

Clarity

Clarity v.2.3 vs v.2.2

Rev. A - 8. July 2004

Phone/Fax: +420 - 251 613 507
Phone/Fax: +420 - 251 612 067
clarity@dataapex.com
www.dataapex.com

© **DataApex Ltd. 2004**
Podohradská 1
155 00 Prague 5
The Czech Republic

Clarity[®], DataApex[®] and [®] are trademarks of DataApex Ltd.
Microsoft[®] and Windows[™] are trademarks of Microsoft Corporation



1	Add On Modules	5
1.1	GPC Module	5
2	Control Modules	6
2.1	Shimadzu GC17A Chromatograph	6
2.2	Agilent 6890 Chromatograph	6
2.3	Agilent 7683 Autosampler.....	6
2.4	LabAlliance HPLC pumps.....	6
2.5	HTA AS300L Autosampler.....	6
3	Measurement.....	7
3.1	Running external programs during acquisition	7
3.2	Auxiliary program for sending commands over a serial line – SendCom.exe	7
3.3	Pulse output in the Event table	7
3.4	Selecting detectors as a part of the method	7
3.5	New variables for filename templates.....	8
3.6	Displaying noise in the Data Acquisition window	8
3.7	New variables in the Run Program field	8
4	Chromatogram	8
4.1	Move and Scale commands in multi-detector chromatograms	8
4.2	Improved Chromatogram List dialog.....	9
4.3	Import RAW command moved	9
5	Calibration	9
5.1	History of all points of the calibration curve	9
5.2	Displaying the Deviation of each calibration point	9
5.3	Displaying the residuum of the calibration curve.....	9
6	Results	10
6.1	Calculating chromatogram noise and drift.....	10
6.2	Calculating signal/noise ratio	10
6.3	The order for displaying Chromatogram/Signal in the Summary Table	10
6.4	Extended number of parameters in the Summary Table.....	10
6.5	Extended options for displaying parameters in the result tables	10
6.6	Enhanced Total row in the Result Table	10
6.7	New Response Base checkbox for unidentified peaks	11



6.8	Selecting the signals in the SST module for multidetector chromatograms	11
7	Print	11
7.1	Printing images	11
7.2	Signal printing options	11
7.3	Black&White printing	11
7.4	Printing multiple chromatograms separately	11
7.5	Printing additional information about a chromatogram	12
7.6	Report Setup – simplified Chromatogram dialog	12
8	Other	12
8.1	Demo mode	12



1 Add On Modules

1.1 GPC Module

You can now extend the Clarity station using the **GPC/SEC** (*Gel Permeating Chromatography/Size Exclusion Chromatography*) add-on module.

This is an analytic technique used to determine molecule weight and its distribution in polymers.

The GPC Module can be purchased along with the station or it can be included later. In either case, the module will be fully integrated within the Clarity station.

The Clarity station with the GPC module is able to evaluate each measured sample using both the standard procedure and GPC calculations.

The GPC Module calculates the following parameters: **Mp**, **Mn**, **Mw**, **Mz**, **Mz1**, **Mv**, **PD**. The following types of calibrations are provided: the method of broad on narrow standard, both in possible combination with universal calibration, and the method of broad on narrow standard.

GPC calculations can contain tools for correcting flow rate changes and delays between detectors.

Chromatograms can easily be displayed together with the GPC calibration curve, distribution or cumulated distribution of the molecule weights curve.

The GPC module can be also used for evaluating chromatograms that have been obtained from other data stations. In this case, only the GPC module with the Clarity Eval version needs to be purchased. The chromatograms acquired from other data system can then be imported using the **Import Chromatogram** command. The system needs to be able to export the chromatogram to a file in a text format (AIA, TXT, etc.).



2 Control Modules

2.1 Shimadzu GC17A Chromatograph

The control module for GC chromatograph **Shimadzu GC17A** has been launched.

2.2 Agilent 6890 Chromatograph

The control module for **Agilent 6890** has been extended by using the new types of inlets: HP/AC (ACI), PCS/SL (GPTV), Manual PCS/SL (MACA), HP-PTV (CIS4), SIMDIST (PCM), CIS4 (CIS3), JIB, Volatiles.

2.3 Agilent 7683 Autosampler

The control module for **Agilent 6890** has been extended by using the direct control of the **ALS 7683** autosampler.

2.4 LabAlliance HPLC pumps

The control module for **LabAlliance** pumps has been extended by using the control of the **Q-grad A** and **Q-grad B** pumps.

2.5 HTA AS300L Autosampler

The control module for **HTA AS300L** autosampler has been launched.



3 Measurement

3.1 Running external programs during acquisition

The Clarity station has been extended to allow external programs to run during acquisition.

The **Event Table** found in the **Method Setup - Acquisition** dialog contains two new columns: **Ext.Prg** and **Params**, for entering the filename of the program and its eventual parameters. In the C:\CLARITY\UTILS subdirectory there are two auxiliary programs:

- SENDCOM.EXE, described in the following chapter
- BEEP.EXE, program that beeps after being invoked.

3.2 Auxiliary program for sending commands over a serial line – SendCom.exe

The SENDCOM.EXE program allows a text string to be sent to a selected serial port. The selection of the COM port and of its parameters is specified in the sendcom.ini file. The text string will be set as a command line parameter or, when using the **Event Table**, it will be sent in the **Params** column. This program is useful for controlling simple devices, e.g. valves, thermostats, simple pumps. This program only communicates one way, i.e. it cannot receive and evaluate text strings from the device.

