Clarity (Lite)

3.0 vs 2.8

ENG

Code/Rev.: M141/30A Date: 19.5.2010

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To facilitate the orientation in the **3.0 vs 2.8** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

Instrument (blue text) marks the name of the window, to which the text refers.

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name (when you already are in the topic describing the window).

WORK1 (capitals) indicates the name of the file and/or directory.

ACTIVE (capital italics) marks the state of the station or its part.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, there are text sections written in format other than normal text. These sections are formatted as follows:

 Note:
 Notifies the reader of possibly interesting information.

 Caution:
 Warns the user of possibly dangerous or very important information.

Marks the problem statement or trouble question.

Description:Presents any closer information on the problem, describes its causes etc.Solution:Marks the response to the question, presents a procedure how to remove it.

1 Preamble

Clarity version 3.0 is focused on the frequently asked improvements and options. More then one hundred new features were made in the User Interface options, Calibration, Sequence, Reports, Import/Export and Event Table. Also the list of Control Modules is extended and some improvements are implemented in Extensions like exporting pictures of graph in PDA extension, etc.

2 General

2.1 User Accounts



Fig. 1: User Accounts dialog

AutoLock 1

The **Instrument** will be locked after a time of computer operator inactivity. Only the current user or **Clarity** user with the *Open User Accounts* privilege could unlock it by entering his/her password. Operation is recorded in **Audit Trail**.

Electronic signature for PDF reports 2

A **PKCS#12** private key certificate file can be defined for the user. PDF documents created from **Clarity** will be then signed automatically with this certificate. As password entry is required for each print, this is not suitable for automated prints from **PostRun**.

2.2 Configuration

Instrument Method Sending options



Fig. 2: Instrument Method Sending dialog

L/min has been added to options for Flow Rate Units in LC Gradient.

Thermostat

Device type Thermostat is now allowed on GC Instrument type.

2.3 Instrument

Project Selection

Login Dialog	X
Choose User Name and Enter Password	
Admin	•
Select Project:	
DEMO_PDA	-
All Possible Instruments	
OK Cancel Help	

Fig. 3: Login Dialog

The project could now be selected in the Login Dialog. Last used project is offered.

Instrument

The *New* (*Method*, *Sequence*, *Calibration*) commands now open the Save As dialog to force the user to name the new file before using it.



Fig. 4: Instrument window

The Project Setup dialog could now be also invoked by clicking the *Project Name* in the status bar ①.

2.4 User Options

General tab

User Options (Admin - Ad	lmin)	
General Graph Axes Appe Graph Axes Appe Show windows on the ta Flay sounds assigned to Request confirmation wh Warn when maximum zo Warn before running alre Recent Files S Maximum Chromatograms in Overlay 20	arance Signals & Curves Gr skbar. selocted events. ccessfully finished sessions. en opening old file formats. om reached. ady measured sequence. Counter (Xn) □ Reset When Instrument Opening Start at: □ 0	adient & Ausiliary Directories Zoom Button C Left Right Left Button Doubleclick Means Unzoom Set Signal to Active Show Properties Dialog Chromatogram Cursors Only Vertical Line Anows Animated Anows
Mouse Wheel Step (in Graphs)	Use Default Font	C Seconds C Minutes C H:M:S

Fig. 5: Mouse Wheel Step option in the User Options dialog

Mouse Wheel Step (in Graphs) 1

Sets the mouse wheel sensitivity on zooming the graphs.

Graph tab



Fig. 6: New options in the Graph tab of the User Options dialog

Peak(s) Selected in the Graph 1

Clicking inside the peak area or selecting several peaks will fill them with the signal color and also mark them in the corresponding *Result Table* lines.

Peak Tags

The peaks could now be labeled with practically all parameters available in the *Result Table*:

Simplified Peaks Tags 2

Enables or disables checkboxes concerning simplified peaks tags.

Enhanced Format... 3

Displays the Peak Tags Format dialog which allows to set custom format of peak tags. Available only if the *Simplified Peaks Tag* checkbox is unchecked.

Peak Tags Format			×
Available Items Reten. Time Start Time End Time End Value End Value Area Area Height Area [2] Height [2] W05 Response Respo	Select Unselect Unselect All	Selected Items Compound Amount Resolution Symmetry/Tailing	 ↑ ↓ ↓ ↓
	OK Cancel	Help	

Fig. 7: Peak Tags Format dialog

Those settings are active only if the *Use User Options* option is selected in the respective graph (Chromatogram or Calibration) properties.

Directories tab

User Options (Admin - Admin)
General Graph Axes Appearance Signals & Curves Gradient & Auxiliary Directories
Print to PDF Directory
Default
Export Directory
Detault
Import Directory
Default
Hint: Specify empty directories to output files to the same directory as chromatograms.
Cancer Apply Help

Fig. 8: Directories in the User Options dialog

Sets the directories that will be used for the automatically created *.PDF files and exported files and where **Clarity** will look for files to import. If the fields are left empty, **Clarity** will use the subdirectory where the exported chromatogram is saved and the *Analysis subdirectory* (DATA by default) of the current project for imports.

