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Iso-Compass User Manual

Isotope Data Reduction Software

(Ver. 1.0)

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1. Software introduction

1.1 Iso-Compass

Iso-Compass is an isotope composition data reduction software developed by the LA-ICP-MS Division of **the State Key Laboratory of Geological Processes and Mineral Resources, China University of Geosciences (Wuhan)**. The software is mainly used for processing raw isotope data in a batch and pattern manner, with the aim of processing the isotope data rapidly and flexibly.

1.2 Software features

1. Reads MC-ICP-MS raw data simply and conveniently; combines graphs and tables to display data intuitively and accurately.
2. Flexibly writes data correction formulas, including instrument mass fraction correction (such as internal standard correction, SSB correction, and external element correction) and interference correction.
3. Satisfies solution MC-ICP-MS data reduction and laser MC-ICP-MS data reduction to achieve batch processing of high-precision isotopic composition absolute and delta data.
4. Quickly formulates the output report format to achieve a formatted report.
5. The software is based on the .Net framework and it can be used independently on the Windows operating system, without installing other commercial software.

1.3 Operating environment

Hardware requirements

• Recommended minimum configuration: Pentium 1 GHz or above, 512 MB RAM or above

• Minimum disk space: x86 – 850 MB; x64 – 2 GB

Applicable software

- Windows XP SP3
- Windows Vista SP1 or above
- Windows Server 2008 (not supported on Server Core roles)
- Windows Server 2008 R2 (not supported on Server Core roles)
- Windows 7 SP1 operating system and above
- Windows Server 2008 R2 SP1 operating system and above

2. Software installation

The Iso-Compass installation package contains the following files. Click "setup.exe" to start the installation.

Figure 2.1 Iso-Compass installation package

When the dialog box displayed in Fig. 2.2 pops up, click "Next."

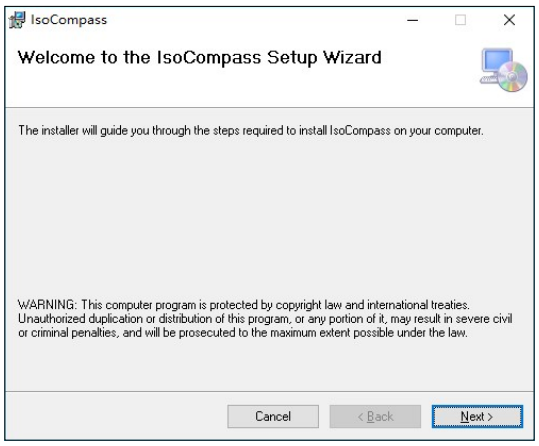


Figure 2.2 Installation process

Click "Browse" and select the software installation path.

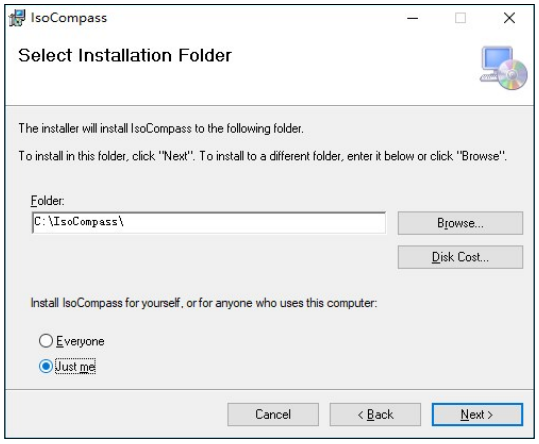


Figure 2.3 Installation process

After selecting the installation path, click "Next." Once the software installation is complete, click "Close" to exit.

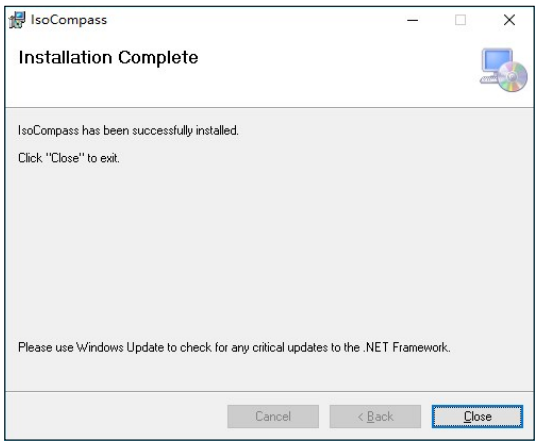


Figure 2.4 Software installation complete

This software comes with the Microsoft .NET Framework 4 installation package. If the installation system finds that the pre-installed Microsoft .NET Framework 4 is missing, the installation system will first install Microsoft .NET Framework 4, and then install the Iso-Compass software.

The Iso-Compass software following installation is illustrated in Fig. 2.5.

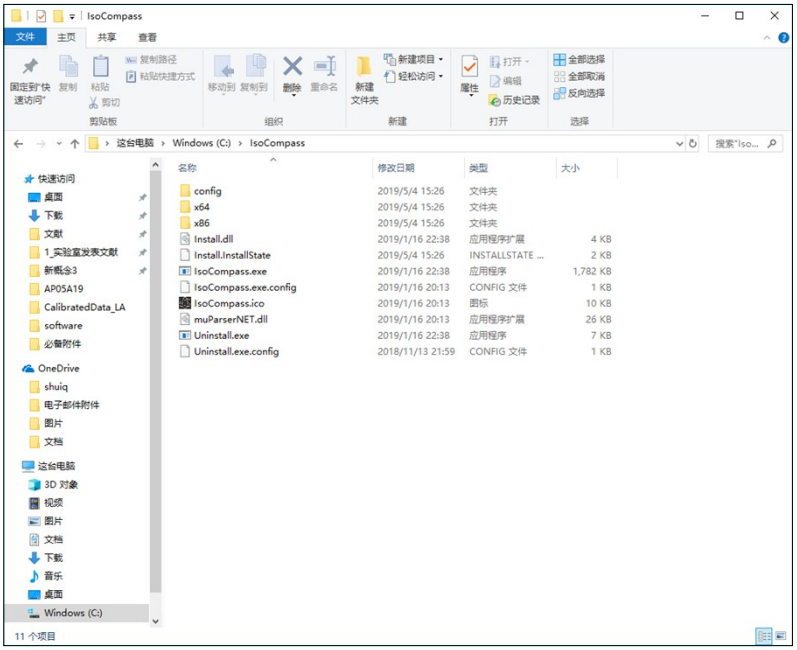


Figure 2.5 Iso-Compass folder

Once the software installation is complete, you need to register. Firstly,

click on the "IsoCompass.exe" file. Please open the file in **“administrator mode.”** If you are using the software for the first time, the following dialog box will pop up:

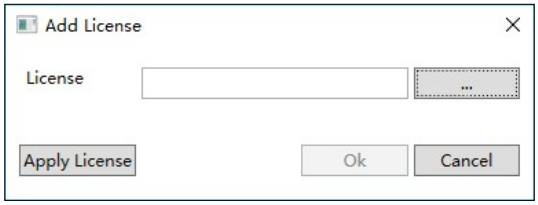


Figure 2.6 Verify software license

Please click "Apply License." The software will generate a document, "Requestcode.txt." Please send this document to the e-mail address "tuyaken@hotmail.com" to apply for a software license from the author. Please search for "Requestcode.txt" in the software installation folder.

After obtaining a valid software license, you can directly find the path where the software license is located. After confirming the license path, the software will prompt the validity period of the license. Please click "OK" to complete the verification.

