User Operation Manual for Isoclock v1.8

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1. Start-up and functional block division

The following steps 1.1.1-1.1.5 is run before Brama runs for the first time.

1.1.1 Python 3.9 is necessary to run the code. Download from https://www.python.org/downloads/ and follow the installation (Fig. 1).

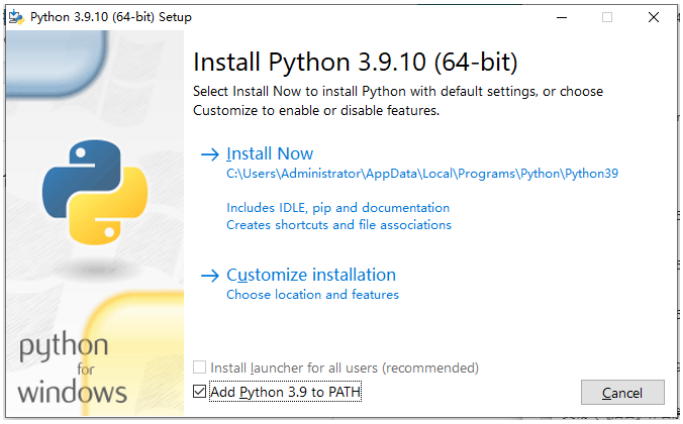

Fig. 1 Install Python 3.9.

1.1.2 Download or clone this repository.

1.1.3 Open terminal/cmd and navigate to the Isoclock folder (Fig. 2).

- `cd path/to/folder/ Isoclock`

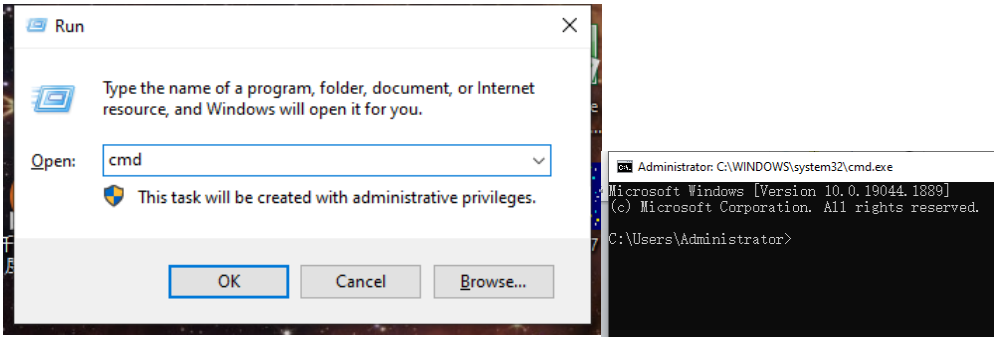

Fig. 2 Open terminal/cmd and navigate to the Brama folder**.**

1.1.4 Instal python libraries required for Isoclock.

- pip install -r requirements.txt

1.1.5 Run Isoclock from python.

- python Isoclock.py

If everything is already installed, follow only steps1.1.5. If you are Windows user, you can also run the Isoclock.exe directly.

The main interface and functional partitions of the program are shown in Fig.3

after starting.