3.3 Pulse output in the Event table

A new type of output called "*Pulse*" has been implemented to the **Event Table**. When activated, the selected digital output will change from its initial state for a selected time and then return back. The default length of the pulse is 100 ms and can be modified in the CLARITY.INI file.

3.4 Selecting detectors as a part of the method

If it is unnecessary to measure on all detectors configured on the device, it will be easy to directly omit unused detectors from the measurement in the method. The **Enabled** checkbox, located above the



Acquisition tab in the **Method Setup** dialog, can omit the currently displayed detector from the measurement.

3.5 New variables for filename templates

Filenames (**FileName** field in the **Single Analysis** dialog or analogous column in the **Sequence** window) can contain the Values from the **Sample** and **Sample ID** fields. The variables are as follows:

%Q (**Sample**) or *%q* (**Sample ID**).

3.6 Displaying noise in the Data Acquisition window

The current values of noise for all measured signals can be displayed in the **Data Acquisition** dialog. The display is enabled using the **Show Noise** checkbox in the **Graph Properties** dialog (**Display-Properties** menu).

3.7 New variables in the Run Program field

The **Run Program** field in the **PostRun** and **Batch** commands can now contain following variables:

%f - the filename of the chromatogram

%e - the filename of the exported file

A typical usage for this is to automatically open exported data in MS Excel.

4 Chromatogram

4.1 Move and Scale commands in multi-detector chromatograms

Shifting of chromatogram and changing of its scale can now be performed for all signals at once in multi-detector chromatograms. To do this, the command has to be invoked while holding down the Shift key.



4.2 Improved Chromatogram List dialog

Active and hidden signals can now be easily distinguished in the **Chromatogram List** dialog. The active signal is highlighted in bold letters. Hidden signals are displayed in grey colour.

4.3 Import RAW command moved

The **Import RAW** command from the **File - Import** menu has been transformed into a **File Type** parameter in the **Save As** dialog. This is invoked using the **File - Import Chromatogram** command.

5 Calibration

5.1 History of all points of the calibration curve

Every calibration curve now contains a historical record of each point. Stored information includes: the name of the calibration standard, retention time, area, height and date of a (re)calibration.

5.2 Displaying the Deviation of each calibration point

A new **Deviation[%]** column has been implemented into the calibration table of individual compounds. The new column displays the deviation of each point from the calibration curve (deviation of amount) in percent.

5.3 Displaying the residuum of the calibration curve

The description of the calibration curve now also provides the residuum of responses of the calibration curve (the sum of squares of deviations of responses of all calibration points from the displayed calibration curve).



6 Results

6.1 Calculating chromatogram noise and drift

The noise and drift over a specified interval can be displayed above the **Result Table**. Use the **Noise Evaluation** and **Drift Evaluation** commands from the **Chromatogram - Noise & Drift** menu to activate the display and select the interval.

6.2 Calculating signal/noise ratio

The signal/noise ratio of any peak can be easily displayed in the **Result Table** using the hidden user column - **Signal/Noise**.

6.3 The order for displaying Chromatogram/Signal in the Summary Table

The order for displaying the Chromatogram / Signal in the **Summary Table** can be altered. It is then easier to compare the signals from a selected detector across all displayed chromatograms.

6.4 Extended number of parameters in the Summary Table

The **Summary Table** can now display the same standard columns as the **Result Table**.

6.5 Extended options for displaying parameters in the result tables

The **Result** and **Summary** tables enable all columns to be displayed, regardless of the selected method of the calculation. E.g. it is possible to display the **Area** and **Height** columns even in the calibrated calculations. The same applies to the custom calculations with these columns.

6.6 Enhanced Total row in the Result Table

The *Total* row in the **Result Table** now also displays the sum for columns with custom calculations.



6.7 New Response Base checkbox for unidentified peaks

When using unidentified peaks, it is possible to select whether the Response Factor calculation will be performed according to the area or height of these peaks.

6.8 Selecting the signals in the SST module for multidetector chromatograms

it is possible to select which signal will be evaluated in the **SST** module. The **Evaluate** field in the SST Table header can be used to select a specific signal or to automatically evaluate the signal which is active in the **Overlay** toolbar.

7 Print

7.1 Printing images

Including the option to print images has enhanced printed reports. Images of any size can be used in the common file formats (BMP, JPG, GIF, WMF, ICO, etc.)

7.2 Signal printing options

When printing multidetector chromatograms the **Result Table** can be printed to all chromatograms, to the active chromatogram or only to the active signal.

7.3 Black&White printing

The Black&White print option optimizes the way coloured chromatograms and tables are printed on black and white printers. Instead of converting to gray levels, all colours will automatically be converted to black or white only.

7.4 Printing multiple chromatograms separately

When printing multiple chromatograms in the Overlay mode it is possible to print in a single graph or separately print a graph for each chromatogram (or even each signal).



7.5 Printing additional information about a chromatogram

The **Report Header** has been extended by the **Last modified** field – the date of last modification of the chromatogram.

7.6 Report Setup – simplified Chromatogram dialog

The **Peak Tags**, **Baseline** and **Labels** checkboxes in the **Report Setup - Chromatogram** dialog have been discontinued. Printing these items is now WYSIWYG, i.e. it depends on whether they are currently displayed in the **Chromatogram** window or not.

8 Other

8.1 Demo mode

The Demo mode does not allow for the importation of chromatograms. It is impossible to work with chromatograms that have been created in the full version in the Demo mode.