

Format of the files used by Pepita

1) Data Files (extension: .XL, .CSV or .TXT)

function:

Stores raw data counts per seconds (or counts) in the measured time slices for each isotope.

Extension:

.XL or .CSV (comma delimited text files)

.TXT (Tab delimited text files)

PEPITA can import text files having very variable formats. The only restriction: the isotopes must form the columns and the time slices the lines. Empty lines between the time slices are not considered.

Intensity Vs Time	Counts Per Second				
Time in Seconds	Li6	Mg24	Al27	Si29	P31
0	3951	239440	2428794	1378444	14307
0	6652	149074	2019309	1377894	14708
0	9903	178964	1907418	1481259	10454
0	7402	100754	1528981	1731036	9303

B11	Sc45	V51	Cr53
50	175	375	200
0	25	375	50
0	50	425	150
25	25	200	150

Examples for data files.

The user can specify the format of the data files and these formats will be saved in the settings. Three parameters can determine the structure of the majority of the table formatted ASCII data files.

A: Number of line that contains the name of isotopes.

B: Number of the line that contains the first time slice (cps or counts data).

C: Number of the column that contains the first isotope.

Customize Import

The import filter can be customized according to the format of the datafiles

Pepita opens text files with CSV, TXT, XL or with user defined extensions. The data should be separated by comma or TAB.

Data must be ordered in a closed table, where the lines are the time slices and columns contain the cps values of the isotopes and time, etc. One line must contain the name of isotopes. The file may contain lines with other content, these will not be considered. The sequence of the isotopes is irrelevant.

The file may contain lines with other content, but these lines will not be considered.

Extension: CSV TXT XL
(comma delimited) (TAB delimited) (comma delimited)

Number of line that contains the name of isotopes: 1 1 2

Number of the line that contains the first time slice (cps data): 2 7 3

Number of the column that contains the first isotope: 1 2 2

an example: 3rd column: first isotope

2nd line: name of isotopes

Sample: from the boss				
Code	Time	201Hg	208Pb	238U
	[m sec]	[cps]	[cps]	[cps]
conditions: Monday morning & rain				
other comments				
my18a11	0	1000	700	66957
my18a11	403	500	600	70172
my18a11	503	500	1100	66856
my18a11	643	100	400	61030

6th line: first time slice

WARNING ! Later modification of these parameters will not allow to open the formerly saved datafiles.

If you change the hardware or you use more ICP-MS devices exporting files with different formats, but with the same extension, then keep the different files separately in different directories and create for these directories different settings files.

Creation of import filter for the own data files (needed to use only once).

2) Standard Composition File (extension: .STC)

function:

Stores the nominal concentration of the isotopes and their error of the reference materials.

how to create:

Use Excel or some other spreadsheet calculator.

- First cell in the first line: comments (do not use comma in the text).
- Write the name of the isotopes in the same format as the mass spectrometer exports them (Cr53 is not equal to Cr-53 or to Cr 53).
- Sequence of the isotopes is not important.
- Type all values in ppm.
- Recommended filename: name of the standard.
- Save it as a "Comma delimited file" with extension of **.CSV**.

- Save it in any directory, but it is recommended to store them together with data files.
- Modify the extension to **.STC**. (*)

first cell in the first line: info about the data

from Pearce et al. 1997		
Ca44	81833	1651
Sc45	441.1	9.6
Ti46	434	14.7

third column: error of concentration in ppm

second column: concentration in ppm

first column: name of the isotope

Structure of the standard composition files.

 (*): How to modify the extension?

It is not very trivial because some comfortable-looking settings of Windows hide the real extension of the files. Thus it is very much recommended to DISABLE the following check box:

My computer / Tools / Folder options / View / Hide file extensions for known file types.

The easiest and most stable way to see the content of directories and modify the filenames can be performed by TotalCommander.

3) Standard Measurement File (extension: .STM)

function:

Stores the average of counts per seconds measured on the standards using the same settings as used at the sample.

how to create (Pepita does it):

- Open the data file, which contains the standard measurement.
- Select "Creating Standard Measurement File" option at the first window.
- Perform time slice selection and the preferred statistical tests/rejections.
- Save the STM file. Recommended filename: name of the standard-date-sequence (e.g.: NBS-621-2004-12-21-A).

first column: name of the isotope

second column: cps

third column: 1 s.e. of cps

La139	4809.292	520.102
Ce140	8855.875	801.618
Pr141	1352.083	258.225

Structure of the standard composition files.

4) Blank File (extension: .BLK)

function:

Stores the average of counts per seconds of blank measurement performed at same settings as the sample.

how to create (Pepita does it):

- Select "Creating Blank File" option at the first window.
- Perform time slice selection and the preferred statistical tests/rejections.
- Save the BLK file. Recommended filename: date-sequence.
(e.g.: 2004-12-21-A)

first column: name of the isotope

second column: cps

third column: 1 s.e. of cps

Ba137	1.316	5.735
La139	0.001	0.001
Ce140	6.579	16.334

Structure of the blank files.

5) Dwell Time File (extension: .DWE)

function:

Stores the dwell times used at the detection of intensities of the isotopes.

how to create:

Use Excel or some other spreadsheet calculator.

- First cell in the first line: comments (do not use comma in the text).
- Write the name of the isotopes in the same format as the mass spectrometer exports them (Cr53 is not equal to Cr-53 or to Cr 53).
- Sequence of the isotopes is not important.
- Type the dwell time in milliseconds into the second column.
- Save it as a "Comma delimited file" with extension of **.CSV**.
- Modify the extension to **.DWE**.

first cell in the first line: info about the data

Dwell times in May 2007	
Fe57	20
Pb208	200
Th232	50

second column: dwell time in ms

first column: name of the isotope