2.5 File Name variables

New variables are available in *Sample*, *Sample ID* and *File Name* fields in *Sequence* table.

- %P Name of the project
- %J Name of the method (without .MET suffix)
- %s Name of the sequence (without .SEQ suffix)

Those variables could be used in the Method Setup, Calculation and Calibration cloning, the %*P* and %*J* are available also in the Single Analysis window. Sample. The Sample ID and File Name fields in Sequence table.

2.6 Fill Series in tables

Using the command *Fill Series*... in the popup menu of the *Sequence*, *Calibration* and *Gradient* table it is possible to fill values in selected range with defined step. This command is also available in the *Edit* menu of **Sequence** and **Calibration** windows.

Fill Series		X			
Fill using in	rement	2 +			
C Replace by value from the first row					
Example:	test-1				
	test-3				
	OK	Cancel			

Fig. 9: Fill Series dialog

As you can see in the **Fig. 9** on pg **7**., by using this function it is possible to fill the selected range of cells with values *test-1*, *test-3*, *test-5*, etc. The number at the end of the first selected cell is automatically detected and incremented when the *Fill using increment* option is selected. For more information about this function, see the **Reference Guide**.

2.7 PostRun and Batch Options

New options are available in the PostRun Setting, Analysis Batch dialogs and Sequence table.

PostRun Setting (For Single Analysis Only) 🛛 🔀
Program to Bun Only with Export
Paramgters
OK Cancel Help

Fig. 10: PostRun Setting dialog

Batch		
1951 1864_3001166a 1864_3001173 1864_3001190 1864_3001205 1864_30012105 1864_3001213 1864_3001213	File Type: Sequence Files Select All Unselect All Sort by: Name © Normal Time © Backward	Options
		Proceed Cancel Help

Fig. 11: Batch dialog

Include chromatogram in SST

Selects whether the batch-processed chromatograms will be included in **SST** ① calculations. In the Batch dialog, the option is called *Include in SST* and available options are *Exclude*, *Include* and *Unchanged* ②.

Open chromatogram with stored calibration

Selects the type of calibration connected to the chromatogram after the reprocess ③. In the Batch dialog, this option is called *Open with*

Calibration and available options are Linked, Stored or Unchanged 4.

Those attributes are set by Sequence table and stored within the chromatogram, thus the *Unchanged* option uses the value stored in *Chromatogram*, while the others will change them also in the *Chromatogram*.

Preserve integration

New option *Preserve Integration* (5) is available for *Reprocess by Instrument Method* or *Complete Processing* options. When active, the integration table in chromatogram will not be updated from the method used for reprocess, so the original integration will be preserved including the hand made modifications in the *Chromatogram*. This option is available only in the Batch dialog.

2.8 Export Data

Export Data					
Export Content Export Content Egestat Table If In Fixed Format Sogcial Results Sogcial Results Column Column	Chrometogram Chrometogram Displayed Data Xavis Ime Step: 0 min. Append Character Encoding: ANSI V	Text Format Fixed Width Deljmited By: <tab> Decimal Separator: <window's locale=""> Automatic Export To Clipboard Text: Fle ✓ Excell ① dgase File (Result table only)</window's></tab>			
Export OK Cancel Help					

Fig. 12: Excel option in the Export Data dialog

Export in MS Excel format

The data could be now exported to formatted MS Excel file ①. The headers are automatically included for the tables. Each selected item in *Export* content is on separate sheet in the Excel file. In case the *Chromatogram* option is checked ②, graph is created from the exported data (no baseline, integration marks and peak tags).

2.9 Registration

E Clarity Registrat	ion 📃 🗖	×
<u>File H</u> elp		
😂 🗙		
	ION	^
- REGIONAN		
* Company:		
* Street:		
* City:		
* ZIP:		
* Country:	(other countries)	
* Name:		
* Your e-mail:		
Phone:		
Fax:		
* Username:		
* Password:		
	You may enter a privacy password below. This provides only mild security, but should prevent others from messing with your subscription. Do not use a valuable password as it will occasionally be emailed back to you in cleartext.:	
* Re-password:		
S/N:	001 - 45635	
	I am DataApex Distributor	
	If you check this field, the User Account registration will be sent to DataApex and processed manually. You will receive an email once the distributor access rights will be authorized.	
	I want to receive product information from DataApex	
	I want to receive email notification about software updates	
	OR	
		\sim

Fig. 13: Clarity Registration

New web based registration form is used. In case the computer is not connected to the Internet, the form could be filled, printed and sent by post or fax.

By registering **Clarity** you get access to direct updates for your chromatography station and also the e-mail support is faster.

