DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

EA EXTENSION

Clarity Extension   ENG

Contents

To facilitate the orientation in the **EA Extension** 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 EA - Elemental Analysis

The **Clarity EA** is an optional **Extension** for the **Clarity Chromatography Station** (from version 2.4). It is intended for data acquisition and evaluation from **Elemental Analyzers** using the technique of combustion/gas chromatography. Any of the **Clarity EA** Instruments can be switched to standard mode for standard chromatography processing, so the user can use both Elemental Analyzer and chromatograph attached to the same software.

EA Extension is also compatible with **Clarity Offline** software.

2 Specification

The **EA Extension** is an optional, fully integrated part of **Clarity** software. It can be ordered as a part of new datastation or as an Extension to existing datastation (p/n A30).

3 Installation

The **EA Extension** is enabled by appropriate user code entered during installation or later by using the *Help - User Code* command from the *Clarity* main window.

To switch an Instrument to *EA mode*, select the **EA** option from the *Instrument Type Setting* dialog.

Instrument Type Setting dialog is invoked by clicking on the ⋯ button in the *System Configuration* dialog.

Options that are technically possible and have been purchased are enabled by default. Otherwise they are automatically disabled.
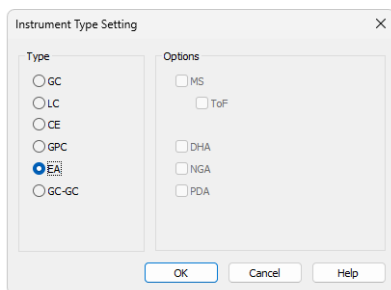
Fig. 1: Switching to the EA mode

4 Key Features

The **EA Extension** brings the following features to the **Clarity** station:

- **Sequence mode only** - since the Elemental analyzers are commonly used for large series of samples, the single analysis mode is not supported to simplify the operation.
- **Standard Table** - the composition of standards used for calibration is stored in an editable **Standard Table** and is automatically transferred to the sequence when the standard is selected.
- **Calibration** - the calibration is created automatically for each new sequence and has the same name as the sequence.
- **Calibration curves** - the calibration curves for the individual elements determined are constructed for amounts calculated from the entered *Sample Amount* and composition of the standard defined in the **Standard Table**.
- **Fixed method from instrument** - to simplify the operation only the template method opened in the *Instrument* window is used for the sample processing (i.e. it is not possible to select different methods for different rows in a sequence).
- **Carbon Ratio** - the column providing the ratio of the respective element to the carbon is present in the **Result Table** and **Summary Table**.
- **Balances** - selected types of analytical balances can be configured to the Instrument, enabling direct transfer of sample amount to the **Sequence Table**.

The following standard **Clarity** features will also help the user to make the best of the **EA** analysis in **Clarity**:

- **User calculations** - the user can define custom calculations in the **Result Table** and **Summary Table**. With the use of the integrated editor you can create your own columns from the original ones and use individual mathematical functions.
- **Reports** - user selectable report sections, WYSIWYG formatting of Graphs and Tables.
- **Batch** - automatic batch processing, display, export or print of any number of chromatograms.
- **Summary Result Table** - displays and prints selected results from all simultaneously displayed chromatograms.

Note: The **Weighting Method** for determining the value of the weight of individual points when calculating the interposing curve has been removed from **EA Extension.** Such method is described in the **Clarity Reference Guide** - chapter **Calibration**, section **Weighting Method**.

4.1 Basic principles and terms

- **Elemental Analysis** (**EA**) is an analytical technique used for determination of elemental composition of various samples. The contents of common elements (C, H, N, O, S) are determined by various methods.
- One of the methods of the **Elemental Analysis** is **combustion** of the sample and separation of the products by **gas chromatography** techniques.
- Dedicated instruments called **Elemental Analyzers** are commercially available.
- **Analytical Balance** are widely used with Elemental Analyzers. **Clarity** with **EA** Extension can automatically transfer the weight from the balance to the **Sequence Table**.

