INAA-INRIM 3.0 software

Vademecum: basic procedure to perform analysis with INAA-INRIM software

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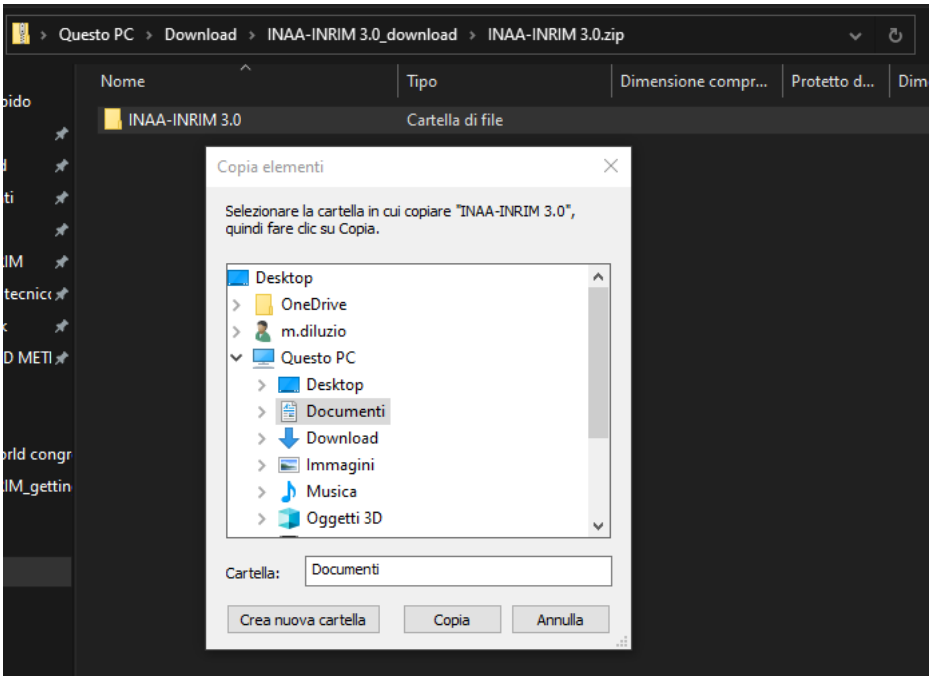
SUMMARY

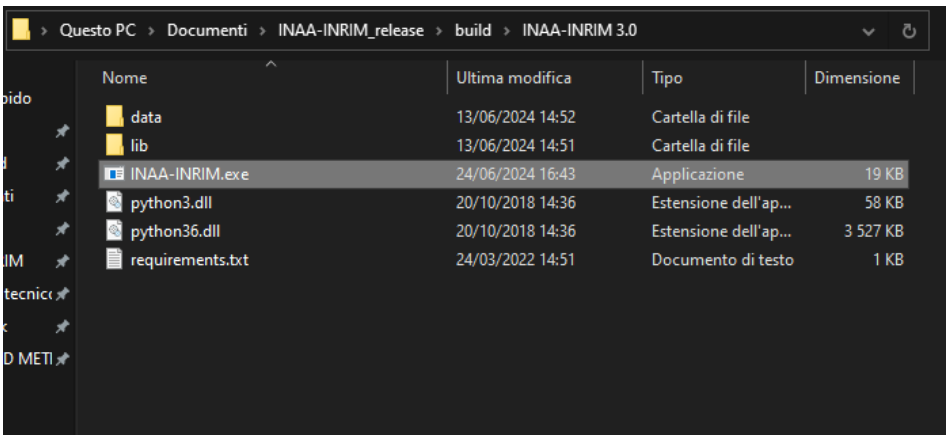
This document does not represent a fully-fledged manual of the software as it only addresses its basic functionalities; Hereafter are reported the actions to perform in order to go through a test analysis from start to finish. Corresponding files recalled here (which are output of the software HyperLab) can be found in the folder “Test spectra”.

1. Software start up

1.1. Access the downloaded zip folder “INAA-INRIM 3.0.zip” and unpack the whole “INAA-INRIM 3.0” folder in a directory of choice (except system restricted directories since INAA-INRIM software needs permission to write and delete files)

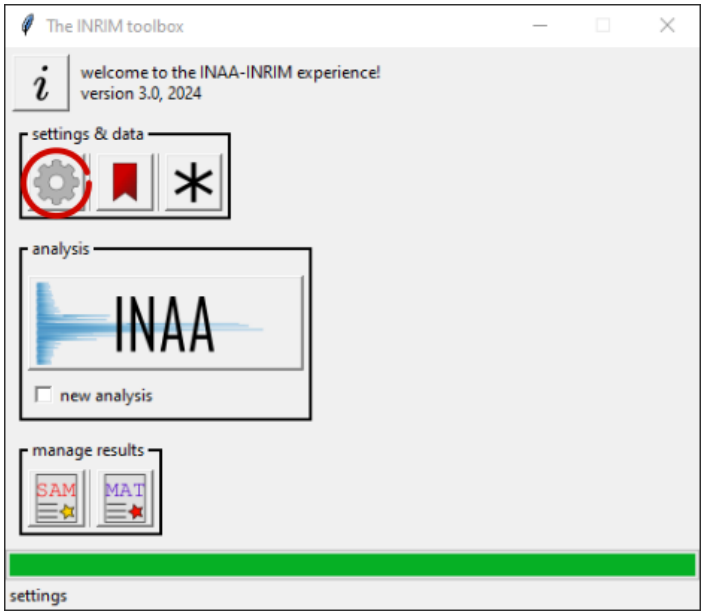


1.2. Open the unpacked folder “INAA-INRIM 3.0” and double click on the “INAA-INRIM.exe” file to start the software

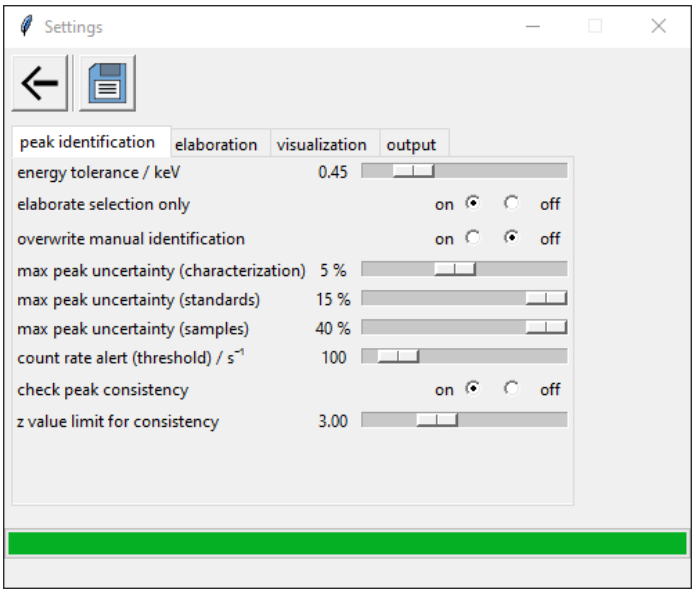


2. Basic settings

2.1. The software starts with a window called the WELCOME window. Main windows names are reported with uppercase letters in the text. Section names are represented with bold-italic font in the text; sections are square portions of a window delimited by a black line, the name of the corresponding section can be seen at the top left of the box. Buttons names are written between double quotation marks in the text and can be seen at the bottom of the window when the corresponding button is hovered with the mouse. The three sections in the WELCOME windows allow to (i) set options and literature data, (ii) perform an analysis and (iii) recall previously saved analysis (as uncertainty budgets object). Click on the "settings" button (the first from left) in ***settings & data*** section to access the SETTINGS window



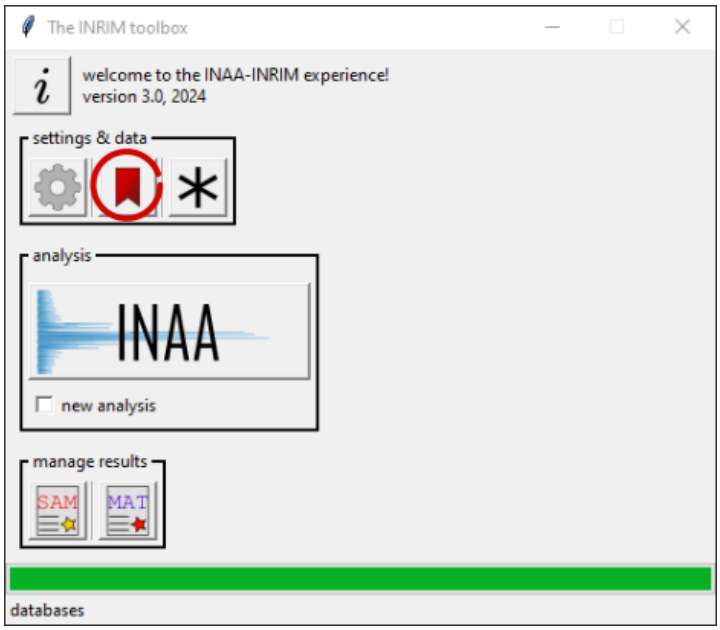
2.2. The four tabs at the top of the SETTINGS window allow to manage various aspects of the software; the *peak identification* tab include conditions to better identify peaks, such as "energy tolerance / keV", "max peak uncertainty"; the *elaboration* tab provides a few options concerning the elaboration algorithms and default values to be used in the calculations; the *visualization* tab allows to modify the aesthetic of the software with options such as "lines in the peaklist window" which has to be changes according to screen size; the *output* tab includes options to modify the style of the output excel files



