

ICPMSDataCal-Py

V1.0

User' Manual

MaoJi (maoji0819@163.com)

**(China University of Geoscience (Wuhan), Crust-Mantle
Interaction and Geodynamics Research Group)**

2024

◆ Please cite the following articles when using the software
to publish data:

**LA-ICP-MS data reduction of elemental content
calibration:**

Liu, Y., Gao, S., Hu, Z. et al., 2009. Continental and Oceanic Crust Recycling-induced Melt–Peridotite Interactions in the Trans-North China Orogen: U–Pb Dating, Hf Isotopes and Trace Elements in Zircons from Mantle Xenoliths[J]. Journal of Petrology, 51(1-2): 537-571.

Liu, Y., Hu, Z., Gao, S. et al., 2008. In situ analysis of major and trace elements of anhydrous minerals by LA-ICP-MS without applying an internal standard[J]. Chemical Geology, 257(1-2): 34-43.

LA-ICP-MS data reduction of zircon U-Pb dating:

Liu, Y., Gao, S., Hu, Z. et al., 2009. Continental and Oceanic Crust Recycling-induced Melt–Peridotite Interactions in the Trans-North China Orogen: U–Pb Dating, Hf Isotopes and Trace Elements in Zircons from Mantle Xenoliths[J]. Journal of Petrology, 51(1-2): 537-571

Catalogs

1 Introduction and Installation	1
1.1 Introduction	1
2 Software Usage Flow	3
2.1 File Import	3
2.1.1 Data import format	3
2.1.2 Analysis type	8
2.1.3 Isotope Ratio Editor	9
2.2 Sequence settings	14
2.3 analysis interface	23
2.3.1 Signal Interface.....	24
2.4 Calibration	35
2.4.1 Calibiration of elemental content	35
2.4.2 U-Pb dating.....	42
2.4.4 Common Pb Correction (Under development)	46
2.4.5 Isotope ratio calculation	46
2.4.5 Figures.....	49
2.4.6 Error propagation.....	51
2.5 Data export.....	53
2.5.1Table Export.....	53
2.5.2Mapping	56
2.5.3 line scan	64
2.6 Setting.....	69
caveat	72
bibliography :	80

1 Introduction and Installation

1.1 Introduction

ICPMSDataCal-Py is developed in Python and runs as a stand-alone package without installation. As the software is currently in the development stage, it only supports the commonly used methods for obtaining primary and trace content, zircon U-Th-Pb dating (including ordinary Pb calibration) and isotope custom calibration, and the developer will add more commonly used functions in the subsequent versions. Compared with other types of data processing software, the software has the following advantages:

- λ Matrix-based calculations greatly improve the speed of operation while supporting multiple batches of data for testing.
- λ For quantitative trace element calculations, the AYCF(Liu et al., 2008) and multiple external standard-single internal standard(Longerich et al., 1997) calculation methods were used to support internal standard-free calibration of the content for

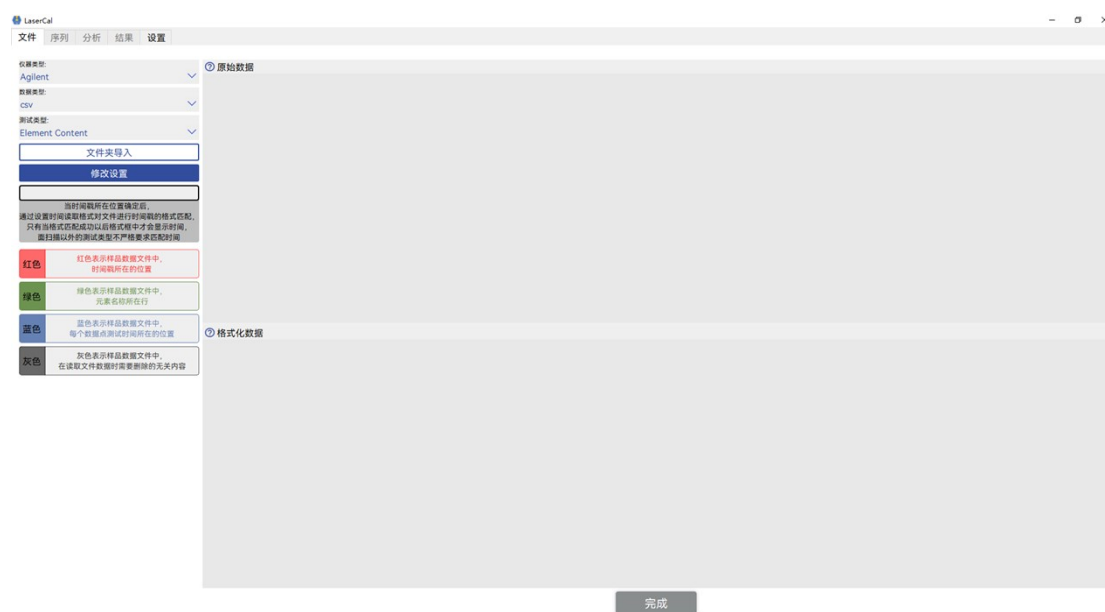
correction calculations for a wide range of mineral types (silicates, carbonates, etc.).

- λ Compatible with the data format of almost all types of instruments, and can be modified and saved according to the actual test situation.
- λ Added algorithms specifically for signal selection as well as outlier rejection and smoothing
- λ Add an isotope method editor for MC-ICP-MS isotope ratio determination, which can be customised to edit the calibration method.
- λ The Common Pb calibration module has been added to support the common ^{204}Pb , ^{207}Pb , ^{208}Pb and Andersen calibrations.
- λ This software does not require any installation steps, just unzip the software installation package and use it normally.

2 Software Usage Flow

2.1 File Import

2.1.1 Data import format



λ Firstly, you need to pre-match the instrument data suffix in the drop-down box according to the instrument type name.

λ To import folder data, please make sure that the imported file has the correct suffix, otherwise the data cannot be imported.。

In this interface is mainly for file import, usually for the data format recognition is automatic, when the automatic recognition fails, the user can custom modify the data format.

Formatted data should have the following flags if the imported data is recognised by the default instrument type selection:

- ✓ A sequence with time as the row name and element name as the column name should appear in the formatted data list.
- ✓ It is preferable not to have nan values in the data (nan means null value, in order not to affect the subsequent image drawing and calculation process, the existence of null values may cause the calculation process to be incorrect).。
- ✓ The correct time format should appear in the Timestamp text box, if no time is displayed it indicates that the timestamp in the file could not be read. This will not affect the test results under common test methods, but mapping may require a timestamp to match the test time.

If there are no problems with the time format, at this point the user just needs to click “sure” button to proceed to the next sequence setting.

The screenshot displays the main data processing window of ICPMSDataCal-Py V1.0. The interface includes a menu bar (文件, 序列, 分析, 结果, 帮助) and a toolbar with buttons for '预览数据导入' (Preview Data Import) and '修改设置' (Modify Settings). The main area shows a data table with columns for '时间 [s]' (Time [s]) and various element concentrations. Annotations with callouts identify key parts of the interface:

- timestamp**: Points to the '时间 [s]' column header.
- Time sequence**: Points to the numerical values in the '时间 [s]' column.
- Element name**: Points to the column headers for elements like Li7, Be9, B11, N423, Mg25, A27, Si29, P31, K39, Yb173, Lu175, Hf178, Ta181, W182, Hg202, Pb208, Bi209, Th232, U238.

When you need to modify the data format, you can click the ‘Setting’ button to modify the format.

The 'Setting' dialog box allows users to configure data processing parameters. It includes the following settings:

- ☐ 单文件模式 (Single File Mode)
- 元素名所在行: 4 (Element Name Row)
- 需要删除的行: 1-3 (Rows to Delete)
- 尾部不读的行数: 1 (Rows not read at the end)
- ☒ 时间戳所在位置: 3,1 (Timestamp Location)
- 时间所在列: 1 (Time Column)
- 需要删除的列: 0 (Columns to Delete)
- 尾部不读的列数: 0 (Columns not read at the end)
- 时间戳格式: %Y/%m/%d %H:%M:%S (Timestamp Format)

Note: If you need to modify the format manually, please read the following operation

settings carefully.

In the time reading format each parameter and its representative meaning are as follows:

One file mode: when the imported data files are located in a single file need to check the mode to re-recognition

Element Row Loc: The row where the element name is located in the original data list, identified by a green area in the original data list.

Time Column Loc: The column where the time is located in the original data list, identified by the purple area in the original data list.

Deleted Rows, Delete Columns: rows and columns in the header of the raw file where other data not related to the information needed for the test (time, signal, element name) are located and are identified by grey areas. (Enter 1 in the input box to indicate that the first row needs to be deleted, 1-3 to indicate that rows 1, 2, and 3 all need to be deleted, and 1-3, 7 to indicate that rows 1, 2, 3, and 7 will be deleted.)

Delete Tail Rows, Delete Tail Columns: indicates that the rows and columns to be deleted at the end of the file have the same setup rules as the rows and columns to be deleted and are identified by grey areas.

Timestamp Loc: indicates the location of the rows and columns where the timestamp of the original data file is located. The time setting can be cancelled in the tick box, in addition to surface scanning in addition

to the common test process, do not need to carry out laser stripping time to match the time of the ablation signal, identified by the red area.

Timestamp format:

**If the user needs to
get the time to
match the ablation**

```
%y Two-digit year representation (00-99)
%Y four-digit year representation (000-9999)
%m Month (01-12)
%d Day of the month (0-31)
%H 24-hour hours (0-23)
%I 12-hour hours (01-12)
%M minutes (00-59)
%S sec (00-59)
%a Local simplified week name (e.g. Monday, Mon)
```

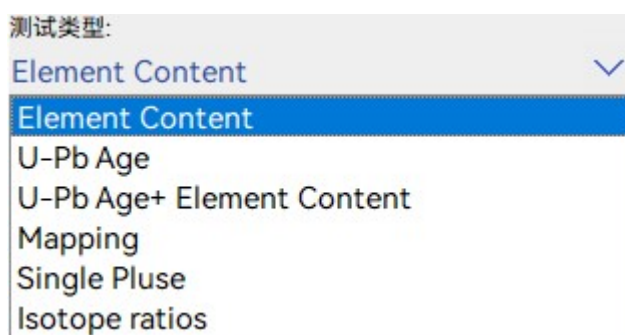
signal with the ablation time during the scanning process, the time of the original data signal acquisition needs to be read accurately. Time format is more complex, in the lower left corner of the interface of the text box on the timestamp format matching function of the parameters are explained, the user can find their own set of timestamp parameters.

For example, in the timestamp '2020-01-11 11:11:11', %Y means year 2020, %m means month 01, and the generic time format should be: %Y%m%d%H%M%S. However, since there are often ':-' and other connectors in the timestamp, the time format is not as simple as it should be. ' and other connectors, the final format plus the connectors after the '%Y-%m-%d %H:%M:%S', in the process the space can

not be omitted. When the format is successfully matched, the date format will be displayed in the text input box of the interface.

After setting the file format, click the OK button, if the format is set correctly, it will automatically jump to the sequence setting.

2.1.2 Analysis type



At present, the software supports Element Content, U-Th-Pb Age and Mapping, which are optimised for

different types of tests, so please choose according to your actual needs.

However, the software does not automatically select and calculate the calibration method for the mapping and single pulse ablation methods, and users need to manually select the method in the calibration interface.

2.1.3 Isotope Ratio Editor

To use the isotope method,

must

Measure Type:
Isotope ratios
Isotope Method:
Rb-Sr dating

▼ Edit

change the analysis type to ‘Isotope ratios’ after importing the data folder, and click the ‘Edit’ button in the calibration method to create and add a new method.

The data file must be imported in advance before proceeding with method editing.

Isotope Approach Editor

Approach: Rb-Sr

RAW Name:

1	2
r_0	83Kr
r_1	83.5
r_2	84Sr
r_3	85Rb
r_4	86Sr
r_5	86.5
r_6	87Sr
r_7	88Sr
r_8	89.868

Formula:

Formula Name	Data Name	Formula	Data Type
f_0	84Sr	$r_2 - r_0 * (57/11.49) - r_1 * (26.978/22.869)$	Normal
f_1	85Rb	$r_3 - r_1 * (14.91/22.869) - r_5 * (2.962/16.103)$	Normal
f_2	87Sr-Rb	$r_6 - r_5 * (33.26/16.103)$	Normal
f_3	86Sr	$r_4 - r_0 * (17.3/11.49) - r_5 * (21.68/16.103)$	Normal
f_4	88Sr	$r_7 - r_5 * (12.996/16.103)$	Normal
f_5	f_Sr	$\ln(8.37521 / ((f_4 / f_3) / \ln(87.90562/85.90927)))$	Normal
f_6	f_Rb	$\ln(0.38571 / ((f_2 - f_3 * 0.705003 / ((87/86) * f_5)) / f_1) / \ln(87/85))$	Normal
f_7	f_Rb/f_Sr	f_6 / f_5	Normal
f_8	87Sr	$(f_2 - f_1 * 0.38571 / ((87/85) * (f_6 * 1.085)))$	Normal
f_9	87Sr/86Sr	$f_8 * ((87/86) * f_5 / f_3)$	Ratio
f_10	84Sr/86Sr	$f_0 * ((84/86) * f_5 / f_3)$	Normal
f_11	Rb/Sr	$(f_1 / f_4) * 1.144$	Normal

Normal Data:

Name	Output
f_0	☒
f_1	☒
f_2	☒
f_3	☒
f_4	☒
f_5	☒
f_6	☒
f_7	☒
f_8	☒
f_10	☒
f_11	☒

Average Parameter:

Name	Reference
------	-----------

Age Parameter:

Name	Ratio Name
f_9	87Sr/86Sr

RAW Name: isotope name refers to the name of the isotope data read in the original data, which is easy

Data Name	Isotope name
r_0	83Kr
r_1	83.5
r_2	84Sr
r_3	85Rb
r_4	86Sr
r_5	86.5
r_6	87Sr
r_7	88Sr
r_8	89.868

to enter when editing the formula and prevents the isotope name from being a number that leads to an error in the formula calculation, so the left side of 'r_*' is used as a substitute.

Formula:

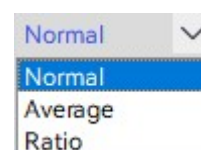
Formula Name	Data Name	Formula	Data Type	
f_0	84Sr	$r_2 - r_0 * (57/11.49) - r_1 * (26.978/22.869)$	Normal	▼
f_1	85Rb	$r_3 - r_1 * (14.91/22.869) - r_5 * (2.982/16.103)$	Normal	▼
f_2	87Sr-Rb	$r_6 - r_5 * (33.26/16.103)$	Normal	▼
f_3	86Sr	$r_4 - r_0 * (17.3/11.49) - r_5 * (21.68/16.103)$	Normal	▼
f_4	88Sr	$r_7 - r_5 * (12.996/16.103)$	Normal	▼
f_5	f_Sr	$\ln(8.37521 / (f_4 / f_3)) / \ln(87.90562/85.90927)$	Normal	▼
f_6	f_Rb	$\ln(0.38571 / ((f_2 - f_3 * 0.705003 / ((87/86)^{f_5}) / f_1)) / \ln(87/85))$	Normal	▼
f_7	f_Rb/f_Sr	f_6 / f_5	Normal	▼
f_8	87Sr	$(f_2 - f_1 * 0.38571 / ((87/85)^{(f_6 * 1.085)}))$	Normal	▼
f_9	87Sr/86Sr	$f_8 * ((87/86)^{f_5}) / f_3$	Ratio	▼
f_10	84Sr/86Sr	$f_0 * ((84/86)^{f_5}) / f_3$	Normal	▼
f_11	Rb/Sr	$(f_1 / f_4) * 1.144$	Normal	▼

λ **Formula name:** Use 'f_*' to refer to the result of each formula line according to the number of lines..

λ **Data Name:** Names used for graphical display of data and export of results.

λ **Formula :** Customised formula editing window. Calculation formulas that can be entered include: Add: '+', Subtract: '-', Multiply: '*', Divide: '/', Exponent: '^', logarithm: "ln"..

λ **DataType:** Each line of the formula is labelled with its data type, which is divided into three categories: 'Normal', 'Average' and 'Ratio'.



“Normal” : Intermediate values generated during the calculation, such as Rb deduction for Sr87, are usually calculated for each cycle, and no averaging operation is performed on the results of the formula for that line.

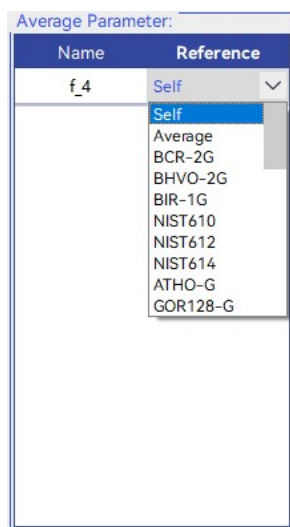
“Average” : The results of the formulae in this row are averaged, either for each sample itself (one column of values), for all samples (one value), or for one of the standard samples of the test procedure (one value). If it is necessary to calculate the isotope fractionation factor using a particular standard and applying it to all samples, this parameter can be set to ‘Average’.

“Ratio” : Ratio calculation of the line formula, the line formula marked as a ratio, the software will automatically identify all the formula ‘/’ and identify the numerator and denominator, so it is recommended to mark the ratio calculation of the formula, in order to prevent the identification of errors, pay attention to the formula in the form of the best for ‘a/b ‘ or ‘(a/c)/(b/d)’.

Normal Data: For each Normal Data, the user can choose whether to export the results or not,

Normal Data:	
Name	Output
f_0	☒
f_1	☒
f_2	☒
f_3	☒
f_4	☒
f_5	☒
f_6	☒
f_7	☒
f_8	☒
f_10	☒
f_11	☒

if exported, the average and error of the Normal Data of all the samples will be calculated and displayed in the graphical interface.