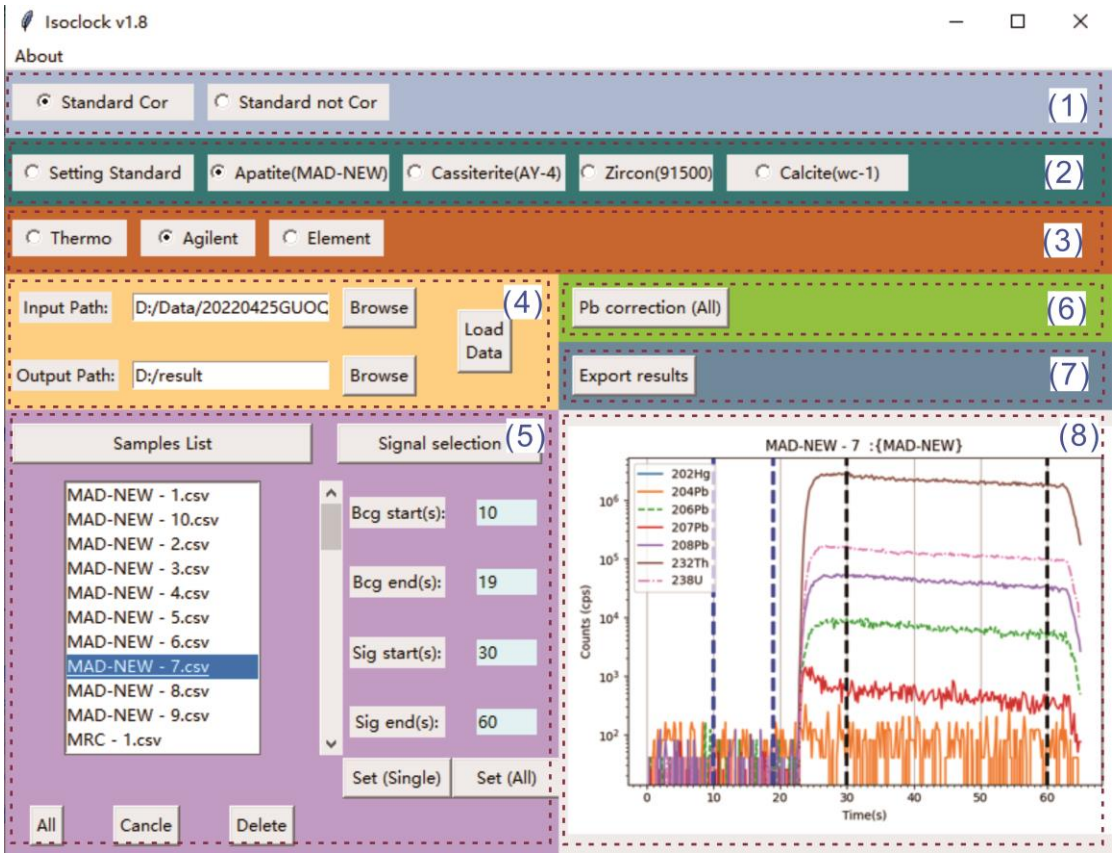

Fig.3 Main interface and function partition

2. General steps of data processing：

The software interface is divided into different functional areas according to color (Fig. 3).

（1）①Select Mode.

Calculation mode selection area (light steel blue): If the standard sample is a mineral containing relatively high common Pb (such as apatite, sphere, wolframite, etc.) which needs to be corrected, select the <standard Cor> button. Otherwise, select <standard not Cor> button (e.g., for most zircon).

（2）②Set standard sample

Standard setting area (turquoise): Select by entering the age or Pb isotopic composition of the reference material.

Note: when selecting the corresponding method directly, it is necessary to ensure that the standard sample name is completely consistent with the software display name.

（3）③Select ICPMS instrument model.

the software provides three formats to choose from:

(a) <**Thermo**> mass spectrometer. The software does not need to provide a “List file”(Excel with two columns of file serial number and sample name), and the software can automatically extract the document serial number and sample name;

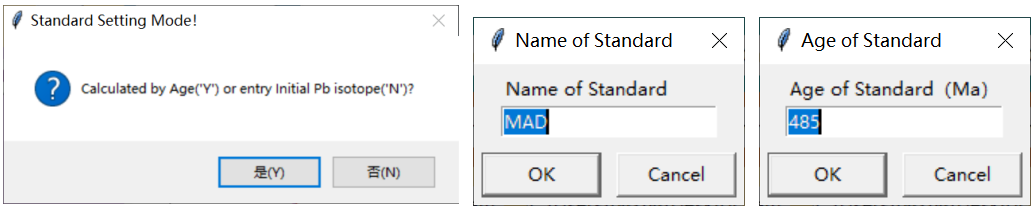

Fig. 3 standard sample selection

(b) <**Agilent**> mass spectrometer. The file is stored in the 'sequence. CSV' file in the 'sequence. D' folder. It is necessary to provide the list format EXCEL file corresponding to the file sequence and sample name (the first column is the folder name, and the second column of the file is the sample or standard sample name);

(c) <**Element**> mass spectrometer. The "*. Fin" format file stores the list sequence file, and the "*. Fin2" format file stores the signal data.

（4）④Date input and output (light yellow):

Select the data input path and output path, and then click the <Load Data> button to import data. If <Agilent> is selected in step (3), the list file should be selected.Select the data input path and output path, and then click the < **Load Data** > button to import data.

Note: If you select **<Agilent>** instrument, you need to select the list file in the pop-up window.

