DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

8.3 VS 8.2

Clarity (Lite)   ENG

Sections of the manual connected only to the **Clarity Full** version are marked with the ✓Full version icon.

Contents

To facilitate the orientation in the **8.3 vs 8.2** 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, 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 Preamble

This document will guide you through the news and improvements in the **Clarity** Chromatography Station version **8.3** compared to version **8.2**.

 The most interesting features of version 8.3 include:

- Method versioning
- Changes in the Calibration - grouped parameters on the tab of a specific compound
- Audit Trail - new columns and icons
- MS Extension enhancements
- New and updated control modules

2 Clarity

2.1 Method versioning

2.1.1 General concepts

It is sometimes necessary to distinguish with what method parameters was a chromatogram acquired. Therefore we have implemented method versioning, just like in the chromatogram.

Method versioning is intended for tracking down changes in the method file (*.met). With each save, a new version of the method is created. These method versions are saved internally into the corresponding method file.

Any existing method (from any previous version of Clarity) will now display version #1, even though it may have been saved with new parameters numerous times before, and now any subsequent method save will create a new version - incrementing the version by +1.

The power of method versioning is that you can go back in time and see what were the parameters at any specific time.

Select Method dialog invoked from the Method Setup window (*Open...* command) now contains *Version* listbox allowing to open any historical version of the method file.
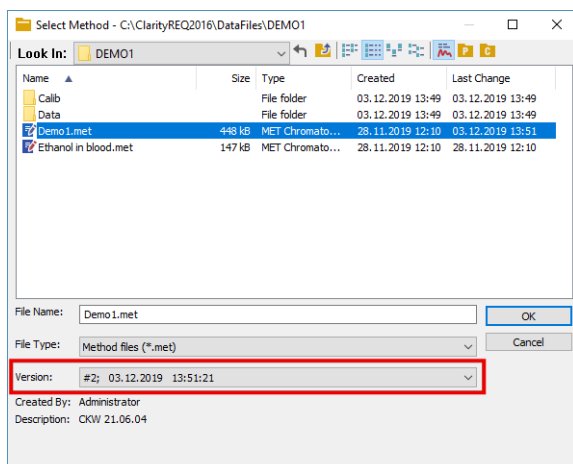

Fig 1: Select Method

To easily track what method version is opened, Method Setup header now displays version number and time of last method save.
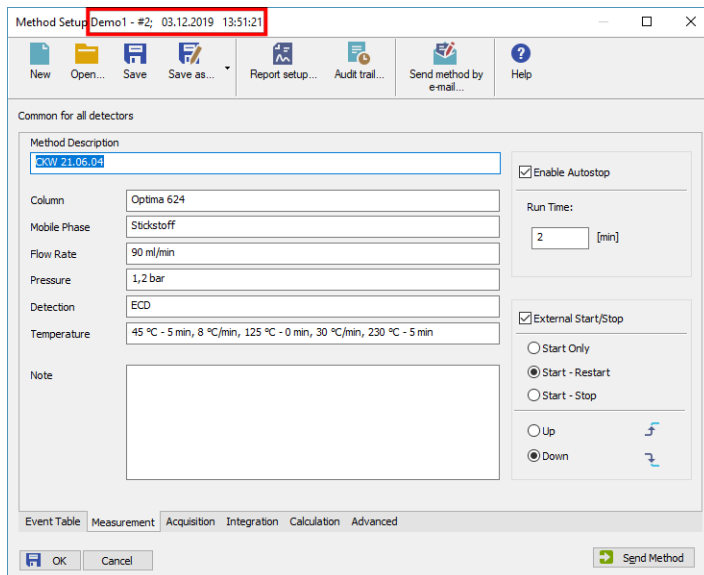
Fig 2: Method Setup

Note: Any historical version of the method will be opened in read-only mode which means it is not possible to change any parameters. To edit historical version you must save it under a new name.

2.1.2 Audit Trail

Changes to the method are logged into the Method Audit Trail, along with the information about the version and save date.