3 Method Setup

3.1 Event Table tab

	Input Output								
Name	Туре	Source	Input	Value	Units	Output Type	Output	Parameter	Store
1	Run Time >			1,000	min	None			N
2	Time Idle >			5,000	min	Command	Start Acq		v
3	Dig. Input Run	53210/532	Ini	Up		Net-PAD	Digital Output 1 👔	Pulse	5
4	Dig. Input Idle	53210/532	Ini	Up		Net-PAD	Digital Output 1	Pulse	v
5	Injection					Run Program	F:\clarity_3_0_0\UTILS\CopyFiles.exe		
6	Close Instrument					Net-PAD	Digital Output 6	Low	
	InpRel Run > InpRel Run < Time Idle > Input Idle > Input Idle <								

Fig. 14: New options in the Type, Input and Output columns in the Event Table

The event table is now active also outside the acquisition during the idle time. The input events are distinguished by the *RUN* and *IDLE* nominations ①. In case the event should be invoked both in *RUN* and *IDLE* stage, it must be entered twice (for each stage separately). Please check the **Help** or **Reference Guide** for detailed description. The *Input* ② and *Output* ③ columns are now displayed with assigned names (instead of numbers).

The Method Setup dialog is now resizable to allow displaying of longer texts and all columns.

Caution: As a consequence, methods from previous versions may show invalid

Time Table – it is necessary to reassign the corresponding inputs and outputs.

3.2 Calculation tab

Method Setup yl9160 (MODIFIED)	
Common for all detectors	
Calibration (Peak Table) test View Parameters Set New Clone None Cloud to the scale Factor Calculations ESTD U Units After Scale factor I Units After Scale f	
Report in Result Table	
C All Peaks in Calibration Event Table Measurement Integration Calculation Advanced OK Cancel Send method Report Audit Trail H	ielp

Fig. 15: Calculation tab of the Method Setup

Calibration Cloning in Sequence

Sets the name for cloned calibration files ① used in the **Standard Addition** calibration method and during the **Safe Calibration** usage and **Calibration Bracketing**. The field enables the use of any text, however it is essential to use %*variables* (added using the button) appropriate to the calibration method.

It is advantageous to use the *Sample ID* (%q) as a part of the variable for the **Standard Addition** measurements, where all lines belonging to one sample (Unknown, possible Blank, all Standards on other levels of the same sample) share the same *Sample ID* in the Sequence window.

For the **Calibration Bracketing**, the use of the Date and Time (in any format) or Line number as a part of the **Calibration Cloning** In Sequence field may be advantageous.

For safe calibration usage (option *Clone on first recalibration* in the Sequence Options dialog), the use of *Date* (%*D*) variable as a part of the cloned calibration name is advantageous.

New calculation modes available 2

- STDADD Standard Addition.
- NORM Normalized calculation

See the Reference Guide for detailed description.

3.3 Advanced tab

Subtraction

Subtraction chromatogram data are now stored in the *.PRM file (it is no more simply linked to it). The changes occurring with the subtraction chromatogram thus do not influence the measured chromatogram from which the background is subtracted. The subtraction, however, does not hold its history - only last subtracted chromatogram's data is saved when it is changed, previous subtraction chromatogram is discarded.

4 Chromatogram

4.1 Result Table

User Columns

Compound in Special Values

A new item **Compound** is available within the Special Values list **1**.

Add Use	r Column						
∐itle	RRT			Units			ОК
	,				Calc	ulate Total	Cancel
Expressio	on:						Help
[Reten.	Time]/[Peak	2,15\$	Reten. Time]				
Opers:	Euncts:	~	<u>C</u> olumns: Reten. Time		~	Variables: Sample Amount	
- * /	acos asin atg		Amount Amount [%] Centroid			Sample Dilution Injection Volume ISTD Amount	
< _	cos exp ln log max min round		Variance Skew Excess Asymmetry Capacity Efficiency Eff/l			Chromatogram # Unretained Peak Column Length Noise ASTM Noise 6-Sigma Noise Drift	Sum Average Std. Deviation Minimum Maximum
	sin	~	Symmetry/Tailine Recelution Special	g Values	<u> </u>		First Last Previous
						-	Next Compound 1

Fig. 16: Adding Special Value to User Column

Clicking the *Special Values* button and selecting the *Compound* command will invoke the dialog window showing list of compounds in the current chromatogram.

Select Compound	
Bromide Chloride Nitrate-N Sulphate	
OK Cancel	Help

Fig. 17: Select Compound

The respective value could then be used in compound specific calculations like is the *Relative Retention Time* or *Amount Ratios* to a specific compound.

Peak Type column

Additional information is shown in the *Peak Type* column.



Fig. 18: Peak Type column in Chromatogram window

Tab 1: Additional information is shown in the Peak Type column:

Value	Description
Ordnr / Ref / ISTD / RISTD / GRP	Peak type.
Error	Value could not be calculated.
Error (Curve Check)	Calibration curve does not met preset criteria.
<lod <loq<="" or="" td=""><td>Value lower then set limits.</td></lod>	Value lower then set limits.
(Forced)	Identification forced by integration table.
(by name)	Another compound calibration data used.
(CF)	Correction factor in calibration applied .

