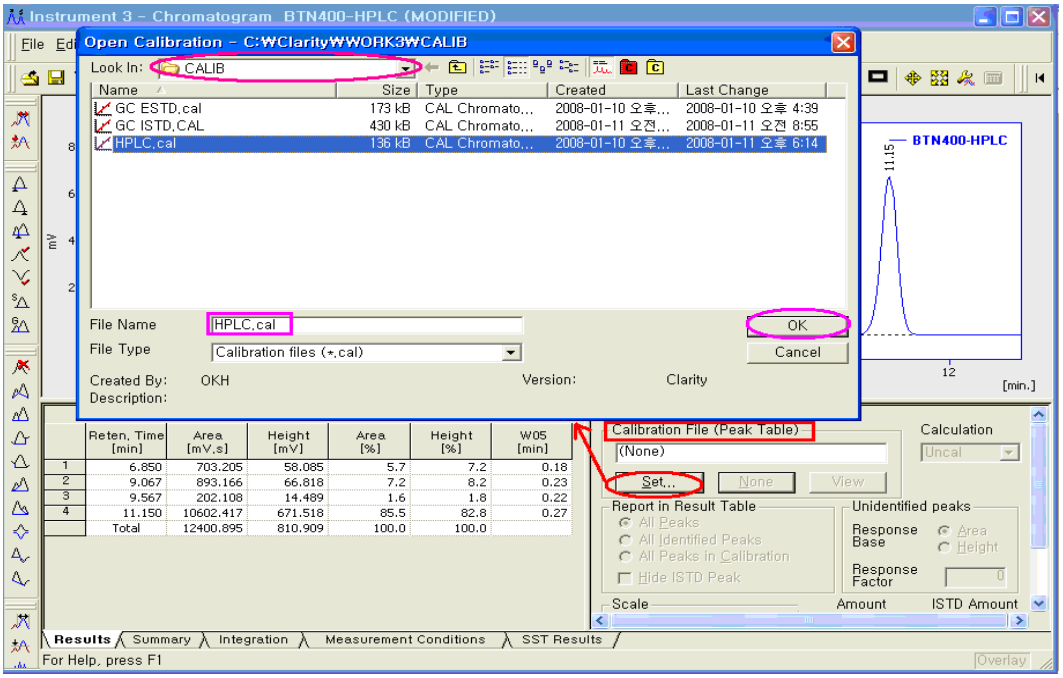
Click open icon  on the Chromatogram Window.

=> Select **Data file** => **OK!** => Chromatogram and result of opened data is displayed.

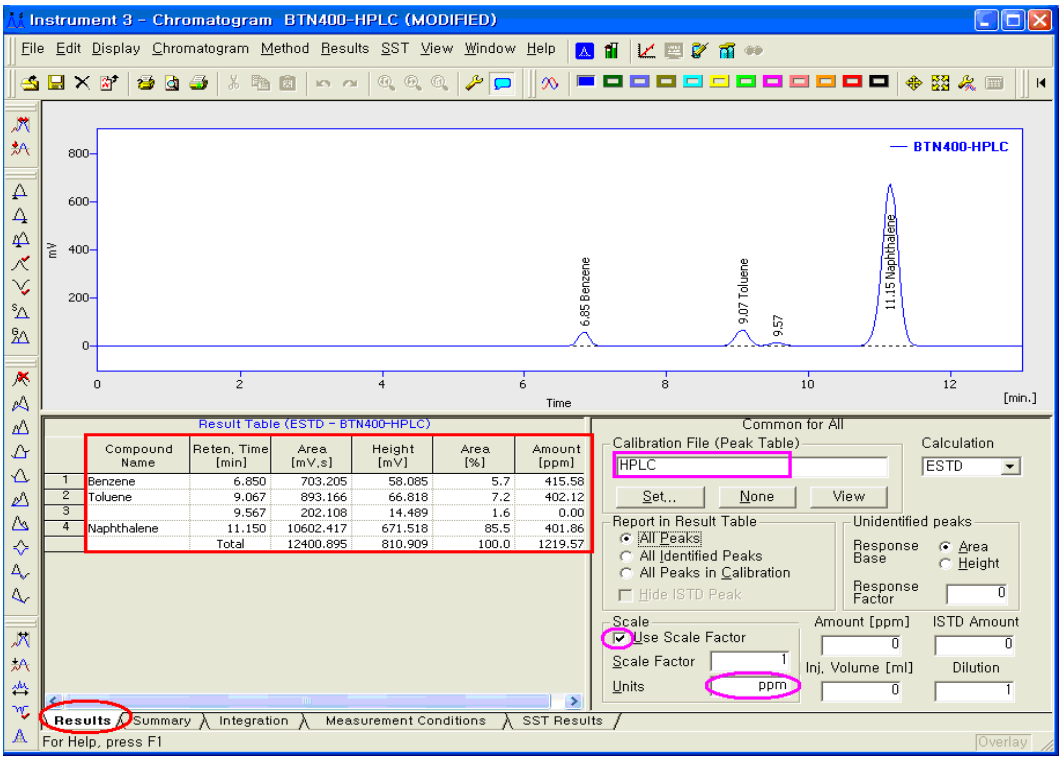


2) Apply calibration file

Click [Set] under the Calibration file(Peak Table) => Select Calibration file to use => OK



Quantification results are displayed as below.

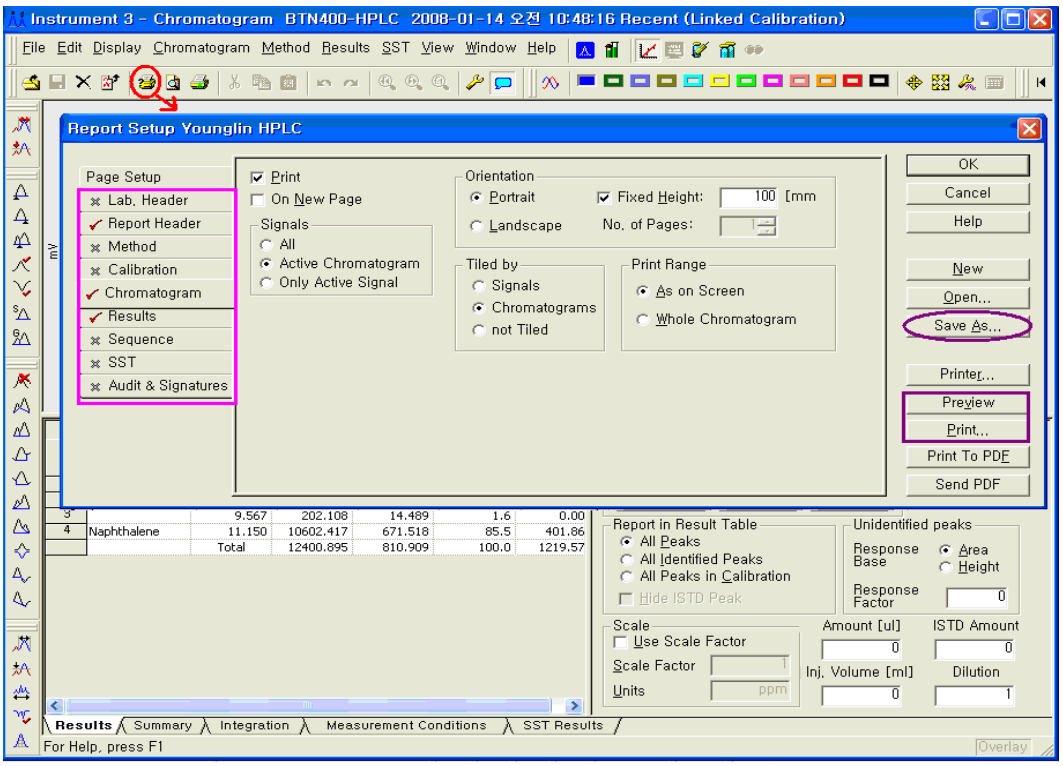


2-10. Print Report

Click report setup icon  on the Chromatogram Window.

=> On the Page Setup, select each option for report and edit report format

=> Click “Save As” => Save Report Style File => Preview  => Print  Click !



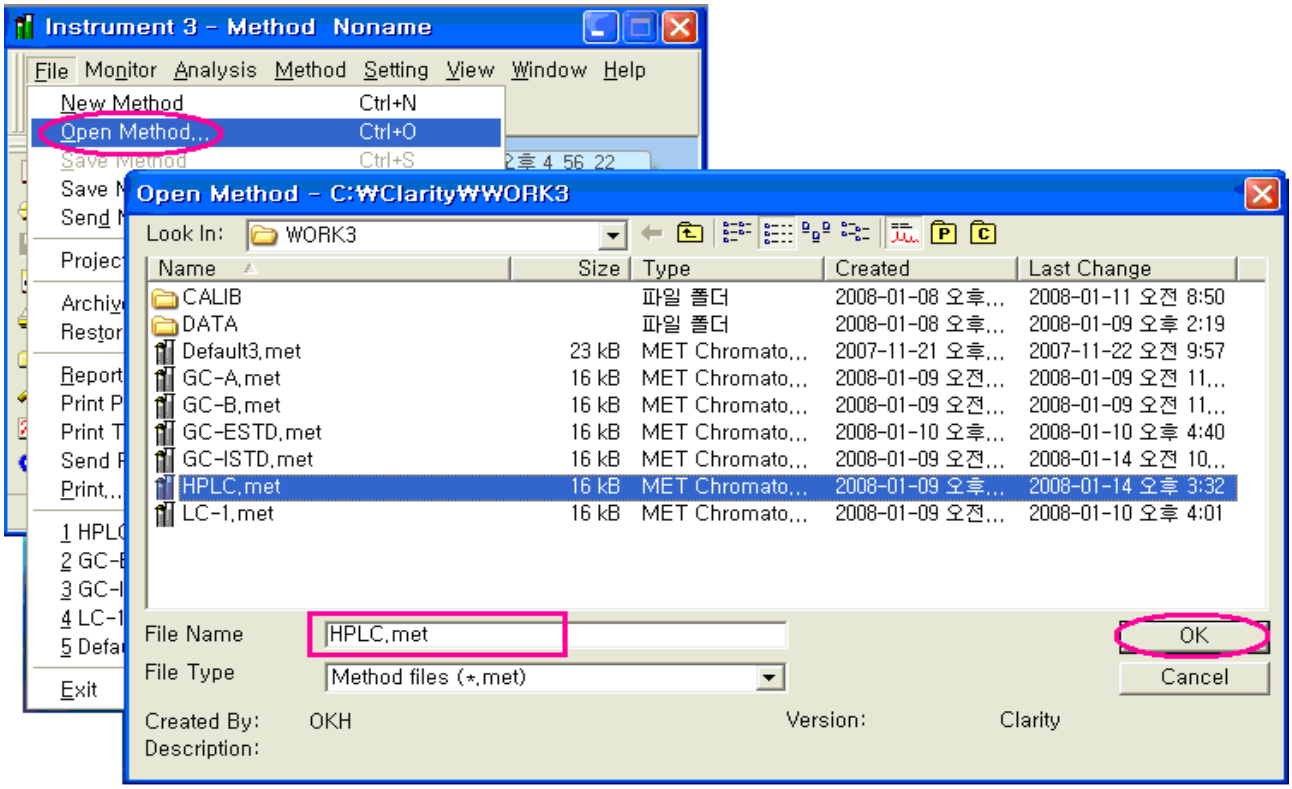
=> Report file is independent file, not related with Method file.

=> Last loaded Sty file is applied to print the report.

2-11. Batch operation(integration, quantification, print report)

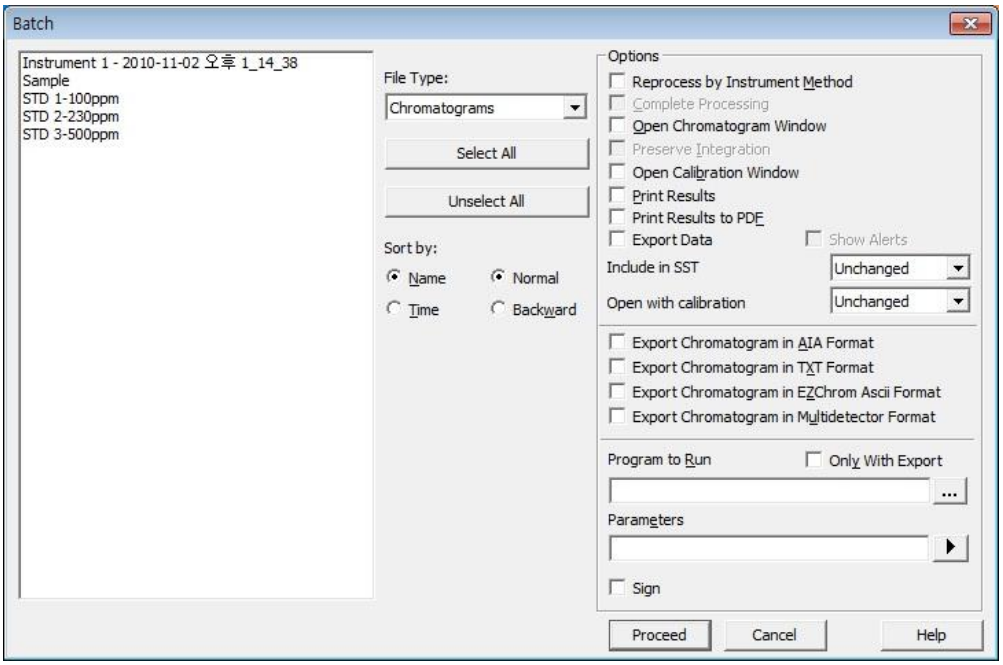
1) Method file(integration event + calibration file) => Save, Report format file(Report sty file) => Load

2) On the Instrument window => File => Open Method => Select Method file => OK



1) Batch analysis

Analysis => Batch => select data files => Options check => Proceed



- You can find the result on the Chromatogram Window.

- Using arrow button  , check all results step by step.

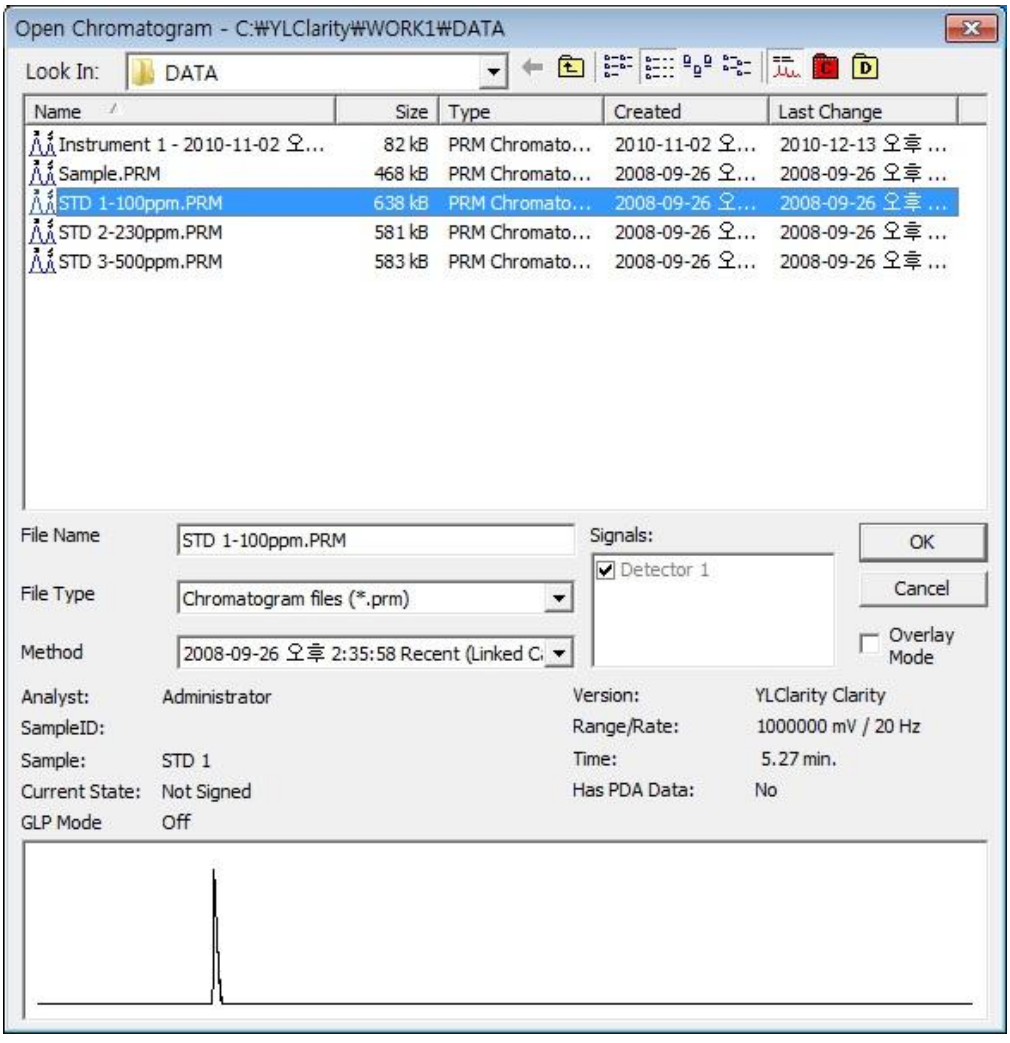
- The data file (PRM file) should be loaded in same project file (PRJ file).

2-11. Chromatogram Overlay and Statistics

1) Open chromatogram

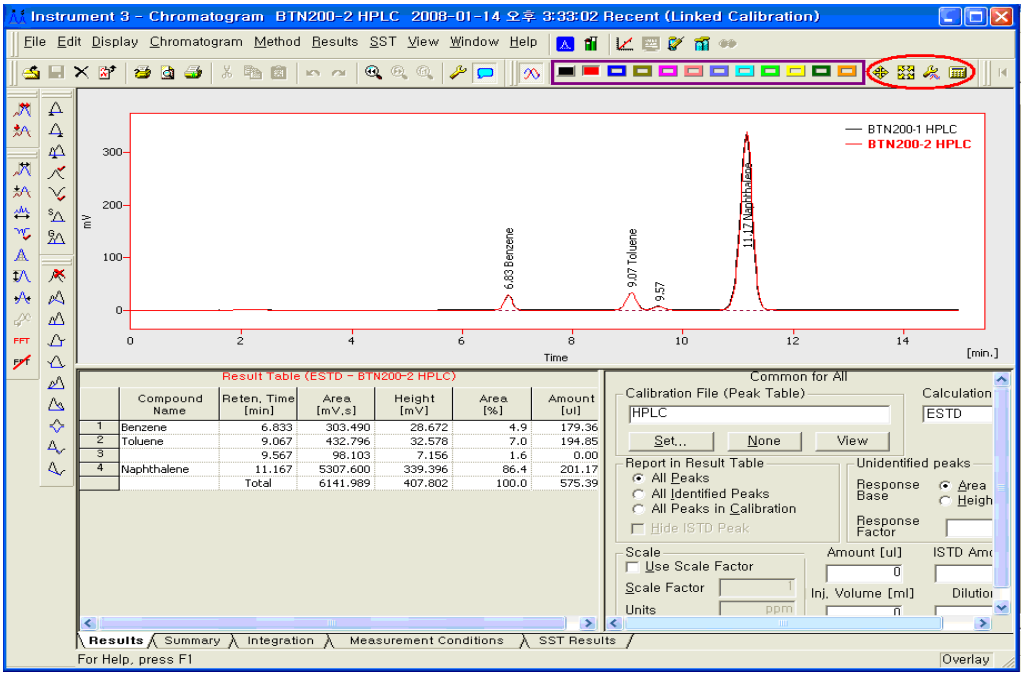
Click Overlay mode icon  on the Chromatogram Window.

=> File => “Open Chromatogram” => Select all data want to compare => OK !



The following overlay chromatogram is displayed.

Useful icon : chromatogram move, zoom in, amplify 



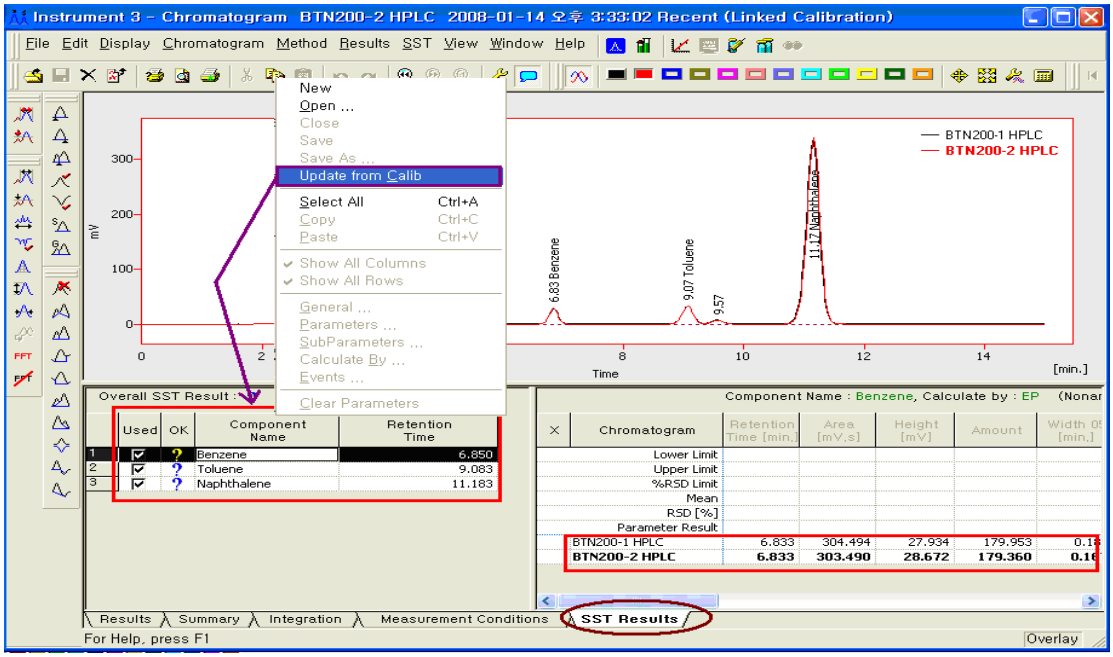
2) Result compare(SST)

Select “SST Result” on the menu => On the lower left window, click right mouse button

=> Click “Update from Calib”

=> The calibrated peak names are displayed on the table.

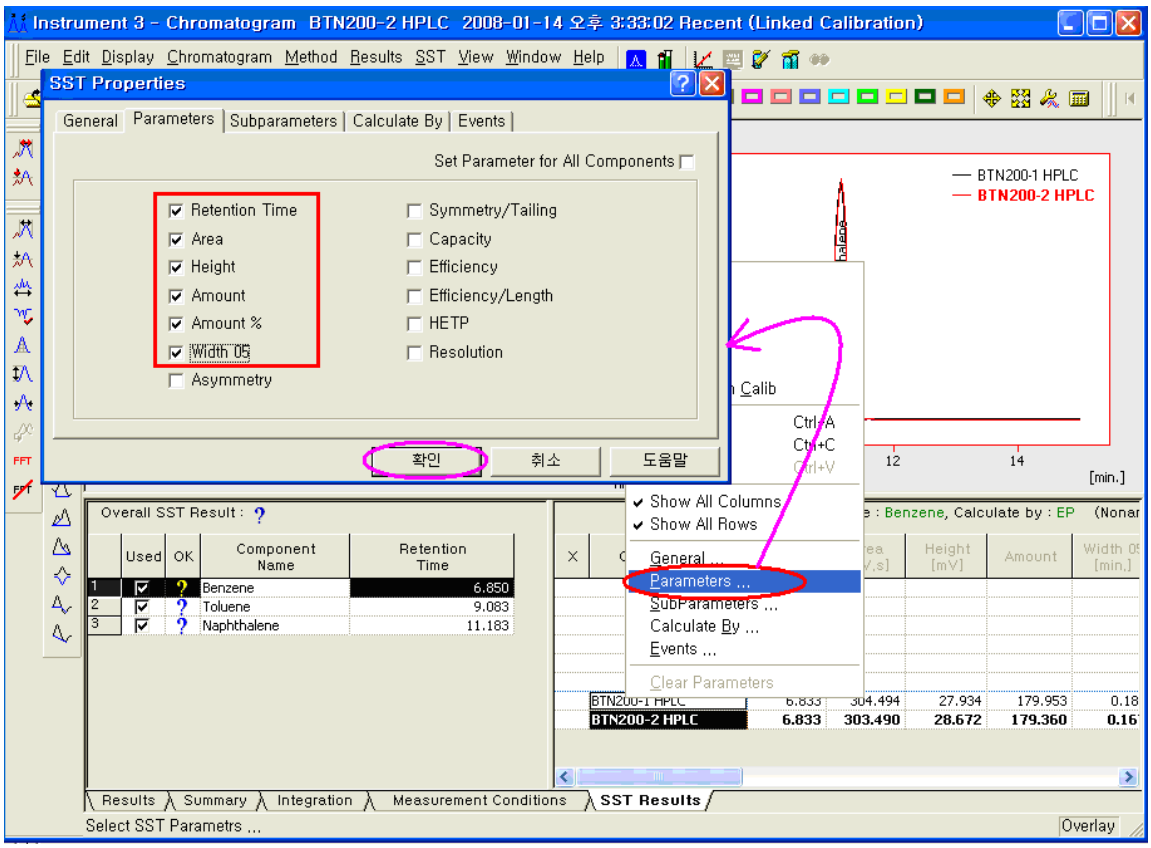
=> If you click “Used”, the results are displayed on the right side table.



Select all **data files** using Ctrl key

Click right mouse button **=> Select "Parameters"**

=> Check the items you want to compare.



=> System Suitability Test results

Component Name : Benzene, Calculate by : EP (Noname

Chromatogram	Retention Time [min,]	Area [mV,s]	Height [mV]	Amount	Width 05 [min,]
Lower Limit					
Upper Limit					
%RSD Limit					
Mean	6.833	303.992	28.303	179.657	0.175
RSD [%]	0.00	0.23	1.84	0.23	6.73
Parameter Result	?	?	?	?	?
BTN200-1 HPLC	6.833	304.494	27.934	179.953	0.183
BTN200-2 HPLC	**6.833**	**303.490**	**28.672**	**179.360**	**0.167**

YL-Clarity

GC

Easy Manual

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

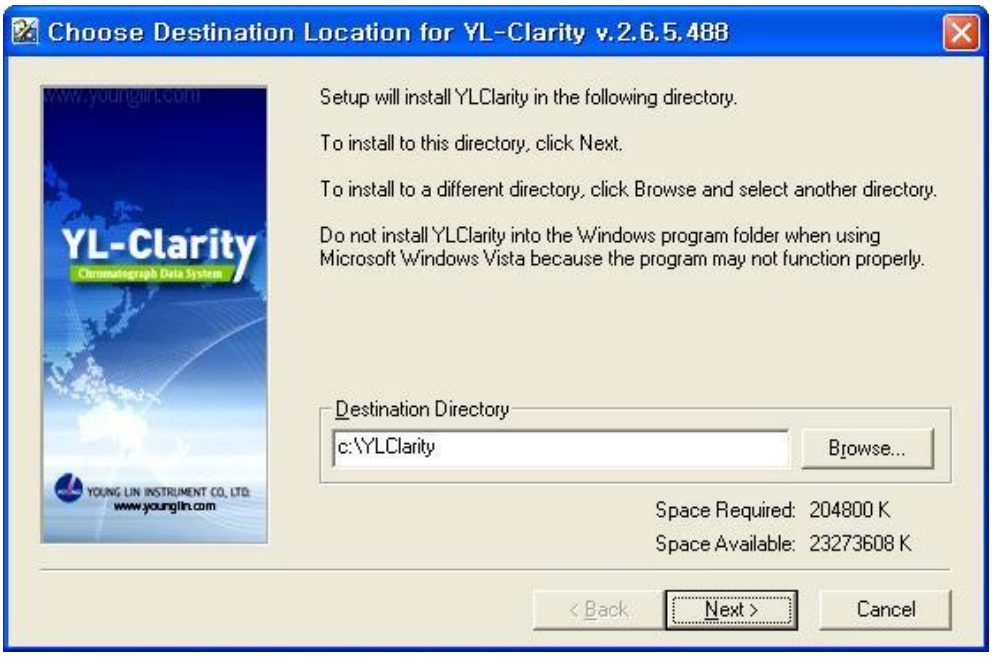
YL INSTRUMENT CO., LTD.

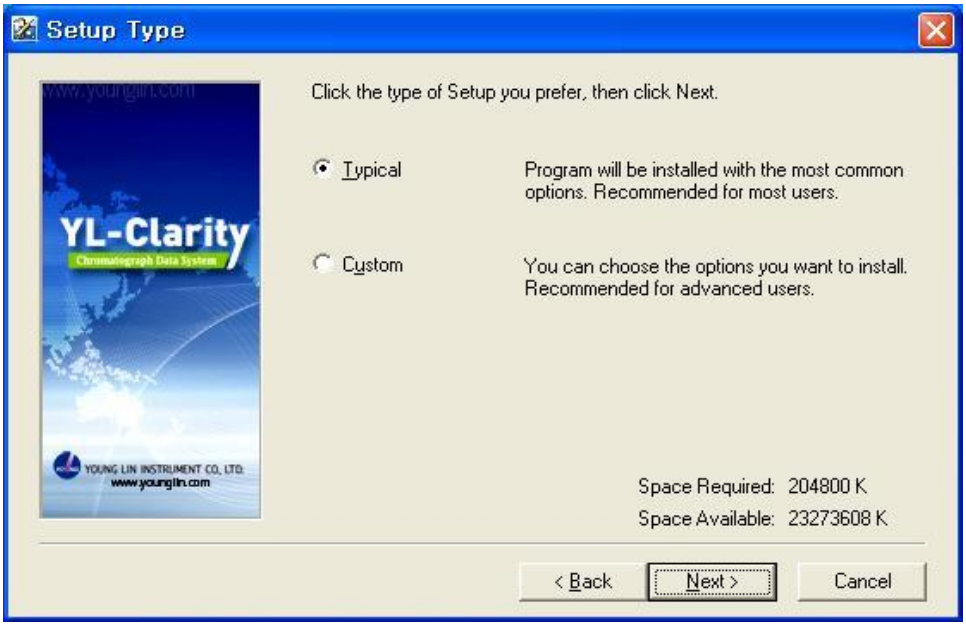
Chapter 1. Installation

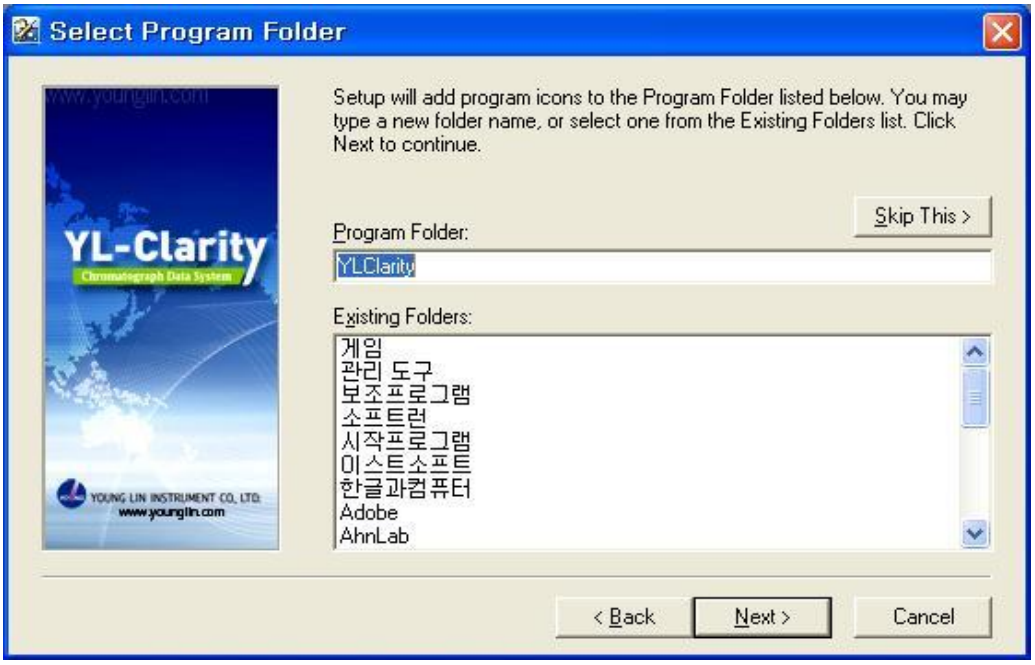
1-1. Installation of YL-Clarity

1) Run **Install.exe** by clinking on  .

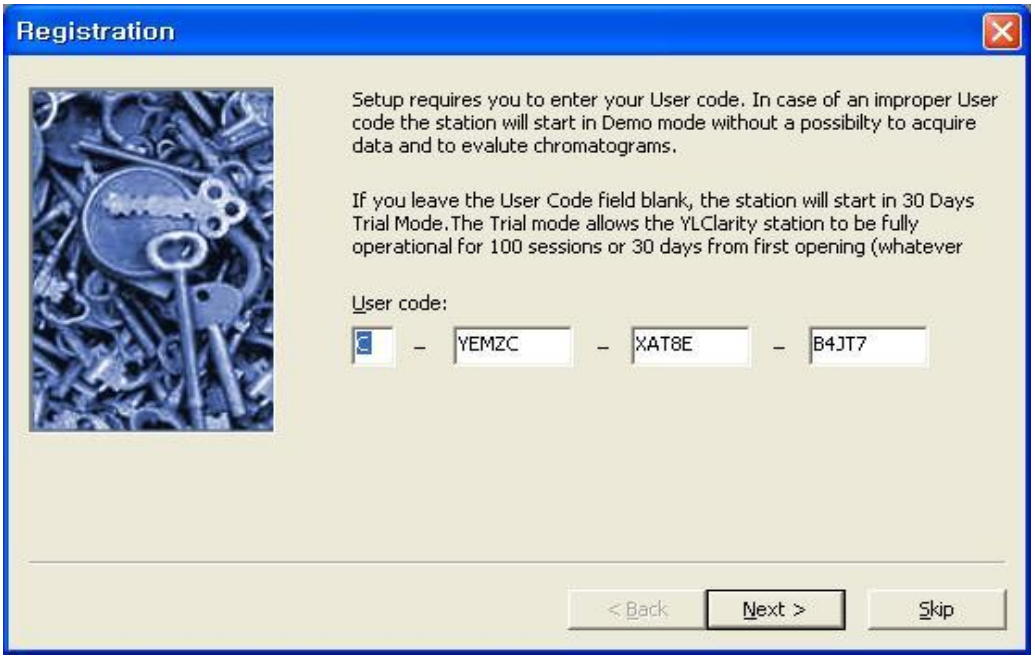
2) Install YL-Clarity by following the installation wizard and click on ***Next*** to go on.

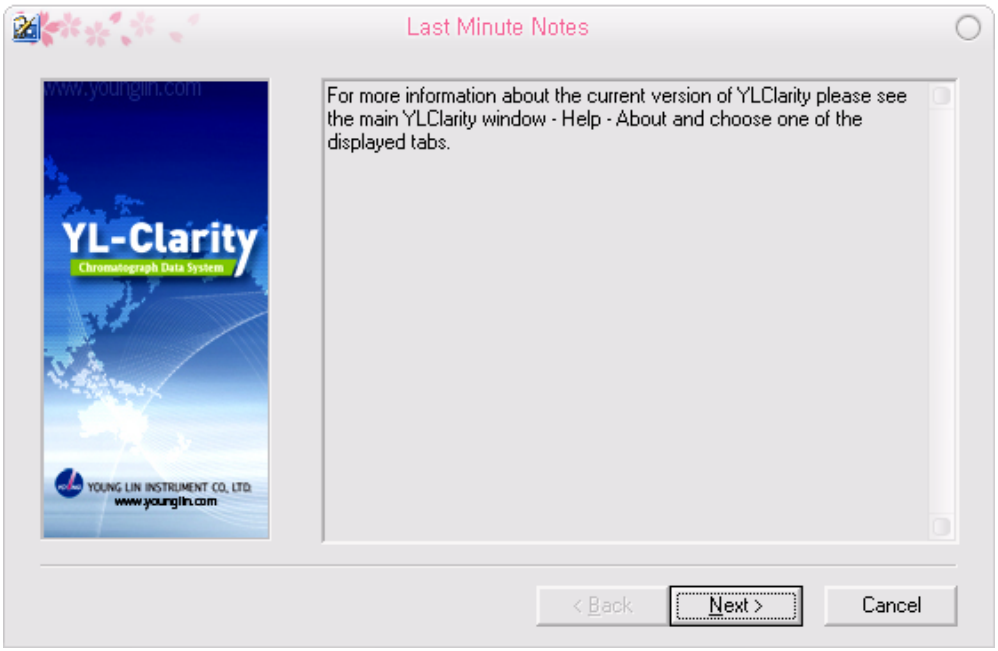


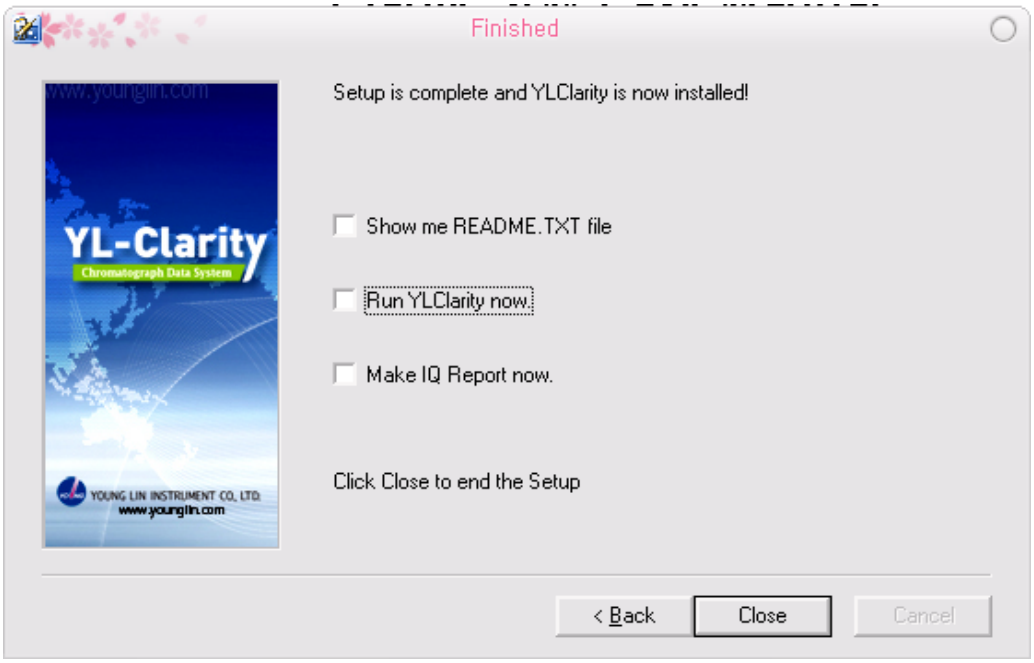




3) Enter the user code given on your CD and click on ***Next*** to go on.




Last Minute Notes
YL-Clarity
Chromatograph Data System
YOUNG LIN INSTRUMENT CO., LTD.
www.younglin.com
For more information about the current version of YLClarity please see the main YLClarity window - Help - About and choose one of the displayed tabs.
< Back
Next >
Cancel

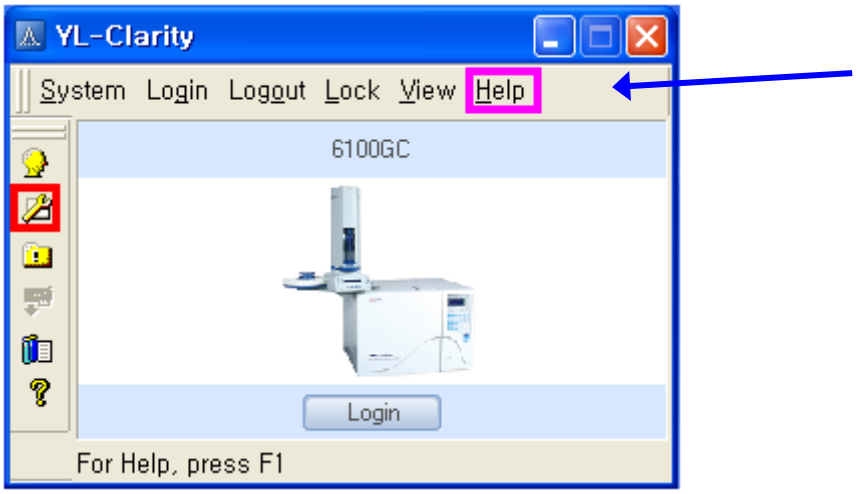

Finished
YL-Clarity
Chromatograph Data System
YOUNG LIN INSTRUMENT CO., LTD.
www.younglin.com
Setup is complete and YLClarity is now installed!
Show me README.TXT file
Run YLClarity now.
Make IQ Report now.
Click Close to end the Setup
< Back
Close
Cancel

Chapter 2. Software Control

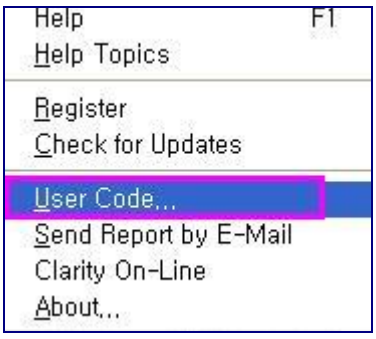
2-1. Entering User Code

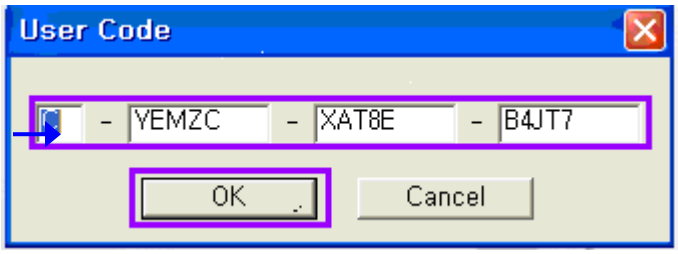
1. Install the Clarity Serial Key on PC, and click the icon 

on the desktop. The screen is shown as below.



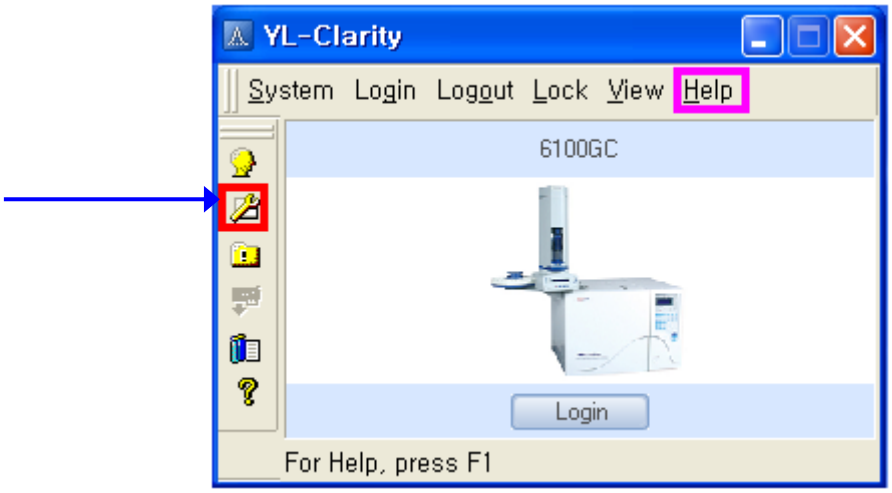
2. Click on **Help** – **User code** on the menu bar.
3. Enter the user code and click on **OK**.

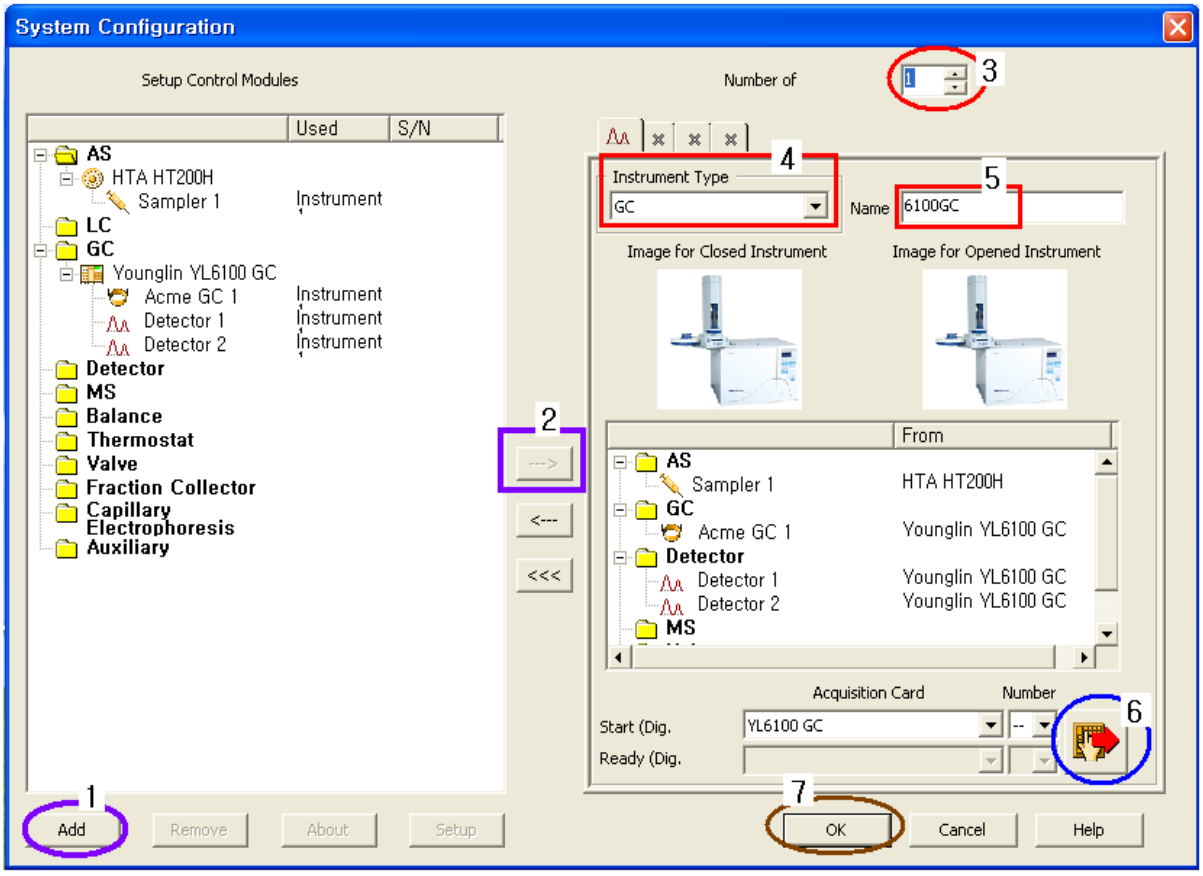




2-2. Instrument setting

1. Click  on the left side of initial screen, the below is shown to set the instruments.



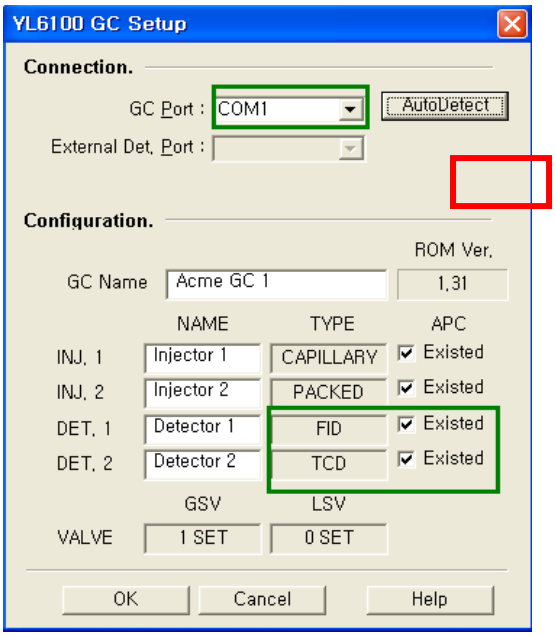


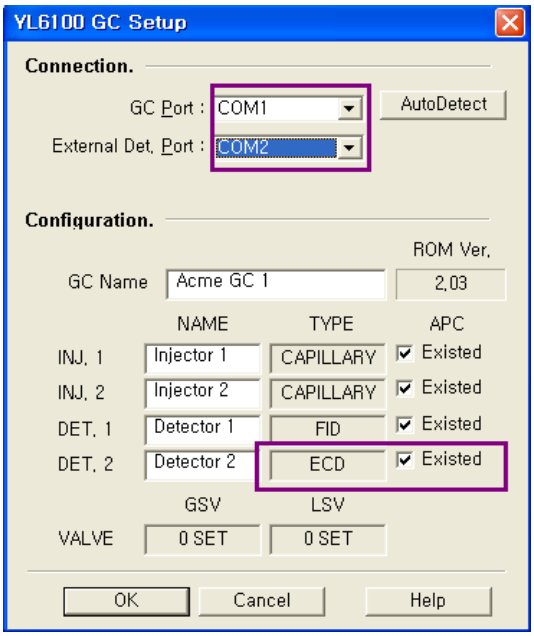
2. Click on **ADD(1)** to add the instrument.

- On the setup control window, On the pop up window, select the GC and input COM Port number

- Click this GC on the left window and move to right window by the **Arrow button(2)**.

ex> **Basic config.** **FID/TCD**(COM Port 1ea) ex> **NPD/ECD/FPD/PDD** (COM Port 2ea)

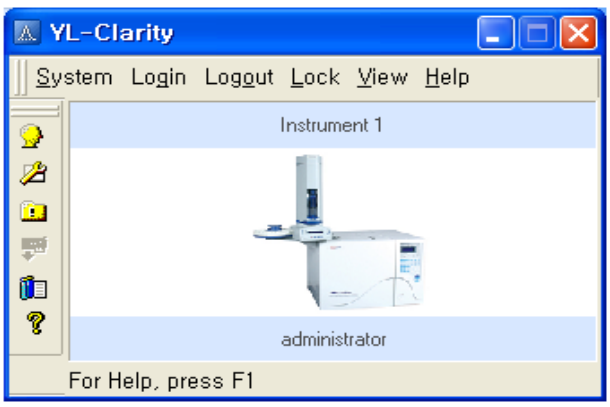




3. Select the number of system **(3)** → Select Instrument Type **(4)** as GC → Input the name of instrument(5)

→ Press the icon  **(6)**, and input the unit, click OK **(7)** button.

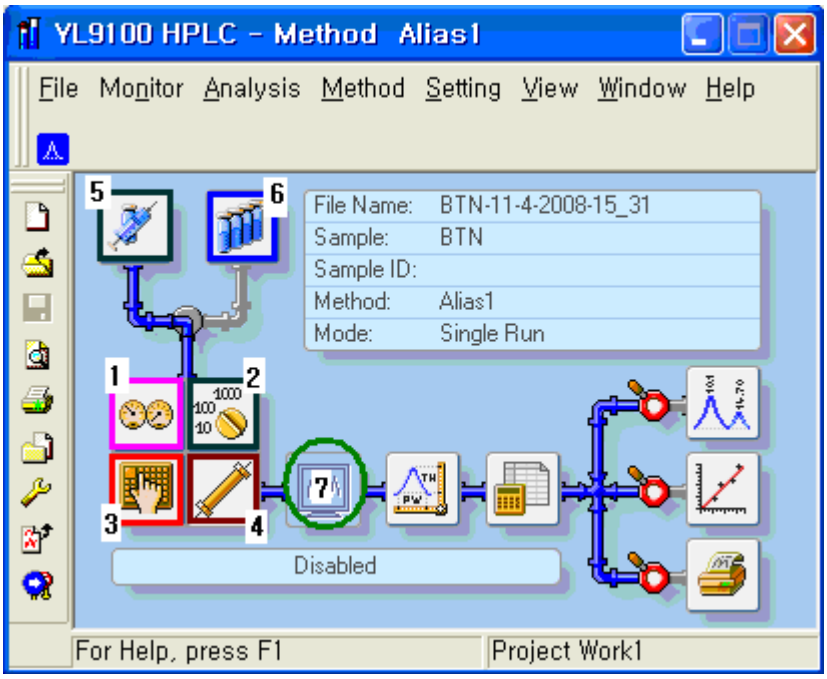
4. Click Log-in on the main window => Following main window and system control window are displayed.



5. If there are already inputted values, it is not necessary to setup System config. again.

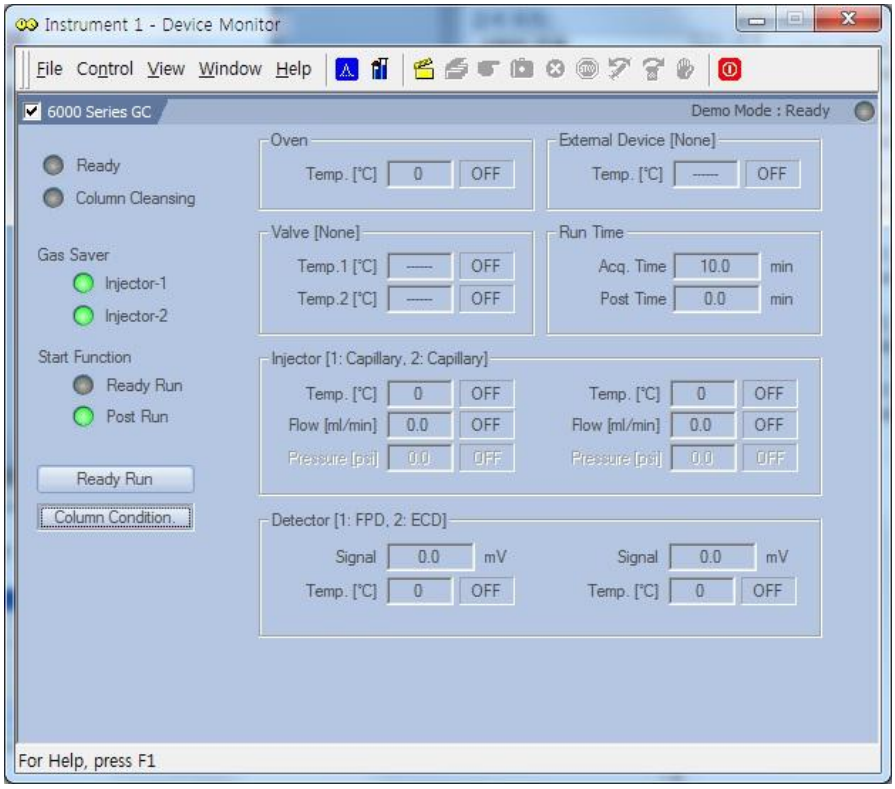
⇨ **Log-in** directly

2-3. System control setup

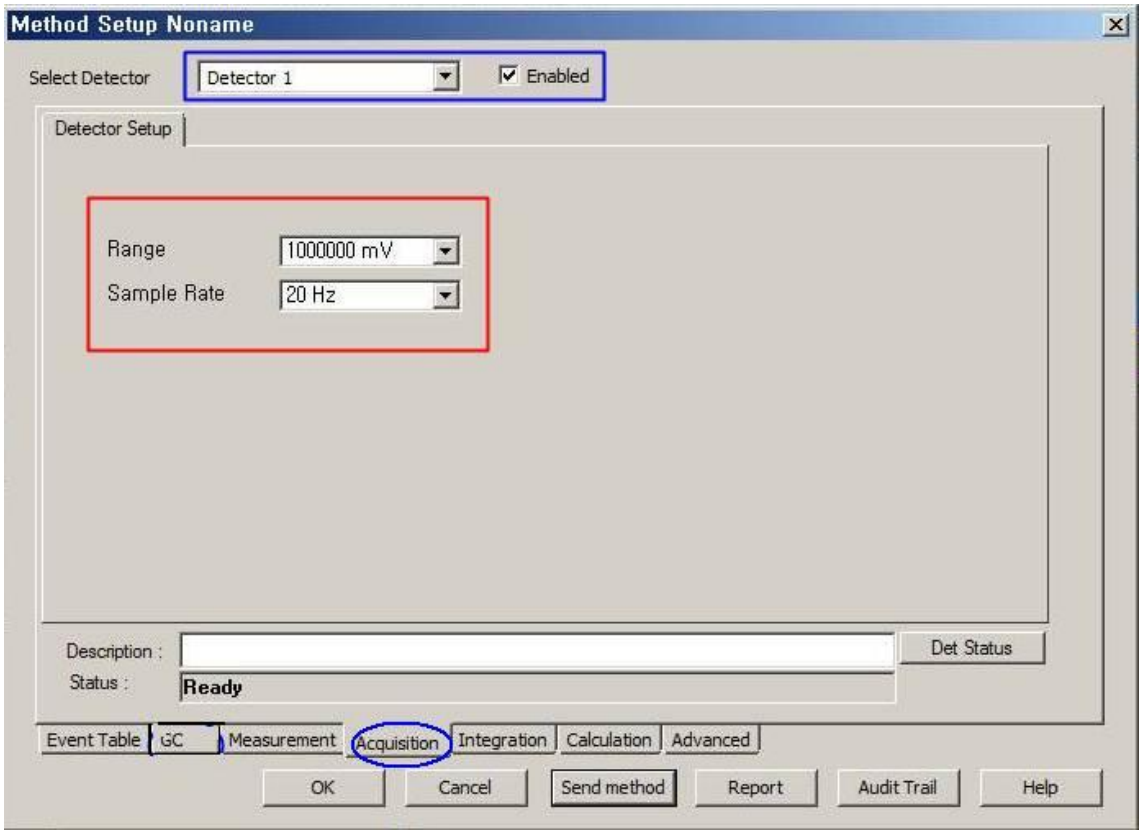


2-3-1. Device Monitor**(1)** Icon

: On this window, you can control simple operation menu as like **Prime Start, Purge**..., and can monitor the system status.