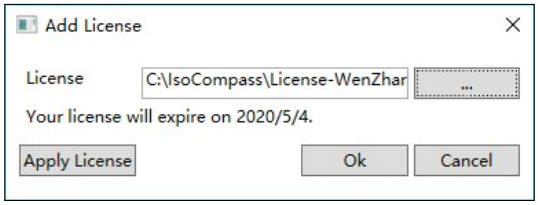
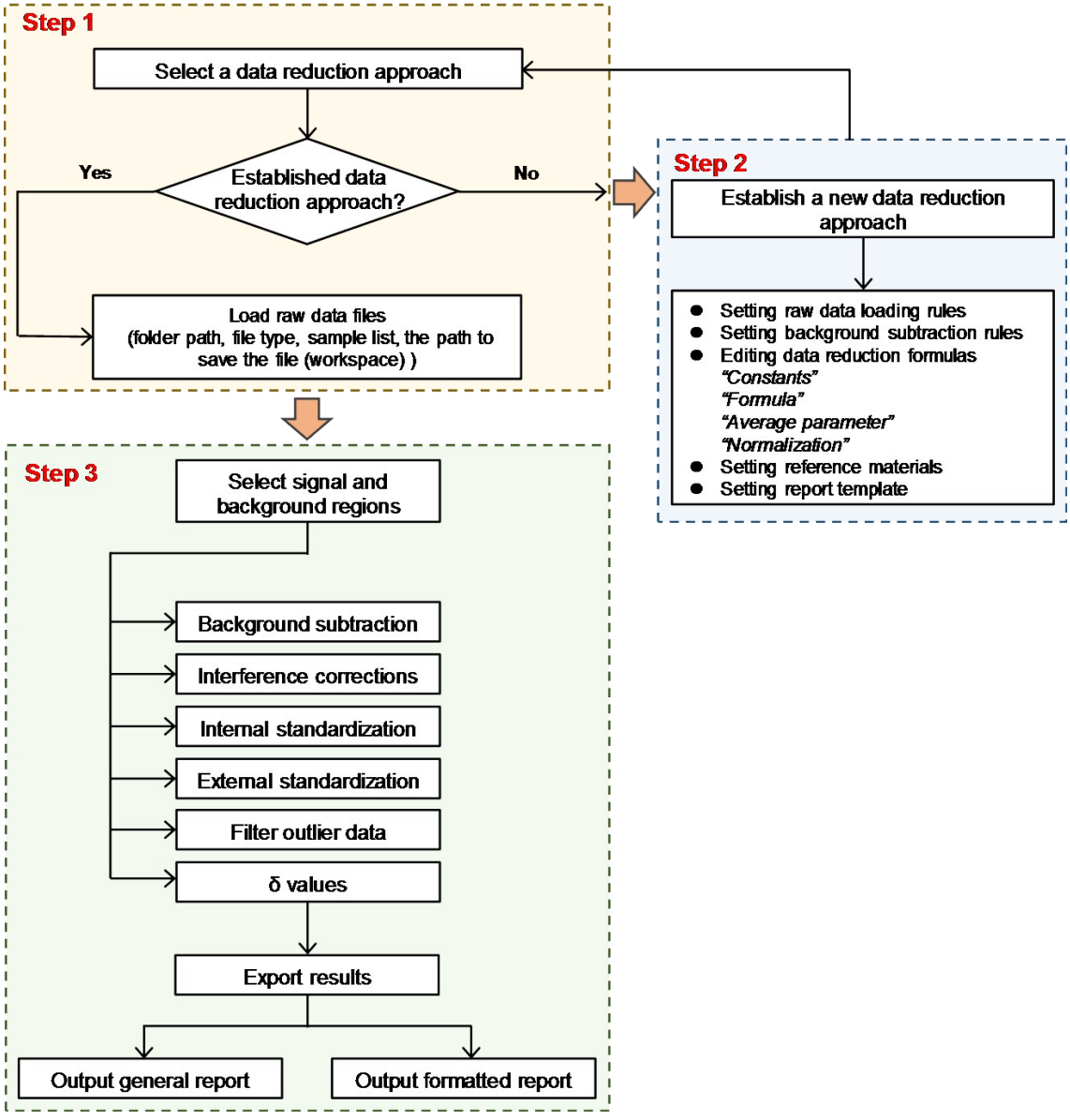


Figure 2.7 Software license verified

If the software license has expired, please send an e-mail to “tuyaken@hotmail.com” to obtain a new license.

3. Software workflow and functions

3.1 Software workflow



3.2 Select initial file information

After clicking the "IsoCompass.exe" file, the welcome screen will appear, followed by the initial dialog box of the software. In the initial dialog, you need to set "Workspace (data storage path)," "Folder (raw data storage path)," "File Type (raw data file format)," "SampleList (raw data list/optional)," and "Approach (Analysis method template)."

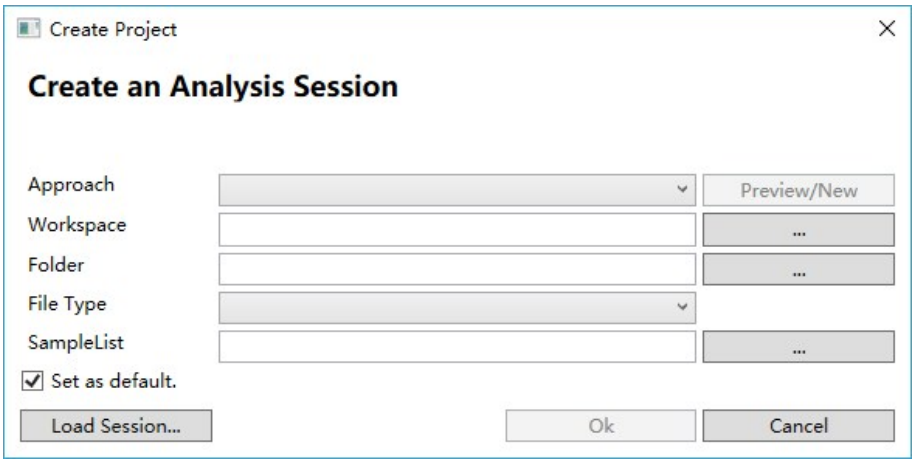


Figure 3.1 Iso-Compass data import interface

Workspace (data save path)

This is used to store all of the data output by the Iso-Compass software, including data reports saved in the output report and data reduction.

Folder (raw data storage path)

The folder in which the data to be processed are located.

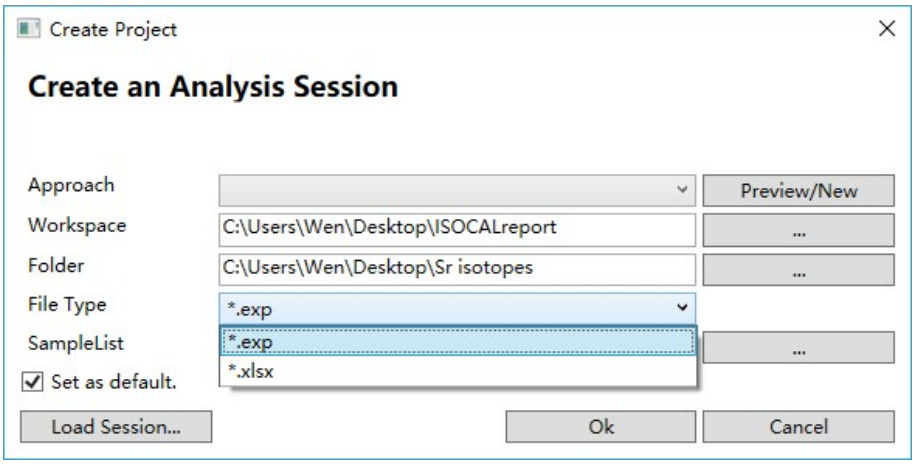


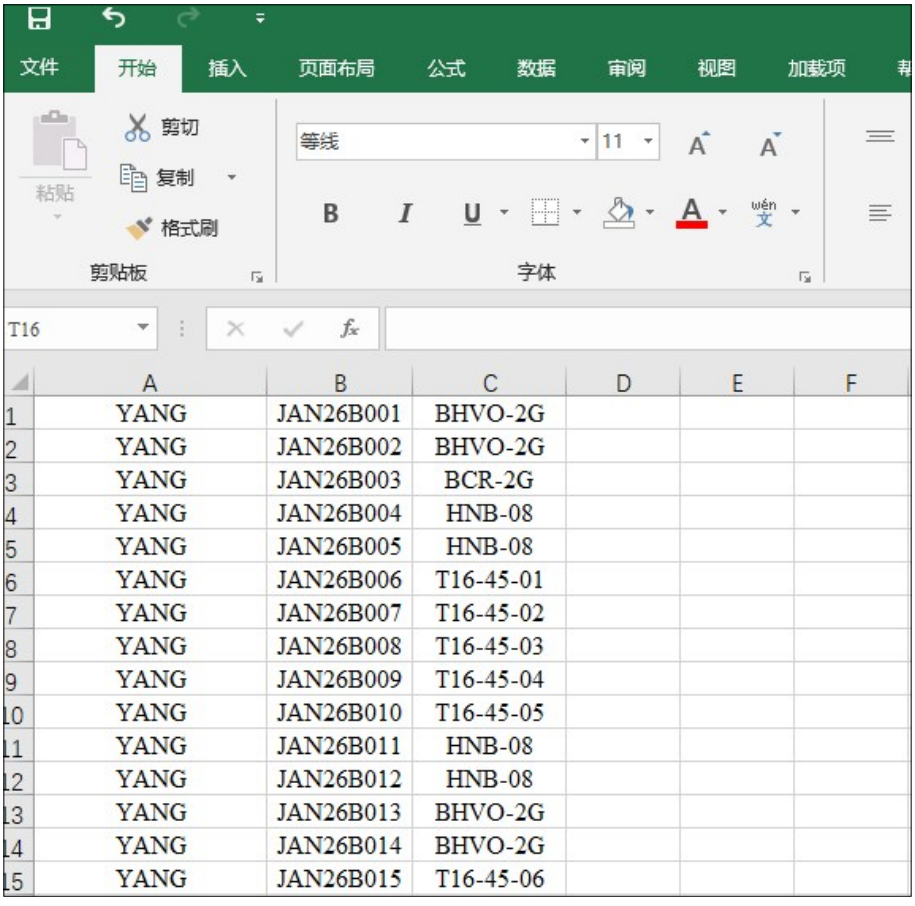
Figure 3.2 Iso-Compass data import interface

File Type (raw data file format)

In the folder where the data to be processed exist, if there are different document types, you can select the file format of the data to be processed. For example, the raw data files exported by Neptune Plus instruments are in the ".exp" format.

SampleList (raw data list/optional)

As Iso-Compass can read all data in the specified file format in "Folder (raw data storage path)," Iso-Compass can read data without relying on "SampleList." However, the data only have the analysis test name, and no sample name. If you need the sample name for external standard calibration, you need to prepare a sample list (Excel format). The sample list needs to be recorded in the specified format, as illustrated in Fig. 3.3. Iso-Compass will depend on the file name in "Folder (raw data storage path)" to find the corresponding sample name in "SampleList."