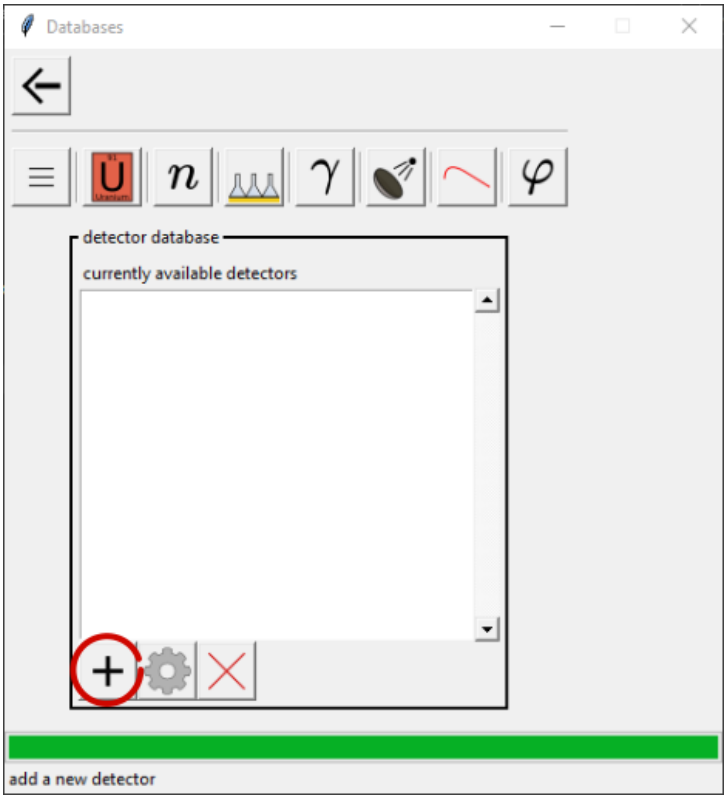
2.3. If modifications have been made, save the settings by clicking on the “confirm changes” button (the second from the left)

3. Set databases prior to characterization/analysis

3.1. To insert information that will be important for the following characterization and analysis, click on the “databases” button, the one at the center found in the ***setting & data*** section in the WELCOME window, to access the DATABASES window



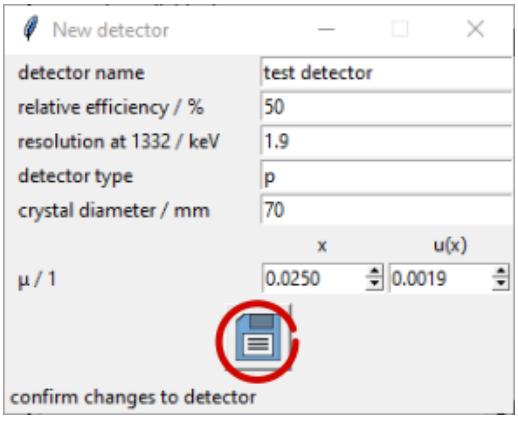
3.2. While in the DATABASES window, click on the “detector database” button (the sixth from the left) to display the list of all currently available detectors; then click on the “add a new detector” button (the first from left in the bottom line) to insert information about the detector that will be used in the following processes



3.3. Once the NEW DETECTOR window is open, insert the information as shown in the following table:

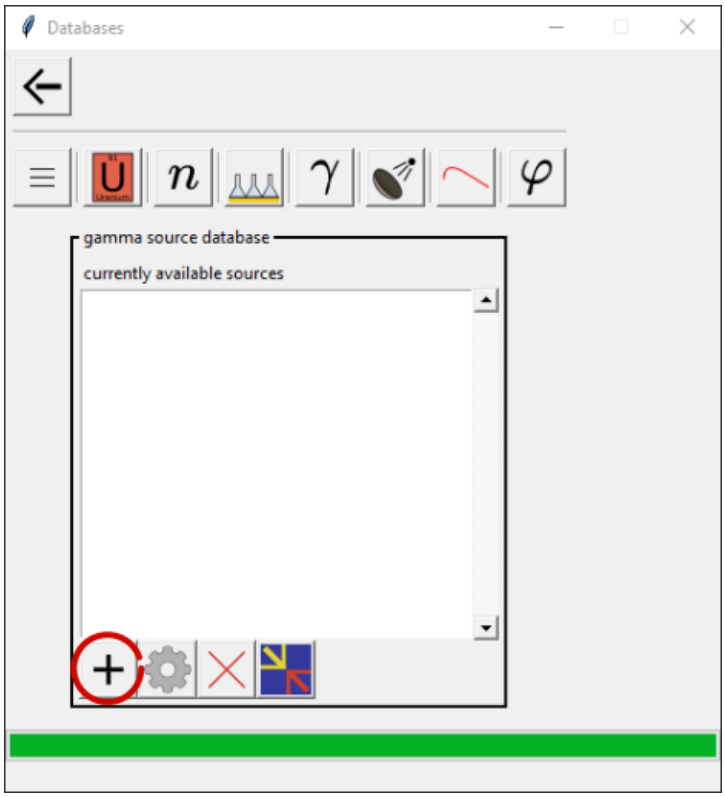
detector name	Test detector	
relative efficiency / %	50	
resolution at 1332 / keV	1.9	
detector type	p	
crystal diameter / mm	70	
	x	u(x)
μ / 1	0.0250	0.0019

3.4. save the entry by clicking on the “confirm changes to detector” button and close the NEW DETECTOR window. The saved entry will appear in the list of available detectors visible in the DATABASES window



3.5. In the DATABASES window, click on the “gamma source database” button (the fifth from the left) to display the list of all currently available gamma sources; then click on the “add a new source” (the

first from left in the bottom line) button to open the NEW/MODIFY SOURCE window and insert information on a new source to be adopted in the characterization process



3.6. Insert the corresponding information concerning the following 9 sources by means of the NEW/MODIFY SOURCE window:

1

source name	Source_Ba
certificate date	05/09/2017 13:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Ba-133	389700	2923	3.330E+08	53.16	0.0214	0.0002	no
Ba-133	389700	2923	3.330E+08	79.61	0.0263	0.0002	no
Ba-133	389700	2923	3.330E+08	81.00	0.3331	0.0002	no
Ba-133	389700	2923	3.330E+08	160.61	0.0064	0.0002	no
Ba-133	389700	2923	3.330E+08	223.24	0.0045	0.0002	no
Ba-133	389700	2923	3.330E+08	276.40	0.0713	0.0002	no
Ba-133	389700	2923	3.330E+08	302.85	0.1831	0.0002	no
Ba-133	389700	2923	3.330E+08	356.01	0.6205	0.0002	no
Ba-133	389700	2923	3.330E+08	383.85	0.0894	0.0002	no

2

source name	Source_Eu
certificate date	25/02/2014 12:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Eu-152	431700	3791	4.266E+08	121.78	0.2841	0.0002	no

Eu-152	431700	3791	4.266E+08	244.70	0.0755	0.0002	no
Eu-152	431700	3791	4.266E+08	295.94	0.0044	0.0002	no
Eu-152	431700	3791	4.266E+08	344.28	0.2659	0.0002	no
Eu-152	431700	3791	4.266E+08	367.79	0.0086	0.0002	no
Eu-152	431700	3791	4.266E+08	411.12	0.0224	0.0002	no
Eu-152	431700	3791	4.266E+08	443.97	0.0312	0.0002	no
Eu-152	431700	3791	4.266E+08	488.68	0.0041	0.0002	no
Eu-152	431700	3791	4.266E+08	563.99	0.0046	0.0002	no
Eu-152	431700	3791	4.266E+08	678.62	0.0047	0.0002	no
Eu-152	431700	3791	4.266E+08	688.67	0.0084	0.0002	no
Eu-152	431700	3791	4.266E+08	778.90	0.1297	0.0002	no
Eu-152	431700	3791	4.266E+08	867.38	0.0424	0.0002	no
Eu-152	431700	3791	4.266E+08	919.34	0.0043	0.0002	no
Eu-152	431700	3791	4.266E+08	964.08	0.1450	0.0002	no
Eu-152	431700	3791	4.266E+08	1005.27	0.0067	0.0002	no
Eu-152	431700	3791	4.266E+08	1085.84	0.1013	0.0002	no
Eu-152	431700	3791	4.266E+08	1089.74	0.0173	0.0002	no
Eu-152	431700	3791	4.266E+08	1112.08	0.1341	0.0002	no
Eu-152	431700	3791	4.266E+08	1212.95	0.0142	0.0002	no
Eu-152	431700	3791	4.266E+08	1299.14	0.0163	0.0002	no
Eu-152	431700	3791	4.266E+08	1408.01	0.2085	0.0002	no
Eu-152	431700	3791	4.266E+08	1457.64	0.0050	0.0002	no

3

source name	Source_Am
certificate date	23/08/2021 12:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Am-241	15090	80	1.365E+10	59.54	0.3590	0.0040	yes

4

source name	Source_Au
certificate date	21/09/2021 17:45:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Au-198	13246	80	2.333E+5	411.8	0.9560	0.0040	yes

5

source name	Source_Cd
certificate date	23/08/2021 12:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Cd-109	34640	870	3.991E+7	88.03	0.0364	0.0016	yes

6

source name	Source_Co
certificate date	23/08/2021 12:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Co-57	10110	60	2.348E+7	122.06	0.8560	0.0017	yes
Co-57	10110	60	2.348E+7	136.47	0.1068	0.0008	no

7

source name	Source_Cr
certificate date	21/09/2021 17:45:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Cr-51	9213	57	2.393E+6	320.08	0.0990	0.0020	yes

8

source name	Source_Cs
certificate date	23/08/2021 12:00:00

emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Cs-137	16220	160	9.483E+8	661.66	0.8510	0.0020	yes

