

Clarity Extensions

Natural Gas Analysis

Extensions

ENG

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To facilitate the orientation in the **Natural Gas Analysis** 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, there are text sections written in format other than normal text. These sections are formatted as follows:

Note: Notifies the reader of possibly interesting information.

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

█ Marks the problem statement or trouble question.

Description: Presents any closer information on the problem, describes its causes etc.

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

1 NGA - Natural Gas Analysis

The **NGA Extension** is an optional **Extension** for the **Clarity Chromatography Station** (from version 2.8). Any **Clarity** Instrument can use *NGA MODE*.

The **NGA Extension** is a tool for Natural Gas and Liquefied Petroleum Gas data processing. The **Clarity NGA Extension** expands the capabilities of **Clarity Chromatography Station** by providing an interactive tool for calculations accordingly to selected norm and its properties.

2 Specification

NGA Extension calculates gas properties in compliance with norms:

Natural Gas

- ISO 6976-95

Natural gas - Calculation of calorific values, density, relative density and Wobbe index from composition.

- ASTM D 3588-98

Standard Practice for Calculating Heat Value, Compressibility Factor, and Relative Density of Gaseous Fuels.

- GPA 2172-09

Calculation of Gross Heating Value, Relative Density and Compressibility Factor for Natural Gas Mixtures From Compositional Analysis.

Liquefied Petroleum Gas

- ASTM D 2421-02

Standard Practice for Interconversion of Analysis of C₅ and Lighter Hydrocarbons to Gas-Volume, Liquid-Volume, or Weight Basis.

- ASTM D 2598-02

Standard Practice for Calculation of Certain Physical Properties of Liquefied Petroleum (LP) Gases from Compositional Analysis.

- ISO 8973-97 / EN589-04

Liquefied petroleum gases - Calculation method for density and vapor pressure

2.1 Calculated properties according to norms

ISO 6976-95

- Compression Factor (for real gas only)
- Mean Molecular Weight
- Relative Density
- Density
- Superior Calorific Value
- Inferior Calorific Value
- Wobbe Index

ASTM D 3588-98 and GPA 2172-09

- Molar Mass
- Molar Mass Ratio
- Compressibility Factor
- Relative Density
- Ideal Heating Value (incl.calculations in BTU - British Thermal Units)
- Real Heating Value (incl.calculations in BTU - British Thermal Units)

ASTM ASTM D 2421-02 and D 2598-02

- Vapor Pressure
- Relative Density
- Motor Octane Number

ISO 8973-97 / EN589-04

- Absolute Vapour Pressure (for Molar and Mass Percent only)
- Gauge Vapour Pressure (for Molar and Mass Percent only)
- Octane Number

3 Installation

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

To switch an Instrument to **NGA MODE**, choose the **NGA** from the *Instrument Type* field in the **System Configuration** dialog.

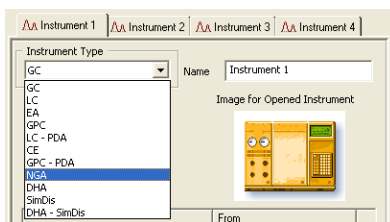


Fig 1: Switching to NGA MODE

4 Description of the NGA Extension

After installation, new functions of the **NGA Extension** will be available. Only features changed or added to the **Clarity** standard mode are listed and described here.

4.1 Calibration

For proper detection of compounds required for gas properties calculations, it is necessary to calibrate the peaks.

- Create a new calibration or for example open the NGA.CAL calibration from the DEMO_NGA project in your **Clarity** installation directory.
- When adding new peaks to the calibration table, use the predefined compound names from the drop-down menu (① in the **Fig 2** on pg 5.) which contains all compound names available in the supported norms and in the **Link Table**. For more details see the chapter **Specification** on pg 2. If you use different compound names, the gas calculations will not work properly.
- **NGA Extension** often uses multi-signal calibrations. It means, that the peaks can be identified on different signals. The calibration table including *Compound Names*, *Response Times* and *Amounts* is common for all signals. It is important that each peak is finally used in one signal only to prevent the **Result Calculations** from warnings. Check the checkbox in the first *Used* column of the calibration table to use the *Compound Name* in the defined signal only. You can change the signal in the *Calibration - Set Signal* menu.