	A	B	C	D	E	F
1	YANG	JAN26B001	BHVO-2G			
2	YANG	JAN26B002	BHVO-2G			
3	YANG	JAN26B003	BCR-2G			
4	YANG	JAN26B004	HNB-08			
5	YANG	JAN26B005	HNB-08			
6	YANG	JAN26B006	T16-45-01			
7	YANG	JAN26B007	T16-45-02			
8	YANG	JAN26B008	T16-45-03			
9	YANG	JAN26B009	T16-45-04			
10	YANG	JAN26B010	T16-45-05			
11	YANG	JAN26B011	HNB-08			
12	YANG	JAN26B012	HNB-08			
13	YANG	JAN26B013	BHVO-2G			
14	YANG	JAN26B014	BHVO-2G			
15	YANG	JAN26B015	T16-45-06			

Figure 3.3 List file writing format

"Set as default"

This sets the parameters set above to the default values.

After setting "Workspace (data storage path)," "Folder (raw data storage path)," and "File Type (raw data file format)," you can select an edited analysis method template in "Approach (analysis method template)" and then click "OK" to start data reduction. You can also click "Preview/New" in "Approach" to view or modify the edited analysis method template.

If no suitable analysis method template is available, you can click "Preview/New" to create a new analysis method template (see following section).

You can click "Load Session" to read the previously saved session data.

3.3 Create analysis method template

3.3.1 Read data

Click "Preview/New" in "Approach" and an initial analysis method template will appear.

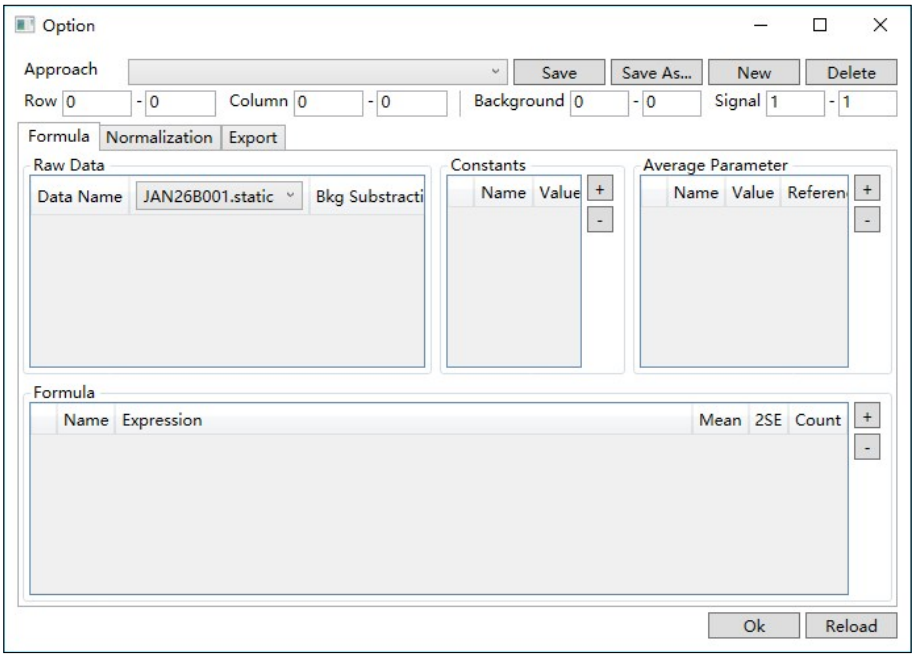


Figure 3.1 Initial analysis method template interface

First click "New" and enter the name of the new analysis method.

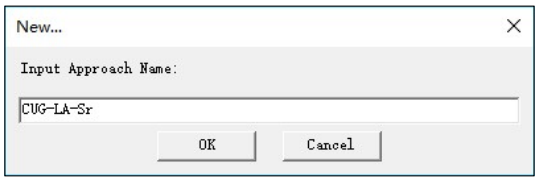


Figure 3.2 Enter name of new analysis method

Thereafter, you need to set the "row" and "column" path of the file data to be processed. You need to open a raw file of the data to be processed, as with the Sr isotope raw data file displayed below:

R152

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Triton Analysis Data Report												
2	Run-Number-View												
3	Filename: F:\2019_LASER\MC19_025_YANGXIAOSONG\JAN26B01.dat												
4	Date: 2019/1/28												
5	Sample ID:												
6	Method Name:												
7	Wheel ID:												
8	Run number: 0												
9	Analysis date: 2019/1/28												
10	Analysis time: 10:59:23												
11	Operator:												
12	Instrument:												
13	Comment:												
14													
15	Cycle	Time	83Kr	167Er++	84Sr	85Rb	85.9	173Yb++	87Sr	88Sr			
16	1	14:39:55:4	1.83E-04	4.57E-05	1.06E-03	1.07E-05	3.10E-04	-7.01E-05	1.33E-04	-8.97E-05			
17	2	14:39:55:9	2.13E-04	-5.38E-05	1.06E-03	-5.66E-06	2.58E-04	-5.56E-05	3.15E-05	5.89E-05			
18	3	14:39:56:5	2.63E-04	2.25E-05	1.06E-03	-4.43E-05	3.41E-04	-5.87E-05	-5.31E-05	5.77E-05			
19	4	14:39:57:0	1.85E-04	1.78E-05	9.78E-04	-5.89E-06	3.46E-04	-6.78E-05	-4.84E-05	1.88E-05			
20	5	14:39:57:5	1.95E-04	-3.55E-06	1.06E-03	-6.72E-05	2.71E-04	-1.60E-05	3.34E-05	1.36E-05			
21	6	14:39:58:0	1.62E-04	2.58E-05	1.12E-03	-4.52E-05	4.80E-04	-2.09E-05	7.61E-07	-5.90E-06			
22	7	14:39:58:6	2.42E-04	8.74E-06	9.92E-04	1.58E-04	2.81E-04	-5.45E-05	-2.12E-05	3.09E-05			
23	8	14:39:59:1	2.31E-04	2.39E-05	1.03E-03	1.14E-04	3.57E-04	-6.72E-06	-6.18E-05	3.35E-05			
24	9	14:39:59:6	3.01E-04	-2.82E-05	1.02E-03	1.06E-04	3.93E-04	-3.66E-05	-2.78E-05	3.75E-05			
25	10	14:40:00:1	2.57E-04	-2.38E-05	1.05E-03	4.41E-06	3.26E-04	-4.73E-05	-2.29E-05	4.06E-05			
26	11	14:40:00:7	1.88E-04	-2.30E-05	1.14E-03	7.58E-05	3.96E-04	-4.62E-05	-5.29E-05	9.83E-07			
27	12	14:40:01:2	1.91E-04	6.69E-06	1.07E-03	-1.08E-05	3.98E-04	-4.83E-05	-1.12E-04	-1.63E-06			
28	13	14:40:01:7	2.54E-04	1.17E-05	1.01E-03	-1.27E-05	2.81E-04	-9.05E-05	-4.21E-07	-8.12E-05			
29	14	14:40:02:3	2.10E-04	2.67E-05	9.91E-04	1.05E-05	3.29E-04	-6.19E-05	9.48E-05	1.08E-04			
30	15	14:40:02:8	2.18E-04	-5.29E-05	9.85E-04	-1.43E-05	3.32E-04	-4.55E-05	-3.99E-05	1.78E-05			
31	16	14:40:03:3	2.35E-04	1.01E-05	1.07E-03	2.36E-05	2.74E-04	-4.06E-05	-9.16E-06	-6.38E-06			
32	17	14:40:03:8	1.83E-04	7.18E-06	1.01E-03	3.13E-05	3.38E-04	-1.83E-05	3.45E-05	9.06E-06			
33	18	14:40:04:4	1.81E-04	-1.84E-05	1.03E-03	7.53E-05	2.52E-04	-2.83E-05	-4.58E-05	-4.70E-05			
34	19	14:40:04:9	2.00E-04	-3.57E-05	1.12E-03	5.92E-05	2.98E-04	-9.55E-06	-3.75E-05	1.43E-05			
35	20	14:40:05:4	1.92E-04	2.55E-05	1.04E-03	9.32E-06	3.27E-04	-6.24E-05	-7.11E-05	7.20E-05			
36	21	14:40:05:9	2.02E-04	1.75E-05	9.43E-04	6.43E-05	3.28E-04	-4.90E-05	-2.48E-05	-5.62E-05			
37	22	14:40:06:5	2.57E-04	7.44E-06	1.03E-03	7.92E-06	3.07E-04	-5.28E-05	-7.22E-05	1.19E-05			
38	23	14:40:07:0	2.61E-04	3.43E-05	9.87E-04	3.83E-05	3.96E-04	-2.86E-05	-1.13E-05	7.10E-05			
39	24	14:40:07:5	1.94E-04	4.27E-05	1.06E-03	-1.97E-05	3.47E-04	-3.31E-05	1.94E-06	-1.04E-05			
40	25	14:40:08:0	2.04E-04	-3.17E-05	9.67E-04	-2.79E-05	4.05E-04	-2.18E-05	-2.71E-05	3.07E-05			
41	26	14:40:08:6	2.02E-04	-6.55E-05	1.03E-03	-3.14E-05	2.45E-04	-4.87E-05	6.38E-05	4.42E-05			
42	27	14:40:09:1	2.29E-04	-3.40E-05	9.76E-04	-2.48E-05	3.50E-04	-7.10E-05	-1.60E-06	2.02E-05			
43	28	14:40:09:6	2.00E-04	1.10E-05	1.09E-03	3.74E-05	2.39E-04	-6.84E-05	-1.28E-04	9.53E-06			
44	29	14:40:10:2	2.50E-04	-9.65E-06	1.02E-03	-1.81E-05	4.43E-04	-2.21E-05	5.49E-06	-5.62E-05			
45	30	14:40:10:7	2.19E-04	-5.22E-05	1.06E-03	4.09E-05	3.44E-04	-1.85E-05	-3.33E-05	3.40E-05			
46	31	14:40:11:2	2.26E-04	-5.29E-05	1.10E-03	-3.32E-06	2.60E-04	-8.96E-05	7.30E-05	5.97E-06			
47	32	14:40:11:7	2.41E-04	1.59E-05	8.98E-04	-1.76E-05	1.59E-04	-3.76E-05	1.35E-05	5.02E-06			
48	33	14:40:12:3	1.68E-04	3.05E-05	9.35E-04	6.60E-05	3.24E-04	-3.98E-06	4.49E-05	-7.36E-05			
49	34	14:40:12:8	1.93E-04	2.32E-05	1.04E-03	1.82E-05	3.46E-04	-6.19E-05	1.38E-05	-4.98E-05			
50	35	14:40:13:3	1.54E-04	1.84E-05	1.09E-03	4.44E-05	3.91E-04	-3.27E-05	-1.20E-04	-3.27E-05			
51	36	14:40:13:8	2.15E-04	-8.23E-06	9.75E-04	7.32E-05	3.54E-04	-4.51E-05	4.66E-05	-1.68E-05			
52	37	14:40:14:4	2.02E-04	-1.50E-05	9.65E-04	-7.42E-07	2.74E-04	5.42E-06	-5.38E-06	-4.44E-05			

