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Last updated: January 20, 2022

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 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. 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.

Governing Equations

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

$$C_i^u = \frac{R_i^u}{S} \quad (1)$$

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 occurring internal standards, S can be defined as:

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

R_i^{std} and C_i^{std} are the count rate 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:

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

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:

$$N_i = \text{median} \left[\frac{cps_i}{cps_{is}} \right] \quad (4)$$

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:

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

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:

$$SE = \frac{\sigma_{N_i}}{\sqrt{n}} \quad (6)$$

σ_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:

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

Detection Limits

Detection limits for each analyte are determined to [Longerich et al. \(1996\)](#):

$$LOD = \frac{3\sigma_b}{\sqrt{n_b}} \sqrt{2}$$

where σ_b and n_b are the standard deviation and total number of observations in the chosen background range, respectively. 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 1):

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-statistic 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

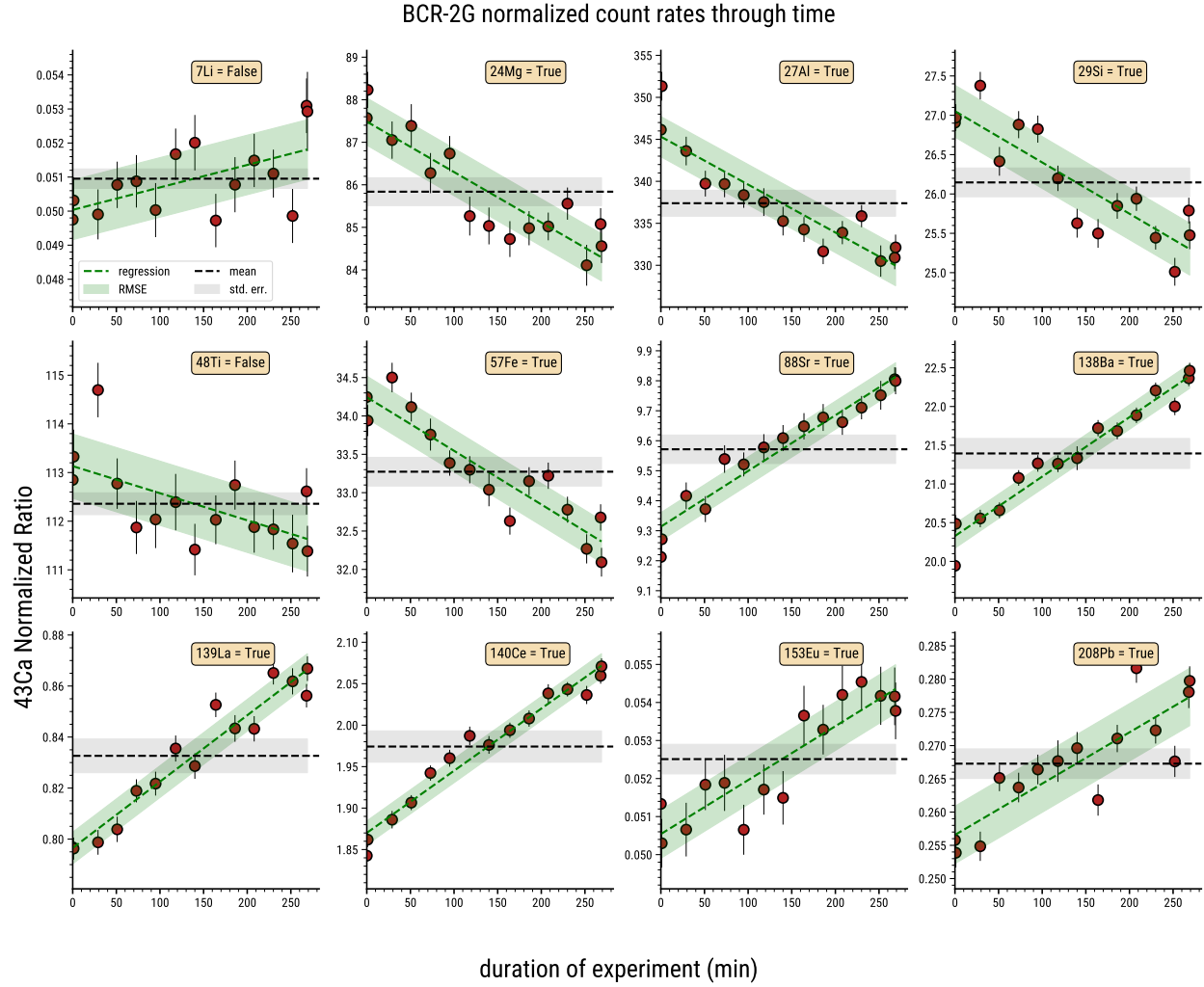


Figure 1: Drift correction test from LaserCalc for a given experiment in which standard reference material BCR-2G was used as the primary standard. We can see here that one experiment may contain analytes that are both drift corrected and not drift corrected.

