



# G.O.Joe: A new software for the evaluation and correction of LA-ICP-MS concentration data

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## Abstract

The software G.O.Joe was developed to calculate trace element concentrations obtained by LA-ICP-MS analysis, offering several types of interference corrections. G.O.Joe operates online and efficiently processes large datasets with the flexibility to change parameters at any stage of the workflow. A series of three self-instructive interfaces guide the user through a straightforward process of data evaluation. Clear visualization of raw data aids the evaluation of each measurement, facilitating the selection of background and sample signals. Concurrently, inclusions or mixed analyses can be excluded. The input of instrument settings and information about the reference material follows the data processing and is used to convert the isotope count rates to element concentrations. Importantly, advanced calculations can be applied to correct the measurements for isobaric interferences and abundance sensitivity. The exported result file (.xlsx) includes calculated element concentrations, relevant statistical parameters, input data, and instrument settings, ensuring a transparent data processing.

## Introduction

Since its introduction in the 1980s, laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) has been developed to an essential instrument offering the simultaneous mass analytical detection at low detection levels in combination with the high-resolution in situ analysis of trace element compositions in solid samples [1,2]. However, determination of the analytical results is still faced with problems regarding isobaric and polyatomic interferences, abundance sensitivity, instrumental sensitivity drift etc. that cannot be resolved instrumentally and must be corrected during subsequent data evaluation [3].

Here we present G.O.Joe, a new software for data reduction and time-resolved analysis of chemical measurements performed by LA-ICP-MS. The most significant advantage over existing software is a fast and comprehensive data evaluation in only three steps (Fig. 1). The features of G.O.Joe are presented by its application on two different types of minerals (scheelite and garnet) including the correction of abundance sensitivity and isobaric interferences.

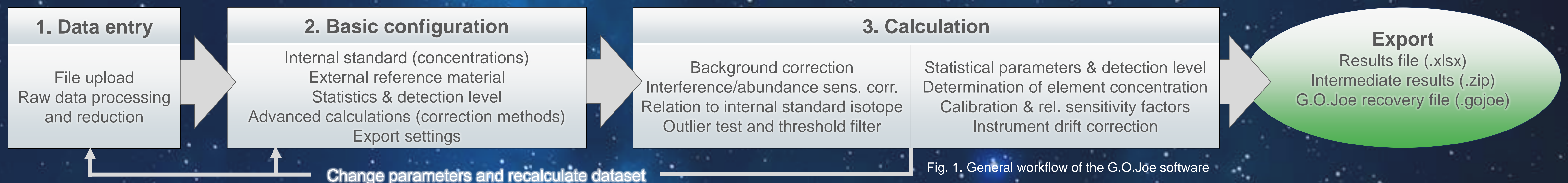


Fig. 1. General workflow of the G.O.Joe software

## Software overview and evaluation procedure

G.O.Joe is an online software written in the Dart programming language using Flutter [4]. The first two steps (Fig. 2 and Fig. 3) of data processing (time-resolved processing for every spot analysis) and configuration (information of the internal standard isotope and external reference material etc.) are done manually. The third step (Fig. 4) comprises the automated calculation of the element concentration following the procedure described in Jochum et al. [5].