Fig 3: Method Setup

2.1.3 Extended functionality of Save as...

Along with method versioning, the *Save As...* functionality has been extended. The default remains the same, clicking directly the *Save As...*

icon invokes dialog to specify the new file name, after that the newly created method is loaded in the Method Setup dialog.

Clicking the small arrow next to the *Save As...* icon reveals the available options:

- Makes a copy of the method along with any changes and opens it (changes in the original method are discarded).
- Makes a copy of the method along with any changes but does not open it and you continue working with the original one.
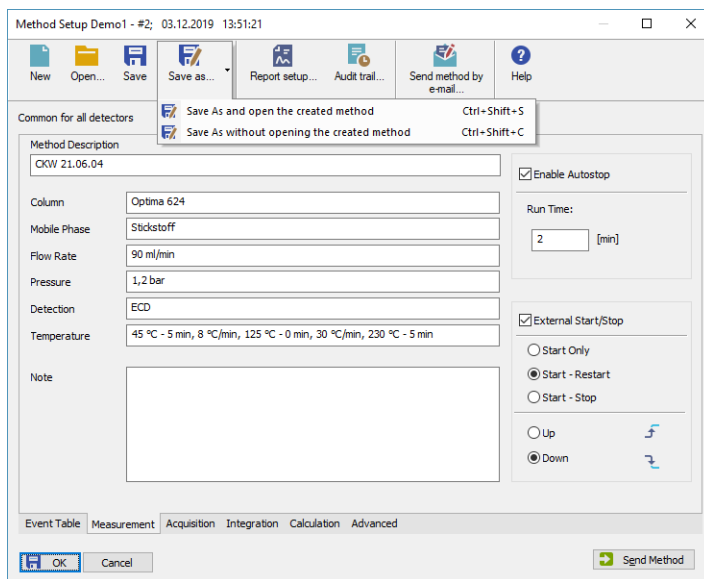

Fig 4: Method Setup

2.2 Calibration

2.2.1 Grouped parameters on the tab of a specific compound

From the identification and quantification point of view, Calibration is perhaps the most important part of data processing. We have redesigned the tab of a specific compound to better distinguish individual dependencies and grouped them into logical units.
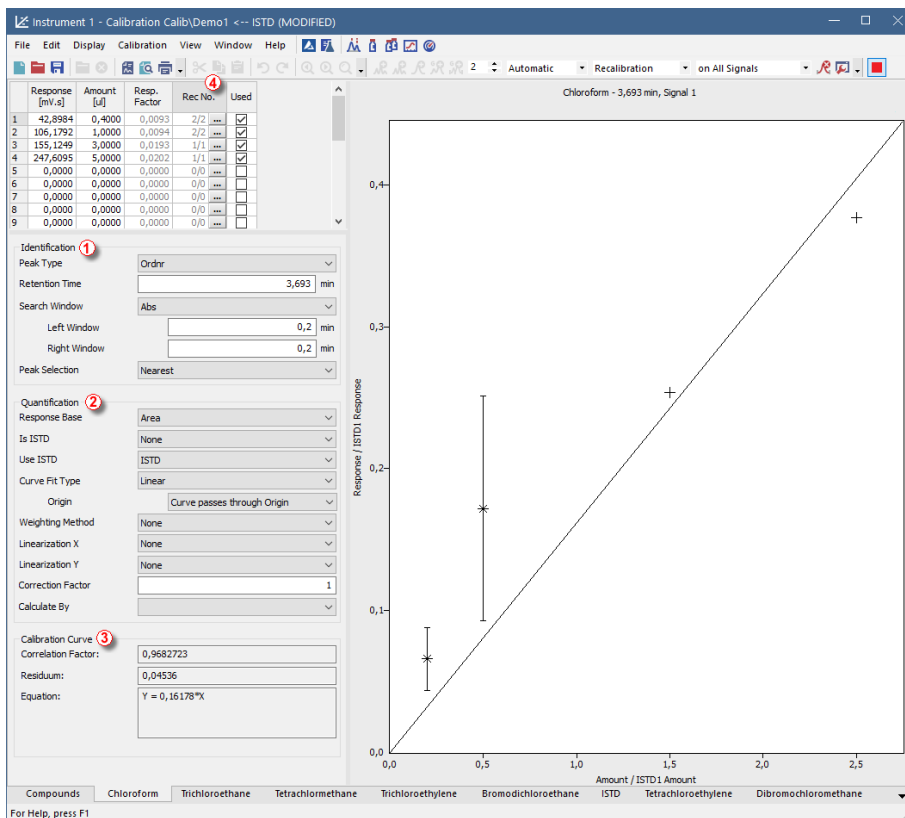

