Clarity

Demo version description

Rev. 23A - 12 July 2004

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1 Brief Description

The **Clarity** chromatographic station is an effective tool for data acquisition, processing and evaluation from any commercially available gas/liquid chromatograph with standard analog output.



Data can also be acquired using the control module from chromatographs with a digital output. The maximum configuration allows for measurement on up to four chromatographs simultaneously, each of which can be equipped with up to 4 detectors.

The station is equipped to automatically support cooperation with chromatographs and autosamplers.

Clarity supports the requirements of the **FDA's 21 CFR Part 11** guideline.

The **Clarity** station will automatically process all data acquired from **CSW** stations.

1.1 Clarity vs Clarity Lite

Smaller laboratories benefit from the **Clarity Lite** station and its reduced set of functions. **Clarity Lite** can only work with a single instrument and does not support the following features: the direct control of chromatography devices using add on modules, Audit Trail, functions supporting 21 CFR part 11, integrated backup and batch reprocessing of chromatograms.

Passages only concerning the full version are distinguished by the following logo Full version in the manual and marked with a grey stripe to the right of the text.

1.2 Clarity Demo version

The **Demo** version which you have received contains all the functions of the full version. The difference is in the word "Demo" found in the header of the main **Clarity** window and on all printed documents. The **Demo** version allows you to try data acquisition procedures even without the converter board because the necessary data are simulated by data files.

1.3 Clarity Evaluation version

The **Clarity Eval** version is a version *without a possibility to acquire data* and serves for evaluation and modification of chromatograms and preparation of measurement methods.

The Eval version reads chromatograms and other files of the Clarity system created by any full version. All files created or modified by the Eval version may be used in a full version.

The **Eval** version can use chromatograms directly from the project of the full Clarity version over local network (LAN).

1.4 Computer and operating system requirements

The **Clarity** station will operate with any of the following Microsoft Windows systems (in any language): 98, Me, NT, 2000, XP.

The equivalent of a Pentium/200 PC with a 32 MB memory is sufficient when using Windows 98/Me. An equivalent to the Pentium/450 PC with 64 MB memory is sufficient when using Windows NT/2000/XP.

The minimum monitor resolution requirement is 800×600 pixels with 256 colours. However, we recommend a 1024×800 resolution with 64K colours (16 bit - High Colour).

2 Key Features

2.1 Clarity and Clarity Lite

- Measuring Simultaneous data acquisition from up to four four-detector chromatographs (4×4 configuration). The Clarity Lite version can measure up to four detectors on a single instrument.
- **Integration** 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 and their mathematical modification for example mutual deductions or derivations of any order.
- Calibration Internal and external standard calculation methods, calibration of groups of peaks and reference peaks method for better identification.
- 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 completion of measurement.
- **Summary result tables** Displays and prints selected results from all simultaneously displayed chromatograms.

- **User settings** User selects parameters for peak display and the specification for axes, including colour from an extensive array of colour settings. Text labels and lines, either as part of the area or anchored to a chromatogram, may also be inserted.
- **Export** Optional exportation of all results with or without the chromatogram, in various formats, into a file or clipboard.
- **Import** Imports chromatograms or mathematical curves, which have been saved in TXT or AIA formats.
- **Method and calibration history** Each chromatogram can easily be displayed under the same conditions as when it was printed, exported or saved.

2.2 Extended functions of the full version



- **Column performance** Calculations of peaks in terms of symmetry, efficiency, resolution; all by several methods (tangent, moments, etc.).
- **Batch** Automatically batch processes, displays, exports or prints any number of 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.
- **User accounts** Sets up access rights and passwords (including their parameters e.g., minimum length, validity, etc.). Each user can define his or her own station appearance.
- Audit trail Records selected events and operations into a special file. Records selected operations directly into a chromatogram.
- **Electronic signature** Each chromatogram can be electronically signed. Signature selection is based on the username or the signature certificate.

2.3 Add on modules



- **SST** (*System Suitability Test*) An integrated module for monitoring the quality of a measurement.
- LC/GC/AS control Integrated add on modules for controlling selected types of chromatographs and autosamplers.
- **PDA** Integrated add on module for evaluating analyses from *Photo-Diode Array* detectors (PDA).
- **GPC** Integrated add on module for evaluating GPC/SEC analyses (GPC = Gel Permeating Chromatography, SEC = Size Exclusion Chromatography).