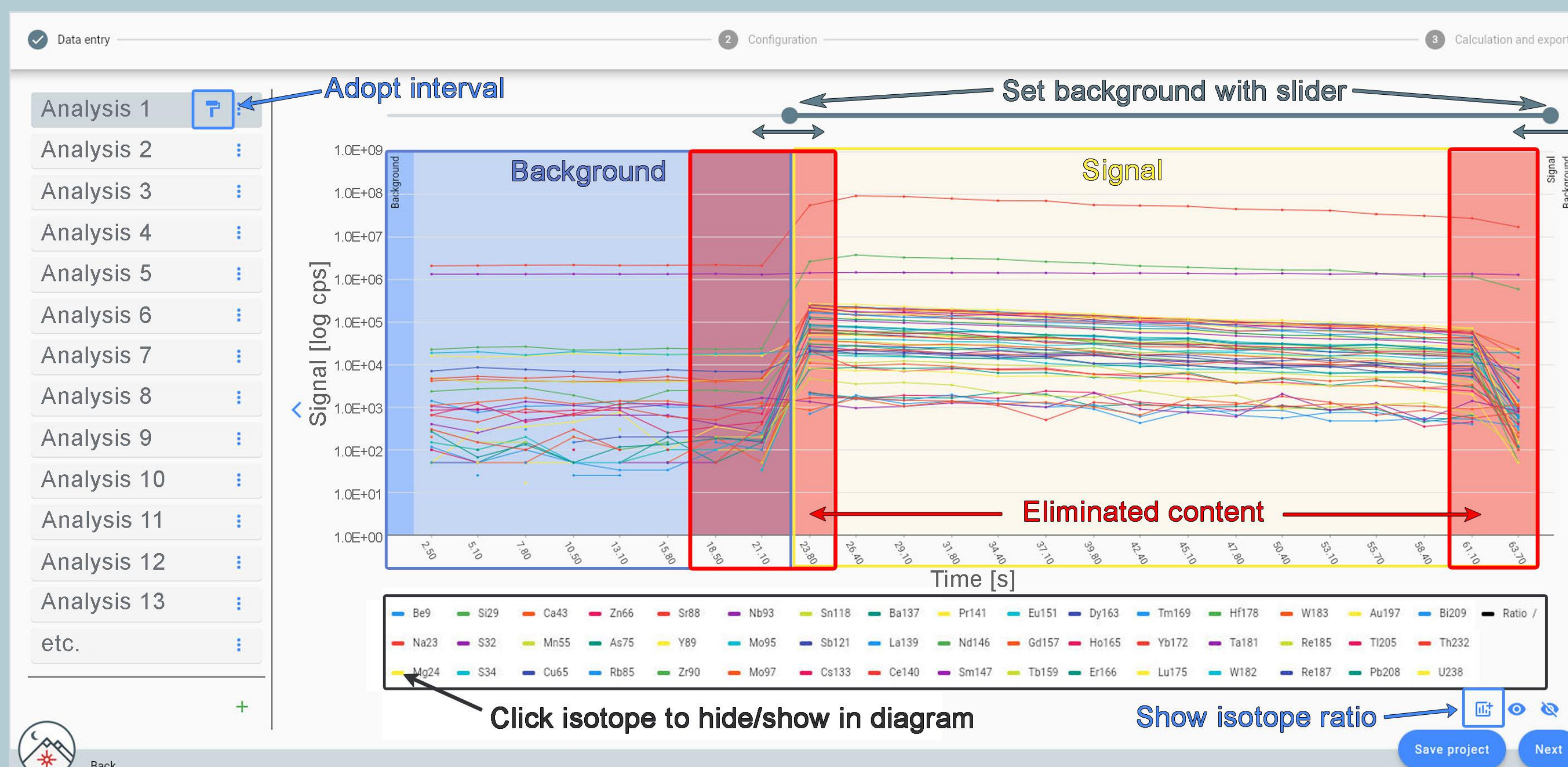


Fig. 2. Graphical user interface of workflow step 1: Overview of the processing options in the data entry-window. The diagram shows the time-resolved intensities of all measured isotopes on a logarithmic scale. The user can click through each analysis individually and specify the desired background (blue area) and signal (yellow area) intervals by using the slider.