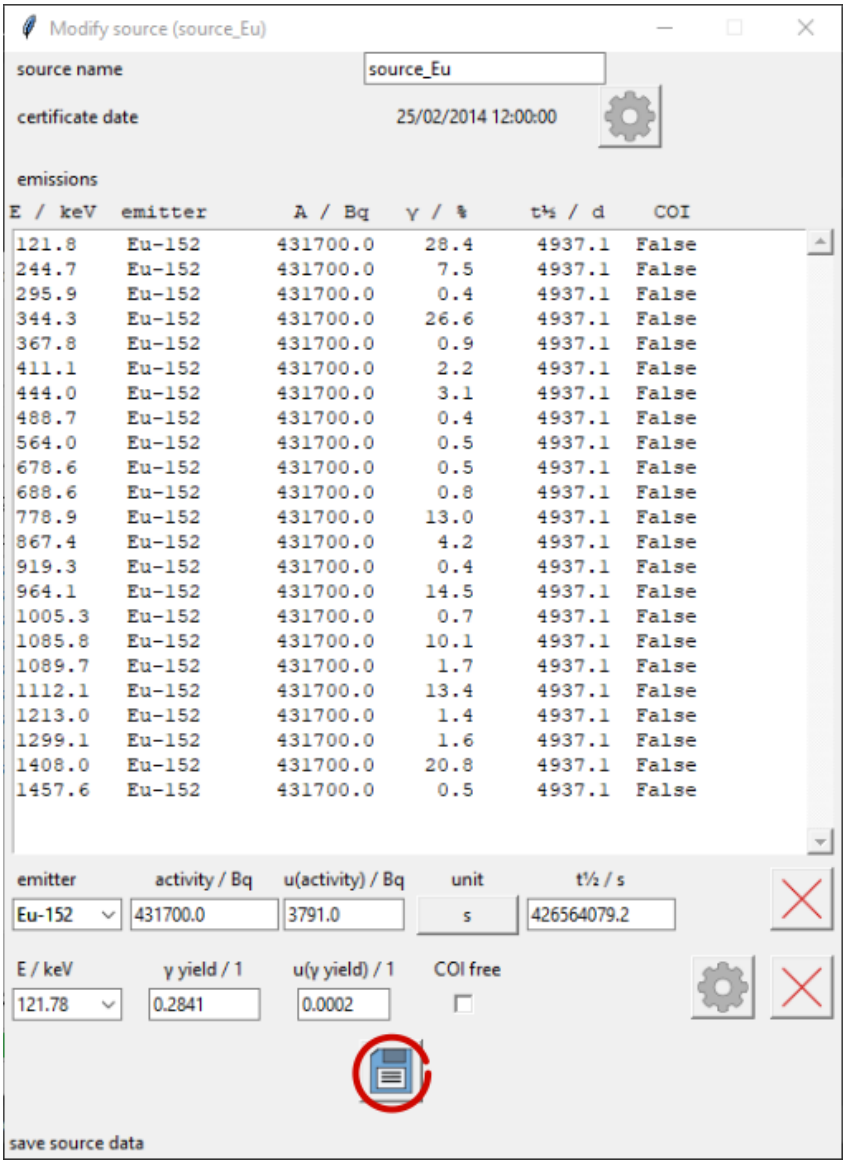
9

source name	Source_Zn
certificate date	21/09/2021 17:45:00

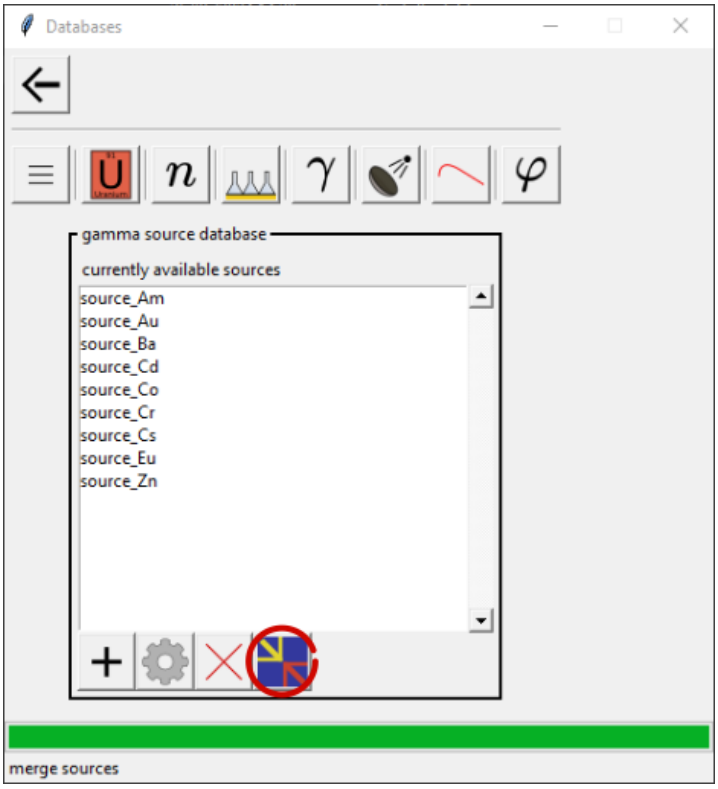
emissions

emitter	activity / Bq	u(activity) / Bq	$t_{1/2}$ / s	E / keV	y yield / 1	u(y yield) / 1	COI free
Zn-65	5462	60	2.108E+7	1115.50	0.5000	0.0020	yes

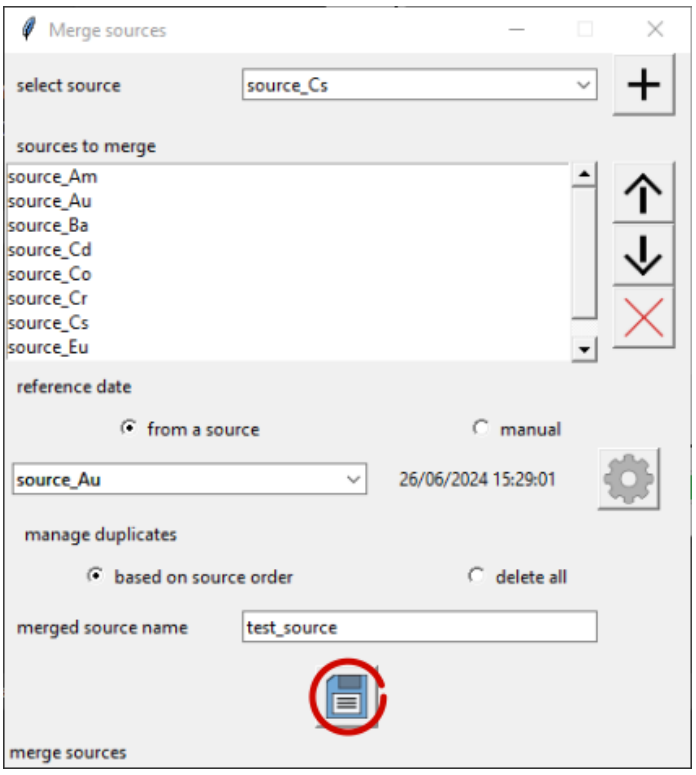
Emissions are added through entries and buttons at the bottom of the NEW/MODIFY SOURCE window: choose or insert the {symbol}-{mass number} of emitter from the drop-down menu under the “emitter” label and fill all the remaining information from both bottom lines according to the previous tables, then confirm by clicking the “add/modify emitter to source” button. To add multiple emissions from the same emitter only update the second line before clicking “add/modify emitter to source” again. To save the current source click the “save source data” and its name will appear in the gamma source database list found in the DATABASES window



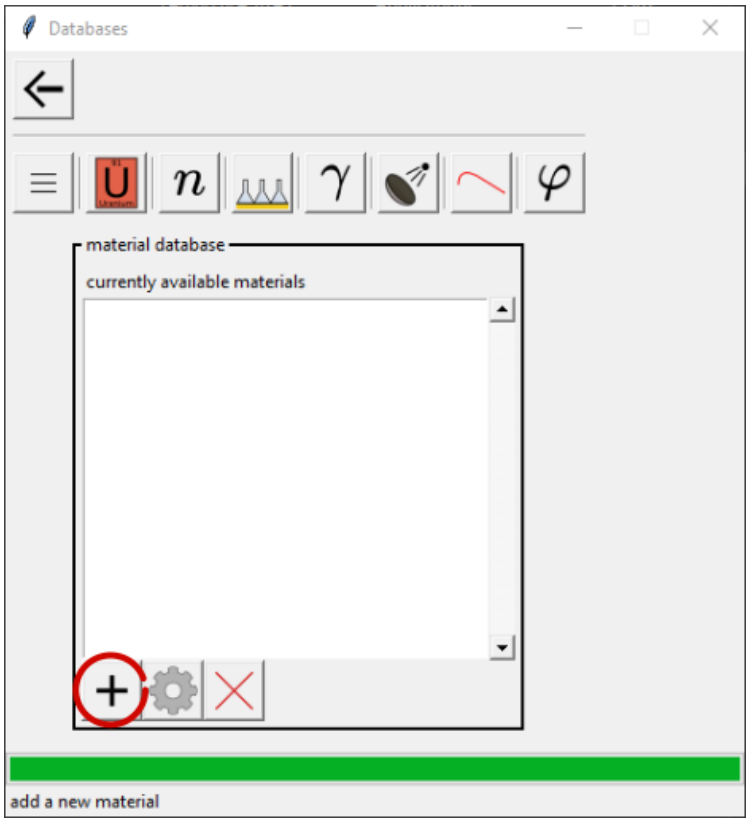
3.7. To use multiple sources for the same detector characterization a merged source has to be created, these objects are cumulated sources that with a single reference date. From the ***gamma source database*** section in the DATABASES window, click on the “merge sources” button (the fourth from the left in the bottom line) to open the MERGE SOURCES window



