DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

10.1 VS 10.0

Clarity (Lite) ENG

Code/Rev.: M254/100B
Date: 2025-05-12

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

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Contents

To facilitate the orientation in the **10.1 vs 10.0** 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 Preamble

This document will guide you through the news and improvements in the **Clarity Chromatography Station** version **10.1** compared to version **10.0**.

Feature highlights include:

- Calibration - Possible to calculate results based on ISTD from different signal.
- Calibration - Determination Coefficient is calculated for calibration curve.
- Installation Qualification - IQ can be launched directly from the Clarity main window.
- GLP - Improvements in signature consistency.
- Chromatogram - When closing multiple chromatograms, changes can be saved or discarded all at once.
- NIST - Search in NIST libraries is now based on NIST23 instead of NIST08.
- MS-MS - A new DEMO project for MS-MS extension available on request.
- DHA - DHA norms originally distributed by DANI are now not visible in new installations.
- New and updated control modules.

The list of all changes is available in the What's New document accessible from the software.

2 Clarity

2.1 Calibration improvements

In **Clarity 10.1** we present several changes in calibration.

2.1.1 Allow ISTD from different signal

In some applications such as ICP-MS speciation some signals may not contain ISTD peaks, while the response of ISTD peak on other signal would be an appropriate replacement. Up to **Clarity** version 10.0 a peak could only use the internal standard which has response on it's own signal, this has now changed.

There is a new option in *Calibration Options* dialog that enables the usage of ISTD peaks that are found on a different signal of the same chromatogram.

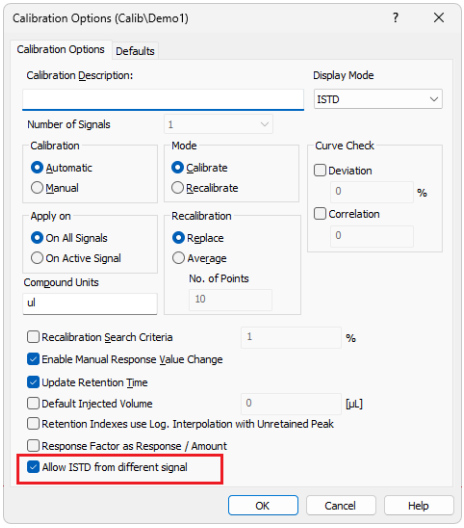

Fig. 1: Allow ISTD from different signal

When the option is not checked, **Clarity** behaves the same as in past with regards to which ISTD peaks can be used by a non-ISTD compound. When checked, the *Use ISTD* column in the **Calibration Summary Table** will contain separate entries for the ISTD peaks defined on particular signals in addition to their generic entries.

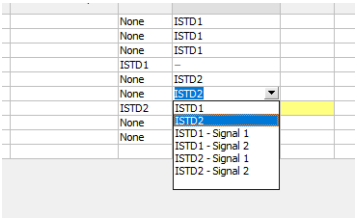

Fig. 2: Possible ISTD peak selections

Generic entries (without the *Signal X* part in the name) mean "use the given ISTD peak on the active signal", while entry with the *Signal X* part in the name means "use the given ISTD peak calibration curve from Signal X, regardless for which signal the results are calculated." Usage of a ISTD peak from specific signal will be visible in the **Calibration Summary Table** (*Use ISTD* column) and **Result Table** (*Peak Type* column).

2.1.2 Calibration warning messages

Clarity provides more warning messages caused by problems while evaluating the calibration, and the displayed warning messages are more specific. When there are problems encountered during the evaluation of the calibration or a chromatogram (e.g. ISTD peak that is needed for the calculation has missing responses in the calibration or is not present in the measured chromatogram), a warning message is displayed in the header of the **Result Table** and/or in the header of the **Calibration Summary Table**.The number of possible warnings has increased for the Result Table and warnings are newly added above **Calibration Summary Table**. The warnings in calibration are displayed regardless of the active signal, while for **Result Table** only warnings relevant to that signal evaluation are displayed. In case more warnings should be displayed, the last row will end with ... sign and all the messages can be accessed on a tooltip over the warning area.