The screenshot shows the 'Instrument 1 - Calibration' window. The title bar indicates the file path: C:\Clarity_27\DEMO_NGA\Calib\nga <-- ESTD. The window contains a 'Calibration Summary Table' with columns for 'Used', 'Compound Name', 'Reten. Time', 'Left Window', 'Right Window', 'Peak Type', 'Peak Color', 'LOD', 'LOQ', 'RB', 'Resp. Factor', and 'Level 1' (subdivided into 'Response', 'Amount', and 'Resp. Fact.'). A drop-down menu is open over the 'Compound Name' column, showing a list of compounds including Nitrogen, Methane, CO2, Ethane, Propane, n-Butane, Neopentane, i-pentane, CO2, hexane, 1,2-Butadiene, 1,3-Butadiene, i-Butene, and 1-cis-Pentadiene. A red circle highlights the drop-down arrow icon.

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Peak Color	LOD	LOQ	RB	Resp. Factor	Level 1		
											Response	Amount	Resp. Fact.
<input type="checkbox"/>	Nitrogen	0,547	0,040	0,040	Ordnr		0,000	0,000	A	0,0000	0,5960	2,520	4,2279
<input checked="" type="checkbox"/>	Methane	0,670	0,040	0,040	Ordnr		0,000	0,000	A	0,0000	1972677,6719	89,560	0,0000
<input type="checkbox"/>	CO2	1,123	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	0,0000	0,993	0,0000
<input checked="" type="checkbox"/>	Ethane	2,183	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	185688,0665	4,990	0,0000
<input checked="" type="checkbox"/>	Propane	4,187	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	56385,7198	0,997	0,0000
<input checked="" type="checkbox"/>	i-Butane	5,873	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	22111,1298	0,301	0,0000
<input checked="" type="checkbox"/>	n-Butane	6,267	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	22857,7375	0,309	0,0000
<input checked="" type="checkbox"/>	Neopentane	7,400	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	8514,4520	0,098	0,0000
<input checked="" type="checkbox"/>	i-pentane	8,123	0,100	0,100	Ordnr		0,000	0,000	A	0,0000	9159,1477	0,101	0,0000
<input checked="" type="checkbox"/>	CO2	8,397	0,100	0,100	Ordnr		0,000	0,000	A	0,0000	9402,1440	0,101	0,0000
<input checked="" type="checkbox"/>	hexane	10,247	0,200	0,200	Ordnr		0,000	0,000	A	0,0000	3636,9920	0,030	0,0000

Fig 2: Calibration window with the drop-down menu

For detailed information about the Calibration, see the chapter "Calibration". in the **Reference Guide** or see the chapter "Calibration window" in the **Getting Started Guide**.

4.2 Chromatogram window

New **NGA Results** and **NGA Summary** tabs are available in the **Chromatogram** window (opened by clicking the  icon). Also, there is the **NGA** menu at the top of the window.