3.8. From the MERGE SOURCES window, create a list including add all the sources previously created by selecting, one by one, the corresponding source names from the drop-down menu labeled “select source” and clicking on the “add source to merge list” button (upper right of the window). Once all the sources appear in the list, select for reference date the date of the Au-198 source by selecting “source_Au” from the drop-down menu labeled “from a source” (alternatively, enter the date 21/09/2021 17:45:00 below the option manual). Choose the name for the merged source and save it by clicking on the “merge sources” button. The merged source is considered as a normal gamma source and its name will be added to the currently available sources in the DATABASES window



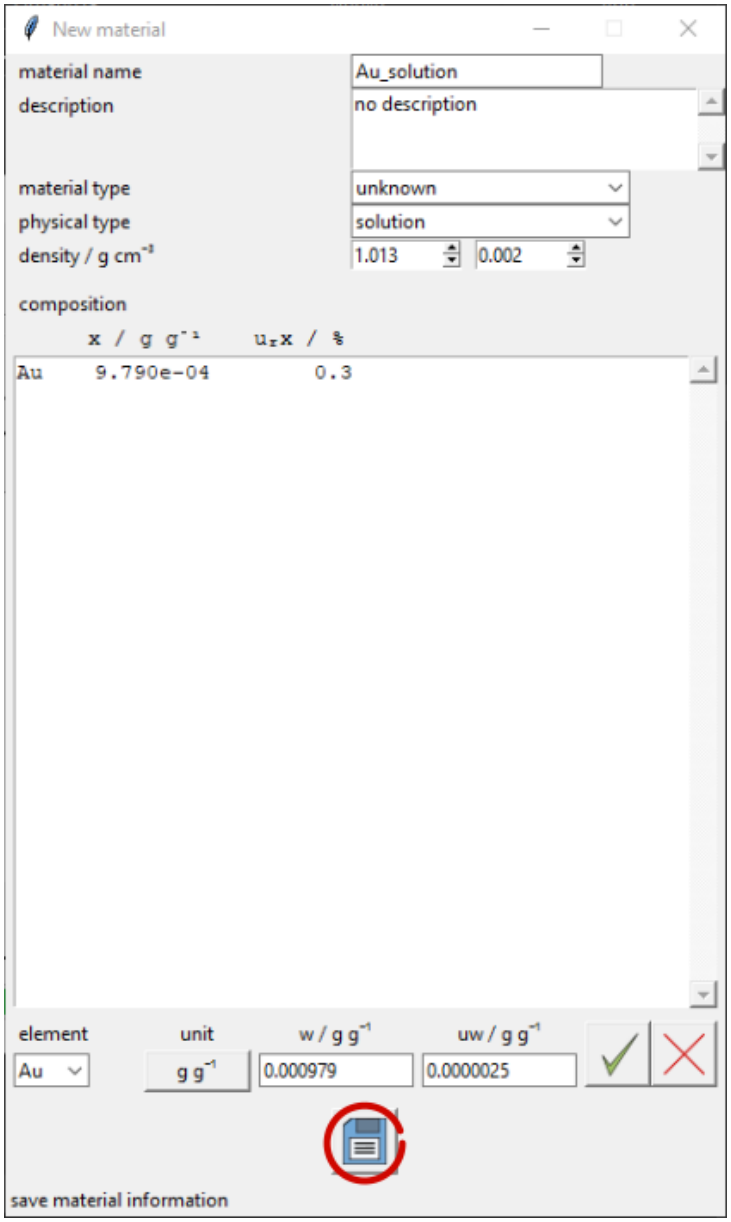
3.9. Material database is where the information about materials used as measurement and standard samples are stored. Access the ***material database*** section in the DATABASES window and click on the “add a new material“ button to access the NEW/MODIFY MATERIAL window



3.10. Use the information reported in the following table to fill the boxes and drop-down menus found at the top of the NEW/MODIFY MATERIAL window

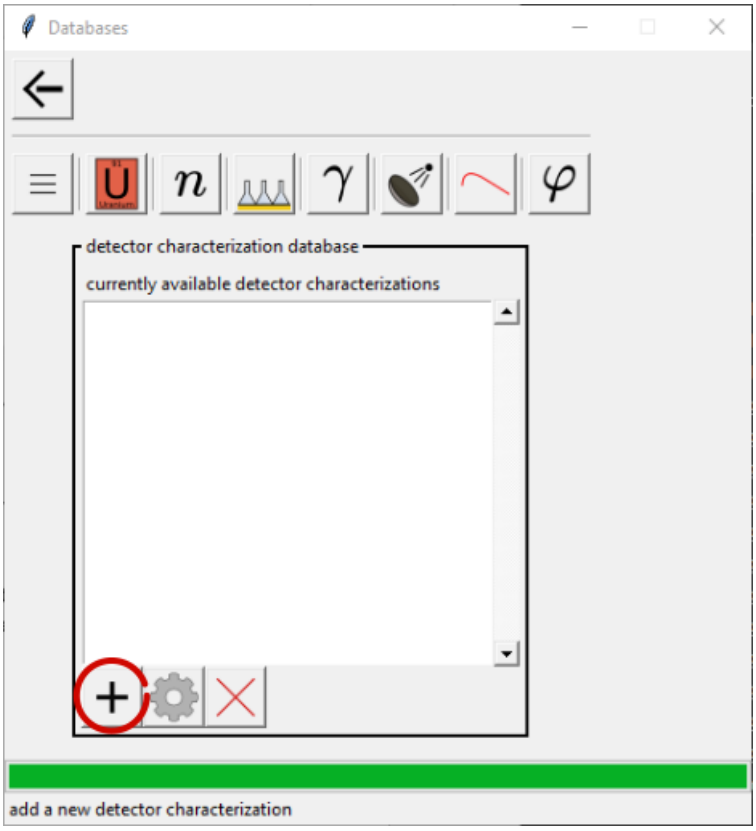
material name	Au_solution	
description	no description	
material type	unknown	
physical type	solution	
density / g cm^{-3}	1.013	0.002

Insert information about mass fraction of Au by selecting the symbol Au from the drop-down menu labeled “element” and typing the values 0.000979 and 0.0000025 in the boxes labeled “w / g g^{-1}” and “uw / g g^{-1}”, respectively. To confirm the data about Au click on the “update element information” button and click the “save material information” button to save the material whose name will appear in the currently available material list in the DATABASES window

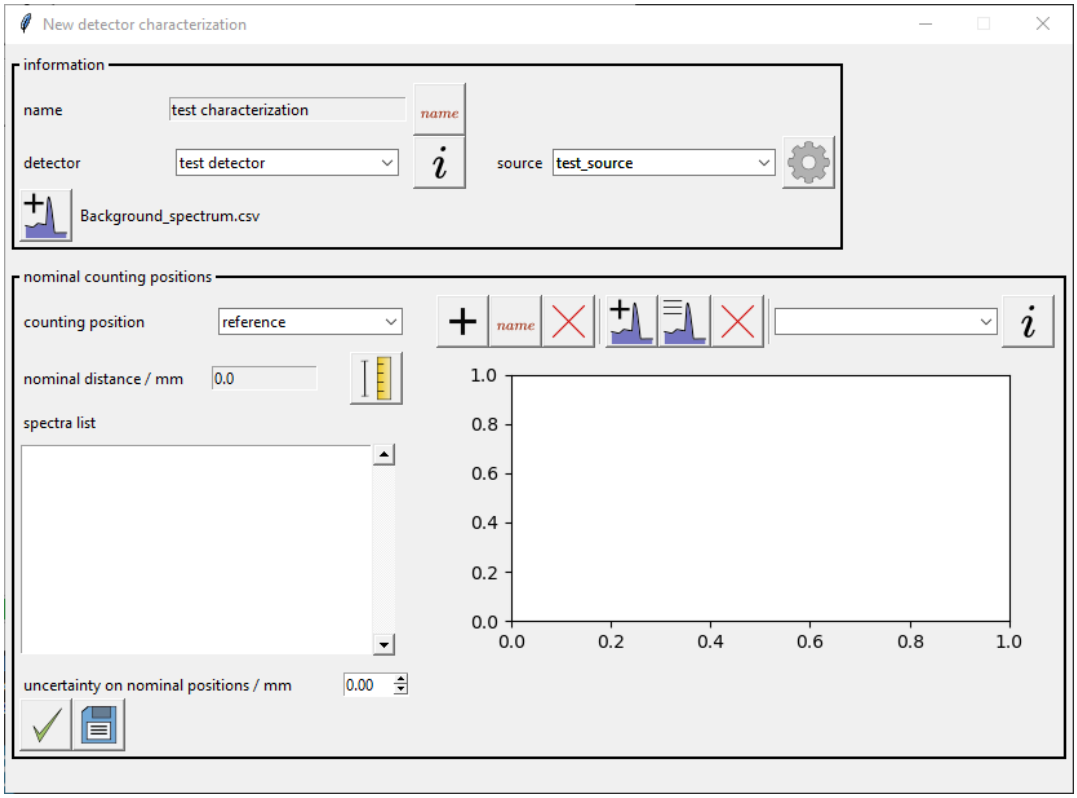


4. Perform detector characterization

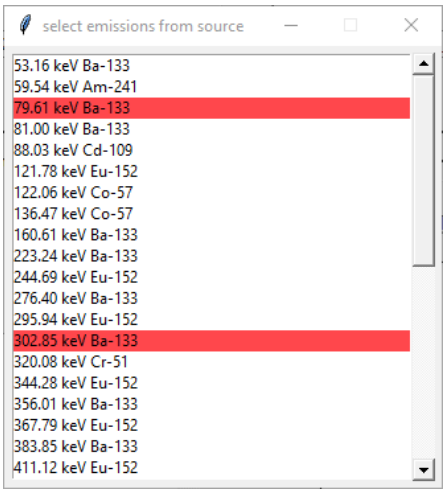
4.1. From the DATABASES window click on the “detection characterization database” button (the seventh from the left) to access the ***detection characterization database*** section where all previously saved characterizations are listed; click on the “add a new detector characterization” button to access the NEW/MODIFY DETECTOR CHARACTERIZATION window to perform a new characterization