2-3-2. Acquisition – Setup Range, sampling rate for detector



Save Method : After setup all conditions, select Save as Method on the top File menu

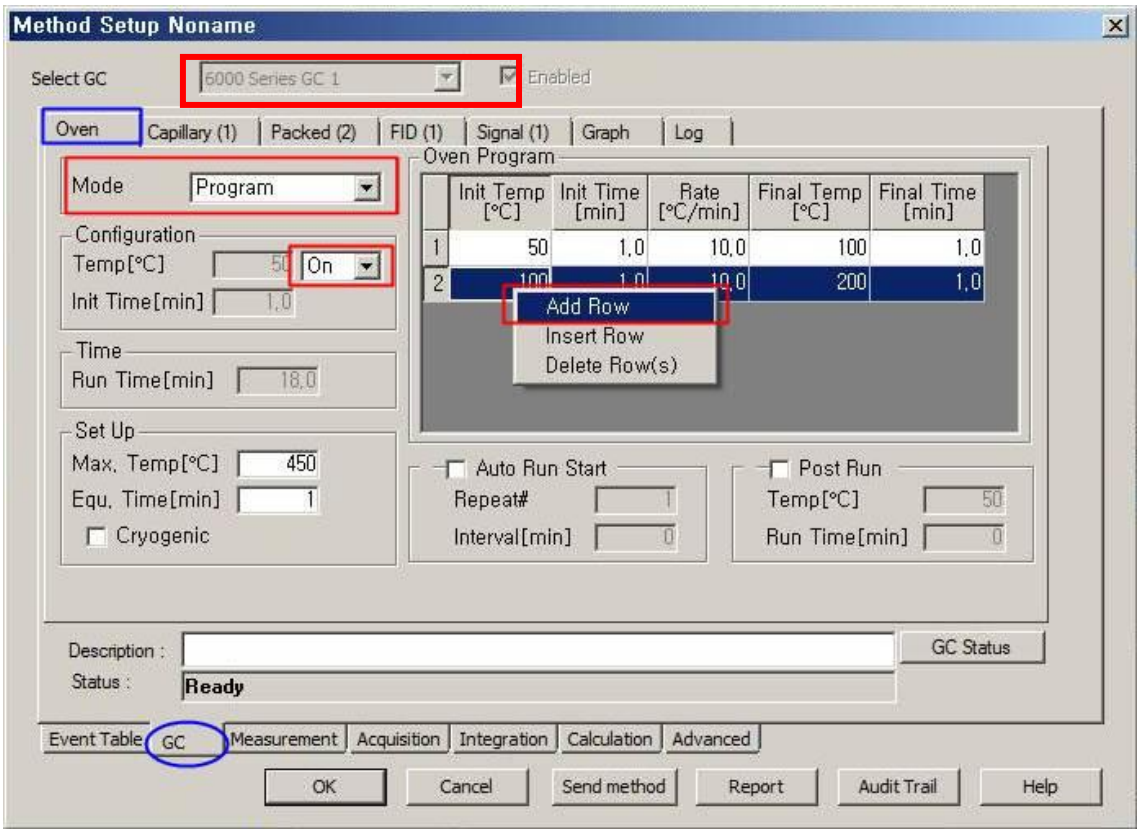
=> save as *.met file

2-3-3. Control

: Set up GC analysis condition - Set Flow or temperature condition of Oven, Injector, Detector, Valve, and Autosampler

1. Oven

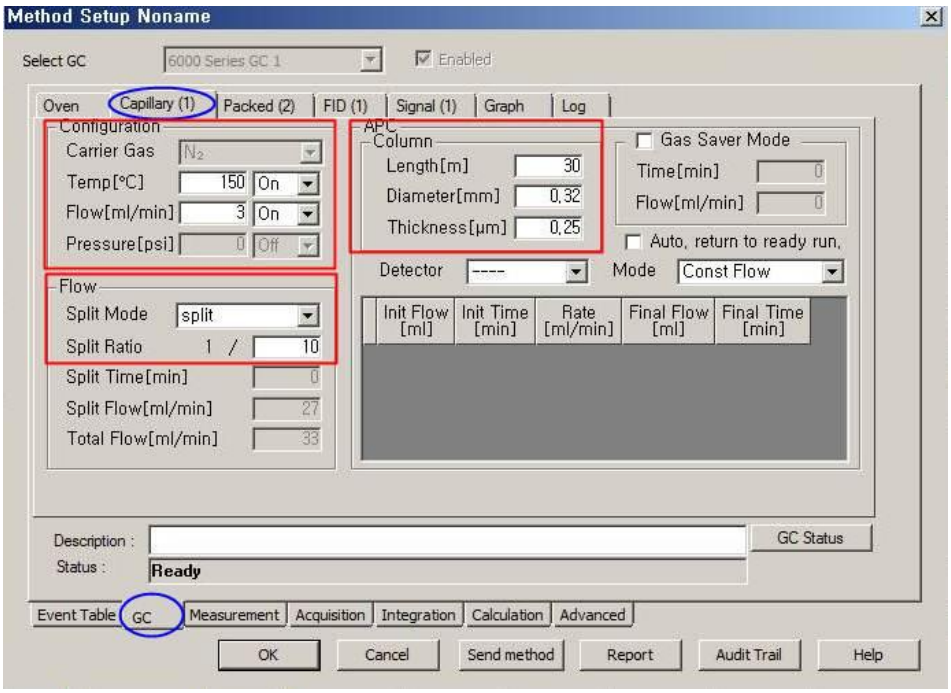
: Set up isothermal/temperature program mode, input the condition



2. Inlet

: Set up column flow, inj. temperature, column dimension and split/splitless

1) Capillary Inlet

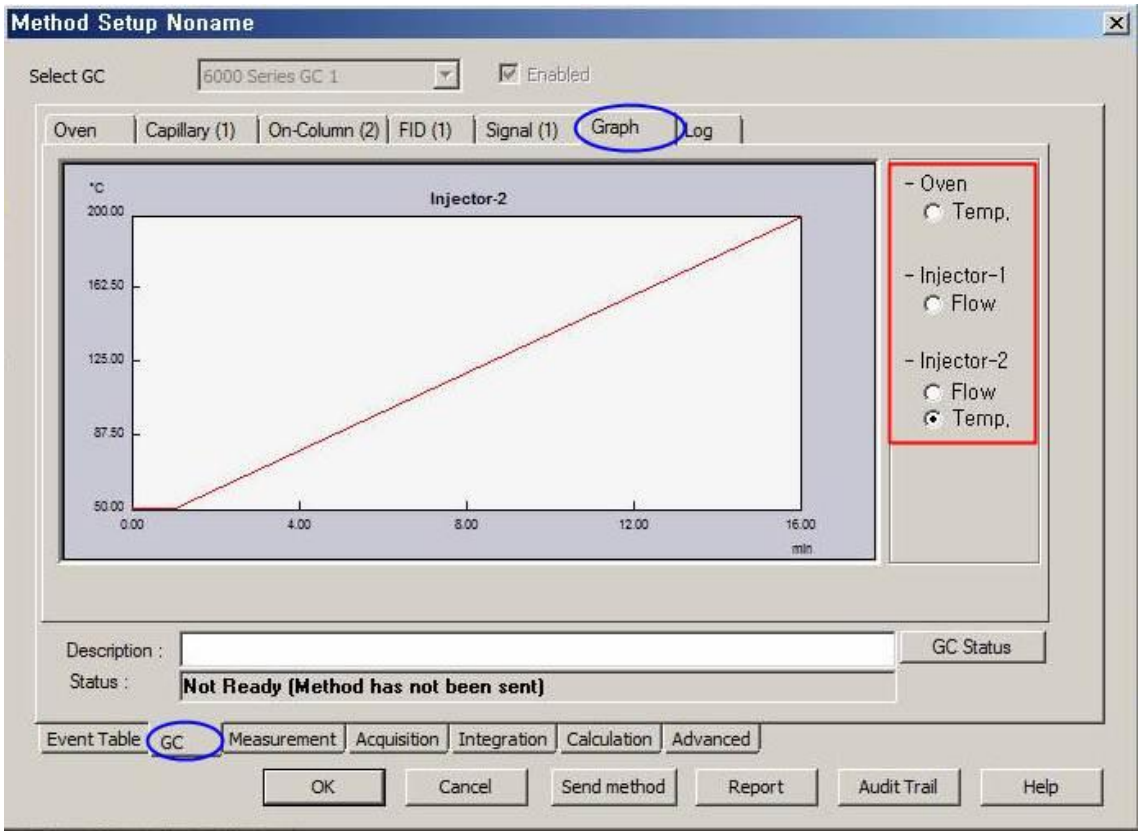


2) Packed Inlet

3) On-Column Inlet

- Temp.mode

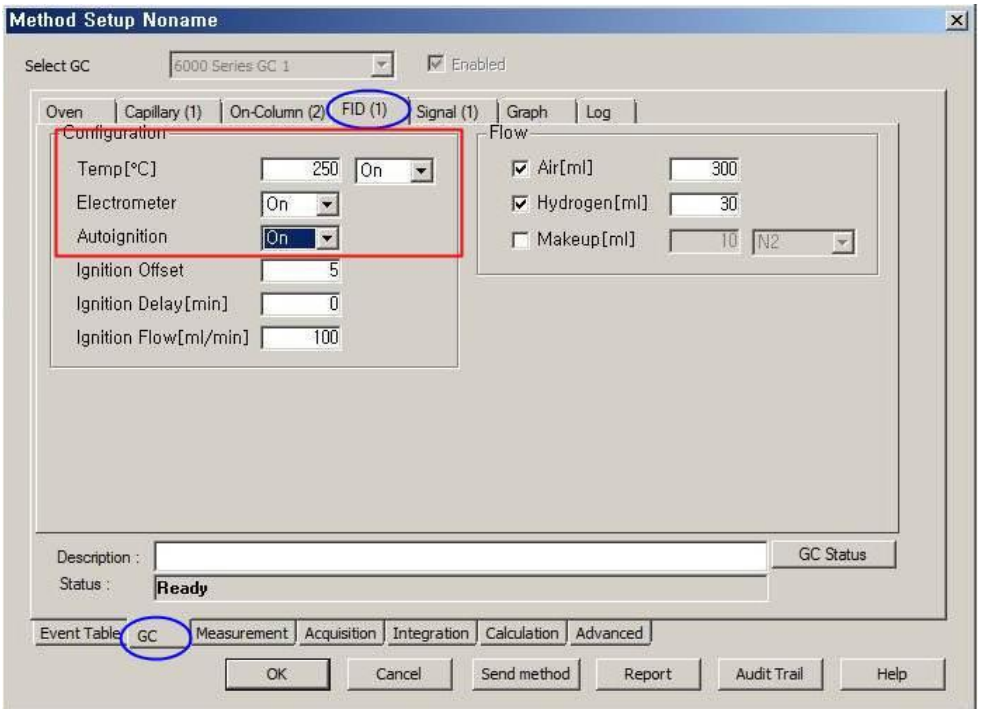
- Isothermal
- Track Oven : Applied same to oven temperature programming
- Program : On-column temp. program, five steps max.

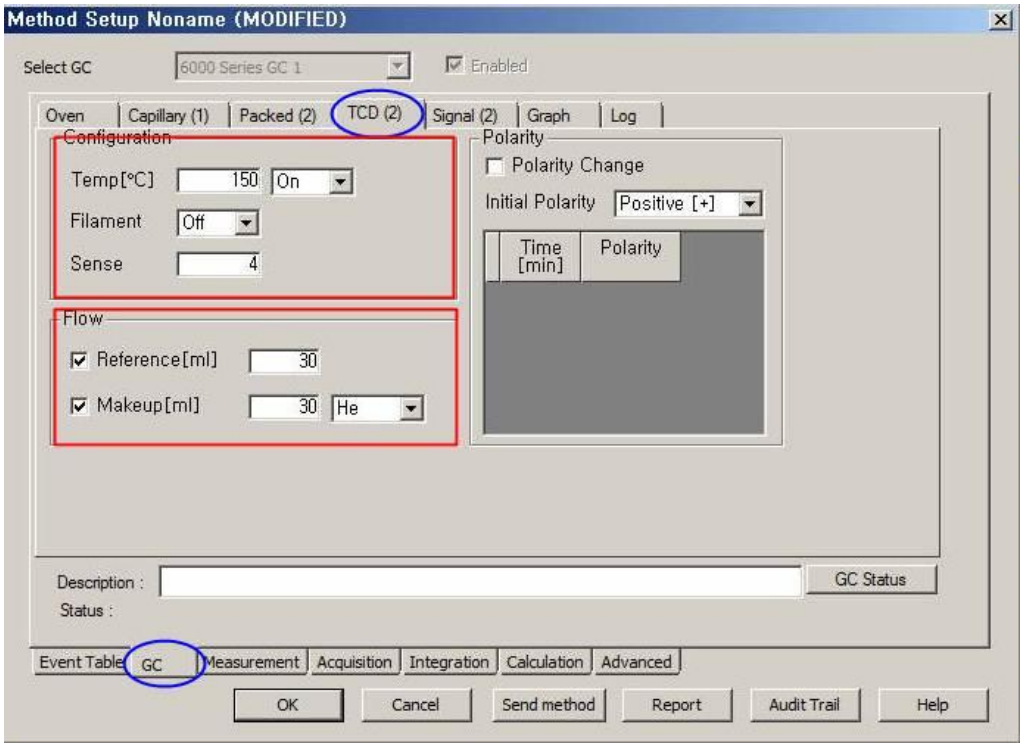


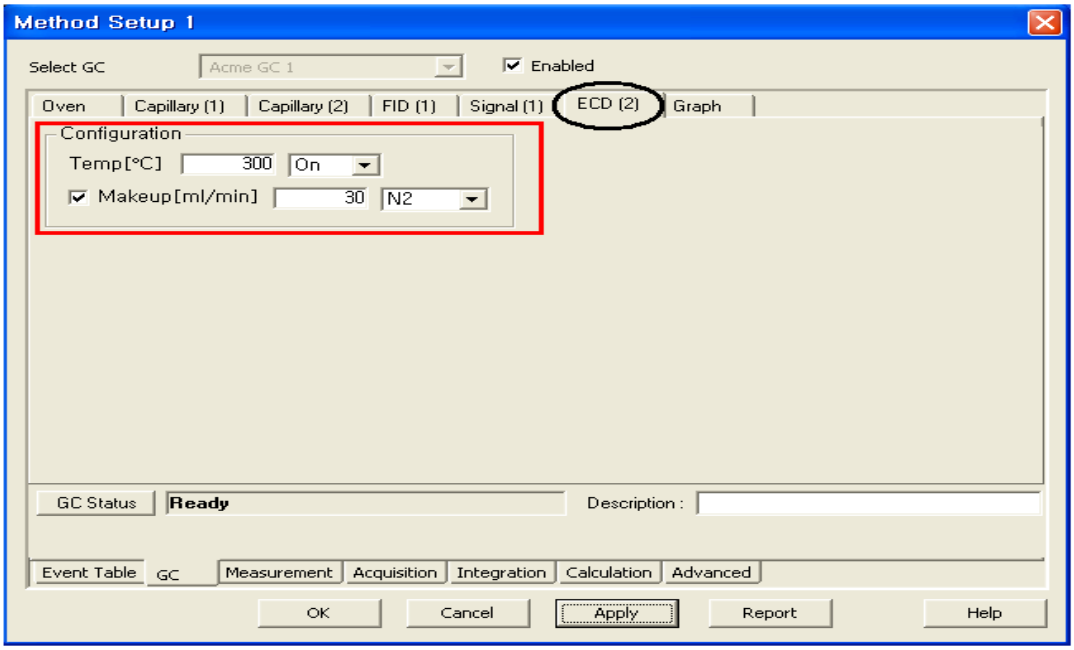
- Temperature programming of on column inlet

3. Detector

: Setup detector gas flow and temperature

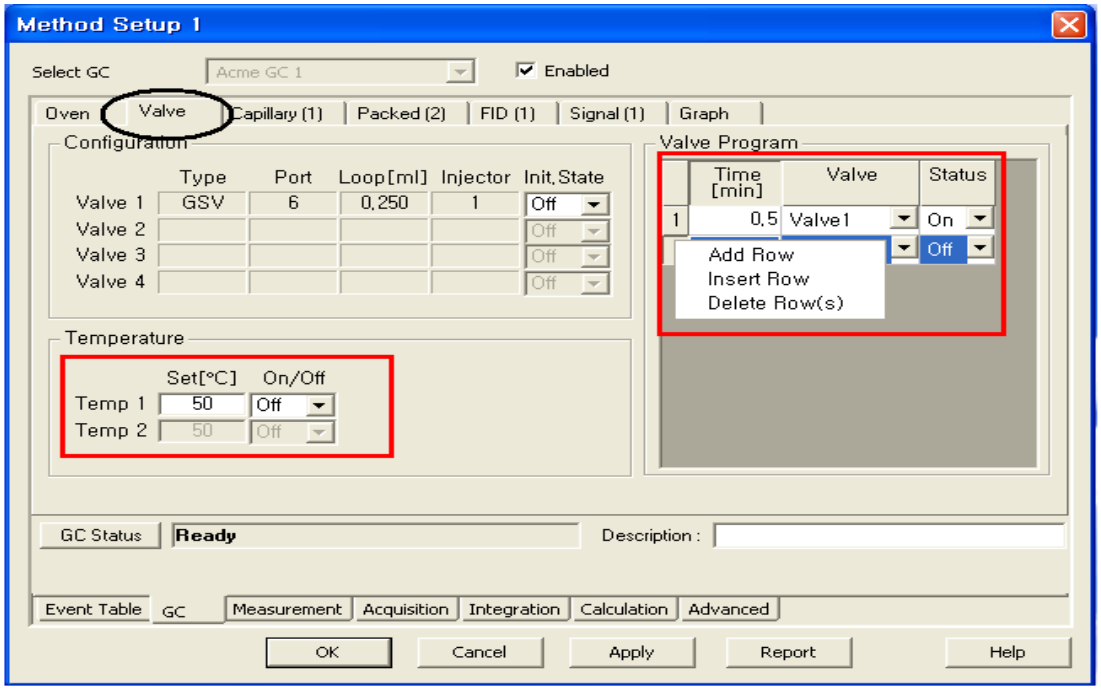






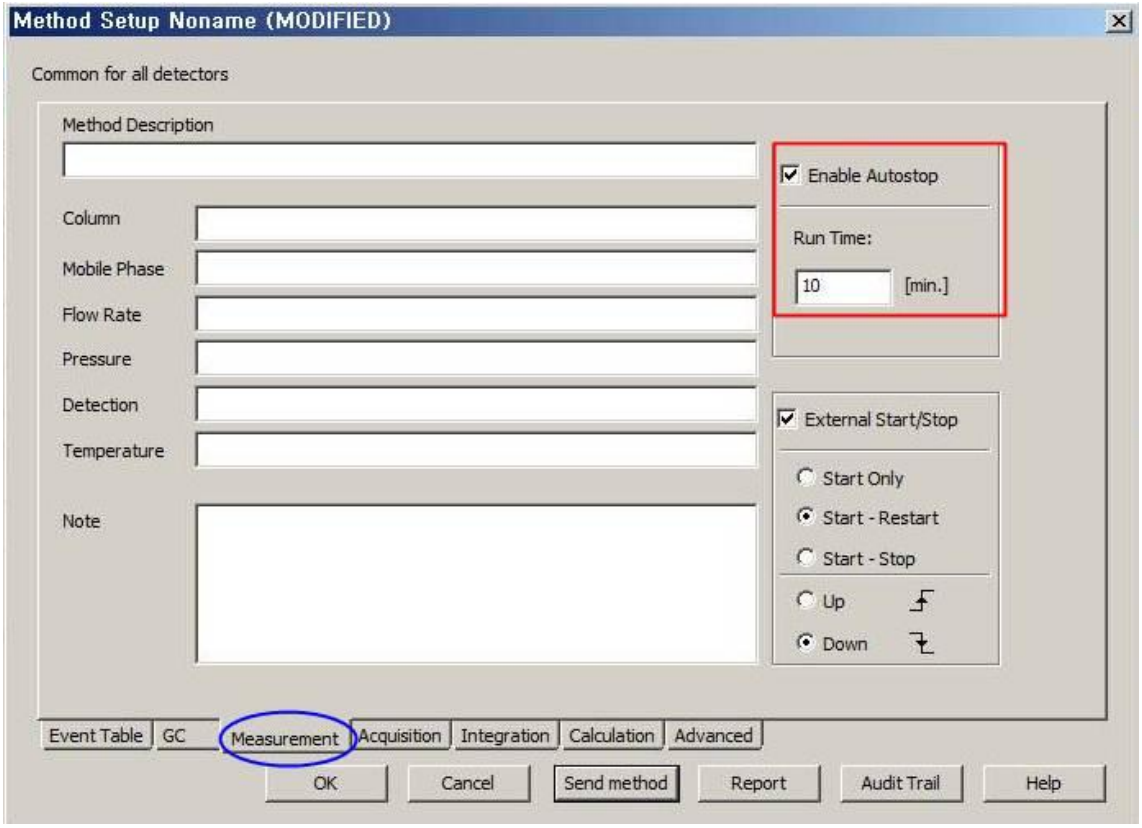
4. The Others

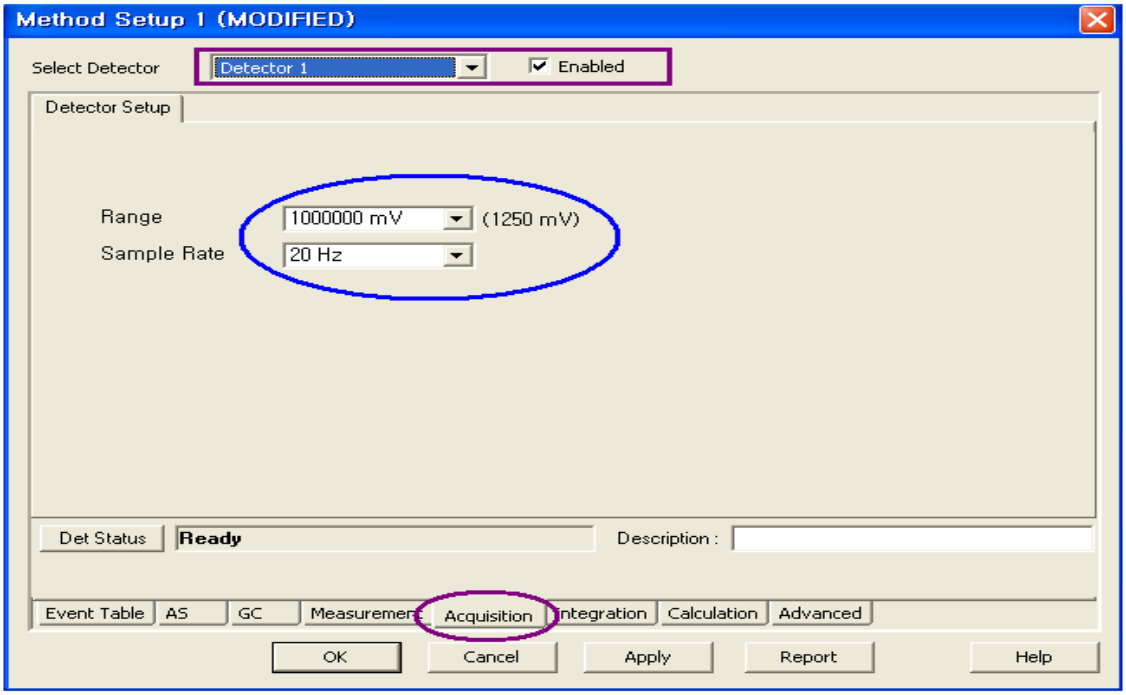
: Setup analysis condition of Valve, Autosampler



2-3-4. Measurement

Setup analysis time and input the condition



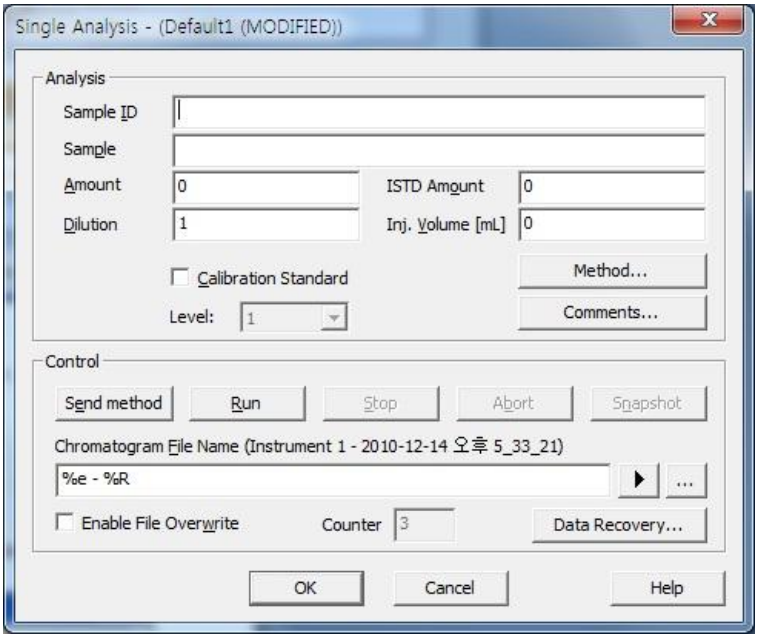


2-4. Sample Analysis

2-4-1. Sample Injection

1. Single Analysis : It is used for injection without autosampler. Click  icon on the control window, input the information of sample(sample name, file name) => OK!

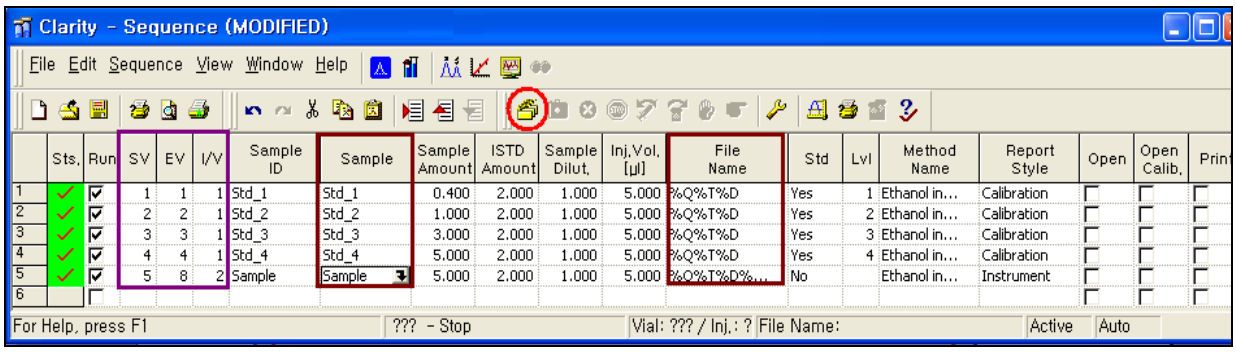
After inject sample using syringe, press Start button on the GC => Start Data acquisition



2) Sequence Analysis : It is used for injection using Autosampler. Click  icon on the control window to open sequence table.

SV : Start Vial number, EV : End Vial number, I/V : Number of injection per each Vial

After setup injection parameters, click  icon to start injection => Start Data acquisition



2-5. Data acquisition

- Click  icon to open acquisition window for monitoring real time data.

- Range of display : Input the Time and Signal on the tool bar.

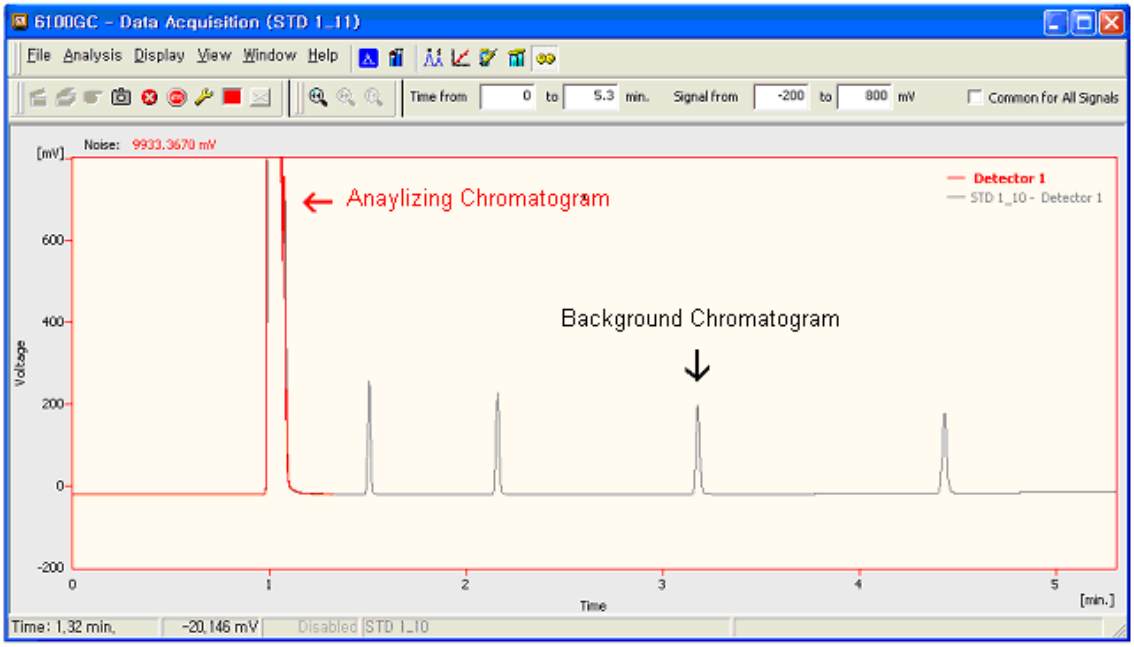
 Snapshot : To check the integration result of present data during acquisition.

 Abort : To stop data acquisition. Data is not saved.

 Stop : To stop data acquisition. Data is saved.

- Back ground chromatogram : File menu => Set Background Chromatogram

=> Select data file want to use for back ground chromatogram.



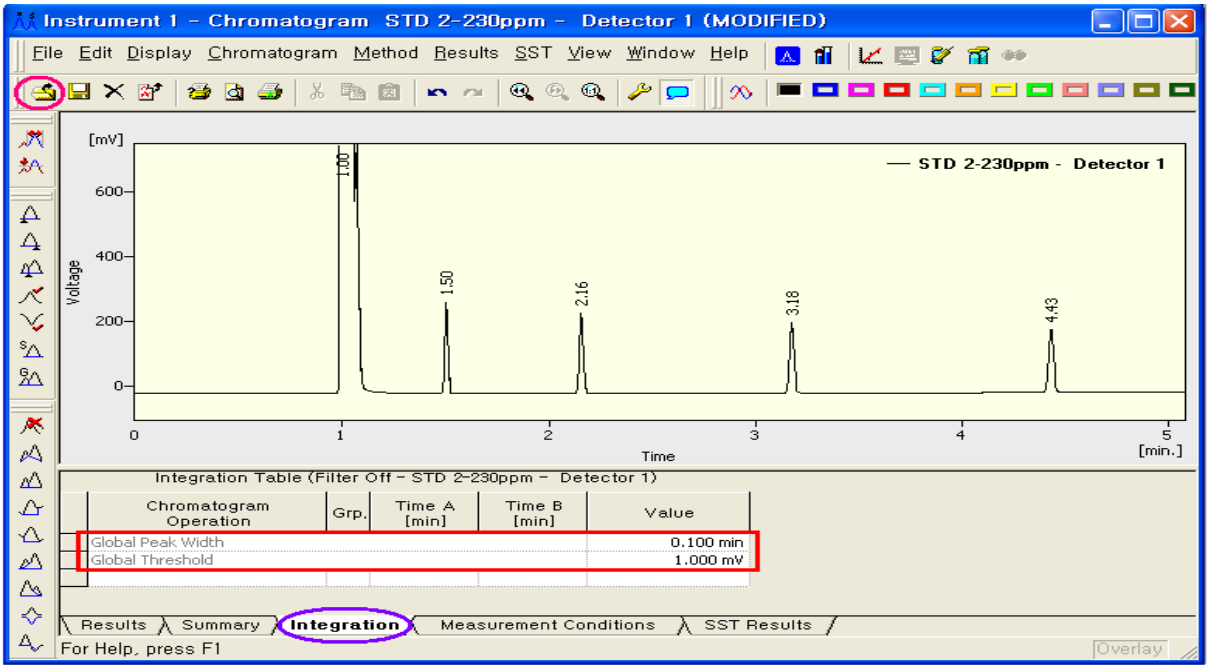
The real time present detector signal is displayed on this window without injection of sample.

The collected data is saved in Data folder, the result can be checked on the chromatogram window  .

2-6. Integration

Click the chromatogram window icon  to integrate acquired data.

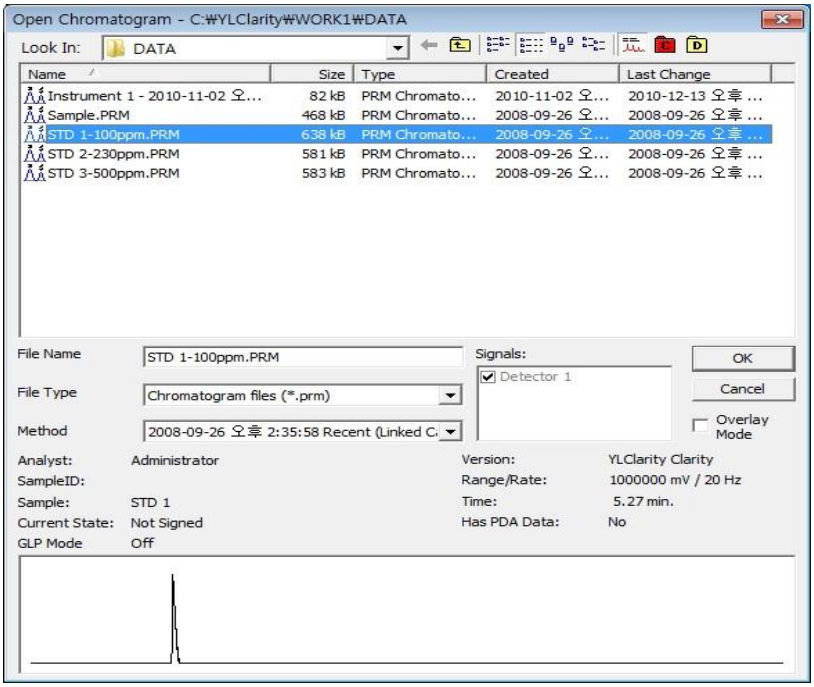
Following window is displayed.



1. Open Data 

On the tool bar, click **“open” icon**  => Select Data file and click OK!

=> The data is displayed on the Chromatogram Window.



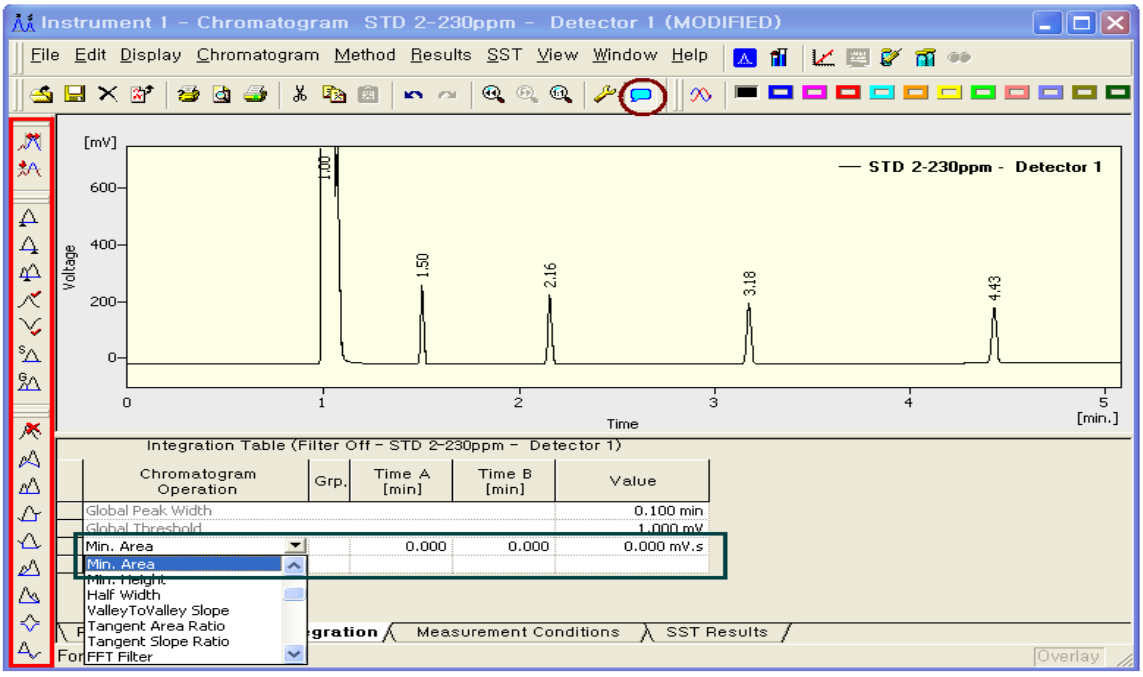
2. Set Integration Factor

   Click Integration tab.

   A. Global setting Factor (Peak width, Threshold) : Input Value and Enter

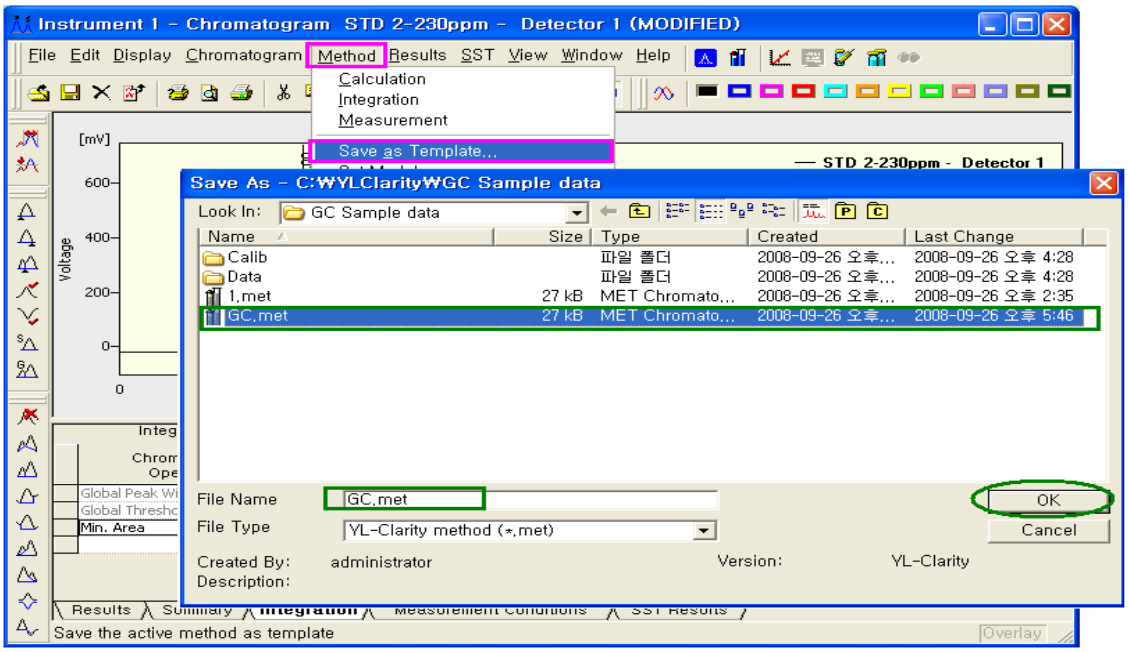
   B. Additional integration Factor : Click integration event table => Select parameter and input Value => Enter

      Or, click  icon => select one of integration event icon want to apply => Drag range want to apply this Factor on the chromatogram



3. Save integration Method

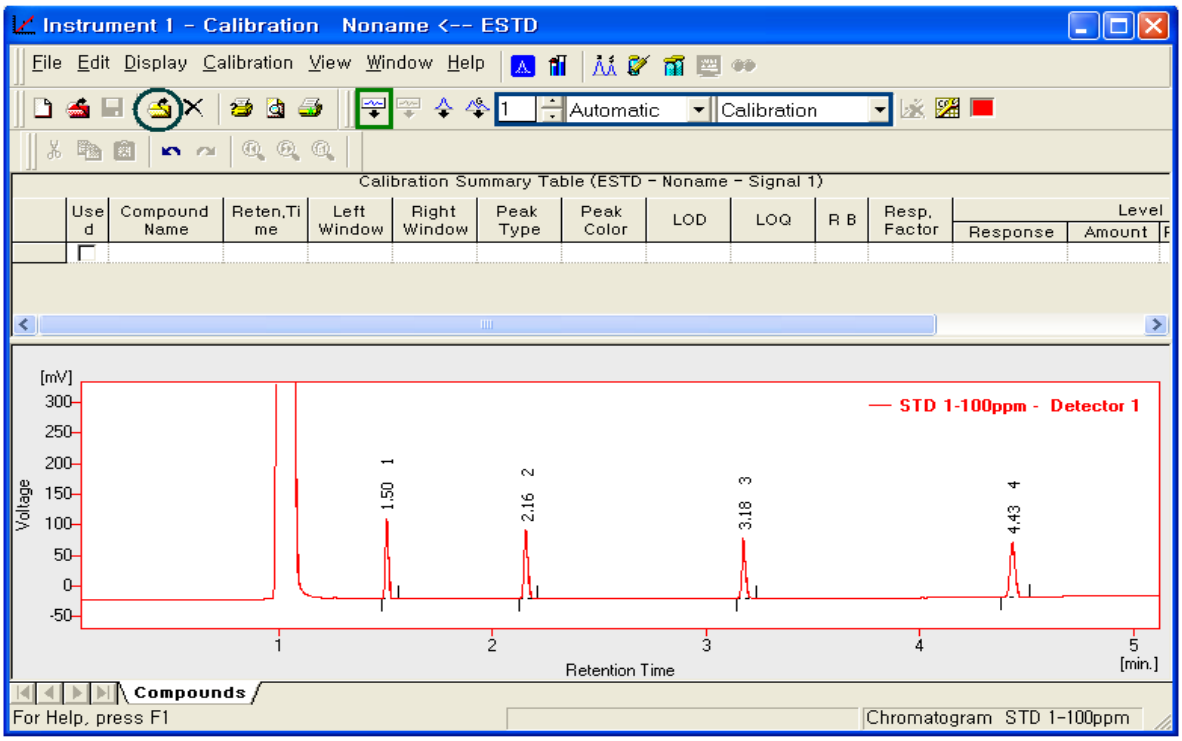
   On the top, **Method** => **Save as Template** => Input **Method file name** => **OK**



2-7. Calibration

Click the calibration window icon  to make a calibration curve.

Following is displayed.



1. Open Data 

   On the tool bar, click “open**” icon**  => Select **Data and OK!**

   ⇨ The integrated peaks are displayed on the **Calibration Window**.

2. Input calibration data 

   Input Level (standard sample concentration level), “Calibration” and click “Add All” icon.

Calibration table shows as below.

Calibration Summary Table (ESTD - Noname - Signal 1)

	Used	Compound Name	Reten,Time	Left Window	Right Window	Peak Type	Peak Color	LOD	LOQ	R B	Resp. Factor	Level 1			
												Response	Amount	Resp. Fac	Rec No.
1	☑	C10	1.505	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	121.5696	100.000	0.8226	1
2	☑	C12	2.159	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	128.2036	100.000	0.7800	1
3	☑	C14	3.178	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	136.6287	100.000	0.7319	1
4	☑	C16	4.433	0.200	0.200	Ordnr		0.000	0.000	A	0.0000	140.6968	100.000	0.7107	1
	☐														

Used : Check it on the compound to use for calibration

Compound Name : Input compound name

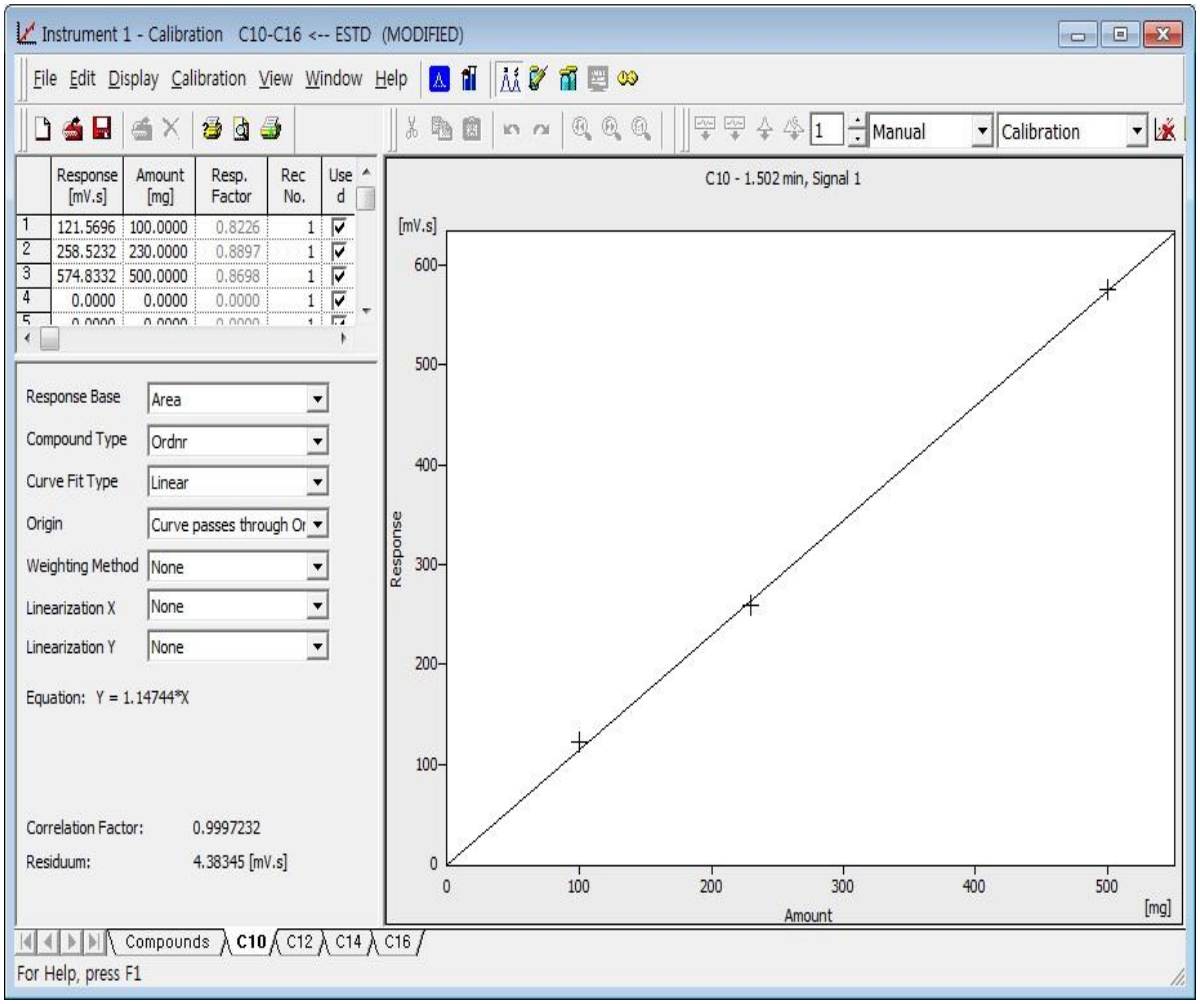
Peak Type : If the compound is ISTD, click and select as a ISTD

Confirm Concentration Level, Response and input Amount => STD Level 1 is finished.

Repeat this procedure for Level 2, Level 3, etc. until all STD results are input.

3. Make a calibration curve

If you click the compound name on the compound line, the calibration curve and related information are displayed.



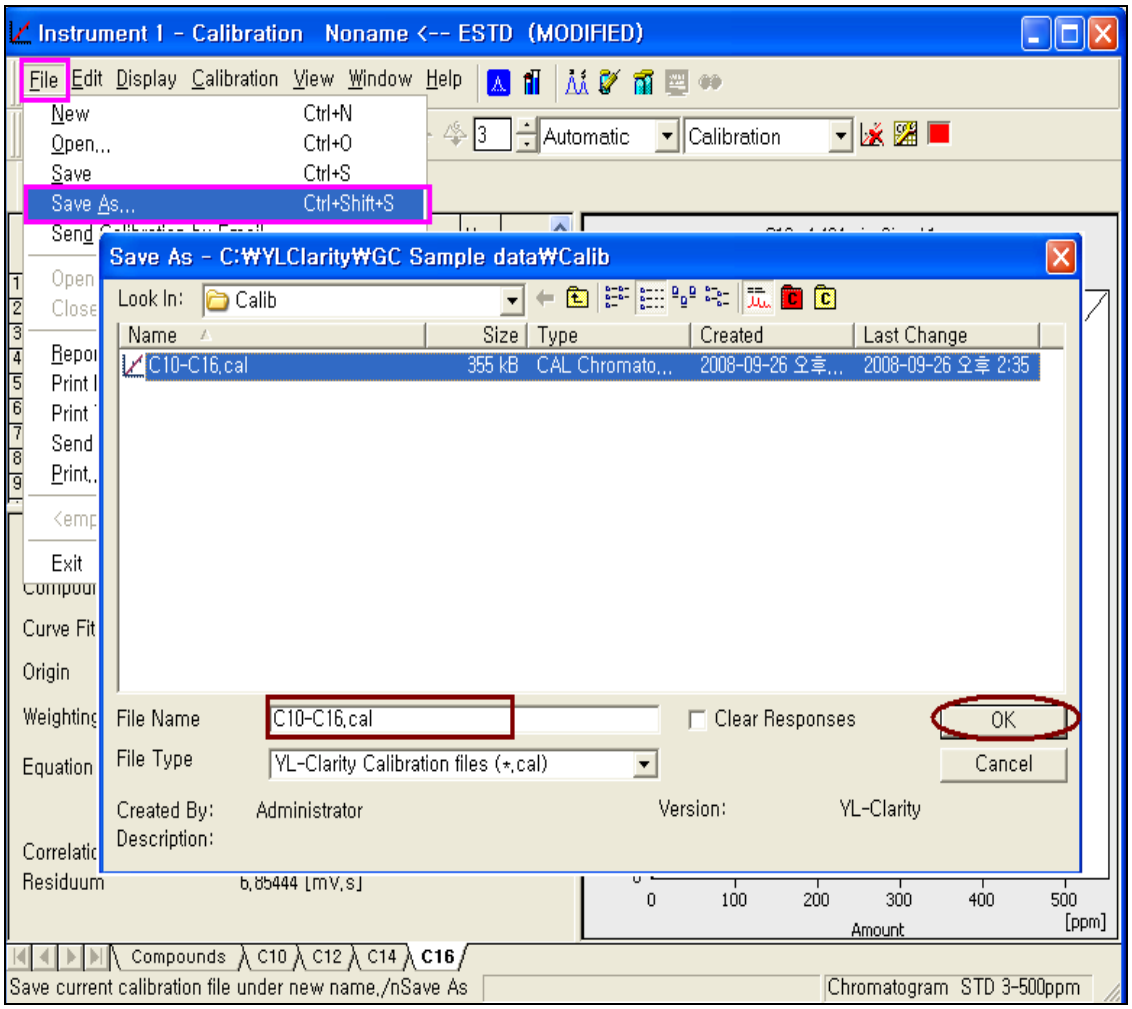
Response Base : Select Area or Height

Origin : Select the way of making curve with the origin point

Correlation Factor : R^2

4. Save Calibration file

On the top menu, **File** => **Save As** => **Input Calibration folder and name** => **OK**

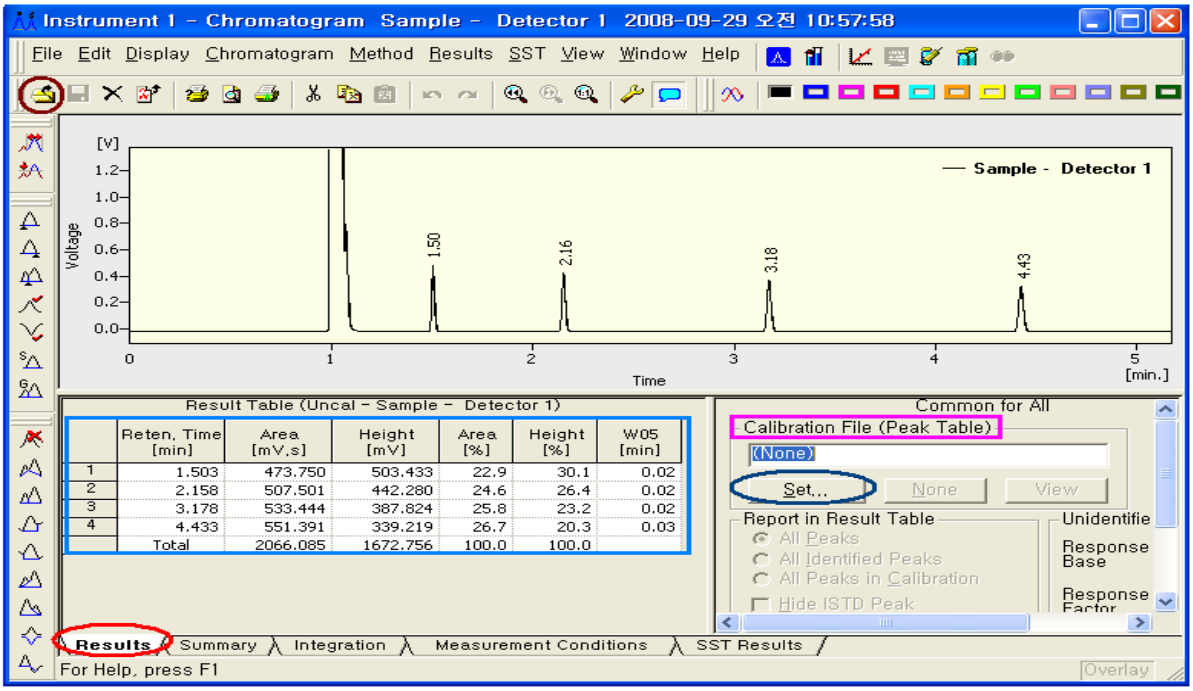


2-8. Quantification

1. Open Data file

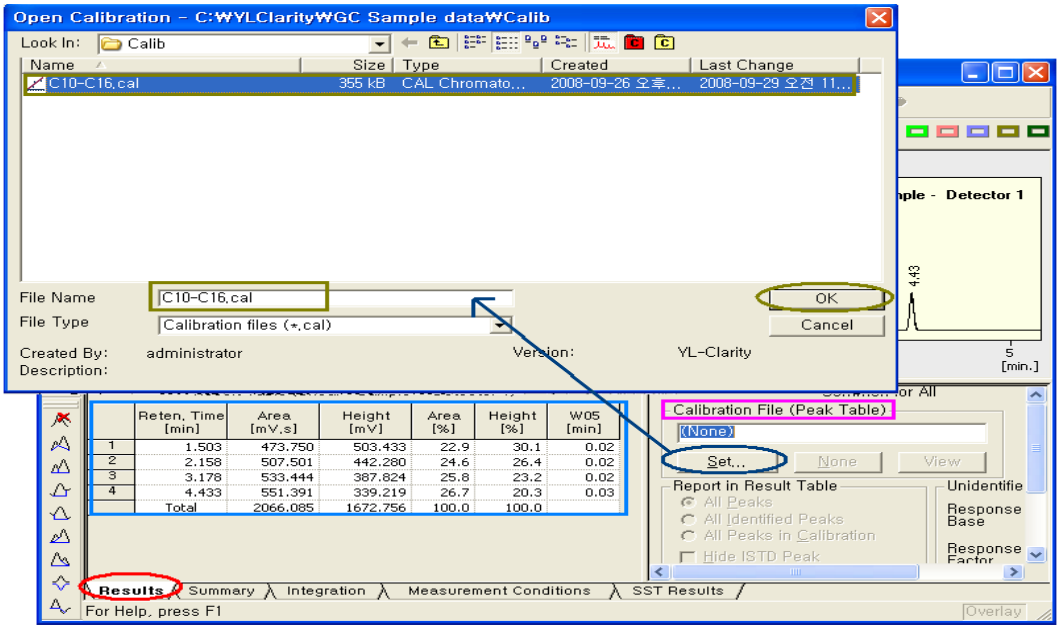
On the **Chromatogram Window, click "open"**  **to open data**

=> Select **Data file and OK!** => Selected data file is displayed as below.

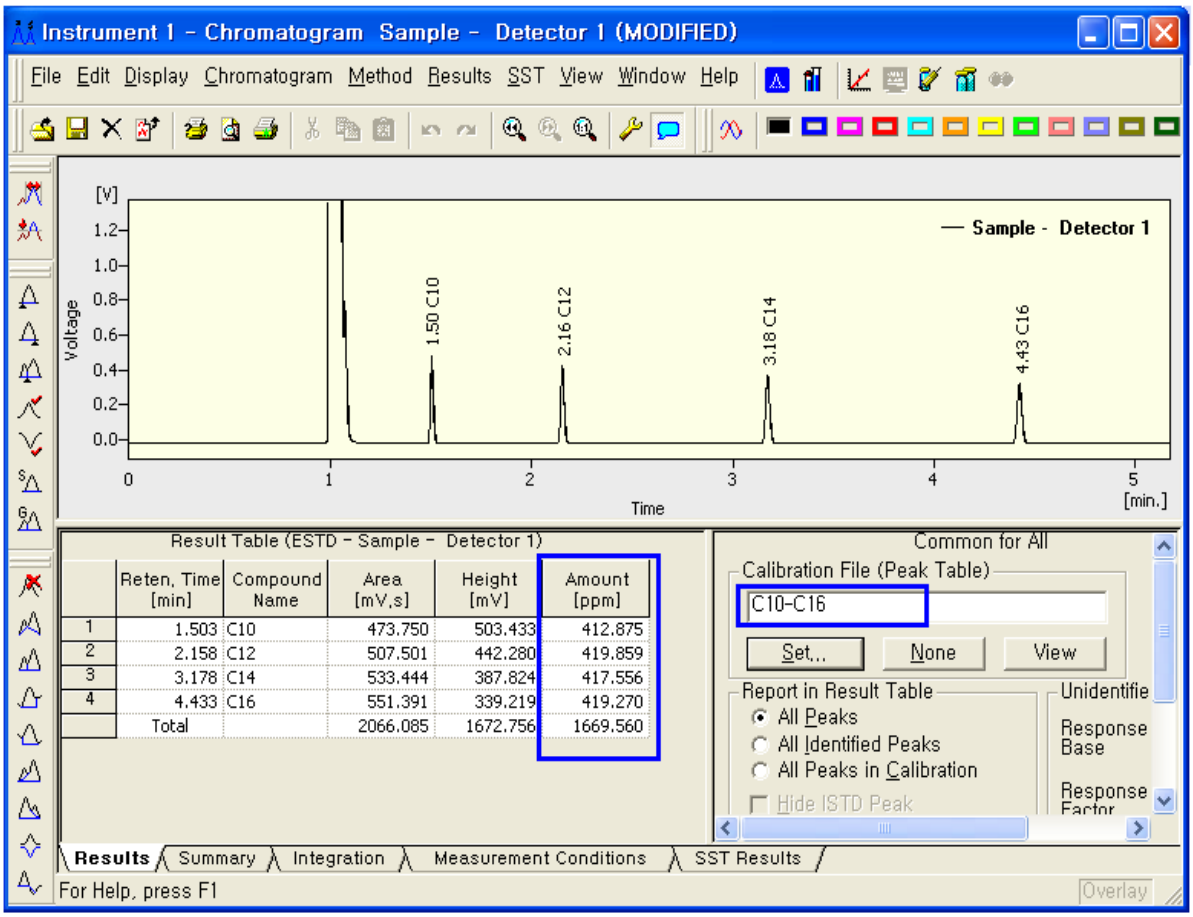


2. Apply Calibration file

Click "Set" of Calibration file(Peak table) menu => Select **"Calibration file"** => **OK**



Following quantification result is displayed.



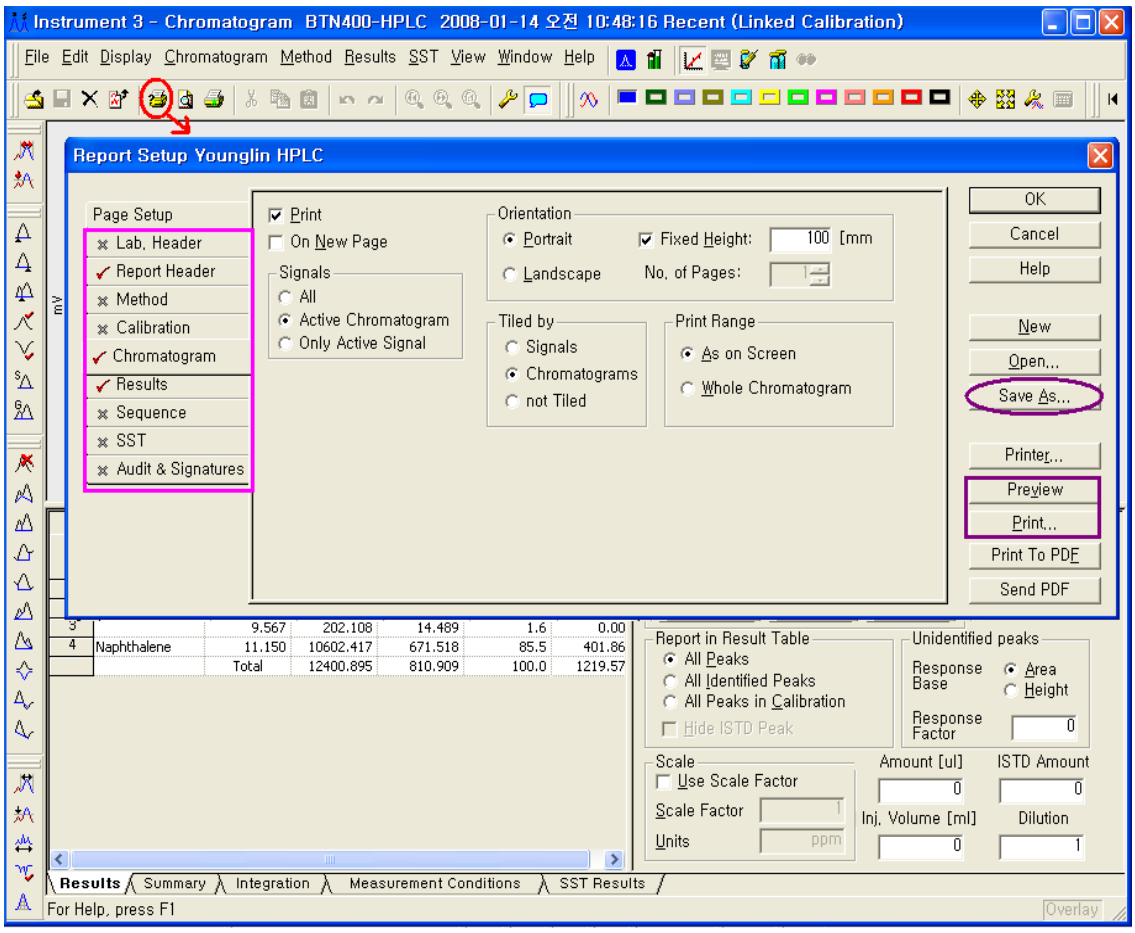
2-9. Print Report

Click “Report Setup” icon  on the **Chromatogram Window tool bar.**

=> Using “Page Setup”, edit report format

=> Save **Report Style File** using **“Save As”** menu => **Preview**  => **Print** 

Click !



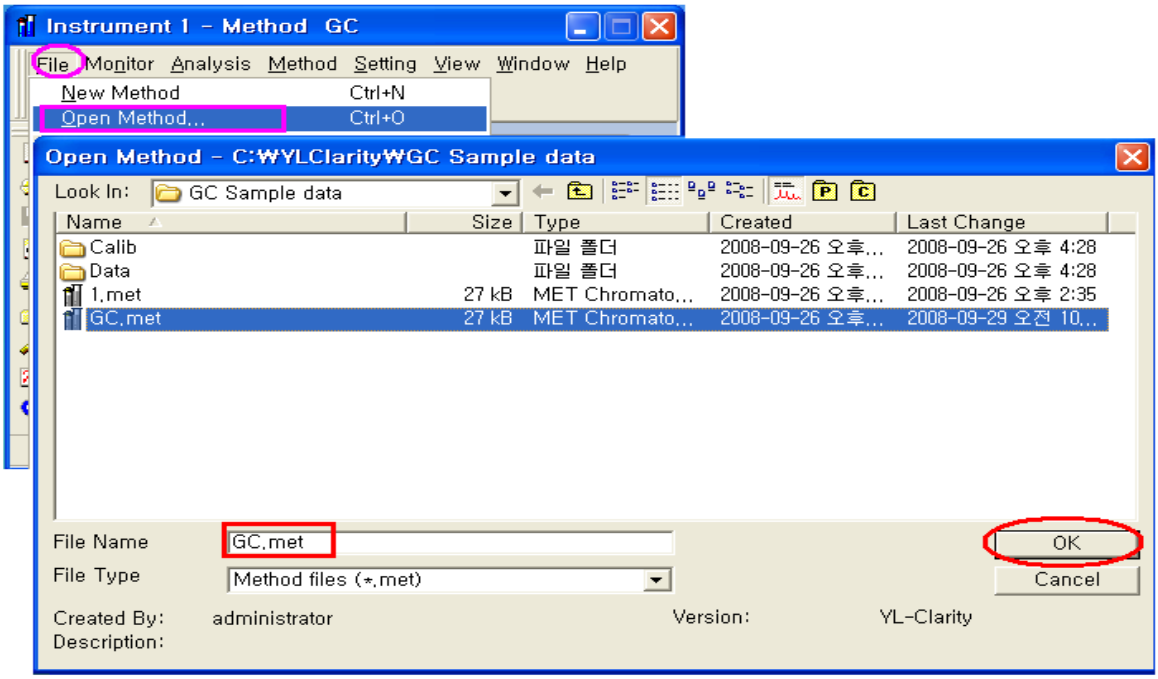
Report Style file is independent with Method file.

=> Using latest Report style file, print the report.