Fig 5: Calibration - tab of a specific compound

The left part of Calibration window is now divided into 3 groups (table with levels is ignored):

- ① Identification - it groups parameters which define conditions under which the peak is recognized.

- ② Quantification - it groups parameters which affect the calculation of the calibration curve.
- ③ Calibration curve - it groups parameters which are calculated from the calibration curve. All parameters displayed here are read-only and cannot be changed.

Some parameters in the groups above are context based, meaning changing the value in one field directly affects other field. Such example is the *Curve Fit Type* which affects whether the option below it will be *Origin*, *Manual Response Factor* or *Ending Point*.
Some Clarity Extensions feature additional amendments but the principle remains the same.

2.2.2 Removed Weight from Calibration Options

Weight option was a historical remain which users found confusing and it was thus removed from the Calibration Options. Any calibration set to *Weight* option will be automatically transferred to *Average* and the change will be recorded in the *Calibration Audit Trail.*

Fig 6: Calibration Options

2.2.3 Improved visibility of recalibrations

*Rec No.*④ (**Fig 5** on pg **5**.) shows number of used recalibrations / total recalibrations on the respective level. Clicking ... invokes the Details of Calibration Point dialog with a detailed log of the selected level of the calibration point. Levels that have not yet been (re)calibrated have default value *0/0*.

2.3 Audit Trail ✓Full version

Audit Trail serves as a log of individual operations of the station. It is required by the GLP practice. It is also useful for onsite troubleshooting and technical support where we can see what was happening on the station.

We have added two more columns:

- *Group* column displays icon and group into which the given audit trail entry falls.
- *Severity* column displays the severity of the logged operation. Severity can be either <empty>, *Warning* or *Error*.

In the future we plan to allow filtering that will enable to easily search for vital information. Therefore the "cleanup" was intended to make better sense of the logged operations.

Fig 7: Audit Trail

2.4 Extension MS ✓Full version

> We continually strive to improve the user experience. This was the main reason for the changes which are described next.

