S. Sykora[1], G. Selva[1], E. M. Vasini[1], M. Abele[2]

[1]Extra Byte, www.extrabyte.eu, email to: info@extrabyte.eu
[2]Evonik Operations Gmbh

Software package TotalXMR to support quantification of total content of X-nucleus from TD-NMR data

and an invitation to collaborate with us in order to solve many elemental analysis problems using your low- or high-field NMR equipment

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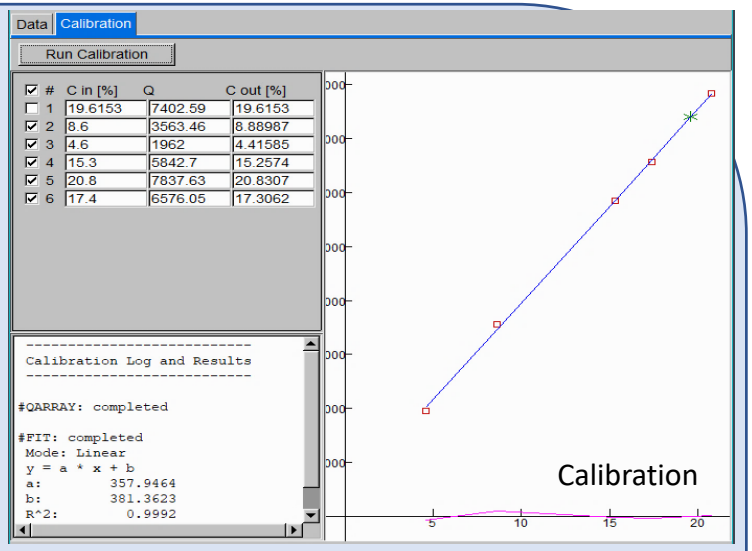
EVONIK Leading Beyond Chemistry

TotalXMR

Loads time-domain NMR data (FID, SE, QSE, CPMG, …) from Bruker or other instruments and provides the user with a set of processing tools needed to

assess the total content of the observed nuclides

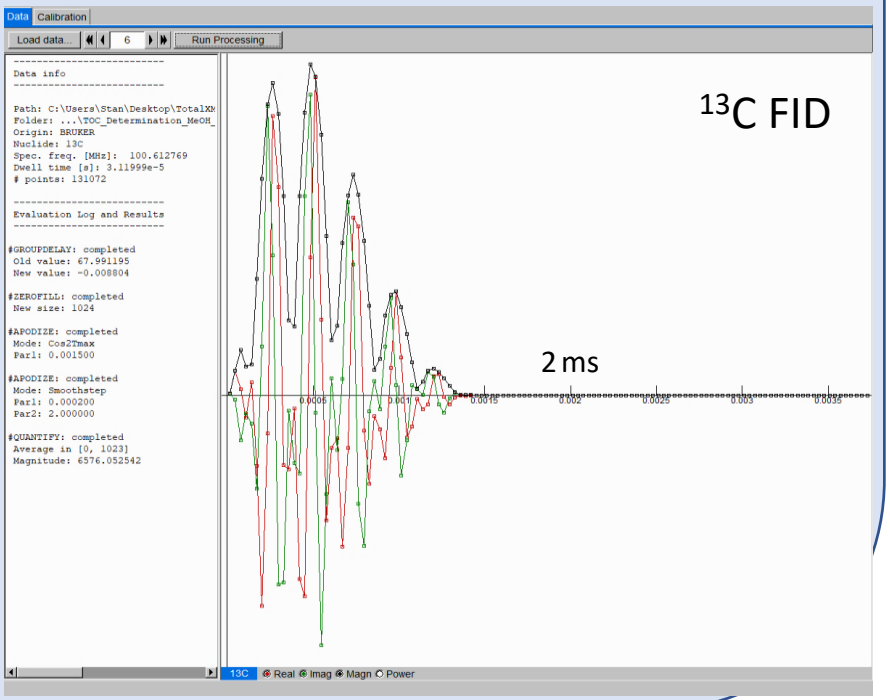
in an unknown sample, regardless of its composition.



Since NMR is intrinsically quantitative, such a task may appear trivial, but in practice it encounters a number of real-life obstacles that are listed in the next slide.

TotalXMR addresses many of these issues. However, it needs to be always combined with a *data acquisition methodology* best suited for each NMR-active nuclide and each context.