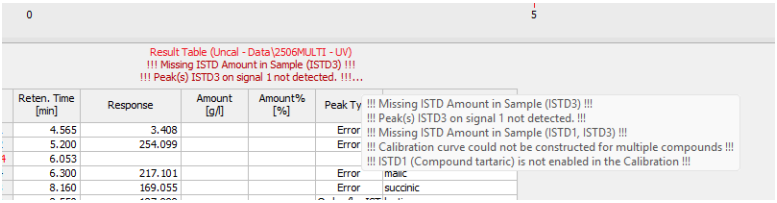

Fig. 3: Warnings over Result Table

2.1.3 Blank

Blank is now ignored for construction of the curve when using *Curve passes through Origin* or *Compute with Origin* options. The only option where blank level is included is *Ignore Origin* for given compound. This column is hidden by default in the **Calibration Summary Table**, but is always visible on the tabs of individual compounds. When the blank level is added to the calibration, the origin handling is changed to *Ignore Origin* for any relevant compounds (present in the blank). If the origin handling is later manually changed on compounds that use the blank level, a warning is displayed over the **Calibration Summary Table**.

In Standard Addition Display Mode, the blank level is never used for construction of the curve as a level with 0 Amount is defined differently.

2.1.4 Determination Coefficient (R^2)

Also referred to as coefficient of determination, is now calculated for calibration curve in addition to Correlation Coefficient. It describes how well the independent variable(s) explain the variability of the dependent variable.

$$R^2 = 1 - \frac{\sum(x_i - y_i)^2}{\sum(x_i - X)^2}$$

where:

x_i - The actual (measured) response at level i.

y_i - The calculated (predicted) response at level i.

X - The mean of all actual responses (including the zero point if *Compute with Origin* or *Curve passes through Origin* is selected, Blank level is ignored when one of these options is selected).

2.2 IQ improvements

Because some information on the station (such as serial numbers of possibly connected A/D Converters) are available only after first **Clarity** start, newly the station must be started at least once before running IQ is possible. IQ can be run directly from the main station window using *Help - IQ Report* command. Option to start IQ directly from the installer has been removed.

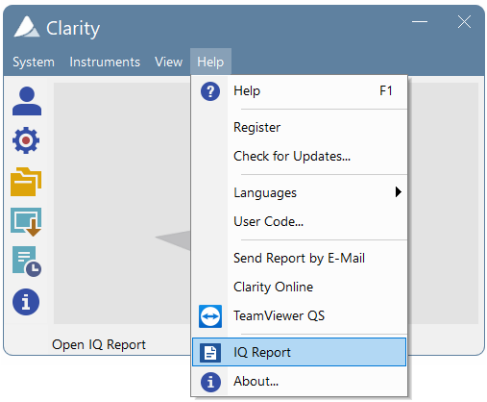

Fig. 4: IQ Report command in the main window

2.3 Signature improvements

For improved signatures consistency, the chromatograms opened with linked calibration have the state of their signature always as "Not Signed". Whenever a chromatogram opened with linked calibration is signed, the opening preference is changed to "Open with Stored calibration" so next time the chromatogram will be opened with the stored calibration by default (showing the actual signature state).

Along with this change, the handling of signature display in non-recent stored versions was amended, historical signed versions no longer state "not current".

3 New and updated control modules

This section contains new and updated control modules introduced in Clarity **10.1**.

3.1 Clarity 10.1

3.1.1 Agilent

Update:

- Agilent ICF control module has been updated to version A.03.04.

3.1.2 Axcend

First Release:

- Axcend FocusArray control module is now available.

Update:

- Axcend Focus LC control module has been updated to version 1.3.5.4.

3.1.3 Coruitech

First Release:

- Corui Module SamplerU and Corui Module ColumnOven control modules are now available through external installer.

3.1.4 Ecom

First Release:

- Ecom ECLM2000 control module is now available.
- Ecom FRC ECVA2000 control module is now available.
- Ecom LED20 control module is now available.

3.1.5 Netel

Update:

- Netel Chrom Plus 6000 control module has been updated to version 1.0.2.44.

3.1.6 Sykam

Update:

- Sykam S1130 control module has been updated to version 2.0.2.6.
- Sykam S4120 control module has been updated to version 1.0.8.1.
- Sykam S5300 control module has been updated to version 2.0.1.4.
- Sykam S6510 control module has been updated to version 1.0.6.1.

3.1.7 Testa Analytical

First Release:

- Testa Analytical Flowmeter control module is now available.

3.1.8 Young In Chromass

Update:

- Young In Chromass YCChroZenGC control module has been updated to version 1.0.2.44.
- Young In Chromass YCChroZenPump control module has been updated to version 1.0.1.22.