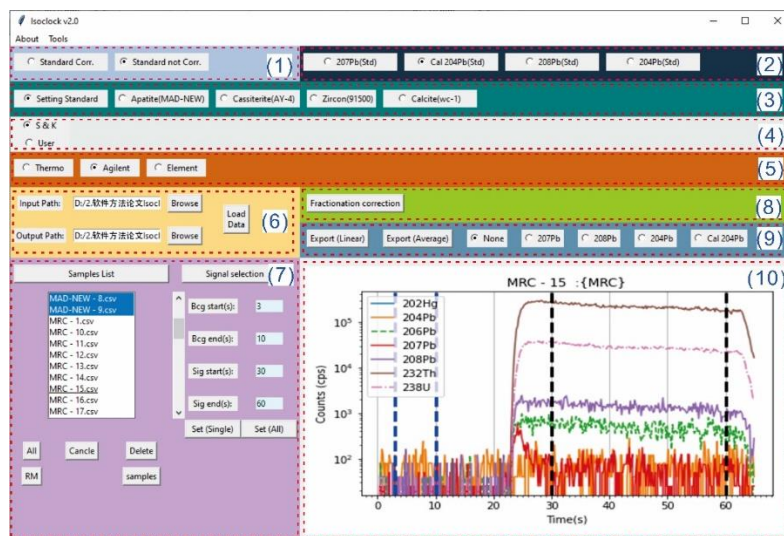




## Hydrothermal/Accessory Minerals U-Th-Pb Data processing for LA-ICPMS

### User Manual of Isoclock 2.0



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## I. Software operation procedures

### 1.1 Start-up and functional block division

Windows users can also download and run the packaged exe file directly.

Download **Isoclock 2.0.exe**:

[https://www.researchgate.net/publication/371012414\\_Isoclock20](https://www.researchgate.net/publication/371012414_Isoclock20).

The demo video is available at:

[https://www.researchgate.net/publication/371039144\\_Demo\\_of\\_Isoclock20](https://www.researchgate.net/publication/371039144_Demo_of_Isoclock20).

The following steps 1.1.1-1.1.5 is run before Brama source code 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.1-1).

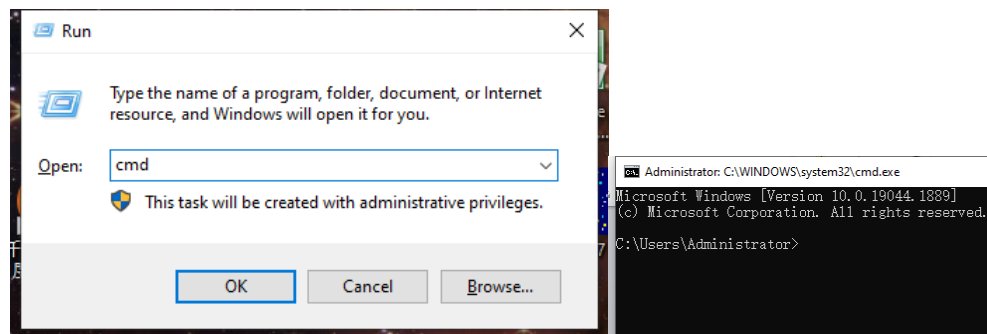


**Fig. 1 Install Python 3.9.**

- 1.1.2 Download or clone this repository (<https://github.com/sndjgm/Isoclock>) .

- 1.1.3 Open terminal/cmd and navigate to the Brama folder (Fig. 1-2).