Figure 3.3 Sr isotope raw data file of Neptune Plus (in ".exp" format)

You should find the start and end numbers of the row and column of the data to read them. For example, the data start at row 16 and end at row 175, and start at column C (column 3) and end at column J (column 10).

Enter the data into "Row" and "Column."

Figure 3.4 Enter row and column numbers of data to read them

You can design the background and signal interval in the imported data in advance. For example, the 1st to 45th data points are background intervals, while the 65th to 140th data points are signal intervals.

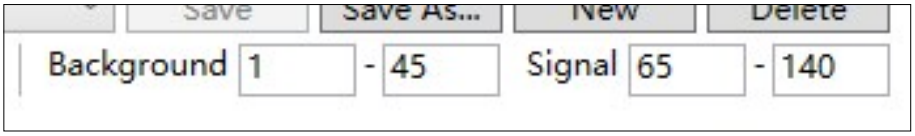


Figure 3.5 Set signal acquisition interval of data

3.3.2 "Formula" module

After setting the “row” and “column” locations of the data, “Raw Data” will display the name of the isotope to be tested for each data column. Note: "r_1, r_2, r_x" are used as the code of the corresponding isotope, which is used for subsequent formula editing.

Check the small box under "Bkg Substraction" and the ticked "Bkg Substraction" box to which it refers will perform background correction. The background deduction principle of the Iso-Compass software is as follows: firstly, select the interval of the background signal through "Background," then remove the 2SD outlier data from the background interval and calculate the average of the remaining data as the "background value." Data with the ticked "Bkg Substraction" box will subtract "background value" from the original data.

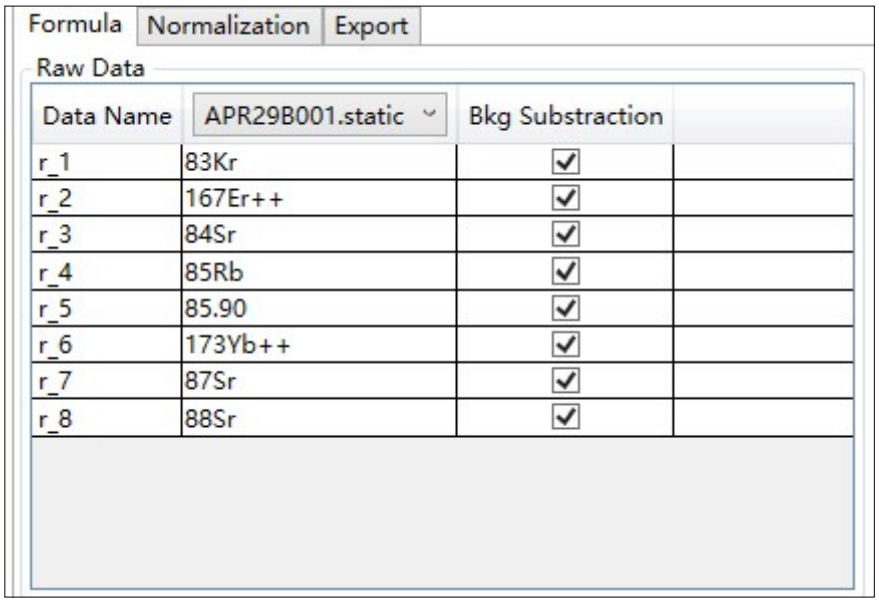


Figure 3.6 Original signal reading and background value subtraction

You can edit formulas in "Formula," including calculation methods such as addition, subtraction, multiplication, division, and exponent. As indicated in the figure below, "f1" refers to a formula code, which can be used for formula calculation. "Name" refers to the actual formula name and it cannot be used in calculations, but it is indicated as the formula name in the following diagrams. You can enter specific formulas in "Expression."

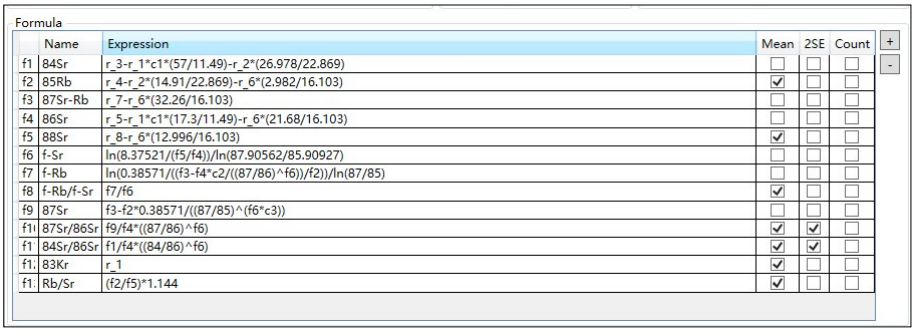


Figure 3.7 Data reduction and editing formulas

For example, the original signal of ^{84}Sr is (r_3), and the interference from $^{83}Kr^{+}$(r_1) and $^{67}Er^{++}$ (r_2) needs to be subtracted. Then, the correction formula is "“r_3-r_1*c1*(57/11.49)-r_2*(26.978/22.869),” where "c1" is a constant parameter set in "Constants." "Constants" can be used to record certain commonly used constant parameters, but the value must be a number and not a formula.

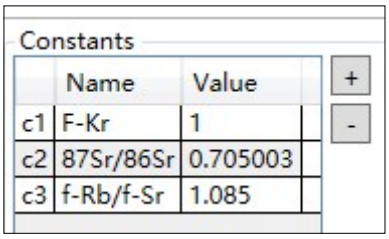


Figure 3.8 Designing constant terms in formula editing

Note: The data in "Formula" are calculated based on the data in each "cycle" (the smallest data unit), following which the average value and relative standard error (2SE) are provided.

Calculations supported by "Formula":

Addition: “+” Subtraction: “-”

Multiplication: “*” Division: “/”

Index: “^” Natural logarithm: “ln()”

Iso-Compass provides a special constant calculation mode, "Average Parameter." The calculation module supports entering a calculation formula to obtain a constant. That is, the user can enter a calculation formula in this module; for example, the calculation formula for calculating the Hf isotope fractionation factor in Hf isotope analysis, and then the formula outputs the average value of the fractionation factor. The user can opt to use the average value of the fractionation factor to correct the mass fractionation or use the fractionation factor in "Formula" to perform a one-to-one mass fractionation correction.

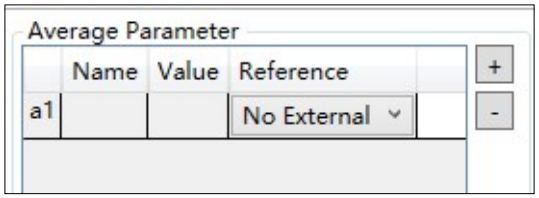


Figure 3.9 Designing variable constants in formula editing

The "Average Parameter" function can also be used. You need to use a calibration parameter in the reference material to correct the data in the actual analysis sample. For example, if you need to correct the interference of Rb on the Sr isotope, you can analyze a reference substance containing Rb before analyzing the actual sample, calculate the Rb isotope fractionation factor from

the reference substance, and then use this isotope fractionation factor for the actual sample. You simply need to select the desired "Reference" name in "Average Parameter" (such as NIST610). This indicates that the constant "a1" is calculated by all selected NIST610 in this data reduction, and this constant can subsequently be used in the "Formula" formula.

