DataApex

Clarity™

CHROMATOGRAPHY SOFTWARE

CLARITY DEMO

Clarity Demo Software   ENG

Author: MP

Contents

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

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.

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

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

[Chromatogram](#) (blue underlined) marks clickable links referring to related chapters.

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

Note: Notifies the reader of relevant information.

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

▌ **Marks the problem statement or trouble question.**

Description: Presents more detailed information on the problem, describes its causes, etc.

Solution: Marks the response to the question, presents a procedure how to remove it.

1 Brief description of Clarity station

This Guide contains walk-through of **Clarity Demo**.

Clarity chromatography station is an effective tool for acquisition, processing and evaluation of data. It permits the collection of data from virtually any gas or liquid chromatograph. It is possible to measure on up to four chromatographs simultaneously, of which each may be equipped with up to 32 detector signals. Each chromatograph may use further add-ons such as Extensions (e.g. **PDA**, **MS**, **CE**, **EA**, **GPC**...) and Controls (**LC**, **GC**, **AS control**...). **Clarity** supports the requirements of the **FDA's 21 CFR Part 11** guidelines.

It is possible to obtain **Clarity Lite Demo** station which does not contain same functions and DEMO examples as is described in this guide for the full version of **Clarity Demo**. For complete overview of the differences, please see D007 datasheet: **Clarity x Clarity Lite Comparison Table** which can be obtained from **DataApex Downoalds** at our website (www.dataapex.com/downloads).

1.1 DEMO version properties

DEMO version which you have received, contains all functions of the full version with the following limitations:

- Not possible to control instruments.
- Not possible to acquire real data.
- Not possible to import chromatograms.
- "**DEMO**" inscription in the header of the main *Clarity* window and in all printed documents.

Clarity Demo version allows you to try data acquisition procedures as it provides simulated data emulation.

Clarity Demo station uses only what is known as "demo data", it cannot process or import real chromatograms.

If you want to try the evaluation of your data, please let us know at sales@dataapex.com. We can prepare Clarity ready chromatograms from AIA FILES (*.CDF) your chromatograms.

Following ASCII text files containing signal values can also be supplied:

- Multidetector files (*.chr)
- Text files (*.txt)
- Comma separated values (*.csv)
- EZChrom ASCII files (*.asc)

1.2 Hardware and software requirements

For details regarding **Clarity** requirements and supported operating system refer to Compatibility Table on our website www.dataapex.com under section *Products - Clarity - Compatible Windows OS and Hardware* or in datasheet D016 (Part of **Clarity** installation or downloadable from www.dataapex.com/downloads).

2 Key features

- **Measuring** - Simultaneous data acquisition from up to four 32- detector chromatographs (4×32 configuration).
- **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 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 color from an extensive array of color settings. Text labels and lines, either as part of the area or anchored to a chromatogram, may also be inserted.
- **Export** - Optional export 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 text or AIA formats, from other programs.
- **Method and calibration history** - Each chromatogram can easily be displayed under the same conditions as when it was printed, exported or saved.
- **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.

2.1 Control Modules

Software modules that provide an interface for chromatography devices such as GC and HPLC systems, Autosamplers, Fraction Collectors and Valves. Direct control allows the device (s) to be controlled and monitored from the **Clarity** environment. The instrument method that controls the device is saved in the measured chromatograms.

2.2 Clarity Extensions

Software modules that enhance the capabilities of the **Clarity** data station. Extensions provide features within **Clarity** that are specific to a given type of analysis or for a specific task. Currently available modules are:

- **SST** (System Suitability Test) - Integrated module for monitoring the quality of a measurement.
- **GPC** - Integrated module for performing and evaluating GPC/SEC analyses (GPC = **Gel Permeating Chromatography**, SEC = **Size Exclusion Chromatography**).

To review the **GPC** Extension open Instrument *My GPC*.

- **PDA** - Integrated module for evaluating analyses from PDA (**Photo-Diode Array**, also called DAD - **Diode Array Detectors**).

To review the **PDA** Extension open Instrument *Agilent 1100 with DAD*.

- **MS** (Mass Spectrometry) - Integrated module for evaluating analyses from MS detectors.

To review the **MS** Extension refer to chapter 8 - **Alternative demo projects**.

- **CE** - Integrated module for performing and evaluating analyses from **Capillary Electrophoresis**. Brings CE terminology to **Clarity**.
- **NGA** (Natural Gas Analysis) - Integrated module for evaluating the calculations according to selected norms in analyses of natural gases and liquefied petroleum gases.

To review the **NGA** Extension refer to chapter 8 - **Alternative demo projects**.

- **EA** - Integrated module for performing and evaluating **Elemental Analyses**.

To review the **EA** Extension refer to chapter 8 - **Alternative demo projects**.

- **DHA** - (Detailed Hydrocarbon Analysis) - Integrated module for determination of individual components in spark ignition engine fuels (PIONA, etc.).

To review the **DHA** Extension refer to chapter 8 - **Alternative demo projects**.

- **GCxGC** - In development - Integrated module for interactive analysis and compound identification in chromatograms measured on any gas chromatograph equipped by two columns and a modulator.

This Extension is accessible only after **Full** installation of **Clarity Demo**. The installation procedure is described in 3 - **Clarity Demo version installation**.

To review the **GC x GC** Extension refer to chapter 8 - **Alternative demo projects**.

3 Demo version installation

The **Clarity Demo** can be acquired in two ways - either on the **USB** or downloaded from the www.dataapex.com/downloads.

- In case of the **Clarity Demo USB**:
  - Plug in the **USB**.
  - Run the INSTALL.EXE file.
- In case of downloaded version:
  - Download the **Clarity Demo version**.
  - If the installation does not start automatically, double click the downloaded INSTALL.EXE file.
- The installation wizard will guide you through the entire installation. After selecting the destination directory, an option of *Typical*, *Custom* or *Full* installation is to be made.
- You can simply select *Typical* and follow the instructions of the installation wizard until the entire installation is completed.

Note: *Typical* installation will provide all of the components needed for a successful DEMO operation, although some of the control modules will be absent. *Custom* installation can be used for selection of files to install.

Caution: It is recommended to uninstall any previous installation of **Clarity Demo** and in the installation wizard select *Overwrite all files without asking* to be able to follow this manual in the chapter **"Tour through the Clarity station"** on pg. **9**.

