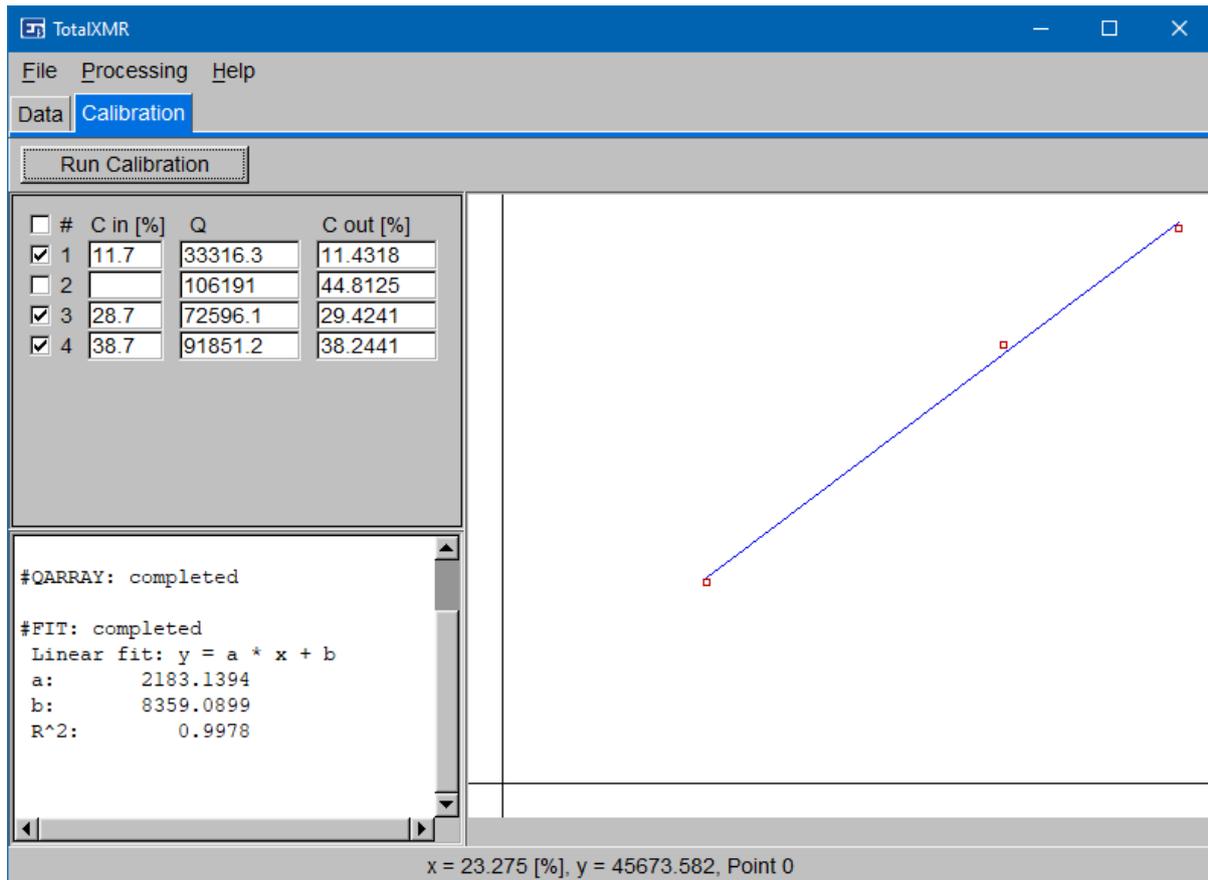


TotalXMR

User Manual

1.0.481





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Overview

TotalXMR main window includes a menu bar at the top (see Figure 1), whose items are: "File", "Processing" and "Help".

