

## **This is product of SISAL workshop 5 – 28<sup>th</sup> February to 4<sup>th</sup> March 2022 – Jerusalem**

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Discussed by all workshop participants

The following document is the wish-list for metadata information for trace element measurements using

- LA-ICPMS
- solution ICPMS
- Synchrotron XRF methods

Provide as much of the following information as possible in the metadata.txt file.

### **Laser Ablation**

#### **Acquisition**

- Image of Laser tracks (Screenshot taken within software )
- Is there a lab methodological paper (put ref)
- Standards used, and also the reference to the standard composition
  - (e.g. NIST612 e.g. from which GRM database version) & also for which Elements (on which mass) is measured
  - List of elements and masses that are measured (and in which acquisition mode)
  - Carrier Gas and Flow rates of Argon, Helium, Nitrogen
  - Could e.g. be retrieved from Igor Metadata export after calibration? (Pauline?)
  - Raster scan or single spot analysis
  - Single spot analysis
    - spot size, form, resolution
    - space in-between
    - crop
    - mean analytical error
    - sample data acquisition time
    - washout time
  - Raster Scan: Laser Pulse rates and scan speed;
  - For spot: spotform and spot diameter. For slit: slit size
  - Pre-ablation: spot diameter, dimension vs measurement spot diameter
- Specify whether unique run, or put in sections, (where are standards)
- One or several line scans, distance between tracks
- Equipment used:
  - Laser system (including specification of Laser wavelength)
  - potential smoothing devices
  - Mass spectrometer
- More suggested parameters, see table from Scholz and Drysdale below

**Table 3**

Operating parameters for the laser ablation systems UP213 and UP193SS.

	UP213	UP193SS
Wavelength/nm	213	193
Pulse length/ns	5	2.8
Fluence/J cm <sup>-2</sup>	8	9
Pulse repetition rate	10	10
Ablation times/s	100	100
Washout times/s	30	60
Spot size/μm	20–110	25–110

Table 1  
Instrumental operating conditions for the LA-ICP-MS.

<i>Agilent 7700x ICP-MS</i>	
Forward power	1300 W
Reflected power	2 W
Sample depth	3 mm
Dwell time	0.01 s
Carrier gas	0.89 L min <sup>-1</sup>
Masses measured (m/z)	<sup>25</sup> Mg, <sup>43</sup> Ca, <sup>88</sup> Sr, <sup>138</sup> Ba, <sup>238</sup> U
<i>Helex laser-ablation system</i>	
Lambda Physik Compex 110 ArF excimer	193 nm
Laser fluence	~5 J cm <sup>-2</sup>
Data collection spot size	7 μm
Data collection repetition rate	5 Hz
Helium gas to cell	500 mL min <sup>-1</sup>
Ablation time	15 s
Final data acquisition window	~5 s

**Data reduction**

- Post-Processing: Which software has been used?
  - Has Background subtraction been done?
  - Has Drift correction been applied?
  - For spot analysis: Have edges of measurement been cropped?
- Masterline:
  - How is Masterline constructed: If several parallel lines have been measured: which line has been selected? Are the lines averaged? What procedure has been used to align the tracks? Have outliers been removed with NA or with data from another line (Outlier treatment)?
- Downsampling:
  - Which strategies are used to downsample? (e.g. running mean..)
  - Depending on your approach, give more properties: bin sizes or filter type, filter width

**Solution ICP-MS****Equipment used:**

- Mass spectrometer
- Sample introduction & Nebulizer system

**-Sample Preparation:**

- which acid and dilution factor is used
- amount of sample

**-Which Standards are used?**

- for in-house standard, report also external calibration
- Analytical method: blanks, how many levels for in-house standard, Frequency of standards between samples, rinse routine

**-Acquisition**

- Basic tuning parameters for each acquisition mode (e.g. NoGas, He, O2)
  - RF Power
  - Carrier Gas and Flow rates
  - Sample depth (for ICP MS)
  - Plasma viewing height (ICP OES - if applicable)
  - sweep time and replicates (if applicable)
- List of measured Elements (and on which mass(es)), with which dwell time, on which mode)
- Report detection limits and analytical uncertainties for measured element ratios

**Data reduction**

- Post-Processing: Which software has been used?
  - Has Background subtraction been done?
  - Has Drift correction been applied?
  - Which Ca-isotope has been used for ratio calculation
  - 
  - 
  - 
  -

**Synchrotron XRF****Equipment used:**

- Synchrotron and synchrotron beamline
- Geometry (45 or 90 degree incident angle)
- XRF detector
- focusing mirror
- incident energy
- beam spot size
- resolution (um)
- dwell time

**-Sample:**

- physical aspect: thin section (specify thickness) and glass composition, or thick slab

- **Data reduction:** - internal elemental calibration
  - data reduction method and software
  - line extraction: software, window width
  - downsampling/filtering/binning