Name	Reference
f_4	Self

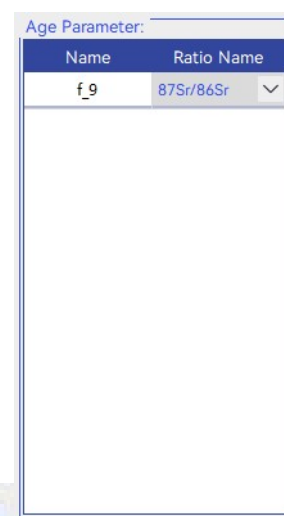
- Self
- Average
- BCR-2G
- BHVO-2G
- BIR-1G
- NIST610
- NIST612
- NIST614
- ATHO-G
- GOR128-G

Average Parameter: Determines the method of calculating the average, with the selection of 'self' meaning that the average of the results of the formula is calculated for each sample individually.

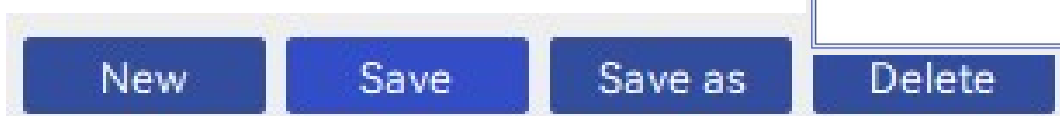
When 'Average' is selected, only one numerical result is produced, and the average result of the

formula is calculated for all samples. When a standard is selected, the average is calculated for the selected specimen and time-drift interpolation is performed on it.

Age Parameter: Calibration of the ratio result for the parameter labelled 'Ratios', select the appropriate ratio name in 'Ratio Name'.



Name	Ratio Name
f_9	87Sr/86Sr

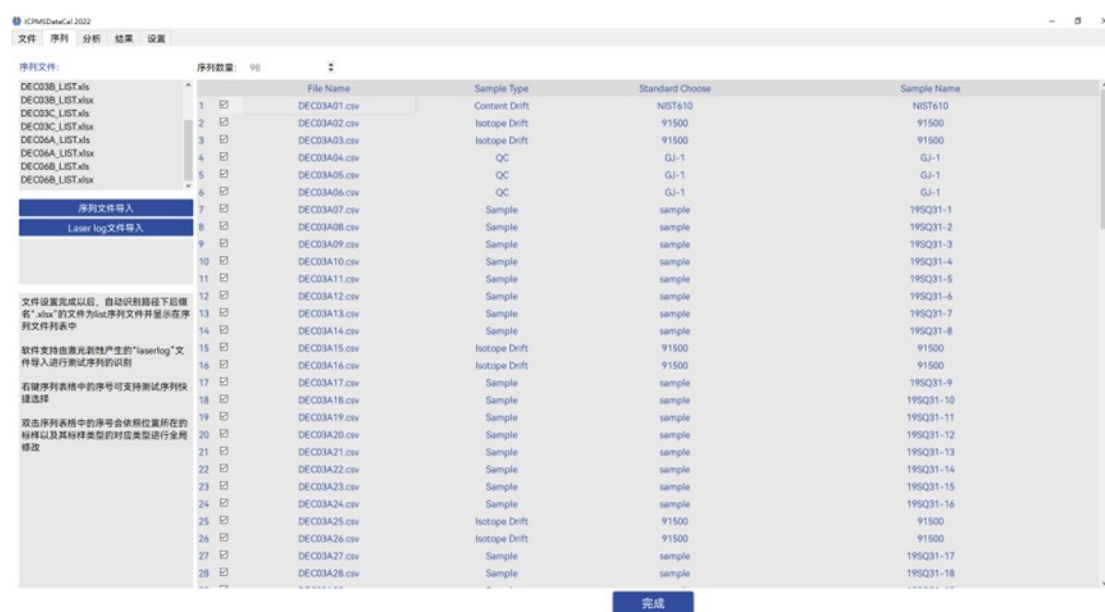


New Save Save as Delete

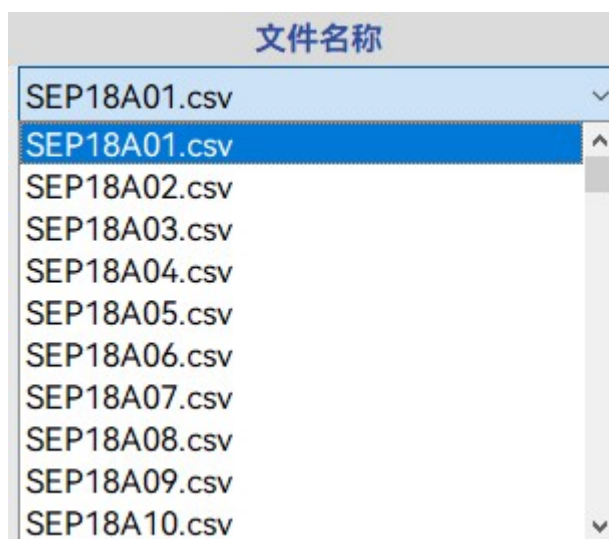
Method additions and deletions: Before you start editing a method, you need to click ‘new’ to create a new method, and then click ‘save’ to save the method, or click ‘save as’ to save the method as a separate file. After modifying an existing method, you can click ‘save’ to save the modification, or click ‘save as’ to save the method as a separate file. ‘Delete’ is to delete the method.

2.2 Sequence settings

In the sequence setting, must set the arrangement of samples and reference materials to be tested. After importing the files, all the data files in the folder will appear in the table, and the software will identify all the files under the path with the same suffix as the data files as data files (when there are other non-data files under the path with the same suffix as the data files (e.g. List files), it is best to move them out of the path).

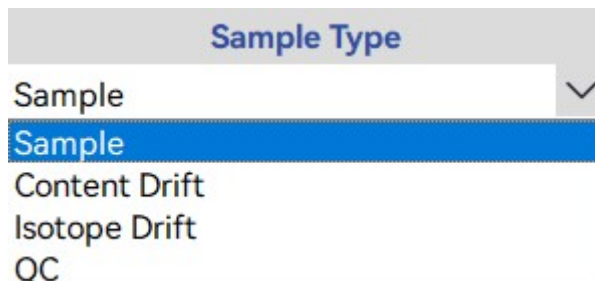


The user can double-click set the columns 'File Name', 'Sample Type', 'Standard Choose', 'Sample Name' and



other columns. The File Name column allows you to set the file source for each sample, allowing the setting to be the same file.

The Sample Type setting classifies samples into four categories: 'Sample', 'Content Drift', 'Isotope Drift', and 'QC'.

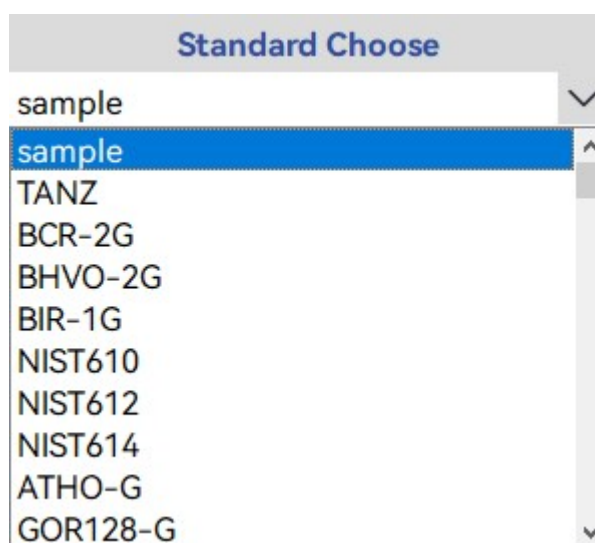


λ **Content Drift:** Reference material used for time drift calibration, elemental content calibration is usually for e.g. NIST 610 glass.

λ **Isotope Drift:** External standard samples for isotope ratio calibration as well as drift correction, e.g. 91500 commonly used in U-Pb testing.

λ **QC:** (Quality Control) reference material

The Reference Standard Selection drop-down box allows the selection of the standard for all samples. Clicking on the drop-down box will bring up the names of all the samples that are



currently available in the software, and if the sample is not a standard, the user will need to switch the sample to ‘Sample’.

In the column of sample name, if the sample name is successfully read from the list file, it will be set according to the list file, otherwise, the software will name the sample according to the naming rule of ‘sample file name + analysis number’.

In order to simplify the operation during the sequence setting process, it supports automatic sequence setting by importing List sequence file or Laserlog file. If there is a file with ‘.xlsx’ or ‘.xls’ extension under the file import path, it will be recognized as a sequence file automatically, and you can

文件导入

D:/办公文件/测试数据/统计测试/测试二类/L19_069_DONGRUIQIAO.b

List序列导入

D:/办公文件/测试数据/统计测试/测试二类/L19_069_DONGRUIQIAO.b/
DEC03A_LIST.csv

Laser log文件导入(.csv)

序列文件:

2019UPbDEC03A_Intensity.xlsx
DEC03A_LIST.xlsx
DEC03B_LIST.xlsx
DEC03C_LIST.xlsx
DEC06A_LIST.xlsx
DEC06B_LIST.xlsx

import the test sequence by double clicking or clicking the available sequence in the sequence file list box and then clicking OK. If the List file cannot be identified in the data folder path, you can click 'List Sequence Import' to import the List file separately. The sequence file is in the same format as the List file in ICPMSDataCal, so after importing the sequence only need to manually modify the sample type and check the test sequence.

Laserlog files are typically generated by the laser and contain information such as the name of the sample for a single stripping and the stripping time, which can also be used in the sequence settings of the software..

Timestamp	Sequence	SubPoint	Vertex	Nus	Comment	X	Y	Intended	Intended	Scan	Veloc	Laser	Stati	Laser	Rep	Spot	Typ
47:10.5	1	1			SRM 610	70186	10909					Off				0	Manual: G
47:10.5						70186	10909					Off				0	Manual: G
47:10.5						70186	10909	70186	10909			Off				0	Manual: G
47:10.5						70186	10909					On				7	Manual: G
47:10.5						70186	10909					On				7	Manual: G
47:40.0						70312	10985	70312	10985			On				7	Manual: G
47:40.0						70312	10985					Off				0	Manual: G
48:08.7	2	1			CPX-2	78490	39953					Off				0	Manual: B
48:08.7					0 CPX-2-1	78490	39953					100	Off			0	Manual: B
48:08.7						78490	39953	78490	39953			Off				0	Manual: B
48:08.7						78490	39953					On				7	Manual: B
48:09.2						78490	39953					100	On			7	Manual: B
48:09.2						78525	39953	78525	39953			On				7	Manual: B
48:09.2						78525	39953					Off				0	Manual: B
48:09.2						78525	39953					100	Off			0	Manual: B
48:09.6					2 CPX-2-2	78309	40023	78309	40023			Off				0	Manual: B
48:09.6						78309	40023					On				7	Manual: B
48:09.6						78309	40023					100	On			7	Manual: B
48:12.1						78553	40023	78553	40023			On				7	Manual: B
48:12.1						78553	40023					Off				0	Manual: B
48:12.1						78553	40023					100	Off			0	Manual: B
48:12.5					4 CPX-2-3	78128	40093	78128	40093			Off				0	Manual: B
48:12.5						78128	40093					On				7	Manual: B
48:12.5						78128	40093					100	On			7	Manual: B
48:16.7						78530	40093	78530	40093			On				7	Manual: B
48:16.7						78530	40093					Off				0	Manual: B
48:16.7						78530	40093					100	Off			0	Manual: B
48:17.1					6 CPX-2-4	77948	40163	77948	40163			Off				0	Manual: B
48:17.1						77948	40163					On				7	Manual: B
48:17.1						77948	40163					100	On			7	Manual: B
48:23.2						78501	40163	78501	40163			On				7	Manual: B
48:23.2						78501	40163					Off				0	Manual: B
48:23.2						78501	40163					100	Off			0	Manual: B
48:23.6					8 CPX-2-5	77767	40233	77767	40233			Off				0	Manual: B
48:23.6						77767	40233					On				7	Manual: B
48:23.6						77767	40233					100	On			7	Manual: B
48:30.7					9	78473	40233	78473	40233			On				7	Manual: B
48:30.7						78473	40233					Off				0	Manual: B
48:30.7						78473	40233					100	Off			0	Manual: B
48:31.1					10 CPX-2-6	77587	40303	77587	40303			Off				0	Manual: B
48:31.1						77587	40303					On				7	Manual: B

The tick box before the file name can be unchecked to exclude a sample from the test sequence.

Double clicking on the sequence number before the tick box will set all samples with the same name in standard choose to the same sample type. To set all NIST610 samples to “QC”, simply switch any

1	☒
2	☒
3	☒
4	☒
5	☒

NIST610 to “QC” and double-click on the serial number in the row.

check selected

uncheck selected

check all

uncheck all

change selected sample type ▶

change selected standard name▶

Right-click to bring up the convenient setting menu:

λ Check selected: Set the checkbox

corresponding to the selected serial number to the selected state, in the selected state, it means participating in the analysis.

λ uncheck selected: Set the tick box corresponding to the selected number to unchecked, i.e. not participating in analysis.

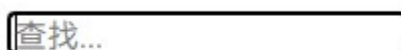
λ Check all: check all samples.

λ Uncheck all: uncheck all samples.

λ Change selected sample type: Setting the sample type of the selected.

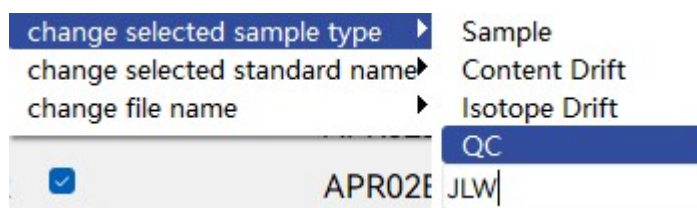
λ **Change selected standard name:** Setting the name of the reference material for the selected samples.

The right-click menu is mainly suitable for the user to manually set up the sequence if the user has not created a List file.



Sequence search: support for sequence name matching search, after the search is complete, you can use 'Ctrl+A' to select all the matching results and then right-click to unify the settings.

It is recommended that manually enter group names in the samples for



the different samples in a sequence, and the software will categorise the samples by group in the plot according to the group..

When the setting is complete, the user needs to click OK to complete the setting and automatically jump to the analysis interface.

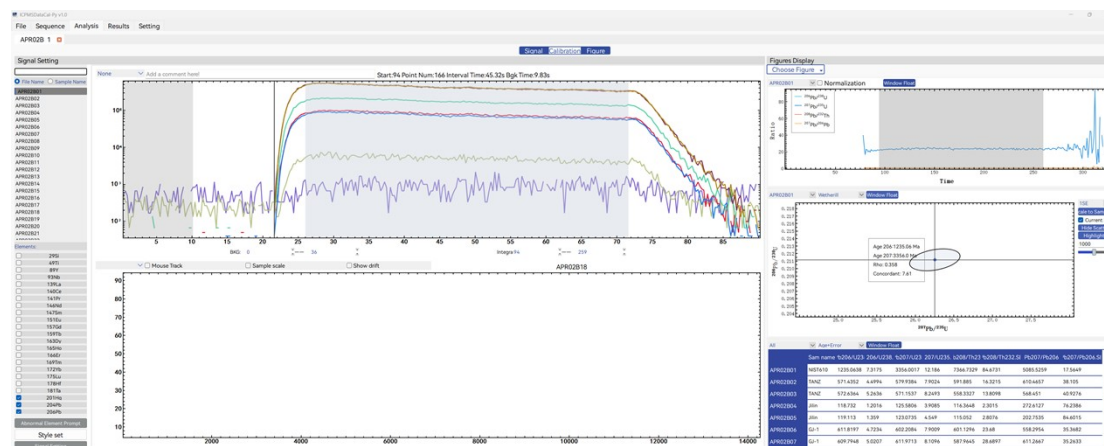
Note: Unlike ICPMSDataCal, the List file used in this software has no requirements for naming or suffixes, and common formats such as ‘.csv’ and ‘.xlsx’ can be imported. At least the file name and sample name columns should be included in the List, the software will automatically extract the file name and sample name and identify the labelled information, but it must be ensured that the file

文件	样品
20210616LDLB_1.csv	SRM 612
20210616LDLB_2.csv	MAD
20210616LDLB_3.csv	MAD
20210616LDLB_4.csv	MAD
20210616LDLB_5.csv	DUR-2-1
20210616LDLB_6.csv	DUR-2-3
20210616LDLB_7.csv	DUR-2-4
20210616LDLB_8.csv	DUR-2-5
20210616LDLB_9.csv	DUR-2-6
20210616LDLB_10.csv	DUR-2-7

name in the sequence file is strictly consistent with the file name of the data file.

Real time flash: In order to obtain calibrated results quickly during sample stripping, the software supports real time monitoring of list files and data files, which must be enabled by setting up the analysis interface and clicking on the ‘Real time flash’ button to turn on the function. Once this function is enabled, any changes made to the test sequence (addition of data files, modification of list files and changes to the sequence setup screen, but not deletion of samples) can be recalculated from existing analyses without the need to set up a new analysis, allowing the instrument's stability to be monitored during the actual test.