At present, there exists no universal data acquisition methodology for elemental analysis that would be applicable to every nuclide and every context.



What makes elemental analysis difficult?

Theoretically, the number of nuclei in the NMR coil is proportional to the FID signal intensity just after the excitation pulse. That sounds simple – so where is the problem? Some answers (though not all):

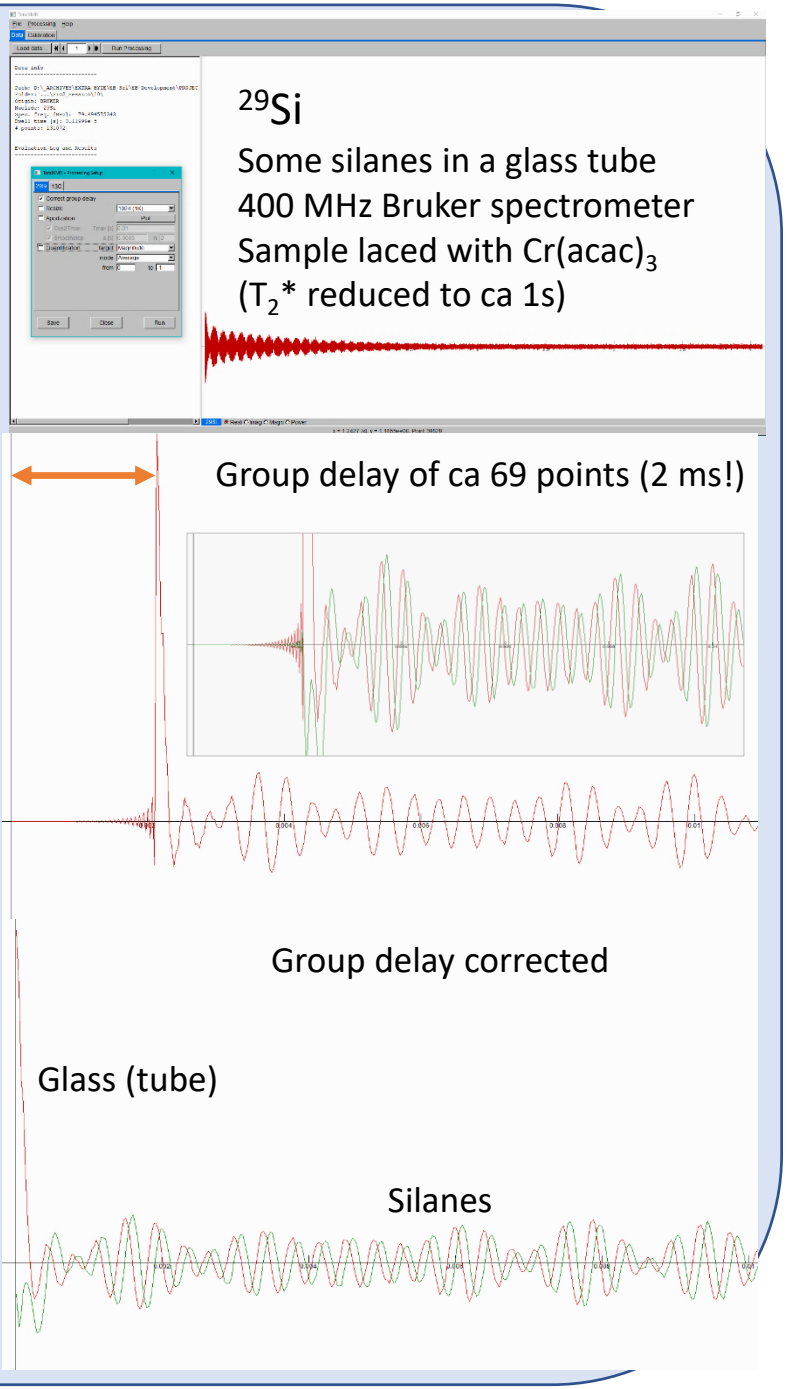
Instrumental artefacts and limits:
- Group delays of digital receivers (see on the right)
- Limited sampling rates (=> SW limits)
- Receiver recovery time
- Probe ringing-down time

Limits imposed by the nuclides (Mother Nature):
- Low sensitivity (S/N ratios) due to low gamma
- Low natural abundance

Strong nuclear interactions (particularly in solids)**:**
- Extreme quadrupole interactions (1 kHz – 5 MHz)
- Strong dipolar interactions (up to 120 kHz)

Very long relaxation times (=> long acquisition times):
- Extremely long T_1's (such as in many ^{29}Si samples), particularly when combined with short T_2* (solids).