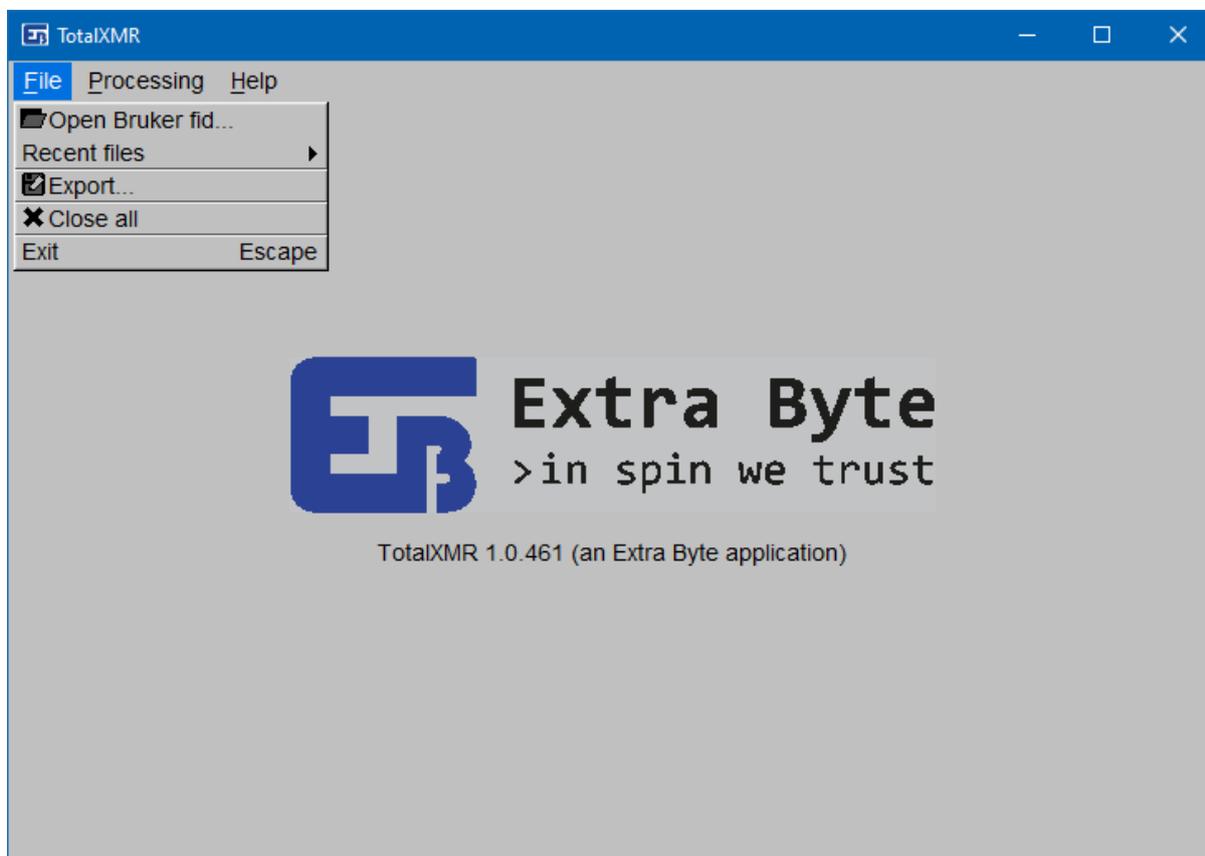


Figure 1. Main window appearance at program launch

File

- "Open Bruker fid..."
Load a Bruker 1D data file (*fid*).
- "Recent files"
Load a recently opened file from a list.
- "Export..."
When data have been loaded, this opens a very simple interface where user can select the destination file format: Scalable Vector Graphic image (.svg), Comma-Separated Values text (.csv) or Bruker TopSpin format.
- "Close all"
Close all the opened file.
- "Exit"
Exit the application (will be asked confirmation).

Processing

- "Setup..."
Open an interface where user can select the processing steps and options (see paragraph [Processing](#) for details).
- "Run"
Run all the operations selected in the Setup to all loaded data starting from the original data.

Help

- "Manual"
A link to this Manual, which must be in the application folder.
- "License"
Show information about license. Also, user can register and activate a license. Registration occurs through email exchange with Extra Byte, which will provide all the payment details. After the payment, user will receive a proper key to activate the license.
- "About"
Open a window with information about this Application and Extra Byte.

Graphic interface

When data are loaded successfully, two overlapping panels appear between the menu bar and the status bar. The first one, labelled as "Data" is for loading and process data, while the second one, labelled as "Calibration", is for building a calibration straight line of data quantifications.