2.3 analysis interface

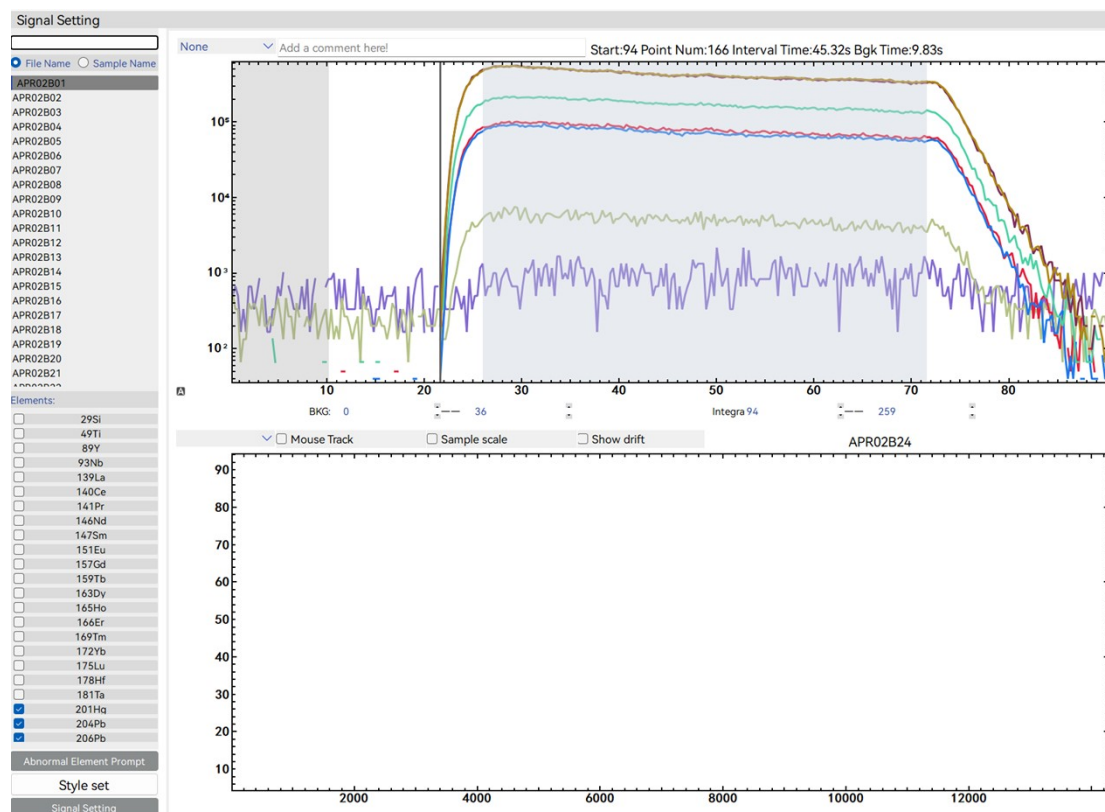


After clicking Confirm in the sequence interface, the test interface will be added automatically for this analysis. Since the software supports adding multiple analyses, users can create a new analysis according to each batch of sequences set up in the sequence setting interface, without having to open the software repeatedly, and an analysis can be deleted by clicking on the ‘×’ in the analysis title bar.

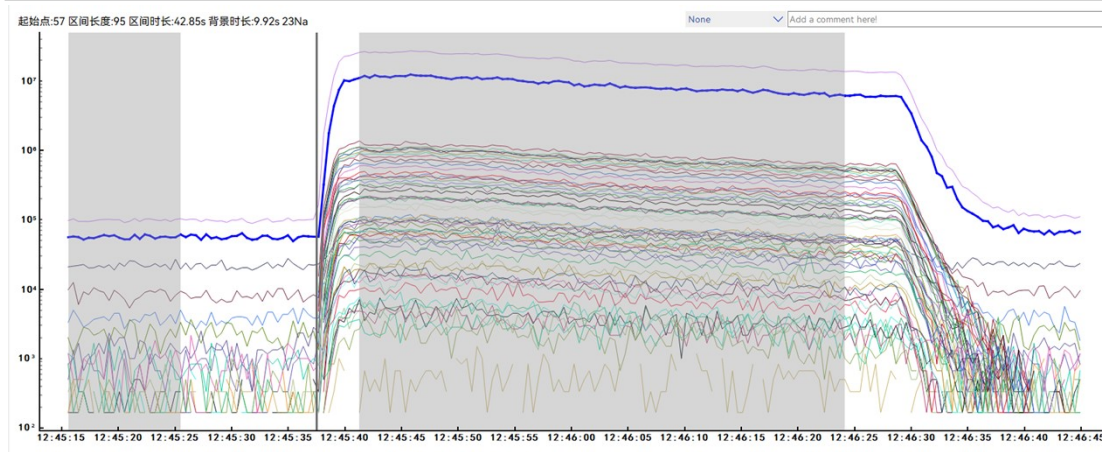
The single analysis screen consists of three pages: Signal, Calibration, and Figure. Signal setup can be switched by clicking on the top button of the analysis screen after the signal setup is complete, signal setup and calibration methods cannot exist at the same time, while the figure can be closed or displayed by clicking on the top figure button.

2.3.1 Signal Interface

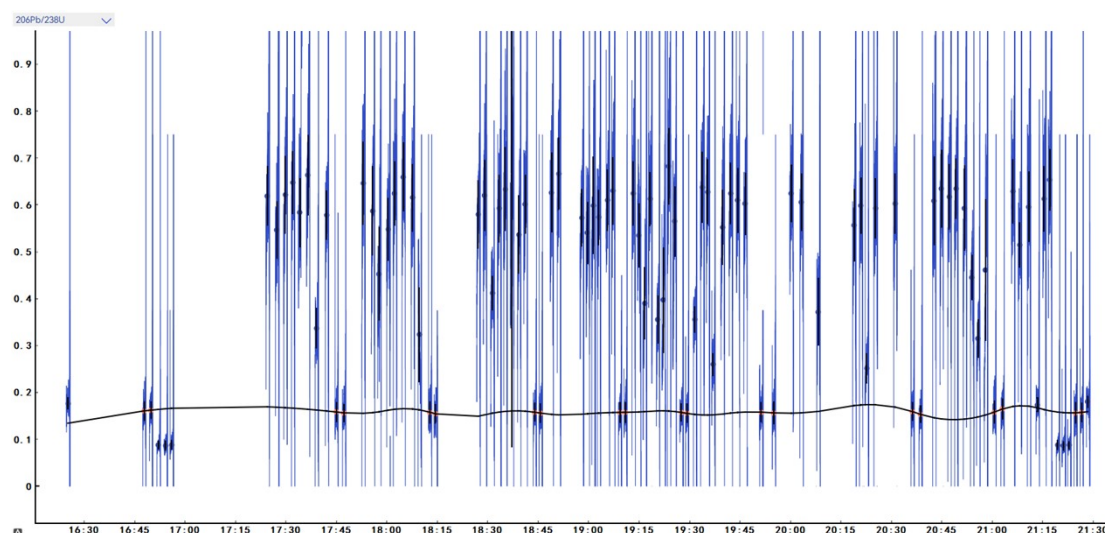
This interface is mainly for observing the signals in the integration interval as well as for shortcut settings.



The Signal interface is divided into Sample View, Drift View, Sample Name List, Element List, Abnormal Element Display button, and Signal Setup button.



Sample view: display all the elemental signals of the currently selected sample, you can click on any line to select the element, the left grey area of the figure for the background interval, the middle grey area for the selected integral interval, the grey line in the middle of the two indicates the position of the laser begins to strip the signal generated, the three software will use algorithms for automatic identification, the user only needs to quickly check the part of the problem samples for the selection of intervals (just mouse interaction in the figure) is all that is required.



Drift view: It is easy for the user to observe and set up the signal drift behaviour of the samples during the test. The black line in the figure shows the drift curve predicted by the software using each drift algorithm.

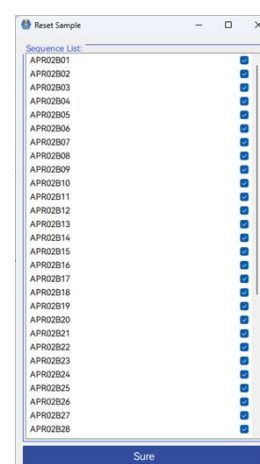


Sample List: The default file name of the sample is displayed, and you can click the Sample Name button to display the name of the sample corresponding to the file name. Click on different samples to switch between the samples displayed in the main view.

Elements:		
☐	140Ce	
☐	141Pr	
☐	146Nd	
☐	147Sm	
☐	151Eu	
☐	157Gd	
☐	159Tb	
☐	163Dy	
☐	165Ho	
☐	166Er	
☐	169Tm	
☐	172Yb	
☐	175Lu	
☐	178Hf	
☐	181Ta	
☒	201Hg	
☒	204Pb	
☒	206Pb	
☒	207Pb	
☒	208Pb	
☒	232Th	
☒	238U	
☐	sum	
☐	206Pb/238U	
☐	207Pb/235U	
☐	208Pb/232Th	
☐	207Pb/206Pb	
☐	238U/232Th	
☐	238U/206Pb	

Elements/ratios list: the left tick box is checked to indicate that the lines of the elements in the main view will be shown, and vice versa will be hidden. The button on the right side indicates the colour of the line of the element corresponding to the button in the main view and in the drift view, which can be switched by clicking on the button. The element will be shown in the main view and the ratio will be shown in the drift view. .

Reset Sample List: During actual testing, when an error occurs in the testing of one or more specimens or samples, the erroneous samples can

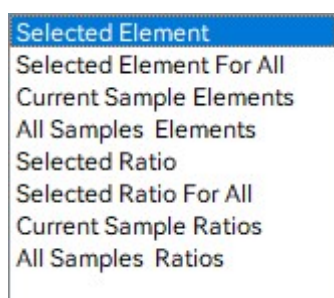


be deleted by resetting the sample list to regenerate the calibration results. There is no need to re-establish the analysis.

signal setting: Clicking the Signal Setting button will bring up the function to set the signal.

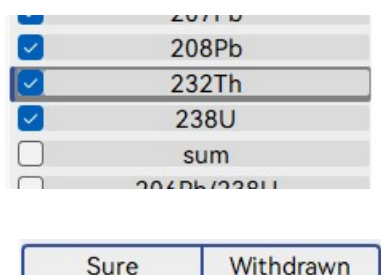
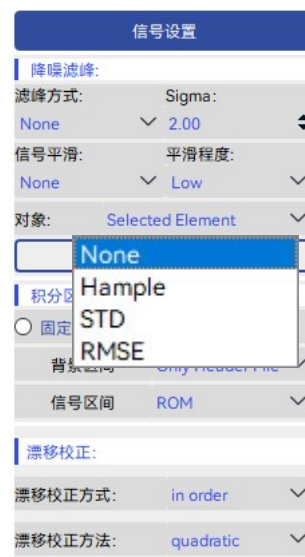
filter mode: The filtering methods include hample filtering, simple outlier filtering, spline filtering and root-mean-square error filtering, usually hample filtering is preferred for the best

filtering effect, and when the effect of hample filtering is unsatisfactory, we can consider replacing other filtering methods.

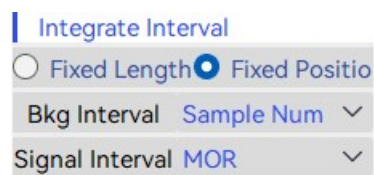


Peak filtering and data smoothing objects: selected elements (ratio), selected elements in all files (ratio), selected files and all files all the

elements (ratio) eight options, the user can choose the appropriate object in accordance with the actual situation, if you need to select a certain element or ratio, in the list of



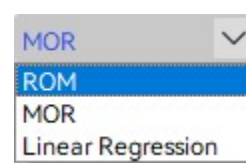
elements / ratios, you need to set the element to the selected state, select a good object and filtering after the way Click on the sure button, if you need to withdraw the filtering operation, click on the withdraw button.



Integrate interval: Clicking on the bkg interval and signal interval buttons only

determines whether the signal interval and background interval are displayed or hidden, and the background interval allows you to select whether all files will be deducted according to the background signal of the first file or whether each file will be deducted individually from the background for the type of analysis.

Signal Integration Mode: The software supports three kinds of integration modes: ROM (Ratio of mean), MOR (Mean of Ratio) and Linear



Regression. Because of the compatibility of the different integration modes, the software supports the calibration of the single pulse ablation , and the software will automatically select the ‘ROM’ integration mode when the calibration method is selected to be single

pulse. User can freely switch the integration method according to different analysis methods. When the integration method is 'Linear Regression', the linear regression calibration figure will appear in the calibration interface.

Error calculation for different integration methods:

If $z=a/b$

For MOR:

$$\sigma_z = \frac{s_z}{\sqrt{n}}$$

S is the standard deviation of z

For ROM :

$$\sigma_z = \left| \frac{a}{b} \right| \cdot \sqrt{\left(\frac{\sigma_a}{a} \right)^2 + \left(\frac{\sigma_b}{b} \right)^2}$$

For LR:

The error of z is the slope error of fit line (SE(z)).

$$\bar{a} = \frac{1}{n} \sum_{i=1}^n a_i$$

$$\text{RSS} = \sum_{i=1}^n (b_i - \hat{b}_i)^2$$

$$S_{aa} = \sum_{i=1}^n (a_i - \bar{a})^2$$

$$\text{MSE} = \frac{\text{RSS}}{n - 2}$$

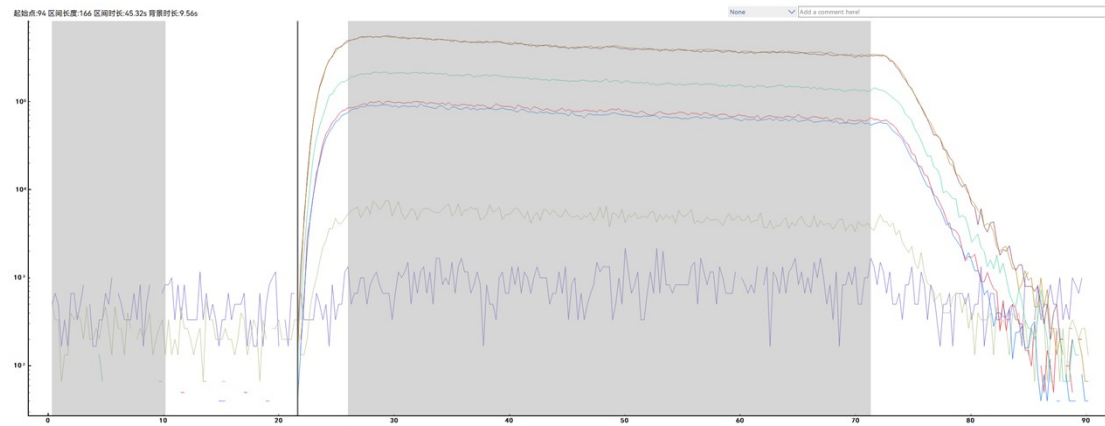
$$z = \frac{\sum_{i=1}^n (a_i - \bar{a})(b_i - \bar{b})}{\sum_{i=1}^n (a_i - \bar{a})^2}$$

$$c = \bar{b} - z \cdot \bar{a}$$

$$\text{SE}(z) = \sqrt{\frac{\text{MSE}}{S_{aa}}}$$

Integral interval selection:

The software contains an automatic integration interval selection function that not only recognizes traditional single-point ablation signals, but also automatically recognizes face-scanning, and single-pulse ablation signals.



λ In order to ensure the accuracy of the integration interval identification and to minimise the impact of depth fractionation on the results, the automatic identification function includes the identification of the start of the ablation (grey vertical line in the figure), while the manual adjustment of the signals includes a fixed length as well as a fixed position.

λ Fixed Length: Set the signal intervals for all samples to have the same length, but ignore the location.

λ Fixed position: not only is the signal interval of all samples set to the same length, but all samples are also kept at the same distance from the start of the laser stripping (grey line in the figure) to ensure that all samples have the same integration interval to the greatest extent possible.

Selection of signal intervals:

In the case of non-mapping analysis, due to the possible fractionation effect caused by the down-hole effect during the ablation process, in order to obtain the optimal signal for the best test results, the signal selection should try to ensure that the samples have the same position of the integration interval.

For common analysis, the following steps should be followed:

- ✓ Since the software automatically recognises the signal interval and the default setting is the same integration interval, the 91500 is first checked for external standard samples such as zircon, and the starting position of laser ablation is determined. Therefore, when analysing external samples such as zircon, first check the 91500, determine the integration intervals and the starting position of the laser ablation, and then check the samples one by one.。**

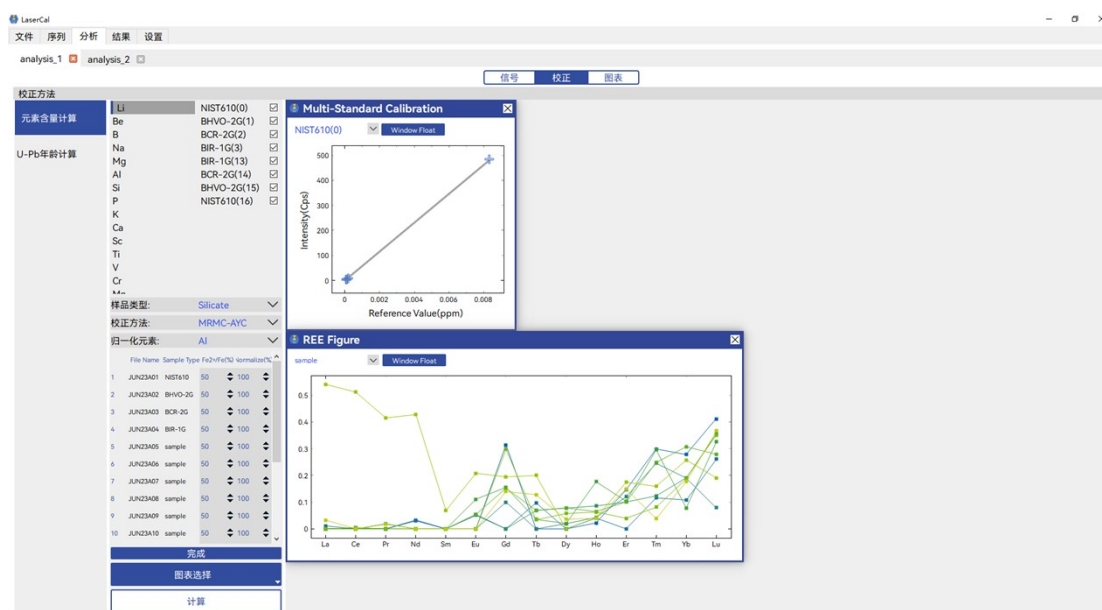
When need to adjust the position of a single integration interval, users need to uncheck ‘fix position’, and after adjusting the appropriate integration interval, turn on the down-hole calibration module in the

calibration method interface, and if modify the integration interval in a holistic way, down-hole calibration module is unnecessary.

2.4 Calibration

When the signal setting is complete, clicking on the calibration method will bring up the calibration interface, which currently only provides four parts: elemental content calculation, zircon U-Pb age calculation and isotope ratio determination, common Pb correction (Still under development).