2-10. Batch operation

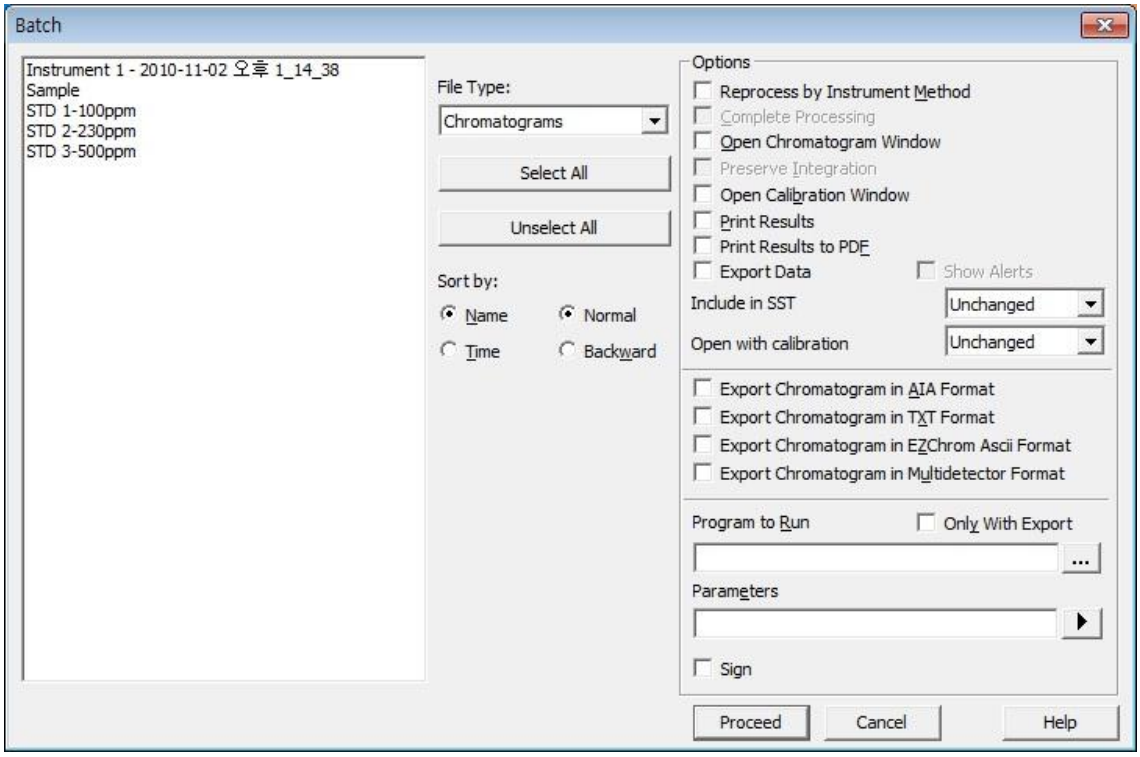
(integration, quantification, print report)

1. Save the Method file with calibration result(integration event + calibration file)
   Load Report sty file want to use
2. On the main control window => “File” => “Open Method” => Select Method file



3. Batch process

Select Analysis => Batch => select all data files want to process => Options check => Proceed



Confirm the result on the Chromatogram Window.

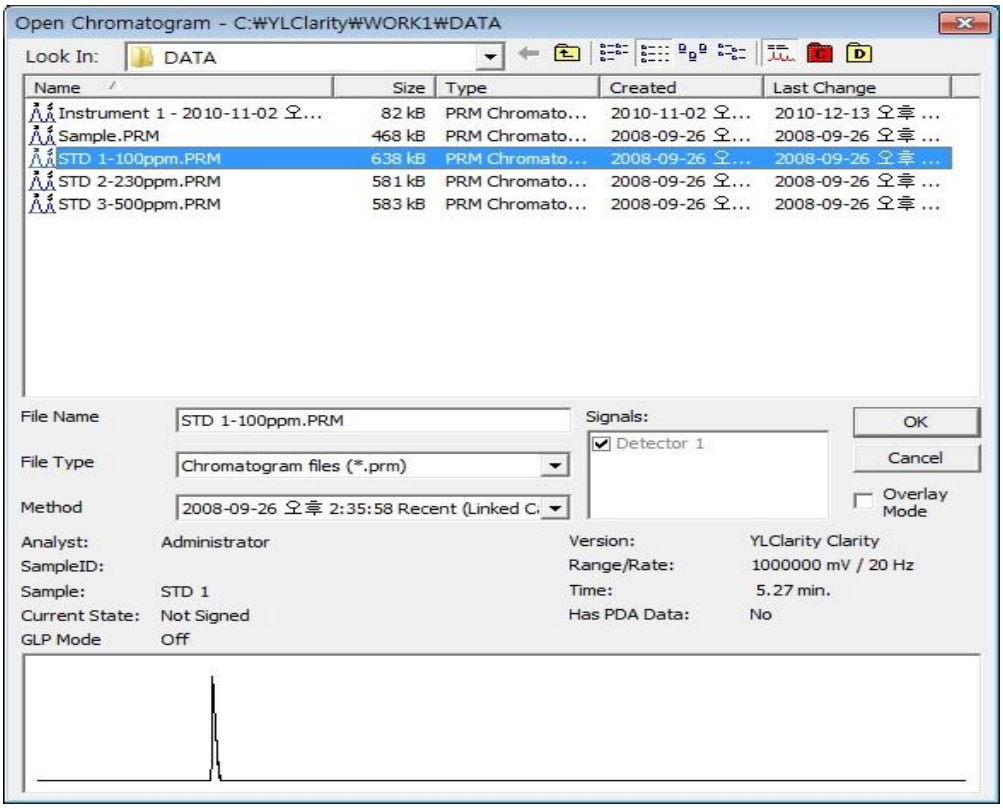
Using  icon, check the result one by one.

2-10. Chromatogram Overlay and Statistics

1. Open chromatogram

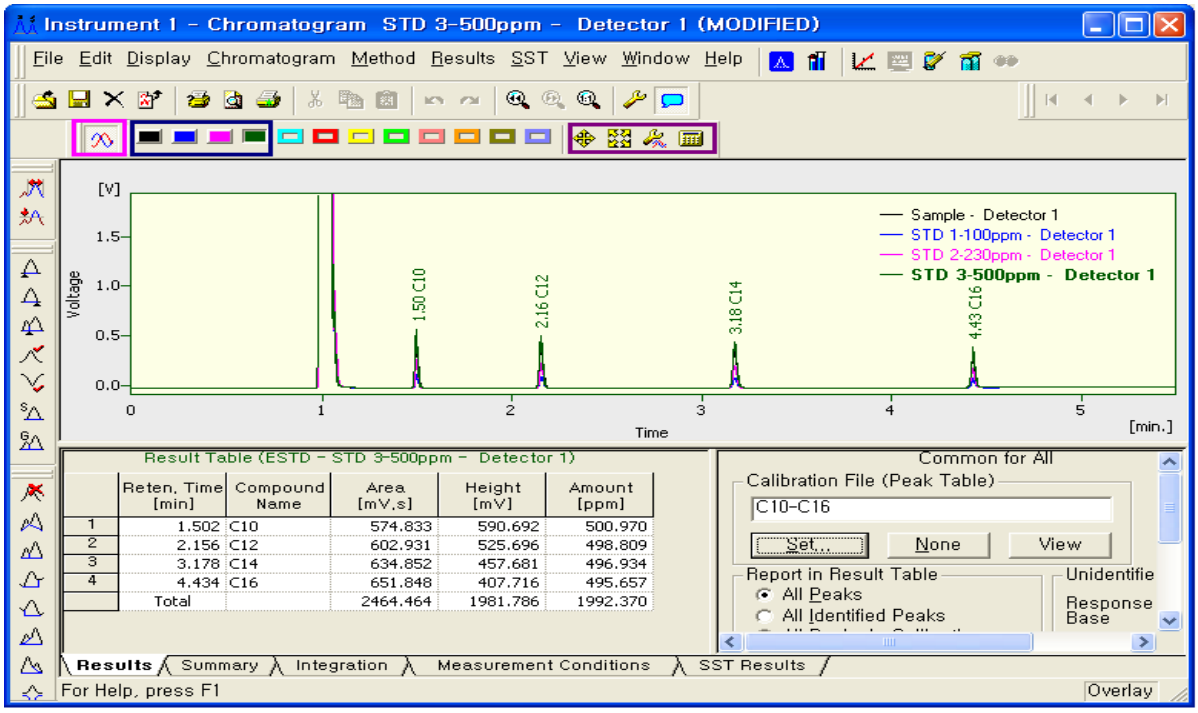
On the Chromatogram Window, click “Overlay mode” icon 

=> File => “Open Chromatogram” => Select all data want to compare => OK !



Following chromatograms are displayed and can choose color for each data.

Additional icon : Chromatogram move, zoom, amplification 



YL-Clarity

User Guide

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

YL INSTRUMENT CO., LTD.

Using this document

The **User's Manual** offers users of the **YL-Clarity** chromatographic station a detailed description of controls, a procedure for processing the first analysis, detailed guidance concerning the fundamental types of analyses and calibrations as well as copious additional information about the options and variants relevant for working with the station. Chapters 1, 2, and 3 are earmarked for beginners who will quickly find the required information there. Once the user has become acquainted with the fundamental procedures of the station, turn to Chapter **10 - Troubleshooting**, for a list of the most common problems encountered when working with the **YL-Clarity** station.

The **Reference Guide** contains summary information regarding all commands and error messages. The User's Manual presupposes that the user is coming to the station with some prior knowledge of the fundamental concepts (such as file, directory, path, etc.) of **Windows** operating systems.

The following fonts are used in the manual to highlight parts of the text:

Open	-	Commands and items - bold
Instrument	-	Window titles - Sans Serif, bold
WORK1	-	Filenames and directories – uppercase lettering
Enter	-	Key designations – Sans Serif, boxed
RUNNING	-	Available states of the station - uppercase, Italics
Istd	-	Values of parameters - Italics.
Full version	-	Passages that do not apply to the Lite version of YL-Clarity

YL Instrument Co., Ltd.

Contents

1 Introduction

1.1 Description of the YL-Clarity Station

The **YL-Clarity** chromatographic station is an effective program used to acquire, process and evaluate data from any standard, commercially available gas/liquid chromatograph. The station can process analyses containing hundreds of peaks with varying widths from tenths of a second to tens of minutes.

Due to the adjustable range (anywhere from ± 156 mV up to ± 10 V) of the inlet A/D converter the station can be directly connected to the output of almost any chromatograph.

YL-Clarity collects chromatographic data independently ("in the background") while the user analyses previously acquired data, corrects the baseline, performs calibrated or uncalibrated calculations, or runs other programs. Results can be printed on any printer, and the printout layout adapted to the user's needs through a host of adjustable parameters. Tables, data and displayed chromatograms can be exported as files or inserted directly to other programs running under **Windows**.

Calibrated calculations by the external or internal standard method may be performed using the calibration files. Each calibration file can contain an arbitrary number of components, each calibrated at up to 20 concentration levels.

YL-Clarity is also equipped to automatically process all data acquired from **CSW** stations.

The full version involves these extra features: Full version

Data can be acquired simply by using the control module from chromatographs with a digital output.

YL-Clarity can be configured to allow measurement on up to four chromatographs simultaneously, each of which can be equipped with up to 4 detectors. **YL-Clarity** is also equipped to support the cooperation between chromatographs and autosamplers, and tools for supporting the requirements of the **FDA**'s **21 CFR Part 11** guideline.

1.2 Updating of program

Updates to the purchased version of **YL-Clarity** are provided free of charge. We are constantly developing the **YL-Clarity** station to meet the needs of our customers. Should you have any problem with the station, please do not hesitate to let us know. Whether it concerns inadequacies in the existing functions or suggestions for improvements, we welcome and take seriously, user opinion as part of our job.

Who's afraid of the Internet?

For easier communication with the developer's team, we have prepared special web sites on which you can learn about a range of interesting information and on which you can inform us of any improvements you would like made, where you can meet other users and mutually exchange experience upon solution of ordinary problems with chromatographic work. All sites are easily accessible from the home page of the **YL Instrument Co., Ltd.** at the address www.ylinstrument.com.

We would like to draw your attention to several sections of the website:

Downloads – Product Updates

Offers updates to the station. Registered users may obtain the latest versions of their station.

Support - Technical Support

The easiest way to connect with our user support is via e-mail. You may of course also contact us by telephone or fax. Technical support enables you to determine the source of a fault and notify us with information we need to be able to help you to solve any problem you may have.

Support – Frequently Asked Questions

The FAQ section summarizes and addresses some of our customers most frequently asked questions and provides the answers.

User Forum

The Users Forum is a place where users are able to exchange experiences they have had with YL chromatographic stations and any connected technical or methodological problems that may have occurred while measuring chromatographic analyses.

Naturally our technicians carefully monitor this forum and answer questions regarding the use of **YL-Clarity**, but it is also not impossible for another user to have had the same problem as you may be experiencing and have an idea of how to solve it.

Automatic check of last available version

Should your computer be connected to the Internet, you may make use of automatic checking of the last available update. In the main **YL-Clarity** window use the **Help** – **Check for Updates** command. The command will compare the number of the last available version on the Internet server with the version you have installed. Should a newer version now be available, a dialog with the number of the new version will appear and you may download the new version.

After downloading, the **YL-Clarity** station will automatically shut-down and run the installation program. The program will take you step-by-step through the installation of the updated version. These updates are only available to registered users. Registration is accomplished by using the **Help - Register** command.

2 Station Control

Although the **YL-Clarity** station operates similarly to other programs that run in **Windows**, we would like to provide brief descriptions of basic **Windows** concepts.

2.1 Windows

Main windows

The **YL-Clarity** station has a hierarchical structure. Instrument consists of up to four major windows; the **Instrument**, **Chromatogram**, **Calibration**, and **Sequence** windows. When any of these windows are opened the corresponding icon along with the name will be displayed in the MS Windows taskbar.

Note: *If you find too many icons displayed in the taskbar distracting, uncheck the **Show Windows on the Taskbar** checkbox from the **User Options - General** dialog (accessible from the **Instrument** window using the **View - Options** command).*

Modal windows

Some open windows - called **modal** windows - prevent the user from working in any other window until the modal window is closed. The **Open File** dialog for selecting files is an example of a **modal** window.

MS Windows shortcuts

The following fundamental key combinations used to facilitate work with windows:

Alt + F4	Closes the current window
Esc	Closes a dialog
Alt + Tab	Switches between windows of all currently running programs
F1	Invokes the context-sensitive online help

2.2 Icons and Toolbars

Icons

Icons are small graphical symbols that facilitate invoking some functions or windows. All icons have the corresponding counterparts in menu commands.

Toolbars

Toolbars are panels containing icons. Toolbars are usually situated below the title bar, but can be moved to any place on the screen.
The **YL-Clarity** station contains several predefined toolbars that may be customised (icons can be added or removed); the user can also create his/her own toolbar.

Scheme of data processing

The **Instrument** windows display a special arrangement of icons that reflect the typical procedure of a measurement and chromatogram processing. The corresponding

commands can be invoked in any order (the displayed arrangement merely facilitates orientation and assists one in following the appropriate procedures for working). Note the three  or  symbols that correspond to the first three items of the **Postrun Setting** dialog.

2.3 Mouse Control

As with most **Windows** programs**,** the **YL-Clarity** station is most easily navigated and controlled using the mouse . **YL-Clarity** makes use of both the left and right mouse buttons, the fundamental concepts of which are explained below.

Clicking

"Clicking" is a term for pressing the left mouse button when the mouse cursor (the arrow) is pointing to the desired location such as an icon, a button, an edit line, etc. In most instances, left clicking will replace the function of the Enter key.

Double-clicking

- Clicking the left mouse button twice in rapid succession in the same location is most often used to select a file or highlight an entire word in the edit line.
- Customized function of the double-click can be set in all graphs using the **Doubleclick means** command from the **User Options – General** dialog (accessible from the **Instrument** window using the **View –Options** command).

Clicking with the right mouse button

- Typically displays the local menu.
- In graphs: Right clicking to zoom can be set using the **Zoom button** command from the **User Options - General** dialog (accessible from the **Instrument** window using the **View –Options** command).

Mouse wheel

The standard scrolling function of the mouse wheel has been extended for the **YL-Clarity** station to facilitate navigation in **Chromatogram**, **Data Acquisition** and **Calibration** graphs.

Wheel only	Shifts a chromatogram cut-out up or down
SHIFT + wheel	Shifts cut-out left/right
CTRL + wheel	Enlarges or reduces a chromatogram cut-out

2.4 Keyboard Control

The station may also be operated strictly from the keyboard. The following is an illustration of the functions of some of the keys and key combinations (striking multiple keys simultaneously).

Keyboard shortcuts of the MS Windows system:

Enter
Applies or implements the selected command. The command that has been selected will be

highlighted in the menu; in a dialog the borderline of the button will be emphasized by a continuous or broken line).

From the menu the required command can be selected using the cursor keys, and from a window using the Tab key.

Esc

In a dialog, the Esc key substitutes for the **Cancel** key and will close a dialog without saving the changes.

Hides an expanded menu.

Tab

Gradual selection of commands, parameters, edit lines and buttons in the active window. A selection is usually completed using the Enter key.

Spacebar

Rapidly switches between selected parameters by checking or un-checking them

Alt

Selects the first menu item.

Alt + letter

Rapidly selects a command or parameter that has the selected letter underscored.

Insert

Switches between the insert and overwrite regimes. When editing text lines you may use Insert to decide whether new characters will be inserted at the cursor position or will overwrite the characters to the right.

Keyboard shortcuts of the YL-Clarity:

Shortcut	Function	Validity
F1	Help	Everywhere
F2	Edit table mode	
CTRL + 1 (2,3,4)	Open instrument (**Login**)	
CTRL + N	New file	
CTRL + A	Select all items in the list/table	
CTRL + O	Open file (**Open**)	
CTRL + S	Save file (**Save**)	
CTRL + W	Close current file (**Close**)	
CTRL + SHIFT + W	Close all opened files (**Close All**)	
CTRL + P	Print (**Print**)	
CTRL + X	Cut (**Cut**)	
CTRL + C	Copy (**Copy**)	
CTRL + V	Insert (**Paste**)	
CTRL + Z	Cancel the last command (**Undo**)	Tables
CTRL + SHIFT + Z	Repeat the last command (**Redo**)	
CTRL + I	Insert and create lines (**Paste Insert**)	
DEL	Erase the table field	
CTRL + -	Display the previous cut-out (**Previous Zoom**)	**Chromatogram**, **Calibration**, **Data Acquisition**
CTRL + +	Display the next cut-out (**Next Zoom**)	

CTRL + *	Display in original size (**Unzoom**)	
CTRL + R	Start an analysis (**Run Single**)	**Data Acquisition**
CTRL + Q or F5	Start a sequence (**Start, Run Sequence**)	**Sequence, Data Acquisition**
CTRL + SPACE	Pause a sequence (**Pause**) / Resume running of a set sequence (**Resume**)	
CTRL + B	Immediately terminate a sequence (**Abort**)	
CTRL + H	Process the sample currently being measured without terminating the analysis (**Snapshot**)	
CTRL + T or SHIFT + F5	Terminate a sequence after the completion of a sample measurement (**Stop**)	
CTRL + Down	Skip the current sample (**Skip**).	**Sequence**
CTRL + Left	Repeat an injection from the current vial (**Repeat Injection**)	
CTRL + E	Reset the flags in the Sts. column (**Reset Status (Sts.)**)	
Insert	Adds the selected device to the instrument ( ). If no device is selected, opens **Add Device** dialog.	**System Configuration**
Delete	Clears the selected device from the instrument ( ).	

2.5 Tables

Because tables in the **Windows** environment are not standardised, the following essential characteristics of tables used in the **YL-Clarity** program are presented below.

2.5.1 Editing

Entering new values

Values can be directly entered in individual cells (provided the table cells are editable).

Note: *Some tables, such as the **Result Table** as well as tables from files that have been opened for reading only, cannot be modified.*

After first clicking a cell, you may then enter a new value that replaces the previous one. By double-clicking or pressing the function key F2 the cell will be transferred to the edit mode.
If, after clicking, an arrow button is displayed, the cell represents a list of values prepared in advance. Click the arrow and select the appropriate value from the list.
Move among the cells by means of the cursor keys.
Once the first cell has been entered the next row will automatically be created.
The row being entered is assessed in its entirety for error during these modifications and can only be abandoned after all errors have been corrected.

If the requested row is not visible, locate it using of the vertical scroll bar displayed on the right or by using the cursor keys. It is also possible to enlarge or maximize a window and display all rows of a table.

Changing values in cells without predefined values

Click anywhere inside the cell and enter the new value (the old value will be erased).
Text can be edited after double-clicking anywhere inside the existing value or pressing F2.

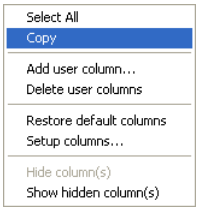
2.5.2 Adding and Deleting Lines

A new line will automatically be created once the first cell has been filled in. The user may edit the new line only after the accuracy of the preceding line has been verified.
The easiest way to delete a line is by first selecting it (using the grey button at the beginning of the row) and then pressing the Delete key.

2.5.3 Local menus of tables

Invoke the local menu by clicking any cell with the right mouse button.
The local menu contains commands from the **Edit** menu:

- The **Select All** command for selecting all cells in the table.
- Fuction **Undo/Redo** for cancelling or renewing applied changes in tables.
- Commands for working with the Clipboard: **Copy**, **Cut**, **Paste**, and **Paste Insert**.
- Commands for configuring the table - **Setup Columns**, **Restore Default Columns**, **Hide Column(s)**, **Show Hidden Column(s)**
- Commands specific for the given table.



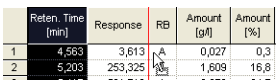
2.5.4 Configuring Tables

All tables enable the user to adjust the width of columns, the order of columns, potentially also the sorting method.

How to change the column width

To change the width of a selected column move the mouse cursor to the right border of the grey field of the heading (the cursor will change its shape to ✣). Click and hold the left mouse button then drag to change the column width.
Double-click at the above location to adjust the column width to accommodate the longest string of text.

Several columns may also be selected at once (changing the width of any one will change the widths of all).



How to change the order of columns

Left click on the grey header of the required column. Click again and hold down while dragging the cursor left or right to the desired location for the column. As soon as a thin red line appears at the location where you want to move the left border of the column, release the left button.

How to sort items in a table

Items (lines) of a column are ordered by default according to the first column or the order in which the lines have been created. To reorder a table according to some other column double-click the heading of that column to sort in ascending order; repeat the process to sort the table

in the descending order. Some tables (e.g. the Integration Table) cannot be reordered, or reordering must be first permitted by the **Enable Sort** command from the local menu.

Displaying and hiding columns

The result tables in the **Chromatogram** window and tables in the **Calibration** window can be extensively reconfigured using the **Setup Columns** command from the local or **Edit** menu. Once invoked, the **Setup Columns** dialog will open. From here, the user can select the columns to be displayed and define their order.

Creating of new column with definition of calculation

Full version

Invoke the **Add Column** command to open the **Add User Column** dialog. Here the user can create a new column for the table using a predefined calculation formula. User columns can be displayed in the **Result** and **Summary** tables.

2.6 Clipboard

Using the clipboard

All data in tables and parameters may be transferred to other locations in the station or even to and from other programs simply using the **Cut**, **Copy** and **Paste** commands.

Within the **YL-Clarity** station it is possible to use the clipboard to copy text labels and lines between chromatograms.

Note: *A typical example of this feature is the use of the table calculator (Excel) to easily prepare an extensive sequence table. This can then be easily transferred using the **Copy** and **Paste** commands into the **Sequence** window.*

Copying data to the clipboard

The values of all parameters and the content of any fields of the tables may be transferred to any other places or other programs of the **Windows** system with the help of the clipboard. The **Clipboard** is a temporary memory that is shared within the entire **Windows** system, into which you enter the selected value using the **Copy** or **Cut** command. You then locate these in another place using the command **Paste**. In some tables you also use the

Paste Insert function (keys Ctrl + I), which does not rewrite the original content of the table but instead adds new lines above the currently selected line.
These commands can be found in either the **Edit** or the local menu of the tables. Also, using the **Copy** (Ctrl + C), **Cut** (Ctrl + X) and **Paste** (Ctrl + V) commands is possible.

Selecting an area to be copied

Use the left mouse button and the grey buttons at the top and to the left of all tables to select a contiguous area. All cells passed by the mouse cursor with the left button held down will be highlighted. The grey buttons to the left select the entire row, those on top select the entire column; the top-left button selects the entire table. To select a contiguous area use a combination of the SHIFT key and the cursor key. The combination Ctrl + A or the command **Select all** from the local menu selects the entire table (see Chapter **2.5.3** - **Local menus of tables**, p. **7**).

Note: *Editable tables are (after selecting all cells of the table) copied to the **Clipboard** without header.*
Non-editable tables are copied with header.

Automatically filling table fields with repeating values.

When entering data into the tables it may occur that you need to fill in an area of the table with periodically repeating information. The **Paste** command automatically supports this need. It is sufficient enough to copy information into the clipboard that is to be repeated and then indicate the area where data is to be inserted using the **Paste** command.

Note: *Automatic data entry applies to both lines and columns. Should you thus wish to insert periodically repeating lines, remember to insert them whole into the clipboard (including any empty columns).*

Deleting values

Often times selected values can be deleted by the **Delete** command or the Del key.

2.7 File Selection

Open any file using the **Open** command. The **Open X** dialog will first be displayed (where X stands for the type of file; a chromatogram, a method, etc.)
A list of all files of the given type from the current directory is displayed on the left (the path is shown in the title bar).

Information about the file

If you click any file and have the panel with a detailed view of the file open by  icon, the items below indicate a detailed description of the file, the name of the author, the version, potentially a preview of the data.

Opening a file

Use the **OK** button or double-click on the filename to display a file. If the station is operating in the password-protected mode and you do not possess the necessary authorisation to access the file, an error message will appear.

Changing the directory

If you wish to open a file from another directory, click the **Look In** (combo box) pull-down menu to inspect and change the current path.

The following icons are displayed in the top-right portion of the window. They allow the user to directly return to the current directory.

 - Current project (storing the template methods).

 - The common project COMMON (storing the report styles)

 - Data subdirectory of the current project (storing chromatograms)

 - Calibration subdirectory of the current project (storing calibration files and standards)

Ordering files

Files are ordered alphabetically by default. To order files either by date/time, size, or when last saved, set a detailed view using the  icon and sort the files by double-clicking the heading of the corresponding column. Double-clicking again will sort the list in reverse order. The ordering mode is indicated by the  icon in the column heading.

Filtering displayed files

While the filename is being entered in the **File Name** field only files beginning in the already entered text will be displayed. If you wish to find files containing a given text not at the beginning of the filename, start by entering either * in the **File Name** item or the corresponding number of question marks.

Filtering file types

The **File Type** field selects the type of files to be displayed.
Selecting *All Files (*.*)* will display all of the files in the current directory regardless of whether they have the same extension that has been ascribed to the relevant file type.

Simultaneous opening of several files

If the *OVERLAY* mode has been enabled, several chromatograms can be selected in the **Chromatogram** window.
To affect a contiguous selection click the first file, then press and hold down the Shift key and click the last file to be selected. All chromatograms will be highlighted and subsequently read in by clicking the **OK** button or striking the Enter key.
Use the Ctrl key to select files other than contiguous files. Press and hold down the Ctrl key while clicking on the files to be selected one by one. Confirm the selection by clicking **OK** or pressing Enter.

2.8 Saving Files

Use **Save** to automatically save changes effected in the file without changing the name or directory of the file.
The **Save As** command saves the file under a different name and/or in a different directory from which the file was opened. When invoked, the **Save As** dialog will display the original filename and directory of the file. Enter a new name in the **File Name** field and select another directory using the **Look In** field (also known as the, “combo box”) and use the **File Type** field to save the file in another format.

Note: *The **File Type** item converts files between the **CSW17 CSW32** and **YL-Clarity** stations in both directions.*

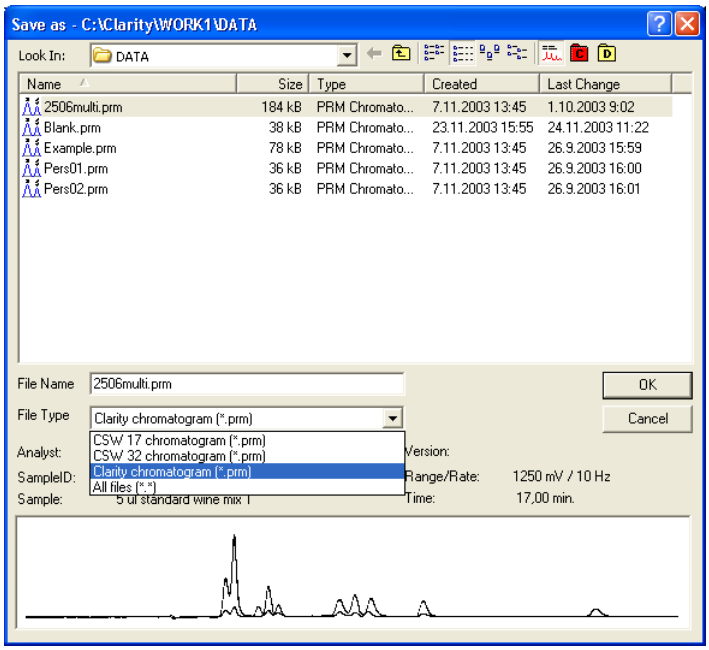


Fig. 1. The Save As dialog

Note: *It is not advisable to save files outside of the current project folder.*

2.9 Recording all station operations (Audit Trail)

Full version

Station Audit Trail

The **YL-Clarity** station keeps a log of all of the operations that it performs. Records of the station's operations are saved in the LOG sub-folder in the station's main folder. All operations performed during a single day (24 hour period) are saved into a file that is named by the date the operation was completed using the LOG suffix. This file can be displayed in the **Daily Audit Trail** tab. The **Session** tab limits the displayed operations only to those that have been performed since last running the session.

Local Audit Trails of individual files

Apart from recording all station operations the station also keeps detailed records of all operations of sequence, calibration and chromatogram files. These records are part of each file and can be displayed using the corresponding **Window - Audit Trail** command from **Sequence**, **Chromatogram** or ***Calibration*** windows.

What are the Audit Trails useful for?

- Logging station activity is one of the essential steps that need to be made in order to fulfill the conditions of *Good Laboratory Practice* (GLP).
- Due to the existence of recorded information in the log table we can easily analyse the conditions that may lead to errors or instability in the station. The program also enables

you to send information regarding system settings and a record of the last two days of station operations when the station has been improperly terminated.

Note: *Before sending an e-mail with information regarding error(s), you have the option to check and modify its content or add comments for our user support. The message will be sent only after you have approved it.*

- The *Audit Trail* also functions as a journal of sorts. If, for example, you are unable to recall the name of a file to which you had exported the results of a performed analysis, you can search for that file in the *Audit Trails* for the given period, arrange the lines according to type of events and check the exports.

3 Structure of YL-Clarity station windows

The following Figure shows the fundamental structure of YL-Clarity stations.

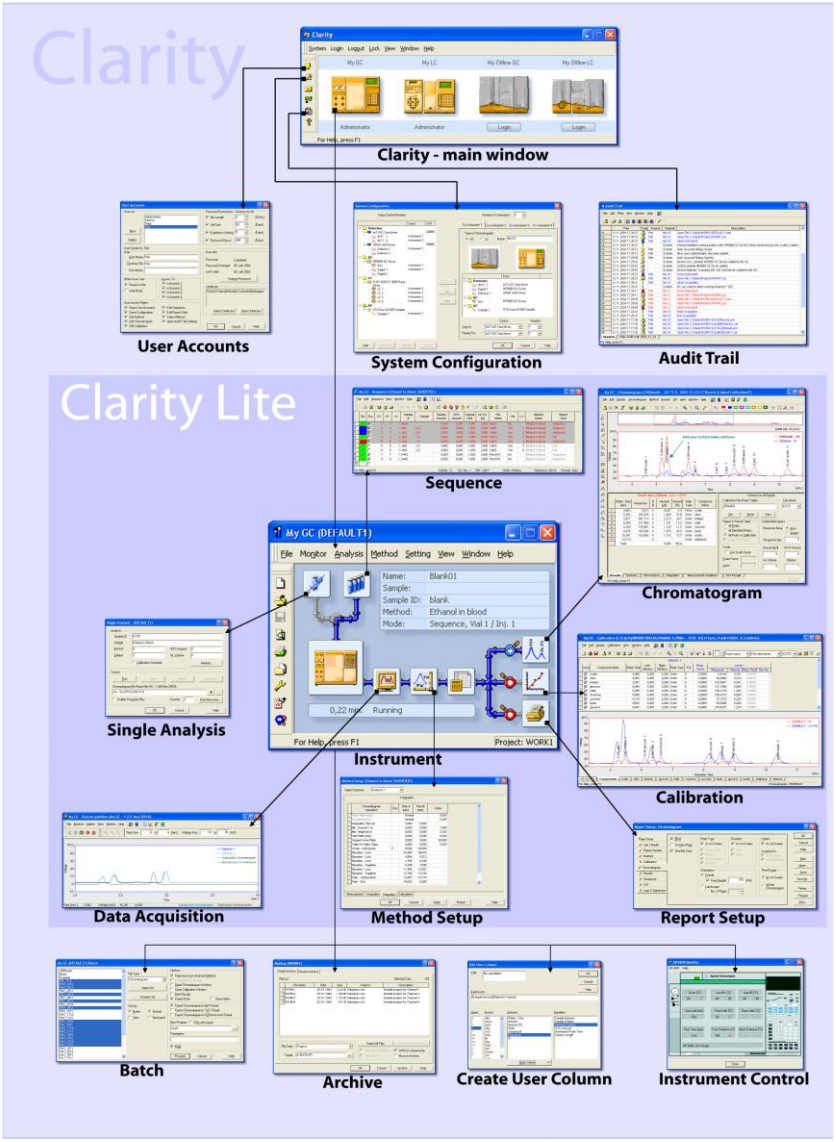


Fig. 2. Fundamental Structure of YL-Clarity Stations

3.1 Structure of YL-Clarity windows

Full version

YL-Clarity stations are organised hierarchically.

The full version can measure on multiple instruments simultaneously. After starting the station the main **YL-Clarity** window will appear and display the symbols of up to four instruments. The **Instrument** window for measuring and processing analyses from connected detectors can be opened by clicking the chromatograph icon and, if need be, entering the user's name and password.

3.1.1 YL-Clarity window

Full version

The fundamental purpose of the main **YL-Clarity** window is to select which instrument is to be used for a particular measurement. The window can be also used to configure the station, select the base directories for data storage, set up the digital outputs, and select the favored method for logging station activities.

Most commands in the main **YL-Clarity** window are enabled only when all **Instrument** windows are closed.

3.1.2 Instrument Window

Full version

All tools necessary for working with a single chromatograph are brought together in the **Instrument** window.

The **Instrument** window contains an information table, status line and analysis-processing diagram.

- Each **Instrument** window opens independent dialogs, so it is possible to control the proceeding of analyses on multiple instruments simultaneously.
- Windows are distinguished by line colour in the analysis-processing diagram and instrument name in the header or potentially in the project (= directory) name in the *Status bar*.

3.1.3 Chromatogram Window

This is the fundamental window for displaying, modifying and evaluating chromatograms. Open the window by clicking the  icon in the **Instrument** window or at the end of menu bars in other **YL-Clarity** windows.

3.1.4 Calibration Window

The **Calibration** window is designed to create, modify and display calibration curves. Open the **Calibration** window using the  icon from the **Instrument** window or using the **Window – Calibration** command from any window. Refer to the **Getting Started** manual for hints on how to create and use a simple calibration.

3.1.5 Sequence Window

This window defines the sequences of multiple analyses. Open the window by clicking on the  icon from the **Instrument** window or the **Window – Calibration** command from any window.

3.2 Structure of YL-Clarity Lite windows

When using the **YL-Clarity Lite** version the **Instrument** window labeled as **YL-Clarity Lite** will appear after starting the station instead of the main window for selecting the instrument.
In contrast to the full version you will find here commands that are in the full version part of the main **YL-Clarity** window:

- In the **File** menu the **Digital Outputs** command
- In the **Help** menu the **Register**, **Check for Updates**, **Send Report by Email**, **User Code**, **YL-Clarity Online** and **About** commands.

For Chromatogram, Calibration and Sequence windows applies the same description like in the full version (chapters **3.1.3** - **3.1.5**).

In contrast to the full version, **YL-Clarity Lite** does not contain the following features:

- Simultaneous measurement on multiple instruments
- Logging of the station's activities - **Audit Trail**
- Advanced setting of access rights, layouts - **User Accounts**
- Setting up the Station - **System Configuration**
- Offline batch processing of multiple chromatograms - **Batch**
- User columns in result tables - **Create User Column**
- Direct control of GC, LC and AS using add on control modules – **GC/LC/AS Control**, **GC/LC Monitor**.
- Backing up of files and projects – **Archive**
- Electronic signatures – **Sign**
- Additional advanced functions useful for working in bigger laboratories

4 Chromatogram Measurement and Evaluation

This Chapter provides a comprehensive review of all the possible ways to measure a single or a series of chromatograms.

4.1 Measurement

A complete measurement is comprised of the data acquisition from a detector, the digital integration of the measured data, and storage of the results on the hard disk.
Individually, an **Instrument** window can be in any one of the following individual states, regardless of the state of other **Instrument** windows:

STOP	-	A measurement is not in progress and may not be started by an external signal.
WAITING	-	A measurement is not in progress and the station is waiting for the external "start" signal before it can begin.
RUNNING	-	An analysis is in progress.
PAUSED	-	Indicates a suspended sequence.
RUNNING/PAUSED	-	The sequence will be suspended after the current analysis has been completed.
IDLE	-	The state of active sequence after the measurement has been finished and before the confirming signal will be sent from the station to the autosampler. The duration of IDLE state can be customized by the user.

Full version

CONTROL	-	Data acquisition has completed and the control program of the directly controlled chromatograph or the LC pumps is concluding its run.
WAITING FOR READY	-	The active sequence has been started, station is waiting for the READY signal from the directly controlled device.

Measurement with the **YL-Clarity** station is comprised of the following steps:

- The A/D converter transforms the analog signal to a 24-bit binary number representing the integral value over a given time.
- Due to the design of the converter, it is possible to obtain a true integral. The YL A/D converter permanently integrates the input voltage while standard sampling converters with approximation transfer, only sample voltage at discrete time intervals.

Full version

Note: *This does not apply to detectors with digital output for which a control module is available (e.g. HP 5890, 6890, etc.) where the data is transferred to YL-Clarity through the RS-232 serial line.*

- The above binary number will then pass through a digital filter that filters out all parasitic components originating, e.g., from power voltage fluctuations.

- Individual binary numbers (data items) are read from the converter at a specified rate. Each partial integral occupies four bytes.
- Data samples are temporarily stored in the operating memory and then sent to the hard disk approximately once per minute as a buffer. In the TMP subdirectory of the main station directory (C:\CLARITY\TMP by default) a file $CHXRUN.RAW (where X stands for the instrument number) is thus created for storing the so-called raw data. This ensures that very long chromatograms can be measured since the capacity of the hard disk is much higher than the capacity of the operating memory.

Selecting the sampling rate

In the field of fast measurements on capillary columns and microcolumns in particular you would be glad to make use of one of the preset sampling rates. The setup is a part of the method file and can be changed using the **Method - Acquisition - Sample Rate** command from the **Instrument** window. Changing the sampling rate affects the chromatogram size.

Note: *The available scopes of sampling speed depend upon the type of converter used.*

4.2 Processing the Analysis

Processing chromatographic data means identification of all peaks in the chromatogram, its identification and quantification and determining the proper baseline. The **YL-Clarity** station is equipped with a standard algorithm for processing chromatographic data. The algorithm requires that the **Peak Width** and **Threshold** parameters be set. These parameters are a part of the template method file and will be transferred to the chromatogram after an analysis is terminated.

Peak Width

The parameter decides on the peak width at half height (expressed in minutes) of peaks occurring in the processed analysis. The value should approximately correspond to the parameter *W05* (peak width at half height). For peaks of different width the value should be set according to the narrowest one.

Threshold

The parameter is entered in millivolts, is independent of peak width and discriminates between a useful signal and noise. If a peak has to be included in integration or measured then the height between the beginning and apex of that peak should be at least twice as high as the value of this parameter.

Both parameters fundamentally influence the quality of the resulting chromatogram with regard of peak detection (determination of peak beginning and end and the correct baseline). Accordingly, in creating a template method used for each class of analyses pay appropriate attention to the optimum setting of the two parameters. Although the setting is not too critical (the result will be the same within a certain range of values), their incorrect selection must be subsequently corrected by operations with the chromatogram (see Chapter **5.4** - **Chromatogram Modifications** on page **39**). These additional operations should not substantially change the selected baseline, rather eliminate some phenomena that the peak detection algorithm is unable to cope with (e.g., tangential separation, identification of the solvent peak, ban on detection during the period of column switching, etc.). Some practical guidelines referring to setting up these parameters are in Chapter **10.4** - **Processing and Displaying Chromatograms** on page **76**. In general, the minimal width of detected peaks (expressed as the distance between the peak start and end) is directly proportional to **Peak Width** and inversely proportional to **Threshold**. Moreover, the **Threshold** parameter prevents erroneous assignment of noise to spurious peaks.

In addition to the above two obligatory parameters stated in the firs two lines of the Integration table, a number of further parameters can be set in the Integration table allowing for automatic integration of complicated chromatograms. These parameters are described in detail in the chapter **5.4** - **Chromatogram Modifications** on pg. **39**

4.2.1 Method

The method file constitutes a tool used to achieve facile description and setting of all measurement conditions and to attain high reproducibility of measurements performed with the **YL-Clarity** station.
The method is divided into a number of sections, of which each is reserved one tab of the **Method Setup** dialog.

Event Table	-	Section for control of the inputs.
Measurement	-	Section with description of measuring conditions and possible setting of length of measurement or automatic subtraction of desired chromatogram.
Acquisition	-	Section with parameters that are related to a signal measurement. This includes attenuation, sampling rate, control of digital outputs through the **Event Table**, etc.
Integration	-	Section with integration parameters for the correct identification of peaks and determination of the baseline.
Calculation	-	Section summarising calculation parameters for setting the type of calibration calculations.
Advanced	-	Section with settings of chromatogram subtraction and column calculations.
		Full version
AS Control	-	Section for potential direct autosampler control.
LC/GC Control	-	Section for potential direct control of a chromatograph or pump

The template method file is accessible from the **Instrument** window using commands from the **File** menu.

Note: *Carefully select the method for measuring a chromatogram, in particular with regard to attenuation, duration of analysis, the limiting integration parameters and the selection of the calibration file. For example the parameters from the **Acquisition** tab should be checked prior to starting an analysis, since they cannot be modified later!*

Once an analysis is terminated, a copy of the method file will be stored with the created chromatogram.

This ensures that most parameters will be available and may be changed in the already measured chromatogram. These are found in the relevant tabs of the **Chromatogram** window using commands from the **Method** and **Results** menus.

Note: *The layout of individual commands does not completely correspond to the tabs of the **Method Setup** dialog. This is mostly due to the fact that parameters from the **Chromatogram - Acquisition** dialog serve for information only and cannot be changed.*

4.2.2 Chromatogram

Raw data processing results in the creation of a chromatogram (file extension *.PRM). Chromatograms consist of three basic parts: a copy of the model method, the raw data, and the chromatogram (with identified peaks and a marked baseline).

Chromatograms can be displayed (in either the **Chromatogram** or the **Calibration** window), printed, and the file contents exported to the Clipboard or to a text file. Chromatograms of individual projects are stored in either the data or the calibration subdirectory. Rapidly switch between the subdirectories using the  and  icons in the **Open Chromatogram** dialog.

Full version

Note: *If you prefer not to have the chromatograms separated in the above manner, select identical names of the two subdirectories (**Analysis Subdir.** and **Calibration Subdir.**) when establishing a new project in the **Project Setup** window.*

To obtain detailed information about the active chromatogram invokes the **Method - Measurement** command from the **Chromatogram** window.

4.3 Fundamental Procedure of Analysis

The following chapters present directives informing about various methods of analysis processing. The basic procedure is also described in the **Getting Started** manual in the **First Analysis** chapter. Additional information is also available in chapter **10.2** - **Signal Displaying and Measurement** on page **75**.

4.3.1 Single Analysis

This chapter describes a comprehensive procedure of analysis processing and takes most options the station has to offer into account. Some additional variants are discussed in subsequent chapters.

Instrument selection

Full version

Click the instrument icon (found in the main **YL-Clarity** window) that represents the chromatograph you wish to use in the analysis. Fill in your name or, while in the protected mode, select your **User Name** and enter the **Password**. Then click the **OK** button to open the corresponding **Instrument** window.

Setting up measurement conditions

All parameters and data items referring to the measurement are summarised in the **Method Setup - Measurement** and **Acquisition** tabs of the template method. These are first displayed using the  and  icons, or by using the **Method - Measurement (Acquisition)**

command from the **Instrument** window. The name of the template method will be displayed in the **Information table**. If you prepare another template method during the measurement, the name of this current template method will be displayed in the header of the **Instrument** window.

Setting up the maximum input voltage

The input range (attenuation) is defined by the **Range** item in the **Method Setup - Acquisition** dialog, and must be higher than the maximum output voltage of the employed detector. On the other hand, it is improper to measure small voltages with, say, the 10-V range, since this would reduce resolution and accuracy of the measurement. If you intend to measure negative voltages,

check the **Bipolar** checkbox in the A/D converter setup dialog (accessible from the **System Configuration** dialog by double-clicking on the A/D converter (INT7, U-PAD, etc.) icon.

Note: *In case of multidetector measurement, it is necessary to set the range values for each detector separately using **Select detector** item in the **Method Setup - Acquisition** dialog.*

Monitoring the baseline drift and noise

Open the **Data Acquisition** window using the icon or the **Monitor – Data Acquisition** command from the **Instrument** window.

The signals from all detectors will automatically be identified and displayed within the range set in the **Time** and **Voltage** fields.

When the displayed range is unsatisfactory, change the values in the **Time** and/or **Voltage** fields and confirm the change by pressing Enter where the signal will be displayed with the new zoom.

Use the left mouse button to zoom in on any one of the cuts.

To resume from the original magnification that was specified in the **Time** and **Voltage** field, double-click the left mouse button.

The station will store selected cuts; to see them use the **Previous** and **Next Zoom**, commands respectively.

Note: *In a zoomed-in cut the window will no longer be automatically redrawn (the same is true when the base range of the window has been exceeded).*

Starting an analysis

Use the icon or the **Analysis - Single** command to open the **Single Analysis** dialog where the analysis can be controlled.

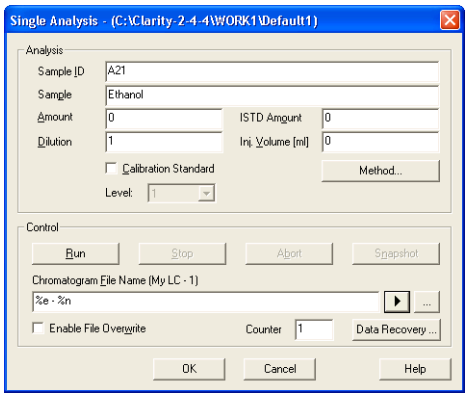


Fig. 3. The Single Analysis Window

Fill in header of the analysis in the **Analysis** group.

If you check the **Calibration standard** checkbox the chromatogram will be automatically stored in the CALIB subfolder.

Check the template method using the **Method** button.

Having injected the sample run the analysis using the **Run** button

The control of an analysis through an external signal is described in chapter **4.3.1.1** - **External Control of Analysis Run** on page **22**.

Note: *Measurement can also be run by using the **Analysis** – **Run Single** command, or using the icon from the **Data Acquisition** window.*

Monitoring the analysis

By default the range of the signals from detectors will not be automatically identified during analysis. The fixed range defined in the **Time… to…** and **Voltage… to…** fields will always be displayed. When the preset values are exceeded the window will not be automatically redrawn.

Note: *The values entered in the **Time** and **Voltage** fields do not in any way limit the scope of the acquired data. The maximum voltage range is defined by the **Range** items from the **Method Setup - Acquisition** dialog. The duration of an analysis may only be restricted by checking the **Enable Autostop** checkbox and setting the **Run Time** field from the **Method Setup - Measurement** dialog.*

Background chromatogram:

Full version

You can also compare the analysis that is in progress to a completed chromatogram by invoking the **File - Set Background Chromatogram** command and selecting the chromatogram that is to be displayed in grey in the background of the **Data Acquisition** window. The chromatogram in the background will only appear after the current analysis has been started.

Automatic subtraction of Chromatogram:

Full version

In addition to comparing the measured signal with the background chromatogram (see above), the **YL-Clarity** station also offers the ability to subtract a chromatogram automatically. Set the desired chromatogram in the **Chromatogram** field and select the

method for automatic subtraction in the **Matching** field from the **Method Setup** – **Measurement** dialog. The station will either simply subtract the chromatogram from the currently measured signal or will attempt to displace the subtracted chromatogram with the measured chromatogram. A more detailed description is provided in the **Reference Guide**.
Display the subtraction chromatogram in the background of the **Data Acquisition** window by using the **File – Show Solvent Chromatogram** command. The status bar of the **Data Acquisition** window will indicate which chromatogram is to be subtracted.

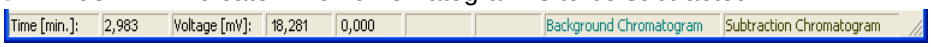


Fig. 4. Status bar of the Data Acquisition window

Setting up the processing parameters

The measured chromatogram will be integrated and evaluated according to the parameters of the template specified in **Method Setup - Integration** and **Calculation** tabs.

Especially check the following parameters:

- **Peak Width** - Enter the width of the narrowest peak expected (in the **Method setup – Integration** dialog)
- **Threshold** - Enter the half height of the lowest expected peak (**Method setup - Integration**)
- **Calibration File** - Set the calibration file that contains the table of compounds used for their identification as well as the calibration curves used to calculate the actual amounts (in the **Method setup - Calculation** dialog).

Preparation for analysis termination

Check the **Setting - Postrun** command from the **Instrument** window regarding which activities will proceed after the processing of measured data.. See Chapter **4.3.1.4 - Automatic Functions after Analysis** on page **24** for additional information.

Invoke the **Analysis - Single** command to open the **Single Analysis** dialog and inspect the **Chromatogram File Name** field.

Up to 254 characters, including spaces and national characters, may be entered. The following characters are however, not allowed: / \ : * ? " < > |.

When employed in the normal operation, the **automated naming** option is very useful. The station uses a set of variables such as the sample number, and current date, etc. that are preceded by the "%"character. Once an analysis has been terminated each such variable will be substituted by the topical value. Variables may be combined and the topical value will be displayed in parentheses above the **Chromatogram File Name** field and in the **Information table** of the **Instrument** window. For additional details refer to the **Reference Guide**, chapter **Single** - in the **Chromatogram File Name** section.

Assistant for setting file name

Click on the icon next to the **File Name** field in the **Single Analysis** dialog to open the assistant that will utilize individual variables to compose file names. Simply select the required function, click on it and the assistant automatically adds the corresponding variable to the file name.

1. *In some instances the application will save the chromatogram under a special name, using the first free eight-digit number starting at 00000000.*. This is designed specifically for situations where a risk that measured data might be lost or existing data overwritten exists:*
   -The user has cancelled the invitation to enter a new chromatogram name using the ***Cancel*** *command.*
   -The application was unable to display a message requesting that the new chromatogram name be entered, since e.g. some other message was displayed at that time.

End of analysis

Activate the **Stop** button in the **Single Analysis** dialog. Depending on the settings affected in the preceding two articles, the analysis will then terminate and the measured data will be saved, potentially evaluated, displayed and printed.

Activation of the **Run** button will terminate the analysis in the same way, run the next analysis and continuously measure a series of analyses.

Note: *An analysis can also be terminated using the* ***Analysis – Stop, Abort*** *commands (, icons) from the* ***Data Acquisition*** *window.*

Displaying results

The ability to have chromatograms automatically displaying in the **Chromatogram** and **Calibration** windows depends on the setting of the corresponding checkboxes from the **Postrun Setting** dialog.

Open the windows manually using the and icons and then have the chromatograms displayed using the **File - Open** or **File - Open Standard** commands.

Data evaluation

Invoke the **Results - Result Table** command to display the table of integration results in the **Chromatogram - Integration** window. See Chapter **6** - **Calculations and Calibration** on page **49** for a detailed description (including the procedure used to obtain calibrated results).

Presentation of results

The results of an analysis can be automatically printed, exported (see Chapter **7** - **Reports** on page **66**) and processed by another program (e.g. Excel), which will be automatically run after termination of the analysis. All based on the settings in the **Postrun Setting** dialog. See Chapter **4.3.1.4** - **Automatic Functions after Analysis** on page **24** for additional details.

4.3.1.1 External Control of Analysis Run

Analyses can also be run and terminated using an external signal: from a chromatograph, an auxiliary button on the cable or a sampling valve (depending on your configuration and program installation). The **External Start/Stop** checkbox from the **Method Setup - Measurement** dialog enables external control. Items in the synonymous section decide on the external control mode.
The **Down** and **Up** items decide whether the station will react to the ascending (leading) or descending (trailing) edge of the external pulse.

The **Start Only** item specifies that the external signal will only start analyses (subsequently manually terminated), either by the **Stop** command or by checking the **Enable Autostop** checkbox.

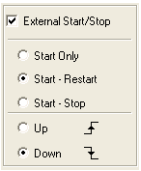


Fig. 5. External Start/Stop section of the Measurement tab

The **Start-Restart** item decides on whether the external signal will stop the currently running analysis and immediately start the next one (continuous series of analyses).
The **Start-Stop** item specifies that the external signal will only terminate the currently running analysis, and the start of the next analysis will wait for an additional external signal.

4.3.1.2 Continuous (Preliminary) Measurement Processing

While an analysis is running the already acquired part can be evaluated (while the analysis continues) using the **Snapshot** command from the **Single Analysis** or **Data Acquisition** windows. This command is almost identical to the **Stop** command but does not stop the analysis. The **Snapshot** is suitable e.g. for a preliminary evaluation of a prolonged analyses.
The **Snapshot** does not increment the counter of the analyses (*%n*) and a warning message regarding an eventual overwrite of the existing chromatogram will be displayed only when the **Snapshot** command has been used in the analysis for the first time. Any changes will then be overwritten by next use of the **Snapshot** command or after the end of the analysis in progress.

4.3.1.3 Control of External Devices

The **YL-Clarity** station (when using A/D converter) is able to control external devices equipped with control inputs (pumps, temperature programmers, autosamplers, etc.). The **Event Table**, included in each method, can control up to eight inputs on the internal or four inputs on the external A/D converter. Each line of the table defines a single condition - event - and, if the condition is satisfied, a set a specified output to the prescribed value. Examples of events: the expiration of a preset analysis time - **Time**, the decrease of a detector signal below or increase

above, a preset value measured either from zero - **Input** or from the value at the start of the current analysis - **Input Rel.**

When contradictory requirements involving a single output occur, the last command issued will be in control.

When using a multi-detector measurement there will be a separate **Event Table** controlling the outputs of the A/D converter and containing the corresponding channel for each detector.

Event Table creation and modification

To display the **Event Table** invoke the **Method Setup – Event Table** dialog command from the **Instrument** window.

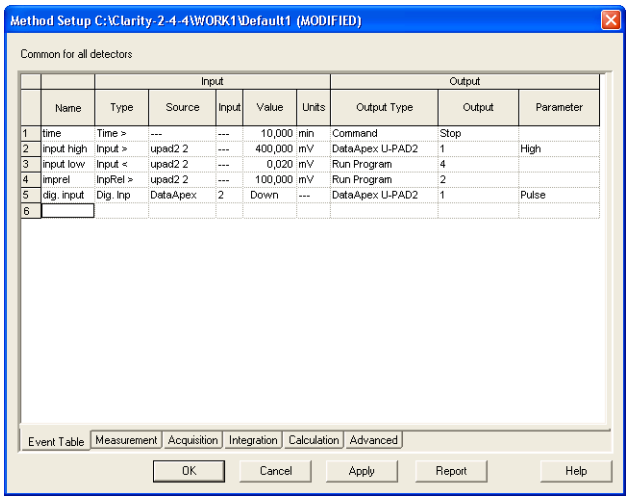


Fig. 6. Event Table

A new line will automatically be appended once the previous line has been correctly filled in.

*Active sequences use some of the digital outputs for synchronising the station with chromatographic equipment. Should you use an active sequence, ensure that you do not use those specific outputs in the Events Table. Active sequences are described in chapter **4.3.2.2 – Active Sequence without Control** on page **26**.*

Manual setting of control outputs

Control outputs can also be manually managed using the **System – Digital Outputs** command. Invoking the command will open the **Digital Output Control XXX Board** dialog (where XXX stands for the name of the A/D board that is used or selected). The first column, **Initial State**, is earmarked to set up the default state of the outputs each time the program is run. The second column, **Current State**, sets the topical state of the outputs and enables the user to change it immediately.

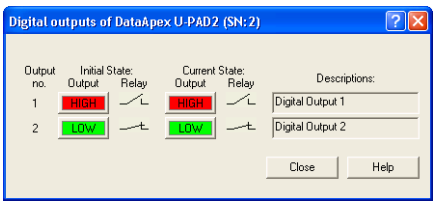


Fig. 7. Digital Output Control for the U-PAD2.

A **Description** column is provided so that notes explaining the meaning of individual digital outputs may be entered.

4.3.1.4 Automatic Functions after Analysis Termination

The station always allows actions to be performed after each analysis has terminated.

Note: Full version

*Similar actions can be performed with batch processed chromatograms using the **Batch** command. See chapter **4.3.3** - **Batch Processing of Analyses** on pg. **30** for additional details.*

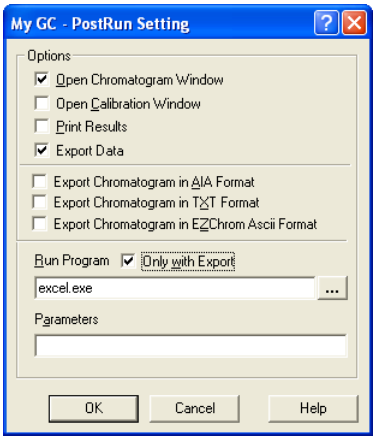


Fig. 8. Postrun Setting

Set up is accomplished using the **Setting - Postrun** command from the **Instrument** window. Invoking the command will open the **Postrun Setting** dialog that contains commands for the automatically displaying the chromatogram, printing a report, exporting the chromatogram, and running another application. The setting of the first three items corresponds to, and can be controlled by, the and "traffic signs" next to the corresponding , and icons in the **Instrument** window.

Automatic displaying of the chromatogram

To set a chromatogram to be automatically displayed in the **Chromatogram** window, check the **Open Chromatogram Window** checkbox from the **PostRun Setting** dialog or switch to the sign next to the icon in the **Instrument** window. If the *OVERLAY* mode is operative, chromatograms will be displayed one by one and overlaid.

To set a chromatogram to be automatically displayed in the **Calibration** window, check the **Open Calibration Window** checkbox from the **PostRun Setting** dialog or switch to the sign next to the icon in the **Instrument** window.

The automatic display will be suspended if the *OVERLAY* mode is not operative and a chromatogram is currently opened that contains some unsaved changes, or if the number of displayed chromatograms has reached the limit (20 by default) set in the **Maximum Chromatograms in Overlay** from the **User Options – General** dialog.

Note: *When the **Maximum Chromatograms in Overlay** limit has been reached the first opened chromatogram will be closed.*

Automated reporting

Use the **Print Results** checkbox from the **PostRun Setting** dialog or the traffic sign next to the icon in the **Instrument** window to enable automatic chromatogram printing. printing will be done according to the report style set by the **File - Report Setup** command from the **Instrument** window. In a sequence analyses, the report style must be defined in the corresponding line of the sequence table. Printing is conditional on both the report style specified in the **Sequence Table** and the checked **Print Results** checkbox.

Automatic export

Check the **Automatic Export** checkbox to have selected data automatically exported to a file or to the **Clipboard**. The export mode depends on the setting in the **Export Chromatogram** dialog (accessible using the **Setting – Export Data** command from the **Instrument** window) or the **File – Export Data** command from the **Chromatogram** window.

Automatic running of another application

If the **Run Program** field contains a name of an application (e.g. EXCEL.EXE) and the **Parameters** field contains optional parameters of that application (for Excel e.g. the name of the working sheet or macro file), that application will automatically be run. Use the ... button to search for the required application including the relevant full path. If the **Only with export** checkbox has been checked, the application will only be run when the **Automatic Export** checkbox has also been checked.

4.3.2 Batch Measurement of Analyses - Sequence

The station enables batch measurement of analyses (also known as sequence measurements or simple sequences) to be performed, in particular in connection with autosamplers. For this it is possible to select an active or passive operation. The running and duration of individual analyses is controlled either by the station (active sequence) or by the autosampler (passive sequence).

4.3.2.1 Passive Sequence

Passive sequences can either be used with autosamplers that decide on the injection time, or by manual injection. In this regime the station will only react to signals that informs about effected injection. This means that there are no special conditions required to make an additional connection between the autosampler and the chromatograph.

Once a sequence has been started using the **Run** command from the **Sequence** window, the sequence will pass from the *STOP* to the *WAITING* state where it awaits the external, starting signal from the autosampler.

Once that signal arrives the analysis starts and the station assumes the *RUNNING* state.

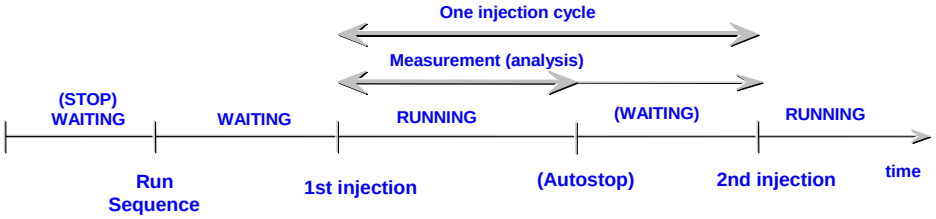


Fig. 9. Time Diagram of a Passive Sequence

If the **External Start/Stop** (from the **Method Setup - Acquisition** dialog of the corresponding template method) has been set to *Start-Restart*, the next external signal will run the following analysis.
An analysis can be also terminated by checking the **Enable Autostop** checkbox in the **Method Setup - Measurement** dialog of the corresponding template method.