4.2 Integration

Force Peak Name



Fig. 19: Force Peak Name function

New command *Force Peak Name...* is available in the Chromatogram window by clicking on the *Chromatogram - Peak* menu or the corresponding icon on the *Peak* toolbar. After selecting the peak in chromatogram, window offering selection of existing peaks in the chromatogram appears. A new name could be filled in or selected. If you select a peak from the list instead of manual filling, the peak will change its name and also the corresponding integration will be used.

Force Peak Name		
actic druc ethanol fructose glucose glycerol ethic metic metic metic metic metic tartaric		
ОК	Cancel	Неір

Fig. 20: Force Peak Name dialog

The purpose of this function is:

- 1. To name peaks in *Chromatogram* without the necessity to create *Calibration* file. Such named peaks could be used in the user column calculations typically for purity determination, where the *RRT* and *%Area* relative to the main component need to be calculated.
- Correct peak identification in some exceptional chromatograms (typically in aminoacid analysis even the peak order may change within series of samples) without the necessity to amend the expected retention times and identification windows in the calibration file.

4.3 Import chromatogram

New options enable simplified import of multiple files in the same format.

Import AIA files

Import AIA Fi	ile 🛛 🔁
1 🔽 Do not sl	how this dialog for remaining files
AIA File	V:\DATA-CLARITY-EXTERNI\CE_koval_05052006\04122041-PDA - 230nm.cdf
 Dimensi Attribut Variable 	ions tes tes
, Chromatogra	am F:\clarity_3_0_0\YL9160\Data\04122041-PDA - 230nm.PRM
	OK Skip Cancel Help

Fig. 21: Import of AIA files

For AIA files, the *Do not show this dialog for remaining files* ① will suppress it for simultaneously imported files.

Import text files

Import Text File			\mathbf{X}
Preset ①	EZ_Chrom		• >
Apply Settings to	C Current File	 All 8 Files Prefer D 	etected Settings
Current Text File	V:\DATA-CLARITY-EXTERN	I\CE_koval_05052006\04	1 Preview 2
Import From Line	8	import To Line	
Separator	; <semicolon> 💌</semicolon>	Decimal Separator	. <dot></dot>
Analyst	Admin		_
Sample ID			-
Sample			-
Sample Date	21.12.2004 💌		
Amount	0		-
Dilution	1		-
ISTD Amount	0		-
Injection Volume	0		
Imported Data 🛛 🔇	Signal + Signal	•	-]
Number of Detectors	1		
Sample Rate [Hz] Signal Unit	Autoscale Signal Nam	e Time Units Y Mult	iplier Data Size
8 mV	AU AU	min 0,001	13683
Save as Chromatogram	F:\clarity_3_0_0\YL9160\D	ata\04122044.PRM	Load Defaults
	OK Skip	Cancel	Help

Fig. 22: Importing text files

Preset 1

When the same type of files are imported frequently, it can be useful to save import settings for further use. In drop-down box a user can select from previously saved presets, by clicking button right to list the presets management menu will open. The menu contains commands for saving current setting (*Create from the Current Settings*), *Rename* or *Remove* presets. Presets are stored as part of *Clarity Desktop* settings.

Preview 2

This button will open the current file in simple text viewer. This can help user to identify exact meaning of particular columns when it's not clear from the file suffix.

Imported data 3

Time + *Signal* + *Time* + *Signal* - Every chromatographic curve is saved in a pair of columns, in which the first one represents a time and the second one a signal.

Signal + Time + Signal + Time - Every chromatographic curve is saved in a pair of columns, in which the first one represents a signal and the second one a time.

Signal only - Every chromatographic curve is saved in one column, where the values represent the signal only. The time basis is obtained from the *Sample Rate* field.

Time + *Signal* + *Signal* - Time base is contained in first column, every next column represents a signal of one detector.

Import CSV files

File type *.CSV are supported in *Import Chromatogram* and *Import Sequence* functions.

4.4 Mathematical Operations

Invert

New function to invert polarity of already measured chromatogram 1.

Operand A Operations Operand A Operand A SolveNT	Operation C Copy Invert 1	Coperand B
	C Differentiate C A + B C A - B	
Result Ainvert	ram	
ОК	Cancel	Help

Fig. 23: Invert function in the Mathematical Operations dialog

4.5 Miscellaneous

- Open Chromatogram Sequentially command is active also in Overlay Mode.
- **CTRL** + *Arrows* keys will move the chromatogram in the graph (when zoomed in).
- The Audit Trail (cleared in previous versions during *Save As*) is preserved.
- File Open dialog includes Overlay Mode checkbox to toggle the Overlay mode on/off directly from this dialog.
- Graph Properties: Show Data Points checkbox to indicate data points in Chromatogram.
- Possibility to make chromatogram active by double clicking the respective row in *Summary* or *SST* table.

- Possibility to highlight peaks and corresponding row in tables by clicking inside the peak area in the chromatogram.
- Last subtraction chromatogram will be stored in chromatogram history.

5 Calibration

New columns in the *Compounds* table. To display them use the Setup columns... command in the pop-up menu of the table.

