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.

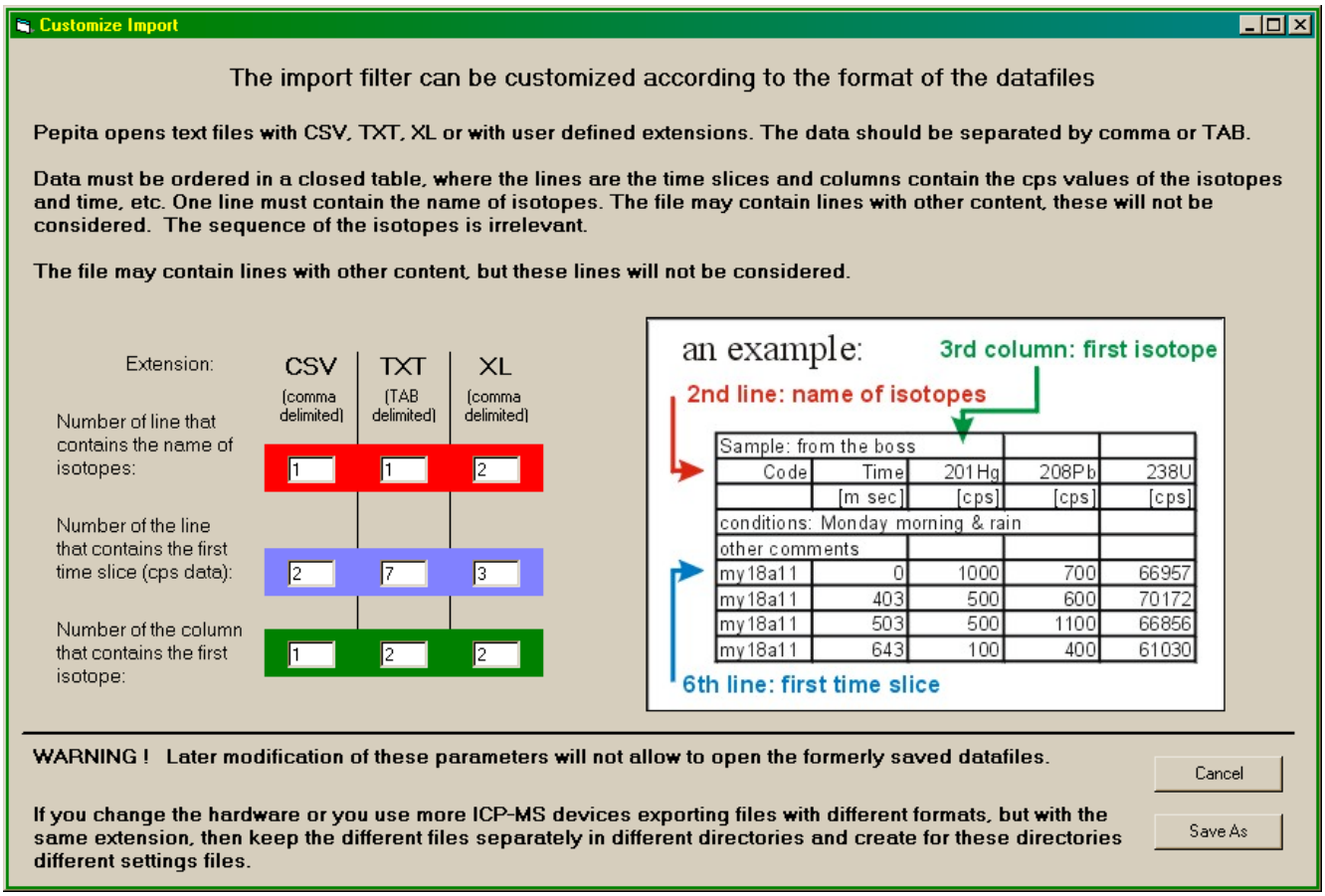
Extension:
.XL or .CSV (comma delimited text files)
.TXT (Tab delimited text files)
PEPITA can import text files having very variable formats. The only restriction: the isotopes must form the columns and the time slices the lines. Empty lines between the time slices are not considered.

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.