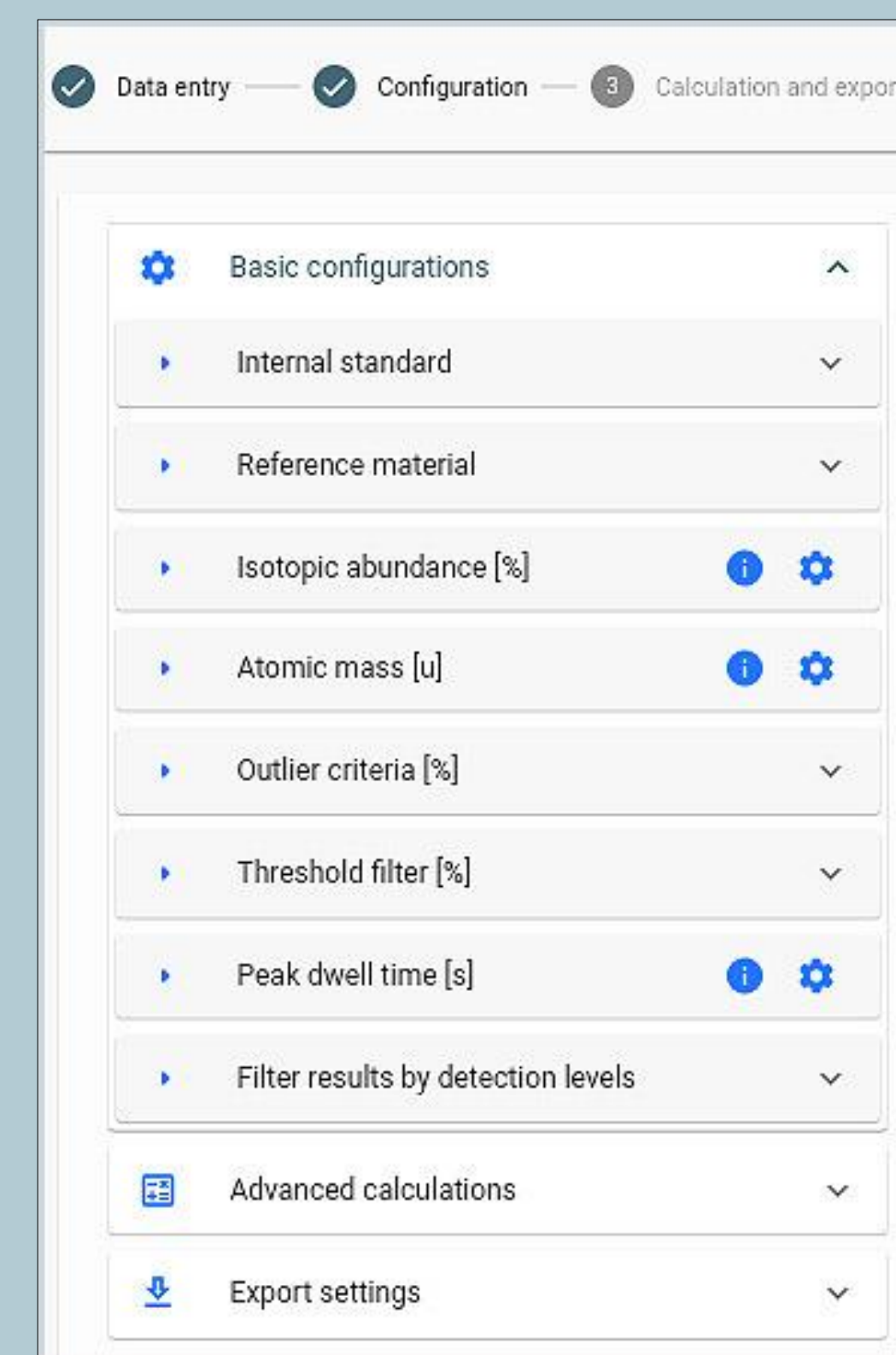


Fig. 3. Workflow step 2: Configuration-window to define essential information and parameters for data calculation.



Fig. 4. Workflow step 3: The automatic calculation is started with just one click and the results can be downloaded immediately as .xlsx file.

## Results

The advantage of G.O.Joe to correct various interferences is presented by its application to different types of minerals:

### Scheelite – $\text{Ca}(\text{WO}_4)$

**Analytical problem:**  $^{181}\text{Ta}$  overlapped by high  $^{183}\text{W}$  content

**Applied correction method:** abundance sensitivity

**Results:** highest correction visible in analyses with lowest Ta concentration (Fig. 5 a) → showing the necessity to correct for abundance sensitivity in W-rich samples with low Ta

### Garnet – $(\text{Fe}^{2+}, \text{Ca}, \text{Mg}, \text{Mn})_3(\text{Fe}^{3+}, \text{Al}, \text{Cr})_2(\text{SiO}_4)_3$

**Analytical problem:**  $^{115}\text{In}$  overlapped by  $^{115}\text{Sn}$

**Applied correction method:** isobaric interference correction

**Results:** uncorrected concentrations of  $^{115}\text{In}$  between 10 and 65  $\mu\text{g/g}$  are corrected to <5 to 10  $\mu\text{g/g}$  (Fig. 6 a); corrected results based on different non-interfering Sn isotopes (i.e.,  $^{117}\text{Sn}$  to  $^{120}\text{Sn}$ ) show deviations of mostly <0.5 %

### Quality control of results – G.O.Joe's accuracy check

Compare calculated element concentrations of secondary reference materials (Fig. 5 b and Fig. 6 b) to preferred literature values from the GeoReM database [6]