Sampling difficulties:
- Example: how to make a representative 1ml sample of, say, the soil in a certain agricultural area.



Some salient features of TotalXMR

- Uses only a brief starting portion of TD-data.
- Automatically removes (known) artefacts.
- Can use both HR- or LR-NMR data.
- Is compatible with the use of relaxation agents to speed the assays.

Special apodization methods:

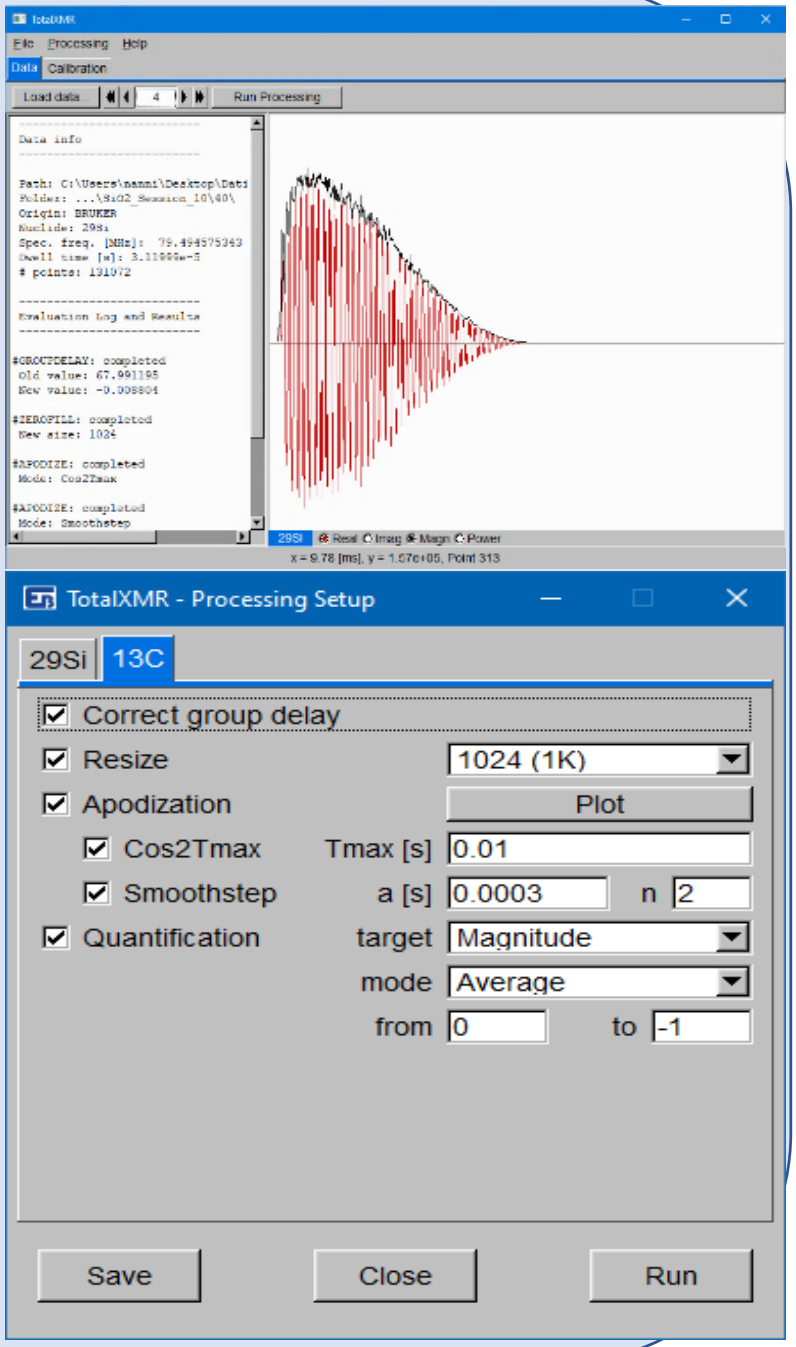
- First suppress the very first (unreliable) points. Follow-up by isolating only a suitable starting portion of the data that makes the result. independent of undesired details of chemical composition.
- If desired, however, leave in *some* chemical discrimination due to either T_2 (solid/liquid) or to a specific shifts range (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