- cd path/to/folder/ Isoclock



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

#### 1.1.4 Instal python libraries required for Isoclock.

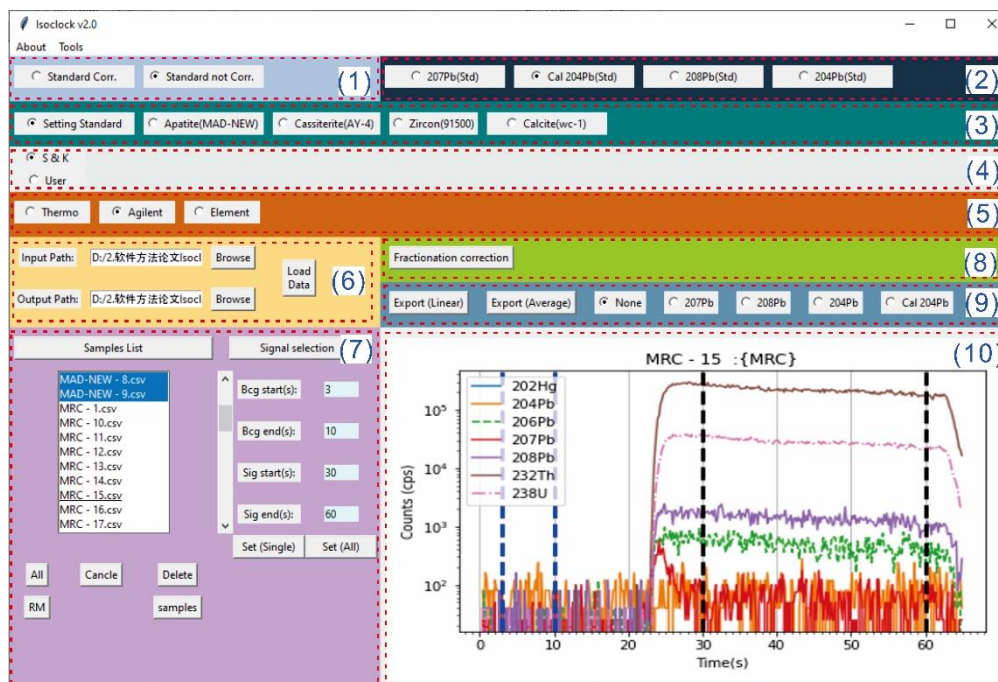
- pip install -r requirements.txt.

#### 1.1.5 Run Isoclock from python.

- python Isoclock.py

If everything is already installed, follow only steps 1.1.5.

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



**Fig. 3 Main interface and function partition**

The software is divided into 7 functional areas. The main functional areas are outlined as follows.

## 2. General steps of data processing:

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

- ❖ (1) ~ (2) Select Mode.

Calculation mode selection area (light steel blue and dark blue): If the standards contain 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).

Dark blue area (2) switches the method of standard common Pb correction methods.

Common Pb correction method based on  $^{207}\text{Pb}$  and  $^{204}\text{Pb}$  derived from [Chew et al. \(2014\)](#).  $^{208}\text{Pb}$  correction method derived from [Zack et al. \(2011\)](#).

(3) ~ (4) Set standard sample

Standard setting area (turquoise and grey): Click the <Setting Standard> button and select "S&k" mode ([Stacey and Kramers, 1975](#)) or "User" mode to set the standard information.

**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.**

❖ (5) Select 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;

(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.

❖ (6) Date 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 <Agilent> is selected, you need to select the list file in the pop-up window.**

❖ (7) Blank 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 (10). Click the button <Set (All)> or <Set (Single)> to change the background and sampling time of selected or all signals.

❖ (8) Isotope ratio calculation (yellow-green):

Click <Fractionation Correction> button to generate the "result\_all. csv" and "Mean\_Cps.csv" file in the output directory.



## ❖ (9) Calculation of age results of samples (Saxe blue):

Click <Export (Liner)> to export the results of the calculated ages and isotope ratios of each sample with Sample-Standard-Bracketing method. No instrument drift correction is performed when the <Export (Average)> button is clicked.

The resulting file is named “cal\_age\_result\_L\*.xls” (Liner) or “cal\_age\_result\_A\*.xls” (average) (Fig. 4).

❖ (10) Signal diagram (white):

When the samples name in step (7) are selected, their signal diagram will be displayed here and automatically saved in the output directory.

