k0-INRIM User's Manual

version 1.0

May 9, 2019

Contents

1 Introduction

A software package, called k0-INRIM, was developed to assist NAA analysts during data elaboration and uncertainty evaluation following the recommendations of the guide to the expression of uncertainty in measurement GUM [1]. The main aim was to make automatic the compiling of the uncertainty spreadsheet for the k_0-NAA method described in [2].

Specifically, the software accepts as an input spectra information and experimental data to obtain the mass fractions of the investigated elements including their uncertainty budgets and detection limits.

The equation model (4) implemented in the present version applies to activation and decay path types I, IIB, IVB and VI defined in [3]. A warning message appears in the case of complex activation decay paths that are not yet implemented. Similarly, the user is informed when non-$1/v$ nuclides requiring the application of Westcott formalism are selected.

It is worth to note that the use of the current version is limited to the particular experimental setup for the gamma counting in which the measurement and standard samples, the first containing the investigated elements and the latter containing the monitor element, have point-like geometry. Moreover, both samples must be located at the same counting position with respect to the detector end-cap.

The calibration of the detection system requires the measurement of a multi-gamma reference source at the counting position of the samples.

Information concerning installation, use and output of the software is given in sections 2, 3 and 4, respectively. It is worth to note that the structure of the section 3 corresponds to the workflow of the analysis. Users can get started with the k0-INRIM software by following step-by-step instructions reported in section 5.

2 Software installation

The k0-INRIM is potentially multi-platform although this version has been tested only on 64 bit Windows systems (versions 7 and 10); this manual specifically refers to the 64 bit Windows.

The software running requires the previous installation of the Python compiler, version 3.6 [4] or higher, freely available at `https://www.python.org/downloads/`. During the Python installation, click the "Add python3.x to PATH" check-box. Moreover, the k0-INRIM uses the additional modules "xlrd", "xlsxwriter", "numpy" and "matplotlib" [5, 6] available by default in the Anaconda package alongside some useful tool for software debugging. The Anaconda package developed for Python 3.7 version is also freely down-loadable at `https://www.anaconda.com/download/`. During the Anaconda installation, click the "Add Anaconda to my PATH environment variable" and "register Anaconda as my default python3.x" check-boxes. Expert users may install each additional module as an alternative to the installation of the complete Anaconda package.

The k0-INRIM is installed by executing the «k0-INRIM_setup.exe». The setup process allows the user to choose any destination for the software main folder. It is recommended to avoid system-reserved destinations, such as the C://Programs path, as this will prevent the writing of working files unless the user has administrator privileges; the «user» or «Documents» folders are suggested.

A successful installation creates the main «k0-INRIM» folder which includes two additional «data» and «classes» folders, and the «k0-INRIM.py» and «user template.xlsx» files.

The «k0-INRIM.py» is the Python script using Python objects defined in the «naaobj.py» supporting script file included in the «classes» folder. The «k0-INRIM.py» and «naaobj.py» are source codes, accessible for expert users for further development. The «user template.xlsx» is an excel workbook for manual spectrum data entries.

The software main settings are defined in the «kimp0-01s.txl» file included in «data» along with the i) «channels», ii) «efficiencies», iii) «irradiations», iv) «k0data», v) «presets», vi) «sources» and vii) «models» folders storing information on i) irradiation channels, ii) energy-FWHM-efficiency calibrations, iii) irradiation data, iv) nuclear data from the k_0 database [7], v) target elements list presets, vi) γ-sources certificates and vii) adopted measurement model, respectively.

3 Use

3.1 Main window

The software main window (Figure 1) is opened by double clicking on the «k0-INRIM.py» file or on the corresponding desktop link. A supporting prompt window is also opened to display user messages and software errors; closing this prompt window stops the program.

The first user action after installation is to set software options by pressing the *Settings* button located in the top-right corner.

Spectrum data are imported manually by pressing the *Input workbook* or automatically by selecting outputs of a gamma spectrum evaluation software (ORTEC GammaVision [8] or HyperLab [9]). The following analysis workflow is suggested by the position of six action buttons placed in descending order at the left side of the window: 1) *Background*, 2) *Calibration*, 3) *Irradiation*, 4) *Sample*, 5) *Standard* and 6) *Detection limits*. Each button identifies a workflow step in a window region bounded by horizontal separators containing spin-boxes, labels and additional action buttons.

The output is finally obtained by pressing the *Elaborate* button located next to the *Input workbook* button in the top-right corner.

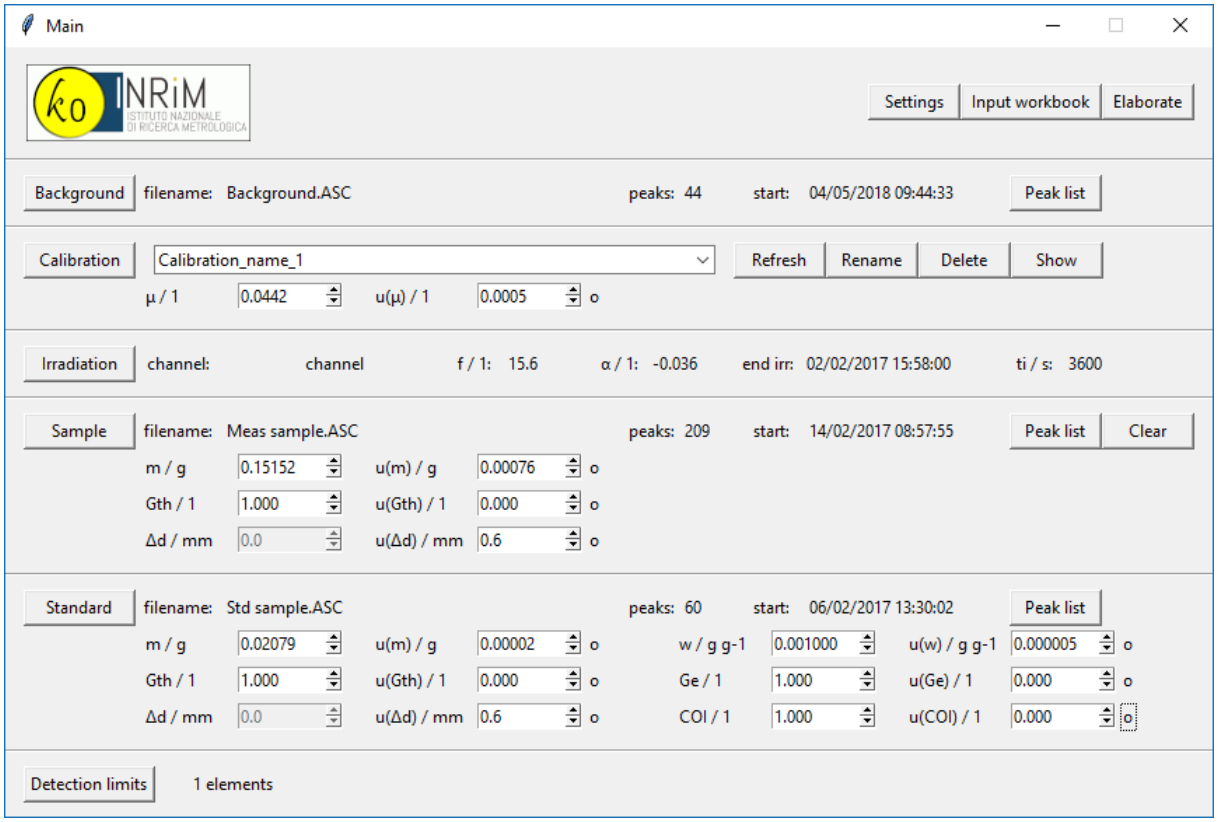


Figure 1: The main window of k0-INRIM software

3.2 Settings

The *Settings* button in the main window allows to set the general behavior of the software (Figure 2). Any change, if confirmed, will automatically make the current settings effective by closing the program.

The first setting is the k_0 database version used to retrieve nuclear data. In the case of release of an updated version, save the new file in the «k0data» folder and replace the current selection with the new filename that appears in the drop-down menu.

The k_0 database installed by default is the most up to date version at the time of writing [7] with a couple of minor but necessary changes. Details of these changes are given in the «README_k0_database.txt» file in the «k0data» folder.

The second setting is the energy tolerance, ΔE, used to identify the gamma peaks of the spectra by comparison with the emission energies reported in the k_0 database, E_p. The software searches for entries satisfying the relationship: $E_\mathrm{p} - \Delta E < E_\mathrm{meas} < E_\mathrm{p} + \Delta E$, where E_meas is the

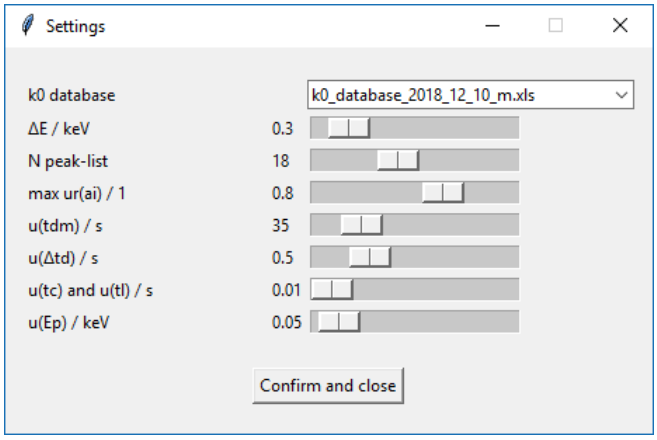


Figure 2: The settings window

energy of the measured peak. The ΔE value shouldn't be neither too low or too high. In the former case the identification fails if the energy calibration is affected by minor biases while in the latter case multiple correspondences are returned. The default 0.3 keV value might be a reasonable compromise.

The third setting affects the visual aspect of the peak list window (see paragraph 3.4) by adjusting the maximum number of listed peaks to appear in the screen.

The fourth setting defines the maximum allowed relative uncertainty for the parameters, a_i, modeling the detection efficiency (see paragraph 3.5).

The last four settings define the default values for the standard uncertainties of the input quantities $t_{\mathrm{d\,m}}$, Δt_{d}, t_{c}, t_{l} and E_{p} (here and hereafter, see the equation model 4 for the adopted symbols of the input quantities).

3.3 Spectrum data input

As a first step of the analysis, spectrum data information is imported for processing either manually by editing a user template workbook (3.3.1) or automatically from outputs obtained with ORTEC GammaVision or HyperLab spectrum evaluation software packages (3.3.2).

3.3.1 Template workbook

The «user template.xlsx» workbook in the «k0-INRIM» folder is manually filled in with spectrum data.

The default workbook includes five worksheets; the first one, «Background», is prepared to add background spectrum data; the second and third ones, «Ref source (1)» and «Ref source (2)», are

prepared to add calibration spectrum data collected with the multi-gamma reference source; the fourth and the fifth ones, «Std sample» and «Meas sample», are prepared to add spectrum data collected with the standard sample and measurement sample, respectively. Whenever required, additional worksheets can be created by duplicating the existing ones.

A spectrum worksheet consists of two regions separated by a vertical solid line as shown in Figure 3.

	A	B	C	D	E	F	G	H	I
1	**Start Acquisition**	04/05/2018 09:44						**Channel / ch**	**Counts / 1**
2	**Real time / s**	256782						0	0
3	**Live time / s**	256681						1	0
4	**Number of channels**	8192						2	0
5	**Channel / ch**	**Energy / keV**	**Net area / 1**	**Std unc (Net area) / 1**	**FWHM / ch**			3	0
6	291.3	72.809886	2381.9	103.2	3.83			4	0
7	299.8	74.940875	4759	121.6	3.83			5	0
8	308.563577	77.13734	790.5	86.6	3.83			6	0
9	339.018617	84.74996	2548.6	123.2	4.57			7	0
10	348.938357	87.229523	1061.1	101.5	4.57			8	0
11	370.200834	92.544347	1489.4	110.2	4.57			9	0
12	743.111357	185.758015	1242.4	134.4	5.02			10	0
13	954.370232	238.564824	3065.1	113.4	4.07			11	0
14	967.613021	241.875025	986.3	87.3	4.07			12	0
15	1180.890822	295.18649	2218.3	99.2	4.53			13	0

Background | Ref source (1) | Std sample | Meas sample

Figure 3: The «Background» worksheet of the «user template.xlsx» file

The first four rows of the left-side region accept the start acquisition, the real time, t_c, the live time, t_l, and the total number of spectrum channels. From the sixth raw downwards, the measured centroid channel, the measured energy, E_{meas}, the net area, n_p, the standard uncertainty of the net area, $u(n_p)$, and the Full Width Half Maximum, FWHM, of the elaborated gamma peaks are sequentially added. The FWHM values are required in a reference source worksheet to evaluate the detection limits (see paragraph 3.9); in the remaining worksheets, the FWHM values are optional.