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:

$$C_i^u = C_n^u \left[\frac{C_i^{std}}{C_n^{std}} \right] \frac{1}{[m_i x + b_i]} N_i^u \quad (8)$$

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 \(1997\)](#) p.61:

$$\sigma_{C_i} = C_i^u \sqrt{\left(\frac{\sigma_{C_u^n}}{C_u^n} \right)^2 + \left(\frac{\sigma_{C_i^{std}}}{C_i^{std}} \right)^2 + \left(\frac{\sigma_{C_n^{std}}}{C_n^{std}} \right)^2 + \left(RSE_i^{std} \right)^2 + \left(RSE_i^u \right)^2} \quad (9)$$

Where RSE_i^{std} is defined as:

$$RSE_i^{std} = \left[\frac{\frac{\sigma_i}{\sqrt{n_i}}}{\mu_i} \right] 100 \quad (10)$$

σ_i and μ_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:

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

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

The easiest way to use LaserTRAM-DB is to use the following link:

- <https://lasertram-db.herokuapp.com/>

Alternatively, LaserTRAM-DB can be installed locally and run by creating a virtual environment. If you are new to python, we recommend doing this through [Anaconda](#).

```
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. For optimal performance, we recommend using the virtual environment option for LaserTRAM-DB. Currently, LaserTRAM-DB is hosted through Heroku with limited computing power. Using through a local machine capitalizes on the computing power of that local device, which in almost all instances will be superior to Heroku. Another thing you will probably notice is that there are both the `requirements.txt` and `local_requirements.txt` file. They are nearly identical with the exception of the `requirements.txt` file containing the package `gunicorn`. This is used in the deployment of the web-app to Heroku and not needed for use on local machines.

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 2). 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 3).

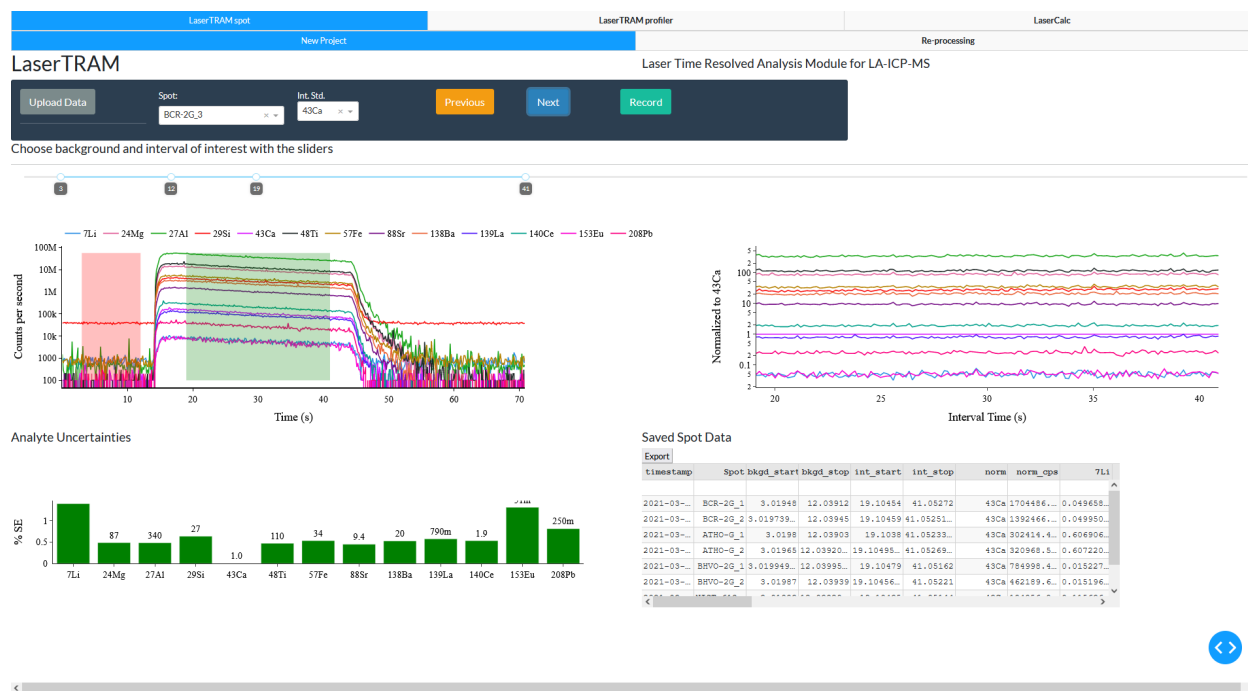


Figure 2: Example of the LaserTRAM New Project tab after data has been loaded in.

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. 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: SiO₂ (e.g., ²⁹Si), CaO (e.g., ⁴³Ca), TiO₂ (e.g., ⁴⁷Ti), Al₂O₃, Cr₂O₃, MnO, FeO, K₂O, Na₂O, 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 ^{29}Si and ^{43}Ca are good options as SiO_2 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.