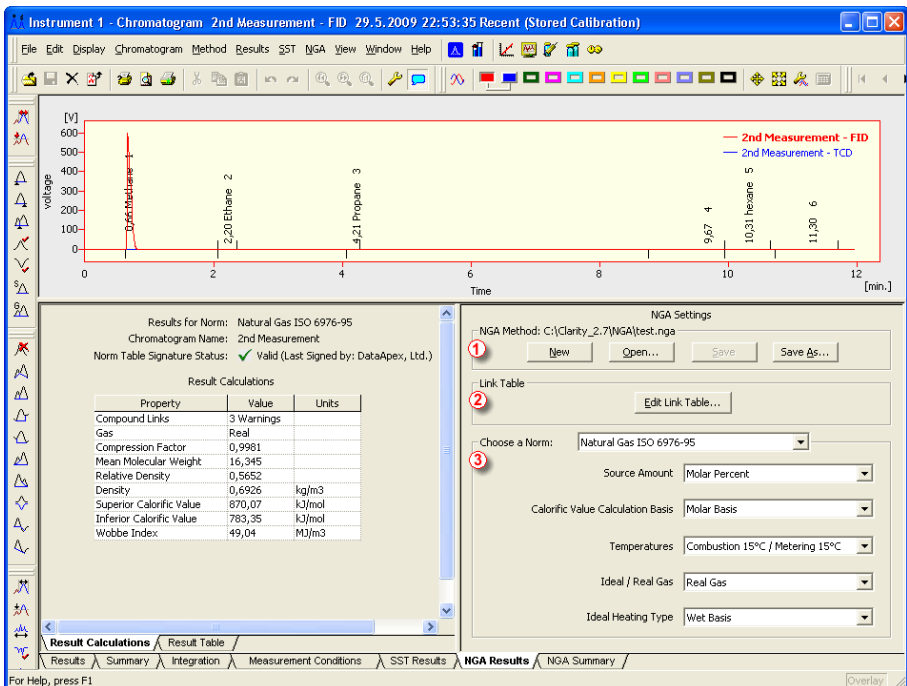
4.2.1 NGA Results

NGA Results tab is divided into two panes:

- Left pane: includes **Result Calculations** and **Result Table** tabs.
- Right Pane: includes **NGA Settings**.

4.2.1.1 NGA Settings


In this pane you can set the **NGA Method** up - choose norm and edit its specific parameters.



The screenshot shows the 'Instrument 1 - Chromatogram' window. The top panel displays a chromatogram with two traces: '2nd Measurement - FID' (red) and '2nd Measurement - TCD' (blue). The x-axis is 'Time [min.]' from 0 to 12, and the y-axis is 'voltage [V]' from 0 to 600. Peaks are labeled with retention times: 2.20 Ethane 2, 4.21 Propane 3, 9.67 4, 10.31 Hexane 5, and 11.20 6.

The bottom panel is split into two sections:

Left Section: Result Calculations

Results for Norm: Natural Gas ISO 6976-95
 Chromatogram Name: 2nd Measurement
 Norm Table Signature Status:  Valid (Last Signed by: DataApex, Ltd.)

Property	Value	Units
Compound Links	3 Warnings	
Gas	Real	
Compression Factor	0,9981	
Mean Molecular Weight	16,345	
Relative Density	0,5652	
Density	0,6926	kg/m ³
Superior Calorific Value	870,07	kJ/mol
Inferior Calorific Value	783,35	kJ/mol
Wobbe Index	49,04	MJ/m ³

Right Section: NGA Settings

NGA Method: C:\Clarity_2.7\NGA\test.nga

Buttons: New, Open..., Save, Save As...

Link Table: Edit Link Table...

Choose a Norm: Natural Gas ISO 6976-95

Source Amount: Molar Percent

Calorific Value Calculation Basis: Molar Basis

Temperatures: Combustion 15°C / Metering 15°C

Ideal / Real Gas: Real Gas

Ideal Heating Type: Wet Basis

Bottom navigation: Results | Summary | Integration | Measurement Conditions | SST Results | **NGA Results** | NGA Summary

Fig 3: Chromatogram window - NGA Results - NGA Settings

NGA Method ①

Currently opened *NGA Method*. All settings in the *NGA Method* are saved in the *.NGA file and it's independent on the Method opened on the [Instrument](#). Last opened *NGA Method* used in the [Chromatogram](#) window is saved in the project file (for more details see also chapter Project).

New

Creates new *NGA Method* with default settings.

Open

Displays the [Open NGA Method](#) dialog where you can open one you want to use.

Save

Saves settings of the current *NGA Method*.

Save As...

Opens the [Save As](#) dialog for saving the *NGA Method* into new file.

Link Table ②

Compound Names for [Result Calculations](#) are retrieved from the *Calibration Table*, it doesn't matter whether the Calibration is saved in the Calibration File or is saved in the *Chromatogram*. How to set the *Calibration* up you can find in the chapter "Calibration" in the **Clarity Reference Guide**. In the Calibration, it is also necessary to set the detection of the peak in one signal only; otherwise you will see warnings in the [Result Calculations](#).

