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# LaserTRAM-DB: A Time Resolved Analysis Module for the complete reduction of Laser Ablation Inductively Coupled Plasma Mass Spectrometry data

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# Summary

LaserTRAM-DB is a dashboard for the complete processing pipeline of Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) data in complex materials such as geologic samples. As LA-ICP-MS data in geologic samples frequently have multiple phases, inclusions, and other compositional complexities within them that do not represent the material of interest, user interaction is required to filter unwanted signals out of the overall ablation signal. LaserTRAM-DB allows the user to filter which portion of the ablation peak is utilized in calculating concentrations, subsequently allowing for more accurate data to be obtained. Furthermore, it allows for the processing of both individual spot analysis data and a line of spots gathered in rapid succession, reducing the time required for data reduction while preserving spatial definition and still ensuring data quality.

# Background

With a wide array of applications in the natural sciences (e.g., Fritz-Endres and Fehrenbacher, 2021; Caricchi et al., 2020; Loewen and Kent, 2012; Lukács et al., 2021), laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is a now a commonplace tool for the gathering of *in situ* trace element (i.e., < 0.1 wt%) data from solid materials. The last two decades have seen significant advances in both instrument capabilities and operating software, allowing users to generate large volumes of *in situ* geochemical data in comparatively little time to previous methodologies (i.e., micro-drilling) while still maintaining high degrees of accuracy and precision.

Raw data output from LA-ICP-MS, however, is in the form of counts per second (cps) for the selected analyte isotopes, not elemental concentrations (e.g. Figure 1). In order to be converted into accurate concentrations, a modest amount of user input and interpretation is required and should not be automated. Currently, there are several proprietary and open-source softwares for LA-ICP-MS data reduction to accomplish this task: SILLS - Guillong et al. (2008); lolite - Paton et al. (2011); LAtools - Branson et al. (2019); Termite - Mischel et al. (2017); GLITTER - Macquarie University GEMOC; and countless other "in house" spreadsheet-based tools. All have their strengths and weaknesses, however, there is yet to be a powerful, web-hosted Graphical User Interface (GUI). Built primarily using Plotly-Dash [Plotly Technologies Inc.], numpy (Harris et al., 2020), and pandas (McKinney et al., 2010), we present a completely open-source dashboard: Laser Time Resolved Analysis Module Dashboard (LaserTRAM-DB) that allows the user to calculate concentrations from raw LA-ICP-MS data with the flexibility of a GUI interface while maintaining the performance of the numerical python ecosystem. Furthermore, by simultaneously displaying both raw data cps and internal standard normalized cps, it allows for rapid decision making about data quality to be determined. Below we outline the theory, workflow, and structure, behind LaserTRAM-DB in an effort to maximize its effectiveness in the petrology and volcanology communities.

# **Governing Equations**

We calculate the concentration of analyte (i) in an unknown material (u) using the following relationship from Longerich et al. (1996):

$$C_i^{\ u} = \frac{R_i^{\ u}}{S} \tag{1}$$

Where  $C_i^{\ u}$  and  $R_i^{\ u}$  are the concentration of analyte and count rate of analyte (i) in the unknown material, respectively, and S is the normalized sensitivity. When using naturally occuring internal standards, S can be defined as:

$$S = \frac{R_i^{std}}{C_i^{std}} \left[ \frac{R_n^{u}}{R_n^{std}} \frac{C_n^{std}}{C_n^{u}} \right]$$
(2)

 $R_i^{std}$  and  $C_i^{std}$  are the count rate and and concentration of analyte (i) in the calibration standard,  $R_n^u$  and  $R_n^{std}$  are the mean count rates of the internal standard in the unknown material and calibration standard,  $C_n^u$  and  $C_n^{std}$  are the concentrations of the internal standard in the unknown material and calibration standard.

Kent and Ungerer (2006) re-arrange this relationship such that the count rate expressions always contain unknown analytes in the numerator:

$$C_i^{\ u} = C_n^{\ u} \frac{\left[\frac{C_i^{\ std}}{C_n^{\ std}}\right]}{\left[\frac{R_i^{\ std}}{R_n^{\ std}}\right]} \frac{R_i^{\ u}}{R_n^{\ u}}$$
(3)

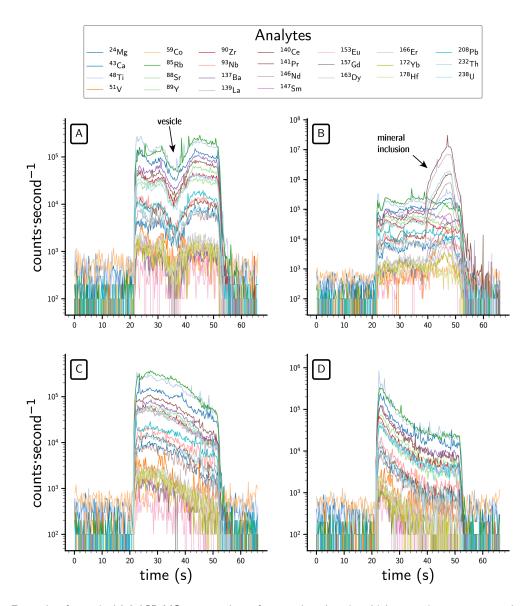


Figure 1: Example of a typical LA-ICP-MS spot analyses from tephra data in which many isotopes are analyzed at once. Data are output from a quadrupole mass spectrometer as counts per second (cps). Elevated values in the center refer to the signal pertaining to the ablated material (e.g., volcanic glass, mineral inclusion, etc.) while lower values on either side refer to background levels of each isotope within the mass spectrometer. Each plot in the panel displays a range of noise where some degree of control over the ablation signal is required for calculating concentrations ranging from significant (A,B) to minimal (C,D). The cause of the noise in A is likely due to different ablation rates in pumice (e.g., the ablation area encountering vesicles) and the noise in B is largely due to the ablation of a mineral inclusion (in this case apatite) part way through the analysis,

### Normalizing to an internal standard

The purpose of LaserTRAM-DB is to give the user complete control over which portion of the analytical spectra gets used in calculating concentrations (e.g., filtering out portions of the signal not reflective of the material under investigation). In complex natural materials, selection of this interval and an overall judgement about data quality require an operator to make a decision. This software is optimized to allow that decision to be made as efficient as possible.

When a given interval from the analytical spectra has been chosen, every analyte is normalized to a chosen internal standard. LaserTRAM-DB allows for any analyte in the experiment to be used as the internal standard (see caveats on this in the walkthrough below). Prior to normalization to an internal standard, raw data first has the background analyte levels subtracted from it. Background is determined by taking the median counts per second value for each analyte over the user specified background range. Once data have been background subtracted, each normalized ratio is calculated the following way:

$$N_i = median \left[ \frac{cps_i}{cps_{is}} \right] \tag{4}$$

Where  $cps_i$  is the background subtracted counts per second data for analyte (*i*), and  $cps_{is}$  is the background subtracted counts per second data for the internal standard. Since counts per second is analogous to count rate above in Equation 3, we can simplify the above relationship to now reflect our  $N_i$  values:

$$C_i^{\ u} = C_n^{\ u} \frac{\left[\frac{C_i^{\ std}}{C_n^{\ std}}\right]}{N_i^{\ std}} N_i^{\ u} \tag{5}$$

Here,  $N_i^{std}$  and  $N_i^{u}$  are the normalized counts per second value of analyte *i* in the calibration standard and unknown, respectively. The uncertainty for any given normalized ratio is expressed as:

$$SE = \frac{\sigma_{N_i}}{\sqrt{n}} \tag{6}$$

 $\sigma_N$  is the standard deviation of a given analyte's normalized ratio for the interval and n is the number of time steps in the interval (i.e., cycles through the mass range). The relative standard error is then:

$$RSE_i{}^u = \left[\frac{SE}{N_i}\right]100\tag{7}$$

### **Detection Limits**

Count rate detection limits for each analyte are determined to Longerich et al. (1996):

$$LOD = 3\sigma_b + b \tag{8}$$

where b is the background median counts per second value for a given analyte. This is standard practice in LA-ICP-MS data reduction. To reflect this in data output, measurements that are below detection limit will have values that say "b.d.l." rather than concentrations.