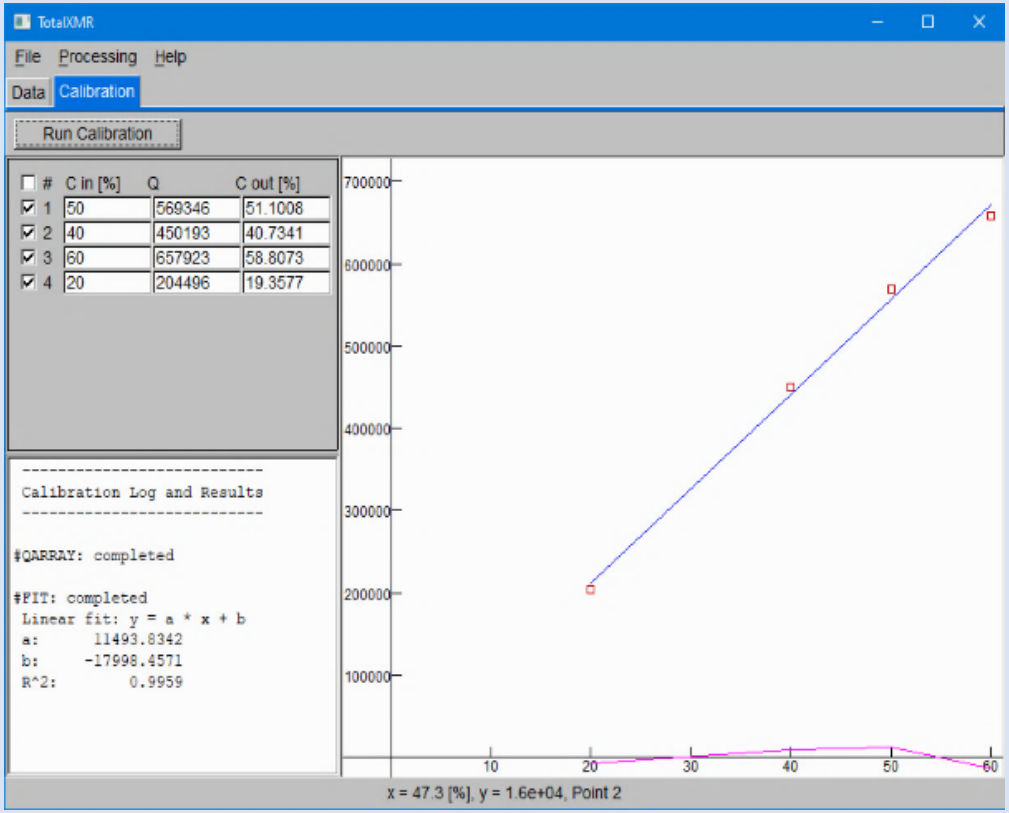
- Data can be windowed.
- Channel (magnitude/power/real).
- Various modes (average/maximum).



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 the Quantify command.

Automatically, all samples will be quantified using a **polynomial-regression**.



Bring-home messages

Any NMR instrument that is capable of measuring an signal of a nuclide, can do so quantitively, but it is not necessarily a trivial task.

The instrument may be low-field, high-field, table-top, full-size, field-cycling, any. TotalXMR needs to read the data that it produces, but we will see to that part.

Field homogeneity is not a problem, within very broad limits. Neither is the lock. Sensitivity, however, is an issue, some nuclei are viable only in high-field.

The acquired data needed for the evaluation are only the initial portions of time-domain signals (either FID's or more sophisticated ones). For good results, acquisition settings are important, and not necessarily matching your "standard" ones.

Many "tricks" regarding pulse sequences and/sample preparation are possible, we have some experience with that and we will be glad to collaborate with you.

Keep in mind that, once you buy a license, we become partners. The core of what we offer is not just the code: it is methodology + consulting + software-as-service.

Nuclei you might be interested in: ^{1}H, ^{2}H, ^{13}C, ^{19}F, ^{31}P, ^{23}Na, ^{14}N, ^{15}N, ^{7}Li, ^{29}Si, …

Typical applications:

Si in silicon glue, **C** in soil, **P** in meat, **N** in an animal feed, **Na** in cheese, **F** in a RedBull,

… … …

Thank You
for Your Attention!

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The team:




In collaboration with

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TotalXMR page: extrabyte.eu/products/totalxmr