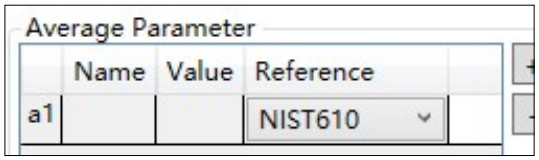


Figure 3.10 Designing variable constants in formula editing

3.3.3 "Normalization" module

The "Normalization" module is used to implement external standard correction. External standard calibration first requires the user to provide an accurate sample name. A reference material data file “ReferenceData.exp” (C:\IsoCompass\config) is provided in Iso-Compass. The user can add the required reference substance name to the database, and enter the isotope name and accurate isotope ratio.

	A	B	C	D	E	F	G	H
1		208Pb/206Pb	207Pb/206Pb	208Pb/204Pb	207Pb/204Pb	206Pb/204Pb	87Sr/86Sr	84Sr/86Sr
2	NIST610	2.169	0.91	36.991	15.515	17.052		
3	NIST612	2.165	0.907	37.02	15.516	17.099		
4	BCR-2G	2.063	0.832	38.709	15.614	18.761	0.705003	0.05657
5	BHVO-2G			38.273	15.591	18.778	0.703469	0.05657
6	BIR-2G						0.703105	0.05657
7	NBS981	2.168	0.915	36.726	15.5	16.942		
8	NBS987						0.710241	0.05657

Figure 3.11 Reference material data file "ReferenceData.exp"

You can find the names of the reference materials in the database in "Reference Materials" of "Normalization" in the software and then select the required reference materials.

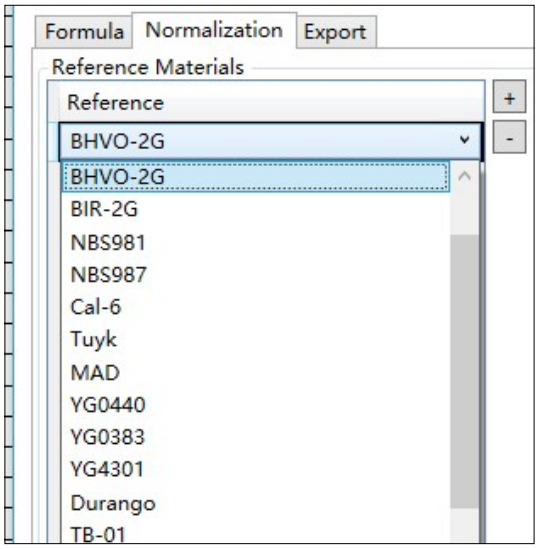


Figure 3.12 Selecting externally calibrated reference substance

In "Corrected Isotopic Ratio," select the isotope ratio of the reference material in the "Reference Isotope" column and then select the name of the formula written in the "Formula" module in the actual analysis in "Measured Data". As indicated in the figure below, $^{87}Sr/^{86}Sr$ is provided to correct the reference value of the reference substance.

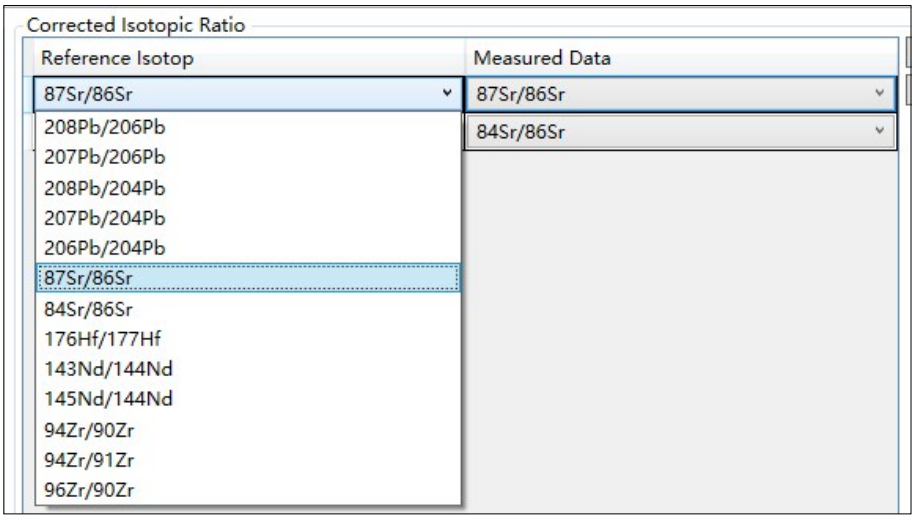


Figure 3.13 Selecting isotope ratio for external calibration

After selecting the ratio of the reference material for the isotope to be corrected, select the correction scheme at the bottom:

No Correction: No external standard correction.

Mean Correction: Use the reference material before and after to calculate

the correction factor, and take the average of the correction factor to correct the unknown sample.

Interpolation Correction: Calculate the average value of the front and back reference material separately. It is assumed that the isotope fractionation changes between the front and back reference materials in a linear manner. The linear interpolation method is used to calculate the correction factor for each unknown sample.

Delta Calculation: After checking "Mean Correction" or "Interpolation Correction," you can also decide whether to calculate the delta value.

Figure 3.14 External correction strategy

3.3.4 "Export" module

You can select the data to be exported in the "Export" module, which uses the parameters edited in "Formula." Select "Add all" and all of the data ticked in the "Mean" column of "Formula" will be listed. These data can be output to "Workspace (data storage path)." "Export Name" is the final export name, which you can edit again.

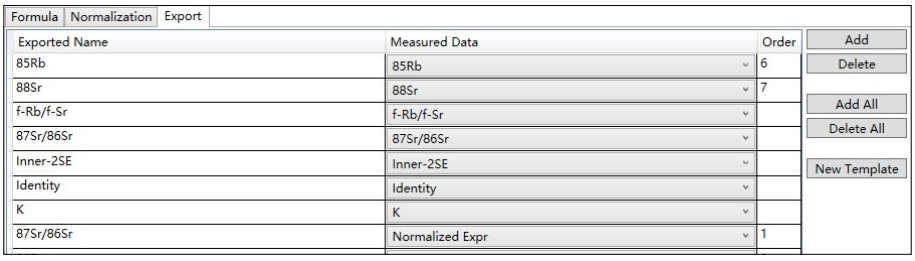


Figure 3.15 Data export

Iso-Compass provides a formatted report "New Template." Prior to formatting the output, you need to perform the following:

(a) Edit and determine the final "Export Name."

(b) Set the data to be output and the data order in the "Order" column. As indicated in the figure below, the data to be output, including “87Sr/86Sr,” “2SE,” “84Sr/86Sr,” and “Rb/Sr,” are numbered in the order of 1, 2, 3...

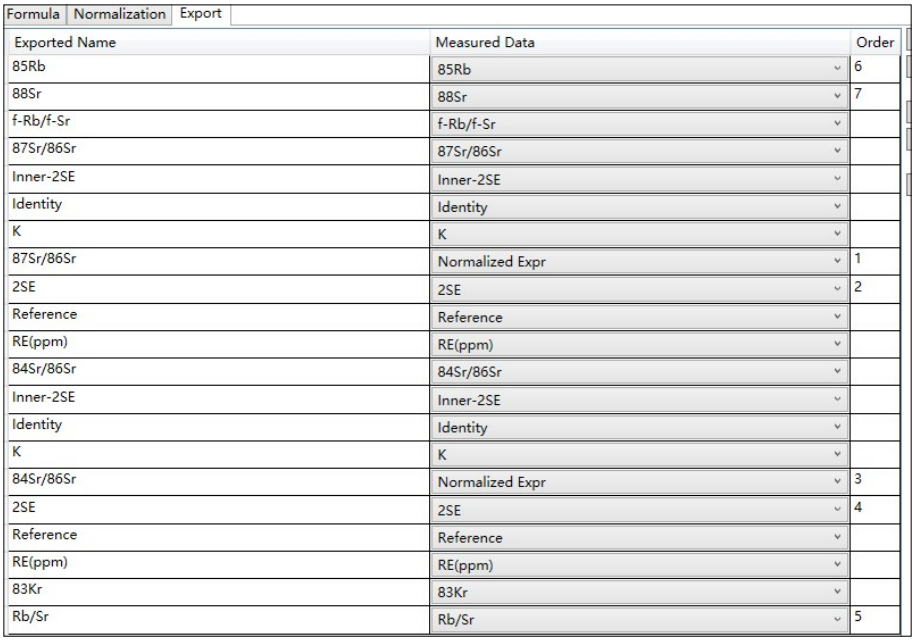


Figure 3.16 Set data export format and edit data export order

(c) Click "New Template" and set a name for the template.

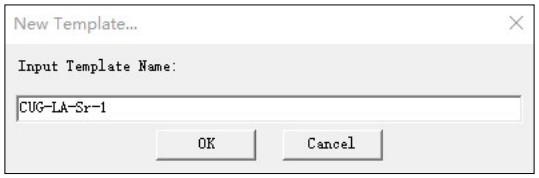


Figure 3.17 Create new format template

(d) An excel file will be opened automatically. Different sheets have been set for the file, including "Front Cover," "Back Cover," and "Data." You can design the document formats in different sheets according to your needs.