# **Drift Correction**

To check for drift in calibration standard normalized ratios over time, a linear regression is applied to the calibration standard for each analyte, where the dependent variable is the count rate normalized to the internal standard and the independent variable is the timestamp associated with each analysis (Figure 2):

We determine the significance of each regression by evaluating following null hypothesis: there is no relationship between a given analyte's internal standard normalized ratio and time. We reject this if both the following conditions are true: The p-value for the coefficient (i.e., slope) is significant; The F-statisic comparing the regression and observed data is greater than the critical F value. By default, we set the threshold for p-value significance at .01 (i.e., we have 99% confidence that we can reject the null hypothesis) in an effort to mitigate

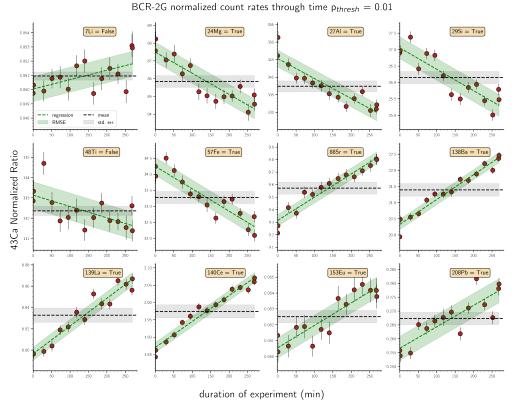


Figure 2: Drift correction test from LaserCalc for a given experiment in which standard reference material BCR-2G was used as the primary standard. We can see here that one experiment may contain analytes that are both drift corrected and not drift corrected.

drift correcting all but the most linear of changes in normalized count rates, but this may be changed by the user. If the null hypothesis for a given analyte is rejected, the analyte is linearly corrected for drift and the regression parameters (e.g., slope and intercept) are used to calculate a normalized count rate for the calibration standard at the point in time where an unknown was analyzed:

$$C_i^{\ u} = C_n^{\ u} \frac{\left[\frac{C_i^{\ std}}{C_n^{\ std}}\right]}{\left[m_i x + b_i\right]} N_i^{\ u} \tag{9}$$

Where m is the regression slope, x is the analysis time, and b is the intercept for analyte i.

### Uncertainties

Calculating concentrations of a given analyte in an unknown material can be considered a series of nested quotients and products. Therefore, we quantify the overall uncertainty of a given analyte as Taylor (1997):

$$\sigma_{C_i} = C_i^{\ u} \sqrt{\left(\frac{\sigma_{C_u^{\ n}}}{C_u^{\ n}}\right)^2 + \left(\frac{\sigma_{C_i^{\ std}}}{C_i^{\ std}}\right)^2 + \left(\frac{\sigma_{C_n^{\ std}}}{C_n^{\ std}}\right)^2 + \left(RSE_i^{\ std}\right)^2 + (RSE_i^{\ u})^2} \tag{10}$$

Where  $RSE_i^{std}$  is defined as:

$$RSE_i^{std} = \left[\frac{\frac{\sigma_i}{\sqrt{n_i}}}{\mu_i}\right] 100 \tag{11}$$

 $\sigma_i$  and  $\mu_i$  are the standard deviation and mean of all of the calibration standard normalized ratios respectively and  $n_i$  is the total number of calibration standard analyses for analyte (*i*).

For analytes where drift correction has been applied,  $RSE_i^{std}$  is replaced with:

$$100 \left[ \frac{RMSE_i}{\mu_i} \right] \tag{12}$$

Where  $RMSE_i$  is the Root Mean Squared Error as specified in the Drift Correction section.

### Concentrations of internal standard in unknown

To calculate concentrations of a given analyte list in an unknown sample, the concentration of the internal standard must be known. LaserCalc takes these concentrations in the form of wt% oxide and utilizes user interaction to input concentrations of the internal standard and its relative uncertainty. A default value of 1% is used for this, but may be updated by the user.

# Installation and Use

# Installation

LaserTRAM-DB can be installed and run two ways. The first is by creating a virtual Python environment. If you are new to Python, we recommend doing this through Anaconda the following way:

```
git clone https://github.com/jlubbersgeo/laserTRAM-DB
cd /path/to/laserTRAM-DB
conda create -n lasertram-db python=3.7.7
conda activate lasertram-db
conda config --append channels conda-forge
conda install --file local_requirements.txt
python lasertram-db.py
```

Once the virtual environment is set up you can also open and run the lasertram-db.py script from any python IDE (e.g., Spyder, IDLE, PyCharm, etc.).

When the program is running, copy and paste the provided link provided in the terminal window into the browser window and the app will run. From now on any time you wish to use the program, simply re-activate the virtual environment and run the script like above.

Alternatively, LaserTRAM-DB has been packaged as a .exe file and may be run by downloading and unpacking the zip file found here. Once unpacked, find the lasertram\_deploy.exe file and run it. A terminal window will pop up and the application will automatically deploy to your default web browser. The .exe file must remain in the lasertram\_deploy folder but you may create a shortcut to it and place that anywhere on your computer (e.g., your Desktop).

#### Walkthrough

Here we will walk through each step of the data processing pipeline in LaserTRAM-DB. In brief, it is comprised of 2 parts:

- 1. Normalizing data to an internal standard
  - LaserTRAM: Choosing an interval of interest from raw cps data in individual spot analyses and normalizing it to an internal standard.
  - LaserTRAM profiler: Functionally the same as LaserTRAM, however has tools that allow for the rapid inspection of a line of spot analyses gathered in quick succession.
- 2. Calculating concentrations from data that has been normalized to an internal standard
  - LaserCalc: Takes the output from either LaserTRAM or LaserTRAM profiler and converts the normalized data into concentrations using the equations outlined above.

#### LaserTRAM: New Project Tab

LaserTRAM is comprised of two tabs:

- 1. New Project tab (Figure 3). This is the default window upon running the software, however none of the figures or tables will be populated yet.
- 2. Re-processing tab (Figure 4).

To begin a new project, simply click on the "Upload Data" button in the upper left portion of the window. A File Explorer/Finder window will prompt the user to choose their file that has been formatted for LaserTRAM (e.g., Table 1). Once the data are loaded in, options will appear in the "Int. Std." dropdown menu. Any analyte in the experiment may be chosen as the internal standard, however in order to calculate concentrations in LaserCalc later only analytes that create the following oxides may be chosen: SiO<sub>2</sub> (e.g., <sup>29</sup>Si), CaO (e.g., <sup>43</sup>Ca), TiO<sub>2</sub> (e.g., <sup>47</sup>Ti), Al<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, MnO, FeO, K<sub>2</sub>O, Na<sub>2</sub>O, NiO. To maximize data quality, it is recommended that the internal standard is an analyte that is already well quantified in the unknown (i.e., in silicate minerals <sup>29</sup>Si and <sup>43</sup>Ca are good options as SiO<sub>2</sub> and CaO are commonly measured accurately via EPMA and are at concentrations in most geologic materials ideal for measurement by LA-ICP-MS). While it is easy to explore many different internal standards and their effect on data quality, only one should be used for recorded intervals that will be used in calculating concentrations later.

timestamp	SampleLabel	Time	24Mg	29Si	 208Pb
Y-M-D HR:MIN:S 2021-03-01 22:18:30	Spotname MQ1	ms 13.24	raw cps 100.04	raw cps 38559.38	  raw cps 100.00

Table 1: Example of input data format for LaserTRAM-DB. Shown is an example row in an input spreadsheet with its units listed above. In this instance, each row represents one cycle through the mass range for a ICP-MS.