2.4 What's new in Clarity

Compared to **CSW32**, **Clarity** contains the following new key features:

 The transition from a channel-based structure to an instrument based structure (i.e. easy multi-detector measuring on one instrument).



- The station includes tools for supporting the FDA's 21 CFR
 Part 11 guideline for electronic records:
 - Implementation of electronic signatures
 - Improved User Accounts
 - Extended Audit Trail
- Each chromatogram contains the entire "method history", including calibration.
- Improved integration algorithm. Now all parameters can be variable in time (particularly Peak Width and Threshold).
- Clicking on the chromatogram, calibration or method file in any file manager automatically opens the **Clarity** station.
- The **Station Configuration** is clearer and corresponds more to the logic of chromatographic equipment.
- Prints only valid calibrated compounds and their valid calibration levels.
- Includes a new Summary table of results in the Chromatogram window.
- **Sigmoid** interlining of the calibration curve, which is suitable for ECD detectors.

3 Demo Version Installation



A minimum 20-35 MB of HDD space (depending on the number of modules you wish to install) is required for program installation.

- Insert the CD.
- If the installation does not run automatically, select and run the INSTALL.EXE file.
- The installation wizard will guide you through the entire installation and will create a Clarity shortcut in the Start
 Programs menu and a Clarity icon on the desktop.

4 Program structure and control

The Clarity station has a hierarchical structure.



After start-up, the main **Clarity** window will be displayed containing the symbols of the connected chromatographs. After clicking on the chromatograph image and entering a username the **Instrument** window will be displayed. This window is used for acquiring and processing data from the chromatograph to which you are connected.

Note:

The Clarity station works with what we call "instruments". All detectors that are connected to the same instrument will share a common time base

4.1 Main Clarity window

√ Full version

The main **Clarity** window is designed to set the station's configuration, select access rights and basic directories for saving data.

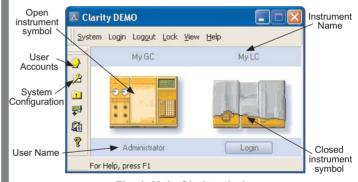


Fig. 1. Main Clarity window

The System Configuration dialog (opened using the Z icon or System - Configuration command) is where number of connected chromatographs, their names, the selection of displayed symbols and the type of directly controlled equipment are all established.

The User Accounts dialog (opened using the picon or System – User Accounts command) is where a name and password for each user is allocated and the extent of authority for individual operation types (access to files, ability to modify a calibration, integration parameters, etc.) are all determined. Each user can adjust the appearance of the station.

Instrument window 4.2

The Instrument window measures and evaluates an analysis from a selected chromatograph.



The window is displayed by clicking on the symbol of the relevant chromatograph in the main Clarity window. Depending on the number of configured instruments being used, up to four independent Instrument windows can be displayed simultaneously.

Windows are distinguished by line colour in the *Scheme* and by the instrument name in the window header.

Note:

The **Clarity** station must be set with as many instruments, as you want to measure independent analyses.

Instrument window contains an Information Table, Status Line and Scheme of data processing.

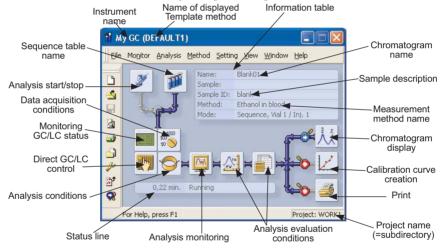


Fig. 2. Instrument window

All dialogs that enable the performance of actions that may be required on a given instrument can easily be displayed from the Instrument window by clicking the corresponding icons in the Scheme or using commands from the menu.

Caution! Sometimes it might happen that you cannot open any other window or the station will not react to your commands. This happens when working with what are known as, "modal windows". A modal window is a window that, while opened, forbids work to be performed in any other window. Particularly windows which are used to select files, set parameters, etc.



4.3 Chromatogram window



The **Chromatogram** window is the central window (opened by clicking the harmonic icon) for displaying, modifying and evaluating chromatograms. Use the icon to open one of the demo chromatograms.