In such situations when Compound Names in norms have different names than the same ones you have saved in your calibrations you can use [Link Table](#) for linking those *Compound Names* and ensure that all compounds are included in selected norm's calculations. For more details see the chapter [Link Table](#) on pg 9.

Edit Link Table...

Opens the [Link Table](#) dialog, where you can edit links between Compound Names in the calibrations and norms.

Choose a Norm ③

Select the norm you want to use for your calculations. Each norm has specific list of parameters that can be changed:

- **ISO 6976-95**

Source Amount

Determines whether the Amount is in mole fractions or in volume fractions. Volume fractions are converted to mole fractions if selected.

Calorific Value Calculation Basis

Determines the units in which to calculate the *Superior* and *Inferior Calorific Values*.

Temperatures

Selects the combustion and metering temperatures.

Ideal / Real Gas

Determines whether the calculations are for *Ideal* or *Real Gas*. For the *Real gas*, the *Compression Factor* is added to the results.

Ideal Heating Type

Determines whether to include a mole fraction of water or not. If water is included in calculations, it is also added to the [NGA Result Table](#).

- **ASTM D 3588-98 and GPA 2172-09**

Ideal Heating Type

Determines whether to calculate *Gross Heating Value* or *Net Heating Value*. For gross calculations, the water condenses to liquid, and, for net calculations, the water remains in the vapor state.

Calorific Value Calculation Basis

Determines the units in which to calculate the *Heating Value*.

Gas Analysis on

Determines whether to include a mole fraction of water or not. If water is included in calculations, it is also added to the [NGA Result Table](#) (but not for **GPA 2172-09**).

- **LPG ASTM D 2598-02 / 2421-02**

Original Basis

Determines the source Amount type. It can be *Liquid*, *Mole*, *Gas*, or *Weight* type. Other types are converted to *Liquid* type.

- **LPG ISO 8973-97 / EN589-04**

Original Basis

Determines the source Amount type. Both Molar and Mass fractions are required for calculations (one is converted into another). If Volume fractions are selected, only the Octane Number can be calculated.

Temperature of Liquid

The approximate temperature of liquid.

4.2.1.2 Link Table

This dialog serves for editing the *Link Table* in the **NGA Extension**. *Link Table* is used in cases, when you have unresolved compound names in the **NGA Result Table**. For example, you are using compound names specific for your language, but in the selected norm there is a different name for the same compound. *Link Table* enables you to use your custom compound names from calibrations and chromatograms in norms repeatedly, without any changes in the norms table.

After you add some link to the **Link Table**, you can add them to the Calibration using the drop-down menu in the Calibration window.

Caution: Detection of compound names is CASE SENSITIVE. "Butane" is not the same as "butane".

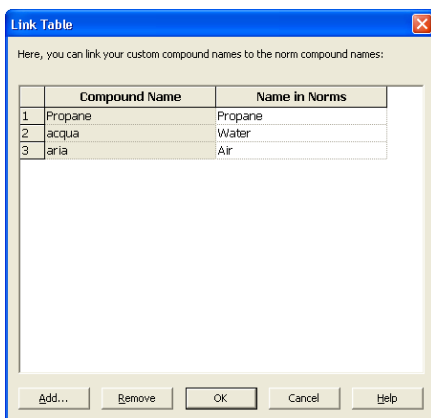


Fig 4: Link Table dialog

1st column in the table

Order number in the *Link Table*.

Compound Name

Compound name in the **Calibration** you want to link with the Name in Norm and thus include it in the **Result Calculations**.

Name in Norms

Compound Names occurring in norms (if the name is in multiple norms, only one occurrence is displayed).

Add...

Displays the **Add Link** dialog for adding a new record to the link table.

Remove

Removes the selected record from the link table.

OK

Saves settings to the link table and exits.

Cancel

Exits the dialog without any changes in the *Link Table*.

4.2.1.3 Add Link

Add Link dialog serves for adding new record to the **Link Table**.

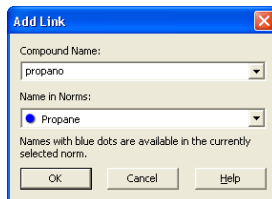


Fig 5: Add Link dialog

Compound Name

Enter the compound name you want to link to a name in norms. Unresolved compounds in the chromatogram are suggested in the drop-down menu.