To populate the graphs and begin processing data, choose a spot from the "Spot" dropdown menu. The first time this is done it may take a few seconds, as the entire project is being loaded in, however it will be relatively instantaneous from there on out. The layout from upper left to lower right:

- Raw data graph: This is the raw signal for each spot being processed. It contains regions indicating the time interval designated for background (red) and signal to be used for concentrations (green).
- Normalized data graph: This graph shows the green region in the raw data graph normalized to the chosen internal standard.
- Analyte uncertainties graph: Bar chart showing the relative standard error (i.e., Equation 10). Values on the top of each bar indicate the median normalized ratio using SI prefixes. If the relative standard error is < 5% the bar will be green, otherwise it will be yellow.</li>
- Saved spot data table: Recorded data for each spot will populate here. Each time the "Record" button is pressed, a new row will be generated. More on this in a bit.

To choose intervals for background and ablation signal, simply drag the handles on the slider bar where it says "Chose background and interval of interest with the sliders". The left two handles are for background and the right two are for ablation signal of interest. All the graphs are linked to the slider, meaning that when the sliders move they will all update in real time to reflect the decisions made by the user. When the sliders are in the desired spot, the "Record" button will save the requisite data to the "Saved Spot Data" table in the lower right. Each row contains the following:

- **Timestamp:** This is a unique time identifier for each spot that is inherited from the raw data. This will be propagated throughout the pipeline to help keep track of sample and monitor for drift in the primary standard over time (i.e. Equation 9).
- **Spot:** This is the name given to each spot in the raw data (i.e., the "SampleLabel" column in Table 1).

- Interval data: These are columns that contain the time information in each analysis for the start and end of both the background and interval of interest. They are bkgd\_start, bkgd\_stop, int\_start, int\_stop.
- Internal standard analyte: The analyte chosen as the internal standard. The "norm\_cps" column contains the median counts per second value of the internal standard over the interval of interest.
- Normalized data: Columns for each analyte's internal standard normalized value. Their header is simply the analyte name. Values that are -9999 denote analytes below detection limit for that spot as dictated by Equation 8.
- Uncertainty data: Columns to the right of the normalized data with the suffix "\_se" contain the relative standard error for each analyte in percent (i.e., Equation 7).

Progressing through all spots in the experiment can be accomplished two ways:

- 1. Using the spot dropdown and picking the spot you wish to process (not recommended).
- 2. Using the "Previous" and "Next" buttons (*recommended*). These will navigate between adjacent spots to efficiently progress through the spot list.

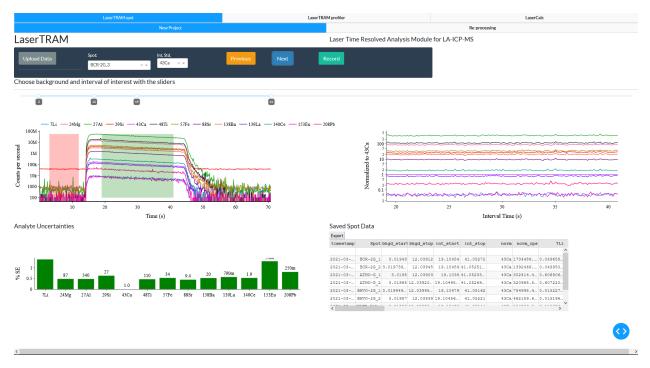


Figure 3: Example of the LaserTRAM New Project tab after data has been loaded in.

When finished, the "Export" button associated with the "Saved Spot Data" table will export the table exactly how it is shown in the browser. It is recommended that in your browser you adjust the file download settings such that they ask for a save location prior to download. This will allow you more control over where the LaserTRAM completed data is stored.

#### LaserTRAM: Re-processing Tab

This tab takes the input and output from the "New Project" tab and re-normalizes the experiment to a newly chosen internal standard. Similar to above, use the upload data in the "New Project" tab to upload raw experiment data. This is the only step that is done in that tab, so now navigate to the "Re-processing" tab. Use the "Upload old LT file" button in the upper left to upload the output for the same experiment you wish to re-normalize. It does not matter if all of the spots in the experiment were processed, LaserTRAM will only re-normalize spots

that have been previously processed. At this point, the "Old normalized Ratios" table on the left will populate with the previously normalized data, as well as a list of potential analytes in the dropdown above to choose for re-normalizing. After the desired analyte is chosen, hit "Re-process!". This will take the interval columns from the old data and use them as bounds for the re-normalization. This should be relatively instantaneous and leave you with something that looks like Figure 4. Similar to the "New Project" tab and everywhere else in LaserTRAM-DB, the table with re-normalized data can be exported using the button attached to the table. It will have the same exact output as the "New Project" tab. If you wish to re-normalize to a few different internal standards, this is easily accomplished by choosing a new analyte in the dropdown menu and hitting "Re-process!".