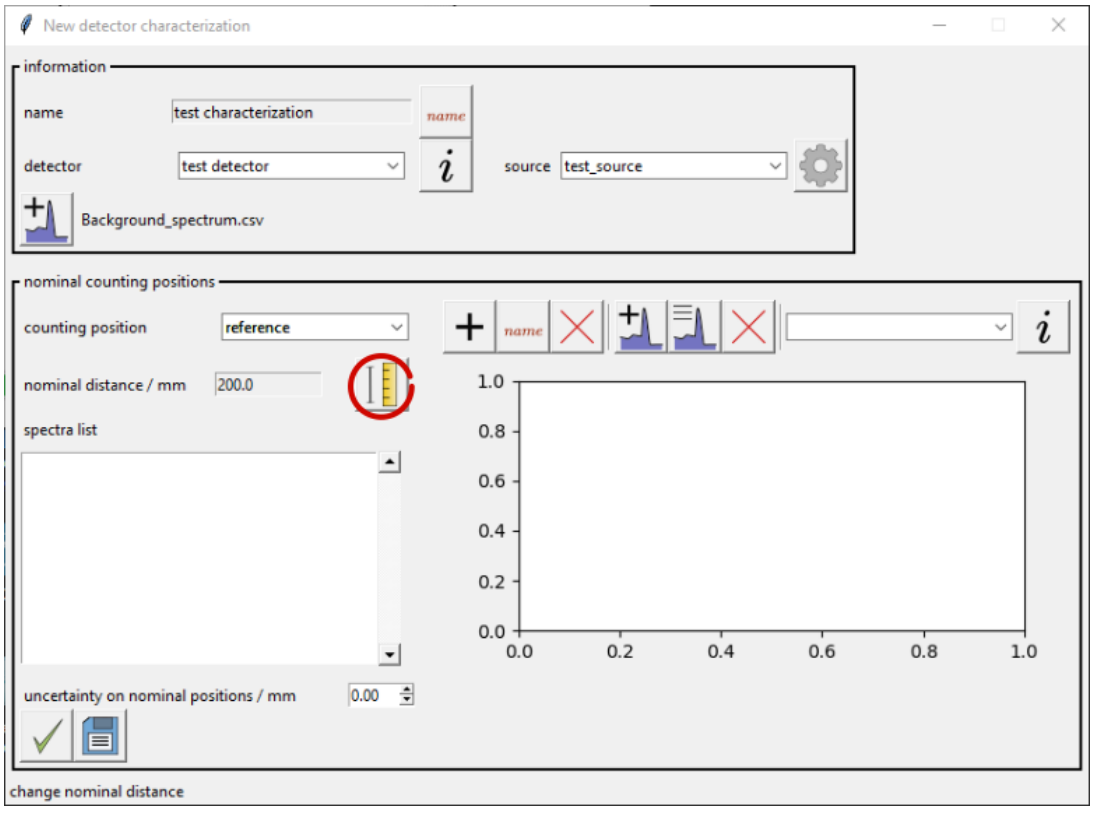
4.2. Fill the required data in the ***information*** section (at the top of the NEW/MODIFY DETECTOR CHARACTERIZATION window): insert the name characterization through the "modify characterization name" button and press enter when done, select "test detector" from the drop-down menu labeled "detector", select "test_source" from the drop-down menu labeled "source", recall the background spectrum named "Background_spectrum.csv" through the "select background spectrum" button



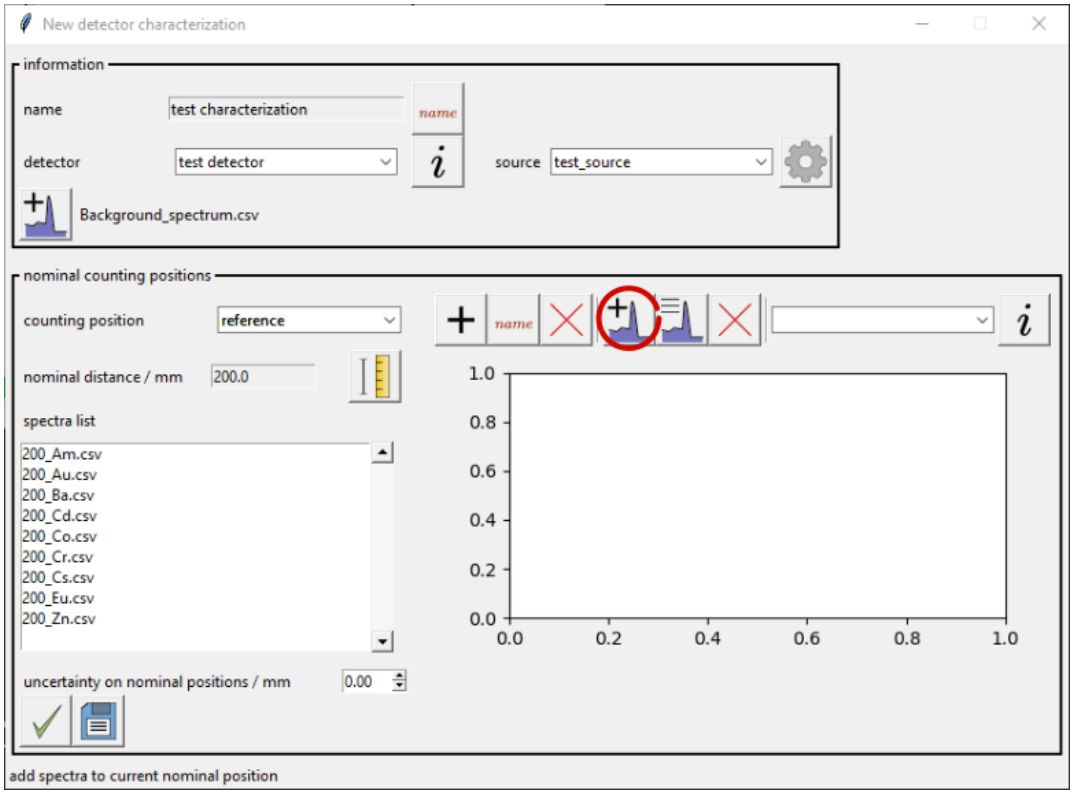
4.3. If needed, selection/deselection of emissions from the adopted source is achieved by clicking on the "select emission from source" button within the ***information*** section of the NEW/MODIFY DETECTOR CHARACTERIZATION window and double clicking on the selected line to make it change color (white=included, red=excluded)



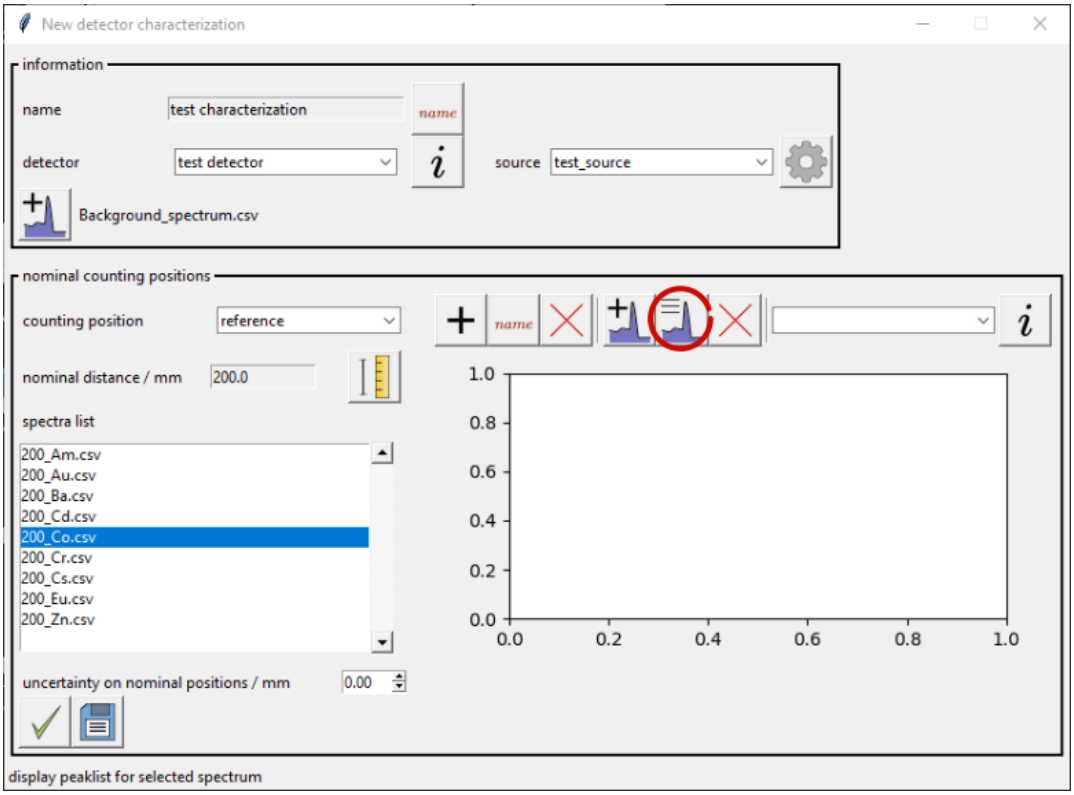
4.4. Back in the NEW/MODIFY DETECTOR CHARACTERIZATION window, select "reference" in the drop-down menu labeled "counting position" in the ***nominal counting positions*** section and insert the value through the "change nominal distance" button next to the label "nominal distance / mm"