4.2 EA-specific terminology

Some of the information fields on the *Method Setup - Measurement* and *Chromatogram - Measurement Conditions* tabs were renamed to better match the **EA** terminology.
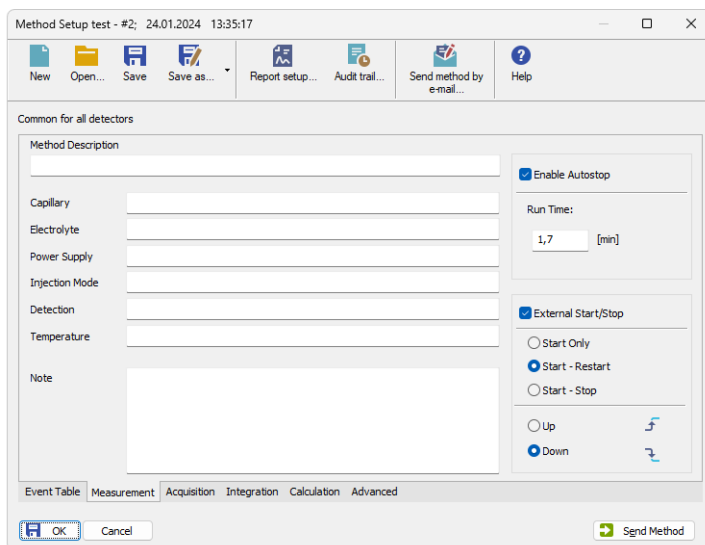

Fig. 2: Method Setup - Measurement

Tab. 1: Renamed existing informational fields:

Default mode	EA mode
Column	GC Column
Mobile Phase	Oven Temperature

Default mode	EA mode
Pressure	Left Furnace Temperature
Temperature	Right Furnace Temperature

5 EA Extension Description

After installation, new functions of the **EA Extension** will be available. Only features changed or added to the **Clarity** standard mode are listed and described here. In general the changes are present in the Instrument window (Single Analysis and Sequence are replaced with just the Sequence window modified to the EA Extension needs), Sequence window itself and Chromatogram Result Table (additional calculation columns). Moreover, peaks in the *Calibration* on the **EA Instrument** must be named exactly the same as components in the Standard Table - this means *Nitrogen*, *Carbon*, *Hydrogen* and *Sulphur* (no localizations, translations etc.) for correct match.

5.1 Instrument window

In the **EA Mode** the *Instrument* window has different appearance.
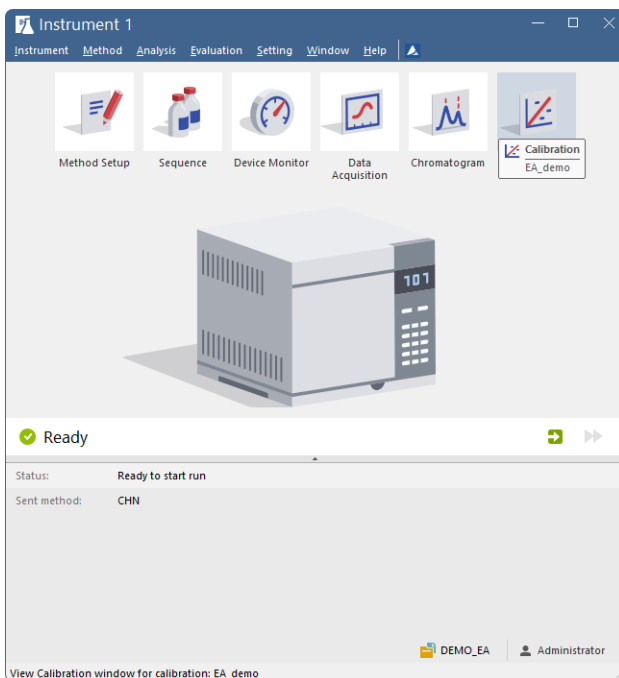

Fig. 3: EA Instrument window

The *Single Analysis* and *Sequence* icons in the **Scheme of Data Processing** have been replaced by a single *EA Sequence* icon. *Calculation* tab has been removed from the *Method Setup* dialog (and from the *Instrument* window menu), the calibration to be applied to the measured chromatograms is defined by the sequence name instead.

5.2 Sequence window

Sequence window now contains new columns of the elemental compound percentages in standards, i.e. *Nitrogen*, *Carbon*, *Hydrogen*, *Sulphur*, *Oxygen*.