2021-0       BCR-0-2       3.0189       11.1374       12.06939       41.0224       281       0.01931       11.1374       12.06939       41.0224       281       0.01931       11.1374       12.06939       41.0224       281       0.01931       0.01931       11.1374       12.06939       41.0224       281       281       0.01931       11.1374       12.06939       41.0224       281       281       0.01931       11.1374       12.06939       41.0224       281       281       0.01931       11.1374       12.06939       41.0224       281       281       0.01931       11.1374       12.06939       41.0224       281       281       0.01931       11.1374       12.06939       41.0224       281       281       281       0.01931       11.1374       11.1354       12.0693       41.0224       281       281       0.01931       11.1374       1.0164       11.0524       281       281       281       0.01931       -999       0.01931       11.1374       1.0184       11.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154       1.0154	start         Int_stop         norm_ope         71.         249/s         27AL           0.0860         41.0572         295.276320         -999.3.23500         12.73500         10.000           0.0980         41.0522         295.276320         -999.3.23500         12.73500         10.000           0.0983         41.0522         295.276320         -999.0.04735         54555         10.000           0.0974         41.0524         295.21398         -999.0.04735         54565         10.000           0.0975         41.0524         295.21398         -999.0.04735         54566         10.000           0.0975         41.0524         295.21398         -9999.0.04735         54566         10.000           0.0975         41.0524         295.21398         -9999.0.04735         54566         10.000           0.0975         41.0524         295.21398         -9999.1.001.574         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.000         10.0000         10.000         10.0000 </th
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Update dull life         293         Reprocess           normalized ratios         Reprocess           ontrol life         30.0146         11.13704         21.0686         11.03704         21.06876         1	08883         41.08272         2981 276320.         -9999 3.238005.         12.73800.           08895         41.0827         2981 281041.         -9999 3.238005.         12.73800.           0797         41.0228         2981 27141.         -9999 0.047936.         8.56853.           1.0994         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2020845         -9999 6.591732.         13.66576           0.0897         41.0524         2981 100404         -9999 1.901574         0.9999 1.905174           0.0894         41.0524         2981 263921         -9999 1.90041         0.9999 1.90041           0.0894         41.0527         2981 265861         -9999 1.90053         12.49420           0.0894         41.0527         2981 271171         -9999 3.100353         12.49420           0.0894         41.0527         2981 271171         -9999 3.200358         12.49420           0.0894         41.0512         2981 271171         -9999 3.200358         12.49420
259         Second         Second <th>08883         41.08272         2981_276320.         -9999_3.238005.         12.73800.           08893         41.08272         2981_2163041.         -9999_3.238005.         12.73800.           08985         41.08282         2981_21741.         -9999_0.047986.         8.56853.           1.0979         41.0829         2981_212393         -9999_0.047986.         8.56853.           0.0974         41.0829         2981_2124393         -9999_0.047986.         8.56853.           0.0974         41.0829         2981_2124393         -9999_0.57756.         8.56853.           0.0974         41.0824         2981_200945         -9999_0.501754.         13.66376.           0.0876         41.0824         2981_3030406         -9999_0.501574.         0.90641.           0.0984         41.0824         2981_265961         -9999_0.190333.         12.4980.           0.0984         41.0827         2981_265961         -9999_0.190333.         12.4980.           0.0897         41.0826         2981_271177         -9999_0.300333.         12.4980.</th>	08883         41.08272         2981_276320.         -9999_3.238005.         12.73800.           08893         41.08272         2981_2163041.         -9999_3.238005.         12.73800.           08985         41.08282         2981_21741.         -9999_0.047986.         8.56853.           1.0979         41.0829         2981_212393         -9999_0.047986.         8.56853.           0.0974         41.0829         2981_2124393         -9999_0.047986.         8.56853.           0.0974         41.0829         2981_2124393         -9999_0.57756.         8.56853.           0.0974         41.0824         2981_200945         -9999_0.501754.         13.66376.           0.0876         41.0824         2981_3030406         -9999_0.501574.         0.90641.           0.0984         41.0824         2981_265961         -9999_0.190333.         12.4980.           0.0984         41.0827         2981_265961         -9999_0.190333.         12.4980.           0.0897         41.0826         2981_271177         -9999_0.300333.         12.4980.
Opt         Description         Description <thdescription< th=""> <thdes< th=""><th>08883         41.08272         2981 276320.         -9999 3.238005.         12.73800.           08895         41.0827         2981 281041.         -9999 3.238005.         12.73800.           0797         41.0228         2981 27141.         -9999 0.047936.         8.56853.           1.0994         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2020845         -9999 6.591732.         13.66576           0.0897         41.0524         2981 100404         -9999 1.901574         0.9999 1.905174           0.0894         41.0524         2981 263921         -9999 1.90041         0.9999 1.90041           0.0894         41.0527         2981 265861         -9999 1.90053         12.49420           0.0894         41.0527         2981 271171         -9999 3.100353         12.49420           0.0894         41.0527         2981 271171         -9999 3.200358         12.49420           0.0894         41.0512         2981 271171         -9999 3.200358         12.49420</th></thdes<></thdescription<>	08883         41.08272         2981 276320.         -9999 3.238005.         12.73800.           08895         41.0827         2981 281041.         -9999 3.238005.         12.73800.           0797         41.0228         2981 27141.         -9999 0.047936.         8.56853.           1.0994         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2813938         -9999 0.047936.         8.56863           0.0992         41.0129         2981 2020845         -9999 6.591732.         13.66576           0.0897         41.0524         2981 100404         -9999 1.901574         0.9999 1.905174           0.0894         41.0524         2981 263921         -9999 1.90041         0.9999 1.90041           0.0894         41.0527         2981 265861         -9999 1.90053         12.49420           0.0894         41.0527         2981 271171         -9999 3.100353         12.49420           0.0894         41.0527         2981 271171         -9999 3.200358         12.49420           0.0894         41.0512         2981 271171         -9999 3.200358         12.49420
	0.883         41.08272         2881 276320         -9999 3.238005.         12.73800           0.8883         41.0827         2981 251041         -9999 3.24887.1         12.9807           0.0893         41.0828         2981 251041         -9999 0.47887.1         12.9807           0.0797         41.0229         2981 251398         -9999 0.047938.6         15.85633           0.0894         41.0124         2981 2020545         -9999 0.04738.6         15.45665           0.0897         41.0524         2981 2020545         -9999 0.891732.1         15.66576           0.0894         41.0524         2981 1303406         -9999 0.491732.1         15.66576           0.0894         41.0524         2981 120221         -9999 0.9999 1.501374         0.9991 1.501374           0.0894         41.0527         2981 669861         -9999 0.900539.12         12.4820           0.0895         41.0527         2981 271187         -9999 0.150339.12         12.4820           0.0897         41.0512         2981 271187         -9999 0.360338.8         8.66071           0.0897         41.0512         2981 271187         -9999 0.36038.8         8.66071
1-03-       BCR-20_1       3.01948       11.3704       21.0880       41.0227       428.1447013       0.049780.       67.17106.       94.1430.24.90       2021-03       BCR-20_1       3.01948       11.13704       21.0880       41.0227       2981.245320       -9999       9.235001         1-03-       BCR-20_1       3.01948       11.13714       21.0888       41.0527       2981.245320       -9999       9.235001       1       -9999       9.235001       -9999       9.235001       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.249501       -9999       9.49951       -9999       9.49951       -9999       4.9951       -9999       4.9951       -9999       4.9951       4.9999       4.9991       4.9991.	0.883         41.08272         2951 276320         -9999 3.28005. 12.73800           0.8883         41.0827         2951 281041         -9999 3.28005. 12.73800           0.8984         41.0820         2951 281041         -9999 0.47856. 8.55653           0.9074         41.0820         2951 2810981         -9999 0.47954         55653           0.9074         41.0820         2951 2020545         -9999 0.47954         516563           0.9074         41.0820         2951 2020545         -9999 0.501754         516563           0.9074         41.0824         2951 2020545         -9999 0.501754         516563           0.9054         41.0824         2951 2020545         -9999 0.501754         500641           0.9054         41.0824         2951 2020245         -9999 0.90093         12.64206           0.9054         41.0824         2951 280221         -9999 0.90093         12.64206           0.9054         41.0827         2951 260861         -9999 0.180033         12.64207           0.9057         41.0512         2951 271187         -9999 0.180033         8.66071           0.9057         41.0512         2951 271187         -9999 0.30033         8.66071<