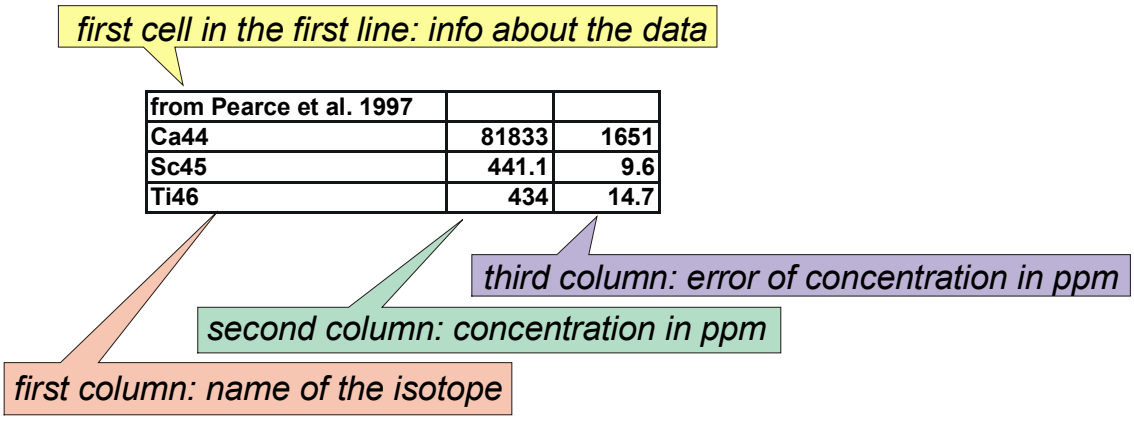
Creation of import filter for the own data files (needed to use only once).

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**. (*)



Structure of the standard composition files.

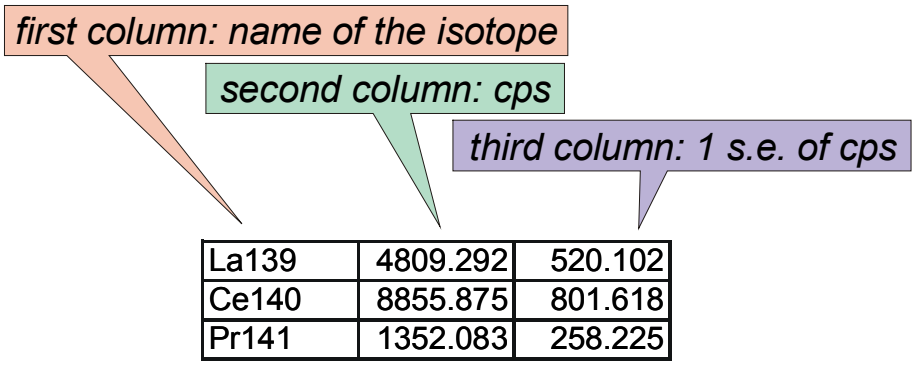
(*): How to modify the extension?
It is not very trivial because some comfortable-looking settings of Windows hide the real extension of the files. Thus it is very much recommended to DISABLE the following check box:
My computer / Tools / Folder options / View / Hide file extensions for known file types.

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).



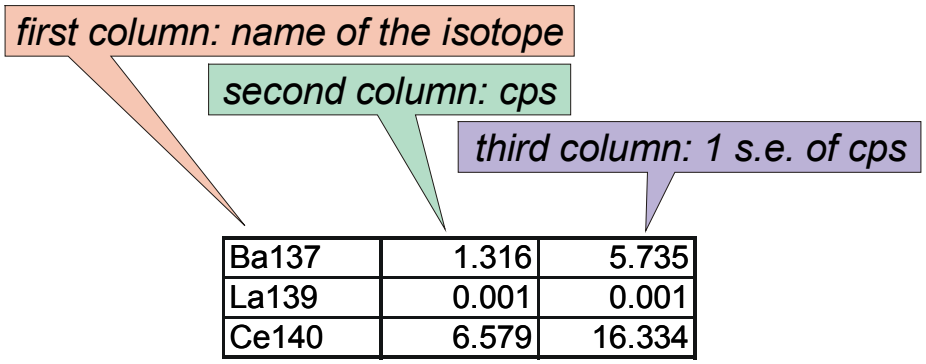
La139	4809.292	520.102
Ce140	8855.875	801.618
Pr141	1352.083	258.225

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)



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 miliseconds into the second column.
- Save it as a "Comma delimited file" with extension of **.CSV**.
- Modify the extension to **.DWE**.