Fig. 4: Sequence window

The *EA Sample Type* column (which replaces the *Sample Type* column in **Clarity** standard mode) specifies the calibration standards, the available entries are:
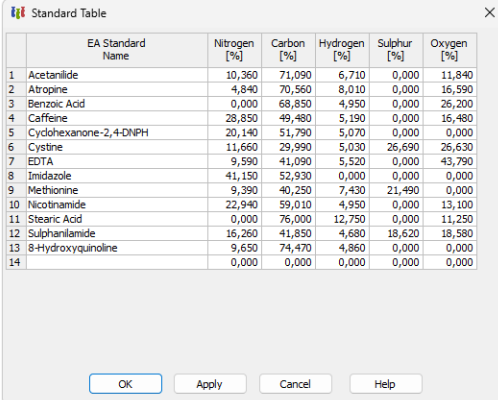
Tab. 2: EA Sample Type entries:

Sample Type	Description
Unknown	For unknown samples.
Standard	For calibration standards. *Sample Amount*, Level (*Lvl.*) and *EA Standard Name* fields must be filled in. The composition columns will be filled automatically from the **Standard Table**.
Blank	For blank samples. The response determined will be used on Level 21 of the calibration with amount *0*, which will be counted to the calibration.
Bypass	Analysis will be performed, but no result chromatogram will be stored. This is useful for running the column-cleaning or equilibrium-setting sample, where results are not desired, but the run must be performed to achieve the required state.

The *Method Name* column contains the method name for the current method. This method is automatically set for all rows in the sequence and can't be changed during the running sequence as the column is disabled.

Note: To change the method while the sequence is running, stop the sequence, change the method in any not measured row and resume the sequence. Only an user with the access right to *Select Method* can select another method.

5.2.1 Standard Table

	EA Standard Name	Nitrogen [%]	Carbon [%]	Hydrogen [%]	Sulphur [%]	Oxygen [%]
1	Acetanilide	10,360	71,090	6,710	0,000	11,840
2	Atropine	4,840	70,560	8,010	0,000	16,590
3	Benzoic Acid	0,000	68,850	4,950	0,000	26,200
4	Caffeine	28,850	49,480	5,190	0,000	16,480
5	Cyclohexanone-2,4-DNPH	20,140	51,790	5,070	0,000	0,000
6	Cystine	11,660	29,990	5,030	26,690	26,630
7	EDTA	9,590	41,090	5,520	0,000	43,790
8	Imidazole	41,150	52,930	0,000	0,000	0,000
9	Methionine	9,390	40,250	7,430	21,490	0,000
10	Nicotinamide	22,940	59,010	4,950	0,000	13,100
11	Stearic Acid	0,000	76,000	12,750	0,000	11,250
12	Sulphanilamide	16,260	41,850	4,680	18,620	18,580
13	8-Hydroxyquinoline	9,650	74,470	4,860	0,000	0,000
14		0,000	0,000	0,000	0,000	0,000
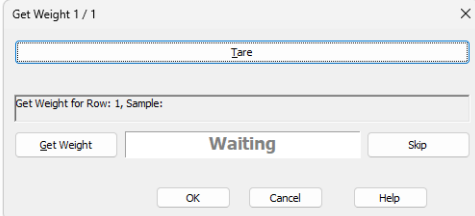
Fig. 5: Standard Table

The *Standard Table* dialog can be invoked using the *Sequence - Edit Standard Table* command or pressing the 📊 icon from the Sequence window switched to the **EA** mode.

Predefined values are listed for commonly used standards. The table can be edited to add other standards or to delete the unused ones.

5.2.2 Get Weight

Clarity with the **EA Extension** can control selected models of balance. The particular Balance Control Module must be configured to the corresponding Instrument in the *System Configuration* dialog. To open the *Get Weight* dialog invoke the *Sequence - Balance* command or use the ⚖ icon from the Sequence window. The numbers behind the "Get Weight" inscription in the dialog header show the number of the sample to be weighted and the total number of samples selected for weighting.

Fig. 6: Get Weight

Tare
Subtracts the weight of an empty container.

Information Panel
Displays messages from the **Sequence Table** indicating current sample.

Get Weight
Transfers the weight from the analytical balance directly into the *Sample Amount* field of the **Sequence Table**.

Status Panel
Displays current status of the analytical balance. Possible states are:

> *Waiting* - Standard state, balance are currently doing nothing or the *Tare* button have been pressed and taring operation is in process.
>
> *Waiting for value* - The balance is measuring the weight of the sample.
>
> *Waiting for calibrate* - Balance is calibrating itself.

Skip
Skips current row in the **Sequence Table**.

5.3 Chromatogram window in EA Extension

The Result Table in the **EA Extension** *Chromatogram* window has two additional columns performing EA calculations. These columns are:

Carbon Amount Ratio
Displays the ratio of the carbon amount to the given row's element amount.

> Carbon Amount Ratio = Carbon Amount / Element (C,H,N,...) Amount

Carbon Response Ratio
Displays the ratio of the given row's element response to the carbon peak response, be it *Area* or *Height*. The column is hidden in the default desktop.