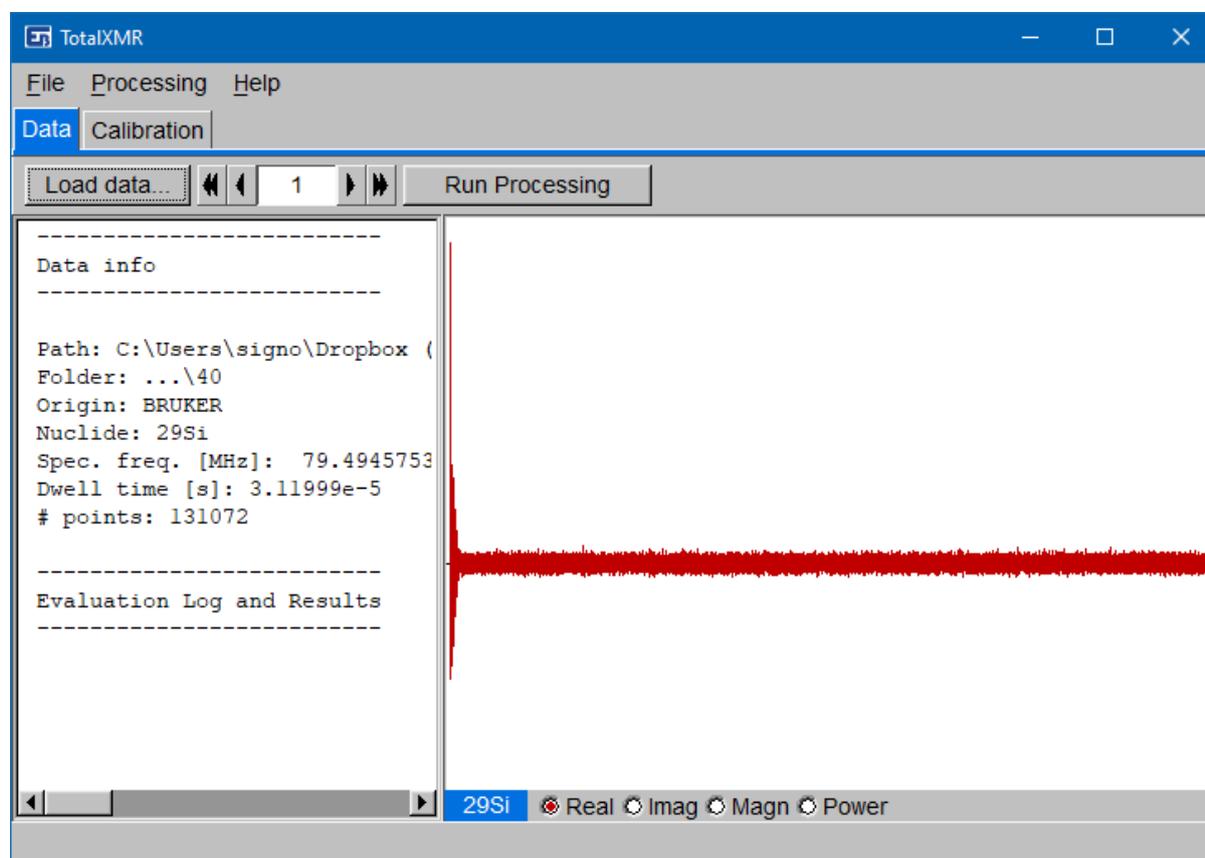


Figure 2. Main window appearance when data are loaded

The first panel (see Figure 2) presents a tool bar in the upper part, that includes a button for load more data, an arrowed widget for navigating through the files, and a button for launching the processing operations to all loaded data (see paragraph Processing). Under the toolbar, the space is divided in two parts: at left, some information about the selected file is shown, along with the evaluation log and results. At right, a canvas shows the graphic plot of raw data and a tool bar at the bottom of it is present. The tool bar shows the name of the nuclide associated to the signal and some buttons to toggle data arrays in the plot (real and imaginary part, magnitude and power). The plot can be zoomed in both horizontal and vertical directions by selecting a rectangle area with the mouse. It can be zoomed out horizontally by dragging the mouse and pressing 'Ctrl', and intensity can be changed with the mouse wheel. Also, the plot can be translated in any direction dragging the mouse together with pressing down 'x' on the keyboard. All zoom states can be reset with a double click. The status bar always shows the mouse position coordinates.