Selection of displayed Switch to other station Work with multiple Custom chromatogram windows detectors/chromatograms label My GC - Chromatogram 2506multi - RI 1.10.2003 10:01:24 Secent (Linked Calibration) Ele_Edit Display Chromatogram Method Results SST Yiew Window Help X B B look Q @ @ D 4 2508multi - LIN This label and arrow are attached to the chromatogram Ψ 2506multi - Ri . × × × × 8558 lactic 7 BD-<u>۾</u> À × W (min.) Δ Δ Calibration File (Peak Table) Calculation Δ 250x8hr1 ESTD Δ 4.56 citric 1,5 Ordnr None 5 423 65 445 0.428 Ordor tertario 0.0065 Report in Result Table Unidentified o All Peaks 44 050 1.037 Ordor matic 0.024 Area 3,7 1,4 4,4 6,8 All Identified Peaks 83,314 0,612 0,0073 <u>H</u>eight All Peaks in Calibration 44 854 0.238 Ordor succinio 0.0053 0,019 37 378 1,125 Ordnr glycero 10.33 35 378 1,2 Ordnr 0,6 Ordnr 0.0058 ISTD Amount 4,079 0,024 Use Scale Factor ₩ 70 14 833 118,373 67,9 Ordnr ethanol 0,094 A Į٨ ement Conditions À SST Results Result table Other table tabs Chromatogram Setting type of result

Fig. 3. Chromatogram window

calculation

The results table for a selected chromatogram can be found in the **Results** tab. If it is not automatically displayed, click on the label of the **Results** tab in the bottom-left corner of the window or use the **Results - Result Table** command. Modification and evaluation of a chromatogram can be found in Chapt. **5.9 - 5.10.**

Tip:

modifications

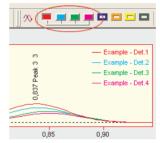


For enlarging a displayed chromatogram:

Use the **Display - Small Graph** command to hide the small orientation graph. Double-click around the splitter (the cursor will change to \downarrow) to enlarge the graph across the whole window. Clicking the Maximize icon in the header enlarges the **Chromatogram** window across the entire screen.

4.3.1 Multi-detector chromatograms

When using a multi-detector measurement, all signals will be saved in one chromatogram.

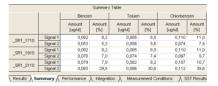


Individual signals from detectors are displayed as independent curves. To work with individual signals it is necessary to select the required signal from the **Chromatogram** menu or by using the coloured symbol in the **Overlay** toolbar. Each signal is independently worked with, just as with a singledetector chromatogram in the Overlay mode.

Caution! Remember that the right part of the Results tab and the **Measurement Conditions** *tab are common for all detectors. On* the other hand, the left part of the **Results** (the **Result Table**), the **Performance** and **Integration** tabs are detector specific.

4.3.2 Summary results table

You will make use of the Summary Table especially for reviewing and processing results from sequences. Here, all results from multiple chromatograms can easily be displayed at one time.





The special add-on SST module (System Suitability Test) is available for statistically processing results and monitoring selected parameters.

4.4 Calibration window



The **Calibration** window (opened by clicking the icon) is used for creating, modifying and displaying calibration curves is.

The global calibration table and calibration standard chromatogram are located in the **Compounds** tab.

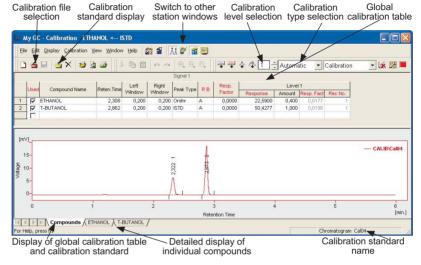
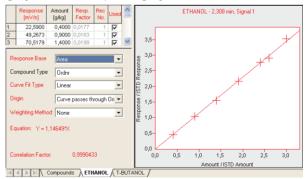


Fig. 4. Calibration window

Switch to the tab with the name of the compound (here displayed as *ethanol*) to display its calibration curve.



Note: The procedure for creating and using a simple calibration is included in the Chapter **Calibration** on pq. **21**.

4.5 Sequence window



The Sequence window (opened using the icon from the **Instrument** window) is used to define the sequential measurement of multiple samples.

Measurements are done individually in the table by row. Each row can define the way multiple samples are measured using the same method for multiple samples and/or by taking multiple injections of one sample.