1-05-         BG-20         5.01279         11.13741         21.06598         41.05221         2015	0.0953         41.0222         2981 21.001         -9999 0.047987         12.9527           0.0777         41.0224         2981 277641         -9999 0.047981.         8.56683           0.0874         10.0129         2981 213938         -9999 0.047984.         8.56686           0.0894         41.0124         2981 201683         -9999 0.79786         15.8668           0.0805         41.0324         2981 201683         -9999 0.619733         15.8668           0.0807         41.0314         2981 1001064         -9999 0.619733         15.00641           0.0904         41.0324         2981 20228         -9999 0.500641         1999 0.00033         12.48420           0.0954         41.0324         2981 202826         -9999 1.03038         12.48420         0.999 1.03038         12.48420           0.0954         41.0324         2981 202826         -9999 1.03038         12.48420         0.999 1.03038         12.48420           0.0954         41.0324         2981 201118         -9999 0.030033         12.48420           0.0957         41.0324         2981 20122         -9999 0.32034         12.48420
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0.8797         41.08234         2981 277641         -9999 0.047931         8.55653           0.898         41.0824         2981 281393         -9999 0.047931         8.55653           0.8992         41.0824         2981 281393         -9999 0.047931         8.55663           0.8992         41.0824         2981 200545         -9999 0.75661         3.55674           0.8876         41.0824         2981 30906         -9999 0.9999 1.501574         0.9999         -9999 1.050574           0.8876         41.0824         2981 30906         -9999 0.9999 1.900541         0.9999 0.90041         0.9991 1.80041           0.9984         41.0822         2981 269661         -9999 0.100303         1.64202           0.8984         41.052         2981 271187         -9999 0.1003033         8.66071           0.8984         41.052         2981 271187         -9999 0.30033         8.66071           0.8984         41.052         2812 271         -9999 0.30033         8.66071
1-03       MTRO-E2       3.01865       11.13727.       21.0589       41.0526       450.275183       0.677584       1.0374.0.1337.271.       151.6       2021-03       MTRO-E2       3.01865       11.13727.       21.0589       41.0526       2051.253       -9999       0.047584         0-3       MTRO-E2       3.01865       11.13727.       21.0589       41.0526       2051.253       -9999       0.047584       -9999       0.047584       -9999       0.047584       -9999       0.047584       -9999       0.047584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.997584       -9999       0.999581       -9999       0.999581       -9999       -9	1.0554         41.0126         2981 2813988         -9999 0.047784         6.54568           0.0502         10.0162         2981 2012653         -9999 6.735661         13.63569           0.0505         41.0014         2981 202654         -9999 6.631732         13.66376           0.0575         41.0014         2981 303046         -9999 6.631732         13.66376           0.0585         41.0014         2981 303046         -9999 9.9991.501374         0.9991 1.00147           0.0584         41.0027         2981 263961         -9999 9.100041         0.9995 1.00041           0.0585         41.0027         2981 263961         -9999 9.1000330         2.48200           0.0587         41.0512         2981 271187         -9999 9.100330         2.482071           0.0587         41.0512         2981 271187         -9999 9.200356         1.24268
$-3 870-26_{1} 3.01994. 11.1360 + 21.0590 + 41.05162 + 430. 52453.4 0.01492. 112.873 + 21.427 + 15.98 + 2021-03 - 870-26_{2} 3.0199 + 11.375 + 21.0587 + 41.0521 + 295 + 202163999 + 6.97364. 1 - 0.0097 + 0.0007 +$	0.8900         41.051.02         2951 201653         -9999         6,795661         13.63960           0.8977         41.0521         2951 200955         -9999         6,891732         13.66376           0.8976         41.0521         2951 200955         -9999         -9999         1.05041           0.8976         41.0524         2951 203725         -9999         -9999         1.80641           0.8986         41.0524         2951 203725         -9999         .1803941         1.04240           0.8986         41.0524         2951 203725         -9999         .180394         1.2.48420           0.8997         41.052         2951 271187         -9999         .806034         1.66671           0.8977         41.052         2951 271187         -9999         .806034         1.2.48420
-3 5870-20_2 3.01997 11.1375 21.05875 41.0522 456 406513.9 0.014699 12.4457 22.9285 16.24 2021-05 870-20_2 3.0199 11.1375 21.05875 41.0522 281 209459999 6.69173. 1 -0 1875-62. 3.0199 11.1375 21.0587 41.0524 40.515 41.0524 291 2091.0 - 1999 6.9173. 1 -0 1875-62. 3.0199 11.1376 21.0587 41.0524 40.515 - 10.024 456. 15376 0.0993 10.516 95.956 0.0993 10.516 95.956 0.0993 10.516 10.5	.08075         41.0521         2951 200645         -9999 6.891732.         13.66376.           .08176         41.0514         2951 3030466         -9999 1.905974.         10.0174           .08084         41.0522         2951 302786         -9999 1.90591         9999 1.00541           .08084         41.0522         2951 269961         -9999 1.80033         12.46420           .08084         41.052         2951 261961         -9999 0.80033         6.66071           .08074         41.052         2951 261237         -9999 0.30033         6.66071
-0 JUST-412. 3.0189 11.1722. 21.0876 41.0814 428 19270.4.0.15976 7.019277.2.9.8931.1977 41.0114 2281 10000 41.0824 430 10000	0.0074         41.0514         2931.330406         -0939         -09391.100374.           0.8054         41.0522         2931.330728         -0939         -09391.40044           0.8054         41.0527         2931.263661         -0939         0.8039         12.6420           0.8054         41.0527         2931.21117         -9999.0.80039         12.6420           0.8054         41.0527         2931.271117         -9999.0.80039         12.6420           0.8057         41.0527         2931.271117         -9999.0.80039         12.6420           0.8057         41.0527         2931.6711         -8999.0.80039         12.6420
-0 MIST-612. 3.01349 11.13772 21.0589 41.0522 440.0 133121.3. 0.116219 0.147278 29.93367.1 9.69 2021-03- MIST-612. 3.0189 11.1376 21.0589 41.0522 2961 33572559999 -9999 1 -05 BCR-20_3 3.01399 11.1376 21.05854 41.0527 4508 1335640. 0.049903 47.00116 343.066 27.37 2021-03- BCR-20_3 3.01399 11.1376 21.0585 41.0527 2951 2689619999 9.16033- 1 -03 ATR0-0_3 3.01399 11.13778 21.0589 41.052 4308 20957.6 0.02359 9.00915 1334.206 152.4 2021-03- ATR0-0_3 3.0199 11.13778 21.0589 41.052 2951 2711179999 0.00033- 1 -03 BCR-20_4 3.0199 11.13778 21.0589 41.052 4308 20957.6 0.02359 9.0915 1334.206 152.4 2021-03- ATR0-0_3 3.0199 11.13778 21.0589 41.052 2951 2711179999 0.00033- 1 -999 0.0003- 1 -990 0.0003- 1 -990 0.	.0890         41.0524         2951         357225         -999         -999         1.50041           .0895         41.0527         2951         268961         -999         9.100335         12.4420           .08564         41.052         2951         171187         -9999         0.50035         8.64671           .08574         41.0542         2951         261227         -9999         0.20036         8.64671
-03- BCR-20_9 1.01389 11.13764 21.05854 41.0527 450a 133540. 0.049903 57.05116 343.6064 77.37 2021-05- BCR-20_3 3.01399 11.1376 21.05854 41.0527 2281 24596419999 3.10339a - 040- ATMO-0_3 3.01999 11.13778 21.05854 41.0524 41.0524 450a 300376. 0.60239- 9.800315 1341.002 12.021-05- ATMO-0_3 3.01999 11.13778 21.05854 41.052 201 2012 11079999 3.100393- 0.000315 -0.5- ECR-20_4 3.01595 11.13771 21.05874 41.0524 450a 3104374-0.000771 107.3507 107.10537 107.0577 41.0512 2012 1079999 3.100395 10.0005 10.00	.05955         41.05267         2951         2689661         -9999         3.180339         12.48420           .05894         41.052         2951         2711187         -9999         0.050033         8.686071           .05877         41.05162         2951         261237         -9999         3.280345         12.62688
03- ATEO-0 3 .0.1999 11.1377E 21.05894 41.052 43Ca 290537.6 0.622359_ 9.809315_1334.206 152.4 2021-03- ATEO-0 3 .0.1999 11.1377E 21.05894 41.052 2951 27111879999 0.050035_ 8 03- BCR-20 4 3.01355 11.13711 21.05877 41.05162 43Ca 13427420.050771 67.35508 339.7267 26.41 2021-03- BCR-20 4 3.01395 11.13711 21.05877 41.05162 2951 26182379999 3.280345_ 1	.05894         41.052         2951         2711187         -9999         0.050033         8.686071           .05877         41.05162         2951         2618237         -9999         3.280345         12.62688
-0 8CR-22 3.01955 11.13711 21.05877 41.05162 49Ca 1342742 0.050771. 87.35508 339.7267. 26.41 2021-05 8CR-22 4 3.01955 11.13711 21.05877 41.05162 2951 2618337	.05877 41.05162 2951 26182379999 3.280345 12.62688