2.4.1 MS Method

> *MS Method* is for the MS extension an important part as it holds information about the evaluation of spectral data. *MS Method* is no more hidden under the *Measurement Conditions* tab. It is on the same level as *Results*, *Summary* and similar tabs. We hope that this change will enable users to access settings of the MS Method more easily and faster.
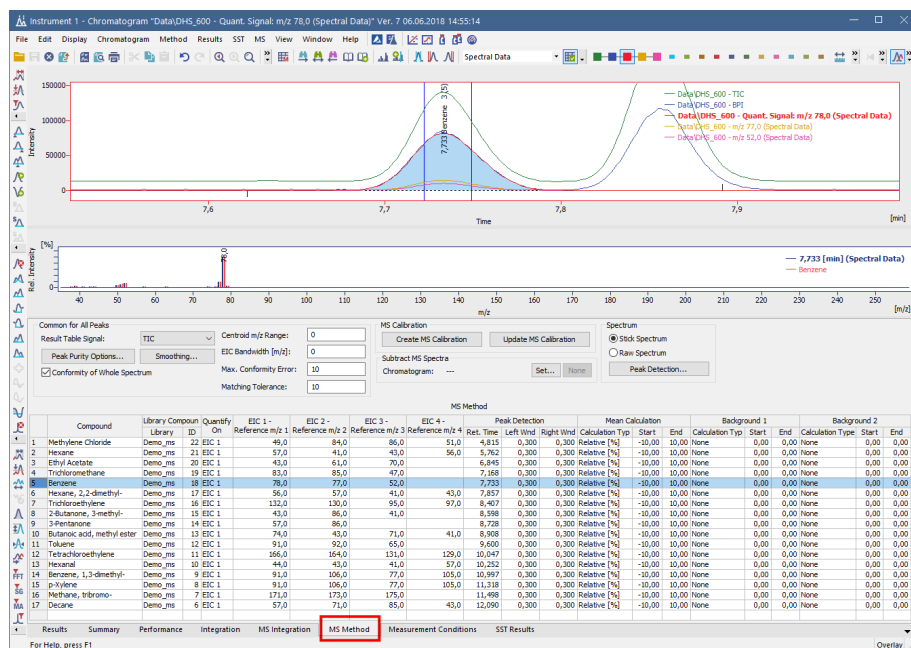
Fig 8: Chromatogram - MS Method tab

2.4.2 MS Integration

> *Integration table* is quite context based - information displayed is based according to which signal is selected. However MS Extension adds one more level of confusion - the quantification signal which can also be integrated.
>
> Therefore the *MS Integration* tab has been isolated from the *Integration* tab. In the *MS Integration* tab only quantification signals are displayed and

can be integrated. To change integration of a quantification signal - from the *Quant. Signal* combobox choose which signal you want to integrate and then continue just as you would in the standard *Integration* table.
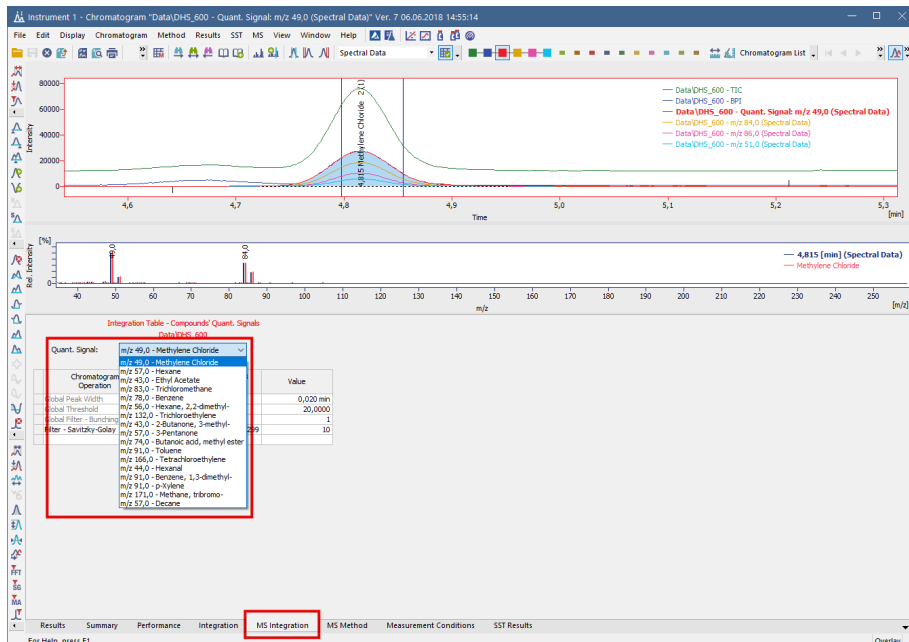
Fig 9: Chromatogram - MS Integration tab