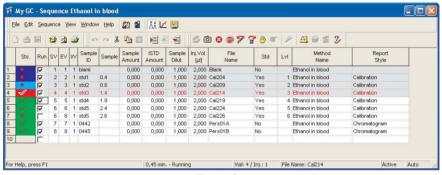


Fig. 5. Sequence window

Both an *active* or a *passive* operation are possible. An *active* sequence means that the station controls both the start-up and duration of individual analyses. In a *passive* sequence they are controlled by the autosampler and chromatograph.

Active sequence:

• increases the reliability of mutual synchronisation between **Clarity**, the autosampler and the chromatograph.



- is required when controlling selected autosamplers through the AS Control module.
- requires the interconnection of a control signal from the Clarity station to the autosampler.

Tip: The results of sequential measuring can be displayed in the Chromatogram window on the Summary tab using the File - Open Chromatogram from Sequence command (see Chapter 4.3.2 - Summary results table on page 11).

4.6 Method Setup dialog

The parameters for determining and describing the conditions for measuring and evaluating are set in the **Method Setup** dialog. These settings are saved in the template method file.



Fig. 6. Method Setup dialog - tabs

The **Method Setup** dialog is divided into tabs that are directly accessible from the **Instrument** window by clicking on one of the following icons:



Measurement – Measurement conditions with optional settings for selecting the duration of a measurement.



Acquisition – Parameters for signal measurement, voltage range, sampling rate, etc.



Integration – Integration table.



Calculation – Parameters for setting the type of calibration calculations.



AS Control – Direct control of the autosampler



LC/GC Control – Direct control of LC or GC chromatograph

Tip:

Control modules in the Demo version are configured on the "MY GC + AS" or "My LC + AS" instruments. The control modules are accessible in demo mode, in which all available control screens are visible.

4.1 Program exit

Using the **System - Exit** command in the **Clarity** (or **Clarity Lite**) window shuts down the program. Before exiting, you will be advised of any running measurements and unsaved files.

5 First "Analysis"

This chapter illustrates an exemplary model analysis that is designed to help demonstrate basic practical work procedures with the **Clarity** station. Naturally however, this model does not address all of the stations capabilities.

5.1 **Program start**

One of the Clarity station's key advantages is its ability to measure immediately without having to make any lengthy preparation or settings.

- Clicking the **M** icon on the desktop or by selecting **Start** - Programs - Clarity - Clarity Chromatography Station starts the program.
- Click on the image of the gas or liquid chromatograph to open the **Instrument** window.

You can immediately run an analysis measurement by clicking the **#** icon and using the **Run** button in the Instrument window. However, in this procedure, we will first explain certain functions before moving on to the measurement.

Note:

After opening the **Instrument** window in the purchased version, measurement can begin immediately upon activation of the start signal, directly from the chromatograph.

5.2 Signal monitoring



- Click the icon to display the current signal from detectors and check for drift and noise (see Fig. 8 on page 17).
- Clicking the icon or by using the File Exit command close the window.

Measurement and evaluation parameters 5.3

Certain parameters (voltage range, sampling rate etc.) must be set prior to measurement.

Caution! Making changes while measuring would render a measurement void and therefore the parameters are blocked.



Placing the cursor over the chromatograph icon will transform the icon into four icons.



Clicking on one of the circled icons will display the contents of the current method in the **Method Setup** dialog (see Chap. 4.6 on page 14 or Fig. 9 on p. 18).

Another method file can be selected using File - Open Method... command or the icon.

5.4 Analysis run



Click the \mathcal{J} icon to open the **Single Analysis** dialog and fill in the header of the measured analysis.

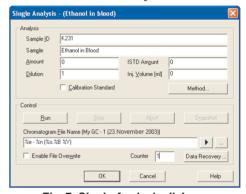


Fig. 7. Single Analysis dialog

Run the analysis using the Run command.

After running, the current measurement time and RUNNING inscription will be displayed in the **Instrument** window in the Status line under the Scheme.



5.5 Analysis monitoring



Click the icon to monitor the analysis procedure again.

Left click the mouse button and drag to select the area to be magnified and then release the button. The original display can be returned by clicking the **Q Unzoom** icon or by double-clicking the left mouse button within the graph area.