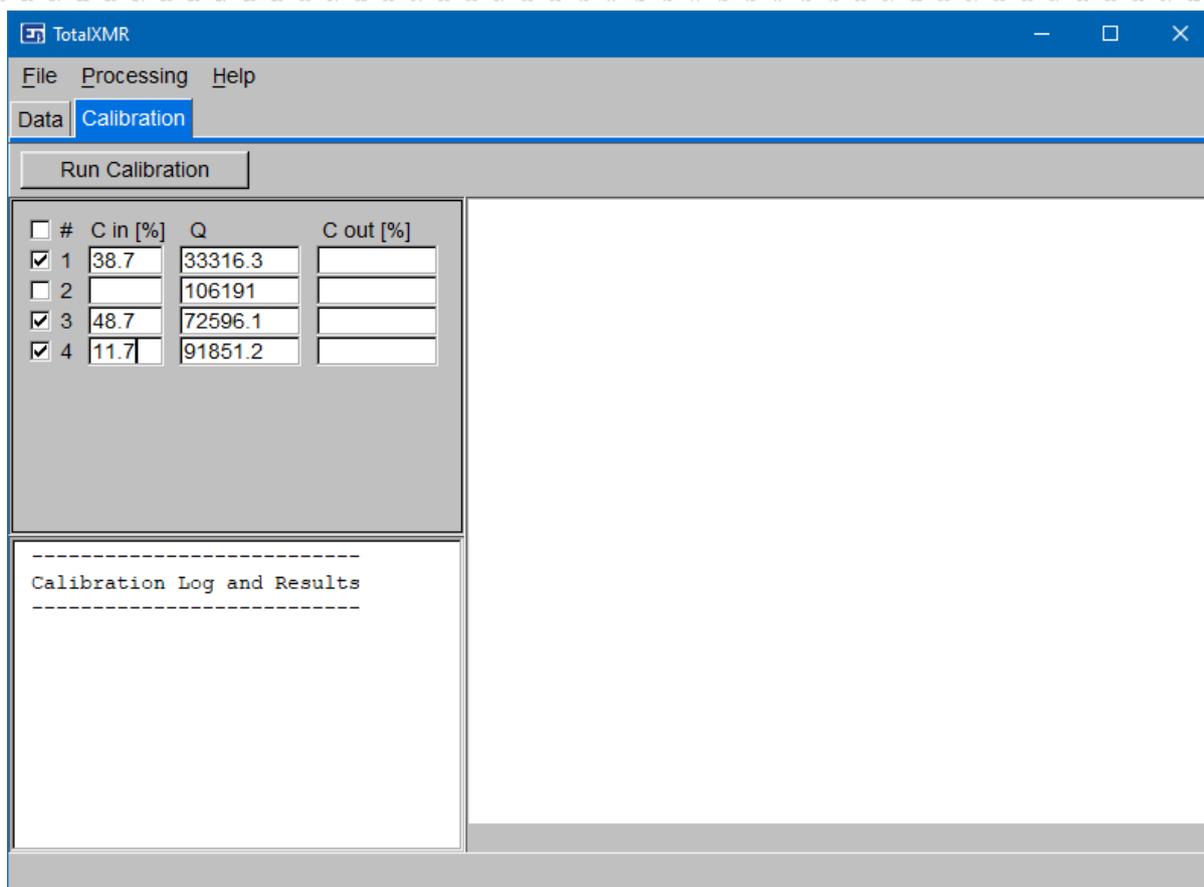


Figure 3. Calibration panel

The second panel (see Figure 3) presents a toolbar in the upper part with one button to run the calibration procedure. Under the toolbar there are three sections: at left, in the upper part, a list of the loaded files can be found and the settings for the calibration can be chosen (see paragraph Calibration). At the bottom results from the calibration are shown in a text display. In the right part, a canvas will show the data (input concentration versus quantification results) and the fit straight line, after the calibration has been finished. The same rules for zooming the plot in the previous panel canvas hold here.

Processing

"Setup" menu item opens a window, as shown in Figure 4, where the processing settings can be prepared.