After installing the software, the installer will create a **Clarity Demo** shortcut in the *Start* menu and a **Clarity Demo** ⬛ icon on the desktop. During the installation a *System configuration* with predefined configuration for 4 instruments was created, offering review of **GC** with autosampler control, **LC** control, **GPC** Extension and **DAD** Extension. Refer to following image.
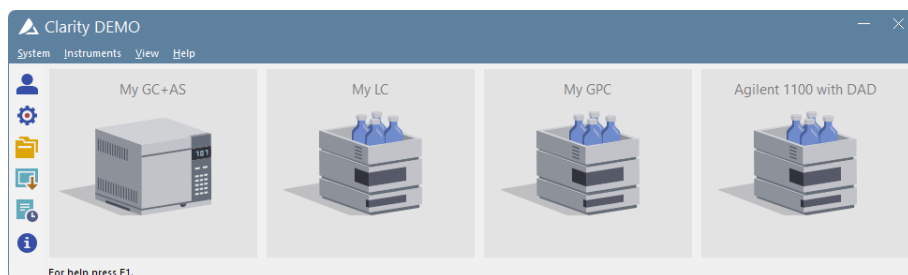

Fig. 1: Clarity Demo

To review other *Clarity* Extensions and projects refer to the chapter **"Alternative demo projects"** on pg. **27**.

4 Program structure and control

Clarity software has a hierarchic structure. After start-up the main *Clarity* window will be displayed with the symbols of configured Instruments.

After clicking on the chromatograph picture and entering the *User Name* (more information on *User Names* can be found in the **Reference Guide**) the *Instrument* window will be displayed. This window is used for acquisition and processing of data using the connected chromatograph.
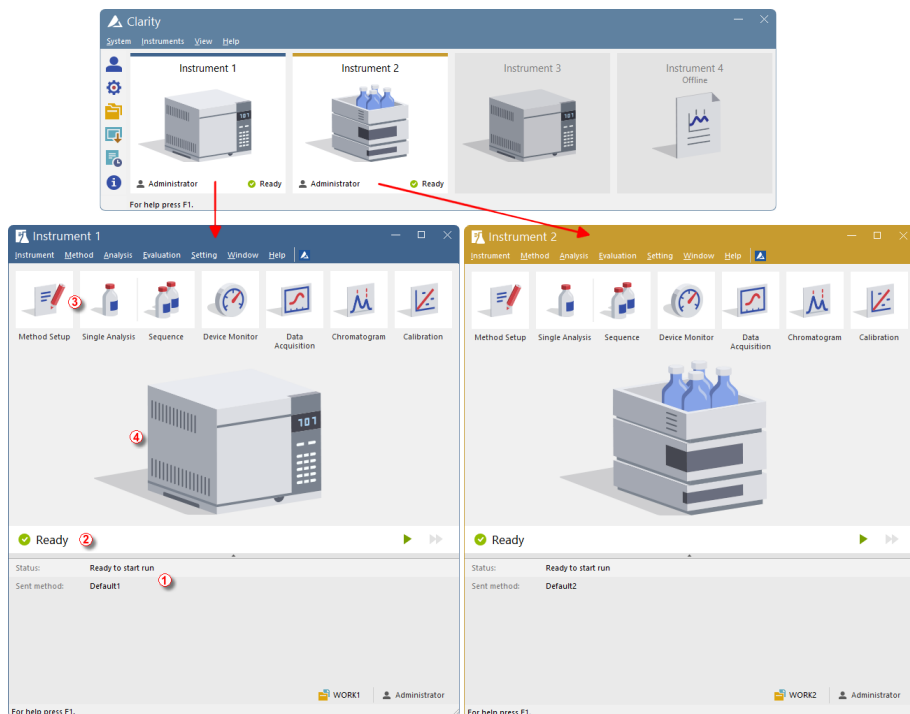

Fig. 2: Clarity and Instrument windows

Note: The **Clarity** station works with so-called Instruments. All detectors connected to the same Instrument share a common time base.

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

The *Instrument* window is used for measuring and evaluating an analysis from a selected chromatograph. The window is displayed by clicking on the symbol of the relevant chromatograph in the station's main *Clarity* window. Depending on the number of the Instruments, up to four independent *Instrument* windows can be displayed.

Each *Instrument* window contains an information table ① , status line ② , icons representing analysis process ③ and instrument image ④ (image is hidden at default window size). Instruments are distinguished by color and instrument name in the header.

All dialogs relevant for performance of actions in the *Instrument* window can be easily accessed from the *Instrument* window by using appropriate commands from the menu or by clicking their icons.

Note: In Tablet mode, processing icon's text description is not visible. Window invoked from Instrument window is indicated by blue frame around the icon.

5 Tour through the Clarity station

The following two sections will show you, step by step, the process of performing a single analysis (the chapter **"Running the Single Analysis"** on pg. **10**.) and sequence measurement (the chapter **"Running the Sequence measurement"** on pg. **17**.). These chapters are shown as a succession of steps, from which all should be performed in the given order. Some sections may be skipped, as we prepared their output for you to be used later. You will be notified of such sections. Also, the whole process presents Notes - the procedures described in them are optional and you don't need to perform them in order to reach the goal.

The **Clarity** software is intuitive and easy to master even without excessive training. The first analysis can be run in less than one minute after installing the station and configuring the hardware.

This tour is primarily designed for the users who installed the **Clarity Demo** version.

Note: Although this is only a tour of the station aimed at beginners with **Clarity**, it assumes users have basic knowledge specific to chromatography principles and basic processes such as calibration.

Note: When in doubts, pressing the F1 key or *Help* button shows help page concerning the specific window or dialog. In the invoked help, the *Index* tab serves for keywords searching, whereas the *Search* tab serves for full-text searching.

6 Running the Single Analysis

There is a simple project DEMO2 aimed on basic functions prepared on the Instrument 2 (labeled **My LC**). It shows the way to start a Single Analysis, monitor the Data Acquisition and process the resulting Chromatogram.