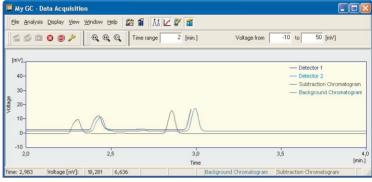


Fig. 8. Data Acquisition window

Data acquisition can be controlled using following icons: Single Run, Sequence Run, Abort and Stop.

The measured chromatogram can be compared to an already completed chromatogram, e.g. solvent, calibration standard, etc.

There are two ways to do this:

- The File Set Background Chromatogram command selects which chromatogram is to be displayed in the background.
- The Show Subtraction Chromatogram command displays the automatically subtracted chromatogram defined in the Method Setup - Measurement dialog.

Note: The chromatogram in the background will only be displayed during data acquisition.

5.6 Preparation for analysis stop



Prior to stopping an analysis, it is advisable to check the integration parameters using the icon or **Method** - **Integration** command.

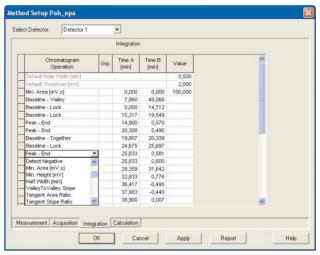


Fig. 9. Method Setup - Integration dialog

The key parameters are **Peak Width** and **Threshold**. Their simplified definitions are:

- The Peak Width parameter determines that all distinctly narrow peaks, compared to the defined value, will not be integrated.
- The Threshold parameter determines the noise threshold, which means that only peaks of at least double the height of the defined value will be detected.

However, in reality the function of the algorithm is more complex because it always combines the mutual effects of both parameters and the shape of the peak.

5.7 Analysis stop

The analysis can be stopped either using the **Stop** command in the **Single Analysis** dialog or will stop automatically after the time set in the **Run Time** field from the **Method Setup – Measurement** dialog has passed (the **Enable Autostop** checkbox must be checked).

At this moment the measured data will be integrated, evaluated and saved.

5.8 Naming the saved chromatogram



In the Single Analysis dialog (see Fig. 7 on page 16) there is a Chromatogram File Name field, which determines the chromatogram name. If a file with the same name already exists, you will be advised at the end of the measurement. Here you can use the automatic chromatogram-naming tool (e.g. ordinal number using %n variable, entering the date using %d variable, etc.).



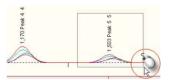
5.9 Chromatogram display and evaluation



The completed analysis will automatically be displayed in the **Chromatogram** window. An automatic display of the chromatogram can be prevented by switching the symbol next to the $\hbar \hat{k}$ icon to the symbol. The **Chromatogram** window can be displayed anytime by clicking directly on the $\hbar \hat{k}$ icon.

The required chromatogram can be selected using the icon from the **Chromatogram** window.

Just as in the window for signal monitoring, any section of the chromatogram can be zoomed to by left clicking, dragging to select the area and then releasing the mouse button.



5.10 Chromatogram modifications



The baseline is automatically generated but you can manually modify the chromatogram whenever you like.

There are two ways to accomplish this:

- interactively, using icons from the three toolbars located on the left edge of the Chromatogram window (or corresponding commands from the Chromatogram Baseline, Peak and Integration submenus). Modifications will be recorded in the Integration table of the Integration tab.
- <u>explicitly</u>, by directly entering and changing parameters in the Integration table of the **Integration** tab.

Tip: The Integration tab in the Chromatogram window is used to modify the <u>already measured chromatogram</u>. The Integration tab in the Method Setup dialog is used to edit the template method for newly measured chromatograms.

5.11 Data update and consistency

The **Clarity** station automatically keeps all data updated and consistent. For example, modification of the baseline will automatically be manifested in the results table. A change of any parameter updates all related calculations and displayed results. Therefore, the station does not need to contain any command such as Integrate, Recalculate, etc.

5.12 Printing





To facilitate printing, all the important windows contain the following icons **Report Setup**, **Print Preview** and **Print**.

- 1. Click the **j** icon in the **Chromatogram** window.
- 2. Select and configure the printer using the **Printer** command on the right-hand side of the **Report Setup** dialog.
- Select a suitable printing style using the **Open** command.
 The report style file actually defines the layout and contents of the printed report.

Information is divided into ten subsections, corresponding to the ten displayed tabs. On each tab a more detailed arrangement can be selected.