Name in Norms

Select the appropriate compound name in norms. Names from all supported norms are available in the drop-down menu. For better orientation, blue dots are displayed at the names, which are in selected norm in the [NGA Settings](#).

4.2.1.4 Result Table

The Result Table contains some of the columns from the standard [Results Table](#), but it also contains additional columns specific for **NGA Extension**.

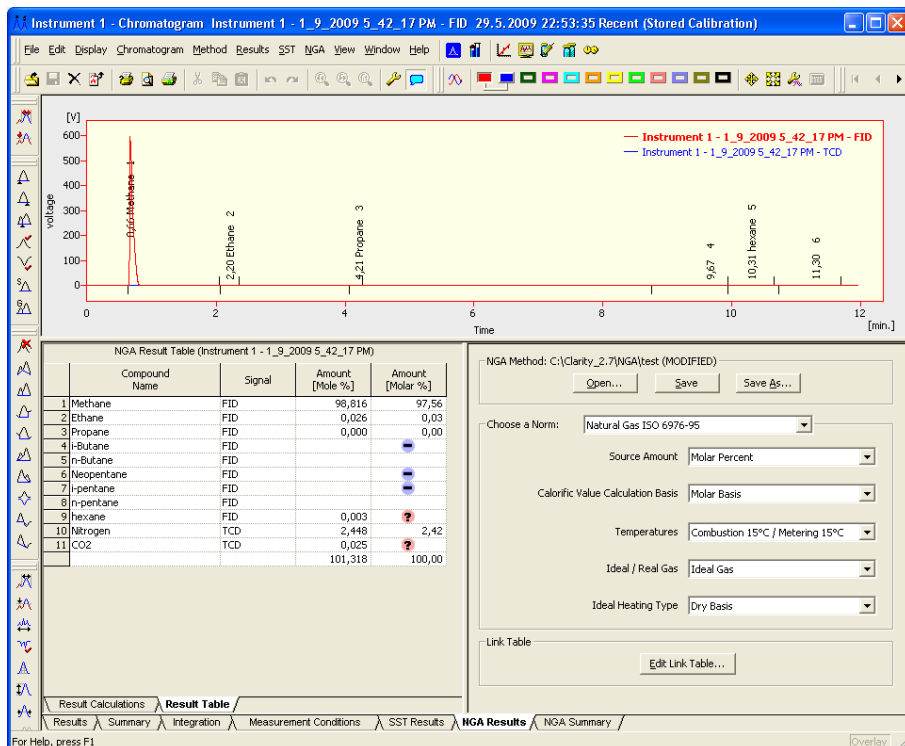


Fig 6: Chromatogram window - NGA Results - Result Table

Compound Name

If the chromatogram contains calibrated peaks or groups, the names are shown in *Compound Name* column. The table contains compounds from all signals of the chromatogram.

Signal

Displays the *Signal* whereon the Compound was detected.

Amount [Mole %]

This column shows the same data as the *Amount* column in the [Result Table](#) (*Results* tab in the [Chromatogram](#) window). This column is informational and isn't important in the **NGA**.

Amount [Molar %]

Contains mole fractions (in percent) or some other fraction type specified in the settings per all signals. The fractions are normalized amounts so

that the total amount is 100%. If a compound isn't linked to a *Name in Norm* (for more details see the chapter **Link Table** on pg 9), its mole fraction will be set to *zero*.

The table can contain a virtual compound *Water*. This one is added when you select *Wet Basis* in the **NGA Settings**.

- The "minus" icon means, that the *Compound Name* from the *Result Table* was not found in the selected norm and it's not needed for calculations.
- The "question" icon means, that the *Compound Name* cannot be found neither in the Norms Table nor in the Link Table. Click the *Edit Link Table...* button and in the desired **Link Table** dialog link the compound name with requested compound name in norm. This icon may appears in such situation, when the *Compound Name* is in the *Result Table* twice or more times. This is caused mostly when you use one calibrated peak in more then one signal in the **Calibration** window. Since the NGA Calculations are performed on all signal in the **Chromatogram**, each Compound can be set in one signal only, see the chapter **"Calibration"** on pg 5.