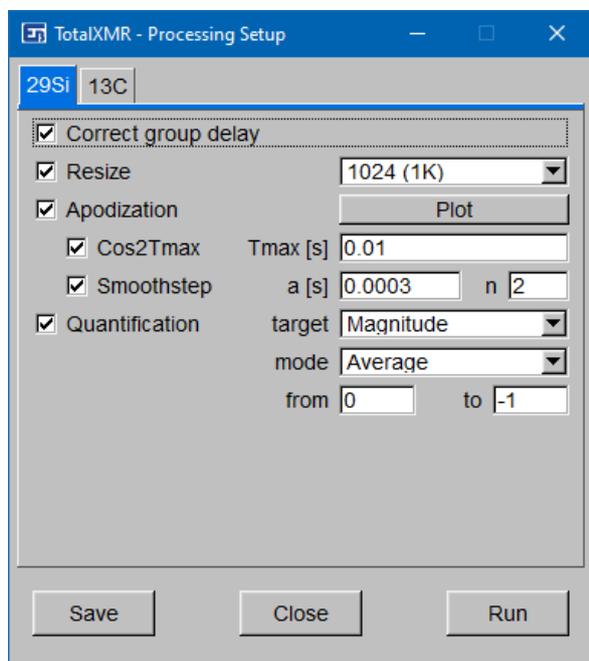


Figure 4. Processing setup interface

A multi-tab panel is shown, one for each nuclide settings. In the current version, only 29Si and 13C are present. The interface is the same, but the parameters may need to be different. When the execution is launched, the program automatically follows the settings corresponding to the correct nuclide. At the bottom of the window, three buttons are present. "Run" button launches the execution (shortcut 'Ctrl'+Enter') with the currently set parameters, even if not saved. "Close" closes the setup and "Save" saves all the setup parameters. Raw data can be restored with 'Ctrl+Z'. During execution, the setup interface can remain opened.

Description of the commands is following.

- "Correct group delay"
Remove the group delay artifact that causes the well-known Bruker spectra wiggings and smileys. This should be always be checked.
- "Resize"
Set a new size for the data. Options are "Current" (which does nothing), "Double" (respect to the original size) or a power of 2. If the new size is greater than the original one, then data are zero filled, otherwise they are truncated.
- "Apodization"
In the current program version, two different apodization modes are available and can be combined. "Plot" button displays the apodization function on the canvas, along with the data. It takes into account the group delay correction shift, if selected. Modes and parameters are described.

- Cos2Tmax

$$A(t) = \begin{cases} \cos^2\left(\frac{\pi}{2} \frac{t}{T_{max}}\right) & \text{for } t < T_{max} \\ 0 & \text{for } t \geq T_{max} \end{cases}$$

Input parameter: T_{max} , that is the time (in seconds) the apodization function reaches value 0.

- Smoothstep

$$A(t) = \frac{\left(\frac{t}{t_{1/2}}\right)^n}{1 + \left(\frac{t}{t_{1/2}}\right)^n}$$

This function has a smoothed step shape: it starts from zero and it grows continuously to one around $t_{1/2}$. Input parameters: time $t_{1/2}$ (in seconds) the function reaches value 0.5 and the steepness parameter n .

This apodization mode is useful to eliminate disturbing signal at the beginning.

- "Quantification"

This command executes the quantification of the signal. The channel to quantify can be chose between the real part, magnitude or power, and the mode (average or maximum value) within a window range set by the points indices. Negative values for these indices stay for default values, that are first and last points. Figure 5 shows the window appearance after running Processing command, including the quantification.