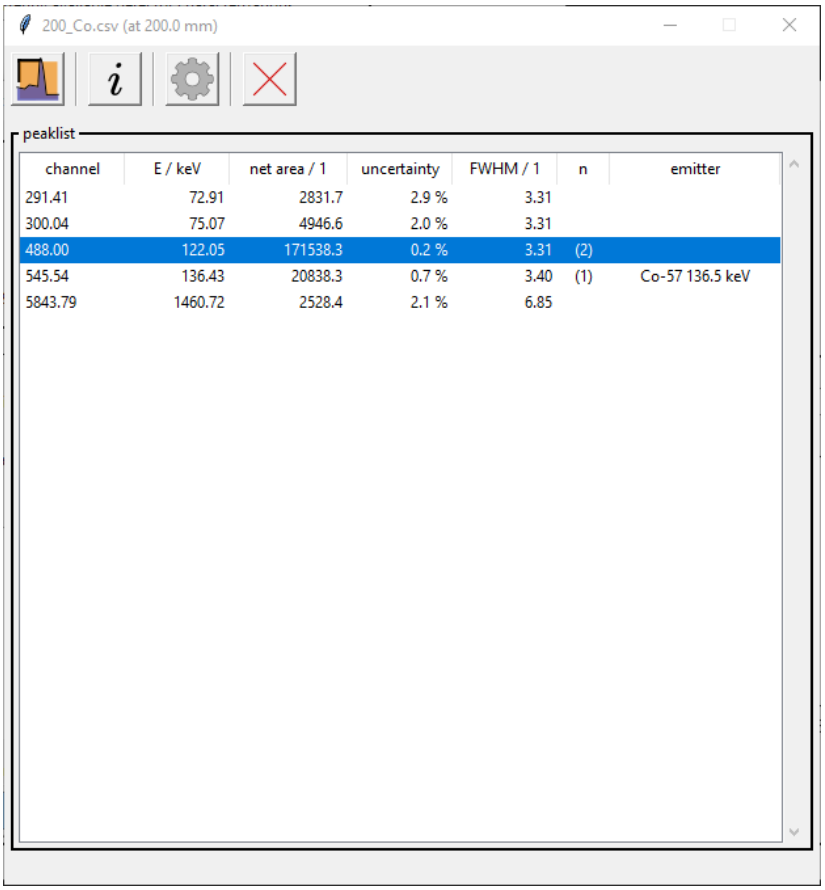
4.5. Recall the spectra of the gamma sources acquired at reference position ("200_Am.csv", "200_Au.csv", "200_Ba.csv", "200_Cd.csv", "200_Co.csv", "200_Cr.csv", "200_Cs.csv", "200_Eu.csv", "200_Zn.csv") through the "add spectra to current nominal position" button in the ***nominal counting positions*** section; their names will appear in the spectra list in the same section



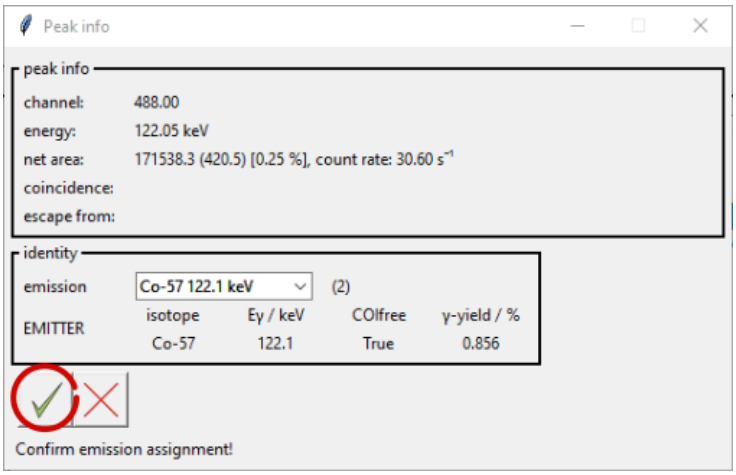
4.6. Select each spectrum from the list and click the “display peaklist for selected spectrum” button to display a PEAKLIST window containing all the relevant information about the spectrum



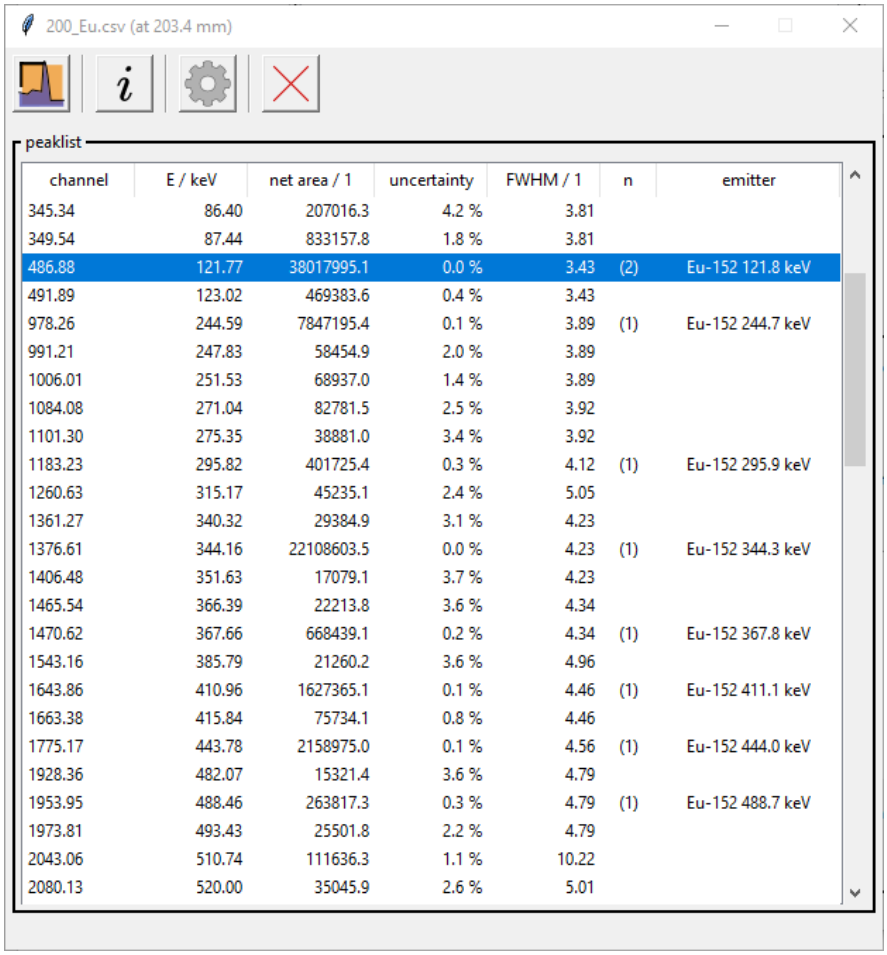
4.7. The PEAKLIST window provides buttons to view the spectrum profile and acquisition information, and a ***peaklist*** section displaying a list of all peaks registered in the spectrum



4.8. Assign the corresponding emitter by double clicking on a line displaying a number in the column “n” in the ***peaklist*** section (or, alternatively by pressing the ”peak information” button in the top line); then select the suitable correspondence from the drop-down menu labeled “emission” in the PEAK INFO window that automatically pops up and click the “Confirm emission assignment” button at the bottom of the PEAK INFO window to confirm the choice

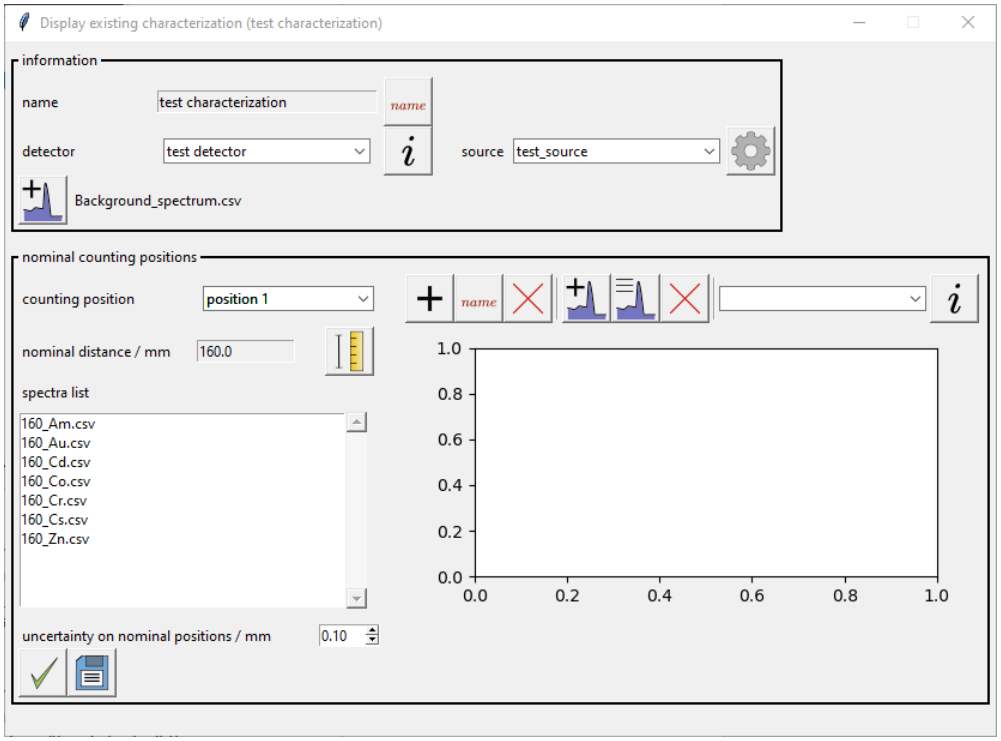


4.9. Check that all emissions from the source are correctly assigned to the corresponding peaks through the ***peaklist*** section of the PEAKLIST window of each spectrum by looking at the text in the column “emitter", especially where the number in the column “n” is 2 (or more) meaning multiple emissions satisfy the searching conditions and the automatic peak assignment is inhibited