> Carbon Response Ratio = Element (C,H,N,...) Response / Carbon Response

The Summary Table in the **EA Extension** *Chromatogram* window now contains the column **Sample Weight** (formerly named as **Sample Amount**).

The Results pane in the **EA Extension** *Chromatogram* window in the Common for All Signals section now contains the field **Sample Weight** (formerly named as **Amount**).

6 Clarity EA operation

The typical operation procedure for **Clarity** in **EA** mode is described in this chapter in logical order. Only topics related to **EA** mode are discussed here, refer to the **Clarity User Guide** for detailed description of operations in standard mode.

6.1 Template Method

The template method parameters need to be set (opened) in the *Instrument* window. These parameters are used for measuring and evaluation of new data and can be edited normally in the *Method Setup* dialog.

Note: Refer to the **Clarity Reference Guide** and **Clarity User Guide** for description of the individual *Method Setup* tabs: *Measurement*, *Acquisition* and *Integration*.

Calibration parameters

The calibration is defined by the sequence and other options are not supported by the instrument using the **EA** mode. The *Method Setup - Calculation* tab is therefore missing.

Integration parameters

The integration parameters in the *Method Setup - Integration* dialog are best set from already measured chromatogram:

- Open the chromatogram in the *Chromatogram* window and switch to the *Integration* tab.
- Select the whole **Integration Table** using the Ctrl + A shortcut and copy its contents to the clipboard using the Ctrl + C shortcut.
- Open the *Method Setup - Integration* dialog.
- Again select the whole **Integration Table** using the Ctrl + A and paste the contents of the clipboard using the Ctrl + V.

Note: The whole operation can be also performed by using the *Method - Save as Template...* command from the *Chromatogram* window. Another filename then the name of the method already opened on any Instrument has to be used for the template method.

6.2 Sequence

- Use the *File - New* command or the ⬜ icon in the *Sequence* window to create a new sequence.
- Name the sequence in the *Save As* dialog.
- The new sequence is created as a copy of the *EATemplate.seq* file stored in the *COMMON* subdirectory of the **Clarity** folder (C:\CLARITY\DATAFILES\COMMON by default). If this file is missing, default program parameters will be used.

Note: You can store the common part of your sequence (most commonly the sequence options and the initial standards with first sample row) to this file.

- Set the method to sequence by using one of the following:
    - After clicking in the cell in the *Method Name* column the ▭▪ icon will appear. Using it invokes the dialog where the method can be selected.
    - The method can be directly input by typing the method's name in the cell in the *Method Name* column.
    - In the *Method Setup* dialog select the desired method and click either *Set To Sequence* or *Send Method*.

Note: Only an user with access right *Select Method* can change the method. The *Set to Sequence* button is disabled when the sequence is running or the method is modified or *noname.met* or when the *Sequence* window is not opened.

- Add new rows to the **Sequence Table** by clicking the checkbox in the *Run* column on the last empty line or editing any of its fields.

Note: Starting vial (*SV*) and End vial (*EV*) fields will be incremented automatically; other fields will be copied from the previous row.

You can also paste the data into the *Sample ID* or *Sample Amount* column. This action will add the corresponding number of rows. Alternatively, the sample information can be imported from a text file generated by a LIMS or Sample Database applications using the *File - Import* command.

6.3 Calibration

For each new sequence a calibration file with identical name (*.CAL) is created in the calibration subfolder (CALIB by default) of the current project.

This calibration will be based on the calibration template EATEMPLATE.CAL file stored in the **Clarity**COMMON folder (C:\CLARITY\DATAFILES\COMMON by default). Display and edit the calibration in the *Calibration* window. Refer to the **Clarity Reference Guide** for detailed description of the *Calibration* window.

Note: The values in the calibration template created during installation for the *Retention Times*, *Identification Windows*, determined elements, calibration curve fits and calibration/recalibration options will have to be adjusted to meet your system performance and your preferences.

The retention times need to be set according to your actual standard - they will differ according to the instrument type and conditions used. The *Identification Windows* should be set wide enough to accommodate the differences in retention times for different element amounts.

The dominant peak (usually carbon) type can be set to *Refer*, the identification windows for other peaks will be shifted accordingly.

Linear Curve Fit Type will usually be used with *Area* as *Response Base*. The *Origin* (zero handling) should be selected according to the spread of the calibration points:

- *Curve passes through Origin* should be selected when one standard with uniform sample amounts is used.
- *Ignore Origin* or *Compute with Origin* should be selected if **Blank** runs are made or the calibration points are spread enough to compute Y axis intercept.