Integration tab (solely in the MS Extension) now displays only signals which come from the *Result Table*. *Signal* combobox lists detector signals only - without quantification signals.
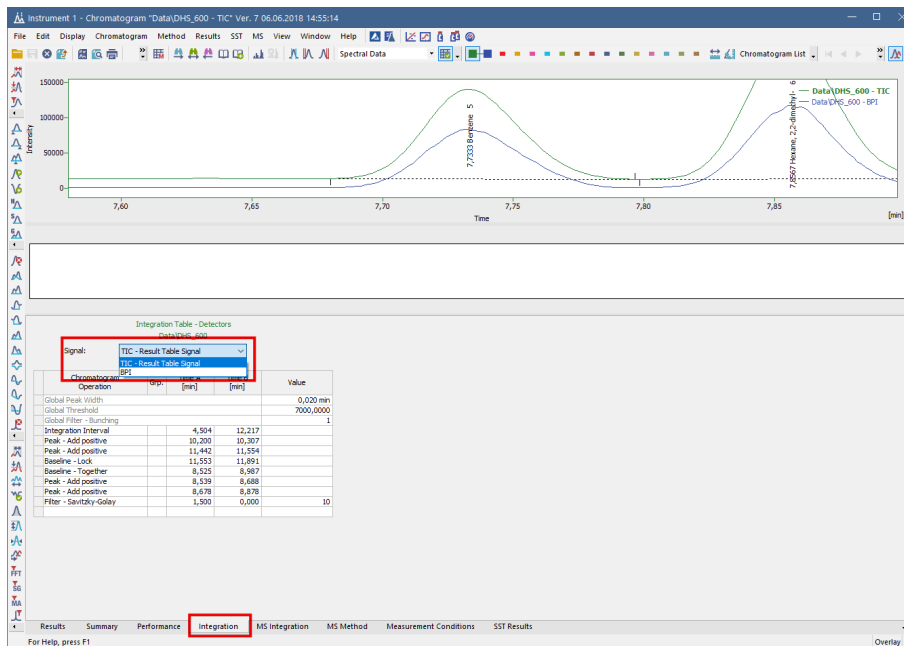
Fig 10: Chromatogram - Integration tab

2.4.3 Report Setup

MS tab in the Report Setup now contains section *MS Integration Table* which allows to select which integration table of quantification signal (option to print all signals is available) will be printed.
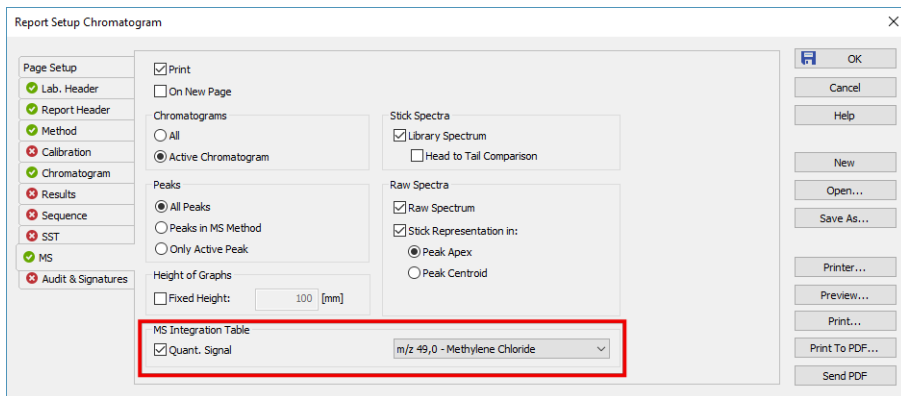
Fig 11: Report Setup - MS tab