The column I in the right-side region accepts the number of counts, n, collected in the corresponding channels indicated in column H. The n values are required in case of a measurement sample worksheet to evaluate the detection limits (see paragraph 3.9); in the remaining worksheets, the n values are optional to display the spectrum profile recalled from the peak list window (see paragraph 3.4).

The filled in user template workbook is selected by pressing the button *Select* from the Select and convert window (Figure 4) opened with the *Input workbook* button in the top-right corner of the main window. The file path is displayed in the select and convert window.

After selection, every worksheet is converted in two spectrum data input files (.csv and .asc) by pressing the *Convert* button. The .csv file contains the Channel, Energy, Net area, Std unc (Net

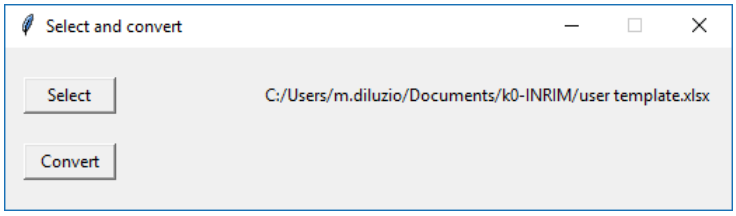


Figure 4: The select and convert window

area) and FWHM data while the .asc file contains the Start Acquisition, Real time, Live time and the n data.

3.3.2 ORTEC GammaVision and HyperLab outputs

The spectrum data input files can be directly created using the ORTEC GammaVision or HyperLab gamma spectrum evaluation software.

The k0-INRIM accepts the ORTEC GammaVision .rpt report and .chn spectrum files, respectively, in alternative to the .csv and .asc files converted from the user template workbook. The .rpt file is obtained from the software main window by selecting the *Entire spectrum in memory...* in the *Analyze* drop down menu (see the GammaVision user manual for further details). The .chn file is the collected integer spectrum file.

In addition, the .csv and .asc files created by the HyperLab software are directly accepted. The .csv file is obtained in the spectrum peak evaluator window by selecting the *Export to CSV file...* in the *File* drop down menu (see the HyperLab user manual for further details).

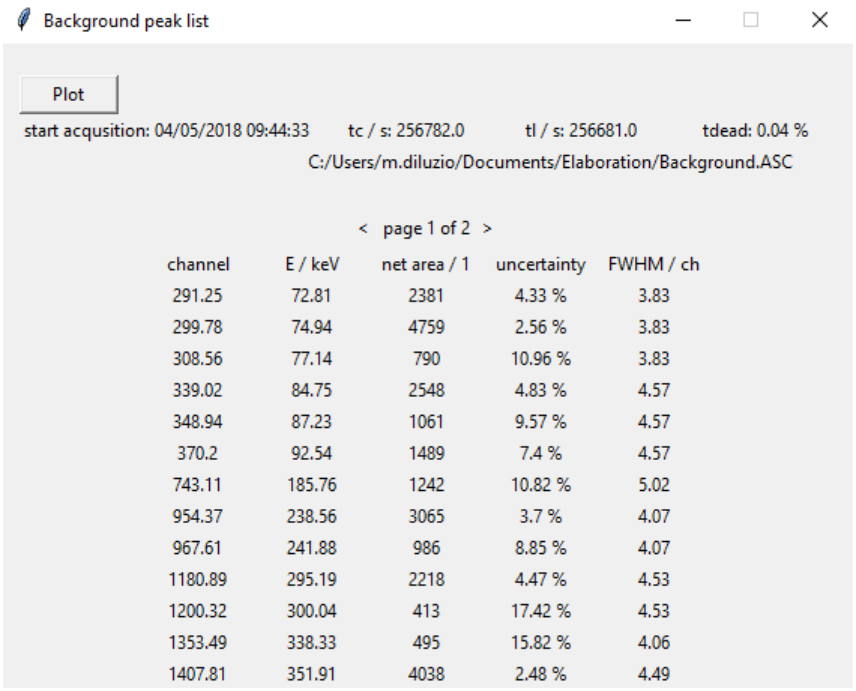
Both the .rpt (or .csv) and .chn (or .asc) files must have the same name in order to be selected in the following workflow steps (see 3.4, 3.5, 3.7 and 3.8) and processed by the k0-INRIM.

It is worth to note that the .csv and .rpt files from ORTEC GammaVision and HyperLab, respectively, must be obtained after the energy and FWHM calibration of the spectrum channels. Peak identification is not required.

3.4 Background

The first workflow step is optional but suggested as a support to the analysis. The background spectrum data are imported by selecting the .csv (or .rpt) file after pressing the *Background* button in the main window; the corresponding .asc (or .chn) file is automatically imported. The .asc (or .chn) filename, the number of peaks and the start acquisition date and time are displayed.

The *Peak list* button opens the background peak list window displaying background spectrum information (Figure 5).



channel	E / keV	net area / 1	uncertainty	FWHM / ch
291.25	72.81	2381	4.33 %	3.83
299.78	74.94	4759	2.56 %	3.83
308.56	77.14	790	10.96 %	3.83
339.02	84.75	2548	4.83 %	4.57
348.94	87.23	1061	9.57 %	4.57
370.2	92.54	1489	7.4 %	4.57
743.11	185.76	1242	10.82 %	5.02
954.37	238.56	3065	3.7 %	4.07
967.61	241.88	986	8.85 %	4.07
1180.89	295.19	2218	4.47 %	4.53
1200.32	300.04	413	17.42 %	4.53
1353.49	338.33	495	15.82 %	4.06
1407.81	351.91	4038	2.48 %	4.49

Figure 5: The background peak list window

The background spectrum profile is plotted in a spectrum window by pressing the *Plot* button (Figure 6); buttons are available to visualize the peaks and save the window.

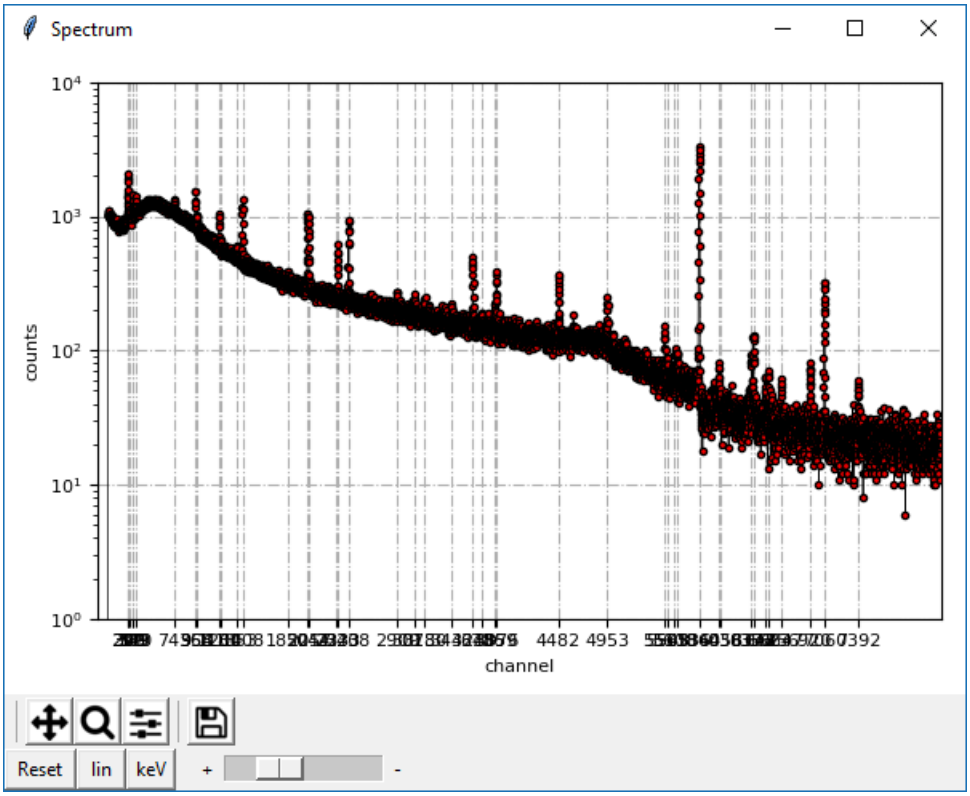


Figure 6: The background spectrum window

The start acquisition, the t_c, the t_l, the relative dead time and the spectrum file path are spotted at the top of the peak list window. The list of the peaks is displayed below including the channel and energy centroid, the net area and relative counting uncertainty, and FWHM (if available). Additional pages are added depending on the total number of peaks and the selected maximum number of listed peaks (see paragraph 3.2).

3.5 Calibration

The second workflow step concerns the detector calibration and is performed in consecutive stages to allow users obtaining a satisfactory result.

The data processing is started using the calibration window opened by pressing the *Calibration* button in the main window (Figure 7).

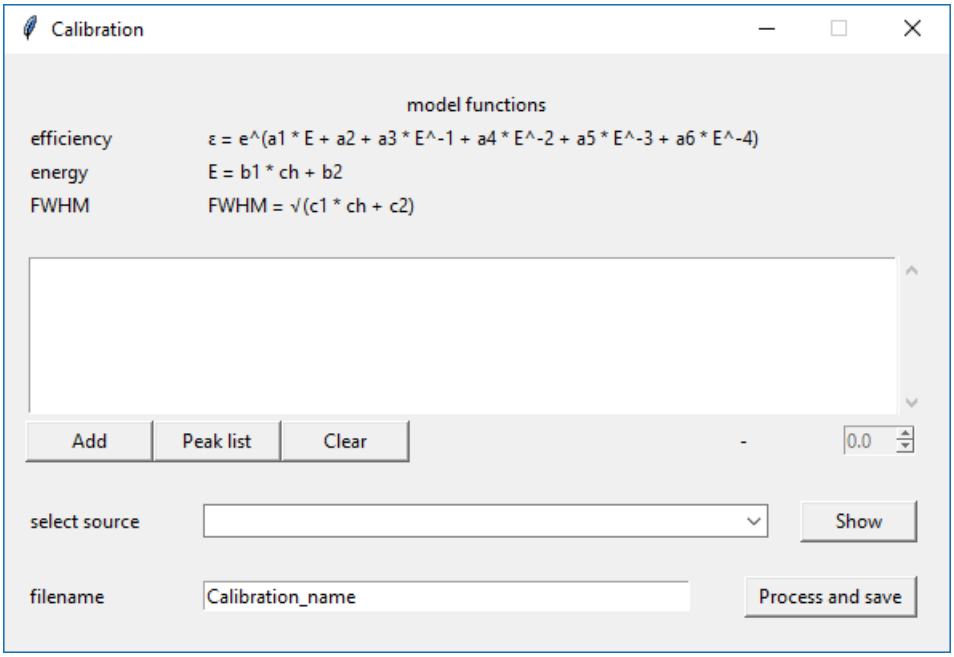


Figure 7: The calibration window

The model functions adopted for efficiency, ε, energy, E, and FWHM calibration are recalled at the top of the window and reported here for user's convenience:

$$\varepsilon = \mathrm{e}^{a_1\,E+a_2+a_3\,E^{-1}+a_4\,E^{-2}+a_5\,E^{-3}+a_6\,E^{-4}}, \tag{1}$$

$$E = b_1\,ch + b_2, \tag{2}$$

$$\mathrm{FWHM} = \sqrt{c_1\,ch + c_2}, \tag{3}$$

where a_1, a_2, a_3, a_4, a_5 and a_6 are efficiency fitting parameters, ch is the spectrum channel, b_1 and b_2 are energy fitting parameters, c_1 and c_2 are FWHM fitting parameters. It is worth to note that the energy and FWHM calibration is only needed for computing detection limits (see paragraph 3.9).