4.3.2.2 Active Sequence without Control

Active sequences are used to increase the reliability of co-operation between the station, autosampler and chromatograph when an autosampler without autonomous control is being employed. An active sequence is also necessary for the intelligent control of some selected autosamplers by means of a special control module (see the next chapter **4.3.2.3** - **Active Sequence** for additional details).
The autosampler must be equipped with one starting input and one confirmation output. Once a sequence has been run using the **Run** command from the **Sequence** window, the station will send an authorising signal and await confirmation from the autosampler. The station will begin a measurement after confirmation has been received. The run will terminate after the time that has been specified in the *Enable Autostop* parameter (from the corresponding method) has expired and the station has remained in the *IDLE* state for the period that has been defined in the *Idle Time* field. Thereafter a new authorisation signal will be sent to the autosampler and the station will await its confirmation.
The above cycle will be repeated for all the measurements listed in the sequence table. If the sequence table has to be updated, a sequence may be suspended using the **Pause** command; the command can be invoked anytime, but the sequence that is in the *RUNNING* state will only be suspended the next time the station switches over to either the *IDLE* or the *WAITING FOR READY* state. Invoke the **Resume** command to continue the sequence.

Conditions underlying start of an active sequence

1. A checked **Active Sequence** checkbox in the **Sequence - Options** dialog.
2. A checked **Enable Autostop** checkbox in each method included in the sequence table.
3. Creation of a logical loop:
   - the relevant digital output should be connected to the confirmation autosampler input,
   - the output signal from the autosampler should be connected to the corresponding external digital output.

The default assignment of digital outputs is as follows:

Instrument	Output	Output pin Nr. on the connector				
		INT5	INT7	UPAD	INT7 Relay	UPAD Relay
1	OUT1	5	11	11	12, 30	8, 27
2	OUT2	23	31	31	13, 32	13, 32
3	OUT3	4	14	-	-15, 33	-
4	OUT4	22	34	-	-16, 35	-
All	DGND	1	19	1		

Note: *Should you be using an active sequence, be sure not to process these outputs in the Events Table.*

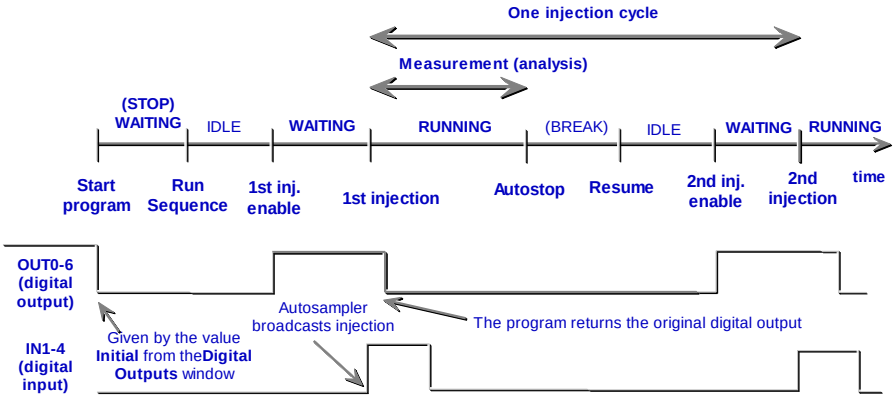


Fig. 10. Time Scheme and Succession of Signals in an Active Sequence

4.3.2.3 Active Sequence with Control

Full version

For selected types of autosamplers we supply a software module that directly selects the injection sequence and time. The interconnection for active sequences is usually then made using a serial communication cable between the PC and the autosampler.
A detailed description will be found in a separate manual.

4.3.2.4 Sequence Table and Its Creation

A sequence measurement is defined in the sequence table, where each line specifies the measurement of one or several samples. The table including the auxiliary data is stored in a sequence file. In order to perform a certain measurement it is sufficient to select a suitable sequence file and start the sequence.

Displaying the Sequence window

To display the **Sequence** window click the icon or invoke the **Analysis - Sequence** command from the **Instrument** window. The last used sequence file will be displayed.

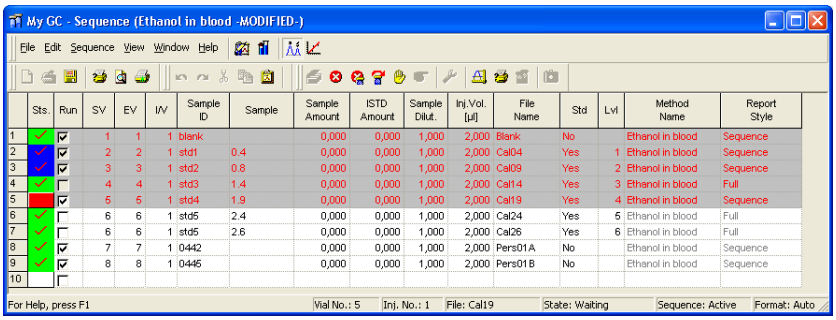


Fig. 11. Sequence

Editing a sequence table

A new line will automatically be appended each time the **SV** (**S**tart **V**ial) cell has been filled in or the **Run** checkbox has been checked.
At the same time, the following remaining mandatory items will be automatically filled in i.e., copied from the preceding line (except for **EV** and **I/V** items):

- **EV** (**E**nd **V**ial) - the last position.
- **I/V** - the number of injections from the position.

- **Sample ID - Inj. Volume** - the values that are included in the chromatogram header.
- **File Name** - the name under which the chromatogram will be saved.
- **Std, Lvl** - the calibration standard and the level to be recalibrated.
- **Method Name** - the name of the method to be used for measuring the analyses performed according to the given line.
- **Report Style** - the name of the report style used.

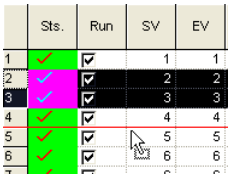
Automatic numbering for multiple measurements from a single line

If more than one sample is to be measured from any given line (**EV** should by at least one higher than the **SV**) or if several injections are to be effected from any given line (**I/V** higher than one), the template of the chromatogram name should contain the **%v** and **%i** variables. In the default set-up the program will automatically add the missing variables. To switch off this automatic correction, change the **Format** item from *Automatic* to *Manual* in the **Options** dialog (**Sequence - Options**).
Save the completed sequence file using the **File - Save** command or **Save As**.

Changing the order of lines

The order of lines in the sequence table can be changed using the drag and drop function with the mouse. Multiple lines can be dragged simultaneously.

- Point the cursor to the number of the line to be dragged. The cursor will change to ➡.
- Left click the mouse button, hold and select the other lines to be dragged
- Release the mouse button then click and hold it again anywhere over the highlighted lines.
- Drag the cursor to the newly desired location of the selected lines. The location will be indicated by a red hairline.
- Release the mouse button.



The lines can also be moved using the **Line Up** and **Line Down** commands from the **Edit** menu.

Selection of lines for measurement

In practice it may happen that you have defined a sequence table for more extensive analyses but you currently only need to use a few lines of this table.
One possibility is to mark the lines in the **Run** column. Larger tables can be edited using the following commands from the **Edit** menu:

Mark for Run - Includes selected lines for measurement – the checkboxes in the **Run** column will be checked.

Clear Run Marks - Excludes the selected lines from the measurement – the checkboxes in the **Run** column will be unchecked.

Invert Run Marks - Inverts the status of the checkboxes in the selected lines. Lines that have been checked will be unchecked and vice-versa.

Another option is to write the individual lines (1,3,7) or groups of lines (1-4, 6-7) in the **Run Lines** field from the **Sequence Options** dialog.

4.3.2.5 Procedure of Sequence Measurements

1. Opening the sequence window

To open the **Sequence** window either click the icon or invoke the **Analysis – Sequence** command from the **Instrument** window.

2. Selecting a sequence file

Open the requested sequence file using the **File Open** command or by clicking the icon.

3. Inspecting the content of the sequence table and the files used

Inspect all parameters in the displayed Sequence Table, eventually also check all method files used: click anywhere in a line with the required template method and display its contents either using the **Sequence - Edit Current Method** command or by clicking the icon.

4. Inspecting the validity of the Sequence Table.

YL-Clarity automatically inspects, whether it will be possible to perform the analyses from the displayed **Sequence Table**. It controls the existence of specified template methods, validity of chromatogram names, the possibility of overwriting files. Invalid lines are indicated with a cross in the **Sts.** column. Point the mouse cursor to the respective cell to display a detailed description of the problem. Detailed description can be also displayed using the **Sequence – Check Sequence** command (icon).

5. Running the sequence

To run the sequence use the command **Sequence – Run Sequence**, (icon) from the **Sequence** or **Data Acquisition** window. The sequence will turn to the *WAITING* state; only then will it be possible to start the measurement of the first sample using an external signal from autosampler.

*If the external signal arrives before the sequence is run using the **Run** command (i.e., in the STOP state), a single analysis will be run according to the setting in the **Single Analysis** dialog.*

6. The measurement process

Measurement proceeds along individual lines of the table. Each line may define several measurements of the same sample in **I/V** item, or measurements of more than one sample under identical conditions - **SV** and **EV** items.

7. Information about the running sequence

Information will both be displayed in the status bar at the bottom of the **Sequence** window and in the **Information table** of the **Instrument** window. Both places will display the name of the analysis in progress, the position of the vial and potentially the serial number of the injection from that position. The **Instrument** window also shows the template method used and the first two items of the chromatogram header, **Sample** and **Sample ID**.

8. Measurement processing in sequence analyses

The template method file listed in the current line of the sequence table in the **Method Name** column determines the method of measurement and sample processing. Printed reports, if requested, are controlled by the **Report Style** cells.

Two conditions must be met for printing:

The report style must be selected in all lines of the Sequence table from which you would like to print report.
The **Print Results** checkbox from the **Postrun Setting** dialog (also indicated and controlled using the sign next to the icon in the **Instrument** window) must be checked.

Note: *All parameters and commands of the **Single Analysis** dialog will be ignored if a sequence is running.*

Displaying chromatograms, printing, exporting and running other applications during the sequence run are also defined in the **Postrun Setting** dialog or by the and signs from the **Instrument** window, and are thus common to the entire sequence.

4.3.3 Batch Processing of Analyses

Full version

The station allows for batch processing already measured chromatograms. Chromatograms selected for batch processing will be subject to operations that are analogous to those included in the **Postrun Setting** dialog.
The **Analysis - Batch** command from the **Instrument** window will open the **Batch** dialog.

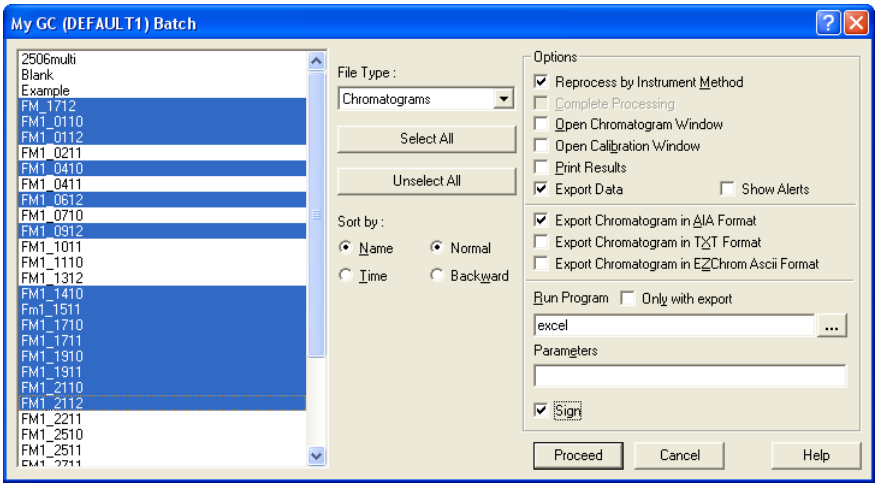


Fig. 12. Batch

The **File Type** command determines what should be processed: chromatograms, calibration standards or sequences. A list of the corresponding files in the current project is then shown in the left column.

Sequence processing

If a sequence is to be batch-processed, all chromatograms measured during the sequence's last run will be included. Any missing chromatograms (not measured, deleted or measured at any of the preceding runs of the selected sequence) will be ignored.

Note: *Chromatograms are sought according to an internal (hidden) list of actually measured chromatograms. It is because the **File Name** column may contain variables that would prevent the relevant chromatogram to be unequivocally identified (date, time, serial number, etc.).*

Also, processing here will only be comprised of the selected operations that are listed in the right-hand part of the **Batch** dialog.

Comprehensive sequence processing

The **Complete Processing** command performs repeated processing according to the topical contents of the sequence table. The headers of all chromatograms will be overwritten and the method actually specified in the sequence table will be employed; recalibration will be carried out if required.

Processing according to the current template method

If you wish to process chromatograms according to the currently opened template method in the **Instrument** window, check the **Reprocess by Instrument Method** checkbox from the **Batch** dialog (all parameters listed in the **Method Setup - Integration** and **Calculation** tabs will be used).

Selection of multiple chromatograms to be processed

To select multiple files, hold down the Ctrl key while left-clicking the mouse on the file name (an second click will cancel the selection). To select a contiguous list of files, left-click the first desired file, hold down the Shift key and click the last desired file - all interjacent files will be selected.
Pay attention to **Select All** (Ctrl + A) and **Unselect All** commands, which are self-explanatory.

Processing order

The items in the list of files can be sorted alphabetically in ascending (item **Normal**) or descending order (item **Backward**) by filename (**Sort by: Name**) or date saved (**Sort by: Time**).

Processing proper

Start the processing using the **Proceed** command. If no chromatogram or sequence has been selected, the command will merely save the current settings of the **Batch** window.
The **Open Chromatogram Window** through **Run Program** checkboxes are the same as those in the **Postrun Setting** window. See Chapter **4.3.1.4** - **Automatic Functions after Analysis** on page **24** for additional details.

4.4 DDE synchronization with other programs

DDE (Dynamic Data Exchange) is a technique the **Windows** system uses for transferring data between individual applications running under **Windows**. By means of DDE another application may follow the status of the **YL-Clarity** station and control a co-operating device accordingly. The **YL-Clarity** station behaves like a *DDE Server*. Other programs can be connected to the **YL-Clarity** station through the following variables:

Service Name : *"Clarity"*
Topic Name : *"Status"*
Item Names : *"Channels"*, *"Channel1"* through *"Channel4"*.

The item "*Channels*" assumes values from 0 to 4 depending on the number of open Instruments.
The items *"ChannelsX"* (with X= 1 - 4) indicate the status of individual instruments as follows:

Value:		Meaning:
-2	-	Instrument not installed
-1	-	Instrument closed
0	-	Instrument is disabled
1	-	Instrument is in *STOP* state
2	-	Instrument is in *WAITING* state

3	-	Instrument is in *RUN* state
4	-	Instrument is in *IDLE* state
5	-	Instrument is in *BREAK* state

You may use one of the following **Clipboard formats** for transferring data: *cf_Text*, *cf_CSV* and *cf_XITable*.

5 Chromatogram

The **YL-Clarity** station enables the user to apply a number of operations to chromatograms. Among them are baseline modification (including the method used for drawing the baseline), shifting peak beginnings and ends, creating new peaks, combining peaks into groups (as well as subsequent joint integration), and selecting limiting parameters for peaks to be included in integration.

The effected operations will be stored with the chromatogram and may be used in subsequent analyses, thus enhancing reproducibility of the obtained results. Because of YL-Clarity's intuitive mouse operations and the auxiliary icons, all operations are simple and facile.

Any part of the chromatogram can be zoomed in to define the exact location of the intended operation. Multiple chromatograms can be simultaneously displayed in the **Overlay** mode and subsequently subjected to mathematical operations.

5.1 Displaying a Chromatogram

Chromatograms are displayed in the **Chromatogram** window, which is opened using the  icon from the **Instrument** window, or the **Window - Chromatogram** command from other windows. It is also possible to have the window open automatically after the completion of a measurement.

Unless the *OVERLAY* mode has been enabled, the chromatogram that is currently displayed will close before another one can be displayed. The size of the chromatogram is such that it will fill the entire area of the graph. To close the displayed chromatogram(s), invoke either of the **File - Close** or **Close All** commands.

Indicative graph

In addition to the main graph, a smaller, indicative graph can be displayed using the **Preview Graph** command from the **Display** menu or through the local menu. The chromatogram will always be shown in the indicative graph at the base magnification and will contain any cut displayed in the main graph.

Zooming in

Point with the mouse to any corner of the cut that is to be zoomed in on. Left click and hold the mouse button then drag the cursor to the opposite corner of the cut. Release the button so as to display the magnified selected cut in the main graph. The station will remember the last cuts so that they can be displayed one by one using the  and  icons or the **Display - Previous (Next) Zoom** commands. The  icon or the **Display - Unzoom** command will display the chromatogram in the original size.

Note: *The implicit size is determined by the **Scale Y Mode** field from the **Graph Properties – Signals** dialog or when the **Range - Fixed** item has been checked using the **From… To…** fields from the **Graph Properties – Axes** dialog.*

5.2 Display Characteristics

In view of the many available options for displaying chromatograms, axes, tags and other information, a separate dialog **Graph Properties** containing several tabs is devoted to these settings. Open the dialog by the command **Display - Properties** from the main menu or **Properties** from the local menu (to pop up the local menu click with the right mouse button). Parameters are organised in several tabs described below.

Global setting

It is convenient to set a number of parameters common to other graphs (chromatograms in other instruments, the **Calibration** and **Data Acquisition** windows); the station therefore offers a global setting for some parameters by the command **View - Options** in the **Instrument** window. The opened **User Options** dialog offers the **Graph**, **Axes Appearance**, **Signals and Curves** and **Gradient** tabs devoted to the setting of graphs. If you check the items **Use User Options** on synonymous tabs in **Chromatogram**, **Calibration** and **Data Acquisition** windows, the corresponding parameters will be taken over from this global setting.

Note: *The setting is stored in a file; in the unprotected mode the file is CLARITY.DSK and is common to all instruments. See Chapter **11.2.8** - **Desktop File (CLARITY.DSK)** on page **84** for additional details.*

5.2.1 Chromatogram Description and Display

Select the information to be displayed in the **Graph Properties - Graph** dialog.

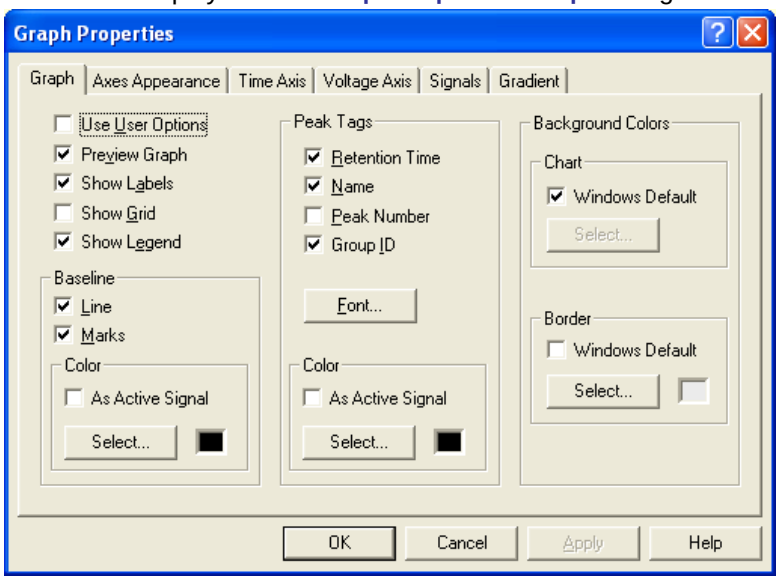


Fig. 13. Graph Properties - Graph

5.2.2 Description and Format of Displayed Axes

The display of axes can be specified in the **Graph Properties – Axes Appearance** dialog.

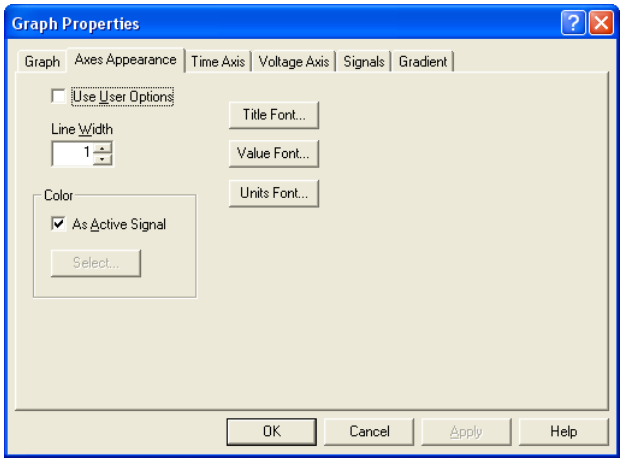


Fig. 14. Graph Properties - Time Axis dialog

The thickness and colour of the axes are set using the **Line Width** and **Color** commands. The **Title Font**, **Value Font** and **Units Font** commands determine which fonts will be used for axes description, values and units.

Note: *Further settings, such as the customisation of descriptive labels, units and determining whether to convert between the original and new units at both axes or display the chromatogram in a fixed rendition (fixed range of the axes), can be set in the **Graph Properties – Time Axis** and **Voltage Axis** dialogs.*

Fixed rendition

Fixed rendition means that both axes will have a fixed range regardless of the actual chromatogram size. The range is always supplied in base units (milivolts and minutes) using the **From…To…** parameters in the **Range** section. The specified values will apply only if the **Fixed** checkbox has been checked.

Axis format:

Select the desired format for the axes in the **Graph Properties – Time Axis** and **Voltage Axis** dialogs.
You may hide the axis by unchecking the **Visible** checkbox. Enter the required title in the **Title** field.
It is possible to shift the axes - **Offset** or change their scale - **Scale**. Using the **Units** field set the units to be displayed on the axes. The units are only displayed on the axes of the main graph and not in the results tables and thus, are for informational purposes only.

How to set actual units on the axis

In chromatographic practice it happens that it may be better to display the absorbency units (AU) instead of voltage. The procedure for setting AU is as follows:

1. Open the **Graph Properties - Voltage Axis** dialog.
2. Verify that the **Visible** checkbox has been checked.
3. Select the name of the axis in the **Title** field, e.g. *"Absorbancy units"* and the abbreviation of units *"AU"* in the **Units Type** field.
4. In the **Units Type** item select whether you wish to display the axis with a fixed scope of values – *Fixed*, or whether the station is to automatically convert values to decimal multiples (these will be expressed by the prefix before the name of the unit e.g. mili, micro, kilo, … etc.) – *Auto*.
5. Ascertain what voltage corresponds to 1 AU and enter its inverse value into the **Scale** field. For example, if 1 AU corresponds to a voltage of 2V, enter the value 0.5 into the **Scale** item.

5.2.3 Descriptive Labels and Lines

The main graph can contain descriptive labels and lines. Both can be situated in the graph area or anchored to the active chromatogram.

Descriptive label location

Invoke the **Chromatogram - Create Label** - **Text** command from the menu or from the local menu to display a dedicated cursor. Move the cursor to the intended location of the new descriptive label. Doubleclick to open the **Text Label** dialog where you can enter the text of the label in the **Text** field, select the font in the **Font** item, and decide which point the nearest chromatogram point or to the graph border will be "fixed" to.

Anchoring to chromatogram

To anchor a label to the active chromatogram, check the **Assign to Active Chromatogram** parameter. Invoke the **Anchor (Text Alignment)** command to decide which point the nearest chromatogram point or to the graph border will be "fixed" to.

Line location

Invoke the **Create Label - Line** command from the **Chromatogram** menu or from the local menu to display a dedicated cursor. Move the cursor to the location of the future line beginning, left click and hold the left mouse button to draw a line. Release the button once the desired end point has been reached and the **Line Label** dialog will open. This is where you can specify the type of line end, as well as the colour and type of the line, and its thickness in **Arrows**, **Line Style** and **Line Width** items.

Note: *Lines with a thickness exceeding one pixel will always be shown as continuous.*

You may anchor the line to the active chromatogram by selecting the **Assign to Active Chromatogram** parameter.

Modifying descriptive labels and lines

A previously created label or line can be modified anytime by double-clicking on it with the left mouse button or right clicking on it with the mouse button. Labels and lines can also be moved or resized using the "handles" (similar to those used in standard drawing applications), which can be invoked by clicking any point on the label or line. Hold down the left mouse button and drag to move the object, and then release the mouse button to drop it at the desired location. The object size can similarly be changed using the relevant handles. When a label height has been changed the font size will adapt accordingly.

Deleting labels and lines

Delete the selected label or line (that with the displayed handles) using the Delete key or the **Remove Labels - Selected** command from the **Chromatogram** menu or the local menu.
To delete all labels and lines from a graph invoke the **Remove Labels - From Workplace** command.
To delete all labels and lines from an active chromatogram invoke the **Remove Labels - From Active Chromatogram** command.
To delete all labels and lines invoke the **Remove Labels - Remove All** command.

Note: *Labels and lines anchored to an active chromatogram will be stored with that chromatogram. Labels and lines attached to the graph area are a part of the desktop file (extension *.DSK).*

Printing descriptions and lines

Set which type of descriptions and lines are to be printed in the print style found in the **Report Setup – Chromatogram** dialog. Either the lines or descriptions that are linked to the chromatogram and/or to the workplace or simply as they are currently displayed on the screen will be printed.

Note: *This feature may also be used for hiding of your working symbols and notes that should not be printed in the final print output.*

5.3 Operations Involving Several Chromatograms - Overlay

The *OVERLAY* mode is where several chromatograms can be simultaneously displayed.

OVERLAY mode enable

To enable the *OVERLAY* mode, use the **Overlay** command from the **File** menu, the icon, or double-click the *OVERLAY* inscription displayed to the right on the status bar.
The active *OVERLAY* mode will be indicated by the activated icon, the coloured , and icons in the **Overlay** toolbar, and the *OVERLAY* inscription in the right-hand part of the status bar.

Displaying multiple chromatograms

A practically unlimited number of chromatograms can be simultaneously displayed using either the **File - Open** command or by clicking the icon. Chromatograms can be displayed by repeatedly invoking the **Open** command or by selecting several chromatograms in the **Open Chromatogram** dialog.
Each chromatogram will be displayed in a dedicated colour. The icons are assigned to the first eight displayed chromatograms. Refer to the **Chromatogram** menu for a comprehensive list of all displayed chromatograms.
To select multiple files hold down the Ctrl key while left clicking the mouse button (a second click will cancel the selection). To select a contiguous sequence of files, left click the first file to be selected with the mouse button, hold down the Shift key and then click on the last file to be selected.

Note: *The number of chromatograms that can be simultaneously opened in the Overlay mode is in fact limited by the **Maximum Chromatograms in Overlay** field from the **User Options – General** dialog. The implicit value is 20 and the maximum can be set to 10,000.*

Active chromatogram

One chromatogram (signal) (usually the last one displayed) - is active, and all displayed information and commands will only refer to that chromatogram. The name of the active chromatogram will be displayed in the title bar of the **Chromatogram** window and in the headers of all tables. The correspondingly coloured icon will be indented. To select another chromatogram as active click on the correspondingly coloured icon or select the chromatogram from the **Chromatogram List** dialog.

Fig. 15. The Overlay Toolbar

Changing chromatogram colour

To change the colour of any of the first eight chromatograms, simply click the icon of the chromatogram whose colour you wish to change and then on an empty icon with the desired colour. The colour of the icons and the chromatogram will change accordingly.

Closing a chromatogram

To close the current chromatogram, invoke the **Close** command from the **File** menu or click the icon.
Invoke the **Close All** command to close all displayed chromatograms.

Disabling the OVERLAY mode

To disable the *OVERLAY* mode, click the **Overlay** command from the **File** menu or the indented icon.
The station will invite you to save modified chromatograms that are about to be closed.

When the *OVERLAY* mode has been disabled only the current chromatogram will be displayed in the graph.

5.3.1 Resizing and Relocating Chromatograms

The current chromatogram can be resized and moved independently in horizontal and vertical directions. This makes it easier to "match" two chromatograms, e.g., to subtract the solvent peak or to modify a chromatogram with erroneous retention times. These modifications are made using the **Move** commands and **Scale** from the **Chromatogram Overlay** submenu or by using the and icons.

Modification procedure

Invoke the command, place the mouse cursor at any part of the main graph, click and hold down the mouse button while slowly dragging in the desired direction (the chromatogram will move and change its size). Once the requested location or size has been reached, release the mouse button.

Displaying/changing values

The values by which the chromatogram has been changed are shown in the **Line Charts** tab of the **Graph Properties** window in parameters **Offset X (Y)** and **Multiplier X (Y)**. The chromatogram can be directly modified by changing the values of these parameters. Invoke the **Origin** command to return to the original size and location.

Saving the effected changes

The chromatogram that has been modified as described above will become a mere graphical curve, i.e., the baseline and the peak descriptions will disappear. To create a full-bodied chromatogram from the curve, invoke the **Overlay - Operation - Copy** command, followed by the **File - Save** command. See Chapter **5.3.2** - **Mathematical Operations** for additional information.

5.3.2 Mathematical Operations

Some basic mathematical operations over chromatograms can be performed using the **Overlay - Operation** command from the **Chromatogram** menu by clicking the icon.

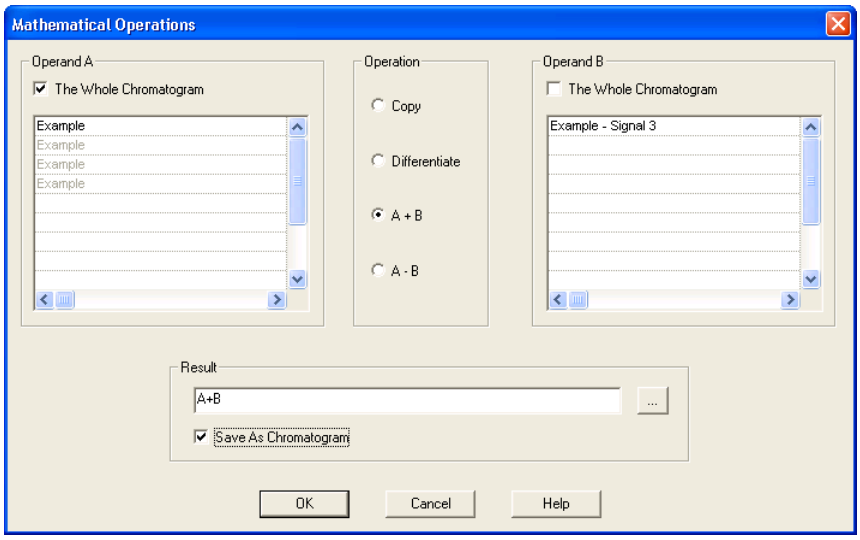


Fig. 16. The Mathematical Operations Dialog

In the opened **Mathematical Operations** dialog, click the colour of the first chromatogram in the left **Chrom A** column, select the required operation in the middle **Operation** column, and select the second chromatogram, if any, in the right **Chrom B** column.

The **Result** field will display the automatically suggested name of the resulting curve.

The created chromatogram will not be saved and will be cancelled when the window is closed. If you want to preserve it, save it using the **Save** or **Save As** command.

If you check the **Save As** checkbox the resulting chromatogram will be automatically saved under the name displayed in the **Result** field, which will be then editable.

The result is automatically integrated and evaluated according to the template method selected in the **Instrument** window.

*The method associated with the original chromatogram will never be used when a copy has been created or differentiation performed using the **Copy** and **Differentiate** commands, respectively. It is only used for a copy that has been created using the **File - Save As** command!*

Any chromatogram created or modified in this way will be labelled in the report with the "*Mathematically reprocessed*" inscription.

5.3.3 Three-dimensional View of Chromatograms

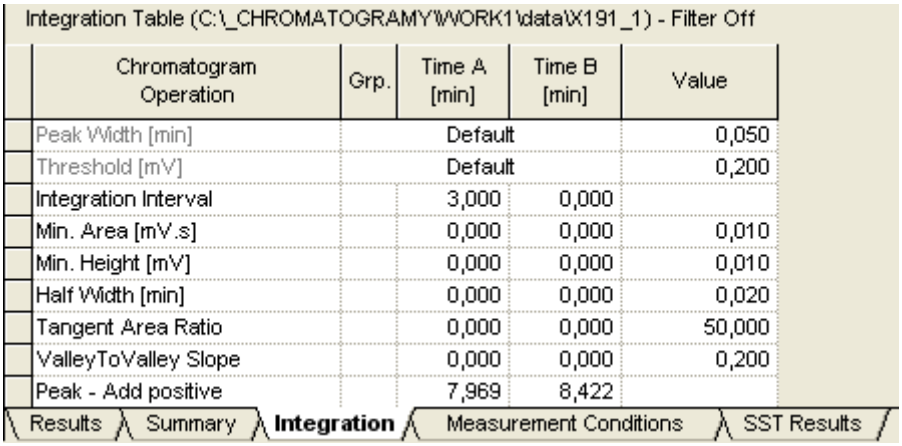
To display chromatograms in a 3-D view invoke the **3D View** command, to cancel the view invoke the **Clear 3D** command, both are from the **Chromatogram - Overlay** submenu. The two straight lines displayed by the **3D View** command are used to set up the angle and depth of the three-dimensional view. All chromatograms will be regularly displaced along the selected line. The displacement is governed by the **Offset X** and **Offset Y** fields from the **Graph Properties** - **Signals** dialog. The **Clear 3D** command zeroes the above offsets and, accordingly, displays all chromatograms in their original positions. The original positions of individual chromatograms are set using the **Original** command, again from the **Graph Properties** – **Signals** dialog.

5.4 Chromatogram Modifications

By default, each chromatogram is integrated according to the parameters from the **Integration Table** displayed in the **Chromatogram - Integration** window. When using multi-detector chromatograms each signal will have its own independent **Integration Table**.

The Integration Table contains all parameters from the template method. These parameters can be modified and filled in either directly in the integration table or using the commands from the **Chromatogram – Baseline**, **Peak** and **Integration** submenus.

Note: *The station automatically checks for instances of baseline crossing. After each operation the baseline will be corrected to prevent baseline crossing (the station either shifts the peak beginning or peak end to the nearest possible point or refuses to perform the requested operation). If the peak's beginning or end has been manually shifted, it may happen that the station refuses to place the point at the requested position, since it detected that the baseline would intersect the signal, and will place the point at the nearest possible location.*


Integration Table (C:_CHROMATOGRAMY\WORK1\data\X191_1) - Filter Off

Chromatogram Operation	Grp.	Time A [min]	Time B [min]	Value
Peak Width [min]		Default		0,050
Threshold [mV]		Default		0,200
Integration Interval		3,000	0,000	
Min. Area [mV.s]		0,000	0,000	0,010
Min. Height [mV]		0,000	0,000	0,010
Half Width [min]		0,000	0,000	0,020
Tangent Area Ratio		0,000	0,000	50,000
ValleyToValley Slope		0,000	0,000	0,200
Peak - Add positive		7,969	8,422	

Results | Summary | **Integration** | Measurement Conditions | SST Results

Fig. 17. Chromatogram - Integration

The order and hierarchy of parameters and commands that affect an integration

1. Peak detection using the **Peak Width** and **Threshold** parameters starts from the time indicated in the **Integration Start** parameter.
2. An attempt then follows to draw the baseline to the valley according to the **ValleyToValley Slope** parameter, followed by automatic tangential separation according to the remaining two parameters of the **Separation** section.
3. The Integration Table is applied.
4. A check of possible baseline/signal intersection is performed.
5. Finally, all peaks that fail to satisfy at least one of the parameters specified in the **Rejections** section are excluded.

Note: *It follows from the above that separation parameters will not be applied, e.g., to manually added peaks and their effect might be suppressed, e.g., by using the **Together** and **Valley** commands specified in the integration table.*

Major commands and global parameters are explained and their effect illustrated in the following chapters.

General modification procedure

Click the corresponding icon on the **Baseline** and **Peak** toolbars or from the **Chromatogram - Baseline (Peak)** menu to initiate the manual chromatogram modification procedure. The mouse cursor will be displayed at approximately the centre of the active chromatogram as a vertical line with an arrow pointing to the signal level. Point the mouse cursor to the location where you wish to effect the requested operation and left click the mouse button. If an interval operation is involved, a second vertical line will appear and the second point can be similarly selected. The user can cancel the operation anytime using the right mouse button or the Esc key.

Repeated usage of selected operation

If you want to use a certain operation several times, it is advantageous to hold Ctrl button before. After selecting the operation and releasing the Ctrl button you will be able to repeat selected operation until you chose another function or press the Esc button.

5.4.1 Baseline Modifications

The **Baseline** submenu and the corresponding toolbar contain the commands used for modifying the baseline operations and eliminating peaks from an integration.

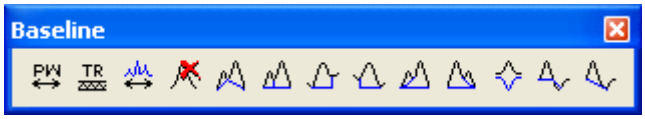


Fig. 18. The Baseline Toolbar

Validity Interval

Two vertical lines delimit the interval of validity. Once the command has been invoked, the left vertical line will appear. Use the mouse to drag the line to the desired position and confirm the move by left clicking the mouse button. Move the right vertical line to the desired position using the same method. The confirmation of the move will invoke the command. The command can be abandoned at anytime by right clicking the mouse button or pressing the Esc key.

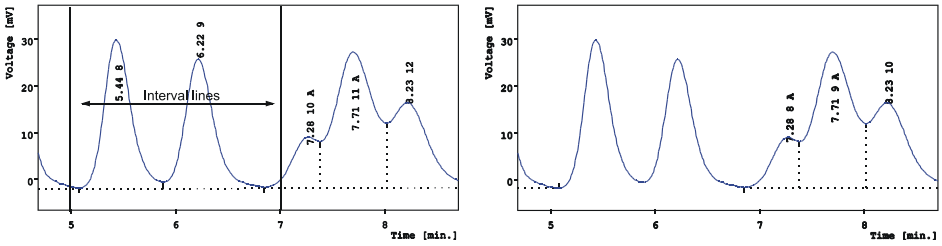
Operations involving peaks will only be performed with peaks that are completely enclosed between the two vertical lines.

Records of modifications

All accomplished modifications will be stored in the integration table, where any operation can be subsequently cancelled or corrected. An integration table from another chromatogram or another method can be also used. See Chapter **5.4.6** - **The Integration** Table on page **48** for additional details.

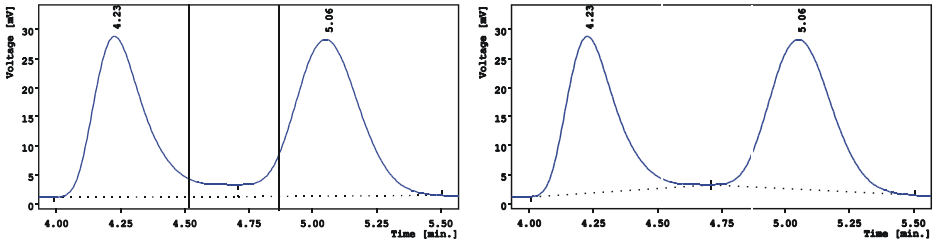
Peak deletion

Using the **Lock** command or icon will exclude all selected peaks from an integration. Only peaks that are completely contained in the selected interval will be excluded.



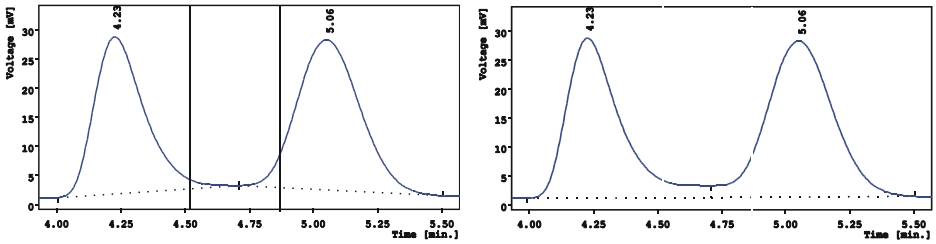
Baseline through a valley

Use the **Valley** command or icon to force the baseline into all the valleys situated between the interval lines. In the event this might result in having the baseline intersect with the signal, the station will prevent the intersection by automatically shifting the peak beginning or end. This operation is opposite to the **Together** command.



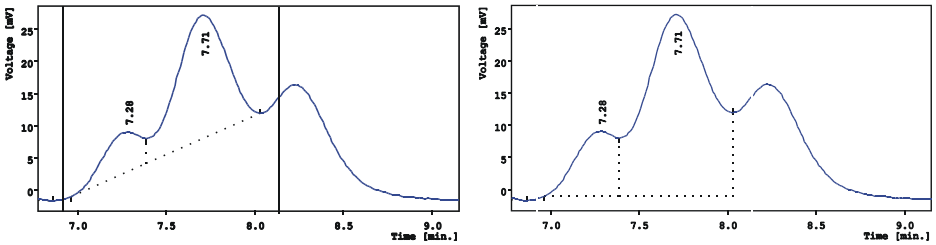
Baseline between separating verticals

The **Together** command or icon introduces separating verticals to all valleys that are situated between the interval lines. This operation is opposite to the **Valley** command.

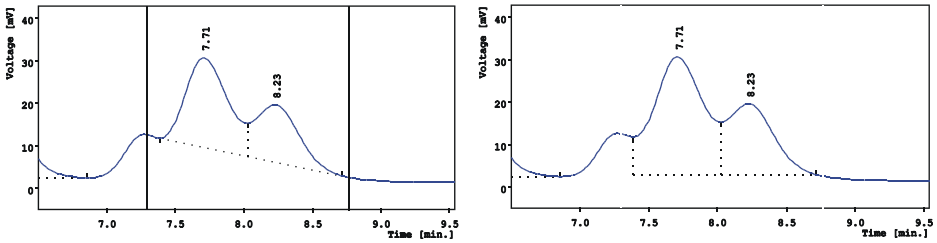


Horizontal baseline

The **Forw. Horizontal** command or icon forces a horizontal baseline from the beginning of the first peak inside the selected interval beneath all peaks inside the interval.



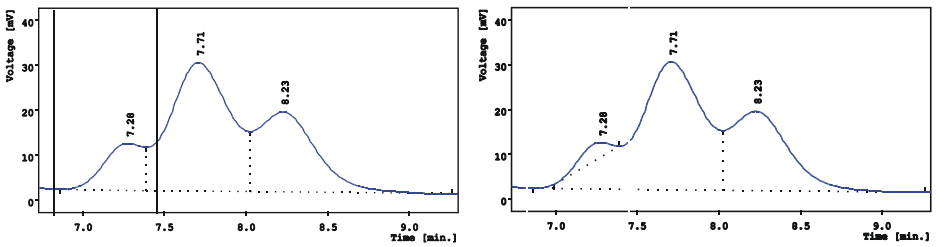
The **Back. Horizontal** command or icon draws a horizontal baseline from the end of the last peak that is inside the selected interval beneath all peaks inside the interval.



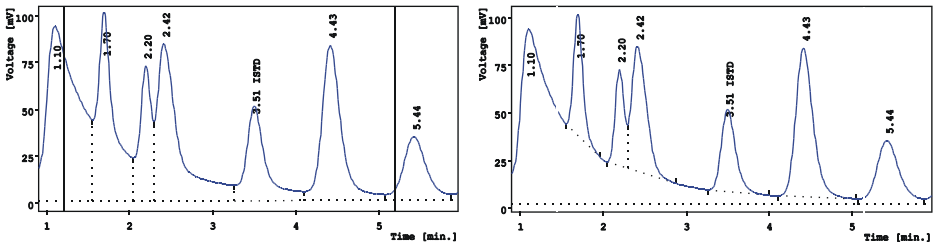
Note: *Should the horizontal baseline intersect the signal inside a peak, no forced horizontal baseline will possible for that peak.*

Tangential separation

The **Front Tangent** command or icon cuts off all of the peaks (riders) that are situated on the leading edge of the first peak and after the selected interval. Place the left interval line to left of the first peak to be cut off, and then place the right interval line inside the starting of the peak from which the cut-off is to be affected.

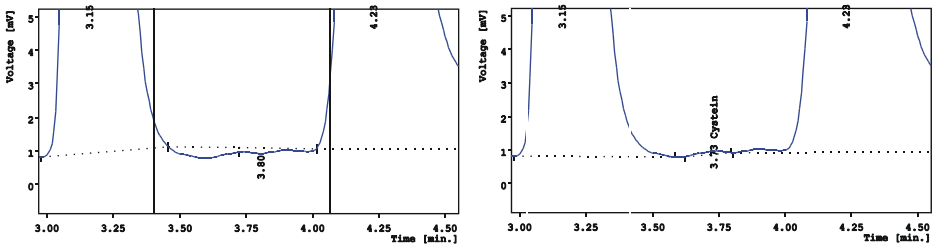


The **Tail Tangent** command or icon cuts off all peaks (riders) that situated on the tailing edge of the last peak and before the selected interval. Place the left interval line inside the peak that carries the tailing riders to be cut off, the right interval line behind the end of the last peak to be so cut off.



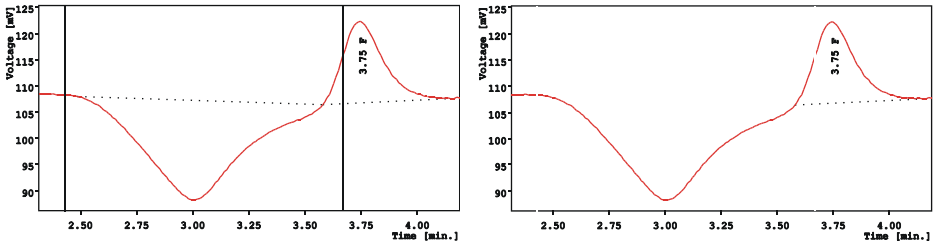
Interchanging positive/negative

The **Clamp Neg.** command or icon interchanges all apexes that are inside the interval to valleys and vice-versa, thus turning negative peaks from a group into positive ones.



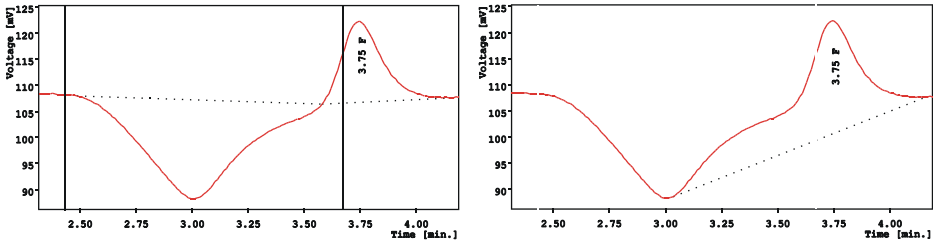
Declaring negative peaks to be disturbances

The **Cut Neg.** command or icon eliminates from integration negative peaks that are in fact disturbances. Neither the beginning nor the end of the preceding positive peak will be affected.



Declaring peaks to be baseline

The **Reject Negative** command or icon excludes negative peaks from an integration without declaring them to be disturbances. The beginning of the subsequent peak or the end of the preceding peak (if any) will be shifted to the original apex of the negative peak.



5.4.2 Peak Modifications

The **Peak** submenu and the corresponding toolbar contain peaks operations with.

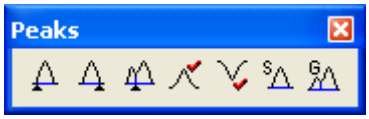


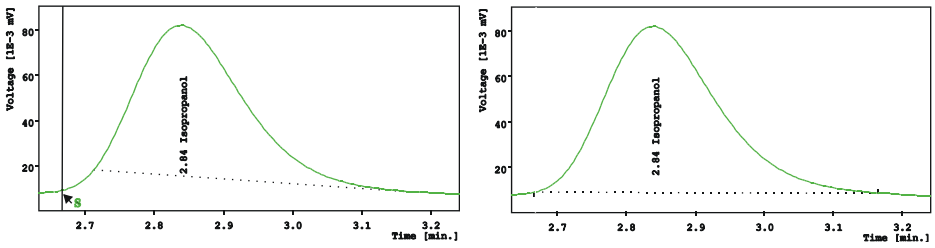
Fig. 19. The Peaks Toolbar

The positions of peak beginnings and ends as well as of valleys or separating vertical lines can be changed. Invoke the command, move the cursor to the required location and click to confirm. Abandon the command may be at anytime by right clicking the mouse button or hitting the Esc key. Since only a single peak beginning or end can be shifted to any place selected on the chromatogram without shifting the apex, it is unnecessary to specify the peak to which the operation refers.

Note: *The preceding sentence does not apply to tangential separations where, if the required location lies inside the main peak, modification of the tangentially separated peaks is given preference.*

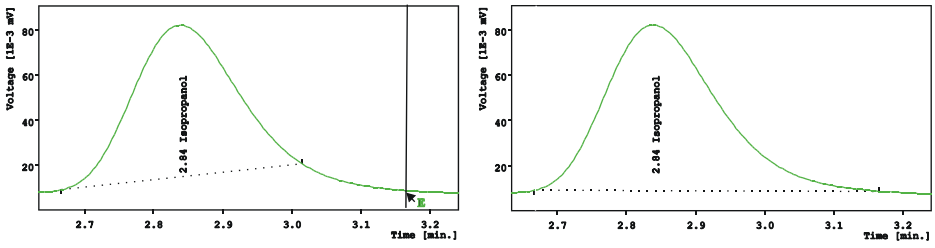
Shifting the peak beginning

The **Start** command or icon defines a new position of the peak beginning. In the event the peak beginning is shifted before the end of the preceding peak, a vertical line will separate those peaks and its position will coincide with the new peak beginning. If the peaks are separated by a vertical line or connected at the valley and the peak beginning is shifted closer to the apex, the peaks will be separated.



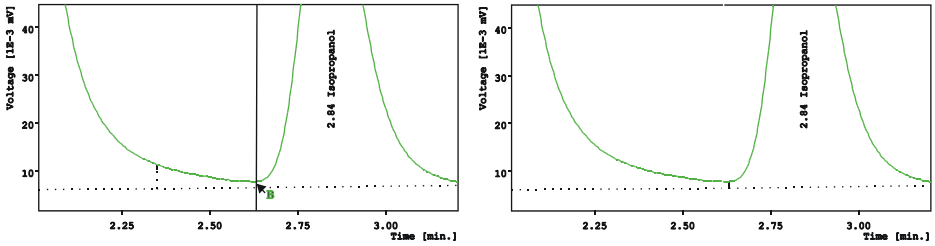
Shifting the peak end

The **End** command or icon defines a new position of a peak end. In the event the peak end is shifted behind the beginning of the following peak, a vertical line will separate those peaks and its position will coincide with the new peak end. If the peaks are separated by a vertical line or connected at the valley and the peak end is shifted closer to the apex, the peaks will be separated.



Change the valley or vertical separating line

The **Both** command or icon defines a new position for a valley or the vertical line that separates the peaks. The common point can be shifted to any location between the apexes of the two peaks. Should the resulting baseline intersect the signal, the peaks will be separated.

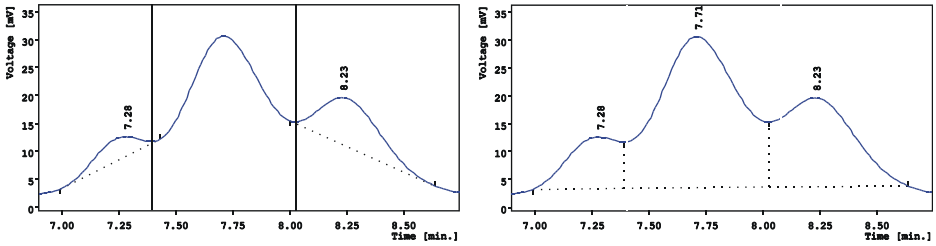


Adding new peaks

Interval lines set the beginning/end of a new peak. The apex is automatically determined at a location between the maximum and minimum (depending on peak orientation) between the peak beginning and end. A new peak cannot be added in the area of tangentially separated peaks.

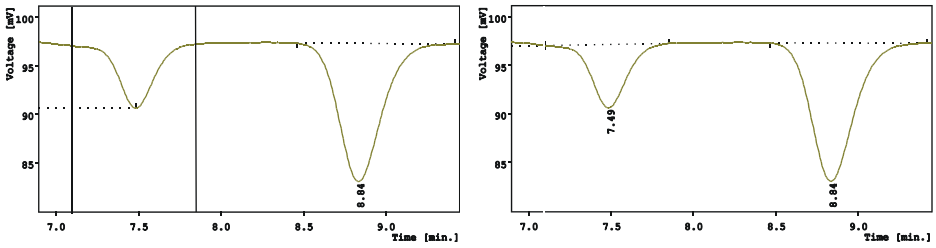
Adding a positive peak

The **Add Positive** command or icon creates a new positive peak. If the beginning or end of the created peak falls inside a neighbouring peak, the peaks will be separated by a vertical line that may either be placed at the beginning or end of the created peak.



Adding a negative peak

The **Add Negative** command or icon creates a new negative peak. If the beginning or end of the created peak falls inside a neighbouring peak, the peaks will be separated by a vertical line that may either be placed at the beginning or end of the created peak.

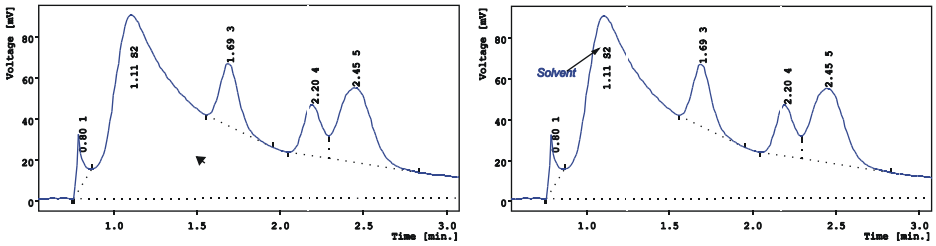


Manual apex determination

Owing to the automatic determination of peak apex, the following procedure must be used to place the apex at a specific location (especially when defining monotonic peaks). First, using the **Lock** command, cancel the peak with the incorrectly assigned apex and add a new peak using the **Add Positive** or **Add Negative** command as required. This is done so that its beginning or end (depending on the position of the maximum of a positive or minimum of a negative peak) will coincide with the position of the intended apex. To finish, shift the beginning or end of the peak to the appropriate location using the **Start** or **End** commands.

The Solvent peak

The **Solvent Peak** command or icon designates a peak to be a solvent peak. The letter "S", before the peak number in the graph, indicates the designation of the peak. Solvent peaks are neither included in integration nor listed in the **Result Table**. More than one peak may be designated as a solvent peak.



Recording accomplished modifications

All operations accomplished will be stored in the integration table and, accordingly, any operation can be cancelled or corrected. An Integration table from another chromatogram or another method can also be used. See Chapter **5.4.6** - **The Integration** Table for additional details.

5.4.3 Working with Groups of Peaks

Peaks can be combined in groups and subsequently integrated together, Each group is assigned a single-letter identifier and, accordingly, the maximum number of groups is 26. The **Chromatogram -Peak- Peak Groups** command or icon from the **Peak** toolbar are earmarked for working with groups and will open the **Groups** dialog.

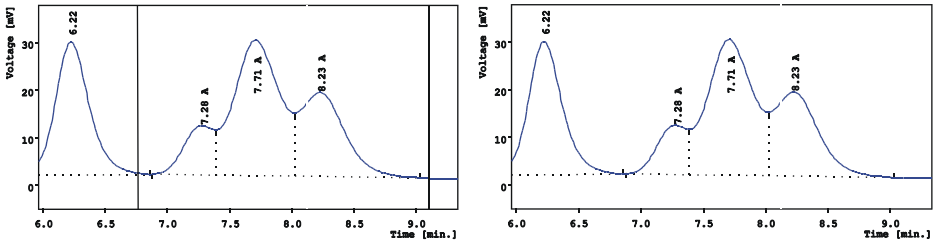
Fig. 20. The Groups Dialog

Adding a peak to a given group

Enter the group identifier in the **ID** field and invoke the **Add** command.
Use the displayed interval vertical lines to select the peak(s) to be included in the group. By repeated use of the command other then neighbouring peaks can be added to a group.

To highlight the fact that a peak is included in a group the corresponding group identifier will be shown after the peak number. The **Result Table** also then comprises the integration results for the created groups. No peak may be included in more than one group.

If a selected peak has been previously assigned to a certain group, it will be transferred to the new group.



Deleting peaks from a group

Enter the group identifier in the **ID** field and invoke the **Delete** command.
Use the displayed interval vertical lines to select the peak(s) to be deleted from the group.
If the selected group is a member of another group, its membership remains intact.

List of existing groups

The **Existing Groups** list specifies all groups containing at least one peak.

Group name

If a calibrated calculation has been enabled and the employed calibration file contains calibrated groups, the list will display their names as defined in the calibration file.

Editing the group name

Group names cannot be changed in the **Groups** dialog since they are derived from the names shown in the calibration file, and can thus be only changed in the main calibration table of the relevant calibration file.

5.4.4 The Selection of Conditions That Restrict Integration

The **Rejection** section in the **Integration** tab can be used to exclude from integration peaks that do not satisfy certain criteria.
All peaks whose **Area**, **Height** or width at half height - **Half Width** are smaller than or equal to the specified values will be excluded from integration, in other words, they are neither displayed in the chromatogram nor included in the **Result Table**.
This way (particularly with the **Height** parameter) you can get rid of small, insignificant peaks that confuse the results without affecting the baseline that runs under the remaining peaks.

5.4.5 Separation Parameters

The **Separation** section in the **Integration** tab can be used to change the baseline below non-separated peaks.
See the **Reference Guide** for additional information.

Valley To Valley Slope – Specifies the maximum slope of the baseline

Tangent Area Ratio – Constitutes the first condition imposed on tangential separation

Tangent Slope Ratio - The condition is satisfied if the ratio of slopes of the second and the first peak exceeds the specified value.

5.4.6 The Integration Table

The **Integration Table** contains a list of "manual" chromatogram modifications, i.e., the commands from the **Baseline, Group, Integration** and **Peak** submenus. Each operation is identified by its name and the range of validity.

For commands with a range of validity that is defined by an interval (**Lock**, **Add Positive**, etc.), the integration table contains the limits of the validity interval.

For commands that are defined by a single point (**Start**, **End** and **Both**), the integration table contains the retention time of the peak that is involved and the new distance relative to the retention time.

Note: *This approach to a certain extent removes any potential inaccuracies that originate from differences in retention times determined in various analyses.*

The Integration Table for new chromatograms:

You can prepare the integration table for new chromatograms before measuring the chromatogram in the **Method Setup** – **Integration** dialog. This dialog you may open using the **Method - Integration** command from the **Instrument** window.

Using an integration table from another method to measure new chromatograms:

Display the integration table in the **Method Setup** dialog using the **Method - Integration** command from the **Instrument** window. Here, the local menu contains the **Copy From** command. After invoking this command, select the corresponding chromatogram or method. This operation is irreversible.

Note: *It is necessary to differentiate between the creation of an entire new method from the current chromatogram using the **Save as Template** command from only copying the integration table using the **Copy From** command.*

Using a method or only the integration table from another chromatogram:

The **Method** menu in the **Chromatogram** window contains amongst other elements, two sets of commands for copying methods or only the integration tables alone from other chromatograms:

Copy (Integration Table) from a Model

Copying a method (or only an integration table) from a chromatogram which was previously indicated as the model using the **Set Model** command. Above all this possibility is used when cloning an integration table from one chromatogram to several various chromatograms.

Copy (Integration Table) from Template Method

Use the method (or only integration table) from a template method. Template methods are saved with the *.MET suffix and are used for measuring new chromatograms.

Copy (Integration Table) from Chromatogram

Use the method (or only integration table) from another chromatogram.

6 Calculations and Calibration

The **YL-Clarity** chromatographic station offers several types of calibration and non-calibration calculations and is able to assess the quality of a measurement using calculated peak and column parameters. Extensive mixtures can be calibrated at up to twenty concentration levels, including the calibration of groups of compounds. Semi-automatic calibration and automated, multiple recalibrations of the same level are also possible (even for sequential analyses). The **YL-Clarity** station incorporates the reference peak method for reliably identifying calibrated compounds.

6.1 Result Table

The Result Table is in the **Results** tab (opened or hidden using the **Results - Result Table** command) and always contains the topical values that refer to the current chromatogram; any changes will immediately be reflected in the table.

Result Table (Pers02) <-- Uncal

	Area [mV.s]	Height [mV]	Area [%]	Height [%]	Reten. Time [min]	W05 [min]
1	0,690	0,138	0,3	0,2	1,195	0,09
2	0,932	0,188	0,5	0,3	1,760	0,09
3	157,639	50,947	77,6	75,8	2,305	0,05
4	1,307	0,270	0,6	0,4	2,557	0,06
5	42,514	15,699	20,9	23,3	2,860	0,04
	203,083	67,242	100,0	100,0	Total	

Results | Summary | Integration | Measurement Conditions | SST F

Fig. 21. Table of Uncalibrated Results

Results are displayed depending on the parameter settings in the right-hand side of the tab. The arrangement of columns is governed using the **Setup Columns** command. In the following text we describe the default layout of the table, which is the result of the **Restore Default Columns** command. Both commands can be found in the **Edit** menu.

In addition to the serial peak number, the retention time and width-at-half-height of all peaks, absolute calibration values and percentages, names and types of compounds, are displayed for uncalibrated results.

By setting the calibration file in the **Calibration File (Peak Table)** field using the **Set** button and selecting one of the calibration calculations in the **Calculation** item, the absolute calibrated values and percentages as well as the names and types of compounds will also be displayed. See Chapter **6.3** - **Types of Integration Calculations** on page **50** and the **Reference Guide** for a more detailed description of individual calibration calculations.

Result Table (2506multi - UV) <-- ESTD

	Reten. Time [min]	Response	RB	Amount [g/l]	Amount [%]	Peak Type	Compound Name
1	4,563	3,613	A	0,027	0,3	Ordnr	oxalic
2	5,203	253,325	A	1,609	16,8	Ordnr	citric
3	5,417	561,713	A	2,372	24,7	Ordnr	tartaric
4	6,300	217,455	A	1,181	12,3	Ordnr	malic
8	8,160	176,947	A	1,125	11,7	Ordnr	succinic
9	8,550	193,934	A	1,970	20,5	Ordnr	lactic
11	10,347	152,602	A	1,312	13,7	Ordnr	acetic
C11	12,710		A			Ordnr	methanol
	Total			9,595	100,0		

Results | Summary | Performance | Integration | Measurement Conditions | SST Results

Fig. 22. Example of Calibrated Results Table

6.2 Table of Peak Parameters

Full version

For the purposes of Good Laboratory Practice and to verify the suitability of the employed system, calculations have been extended to include some special parameters such as asymmetry, the capacity factor, column efficiency, and resolution. These calculations can be found in the Performance tab. This tab is implicitly hidden, use the **View – Show Tables – Performance Tables** or **Results – Performance Table** commands to display it.