2.4.1 Calibration of elemental content



λ **Element list:** The element list contains all the test elements. By clicking on the different elements, you can observe the

Li	NIST610(0)	☒
Be	BHVO-2G(1)	☒
B	BCR-2G(2)	☒
Na	BIR-1G(3)	☒
Mg	BIR-1G(13)	☒
Al	BCR-2G(14)	☒
Si	BHVO-2G(15)	☒
P	NIST610(16)	☒
K		
Ca		
Sc		
Ti		
V		
Cr		

sample signal/recommended value and calibration curves of the different elements in the calibration graph.

λ **RMs list:** All reference materials identified by the software, the tick box behind it can decide whether a specimen of the element is involved in the calibration process or not, if it is necessary to add or delete a specimen for several or all elements, you can select several elements in a row or use 'Ctrl+A' to select all the elements for adding or deleting a RM, if it is necessary to set up the addition or deletion of several RMs at the same time, the steps are the same. If you need to add or delete multiple RMs at the same time, the steps are the same. For example, if want to delete NIST610 for all elements. Firstly, choose all elements use "Ctrl+A", then choose all NIST610, finally, unchecked NIST610.

λ **Sample parameter settings:** For the calibration method with multiple external standards and no internal standard, the sample needs to be set with the proportion of divalent iron (Fe²⁺/Fe Total), the normalised value of the total amount (Normalize (%)) and the compound type. For calibration methods with multiple external

standards and single internal standard, the content of the internal standard is set.

	Sample Name	Sample Type	Fe2+/Fe(%)	Normalize(%)	Compound Type
JUN23A01	NIST610	NIST610	50	100	Silicate
JUN23A02	BHVO-2G	BHVO-2G	50	100	Silicate
JUN23A03	BCR-2G	BCR-2G	50	100	Silicate
JUN23A04	BIR-1G	BIR-1G	50	100	Silicate
JUN23A05	MongOL sh11-2	sample	50	100	Silicate
JUN23A06	EM57-1-0001_1	sample	50	100	Silicate
JUN23A07	EM57-1-0001_2	sample	50	100	Silicate
JUN23A08	EM57-1-0001_3	sample	50	100	Silicate
JUN23A09	EM57-1-0001_4	sample	50	100	Silicate
JUN23A10	EM57-1-0001_5	sample	50	100	Silicate
JUN23A11	EM57-1-0001_6	sample	50	100	Silicate
JUN23A12	EM57-1-0001_7	sample	50	100	Silicate
JUN23A13	EM57-1-0001_8	sample	50	100	Silicate
JUN23A14	BIR-1G	BIR-1G	50	100	Silicate
JUN23A15	BCR-2G	BCR-2G	50	100	Silicate
JUN23A16	BHVO-2G	BHVO-2G	50	100	Silicate
JUN23A17	NIST610	NIST610	50	100	Silicate

	File Name	Sample Type	IS ElementAl(ppm)
1	JUN23A01	NIST610	10795.68
2	JUN23A02	BHVO-2G	71971.2
3	JUN23A03	BCR-2G	70912.8
4	JUN23A04	BIR-1G	82026.0
5	JUN23A05	sample	
6	JUN23A06	sample	
7	JUN23A07	sample	
8	JUN23A08	sample	
9	JUN23A09	sample	
10	JUN23A10	sample	

完成

λ **Sample type:** The default sample type is silicate, and the user needs to change it according to the actual sample type. The software supports most common sample types such as carbonates (Chen et al., 2011) , sulphides, metals, phosphates, chlorides, etc., and the user can set the compound type for each sample individually.

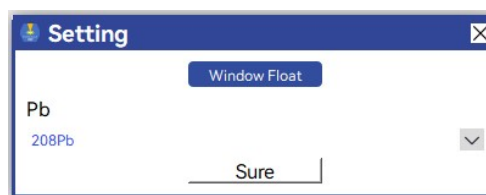
λ **Note:** When using sulphide calibrations the atomic ratio of S/Fe is entered in (Compound Type).

λ **Calibration method:** The software defaults use MRMC-AYCF(Liu et

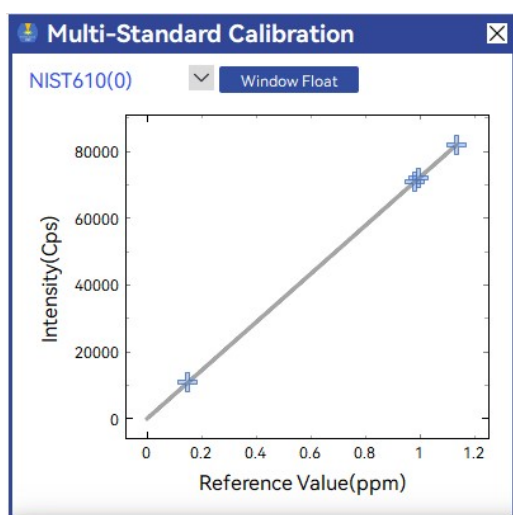
MRMC-AYC
MRMC-ISN
MRMC-Simple

al., 2008) method、 users can change to MRMC-ISN(Longerich et al., 1997) and MRMC-Simple。

Isotopic choose: In content calculations, only one isotope of an element must be selected for the



calculation of the result if more than one isotope of the element is determined, since the total normalisation method is used. For example, in the case of U-Pb testing, the appropriate Pb isotope must be selected in order to accurately obtain the Pb content.



Multi-Standard Calibration: The blue crosses in the figure represent the calibrated samples in the current elemental calibration process. You can click on the elemental list to switch samples, and

tick the samples in the list of samples to change the calibration curve.

Note:

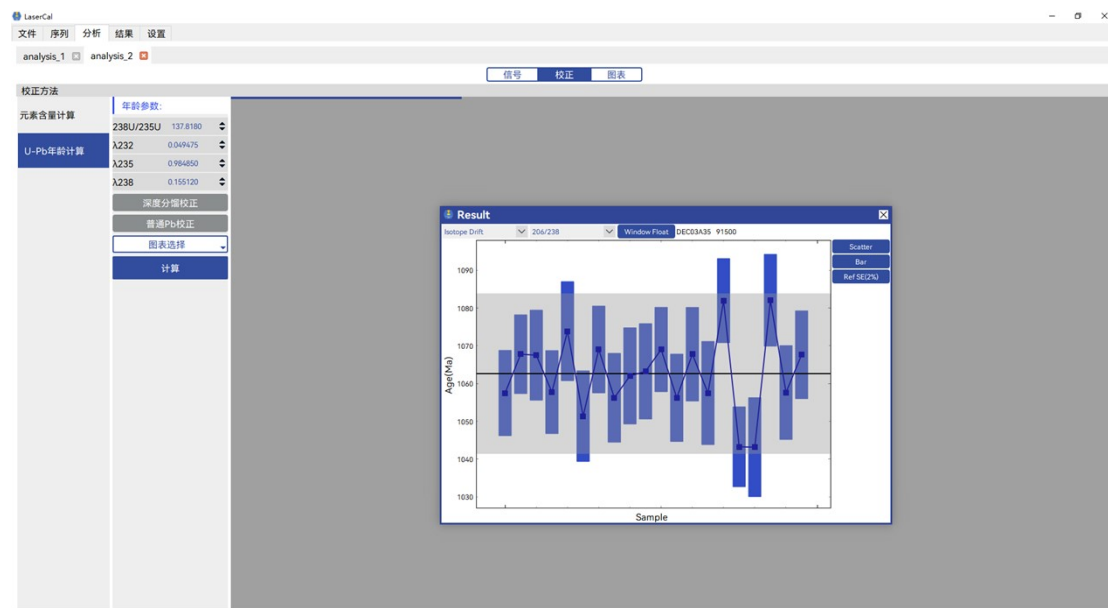
- λ If multiple isotopes are present in an element, the appropriate isotope must first be checked and selected before obtaining the correct calibration.**
- λ The use of the multiple external standard - no internal standard method requires the selection of the normalizing element, which is usually an element with a stable signal and a high content in the sample. It is also necessary to vary the sample type, the proportion of Fe²⁺ to total iron in the specimen and the normalized value for each sample according to the actual situation.。**
- λ The use of multiple external - single internal standards requires the selection of the internal standard element, which is usually the primary element and whose content in the sample has already been obtained by other means and needs to be entered in the form. The content of the internal standard element is known and to reduce the workload, the same sample type can be set to the same value by double clicking on the sample type. The result is only calculated if all the values of the internal standard elements are not null.**
- λ The naming rule of the RMs list is RMs name + (sample test**

number). Clicking on the element list will change the element calibration curve image, by checking or unchecking the RMs, users can decide whether or not the RMs will participate in the calibration curve building process, both the element list and the RMs list support multiple selections as well as CTRL+A for selecting the whole list, double clicking on the name of the RM will check the list of all the RMs with the same name, and by selecting more than one of the elements and RMs, you can decide whether or not more than one of the samples in the sample will participate in the calibration at the same time.

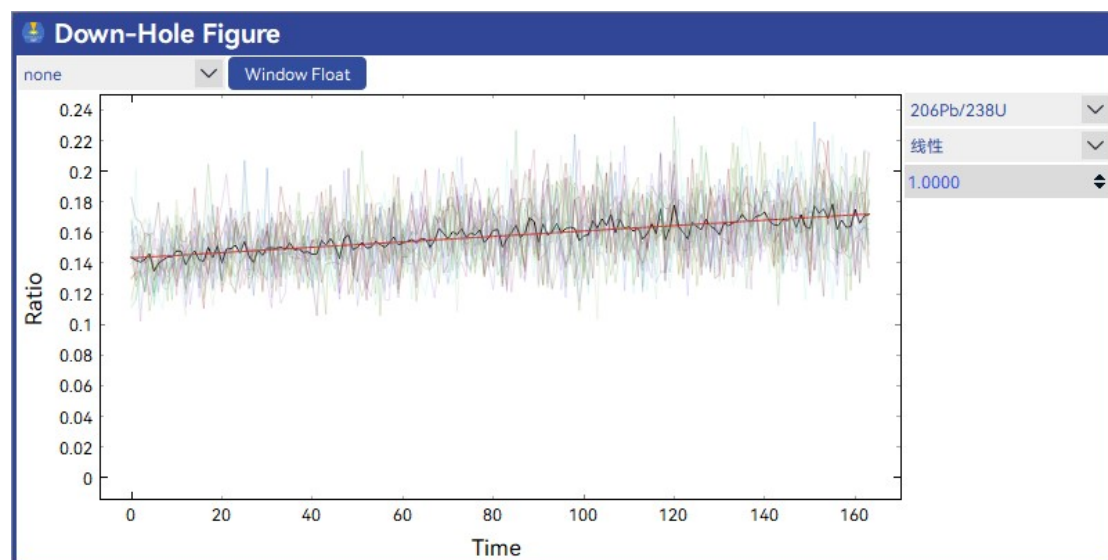
λ The limit of detection (LOD) is calculated as the concentration value corresponding to three times the standard deviation of the background signal and is given by the formula:

$$\left\{ \begin{array}{l} LOD = 3 \times \sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \times (l_{rm}^i \times l_{sam}^{is} / l_{rm}^{is}) \\ l^i = \frac{C^i}{cps^i} \end{array} \right.$$

2.4.2 U-Pb dating



年龄参数 Change $^{238}\text{U}/^{235}\text{U}$ value and change decay constants for U-



Th.

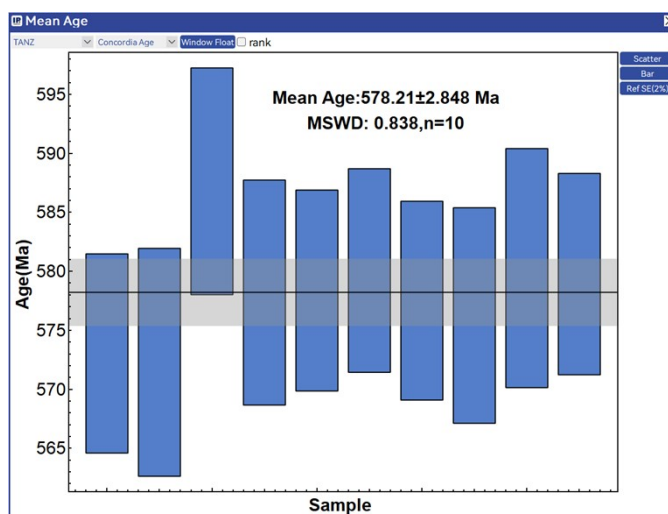
Down-hole correction: Correction for possible down-hole fractionation of U-Pb with denudation, the main principle of the correction is derived from Paton et al. (2010), which allows the down-

线性
二次
三次
指数
样条插值

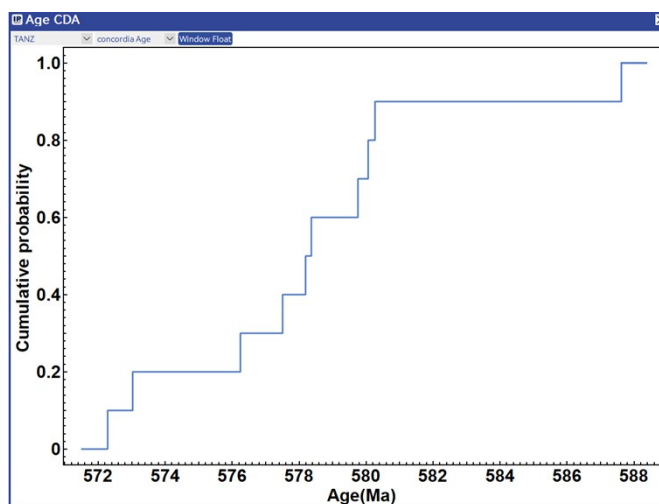
hole fractionation curve of the external standard to be fitted in a number of ways (red lines in the figure) and the results of the fit to be used to calibrate the fractionation behavior of the sample (required).



Figure choose: current support mean age、CAD and KDE.

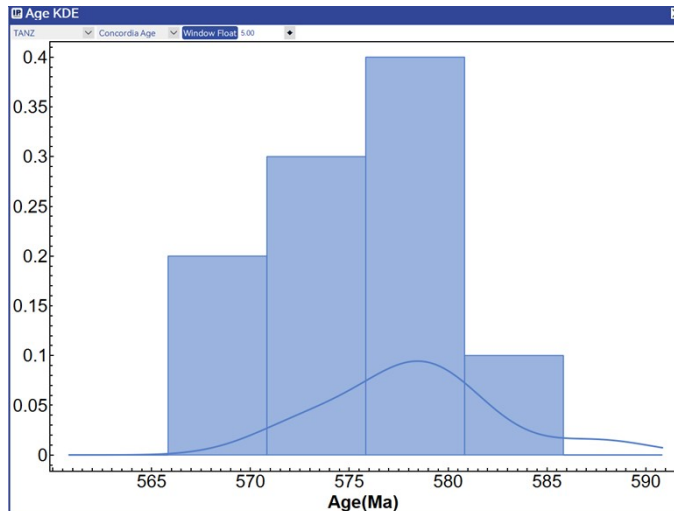


Mean Age: Users can select bar graphs as well as line graphs to display test results for different types of samples, with gray areas indicating the margin of error and black lines indicating the average age.

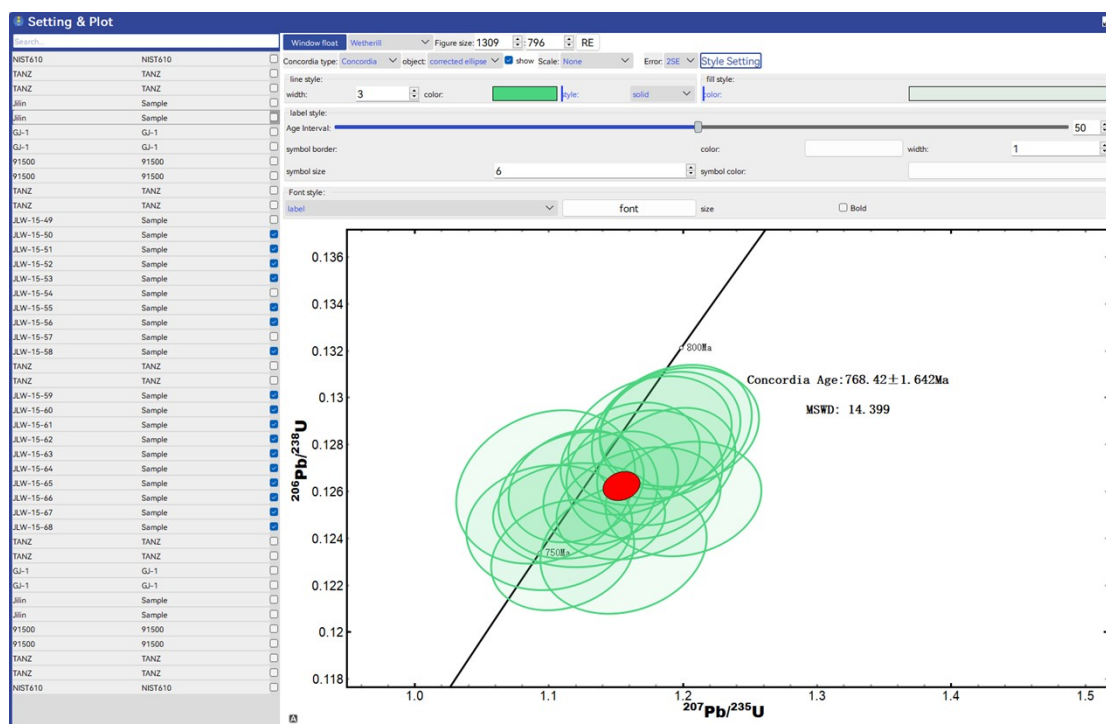


CAD: This graph shows

the cumulative density distribution of the data



KDE: This figure shows the kernel density distribution of age



Concordia Plot: The software supports the plotting of concordia and isochronous ages and the customization of chart styles. Users can preset the styles of real-time processing results and export the charts

directly with publishable quality. will be reproduced the next time you turn on the software.