6.1 Instrument window

- Start the **Clarity Demo** station. The *Clarity* main window will display, showing four configured Instruments.
- Open the second Instrument (labeled **My LC**) by clicking on its icon. *Login Dialog* will open. Choose the Project DEMO2.
- *Administrator* user name is pre‑selected. This User Account needs no password, thus proceed by clicking the *OK* button. The dialog about Method adaptation may be displayed (if there was change to configuration). Click *Yes* and adapt the Method in the *Method Setup* dialog. In case you are using DEMO2 project, just click on the *OK*. Alternatively you can click *Help* to learn more about method adaptation. Now the **Instrument** window will be displayed.

Note: You can create your own User accounts from the main *Clarity* window using the *System - User Accounts...* command.
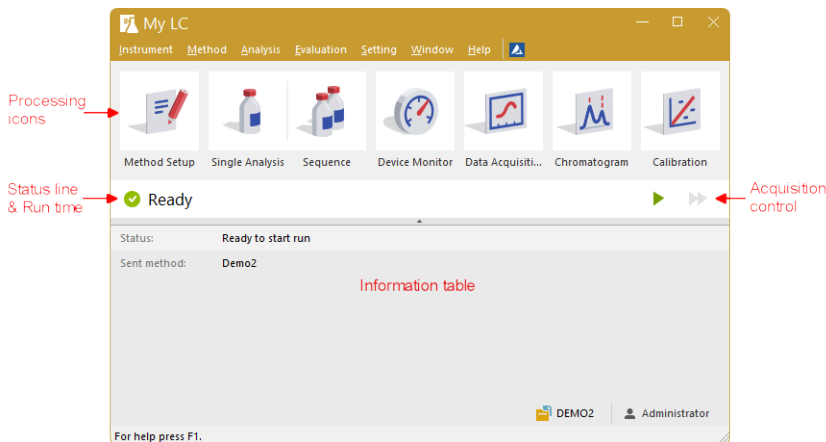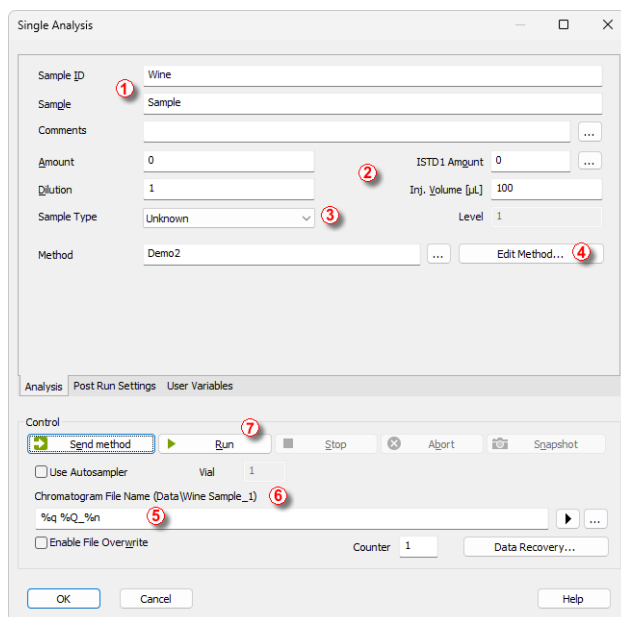
Fig. 3: Instrument window

6.2 Single Analysis dialog

Use the *Single Analysis* 🛅 icon in the *Instrument* window to open the *Single Analysis* dialog.

Fig. 4: Single Analysis dialog

- Fields in the *Analysis* tab carry the information about the sample. All necessary parameters are already set for you, but we will browse through them nonetheless.
- *Sample ID* and *Sample* fields ① are purely informational and can be propagated to chromatogram name, whereas the data in *Amount*, *Dilution*, *ISTD Amount* and *Inj. Volume* fields ② are used for further calculations.
- Choosing the *Standard* from the *Sample Type* drop-down ③ would mark this sample as a calibration standard and save the chromatogram into the CALIB subdirectory. Filling a value in the *Level* field would also automatically fill this chromatogram to the calibration which is linked in the used method.
- The measurement of the sample will be performed according to the template method selected in the *Method* field. Method can be selected by using ⋯ button. The *Edit Method...* button ④ serves to change the parameters of the selected template method. Click the button to open the *Method Setup* dialog and check the setting of the *Autostop* parameter (*Autostop* is enabled and

Run Time is set to 7.5 minutes). Return to the ***Single Analysis*** dialog by pressing *OK* button.

- The *Chromatogram File Name* field ⑤ serves to enter the file name of the resulting chromatograms. It is possible to use plain text together with variables adding the time, date, sample ID or other parameters to create unique chromatogram name. The resulting name can be seen just above the field ⑥ in parentheses.

Note: The complete set of available variables can be seen after clicking in the field and selecting the ▶ icon.

- Run the analysis by clicking the *Run* button ⑦ . The ***Single Analysis*** dialog will close now, but if you open it again, you will see three more buttons (*Stop*, *Abort*, *Snapshot*) accessible, allowing you to stop or abort the analysis or take snapshots (see the chapter **"Data Acquisition window"** on pg. **13**.).
- Close the ***Single Analysis*** dialog and return to the *Instrument* window.

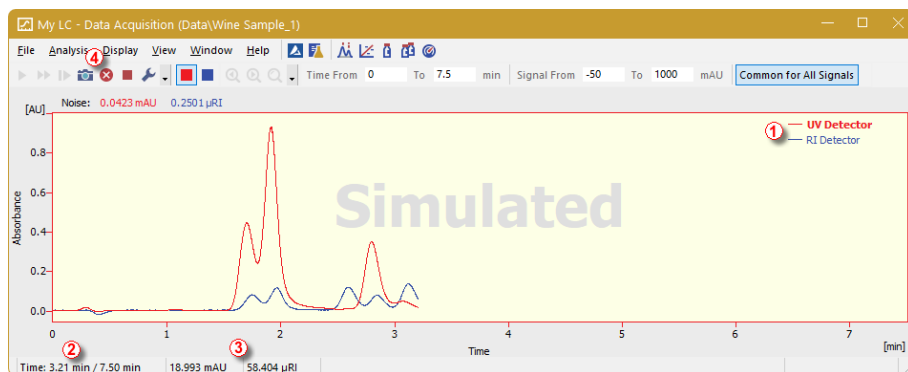## 6.3 Data Acquisition window

- In the *Instrument* window, look at the *Status line* (see **Fig. 3** on pg. **10**.). The acquisition is now signaled by the *RUNNING* state and the actual run time is displayed there.
- To see the data acquisition in process and possibly control it, use the *Data Acquisition* 📈 icon (see **Fig. 3** on pg. **10**.) to enter the **Data Acquisition** window.
- In the **Data Acquisition** window two signals can be seen. This is because the analysis is set as two-detector ① analysis.