(e) Close the file after saving the Excel file. The template is created successfully and it is saved in the “IsoCompass\template” folder. The data reporting section that follows describes how to use this template.

3.4 Data reduction

After correctly setting the folder path, calibration method template, and sample list of the sample to be processed, click "OK" on the "Create an Analysis Session" page to enter the data reduction page.

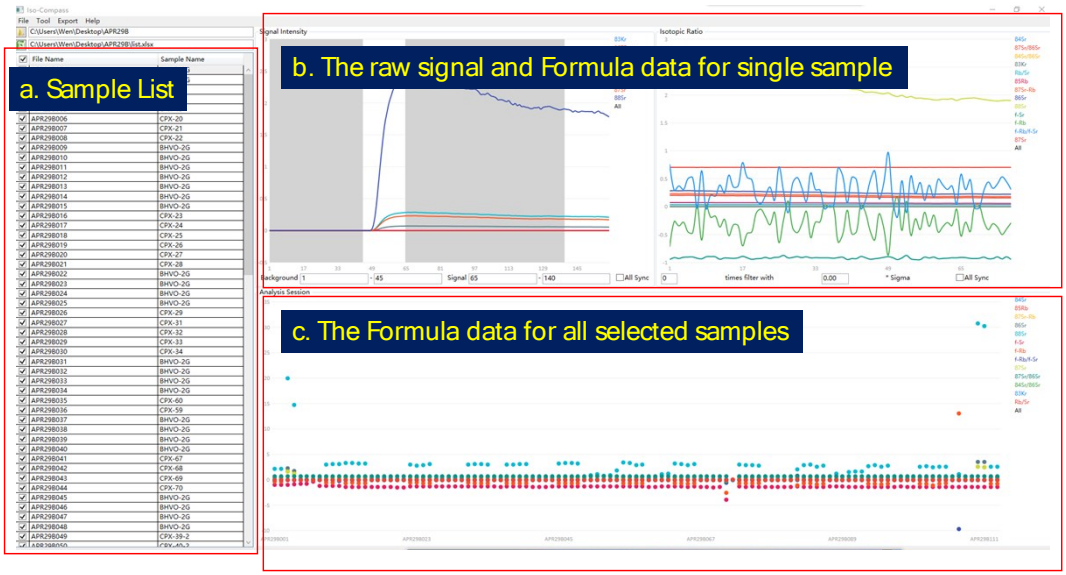


Figure 3.18 Data reduction interface

Tool—Option (Fig. 3.19).

The data reduction page includes three major modules:

(a) Sample List. The File Name of the Sample List is the name of all ".exp" files in the folder set by the user, and the Sample Name comes from the List file provided by the user. If the name of the ".exp" file does not correspond to the file name in the list, the Sample Name of the ".exp" file will be replaced with the File Name. You can select the file to be processed by ticking the small box in front of the file. Ticking the small box before File Name selects all data.

(b) After selecting a file, the two graphs on the upper right side display the signal distribution of the original sample data and all of the data written during the formula editing. In the original signal map, the two shaded areas are the background signal interval and data signal interval. You can directly select the signal interval manually by dragging the shadow or by entering the required signal interval below. One of the small boxes "All Sync" refers to whether global signal interval selection is performed.

The Formula chart includes a data filtering function. "X" times filtering with "x" sigma means the data culling operation is performed x times. In general, you can tick "All Sync" at the back and fill in "2" times filtering with "2" sigma, which means a 2-times 2x sigma discrete data deletion will be performed on the global sample.

(c) The formula data of all the selected samples are displayed in the lower right part to observe the global data.

You can also enter the Formula module from the data reduction page to make real-time changes to existing calibration methods: Tool—Option.

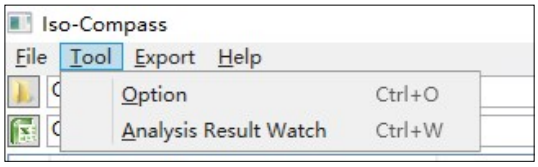
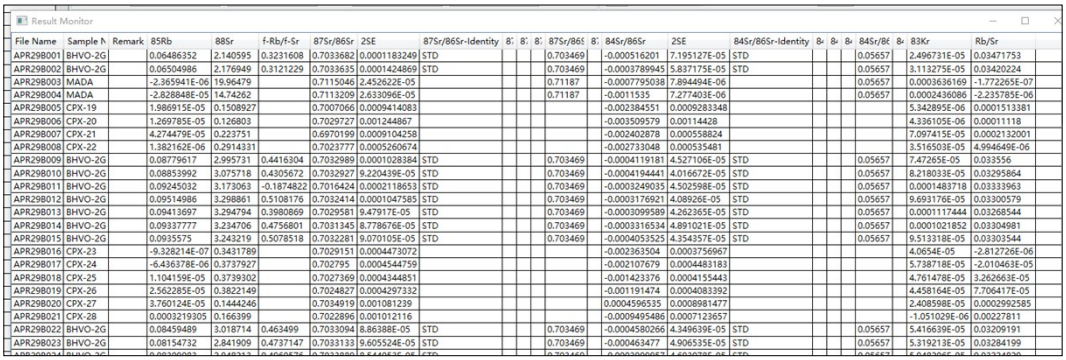


Figure 3.19 Data reduction interface: Tool toolbar

You can click the "Result Monitor" window in "Analysis Result Watch" in the Tool toolbar to view the correction data in real time. Only data with "Mean," "2SE," and "Count" ticked in the "Formula" module will be displayed in the "Result Monitor" window. The "Result Monitor" window also provides a "Remark" column to record problems with this data during processing.



File Name	Sample N	Remark	85Rb	88Sr	f-Rb/f-Sr	87Sr/86Sr	2SE	87Sr/86Sr-Identity	8'	8'	8'	87Sr/86S	8'	84Sr/86Sr	2SE	84Sr/86Sr-Identity	8-	8-	8-	84Sr/86	8-	83Kr	Rb/Sr
APR29B001	BHVO-2G		0.06486352	2.140595	0.3231608	0.7033682	0.0001183249	STD				0.703469		-0.000516201	7.195127E-05	STD				0.05657		2.496731E-05	0.03471753
APR29B002	BHVO-2G		0.06504986	2.176949	0.3121229	0.7033635	0.0001424869	STD				0.703469		-0.0003789945	5.837175E-05	STD				0.05657		3.113275E-05	0.03420224
APR29B003	MADA		-2.365941E-06	19.96479		0.7115046	2.452622E-05					0.71187		-0.0007795038	7.894494E-06					0.05657		0.0003636169	-1.772265E-07
APR29B004	MADA		-2.828848E-05	14.74262		0.7113209	2.633096E-05					0.71187		-0.0011535	7.277403E-06					0.05657		0.0002436086	-2.235785E-06
APR29B005	CPX-19		1.986915E-05	0.1508927		0.7007066	0.0009414083							-0.002384551	0.0009283348							5.342895E-06	0.0001513381
APR29B006	CPX-20		1.269785E-05	0.126803		0.7029727	0.001244867							-0.003509579	0.00114428							4.336105E-06	0.00011118
APR29B007	CPX-21		4.274479E-05	0.223751		0.6970199	0.0009104258							-0.002402878	0.000558824							7.097415E-05	0.0002132001
APR29B008	CPX-22		1.382162E-06	0.2914331		0.7023777	0.0005260674							-0.002733048	0.000535481							3.516503E-05	4.994649E-06
APR29B009	BHVO-2G		0.08779617	2.995731	0.4416304	0.7032989	0.0001028384	STD				0.703469		-0.0004119181	4.527106E-05	STD				0.05657		7.47265E-05	0.033556
APR29B010	BHVO-2G		0.08853992	3.075718	0.4305672	0.7032927	9.220439E-05	STD				0.703469		-0.0004194441	4.016672E-05	STD				0.05657		8.218033E-05	0.03295864
APR29B011	BHVO-2G		0.09245032	3.173063	-0.1874822	0.7016424	0.0002118653	STD				0.703469		-0.0003249035	4.502598E-05	STD				0.05657		0.0001483718	0.03333963
APR29B012	BHVO-2G		0.09514986	3.298861	0.5108176	0.7032414	0.0001047585	STD				0.703469		-0.0003176921	4.08926E-05	STD				0.05657		9.693176E-05	0.03300579
APR29B013	BHVO-2G		0.09413697	3.294794	0.3980869	0.7029581	9.47917E-05	STD				0.703469		-0.0003099589	4.262365E-05	STD				0.05657		0.0001117444	0.03268544
APR29B014	BHVO-2G		0.09337777	3.234706	0.4756801	0.7031345	8.778676E-05	STD				0.703469		-0.0003316534	4.891021E-05	STD				0.05657		0.0001021852	0.03304981
APR29B015	BHVO-2G		0.0935575	3.243219	0.5078518	0.7032281	9.070105E-05	STD				0.703469		-0.0004053525	4.354357E-05	STD				0.05657		9.513318E-05	0.03303544
APR29B016	CPX-23		-9.328214E-07	0.3431789		0.7029151	0.0004473072							-0.002363504	0.0003756967							4.0654E-05	-2.812726E-06
APR29B017	CPX-24		-6.436378E-06	0.3737927		0.702795	0.0004544759							-0.002107679	0.0004483183							5.738718E-05	-2.010463E-05
APR29B018	CPX-25		1.104159E-05	0.3739302		0.7027369	0.0004344851							-0.001423376	0.0004155443							4.761478E-05	3.262663E-05
APR29B019	CPX-26		2.562285E-05	0.3822149		0.7024827	0.0004297332							-0.001191474	0.0004083392							4.458164E-05	7.706417E-05
APR29B020	CPX-27		3.760124E-05	0.1444246		0.7034919	0.001081239							0.0004596535	0.0008981477							2.408598E-05	0.0002992585
APR29B021	CPX-28		0.0003219305	0.166399		0.7022896	0.001012116							-0.0009495486	0.0007123657							-1.051029E-06	0.00227811
APR29B022	BHVO-2G		0.08459489	3.018714	0.463499	0.7033094	8.86388E-05	STD				0.703469		-0.0004580266	4.349639E-05	STD				0.05657		5.416639E-05	0.03209191
APR29B023	BHVO-2G		0.08154732	2.841909	0.4737147	0.7033133	9.605524E-05	STD				0.703469		-0.000463477	4.906535E-05	STD				0.05657		5.319213E-05	0.03284199

Figure 3.20 Data display interface after processing

The Export toolbar includes two data export modes: one is the ordinary "Export," which exports all of the data added in the "Export" module, while the other is the templated data export mode, "Formatted Export," Which uses an edited template to output the data. All exported data is saved in "Workspace (data save path)."