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.
- **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.
- **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.
- **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.

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 3. 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!”.

LaserTRAM spot

New Project

LaserTRAM profiler

Re-processing

LaserCalc

LaserTRAM Re-processing

Re-process an old experiment using a new internal standard

Upload old LT file

Internal Standard: 29Si

Re-process!

Old normalized ratios

Re-normalized data

Export

timestamp	Spot	bkgrd_start	bkgrd_stop	int_start	int_stop	norm	norm_ops	7Li	24Mg	27Al	29
2021-03-...	BCR-26_1	3.01948	11.13704	21.05863	41.05272	43Ca	1467013...	0.049750...	87.57106	346.1430	26.90
2021-03-...	BCR-26_2	3.019739...	11.13741	21.05893	41.05251...	43Ca	1364077...	0.050314...	88.23107	351.3262	26.97
2021-03-...	ATMO-5_1	3.0198	11.13702	21.05797	41.05233...	43Ca	270495.3...	0.067011...	9.797868	1345.794	157.2
2021-03-...	ATMO-5_2	3.01965	11.13727...	21.0594	41.05269...	43Ca	279183.3...	0.067884...	9.747460	1337.271	155.6
2021-03-...	BRVO-26_1	3.019949...	11.13804	21.05902	41.05162...	43Ca	524353.4...	0.014921...	112.4873	217.4247	15.98
2021-03-...	BRVO-26_2	3.01987	11.1375	21.05875	41.05221...	43Ca	406813.9...	0.014699...	112.4457	222.8925	16.24
2021-03-...	NIST-612	3.01983	11.13722	21.05876	41.05144...	43Ca	192470.4...	0.115396...	0.150267	29.89531	19.79
2021-03-...	NIST-612	3.01969	11.13726	21.05904	41.05224...	43Ca	193181.3...	0.116219...	0.147278	29.93367	19.69
2021-03-...	BCR-26_3	3.01959	11.13764	21.05954	41.05247...	43Ca	1333640...	0.049903...	87.05114	343.4064	27.37
2021-03-...	ATMO-5_3	3.01999	11.13778	21.05894	41.052	43Ca	280537.6...	0.060259...	9.809315	1334.206	152.4
2021-03-...	BCR-26_4	3.01955	11.13711	21.05877	41.05162...	43Ca	1342742...	0.050771...	87.38508	339.7267	26.41
2021-03-...	ATMO-5_4	3.01916	11.13707	21.05851	41.05153...	43Ca	177333.6...	0.074540...	8.86750	1016.506	151.7

Export

timestamp	Spot	bkgrd_start	bkgrd_stop	int_start	int_stop	norm	norm_ops	7Li	24Mg	27Al	29
2021-03-...	BCR-26_1	3.01948	11.13704	21.05863	41.05272	29Si	2763520...	-9999	3.235005	12.73500	...