There are two calibration approaches available for the user based on i) single spectrum acquisition of the source at the counting position of the samples, or ii) multiple spectra acquisitions of the source located in equally spaced points at the counting position of the samples. The first approach requires previous knowledge of the relative variation of efficiency per mm on E at the calibration position, $\delta\varepsilon_\mathrm{r}$ [2].

3.5.1 Single reference source spectrum

A single spectrum of the reference source is collected at the distance where the samples are counted.

The calibration spectrum data are imported by selecting the .csv (or .rpt) file after pressing the *Add* button; the corresponding .asc (or .chn) file is automatically imported. The filename is displayed in the calibration window together with the spin-box where the user can enter the $\delta\varepsilon_r$ value (Figure 8). Since this parameter depends on the emission energy, the entered value might require adjustments in the output uncertainty spreadsheet.

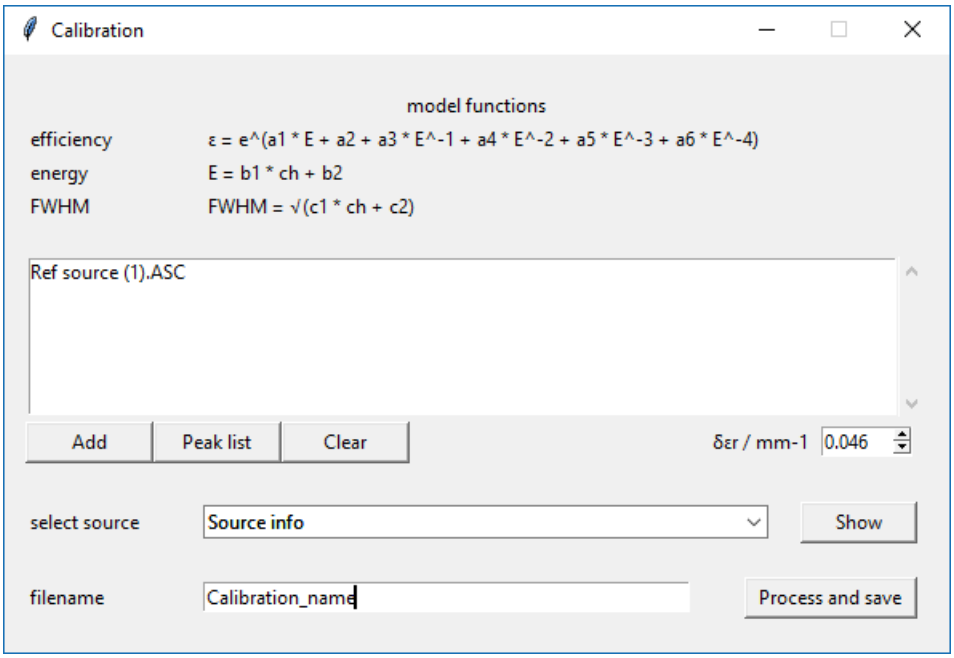


Figure 8: The calibration window

The *Peak list* button opens the calibration peak list window to display calibration spectrum information. The calibration peak list window layout corresponds to the background peak list window layout (see paragraph 3.4) with a single exception. Specifically, the user can show or hide the background spectrum profile (if previously selected) by pressing the additional *+BG/-BG* buttons (Figure 9).

The added spectrum can be removed by pressing the *Clear* button in the calibration window.

The select source drop-down menu allows selecting among the γ-source certificate data saved in the «sources» folder. The default Source template corresponds to the «Source template.sce» file, available for user's customization (see the «README_filesources.txt» file in the «sources» folder for further details). The source window is displayed by pressing the *Show* button (Figure

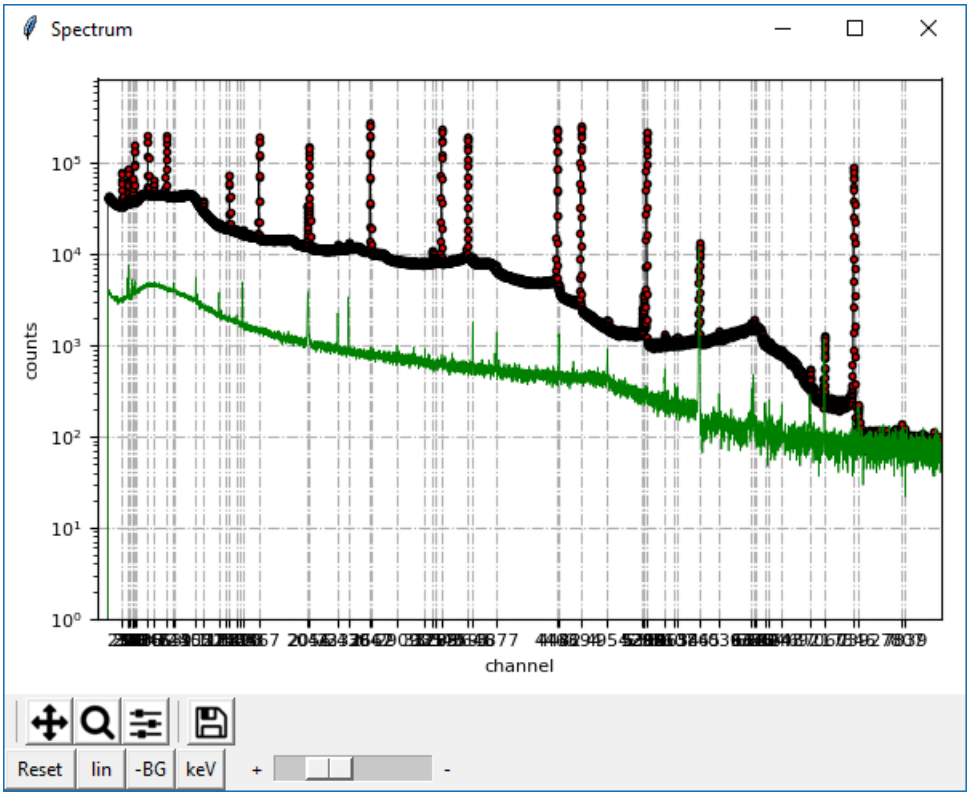
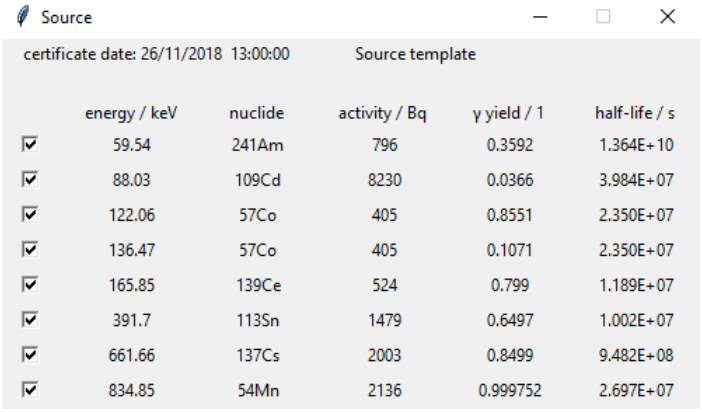


Figure 9: The calibration spectrum window

10). By default, all the certified emissions are selected; the user may deselect the unwanted ones.

After entering the calibration filename in the calibration window, calibration data are processed and the result is saved by pressing the *Process and save* button; the algorithm calculates the fitting parameters of ε, E and FWHM. The calibration processing window is automatically opened (Figure 11) with a title bar showing the calibration filename with a progressive number corresponding to the current processing stage.



	energy / keV	nuclide	activity / Bq	γ yield / 1	half-life / s
☑	59.54	241Am	796	0.3592	1.364E+10
☑	88.03	109Cd	8230	0.0366	3.984E+07
☑	122.06	57Co	405	0.8551	2.350E+07
☑	136.47	57Co	405	0.1071	2.350E+07
☑	165.85	139Ce	524	0.799	1.189E+07
☑	391.7	113Sn	1479	0.6497	1.002E+07
☑	661.66	137Cs	2003	0.8499	9.482E+08
☑	834.85	54Mn	2136	0.999752	2.697E+07

Figure 10: The source window

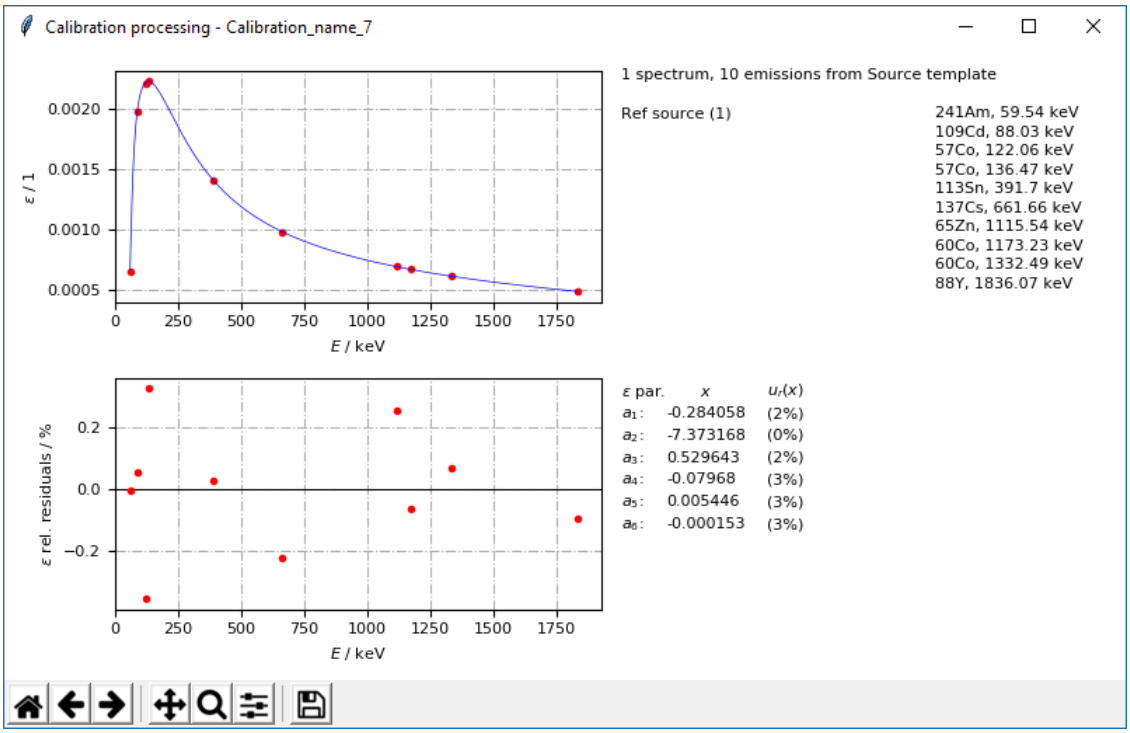


Figure 11: The calibration processing window

The efficiency curve is plotted in the upper graph. The blue solid line is obtained by fitting the efficiency model function (1) to the efficiency values calculated at the certified emissions (red dots) and adopted for calibration; the counting position of the source is called calibration position.

The calibration relative residuals are plotted in the lower graph. Additional information is given to the right side, including the fitted efficiency parameters values with their relative standard uncertainties.

The user may save the current calibration processing window for future record by pressing the *Save the figure* button or, in the case of a unsatisfactory result, repeat the calibration by adjusting the current selection of the certified emissions in the source window.

The *Refresh* button in the main window adds the saved calibration stages to the calibration drop-down menu. The selected calibration is renamed or deleted by pressing the *Rename* or *Delete* buttons. The outcome is displayed in the calibration result window by pressing the *Show* button (Figure 12).