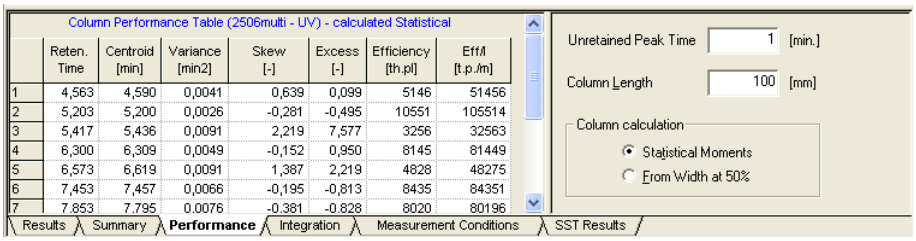


Fig. 23. Table of Peak Parameters

Calculation method

Use the **Column Calculation** parameter from the **Performance** tab to select one of the two available calculations:

1. According to statistical moments - Statistical Moments

This constitutes the most accurate integral calculation based directly on the values measured for a given peak. The calculation provides top-quality results for well-separated peaks at a reasonable signal-to-noise ratio and sufficient number of partial integrals for individual peaks. The underlying formulae are listed in the **Reference Guide**.

2. From width-at-half-height - From width at 50 %.

This represents the standard calculation method based on the measured width-at-half-height and the assumed Gaussian peak shape. This method often leads to deviations from the actual efficiency for real chromatographic peaks.

Note: *To ensure that the capacity factor has been correctly calculated, do not forget to specify the dead retention time - (**Unretained Peak Time**) and also the column length necessary for calculating the relative efficiency (**Column Length**).*

6.3 Types of Integration Calculations

Generally speaking, the result of a chromatographic analysis, representing the amount of a compound, is either the area or height of the corresponding chromatographic peak or group of peaks. However, the same amounts of different compounds elicit different detector responses. To take this fact into account while calculating the amount, one must know the detector sensitivity under the given measurement conditions. In other words, the calibration curve of the compound in question, representing the response as a function of the amount of the compound.

Calibration curves are stored in a calibration file; the latter can contain an arbitrary number of calibration curves that correspond to the compounds that are present in a mixture. The **Calibration** window is earmarked for creating and modifying calibration curves. Calibration calculations respect the differences in detector sensitivity vis-à-vis individual compounds at various concentrations. Concurrent calibration of several compounds from a single injection may register potential interactions between the calibration compounds as well. If a tentative evaluation of the amount of the compound is sufficient for your purposes, use the uncalibrated calculation where no calibration curve is required.

The **YL-Clarity** station offers two fundamental calibration calculations - the external standard method (ESTD) and the internal standard method (ISTD). Each can be based on peak height or peak area. It is always mandatory to select the appropriate calibration file and enter any additional parameters that are necessary for the selected type of calculation. This can be done either, in advance in the template method (**Method Setup - Calculation** dialog), or in the right-hand section of the **Chromatogram - Results** window for already measured chromatograms.

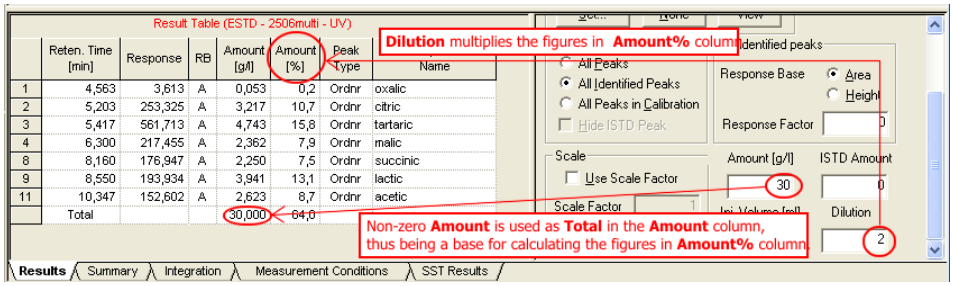
Note: *The calculation method is defined using the **Calculation** item in the right-hand section of the **Results** tab and not by the **Display Mode** parameter from the calibration file (in the **Calibration Options** dialog), since the latter merely decides on how the calibration curves are displayed. Regardless, the calibration file always contains all data necessary for any type of calculation.*

Calculation of percentages

The ratio of **Amount** and **Dilution** fileds from the chromatogram header (specified in **Single Analysis** or **Sequence** windows) specifies the overall amount of components in calculation of percentages in Chromatogram – Results window. These parameters can also be modified later in the right part of the **Chromatogram – Results** window.

If the Amount field is left blank (= 0), the total amount (Total row value of **Amount** column in the **Results** table) will be computed as the sum of calibrated amounts of all compounds (also including unidentified compounds, if **Response Factor** from **Unidentified Peaks** field is non-zero).

If the **Amount** field is provided (non zero) its value will be substituted for the Total row value of Amount column in the **Results** table. The **Amount%** column values will be then calculated with it as a base. The **Dilution** field multiplies the values in the **Amount** column.



Thus, if the sample weight will be entered in the **Sample** field and the volume used for dissolving the sample in the **Dilution** field, using the same units as are used in the calibration (i.e. calibration is in mg/l, weight in mg, solvent volume in litres) the user will get the percentage of compound in the original sample in the **Amount%** column of the **Results** table.

For example:

The amount 5 mg/l was found for 100 mg sample dissolved in 100 ml (0,1 l).

The result in the **Amount%** column will be: **5** *mg/l* *** 0,1** *l* / *100 mg* = **0,5***%*

Attention! *In evaluation of peak groups the total response used in the calculation of percentages includes contributions from individual groups and separate peaks (i.e., peaks not included in any group). It is important to keep this fact in mind when some peak is calibrated separately as well as a part of some group.*

Calculation of unidentified peaks

For peaks that are not identified in the calibration file the **Response Factor** parameter is used in the calculation instead of a value read off the calibration curve. The default value is *0*, so the unidentified peaks will not be applied.

6.3.1 Non-calibrated Calculations - Uncal

Without a calibration file the amounts can be only expressed as percentages of the overall area or height of all chromatograms.

The two types of non-calibrated calculations assume that the detector sensitivity is the same for all compounds and that all compounds present in the injected sample were actually detected. Since the first assumption is very rarely met, non-calibrated calculations are primarily used to obtain a preliminary, semi-quantitative result.

Note: *Non-calibrated calculations are also used by default in instances where a calibrated calculation has been selected but not all required conditions have been met, no calibrated compound was identified in the chromatogram or the requested calibration file was not found. The type of calculation that is actually being employed will always be indicated in the header of the table of integration results (**Results**) together with a reason for why the required calculation could not be performed.*

6.3.2 External Standard Method - ESTD

Calculating using the external standard method respects differences in detector sensitivity to various compounds, and provides the amounts of individual compounds and their percentages in the injected sample.

The drawback of the external standard method is that it is extremely sensitive to both the injected amount and measuring conditions. To eliminate any possible errors it is mandatory to maintain the highest precision of injected amounts (autosamplers) and frequently rebuild the calibration files using recalibration so that they reflect potential changes in characteristics of the detector and the chromatographic system as a whole. The above drawbacks are in part removed in the internal calibration methods.

6.3.3 Internal Standard Methods - ISTD

Calculations that use the internal calibration method respect the different detector's sensitivity to various compounds and to a certain extent, eliminate errors that originate from differences in the injected amount. The methods provide the amounts of individual components present in the sample and their percentages.

In the internal standard method, a compound - internal standard - will be added to the calibration mixture. That compound is known as the internal standard. A known amount of the internal standard must be then added to each analysed sample. It thus follows that the internal standard itself must not be originally present in the calibration mixture or in the analysed sample.

Note: *In selecting the internal standard take into account the sample composition and the chromatographic conditions. The internal standard should be very pure and stable, must not react with any analyte, and should provide a well-separated peak. Furthermore, it must be soluble in the sample and the sensitivity of the detector vis-à-vis the internal standard and other components of the sample should be similar.*

Since the internal standard is present in the calibration mixtures and in each sample, changes in chromatographic conditions and in the injected amount affect the peak of the internal standard in the same manner as the peaks of other injected compounds. This circumstance is taken into account in the calculation and ensures high reproducibility of the obtained results.

The YL-Clarity station uses two procedures for calculating the internal standard method. The appropriate method is automatically selected depending on whether the same amount of the internal standard in all calibration standards and in unknown samples is being used.

a) The same amount of the internal standard is used and it is neither specified in an unknown sample nor in the calibration file

A relative calibration curve is compiled and used in the calculation, where the ratio of responses of the compound in question and the internal standard is plotted against the internal standard response on the vertical axis and the **Amount** of the compound on the horizontal axis.

b) The different amount of the internal standard has been set both in unknown sample and in calibration file

The actual amounts are calculated from a relative calibration curve, where the ratio of responses of the analyte and the internal standard on the vertical axis is plotted against the ratio of the amount of the analyte and the amount of the internal standard on the horizontal axis.

Note: *The compilation of both types of variables requires that the calibration file contains at least one level at which both the analyte in question and the internal standard have been measured. If this condition is not met the relative calibration curve cannot be compiled and the N/A (not available) inscription will be displayed instead of results in all chromatograms that have been evaluated according to this calibration.*

Note: *If the amount of internal standard was only filled-in on one side (the **ISTD Amount** parameter is left blank in the header of the relevant chromatogram or the **Amount** column in the internal standard compound in the calibration file), the internal standard method cannot be applied. In all chromatograms that have been evaluated according to this calibration, only the **uncalibrated calculation** will be used.*

6.4 Description of the Calibration File

The calibration file contains data items needed for the compilation of calibration curves. In addition to the table of amounts and responses, other information , like the compound name, retention time, number of recalibrations, etc. is listed for each compound. The data contained in the calibration file is presented in two tables. The main calibration table lists data of all compounds that are common to all calibration levels, while the compound tables contain data referring to individual compounds at all levels, including the calibration curve.

Note: *All data items that are stored in several locations will always be updated after each change. Naturally, when a modified calibration file is used to process the displayed chromatogram, the changes will immediately be taken into account.*

Multidetector calibration

For multidetector chromatograms the calibration file can simultaneously contain a set of calibration curves for up to four signals. The number of displayed signals can be set in the **Number of Signals** item from the **Calibration Options** dialog. All displayed figures apply to the current signal whose name will be displayed in the header of the global calibration table or in the header of the graph of the calibration curve. Select the desired signal using the **Calibration – Set Signal** command or the coloured button from the toolbar. The figures that are common to all signals will be displayed in black. The figures that are specific for each detector will be displayed in the colour of the appropriate signal.

6.4.1 Main Calibration Table

The global calibration table is available from the **Compounds** tab of the **Calibration** window.

Open the window using the **Window - Calibration** command or the  icon. The table summarises data about all compounds that are common to all levels: The name of the compound, retention time, the two identification time windows, compound type (**Peak Type**),

global response coefficient (**Response Factor**) used in free calibration. The columns labelled **Level X** contain data of the current calibration level.

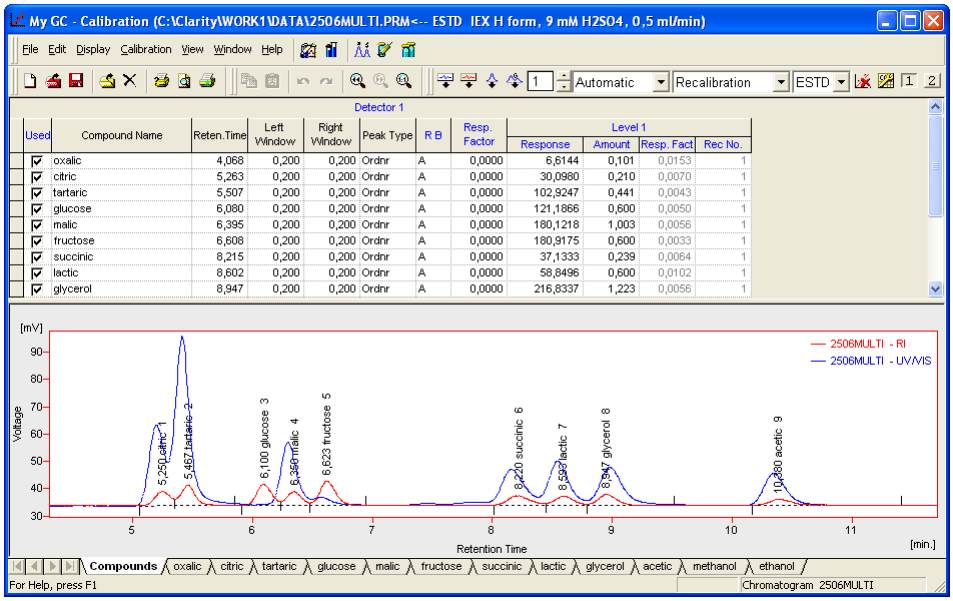
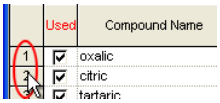


Fig. 24. The Main Calibration Table

The table can be displayed above or below the calibration standard graph - see the **View - Table Up** command.

6.4.2 Compound Calibration Tables



Calibration tables of individual compounds are available - together with the calibration curves and other parameters - from tabs of individual compounds in the **Calibration** window. Display the relevant tab by double-clicking its name or the first grey field of the corresponding line in the main calibration table.

The table lists values for all levels of the relevant compound: level number in the first column, responses in the **Response** column, and amounts at individual levels in the **Amount** column. The **Response Factor** column contains level-specific response factors equal to the amount divided into the response at that level. The **Rec. No.** column displays the number of eventual recalibrations of the point.

Note: *The level-specific **Response Factor** is merely an indicative value. When the free calibration is to be employed the global response factor taken from the main calibration table will always be used.*

Display and calculate areas or heights?

The base (either the peak area or peak height) of the displayed response, of the level response factor, of the correlation equation and of the displayed curve is determined by the **Response Base** field.

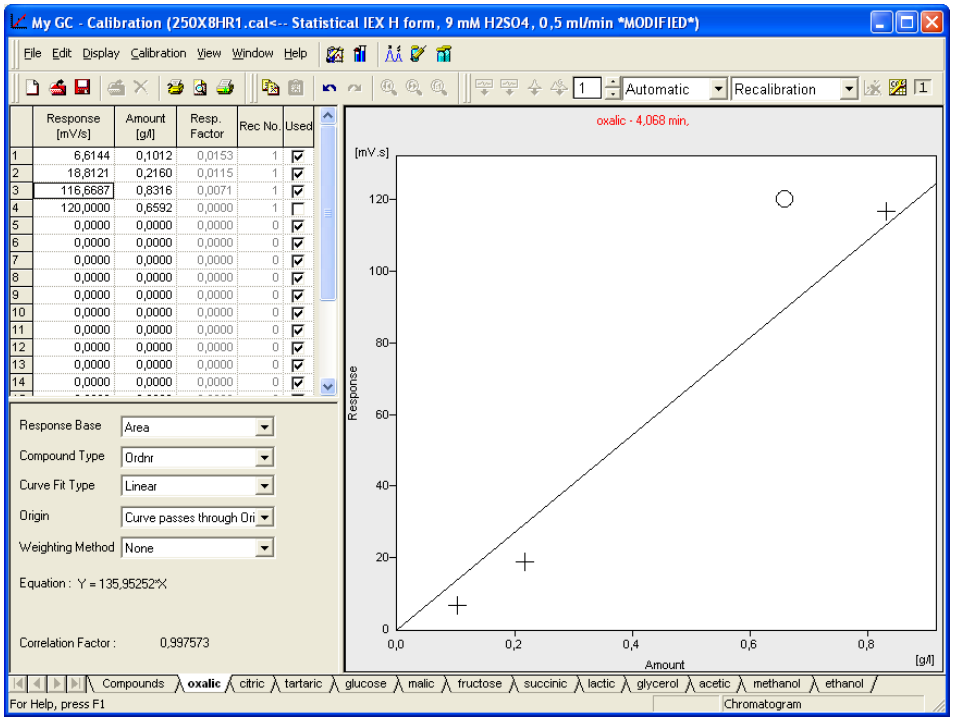


Fig. 25. The Compound Calibration Table

Optional validity of points:

Individual points may be temporarily left out or on the other hand included into the calculation of the calibration curve. A point is omitted from the calculation by cancelling the indication in the **Used** column in the calibration table of substance. An invalid point is illustrated in the graph by a circle.

Note: *An invalid point in the calibration curve behaves as if it were not present. For example, indicating an invalid point at the end of the curve will change the scope of the axes. This will cause the circle, representing an invalid point, to be shown outside of the displayed area of the graph. Only the circles of those invalid points, behind which will still be at least one valid point (cross), can be seen.*

6.4.3 Calibration Curve

The calibration curve is displayed together with the compound calibration table. The curve is plotted as the dependence of the response on the amount. The curve will be not displayed, though, if the correlation equation cannot be compiled for the selected type of correlation. Each calibrated level is displayed using a cross in the graph; points for recalibrated values at some levels, if any, will be displayed with asterisks (the number of recalibrations is apparent from the **Rec. No.** column.)

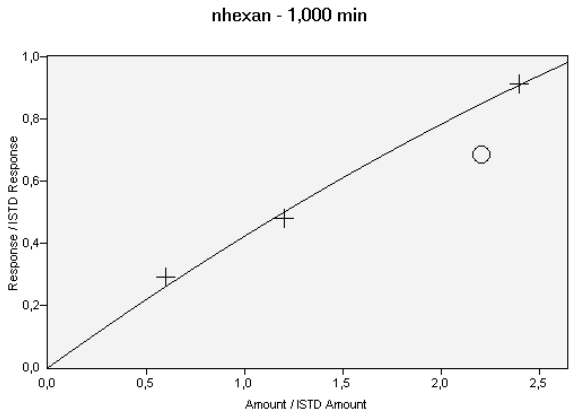


Fig. 26. Example of Relative Calibration Curve for the ISTD Method

Any part of the curve can be zoomed in using the left mouse button; return to any of the previous magnifications or to the original cut using the **Previous Zoom** commands (icon), **Next Zoom** (icon) or **Unzoom** (icon), respectively, or display a grid using the synonymous command. All the above graphical functions are the same as in the **Chromatogram** or **Data Acquisition** windows (e.g. Chapter **5.1** - **Displaying a Chromatogram** on page **33**).

Type of curve fit equation

The type of correlation is defined in **Curve Fit Type** item; **Origin** item decides on how the co-ordinates of the origin will be handled: the *Ignore Origin* option ignores the origin while with the *Compute with Origin* option the origin is considered to be one of the calibration points; this means that the resulting curve is influenced by, but need not pass through, the origin; the *Curve Passes Through Origin* option will always force the correlation curve to pass through the origin.

Correlation equation

The **Equation** item displays the plot of the calibration curve and the corresponding correlation equation (except for the *Point to Point* segmented line type of fit, *Free Calibration* and Sigmoid interlining), with X representing the amount and Y the response. The curve and the corresponding equation need not to always be displayed and, especially in instances of third-order polynomial correlation, the algorithm that is used to calculate the coefficients of the equation, may fail for some extreme values of amounts and responses. To remedy such situations, use another curve fit type or normalise the entered values.

Tightness of fit

The **Correlation Factor** item contains the calculated correlation coefficient - a number from the interval **<0; 1>**, characterising the tightness of fit.

Note: *In the event that the degree of the correlation equation is the same as the number of calibration levels (for the* Ignore Origin *option already for a degree less by one) the correlation coefficient will be one (1) since such a curve will pass through all points.*

Weighting

This method can increase the influence of points with lower concentration on the calculation of the interlined curve. Weighting can be related to either the amount of compound in the given point of calibration curve (1/Amount or $1/Amount^2$) or to the response of the compound in the given point of the calibration curve (1/Response or $1/Response^2$).

6.5 How to Create Calibration

The following chapters describe the procedure used to create and modify calibration files. The station provides for both automatic and manual calibration and recalibration of individual peaks or groups, or jointly for all compounds (peaks and groups).

1. Create the calibration file

Create a new calibration file using the **File - New** command from the **Calibration** window.

2. Display a calibration standard

Unless you intend to create an "artificial" calibration, you must display in the calibration window, the relevant calibration standard at a certain level. To do that, invoke the **Open Standard** command or click the icon to display a list of all chromatograms from the calibration subdirectory of the current project. Use the icon to display chromatograms from the data subdirectory.

3. Selecting calibration parameters

Check the toolbar to determine whether has been set. 

The number box indicates the calibration level. **Automatic** means that data for individual compounds will automatically be transferred to the calibration table and **Calibration** indicates the calibration regime (contrary to recalibration regime).

4. Transferring individual compounds data to the calibration table

Use any of the following commands from the **Calibration** submenu or the corresponding icon to transfer compound data contained in the calibration standard to the calibration file:

Add All	-	Add all peaks identified in the calibration standard.
Add Existing	-	If the calibration table is empty, all peaks and groups from the calibration standard will be calibrated. If the calibration table already contains compounds, then only these compounds will be calibrated.
Add Peak	-	Only the selected peak will be calibrated.
Add Group	-	Only the group containing the peak selected using the cursor will be calibrated.

5. Supplying known amounts and other data items

Enter all known amounts for all compounds in the **Amount** column below the calibration level - **Level 1**.
Update the compound name in the **Compound Name** column.

6. How to display and check the calibration curve?

Click the tab with the name of compound whose calibration curve you want to see; the calibration table, the calibration curve and parameters of that compound will be displayed.

7. How to redisplay the main calibration table and the standard?

Click the **General** tab.

8. Saving the calibration file

To save the calibration file invoke the **File - Save** command.

9. How to use the calibration file?

Open the **Chromatogram** window using the **Window - Chromatogram** command or the  icon.
Open the chromatogram to be evaluated using the calibration that has just been created.
Set the created calibration file using the **Set** command in the right-hand side of the **Results** tab.
Do not forget to set the appropriate type of calibration calculation in the **Calculation** item.
If all went well, the **Amount** column of the result table should now contain the amounts for all calibrated and identified peaks.

6.6 Creating Additional Concentration Levels

Once the first calibration level has been created, continue to calibrate at the next levels. Any number of compounds can be calibrated at each level regardless of whether or not they have been calibrated at the lower levels. Moreover, compounds from different calibration standards can be calibrated at a single level.

1. How to set another calibration level?

Each time a calibration file is opened the first calibration level will always be selected.

Use the  arrows from the toolbar or **Calibration – Set Level** command to change the calibration level. If the **Automatic - Calibrate** regime has been enabled, the current calibration level will change in conformity with the following rules:

- The **Add All** and **Add Existing** commands set and calibrate the first completely free level.
- The **Add Peak** or **Add Group** commands always set and calibrate the first free level of the relevant compound.

To prevent the program from automatically selecting calibration levels, enable the **Manual Calibration** regime on the toolbar. See Chapter **6.7** - **Manual Calibration** for additional details.

2. Reading in another calibration standard

Invoke the **Open Standard** command to select and display another calibration standard corresponding to the preset calibration level.

3. Transferring compound data to the calibration table

Invoke any of the following commands:

	**Add All**	- Add all peaks identified in the calibration standard.
	**Add Existing**	- If the calibration table contains compounds already calibrated on previous level, it will look for and eventually calibrate these compounds also at the current level.
	**Add Peak**	- Only the peak selected using the cursor will be calibrated.
	**Add Group**	- Only the group containing the peak selected using the cursor will be calibrated.

4. Supply known amounts

Enter all known amounts for all compounds in the **Amount** column below the calibration level - **Level x**.

5. Repeat steps 2 to 4 for all calibration levels required

Note: *Thanks to the character of the **YL-Clarity** station, any change in the calibration file will immediately be reflected in the result tables of all chromatograms that use it. In other words, it is not necessary to save changes using the **File - Save** command to update the result table.*

6. How are peaks assigned to compounds in the calibration table?

The retention time of each peak you wish to calibrate using the **Add Peak** command will be compared with the identification windows of already calibrated compounds. If identified with any of them (i.e., if the retention time lies within the interval **< Ret. Time - Left Window**; **Ret. Time + Right Window**>, its retention time will be added at the next level. Otherwise a new calibrated compound will be established.

If the calibration proceeds under the **Add Existing** command, only identified compounds will be calibrated in the above manner, in other words, you cannot add new compounds in this manner. Identifying a calibration using the **Add Group** command will only proceed according to the group identifier.

7. Updating retention times of compounds

The retention time of any compound can be changed manually in the **Retention Time** column at anytime.

The retention time is also automatically updated during each new calibration or recalibration of the compound in question. The updated retention time is taken as the arithmetic mean of all values established using existing (re)calibrations of that compound.

The automatic update can be switched off by unchecking the **Update Retention Time** item in the **Calibration Options** dialog.

6.7 Manual Calibration

If you wish to acquire full control over the calibration process, reset the *Automatic* parameter to *Manual* in the toolbar.

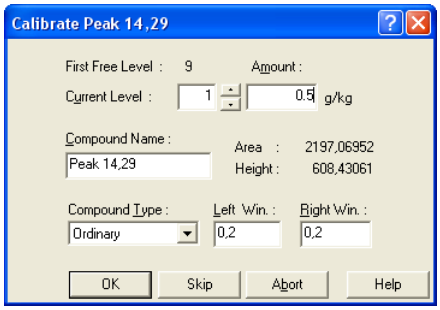


Fig. 27. The Calibrate Peak Dialog

After using certain of the **Add All**, **Add Existing, Add Peak**, **Add Group** commands in the manual regime, the **Calibrate Peak (Group)** dialog will be displayed for each compound, in which you may immediately amend and enter all data on the calibrated compound. For the **Add All** command you can then skip the calibration of the currently displayed compound using the **Skip** button. The **Abort** button terminates the whole calibration process. The amount of the calibrated compound is entered in **Amount** field in the displayed dialog.

6.8 Recalibration

The **YL-Clarity** station provides for facile recalibration (modification of calibration files). The procedure is similar to that which has already described for calibration.

What does recalibration mean?

Recalibration means repeated calibration at a given concentration level. The purpose is either to update the calibration points or increase precision by repeated averaging at individual calibration levels.

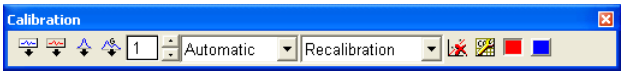


Fig. 28. The Calibration Window Toolbar

How is the recalibration mode set?

The mode of recalibration is set in **Mode - Recalibration** field in the **Calibration Options** dialog. The command can be opened by invoking the **Calibration - Options** command, using the  icon, or directly in the main toolbar of the calibration window.

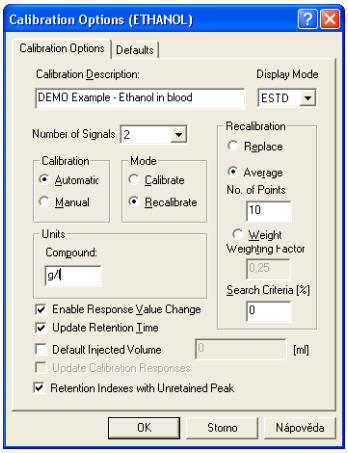


Fig. 29. The Calibration Options Dialog

How to set the recalibration mode?

Set the recalibration mode in the **Recalibration** section of the aforementioned **Calibration Options** window. The result of recalibration can be either the arithmetic mean of all previous values and the new value - **Average**, a weighted mean of the original and the new value – (**Weight**) or, finally, the old value can be replaced by the new one –(**Replace**).

How to prevent recalibrating using incorrect values?

The maximum allowable difference in per cent between the new and the existing value can be specified in the **Search Criteria** field; in this manner you can forbid automatic recalibration using values that fall outside the permitted range. In manual recalibration the *Over* message in **Departure** column will appear if the permitted difference has been exceeded. Enter zero to disallow the condition.

6.9 Manual Recalibration

As with calibration you may choose between manual and automatic recalibration. In the former instance the appropriate **Recalibrate Peak (Group)** dialog containing all data that can be changed directly will open each time a compound has been selected.

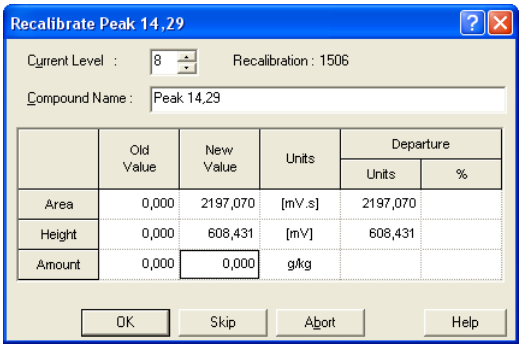


Fig. 30. The Recalibrate Peak Dialog

The window offers a selection of the recalibrated level and contains the compound name, the total amount of recalibrations already effected, and the recalibration table. The first calibration of the compound is included in the number of recalibrations, and is reset to 1 each time recalibration of the **Replace** type has been undertaken. The **Cancel** command will skip the recalibration of the currently displayed compound, and the **Abort** button will terminate the recalibration of all compounds.

The recalibration table contains the previous and current values of the two responses, the amount (including the units), and the absolute and relative deviations. A differing amount (if any) will be recalibrated in the same manner as the responses. The **Default Injected Amount** item offers a more suitable method for correcting differences in the injected amount - see Chapter **6.12**.

The *Over* message will appear in the **Departure** column each time a permitted deviation (set in the **Search Criteria** field) has been exceeded.

6.10 Multidetector calibration

Calibration and recalibration for multidetector measurement is performed in the same way as the single-detector described in the previous chapters. When the multi-detector calibration standard has been loaded and the calibration of the first signal has been calibrated another signal may be selected using the **Calibration – Set Signal** or using corresponding colour symbol from the toolbar. It is not necessary to fill in all figures for each signal. For example, the **Compound Name**, **Retention Time** and **Amount** are common for all signals. Common columns are displayed in black type.

Note: *A multidetector calibration can also be created using the single-detector calibration standards. Then you will have to enable the calibration of further signals in the calibration file using the **Number of Signals** command from the **Calibration Options** dialog.*

6.11 Calibration File Modification

All data in calibration files can be changed unless dimmed.

The manual modification of responses

The **Enable Response Value Change** checkbox from the **Calibration Options** dialog must be checked prior to any manual modification of the values of responses. The number of recalibrations is reset to one (1) when a response has been manually changed.

Deleting a compound

To delete a compound invoke the **Calibration - Delete Compound** command or click the icon.

"Artificial" calibration

It is not a problem to create a calibration curve from the known response factor or response without using a calibration standard. Add a new compound to the global calibration table by simply filling in any cell in the last free line. Once the entry has been confirmed using the Enter key, the remaining data will be automatically supplemented and can be subsequently modified.

6.11.1 Default Parameter Settings

Invoke the **Calibration - Options** command to open the **Calibration Options** dialog, and then click the **Defaults** tab.

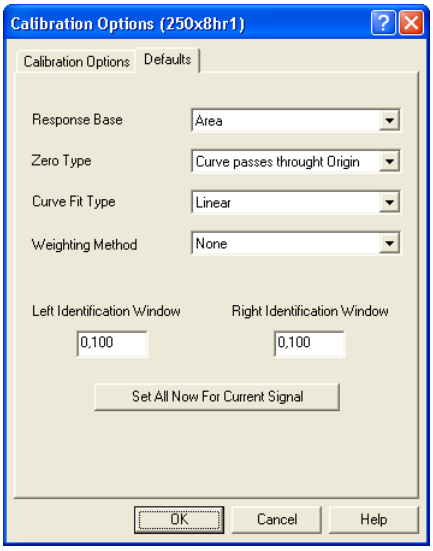


Fig. 31. The Calibration Options - Defaults Dialog

Default values of some selected parameters for new compounds in the current calibration file can be selected here.

6.11.2 Response Factor and Free Calibration

The calibration file lists two response factors for each compound.

Level-specific response factor

For each calibrated level the compound table lists the response factors in the synonymous item. The factor is calculated as amount divided into response at a given level and is only indicative.

Global response factor

The main calibration table contains the column for setting the global response factor – (**Response Factor**), used instead of values calculated from the calibration equation when the *Free Calibration* applies.

Free calibration can be selected in the selected compound tab of the **Curve Fit Type** item. Free calibration is indicated with the *Free* inscription in the **Peak Type** column from the **Result** table in the **Chromatogram - Results** window.

6.11.3 Selection of Calibration Units

The amount entered in the calibration table can be expressed in any units. The type of units is specified in the **Units - Compound** field of the **Calibration Options** dialog.

The units stated there will be shown at all amounts in the table, in the graph and also in the **Results table** in the **Chromatogram** window.

Note: *The user can specify their own units in **Units after Scaling** item of the **Results table**.*

6.12 Correction for Differences in Injected Amount

Different injected amounts of both the calibration and unknown samples can be adjusted to a common value. If the **Default Injected Volume** checkbox has been checked and a value has been entered in the **Calibration Options** dialog, each response used in calibration, recalibration or evaluation will be multiplied by a correction factor calculated as the ratio of the above value and the value of **Inj. Volume** from the chromatogram header.

Unless the **Default Injected Volume** checkbox has been checked, the **Inj. Volume** parameter serves for informational purposes only.

If you change the entered value, you can invoke the **Update Calibration Responses** command to recalculate all responses by multiplying them by the ratio of the old and the new value.

If the **Default Injected Volume** checkbox has been unchecked, the last recalculated values of responses will remain valid regardless of any changes made in **Inj. Volume** item.

Owing to the linear interpolation that replaces the actual dependence between the amount and the response, it is advisable to only use the above correction for small deviations originating, e.g., from the difficulty of achieving a reproducible injection in gas chromatography.

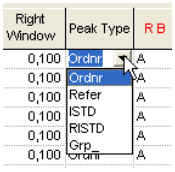
6.13 Peak Identification in Calibrated Calculations

This chapter deals exclusively with the identification of separate peaks, since the identification of peak groups proceeds according to respective single-letter identifiers.

One may reasonably expect that compounds contained in a calibration file will be identified with peaks in the measured chromatogram. To this end the user specifies identification windows relative to the relevant retention time for each compound in the calibration file. If a peak exists in the chromatogram whose retention time falls within the identification window, it will be assigned to the corresponding compound from the calibration file. In calibrated calculations, the calibration curve for that particular compound will subsequently be used for the peak thus identified. If there are several peaks inside the identification widow, **the peak whose retention time is the closest to the retention time of the calibrated compound will be identified**.

Peak identification is used not only in calibrated calculations but in recalibration and multilevel calibration as well. Chapter **6.13.2** explains how the station resolves possible instances of overlapping identification windows.

6.13.1 "Reference Peak" Method



The process of peak identification may sometimes be complicated with changes in retention times brought about by changes of measurement conditions, use of different methods, changes in characteristics of the chromatographic system, or simply by random error. The method of reference peaks eliminates a substantial part of these complications, resulting in reliable identification of peaks in the chromatogram.

Compounds marked as reference in the calibration file will be identified first. The difference between the retention time of a reference compound and that of the corresponding reference peak in the chromatogram is then used to correct the retention times of the other (non-reference) compounds listed in the calibration file. The non-reference compounds are then identified according to the retention times so corrected.

The reference peak method will automatically be applied if at least one compound in the calibration file has been marked as reference, either in the main calibration table, the **Peak Type** item, or in the tab of the relevant compound of the **Compound Type** item accessed by selecting *Refer.* The peak of the internal standard can also be marked as reference peak by selecting *RISTD*.

If several peaks fall within the identification window of the reference peak, the largest of them (determined according to how the peak area or height has been set in the **Response Base** item) will be identified.

A reference peak not originally identified in the chromatogram cannot be subsequently identified inside the newly calculated intervals.

The method used to correct the retention times of the non-reference peak is apparent from the following Figure:

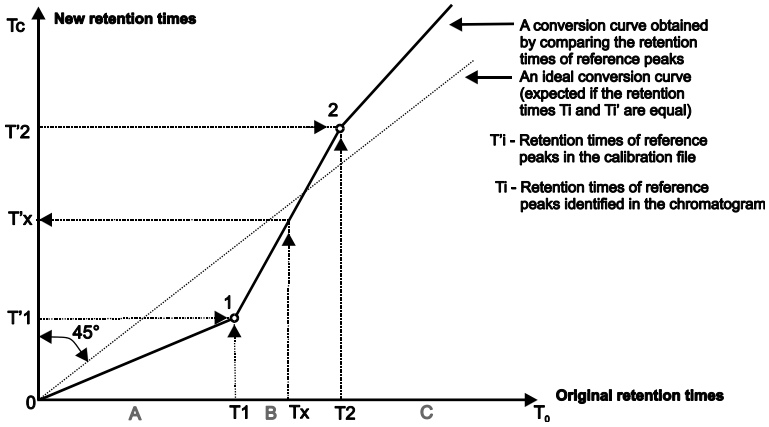


Fig. 32. Scheme of the Reference Peak Method

The difference between the actual retention times of reference peaks, Ti, and the retention times listed in the calibration file, T'i, is used to determine, by linear interpolation (linear extrapolation for non-reference peaks past the last reference peak), the correction that is to be applied to the retention times of non-reference peaks.

The following relations apply to the i-th peak in individual segments between the A, B, C etc. reference peaks:

In segment A (before the first reference peak) $Tc_i = To_i \cdot \frac{T'1}{T1}$

In segment B (between two reference peaks) $Tc_i = T'1 + (To_i - T1) \cdot \frac{T'2 - T'1}{T2 - T1}$

In segment C (behind the last reference peak) $Tc_i = To_i \cdot \frac{T'2}{T2}$

To_i - Original retention time of peak i

Tc_i - Corrected retention time of peak i

T'_i - Retention time of the reference peak in the calibration file

T_i - Retention time of the reference peak in the sample.

Identification windows relative to the retention times so corrected are used to identify non-reference peaks. The method used to resolve overlapping identification windows construed in the above manner is described in the following chapter. The reference peak method will provide the most reliable results if reference peaks are distributed fairly uniformly across the entire chromatogram.

The calculated, corrected retention times of non-reference peaks apply only to identification during calibration, recalibration or calibrated calculations, and are not substituted for retention times of compounds in the calibration file or the sample. Updating retention times of compounds included in the calibration file is described in Chapter **6.13.3**

6.13.2 Resolving Instances of Overlapping Identification Windows

It is not necessary to monitor whether or not the neighbouring identification windows overlap. Prior to the identification process proper, the **YL-Clarity** station will check the identification windows of individual compounds and resolve instances of overlapping by reducing some identification windows.
This method is elucidated in the following Figure.

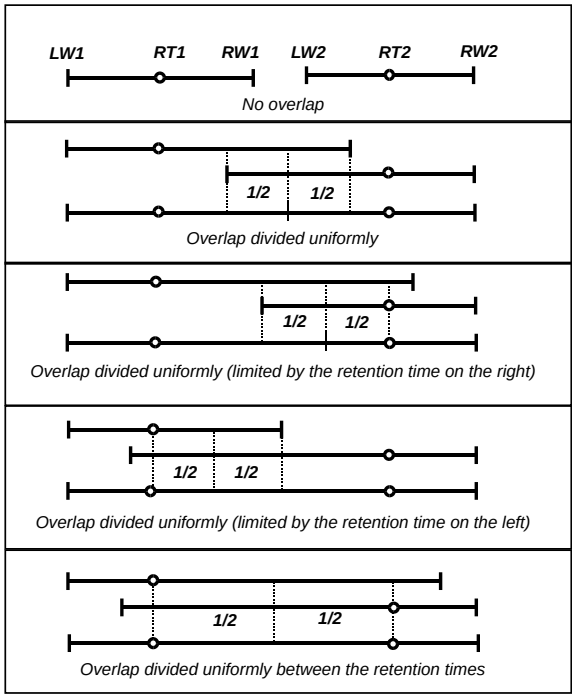


Fig. 33. Resolving Overlapping Identification Windows

The corrected identification windows remain in effect only during the identification process and do not replace the windows specified in the calibration file.

6.13.3 Updating Retention Times

Retention times of compounds tend to eventually shift and, accordingly, difficulties with the identification of calibrated compounds in the chromatogram may sometimes be encountered. To avoid this problem, the **YL-Clarity** station provides for an automatic update of the retention times of calibrated compounds in each subsequent (re)calibration by registering any potential shifts in retention time. This process results in the reliable identification of calibrated compounds. Enable the automatic update by checking the **Update Retention Time** checkbox in the **Calibration Options** dialog. The retention times listed in the calibration file will be updated as an arithmetic mean of the new time and all times established in previous (re)calibrations of the given compound.

7 Reports

The **YL-Clarity** station provides for an arbitrary part of the obtained results to be printed at any printer registered in the **Windows** environment.

7.1 Reporting Procedure

1. Where to initiate a report?

The **YL-Clarity** station enables reports to be printed from many dialogs. The menus of most windows contain the **Report Setup** command , icon or the **Report** button. Always select the window that contains the data you wish to include in the report. Different report styles are preset in each dialog, but can be modified or replaced at will.

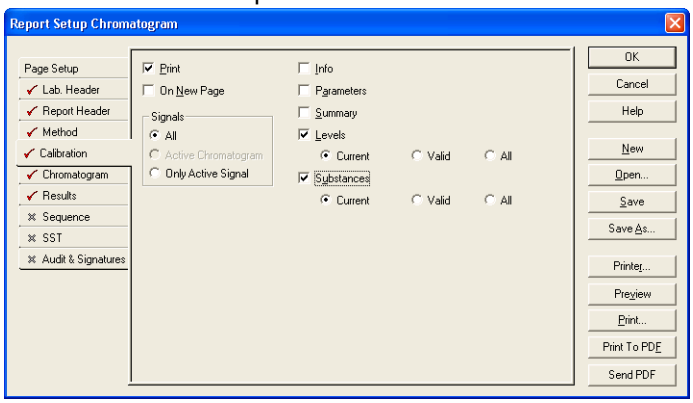


Fig. 34. The Report Setup Dialog

2. Selecting a printer

Check and, if need be, select a printer using the **Printer** command, including setting the quality and size of the printout.

3. What will be printed?

Look through all tabs in the left-hand side of the **Report Setup** window and check or change what will be printed. The name of the report style containing these settings will be displayed in the title bar of the window.

4. Selecting a different report style

In some instances it is more convenient to use a different report style instead of modifying the current report style. Invoke the **Open** command to list all the report styles that are stored in the COMMON directory.

5. How will the printout look?

Use the **Preview** command to see what will be actually printed.

6. Printing reports

To start printing the report, invoke the **Print** command. The dialog showing the printer settings will appear once again to enable the user to verify that the settings are correct, determine the number of copies to be printed, select the scope of printed pages, etc.

7.2 Report Style Files

A report style is really a template that contains a list of all the sections to be printed and the report layout (size and type of the font, borders, spaces, etc.). During the printing process proper, the actual values or files are merely inserted into the corresponding sections. Each report style is then stored in the corresponding report style file where its contents can be displayed and modified. The adapted report style can be saved under the same or different name as a new report style. All activities are concentrated in the **Report Setup** dialog. Report styles are stored in the COMMON subdirectory and are common to all instruments and projects.

7.3 Printer Selection

Printer selection is the only part of the **Report Setup** dialog that is not included in the report style and is shared by the whole station; in other words, it is not possible to set different printers or different print quality at individual parts of the station. The list of available printers, their set-up and the connection with the computer all constitute a part of the **Windows** system and the station takes it over in its entirety.

Start the selection using the **Printer** command. Select the appropriate printer using the button; this will display a list of all printers that are registered with the **Windows** operating system. While the station is running, click the line that contains the requested printer to make it the current printer. The **Properties** command, beside the line with the printer name, opens a dialog where the print size, quality and other parameters can be set. The layout of the window differs among individual printers.

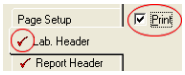
7.4 Report Style Selection

The name of the preset report style is displayed in the title bar of the **Report Setup** dialog. Invoke the **Open** command to see a list of all the available report styles. Click the name of the report style to display some additional data items, like the author's name in the **Created By** field or a description of the report style in the **Description** field. Select the style either using the **OK** button or directly by double-clicking the style name. Alternatively, you can enter the name of the style in the **Filename** field. The **New** command creates a new, empty style.

7.5 Report Style Modification

Each report style is divided into individual segments, and a separate tab is reserved for each such segment to the left of the **Report Setup** window.

Segments preceded by the ✓ symbol will be printed. Double-click the tab of the corresponding tab to include or exclude that segment from the report. The ✓ symbol corresponds to the **Print** item in the top-left corner of each tab.



Most segments are further subdivided. The **On New Page** checkbox decides whether the segment will be printed on a new page or not.

Global parameters that apply to all segments

The first tab, **Page Setup**, defines the parameters common to the printout in its entirety.

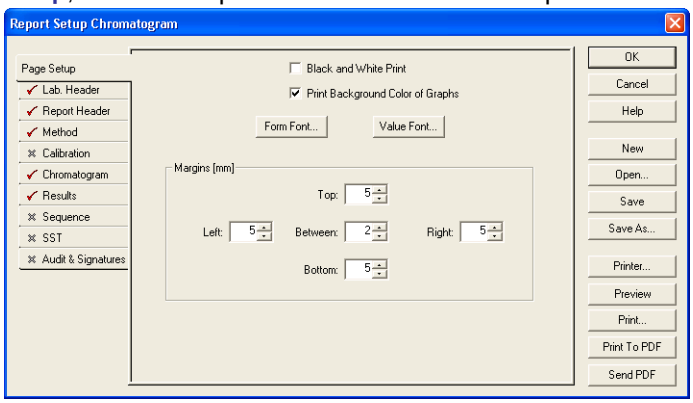


Fig. 35. The Page Setup tab

Use the **Form Font** commands and the **Value Font** to select the type, size and properties of the employed font: **Form Font** will be used to print headings, **Value Font** for the data items proper. The commands in **Margins** section decide on the page margins, the **Between** command specifies the space between individual parts of the printout; all parameters are in millimetres.

Heading

The second tab, **Lab. Header**, contains the laboratory header. Up to ten lines of text can be entered and will appear in the header of the first page or alternatively in the header of all pages in the printout, according to how the **On 1st Page Only** item has been set. The header can be framed (using the **Border** item) and printed on grey background (using the **Grey Background** item). The **Number of Lines** field specifies the number of lines per page. A separate font type, font size and characteristics can be selected for each line using the A icon, and the text aligned using the , , and icons.

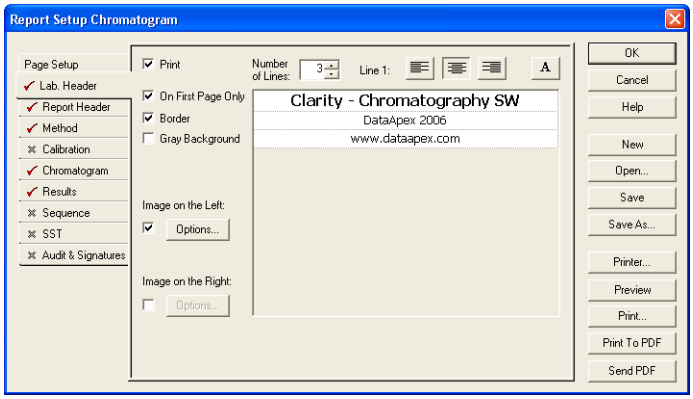


Fig. 36. An Example of a Laboratory Header

The contents of all printed segments outside the **Report Header** can be specified in more detail in the corresponding tab. The **Method** and **Sequence** segments always comprise several parts of the relevant files. The **Results** segment enables the user to decide whether the table of integration results, summary table or the table of column parameters will be printed. The **Calibration** segment allows the user to decide whether all valid or only current level and calibrated compounds will be printed.

Printing the chromatogram

Parameters from the **Chromatogram** segment define the orientation and size of the printed chromatogram. **Orientation** item is used to select the orientation, location and size of the chromatogram. When the **Portrait** item has been selected, the chromatogram will be printed across the page (with the time axis parallel to the text). The chromatogram will occupy the entire page width and, unless a fixed height is specified by the **Fixed Height** command, the default height will be 2/3 of the page. When the **Landscape** item has been selected, the chromatogram will be printed on a separate page with the time axis along the longer side of the page. Use the **No. of Pages** parameter to print the chromatogram on several pages.

Printing in Colour

The station is able to print on colour printers. Chromatograms, descriptive labels and lines will be printed in colour.

8 Import

The YL-Clarity station provides complex possibilities for chromatogram imports in the following *AIA*, *TXT* and *EZ Chrom* formats. Importation can be performed using the **File – Import Chromatogram** command from the **Chromatogram** window. Select the desired directory and file(s) to import in the **Open Files to Import** dialog. Files can be filtered to display only the files of a selected type using the **Files of Type** listbox.

Attention! *Imported chromatograms will be processed using the current template method opened in the Instrument window and not using the method of the currently opened chromatogram!*

Importation of multiple files at once

Multiple files can be selected at once in the **Open Files to Import** dialog. A separate dialog window will subsequently be opened for each imported file.

AIA format

The format of AIA files is quite strict in the form but the content is not fixed. Thanks to this the AIA file may contain various customized items. The Import AIA File dialog is designed to include an unpacking tree to make it easier to verify which items are present in the file. The AIA format is designated for single-detector chromatograms only.

Text format

A chromatogram saved in the text format may (but does not have to) contain a header that describes the conditions of the measurement and (obligatory) data of up to four subsequent chromatographic curves which come one after another. Data can be in one column (voltage) or in two columns (time and voltage). The conversion program determines, according to the content of the individual imported text files, the most appropriate settings for importation. The automatic setting can be manually modified.

Text format EZChrom ASCII

This format utilizes the *.ASC suffix and from the text format used by the YL-Clarity station only differs in the header with different names of individual items.

9 Export

The **YL-Clarity** station allows conjoint text export of results and chromatogram to either the Clipboard or a file, export of results to a database file, text export of the summary table. It is also possible to export the chromatogram in various formats (AIA, Text, EZChrom ASCII); moreover, chromatograms can be exported in the vector picture format.

9.1 Conjoint text export of Chromatogram and the Corresponding Results

The **Export Data** command (invoked by clicking the icon from the **Instrument** window or in the **Chromatogram** window) is used to export data as text.

In the **Instrument** window, the **Export Data** command will only set up the mode to export automatically (**Postrun** function) after an analysis has terminated. The **Export** command in the **Chromatogram** window is earmarked for manually exporting the active chromatogram. In both instances the **Export Data** dialog will open.

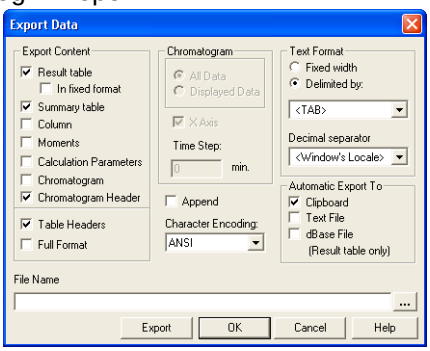


Fig. 37. The Export Chromatogram Dialog

What may be exported?

The **Export Data** command enables the user to export data from the **Results Table** (**Result table** checkbox), from the column parameters table (**Column** item), chromatogram header (**Chromatogram Header** checkbox), calculation parameters (**Calculation parameters** checkbox), statistical moments (**Moments** checkbox) and also the chromatogram (**Chromatogram** checkbox), all in a user-defined format. When a chromatogram is to be exported, the Chromatogram section will be made available where the user can select the time axis (**X Axis** checkbox) and either the chromatogram in its entirety or only the currently displayed part (**All Data** or **Displayed** items) to be exported.

In what format is the chromatogram exported?

The chromatogram is exported as one or two columns of values separated by a character selected from **Text Format** item. The **Fixed** format adds the required number of spaces between values of different length to ensure that they are properly aligned in columns of equal width.

The first column contains time in minutes, the second column voltage in mV. The time increment is taken from **Time Step** field. Each voltage is calculated as arithmetic mean of all voltages within the specified time increment. If zero has been entered, the data will be transferred with the minimum time increment of the chromatogram in question (defined by the sampling rate - **Sample Rate**). If a value larger than the chromatogram duration has been specified as the time

increment, the result will be a single number representing the voltage that is averaged over the entire chromatogram.
No other data (baseline, marks, retention times, descriptive labels) are exported. In this instance the **Headers** checkbox will insert headings of individual columns. The **Full Format** checkbox will insert the chromatogram header at the beginning of the exported text.

In what format is the Results Table exported?

A character taken from the **Text Format** item will separate the values of individual cells of the table. The **Fixed** format adds the required number of spaces between values of a different length in order to align them into columns of equal width.
The **Headers** item adds headers to individual table columns. The **Full Format** item appends the name, date and time of chromatogram creation to each line of the table.

Which characters may be used as separators?

Characters for separating individual columns are selected in the **Text Format** item. If the **Delimited by - Comma**, **Delimited by - Semicolon** or **Delimited by - Tab** item has been selected, the corresponding separator will be inserted between individual data items. To preserve the layout of the table use the **Fixed** format; this format inserts the number of spaces necessary for properly aligning values (unless a proportional font such as the *System* font, is being used) between individual data items. This selection is suitable for exporting data to text editors when creating final reports.

Note: *The **Fixed** format is suitable when a document is to be left "as it is", without further amendments. To classify sections of reports into a document in the text editor, create a separate style, which, for example, could be named "YL-Clarity report" and will use a disproportionate type font. Then apply this style to passages that have been copied from the report of the station. On the other hand, the **Delimited** format is more suitable if further amendments to the report are to be made by removing or adding lines in tables etc. Most of the advanced text editors contain a function that formats text that is separated by a selected symbol into a table.*

Destination of exported data

The **Clipboard** item exports the data to the **Windows Clipboard**. To export to a text file, select the **File** item and specify the filename in the **File Name** field. If you wish to enter the name of an existing file, invoke the **Browse** command to search for the file.

Automatically assigned filenames

If the **File Name** field has been left blank, data will be transferred to a file of the same name as a chromatogram with the *.TXT extension.

Target directories for export

If **File Name** field does not specify a path, the text file will be stored in the same directory as the exported chromatogram.

Export to a single file

The user can append the exported data at the end of an existing file; to do that check the **Append** item.

9.2 Exporting results to a database

If **dBase File** item from the **Export Data** dialog has been checked, the data will be exported in the *.**DBF** format. In this case, only the **Results Table** will be exported to the file in the full format regardless of whether or not **Full Format** has been checked.

9.3 Exporting the Summary table

The **Export Summary Table** command will invoke the **Open File to Export Summary Table** dialog for entering the filename and directory.
Individual items of the summary table are found separated by a tab in the exported file.

9.4 Exporting a chromatogram

Exportation of the chromatographic curve to the *AIA (*.CDF)*, *text (*.TXT)*, *Multidetector text format (*.CHR)* or *EZChrom ASCII (*.ASC)* format. The **Export Chromatogram** command invokes the **Export Chromatogram** dialog where the file format, detector, and target directory are to be entered.

Note: *If you do not set any filename, the name of the exported chromatogram with the appropriate suffix will be used as default.*

9.5 Exporting Chromatograms as Vector Pictures

The **Export - Export As Picture to File** or **Export As Picture to Clipboard** commands export all displayed chromatograms including all descriptive labels, headers and lines in the vector format *.WMF (Windows metafile).

What is a vector format?

In the vector format a chromatogram can easily be incorporated, modified and printed at a high quality using a text editor or a graphical application (**Word, Excel, Corel Draw, etc.**), since it is exported as a set of individual line segments connecting all its points.

What are the advantages of the vector format over the bitmap format?

Displaying and printing a vector picture is not restricted by the size of the graph in the **Chromatogram** window, which otherwise affects the quality and size of data exported as a bitmap. The size of the exported *.WMF file will be smaller than the size of the bitmap file.

Note: *In other words, contrary to a bitmap, a vector picture can be arbitrarily magnified and contracted without any adverse effect on its quality or file size.*

A detailed procedure for copying a chromatogram to an MS Word document

1. Display the requested chromatogram in the **Chromatogram** window.
2. Invoke the **Export - Export as Picture to Clipboard** command.
3. Run **MS Word** and open the target document.
4. Point the cursor to the location where the chromatogram picture is to be inserted and select **Edit - Insert** from the main menu.

The inserted picture can be magnified or contracted and modified once double-clicked.

10 Troubleshooting

This chapter summarises problems most often encountered when working with the **YL-Clarity** station. Problems are listed in chronological order in which they might occur in a typical working procedure.

10.1 Running the Program

10.1.1 YL-Clarity Lite

Demo inscription in the header of the Instrument window

The demonstration version of the program has mistakenly been run. The demonstration version will have the serial number displayed in the **About** dialog in the form 99-999. Open the window using the **Help - About** command.

Message Demo - Wrong S/N in the Instrument window

The serial number of the station listed in the **About** dialog (open the dialog using the **Help - About** command) differs from the number on the **A/D Converter** board.

Message Demo - Missing HW in the Instrument window

- The **A/D board** has either not been found or has been damaged.
- **INT7** board driver has either not been installed or is inoperative.

10.1.2 YL-Clarity

Full version

Demo inscription in the header of the main station window

The demonstration version of the program has mistakenly been run. The demonstration version will have the serial number displayed in the **About YL-Clarity** window in the form 99-999. Open the window using the **Help - About** command from the main **YL-Clarity** window.

Message Demo - Wrong S/N in the main station window

The serial number of the station listed in the **About** dialog (open the window using the **Help - About** from the main **YL-Clarity** window command) differs from the number on the **A/D Converter** board or in the protective **Sentinel** key.

Message Demo - Missing HW in the main station window

- The **A/D board** or the protective **Sentinel** key has either not been found or has been damaged.
- **INT7** board driver or the protective **Sentinel** key has either not been installed or is inoperative.
- The driver module of the **A/D board** or the protective **Sentinel** key has not been registered.
- The **A/D board** driver has not been activated.
- The driver of the **INT5** board has not been configured.
- A different base address or interrupt has been set on the board and in the **INT5** driver.

- A conflict has occurred between the base address or the interrupt of the **INT5** board and the base address or the interrupt of some other computer device.
- The interrupt set on the **INT5** board is not reserved for ISA slots in the BIOS setting of the PC.

You have either forgotten the password or intend to cancel the password-protected mode

If the station is operating in the protected mode and you have forgotten the password, copy the original CLARITY.PSW file from the PGM subdirectory of the installation CD to the main station directory. This will shift the station to the unprotected mode, but be aware that all the settings in the **User Accounts** dialog will be lost.

10.2 Signal Displaying and Measurement

The icon is dimmed and accompanied by the Disabled message, and the Data Acquisition command is inoperative. Full version

- No source for the detector signal has been assigned to the instrument (usually a channel of the A/D converter board). Open the **System Configuration** dialog using the **System - Configuration** command and select the appropriate signal source on the **Instrument1 (2-4)** tab in **Acquisition** item.
- The instrument you are you using has exceeded the number of instruments purchased (e.g., it is impossible to measure on a third instrument if only two have been purchased).
- You are using the **Offline** version of YL-Clarity. Invoke the **Help - About** command from the main **YL-Clarity** window to display the **About** dialog and check the serial number. The serial number format of the **Offline** version is **98-XXX…**

No signal is being displayed in the Data Acquisition window.

- Probably an incorrect range has been selected, so that the current value of the signal lies outside the displayed range. Change the **Time and Voltage** parameters, preferably to their respective maximum values. Alternately, you may select the floating range using the **View - Floating Axes** command, which enables the station to choose the appropriate setting for displaying the signal.
- A cut that lies outside the signal is being displayed. Cancel the cut by using the **Unzoom** command (Ctrl + * or the icon).
- You have mistakenly set the same colour for both the curve and the background. Invoke **Properties** from the local menu and check the assignment of colours.

Data acquisition terminated prematurely.

Verify that the **Enable Autostop** has not been enabled in the **Method Setup - Measurement**.

Data acquisition has prematurely terminated or started repeatedly.

Probably a false start signal has occurred in the instrument where an external signal start has been enabled - contact your vendor.

Redeeming data from an analysis.

An emergency situation might occur during while acquiring data (power failure, computer malfunction, disk error, disk full etc.) causing an interruption. If you consider data from the interrupted analysis to be important, you can redeem it. First remove the cause of the underlying failure, and then invoke the **Data Recovery** command from the **Single Analysis** dialog. The interrupted analysis will then be saved as a valid chromatogram.

Disk full

If a requested operation cannot be performed because the disk is full, you have several options:

- Delete files that are no longer needed from any directories other than **YL-Clarity**.

Full version

- Archive or delete unnecessary chromatograms or entire projects. With the **Archive** command in the **Instrument** window, open the **Backup – Create Archive** dialog. Either archive the older chromatograms on another disk or erase them using the **Delete Selected Files** command.

10.3 Sequence

The Run command and icon are inactive (dimmed)

A Single Analysis is running. Check the status in the **Instrument** window. Single Analysis can be terminated from the **Single Analysis** dialog or **Data Acquisition** window.
See the first bullet of the chapter **10.2** - **Signal Displaying and Measurement**.

10.4 Processing and Displaying Chromatograms

A saved chromatogram has been "lost".

Chromatograms are either stored in the data or calibration subdirectory depending on the setting of the **Calibration Standard** parameter in the **Single Analysis** dialog. When selecting a chromatogram do not forget to display the corresponding subdirectory using the D or C icons.

A file contains an incorrect chromatogram

- Verify that the correct project has been selected, since files of identical names can exist in several directories.
- Maybe you have overwritten the original chromatogram using another one by entering the name of an already existing chromatogram in the **Chromatogram File Name** field (inadvertently ignoring the warning against possible overwrite). It is essential to keep in mind that, when the **Enable Overwrite** toggle in the **Single Analysis** dialog has been checked, newly created files will overwrite any old ones.

A completed chromatogram appears clipped from above or from below

- First verify that the chromatogram is not clipped only clipped on the monitor because of the **Properties - Axes - Range - Fixed** command.
- If the chromatogram is clipped from above, the detector signal was apparently cut off either because of a too low range setting in the **Range** item of the **Method Setup - Acquisition** dialog, or was already cut off in the detector because of an excessive preset range or the injection of an extremely concentrated sample.

- If negative voltage values are missing from the chromatogram, the **Bipolar** item in the **Method Setup - Acquisition** dialog was probably left unchecked; this item enables the measurement of a negative detector signal.

There is an excessive noise in the chromatogram

A measurement was possibly made using an unsuitable connection between the chromatograph and the computer (e.g., the detector cable of the **YL-Clarity** station was not shielded). Another reason might be a defective chromatograph or converter board. Check the chromatograph (e.g. using a recorder), or contact your vendor.

Small peaks exhibit a staircase shape or excessive noise

Possibly the full measuring range of the converter is not being utilised. If the voltage of the maximum peak of interest is at least 10x smaller that the voltage range set in the **Range** item in the **Method Setup - Acquisition** dialog, use a lower range.

