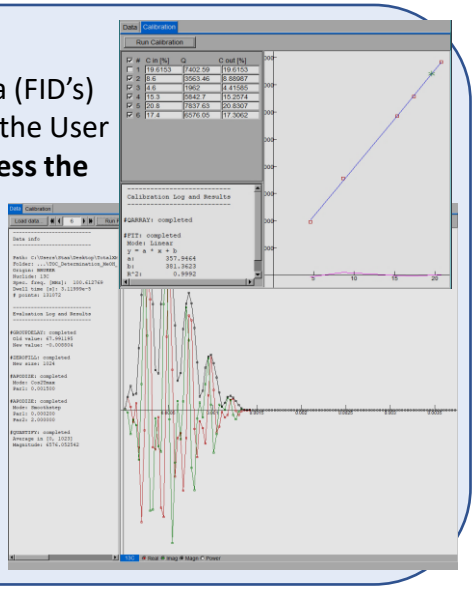
TotalXMR

A tool for quantitative NMR assays of nuclei

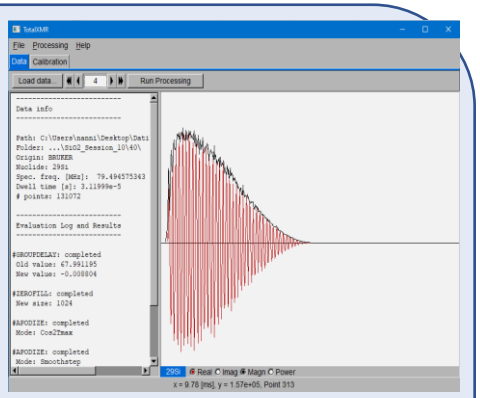
A new software Utility!

TotalXMR loads time-domain NMR data (FID's) from Bruker or other OEM's and offers the User a set of processing tools needed to **assess the total content of the observed nuclides** in an unknown sample, regardless of its chemical composition.
NMR being intrinsically quantitative, such a task may appear trivial, but in practice it encounters a number of serious obstacles which this Utility addresses and, in combination with empirical calibration, solves better than earlier "absolute" approaches.



Salient features:

- ✓ Uses only a brief starting portion of time-domain data (FID's).
- ✓ Automatically removes any acquisition artefacts such as the group delay.
- ✓ Can use both HR- or LR-NMR data.
- ✓ Is fully compatible with the use of relaxation agents to speed the assays.

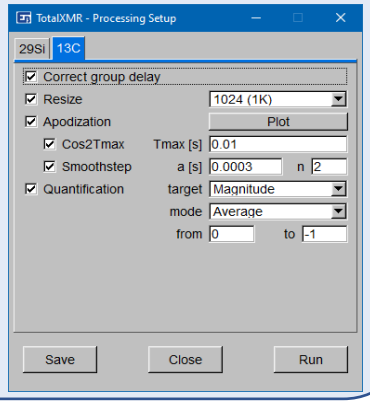


Special apodization methods

- ✓ Suppress very first (unreliable) points with a sharp step-like function
- ✓ Follow-up by isolating only a suitable starting portion of the FID that makes the result independent of undesired chemical composition details.
- ✓ If desired, however, leave in *some* chemical discrimination due to either T_2 (solid/liquid) or by shifts range (e.g., aliphatic/aromatic).

Parameter settings:

- ✓ Very intuitive, User-friendly GUI.
- ✓ Allows separate settings for each nuclide.
- ✓ The setup can be saved and reused later.

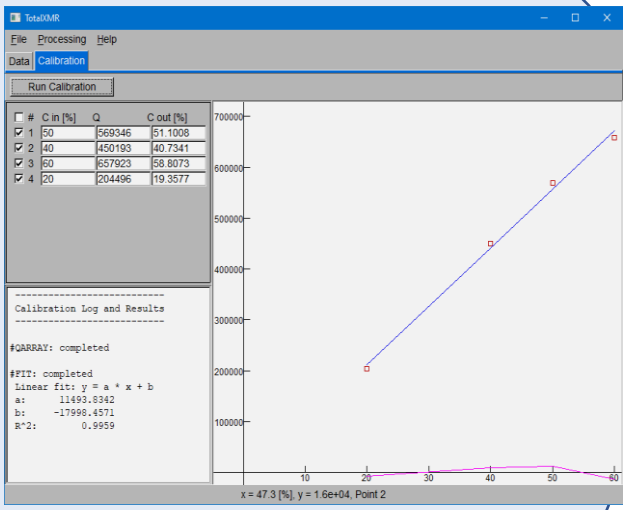


FID quantification selections

- ✓ Data window in terms of data points.
- ✓ Channel (Magnitude/Power/Real).
- ✓ Mode (Average/Maximum).

Calibration procedure:

- ✓ Load FID's of samples with either known or unknown concentrations.
- ✓ Set the desired parameters (or load them from a file)
- ✓ Input the concentrations or quantities of the calibration reference samples.
- ✓ Apply a Quantify command. Automatically, all samples will be quantified using a polynomial-regression.



In case of any problem we are ready to help (free of charge)

Extra Byte

> in spin we trust <

We specialize in rapid development of **STEM software applications**, particularly (but not only) in of **Magnetic Resonance** (MR), and in **MR consulting** & **software/hardware feasibility studies**

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