4.2.1.5 Result Calculations

In *NGA Results - Result Calculations* tab you can find the table containing result calculations for selected norm. Results are automatically recalculated each time you open or change the chromatogram or select different norm (or its parameters).

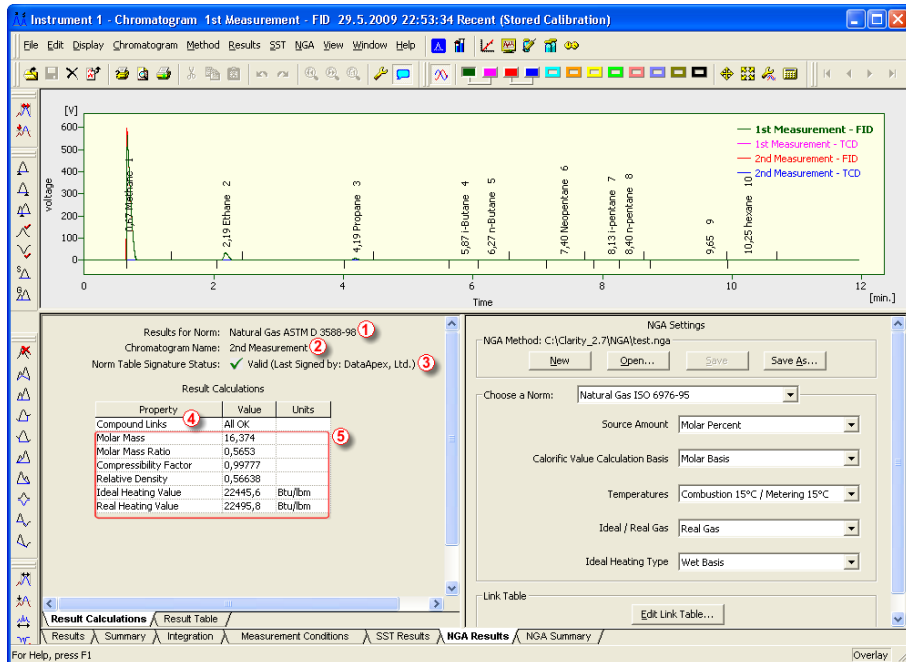


Fig 7: Chromatogram window - NGA Results - Result Calculations

Results for Norm ①

Displays the information which norm the calculations are performed from.

Chromatogram Name ②

Displays the information what chromatogram is selected for the result calculations. It is helpful especially if you have opened multiple chromatograms in *OVERLAY MODE*.

Norm Table Signature Status ③

Information about the validity of the **Norms Table** file, where the data required for the calculations are saved. This file is provided by **DataApex** and is digitally signed. If somebody changes the Norm Table file, the signature will be no longer valid.

Note: For any update request in the *Norm Table*, contact DataApex Support at www.dataapex.com.

Result Calculations

Compound Links ④

Information about the peak detection in the *Result Table* (for more details see the chapter **Result Table** on pg 11). Those reported values may appear:

- *All OK*: There are no errors and warnings in the *Result Table*.
- *X Errors*: The X is number of the unresolved *Compound Names* in the *Result Table*.
- *X Warnings*: The X is number of the compounds not found in *Norms Table* nor in the *Link Table*. Warning may occur if you have set detection of the same peak in more then one signal. For more details see also chapter Calibration.

Other rows in the table are respective to the selected norm ⑤

What properties are calculated in each norm you can find in the chapter "**Specification**" on pg 3.

4.2.2 NGA Summary

Displays the Result Calculations for all chromatograms opened in the *OVERLAY MODE* (for more details see the chapter **Result Calculations** on pg 13).