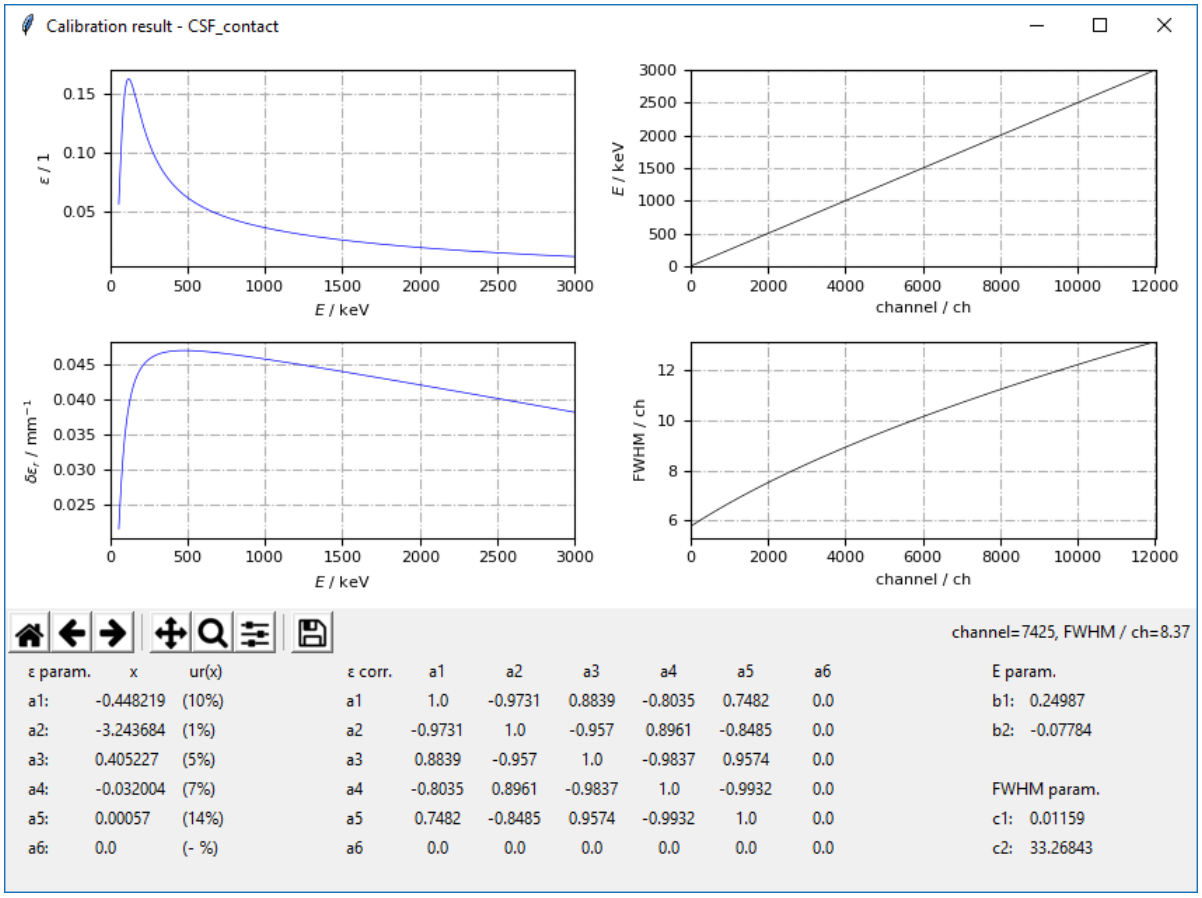


Figure 12: The calibration result window

The ε and $\delta\varepsilon_r$ curves are plotted in the left graphs while the E and FWHM curves are plotted in the right graphs. Efficiency, energy and FWHM parameters are displayed below, including the

efficiency parameters correlation matrix.

The calibration selected in the calibration drop-down menu of the main window is adopted for the analysis. Two additional spin-boxes are available to enter the excess counting loss constant, μ, and its standard uncertainty, $u(\mu)$ [2]; in the case that the available uncertainty information is based on a priori rectangular or triangular probability distribution [1], the corresponding half-width interval is entered in the uncertainty window displayed by pressing the small open circle (Figure 13).

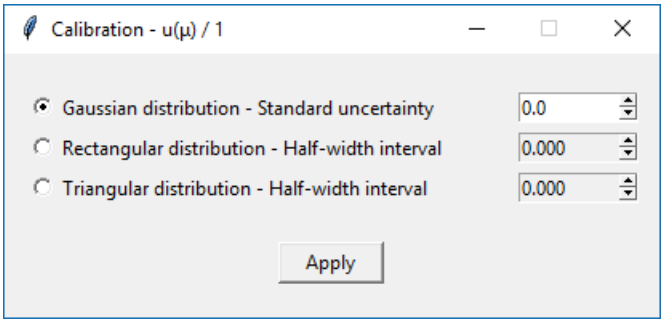


Figure 13: The uncertainty window

The uncertainty window is available for other uncertainty spin-boxes in the program interface.

3.5.2 Multiple reference source spectra

Multiple spectra of the reference source are collected in equally spaced points in a range centered at the counting position of the samples.

The minimum number of points is two, located at the same distance above and below the counting position of the samples (Figure 14). The maximum gap between the counting points, Δg, (mm) should be limited by taking into account non-linearities of vertical efficiency variation.

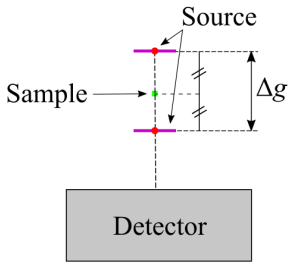


Figure 14: The calibration setup

After importing the collected multiple spectra, the $\delta\varepsilon_r$ spin-box is replaced by the Δg spin-box where user can enter the corresponding value (Figure 15).

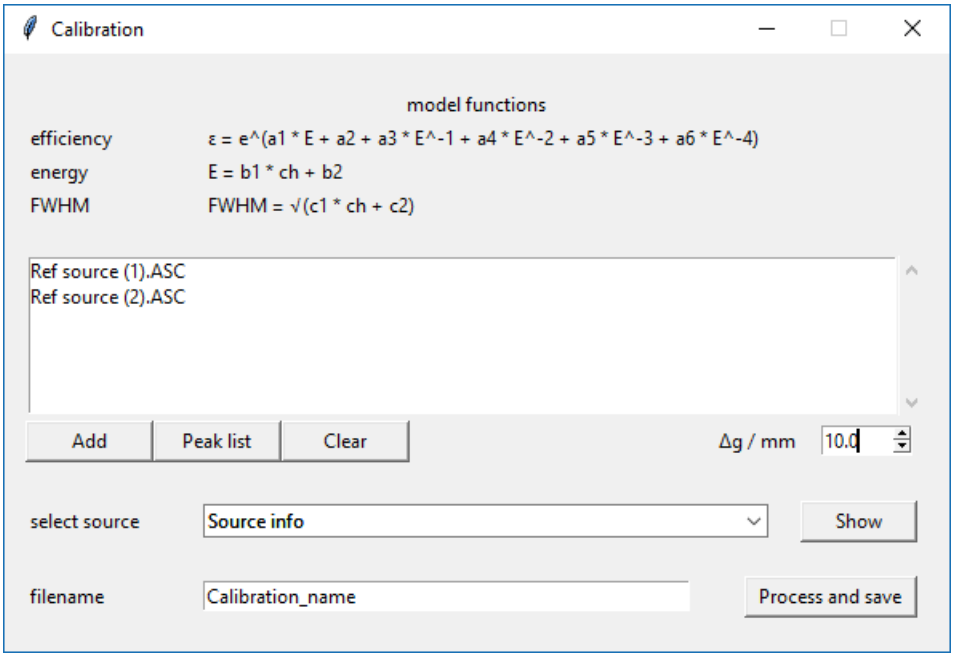


Figure 15: The calibration window

The peak list window opened by the *Peak list* button includes the additional possibility to browse the select multiple spectra (Figure 16).

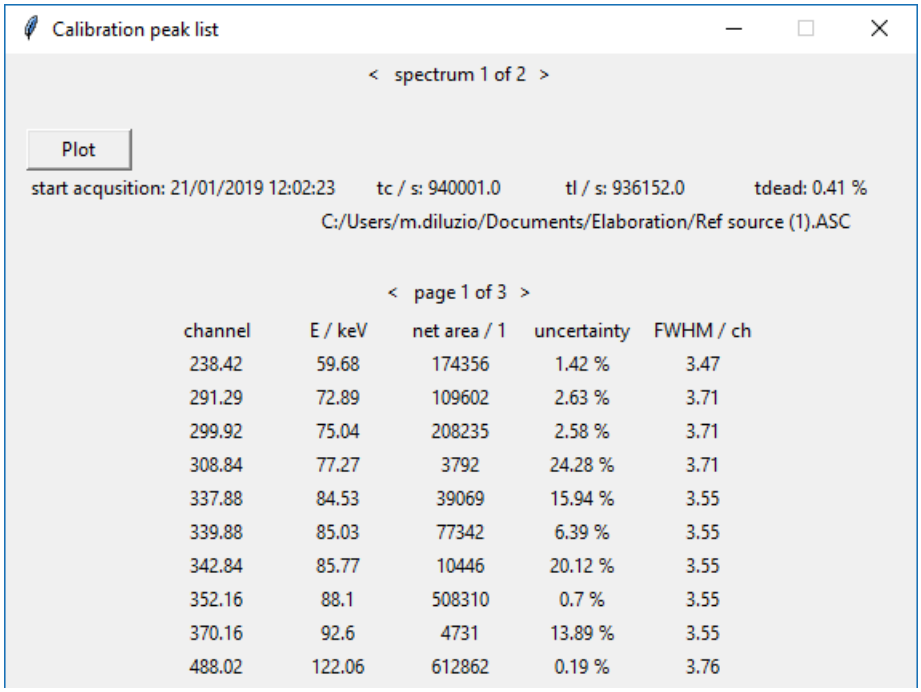


Figure 16: The calibration window

The processing algorithm calculates the $\delta\varepsilon_r$ in addition to the fitting parameters of ε, E and FWHM.

Multiple efficiency curves are plotted in the upper graph of the (Figure 17). Dashed lines curves and open circles refer to the efficiencies at the multiple counting positions of the reference source. The blue solid line is obtained by fitting the efficiency model function (1) to the average of the efficiency values calculated at the certified emissions (red dots) and adopted for calibration at the counting position of the samples.

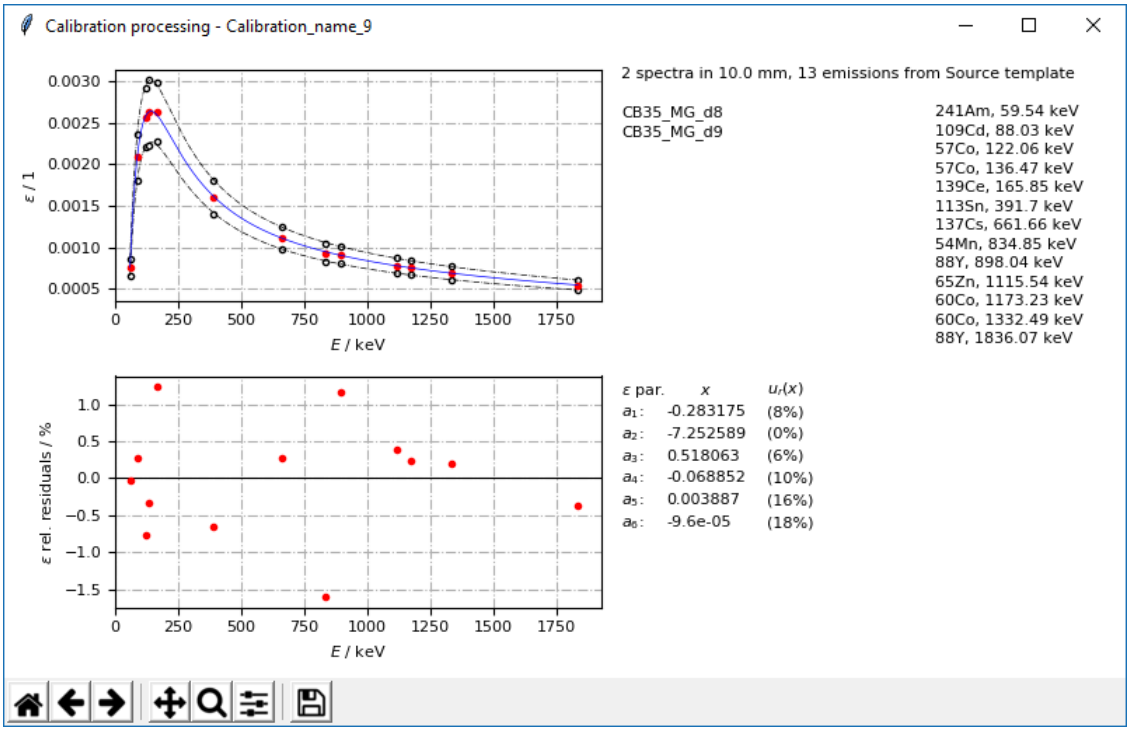


Figure 17: The calibration processing window

3.6 Irradiation

The irradiation data are entered in the irradiation window opened by pressing the *Irradiation* button in the main window (Figure 18).