Fig. 5: Data Acquisition window

- In the *Status bar* on the bottom of the **Data Acquisition** window, the time of the analysis ② can be seen, as well as the signal for each detector ③ in its particular units.

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Note: If the detector range exceeds the tolerance limit by ± 1.285%, the OVER string in red lettering will be displayed in the part of the status bar corresponding to the detector.

- *Stop* ■ and *Abort* ✖ icons ④ allow for canceling the analysis. In the case of stopping, **Clarity** will save all data acquired so far and cancel the analysis, while aborting cancels the acquisition without saving any data.

- *Snapshot* icon 📷 is also available for creating the preview of already measured data. After clicking it, the *Chromatogram* window will open with the chromatogram file corresponding to the part of the data already measured (more information on the *Chromatogram* window can be found in the chapter **"Chromatogram window"** on pg. **15**.). If the **Snapshot chromatogram** is to be preserved, it must be saved under a different name

(*File - Save As*), as it would be overwritten by the real chromatogram at the end of the analysis.

- After 7 minutes 30 seconds (the time set in the template method used for the measurement), the analysis will automatically stop and the *Chromatogram* window will open.

Note: You can stop current analysis anytime by pressing the *Stop* or *Abort* ④ icons

- The *Chromatogram* window opens because the station is set to do so. These settings are available in the *Single Run* window in *Post Run Settings* tab. Other post run actions including export of data or running external program can be set there as well.

6.4 Chromatogram window

- The *Chromatogram* window can be opened manually by clicking on the *Chromatogram* 🏔 icon in the *Instrument* window.
- The *Chromatogram* window is divided into two halves: the *Graph* pane and the *Results* pane.
- Enlarge any part of the graph by selecting the area to enlarge while holding the left mouse button. Return to the view of the entire chromatogram by double-clicking in the graph.
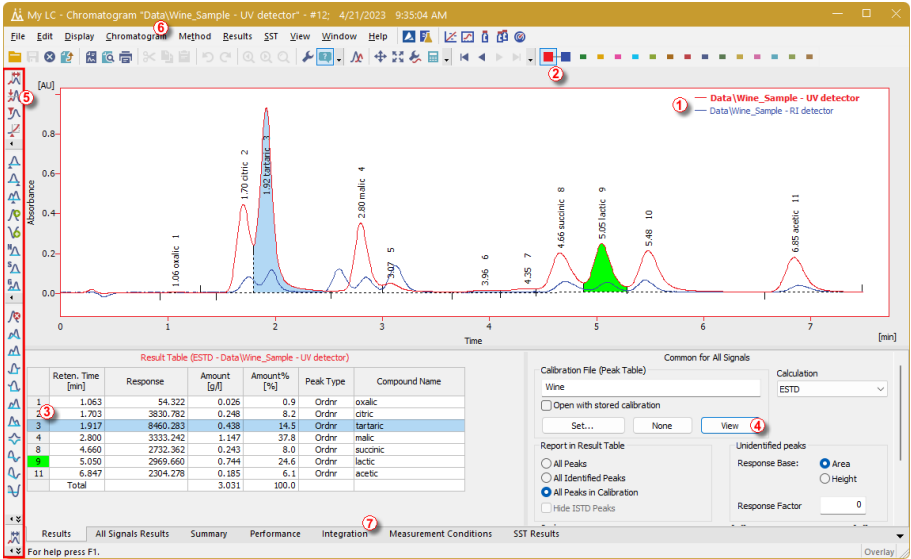

Fig. 6: Chromatogram window

- Only one signal of the chromatogram can be active at a time. The active signal can be recognized from the legend section ① in the upper right corner of the graph (active signal is set in bold), from the icons in the *Overlay* toolbar ② (the active signal has the highlighted 🔴 icon) or from the graph outline color and table headers color. Values inside the tables change by changing the active signal.
- Change the active signal by double clicking on its name in the legend section ① . Change the color of the currently active signal to another one by clicking on the *Not used color* 🟦 icon in the *Overlay* toolbar. All parts of the *Chromatogram* window mentioned in the previous step will change color.

- Click in any row in the *Result table* ③ . The peak (or peaks) corresponding to the row you just clicked into will change color according to the color of the signal. This change will last until the focus in the *Result table* is canceled.

- To add permanent color to the peak, click the *View* button ④ in the right side of the *Results* tab. This will get you to the linked calibration file. There, in the *Calibration Summary Table*, find the *Peak Color* column (see **Fig. 9** on pg. **21**.). In the row corresponding to the peak to be colored select the appropriate color and click *OK*. Return to the **Chromatogram** window by using the 👁 icon in the toolbar. The selected peak is now colored according to the color selected in the **Calibration** window (green in our case).

- You can change the integration of peaks by using the interactive icons in the toolbars on the left side of the **Chromatogram** window ⑤ , by using commands from *Chromatogram* menu ⑥ or directly in the *Integration* tab ⑦ . Any changes made either way will change the **Integration table** and can be copied to the template method. To do so, click on *Method - Save as Template...* menu command.

Note: If you want to measure chromatograms with altered integration table, copy the **Integration table** and paste it into the template method. New chromatograms will be automatically integrated according to these changed parameters. Already measured results can be reprocessed (for more details see the chapter **Linking the calibration to the method** on pg. **24**).

- Before you proceed to work with Instrument 1 (My GC+AS), close the window of Instrument 2 (My LC). It is not mandatory, but it will be less confusing to work with one **Instrument** at a time only. You will be asked to save any unsaved files.

7 Running the Sequence measurement

Sequence operation allows automated measurement of large number of samples for chromatographs equipped with autosamplers. **Clarity** provides the possibility to select an *ACTIVE* (start controlled by the station) or *PASSIVE* (start controlled by the autosampler) sequence. It is also possible to re-process already measured sequences.

Note: It is not necessary to have the **AS Control** module to use the autosampler; start synchronization can be performed even without it. However, the control module can add direct control from **Clarity** for automated sending of vial positions, injection volumes, etc., without the need to program the AS itself.