Figure 4: Example of the LaserTRAM reprocessing tab after data has been loaded in.

#### LaserTRAM profiler

LaserTRAM profiler is functionally the same as the "New Project" tab in LaserTRAM. It takes in raw data through upload button, has a dropdown for the internal standard, a button for recording the data for a given spot, and all of the quadrants have the same display. The major differences are as follows (Figure 5):

- The addition for a "step size" numeric input box.
- Rather than "Next" and "Previous" buttons to move between spot analyses, we have "Forwards" and "Backwards" buttons. These will step the green interval of interest by the value in the "step size" input box. This can be used in conjunction with the range sliders directly below the buttons to efficiently jump from one peak to the next in the line of spots.
- Unlike the individual spot reduction, the "Saved Spot Data" table in LaserTRAM profiler will have rows that pertain to each spot in the line of spots. They will be named accordingly following the naming scheme: "transectname\_spotnumber".

It is recommended that after each line of spots is processed it is exported and saved as its own spreadsheet. They can then be later combined in order for LaserCalc.

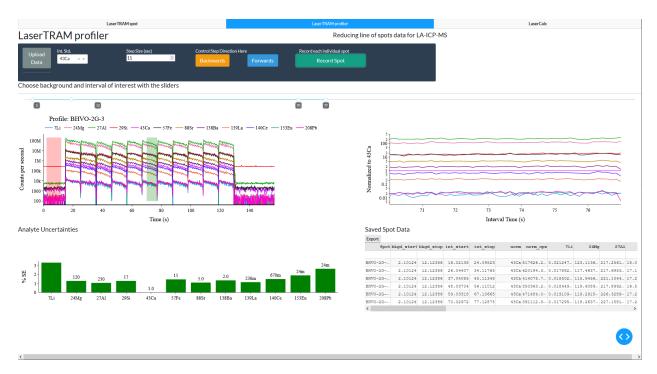


Figure 5: Example of the LaserTRAM profiler illustrating how the software can easily normalize a line of spots gathered in rapid succession to one another.

#### LaserCalc: Concentrations Tab

This tab takes the output of either the spot or profile versions of LaserTRAM and a spreadsheet of published concentrations for standard reference materials that can be found here under the file laicpms\_stds\_tidy.xlsx. Begin by uploading the output from LaserTRAM using the "Upload Data" button. This will populate the "Internal Std. Concentrations" table with a column for the spot name, concentration for the internal standard in wt% oxide, and a column for the relative uncertainty for the internal standard concentration. This concentration is analogous to  $C_n^u$  in Equation 3. By default it is 10 wt% regardless of the internal standard chosen, however it can be updated later to reflect more accurate concentrations.

LaserCalc will also search the spot names and determine potential calibration standards based on spot name. In order for this to work spot names in your experiment for standard reference materials **must** match those found within the laicpms\_stds\_tidy spreadsheet at least somewhere in the spot name (e.g., BHVO-2G\_1, BCR-2G\_23, ATHO-G\_replicate). There may be extra characters but at a minimum they must contain the proper standard name. Based on the results of this search, the "Calibration Standard" dropdown will populate with options for potential calibrations standards. Data pertaining to these analyses correspond to the  $N_i^{std}$  term in Equation 5.

Once a calibration standard is chosen, hit "Calculate!". LaserCalc will apply Equation 5 or Equation 8 to the data on an analyte by analyte basis based on whether or not it needs to be drift corrected. This is relatively quick and upon completion the "Calculated Concentrations" tab will populate with calculated concentrations for all spots in the experiment (Figure 6). These, by default will be incorrect for all unknown analyses as they are using the default concentration for the internal standard. You may now adjust the values in the "Internal Std. Concentrations" table to reflect the actual concentration and uncertainty of the calibration standard for each spot. While doing this, you will notice that the "Calculated Concentrations" table will update in real time to reflect the choice made. You may also change the value for the calibration standard dropdown menu at this time and the concentrations will adjust to reflect that decision. This makes it relatively easy to calculate concentrations using a variety of calibration standards if they exist in enough abundance within your experiment. When complete, export the "Calculated Concentrations" table to the desired directory. It is recommended the calibration standard is somewhere in the file name so as to help keep track of decisions made in the data processing pipeline.

	LaserTRAM spot		LaserTRAM	A profiler									LaserCalc			
										Primary Star	dard data					
aserCalc				Calculating	concentratio	ns for LA-ICF	-MS spot	data								
Upload Data Calbra BCR-2 Upload Stds	ion Standard: G	Dvitt significance threshold: K =	Talculate!													
ternal Std. Concentrations:				Calculated	Concentratio	ns:										
Spot	CaO wth	CaO 1stdevb		Export												
BCR-2G_1	10	1 ^		Spot	Ca0 wt% Ca0 1s	tdev 71.	L 2416g	27A1	2991	43Ca	4071	57Fe	0021	130Ba	13914	140Ce
BCR-20_2	10	1		NQ1_1	10	1 18,10907	58.18290.	215109.9.	459152.4.	71469.50_	349.7500	2062.915.	600.6298	352.7469	14.50718	19.06096
ATRO-G_1	10	3		NQ1_2	10	1 16,80343	57.93984	237916.7.	531804.5-	71469.58-	348.2313	2152.000	729.5783	298.0370	12,53372	16.05919
ATHO-G_2	10	1		Mg2_1	10	1 21,63722	73.44634-	172789.9-	341036.3-	71469.58-	356,6212-	1696.748-	844.6120	477.2083	28,71922	45.52298
BHVO-2G_1	10	1		MQ2_2	10	1 25.61659-	73.26569-	158184.2-	287556.4-	71469.58-	383.7266-	1781.801-	757.3847	381.1427	16,92835	21.27162-
BHV0-20_2	10	1		NQ2_3	10	1 31,21556	71.69828	175238.3.	344890.0_	71469.50_	363.2828.	1764.076	036.6915	403.0769	20.64517	25.44392
NIST-612_1	10	1		NQ3_1	10	1 32,37537										
NIST-612_2	10	1		MQ3_2	10	1 25,25890-	69.04056-	204643.8-	433292.5-	71469.58-	349,2398-	1998.312-	858.5848	457.8506	12,98090	16,67216
BCR-2G_3	10	1		MQ3_3	10	1 14.15063	63.33684	202955.6-	425669.8-	71469.50-	349.7748-	1973.927	751.0317	433.9280	14.41089	18.40770
ATH0-0_3	10	1		NQ4_1	10	1 26,60242										
BCR-26_4	10	1		MQ4_2	10	1 26,98704										
ATHO-G_4	10	1		MQ5_1	10	1 34,03339										
				M15.2		1 19 10213	67 90978	196821-8	407941 7	71469 84	354 9595	1951 271	829 2177	521 0244	18 91517	18 91100

Figure 6: Example of the LaserCalc Concentrations tab where concentrations can be calculated using the output from LaserTRAM and published values for standard reference materials.

### LaserCalc: Primary Standard Tab

This tab is solely devoted to inspecting data pertaining to the chosen calibration standard throughout the course of the experiment as calibration standard data quality greatly influences the calculated concentrations quality. It is designed to help one maximize the quality in their data by having insight into the temporal evolution of the normalized values of each analyte. Both the graph and the table will populate after data are uploaded and a calibration standard is chosen from the dropdown menu in the LaserCalc "Concentrations" tab. It is comprised of two parts (Figure 7): a graph showing the normalized ratio for a given analyte over time on the top and a table with information pertaining to each calibration standard analysis on the bottom. To view different analytes in the graph, use the dropdown at the very top of the screen.

Annotated on the graph are the relative standard error of the mean for a given analyte (i.e., Equation 10), the relative RMSE of the regression for that analyte over time, other descriptive statistics used in checking for drift (i.e., the p-value for the slope of the regression, the F-statistic, and critical F-value), and whether or not it has been drift corrected. If a given analyte has been drift corrected, the linear relationship describing the drift correction will be displayed on the chart. Lines for the regression and mean of the values are also displayed. Remember, drift correction only happens when **both** the p-value and F statistic are significant. To adjust the significance threshold of the p-value you may adjust the value in the input area of the "Concentrations" tab that says "Drift significance threshold". If this change in value changes whether or not an analyte is drift corrected, the "Calculated Concentrations" table will update in real time to reflect those changes. For example, if the p-value for a certain analyte is at 0.03, by default it will not be drift corrected by the software as the default threshold is 0.01. Based on the data in the "Primary Standard" tab, you may wish to force this drift correction to happen based on outlier measurements. Adjusting the threshold value to 0.04 will accomplish this. We advise adjusting this value with caution and keeping track of this decision along with the other metadata in the data reduction pipeline (e.g., internal standard, calibration standard, etc.).