Data are stored with the irradiation code added in the drop-down menu. Pressing the *Delete* button eliminates data referred to the irradiation code selected from the drop-down list.

The information concerning irradiation channel name, f and α values, and uncertainties are added in the corresponding drop-down menu and spin-boxes, respectively. Irradiation channel data are saved or deleted by pressing the *Save* or *Delete* buttons, respectively.

The irradiation time, t_{i}, its uncertainty, $u(t_{\mathrm{i}})$, and the irradiation end are entered in the remaining spin-boxes.

Data are imported for the analysis by pressing the *Confirm* button; the channel name, f and α values, the irradiation end and t_{i} are displayed in the main window.

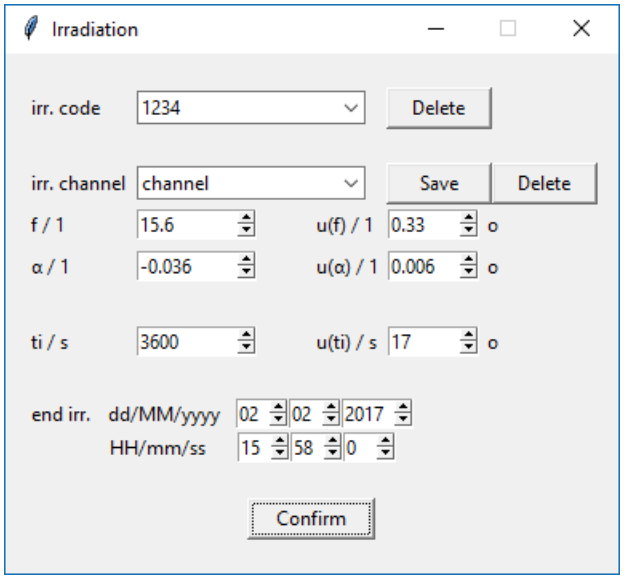


Figure 18: The irradiation window

3.7 Sample

The sample spectrum data are imported in the fourth workflow step by selecting the .csv (or .rpt) file after pressing the *Sample* button in the main window; the corresponding .asc (or .chn) file is automatically imported. The selected filename, the number of peaks and the start acquisition date and time are displayed. In the case of multiple sample files selection, only the number of spectra is displayed instead of the filename and the remaining fields are unfilled.

The *Peak* list button opens the sample peak list window displaying sample spectrum information (Figure 19).

The sample peak list window layout corresponds to the background peak list window layout (see paragraph 3.4) with additional features for the identification of the investigated elements.

As in the calibration step, the user can select multiple spectra and, in the spectrum plot, show or hide the background spectrum profile by pressing the *+BG/-BG* buttons (Figure 9).

An emission drop-down menu connected to *X* and *Info* buttons is available for each elaborated and imported peak. The drop-down menu is activated for those peaks whose energy has an agreement with the emissions reported in the k_0 database within the tolerance, ΔE, defined in the settings window (3.2); the resulting (gamma) emitters and their emission energies (keV) are included in the drop-down menu.

The user can reset the menu by pressing the *X* button or open an information window for the selected emission by pressing the *Info* button. The information window displays data retrieved

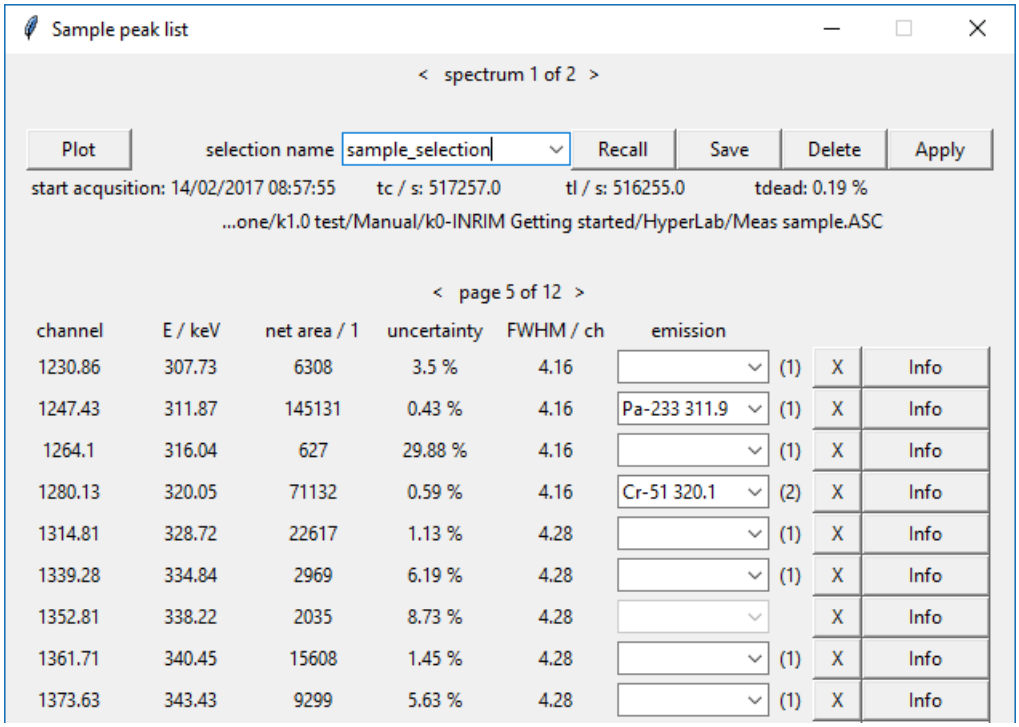


Figure 19: The sample peak list window

from the k_0 database (Figure 20); the target element, the target isotope, the Q_0 and $\bar{E}_r$ values (with relative uncertainties) are in the first row; the selected emitter, the energy, E_p, the k_0 value (with relative uncertainty), $k_{0\,\mathrm{Au}}$, coincidence warning and the gamma yield are in the second row; the decay type and the cascade nuclides are in the third row. Further emissions (with the gamma yield) from the emitter and further emitters (with the emission energy) from the target are displayed in the left-side and right-side list boxes, respectively. Additional notes are shown at the bottom of the window.

Users might take advantage of comparing background with sample peaks in the spectrum window and knowing the list of emitters displayed in the activated drop-down menus to check possible peak interferences. Additionally, the information data might help to confirm the identity of the investigated elements.

The emissions selected in the sample peak list window are finally considered for the analysis. The current selection can be named by editing in the selection name drop-down menu, recalled, saved, and deleted using the *Recall*, *Save* and *Delete* buttons, respectively. The selection name drop-down menu includes by default the " " selection to clear, if recalled, all the selected emissions. In case multiple spectra, the *Apply* button allows to copy the current selection to all the imported

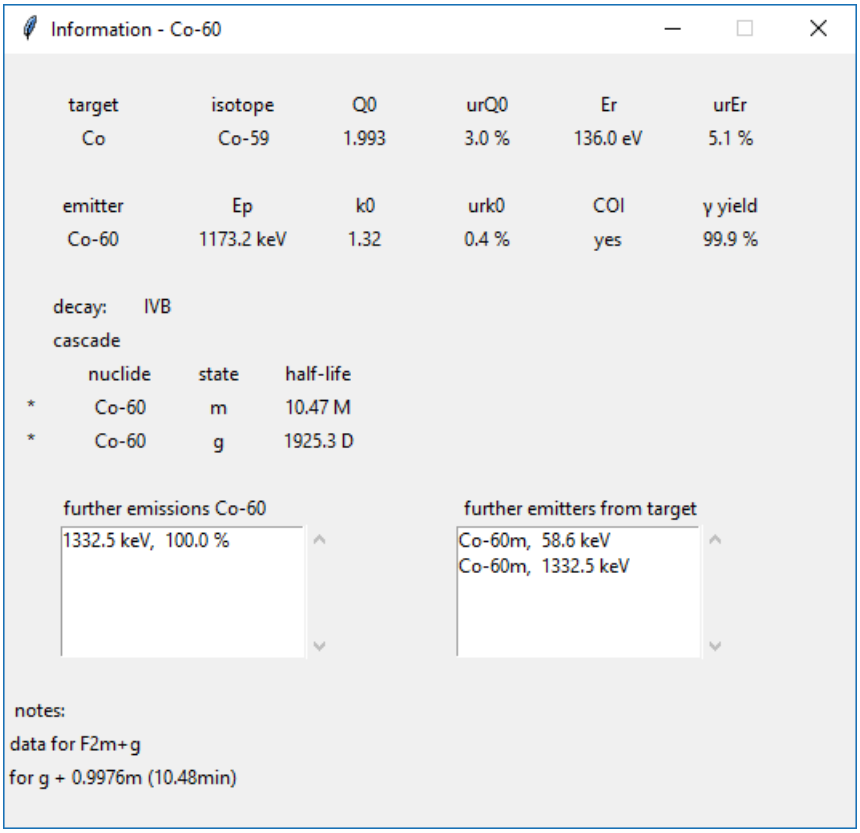


Figure 20: The info window

peak lists.

Spin-boxes are available in the sample region of the main window to enter the measurement sample mass, m_{sm}, the thermal self-shielding factor, $G_{\mathrm{th\,a}}$, and the vertical distance between the counting position of the measurement sample and the calibration position, Δd_{a} (see paragraph 3.5); standard uncertainty spin-boxes and the corresponding small open circles are available for these parameters. Since the measurement sample must be located as close as experimentally possible to the calibration position (see paragraph 1), the Δd_{a} spin-box is nominally fixed to zero and disabled. In addition, the sample epithermal self-shielding, $G_{\mathrm{e\,a}}$, and coincidence factor, $\mathrm{COI_a}$, are not displayed in the software interface and by default fixed to the unity value with zero uncertainty. The user can manually modify these values in the uncertainty spreadsheet budget outputs.

3.8 Standard

The standard spectrum data are imported in the fifth workflow step by selecting the .csv (or .rpt) file after pressing the *Standard* button in the main window; the corresponding .asc (or .chn) file is automatically imported. The selected filename, the number of peaks and the start acquisition date and time are displayed.

The *Peak list* button opens the standard peak list window displaying the standard spectrum information (Figure 21).

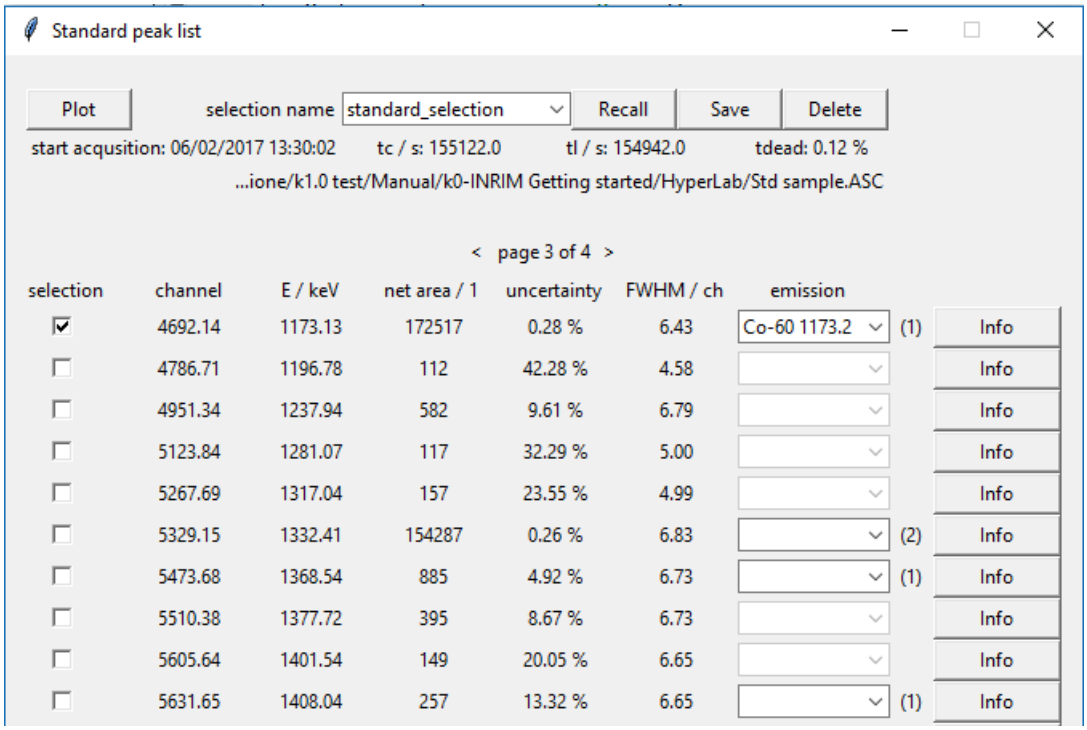


Figure 21: The standard peak list window

The standard peak list window layout corresponds to the sample peak list window layout (see paragraph 3.7) with the addition of a selection check-box for each elaborated peak. The user identifies and selects the emission of the adopted monitor element from the correspondent drop-down menu, then confirms the selection in the selection check-box. Full functionalities for peak identification are still available.