This chapter and the Clarity demo project prepared on the **Instrument 1** (named My GC + AS) will lead you through *Sequence*, *Calibration* and *Method Setup* windows used for automated measurement and preparation of template methods.

7.1 Sequence window

- In the main *Clarity* window, open Instrument 1 (With the label **My GC + AS**).
- In the displayed *Login* dialog with the pre-selected *Administrator* user, click the *OK* button.
- Use the *Sequence* button in the *Instrument* window to enter the *Sequence* window.

Note: *Sequence* window contains similar setting to *Single Analysis* dialog, but they are organized into separate columns.
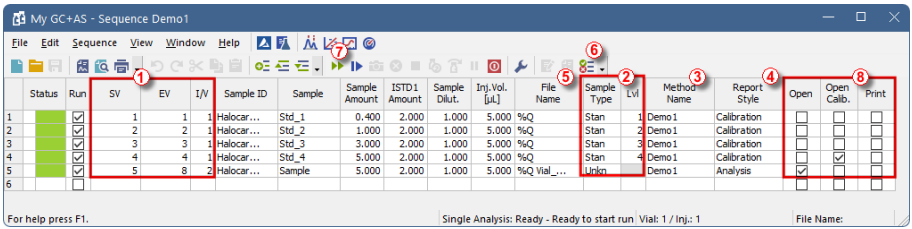

Fig. 7: Sequence window

- Look at the *Sequence Table*. Each row of this table defines one or more analyses, depending on fields *SV* (Starting vial), *EV* (Ending vial) and *I/V* (Injections per vial) ①. As it can be seen, the first four rows each present a single measurement (*SV* and *EV* is the same, *I/V* is *1*), while row 5 represents eight analyses (*SV* is *5*, *EV* is *8*, thus measuring 4 samples from 4 successive vials, and *I/V* parameter is *2* - each sample will be measured twice).

- Also, note that in the *Sample Type* and *Lvl* fields ② the first four samples are marked as standards on levels 1-4. These will be used for automatic making of the calibration (or its recalibration, if there already were any data in the calibration).

- The *Method Name* column ③ sets the template method used for measuring the sample. The *Report Style* column ④ sets the print style used for reporting the measurement. Each row can have its own template method and report style; it is thus possible to measure according to several template methods in one sequence.

- In the *File Name* column ⑤ , the name of the resulting chromatogram file is specified. It is possible to use variable parameters to form the chromatogram filename, for example **%Q** means that the file name will use the text from the *Sample* field. It is possible to combine several of these variables with plain text or symbols to create a unique file name for each chromatogram. The complete set of available variables can be seen after clicking in the field and selecting the 📥 icon.

- To check the sequence, click the 🔳 icon ⑥ . **Clarity** station will keep all symbols at the beginning of the row green (▮▮▮▮) meaning the row is ready or issue an error/warning 🔴⚠ message listing what should be corrected on which row to be able to proceed.

Note: For demonstration purposes only, try to make a mistake and check the sequence once more. For example, on row number **3**, change the text in the *Sample* column to *Std_1*, you can immediately see that a warning sign appeared on the corresponding rows - *1* and *3*. After pressing the 🔳 icon, warning message appears telling that there are two rows which would produce chromatogram with the same file name. Holding the mouse above either field will display the tooltip with the cause of the problem. Set the sequence back to its original state and continue to the next step.

- Start measuring the sequence using the ⏩ icon ⑦ . The state of the *ACTIVE* sequence will change to *WAITING FOR INJECTION* and as soon as the *Start* signal from the autosampler is detected, the measurement will start.

Note: Even if the autosampler is not connected, **Clarity Demo** will get the *Start* signal, thus starting the sequence. However, it is not possible to give its own demo data for each chromatogram, so all chromatograms would be the same. All files are already prepared for you. You may stop or abort the sequence now or later either from the *Data Acquisition* window or directly from the *Sequence* window.

- After the first row of the *Sequence table* (controlling one analysis) is measured, the Instrument will once again switch to the *WAITING FOR INJECTION* state and the autosampler will start a new measurement by

sending the *Start* signal. Stop the sequence from the *Data Acquisition* window or *Sequence* window at any time by pressing the *Stop* ■ button (single-click means that the currently measured Chromatogram will finish and the sequence will stop subsequently, after second click the sequence will stop immediately). All data measured will be saved. Or abort the measurement with *Abort* ✖ button (does not produce any chromatogram).

- Already measured rows will change *Status* from green field (▬▬) to icon with small chromatogram (〜▾). If there is a chromatogram resulting from this row, small triangle will appear in the icon - 〜▾ . Left mouse click on the triangle will reveal option to open the chromatogram(s). You can click on the name of the chromatogram to open it or select option to open all chromatograms in overlay.

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Note: It is possible to edit the sequence even during the measurement.

- On the right side of the *Sequence Window* you can check at each row whether corresponding chromatogram should be opened, printed or loaded into the calibration window.

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Note: There are many more hidden columns, they can be displayed by right-clicking the sequence table and selecting *Setup Columns*. In the following dialog move columns that should be displayed to *Show Columns* list.

7.2 Calibration window

The following section describes how to make a calibration. Calibration can be pre-filled automatically when using *Standard Sample Type* and filling *Lvl* field, but it can also be modified or fully created manually which is described below.

- Use the Calibration ⬚ button in the *Instrument* window to open the *Calibration* window.

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Note: If you wish to skip the following section about creating a new calibration, you can open (via the *File - Open...* command) the calibration file DEMO1.CAL we prepared for you instead and test the functions of the *Calibration* window on it. In this case you can continue with the chapter **"Linking the calibration to a chromatogram"** on pg. **23**.
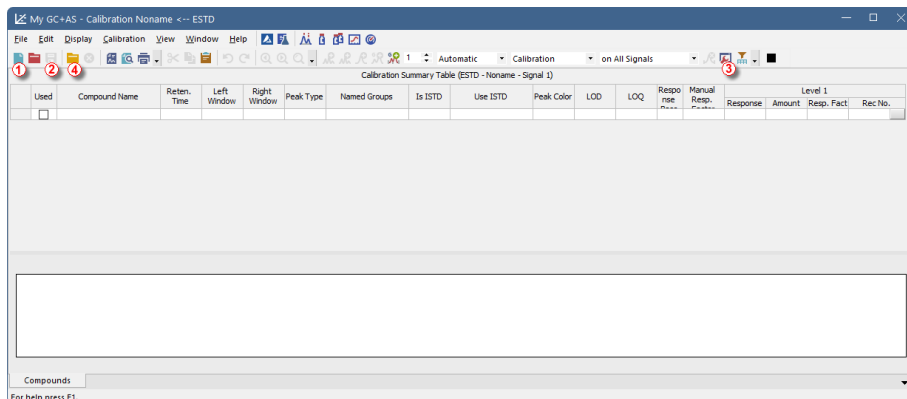
Fig. 8: Calibration window - empty

- It is necessary to create a new calibration. Use the *New Calibration* ![icon] icon ① to create new calibration file. Save the calibration under CALIBDEMO for example.