SampleName	207Pb/235U	207Pb/238U	207Pb/232Th	208Pb/232Th	208Pb/204Pb	232Th/204Pb	208Pb/204Pb
GBW04420	0.04865	0.00073	0.01033	0.00027	0.06943	0.00207	-0.00015
GBW04420	0.04903	0.00073	0.01013	0.00026	0.06848	0.00203	-8.4E-05
GBW04420	0.0487	0.00072	0.01119	0.00029	0.07517	0.00225	-0.00013
GBW04420	0.04803	0.00069	0.01111	0.00031	0.0736	0.00232	#NUM!
GBW04420	0.04822	0.0007	0.01065	0.00022	0.0723	0.00179	-0.00017
GBW04420	0.04878	0.0007	0.00895	0.00019	0.06022	0.00152	-5.5E-05
GBW04420	0.04838	0.00076	0.01027	0.00015	0.06851	0.00145	-0.00029
GBW04420	0.04856	0.00068	0.00862	0.00029	0.05775	0.0021	-0.00033
GBW04420	0.04847	0.00064	0.01097	0.00026	0.07328	0.00198	#NUM!
GBW04420	0.0491	0.0007	0.01134	0.00032	0.07679	0.00241	-4.8E-05
GBW04420	0.04896	0.00072	0.01112	0.0003	0.0751	0.00228	-7.1E-05
GBW04420	0.04808	0.00074	0.01085	0.00023	0.07189	0.00189	-0.00017
GBW04420	0.04835	0.00066	0.01088	0.00032	0.07254	0.00233	-0.00034
GBW04420	0.0488	0.00068	0.01173	0.00029	0.07896	0.00223	-0.00017
GBW04420	0.04815	0.00078	0.01085	0.00023	0.07203	0.00187	-7.7E-05
GBW04420	0.04845	0.00072	0.01103	0.00027	0.0737	0.00211	-6.4E-05
GBW04420	0.04841	0.00064	0.011	0.00022	0.07344	0.00177	-0.00015
GBW04420	0.04781	0.00067	0.01176	0.00032	0.07753	0.00238	-6.1E-05
GBW04420	0.04819	0.00071	0.01066	0.00025	0.07085	0.00195	-0.00013
GBW04420	0.04788	0.00062	0.01143	0.00025	0.07543	0.00189	-0.0002
GBW04420	0.04913	0.00073	0.01175	0.00023	0.0796	0.00194	-0.00012
GBW04420	0.04834	0.00075	0.01121	0.00025	0.07468	0.00199	-6.7E-05
GBW04420	0.04881	0.00061	0.01094	0.00028	0.07364	0.00207	-0.00018
GBW04420	0.04889	0.00063	0.01065	0.00021	0.07181	0.00165	-0.0002