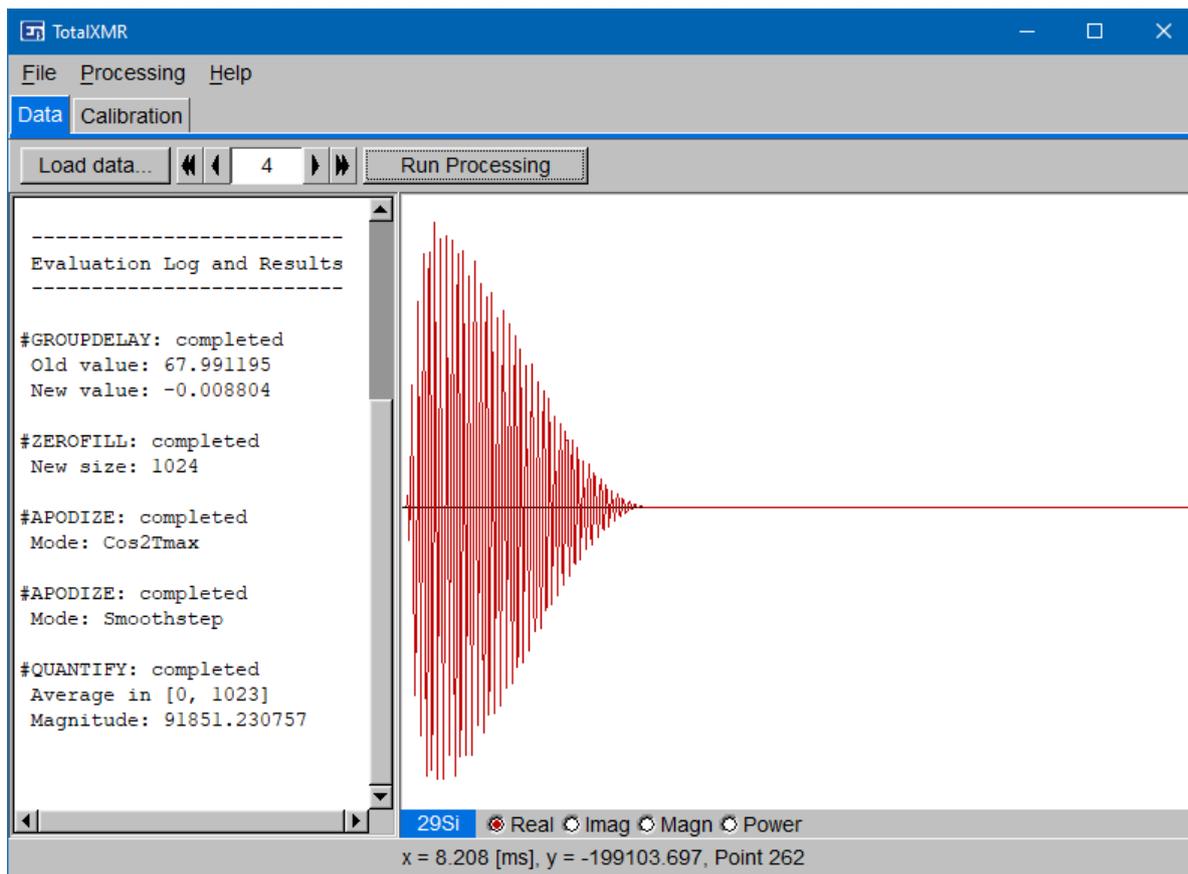


Figure 5. Display after running the signal quantification

Calibration

In the "Calibration" panel, user can see the list of all the loaded data, sorted by loading order. Each one is accompanied with a field for the concentration (C in [%]), which need to be input by the user for known samples. Also, there are the quantification (Q) and the extrapolated concentration (C out [%]). The quantification field is filled automatically with the results of the Processing procedure. User can select the data to use for calibration by clicking on the relative checkbox and he can manually input the concentration of the sample.

Then, the calibration procedure is ready to be launched through the button "Run calibration". This command creates an array with the selected data and perform a linear regression. The results are shown in the section in the window below the list of data, along with the statistical coefficient of determination R^2 (see Figure 6). Also, the concentrations calculated by the fit function are automatically extrapolated for all data, either used and not used for the fit, and shown in the proper field in the upper section.