Note: To save the calibration now, it would be necessary to change its name (no calibration can be saved under the name NONAME.CAL) which can be done using *File - Save As...* command. *Save Calibration* ![icon] icon ② and *File - Save* command are enabled after first change to calibration has been made.

- Use the *Calibration Options* ![icon] icon ③ and change the *Display Mode* (top right corner of the dialog) to *ISTD*, then press *OK* button.
- Now, the calibration standards have to be imported to the calibration. Use the *Open Standard* ![icon] icon (yellow) ④ to open the STD 1.PRM data file. The lower part of the *Calibration* window now displays the chromatogram of the calibration standard.
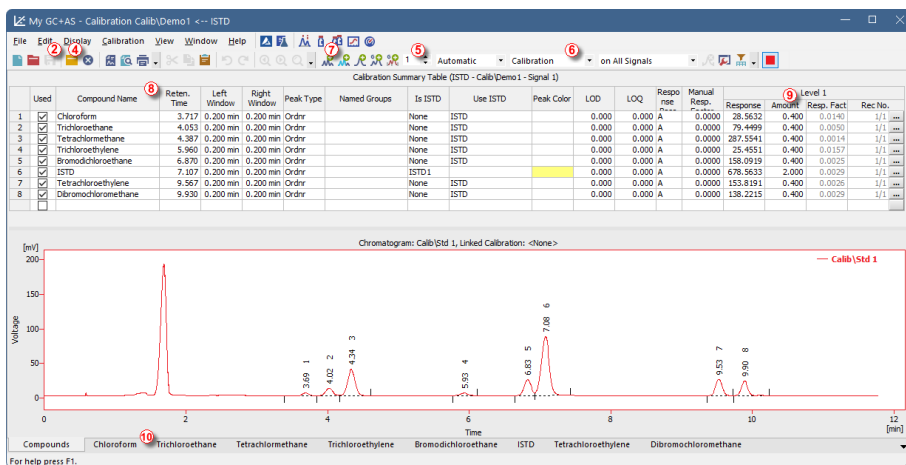
Fig. 9: Calibration window - loaded standard

- It's recommended to check that the *Current Level* field ⑤ is set to *1*, however, this is only for your orientation, because when *Calibration* option ⑥ is selected response is added to the first empty level regardless of which one is displayed. It is important to be on correct level when using *Recalibration* option. Use the *Add All* icon (blue) ⑦ to move all identified peaks to the calibration table. The Calibration table appears in the *Calibration* window, ready to be completed as seen on **Fig. 9** on pg. **21**.
- As it can be clearly seen in the calibration, particular peaks are now identified according to their retention times only. Click and edit the fields in the *Compound Name* column ⑧ to those seen on **Fig. 9** on pg. **21**. You may also set the peak color for some peak, for example the ISTD peak, in the *Peak Color* column.
- Fill the *Amount* column ⑨ with the concentration of the particular compounds. In this standard mixture, all compounds except for the peak number 6 have concentration of *0.4*.
- Peak number 6 is marked as an ISTD peak. In the *Is ISTD* column, change its type to ISTD1 and then set its amount in the *Amount* column to *2*.
- The first calibration level is now set. On the tabs of the individual compounds ⑩ (named according to the *Compound Name* field) the graph with single-point linear calibration can be seen.
- Proceed to setting the other calibration levels. The operation is quite simple and straightforward - use the *Open Standard* icon (yellow) ④ again to open another calibration standard named STD 2.PRM. Use the *Add All*

icon (blue) ⑦ . Fill in the *Amount* column with *1.0* values (except for the ISTD peak, in which the *2* value should be used again).

- Set the third calibration level accordingly using the STD 3.PRM file and *Amount* of *3.0* and the fourth level (file STD 4.PRM, *Amount 5.0*) except for the ISTD peak (*Amount 2* every time). On the tabs of the individual compounds ⑩ , the linear four-point calibration can be seen. Save the calibration file now using the *Save Calibration* 🖫 icon ② under the name CALIBDEMO.CAL into the default directory.

7.3 Linking the calibration to a chromatogram

- Any chromatogram can be linked to a calibration file, thus automatically giving calibrated results. In the *Instrument* window, use the *Chromatogram* icon to open the *Chromatogram* window.

- Use the *Open Chromatogram* icon to open chromatogram data based on the calibration you have just created. Use the SAMPLE_VIAL_6-1.PRM file saved in the default directory. Other files in the directory are uncalibrated too, but they will be used later.

- The data are uncalibrated and no information about the names of individual compounds is available, peaks in the **Result Table** are just described according to their retention times. To change this, the appropriate calibration should be linked to this chromatogram.

- Select the *Results* tab and look at the section on the right side of the screen. Use the *Set...* button in the *Calibration File (Peak Table)* section to select the calibration file (CALIBDEMO.CAL) created in the previous chapter. Any peaks present in calibration are now identified with their names.

Note: In case you skipped the process of making your own calibration, please use the pre-prepared DEMO1.CAL instead of CALIBDEMO.CAL.

7.4 Linking the calibration to the method

In case of large number of chromatograms, linking the calibration to each file separately would be a time-consuming process. To avoid this, the calibration may be linked to the resulting chromatograms automatically.