Sample number column

Isotope ratio and error column

206Pb/238U	207Pb/235U	208Pb/232Th	Corrected 206U	Rad 206Pb/2s	Terra-Wasserburg Plot	238U/204Pb 2s error	207Pb/204Pb 2s error	Plotting p	207Pb/232Th 2s error	206Pb/232Th 2s error	rho	208Pb/232Th 2s error	208Pb/204Pb 2s error
66.956	1.70422	68.1599	2.03365	-0.30266	1.9987	0.00156	86.2696	2.61714	0.009432	0.002072	0.010351	0.000409	0.906212
64.9663	1.65440	67.2540	1.99345	-0.16695	0.91543	0.00205	64.834	2.55134	0.008478	0.00203	0.010129	0.000399	0.904995
71.7619	1.86005	73.5901	2.20051	-0.25646	1.91026	0.00163	71.6457	2.84376	0.009479	0.00203	0.010129	0.000399	0.904995
61.4765	1.59233	62.9458	1.80596	-0.06802	1.05976	0.00126	61.3997	2.43354	0.008384	0.00183	0.009562	0.00038	0.92239
71.2511	2.00973	72.106	2.27422	#NUM!	#NUM!	0.00078	71.1961	2.93168	0.007358	0.00221	0.011114	0.000458	0.916234
57.5541	1.2701	56.5362	1.62017	-0.18774	2.76541	0.00201	57.2991	2.14333	0.009387	0.001943	0.008937	0.000333	0.864735
68.3169	1.4578	70.8806	1.75934	-0.34763	2.77722	0.00226	68.162	2.4808	0.007358	0.00221	0.011114	0.000458	0.916234
57.4608	1.20966	59.3723	1.49773	-0.11071	0.6113	0.00172	57.3623	2.1023	0.009387	0.001943	0.008937	0.000333	0.864735
65.8742	0.97511	67.2888	1.42677	-0.59313	4.20664	0.00122	65.7941	2.20103	0.009387	0.001943	0.008937	0.000333	0.864735
55.3591	1.86733	57.0081	2.06992	-0.66193	3.52709	0.00145	55.2769	2.4954	0.009387	0.001943	0.008937	0.000333	0.864735
70.3025	1.6736	71.8042	1.94047	#NUM!	#NUM!	0.00133	70.2094	2.68886	0.009387	0.001943	0.008937	0.000333	0.864735
72.7157	2.04071	75.1266	2.36005	-0.69799	1.0747	0.00213	72.5616	2.96701	0.009387	0.001943	0.008937	0.000333	0.864735
71.3182	1.92207	73.5252	2.23712	-0.1432	1.03479	0.00196	71.1797	2.87053	0.009387	0.001943	0.008937	0.000333	0.864735
69.5382	1.50433	70.4944	1.85489	-0.35183	2.6082	0.00084	69.4801	2.56962	0.009387	0.001943	0.008937	0.000333	0.864735
69.7651	2.04065	71.1024	2.28358	-0.693	3.66632	0.00118	69.6831	2.9197	0.009387	0.001943	0.008937	0.000333	0.864735
75.2034	1.86343	77.1647	2.17656	-0.35119	1.81365	0.00175	75.0723	2.92105	0.009387	0.001943	0.008937	0.000333	0.864735
69.5569	1.44387	70.6199	1.8331	-0.15617	7.59162	0.00093	69.4022	2.53518	0.009387	0.001943	0.008937	0.000333	0.864735
70.7332	1.74893	72.2044	2.06404	-0.12941	87.4833	0.00131	70.6413	2.74684	0.009387	0.001943	0.008937	0.000333	0.864735
70.5428	1.43825	71.9587	1.73436	-0.30354	2.40237	0.00126	70.4546	2.55611	0.009387	0.001943	0.008937	0.000333	0.864735
75.3779	2.07357	75.8161	2.32633	-0.12366	1.02403	0.0005	75.3406	3.0666	0.009387	0.001943	0.008937	0.000333	0.864735
68.3709	1.61321	69.508	1.91454	-0.25452	1.18217	0.00099	68.3037	2.60695	0.009387	0.001943	0.008937	0.000333	0.864735
73.2408	1.59052	73.8399	1.83366	-0.41418	28.3883	0.00059	73.1979	2.71089	0.009387	0.001943	0.008937	0.000333	0.864735
75.2997	1.4834	77.765	1.89496	-0.24398	19.142	0.00217	75.1371	2.69657	0.009387	0.001943	0.008937	0.000333	0.864735
71.8332	1.58215	73.1513	1.9407	-0.01346	2261.8	0.00117	71.7498	2.67032	0.009387	0.001943	0.008937	0.000333	0.864735
70.1567	1.78153	72.153	2.02578	-0.37151	20822.1	0.00176	70.0109	2.75264	0.009387	0.001943	0.008937	0.000333	0.864735
68.3018	1.31041	70.2414	1.61651	-0.40019	28800.3	0.00187	68.115	2.5257	0.009387	0.001943	0.008937	0.000333	0.864735

Age and error column

Corrected  $^{206}\text{Pb}/^{238}\text{U}$  age and error

Isotope ratio and error (Terra Wasserburg diagram)

Isotope ratio and error (Wetherill diagram)

Isotope ratio and error ( $^{208}\text{Pb}/^{206}\text{Pb}$  vs  $^{208}\text{Pb}/^{232}\text{Th}$ )

Fig. 4 description of software data processing results

### Other Notes:

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  $^{204}\text{Pb}$ ,  $^{206}\text{Pb}$ ,  $^{207}\text{Pb}$ ,  $^{208}\text{Pb}$ ,  $^{232}\text{Th}$  and  $^{238}\text{U}$  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
7. 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".

### Reference

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- Zack, T., Stockli, D.F., Luvizotto, G.L., Barth, M.G., Belousova, E., Wolfe, M.R., Hinton, R.W., 2011. In situ U–Pb rutile dating by LA-ICP-MS: 208Pb correction and prospects for geological applications. *Contributions to Mineralogy and Petrology* 162, 515-530.