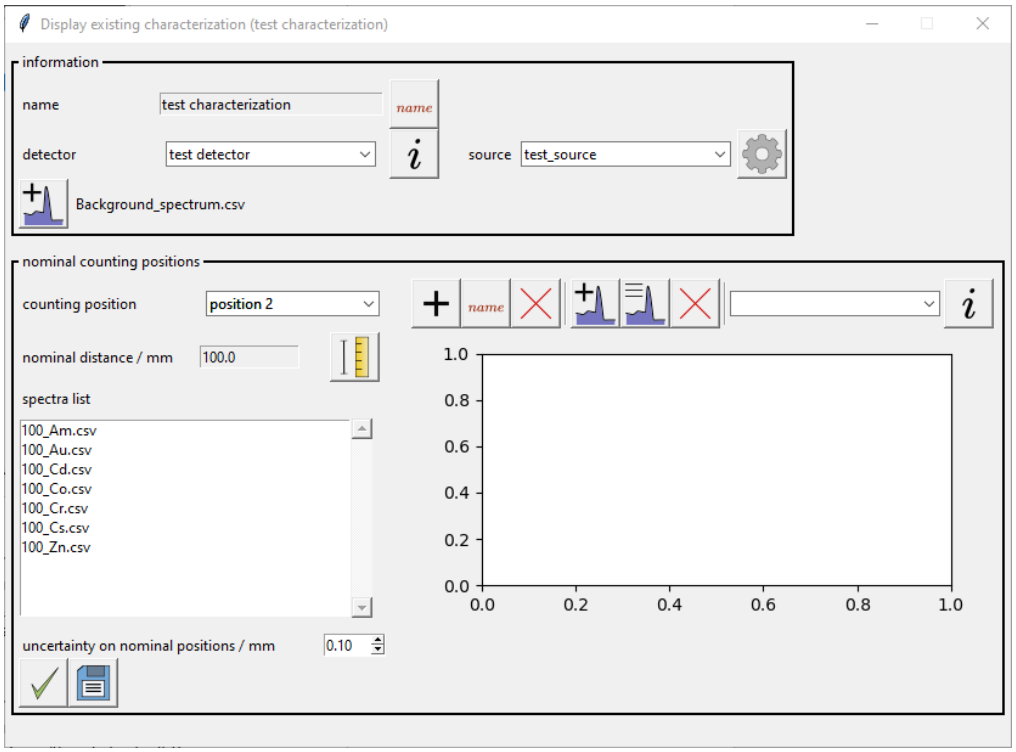


channel	E / keV	net area / 1	uncertainty	FWHM / 1	n	emitter
345.34	86.40	207016.3	4.2 %	3.81		
349.54	87.44	833157.8	1.8 %	3.81		
486.88	121.77	38017995.1	0.0 %	3.43	(2)	Eu-152 121.8 keV
491.89	123.02	469383.6	0.4 %	3.43		
978.26	244.59	7847195.4	0.1 %	3.89	(1)	Eu-152 244.7 keV
991.21	247.83	58454.9	2.0 %	3.89		
1006.01	251.53	68937.0	1.4 %	3.89		
1084.08	271.04	82781.5	2.5 %	3.92		
1101.30	275.35	38881.0	3.4 %	3.92		
1183.23	295.82	401725.4	0.3 %	4.12	(1)	Eu-152 295.9 keV
1260.63	315.17	45235.1	2.4 %	5.05		
1361.27	340.32	29384.9	3.1 %	4.23		
1376.61	344.16	22108603.5	0.0 %	4.23	(1)	Eu-152 344.3 keV
1406.48	351.63	17079.1	3.7 %	4.23		
1465.54	366.39	22213.8	3.6 %	4.34		
1470.62	367.66	668439.1	0.2 %	4.34	(1)	Eu-152 367.8 keV
1543.16	385.79	21260.2	3.6 %	4.96		
1643.86	410.96	1627365.1	0.1 %	4.46	(1)	Eu-152 411.1 keV
1663.38	415.84	75734.1	0.8 %	4.46		
1775.17	443.78	2158975.0	0.1 %	4.56	(1)	Eu-152 444.0 keV
1928.36	482.07	15321.4	3.6 %	4.79		
1953.95	488.46	263817.3	0.3 %	4.79	(1)	Eu-152 488.7 keV
1973.81	493.43	25501.8	2.2 %	4.79		
2043.06	510.74	111636.3	1.1 %	10.22		
2080.13	520.00	35045.9	2.6 %	5.01		

4.10. Add a new counting position by clicking on the “add a new nominal position” button, insert 160.0 as nominal distance, recall the corresponding spectra (“160_Am.csv”, “160_Au.csv”, “160_Cd.csv”, “160_Co.csv”, “160_Cr.csv”, “160_Cs.csv”, “160_Zn.csv”) and check all the gamma source emissions are correctly accounted for through the PEAKLIST windows

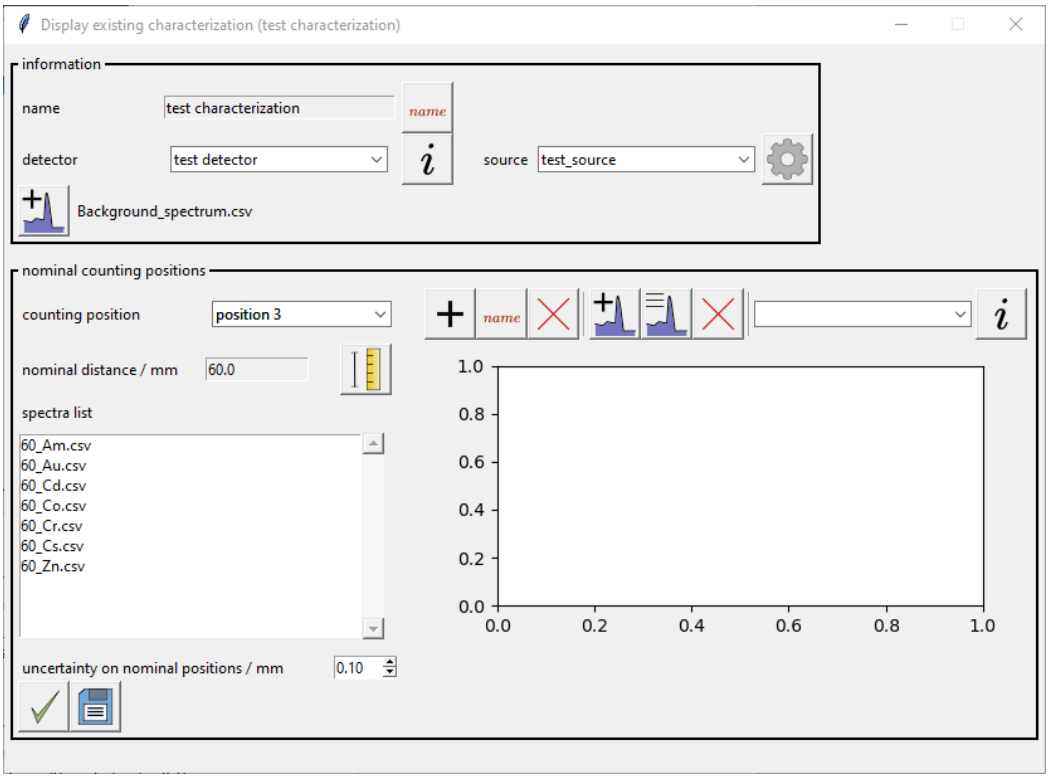


4.11. Add a new counting position by clicking on the “add a new nominal position” button, insert 100.0 as nominal distance, recall the corresponding spectra (“100_Am.csv”, “100_Au.csv”, “100_Cd.csv”, “100_Co.csv”, “100_Cr.csv”, “100_Cs.csv”, “100_Zn.csv”) and check all the gamma source emissions are correctly accounted for through the PEAKLIST windows