- Return to the *Instrument* window and Click on the *Method - Calculation* 🔢 menu command to open the *Method Setup* dialog directly on the *Calculation* tab ① . Alternatively, you can use other commands such as the *Integration* 📐, *Measurement* 📝 or *Acquisition* 〰️ . All of these sections (and some others) are part of the template method; thus they are present within the same dialog but on different tabs.
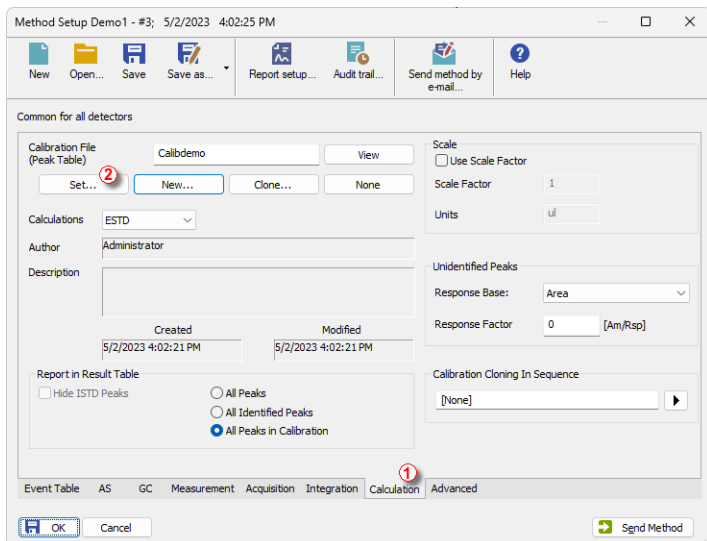

Fig. 10: Method Setup - Calculation dialog

- Use the *Set...* button ② to select the calibration file and link it to the method.
- Exit the *Method Setup* dialog using the *OK* button. Clicking this button applies and saves this change to the template method.
- Any chromatograms measured with this template method in the future will have the actual calibration linked.

7.5 Linking the calibration to a series of already measured chromatograms

In case you have already measured chromatograms and you want to change/update the calibration linked to it, it can be done with a single click using the *Batch* reprocess.

This command is especially useful when you have large number of already measured chromatograms and you want to modify them somehow.

Steps below will describe how to change the calibration in already measured chromatograms.

- Go to the *Instrument* window and use the *Analysis - Batch* command.
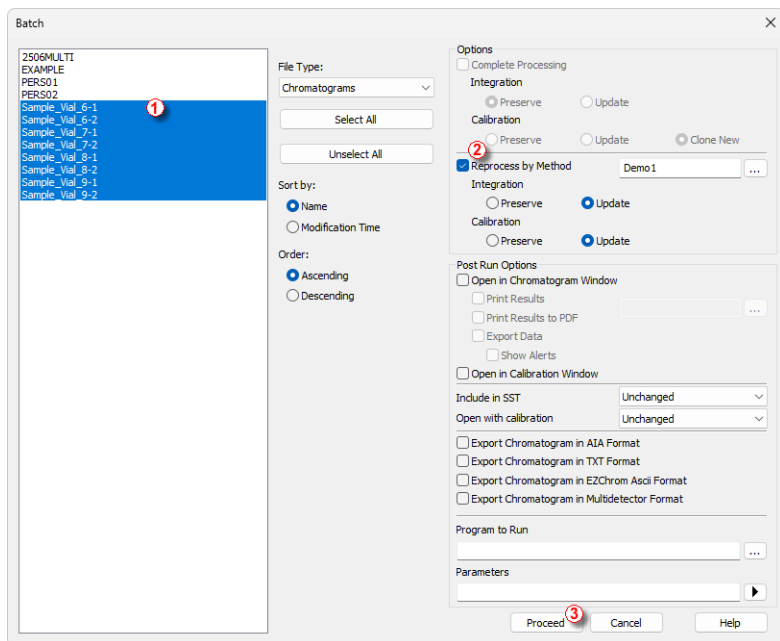
Fig. 11: Batch dialog with selected chromatograms

- Select files to be reprocessed in the left part of the dialog ① ; multiple files can be selected by left-clicking them while holding the **Ctrl** or **Shift** key. Mark all files with the names SAMPLE_VIAL_X-Y in the DATA directory to be reprocessed, check the *Reprocess by Method* ② checkbox and click the *Proceed* ③ button. All selected chromatograms will now have the calibration, according to the selected method, linked to it.

Note: Chromatograms to be batch processed need to be saved in the current project directory.

- Open the **Chromatogram** window and load any reprocessed file (e.g. SAMPLE_VIAL_7-2.PRM) and look at the *Result table*. All peaks present in the calibration are now identified and calibrated.
- Multiple chromatograms may be displayed at once. Use *File - Open Chromatogram* command or the *Open Chromatogram* 📁 icon and select several files to be opened in the **Open Chromatogram** dialog (*Open* button changes to *Open in Overlay*). *Overlay* mode can be toggled any time in *Chromatogram* window by using *Overlay* 📈 icon found in the *Overlay* toolbar.

8 Alternative demo projects

Clarity Demo opens with four default projects: **GC**, **LC**, **GPC** and **PDA**. The **GC** and **LC** projects have been described in previous chapters of this manual. Additionally there are projects **EA** (**Elemental Analysis**), **NGA** (**Natural Gas Analysis**), **DHA** (**Detailed Hydrocarbon Analysis**), **MS** (**Mass Spectrometry**) and **GCxGC** (**Two-dimensional Gas Chromatography** only available in Full installation).

To review the additional projects use:

- *Launch Manager* to set Clarity Demo to corresponding state.
- Refer to the corresponding manual that you can find
    - on the Installation USB media (All *Clarity* Manuals/Extensions)
    - download from our website www.dataapex.com/downloads

Launch Manager

1. Invoke the *Launch Manager* available in the Windows *Start Menu* or in BIN subfolder of Clarity Demo installation.
2. The *Select Clarity Profile* dialog will open.
3. Select the desired project and click the *Launch* button ① .
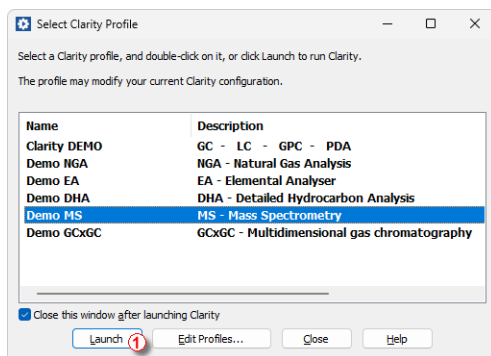
Fig. 12: Launch Manager

8.1 Demo GPC Project

The abbreviation **GPC** stands for the **Gel Permeation Chromatography** (also called **SEC - Size Exclusion Chromatography**). The **Clarity** station provides the means to perform the **GPC** analyses with several modes of calibration (Narrow, Broad, Broad on Narrow).