The table below the graph essentially extracts the information from the input into the "Concentrations" tab for all the chosen calibration standards. It then also adds on a bottom row that shows the mean values for all analytes. Similar to all tables, this can also be exported and saved as an Excel spreadsheet to help keep track of decisions made in the data processing pipeline. The data in this table will allow you re-create the observed regression and its various statistics should you desire to do so (i.e., making publication quality figures).

		LaserTRAM spot				LaserTRAM profiler			
			Concentrations data						
Choose	an analyte to in	spect!							
885r			× <b>*</b>						
									0 .+ 00 D DX-
	Normalized ra	tios for BCR-2G over time							
	. Err. of mean %: 0.478	Regression stats: RMSE % : 0.489	Feat: 173.446		Drift Corrected: True y = 0.0x + -49971.93				regre
9.8		D: 0.000000E+00	Fent: 3.698		y = 0.0x + -499/1.93				ingre-
9.7	Mean							•	
9.6					• • • • • • • • • • • • • • • • • • • •				
9.5 9.4									
8 9.4									
			•						
9.3	<b>*</b> ****								
9.3		-							
	•		50		100	10	200	240	
	0	-	50		100	150	200	250	
9.2	0		50			150 Time in experiment (min)	200	250	
9.2	0			000 0000 000 °71		Time in experiment (min)	200	250	
9.2	0 Spot timestamp	index.bkgd_start bkgd_stop int_start	int_stop ne	orm sorm_cps 72.1	2400y 27Al 2951	Time in experiment (min)	200	250	
9.2 - Standard BCR-26	BCB-2G_1 2021-03	index.bkgd_start bkgd_stop int_start 1 3.01548 11.13704 21.05863	int_stop ne 41.05272 4:	3Ca 1467013 0.049750_ 87.5	<b>26mg 27A1 2951</b> 57106_ 346.1430_ 26.90601_	Time in experiment (min) 430a 4871 1112.4844.^	200	250	
9.2 - Standard BCR-26 BCR-20	BCR-2G_1 2021-03 BCR-20_2 2021-03	index blog_start blog_stop int_start i 3.01540 11.13704 21.0560 2 3.01974 11.13741 21.05693	int_stop n 41.05272 42 41.05252 42	3Ca 1467013 0.049750 87.5 3Ca 1364077 0.050314 88.5	24mg         27AL         2951           557106         346.1430         26.590601           23107         351.3262         26.97051	Time in experiment (min)	200	250	
9.2 Skport Standard BCR-25 BCR-20 BCR-20 BCR-20	BCR-20_1 2021-03 BCR-20_2 2021-03 BCR-20_3 2021-03	index.bkgd_start bkgd_stop int_start 1 3.01548 11.13704 21.05863	int_stop m 41.05272 4 41.05252 4 41.05252 4	30a 1467013 0.049750 87.5 30a 1364077 0.050314 88.5 30a 133640 0.049903 07.0	26mg         27AL         2951           57106346.14.3026.50601         26.50601           .23107351.326226.97051         343.606427.37654	Time in experiment (min)	200	259	
9.2 Standard BCR-26 BCR-20 BCR-20 BCR-26	BCR-2G_1 2021-03 BCR-20_2 2021-03 BCR-20_3 2021-03 BCR-2G_4 2021-03	index Dagi start blagi stop int start 1 3.01940 11.13704 21.05863 2 3.01959 13.13741 21.05893 9 3.01959 13.13745 21.05955	int_stop m 41.05272 42 41.05252 42 41.05252 42 41.05267 42 41.05162 42	3Ca 1467013         0.049750         87.9           3Ca 1364077         0.050314         88.2           3Ca 1364077         0.049903         87.9           3Ca 1342742         0.050711         87.9	2600         27AL         2951           57105         346.1435         26.90601           23107         351.3262         26.97051           0313         351.0264         27.37544           30504         339.7267         26.41470	Time in experiment (min) 430a 4971 1112.4444. 1113.2564. 1114.4994.	200	230	
9.2- Standard BCR-26 BCR-20 BCR-20 BCR-26 BCR-26	BCR-20_1 2021-03+ BCR-20_2 2021-03+ BCR-20_3 2021-03+ BCR-20_4 2021-03+ BCR-20_5 2021-03+	<b>Index XXed_start XXed_stop Int_start</b> 1 3.0146 11.13704 21.05851 2 3.01574 11.13714 21.05855 9 3.01599 11.13745 21.05955 11 3.01555 11.13712 21.05875 20.05595 11.13712 21.05959	int_stop In 41.05272 4: 41.05252 4: 41.05252 4: 41.05267 4: 41.05162 4: 41.0535 4:	Sca 1467013 0.049750 07.9 Sca 1364077 0.050314 08.0 Sca 1333640 0.049903 07.0 Sca 1342742 0.050771 07.3 Sca 1298515 0.050875 06.0	26%         274         2951           5710         46.1450         26.99601           23107         351.3262         26.97051           30316         332.6064         27.37554           30506         339.6058         26.41470           27551         339.6058         26.68060	Time in experiment (min)           452a         4871           1         1124984^           1         1132986           1         1144954           1         1114954           1         1114954	200	259	
9.2- Standard BCR-26 BCR-20 BCR-20 BCR-20 BCR-20 BCR-20 BCR-20	BCR-2G_1         2021-03         BCR-2G_2         2021-03         BCR-2G_3         BCR-2G_3	ID58x3Mpd_start Mod_stop ID4_start 1 3.01548 11.13764 21.05660 2 3.01974 11.13784 21.05660 3 3.01959 11.13782 21.05957 11 3.01959 11.13772 21.05957 13 3.01952 11.13772 21.05957 15 3.01942 11.13742 21.05959	int_stop n 41.05272 42 41.05252 43 41.05257 44 41.05162 44 41.05162 44 41.0535 44 41.05211 45	Sca 1467013 0.049750 07.6 Sca 1364077 0.050314 08.6 Sca 1333640 0.049903 07.0 Sca 1342742 0.050771 07.3 Sca 1290515 0.050875 06.7 Sca 1318449 0.050030 06.7	26mg         27AL         299L           3210-         364.0450-         26.90601-           33110-         391.3262-         26.97061-           3013-         39.7262-         26.41470-           3955-         39.7262-         26.41470-           73465-         26.9262-         26.4247-	Time in experiment (min)	200	250	
9.2- Standard BCR-26 BCR-20 BCR-20 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26	BCR-2G_1         2021-03           BCR-20_2         2021-03           BCR-20_3         2021-03           BCR-2G_4         2021-03           BCR-2G_5         2021-03           BCR-2G_6         2021-03           BCR-2G_7         2021-03	<b>Index XXed_start XXed_stop Int_start</b> 1 3.0146 11.13704 21.05851 2 3.01574 11.13714 21.05855 9 3.01599 11.13745 21.05955 11 3.01555 11.13712 21.05875 20.05595 11.13712 21.05959	int_stop m 41.05272 42 41.05282 44 41.05287 44 41.05182 44 41.05182 44 41.05185 44 41.05211 44	Sca 1467013 0.049750 07.9 Sca 1364077 0.050314 08.0 Sca 1333640 0.049903 07.0 Sca 1342742 0.050771 07.3 Sca 1298515 0.050875 06.0	26mj         27AL         295L           57106         366.1430         26.9605           301.3262         26.9905           301.3262         26.9051           301.3262         26.41470           359.6383         39.4287           2755L         39.4658         26.41470           39.4383         26.42800           73463         39.4385         26.42801	Time in experiment (min)           452a         4871           1         1124984^           1         1132986           1         1144954           1         1114954           1         1114954	200	259	
9.2- 5tandard BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26	BCR-2G_1 2021-03 BCR-20_2 2021-03 BCR-20_3 2021-03 BCR-2G_2 2021-03 BCR-2G_6 2021-03 BCR-2G_6 2021-03 BCR-2G_6 2021-03 BCR-2G_6 2021-03	1000x100g_start 100d_stop int_start 1 5.01540 11.13794 21.05601 2 5.01994 11.03794 21.05691 9 5.01999 11.13794 21.05693 11 5.0195 11.13712 21.05693 15 5.01962 11.13712 21.05693 15 3.0197 11.13674 21.05693	int_stop in 41.05272 44 41.05272 44 41.05272 44 41.05282 44 41.05385 44 41.05385 44 41.05211 44 41.05211 44	Sca 1467013.         0.049750.         07.3           Sca 1364077         0.050314         08.4           Sca 1333640         0.049950         07.4           Sca 1323742         0.050711         07.3           Sca 129515         0.050715         07.3           Sca 1318449         0.050715         07.3           Sca 129515         0.050670         08.7           Sca 1218449         0.050071         07.3           Sca 1218449         0.050071         07.3           Sca 1218449         0.050071         07.3           Sca 1218449         0.050071         07.3           Sca 1270033         0.050172         05.3	26bg         27AL         295L           57104         346.1430.         26.9905L           31307         393.3262.         26.9905L           31314         34.0464.2         37.9764L           3359.227.         26.41470.         27.9754.3           359.39.258.3         39.7267.2         24.1470.           77469.3         39.7267.2         24.1470.           27321.339.458.3         24.9905.3         24.9905.3           337.9272.337.326.335.2         24.14854.3         24.3245.3	Time in experiment (min)	200	250	