2021-03-...	BCR-26_2	3.01974	11.13741	21.05893	41.05252	29Si	2815041...	-9999	3.249927	12.95827	...
2021-03-...	ATMO-5_1	3.0198	11.13702	21.05797	41.05234	29Si	2776411...	-9999	0.047931	8.556533	...
2021-03-...	ATMO-5_2	3.01965	11.13727...	21.0594	41.05269	29Si	2813938...	-9999	0.047956	8.545669	...
2021-03-...	BRVO-26_1	3.01995	11.13804	21.05902	41.05162	29Si	2021653...	-9999	6.795661	13.63969	...
2021-03-...	BRVO-26_2	3.01987	11.1375	21.05875	41.05221	29Si	2009545...	-9999	6.891732	13.66376	...
2021-03-...	NIST-612	3.01983	11.13723	21.05876	41.05144	29Si	3309406...	-9999	-9999	1.501574	...
2021-03-...	NIST-612	3.01969	11.13726	21.05904	41.05224	29Si	3357225...	-9999	-9999	1.500641	...
2021-03-...	BCR-26_3	3.01959	11.13765	21.05955	41.05247	29Si	2689861...	-9999	3.180339	12.48420	...
2021-03-...	ATMO-5_3	3.01999	11.13778	21.05894	41.052	29Si	2711187...	-9999	0.050033	8.686071	...
2021-03-...	BCR-26_4	3.01955	11.13711	21.05877	41.05162	29Si	2610237...	-9999	3.280345	12.62688	...
2021-03-...	ATMO-5_4	3.01916	11.13707	21.05851	41.05153	29Si	1781411...	-9999	0.05193	8.410508	...

Figure 3: 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 4):

- 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.

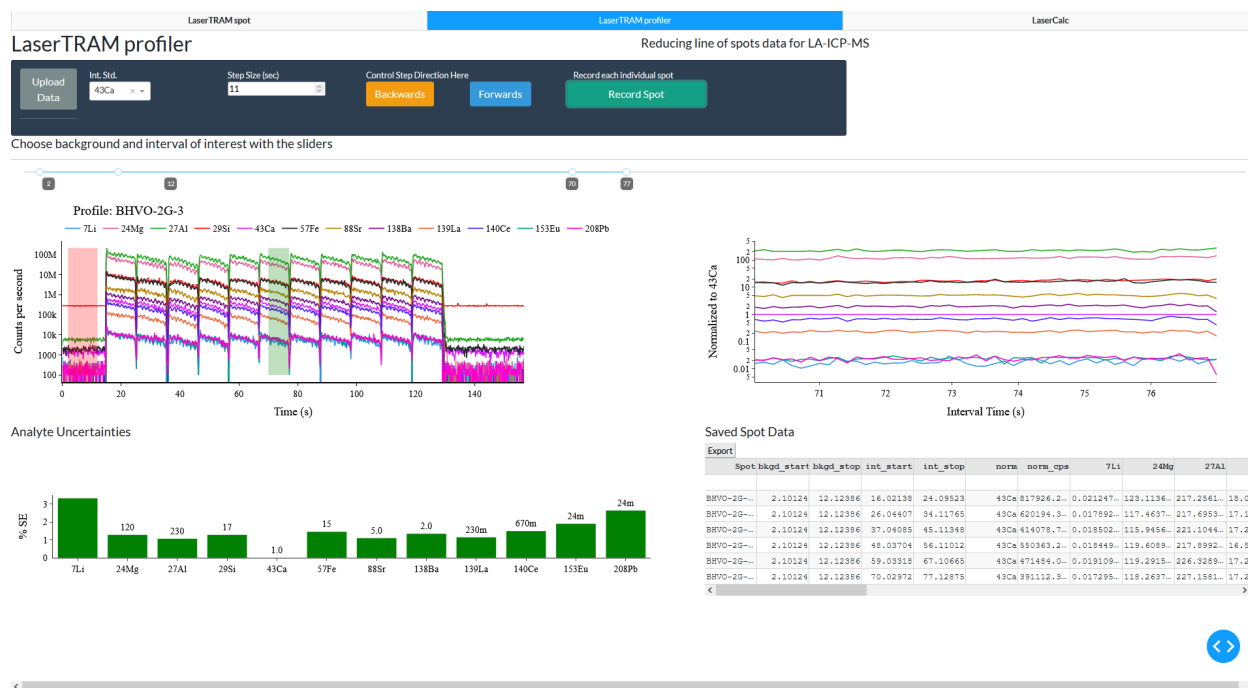


Figure 4: Example of the LaserTRAM profiler illustrating how the software can easily normalize a line of spots gathered in rapid succession to one another.

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 5). 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,

LAerTRAM spot

Concentrations data

Upload Data

Calibration Standard

ICR-20

Drift significance threshold

0.05

Calculate!

Upload Data

Internal Std. Concentrations:

Spot	Conc. wt%	Conc. Isotopes
ICR-20_1	10	1
ICR-20_2	10	1
ATRO-20_1	10	1
ATRO-20_2	10	1
BBVO-20_1	10	1
BBVO-20_2	10	1
WIST-20_1	10	1
WIST-20_2	10	1
ICR-20_3	10	1
ATRO-20_3	10	1
ICR-20_4	10	1
ATRO-20_4	10	1

LAerTRAM profile

Primary Standard data

Calculating concentrations for LA-ICP-MS spot data

Calculated Concentrations:

Spot	Conc. wt%	Conc. Isotopes	TLI	204p	27Al	28Al	43Ca	49Ti	57Fe	88Sr	138Ba	139La	140Ce
MDL_1	1	1	1.19.10951	58.18290	231079.9	431812.4	71649.58	149.7050	2042.615	488.4296	32.7469	14.50718	19.40696