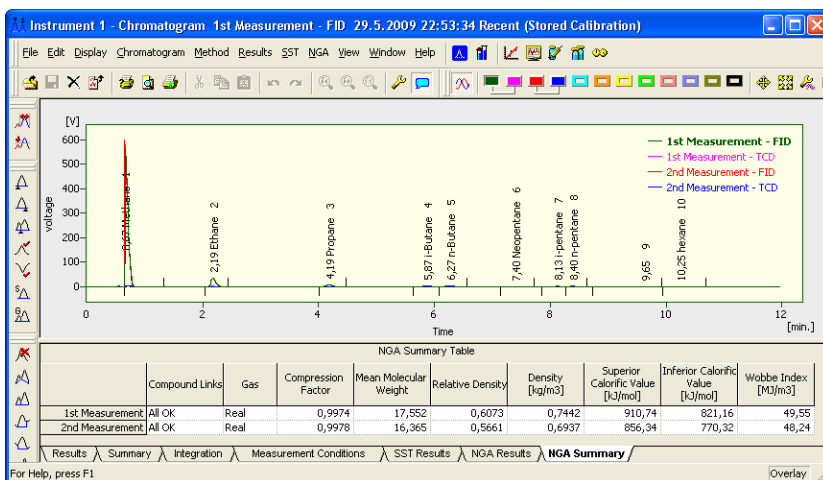


Fig 8: Chromatogram window - NGA Summary

NGA Summary Table

In this table you can find result calculations transformed into rows per chromatogram.

1st column

Name of the chromatogram

Other columns

List of columns is identical to [Result Calculations](#), but performed on all chromatograms opened in the *OVERLAY MODE*. You can find detailed description of the calculated properties in the chapter "[Specification](#)" on pg 3.

User Columns

You can create User Columns by clicking the right button of the mouse. For more details see also chapter Setup Columns... in the [Clarity Reference Guide](#).

4.3 Report Setup

In [Report Setup Instrument](#) dialog, tab *NGA* you can set the printing options of data in the **NGA Extension**.

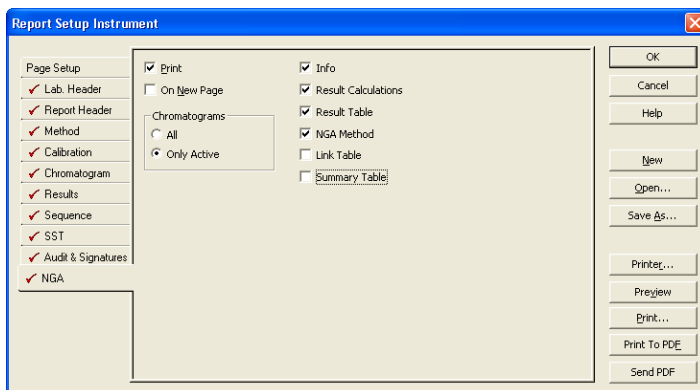


Fig 9: Report Setup Instrument dialog

Print

Allows/disallows the printing of the **NGA**. If checked, the symbol ✓ will be shown before the tab name and other fields on the tab will become editable.

On New Page

If checked, the **NGA Section** is printed on a new page.

Chromatograms

All

Prints the *Result Calculations* and the *Result Table* of all chromatograms opened in the *OVERLAY MODE*.

Only Active

Prints the *Result Calculations* and the *Result Table* of the *ACTIVE Chromatogram* only.

Info

If checked, prints the *NGA Info* including the *Norm Name* and the *Norm Table Signature Status*.

Result Calculations

If checked, prints the [Result Calculations](#).

Result Table

If checked, prints the [Result Table](#).

NGA Method

If checked, prints the [NGA Method Settings](#).

Link Table

If checked, prints the [Link Table](#).

Summary Table

If checked, prints the [Summary Table](#).

4.4 Export Data

In the [Export Data](#) dialog you can set, whether **NGA Result Table** and **NGA Summary Table** will be included in the exported data. For more details see also chapter Export Data in the **ClarityReference Guide**.

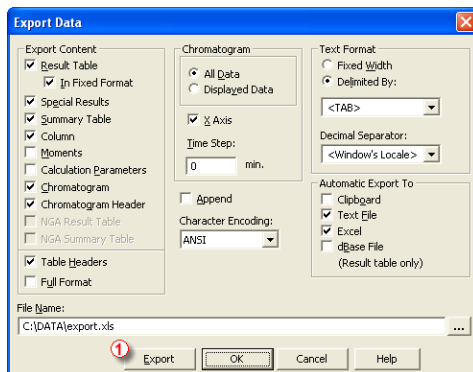


Fig 10: Export Data dialog

5 How to try the extension

5.1 How to perform first calculations

In this chapter you can find information, how to try the **NGA Extension** on the **NGA DEMO** Project for the first time.