The project on the Instrument 3 (labeled **My GPC**) allows to test the capabilities of the **Clarity** station with the **GPC** Extension. Twenty chromatograms and five calibration files are prepared for testing. For more information on the functions of the **GPC** module, see the **GPC** Extension manual (downloadable at www.dataapex.com).

8.2 Demo PDA Project

Clarity station is able to handle data collected from **PDA** (**Photo Diode Array**) detectors, sometimes also called **DAD** (**Diode Array Detectors**). The third dimension of the spectral data can be displayed in a number of ways, including 3D rendering.

The project on the Instrument 4 (labeled **Agilent 1100 with DAD**) enables to test the capabilities of the **Clarity** station with the **PDA** Extension. Several chromatograms and two calibrations are prepared for testing. For more information on the functions of the **PDA** module, see the **PDA** Extension manual (downloadable at www.dataapex.com).

8.3 Demo NGA Project

Clarity station can contain a software module called **NGA** (**Natural Gas Analysis**) for Natural Gas and Liquified Petroleum Gas data processing. You no longer need an external tool for gas properties calculations since the Clarity contains the complete workflow of data acquisition, peak calibration, gas properties calculations based on supported norms and reporting. It is possible to perform summary calculations of gas properties from multiple signals and chromatograms. Calculations in the NGA Extension currently supports these forms:

Natural Gas
- ISO 6976-95
- ASTM D 3588-98
- GPA 2172-09

Liquified Petroleum Gas
- ASTM D 2421-02
- ASTM D 2598-02
- ISO 8973-97 / EN589-04

The project (instrument labeled as **NGA**) enables to test the capabilities of the **Clarity** station with the **NGA** Extension. Two chromatograms and one calibration are prepared for testing. For more information on the functions of the **NGA** module, see the **NGA** Extension manual (downloadable at www.dataapex.com).

8.4 Demo EA Project

Clarity station contains a software module called **EA** (**Elemental Analysis**) for determining the Carbon, Hydrogen, Nitrogen, Oxygen, and Sulphur (CHNS-O) content of unknowns that is one of the most basic and essential needs of any chemist. EA Extension provides a simplified version of the Clarity user interface that speeds up the workflow with elemental analyzers equipped by autosamplers. EA Extension is an optional addition to Clarity software, it cannot be used as a standalone program. Its user interface is optimized for maximum efficiency in repetitive tasks. Using features that are specific to EA Analysis, such as Standard

Table, automatic weight input from analytical balance and other improvements, EA Extension provides an interactive and automated tool for determining the Carbon, Hydrogen, Nitrogen, Oxygen, and Sulfur (CHNS-O) content of unknowns.

The project (instrument labeled as **EA**) enables to test the capabilities of the **Clarity** station with the **EA** Extension. Several chromatograms and one calibration and a sequence are prepared for testing. For more information on the functions of the **EA** module, see the **EA** Extension manual (downloadable at www.dataapex.com).

8.5 Demo DHA Project

Clarity station contains a software module called **DHA** for Detailed Hydrocarbon Analysis. It allows the determination of individual components in spark ignition engine fuels. Clarity brings you the ability to calculate the properties of the samples directly in the data station with the complete workflow of data acquisition, peak calibration, DHA calculations based on supported norms and reporting. These methods are often referred to as PONA, PIONA, O-PONA, etc. It is possible to create a custom norm which will meet the conditions in your laboratory. Calculations in the DHA Extension currently supports these forms:

- ASTM D-6730
- Custom Method - Allows you to create custom norm which will meet the conditions in your laboratory.

The project (instrument labeled as **DHA**) enables to test the capabilities of the **Clarity** station with the **DHA** Extension. Several chromatograms and two calibrations are prepared for testing. For more information on the functions of the **DHA** module, see the **DHA** Extension manual (downloadable at www.dataapex.com).

8.6 Demo MS Project

The **Clarity MS** (**Mass Spectrometry**) Extension is a tool that is used for processing data that has been acquired from selected Mass Spectrometry detectors. Spectral data, together with chromatograms, add a third dimension to analytical data analysis.

The **MS** Extension expands the capability of **Clarity** by providing interactive spectral analysis, peak purity analysis and compound identification that is based on a spectral library search. The Extension is prepared to function with single quadrupole MS detectors and TOF MS detectors. The **Clarity** is designed to acquire and evaluate data from up to four chromatographs at a time (multi-detector measurement support). Any Instrument within the **Clarity** can use the **MS** Extension.

All data is saved in a single file; a chromatogram at any m/z value or even only a spectrum can simply be recalled for review after an analysis. MS spectra, acquired using a MS detector, may be interactively selected from a chromatogram signal for visual inspection and comparison. The spectra may also be used for peak purity

determinations and component identification through spectral libraries. It is possible to import MS data in AIA (cdf), mzXML, MzML and mzData formats.

The project (instrument labeled as **MS**) enables to test the capabilities of the **Clarity** station with the **MS** Extension. Several chromatograms and one calibration are prepared for testing. This set contains data acquired using TOF MS detector with unity precision. For more information on the functions of the **MS** module, see the **MS** Extension manual (downloadable at www.dataapex.com).

8.7 Demo GCxGC Project

The **Clarity GCxGC** (**Two-dimensional gas chromatography**) Extension is still in development and it is not fully finished. It is a tool developed for visualizing and processing two-dimensional chromatographic data. It expands the capability of **Clarity** by providing interactive analysis and compound identification in chromatograms measured on any gas chromatograph equipped by two columns and a modulator.

In a typical GCxGC system, the separation in the first column is based on boiling point, while separation in the second dimension is determined by the polarity of compounds. This will generate highly structured two-dimensional chromatograms.

The project on the Instrument labeled **My GCxGC** enables to test the capabilities of the **Clarity** station with the **GCxGC** Extension. Several chromatograms and one calibration are prepared for testing. For more information on the functions of the **GCxGC** module, see the **GCxGC** Extension manual (downloadable at www.dataapex.com).