（5）⑤Blank and sampling time settings (light purple):

Click the sample list on the left side of this area, and the signal diagram of the selected sample will be drawn in the area (8). Click the button <Set (All)> or < Set (Single)> to change the background and sampling time of selected or all signals (Fig. 4)

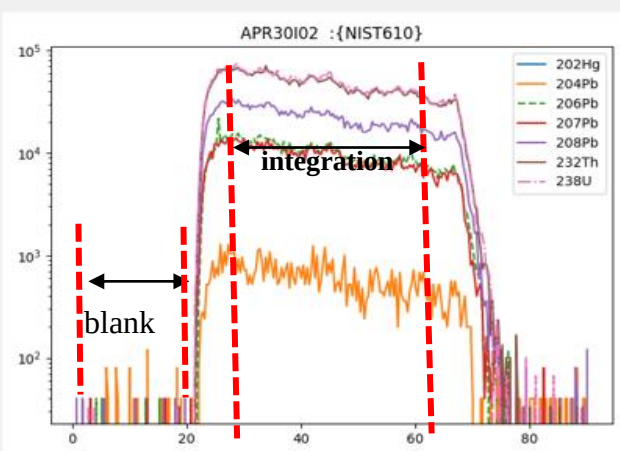

Fig. 4 sample signal diagram display

（6）⑥Isotope ratio calculation (yellow-green):

Click <Pb correction (all)>button to generate the "result_all. csv" file in the output directory. This file contains U-Th-Pb isotope ratios without fractionation correction.

（7）⑦Calculation of age results of samples (Saxe blue):

Click <Export results> to export the results of the calculated ages and isotope ratios of each sample with sample-standard-bracketing method. The resulting file is named “cal_age_result_L*.xls”(Fig. 5).

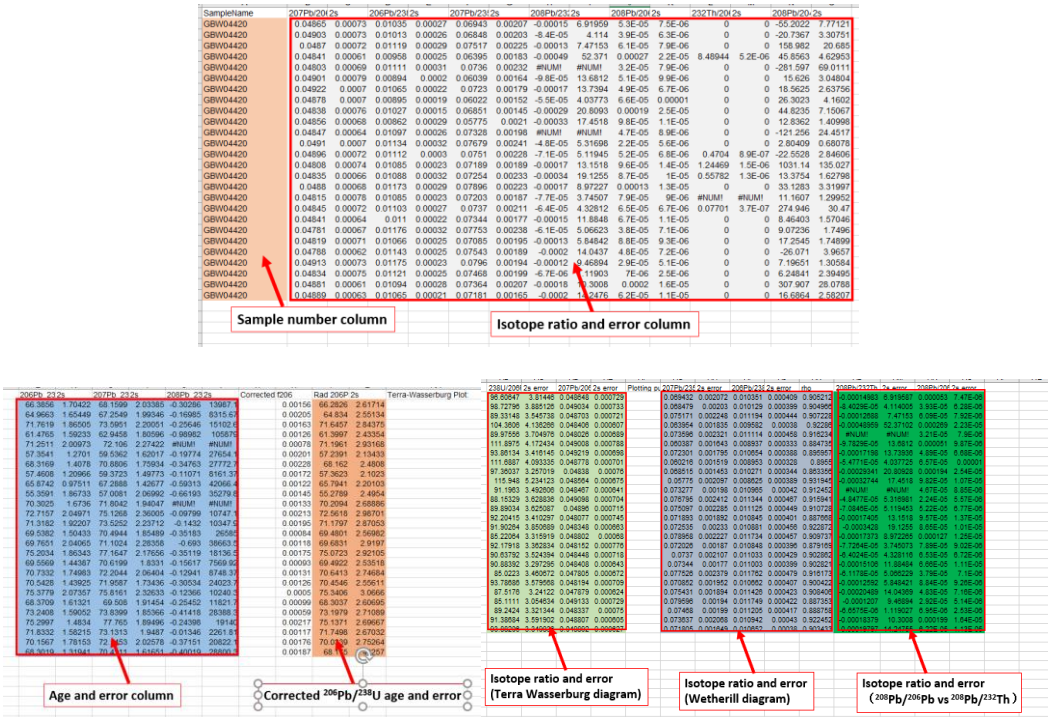

Fig. 5 description of software data processing results

（8）⑧Signal diagram (white):

When the samples in step (5) are selected, their signal diagram will be displayed here and automatically saved in the output directory.

3. Other considerations:

（1）Input folder and output folder cannot be the same；

（2）Only the original data is stored in the input folder, and there can be no other data files(such as CSV file of non-signal data), otherwise the program will report an error!

（3）After processing one sample at a time, restart the program and replace with a new output folder directory.

（4）Note that ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{232}Th and ^{238}U are required items, otherwise an error will be reported.

（5）The first line of the “result_all.csv” file is the header, and the rest are in digital format.

（6）When selecting the "Agilent" instrument, it is required to select the list file when loading data. the first column is the folder name, the second column is the sample name, and the name of the list file worksheet must be "Sheet1".

（7）If the data format is inconsistent or the name and age of other mineral standard samples are added, please contact the author.