K)	nstru	ument 1 - C	alibratio	n 250X	8HR1 <	ESTD					×
<u> </u>	<u>E</u> di	t <u>D</u> isplay <u>C</u>	alibration (∥iew <u>W</u> ind	ow <u>H</u> elp	🔺 🖬	👬 🖉 🕇	ñ 🕎 (5 9		
ľ			< 🔁 🖁	à 🥔	X 🖻 🖬) n o	r @, @	0	*	🔤 🔶 4	\$~
										22 📕 📘	
			Calibra	tion Summa	ry Table (ES	TD - 250X8H	HR1 - Signal	1)			
	Used	Compound Name	Reten. Time	Search Window	Left Window	Right Window	Peak Selection	Peak Type	Peak Color	Reten. Index	
1	•	oxalic	4,561	Abs	0,100 min	0,100 min	Ngorst	Ord		0,000	
2		citric	5,203	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
3	☑	tartaric	5,423	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
4		glucose	6,053	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
5		malic	6,303	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
6		fructose	6,577	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
7	5	succinic	8,177	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
8		lactic	8,550	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
9		glycerol	8,900	Abs	0,100 min	0,060 min	Nearest	Ord		0,000	
10	∇	acetic	10,337	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
11		methanol	12,710	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
12	F	ethanol	14,833	Abs	0,100 min	0,100 min	Nearest	Ord		0,000	
<								1			>
I≪ ≪ For H	elp, p	Compo ress F1	unds (o	:alic ∕ citri	c) tartari	:) glucos	æ} malic	} fruct	ose)	succinic)	lac

Fig. 24: Search Window and Peak Selection columns in the Compounds table

New columns *Search Window* and *Peak Selection* enable more flexibility in compounds identification.

Search Window 1

Defines whether the *Left Window* and *Right Window* content will be inserted in *Abs* (absolute - set in minutes) or *Rel* (relative - set in percents of the *Reten. Time*) values.

Peak selection 2

Defines the way the correct peak is matched with the Retention time when several peaks are present in the same identification window. The options available are Nearest (closest possible to the selected retention time - default for standard peaks), *First, Last* and *Biggest* (default for *Reference* peaks).

L II	nstrumen	it 1 - (Calibratio	n 250X	8HR1 <	ESTD (MODI	TED)		
Eile	<u>E</u> dit <u>D</u> is	play 🤇	alibration	/iew <u>W</u> ind	ow <u>H</u> elp	🔼 📶 👗	🖉 📶 🖉	j 00	
ĨD	4 🖬	S	× 🗃 🛙) 🍠 📗	X 🖪 🛙	n 2	8, 6, 6		₩ 4 4 2 -
			Calibra	tion Summa	y Table (ES)	TD - 250X8HR1 ·	Signal 1)	14	
	LOQ	RB	Factor	Factor	By	Response	Amount	Resp. Eart.	Rec No.
1	0,000	A	0,0000	1,0900	0	3,6130	0,101	0,0280	0
2	0,000	A	0,0000	1,30	- (4)	36,2510	0,210	0,0058	0
3	0,000	A	0,0000	1,0000	ethanol	98,5410	0,441	0,0045	0
4	0,000	A	0,0000	1,0000		0,0000	0,600	0,0000	0
5	0,000	A	0,0000	1,0000		217,4548	1,003	0,0046	0
6	0,000	A	0,0000	1,0000		0,0000	0,600	0,0000	0
7	0,000	А	0,0000	1,0000		31,5600	0,239	0,0076	0
8	0,000	A	0,0000	1,0000		51,3650	0,600	0,0117	0
9	0,000	A	0,0000	1,0000		0,0000	1,223	0,0000	0
10	0,000	А	0,0000	1,0000		24,9850	0,202	0,0081	0
11	0,000	A	0,0000	1,0000		0,0000	0,104	0,0000	0
12	0,000	A	0,0000	1,0000		0,0000	10,847	0,0000	0
<		1)>
For He	elp, press F	Compo 1	ounds / 💿	:alic ∕ citri	tartari	c λ glucose λ	_malic ∕fi	ructose) s	uccinic 👌 lac

Fig. 25: Correction Factor and Calculated By columns in the Compounds Table

New columns *Correction Factor* and *Calculate By* enable to use another compound response or calibration curve for quantification

Correction Factor 3

Allows for the correction of amount due to the lower recovery, etc. The *Amount* value is multiplied by the *Correction Factor* to calculate the final *Amount*. The use is indicated in the *Peak Type* column in the *Result* table in the Chromatogram window, see the **Reference Guide**.

Calculate By 4

Clicking the field of this column on a given row opens the Calculate By dialog, which allows to set a compound whose *Response* will be used for the *Amount* calculation for a given compound. Use is indicated in the *Peak Type* column in the *Result* table in the Chromatogram window, see the **Reference Guide**.

Those *Calibration Curve* parameters are now available directly from the *Compounds* - *Calibration table* as columns (display them by using the *Setup Columns...* in the pop-up menu of the table).