Step 1

In the **System Configuration** window (menu *Clarity - System...*), select the **NGA** in the *Instrument Type* combo box, for example on the *Instrument 1*. For more details see the chapter **Installation** on pg 4.

Step 2

After saving and closing the **System Configuration** window, open the appropriate **Instrument**. Now open the **NGA DEMO** Project: Click the *File - Project...* and in the desired window click the *Open...* button to open the project. Select the **DEMO_NGA** in the list and click the *OK* button.

Step 3

Open the **Chromatogram** window (it can be opened by clicking on the menu *Window - Chromatogram*). In the lower part of the **Chromatogram** window you can see the new *NGA Results* and *NGA Summary* tabs. If you can't see any chromatogram, using the *File - Open Chromatogram...* menu open a chromatogram from the DEMO_NGA\DATA folder located in your **Clarity** Installation directory (by default C:\CLARITY).

Step 4

Click the *NGA Results* tab and on the right side of the pane you can see the *NGA settings*, where you can set the calculations parameters. They are saved in special .NGA file which enables repeatedly use of the **NGA settings** on multiple **Chromatograms**. By clicking the *Open...* button you can browse to the **Clarity Installation** directory (by default C:\CLARITY) and in the DEMO_NGA subdirectory select the DEMO_NGA.NGA file. **NGA Method** is then loaded and *ACTIVE Chromatogram* is automatically recalculated even if you select different norms or parameters. For more details see the chapter **NGA Settings** on pg 6.

Step 5

On the left side of the pane, the *Result Calculations* tab shows the **Calculations**, in the *Result Table* tab you can see what calibrated peaks was processed by the **NGA Extension**. It depends on the selected norm in the *NGA Settings* and whether all calibrated peaks are found in the norm. You can find detailed description of the norms supported by the extension in the chapter "**Specification**" on pg 2. More details you can find in the chapter "**Result Calculations**" on pg 13. and in the chapter "**NGA Results**" on pg 6.

Step 6

All compounds required for the *NGA Calculations* are saved in the norm table. It may happens, that you can use different compound name for the same peak which is in the norm table (for example, compound names are case sensitive) but is not processed. In the *NGA Settings* click the *Edit Link Table...* button to link calibrated compound name with the compound name in the norm. Results are then automatically recalculated after any changes in the [Link Table](#) window. *Link Table* is used for all chromatograms, so you need to set it once only.

For more details see the chapter **Link Table** on pg 9.

Step 7

In case you have analysis divided into multiple chromatograms, open them in the *OVERLAY* mode and click the *NGA Summary* tab, where you can see the *Result Calculations* of all opened chromatograms in the table. For more details see the chapter **NGA Summary** on pg 14.

5.2 How to print and export results

Ensure that you have selected the **NGA Instrument Type** in the [System Configuration](#) window as described in the chapter "**How to try the extension**" on pg 17.

Print

To print the data from the **NGA Extension**, open the [Report Setup](#) window by clicking the menu *File - Report Setup...* in the [Instrument](#) window or in the [Chromatogram](#) window.

On the left side, select the *NGA* tab. By clicking the *Print* check box you enable other controls of the pane. By selecting other options you can configure what information are printed.

Settings from the [Report Setup](#) are then used in the print output and preview which is accessible from the *File* menu of the [Instrument](#) window and the [Chromatogram](#) window.

For more details see the chapter **Report Setup** on pg 15.

Export

Open the *Setting - Export Data...* menu in the [Instrument](#) window. Set the *NGA Result Table* and *Summary Table* check boxes if you want to include those tables in the exports. Settings in this window are then used in the [PostRun Setting](#) dialog accessible from the *Setting - Postrun* menu of the [Instrument](#) window.

For more details see the chapter **Export Data** on pg 16.