MDL_2	1	1	1.16.81061	57.03984	37974.7	51304.3	71649.58	368.213	2181.080	719.5703	286.0390	12.53751	16.19519
MDL_3	1	1	1.21.43722	73.44434	137879.9	341036.3	71649.58	356.4212	1498.744	744.4125	477.2051	28.70255	45.22395
MDL_2	1	1	1.25.45619	73.26469	38184.2	287556.4	71649.58	383.7626	1781.851	757.3847	381.8421	16.51828	21.27142
MDL_3	1	1	1.31.21556	71.49328	17523.3	344839.6	71649.58	363.2828	1744.076	316.4515	43.87676	20.44317	25.44392
MDL_1	1	1	1.32.75972	47.45468	177487.7	757122.7	71649.58	354.8186	1740.795	338.2254	490.3276	12.44884	21.44884
MDL_2	1	1	1.23.25890	69.04454	246443.5	412392.3	71649.58	339.2638	1399.312	647.8506	12.90980	14.67212	21.3
MDL_3	1	1	1.24.15063	63.33684	202935.6	425669.8	71649.58	349.7748	1973.927	751.0217	43.82810	14.42688	14.40770
MDL_1	1	1	1.26.40242	102.1942	131110.7	331313.3	71649.58	364.1762	2042.685	780.3748	35.4372	13.41049	21.48846
MDL_2	1	1	1.26.88788	92.00993	140994.4	297841.7	71649.58	362.8629	1599.260	259.6465	293.4445	11.08306	26.18525
MDL_3	1	1	1.26.23335	70.17074	162618.6	446489.9	71649.58	357.3512	1944.398	889.2571	605.7946	12.78274	25.59704
MDL_1	1	1	1.28.12213	92.30734	136213.8	407941.3	71649.58	354.8608	1483.371	674.7197	401.0242	14.00309	18.56105

LaserCalc: Primary Standard Tab

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 it has been drift corrected the equation for 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 .03, by default it will not be drift corrected by the software. 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 .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.).

9

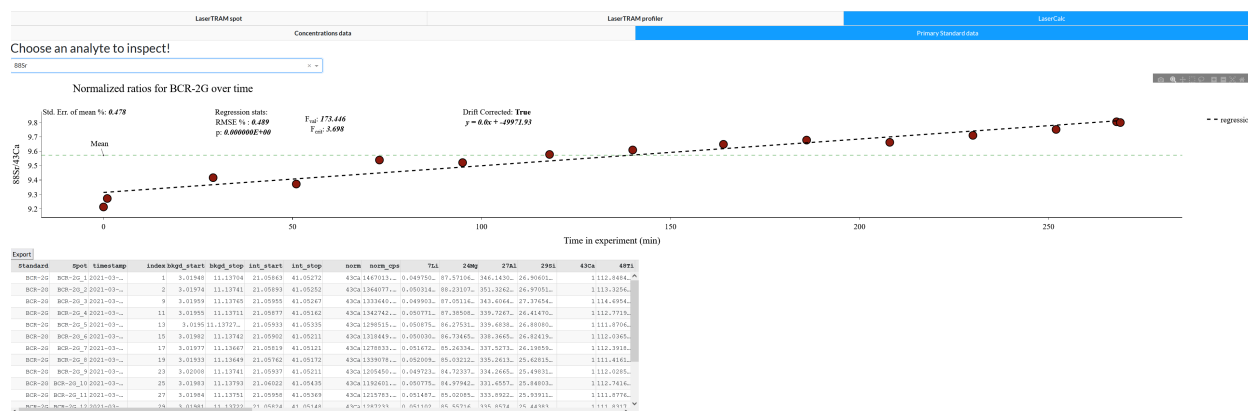


Figure 6: Example of the LaserCalc Primary Standard tab that shows data for the chosen calibration standard both graphically and in a table.

Video Demos

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

- [LaserTRAM video](#)
- [LaserTRAM profiler 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}
}
```

Acknowledgements

We express our gratitude to the W.M. Keck Foundation for helping foster the laboratory environment that led to the genesis of this software, the open-source coding community for developing the tools that made this all possible, and NSF project grants 1763639, 1948862, 1654275.

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