Note:

- ✓ In order to minimize the possible influence of the shunt effect on the test results during the test process, try to have consistent signal intervals for each sample and RMs.
- ✓ The calibration of zircon U-Pb ages for the software is derived from (Liu et al., 2009) The drift in the ratios is mainly calibrated by a linear drift in the quality control RMs.
- ✓ The software in the uncertainty transfer process does not currently support the transfer of decay constant errors, and the errors in the recommended values of the RMs use their 1σ .
- ✓ This software provides the results of the error correlation coefficient (rho), which is calculated as follows:

$$\text{rho} = \text{cov}(^{206}\text{Pb} / ^{238}\text{U}, ^{207}\text{Pb} / ^{235}\text{U}) / (\sigma_{^{206}\text{Pb}/^{238}\text{U}} \sigma_{^{207}\text{Pb}/^{235}\text{U}})$$

U-Pb dating calibration strategy and error transmission:

The calibration formula as well as the error transfer

formula are described in Liu et al. (2009).

Calibration formula:

$$R_{cor}^{sam} = R_{mea}^{sam} \times R_{ref}^{std} \times \left(\frac{1}{R_{mea1}^{std}} \times \left(1 - \frac{t_{mea1}^{sam} - t_{mea1}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}} \right) + \frac{1}{R_{mea2}^{std}} \times \left(1 - \frac{t_{mea2}^{sam} - t_{mea2}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}} \right) \right)$$

Uncertainty propagation:

$$\sigma_{R_{cor}^{sam}} = R_{cor}^{sam} \times \sqrt{\left(\frac{\sigma_{R_{mea}^{sam}}}{R_{mea}^{sam}} \right)^2 + \left(\frac{\sigma_{R_{ref}^{std}}}{R_{ref}^{std}} \right)^2 + \frac{\left(\left(1 - \frac{t_{mea1}^{sam} - t_{mea1}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}} \right) \times \frac{\sigma_{R_{mea1}^{std}}}{R_{mea1}^{std}} \right)^2 + \left(\frac{t_{mea2}^{sam} - t_{mea2}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}} \times \frac{\sigma_{R_{mea2}^{std}}}{R_{mea2}^{std}} \right)^2}{\frac{1 - \frac{t_{mea1}^{sam} - t_{mea1}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}}}{R_{mea1}^{std}} + \frac{\frac{t_{mea2}^{sam} - t_{mea2}^{std}}{t_{mea2}^{std} - t_{mea1}^{std}}}{R_{mea2}^{std}}}}$$

2.4.4 Common Pb Correction (Under development)

2.4.5 Isotope ratio calculation

Background deduction: Decide whether to background deduct the signal.

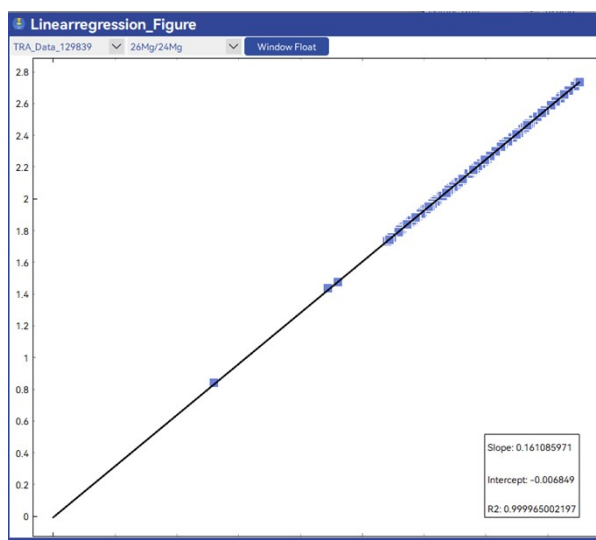
Signal Integration Method: When editing the isotope ratio method, the software automatically labels the numerator and denominator of the ratio formula. Therefore, ratio calculations can be performed by selecting the appropriate ratio integration method to obtain the correct result.

Mean of Ratio: The average of the ratios was calculated for each cycle (the smallest data unit, each count of its isotope for each sample) after calculating the ratios and then calculating its average as the isotope ratio of the sample.

Ratio of mean: The ratio of the mean values is calculated by first calculating the isotope and its signal mean, and then the ratio of the mean values is used as the

isotope ratio of the sample.

Linear of regression: A linear fit to the numerator



denominator of the isotope ratio is performed and the slope is used as the isotope ratio. Depth fractionation correction is not available when this method is selected.

SUM: As a complement to Ratio of mean , the integral intervals are summed and then the ratio is calculated as the isotope ratio.

Down-hole

Fractionation

Correction: The

isotope ratios were

corrected for depth

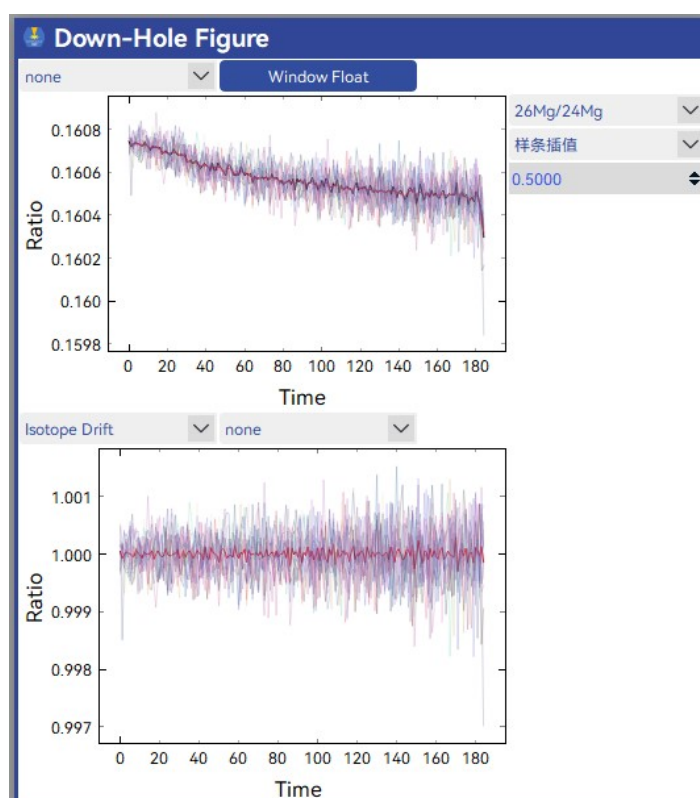
fractionation by

choosing different fits,

and the following figure

shows the corrected

ratio image.



2.4.5 Figures

In order to help users better select data and

observe the quality of data, there are

currently six types of charts supported. After

user has set the analysis type, the software will

automatically display different charts according to the actual

situation. All chart data will be fed or refreshed in real time according

to the user's choice.

Concordia: U-Pb

concordance plot, real-

time display of the

current U- Th-Pb ratio

results. Users can display

the size of the error

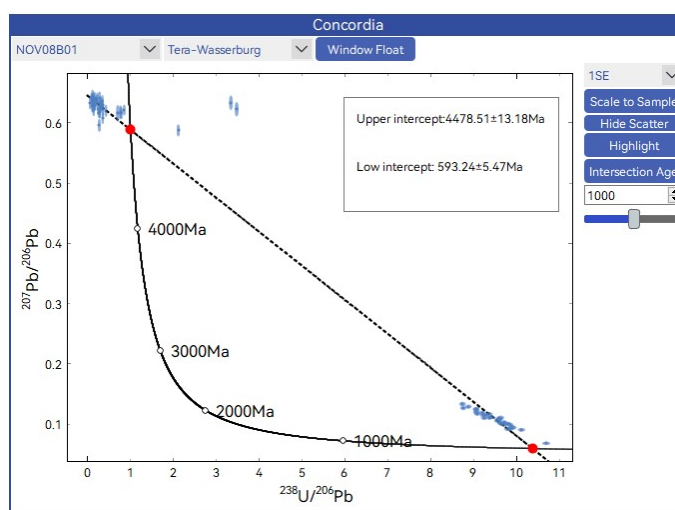
ellipse, the graph display range Scale to sample, Hide / Show. Users

can adjust the size of error ellipse, scale to sample, hide/show the

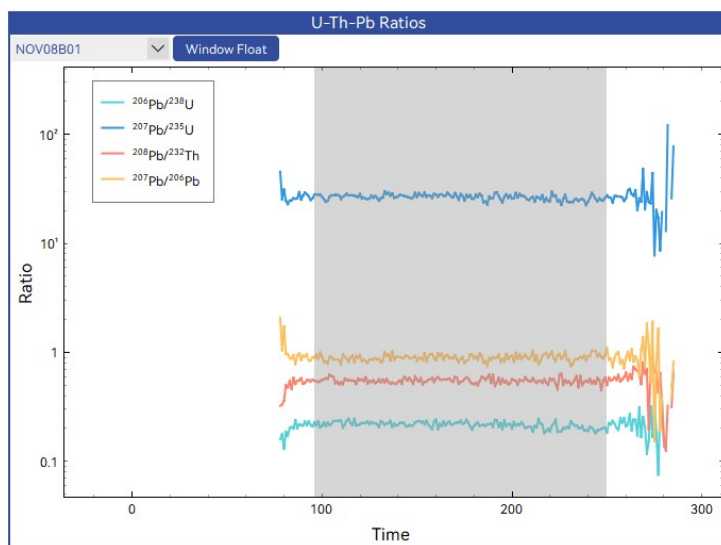
center of the error ellipse, highlight the current

Standards Content Result
Content Result Table

✓ U-Th-Pb Ratios
✓ U-Pb Result Table
Single File Concordia
✓ Concordia

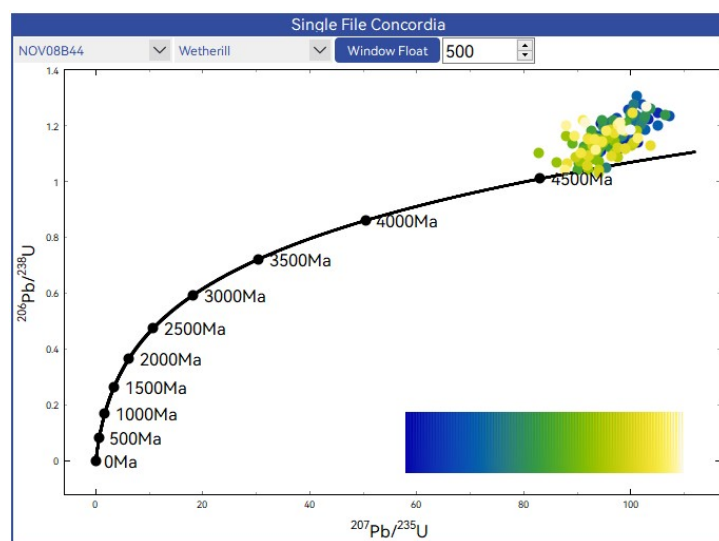


sample(Highlight), calculate the age of all samples in the intersection
line(Intersection Age) and adjust the age label.

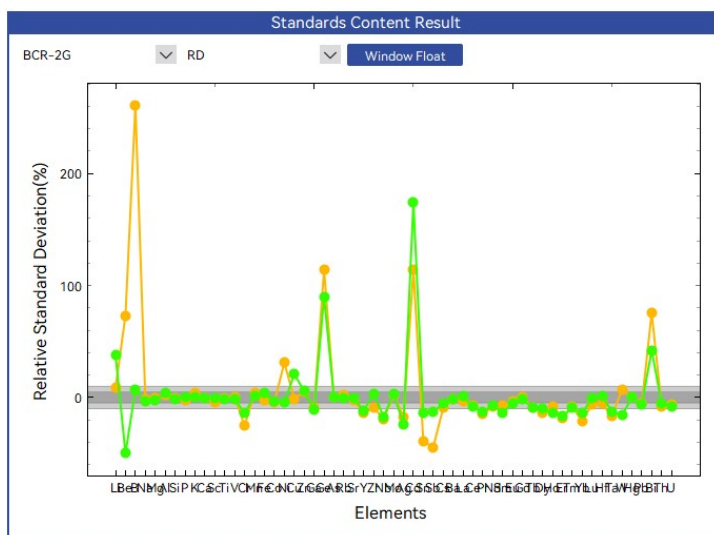


U-Th-Pb Ratios: Show
s $^{206}\text{Pb}/^{238}\text{U}$, $^{207}\text{Pb}/^{235}\text{U}$, $^{208}\text{Pb}/^{232}\text{Th}$, and $^{207}\text{Pb}/^{206}\text{Pb}$
Pb, with the ability to cl
ick on the legend to hide
or show the lines

Single File Concordia:A
single-file concordance
graph that plots all
points in the current
file's point interval on a
concordance graph,



changing from blue to yellow to represent the time change from the start to the end of the point interval.



Standards Content Result: Plot of reference materials content results, test results of all specimens during the test, and RD (Relative Deviation), with

gray areas indicating 5% and 10% error ranges.

2.4.6 Uncertainty propagation

Elemental content: The uncertainty transfer equation for the internal standard calibration method is derived from (Longerich et al., 1997), while the sum normalized method adds the sum value as a total constraint (usually 100%) without the internal standard element, so its uncertainty calculation process is comparable to the internal standard method, and because the total value is usually entered manually without error, its final error may be smaller relative to the internal standard method.

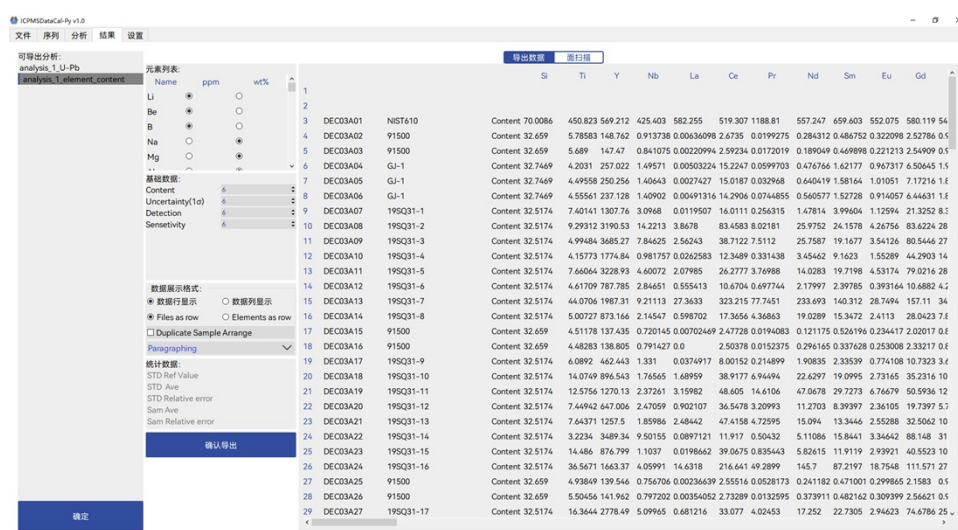
Details for U-Pb dating error propagation in section 2.4.2.

Isotopic editor: isotope correction methodology cannot provide a comprehensive error propagation formula for specific correction methods due to the implementation of customized editors. Consequently, our approach employs a Monte Carlo simulation-like procedure utilizing data from the integration interval itself. The simulated dataset size is determined by the length of the integration interval for each sample. Statistical analysis of the resulting data yields mean values with standard error (SE) as the measurement uncertainty. However, this methodology presents a limitation in its inability to incorporate fixed constant errors, such as those associated with decay constants and their inherent uncertainties. Nevertheless, given that the systematic errors from these constants generally exhibit negligible magnitudes (typically <1% relative uncertainty), the overall reliability of the error estimates derived through this computational strategy remains statistically valid.

2.5 Data export

2.5.1 Table Export

In the data export screen, all the data that have been processed will be displayed in the list on the left, with the naming convention of test name (analysis_?) + Calibration type.



Element List: When the calibration type is content test (element_content), the user can add and remove operations to determine whether the element passes the compound percent content or displays the element content in ppm.

Basic data: You can decide whether the element content, content uncertainty, detection limit, and Sensitivity are displayed or not. The

number of valid bits (1-10) that can be retained for each item can also be determined by changing the value ..

Data presentation format: The data row display indicates the element name in horizontal coordinates and the sample name in vertical coordinates, while the column display indicates the opposite..

Arrangement of duplicate

☐ Duplicate Sample Arrange

samples: In the actual

testing process, it may be necessary to focus on duplicate samples for the evaluation of results, so all samples can be arranged in a duplicate grouping.

The software at the end of the results table provides the results of the relative deviation (RD%) for all replicate samples.

134	DEC03A02	91500 (RD%)	-0.4619	-2.242	1.734	-5.241
135	DEC03A03	91500 (RD%)	0.463	2.208	-1.731	5.119
136	DEC03A15	91500 (RD%)	0.4324	1.611	0.2367	4.358
137	DEC03A16	91500 (RD%)	-0.4313	-1.62	-0.232	-4.427
138	DEC03A25	91500 (RD%)	0.9398	-0.4939	-0.3936	-3.254
139	DEC03A26	91500 (RD%)	-0.9399	0.5093	0.3982	3.244
140	DEC03A35	91500 (RD%)	0.624	0.7352	-3.826	1.053
141	DEC03A36	91500 (RD%)	-0.6232	-0.7228	3.823	-0.9972
142	DEC03A45	91500 (RD%)	-0.0783	-0.3548	1.033	-0.1324
143	DEC03A46	91500 (RD%)	0.07969	0.3715	-1.029	0.1947
144	DEC03A55	91500 (RD%)	0.5712	0.5883	5.925	0.3776
145	DEC03A56	91500 (RD%)	-0.5704	-0.5737	-5.938	-0.3152
146	DEC03A65	91500 (RD%)	0.4682	1.17	4.404	1.645
147	DEC03A66	91500 (RD%)	-0.4671	-1.166	-4.409	-1.6
148	DEC03A75	91500 (RD%)	1.811	2.6	-2.487	4.602
149	DEC03A76	91500 (RD%)	-1.815	-2.655	2.488	-4.688
150	DEC03A85	91500 (RD%)	-1.713	-0.345	-2.256	3.047
151	DEC03A86	91500 (RD%)	1.71	0.3617	2.258	-3.048

2.5.2 Mapping

Theoretically, the signal form and correction process of the mapping analysis is not different from that of a normal point analysis; the main difference is in the presentation of the data results. The main difference lies in the presentation of the data results, which is therefore included as part of the data export.