- Curve Fit Type
- Origin
- Ending Point
- Weighting Method
- Linearisation X
- Linearization Y
- Lin Response
- Lin Amount

5.1 Calibration Options



Fig. 26: Calibration Options

Display Mode

New items *NORM* and *STDADD*. For more details see the chapter **Standard Addition Calculation** on pg **29**. and the chapter **"Normalization Calculation"** on pg **30**.

Curve Check

The parameters of calibration curve could be checked against the set limits.

Deviation

In % as displayed in the *Deviation* column in the Calibration and *Compound* table.

Correlation

The correlation factor displayed under the calibration curve equation with values between 0 and 1.

Failure to comply is indicated in the *Result Table - Peak Type* column by Error (Curve Check).

Response Factor as Response/Amount

Option to display the *Response Factor* as Response/Amount (inverted value to the default Amount/Response).

In calculations the Amount/Response value is used in both cases, the checkbox only influences the display of the *Response Factor* in the Calibration or *Result Table*. Useful in case the Response Factor is a small

number and the valid digits could not be properly displayed due to the decimals limitation.

The used option is indicated in the column header tooltip.

Miscellaneous

- Open Standard as Chromatogram command will open the standard in the Chromatogram window.
- Link Calibration to Standard command in the File menu. Links currently opened chromatogram of standard to calibration file in which this standard is used. This will enable showing the names of peaks, as they were coined in the calibration file.
- Bubble hint in the graph of calibration standard for Add Peak function.

5.2 Calibration Options - Defaults

Identification Windows.

Calibration Options (PA	H_EPA)	? 🗙
Calibration Options Default	3	
Response Base	Area	•
Origin	Curve passes through Origin	•
Curve Fit Type	Linear	•
Weighting Method	None	•
Linearization X	None	•
Linearization Y	None	•
Identification Windows Search Window 1		
Left Window	0,200 min 10,000	%
Right Window	0,200 min 10,000	*
Peak Selection	Nearest	•
Set All N	ow For Current Signal	
	OK Cancel	Help

Fig. 27: Identification windows in the Calibration Options dialog

A user can select between absolute (*Abs*) and relative (*Rel*) values and set values for both of them independently. **1**.

Curve Fit Type

Calibration Options (PA Calibration Options Default	H_EPA) ? 🗙
Response Base	Area
Origin	Curve passes through Origin 📃
Curve Fit Type	Linear 🔹 💌
Weighting Method	Free Calibration
Linearization X	Linear Quadratic
Linearization Y	Cubic Sigmoid
Identification Windows	log10 exp
Search Window	pow10 Hyperbola
Left Window	Half Sigmoid
Right Window	0,200 min 10,000 %
Peak Selection	Nearest
Set All N	ow For Current Signal
	OK Cancel Help

Fig. 28: Curve Fit Type in the Calibration Options dialog

New Curve Fit types 2:

- In
- log10
- exp
- pow10
- Hyperbola
- Half Sigmoid

For more details see chapter Calibration in Reference Guide.

Calibration Options (te Calibration Options Defaul	st) Its	?
Response Base	Area	¥
Origin	Curve passes through Origin	•
Curve Fit Type	In	-
Weighting Method	None	-
Linearization X	None	•
Linearization Y	None (3)	-
Identification Windows Search Window Left Window Right Window	None 1/Response 1/Response) sqt(Response) 1/sqt(Response) Response 0.200	× *
Peak Selection	Nearest	•
Set All N	ow For Current Signal	
	OK Cancel	Help

Linearization X & Linearization Y

Fig. 29: Linearization X and Linearization Y in the Calibration Options dialog

Sets the axis linearization for the calibration curve calculation @. The function and its possible options are described in the chapter **Calibration** in the **Reference Guide**.

5.3 Graph Properties

Graph Properties			
Use Liser Options Show Grid Logarithmic Amount Logarithmic Amount Source Comparithmic Amount Show Recalibration Points For Show Linearized Values Thow Linearized Values	Color Color As the <u>Active</u> Signal Select	Axes Line Width I = TRIE Font Value Font Links Font	Background Colors Chart Windows Default Select Border Windows Default Select
	OK Cancel	Help	

Fig. 30: Graph Properties dialog

The checkbox *Show Linearized Values* ① toggles the display of original and linearized values in the calibration curve graph. The choice is indicated in the Axis description.

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Fig. 31: Calibration window without linearized values

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Linearization Y	In(Response)	•					1	-		
Equation: Y = 0,	8602*X + 4,10352									
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Fig. 32: Calibration window with linearized values

The linearized values are displayed in the *Lin Response* and *Lin Amount* columns on the compound tab.

5.4 Standard Addition Calculation

New **Standard Addition** calculations has been added. The following order of measurements is used: *Blank* (optional), *Unknown*, *Unknown*, *with Standard Addition1*, *Unknown with Standard Addition2*, etc.