9.2 5tandard BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26	BCR-25_1 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03	LORX/MUT_flatt         Modflag         Dist_station           1         -0.1540         21.13744         21.0560           2         -0.0574         11.13744         21.0560           3         -0.0593         11.33741         21.0596           3         -0.0593         11.33741         21.0593           10         -0.0515         11.33742         21.0593           15         -0.0193         11.33742         21.0593           16         -0.0193         11.34842         21.0582           19         -0.0193         11.34842         21.0582           19         -0.0193         11.13442         21.0582	int_stop n 41.05272 44 41.05272 44 41.05282 44 41.05282 44 41.05283 44 41.05283 44 41.05281 44 41.05281 44 41.05212 44	Sca. 1447013         0.494750         87.3           Sca. 13364077         0.496934         88.4           Sca. 1336440         0.496903         87.4           Sca. 1336449         0.496903         87.4           Sca. 1336449         0.496903         87.4           Sca. 1296515         0.656971         87.4           Sca. 1298515         0.4969030         86.7           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298545         0.491721         87.4           Sca. 1299455         0.491721         84.7	2600         27AL         25921           57104         346,1450.         26,40601.           20109         501,326.         26,9205.           5014         343,4064.         27,9764.           3506         359,4263.         26,4000.           27531         339,4683.         26,4000.           27543.         39,4683.         26,4000.           27533.         33,4664.         24,923.           20343.         23,523.         24,2683.           20323.         35,2653.         26,4835.           20323.         35,2654.         26,4835.	Time in experiment (min) <b>USE 4994</b> , ** 1122494, ** 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314395, 11314355, 11314555, 11314555, 113145	200	230	
9.2 5tandard BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-26 BCR-20 BCR-26 BCR-20 BCR-26	BCR-20_1 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03	Lobelbagi Start Magi Joop Int_start 1 Julies ULL178 (2009) 2 Julies ULL178 (2009) 3 Julies ULL178 (2009)	int_stop         m           int_05272         41           41.05272         42           41.05274         42           41.05162         42           41.05162         42           41.0517         42           41.0511         42           41.0512         41           41.0512         42           41.0512         42           41.05212         43           41.05213         42	Sci 1447013.         0.49750.         87.5           Sci 154407         0.409750.         87.5           Sci 1544742.         0.60971.         87.5           Sci 1344742.         0.60971.         87.5           Sci 1344742.         0.60077         87.5           Sci 1344742.         0.60077         87.5           Sci 1245745         0.60075         86.5           Sci 1234474         0.60075         86.5           Sci 123459         0.60075         86.5           Sci 123459         0.60075         86.5           Sci 123459         0.60075         86.7           Sci 123459         0.60075         86.7           Sci 123459         0.60175         86.7           Sci 123450         0.60175         84.7	2000         27AL         2596L           37106.         16.4.1450.         26.5906L           3107.         35.1.362.         26.49705L           3107.         35.9.7262.         26.41705L           3107.         35.9.7267.         26.41805L           3107.         35.9.462.         26.42805L           3107.         35.9.662.         26.42805L           3108.         37.9.726.         26.42815L           3004.         37.0.727.         26.42815L           3014.         37.0.527.         26.42815L           3014.         37.0.527.         26.42815L           3014.         37.0.527.         26.42815L           3014.         37.0.527.         25.42815L           3014.         37.0.527.         25.44815L           3014.         37.0.525.         25.448012	Time in experiment (min) <b>UP</b> 1112-044. A 1112-045. A 112-045. A	200	239	
9.2 Standard BCR-26	BCR-25_1 2021-03 BCR-20_2 2021-03 BCR-20_2 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03 BCR-25_6 2021-03	LORX/MUT_flatt         Mod_sfor         Dist_set           1         -0.1540         21.13744         21.0560           2         -0.0574         11.13744         21.0560           3         -0.0593         11.33741         21.0560           3         -0.0593         11.33741         21.0580           10         -0.0515         11.33742         21.0580           10         -0.0511.13722         21.0580         11.3344         21.0580           10         -0.0511.13722         21.06803         11.3344         21.05803           10         -0.0511.13722         11.05802         21.05803         21.05803           10         -0.0511         11.03442         21.05803         21.05803	int_stop PM 41:05272 44 41:05252 44 41:05252 44 41:05252 44 41:05253 44 41:05253 44 41:05231 44 41:05211 44 41:05211 44 41:05211 44 41:0523 44 41:0523 44	Sca. 1447013         0.494750         87.3           Sca. 13364077         0.496934         88.4           Sca. 1336440         0.496903         87.4           Sca. 1336449         0.496903         87.4           Sca. 1336449         0.496903         87.4           Sca. 1296515         0.656971         87.4           Sca. 1298515         0.4969030         86.7           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298515         0.4910930         87.4           Sca. 1298545         0.491721         87.4           Sca. 1299455         0.491721         84.7	2 (39)         27(A)         2 (39)           57146.         36 (4.13%).         26.1905).           511.0         26.1905).         26.1905).           511.0         26.1905).         27.1764.           511.0         31.9.4931.         26.1905).           519.2         27.4176.         27.1905.           201.2         24.1905.         26.1910.           201.3         37.5713.         26.4085.           201.3         37.5713.         26.4085.           201.3         37.5713.         26.4085.           201.3         37.5713.         26.4085.           201.3         37.643.         26.4085.           201.3         37.643.541.         36.4085.           201.3         37.643.541.         36.4085.           201.3         37.643.541.         37.6439.5           201.3         37.645.7.541.         27.4095.541.           201.3         37.645.7.54.991.         27.4095.541.	Time in experiment (min)	200	230	

Figure 7: Example of the LaserCalc Primary Standard tab that shows data for the chosen calibration standard both graphically and in a table.

# Video Demos

Video tutorials on how to use each piece of software can be found at the following links:

- LaserTRAM video
- LaserCalc video

# Citing

If you use this software for your research, first off, we hope that it helps bring clarity and efficiency to your LA-ICP-MS data processing life. If there are features you would like to see that are not *totally* unreasonable, please do not hesitate to reach out!

Secondly, we would appreciate that you cite our work accordingly:

- In text: Lubbers et al. (2021)
- bibtex:

```
@misc{lubbers2021lasertram,
author = {
    Jordan Lubbers and
    Adam Kent and
    Russo Chris
    },
title = {LaserTRAM-DB},
month = {10},
year = {2021},
doi = {10.5281/zenodo.5620857},
url = {https://github.com/jlubbersgeo/laserTRAM-DB}
}
```

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