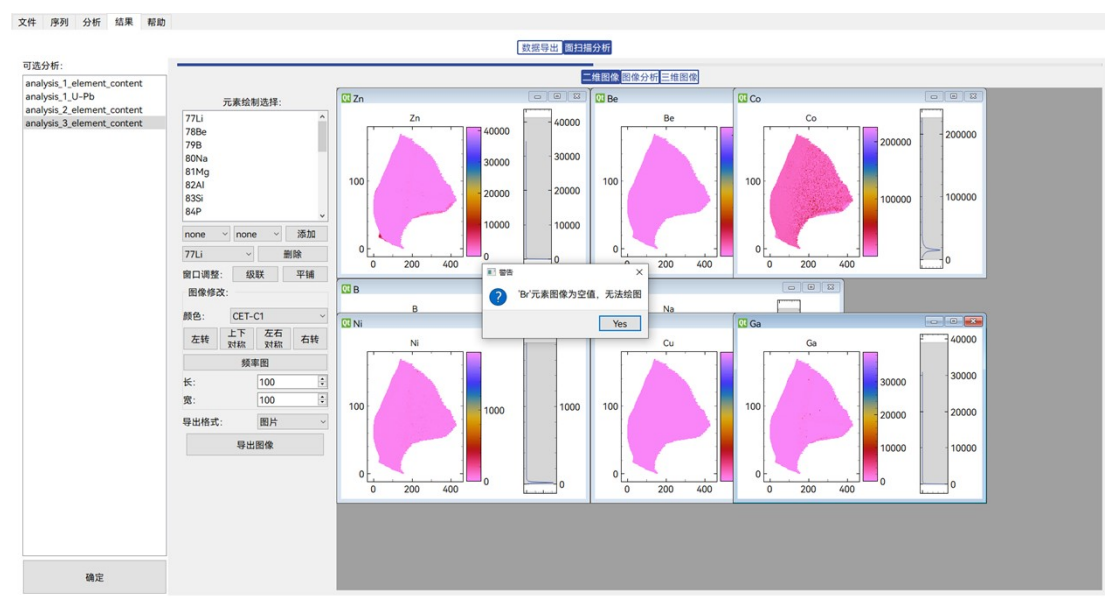
When exporting the results of mapping, the software supports any calibration method and any shape of data export, the calibration process will retain all the calculations in the interface of the analysis method and carry out the same calculation process for all the data points of mapping, mapping analysis including two-dimensional images, three-dimensional images, and three kinds of functions of the image analysis, clicking on the function buttons for switching.



2.5.2.12D image interface

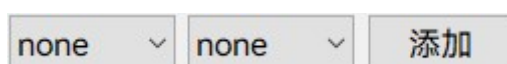
Click the mapping button, select the optional analysis list and click OK to start the image drawing of the 2D plane, the default is to draw the

image of all elements, when an element is a null value signal, the element will not be drawn. When an element is a null signal, the element will not be plotted. In the element plotting selection list, the naming rule of each chart name is chart serial number + element name.。

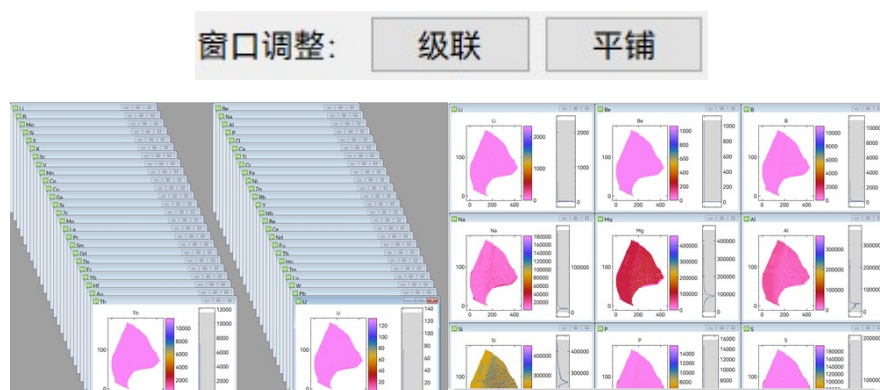


When plotting content tests, all elemental corrections are plotted by default, whereas age results are plotted for U-Pb dating.

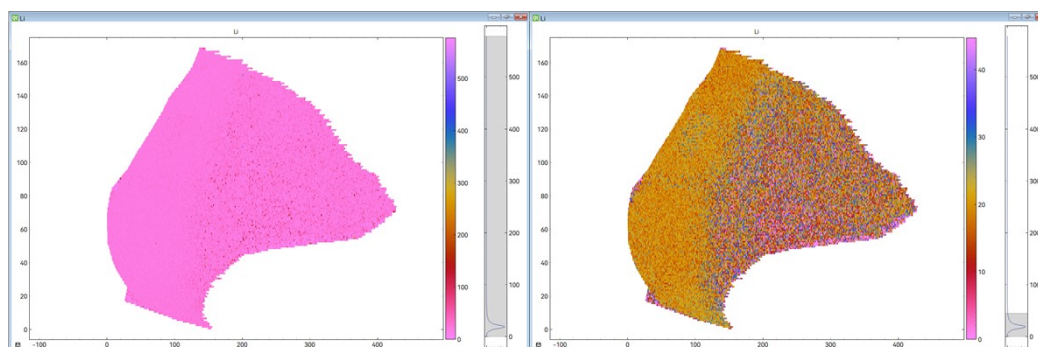
In addition to the elemental drawing results, the user only needs to switch none to any two elements, you can add your own elemental ratio image results, any one of them is none when only a single-element image drawing.。



To facilitate the display of multi-element images, cascading(left) as well as tiling (right) can be selected.。



In addition to the drawing area and colorbar in a single image, there is also a frequency distribution image of the image. By adjusting the size range of the gray area in the frequency distribution image, you can change the color distribution range of the image.



When exporting data, you can export scanned surfaces as images, svg files, and table data. Images include.png\jpg\tifthree kinds, table data exported in the form of .xlsx.

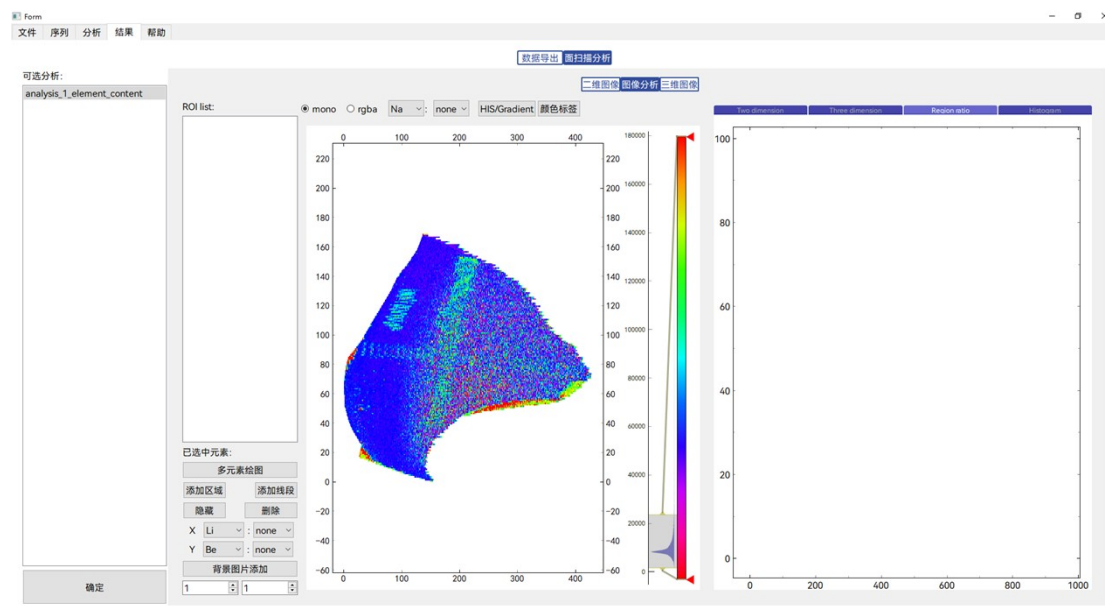
2.5.2.2 3D image drawing

When drawing 3D images, considering the speed of image drawing, users are required to add single element or element ratio images on their own, and the same as 2D image drawing, images can be added, multiple images can be arranged, and images can be deleted..

The information displayed in the 3D image is basically the same as the 2D plane, but the signal of a point in the 3D image is not only displayed by the color, the height of Z-axis can also represent the signal strength of the point. In the chart, there are X, Y, Z, M, A, V parameters, X, Y, Z indicates that the 3D image is displayed in X, Y, Z axes, M(Main) indicates that image is displayed in main view, A(Axis) indicates whether to add the axes, V(Value) indicates whether to add the axes.

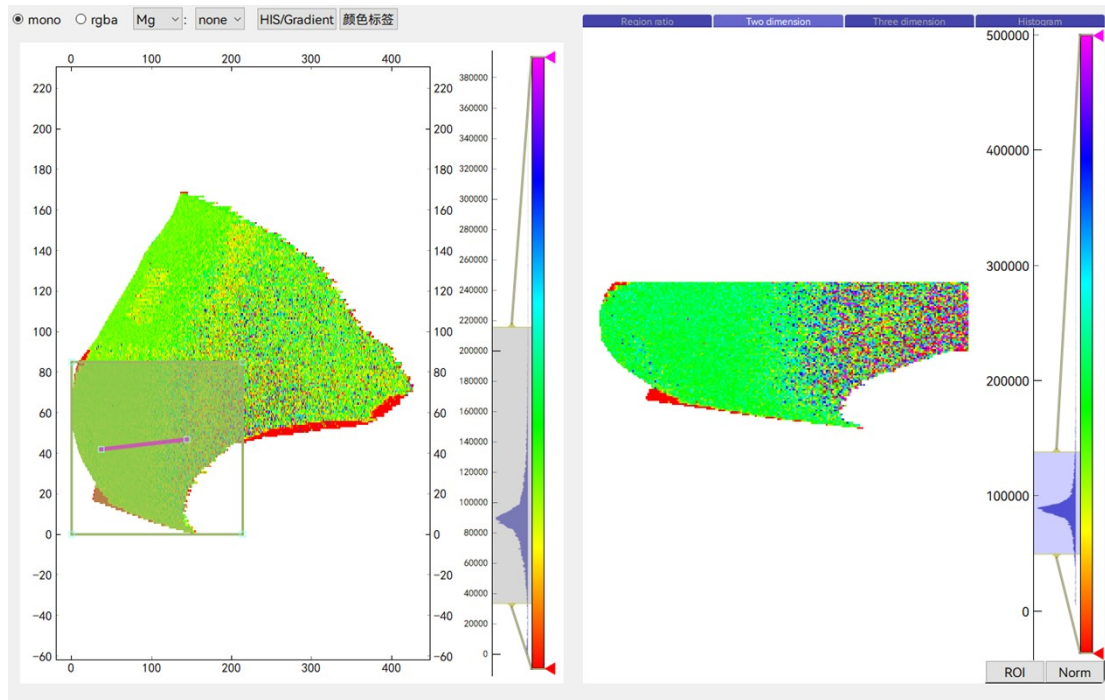
In the image modification settings, it supports users to modify the length, width and height ratio of the image by changing the length, width and height values, and changing the internal legend size parameter can modify the size of the legend in the chart. Click the Colorbar button or Histogram button to select the colorbar or histogram to show or hide in the chart..

2.5.2.3 image analysis

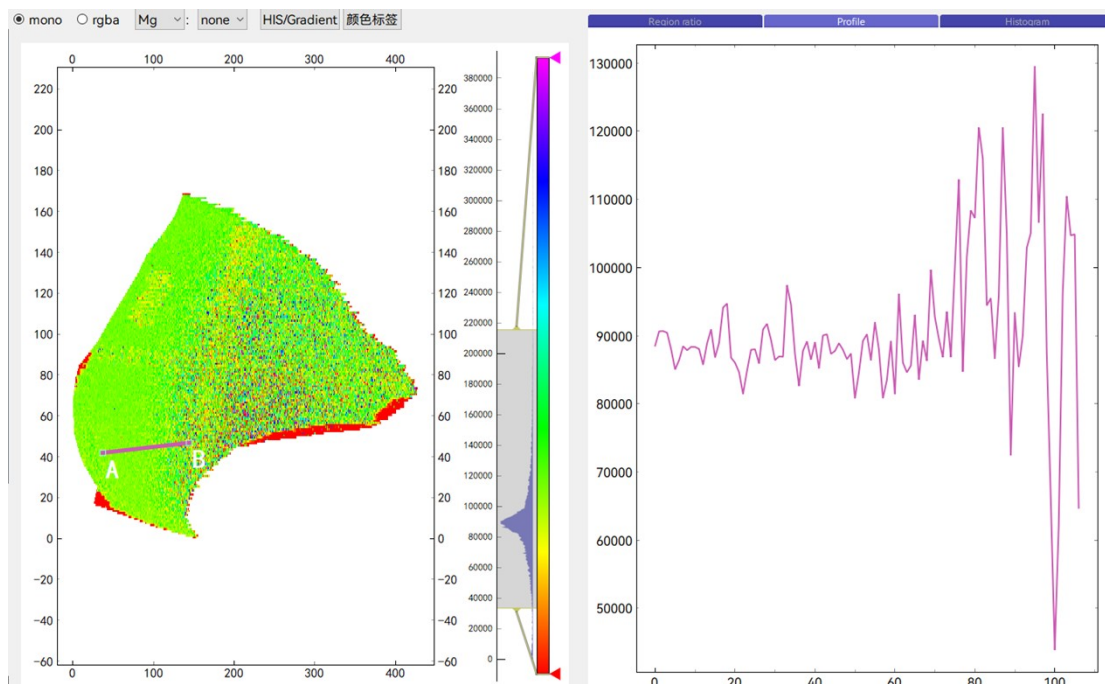


In the image analysis interface, you can add a ROI (region of interest) region by clicking Add Region, which is a rectangular region by default, and you can change the shape and size by dragging and dropping the edges. After adding ROIs, the Histogram, Ratio image, 2D image of the ROI region and 3D image of the ROI region will be drawn automatically.

The X and Y axis data of the ratio image can be either elemental content or elemental content ratio, and the data can be switched by the X and Y on the left side.

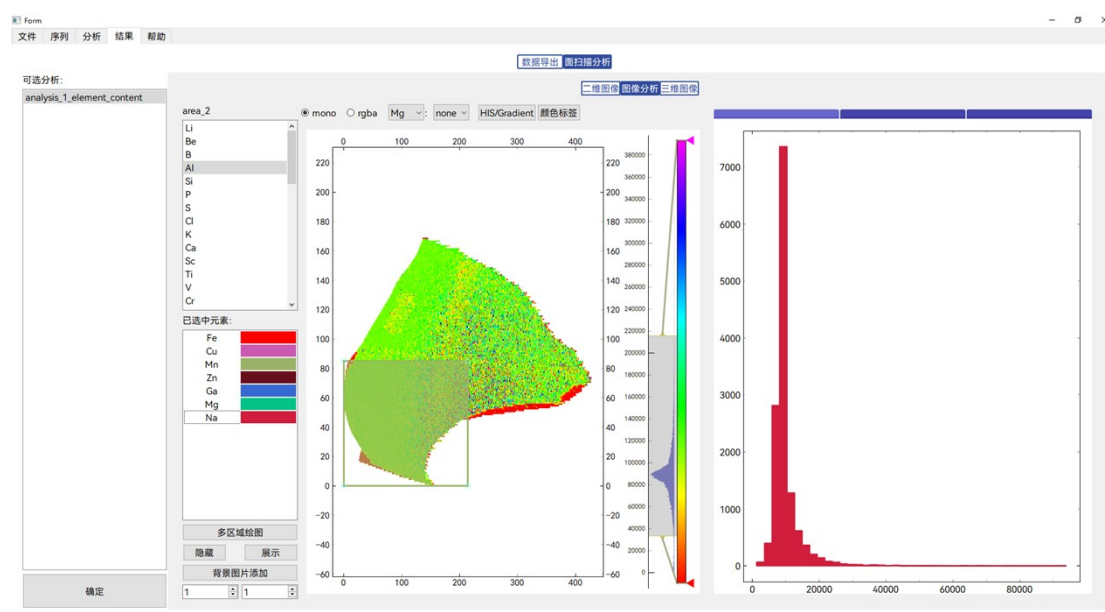


In addition to adding ROIs, it also supports the addition of line segments, which are generated when the segments are added, and generates an elemental profile, a Histogram, and a ratio image.



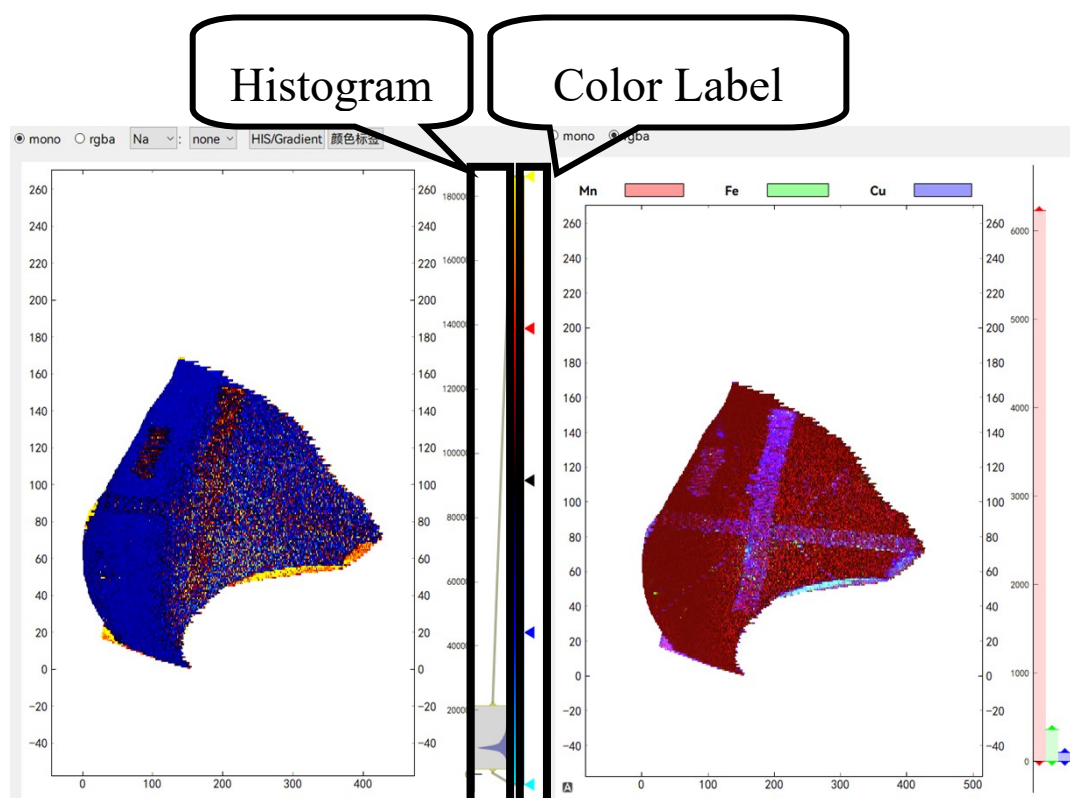
The ROI list displays the currently added ROI areas or segments. By clicking on the Color button you can change the color of the ROI area or segment and its color in the chart. The Hide and Delete buttons allow you to hide or delete a segment or ROI area.