To include the entire section in the report, check the **Print** checkbox in the top-left corner of the tab. The selected section will be marked with a checkmark on the tab label

Tip: A tab can also be selected by double-clicking the left mouse button on the tab label.

4. Using the **Print Preview** icon a print preview can be displayed. Use the **Print** icon to print.

Note:

By default different report styles are predefined in all major windows to print information that is most pertinent to the dialog from which printing commands have been invoked. Report styles can easily be customized according to the preference of the user.

5.13 Calibration



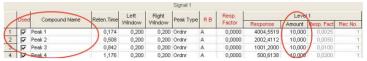
The creation and use of calibration curves is an extensive part of the **Clarity** station. Calibration curves created from calibration standards are saved in separate calibration files. Each file can contain a virtually unlimited number of curves, which then can be calibrated at up to twenty concentration levels.

Calibrated results are obtained by creating calibration curves, saving them in a calibration file and then subsequently linking a calibration file to a chromatogram, and setting the required type of calculation (external or internal standard).

5.13.1 Creating a calibration curve

- Click the icon or use the Window Calibration command.
- In the Calibration window, click the New Calibration icon or use the File - New command to create a new calibration file.
- Click the yellow Open Standard icon (a red icon would open a calibration file) or use the File Open Standard command to open an integrated chromatogram representing a calibration standard.
- 4. Click the icon to automatically transfer available data about each peak to the calibration table.

5. Modify compound names in the first column of the Calibration table (displayed below). Table fields can be edited after clicking on them with the mouse.



- 6. Fill in the known quantity of each compound in the Amount column under the number of the current calibrated level. After clicking on the tab of the required compound you should obtain a straight line, single-point calibration curve (if the described operations have been performed correctly).
- Finally, save the created calibration curves to a file under a selected name using the File - Save command.

Note:

The station also allows for calibration to be done at multiple levels with multiple recalibrations from a user-determined algorithm. This can be done automatically or manually. In the manual regime individual compounds can be reviewed and potentially modified. The method of interlining a curve, type of reaction, size of identification windows and improved identification by the method of reference peaks can also be selected for all compounds.

5.13.2 Calibration curve use

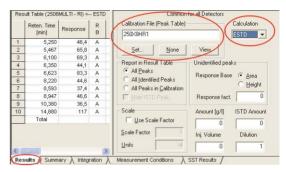
The simplest way of verifying that the calibration has been correctly performed is to link it to the chromatogram from which it was created.

- 1. Go to the **Chromatogram** window (e.g. the $\hbar \frac{1}{\hbar}$ icon).
- Here, click the Open Chromatogram icon to invoke the Open Chromatogram dialog.
- Because the calibration standards are saved in CALIB subdirectory, select this calibration subdirectory first (e.g. using the Calibration Directory icon in the top-right corner of the Open Chromatogram dialog). Here, select the chromatogram from which you created the calibration curves.



Further, set the calculation method:

- 4. Display the **Results** tab.
- 5. In the right-hand section, use the **Set** button to select your calibration file and then select ESTD in the Calculation item



Now the **Result Table** should display known quantities for compounds that you have entered, including the names and percentage ratios.

For peaks where no calibrated compound was found (based on correspondence of the retention time), the quantity will be zero. If the calibration compound is found and allocated but no calibration curve exists, the **Peak Type** column will display the Error inscription.

Caution! The chromatogram typically uses calibration curves from the calibration file whose name is shown in the righthand section of the Chromatogram - Results window. This will be a linked calibration by reference. Its advantage lies in its easy recalibration and changes when using single calibration file for multiple chromatograms.

> Nevertheless, all calibration curves are also saved directly in the chromatogram, including their history. Results pertaining to these saved calibration curves (including the then valid chromatogram modifications) can be recalled if you select the relevant method in the Open Chromatogram dialog in the Method field.



6 Conclusion

The **Clarity** station and our team of designers draw on years of experience in the development and testing of chromatographic stations for commercial laboratories, scientific facilities and universities.

Its functionality has been discussed and reliability carefully tested by many external consultants.

Because we like to have a close co-operation with our users we are appreciative of any comments, queries and ideas that you may have regarding the **Clarity** station, its demo version and this text.

If you have any problems in understanding this manual, or are not sure whether the **Clarity** station meets your laboratory requirements, please, contact us or your nearest distributor. A list of all our distributors can be found at **www.dataapex.com**.