Spin-boxes are available in the standard region of the main window to enter the standard sample mass, m_{std}, the mass fraction of the monitor element in the standard sample, w_{m}, the thermal self-shielding factor, $G_{\mathrm{th\,m}}$, the epithermal self-shielding factor, $G_{\mathrm{e\,m}}$, the vertical distance between the

counting position of the standard sample and the calibration position, Δd_{m} (see paragraph 3.5) and the coincidence factor, $\mathrm{COI}_{\mathrm{m}}$; standard uncertainty spin-boxes and the corresponding small open circles are available for these parameters. Since the standard sample must be located as close as experimentally possible to the calibration position (see paragraph 1), the Δd_{m} spin-box is nominally fixed to zero and disabled.

3.9 Detection limits

The sixth and last workflow step is optional to evaluate the Currie's detection limits [10]. The element selection window is opened by pressing the *Detection limits* button in the main window (Figure 22).

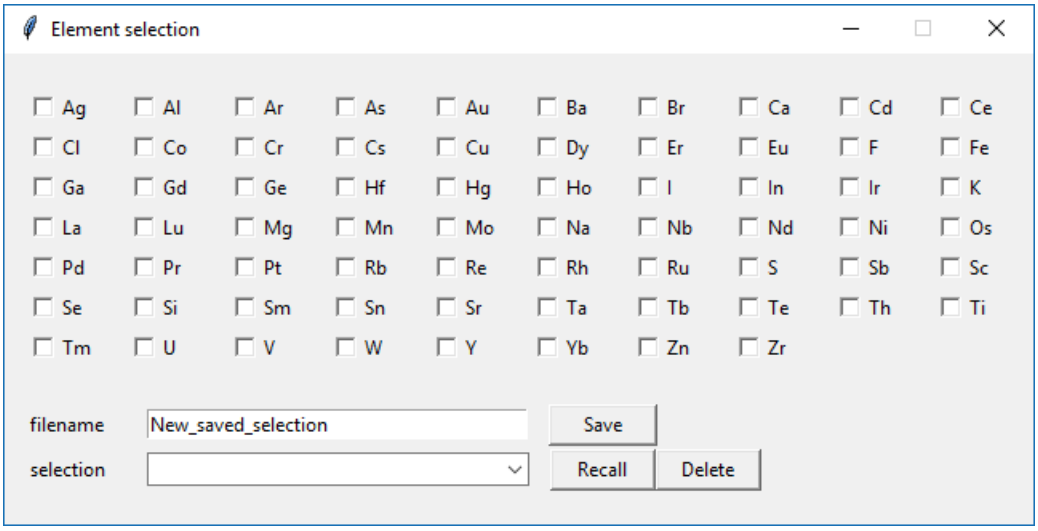


Figure 22: The element selection window

The elements for which the detection limits are evaluated can be manually selected by clicking on the correspondent element check-box. The current selection is named by editing in the filename box, saved, recalled and deleted using the *Save*, *Recall* and *Delete* buttons, respectively. The selection drop-down menu includes by default five selections: i) "all", ii) "medium and long-lived", iii) "rare earths", iv) "short and medium-lived" and v) " "; the " " selection, if recalled, clears all the element check-boxes.

4 Output

4.1 Elaborate

The output is obtained by pressing the *Elaborate* button in the upper-right corner of the main window and a message window "Results file successfully created!" is opened.

The program creates an Excel workbook file named by the user and consisting of multiple worksheets. The first, «Analysis», is an overview of the results, and the following are uncertainty budgets, «(i)_UncBud_te(j)», and detection limits, «(i)_DetLim_te(j)», respectively; where te is the target element symbol, e.g. Au, i is the index referring to the measurement sample spectrum and j is the index referring to the selected gamma emission.

The «Analysis» worksheet is shown in Figure 23. General information is reported including the target monitor element (in the Standard section) and a summary of the results obtained for the investigated elements (in the Sample section). Quantifications and detection limits are given in mass fractions; in the first case values include the combined (absolute and relative) uncertainties whereas, in the latter case, the lowest detection limit.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Irradiation end		t_i / s		Channel	f / 1	α / 1		Calibration name					
2	02/02/2017 15:58		3600		channel	15.6	-0.036		Calibration_name_1					
3														
4	**Standard**		**C:/Users/m.diluzio/Documents/Elaborazione/k1.0 test/Manual/Elaboration example/Std sample.ASC**											
5	Start acquisition		t_c / s	t_l / s	t_{dead}	t_d / s								
6	06/02/2017 13:30		155122	154942	0.12%	336722								
7														
8	Target	Isotope	Emitter	Half-life	E_p / keV	n_p / 1	FWHM / ch	Coincidence	m_{std} / g	Decay type		w_m / g g^{-1}	$u(w_m)$ / g g^{-1}	$u_r(w_m)$
9	Co	Co-59	Co-60	1925.3 D	1173.2	172517.7	6.43	yes	0.02079	IVB		0.001	0.000005	0.50%
10														
11														
12	**Sample**		**C:/Users/m.diluzio/Documents/Elaborazione/k1.0 test/Manual/Elaboration example/Meas sample.ASC**											
13	Start acquisition		t_c / s	t_l / s	t_{dead}	t_d / s								
14	14/02/2017 08:57		517257	516255	0.19%	1011595								
15														
16	*Quantifications*													
17	Target	Isotope	Emitter	Half-life	E_p / keV	n_p / 1	FWHM / ch	Coincidence	m_{sm} / g	Decay type		w_a / g g^{-1}	$u(w_a)$ / g g^{-1}	$u_r(w_a)$
18	Sc	Sc-45	Sc-46	83.83 D	889.3	743458.9	5.71	yes	0.15152	IVB		8.49E-06	3.50381E-07	4.13%
19	Cr	Cr-50	Cr-51	27.7 D	320.1	71132.8	4.16	no	0.15152	I		7.1E-05	3.04687E-06	4.29%
20	Co	Co-59	Co-60	1925.3 D	1332.5	31878.7	6.83	yes	0.15152	IVB		8.46E-06	3.44801E-07	4.08%
21	Zn	Zn-64	Zn-65	244.3 D	1115.5	14962.5	6.37	no	0.15152	I		0.000104	4.47855E-06	4.30%
22	Sb	Sb-123	Sb-124	60.2 D	1691	4124.9	7.79	yes	0.15152	VI		1.72E-06	9.36307E-08	5.44%
23	Cs	Cs-133	Cs-134	2.0644 Y	795.9	42033.7	5.66	yes	0.15152	IVB		5.35E-06	2.50932E-07	4.69%
24	La	La-139	La-140	1.678 D	1596.2	29436.6	7.35	yes	0.15152	I		2.81E-05	1.28135E-06	4.57%
25	Ce	Ce-140	Ce-141	32.51 D	145.4	120978.2	3.56	no	0.15152	I		5.95E-05	2.65709E-06	4.46%
26	Nd	Nd-146	Nd-147	10.98 D	531	4956.3	5.03	yes	0.15152	I		2.64E-05	1.73044E-06	6.56%
27	Tb	Tb-159	Tb-160	72.3 D	879.4	10944.1	5.71	yes	0.15152	I		6.39E-07	3.26747E-08	5.11%
28	Yb	Yb-174	Yb-175	4.185 D	396.3	19148.1	4.44	yes	0.15152	IVB		2.2E-06	9.68352E-08	4.40%
29	Hf	Hf-180	Hf-181	42.39 D	482.2	52459.9	4.7	yes	0.15152	I		4.91E-06	2.08225E-07	4.24%
30	Ta	Ta-181	Ta-182	114.4 D	1221.4	6498.6	6.61	yes	0.15152	IVB		7.35E-07	1.10341E-07	15.01%
31	Th	Th-232	Pa-233	26.97 D	311.9	145131	4.16	yes	0.15152	IIB		8.15E-06	3.74806E-07	4.60%
32														
33	*Detection limits*													
34	Target	Isotope	Emitter	Half-life	E_p / keV	n_p(Currie)	FWHM / ch	Coincidence	m_{sm} / g	Decay type		(<)w_a / g g^{-1}		Lowest de
35	Au	Au-197	Au-198	2.695 D	411.8	49438	14	no	0.15152	I		3.17E-09		3.17E-09

Analysis | (1)_UncBud_Sc(1) | (1)_UncBud_Cr(1) | (1)_UncBud_Co(1) | ...

Figure 23: The «Analysis» worksheet

The «(i)_UncBud_$te(j)$» uncertainty budget worksheet implements the spreadsheet technique adopted to evaluate the uncertainty of the quantified mass fraction [2].

According to the GUM recommendations the following measurement model [11], adopted for computations, is displayed in the worksheet:

$$
\begin{aligned}
w_{\mathrm{a}} = & \frac{\lambda \frac{(n_{\mathrm{p}}/COI)(t_{\mathrm{c}}/t_{\mathrm{l}})e^{-\mu(1-t_{\mathrm{l}}/t_{\mathrm{c}})}}{(1-e^{-\lambda t_{\mathrm{i}}})(1-e^{-\lambda t_{\mathrm{c}}})}\Big|_{\mathrm{a}}}{\lambda \frac{(n_{\mathrm{p}}/COI)(t_{\mathrm{c}}/t_{\mathrm{l}})e^{-\mu(1-t_{\mathrm{l}}/t_{\mathrm{c}})}}{(1-e^{-\lambda t_{\mathrm{i}}})(1-e^{-\lambda t_{\mathrm{c}}})}\Big|_{\mathrm{m}}} e^{(\lambda_{\mathrm{a}}-\lambda_{\mathrm{m}})t_{\mathrm{d\,m}}+\lambda_{\mathrm{a}}\Delta t_{\mathrm{d}}} \\
& \times \frac{k_{0\,\mathrm{Au}}(\mathrm{m})}{k_{0\,\mathrm{Au}}(\mathrm{a})} \frac{G_{\mathrm{th\,m}} + \frac{G_{\mathrm{e\,m}}}{f}\left(\frac{Q_{0\,\mathrm{m}}-0.429}{\bar{E}_{\mathrm{r\,m}}^{\alpha}} + \frac{0.429}{0.55^{\alpha}(1+2\alpha)}\right)}{G_{\mathrm{th\,a}} + \frac{G_{\mathrm{e\,a}}}{f}\left(\frac{Q_{0\,\mathrm{a}}-0.429}{\bar{E}_{\mathrm{r\,a}}^{\alpha}} + \frac{0.429}{0.55^{\alpha}(1+2\alpha)}\right)} e^{\sum_{i=1}^{h} a_i (E_{\mathrm{p\,m}}-E_{\mathrm{p\,a}})^{2-i}} \frac{(1-\delta\varepsilon_{\mathrm{r\,m}}\Delta d_{\mathrm{m}})}{(1-\delta\varepsilon_{\mathrm{r\,a}}\Delta d_{\mathrm{a}})} \frac{m_{\mathrm{std}}}{m_{\mathrm{sm}}} w_{\mathrm{m}},
\end{aligned}
\tag{4}
$$

where subscripts a and m refer to the analyte and monitor, respectively, and the input quantities:

- $\lambda = \ln(2)/t_{1/2}$ is the decay constant of a radionuclide having an half-life time $t_{1/2}$,
- n_{p} is the number of counts in the full-energy γ-peak,
- COI is the true-coincidence correction factor,
- t_{c} and t_{l} are the counting and live times of the detection system,
- $t_{\mathrm{d\,m}}$ is the decay time of the monitor,
- $\Delta t_d = t_{\mathrm{d\,a}} - t_{\mathrm{d\,m}}$ is the difference between the analyte and monitor decay times at their acquisition start times,
- t_{i} is the neutron irradiation time,
- μ is the excess counting loss constant of the detection system,
- $k_{0\,\mathrm{Au}}$ is the k_0 factor,
- G_{th} and G_{e} are the thermal and epithermal neutron self-shielding correction factors,
- f is the (conventional) sub- to epi-cadmium neutron flux ratio,
- α is the epi-cadmium neutron shape factor,
- Q_0 is the ratio of the resonance integral (for a $1/E$ neutron spectrum in the epi-cadmium region) to the thermal cross section,
- $\bar{E}_{\mathrm{r}}$ is the effective resonance energy,
- E_{p} is the energy of the γ-peak,

- a_i are the h parameters of the model adoped to describe the full-energy γ-peak detection efficiency at the counting position, $\varepsilon_{\mathrm{p}} = e^{\sum_{i=1}^{h} a_i E^{2-i}}$, with $h = 4$, 5 or 6,

- $\delta\varepsilon_{\mathrm{r}}$ is the relative variation of detection efficiency per unit of vertical position,

- Δd is the vertical position difference between the sample and the reference source used for efficiency calibration at the counting position, and

- m_{std} and m_{sm} are the standard and sample masses, respectively.