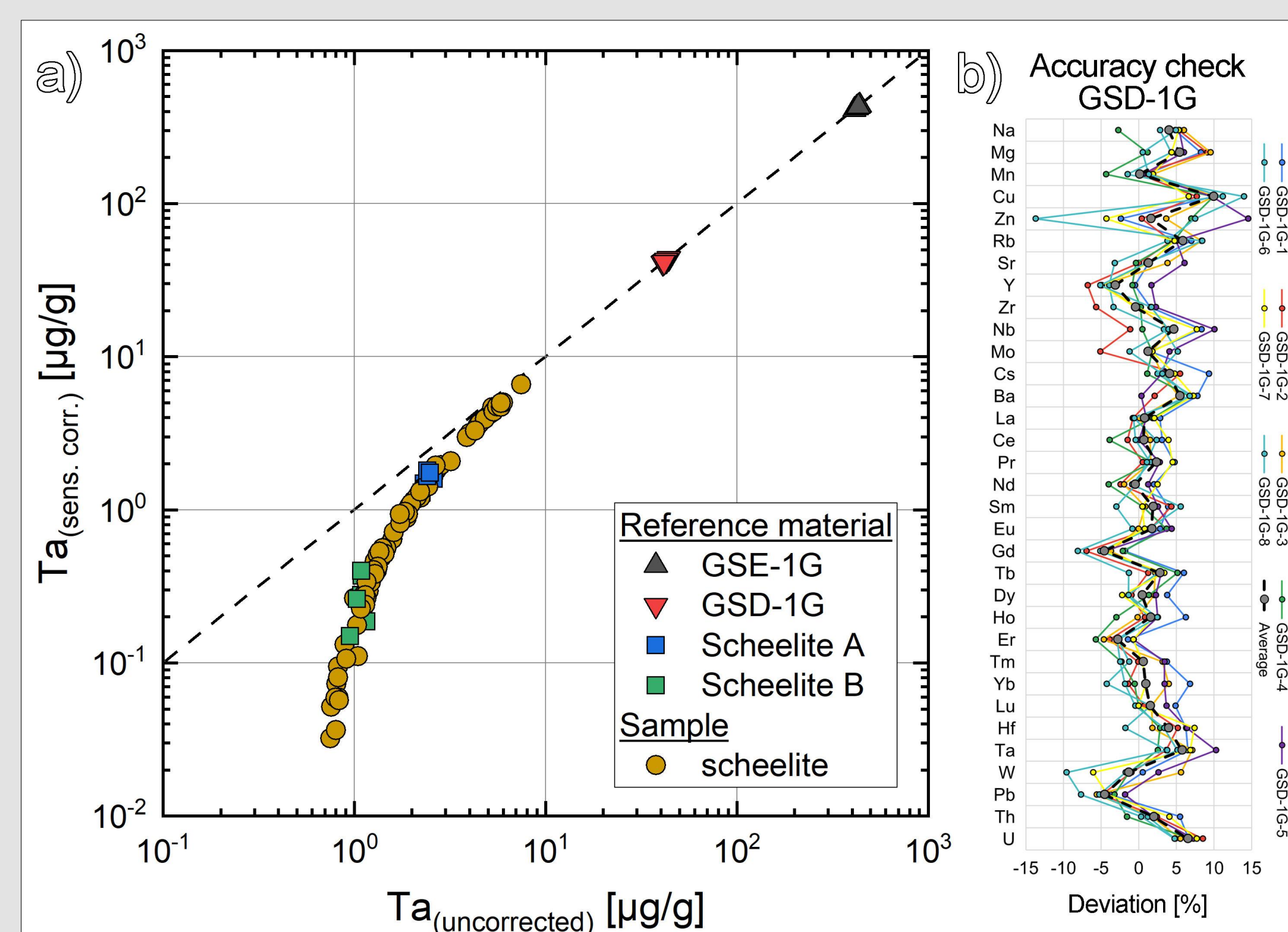


Fig. 5. a) Results of the abundance sensitivity correction ( $^{183}\text{W} \rightarrow ^{181}\text{Ta}$ ) applied on scheelite. b) Accuracy check of the secondary reference material GSD-1G. Deviation [%] = (measured value - literature value) / literature value \* 100.