6.4 Typical operation steps

Chapters about typical operation steps.

6.4.1 Sequence setup

- Create new sequence as described in the chapter **"Sequence"** on pg. **11**.
- Fill in the standards and samples to be measured.

It is suggested to create a new sequence for each set of measurements (daily work, series of samples).

All the samples in the sequence refer to a single common calibration file.

When acquired, the sequence will remember the chromatograms measured during the last run, thus they can be opened using the *File - Open from Sequence* command in the *Chromatogram* window or reprocessed (after changing integration parameters or calibration options) by the *Analysis - Batch...* command (icon) from the *Instrument* window.

6.4.2 Calibration setup

In common practice, several standards are run at the beginning of the sequence and then additional standards are run after certain number of samples. In case there are no significant trends in response observed during a sequence, the calibration is best calculated from all measured standards.

6.4.3 Sequence measurement

- Start the **Clarity** Instrument on which the **Elemental Analyzer** is configured and run the prepared sequence (using the *Run Sequence* command (or ▶▶ icon) from the *Sequence* window) to process the samples.
- New rows can be added to the table and the not yet measured rows can be edited during the sequence run.

6.4.4 Results presentation

For results presentation it is advantageous to:

- Set the **Overlay Mode** by the *File - Overlay Mode* command or icon ① in the *Chromatogram* window.
- Open all desired chromatograms using the *File - Open* command (or icon) ② . You may hold Ctrl key to select multiple files.
- Switch to the *Summary* ③ tab.

- Customize the **Summary Table** to display the desired information in a suitable layout. This can be done by right clicking the table and selecting the *Summary Options...* ④ or *Setup Columns...* ⑤ commands.
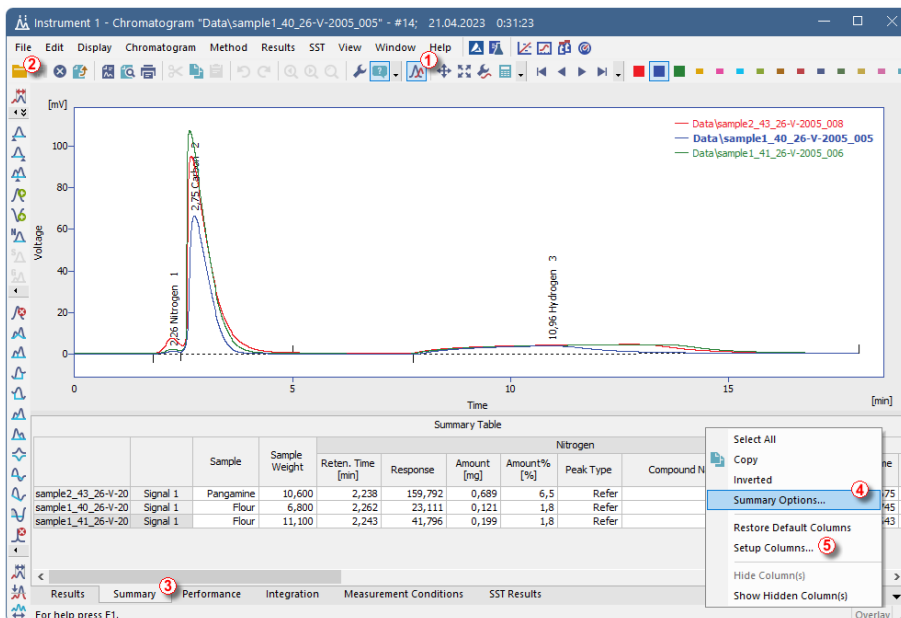

Fig. 7: Chromatogram - Summary

You can select which information will be printed in the report using the *Report Setup* dialog.

The **Summary Table** can be also exported in *.TXT format (*File - Export - Export Summary Table* command in the *Chromatogram* window) and the data thus easily transferred to other programs for further evaluation.

6.4.5 Reprocessing the results

If there were some problems encountered during the sequence acquisition, the whole sequence or selected chromatograms can be reprocessed to correct those problems. Commonly encountered problems are incorrect integration or identification of the peaks, interferences or ghost peaks in the chromatograms or errors entered in the *Sample Amount* column.

Note: Take care when using the *Complete Processing* option in the **Batch** dialog (available for the reprocessing of whole sequences). This option is not suitable if any manual changes to the integration has been performed on individual chromatograms. In the **EA** mode, some chromatograms will probably need manual integrations.