See [2] for details

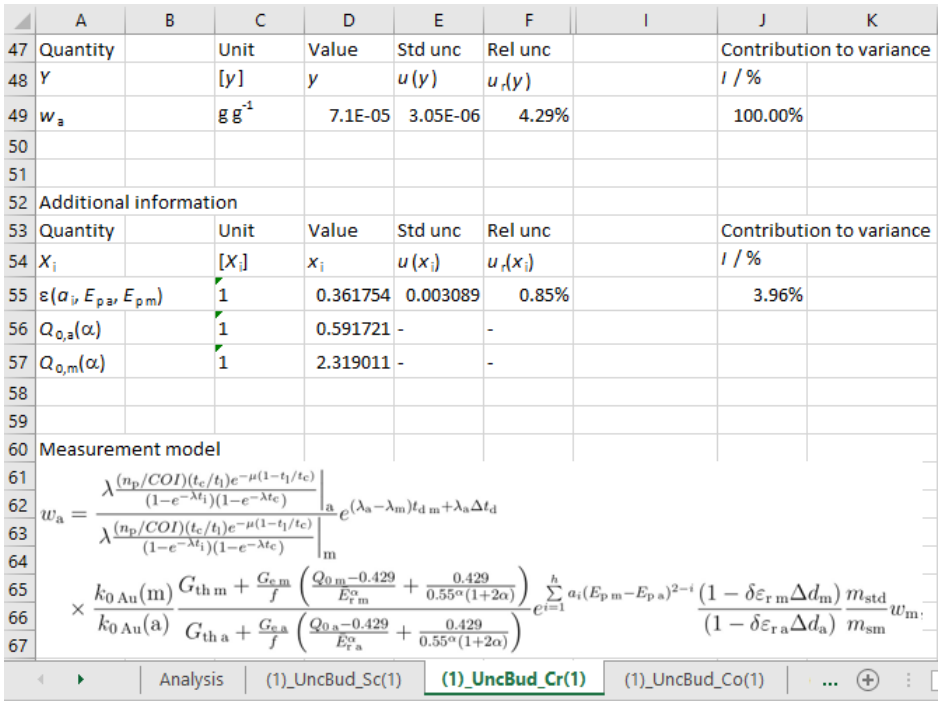
For each input quantity, X_i, the unit, $[X_i]$, the value, x_i, the standard uncertainty, $u(x_i)$, the relative uncertainty, $u_r(x_i)$, the sensitivity coefficient, c_i, and the contribution to the variance, I / % are given at the top-left of the worksheet (Figure 24). The sensitivity coefficient is obtained by calculating the equation model increasing and decreasing x_i to $x_i+u(x_i)$ and $x_i-u(x_i)$, respectively, to account for possible model non-linearity.

	A	B	C	D	E	F	I	J	K
1	Isotope	**Cr-50**	Emitter	**Cr-51**	E_p / keV	**320.1**			
2									
3	Quantity		Unit	Value	Std unc	Rel unc	Sensitivity coef.	Contribution to variance	
4	X_i		$[X_i]$	x_i	$u(x_i)$	$u_r(x_i)$	c_i	I / %	
5	t_i		s	3600	17	0.47%	1.01368E-11	0.00%	
6	n_{pa}		1	71132.8	417.9	0.59%	9.98613E-10	1.88%	
7	λ_a		s^{-1}	2.9E-07	2.51E-11	0.01%	-155.3684211	0.00%	
8	Δt_d		s	674873	0.5	0.00%	2.05731E-11	0.00%	
9	t_{ca}		s	517257	0.01	0.00%	1.6088E-11	0.00%	
10	t_{la}		s	516255	0.01	0.00%	-1.43665E-10	0.00%	
11	COI_a		1	1	0	0.00%	-7.10342E-05	0.00%	
12	m_{sm}		g	0.15152	0.00076	0.50%	-0.000468822	1.37%	
13	$k_{0Au}(a)$		1	0.00262	1.31E-05	0.50%	-0.027112956	1.36%	
14	G_{tha}		1	1	0	0.00%	-6.84382E-05	0.00%	
15	G_{ea}		1	1	0	0.00%	-2.59593E-06	0.00%	
16	Q_{0a}		1	0.53	0.106	20.00%	-6.05026E-06	4.43%	
17	E_{ra}		eV	7530	828.3	11.00%	-2.93249E-12	0.00%	
18	n_{pm}		1	172517.7	476.6	0.28%	-4.11753E-10	0.41%	
19	λ_m		s^{-1}	4.17E-09	6.49E-13	0.02%	17017.68295	0.00%	

Analysis | (1)_UncBud_Sc(1) | **(1)_UncBud_Cr(1)** | (1)_UncBud_Co(1) | ...

Figure 24: The «(i)_UncBud_$te(j)$» worksheet zoom, input quantities

The resulting mass fraction, Y, the unit, $[Y]$, the value, y, the standard uncertainty, $u(y)$, the relative uncertainty, $u_r(y)$, and additional information, e.g. value, uncertainty and contribution to the variance of the efficiency calibration ratio, $\varepsilon(a_i, E_{\mathrm{p\,a}}, E_{\mathrm{p\,m}})$, are displayed at the bottom-left (Figure 25) of the worksheet. The adopted equation model is also displayed at the bottom.



	A	B	C	D	E	F	I	J	K
47	Quantity		Unit	Value	Std unc	Rel unc		Contribution to variance	
48	Y		$[y]$	y	$u(y)$	$u_r(y)$		I / %	
49	w_a		g g^{-1}	7.1E-05	3.05E-06	4.29%		100.00%	
50									
51									
52	Additional information								
53	Quantity		Unit	Value	Std unc	Rel unc		Contribution to variance	
54	X_i		$[X_i]$	x_i	$u(x_i)$	$u_r(x_i)$		I / %	
55	$\varepsilon(a_i, E_{\mathrm{p\,a}}, E_{\mathrm{p\,m}})$		1	0.361754	0.003089	0.85%		3.96%	
56	$Q_{0,a}(\alpha)$		1	0.591721	-	-			
57	$Q_{0,m}(\alpha)$		1	2.319011	-	-			
58									
59									
60	Measurement model								

$$w_{\mathrm{a}} = \frac{\lambda \frac{(n_{\mathrm{p}}/COI)(t_{\mathrm{c}}/t_{\mathrm{l}})e^{-\mu(1-t_{\mathrm{l}}/t_{\mathrm{c}})}}{(1-e^{-\lambda t_{\mathrm{l}}})(1-e^{-\lambda t_{\mathrm{c}}})}\Big|_{\mathrm{a}}}{\lambda \frac{(n_{\mathrm{p}}/COI)(t_{\mathrm{c}}/t_{\mathrm{l}})e^{-\mu(1-t_{\mathrm{l}}/t_{\mathrm{c}})}}{(1-e^{-\lambda t_{\mathrm{l}}})(1-e^{-\lambda t_{\mathrm{c}}})}\Big|_{\mathrm{m}}} e^{(\lambda_{\mathrm{a}}-\lambda_{\mathrm{m}})t_{\mathrm{d\,m}}+\lambda_{\mathrm{a}}\Delta t_{\mathrm{d}}} \times \frac{k_{0\,\mathrm{Au}}(\mathrm{m})}{k_{0\,\mathrm{Au}}(\mathrm{a})} \frac{G_{\mathrm{th\,m}} + \frac{G_{\mathrm{c\,m}}}{f}\left(\frac{Q_{0\,\mathrm{m}}-0.429}{E_{\mathrm{r\,m}}^{\alpha}} + \frac{0.429}{0.55^{\alpha}(1+2\alpha)}\right)}{G_{\mathrm{th\,a}} + \frac{G_{\mathrm{c\,a}}}{f}\left(\frac{Q_{0\,\mathrm{a}}-0.429}{E_{\mathrm{r\,a}}^{\alpha}} + \frac{0.429}{0.55^{\alpha}(1+2\alpha)}\right)} e^{\sum_{i=1}^{h} a_i (E_{\mathrm{p\,m}}-E_{\mathrm{p\,a}})^{2-i}} \frac{(1-\delta\varepsilon_{\mathrm{r\,m}}\Delta d_{\mathrm{m}})}{(1-\delta\varepsilon_{\mathrm{r\,a}}\Delta d_{\mathrm{a}})} \frac{m_{\mathrm{std}}}{m_{\mathrm{sm}}} w_{\mathrm{m}}$$

Analysis | (1)_UncBud_Sc(1) | (1)_UncBud_Cr(1) | (1)_UncBud_Co(1) | ...

Figure 25: The «(i)_UncBud_$te(j)$» worksheet zoom, results and additional information

Finally, the correlation matrix of the input quantities is shown at the right-side (Figure 26) of the uncertainty budget.

	L	M	N	O	P	Q	R	S	T
4	Corr. Matrix	t_{l}	$n_{\mathrm{p,a}}$	λ_{a}	$t_{\mathrm{d,a}}$	$t_{\mathrm{c,a}}$	$t_{\mathrm{l,a}}$	COI_{a}	m_{a}
5	t_{l}	1	0	0	0	0	0	0	0
6	$n_{\mathrm{p,a}}$	0	1	0	0	0	0	0	0
7	λ_{a}	0	0	1	0	0	0	0	0
8	$t_{\mathrm{d,a}}$	0	0	0	1	0	0	0	0
9	$t_{\mathrm{c,a}}$	0	0	0	0	1	0	0	0

Figure 26: The «(i)_UncBud_$te(j)$» worksheet zoom, correlation matrix

It is worth to note that the program creates an uncertainty budget worksheet which calcu-

lates the sensitivity coefficients, the mass fraction and the combined uncertainty based on the measurement equation (4) by taking into account the covariances. Matrix formalism is adopted for computation. Users are free to manually modify the values, uncertainties and correlations of input quantities. The results are automatically updated. This makes the output worksheet as a stand-alone template based on the spreadsheet technique [2].

Finally, the «(i)_DetLim_te(j)» worksheet implements the model equation to compute the detection limit based on the Currie's limit count instead of the peak net area, $n_{\mathrm{p\,a}}$.

5 Getting started with k0-INRIM

User can get started with the software by following the examples given as step-by-step instructions hereafter reported to obtain the output Excel workbook file starting from experimental data included in the compressed «k0-INRIM_get_started.zip» file given alongside the «k0-INRIM_setup.exe». The compressed file includes the folders «User template workbook», «ORTEC GammaVision» and «HyperLab».

Depending on the method adopted to import spectrum data information, refer to 5.1 in case of manual editing of the «user template.xlsx» workbook or to 5.2 in case of use of ORTEC GammaVision or HyperLab.

The experimental γ spectra files («Background.chn», «Ref source (1).chn», «Meas sample.chn» and «Std sample.chn») adopted for these examples, were collected with ORTEC GammaVision and included in the «ORTEC GammaVision» folder. For convenience, the calibration file «Ref source (1).Clb» is also provided.

Finally, the input quantities of the measurement model are listed in Table 2 and grouped depending on the source of their values and uncertainties. It is worth to note that spectrum information are imported from the template worksheet or outputs of the ORTEC GammaVision and Hyperlab. The remaining data are manually added by the user in the input fields of the software interface or automatically recalled from a code predefined dataset, the k_0-database and intermediate computation results.