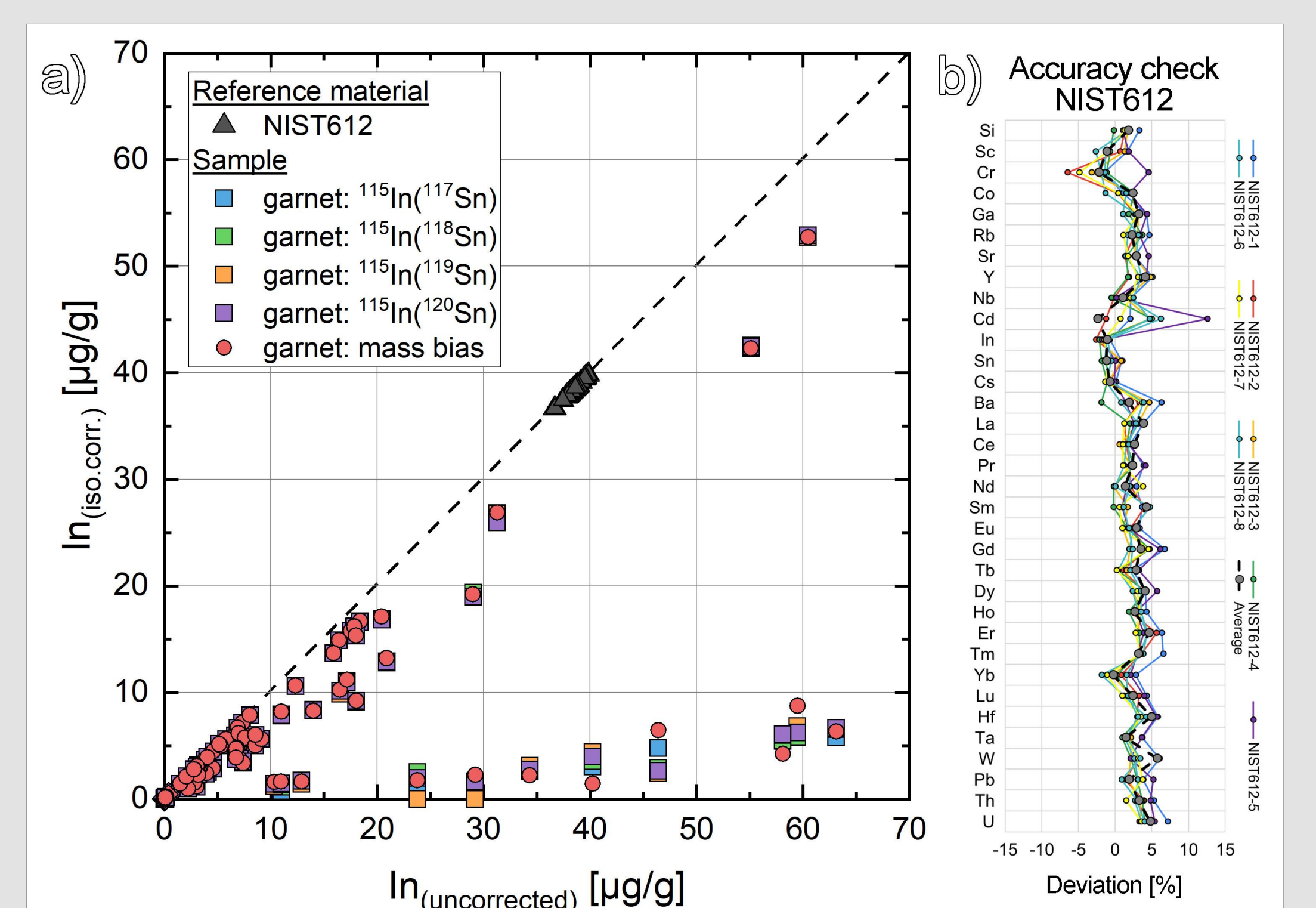


Fig. 6. a) Results of the isobaric interference correction ( $^{115}\text{Sn} \rightarrow ^{115}\text{In}$ ) applied on In-bearing garnets using different Sn isotopes and considering mass-based fractionation of Sn isotopes. b) Accuracy check of the secondary reference material NIST612.

## Discussion and Conclusion

- G.O.Joe is a new software for the evaluation of LA-ICP-MS analysis that includes different methods of interference correction and is planned as a non-commercial software that does not require installation.
- This time-efficient, transparent and easy-to-use tool for trace element analysis is appealing to both experts and newcomers to LA-ICP-MS.
- The examples of scheelite and garnet analyses show that interference corrections on individual elements can be carried out without great effort and that therefore the G.O.Joe software makes a significant contribution to the improvement of the data quality in various trace element studies using LA-ICP-MS.

## Outlook

- G.O.Joe is of course constantly evolving and some interference problems have not yet been fully resolved.
- We invite everyone to get in touch with us to further develop the software by expanding the scope and implementing more features.
- A first version of G.O.Joe is currently in the final stages of development and will be made available alongside detailed information at <https://www.gojoe.software>.

## References

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