Some peaks are not being detected

- Check whether the limiting integration conditions are improperly set using the **Rejection** item in the **Integration** tab of the **Chromatogram** window. These parameters are included in the method file and might even prevent integration of correct peaks if the selected method is inappropriate.
- If you use the integration algorithm with the default values (*Peak Width* = 0.1 min., *Threshold* = 0.1 mV), the very narrow peaks occurring at the beginning of analysis might be ignored. Try reducing the **Peak Width**. If this leads to the detection of many small, spurious peaks, set the **Threshold** to a value higher than the height of these spurious peaks. It must be stressed that the detection of peaks always depends on an interplay of the above two parameters, and changing only one of them not always produces the expected results (see Chapter **4.2** for additional details).
- If none of the above two remedial measures was successful in recognising some undetected peaks, the peaks involved are probably highly distorted so that their shape fails to satisfy the elementary conditions for peak detection. In this event use manual integration (**Chromatogram - Peak - Add Positive (Negative)**).

Too many peaks are detected

For a very noisy signal the algorithm might erroneously interpret the noise as a high number of small peaks. Working with such chromatograms is very confusing and the speed of all operations decreases dramatically.

- Increase the value of **Threshold**.
- Make the chromatogram more lucid by reducing the number of detected peaks using the **Rejection** command to appropriately set the integration conditions.
- In some instances it might be advisable to ban undesirable peaks using the **Baseline - Lock** command.

Incorrectly detected peaks

- When the **Threshold** value is too high, the beginning of some peaks might be placed too high on the leading peak edge. This can be corrected using the **Chromatogram - Peak Start** command. An alternative automatic remedy may be tried by entering a lower value in the **Threshold** field.

- When the **Threshold** value is too high, the narrow peaks may not be detected or a group of unseparated peaks may be integrated as a single peak. If this happens, decrease the value of the Peak Width parameter. With very narrow peaks it is advisable to verify that the chromatogram was not measured with a too low sampling rate (**Sample Rate**). E.g. when the chromatogram has been measured using a 10 Hz sampling rate, the decreasing of the **Peak Width** parameter under the value 0.07 min will have no effect. It is then necessary to measure the chromatogram again with an increased sampling rate.
- If the **Peak Width** parameter is too low, a group of peaks might be separated (the peaks in the group are not separated by a vertical line). If this is the case, raise the value of the **Peak Width**.

In general, the width of detected peaks (measured as the distance between the peak beginning and end) is proportional to the value of the **Peak Width** and inversely proportional to the value of the **Threshold** (see Chapter **4.2** - **Processing the Analysis** for additional details).

10.5 Chromatogram Modification

Added peaks or other chromatogram modifications have been "lost"

- You have probably failed to save the chromatogram after effected modifications.
- The integration table was mistakenly deleted or replaced by another one.

The "manual integration" procedure

In the event that manual integration commands have been invoked (**Chromatogram - Peak Add Positive (Negative)**), keep in mind that the manually added peaks will be stored exclusively in the integration table, just like all other chromatogram modifications.

How to shift the peak apex

As the peak apex location is automatically determined, no instruments will be available for shifting it. If it is still necessary to shift the peak apex to some other location, use the procedure described at the beginning of chapter **5.4.2** - **Peak Modification** on page **43**.

Dividing the chromatogram into regular integration areas (slices)

In connection with some types of data evaluation it is necessary to divide the chromatogram into segments of equal length and integrate them separately. The simplest way to achieve this is to forbid all existing peaks across the chromatogram using the **Baseline - Lock** command then divide the chromatogram into individual segments by repeatedly invoking the **Add Positive (Negative)** command and "tune up" the segments by editing the integration table. In some instances the commands for baseline modification may be needed.

The peak beginning/end cannot be shifted to the requested location, or the required baseline modification cannot be accomplished

A command aimed at baseline or peak modification will sometimes not conform to the user's desire because the algorithm employed for automated baseline modification will not allow it. The reason for this is that the station has detected an attempt that would cause the signal to cross the baseline and so it automatically shifts the point in question out of the way.

A new peak cannot be added

There was probably an attempt to add a new peak to an area occupied by the apex of another peak or to the region of tangential separation.

Cancellation of a command in the integration table had unexpected consequences

All of the commands involving baseline or peak modification, including those that do not have the required effect, are incorporated in the integration table. At the moment a command is cancelled, the originally ineffective commands may assert themselves. It is therefore recommended to maintain only functional commands in the integration table. In this manner the table will also be kept within manageable limits, a feature that will effect the speed of additional modifications.

10.6 Calibration

Some peaks have not been calibrated

New peaks can be added to an already calibrated file only by using the **Add Peak** or **Add Group** commands but not by using the **Add All** command. The latter only calibrates all peaks from the calibration standard for an empty calibration file; in other instances the command only calibrates the already existing peaks.

A peak has been erroneously calibrated as a new compound.

The deviation in the retention time of the affected peak exceeds the size of the identification window. Increase the values stored in the **Left (Right) Window** items or, alternately, use the reference peak method (see Chapter **6.13.1** - **"Reference Peak" Method** on page **63**).

Note: *When applying the reference peak method keep in mind that the modified retention time of a compound might differ significantly from the retention time actually measured. Thus, also if two original retention times are identical, the peak identification could fail because the modified retention time may wander outside the limits given by the identification window.*

Neither the calibration curve nor the corresponding calibration equation is displayed

- The **Curve Fit Type** item is set to *Free Calibration*. (The curve fit for new compounds is set using the **Curve Fit Type** parameter in the **Calibration Options - Defaults** dialog.)
- The system was unable to compile the calibration equation for the given type of curve fit. Change the type or normalise all amounts (e.g. by dividing/multiplying all values entering the calibration by 100 and then specify the **Scale Factor** = 100 or 0.01 in each affected chromatogram).

10.7 Calibrated Calculations

The requested type of calibrated calculation was not used

If the required type of calculation is not specified in the **Results** table, all the conditions that underlie its use have probably failed to be satisfied. See Chapter **6.3.3** - **Internal Standard Methods - ISTD** on pg. **52** and the **Reference Guide** for additional details.

The following are the most often encountered underlying errors:

- Use of the incorrect calibration file or too narrow identification windows.
- For an **ISTD** calculation the calibration file must contain the compound marked *ISTD*.
- In **ISTD** calculations with different amounts of internal standard when it has either been set in only an unknown sample or only in the calibration file. The station will then not be able to recognize whether it is missing from one or is surplus of another. Therefore, YL-Clarity would rather choose an uncalibrated calculation instead of an incorrect variant of the ISTD calculation.

- In **ISTD** calculations with the same amount of internal standard when it has either been set in only an unknown sample or the calibration file. The station is then not able to recognize whether it is missing from one or is surplus of another. So YL-Clarity would rather choose an uncalibrated calculation instead of an incorrect variant of the ISTD calculation.

The type of a peak is displayed as Free in the Results Table

- The free calibration has been used in the **Fit Type** item of the relevant compound. This means that the amount of the relevant compound has not been read off the calibration curve; instead, the global response factor –(**Resp. Factor**) from the main calibration table was used.

11 YL-Clarity Files and Directories

Since the chromatographic station uses a relatively large number of directories and files of various types, and moreover these can be shared in several windows, it is prudent to present an overview.

11.1 Directories

The **YL-Clarity** station can be installed in any directory on any hard disk. After an installation has completed, the main directory will contain the following fundamental files:

CLARITY.EXE	The executable program of the YL-Clarity station.
Clarity Lite.EXE	The executable program of the YL-Clarity Lite station.
*.DLL	Dynamically loaded auxiliary libraries, that contains in particular modules for data acquisition and direct chromatograph control.
*.HLP, *.CNT, *.GID	Online help files.
*.DTA	Data files of simulated analyses used in the demo version.
CLARITY.PSW	The file that summarises the access rights of all users including their passwords.
CLARITY.CFG	The configuration file of the station.
CLARITY.DSK	A default station desktop file.
*.DSK	A station desktop files of individual users.
*.TXT	A text file that contains topical information.

The main directory contains the following subdirectories:

COMMON	A subdirectory that stores common methods and report styles.
PROJECTS	A subdirectory that contains a list of all projects.
BACK	A subdirectory with backup copies of configuration files of the previous version (after updating the station).
DOCPDF	A directory with an electronic version of all manuals in *.PDF format.
CB20, INT7, UPAD, SENTINEL	Directories with backup copies of PnP device drivers.
IMAGES	A directory with symbols of the selected chromatographs
SOUNDS	A directory with the default sounds assigned to selected events.
TMP	The directory for storing temporary data during acquisitionand backup copies of the last two measured chromatograms from each instrument.
WORK	The basic project directories, assigned to one station instrument.

Full version

LOG	A directory with the station audit trail files.

Each project directory can contain the following files:

*.MET	Template methods.
*.SEQ	Sequence files.
DATA	Data subdirectory containing the following files:
*.PRM	Chromatograms
CALIB	Calibration subdirectory containing the following files:
*.PRM	Calibration standards
*.CAL	Calibration files

A more detailed description of the structure of subdirectories can be found in Chapter **13** - **Working with Directories and Projects** on page **91**.

11.2 Files

11.2.1 Chromatograms (*.PRM)

Each chromatogram contains the following:

- A header that specifies the date and time of an analysis, name of the analyst and the parameters of the sample.
- Original raw data of the whole analysis from up to four detectors.
- Chromatograms from up to four detectors with the originally detected baseline
- Method describing the progress of a measurement, its modifications and evaluation.
- A link to the name of the calibration file being used.
- Storage of all methods including the calibration files from all the states in which they were ever saved, printed or exported.
- Descriptive labels and lines (only those attached to the signals).

Full version

- A record of all chromatogram changes – **Chromatogram Audit Trail**
- An electronic signature.

11.2.2 Template Method Files (*.MET)

Each template method file specifies the conditions under which the chromatogram will be measured and evaluated.
The content of the template method file is copied to each chromatogram at the moment an analysis is terminated.
The Template Method File contains the following:

- Indicative information (the column and mobile phase used, the type of detector employed and its settings, etc.).
- Parameters of the input converter, detector selection and a table for controlling the control outputs according to defined events for up to four detectors.
- An integration table for up to four detectors.
- The name of the calibration file and calculation parameters.

Full version

- The parameters used for direct chromatograph and autosampler control (optional).

11.2.3 Calibration Files (*.CAL)

The calibration files contain calibration curves for a practically unlimited number of compounds for up to four detectors.
Any calibrated chromatogram contains a link to the calibration file and also a copy of all the calibration files that where present at the moment of saving, printing or exporting changed comparing to the last saved version.

Full version

Note: *The calibration file also contains a record of all the changes performed:* ***Calibration Audit Trail****.*

11.2.4 Sequence Files (*.SEQ)

The sequence files enable one to perform a series of measurements. Each sequence file contains the relevant sequence table and some auxiliary parameters. Each line of the sequence table in fact describes the method of measurement and evaluation to be used for one or more injected samples.

Full version

Note: *The sequence file also contains a record of all performed changes in the **Sequence Audit Trail**.*

11.2.5 Report Style Files (*.STY)

A report style decides what will be printed and how. The following information can be printed as part of a report:

- The measurement description and conditions.
- The chromatograms and calibration curves.
- Tables of results.
- Sequence tables.

The user can also:

- Select page characteristics (borders, numbering) and font.
- Define the headers printed on individual pages.

The station is supplied with a number of pre-defined report styles. The user can modify them at will or create his or her own.

11.2.6 Password File (CLARITY.PSW)

Full version

Access rights of all users are stored in this file, provided the station operates in the protected mode. To change the access rights invoke the **User Accounts** command from the main YL-Clarity window. Refer to Chapter **12.2** - **User Accounts - Protected Mode** on page **88** for additional details.

11.2.7 Configuration File (CLARITY.CFG)

This file stores the current settings, especially the hardware configuration of the YL-Clarity station.

Full version

Note: *A backup copy - BACKUP.CFG - is created during station installation. In the event the CLARITY.CFG file is for any reason damaged, you will be notified and the backup copy will automatically be used.*

It contains:

- The number of displayed instruments and their names.
- The list and configuration of the installed A/D and D/A converters, modules for direct control of chromatographs, pumps and autosamplers.
- Assignment of the above devices to individual instruments.
- Configuration (appearance) of the main **YL-Clarity** window.

11.2.8 Desktop File (CLARITY.DSK)

The CLARITY.DSK file contains the following:

- Settings referring to size, visibility and location of all non-modal (non-dialog) windows of the station.
- A configuration of all graphs and tables.
- A user-specific configuration of the station, available from the **User Options** dialog.
- Name of the project to be opened (.prj).
- Print styles. These are not dependent on the project, you may use the same print style in several projects.

The full version features: Full version

- In the protected mode any user can use his or her own, dedicated DSK file. The filename is specified in the **Desktop File** item of the **User Accounts** dialog.

11.2.9 Archive Files (*.DGZ) Full version

The *.DGZ archives are files to which all the archived data are compressed. *.DGZ archive is not the same as *.ZIP archive in the fact that files cannot be added to it. Instead, the files from the archive have to be extracted, the old archive must be deleted and finally a new one with the original and added files should be created.

11.2.10 Project Files (*.PRJ)

These files contain the information on the directories to which the user files will be stored, as well as on recently opened files.

11.3 File Sharing

The **YL-Clarity** station allows files to be shared with another station. Sharing means that the station that first opens the file can modify it. In all other stations the file will be opened only for reading (indicated by an READ ONLY inscription after the filename).

How to facilitate file sharing over a LAN network?

For the occasional display of individual files from other YL-Clarity stations it is sufficient to use the standard **Open File** dialog, manually navigate to **My Network Places** and to then select the desired computer.

Full version

For a regular access of files over the network it is better to use the **System – Directories** command from the main **YL-Clarity** window. In the displayed dialog use the ... button next to the desired instrument to select the main directory of the distant station. When opening this instrument you will only have to select the desired project.

Note: *Files cannot be shared among instruments within a single station. The only exception is files of the report styles, which can be shared.*

Note: *Since files are stored in project directories, the same name of a file that is open in several instruments does not necessarily mean that the files are identical, since in most instances each instrument has its own project directory. The same holds true of chromatograms in the data and calibration subdirectories.*

11.4 File Locking

In some instances the ability of the station to work with certain files is restricted to prevent a collision that may corrupt measured data.

- The parameters of the current template method from the tab in the **Method Setup** – **Acquisition**, **LC**, **GC** or **AS** dialogs cannot be modified while an analysis is in progress.
- While a sequence is in progress, all already measured calibration files, including the one in progress, will be locked.

11.5 Marking Changes in a File Not Yet Saved

For most files the *MODIFIED* notice after the filename indicates that the effected modifications have not yet been saved. The station always alerts to situations where such changes may be lost (e.g., when the station is closed or when a new file is being opened), and will offer the option to save the changes.

12 Station Settings

Full version

In the interest of extensive utilisation the station contains a number of commands that allow settings to be customised. These features include everything from selecting the number of instruments and connected detectors, to creating users' access rights, customising the desktop appearance and configuring the settings of individual instruments and current projects.

12.1 System Configuration Setting

Invoke the **System - Configuration** command from the main window to display the system settings of the **YL-Clarity** station saved in the CLARITY.CFG file. A foundation set-up will have already been made during the installation procedure.

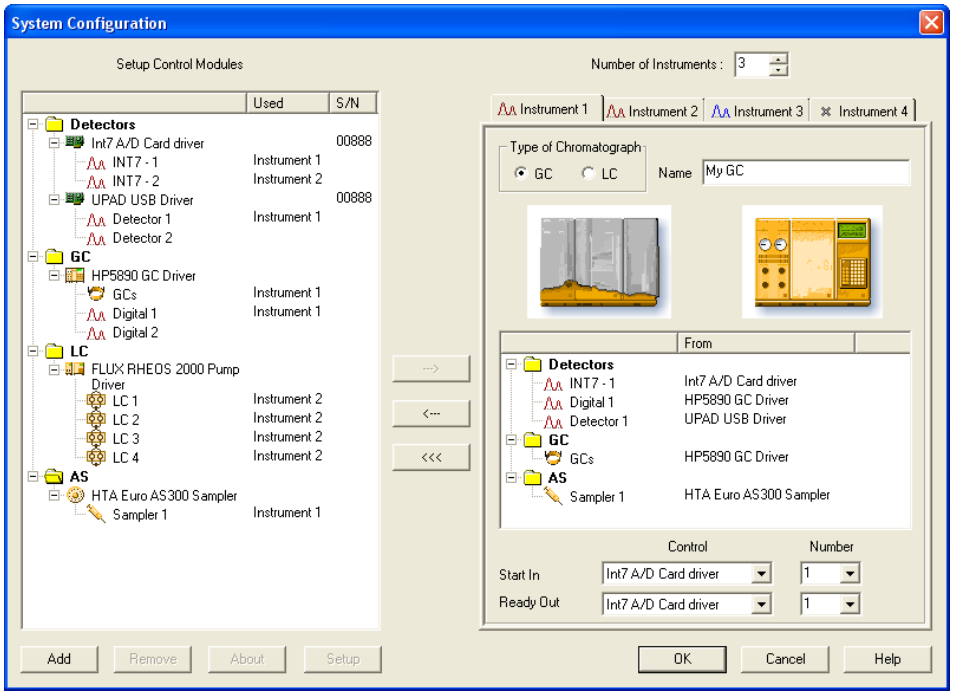


Fig. 38. The System Configuration dialog

The command opens the **System Configuration** dialog. Using this command will display a list of all installed and configured devices and control modules in the left and the configuration of individual instruments in the **Instrument 1 – 4** tabs in the right.

How to add a device to the left list?

Below the list (**Setup Control Modules**) is the **Add** button, which displays the list of all currently available device drivers in the **Available Control Modules** dialog. The dialog contains all drivers that you have installed including those you can't use due to licenses not purchased. Click the **Add** button or double-click the name of a device to transfer it to the list.

Note: *Being listed in the file does not necessarily imply that the device is present, correctly installed or properly connected.*

The configuration dialog of the device involved will open first. If an A/D or D/A converter is involved the station will attempt to find the converter during the set-up. If the attempt to communicate with the converter has been successful, the configuration dialog of the converter is shown, allowing the user to enter custom signal names and units. Then the device is shown in

the left-hand list of the **System Configuration** dialog and its free channels can be assigned to individual instruments of the station.

Note: *Communication with modules for direct control of chromatographs, digital pumps and autosamplers will only be checked when the instrument from which the user would like to control these devices is being opened. Accordingly, during the configuration process, one cannot establish whether the communication set-up is correct.*

How to assign individual devices to station instruments?

Switch to the corresponding instrument tab in the right part of the **System Configuration** dialog.
In the **Setup Control Modules** list (on the left) select the desired device and add it to the instrument using the ---> button or the mouse to drag and drop the device.
Each station instrument you wish to use for measuring chromatograms must have the correct signal source assigned:

- Channel(s) of the A/D converter (internal INT5/INT7 or external U-PAD).
- A digital output(s) from the chromatograph to which an available control module has been connected (e.g. HP 6890, etc.).

How to remove the device?

Select the device to be removed from the list in the corresponding **InstrumentX** tab of the **System Configuration** dialog.
Use the <--- button or drag and drop with mouse to remove the selected device from the displayed instrument.
Use the <<< button to remove all devices from the displayed instrument.

INT5 board setup

The ISA board of A/D converters (INT5) is not equipped with a Plug and Play system and so the configuration has to be done manually. Specify the connection between **YL-Clarity** and the A/D converter board **Interrupt** and **Base Address** items. The values set here must coincide with the setting of the jumpers on the converter board, otherwise data acquisition will be inoperative. It is recommended that you note these parameters, e.g., in the corresponding table provided at the end of the **Reference Guide**.

12.1.1 Number of Instruments

Up to 4 instruments may be set in the **No. of Instruments** item regardless of the number of instruments in your version. The excess instruments (so called Offline instruments will be fully functional for evaluating analyses that are proceeding in other instruments (although not for data acquisition).

12.1.2 Description of Instruments and graphical symbols

To make the work with the station more comprehensible the user can assign a name to each instrument (using the **Name** field), select the type of attached chromatograph (in the **Type of Chromatogram** item) and assign arbitrary images to represent opened and closed chromatographs by clicking the images below the **Image for Closed (Opened) Chroamtogram** inscriptions.
Once the configuration is saved, the main **YL-Clarity** window will display the assigned names and the symbol of each instrument.

12.2 User Accounts - Protected Mode

The station can operate what is known as the protected mode. Advantages of the protected mode include the following:

- The data and station configuration are protected against intervention from unauthorised or inexperienced persons.
- The station can be locked during a proceeding measurement to protect it from being used by unauthorised persons.
- Several users can work with the station simultaneously and independently,
- Customised settings can be saved for each user.
- Ability to electronically sign a chromatogram

Invoke the **System - User Accounts** command from the main **YL-Clarity** window to open the **User Accounts** dialog where changes can be made and the protected mode set.

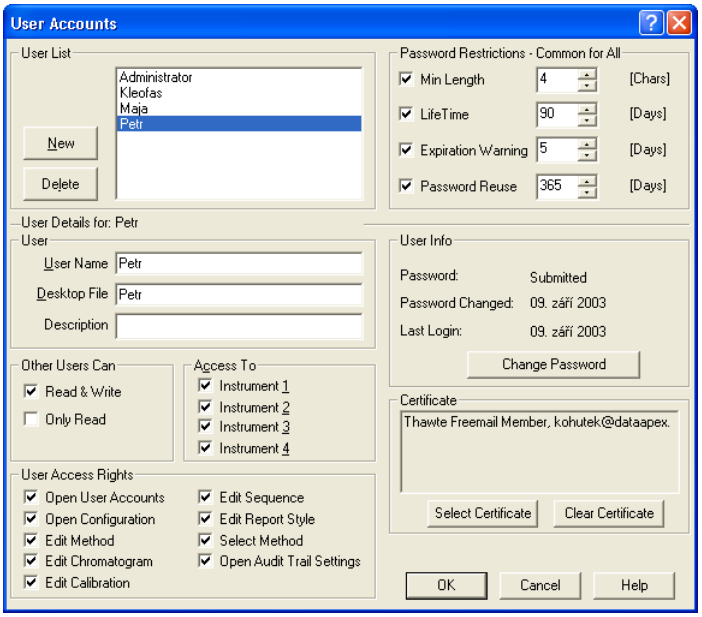


Fig. 39. The User Accounts Dialog

How to establish a new user account?

Open the **User Accounts** dialog.
Press **New**.
Fill in the following items:

User Name

The name of the analyst entered here will be stored in all files created by that user.

Desktop File

The name of the customised desktop file is entered here. Several users may share the file.
If no name is entered, the desktop file created by copying the CLARITY.DSK file will have its name entered in **User Name** field.
Each newly created desktop file is a copy of CLARITY.DSK file.

What activities should be banned/allowed?

Once a new user's account is established, that user can enjoy all rights. Some access rights or rights for modifying specified parts of the station can be banned in the **User Access Rights** section. It is advisable to ban standard users from accomplishing the following activities:

- Access to setting user passwords - **User Accounts**
- Access to system configuration of the station - **Configuration**
- Access to setting the station log output – **Audit Trail**.

On the contrary, any ban on chromatogram modification (**Chromatogram)** is unnecessarily restrictive.

How to allow certain users to only work with certain instruments?

It is possible to allow certain users only to work with certain instruments by using the **Access to** item.

How to restrict certain users from using or updating files?

Permit files to only be read using the **Read Only** item or to be read and updated using the **Read/Write** item. If no item is checked your files will be inaccessible to other users.

Under which conditions do files cease to be protected?

- Files are protected as long as your account exists and cease to be protected once the mode has been changed to the unprotected state.
- Files read into another **YL-Clarity** station where you do not have an account will be accessible.

How to cancel an existing account?

Select the name of the user to be eliminated from the list in **User List**.
Invoke the **Delete** command. (It is still possible to cancel elimination from the list by striking the **Cancel** button.)
All files created by the eliminated user will then be accessible to all users after the station is run for the next time.
If all users are eliminated the station will pass to the unprotected regime when run for the next time.

How to change the access rights of a user?

Select the name of the user whose rights you wish to modify from **User List**. All items will then refer to that user and can be changed.
The effected change may still be cancelled using the **Cancel** command.

How to transfer the station to the unprotected mode?

Eliminate all users one by one from the list using the **Delete** command. When the window is then closed the station will be unprotected and files with originally restricted access will now be accessible.

What if you forget the password?

In this instance transfer the station to the unprotected mode by copying the CLARITY.PSW file from the PGM directory on the installation disk to the main station directory. This remedy however cancels all user access rights previously set.

12.3 Instrument Locking

In the protected mode any open instrument can be locked to protect it against unauthorised intervention during the user's absence. To lock an instrument, invoke the **Lock** command from

the **Lock** menu in the main **YL-Clarity** window. All activities (running a sequence, printing a report, batch processing, etc.) will continue unabated in the locked instrument.
Unlock the instrument by either repeatedly invoking the **Lock** command or by clicking on the chromatograph symbol and entering the password of the user who opened that instrument.

12.4 User Settings

The station automatically saves the settings of visibility, size and location of all non-modal windows, the configuration of all graphs and tables, and all user-specific settings available from the **User Options** dialog.
The settings are saved in the CLARITY.DSK desktop file. In the protected mode the settings are saved in the file specified in **Desktop File** field for each user listed in the **User Accounts** dialog. Thus, in the protected regime each user can have his or her station appearance settings customised.
The settings of all windows, graphs and tables are instrument-specific.
The parameters specified in the **User Options** are common to all instruments used by a user.

13 Working with Directories and Projects

The station enables a base directory to be assigned to each instrument as well as for the storage of analyses in different projects.

13.1.1 Instrument Directory Selection

Invoke the **Directories** command in the **Main station** window to specify a different base directory for storing projects for each instrument. The above command is especially suitable if the **YL-Clarity** station is a part of a computer network where either several stations or several "**YL-Clarity Offline"** evaluation programs are operative.

By default, all instruments use the main station directory, usually C:\CLARITY. Instrument directories are stored in the CLARITY.CFG configuration file.

At least one project directory is assumed to exist in the instrument directory; the former is described in PROJECT subdirectory. If no instrument directory, no PROJECT subdirectory and no project directory exists you will be queried as to whether or not you wish to create the corresponding directory or project.

13.1.2 Projects

A project is an ensemble of different analysis data and accessories, used as basic organisation unit for sorting data and auxiliary files.

For example, it may be used for sorting data of certain compound determination, for different series of samples, or for data from certain time period.

Whenever an instrument starts, it opens that project which was used the last time by any user on this instrument. Projects contain paths to last opened chromatograms, calibrations, reports, sequences and methods. When a project is opened by any user, these last opened files are opened automatically.

***.prj file:**

The project files are named as *.prj. They are contained in the PROJECT directory, situated in the working directory (by default "CLARITY"). The main function of the project file is to specify another directory, having the same name and containing relevant stored data.

Project directory:

The project directory contains template methods, sequence files, report styles and also two subdirectories, DATA and CALIB. The data subdirectory stores chromatograms, the calibration subdirectory stores calibration standards and calibration files. To switch between the calibration and data subdirectories when selecting files click either of the  and  icons in the **File Open Chromatogram** dialog.

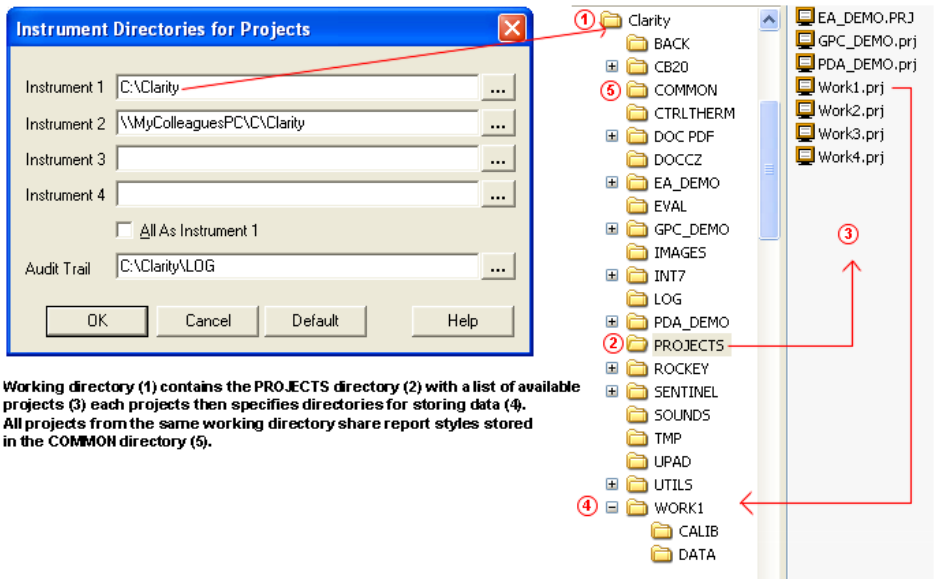
By default, files from the current project are displayed in each instrument. Use the icons and commands from the **File Open** dialog to select a file from any other directory.

To facilitate sharing files common to several projects (e.g. report styles) the station contains the COMMON directory. Click the  icon in the **File Open** dialog to switch to the COMMON directory.

Instrument directories:

There is a possibility to set different working directories for different instruments. This can be done in the **Instrument Directories for Projects** dialog, which is opened by the **System**

Directories command in the **YL-Clarity** window. The directories specifications are stored in configuration file (clarity.cfg) and are common for all users.



Working directory (1) contains the PROJECTS directory (2) with a list of available projects (3) each projects then specifies directories for storing data (4). All projects from the same working directory share report styles stored in the COMMON directory (5).

Note: *In the above image the Instrument 2 shares projects with another YL-Clarity station that has been installed on a networked computer named MyColleaguesPC.*

Each item specifies the working directory for the corresponding instrument. If an item is left blank, the working directory will be set to the directory from which the executable file CLARITY.EXE was run (C:\CLARITY by default). This directory may be set any time by the command Default.

How to establish a new project?

Create a new project in the **Instrument** window using the **File – Project** command, which opens the **Project Setup** dialog, and in this dialog press the **New** button.

After first entering the project name you may then modify the names of the data and calibration subdirectories.

How to store chromatograms and calibration standards in the same directory?

Select the same name for the two subdirectories in the **Project Setup** dialog (the **Analysis** and **Calibration Subdir** items).

How to open another project?

Select a new project using the **File - Project - Open** command. A project can be opened in several instruments and can be shared by other **YL-Clarity** programs across a computer network.

14 Backing up and Restoring Files and Projects

Full version

The **YL-Clarity** station provides tools for backing up and restoring all data and working files.

14.1.1 Backup

The **File - Archive** command from the **Instrument** window is earmarked for backing up data. When invoked the command will open the **Archive** tab of the **Backup** dialog.

How to select the type of files to be archived?

The type of files to be archived is specified using the **File Type** item. Also in addition to all the **YL-Clarity** files, entire projects can be archived (i.e., all files identified in a specified project directory and all its subdirectories).

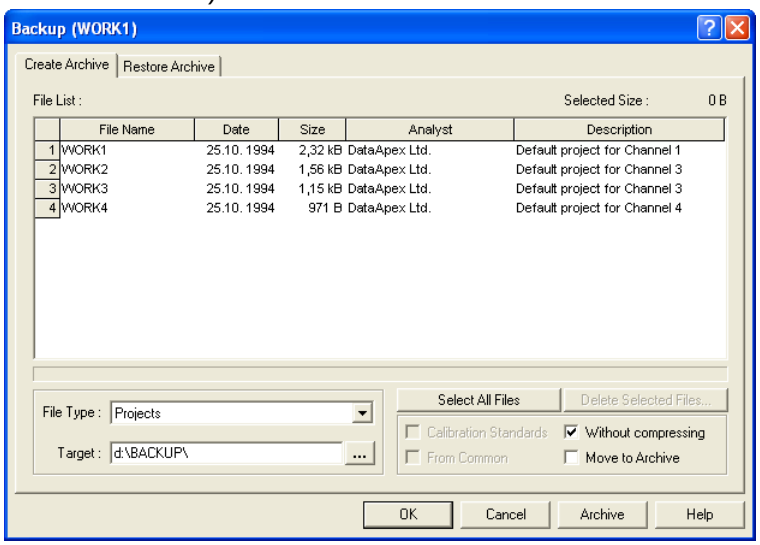


Fig. 40. The Backup – Create Archive Dialog

How to select files to be archived?

The list shown in the upper part of the **Archive** tab contains all the files of the selected type from the current project.

Select a file by clicking the filename. Several files can be selected by clicking their names one by one while holding down the Ctrl key.

The meaning of the **Select All Files** button should be self-evident.

Where will the files be archived?

Specify the destination (another directory, disk or computer) in the **Target** item. The path can either be entered directly or selected using the ... button.

In what format are files stored in the target location?

If the **Without Compressing** item has been checked, files will be stored unchanged as individual files, otherwise all archived files will be compressed and stored as a single file under a selected name.

Will the files be copied or moved?

If the **Move to Archive** item has been checked, the file(s) will be moved to the destination specified in the **Target** field (i.e., deleted from the original directory).

What is the total size of files to be archived?

The overall size is indicated above the list of the selected files, in the **Selected Size** item.

How to sort files in the list?

Double-click the header of each column to sort the entire table according to that column. Double-click again to sort the files in the reverse order.

Backing up calibration standards

If chromatograms are to be archived, the **Calibration Standard** item displays the contents of the calibration subdirectory.

Archiving files from the COMMON directory

Check **From Common** item to archive files that are stored in the COMMON directory.

How to delete files?

Invoke the **Delete Selected Files** command. This command cannot be reversed from within the **YL-Clarity** station!

14.1.2 Restoring Files

The **File Restore** command from the instrument window restores files from any directory to the current project. When invoked, the **Restore Archive** tab from the **Backup** dialog opens. This is very similar to the **Create Archive** tab.

To which location will be files restored?

The **Restore** command always restores files to the current project whose name is shown in the title bar of the **Backup** dialog.

From which location will be files restored?

The source location (other directory, disk, or computer) can be specified in the **Source** item. Either enter the path directly or use the ... button to browse.

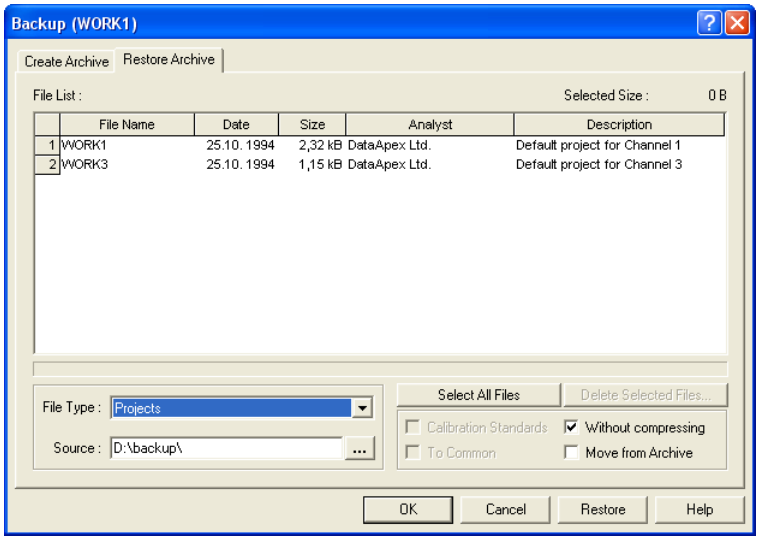


Fig. 41. The Backup – Restore Archive dialog.

The other items and commands are analogous to those listed in the **Archive** tab described in Chapter **14** - **Backing up and Restoring Files and Projects** on page **93**.

15 Glossary

The following list of often used or differing terms is providing to prevent misunderstandings and errors .

21 CFR Part 11

This is a directive stipulating the conditions under which a company may use electronic records and signatures. The directive is mandatory for companies that use computer system designed for manufacturing or distributing products that are subject to regulation by the FDA (known as, “regulated products”).

Access rights

A system that governs the activities that specified users are allowed to perform. Among other things, a user may be restricted in their authorisation to change fundamental station settings, access certain instruments, inspect or change the data of other users, etc.

Active chromatogram

The chromatogram name that is displayed in the header of the **Chromatogram** window. All data being displayed and operations performed will only relate to this active chromatogram. The name of the active chromatogram is highlighted in the key by bold letters.

Active chromatogram signal

When performing a multi-detector measurement, each chromatogram file may contain a record from up to four detectors (this is what we call “signals”). The active signal in the chromatogram is the signal whose name is being displayed behind the name of the chromatogram in the window header and header of the tables (divided by a hyphen).

The name of the active signal together with the name of the chromatogram will be highlighted by bold letters in the legend of the graph.

Active calibration signal

When performing a multi-detector measurement, each calibration file may contain calibration curves for up to four signals.

The active signal (i.e. its table or curve) of the calibration will be highlighted in the header of the calibration table or curve by its name. At the same time, all values that are signal specific will be displayed in the same colour as the active signal.

Active detector

A detector whose measurement and calculation parameters are displayed in the **Acquisition** or **Calculation** tabs in the **Method Setup** dialog with the help of the **Select Detector** field. The field is only visible when performing a multi-detector measurement.

Calibrated group

A group of peaks calibrated as a single component.

Calibration file (Calibration)

Contains calibration curves and further data for calibrated calculations. When performing a multi-detector measurement, each substance will have its own calibration curves for all detectors.

Calibration standard

A chromatogram containing known amounts of some compounds that is used to calibrate/recalibrate at a specified calibration level.

Channel

Part of the converter that enables the independent collection of data from one single detector.

YL-Clarity Offline (Eval, Lock, Evaluation Version, etc.)

A version of the **YL-Clarity** station that, although otherwise fully functional, does not allow for data acquisition. This version utilises a protective key that is inserted in the printer or USB port of the computer.

Clipboard

A **Windows** tool that uses the **Copy, Cut** and **Paste** commands for the simple transfer of data between items, including those in other applications.

Closed window

A closed window is invisible and its activity has been terminated. A window is usually closed using the **Close** command (cf. **Hidden** window).

Configuration of the station

Sets the number of instruments and their allocation to the A/D converter, directly controlled chromatographs and autosamplers and pumps.

Data processing string

A series of operations comprising the entire procedure used for everything from processing data from an analysis to printing the report. This procedure is graphically displayed in the **Instrument** window using icons that represent the main commands.

Desktop file - extension DSK

A file used to store the size, location and appearance of all windows and parameters of the instruments.

Direct control of chromatograph (autosampler, pumps)

An integrated additional module for selected chromatographs (pumps and autosamplers) enabling the direct control and monitoring of selected parameters.

Electronic signature

An electronic signature is an analogy for doing to electronic documents what we do to paper ones and must fulfil the same function as a handwritten signature. Meaning that it is a similar process of marking a document for protection and that it must be unique, clear and ensure the immutability of the document.

File sharing

YL-Clarity enables file sharing between multiple stations. Any changes (saving) of such files are enabled only in the station that first opened it. Modifications performed with the shared file will take effect in the other stations only after the file has been reloaded.

YL-Clarity does not enable file sharing between instruments of a single station.

YL-Clarity does enable projects to be shared between multiple instruments of the same station.

Attention! *Using the same file name in multiple instruments at once does not mean that you are using the same file, because each instrument must have a different project directory. In other words it is not possible to share projects or files among instruments of the same station.*

GLP

Good Laboratory Practice (GLP) is an internationally agreed upon system for ensuring and monitoring the quality of laboratory work. This is verified and its fulfilment confirmed by the issuance of a certificate.

Hidden window

A window that is not visible or has been “hidden”. Its activity has not been terminated but rather suspended or is proceeding in the background. Click the minimise button  to hide a window (cf. **Closed** window).

Information table

A table in the **Instrument** window displaying the name, the measurement methods, and the identification of the measured chromatogram.

Instrument

(a) A part of the program designated to measure and evaluate analyses that share a common time base (from one chromatograph). The instrument is indicated by the **Instrument** window (see chapter **3.1.2** - **Instrument Window** on pg. **13**.), from which further windows can be opened, e.g. **Chromatogram**, **Calibration**, etc. Detectors and control modules can be configured into individual instruments (see).

(b) Sometimes also a chromatograph.

Instrument directory

The directory identified in the main **YL-Clarity** window for each instrument, where projects (i.e. project directories) are sought.

Integration Table

Constitutes a part of the method and contains a list of all modifications of the baseline or peaks that have been or will be affected in the chromatogram measured by that method.

Locked file (READ ONLY)

A file that can only be read and never modified.

Locked instrument

An instrument in the protected mode with locked control. Lock mode can be activated using a command from the **Lock** submenu in the main **YL-Clarity** window. An instrument is both locked and unlocked by the same password.

Main station directory

The directory where the executable file of the station (CLARITY.EXE) is stored (C:\CLARITY by default). The same directory contains the project directories, including the project directory PROJECTS, the common directory COMMON, and all configuration files.

Method file - extension MET

A template method file with a description of all parameters affecting an analysis.

Model method

A chromatogram method marked as **Model Method** that can be easily used with other chromatograms by invoking the **Copy from Model** command.

Multi-detector configuration (measurement)

The ability to measure, save and evaluate a single analysis by simultaneously using a signal from multiple detectors.

Password

A string of a maximum of eight characters that are necessary for working in the protected mode with the station.

Printout

The layout of individual parts of analysis results and the setting of parameters controlling the resulting report. The layout is defined by the employed report style.

Project directory

Used to store all working files of an instrument in which the homonymous project has been opened.

Project file - extension PRJ

The file specifies the directories in which all user files will be stored.

Protected mode

A regime that enables only authorised users (users who have an account assigned in the **User Accounts** dialog) to work with the station and access data.

Raw data file - RAW

A file used in previous versions of the CSW10 - 17 and for the external PAD unit containing non-analysed and non-adjusted data of the analysis. The CSW32 and YL-Clarity stations save raw data directly into the chromatogram file.

Report style

An outline determining which and how analytical results will be incorporated into a report and subsequently printed. Each report style will be stored in a separate report style file.

Report style file - extension STY

A file storing information that determines what to print and how to print it.

Sequence file - extension SEQ

A file that defines an automatic sequence of analyses.

Splitter

A resettable bar that divides certain windows (e.g., the **Chromatogram** or **Calibration** windows) into individual panes. The bar can be moved to change the size of individual panes.

SST

The **System Suitability Test** is an integrated module designated to validate the chromatographic system on the basis of evaluation of chromatograms obtained from the **YL-Clarity** station.

Station configuration

Determines the number and arrangement of instruments and their interconnection to the A/D converter board, directly controlled and description of connected detectors.

Status table

A table displayed in the **Instrument** window, containing the names of system files, the status of the analysis currently in progress, potentially the retention time and identification number of a sample.

System files

The decisive files for working with the station and individual data files: project, method, report style, sequence and calibration files.

Tabs

A tab is where several windows are "stacked". The system is frequently used in dialogs and also in the **Chromatogram** and **Calibration** windows. Click the corresponding tab to switch over to another tab.

Template method

A method file that serves as a template for new analyses. It is always stored directly in the project directory. Its name is displayed in the *Information Table* and its contents are always copied to the newly created chromatogram.

Toolbar

A block of icons that lead to commands. Each toolbar can be situated anywhere on the screen and be configured by accessing the **View - Customize** command in the window or by right clicking the mouse button to access the local menu.

Unprotected mode

A regime of the station that enables any user to work with the station and access its data.

Window title bar

Title bar is the upper band of each window. It is comprised a button to used activate the control menu of the window, the window name, and the minimise and maximise buttons.

16 List of Pictures

17 Index

YL-Clarity Extensions

PDA

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

YL INSTRUMENT CO., LTD.

1 PDA Extension

The **PDA module** is optional extension for the **YL-Clarity Chromatography Station** (from version **2.4**). Any Instrument within YL-Clarity station can use the **PDA Extension**.

PDA module is compatible also with **YL-Clarity EVAL** software.

The **YL-Clarity PDA Extension** is a tool that is used for processing data that has been acquired from selected photo diode detectors (PDA/DAD). Spectral data together with chromatograms add a third dimension to analytical data analysis.

The **YL-Clarity PDA Extension** expands the capability of **YL-Clarity Chromatography** software providing interactive spectral analysis, peak purity analysis and compound identification that is based on spectral library search. PDA data can be displayed in a set of optional views including 3D rendering.

1.1 Availability

The **PDA Extension** is an optional, fully integrated part of **YL-Clarity** data station. It can be ordered as a part of new data station or as an extension to existing data station (p/n **A29**).

1.2 Installation

The **PDA Extension** is enabled by appropriate user code entered during installation or later by using the **Help - User Code** command from the **YL-Clarity** main window.

Caution! ***PDA** mode is available only on **YL-Clarity Instruments** of **LC Type**.*

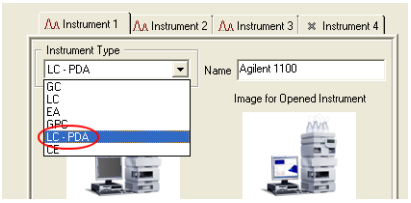


Fig. 1. System Configuration – Instrument Type

Set the type of **Instrument** to **LC-PDA**, open the **System Configuration** dialog and select the **LC-PDA** option in the **Instrument Type** group.

2 Key Features

- **Import/Export Data:** Spectral data can be imported/exported in ASCII text formats to or from the **YL-Clarity** software.
- **Reports:** Users can easily include PDA options such as data 3D Display, Isoplot, Spectra, Peak Purity and Library Search results in reports using the intuitive Report Setup Dialog.
- **Instrument Control** – A control module for Agilent 1100 DAD is available. Additional control modules for other PDA detectors can be developed upon request.

2.1 Basic Principles and Terms

- **PDA View:** The **PDA** window is customizable; up to four views can be displayed at one time (Any combination from the following views may be selected: Isoplot, Chromatogram, Spectral, 3D Display, Peak Purity, Peak Purity Spectra, Spectral Library and Spectral Search Results). The user can easily extract chromatographic signals from PDA data to determine the optimal detection wavelength for each peak.
- **PDA Method:** The YL-Clarity PDA method includes an option for **spectral library search** and **peak purity analysis**.
- **Spectral Library:** The **YL-Clarity** software compares the peak spectra with the spectra of an unlimited number of spectral libraries. Spectra stored in a **Spectral Library** include retention times and analysis parameters (optional). The **Spectral Library Search** can perform automatic identification of integrated/calibrated components (peaks). The library search may be constrained by the **RT Window** and by **Wavelength Range**. Either the **Least Square**, the **Weighted Least Square** or the **Correlation Method** is used for calculating library search matches. A **Background Correction** option is also available.
- **Peak Purity:** This analysis helps to discover hidden impurities. **Peak Purity** test is applied to all integrated/calibrated peaks in the active signal. Purity is calculated from *5* or *all spectra* within the peak. The similarity curve is displayed in the **PDA** window. **Peak Purity** analysis can be optimized by setting custom preferences relating to the purity threshold, wavelength restriction and absorbance threshold.

3 PDA Extension description

After installation, new functions of the **PDA Extension** will be available. Only changed or additional features to the standard **YL-Clarity** mode are listed and described here.

3.1 Instrument window

In the **Instrument** window the new **Method – PDA Method** command opens the **Method Setup – PDA Method** dialog.

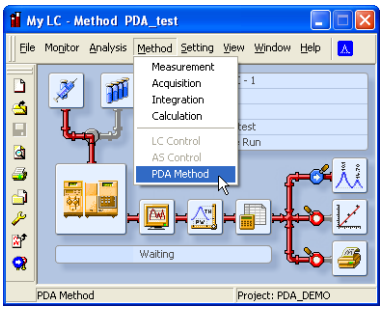


Fig. 2. Instrument window

3.2 Method Setup – PDA Method

In the **Method Setup** dialog, new **PDA Method** tabs is available.

Peak Purity Options

Restrict Wavelength Range

Compares the spectra only in specified range

Purity Threshold

Restricts spectra with match factor bellow this value from the **Peak Purity** average value calculation.

Absorbance Threshold

Defines the start and end spectrum for peak purity evaluation in % of detected peak height.

Available values: 1 – 100%

Used Points

All spectra or only the five significant points (start, inflexes, apex, end) are used for peak purity value. The Absorbance and Purity Thresholds are not used in Five point calculations.

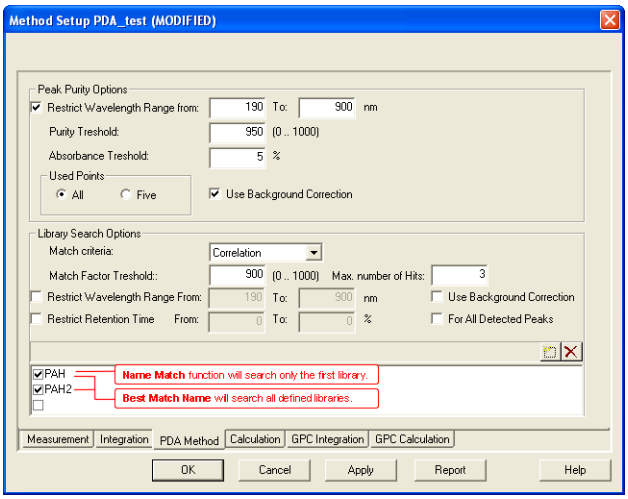


Fig. 3. Method Setup

Use Background Correction

The baseline (background) for individual wavelengths is interpolated between peak start and peak end points.

With **Background Correction** the spectra are measured against this surface.

Library Search Options

Match Criteria

Correlation, Least square, Weighted least square - selection of different types of Match factor calculations.

Match Factor Threshold

Only hits with match factor above this value will be displayed

Max. Number of Hits

Limits number of displayed spectra found by matching with the other criteria

Restrict Wavelength Range

The spectra comparison will be limited to the specified range (the whole overlapping range is compared, when not specified.

Restrict Retention Time

Limits the found spectra only to those with RT within specified range (in % of peak RT)

Use Background Correction

The baseline (background) for individual wavelengths is interpolated between peak start and peak end points. With **Background Correction** the spectra are measured against this surface

For All Detected Peaks

Performs the library search for all detected peaks when checked, otherwise only identified peaks are evaluated.

3.3 Chromatogram

The **Chromatogram** window is enhanced by PDA related features in the **Results**, **Summary** and **Measurement** tabs.

3.3.1 Results

The **Result table** is in PDA mode enhanced by the following columns: **Peak Purity**, **Name Match**, **Best Match Name**, **Best Match**.

It is possible to change the order of the columns or hide some of them using the **Edit - Setup Columns** command.

Peak Purity

Displays the **Peak Purity** value of the peak.

Name Match

Displays the match factor of the spectrum that was found in the first used **Spectral Library** based on the name of the Peak from the **Calibration Table**.

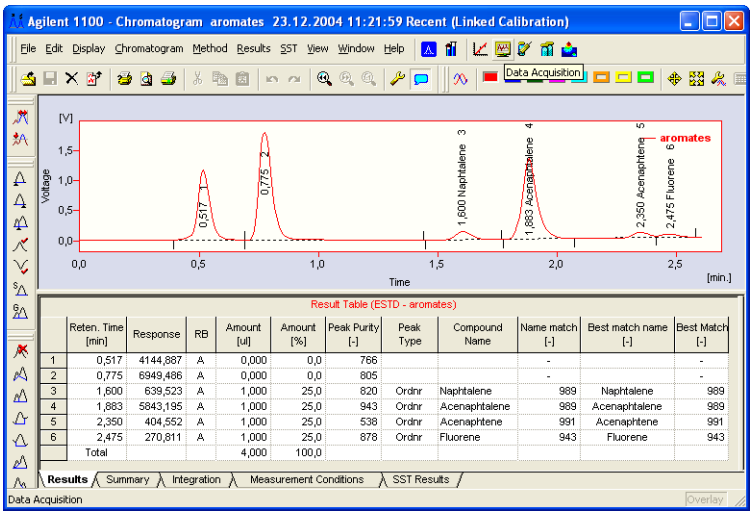
Caution! *If there are multiple libraries specified in the PDA method (**Chromatogram – Measurement Conditions – PDA**), the **Name Match** will search only the first **Library**.*

Best Match Name

Displays the name of the spectrum found according to the method Library search options.

If there are more libraries specified in the PDA method (**Chromatogram – Measurement Conditions – PDA**), **Best Match Name** will search ALL libraries.

The library name is displayed as a tool tip over the result table cell.



	Reten. Time [min]	Response	RB	Amount [ul]	Amount [%]	Peak Purity [-]	Peak Type	Compound Name	Name match [-]	Best match name [-]	Best Match [-]
1	0,517	4144,887	A	0,000	0,0	766			-		-
2	0,775	6949,486	A	0,000	0,0	805			-		-
3	1,600	639,523	A	1,000	25,0	820	Ordnr	Naphtalene	989	Naphtalene	989
4	1,883	5843,195	A	1,000	25,0	943	Ordnr	Acenaphtalene	989	Acenaphtalene	989
5	2,350	404,552	A	1,000	25,0	538	Ordnr	Acenaphtene	991	Acenaphtene	991
6	2,475	270,811	A	1,000	25,0	878	Ordnr	Fluorene	943	Fluorene	943
	Total			4,000	100,0						

Fig. 4. Chromatogram - Results

Best Match

Displays the **Match Factor** of the Compound from the **Best Match Name** column.

3.3.2 Measurement

The **Chromatogram – Measurement Conditions** dialog contains additional **PDA** subtab with PDA related parameters of the chromatogram.

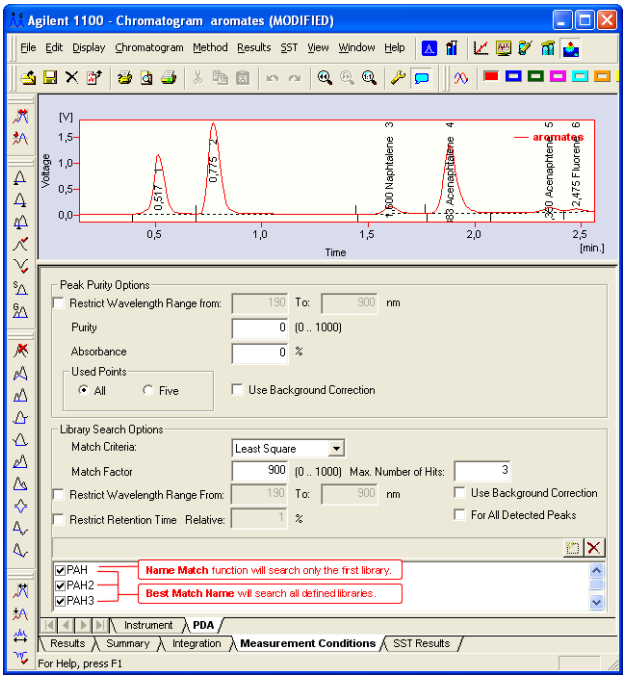


Fig. 5. Chromatogram – Measurement Conditions - PDA

The individual items correspond to the **Method Setup – PDA Method** dialog (see **3.2** - Method Setup – PDA Method on pg. **4**).

The **Method Setup - PDA Method** dialog displays the parameters of the *Template method* that will be applied to new chromatograms.

The **PDA** tab in the **Chromatogram – Measurement Conditions** dialog displays the PDA method of the selected chromatogram.

3.4 Open Chromatogram

The **Open Chromatogram** dialog indicates whether the chromatogram contains PDA data in the **Information Pane** item **Has PDA Data**.

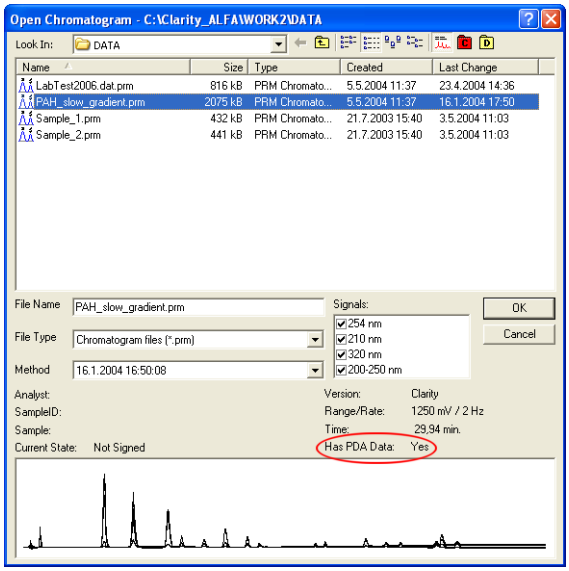


Fig. 6. Open Chromatogram

3.5 PDA Chromatogram window

The PDA window is accessible from the **Chromatogram** window using the **Window – PDA Window** command.

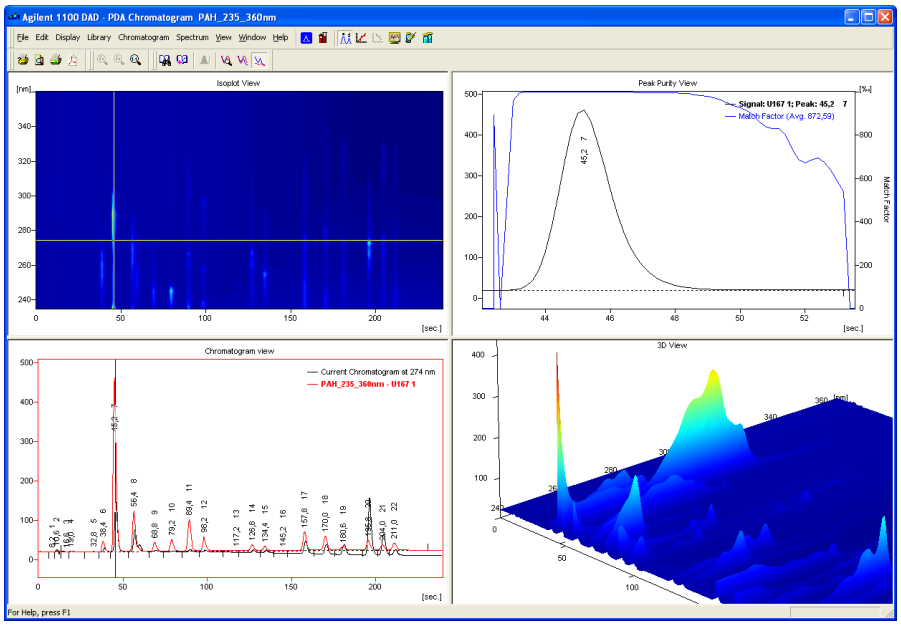


Fig. 7. PDA window

3.5.1 Panes

The **PDA** window can display single view or it can be split into two or four panes. Each pane can display any of the following views: **Isoplot, Chromatogram, Spectral, 3D Display, Peak Purity, Peak Purity Spectra, Spectral Library** and **Spectral Search Results.** The size and position of the panes can be controlled by the commands from **View** menu and by holding and dragging sliders between the panes with the mouse. To display any of the views in a particular pane click the right mouse button to display local menu and select the desired view from the list.

- As there are more available views than panes, it is not possible to see all the views at once. However all user operations with the hidden view are still enabled (e.g. user can open and work with spectral library even if **Spectral Library View** is hidden).
- Specific view can be displayed only in one pane at the time. Selecting a view (e.g. **Isoplot**) that is already displayed in another pane will result in switching the positions of the views (selected view could not be displayed at once in both the original and the new pane). Selecting a view that is not yet displayed will result in hiding the original view and displaying the selected one in the pane.

3.5.2 Markers

Isoplot, **Chromatogram**, **Spectral** and **3D Display** views feature one or two **markers** (thin lines of inverse color crossing the data plot) depicting **current position** in the data.

For many operations (e.g. adding spectrum to library, adding signal, selecting peak, etc.) current time or wavelength serve as a point where the operation takes place.

Markers also specify slices of 3D data that are displayed as curves in **Chromatogram** and **Spectral** views (see below).

- **Time marker** (vertical marker shown in **Isoplot** and **Chromatogram** views) moves over time axis and depicts spectrum currently displayed in the **Spectral** view.
- **Wavelength marker** (horizontal in **Isoplot**, vertical in **Spectral** view) moves over wavelength axis depicting current chromatogram curve in the **Chromatogram** view.
- Markers can be moved by holding left mouse button while cursor is over the marker (cursor changes to ⟷) and dragging it with the mouse.
- Another possibility is to use **Move marker(s) here** function on context menu of the view. The function moves one or both markers to position of the right mouse click that popped up the menu. This is useful while the view is zoomed and marker(s) may not be visible. With **Move Marker(s) Here** marker(s) can always be brought within visible range.

3.5.3 File

Open Chromatogram	Opens the chromatogram that contains PDA Data. (Ctrl+O)
Save Chromatogram	Saves current chromatogram. (Ctrl+Alt+S)
Close Chromatogram	Closes current chromatogram. (Ctrl+Alt+W)
Import 3D	Imports 3D data.
Export 3D	Exports PDA data to EZ Chrom format.
Report Setup	Opens the **Report Setup – PDA** dialog for setting the reporting options. (Ctrl+Alt+P) See the chapter **3.7.1** - Report Setup - PDA on pg. **21.**
Print Preview	Displays the onscreen print preview (Ctrl+SHIFT+P)– consult the **YL-Clarity Reference Guide**.
Print to PDF	Prints report directly to PDF file.
Send Printed PDF	Sends printed PDF as email attachment.
Print	Prints the selected report – consult the **YL-Clarity Reference Guide**. (Ctrl+P)
Exit	Closes the **PDA Chromatogram** window.

3.5.3.1 Import 3D

Imports the 3D PDA data from a txt file. The format is compatible with the EZ Chrom 3D.asc exports.

In general, the imports/exports contain only the matrix of signal values where:

- **Rows** represent time points at the time intervals corresponding to the **Sample Rate**
- **Columns** represent individual wavelengths for the respective range as specified by the **Wavelength From** and **To** fields.

3.5.3.2 Export 3D

Export format is based on export format EZChrom. See ch. **3.8.1** - **Export format** on pg. **22**.

3.5.3.3 Send Printed PDF

Prints report to PDF file then creates a new email message in the default email client and adds the printed PDF file as an attachment.

The name of the PDF file will be derived from the name of the chromatogram.

3.5.4 Edit

Undo	Cancels adjustments in the tables. (Ctrl + Z)
Redo	Redoes the last Undoed operation (Ctrl + Shift + Z)
Copy	Copy to Clipboard. (Ctrl + C)
Paste	Pastes from Clipboard. (Ctrl + V)
Delete	Deletes the selected item. (Del)
Select All	Selects all items. (Ctrl + A)

3.5.4.1 Undo

Cancels adjustments in the tables. This may be used repeatedly as the station remembers all adjustments made to tables from its initial start-up. The history of commands only applies within the framework of the table and each table maintains its own independent list of operations. The command can also be selected using the CTRL + Z shortcut.

3.5.4.2 Redo

Countermands the **Undo** command, which can be invoked repeatedly. The station remembers all modifications made in tables during the last session. The history of commands applies within the framework of the table and table of each signal maintains its own independent list of operations. Commands can also be selected using the CTRL + SHIFT + Z shortcut.