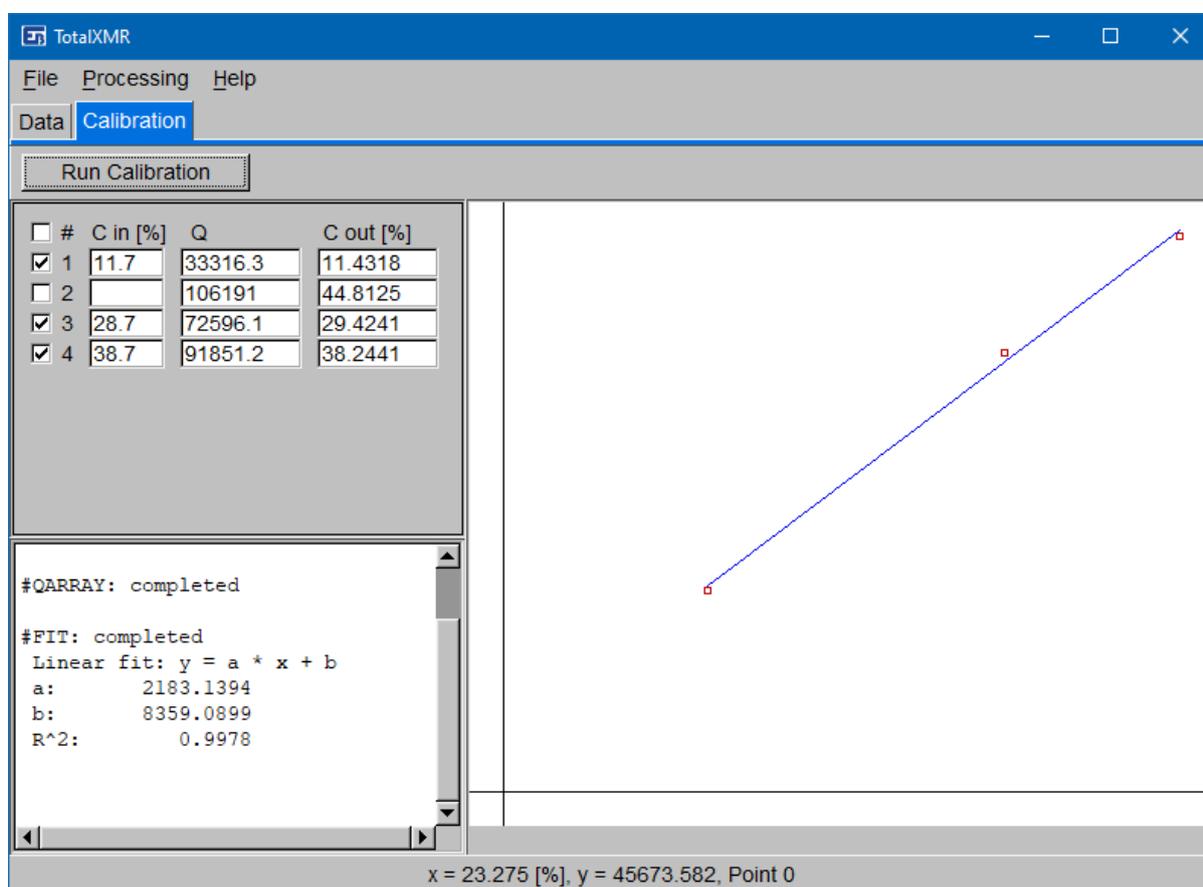


Figure 6. Appearance after calibration procedure

License

How to activate a license

Each Extra Byte Application, once installed, provides 30 days of free trial period starting from the first access. When the trial period is about to expire (<10 days left) the program sends a warning message about that at its launch.

When the trial period is over, the Application opens the Licensing interface. The same can be whenever opened by the user from the program main menu bar under the *Help* item. The License interface shows all the information about the user license: the personal data, if already registered, the *Computer ID*, the license key, if activated, the number of days left. Here user can activate a license by inserting a key. The key is provided by Extra Byte through an email exchange, after that the user has been registered and has made the payment, if required. A key can be used to activate a license on a unique computer.

The License interface allows user to register, by filling in the form with the proper entries (*Name, Surname, Institution/Organization, Email address*), and to send automatically an email, by clicking on the *Get key* button. This button opens the email client and prepares a new message to licensing@ebyte.it with a formatted text. If this should not happen, user has to send the message manually, inserting all the info above, included the *Computer ID* and the number of the Application version.

After sending the license key request, Extra Byte will reply to the user, providing invoice and payment details, if necessary. After payment, user will receive an email with an attached text file containing the key. He or she has to copy and paste it into the proper field in the License interface, then click the *Activate* button. The program notifies if the activation has been made successfully or not. In the next sessions, the program warns the user when the license is about to expire (<30 days left).

User is recommended to never modify the system time after the installation. This guarantees a correct execution of the program.