3.5 Saving data and exporting reports

All corrected parameters can be saved in "Save Session" in the File toolbar. The saved file can be read directly. However, the saved session can only be observed and cannot be edited. The file is saved in "Workspace (data save path)."

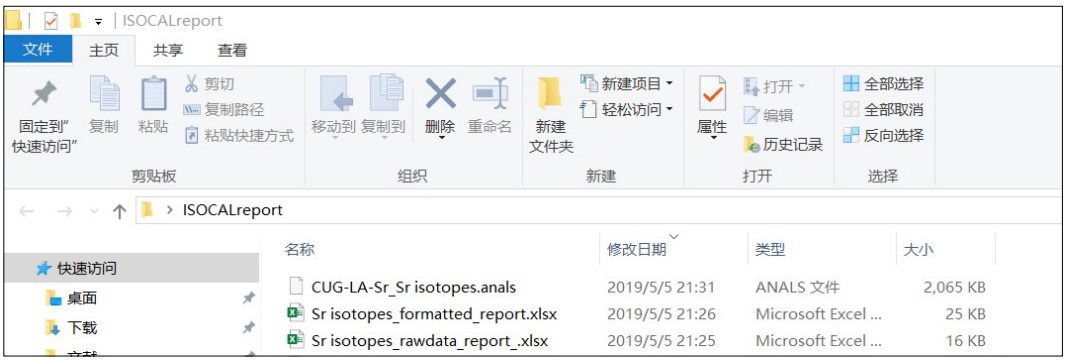


Figure 3.21 Saved session

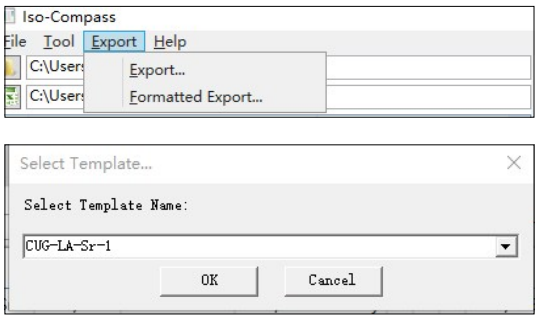


Figure 3.22 Formatted data export mode

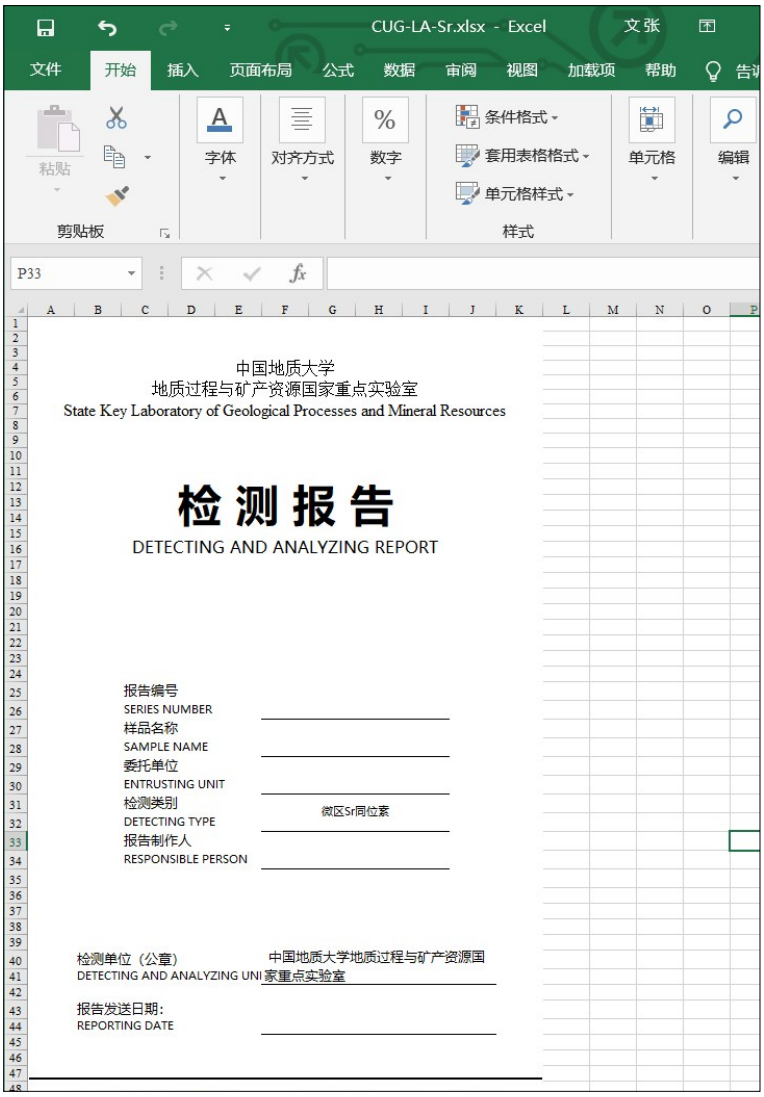


Figure 3.23 Formatted data export cover

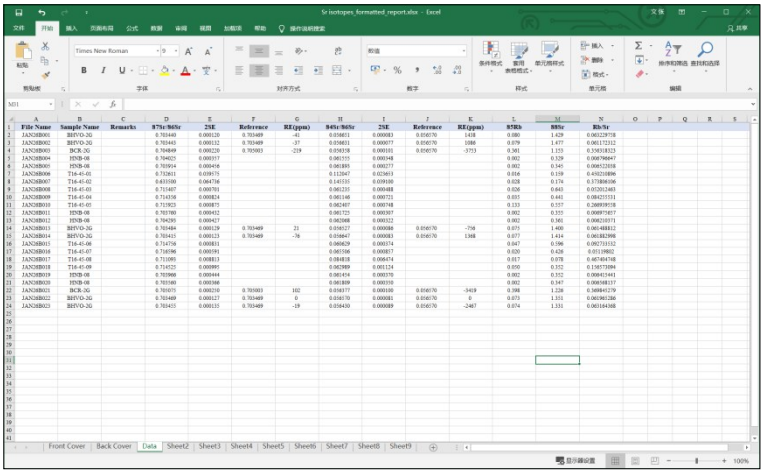


Figure 3.24 Formatted data export: data page

4. Laser MC-ICP-MS data reduction

Example: zircon Hf isotope

The zircon Hf isotope is an important research object in micro-area isotope analysis. In this section, the zircon Hf isotope is used as an example to explain to the reader in detail how to use Iso-Compass to carry out micro-area isotope data reduction.

4.1 Data preparation

Prepare a zircon Hf isotope data folder, which contains raw data (“.exp” format). All of the isotope signals to be tested are required to appear in the raw file. An edited list of data names in the form of APR27C_LIST.xls is required.

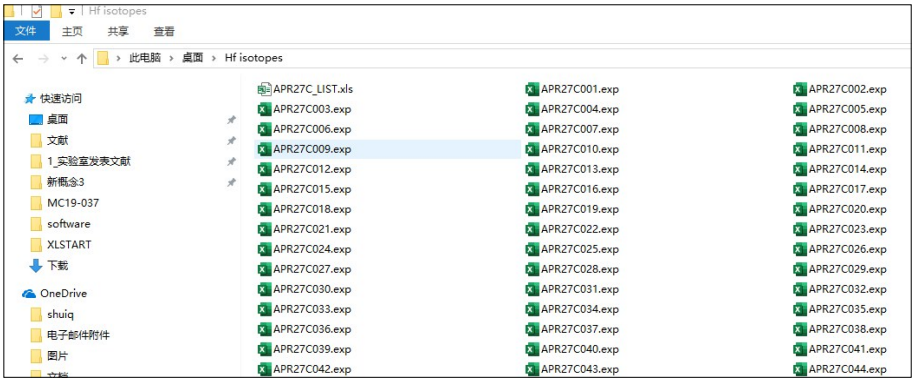


Figure 4.1 Raw data folder

4.2 Data import

Open the Iso-Compass software. Set the working folder path "Workspace," raw data folder path "Folder," file type "File type," and sample name list path "SampleList."