3.5.4.3 Copy

Copies the selected text to the Clipboard (CTRL + C).

3.5.4.4 Paste

Copies the Clipboard content to the desired location (CTRL + V).

The **Paste** function automatically inputs the content of the clipboard into the desired fields of tables. If the area is larger than the content, the content will be tiled.

You may make use of this characteristic if you wish to insert a larger quantity of identical fields into a table or several periodically repeating fields.

3.5.4.5 Delete

Deletes all individually selected table cells.

3.5.4.6 Select All

Selects all table cells (CTRL + A).

3.5.5 Display

Unzoom	Cancels all cuts. (CTRL + *)
Previous Zoom	Restores the previous chromatogram cut (CTRL + -)
Next Zoom	Restores the original cut abandoned by the **Previous Zoom** command. (CTRL + +)

Properties	Invokes the **PDA Properties** dialog for the settings of the graph properties.

3.5.5.1 PDA Properties

There is one new tab (**Chrom&Spectrum View**) in the **PDA Properties** dialog.
The other tabs correspond to the tabs of the **Graph Properties** dialogs in other **YL-Clarity** windows.

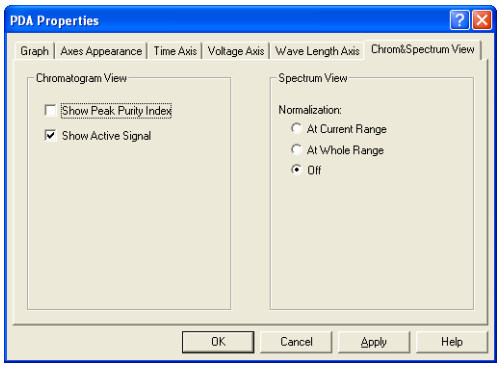


Fig. 8. PDA Properties - Chrom&Spectrum View

Chromatogram View

Show Peak Purity Index

Shows the peak purity across whole chromatogram. The line varies between 80 and 100% of the Y axis

Show Active Signal

Shows the active signal from the chromatogram (including labels)

Spectrum View

Normalization:

- At Current Range
- At Whole Range
- Off

See the description in chapter **3.6.3** - Spectral on pg. **18**

3.5.6 Library

This menu serves for creating and editing **Spectrum Libraries**.

Note: *The **Spectrum Search** is performed in libraries specified in the **Spectral Library Search Options** dialog available by the **Spectrum - Search in Library…** command.*

New	Creates a new empty spectral library. (CTRL + ALT + N)
Open	Opens spectral library file. (CTRL + ALT + O)
Save	Saves spectral library. (CTRL + ALT + S)
Save As	Saves spectral library under different name. (CTRL + SHIFT + S)
Options	Displays the **Spectral Library Options** dialog.
Close	Closes the spectral library. (CTRL + ALT + W)

3.5.6.1 Options

The **Spectral Library Options** defines whether the **Spectral Library** should use the background correction (**Use Background Correction**) and enables to save a **Description** of the library.

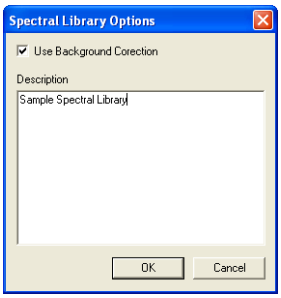


Fig. 9. Spectral Library Options

Caution! *Use the background correction consistently, either always and everywhere ON, or always OFF.*

Use Background Correction

Toggles the use of the background correction.

The baseline (background) for individual wavelengths is interpolated between peak start and peak end points.

With **Background Correction** the spectra are measured against this surface.

Description

Stores the description of the Spectral Library.

3.5.7 Chromatogram

Add Signal	Add (replace) chromatogram signal to Library.
Display Peak Purity	Selects peak to be displayed in **Peak Purity** and **Peak Purity Spectra** views (CTRL + D).

3.5.7.1 Add Signal

Stores selected wavelength/range of wavelengths as a signal in a chromatogram.

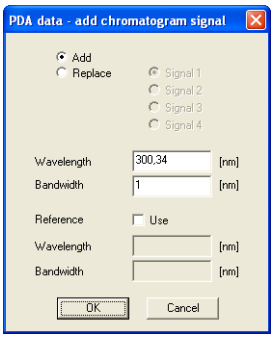


Fig. 10. PDA data – add chromatogram signal

Add

Adds chromatogram to opened **Spectral Library**.

Replace

Replaces the checked **Signal X** in the opened **Spectral Library** by the current chromatogram signal.

Wavelength
Displays the wavelength of current signal.
It can be modified.

Bandwith
Edits the Bandwith of current signal.

Reference
If the **Use** checkbox is checked the Reference signal will be used.

Wavelength
Edits the wavelength of reference signal.

Bandwith
Edits the Bandwith of the reference signal.

3.5.7.2 Display Peak Purity

Selects peak to be displayed in Peak Purity and Peak Purity Spectra views (CTRL + D).

When the time marker is over detected peak in **Chromatogram** or **Isoplot** views, **Display Peak Purity** function selects this peak to be displayed in **Peak Purity** and **Peak Purity Spectra** views.

Invoking the function when marker is not over any peak clears the views, which then display "*No peak selected*" label.

3.5.8 Spectrum

Add to Library	Adds selected spectrum to spectral library.
Search Library	Searches the library for matching spectrum (Ctrl + F).
Normalize Zoomed	Normalizes to zoomed range. See **3.6.3** - **Spectral View** on pg. **18**.
Normalize Whole	Normalizes to whole wavelength axis range. See **3.6.3** - **Spectral View** on pg. **18**.
Normalization OFF	Turns Normalization OFF.

3.5.8.1 Add to Library

Adds selected spectrum to spectral library.

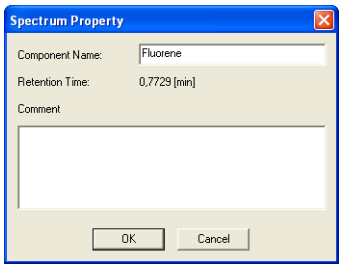


Fig. 11. Spectrum Property

Component Name
Sets the name of the component.

Retention Time
Displays the Retention Time of the selected spectrum.

Comment
Provides place for custom comments.

3.5.8.2 Search Library

The **Spectral Library Search** (Ctrl + F)can perform automatic identification of integrated/calibrated components (peaks).

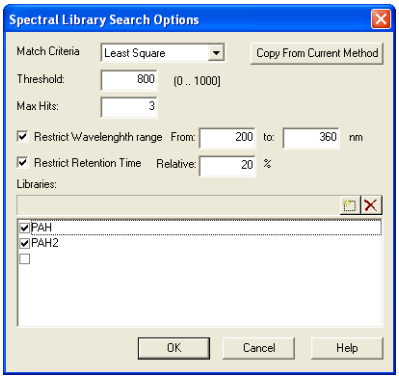


Fig. 12. Spectral Library Search Options

Match Criteria

Sets one of the **Least Square**, the **Weighted Least Square** or the **Correlation Method** for calculating library search matches.

Threshold

Only hits with **Match Factor** above this value will be displayed.

Max. Hits

Restricts the number of displayed hits, this can reduce the search time.

Copy From Current Method

Copies the settings from the PDA method of the active chromatogram (= settings from the **Chromatogram – Measurement Conditions – PDA** see chapter **3.3.2** - Measurement on pg. **7**.)

Restrict Wavelength Range

Restricts the search to the wavelength specified in the **From** and **To** fields.

Restrict Retention Time

Restricts the search to peaks with retention times that do not exceed the specified relative deviation from the spectra retention time.

Libraries

Specifies the libraries to be searched.

Click the button to add new line to the list, in this new line click the … button to invoke **File Open** dialog where you can select the **Spectral Library** to be opened.

Uncheck the checkbox next to the library to omit it from the Search.

3.5.9 View

Toolbar	Displays/hides the toolbars.
Customize	Lets the user to customize toolbars (see the **YL-Clarity Reference Guide** for details).
Reset All	Reset all toolbars to the default state. It is recommended to use this command after installation of updates to display eventual new icons.
View Library	
Maximize View	Maximizes selected view.
Restore Views	Restores layout of PDA window.
Two Vertical Panes	Displays two vertical panes.
Two Horizontal Panes	Displays two horizontal panes.

Four Panes	Displays four panes.

3.5.9.1 Maximize View

Maximizes selected view either in its own pane if it is already displayed or in top left pane if it has been hidden so far.

3.5.9.2 Restore Views

Restores the layout of the views (panes) in the **PDA** window to the state before the **Maximize View** command was used last.

3.5.9.3 Two Vertical Panes

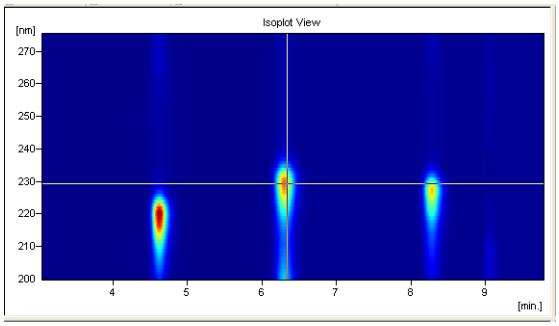
When switching from four panes layout, views from left panes are displayed.

3.5.9.4 Two Horizontal Panes

When switching from four panes layout, views from top panes are displayed.

3.6 PDA Chromatogram views

3.6.1 Isoplot



The **Isoplot** view is the basic view of PDA spectral data. It displays the spectral data viewed “from the top” with absorbance value distinguished by color. The lowest values are represented by dark blue, rising over light blue, green, yellow up to red and dark red being the highest.

3.6.2 Chromatogram

The **Chromatogram** view displays slice of 3D data defined by actual position of the wavelength marker. It can also display active signal from the **Chromatogram** window and/or peak purity (match factor) curve for that signal.

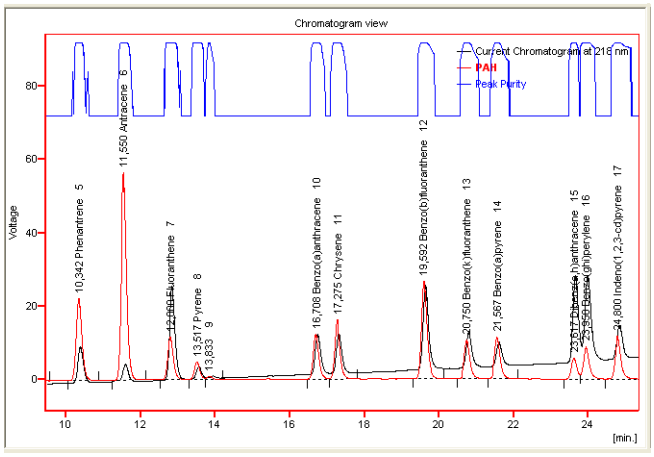


Fig. 13. Chromatogram View

- Display of active signal and peak purity curves is controlled either on **Chrom&Spectral Views** tab in **PDA Properties** dialog or with **Show Active Signal** and **Show Peak Purity** functions on the context menu.
- Appearance of the active signal curve can be tailored exactly the same way as in **Chromatogram** window on **Graph** tab of **PDA Properties** dialog.
- Peak Purity curve is shown in upper part of the view so that it doesn't interfere with displayed signals. It is in per mille units. Peak purity curve for particular peak can be viewed in more detailed way using Peak Purity View and **Display Peak Purity** function.

3.6.3 Spectral View

Spectral view visualizes slice of 3D data defined by actual position of the time marker along with depicted spectra from **Spectral Library** and **Spectral Search Results** views.

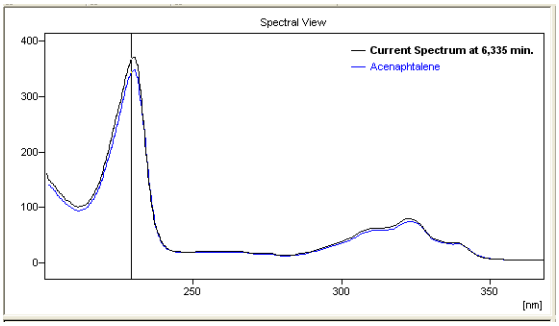


Fig. 14. Spectral View

Spectra can be overlaid in the graph using three different modes:

- **Normalized to whole wavelength axis range:**

  All spectra are re-scaled (the display only, spectral data stay the same) so that their respective lowest and highest points throughout the whole graph appear at the same level.

  It is convenient for visual comparison of peak spectra as the shape of the spectra curve does not depend on peak height in this mode.

  Vertical axis on the left displays values for currently active curve only (its label is appearing bold in the graph legend).

- **Normalized to zoomed range:**

  This is more advanced variety of the previous mode – spectra appear normalized as well, but this time lowest and highest **visible** points appear at the same level.

  Only characteristic regions of spectra can be easily compared in this view.

- **With normalization turned off:**

  In this mode all spectra appear in their respective scales.

  Mode can be chosen using functions **Normalize Zoomed**, **Normalize Whole** and **Normalization OFF** in the **Spectrum** menu.

3.6.4 3D View

This view shows three-dimensional plot of PDA data with **Time** and **Wavelength** being the horizontal axes and height (and color) depicting **Absorbance Value**.

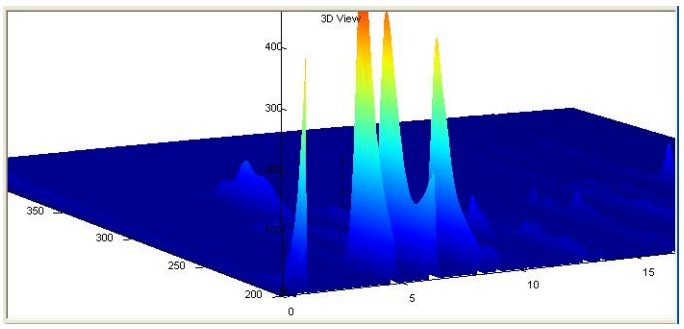


Fig. 15. 3D Plot

Caution! *The 3D Plot can take some time to display depending on the amount of data and the speed of your graphics card.*

The view also contains both markers (cursor Lines), though they may be hidden beneath the surface of the data, being visible only from one side of the 3D plot.

Projection of the plot is always centered on the crossing point of the markers.

The plot can be moved, rotated and zoomed using the mouse.

- In the **Move** mode () holding left mouse button and dragging the mouse moves the plot with the cursor. Note that markers move as well, as the view is always centered on the crossing point. Move mode can be set with **Smart Move Graph Mode** function on context menu.
- In the **Rotate** mode () holding left mouse button and dragging the mouse rotates the plot. Moving the mouse horizontally rotates the plot along the vertical (absorbance) axis, moving the mouse vertically rotates the plot along horizontal axis of the view. The **Rotate** mode can be achieved with **Rotate Graph Mode** function on context menu or by holding the Shift key while moving the mouse in **Move** mode.
- In the **Zoom** mode () holding left mouse button and dragging the mouse zooms the plot. Moving towards the center of the view shrinks the plot while moving away from the center enlarges in. The **Zoom** mode can be set with **Zoom Graph Mode** function on context menu or by holding the Ctrl key while moving the mouse in **Move** mode. The plot can also be zoomed in any mode using mouse wheel.
- Function **Restore Default View** on context menu restores default projection of the 3D plot.

3.6.5 Peak Purity

The **Peak Purity** view displays peak previously selected with **Display Peak Purity** in **Chromatogram** or **Isoplot** views and its **Match Factor**. If no peak has been selected, label "*No peak selected*" is displayed instead.

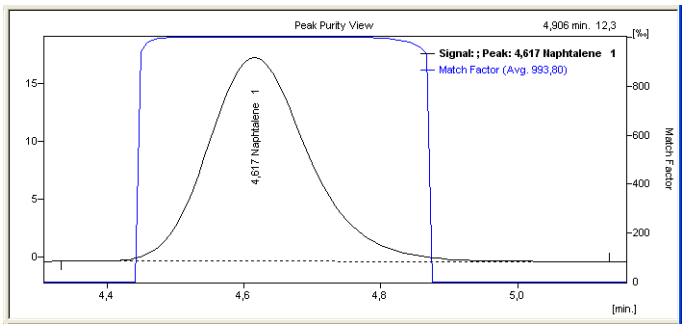


Fig. 16. Peak Purity View

- Menu item **Toggle to Spectra** on context menu switches view in the pane to **Peak Purity Spectra** view of the same peak.
- The **Peak Purity** is performed according to the settings from the PDA method of the chromatogram that can be displayed/edited in the **Chromatogram – Measurement Options – PDA** dialog (see **3.3.2** - **Measurement** on pg. **7)**.

3.6.6 Peak Purity Spectra

The **Peak Purity Spectra** view displays spectra in significant points of peak selected in **Peak Purity** view. These points are both threshold points (first and last point in which match factor is computed for given peak), both inflex points and apex.

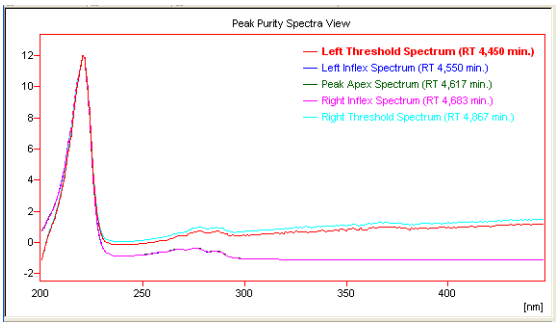


Fig. 17. Peak Purity Spectra View

- All spectra in the **Peak Purity Spectra** view are always normalized to current cut regardless of spectrum normalization settings.
- Menu item **Toggle to Match Factor** on context menu switches view in the pane to **Peak Purity** view of the same peak.

3.6.7 Spectral Library

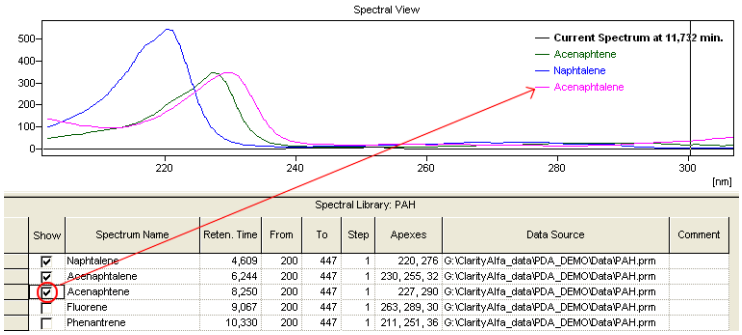


Fig. 18. Spectral Library View

- The **Spectral Library** view displays the spectra information from the currently opened spectral Library.
- The **Spectrum Name** and **Comment** columns can be edited.
- To delete a spectrum from **Library**, select its line and press the DEL key.
- To add spectrum to library, use the **Spectrum - Add to Library** command see **3.5.8** - **Spectrum** on pg. **14**.
- The spectra may be overlaid to the current spectrum in the **Spectral** view by checking the checkbox in the Show column. To hide the spectrum, uncheck its checkbox. The overlaid spectra will be hidden automatically when another library will be opened.

3.6.8 Spectral Search Results View

The **Spectral Search Results** view displays the matching spectra information found by the current **Search in Library** command.

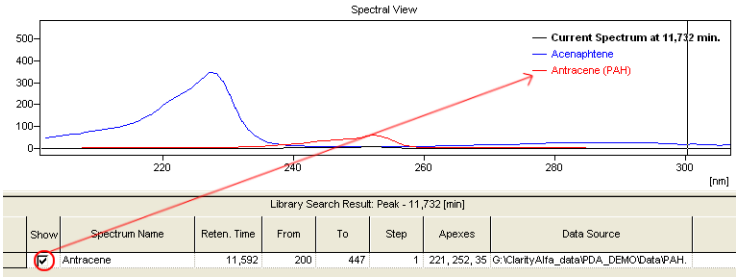


Fig. 19. Spectral Search Results view

- The spectra may be overlaid to the current spectrum in the **Spectral** view by checking the checkbox in the Show column. To hide the spectrum, uncheck its checkbox. The overlaid spectra will be hidden automatically when a new search is performed or the chromatogram changed.

3.7 Printing

The **Report Setup** command in the **PDA** window opens the **Report Setup - PDA** dialog.

3.7.1 Report Setup - PDA

Print

Allows/disallows printing the relevant part. If allowed the symbol ✓ will be shown before the tab name.

On New Page

If checked, the relevant part will be printed on a new page.

Signals

Sets which signals will be included in the report:

All – Active Chromatogram – Only Active Signal

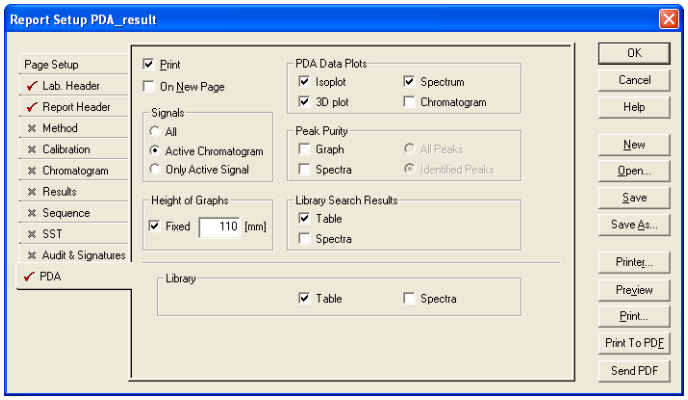


Fig. 20. Report Setup – PDA

Height of Graphs

Prints the graphs with vertical size scaled to the specified dimension in millimetres.

PDA Data Plots

Enables the printing of the selected data plots: **Isoplot** - **3D plot** – **Spectrum** – **Chromatogram.**

When the report setup has been invoked from the **PDA** window **Spectrum** and **Chromatogram** parameters will be printed WYSIWYG (including spectra overlays).

Peak Purity

Enables the printing of the selected items:

Graph – Spectra – All Peaks – Identified Peaks

Library Search Results

Enables the printing of the selected items:

Table – Spectra – All Peaks – Identified Peaks

Library

Enables the printing of the selected items:

Table - Spectra

Caution! *The **Spectra** items will be printed only from the **PDA** window.*

3.8 Export and import format of PDA (3D) data

3.8.1 Export format

Export format is based on EZChrom export format. Resultant file has following parameters:

- text file format
- the name of file listed in **Export Chromatogram** dialog is in the case of 3D data extended with "-3D" inscription at the end of the respective nameto enable conjoined export of signals and 3D data.
- 8-bit coding ASCII, code page according to settings of the operation system
- field separator is tabulator (ASCII code 0x09)
- new lines separator is sequence CR, LF (ASCII codes 0x0D, 0x0A)
- text values are quoted (xxx) with tabulators and ends of lines, tabulator and end of line symbols are not allowed
- real numbers are in decimal or in science-technical notation (1.2345e+6), it depends on which one is shorter; decimal delimiter is "."
- date and time are formatted according to settings in the operation system

Caption is formed from a few lines in format:

- <field name>:<tabulator><field value><end of line>

Individual fields in caption are:

Version	number of export version, always "3"
Sample ID	content of the **Sample ID** field in **Single Analysis** dialog or from the **Sequence** table
Data File	implicit path to exported .prm file
Method	name of the used template method (without file path and extension), provides the info from **Chromatogram - Measurement Conditions - Instrument - Acq. Method**. dialog
User Name	author of the chromatogram; content of the **Analyst** field in **Chromatogram - Measurement Conditions - Instrument** dialog
Acquisition Time	time and date of acquisition; content of the **Acquired** field in the **Chromatogram - Measurement Conditions - Instrument** dialog
Sample Rate (Hz)	sampling frequence in Hz
Number of Points	number of spectrums in chromatogram; number of samples on time axis; number of lines with values
Wavelength Start (nm)	minimal wavelength of measured spectrums in nm
Wavelength End (nm)	maximum wavelength of measured spectrums in nm
Wavelength Step (nm)	length of step in nm between two sequential points in spectrum
Points per Spectrum	number of points in spectrum; number of fields in one line of values; there is a formula: (Wavelength End - Wavelength Start) / Wavelength Step = Points per Spectrum
Absorbance Units	units of data values (after including the **Absorbance Multiplier** field,values can be in "µAU", "mAU" or "AU"
Absorbance Multiplier	coefficient transferring (integral) values in lines of values to real value in listed units ("Absorbance Units"); value is chosen closest to value 1 so that all values in lines of values were integral; there is a formula: <value> * Absorbance Multiplier = <real value in Absorbance Units>

The rest of the file contains lines of values. Individual values are integral numbers with sign, separated with tabulator. Lines contain spectrums,

columns signals in time for specific wavelength. First value on the first line corresponds to time 0.0 min and minimal wavelength.

3.8.2 Import format

Import format is the same as export format with the following changes:

Version	must be “2“ or “3“
Data File	value is ignored, name of file fills user during import
Method	value is ignored
Number of Points	value is ignored, the real number of lines of values is used
Points per Spectrum	value is ignored, the real number of values in 1. line of values is used
Absorbance Units	allows to set even “u“ and “micro“ in place of “µ“, “mili“ in place of “m“ and “V“ in place of “AU“, farther ignores symbols “[“, “]”, “ “ and “-“
Volume (uL)	after conversion of units fills field “Inj. Volume [ml]” on “Results” tab of chromatogram

Caption can also contain any other parameters, these will be ignored. For known parameters it is necessary to keep upper and lower case letters otherwise the values will be ignored. Between caption and lines of values can be any number of empty lines.

YL-Clarity Extensions

GPC

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

YL INSTRUMENT CO., LTD.

1 GPC - Gel Permeation Chromatography

The **YL-Clarity GPC** is an optional **Extension** for the **YL-Clarity Chromatography Software** (from version 2.3). The **YL-Clarity Chromatography Station** can acquire data from any *GPC system* with standard analog output. Any YL-Clarity Instrument can use **GPC mode**.

GPC extension provides interactive and automated GPC analysis including recalibration and GPC reporting, simplifies retrieval of GPC data. It also allows flow rate and multi-detector delay corrections and includes *Narrow*, *Broad* and *Broad on Narrow* calibrations.

GPC Extension is also compatible with **YL-Clarity Offline** software.

1.1 Availability

The **GPC Extension** is an optional, fully integrated part of **YL-Clarity** software. It can be ordered as a part of new datastation or as an extension to existing datastation (p/n A28).

1.2 Installation

The **GPC Extension** is enabled by appropriate user code entered during installation or later by using the **Help - User Code** command from the **YL-Clarity** main window.

To switch an instrument to **GPC mode**, choose the **GPC - Instrument Type** in the **System Configuration** or the **Setting - GPC mode** command in the **Instrument window**.

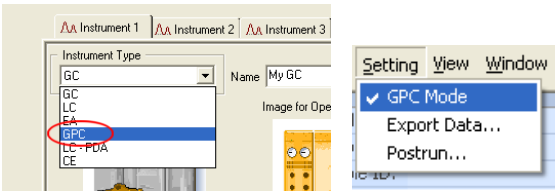


Fig. 1. Switching to the GPC mode

2 Key Features

- **Measuring** – Simultaneous data acquisition from up to four twelve-detector chromatographs (4×12 configuration).
- **Evaluation** – The same chromatograms can be evaluated both in standard and GPC mode.
- **GPC Integration** – Separate integration tables for GPC and standard evaluation are used. There are extensive possibilities for modifying chromatograms. The chromatogram can be changed by entering global parameters or interactively, through the direct graphical modification of the baseline.
- **Overlay** – Simultaneously displays a virtually unlimited number of chromatograms. Molecular weight and cumulative molecular weight distributions can be easily compared.
- **GPC Calibration** – Narrow or Broad standard calibration methods (see chapter **2.1** on pg. **2**) combined with flow rate correction and Universal calibration. Manual calibration or automated recalibration from sequence. Multiple broad standards can be used.
- **GPC Results table –** Displays molecular weight averages together with peak details for active signal. Multiple peaks can be evaluated from one chromatogram.
- **GPC Summary result tables** – Displays and prints selected results from all simultaneously displayed chromatograms.
- **User calculations** – User can define custom calculations in the **Result** and **Summary** tables. Using the integrated editor you can create your own columns from the original columns and individual mathematical functions.
- **Reports** – User selectable report sections, WYSIWYG formatting of Graphs and Tables.
- **Automated measuring support** – Sequence tables for any set of samples with or without an autosampler.
- **Postrun** – Automatically displays, prints, exports and starts other programs after completing the measurement.
- **Batch** – Automatically batch processes, displays, exports or prints any number of chromatograms.
- **Fraction Collectors** – GPC offers support for fraction collectors controlled by **Collect/Waste** and **Next** signals.

2.1 Basic Principles and Terms

- *Gel Permeation Chromatography* (**GPC**) or *Size Exclusion Chromatography* (**SEC**) is a specialized chromatography technique for determination of molecular weight distribution in polymers. Sample of polymer solution, containing mixture of molecules differing in size, is separated on column. Under conditions used for this chromatography mode, the molecules are separated according to size, the larger molecules emerging first and the smaller later. With appropriate polymer standards with known molecular weights, calibration curve describing the dependence between molecular weight and elution volume can be constructed.
- **Narrow standard** calibration is the most commonly used, when polymer standards with narrow molecular weight distribution are available. Calibration curve is constructed from detected peak maximum retention times and known *Mp* values. Alternatively, *(Mw.Mn)^1/2* values can be used, if *Mp* values are not declared.
- **Broad standard** calibration is used, when only polymer standards with broad molecular weight distribution are available. **YL-Clarity GPC** extension uses three types of Broad standard calibration

- **Broad linear** – assuming linear calibration curve for broad peak concerned. Linear calibration equation is calculated from the standard peak elution profile and declared **Mn** and **Mw** values. Multiple Broad Standards can be used to construct a result calibration curve.
- **Broad integral** – a calibration curve is constructed from the standard peak elution profile and a table of declared cumulative molecular weight distribution values. Multiple Broad Standards can be used to construct a calibration curve.
- **Broad on narrow** – appropriate **K** and **Alpha** values are sought for polymer standard with declared **Mn** and **Mw** values, to fit the standard peak elution profile to existing narrow standard calibration curve.
- **Flow rate correction** – the elution volumes are calculated from retention time and flow rate. Small variations in flow rate have tremendous effect on the correctness of calculated molecular weights. A low molecular weight compound (flow rate marker) can be added to the standards and samples, the retention times in different chromatograms can than be normalized to common base. Flow rate correction can be used with every calibration type.
- **Universal calibration** – the separation of polymer molecules on column is governed by molecular size, not molecular weight. The polymer molecule size is besides its weight dependent on the molecule structure (linear, branched, starlike) and conformation (given by solvent and temperature). A dependence (*Mark-Houwink equation*) can be used to calculate molecular weights for molecules of the same size, provided the constants **K** and **Alpha** of the *Mark-Houwink equation* are known for both polymers. Universal calibration can be used with every calibration type, except *Broad On Narrow*.

3 GPC extension description

After installation, new functions of the **GPC extension** will be available. Only changed or additional features to the standard **YL-Clarity** mode are listed and described here.

3.1 Instrument window

In the **Instrument** window the new **Setting - GPC Mode** command enables the switching between standard and GPC evaluation mode on the selected instrument. The **GPC mode** is indicated by the "**GPC:**" inscription preceding the *Instrument* and *Method* names in the **Instrument** window title bar.

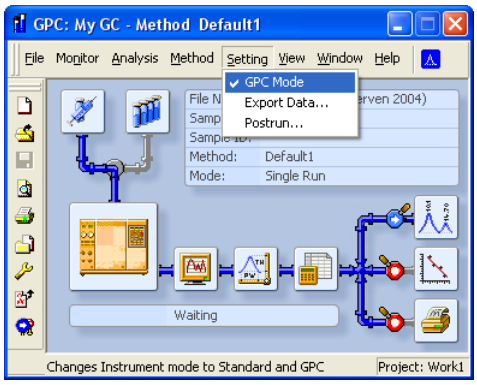


Fig. 2. Instrument window

3.2 Single Analysis window

In the **Single Analysis** dialog the new fields named **K** and **Alpha** enable the entering of the *Mark-Houwink parameters* used for universal calibrations. The default values *14.1* and *0.7* are valid for *linear polystyrene in tetrahydrofurane at 25℃*.

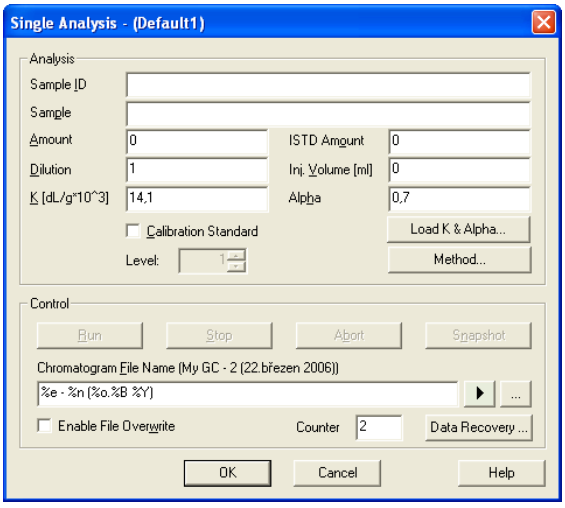


Fig. 3. Single Analysis

The **Load K & Alpha** button enables entering those values from user editable table.

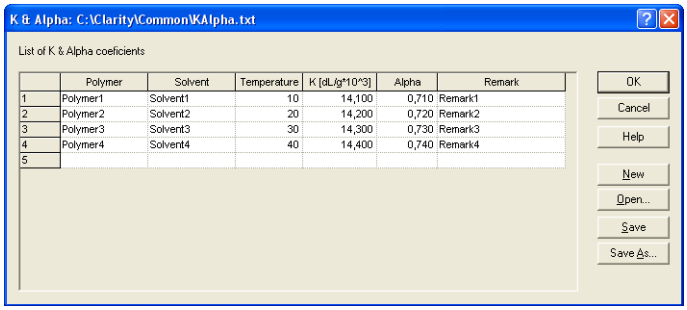


Fig. 4. K & Alpha

3.3 Sequence window

In the **Sequence** window new columns for entering **K** and **Alpha** values are available. The values can also be entered from editable table using the **Load K & Alpha** command available in local menu. **GPC Std Type** and **GPC Std No** columns serve for automatic recalibration of GPC calibration during sequence runs. The columns to be displayed can be selected by using the **Hide Columns** and **Show Hidden Columns** commands from local menu (right mouse click in table area).

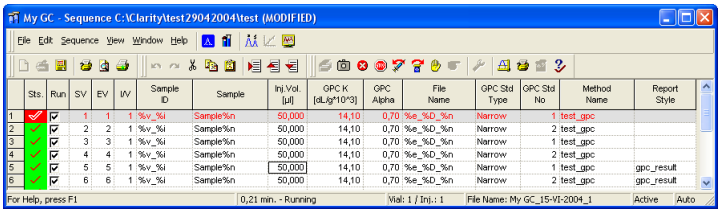


Fig. 5. Sequence window

Note: *Only relevant parts of report for the actual mode selected (Standard or GPC) will be printed from the Report Style selected in Sequence.*

3.4 Method Setup dialog

In the **Method Setup** dialog, new **GPC Integration**, **GPC Calculation, GPC Advanced** and **GPC Ranges** tabs are available. Different parameters for standard and **GPC mode** can be set for automatic chromatogram integration and calculations after acquisition. However, the evaluation and display of results for measured chromatograms is possible only according to the mode (GPC or standard) selected.

Caution! *Performing **Reprocess by Instrument Method** or **Complete Reprocessing** in the **Batch** dialog will always reprocess both standard and GPC parts of the method.*

3.4.1 GPC Integration

The **Method Setup – GPC Integration** dialog is similar to the **Method Setup – Integration** dialog.

There are three differences between the parameters in the **Method Setup - GPC Integration** dialog and the standard **Method Setup - Integration** dialog.

- The **Solvent Peak** operation excludes selected integrated peaks from evaluation.

  It is useful for low molecular weight impurities, which need to be integrated to get correct baseline, however the results are not desired. In GPC mode solvent peaks are identified differently than in normal mode. Peaks are marked as solvent if they are found in the selected intervals.
- The **Flow Marker Peak** designates a peak to be used for flow rate corrected calculations. Only one peak in chromatogram can be used as

flow marker, the last occurrence of this operation in integration table will be used.

Note: *The **Use Flow Rate Correction** check box must be checked in the used calibration in addition to the selected **Flow Marker**, otherwise the correction will not be performed.*

- The **Group** operation is not available in GPC mode.

  To get averaged values for multimodal Mw distribution polymer, integrate the peaks as a single one using **Baseline Lock** and **Add Positive** functions.

  It is possible to set different settings in both dialogs to have the chromatogram evaluated as both standard mode and in GPC mode.

3.4.2 GPC Calculation

The **Method Setup – GPC Calculation** dialog is analogical to the **Method Setup – Calculation** dialog.

The **Parameters** and **Report in Result Table** sections are disabled in GPC Calculation.

It is possible to set different settings in both dialogs to have the chromatogram evaluated as both standard mode and in GPC mode.

3.4.3 GPC Advanced

The **Method Setup - GPC Advanced** dialog is identical with the **Method Setup - Advanced** dialog.

It is possible to set different settings in both dialogs to have the chromatogram evaluated as both standard mode and in GPC mode.

3.4.4 GPC Ranges

GPC ranges serves for calculation of peak area percentage for defined ranges of molecular weights or average molecular weight for selected area percentage ranges.

Ranges Type

Select *Percent* or *MW*.

Low Percent

For percent range type set the start of range in % of peak area from start.

High Percent

For percent range type set the end of range in % of peak area from start.

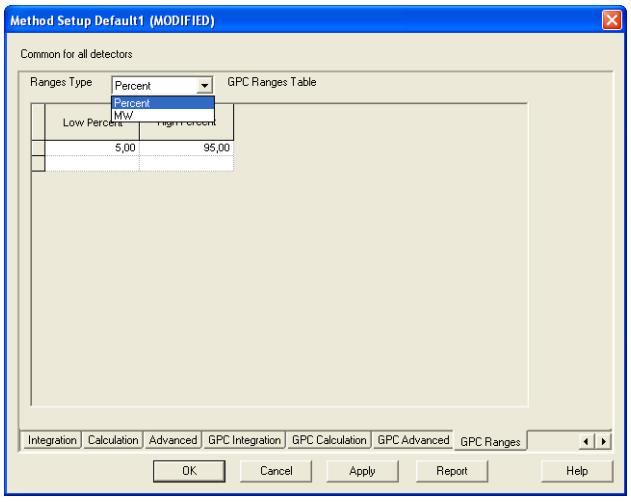


Fig. 6. Method Setup – GPC Ranges

High MW
For MW range type; set the start of range in MW

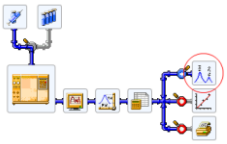
Low MW
For MW range type; set the end of range in MW

Note: *For the last 10% of peak area enter range 90 to 100.*
Multiple ranges of the same type can be set.

Result average molar weight is calculated by following algorithm:

$$MW = \frac{\Sigma\left(response \times M^2\right)}{\Sigma\left(response \times M\right)}$$

3.5 Chromatogram window



The **Chromatogram** window is the central window (opened by clicking the icon) for displaying, modifying and evaluating chromatograms.

In the **Graph pane**, alternatively a **Chromatogram** (or chromatograms) overlaid by a calibration curve, **MW Distribution** or **Cumulative MW Distribution** tabs can be displayed using the appropriate tabs.

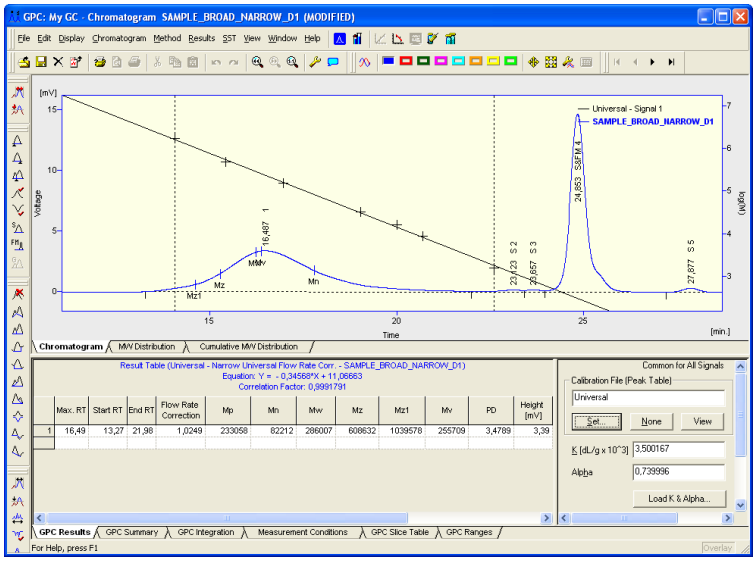


Fig. 7. Chromatogram window

In the **Tables pane**, any of the **GPC Results**, **GPC Summary**, **GPC Integration**, **Measurement Conditions**, **GPC Slice Table** and **GPC Ranges** can be displayed using the appropriate tabs or commands from the **Method** and **Results** menus.

3.5.1 GPC Results

The results for a selected chromatogram can be found in the **GPC Results** tab. The table appearance – (displayed columns) can be modified using the **Setup columns** command from the local menu (opened by right mouse button click in the table area).

On the right side, the used calibration file and *Mark-Houwink parameters* can be set or changed.

Following columns can be displayed in tables

Max. RT	Retention time of peak maximum
Start RT	Retention time of peak integration start
End RT	Retention time of peak integration end
Mp	Molecular weight at peak maximum
Mn	Molecular weight number average
Mw	Molecular weight weight average
Mz	Molecular weight z average
Mz1	Molecular weight z+1 average
Mv	Molecular weight viscosity average
PD	Polydispersity (Mw/Mn)
Flow Rate Correction	Flow rate correction factor
Height [mV]	Peak height
% Height	Percentage of total height of evaluated peaks
Area [mV.s]	Peak area
% Area	Percentage of total area of evaluated peaks

Additional columns can be displayed or calculated using the **Add User Column** command from the local menu.

3.5.2 GPC Summary

Using the **GPC summary** tab, a summary results table for all displayed signals is accessible. Its appearance can be customized using the **Setup Columns** and **Summary Options** commands from local menu.

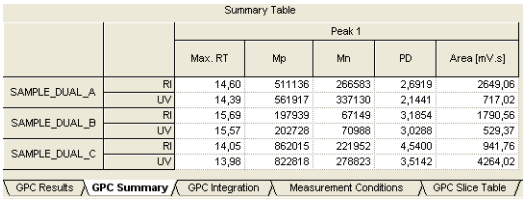


Fig. 8. GPC Summary

3.5.3 GPC Integration

In the **GPC Integration** table all operations used for the GPC peak integration are displayed and editable. The operations can be entered directly in the table or interactively on the chromatogram in the Graph pane using the **Peak**, **Baseline** and **Integration** toolbars.

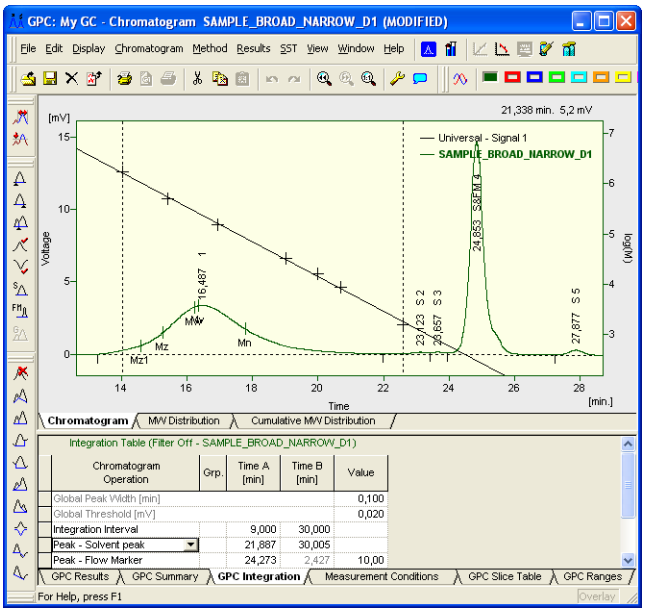


Fig. 9. Chromatogram – GPC Integration

Most operations are common for standard and GPC mode and are described in the **YL-Clarity User** and **YL-Clarity Reference** Guides. For differencies see chapter **3.4.1** on pg. **5**.

3.5.4 Measurement Conditions

The **Measurement Conditions** tab is common both for normal and GPC mode.

3.5.5 GPC Slice Table

The **GPC Slice Table** displays the cumulative molecular weight distribution table for the active peak. In signals with multiple evaluated peaks, the peak is set active by clicking on its row in the results table for the respective signal. The table appearance can be modified using the **Setup columns** command from local menu.

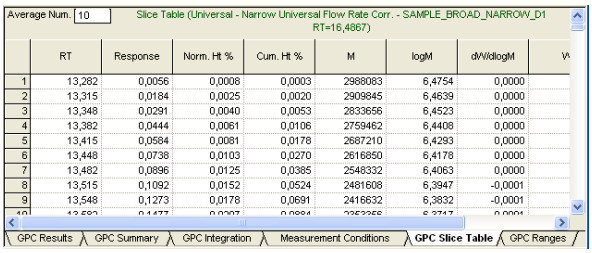


Fig. 10. Chromatogram – GPC Slice Table

The number of slices depends on the peak length and **Peak Width** value used in **GPC Integration** table. The slices can be averaged by entering a number (1-100) to the **Average Points** field in the table title line.

For the integrated peak, following values are available for the specified time intervals (slices):

RT

Retention time of slice (averaged)

Response

Peak height (averaged)

Norm Ht %

Percentage of Slice Height from total of all slices height (summed to give total 100%)

Cum Ht %

Cumulative percentage of Slice Height from total of all slices height (averaged)

M

Molecular weight corresponding to slice RT (averaged)

Log M

Log of molecular weight corresponding to slice RT (averaged)

Outside Calib

Flag for slices outside (value = 1) or inside (value = 0) the used calibration RT range

Norm. Ht

Normalized slice height (summed)

Cum. Ht

Cumulative slice height (averaged)

Cum Ht % Graph

Cumulative percentage of Slice Height from total of all slices height in inverse order (increasing with increasing M) (averaged)

W

Normalized slice height used for MW distribution calculation.

dW/dlog M

Normalized distribution of slice molecular weights used for the graph in **MW distribution** tab.

3.5.6 GPC Ranges

This tab presents the same parameters as on the **Method Setup – GPC Ranges** tab (see pg. **6**) along with the computed results. For *MW* mode, **Result Percent** field is calculated, while for *Percent* mode, **Result MW** is shown.

Result MW

Displays the average of MW values for the percent range set.

Result Percent

Displays the peak area percentage for the MW range set.

Note: *The **GPC Ranges** table setings are stored in the chromatogram. You can change them on the **GPC Ranges** tab for the current chromatogram. Alternatively you can change them in the template method and batch reprocess the respective chtromatograms with this method.*

Note: *Multiple ranges of the same type can be set. For MW ranges not containing any peak points no value is calculated.*

Note: *For chromatograms with multiple peaks the table is shown for the active peak (as selected in the **Results table** tab). Its retention time is indicated in table header.*

3.5.7 Chromatogram

The chromatogram or chromatograms are displayed in the **Graph** pane of the **Chromatogram** window on the **Chromatogram** tab. The window properties including the **Overlay** and **Graph Properties** are essentially the same as in normal mode and are described in the **YL-Clarity User** and **YL-Clarity Reference** Guides. The **Peak Name** and **Group Peak** tags are not available in GPC mode.

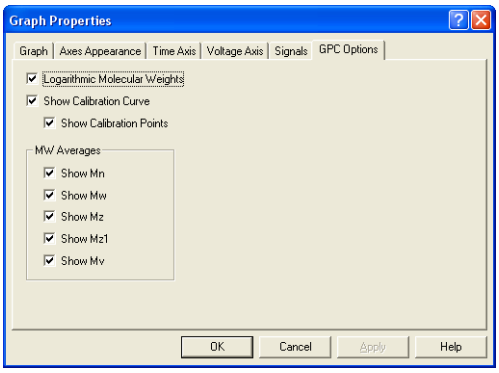


Fig. 11. Graph Properties – GPC Options

The overlaid GPC calibration curve for active signal or its points can be switched off in the **Graph Properties - GPC Options** dialog (available from local menu). The **Log M** axis of the curve is fixed regardless of the zoom in the **Chromatogram** window. The labels of this axis can be displayed in **M** or **Log M** format. The **MW Averages** can be displayed or hidden using the **MW Averages** checkboxes. The setting is common for chromatogram and **MW Distributions** graphs.

3.5.8 Mw distribution

The **MW Distribution** tab in the **Graph** pane of **Chromatogram** window shows the molecular weight distribution of the active peaks from the overlaid signals or chromatograms.

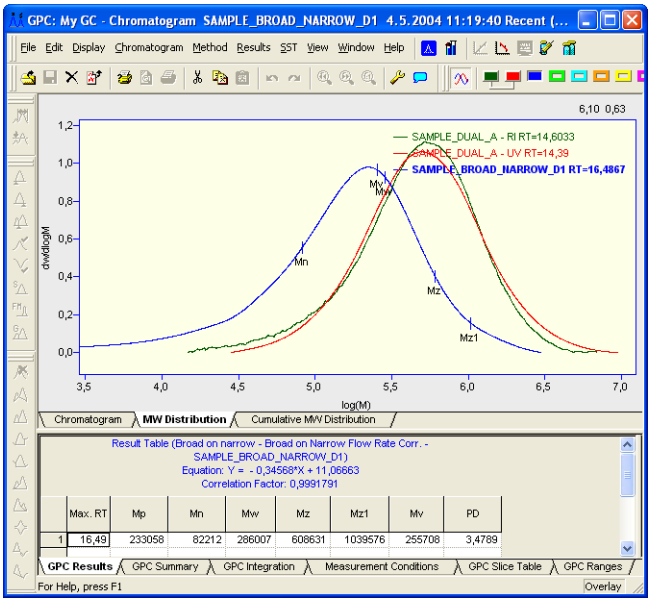


Fig. 12. Chromatogram – MW Distribution

In signals with multiple evaluated peaks, the peak is set active by clicking on its row in the **Result Table** for the respective signal. The active peak RT is indicated at the end of its legend in the **Graph** pane.

3.5.9 Cumulative MW distribution

The **Cumulative MW Distribution** tab in the **Graph** pane of **Chromatogram** window shows the cumulative molecular weight distribution (in %) of the active peaks from the overlaid signals or chromatograms. In signals with multiple evaluated peaks, the peak is set active by clicking on its row in the results table for the respective signal.

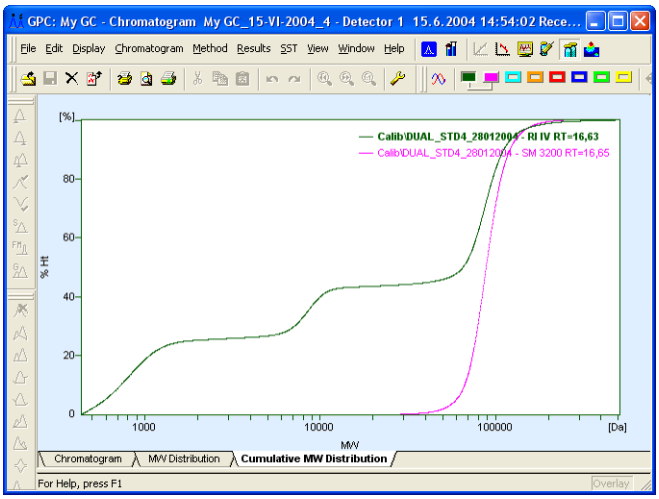


Fig. 13. Chromatogram – Cumulative MW Distribution

Note: *By integrating multiple peaks as single one it is possible to get a single molecular weight distribution curve for multi-modal polymer samples.*

3.6 Calibration window

The **GPC: Calibration** window (opened by clicking the icon) is used for creating, modifying and displaying calibration curves.

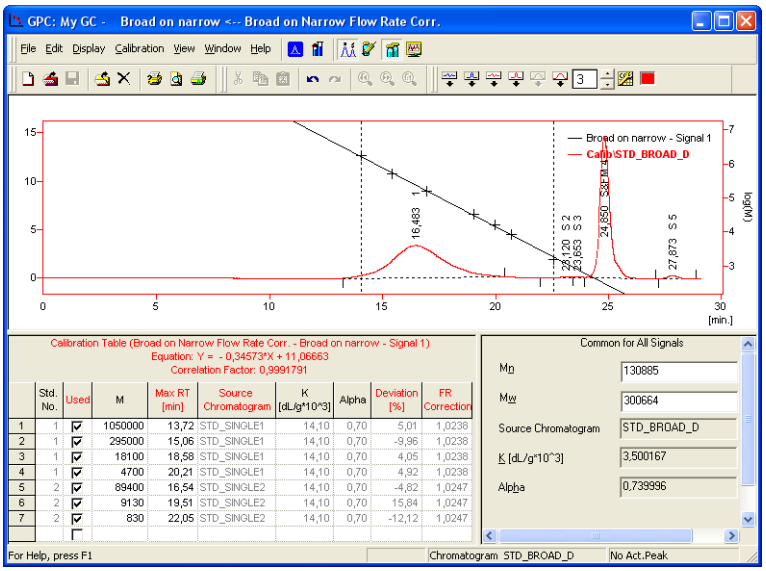


Fig. 14. GPC Calibration

In the **Graph** pane of the **Calibration** window the standard chromatogram with the calibration curve is displayed. Its appearance can be modified using the **Graph Properties** dialog from the local menu

In the **Table** pane of the **Calibration** window the **Calibration Table** is displayed. Its appearance depends on the selected calibration type.

3.6.1 GPC Calibration Options

When creating a new Calibration, the **GPC Calibration Options** dialog will be displayed first, enabling the selection of new calibration type.

Caution! *The calibration type can not be changed later.*

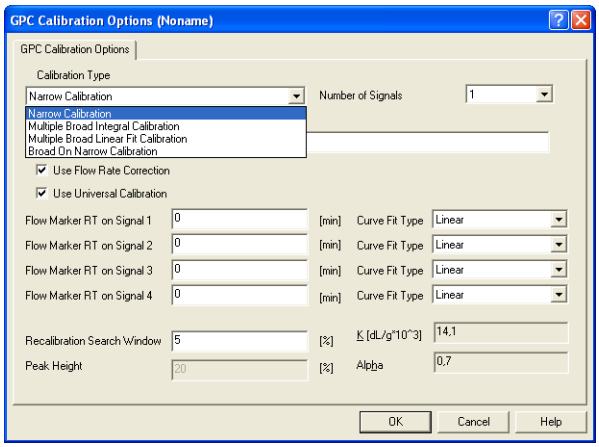


Fig. 15. GPC Calibration Options

The following calibration types can be selected:

- Narrow Calibration
- Multiple Broad Linear Calibration
- Multiple Broad Integral Calibration
- Broad on Narrow Calibration

The type of calibration used is indicated in the **Calibration Table** title line as well as in the chromatogram **Result Table** title line.

- The **Use Flow Rate Correction** checkbox will amend the calibration curve and calculations respectively, if the **Flow Marker Peak** was identified for standards and sample. The use is indicated in the **Calibration Table** title line as well as in the chromatogram **Result Table** title line by the inscription "*Flow Rate Corr*". In such case the calibration curve is constructed for each chromatogram separately.
- The **Use Universal Calibration** checkbox will amend the calibration curve and calculations according to the *Mark-Houwink* parameters entered for standards and sample. The use is indicated in the **Calibration Table** title line as well as in the chromatogram **Result Table** title line by the inscription "*Universal*". In such case the calibration curve is constructed for each chromatogram separately.
- The **Number of Signals** field value determines, for how many signals the calibration curves are constructed and displayed. It is increased automatically according to the number of signals in chromatograms used for calibration.
- The **Flow Marker RT on Signal X** fields are filled with values from the first standard chromatogram and are used as a base for all subsequent standards and samples. The field can be edited and the value is then applied as a base for all chromatograms (including the first one).
- The **Curve Fit Type** can be selected from polynomial regression with **n** between *1* and *5*.
- The **Recalibration Search Window** gives (in %) the maximum deviation of standard peak RT from the stored value to perform the recalibration.
- **K** and **Alpha** fields give the *Mark-Houwink* parameters used for universal calibration. Default values are used to display the calibration curve, if no

chromatogram is opened (otherwise the **K** and **Alpha** from the actual chromatogram are used).

- The **Peak Height (%)** value determines the position of points used for construction of calibration curve in case multiple broad standards with *Hamielec linear fit* are used.

Caution! *Change in this value will have effect only after recalibrating by the **Set Broad Peak** command.*

Note: *Some fields may be unavailable or not editable depending on the calibration type selected.*

3.6.2 Narrow Calibration

Narrow calibration can be used, if narrow molecular weight distribution standards (*polydispersity < 1.2*) are available for given polymer. Calibration curve is constructed from detected peak maximum retention times and known **Mp** values. Alternatively, *(Mw.Mn)^1/2* values can be used, if **Mp** values are not declared.

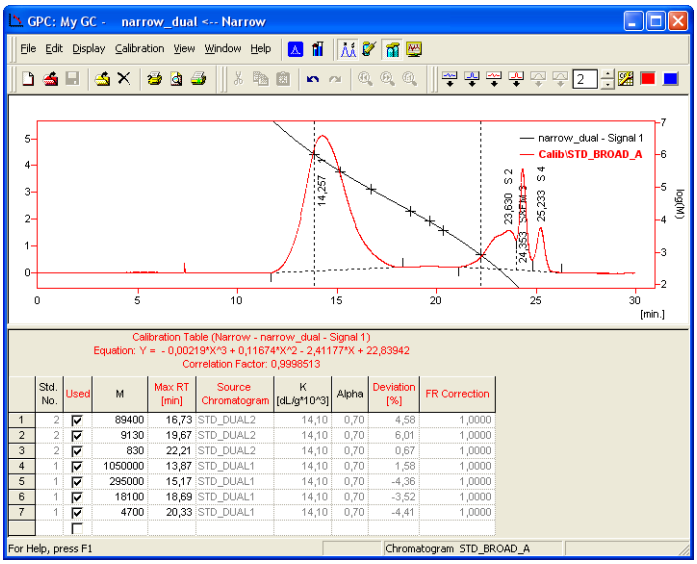


Fig. 16. GPC Calibration (Narrow)

After selecting the calibration type, a standard chromatogram can be opened. The **Add all Narrow Peaks** icon will transfer the integrated peaks data to the **Calibration Table**, setting a new standard number for each standard chromatogram opened and creating a new line for each peak in the standard. The **Add Narrow Peak** icon will perform this peak by peak.

For multi-signal standards the **Set RT To All Narrow Peaks** icon is used for transferring the **RT** on subsequent signals to calibration for peaks where **RT** is not used. Operation is performed only for peaks with **Std No.** value equal to current **Std No.** indicated on **Calibration** window toolbar. This command can also be used for recalibration by selected standard. In this case **RT** of standard peak must match **Std No** values as described and also match **Recalibration Search Window** of peak being recalibrated (see **3.6.1 - GPC Calibration Options** on pg. **14**). The **Set RT To Narrow Peak** performs this operation peak by peak.

Caution! *The calibration curve and equation will not be displayed, if the equation could not be constructed using all the points marked as used. Please check, that you have entered retention times and molecular weights for all points to be used in the calibration.*

Note: *Calibration curve is cut off on nearest local extreme outside the minimum and maximum RT to assure it is monotonous on definition interval. Definition interval is checked during all computations.*

Note: *If local extreme occurs between the minimum and maximum RT, "**Invalid points to construct curve**" error is reported. Check the correctness of your data (typing mistake in **Mp** value is a typical problem) or decrease the polynomial fit degree.*

3.6.3 Multiple Broad Linear Calibration

This method utilizes **Broad Standards** with solely known **Mn** and **Mw** values. The *Hamielec method* assumes that the calibration can be approximated by straight line in the area of Broad Peak being calibrated. The software uses numeric *Newton method* for calculating **A** and **B** parameters of linear calibration curve of given peak. Accuracy of **Mn** and **Mw** values calculated is about 1e-5 in comparison to **Mn** and **Mw** values documented for the standard. **Multiple Broad Peaks** can be used subsequently to extend area of calibration reliability. Three points for each peak are used to construct a result (non)linear calibration curve. One point is peak **Max RT**, the others are computed in **Peak Height (%)** entered in the **GPC Calibration Options** dialog.

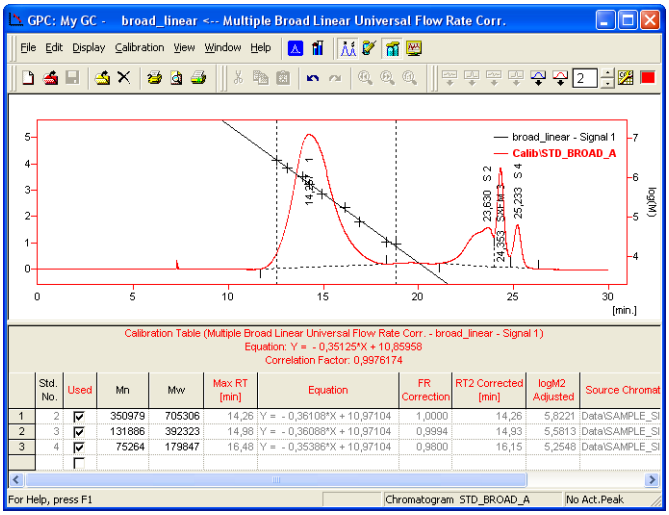


Fig. 17. GPC Calibration (Broad Linear)

After selecting the calibration type, a standard chromatogram can be opened. The **Add Broad Peak** icon will transfer the integrated peak data to the **Calibration Table**, setting a new standard number and creating a new line for each peak.

For multi-signal standards the **Set Broad Peak** icon is used for transferring the peak data on subsequent signals to calibration. Operation is performed only for peak with **Std No.** value equal to current **Std No.** indicated on **Calibration** window toolbar.