First calibration level in *Calibration Table* is used for *Unknown*, the other levels are shifted accordingly. Calibration curve is constructed using the Standard Additions concentrations (assuming Unknown concentration = 0) and the Unknown concentration is determined as an intercept of this curve with the zero response line.

In case a *Blank* is used, its response will shift the zero line used for determination of the intercept.



Fig. 33: Standard Addition

Unknown

Specifies the method for including the unknown sample into the calibration curve calculation in the Standard Addition mode. This value is individual for each signal.

Without Unknown Sample

The Unknown sample is not used in calibration curve calculation.

Compute with Unknown

Considers the Unknown sample to be one of the calibration points with *Amount=0*.

Curve passes through Unknown

Always passes the calibration curve through the Unknown sample for *Amount=0*.

Blank

In standard addition calculation the response for blank (Calibration *Level* 21 is used to shift the zero response level used to calculate the *Unknown* concentration.

5.5 Normalization Calculation

New **NORM** calculation has been added. This calculation type performs the calculations identically to the **ESTD** calculations according to the actual calibrations settings. The desired *Norm%* results are displayed in the *Amount%* column, the calculation checks the condition that all identified peaks are calibrated and all peaks in calibration were identified in the chromatogram. No results and warning message in *Result Table* header are given in opposite case. It means that *Peak Type* would be *ERROR* and *Amount%* zero.

5.6 Calibration Curve Export

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Fig. 34: Exporting the calibration curve

Using the menu *File* - *Export* or popup menu of the calibration curve area ① it is possible to perform new export functions.

Export as Picture to Clipboard

This command will copy the calibration curve to Windows clipboard. It allows user to quickly utilize picture in another program using the *Paste* command.

Export Calibration Curve as Picture...

This command will open the Save As... dialog, which will save the calibration standard curve into **Enhanced Metafile** format supported by Microsoft Windows and Microsoft Office.

6 Sequence

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Fig. 35: Sequence window

Sample ID

This field is now limited to 64 characters (was limited to 20).

File name variables

New variables are available in *Sample*, *Sample ID* and *FileName* columns.

- %P Name of the project
- %J Name of the method (without path and .MET suffix)
- %s Name of the sequence (without .path and .SEQ suffix)

Std

Specifies/Sets the type of the sample being measured instead if the previously used YES/NO. The possible options are:

Unknown

Denotes an unknown sample.

Standard

Specifies the calibration standard. Samples marked as *Standard* must have the calibration level filled in the *Lvl* column. Chromatograms created on the sequence rows marked as calibration standards will be stored in the calibration subdirectory (CALIB by default) instead of the analysis subdirectory (DATA by default).

Bypass

This *Std* type allows for performing an analysis in the *ACTIVE* sequence with controlled autosampler without actually injecting a sample. This may be useful for system clean-up, etc.

Blank

In fact a calibration standard with no amount of added sample. The *Blank* is thus one point of a calibration curve (with the *Amount* of 0, used on calibration *Level 21*).

Post run columns

New PostRun columns has been added. To display them, use the *Setup Columns...* in the pop-up menu of the *Sequence* table.

T	la	bal	l - Seq	uenc	e postrun									
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1		/	Unkn		yl9160	Instrument	v	Г	Г	•			1	
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Fig. 36: New PostRun columns

Include in SST

This checkbox allows user to set whether the particular chromatogram will be included in the SST calculations or not.

Close All

This checkbox allows user to close all currently opened chromatograms. Those options enable to create a specific summary reports during sequence run. Opening of the chromatogram measured in the same line of sequence is not influenced by this setting, it follows setting of Open checkbox only.

Stored Calib.

This checkbox causes the chromatogram will be opened with the stored version of the calibration file, as opposed to the linked calibration when not checked. As the use of linked calibration is preferable, should be used exceptionally.

6.1 Sequence Options

Sequence Options	
☑ Active Seque ☐ Idle Time bel Idle Time	nce fore First Injection 0 [min.]
1-3	
Counter (%n) Start © 0 © 1 Reset when: © Run Sequence © Open Instrument © Never Current Value 6	Format C Automatically C Manually Inj. Volume Units C µL C mL
Calibration and Sequence Usage () Calibration used as specifie Calone on first recalibration (Calibration Measure Calibration Bracketing Description:	d by user safe calibration usage) ment
ОК	Cancel Help

Fig. 37: Sequence Options

Calibration and Sequence Usage

Selects the mode of the calibration and sequence usage. With exception of the first option, suitable calibration file *Cloning* in Method Setup - Calculation should be set, see pg **12**.

Calibration used as specified by user

Sets the sequence and calibration to the standard **Clarity** use (the only way available to version **2.8**). The calibration set in the Method Setup - Calculation dialog is used for calibration and recalibration, no calibration cloning is performed.

Clone on first recalibration (safe calibration usage)

Sets the sequence and calibration to the safe calibration usage mode. The calibration will be cloned at each start of the sequence and at each start of a new sequence. Setting this options *ON* prevents from situations when new measured standards with different responses may devaluate already measured standards because all chromatograms are linked to the created calibration.