After setting the appropriate ROI area or line segment, you can click the Multi-Element Plot button to compare the results of different elements after selecting the ROI area or line segment.



Two-dimensional plane drawing includes two modes, mono and rgba, in the commonly used mono mode, the main view of the chart can be drawn as a single element or element ratio for the image, by clicking on the HIS/Gradient button users can choose the color drawing of the HIS is hidden or not, and the Color Label button determines whether

the color labels are hidden or not(adding as well as moving the Color Label button in HIS image can change the color distribution pattern of the image).Selecting three elements at the same time in the selected element draws their rgba image by clicking on the rgba button above the image. The three elements are represented by red, green and blue in the rgba image, which shows the abundance of the three elements in a two-dimensional image, and better compares the distribution of the elements in the plane.



After the image has been drawn, you can choose to add a background image to add a specular or backscattered image of the mineral as a background and compare it to the 2D image.

2.5.3 line scan

data selection: Similar to the mapping setup, Line Scan provides plotting of each line scan result as well as data export. By default, all samples are selected for plotting. Users can freely select the objects to be plotted according to your specific needs.

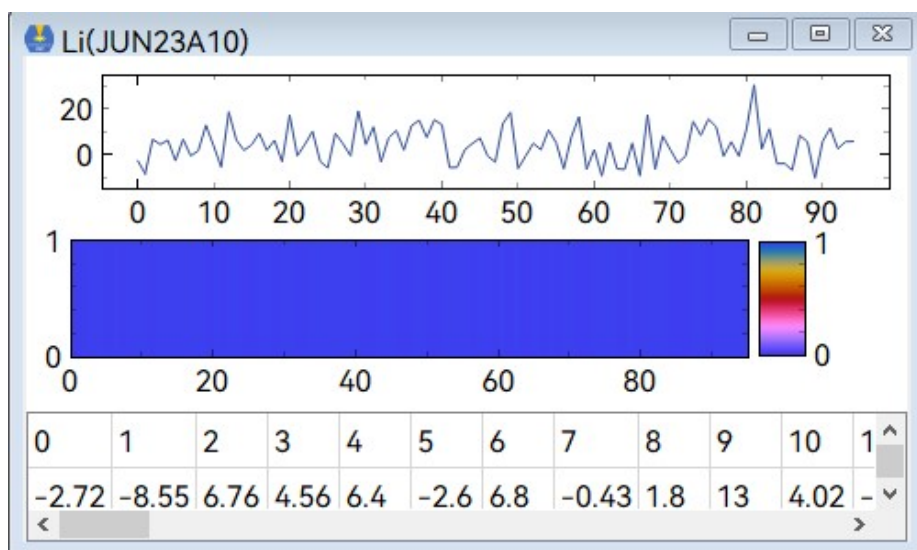
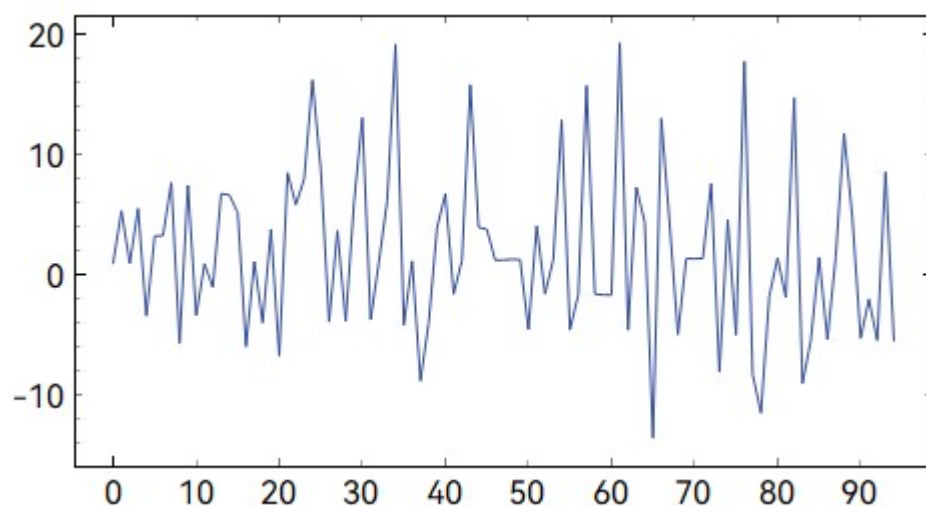
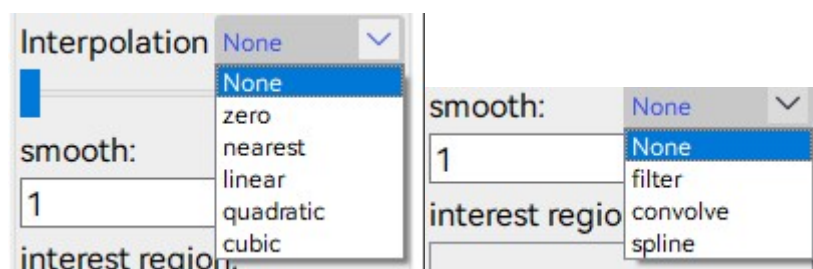
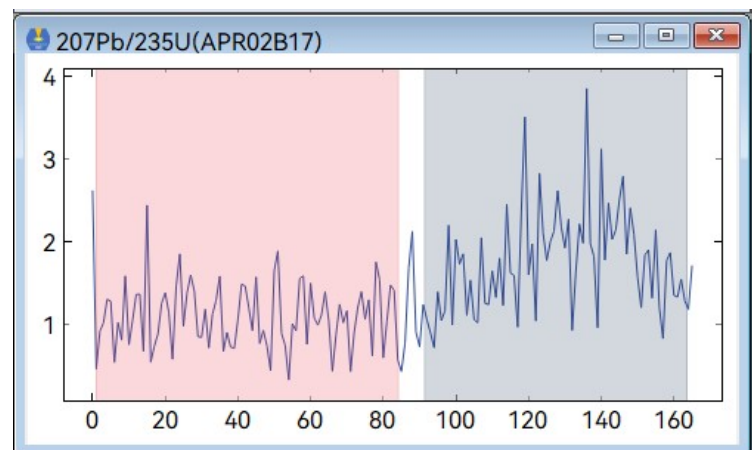
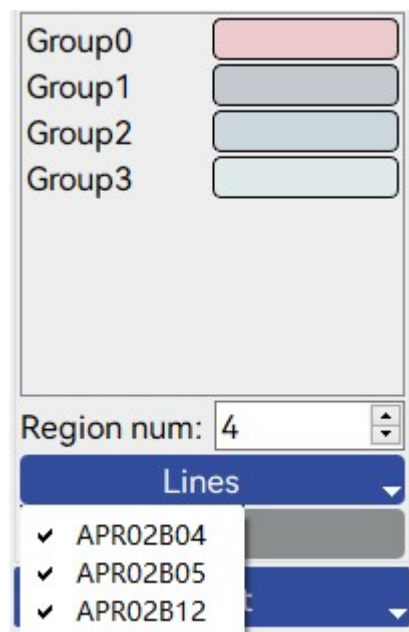
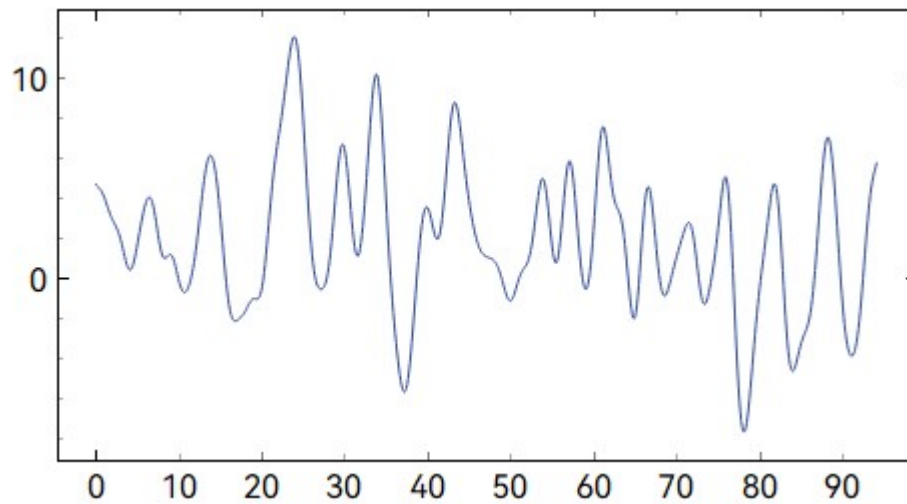


image display: A single file can consist of three parts: a line graph, a surface plot, and a table of results; the surface plot and the table of data are not displayed by default.◦

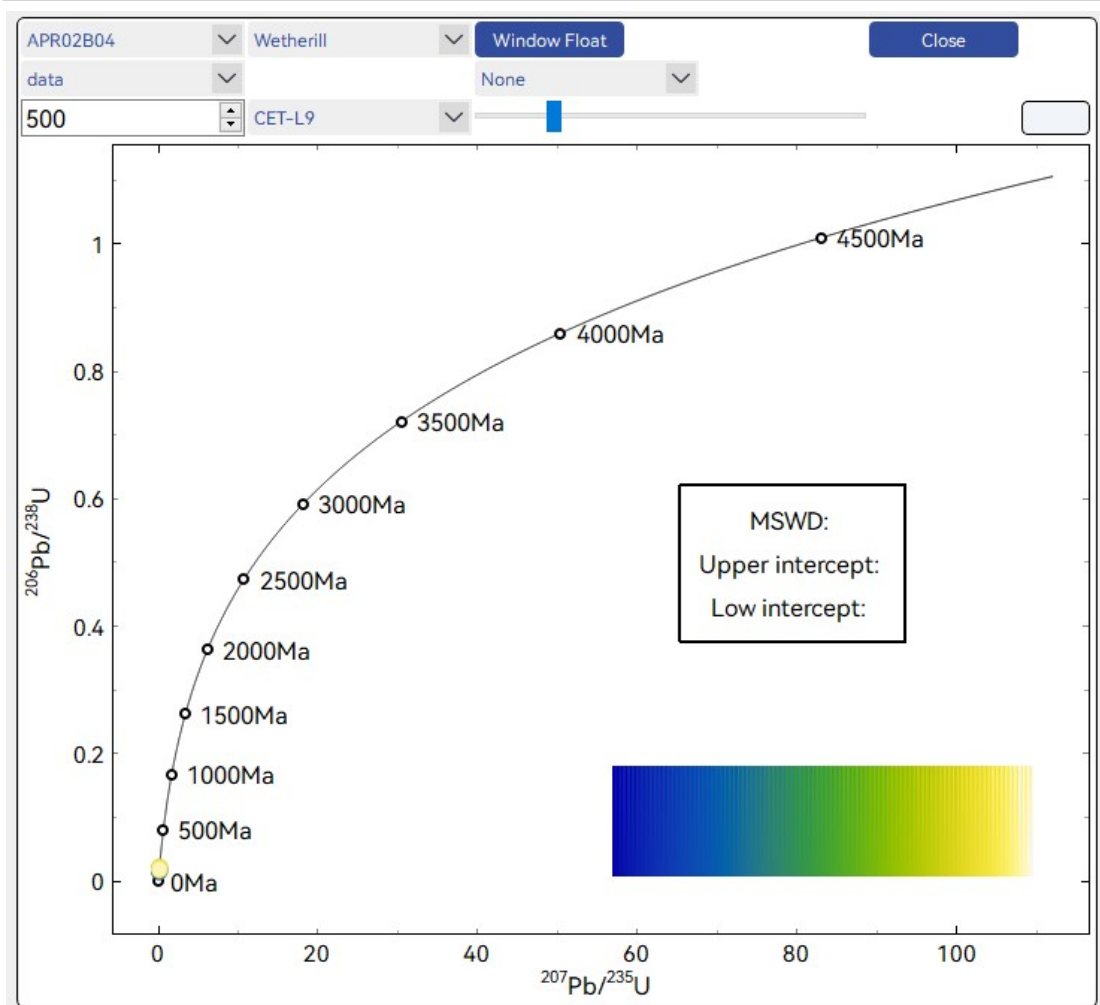
Data interpolation and smoothing: Data results can be recalculated using interpolation or smoothing functions



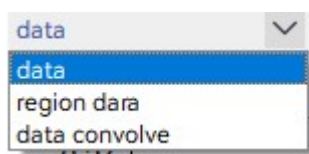


AddROI: Grouping of sample line scan
results with customizable group colors

U-Pb 年龄结果:

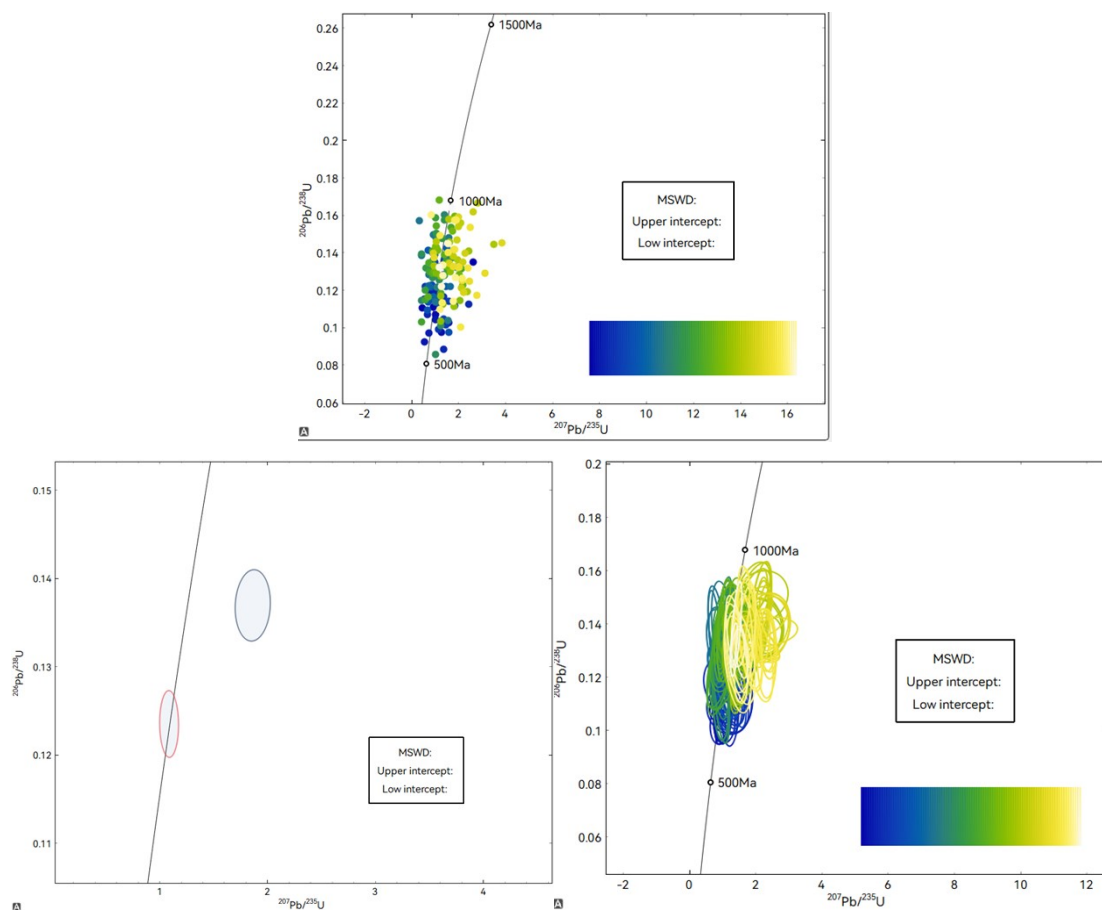


Individual sample line sweeps can be imaged, with a change in legend color indicating the order of the data as a function of stripping time.

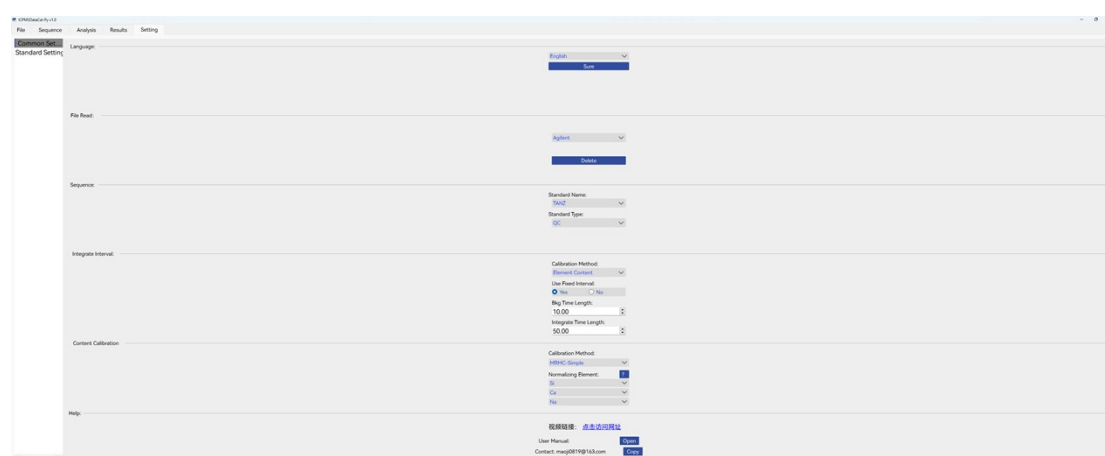


, The data plotting object, which can use data (which results in a scatterplot), region data (which plots the results in groups), and data convolve (which groups the results in fixed steps) to

compute the results and plot the image, supports both harmonic and disjunctive age image plotting.