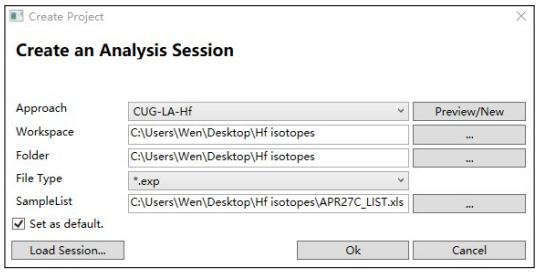


Figure 4.2 Data import

Select the Hf isotope data reduction method "Approach" – "CUG-LA-Hf." After selecting the method, click "Preview/New" to check the method.

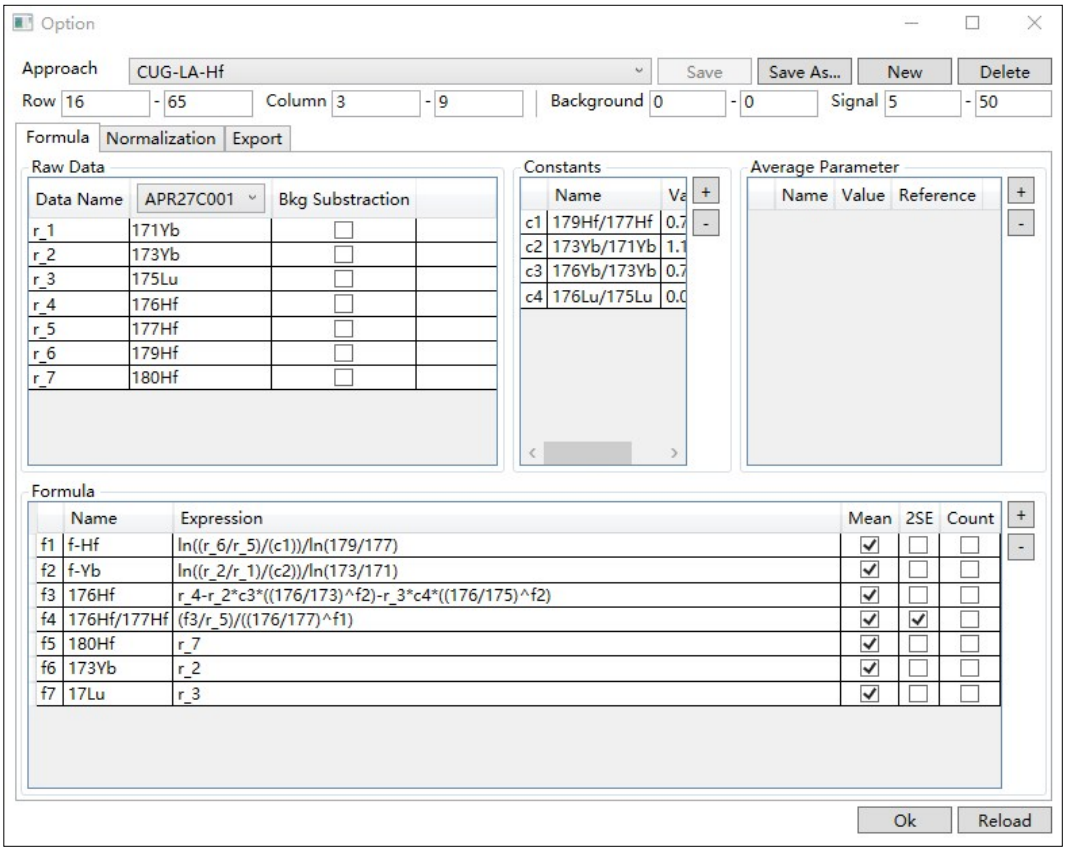


Figure 4.3 Checking data reduction

4.3 Data reduction

After confirming that the data reduction method is correct, click "OK" to enter the data reduction page.

On the data reduction page, you need to check the signal interval of each

data point individually to verify the precision of the data and accuracy of the reference substance.

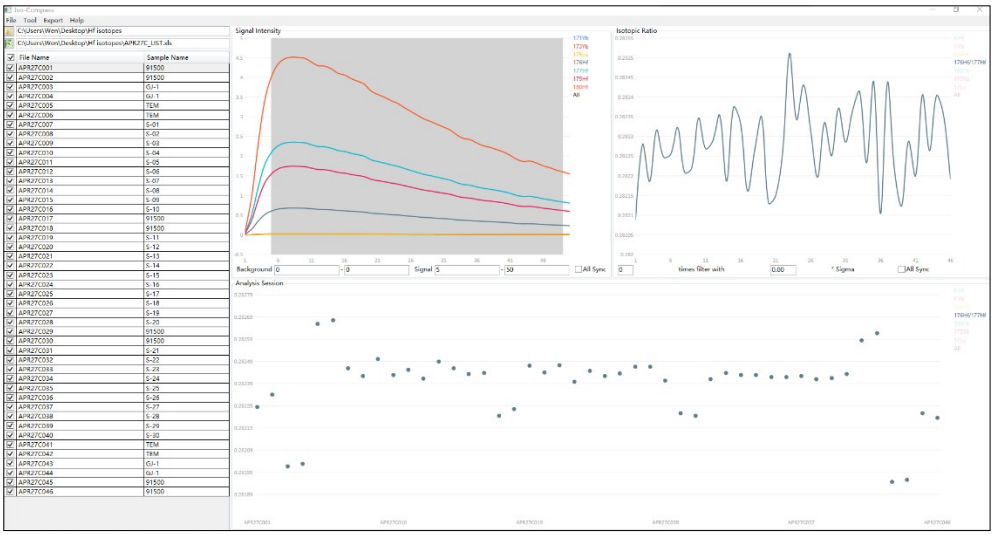


Figure 4.3 Raw data reduction interface

4.4 Data export

After completing the data check, select "Export" – "Formatted Export" and use the established data export template to export the currently processed data in a formatting scheme.

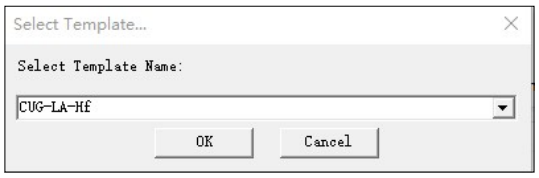


Figure 4.4 Data export

You can then obtain the final formatted data:

中国地质大学
地质过程与矿产资源国家重点实验室
State Key Laboratory of Geological Processes and Mineral Resources

检 测 报 告
DETECTING AND ANALYZING REPORT

报告编号 SERIES NUMBER	MC19_024_ZHANGWEN
样品名称 SAMPLE NAME	锆石
委托单位 ENTRUSTING UNIT	中国地质大学（武汉）
检测类别 DETECTING TYPE	微区锆石Hf同位素
报告制作人 RESPONSIBLE PERSON	张文
检测单位（公章） DETECTING AND ANALYZING UNIT	中国地质大学地质过程与矿产资源国家重点实验室
报告发送日期： REPORTING DATE	2019/8/16

File Name	Sample Name	Remarks	176Hf/177Hf	2SE	Reference	RE(ppm)
APR27C001	91500		0.282295	0.000030	0.282302	-25
APR27C002	91500		0.282343	0.000037	0.282302	144
APR27C003	GJ-1		0.282041	0.000024	0.282013	101
APR27C004	GJ-1		0.282031	0.000023	0.282013	63
APR27C005	TEM		0.282684	0.000024	0.282686	-7
APR27C006	TEM		0.282683	0.000027	0.282686	-12
APR27C007	S-01		0.282478	0.000036		
APR27C008	S-02		0.282449	0.000037		
APR27C009	S-03		0.282533	0.000039		
APR27C010	S-04		0.282454	0.000045		
APR27C011	S-05		0.282489	0.000047		
APR27C012	S-06		0.282416	0.000039		
APR27C013	S-07		0.282493	0.000047		
APR27C014	S-08		0.282476	0.000038		
APR27C015	S-09		0.282443	0.000024		
APR27C016	S-10		0.282448	0.000042		
APR27C017	91500		0.282286	0.000024	0.282302	-58
APR27C018	91500		0.282337	0.000031	0.282302	124
APR27C019	S-11		0.282514	0.000037		
APR27C020	S-12		0.282489	0.000042		
APR27C021	S-13		0.282513	0.000037		
APR27C022	S-14		0.282435	0.000039		
APR27C023	S-15		0.282499	0.000042		
APR27C024	S-16		0.282466	0.000036		
APR27C025	S-17		0.282471	0.000036		
APR27C026	S-18		0.282506	0.000044		
APR27C027	S-19		0.282486	0.000034		
APR27C028	S-20		0.282435	0.000042		
APR27C029	91500		0.282316	0.000030	0.282302	49
APR27C030	91500		0.282294	0.000030	0.282302	-29
APR27C031	S-21		0.282471	0.000032		
APR27C032	S-22		0.282483	0.000035		
APR27C033	S-23		0.282494	0.000031		
APR27C034	S-24		0.282467	0.000037		
APR27C035	S-25		0.282470	0.000037		
APR27C036	S-26		0.282484	0.000043		
APR27C037	S-27		0.282489	0.000042		

Figure 4.5 Formatted data export results