Note: *Calibration curve is cut off on nearest local extreme outside the minimum and maximum RT to assure it is monotonous on definition interval. Definition interval is checked during all computations.*

Note: *If local extreme occurs between the minimum and maximum RT, "**Invalid points to construct curve**" error is reported. Check the correctness of your data (typing mistake in **Mn** and **Mw** value is a typical problem) or decrease the polynomial fit degree.*

Note: *The last **Broad Peak** is temporarily remembered and used in subsequent recalculations. **Current Broad Peak** is indicated in right lower corner of the **Calibration** window.*

3.6.4 Multiple Broad Integral Calibration

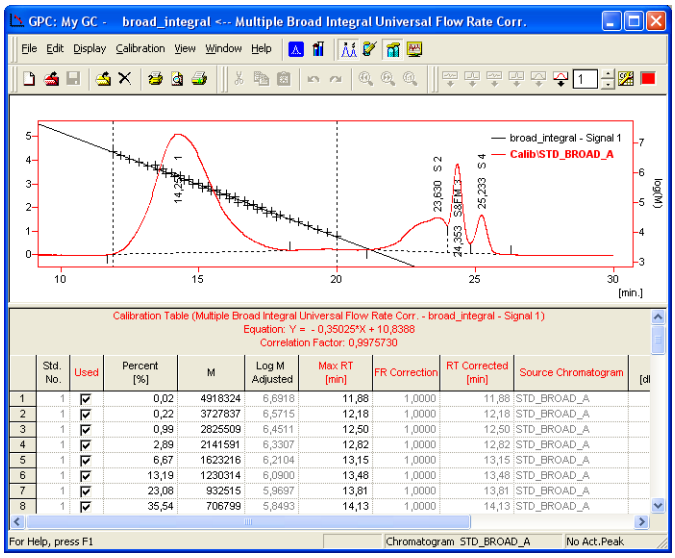


Fig. 18. GPC Calibration (Broad Integral)

The standard to be used will have a table detailing the **% Cumulative Weight Fraction** (**Percent [%]** in YL-Clarity) and **Molecular Weight** (**M**) values supplied by the manufacturer of standard. **Multiple Broad Peaks** can be used subsequently to extend the area of calibration reliability.

After selecting the calibration type the **Percent [%]** and **M** parametres must be entered manually. Standard chromatogram should be opened next. The **Set Broad Peak** icon will recalculate the **% Cumulative Weight Fraction** values entered into **RT** using the peak being calibrated. Operation is performed only for rows with **Std No.** value equal to current **Std No.** indicated in the **Calibration** window toolbar.

The **% Cumulative Weight Fraction** and **Molecular Weight** values are common for all signals. If this type of calibration is to be used for multi signal chromatograms, the **Detector Delay** function should be used to put the signals on a common time base.

Note: *Calibration curve is cut off on nearest local extreme outside the minimum and maximum RT to assure it is monotonous on definition interval. Definition interval is checked during all computations.*

Note: *If local extreme occurs between the minimum and maximum RT, "**Invalid points to construct curve**" error will be reported. Check the correctness of your data (typing mistake in **Percent** or **M** value is a typical problem) or decrease the polynomial fit degree.*

Note: *The last Broad Peak is temporarily remembered and used in subsequent recalculations. Current Broad Peak is indicated in right lower corner of **Calibration** window.*

3.6.5 Broad On Narrow Calibration

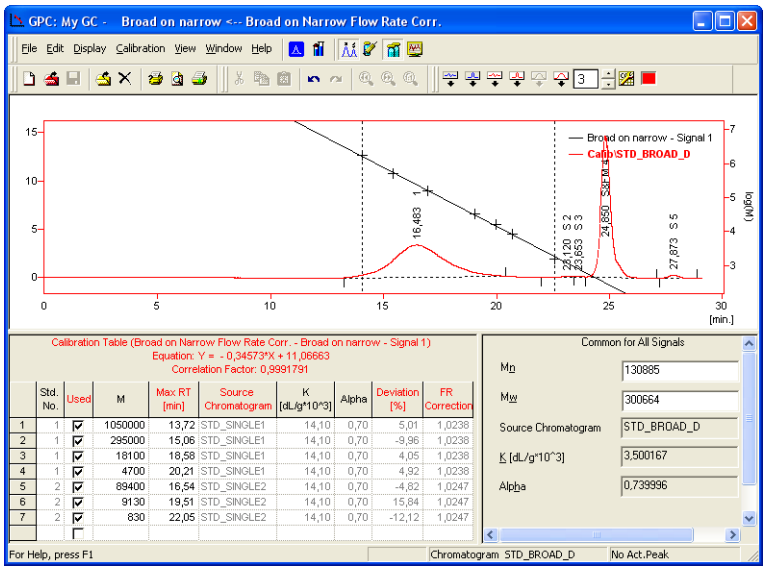


Fig. 19. Broad on Narrow Integration

This method first requires the calibration of the column with a series of *Narrow Standards* and then a calibration with a *Broad Standard* with known **Mn** and **Mw**. It relies on a principle that *Narrow Standards* are used to characterize the shape of the calibration curve, while the *Broad Standard* is then run to compute suitable **K** and **Alpha** using numeric *Newton method*. Accuracy of **Mn** and **Mw** values calculated is about 1e-5 in comparison to **Mn** and **Mw** values documented for the standard.

After selecting the calibration type, a narrow standard chromatogram can be opened. The **Add All Narrow Peaks** icon will transfer the integrated peaks data to the **Calibration table**, setting a new standard number for each standard chromatogram opened and creating a new line for each peak in the standard. The **Add Narrow Peak** icon will perform this peak by peak.

For multi-signal standards the **Set RT To All Narrow Peaks** icon is used for transferring the **RT** on subsequent signals to calibration for peaks where **RT** is not used. Operation is performed only for peaks with **Std No.** value equal to current **Std No.** indicated on **Calibration** window toolbar. This command can also be used for recalibration by selected standard. In this case **RT** of standard peak must match **Std No.** values as described and also match **Recalibration Search Window** of peak being recalibrated (see **3.6.1 - GPC Calibration Options** on pg. **14**). The **Set RT To Narrow Peak** performs this operation peak by peak.

Broad Standard chromatogram can be opened next and **Mn** and **Mw** values should be entered. The **Set Broad peak** icon will compute desired **K** and **Alpha** values and display them in appropriate input boxes.

Keep in mind that:

- The calibration curve and equation will not be displayed, if the equation could not be constructed using all the points marked as used. Please check that you have entered retention times and molecular weights for all points to be used in the calibration.
- Calibration curve is cut off on nearest local extreme outside the **Minimum RT** and **Maximum RT** to assure it is monotonous on definition interval. Definition interval is checked during all computations.

- If local extreme occurs between the **Minimum RT** and **Maximum RT**, "**Invalid points to construct curve**" error will be reported. Check the correctness of your data (typing mistake in **Mp** value is a typical problem) or decrease the polynomial fit degree.
- The last **Broad Peak** is temporarily remembered and used in subsequent recalculations. **Current Broad Peak** is indicated in right lower corner of the **Calibration** window.
- The **Universal Calibration** cannot be used for **Broad On Narrow** because computed **K** and **Alpha** values will be overwritten by **K** and **Alpha** of unknown sample. If you know **K** and **Alpha** of unknown sample, use **Narrow Universal Calibration**.
- When **Broad On Narrow** calibration type is used, the **K** and **Alpha** values fields in the **Chromatogram - GPC Results** tab are inactive, because these values are loaded from the calibration results.

3.7 Export

To transfer data from **YL-Clarity** to other programs, the simplest way is through the **Windows Clipboard**, i.e. using the **Copy** (Ctrl + C) and **Paste** (Ctrl + V) commands on the selected table area.

3.7.1 Export of Graphs

The Chromatogram (including overlaid calibration curve), **Mw Distribution** or **Cumulative Mw Distribution** graphs can be transferred to other programs using the **Export**, **Save As Picture to Clipboard** or **Save As Picture to File** commands. The actually displayed graph pane will be copied to clipboard or saved into a file in an *.EMF vector graphic format and can be pasted or inserted to any **MS Office** document. It is advisable to apply all desired formatting to the picture (fonts, sides ratio, etc.) completely in **YL-Clarity** prior to performing the export command.

3.7.2 Export of Data

The **Export Data** dialog accessible using the **Setting - Export Data** command from the **Instrument** window will change to **Export GPC Data** in GPC mode. The same dialog opens also using the **File – Export - Export Data** command in the **Chromatogram** window. Settings made in the **Export GPC Data** dialog will be used during automated processing for the checked **Export Data** checkbox in the **PostRun Setting** and **Batch** dialogs.

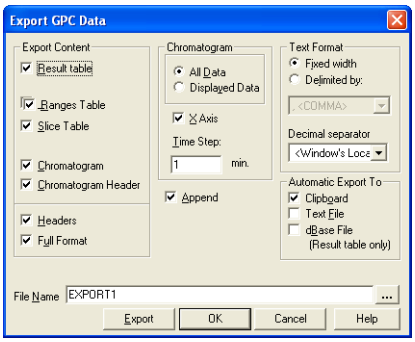


Fig. 20. Export GPC Data

Caution! *Only commands different from the standard **Export Data** dialog will be described here.*

Result Table

Exports all the columns available for **Result Table**, each peak on separate line.

Slice Table

Exports all the columns available for **Slice Table**, continuously for all peaks. (**Peak No.** will be exported as one of the columns)

Ranges Table

Exports the **Ranges Table**.

Chromatogram

Exports the time/signal values according to the settings in the Chromatogram area.

Chromatogram Header

Exports the chromatogram information including the calibration file details.

All other options behave in the same way as in standard mode, see the **YL-Clarity Reference Guide** chapter **2.6.1** – **Export Data**.

3.7.3 Export Summary table

The summary table is exported as a *.TXT file from the **Chromatogram** window using the **File – Export - Export Summary Table** command. The export is performed according to the actual setup used for the **Summary** tab. The setup can be changed using the **Setup Columns** and **Summary Options** commands from the table local menu.

3.7.4 Export Chromatogram

The **Export Chromatogram** options are the same as in standard mode, see the **YL-Clarity Reference Guide** chapter **3.1.12** – **Export Chromatogram**.

3.8 Printing

The **Report Setup** command in the **GPC mode** opens the **Report Setup** dialog. Only the **Method**, **Chromatogram** and **Results** tabs are different from standard mode and will be described here.

3.8.1 Report Setup - Method

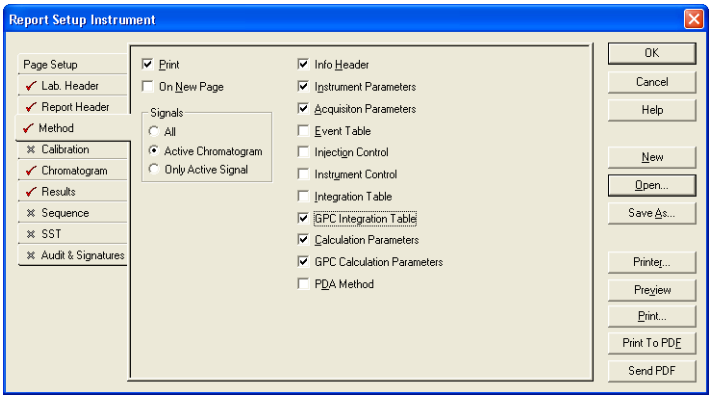


Fig. 21. Report Setup - Method

The added **GPC Integration Table** and **GPC Calculation Parameters** correspond to the new **GPC Integration** and **GPC Calculation** tabs in the **Method Setup** dialog.

3.8.2 Report Setup - Chromatogram

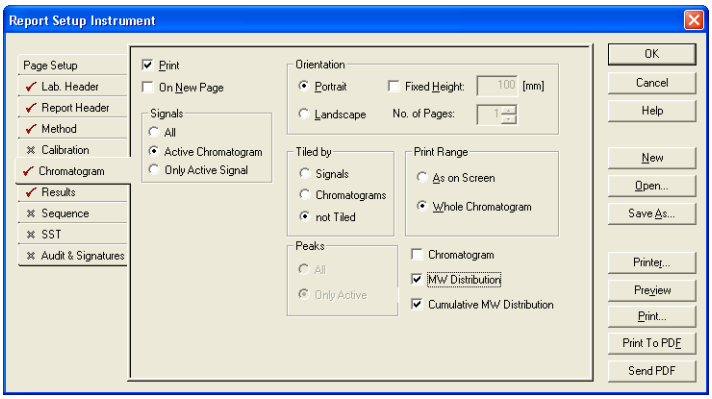


Fig. 22. Report Setup - Chromatogram

The printing of **Chromatogram**, **MW Distribution** or **Cumulative MW Distribution** can be individually selected by the appropriate checkboxes. All graphs are printed using the common **Orientation** settings.

The **Peaks** option set will be active only if the **Tiled by Signals** option has been selected. It will then print the **MW Distribution** and **Cumulative MW Distribution** graphs for all or only for active peak in each signal.

Other options are the same as in standard mode, see the **YL-Clarity Reference Guide** chapter **8.6** - **Chromatogram**.

3.8.3 Report Setup – Results

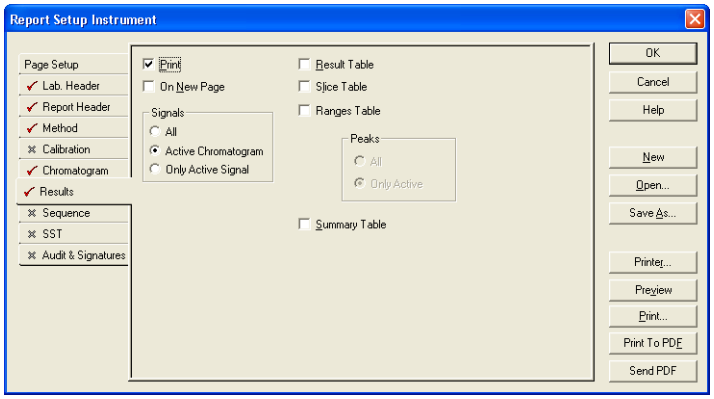


Fig. 23. Report Setup – GPC Results

The printing of **Result Table**, **Slice Table, Ranges Table** or **Summary Table** can be individually selected by the appropriate checkboxes. The **Slice Table** and **Ranges Table** can be printed for the active peak or for all peaks from the given signal. This setting is common for both tables and can be set in the **Peaks** area.

Note: *The peak is set active by clicking on its row in Results table. During automatic printing (from postrun, sequence or batch), the first peak is considered as active.*

The tables are printed as configured on the display (with exception of fonts). The setup can be changed using the **Setup Columns** command from the table local menu, eventually by the **Summary Options** command for the **Summary Table.**

YL-Clarity Extensions

SST

ENG

Tel: +82-31-428-8700
Fax: +82-31-428-8779
Email: export@younglin.com
www.ylinstrument.com

Young Lin Bldg., 899-6, Hogye-dong,
Anyang, 431-836
The Republic of Korea

YL INSTRUMENT CO., LTD.

1 SST System Suitability Test

1.1 What is the SST Module?

The *System Suitability Test* (**SST**) is an integrated module designed to validate a chromatography system based on the evaluation of chromatograms that have been acquired from the **YL-Clarity** station.

Validation is a process that determines whether certain components (peaks or groups of peaks) from a chromatogram, comply with selected parameters (calibrated quantity, retention time, asymmetry, etc.).

YL-Clarity permits both individual and batch validations of either individual chromatograms or a group of them. The user can easily change the number of validated components, sets of validation parameters, values of validation limits and the type of calculation methodics. It is also possible to choose between testing mean of all values or individual results within a group of chromatograms.

Even though validation primarily focuses on testing system reliability, it can also be used in many other ways.

Validation can be run during measurements, or additionally, using batch processing. Validated data can be automatically saved to a database file for further processing.

In connection with a sequence, the **SST** module can even pause a sequence when a specified value has been exceeded or to perform predefined functions.

1.2 How to get SST Module?

SST is an optional part of the **YL-Clarity** station. By purchasing the **SST** together with the station this optional software feature will automatically be installed.

Additionally, by purchasing the **SST**, you will be provided with a new user code. Entering this new user code into the **YL-Clarity** station will allow access to the integrated **SST** module.

1.3 System Suitability Testing

A key **GLP/GMP** requirement in analytical laboratories is validation. This requirement is divided into the validation of equipment (chromatograph and PC) and of methods. **SST** verifies the parameters achieved by measuring on a validated instrument using a validated method.

The most frequent parameter monitored is *analysis reproducibility*, where the standard deviation of monitored parameters must not exceed the specified range.

SST module provides tools for *Performance Qualification* (**PQ**) and together with **Validator** also for *Operational Qualification* (**OQ**).

2 How to Set the SST?

This chapter includes practical procedures for setting the **SST** module to suit your individual requirements.

2.1 Conditions for SST Use

The following requirements must be fulfilled in order to start a validation:

Setting the *SST method* on an instrument

You can either open an existing **SST** method using the **SST – Open** command in the **Chromatogram** window, or create a new **SST** method using the **SST – New** command.

Calibrated chromatograms

Components in validated chromatograms are identified according to the component name (i.e. you can only validate identified components).

Opening a chromatogram(s) in the Chromatogram window

Validation calculations will automatically run after a chromatogram has been opened in the **Chromatogram** window. (It is not necessary to press any button.)

Remember that, when recording validation results in a database file, they will only be recorded when the chromatogram closes.

Note: *Chromatograms are closed using the **Close**, **Close All** commands or by closing the **Chromatogram** window. If the **Overlay** mode has been disabled, loading a new chromatogram will close the previous one.*

2.2 Creating SST method

- Open the **Chromatogram** window.
- Click on the **SST Result** tab.
- Open any calibrated chromatogram.
- Use the **Update from Calib** command in the **SST** menu. This will transfer the list of all components from the linked calibration into the **component table** (on the left), regardless of whether they are identified in the current chromatogram.

Note: *This command is also accessible in the local menu after clicking the right mouse button on the **SST Result** tab.*

- Using the checkboxes in the **Used** column of the **component table**, select the components to be included in the validation.

Note: *Components can be eliminated from a validation using the **Delete Component** command. Thereby you can eliminate components which will not be used and which would only make the **component table** too complex.*

- Specify which parameters are to be monitored using the **SST - Parameters** command.
- Switch to the next tab **SST Properties** – **Subparameters** dialog. Here, specify the limit values from which parameters are to be evaluated.
- In the other tabs, select the method for calculating parameters (**Calculate By**), user-defined events for exceeded limits (**Events**) and finally, whether validation results are to be saved in the database file (**General**).
- Close the **SST Properties** dialog by clicking **OK**.
- In the **component table**, mark the component for which you want to enter a limit value.
- In the **parameters table** (on the right), fill-in the limit values.

Note: *Each component may be validated according to different parameters. For example; one may be validated according to the amount of a component (**Amount**), while another is validated according to the peak height (**Height**).*

- Then, from the **component table**, select another component and enter its values in the **parameters table**.

- Repeat this procedure for all components that you want to include in the validation.

Note: *Parameters can easily be added or removed from a validation by double-clicking on the header of the relevant parameter column in the **parameters table**.*

- Save the **SST** method using the **Save** command.

Note: *You can make the **parameters table** more synoptic by hiding unused (grey) columns and rows using the **Show All Columns** and **Show All Rows** commands in the **SST** main menu. In this case, columns/rows cannot be activated or deactivated by double-clicking on them.*

2.3 Step-by-step validation

Prior to running validation, the following points must be made clear:

What do I want to validate?

- Individual chromatograms – monitor whether or not the values of individual parameters meet specified criteria – the **Overlay** mode must be disabled.
- Chromatographic system – monitors whether the mean values or standard deviations of individual parameters fall between specified limits - the **Overlay** mode must be enabled.

b) When do I want to validate?

- During analysis (online) – results are automatically loaded to **Chromatogram** window from single runs or from sequence.
- Subsequently (offline) – chromatograms measured earlier are either loaded manually into the **Chromatogram** window or batch processed using **Batch** command.

Note: *In the **YL-Clarity** station the **Overlay** mode allows more chromatograms to be simultaneously opened in the **Chromatogram** window. When the **Overlay** mode is switched off, only the currently open chromatogram will be validated against specified limit values.*

Note: *Certain terms are explained in Chapter **3** - **Reference Description**.*

2.3.1 Validation of the chromatographic system

When validating a chromatographic system we monitor whether or not the mean values or standard deviations of monitored parameters of are complying with specified criteria.

OK	Chromatogram	Retention Time [min.]	Area [mV.s]
	Lower Limit	6,600	560,000
	Mean	6,618	556,748
	RSD [%]	0,19	13,51
	Parameter Result	✓	✗
✓	C:\CSW32\WORK1\WORK1\data\SR1_0612	6,630	629,507
✗	C:\CSW32\WORK1\WORK1\data\SR1_0710	6,598	394,989

Note: *When validating a chromatographic system, the results of individual chromatograms found in the list of validated chromatograms under the bold line in the **parameters table** are irrelevant.*

✗	C:\CSW32\WORK1\WORK1\data\SR1_2711	8,207	1133,460
?	C:\CSW32\WORK1\WORK1\data\SR_1712	-	-
✓	C:\CSW32\WORK1\WORK1\data\SR1_0110	8,223	1592,070
✓	C:\CSW32\WORK1\WORK1\data\SR1_0112	8,227	1620,718
✓	C:\CSW32\WORK1\WORK1\data\SR1_0211	8,221	1623,894

A chromatographic system can be validated *online* (running) or *offline* (loading of earlier measured chromatograms into the **Chromatogram** window).

2.3.1.1 Online – Sequence (or Single Run)

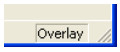
During an online validation, the measured chromatograms will gradually and automatically be opened in the **Chromatogram** window.

Validation results will automatically be updated with every new chromatogram.

- In the **Chromatogram** window switch to the **SST** tab and open the **SST** method using the **SST – Open** command.

Note: *If it is not available yet, create a new one, see **2.2** - Creating SST method on pg. **2**.*

- Close any chromatograms that are still open in the **Chromatogram** window using the **File – Close All** command.
- Check that the **Overlay** mode has been enabled. E.g. in the bottom-right corner of the **Chromatogram** window.



Note: *If **Overlay** has been disabled (the word "Overlay" is shaded grey), enable it by double-clicking on it.*

- Ensure that automatic loading of measured chromatograms into the **Chromatogram** window has been enabled; see the instrument in **PostRun Settings** (opened using the **Setting – PostRun** command in the **Instrument** window). There must be the symbol in front of the chromatogram icon in the flowchart of the **Instrument** window. If this is not the case, then switch it on by clicking the symbol.
- Switch to the **Sequence** window and run the prepared sequence. When running a single analyses, gradually run them in the **Single Run** dialog.
- All measured chromatograms will automatically be opened in the **Chromatogram** window and added to the validation.
- After measuring the final sample, switch to the **Chromatogram** window, then switch to the **SST** tab and check the validation results.

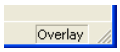
2.3.1.2 Offline - Manual

Manual validation can be performed on already measured chromatograms. The advantage is that these chromatograms may be measured in various sequences. Manual validation is used for "ex-post" verification of system suitability.

- In the **Chromatogram** window switch to the **SST** tab and open the SST method using the **SST – Open** command.

Note: *If it is not available yet, create a new one, see **2.2** - Creating SST method on pg. **2**.*

- Close any still open chromatograms in the **Chromatogram** window using the **File – Close All** command.
- Check that the **Overlay** mode has been enabled. E.g. in the bottom-right corner of the **Chromatogram** window.



Note: *If the **Overlay** has been disabled (the word "Overlay" will be shaded grey), switch it on by double-clicking on it.*

- Using the **File – Open** command open all the chromatograms that are to be included in the validation.

Note: *More files can be selected simultaneously by left-clicking on them while holding down on the CTRL key (file-by-file selection) or SHIFT key (continuous selection). You can select all files in the directory using the CTRL + A keyboard shortcut. For details see **Reference Guide** Chap. **3.1.2** – **Open**.*

- Check the validation result in the **SST** tab.

2.3.1.3 Offline - Batch reprocess

Batch opening and processing of chromatograms can be used for "ex-post" validation that works similarly to simple opening of chromatograms in the **Chromatogram** window with the **Overlay** mode enabled.

Note: *Use batch opening if you want to batch adjust opened chromatograms prior to a validation, otherwise opening chromatograms in the **Chromatogram** window is more suitable, see Chapter **2.3.1.2**.*

- Open the **SST** method in the **Chromatogram** window using the **SST – Open** command.

Caution! *The **Overlay** mode in the **Chromatogram** window must be enabled.*

- Switch to the **Instrument** window and open the **Batch** dialog using the **Analysis - Batch** command.
- In the **Batch** dialog, select the chromatograms intended for validation.

Caution! *The **Open Chromatogram Window** item must be selected!*

Note: *The **Reference Guide** contains a detailed description of the **Batch** dialog.*

- Using the **Proceed** button will run a batch processing of selected chromatograms.
- All batch-processed chromatograms will automatically open in the **Chromatogram** window.
- You can view the validation result in the **SST Result** tab.

2.3.2 Chromatogram validation

During a chromatogram validation, it is determined whether or not the parameters of individual chromatograms meet specified criteria.

Individual chromatograms can be validated either *online* (running) or *offline* (loading of earlier measured chromatograms into the **Chromatogram** window).

With the **Overlay** mode disabled, the **Chromatogram** window will always show only one chromatogram. Regardless of from where we open a chromatogram (**Single Run**, **Sequence**, **Open Chromatogram**, **Batch**), every result will always be related to the current chromatogram.

Note: *The overall validation result indicates whether or not the chromatogram has complied with all criteria for all components; the **component table** displays results for individual components.*

- Open the SST method in the **Chromatogram** window using the **SST – Open** command.

Caution! *The **Overlay** mode in the **Chromatogram** window must be disabled.*

- Using any arbitrary method (from an analysis or, additionally, from a file), open a chromatogram in the **Chromatogram** window.
- All data in the **SST Result** tab relate to the currently opened chromatogram.

2.3.3 Summary table of validated chromatograms

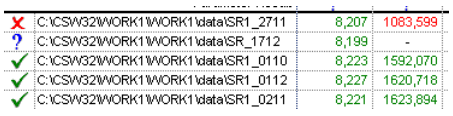
In the summary table of validated chromatograms, one can easily and quickly determine if a chromatogram is deviating out of line.

The procedure for setting the **SST** method is the same as a chromatographic system validation.

Caution! *The **Overlay** mode in the **Chromatogram** window must be enabled.*

In the parameters table you can set limit values for the measured results to comply with.

Only the list of chromatograms in the **parameters table** and icons to the left of it are relevant.



✗	C:\CSW32\WORK1\WORK1\data\SR1_2711	8,207	1083,599
?	C:\CSW32\WORK1\WORK1\data\SR_1712	8,199	-
✓	C:\CSW32\WORK1\WORK1\data\SR1_0110	8,223	1592,070
✓	C:\CSW32\WORK1\WORK1\data\SR1_0112	8,227	1620,718
✓	C:\CSW32\WORK1\WORK1\data\SR1_0211	8,221	1623,894

Note: *All other results (overall validation result, results in the component table, as well as results in the **parameters table** - above the bold line) refer to the chromatographic system validation.*

Chromatogram	Retention Time [min.]	Area [mV.s]	Height [mV]
Lower Limit	8,100	1100,000	
Upper Limit	8,300	1400,000	
%RSD Limit			
Mean	8,221	1517,531	423,708
RSD [%]	0,20	14,08	14,07
Parameter Result	✓	✗	?

2.3.4 Storing results in DBF

Results saved in a database file can be freely used, for example, a system validation according to special validation methods, to monitor trends in results, etc.

Note: *Setting of the **Overlay** mode has no affect on results saved in the database file.*

- Open the **SST** method in the **Chromatogram** window using the **SST – Open** command.
- Open the **SST Properties - General** dialog, in the **Chromatogram** window using the **SST – General** command.
- Here, select the **Log SST Result into DBF file** and fill-in the database file name in the **File Name** item.
- Use the **YL-Clarity** station either *online* (measuring) or *offline* (opening saved chromatograms).

Note: *Only chromatograms opened in the **Chromatogram** window will be saved in the database file.*

…

- Open the created database file in the database program. The database file is automatically created in the current project directory.

Caution! *If you open the database file in another program, the **SST** module cannot write into it. Work with the database file only after completing work with the **YL-Clarity** program, thereby avoiding an unwanted locking of the file while saving results.*

3 Reference Description

The **SST** module is represented in the **YL-Clarity** station as the **SST Result** tab in the bottom part of the **Chromatogram** window.

3.1 Chromatogram – SST Result

The **SST** tab in the **Chromatogram** window contains two tables used for setting validation parameters – **component table** (on the left) and **parameters table** (on the right) of a selected component.

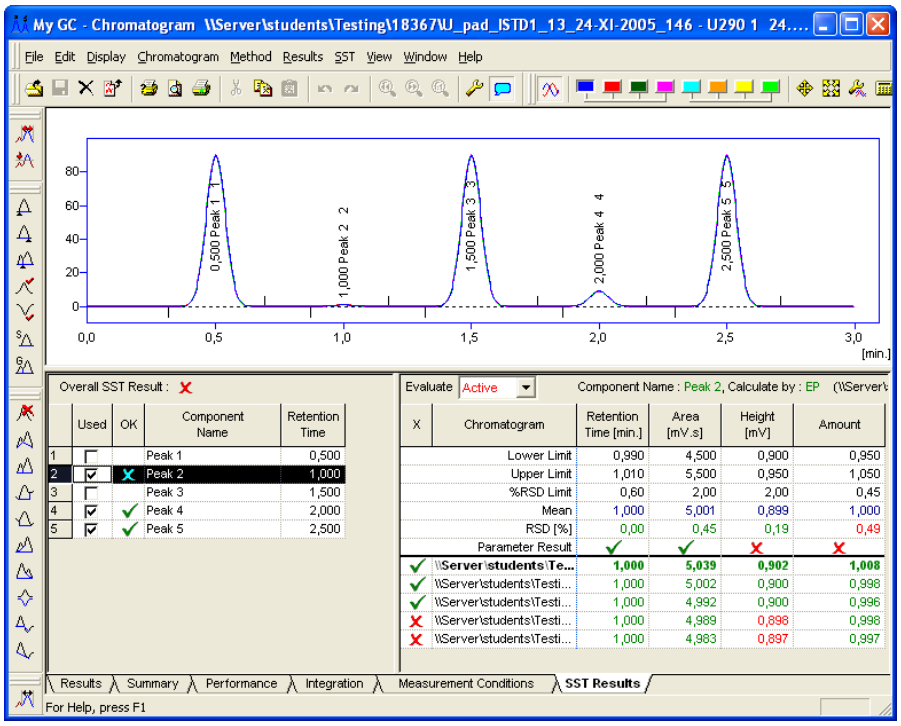


Fig. 1. Chromatogram – SST Result

Tables in the **SST** module use graphical symbols depicting the validation result at individual levels:
parameter, chromatogram, component, overall validation.

Symbol meanings are as follows:

✓ Validation was successful

? Validation could not be run (e.g. no parameters specified) – validation result unknown

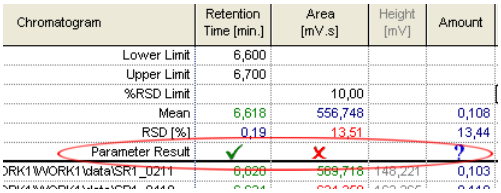
✗ Validation was unsuccessful

3.1.1 Validation results hierarchy:

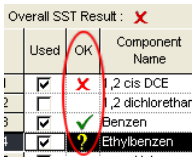
Validation results are created hierarchically. Arranged in ascending order: *parameter -> component – overall evaluation*.

Note: *Chromatogram validation is not subject to this hierarchy when system validation does not involve individual chromatograms-"Mean of all values" is selected in Subparameters of SST Properties.*

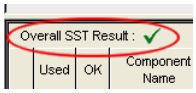
- **Parameter**
  Validation results for individual parameters are found in the **parameters table** on the **Parameter Result** line. For successful validation, the mean value (or standard deviation) must lie within specified limits.



- **Component**
  The validation result for a component is found in the **component table** in the **OK** column. For successful component validation, all component parameters must be successfully validated.



- **Overall validation**
  The overall validation result (**Overall SST Result**) is found in the **component table**. For successful overall validation all components in all monitored parameters must be successfully validated.



One unsuccessfully validated *parameter* will cause an unsuccessful *component* validation and therefore, an unsuccessful *overall validation*.

If at least one parameter is validated with an unknown result, then the component validation and overall validation results will also be unknown.

An *unsuccessful validation* is of a higher priority than an *unknown validation result*. Consequently, if one parameter is validated as unsuccessful and another as unknown, the component validation result will be unsuccessful.

To perform a validation, the **SST** method must be opened (defined) on the instrument.

As soon as you open a chromatogram in the **Chromatogram** window, validation calculations will automatically be made.

3.1.2 Validating multi-detector chromatograms

When using multi-detector chromatograms it is possible to select which signal has to be used for SST evaluation.

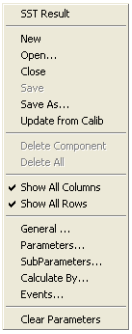
Evaluate

In the header of the parameters table in the SST tab will appear an **Evaluate** combo box with following options: **Active**, **Signal 1**, .., **Signal n**.

The default **Active** option will evaluate the signal that is currently active in the **Chromatogram** window.

Note: *The name of the active signal is indicated in the window header and its description in the graph legend is highlighted in bold letters.*

3.1.3 SST menu



In the main **SST** menu in the **Chromatogram** window, you can access all the **SST** module functions and settings.

Note: *Most commands from the main **SST** menu can also be accessed through the context menus which are opened by right clicking the on the **SST** tab.*

SST Result

Switch to the **SST Result** tab.

(*Click on the tab name at the bottom of the **Chromatogram** window.*)

New

Creating a new **SST** method.

During the initial file saving you will be prompted to enter a filename.

Note: *The filename "NONAME" is reserved and cannot be used.*

Open

Opening a saved SST method.

Close

Closing an open SST method. If the file contains any unsaved changes, you will be prompted to save them.

Save

Saving an SST method.

Save As

Saving a copy of the current SST method under a new filename.

Update from Calib

Transferring data on components (known as the Peak Table) from the current chromatogram.

The chromatogram must be calibrated.

Components are selected by the name not the retention time.

Note: *All components will be transferred from the calibration, even those not identified in the current chromatogram.*

Delete Component

Removing a component from the **SST** method.

Note: *If you do not want to validate a specific component you do not have to remove it, just uncheck the **Used** column in the **component table**.*

Delete All

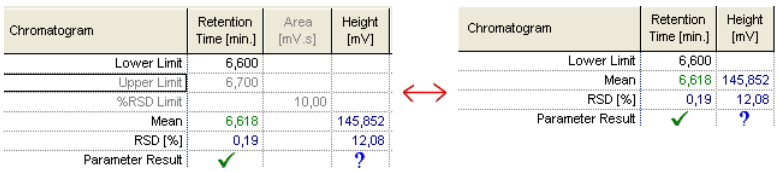
Removing all components from the **SST** method.

Show All Columns

Showing / hiding unused (shaded) columns in tables.

Show All Rows

Showing / hiding unused (shaded) rows in tables.



Chromatogram	Retention Time [min.]	Area [mV.s]	Height [mV]
Lower Limit	6,600		
Upper Limit	6,700		
%RSD Limit		10,00	
Mean	6,618		145,852
RSD [%]	0,19		12,08
Parameter Result	✓		?

Chromatogram	Retention Time [min.]	Height [mV]
Lower Limit	6,600	
Mean	6,618	145,852
RSD [%]	0,19	12,08
Parameter Result	✓	?

General

General description of the **SST** method and setting saving of results in the database file.

See 3.2 - SST Properties – General on pg. 13.

Parameters

Selecting parameters for validation (e.g. Retention Time, Area, …).

See 3.3 - SST Properties - Parameters on pg. 15.

Subparameters

Selecting limits according to which parameters will be evaluated (Lower Limit, Upper Limit, %RSD Limit).

See 3.4 - SST Properties - Subparameters on pg. 17.

Calculate By

Selecting the calculation method according to which parameters will be calculated (EP, USP, JP).

See 3.5 - SST Properties – Calculate By on pg. 18.

Events

Setting special events depending on validation results (e.g. pause sequence).

See 3.6 - SST Properties - Events on pg. 18.

Clear Parameters

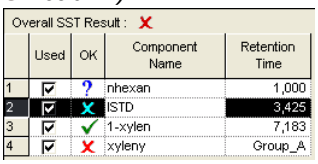
Deleting all set limiting parameters in the **parameters table**.

Applied to the currently displayed component.

3.1.4 Component table (left)

The left section contains a table of results for all components included in a validation . By selecting or deselecting a component in the **Used** column you determine whether or not a component will be included in the overall validation.

Note: *The overall validation result (**Overall SST Result**) is displayed above the **component table.** The validation results for individual components are in the **component table** (in the **OK** column).*



Overall SST Result:

The overall validation result will be marked as successful (✓) only if all components were validated successfully in all monitored parameters.

Used

By selecting/deselecting a component you include it in or exclude it from a validation.

Note: *By right clicking on the **component table** and selecting the **Delete Component** command you can delete a component from a validation. Deleting unnecessary components will make the **component table** synoptic.*

OK

This symbol marks the validation result for a specific component. A component is validated successfully if all monitored parameters are complied with.

Component Name

The name of a monitored component taken from a calibration.

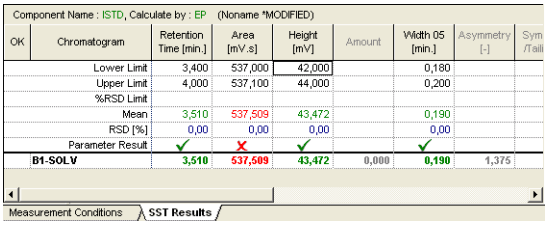
Retention Time

The retention time of a monitored component taken from calibration.

Caution! *In validated chromatographs, components are identified by name and not by retention time.*

3.1.5 Parameters table (right)

The table on the right shows a detailed breakdown of the validation of individual parameters of the component which has been selected in the **component table** on the left.



Note: *You can hide or show unused columns and rows (shaded) using the **Show All Columns/Rows** command in the context menu, which is accessible after right clicking on the **parameters table**.*

The name of the current component (**Component Name**), parameter calculation method (**Calculate By**) and the name of the current **SST** method (in parenthesis) are displayed above the **parameters table**.

Note: *If you have changed the **SST** method and not saved it yet, it will be so indicated by the "*MODIFIED" inscription.*

Individual validation parameters are set in the top section of the **parameters table** (down to the bold line). The mean values for all loaded chromatograms are displayed below them. A list of validated chromatograms is below the bold line.

1. Limiting parameters - Lower, Upper, %RSD Limit

For a detailed description of parameters see 3.4 - SST Properties - Subparameters on pg. 17.

Note: *If more limits are entered for one parameter, then all conditions must be complied with for a successful validation to occur. Limit values are entered directly into the **parameters table** and can differ from component to component.*

2. Summary values – Mean, RSD[%]

Mean – arithmetic mean of monitored parameters from all loaded chromatograms.

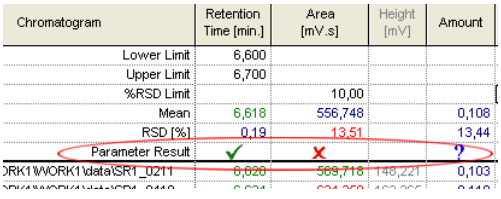
RSD[%] – percentage standard deviation (variation coefficient) of a parameter of the displayed components for all loaded chromatograms. A formula is shown in Chap. 5- Appendix – Mathematical Formula on pg. 23.

Note: *These parameters are useful only when you validate more chromatograms simultaneously. The **Overlay** mode must be enabled.*

The validation procedure is described in detail in Chapter 2.3.1 - Validation of the chromatographic system on pg. 3.

3. Parameter Result

The result of the validation of a specific parameter. If more chromatograms are validated then the more a validation result will relate to the mean parameter value of all validated chromatograms.



4. List of validated chromatograms

A bold line, followed by a list of validated chromatograms completes **parameters table** header. An icon indicating the validation result for a specific chromatogram is displayed in the **OK** column.

✓ - Chromatogram validation was successful (i.e. all values met the defined criteria).

✗ - Chromatogram validation was unsuccessful (i.e. at least one parameter did not meet the defined criteria).

? - The validation result could not be determined (i.e. at least one parameter could not be determined – e.g. parameter was not found in the chromatogram or at least one parameter limit value was left un-entered - **Subparameter**).

X	Chromatogram	Retention Time [min.]	Area [mV.s]	Height [mV]	Amount
	Lower Limit	0,990	4,500	0,900	0,950
	Upper Limit	1,010	5,500	0,950	1,050
	%RSD Limit	0,60	2,00	2,00	0,45
	Mean	1,000	5,001	0,899	1,000
	RSD [%]	0,00	0,45	0,19	0,49
	Parameter Result	✓	✓	✗	✗
✓	**\\Server\students\Te...**	**1,000**	**5,039**	**0,902**	**1,008**
✓	\\Server\students\Testi...	1,000	5,002	0,900	0,998
✓	\\Server\students\Testi...	1,000	4,992	0,900	0,996
✗	\\Server\students\Testi...	1,000	4,989	0,898	0,998
✗	\\Server\students\Testi...	1,000	4,983	0,897	0,997

Fig. 2. Validate individual values

X	Chromatogram	Retention Time [min.]	Area [mV.s]	Height [mV]	Amount
	Lower Limit	0,990	4,500	0,900	0,950
	Upper Limit	1,010	5,500	0,950	1,050
	%RSD Limit	0,60	2,00	2,00	0,45
	Mean	1,000	5,001	0,899	1,000
	RSD [%]	0,00	0,45	0,19	0,49
	Parameter Result	✓	✓	✗	✗
	\\Server\students\Te...	**1,000**	**5,039**	**0,902**	**1,008**
	\\Server\students\Testi...	1,000	5,002	0,900	0,998
	\\Server\students\Testi...	1,000	4,992	0,900	0,996
	\\Server\students\Testi...	1,000	4,989	0,898	0,998
	\\Server\students\Testi...	1,000	4,983	0,897	0,997

Fig. 3. Validate mean of all values

Then the chromatogram name follows along with a summary of values for individual parameters.

Successfully validated values are in green, and values not complying with criteria are in red, while blue values indicate that a result cannot be determined.

	Parameter Result	✓	✗	?
:K1\WORK1\data\SR1_0612		6,630	629,507	162,058

3.2 SST Properties – General

In the **General** tab, you will find information about the **SST** method, edit its description and set it so that results will be saved in a database file.

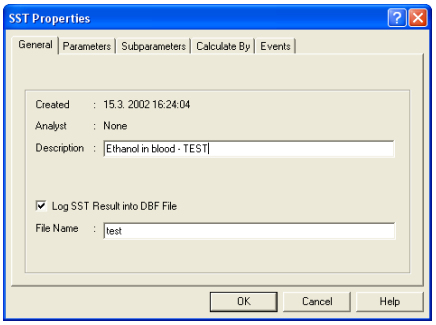


Fig. 4. SST Properties - General

Created

Date of creation of a **SST** method file. Cannot be edited.

Analyst

Name of user who created the **SST** method. The name you enter when opening an instrument will be used. Cannot be edited.

Description

Space to input a personal description of the **SST** method.

Log SST Result into DBF file

The **YL-Clarity** station can save all validation results into an independent database file.

Select **Log SST Result into DBF File** and enter the file name in **File Name** (can be without suffix).

The database file will automatically be created in the current project directory. Then it can be processed further in any arbitrary database program or in Excel, e.g. using contingency tables and graphs (see 4.1 - Using DBF in MS Excel on pg. 20).

Caution! *Validation results for a chromatogram are saved when the chromatogram is closed using the **Close** command or after opening another chromatogram in the **Chromatogram** window.*
*The same applies in the **Overlay** mode – files are saved gradually after closing.*

Caution! *Make sure that the database file is not open at the same time in another program. In this case it is not be possible to save validation results in it!*

3.2.1 DBF file structure:

Each validated chromatogram is saved separately, a separate row is created for each monitored parameter. Columns irrelevant to a given parameter remain empty.

Note: *The database file is automatically created in the current project directory.*

Description of individual columns (category):

- CHROM_NAME
  Chromatogram name (including path, if applicable)

Caution! *The CHROM_NAME field is designed for 256 characters, so the entire name will fit. It can, however, happen that in MS Excel, for example, only the first column of an open *.dbf will be displayed – other columns being beyond the screen size.*

- DATE
  Date of validation
- COMPONENT
  Component name
- PARAM_NAME
  Parameter name
- LO_LIMIT
  Lower limit
- HI_LIMIT
  Upper limit
- VALUE
  Parameter value
- RESULT
  Validation result (PASS, FALL, UNKNOWN)

Note: *Working with *.dbf files in Excel is described in detail in Chapter **4.1** - **Using DBF in MS Excel** on pg. **20**.*

3.3 SST Properties - Parameters

The parameters to be displayed in the **parameters table** and used in a validation are defined by selecting individual items in the **SST Properties – Parameters** dialog.

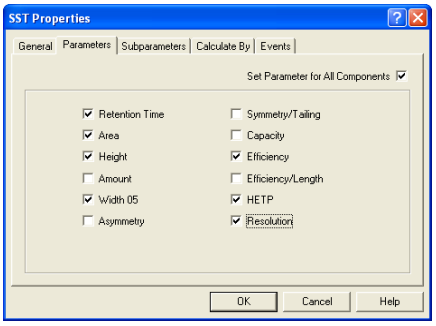


Fig. 5. SST Properties - Parameters

Parameters are included or excluded from a validation by checking the corresponding checkbox.

The list of parameters used in validation is part of the **SST** method file.

Note: *Selecting or deselecting a parameter can be replaced by double-clicking on the header of the respective column in the **parameters table** (on the right)*

Note: *Mathematical formulas for parameter calculation according to selected methods are found in Chapter **5** - **Appendix – Mathematical Formula** on pg. **23**.*

Set Parameters for All Components

An option to select whether the list of used parameters should be applied to all validated components or only to the currently selected component (= component highlighted in the **component table**).

Retention Time

Retention time of validated component.

Area

Component peak area.

Height

Component peak height.

Amount

Calibrated amount of component.

Width 05

Peak width at half its height.

Asymmetry

Peak asymmetry.

Symmetry/Tailing

Calculation of symmetry.

Note: *The name depends on the selected calculation method that is set in the **Calculate By** tab.*

Capacity

Capacity ratio.

Efficiency

Column efficiency.

Note: *The calculation method depends on the selected calculation method that is set in the **Calculate By** tab.*

Efficiency/Length

Length efficiency of the column.

Note: *(The value depends on the selected calculation method that is set in the **Calculate By** tab.*

HETP

Height equivalent to a theoretical plate.

Note: *The value depends on the selected calculation method that is set in the **Calculate By** tab.*

Resolution

Resolution relating to the previous peak (even non-calibrated).

Note: *The value depends on the selected calculation method that is set in the **Calculate By** tab.*

3.4 SST Properties - Subparameters

In the **Subparameters** tab you select which limit values can be entered in the **parameters table**, i.e. whether to check the lower or upper limits or the variation coefficient.

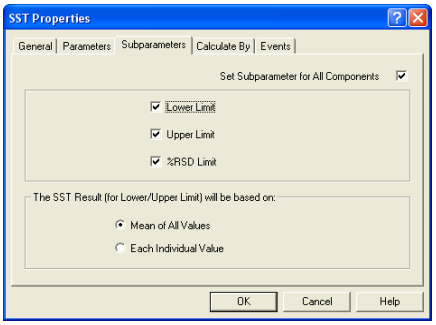


Fig. 6. SST Properties - Subparameters

For a successful validation, at least one of the three offered limit items must be selected.

Note: *You can also enable/disable items directly in the **parameters table** by clicking on their names.*

Set Subparameter for All Components

An option to select whether the list of used parameters should be applied to all validated components or only to the currently selected component (= component highlighted in the **component table**).

X	Chromatogram	Retention Time [min.]	Area [mV.s]	Height [mV]	Amount
	Lower Limit	0,990	4,500	0,900	0,950
	Upper Limit	1,010	5,000	0,950	1,050
	%RSD Limit	0,60	2,00	2,00	2,00
	Mean	1,000	5,001	0,899	1,000
	RSD [%]	0,00	0,45	0,19	0,49
	Parameter Result	✓	✗	✗	✓
✗	\\Server\students\Te...	**1,000**	**5,039**	**0,902**	**1,008**
✗	\\Server\students\Testi...	1,000	5,002	0,900	0,998
✓	\\Server\students\Testi...	1,000	4,992	0,900	0,996
✗	\\Server\students\Testi...	1,000	4,989	0,898	0,998
✗	\\Server\students\Testi...	1,000	4,983	0,897	0,997

Lower Limit

Minimum arithmetic mean value of all loaded chromatograms.

Upper Limit

Maximum arithmetic mean value of all loaded chromatograms.

Note: *If a single chromatogram is validated then the current value will be equal to the mean value. It follows that exceeding the parameter limit value will immediately be visible in the overall validation result (**Overall SST Result**).*

%RSD Limit

Maximum value of the percentage standard deviation (variation coefficient) of a parameter of the displayed component for all loaded chromatograms.

A formula for *%RSD Limit* is available in Chap. **5** on pg. **23**.

The SST Result (for Lower/Upper Limit) will be based on:

Mean of All Values

The **SST** module will compare the Mean of all evaluated values with the **Upper Limit** or **Lower Limit**.

It is not necessary to have all values within the limits to receive successful validation result.

Each Individual Value

The **SST** module will compare each evaluated value with the **Upper Limit** or **Lower Limit**.

Every single value must be within the limits to receive successful validation result.

3.5 SST Properties – Calculate By

The method of an individual parameter calculation is selected in the **Calculate By** tab. The selection of the calculation method effects the following parameters: efficiency (**Efficiency**), length efficiency (**Efficiency/Length**), floor height (**HETP**) and resolution (**Resolution**).

Note: *A mathematical formula for parameter calculation according to selected calculation methods are found in 5 - Appendix – Mathematical Formula on pg. 23.*

EP (European Pharmacopoeia)

Calculation of efficiency and related parameters based on the *width at half height*.

USP (United States Pharmacopoeia)

Calculation of efficiency and related parameters based on *width given by intersection of tangents with baselines*.

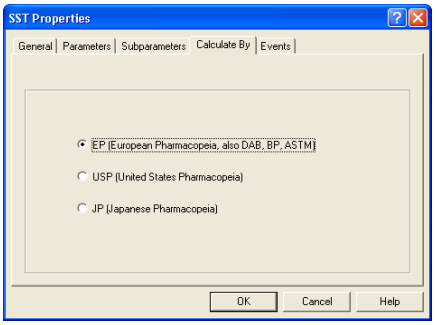


Fig. 7. SST Properties – Calculate By

JP (Japanese Pharmacopoeia)

Calculation of efficiency and related parameters based on *width given by intersection of tangents with baselines*.

3.6 SST Properties - Events

In dependence on **SST** validation results you can use the **Events** tab to set running of other events like sequence pause or running an external program.

On SST Result OK

Once a successful validation result (✓ - **OK**) has occurred, the selected event will be run.

- **Pause Sequence**
  Pausing a running sequence.
- **Run External Program**

Note: *You can also use the **Run External Program** function to for example send a message to an e-mail, SMS or pager. (E.g. see **4.2.1** - **Automatic e-mail sending (SMS)** on pg. **21**.*

On SST Result Unknown

Once an unknown validation result (? **Unknown**) has occurred, the selected event will be run.

- Pause Sequence (see above)
- Run External Program (see above)

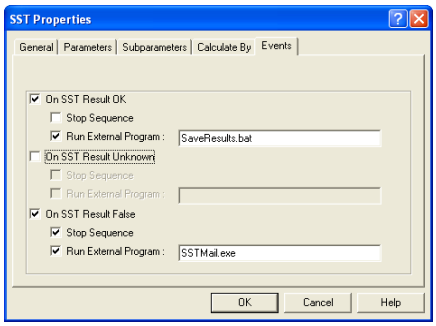


Fig. 8. SST Properties - Events

On SST Result False

Once **False** an unsuccessful validation result has occurred, the selected event will be run.

- Pause Sequence (see above)
- Run External Program (see above)

3.7 Report Setup – SST

The print output properties are set in the **Report Setup** dialog. Settings for printing **SST** validation results are in a separate tab.

Print

Selecting **Print**, will include the **SST** validation results in the report printout. An included tab is highlighted in colour and an excluded tab is shaded grey. The same can be achieved by clicking on the tab name.

Note: *If you only want to print validation results, then you have to disable all other tabs.*

Note: *You can save the printing style for further use by pressing the **Save As** button.*

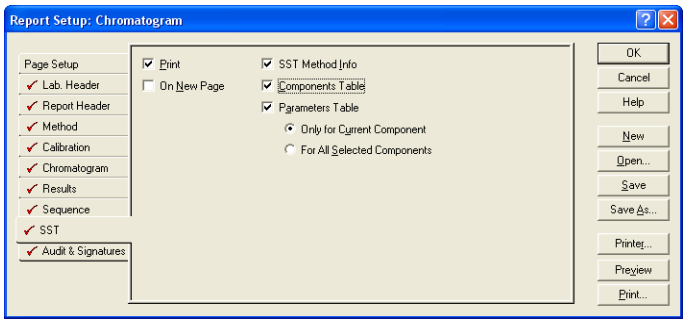


Fig. 9. Report Setup - SST

On New Page

Printing of the respective section (tab) will begin on a new page.

SST Method Info

Current method description – name, date of last save, and a description.

Components Table

Printing the **component table**.

Parameters table

Printing the **parameters table**

- **Only for selected component**
  Printing the parameters of a currently selected component.

Note: *The selected component is highlighted in the **component table**.*

- **For All Selected Components**
  Printing parameters for all monitored components, regardless of which is currently selected.

4 Workarounds

4.1 Using DBF in MS Excel

An experienced user can program selected reports in a database program (Access, dBase, FoxPro, SQL). However, not everyone is a database-programming expert. What if we open a database file containing validation results in a common application, for example **Microsoft Excel**? At first, a complex table will be displayed. Can it be processed in such a way to make it useful?

One option of working with an **SST** dbf file in **Excel** is to use what are known as, **Contingency tables**:

- Select the whole table in MS Excel, e.g. by using the CTRL + A key combination.
- Select the **Contingency tables and graphs** command in the **Data** menu.
- A "*Contingency table wizard"* will appear to help you prepare the table (and graph, if applicable).
- In the wizard, you gradually select the required data (database) and location where the contingency table and graph should be created (a new spreadsheet is a suitable option).
- In the last step (3/3) click the layout button and drag the field names onto the table picture to determine the look of the table layout.
- Using the **Finish** button, create the contingency table and graph.

Note: *This procedure was created for use with MS Excel 2000 and may vary for other versions.*

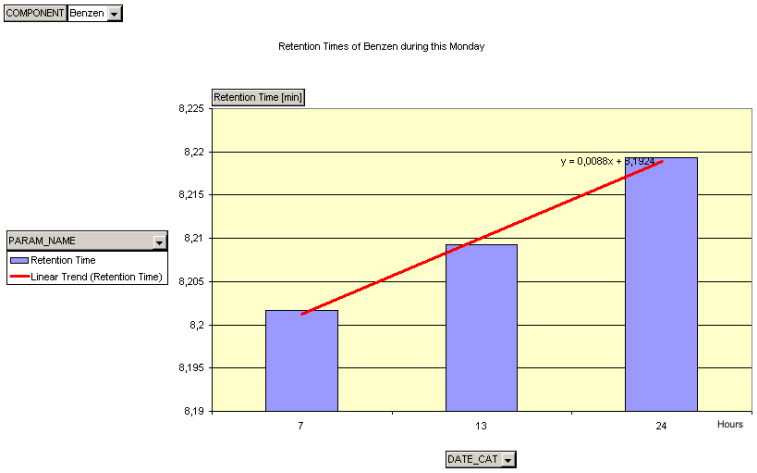


Fig. 10. Example of a contingency graph in Excel

Using a contingency table you can, for example, display a detailed overview of the amount of monitored component in chromatographs.

Or you can have data sorted according to the validation date to compare results for various measurements (e.g. for periodically repeated measurements, or to monitor trends), and so on. Graphs can also be generated simply from the contingency tables using the wizard.

Note: *Detailed information on working with contingency tables is found in the **MS Excel** online help section.*

4.2 Pausing a running sequence

- To set a sequence follow the same procedure as in Chapter **2.3.1.1** - **Online – Sequence** on pg. **3**, inserting the following between steps **4**. and **5.**:

- Select the **SST – Events** command in the **Chromatogram** window.
- In the displayed **SST Properties – Events** dialog select the **Pause Sequence** in item **On SST Result False** parameter.

Note: *Pausing a sequence can also be done along with a pre-defined event (e.g. running a program, sending an e-mail, etc.)*

4.2.1 Automatic e-mail sending (SMS)

If a problem occurs during prolonged analyses, the time lost is usually worse than the material wasted. If your computer is connected to the Internet, then you can easily have the **YL-Clarity** station send an e-mail to your office or a message to a mobile phone.

Lets have a look at how this works in an **MS Outlook** example:

First, a macro must be created using **MS Visual Basic**. This macro is saved as an executable file which is then run from the **YL-Clarity** station.

Note: *We presume that you do have MS Visual Basic installed. This example is prepared for MS Outlook 2000; it should work similarly in other versions.*

Note: *If you are not able to create a similar macro, have it done by your network administrator or you can use the ready **SSTMail** freeware (see below).*

Create a new project in **Visual Basic** and write the following code down:

```
Sub Main()
Set myOLApp = CreateObject("Outlook.Application")

   Set myOLItem = myOLApp.CreateItem(olMailItem)
   With myOLItem
      .Subject = "SST REPORTS ERROR"
      .Body = "Hurry to the laboratory, the test-tubes are lonely!"
      .To = "me@myemail.com"
   End With
   myOLItem.Send

End Sub
```

Note: *Change the text highlighted in yellow as needed. The subject of the e-mail message is entered in the first line, the text in the second and the e-mail address in the third.*

Note: *Sending an SMS message as an e-mail using what is known as an "SMS Gate" is quite common today. If you are not sure whether your operator supports this service or how to activate it, contact you operator's customer support centre.*

Completed macros must be saved as executable files (suffix *.exe).

SSTMail

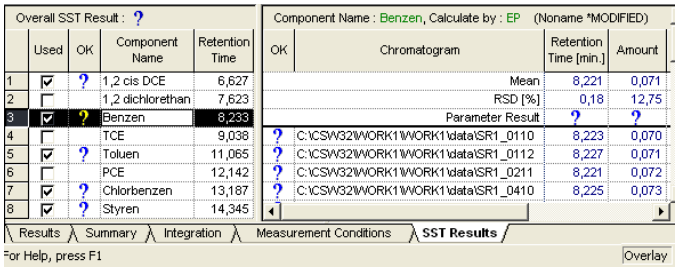
You can also use the ready **SSTMail** freeware utility which is found in the \UTILS\SSTMAIL subdirectory of the main **YL-Clarity** directory. Then simply open the SENDEMAIL.INI file in a text editor (e.g. **Notepad**) and fill-in your own data.

4.3 Sequence summary table

Outputs from **SST** can, to a certain extent, replace the summary tables function for measuring sequences. The means and standard deviations of monitored parameters are calculated directly in the **SST** module of the **YL-Clarity** station.

A separate table, containing summaries of individual parameters, is prepared for each component.

If the **SST** module is only used for summary results, no limit values need be filled-in you simply have to determine which components are to be monitored.



- Open all measured chromatograms in the **Chromatogram** window.

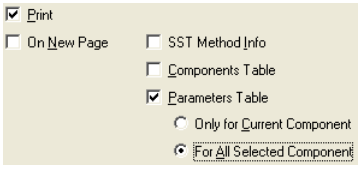
Caution! *The **Chromatogram** window must be switched to the **Overlay** mode.*

- Further, continue only after at least one chromatogram has been opened in the **Chromatogram** window.
- Switch to the **SST Result** tab.
- Create a new **SST** method using the **SST – New** command.
- Using the **SST - Update from Calib** command, transfer components from the calibration connected to the current chromatogram, into the **SST** method.

Caution! *Chromatograms must be calibrated.*

- In the **Used** column of the **component table**, select which components are to be summarised.
- Select which parameters are to be monitored using the **SST – Parameters** command.
- Switch to the **Subparameters** tab and uncheck the selection of all three items.
- Close the **SST Properties** dialog using the **OK** button.

- Using the **SST – Show All Columns** and **Show All Rows** commands you can hide inactive rows and columns in the **parameters table**.
- Now the **parameters table** will display a summary table of all loaded chromatograms for the currently selected component in the **component table**.
- Using the **File – Report Setup** command, open the **Report Setup** dialog and switch to the **SST** tab.
- Select the **Print** command in the top-left corner.
- Select the **Parameters Table**.



- Select the **Only Current Component** to print only the summary table for the currently selected component or select the **For All selected Components** to print all summarised components (see above).

5 Appendix – Mathematical Formulas

	USP	EP	JP
Efficiency$_i$	$16\left(\frac{RT_i}{W_i}\right)^2$	$5{,}54\left(\frac{RTi}{W05i}\right)^2$	$5{,}55\left(\frac{RTi}{W05i}\right)^2$
Asymmetry$_i$	$\frac{b_i}{a_i}$		
Symmetry/ Tailing	$\frac{A05_i + B05_i}{2 \times A05_i}$		
Capacity$_i$	$\frac{RT_i - T_M}{T_M}$		
Eff/l$_i$	$\frac{Efficiency_i}{ColumnLenght}$		
HETP$_i$	$\frac{ColumnLenght}{Efficiency_i}$		
Resolution$_i$	$2\frac{RT_i - RT_{i-1}}{(W_{i-1} + W_i)}$	$1.18\frac{RT_i - RT_{i-1}}{(W05_i + W05_{i-1})}$	

Fig. 11. Formula for parameter calculation

RT_i - Component retention time
$W05_i$ - width at half height
W_i - Baseline width
a_i - Left half-width at 10% height
b_i - Right half-width at 10% height
$A05_i$ - Left half-width at 5% height
$B05_i$ - Right half-width at 5% height
T_M - Retention time of the unretained solute.

RSD [%]

Percentage standard deviation (variation coefficient).

$$RSD[\%] = \frac{\sqrt{\left[\frac{1}{n-1}\sum_{i=1}^{n}\left(X_i - \overline{X}\right)^2\right]}}{\overline{X}} * 100$$

where:

n – number of validated (loaded) chromatograms

X_i – the value of a monitored parameter of the i-th chromatogram

$\overline{X}$ - arithmetic mean of a monitored parameter of all validated (loaded) chromatograms

YL INSTRUMENT

Young Lin Bldg.,899-6, Hogye -dong,
Anyang, 431-836, Korea
Tel : +82-31-428-8700 Fax : +82-31-428-8779
E-mail : export@younglin.com
Homepage : www.ylinstrument.com