2.6 Setting

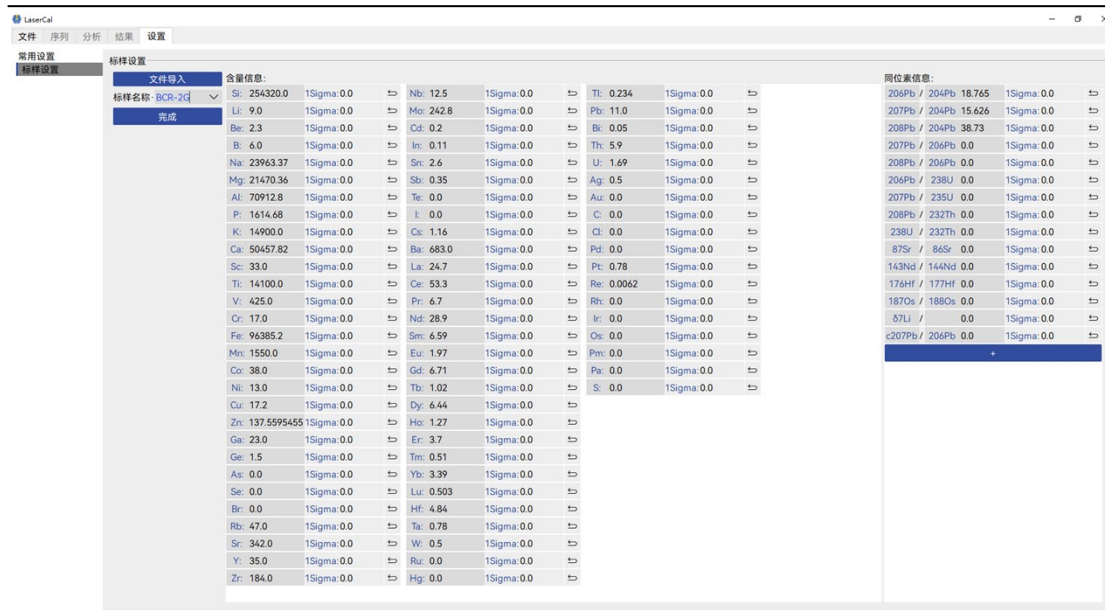


Users can modify the default settings of the software and add markers in the setup interface.

Common Settings:

- λ **Language Selection:** The current software supports switching between English and Chinese.
- λ **Sequence:** Select a specimen and set its default sample type, when the software recognizes a specimen during the sequence setting process, it will set the specimen as its default sample type.
- λ **Integration Interval:** Sets whether a fixed integration interval is used for a test type, as well as the default background interval and integration interval time length.
- λ **Content calibration:** Set the default calibration method used for content calibration and the preferred internal standard or normalizing element.
- λ **Help:** Open the user manual and contact the author.

RMs setting:



The software supports the modification and addition of reference materials

File import: supports the import of ".json" sample files from iolitev4.

Specimen modification: manually modify the element content or isotope ratio, when the isotope ratio does not exist in the list of isotope ratios, you can click on the plus sign to add.

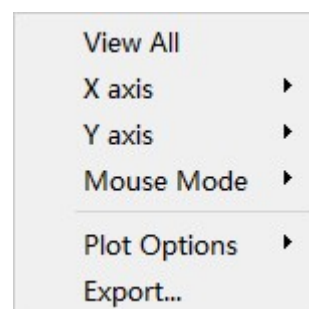
Specimen addition: manually modify the specimen name in the specimen name drop-down list and add the recommended value.

Note: Additions and modifications to the specimen data must be clicked on the **Finish** button to be saved.

caveat

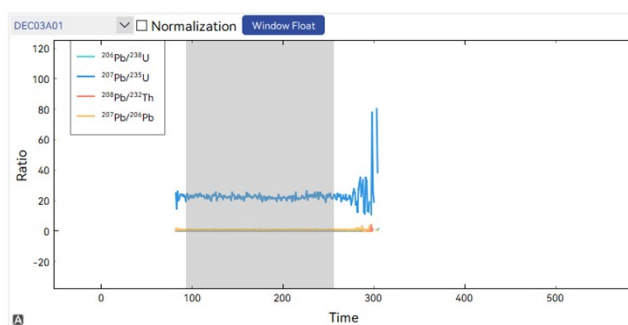
1. Interaction and manipulation

λ The drawing module used by the software has powerful interactive capabilities. The visualization range of the image can be changed using the mouse wheel and drag-



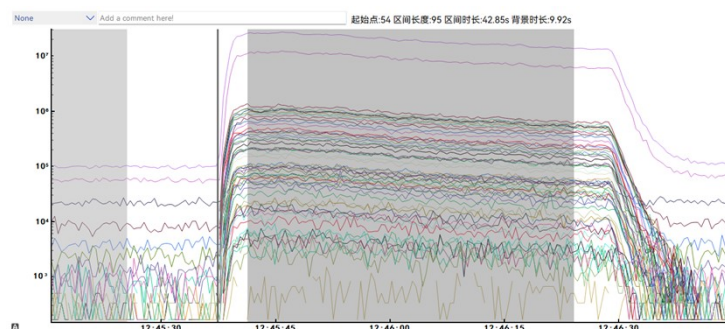
and-drop operations. Right-click to bring up the settings menu, which allows you to modify the visualization range, the mouse interaction mode, the table style, and to export the chart separately.

λ Due to the high interactivity when the user adjusts the image if you need to return to the



original image range, users can click on the black letter A in the lower right to quickly return to the initial state. .

2.Signal Selection Issues



It is recommended that the integration interval (gray shaded area on the right) does

not extend beyond the laser ablation starting point (black line) during signal selection

3.Differences in different calibration methods

The software has different optimization processes for different calibration methods in order to facilitate the user to obtain higher quality data results.

- λ Element Content(Element Content Test):its integral interval uses fixed position by default, and its integral method uses ROM by default.
- λ U-Pb dating: its integration interval uses a fixed position by default, and the integration method uses MOR by default.

Element Content+U-Pb Age (U-Pb age and element content are acquired simultaneously):

Its integration interval uses fixed position by default, and the integration method uses MOR by default. Under this test method, the content acquisition uses the internal standard method by default. Since the use of this method is generally zircon, the default internal standard element of the sample is Si, and the content of the internal standard element of the sample is 153000 ppm.

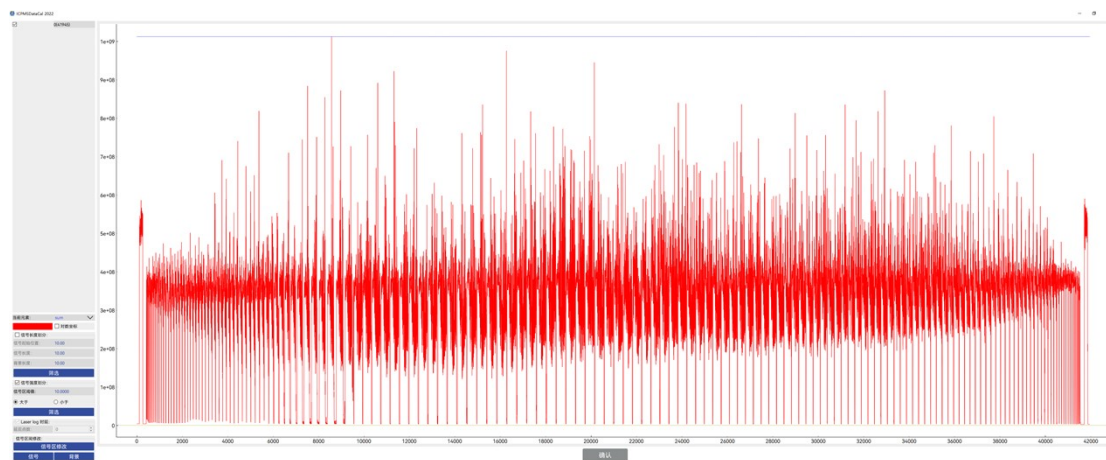
λ Single Pulse: Its integration interval is not fixed, and the integration method uses ROM by default. Since single-pulse stripping is only a change in stripping method and does not specify the calibration method, it is necessary for the user to select the calibration method by self.

λ Mapping: Since face-scan image plotting requires determining the location of each point in the image (unless the sample stripping area is rectangular). Therefore, the most logical approach to face-scanning exfoliation requires time-

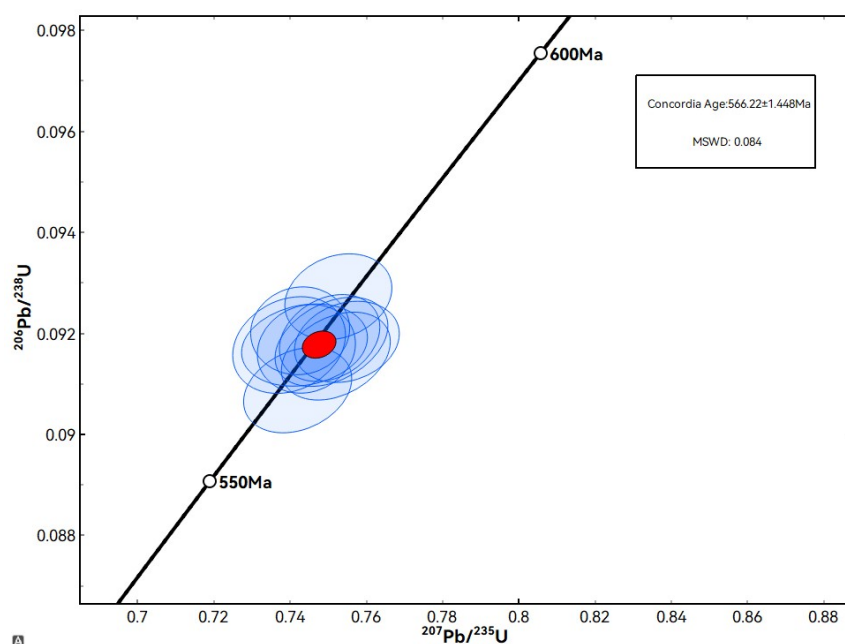
matching the log files of the laser exfoliation as well as the raw data files to determine the location of each point in the face-scan image.

4 Data reading for mapping

When the mapping area is rectangular, if the timestamp format matching fails or the laser fails to give a log file, the software will automatically pop up the setup screen for manually selecting the integration interval after the sequence setup is completed.



5. Plot of U-Pb dating:

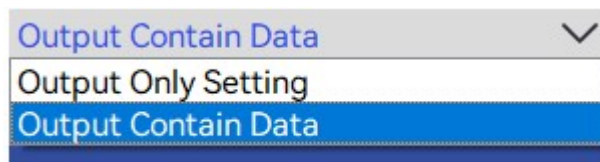


In the software, the U-Pb ratio calculation includes U-Pb age calculation and common Pb correction. The U-Pb age calculation module is suitable for real-time calculation of the results, so that the user can adjust the signal and other parameters according to the real-time feedback of the results, while the common Pb correction process may involve iterative calculations, and therefore the results cannot be refreshed in real time. The results cannot be refreshed in real time because of the iterative calculations that may be involved in the ordinary Pb correction process, but this also facilitates the drawing of a more beautiful image. Once the parameters have been determined, the normal Pb correction module can be clicked on to select the

appropriate samples for plotting. The calculation and plotting methods are from ISOPLOT.(Ludwig, 2003)。

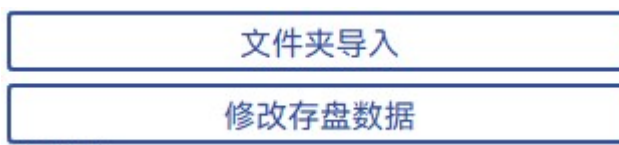
6. Importing, exporting and modifying saved data.

When exporting data results(note that it is not the result of surface scanning or line scanning), the

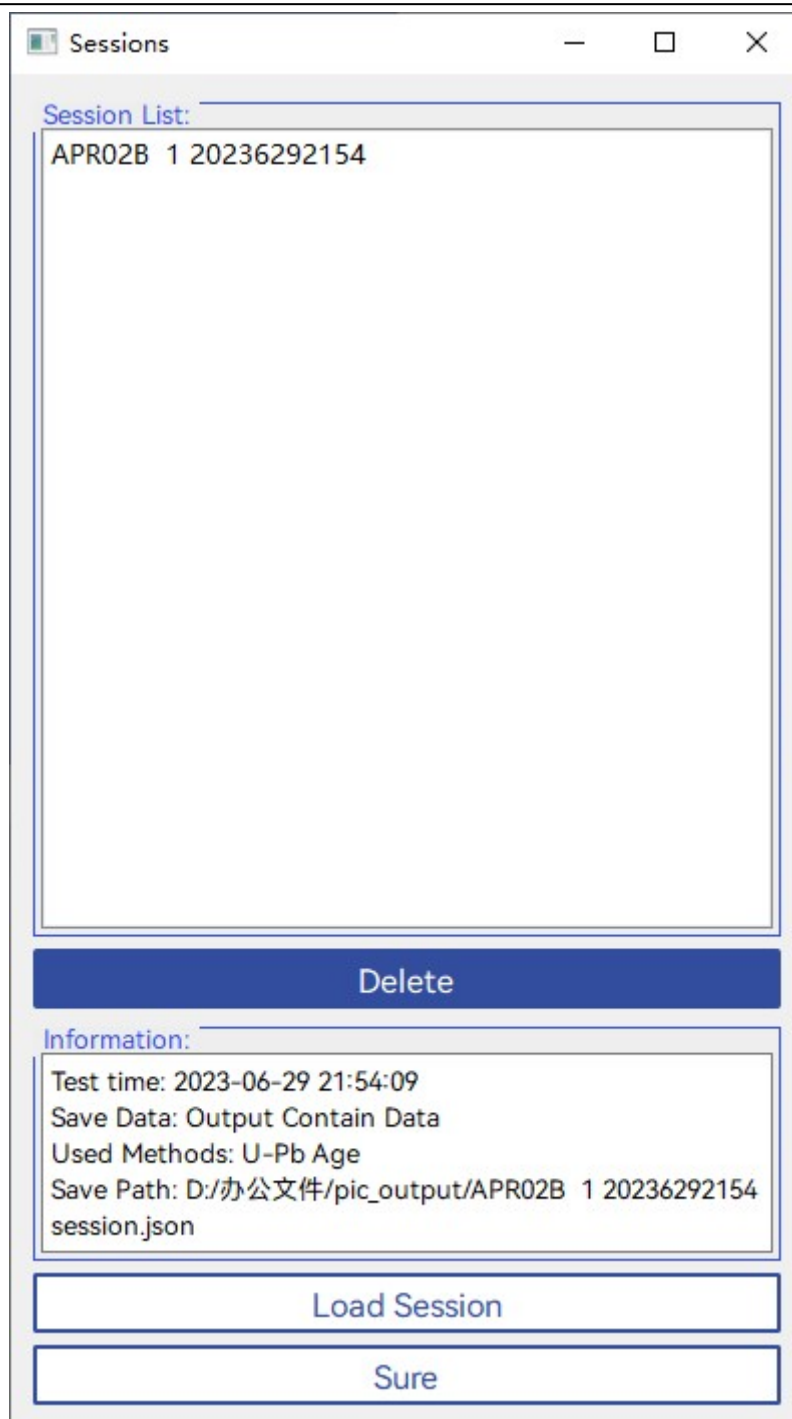


parameter file of the data processing process will be exported under the path at the same time, and

there can be two forms of export, if only the parameter



file is exported (only setting, with .json suffix), or it can be exported together with the original data (contain data with a .npz extension).To read the saved data, click Modify saved data in the data import interface and select the appropriate session.,



If only the parameter file exists, there is no need to import the data file when the original data file has not been migrated, if the data has been migrated or you need to change the computer to open it, then you need to import the correct data file before selecting the sequence file, if the

session file is exported together with the original data, you just need to make sure that the ".json" and ".npy" in the two in the same path to recover the stored data.

7.Problem solving

The software is currently in the development stage, in order to better improve the user experience. If you have any problems send an e-mail tomaoji0819@163.com Contact the author of the software.

bibliography :

- Chen, L. et al., 2011. Accurate determinations of fifty-four major and trace elements in carbonate by LA-ICP-MS using normalization strategy of bulk components as 100%. *Chemical Geology*, 284(3): 283-295.
- Liu, Y. et al., 2009. Continental and Oceanic Crust Recycling-induced Melt-Peridotite Interactions in the Trans-North China Orogen: U-Pb Dating, Hf Isotopes and Trace Elements in Zircons from Mantle Xenoliths. *Journal of Petrology*, 51(1-2): 537-571.
- Liu, Y. et al., 2008. In situ analysis of major and trace elements of anhydrous minerals by LA-ICP-MS without applying an internal standard. *Chemical Geology*, 257(1-2): 34-43.
- Longerich, H.P., Jackson, S., Günther, D., 1997. Laser-Ablation Inductively Coupled Plasma-Mass Spectrometric transient signal data acquisition and analyte concentration. *J. Anal. At. Spectrom.*, 12.
- Ludwig, K.R., 2003. Isoplot/Ex, a geochronological toolkit for Microsoft Excel, Version 3.00. Berkeley Geochronology Center.
- Paton, C. et al., 2010. Improved laser ablation U-Pb zircon geochronology through robust downhole fractionation correction. 11(3).