5.1 Template workbook instructions

1) - Press the button *Input workbook* in the main window to select and convert the file «user template.xlsx» in the folder «User template workbook». The eight files «Background», «Ref source (1)», «Std sample» and «Meas sample» in both the .csv and .ASC extensions are created in the selected folder.

2) - Press the *Background* button in the main window to select the converted «Background.csv» file.

3) - Copy the «source info.sce» file located in the «User template workbook» folder and paste it to the «k0-INRIM/data/sources» folder.
- Press the *Calibration* button in the main window to open the calibration window.
- Press the *Add* button to select the converted «Ref source (1).csv» file.
- Enter the value 0.0046 in the $\delta\varepsilon_{\mathrm{r}}$ / mm^{-1} spin-box.
- Select source info from the select source drop-down menu.
- Press the *Process and save button*.
- Press the *Refresh* button in the main window and select calibration_name_1 in the calibration drop-sown menu.
- Enter the value 0.0442 in the μ / 1 spin-box and the value 0.0005 in the $u(\mu)$ / 1 spin-box.

4) - Press the *Irradiation* button to open the irradiation window.
- Enter the name "Channel" in the irr. channel drop-down menu.
- Enter the values 15.60 and 0.33 in the f / 1 and $u(f)$ / 1 spin-boxes.
- Enter the values -0.036 and 0.006 in the α / 1 and $u(\alpha)$ / 1 spin-boxes.
- Enter the values 3600 and 17 in the t_{i} / s and $u(t_{\mathrm{i}})$ / s spin-boxes.
- Enter the irradiation end date 02/02/2017 and time 15:58:00 in the corresponding end irr. spin-boxes.
- Press the *Confirm* button.

5) - Press the *Sample* button in the main window to select the converted «Meas sample.csv» file.
- Press the *Peak list* button to open the sample peak list window.
- Select the emitters and the corresponding γ-energy reported in Table 1 from the emission drop-down menus.
- Enter the values 0.15152 and 0.00076 in the m / g and $u(m)$ / g spin-boxes in the sample region of the main window.
- Enter the values 1.000 and 0.000 in the G_{th} / 1 and $u(G_{\mathrm{th}})$ / 1 spin-boxes.
- Enter the value 0.6 in the $u(\Delta d)$ / mm spin-box.

6) - Press the *Standard* button in the main window to select the converted «Std sample.csv» file.

Target	Emitter	Emission / keV
Ce	Ce-141	145.4
Th	Pa-233	311.9
Cr	Cr-51	320.1
Yb	Yb-175	396.3
Hf	Hf-181	482.2
Nd	Nd-147	531.0
Cs	Cs-134	795.5
Tb	Tb-160	879.4
Sc	Sc-46	889.3
Zn	Zn-65	1115.5
Ta	Ta-182	1221.4
Co	Co-60	1332.5
La	La-140	1596.2
Sb	Sb-124	1691.0

Table 1: Emitters and emissions list.

- Press the *Peak list* button to open the standard peak list window.
- Select the Co-60 emission at 1173.2 keV γ-energy from the emission drop-down menu and click the corresponding selection check-box.
- Enter the values 0.02079 and 0.00002 in the m / g and $u(m)$ / g spin-boxes in the standard region of the main window.
- Enter the values 0.001000 and 0.000005 in the w / g g^{-1} and $u(w)$ / g g^{-1} spin-boxes.
- Enter the values 1.000 and 0.000 in the G_{th} / 1 and $u(G_{\mathrm{th}})$ / 1 spin-boxes.
- Enter the values 1.000 and 0.000 in the G_{e} / 1 and $u(G_{\mathrm{e}})$ / 1 spin-boxes.
- Enter the value 0.6 in the $u(\Delta d)$ / mm spin-box.
- Enter the values 1.000 and 0.000 in the COI / 1 and $u(COI)$ / 1 spin-boxes.

7) - Press the *Detection limits* button in the main window to open the element selection window and click the Au element.

8) - Press the *Elaborate* button. The output Excel workbook should correspond to the «Output workbook TL.xlsx» located in the «User template workbook» folder.

5.2 ORTEC GammaVision and HyperLab instructions

1) - Press the *Background* button in the main window to select the «Background.rpt» (or «Background.csv») file located in the «ORTEC GammaVision» (or «HyperLab») folder.

2) - Copy the «source info.sce» file located in the «ORTEC GammaVision» (or «HyperLab») folder and paste it to the «k0-INRIM/data/sources» folder.
   - Press the *Calibration* button in the main window to open the calibration window.
   - Press the *Add* button to select the «Ref source (1).rpt» (or «Ref source (1).csv») file.
   - Enter the value 0.0046 in the $\delta\varepsilon_{\mathrm{r}}$ / mm^{-1} spin-box.
   - Select source info from the select source drop-sown menu.
   - Press the *Process and save button*.
   - Press the *Refresh* button in the main window and select calibration_name_1 in the calibration drop-sown menu.
   - Enter the value 0.0442 in the μ / 1 spin-box and the value 0.0005 in the $u(\mu)$ / 1 spin-box.

3) - Press the *Irradiation* button to open the irradiation window.
   - Enter the name "Channel" in the irr. channel drop-down menu.
   - Enter the values 15.60 and 0.33 in the f / 1 and $u(f)$ / 1 spin-boxes.
   - Enter the values -0.036 and 0.006 in the α / 1 and $u(\alpha)$ / 1 spin-boxes.
   - Enter the values 3600 and 17 in the t_{i} / s and $u(t_{\mathrm{i}})$ / s spin-boxes.
   - Enter the irradiation end date 02/02/2017 and time 15:58:00 in the corresponding end irr. spin-boxes.
   - Press the *Confirm* button.

4) - Press the *Sample* button in the main window to select the «Meas sample.rpt» (or «Meas sample.csv») file.
   - Press the *Peak list* button to open the sample peak list window.
   - Select the emitters and the corresponding γ-energy reported in Table 1 from the emission drop-down menus.
   - Enter the values 0.15152 and 0.00076 in the m / g and $u(m)$ / g spin-boxes in the sample region of the main window.
   - Enter the values 1.000 and 0.000 in the G_{th} / 1 and $u(G_{\mathrm{th}})$ / 1 spin-boxes.

- Enter the value 0.6 in the $u(\Delta d)$ / mm spin-box.

5) - Press the *Standard* button in the main window to select the «Std sample.rpt» (or «Std sample.csv») file.
   - Press the *Peak list* button to open the standard peak list window.
   - Select the Co-60 emission at 1173.2 keV γ-energy from the emission drop-down menu and click the corresponding selection check-box.
   - Enter the values 0.02079 and 0.00002 in the m / g and $u(m)$ / g spin-boxes in the standard region of the main window.
   - Enter the values 0.001000 and 0.000005 in the w / g g^{-1} and $u(w)$ / g g^{-1} spin-boxes.
   - Enter the values 1.000 and 0.000 in the G_{th} / 1 and $u(G_{\mathrm{th}})$ / 1 spin-boxes.
   - Enter the values 1.000 and 0.000 in the G_{e} / 1 and $u(G_{\mathrm{e}})$ / 1 spin-boxes.
   - Enter the value 0.6 in the $u(\Delta d)$ / mm spin-box.
   - Enter the values 1.000 and 0.000 in the COI / 1 and $u(COI)$ / 1 spin-boxes.

6) - Press the *Detection limits* button in the main window to open the element selection window and click the Au element.

7) - Press the *Elaborate* button. The output Excel workbook should correspond to the «Output workbook GV.xlsx» (or «Output workbook HL.xlsx») located in the «ORTEC GammaVision» (or «HyperLab») folder.

5.3 Sources of input quantities

Source		X_i
User template / GV[1)] / HL[2)]	x_i	$n_{\mathrm{p\,m}}$, $n_{\mathrm{p\,a}}$, $t_{\mathrm{c\,m}}$, $t_{\mathrm{c\,a}}$, $t_{\mathrm{l\,m}}$, $t_{\mathrm{l\,a}}$
	$u(x_i)$	$n_{\mathrm{p\,m}}$, $n_{\mathrm{p\,a}}$
Interface input fields	x_i	t_{i}, COI_{m}, μ, $G_{\mathrm{th\,m}}$, $G_{\mathrm{th\,a}}$, $G_{\mathrm{e\,m}}$, α, f, m_{m}, m_{a}, w_{m}
	$u(x_i)$	$t_{\mathrm{c\,m}}$, $t_{\mathrm{c\,a}}$, $t_{\mathrm{l\,m}}$, $t_{\mathrm{l\,a}}$, t_{i}, COI_{m}, μ, $G_{\mathrm{th\,m}}$, $G_{\mathrm{th\,a}}$, $G_{\mathrm{e\,m}}$, α, f, Δd_{m}, Δd_{a}, m_{m}, m_{a}, w_{m}, Δt_{d}, $t_{\mathrm{d\,m}}$, $E_{\mathrm{p\,m}}$, $E_{\mathrm{p\,a}}$
Code predefined dataset	x_i	Δd_{m}, Δd_{a}, COI_{a}, $G_{\mathrm{e\,a}}$
	$u(x_i)$	$\delta\varepsilon_{\mathrm{r\,m}}$, $\delta\varepsilon_{\mathrm{r\,a}}$, COI_{a}, $G_{\mathrm{e\,a}}$
k_0-database	x_i	$k_{0\,\mathrm{Au}}(\mathrm{m})$, $k_{0\,\mathrm{Au}}(\mathrm{a})$, $\bar{E}_{\mathrm{r\,m}}$, $\bar{E}_{\mathrm{r\,a}}$, $Q_{0\,\mathrm{m}}$, $Q_{0\,\mathrm{a}}$, λ_{m}, λ_{a}, $E_{\mathrm{p\,m}}$, $E_{\mathrm{p\,a}}$
	$u(x_i)$	$k_{0\,\mathrm{Au}}(\mathrm{m})$, $k_{0\,\mathrm{Au}}(\mathrm{a})$, $E_{\mathrm{r\,m}}$, $E_{\mathrm{r\,a}}$, $Q_{0\,\mathrm{m}}$, $Q_{0\,\mathrm{a}}$, λ_{m}, λ_{a}
Computation results	x_i	a_i, $\delta\varepsilon_{\mathrm{r\,m}}$[3)], $\delta\varepsilon_{\mathrm{r\,a}}$[3)], Δt_{d}, $t_{\mathrm{d\,m}}$
	$u(x_i)$	a_i[4)]

Table 2: Input quantities, X_i, grouped depending on the input source of their values, x_i, and uncertainties, $u(x_i)$. [1)] ORTEC GammaVision, [2)] HyperLab, [3)] the source is the software interface if a single spectrum of the reference source is collected, [4)] the correlation matrix is included.

6 Bibliography

References

[1] JCGM, *Evaluation of measurement data – Guide to the expression of uncertainty in measurement.* BIPM, 2008.

[2] G. D'Agostino, M. Di Luzio, and M. Oddone, "An uncertainty spreadsheet for the k_0-standardisation method in Neutron Activation Analysis," *J Radioanal Nucl Chem*, vol. 318, pp. 1261–1269, 2018.

[3] F. De Corte, *The k_0-standardization method.* 1987.

[4] G. Van Rossum, *Python 3 Reference Manual.* Paramount, CA: CreateSpace, 2009.

[5] T. E. Oliphant, *A guide to NumPy.* USA: Trelgol Publishing, 2006.

[6] J. D. Hunter, "Matplotlib: A 2d graphics environment," *Computing In Science & Engineering*, vol. 9, no. 3, pp. 90–95, 2007.

[7] "k_0 database, http://www.kayzero.com/k0naa/k0naaorg/nuclear_data_sc/entries/2018/12/10_update_of_k0-database.html."

[8] ORTEC, "GammaVision for windows."

[9] HyperLabs Software, "Hyperlab software 2014."

[10] L. A. Currie, "The measurement of environmental levels of rare gas nuclides and the treatment of very low-level counting data," *IEEE Trans on Nucl Sci*, vol. 19, pp. 119–126, 1972.

[11] G. D'Agostino, M. Di Luzio, and M. Oddone, "The k_0-INRIM software: a tool to compile uncertainty budgets in Neutron Activation Analysis based on k_0-standardisation," *submitted to Measurement Science and Technology*, 2019.