Standard Addition Measurement

Sets the sequence and calibration to the Standard Addition mode use. As each unknown sample will use one calibration file, calibration will be cloned from the original calibration file whenever an unknown sample or blank follows the calibration standard. All responses are cleared from a newly cloned calibration. For more information, see the **Reference Guide**.

Calibration Bracketing

Sets the sequence and calibration to the *Calibration Bracketing* mode use. As every unknown sample series is demarcated by calibration standards and as such uses a single calibration file, calibration will be cloned from the previous calibration clone whenever an unknown sample or blank follows the calibration standard. The unknown samples are calculated against the standards immediately preceding and following them. All responses are cleared from a newly cloned calibration and preserves just the last recalibration responses.

7 Report

Order of the report sections could be modified in the Report Setup dialog.

Report Setup Instru	ment		
Page Setup Lab. Header Report Header Me Move to the Ce Move Up	Print On New Page Signals Top P Chromatogram	Info Header Info Instrument Parameters Acquiston Parameters GLP Info Event Table	OK Cancel Help
Cr Move Down Move to the X Se X SST	Bottom Active Signal	Injection Control Instrument Control Integration Table Calculation Parameters	Open Save As
X Audit & Signatures		PDA Method	Printer Preview Print Print To PDF Send PDF

Fig. 38: Popup menu of tabs in the Report Setup

The report is printed in order respective to tabs order on the left. By right click on the tab you can move the tab up or down. The order of *Page Setup* and *Audit & Signatures* can't be changed since they don't represent the print section.

Electronic signature for PDF

Electronic signature for PDF reports (used for GLP). For more details see the chapter **General** on pg **2**.

8 Control Modules

New Control Modules has been added.

Agilent 1200

- Testing.
- Only the G1315D Diode Array Detector is currently supported. It has to be controlled by one separate LAN communication line using the 1200 Control Module and the rest of the 1100/1200 system by other LAN or GP-IB communication line using the 1100 Control Module on the same Clarity Instrument.

Agilent 7890

• Testing.

Sedere ELSD LT80/LT85

• Testing.

Esa Coulochem II

• Testing.

Currently not supported:

- Scan Mode.
- RS 232 (only the USB communication is supported).
- Not possible to control more than one detector at once.
- *Rate* and *Range* are shared in *DC* and *Pulse* Mode due to restriction in **Clarity SDK**.
- Time Table is not yet implemented.

8.1 LC Control

- Method Setup *LC Gradient*: new option *Initial Standby* in the *Idle State* group enables to set different flows at sending the method and after finishing the analysis. Grayed out for modules not supporting this option.
- Method Setup Valves new Set Home position on Close instrument checkbox.

8.2 FC Control

The Fraction Collector (FC GP driver)

• New checkbox *Collect All* in the Method Setup - FC - Vial Numbers dialog for FC without diverter value.

• New option *Delay Volume 2* in the Method Setup - *FC* - Fraction Table dialog enables to compensate for volume between valve and collection point.

9 Extensions

9.1 GPC

• Calibration broad on narrow - changes of *K* and *Alpha* values will be recorded in the Chromatogram Audit Trail.

9.2 PDA

Export Picture



Fig. 39: Export picture in PDA Window

Copy to Clipboard

Available from context menu in the Graph Panes in PDA View window 1.

Save as Picture...

Available from context menu in the Graph Panes in PDA View window ①.

Spectral Library

Add All Identified Peaks

Using the menu *Spectrum - Add All Identified Peaks* ② will add spectra of all identified peaks in chromatogram to a **Spectral Library**.

Confirmation window will appear:

Clarity		×
?	Add spectra of these peaks to library /C:\Clarky_30\DEMO_PDA\Calib\PAH7 4.62 min Naphtalene 6.28 min Acenaphtane 9.38 min Euroane 10.34 min Phenantrene 11.55 min Atricacene 12.200 min Fluoranthene 13.71 min Physeine that acene 13.72 min Chrysene 13.75 min Benzol\filuranthene 20.75 min Benzol\filuranthene 23.55 min Benzol\filuranthene 23.55 min Benzol\filuranthene 23.55 min Benzol\filuranthene 23.55 min Benzol\filuranthene 23.55 min Benzol\filuranthene 23.56 min Benzol\filuranthene 24.80 min Indeno(1,2,3-cd)pyrene 24.80 min Indeno(1,2,3-cd)pyrene	

Fig. 40: Question before all identified peaks are added to the library

Spectrum Overwriting

Warning Window will appear upon attempt to add duplicate spectrum name in library.



Fig. 41: Warning before duplicate spectrum is added to the spectrum library

10 Other

CopyFiles

Standalone utility "CopyFiles" to copy selected file types to specified directory (available in the UTILS subdirectory of **Clarity** installation folder).

By using this utility in the PostRun Setting dialog it is possible, for example, to additionally copy files such as PDF documents to another network destination. If the network directory is not currently accessible, the **Clarity** will still works without any exception.