2.5 Other changes

- Audit Trail: AreaEN and DescriptionEN columns will be filled even when the station is switched into English.
- Audit Trail: Audit Trails created with version 8.3 cannot be opened in previous versions due changes in the internal format.
- Chromatogram: Enabled a limited support for Paste operation into the Integration table.
- Chromatogram: Improved Asymmetry calculation in case of too few datapoints.
- GLP: New item "Disallow Chromatogram Merge Operation" in the GLP Options dialog.
- IQ: Reorganized IQ to better distinguish between control modules installed by Clarity and by 3rd parties.
- Installation: Installer step for selecting acquisition device was removed from the installation as it confused many users. This removal will not affect any existing installations.
- Installation: Entering User Code (U/C) step was moved almost to the end. Once the U/C is entered, the installation jumps to the last step where the user may start Clarity or simply end the installation process.
- OQ Validation: Instead of Knauer Virtual Detector a new OQ Validation detector by Ruby script is used.
- PDA Extension: Changes in Peak Purity calculations. The reference spectrum now is peak apex in the spectrum (previously in the active signal, which may have been shifted). In case the calculated correlation is negative, it is replaced by zero (previously absolute value was used). Corrected calculation of absorbance threshold.

3 New and updated control modules ✓Full version

This section contains new and updated control modules introduced in Clarity **8.3**.
Testing state is dedicated for new control modules.
Ready state is dedicated for existing control modules that have been updated or somehow improved.

3.1 Agilent

New:

- Agilent 8860, 8890 and Intuvo 900 GC control modules are now in the Testing state.

Updated:

- Agilent ICF libraries updated to version A.02.06.DU3.

Removed:

- Agilent 1200 control module supporting G1315C, G1315D, G1321B detectors was removed from installation. In order to continue using Agilent 1200, please use the Agilent ICF LC driver.

3.2 Analytik Jena

New:

- Analytik Jena PQ LC / IC control module is now in the Testing state.

3.3 Antec

Updated:

- Antec Decade Elite control module - added support for pulse mode 2. See respective manual for further details.
- Antec AS 110 control module was replaced by Alias II. control module - the functionality remained the same.

3.4 CQS

Updated:

- Climax HPLC system control module is now in the Ready state.

3.5 Dani

Updated:

- Dani Master GC control module updated to version 1.6.11.0.

3.6 Esensing

Updated:

- MassChrom1299 HPLC system control module is now in the Ready state.

3.7 Fuli

Updated:

- GC 9720 Plus control module is now in the Ready state.
- GC 9790 Plus control module is now in the Ready state.

3.8 JAI

Updated:

- JAI FC-7000 control module is now in the Ready state.

3.9 Futecs

New:

- Futecs CD-6000, CT-6000, P-6000 and RI-6000 control modules are now in the Testing state.

3.10 Knauer

Updated:

- Knauer HPLC control module updated to version 8.1.0.6036.

3.11 Sedere

Updated:

- Sedere Sedex 85/90 and ELSD USB drivers updated to version 1.3.
- Sedere Sedex LC/FP 100 USB drivers updated to version 1.2.

3.12 Shimadzu

Updated:

- Shimadzu GC2010 control module is now in the Ready state.

3.13 Spark

New:

- Spark LC1299 and LC1299 Plus HPLC systems control modules are now in the Testing state.

Updated:

- Spark Symbiosis ACE - added support for new options for addressing cartridges.

3.14 Sykam

New:

- Sykam S4120 control module is now in the Testing state.
- Sykam S150 control module is now in the Testing state.

Updated:

- Sykam S6510 control module is now in the Ready state.
- Sykam S1130 control module updated to version 2.0.1.5.
- Sykam S5300 control module updated to version 2.0.0.13.

3.15 VICI Valco Instruments

Updated:

- VICI Valco TCD3 Thermal Conductivity detector control module is now in the Ready state.
- VICI Valco valves - option to set position while closing Instrument has been moved from Method Setup to System Configuration of the respective valve.

3.16 Watrex

New:

- Watrex Streamline CT1, IC1, P1m and P1s control modules are now in the Testing state.

Updated:

- Watrex Streamline AS1, AS2 and UV1 control modules are now in the Ready state.

3.17 Young In Chromass

New:

- Young In Chromass ChroZen GC control module is now in the Testing state.

Updated:

- Young In Chromass YL9130 control module updated to version 4.0.1.12.
- Young In Chromass YL9150 Plus control module updated to version 1.0.0.6.