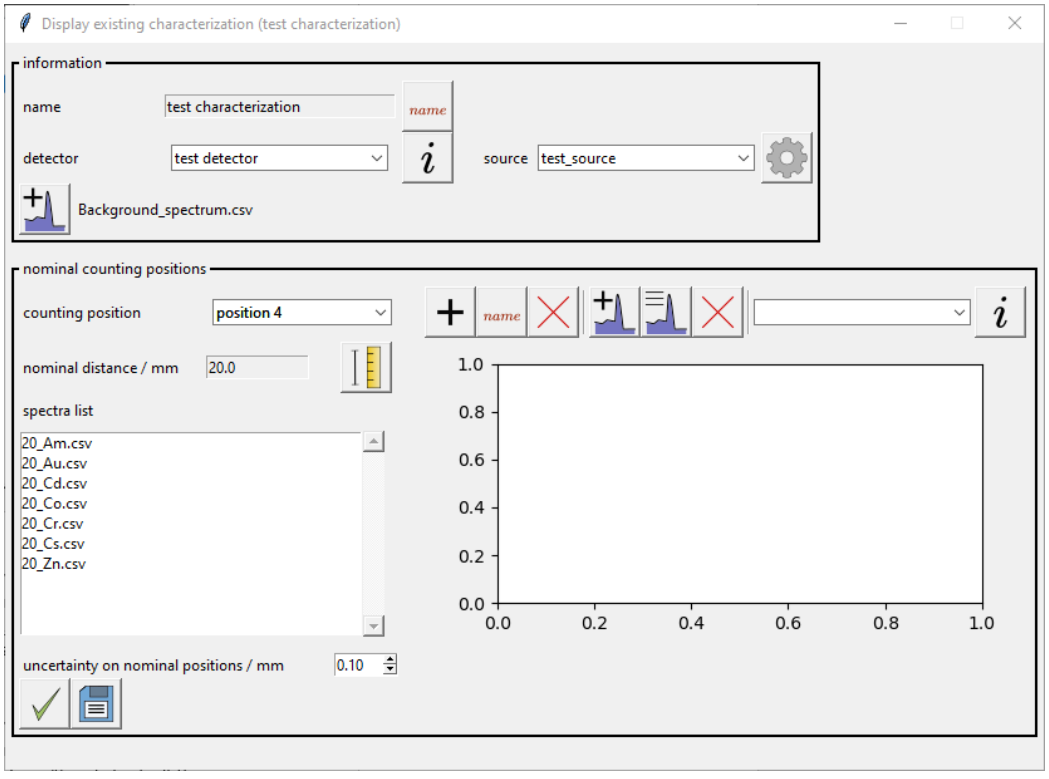


4.12. Add a new counting position by clicking on the “add a new nominal position” button, insert 60.0 as nominal distance, recall the corresponding spectra (“60_Am.csv”, “60_Au.csv”, “60_Cd.csv”,

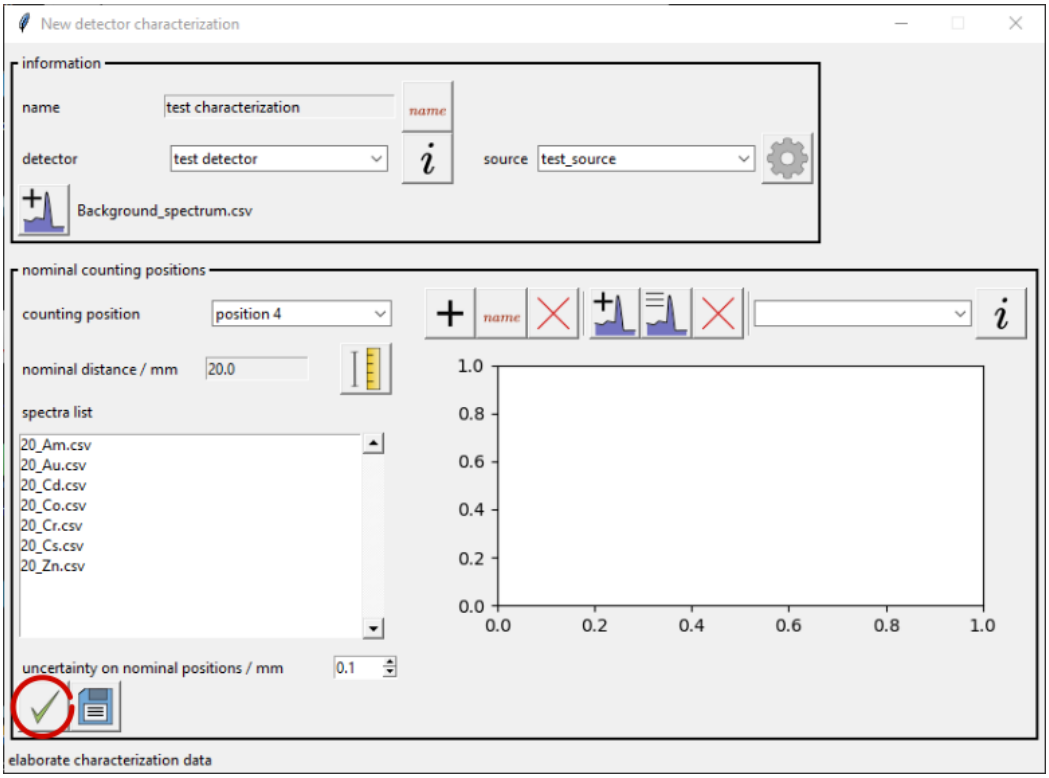
“60_Co.csv”, “60_Cr.csv”, “60_Cs.csv”, “60_Zn.csv”) and check all the gamma source emissions are correctly accounted for through the PEAKLIST windows



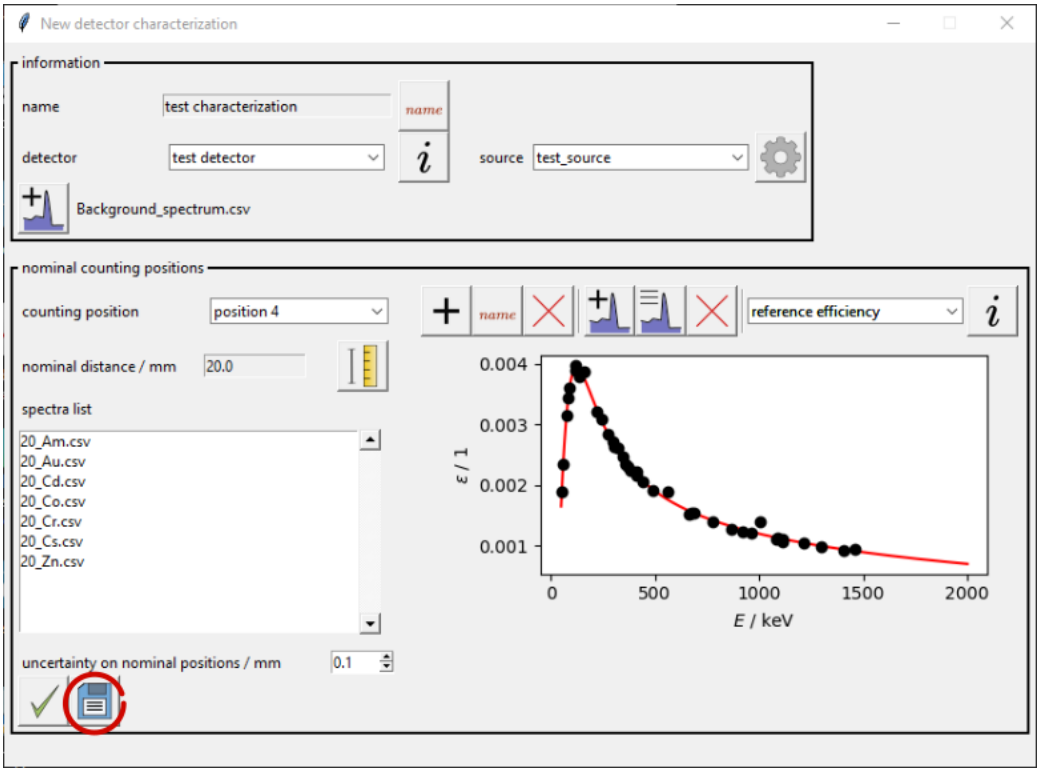
4.13. Add a new counting position by clicking on the “add a new nominal position” button, insert 20.0 as nominal distance, recall the corresponding spectra (“20_Am.csv”, “20_Au.csv”, “20_Cd.csv”, “20_Co.csv”, “20_Cr.csv”, “20_Cs.csv”, “20_Zn.csv”) and check all the gamma source emissions are correctly accounted for through the PEAKLIST windows



4.14. Insert the value 0.1 in the spinbox labeled “uncertainty on nominal positions / mm” and click the “elaborate characterization data” to perform the necessary calculations to get the fit parameters

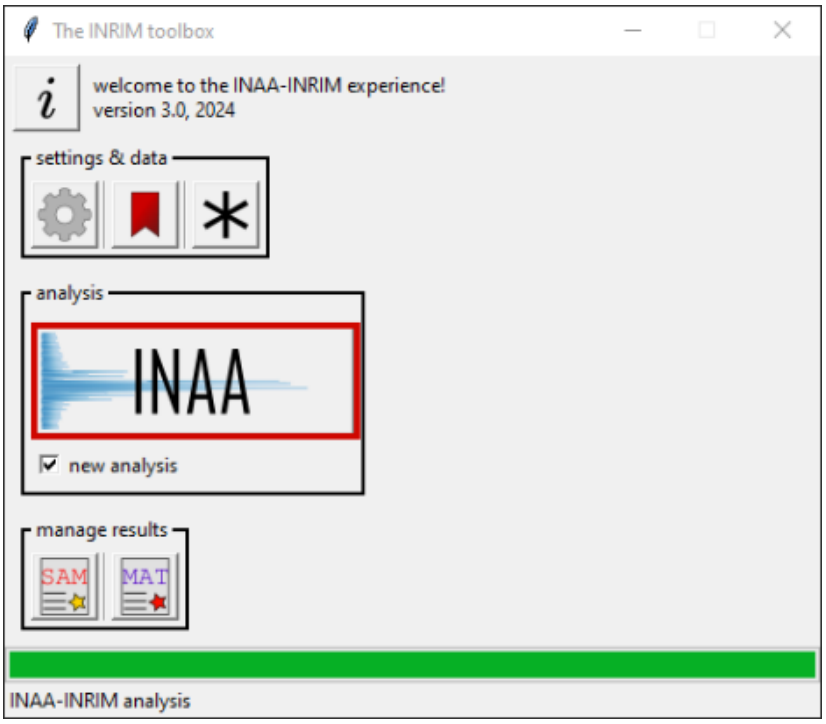


4.15. Browse and visualize the obtained fits from the drop-down menu at the top right of the ***nominal counting positions*** section; if satisfied, click on the “save characterization data” button (the second from left at the bottom of the window) to store the characterization for future use. The saved characterization will appear in the currently available detector characterization list in the DATABASES window

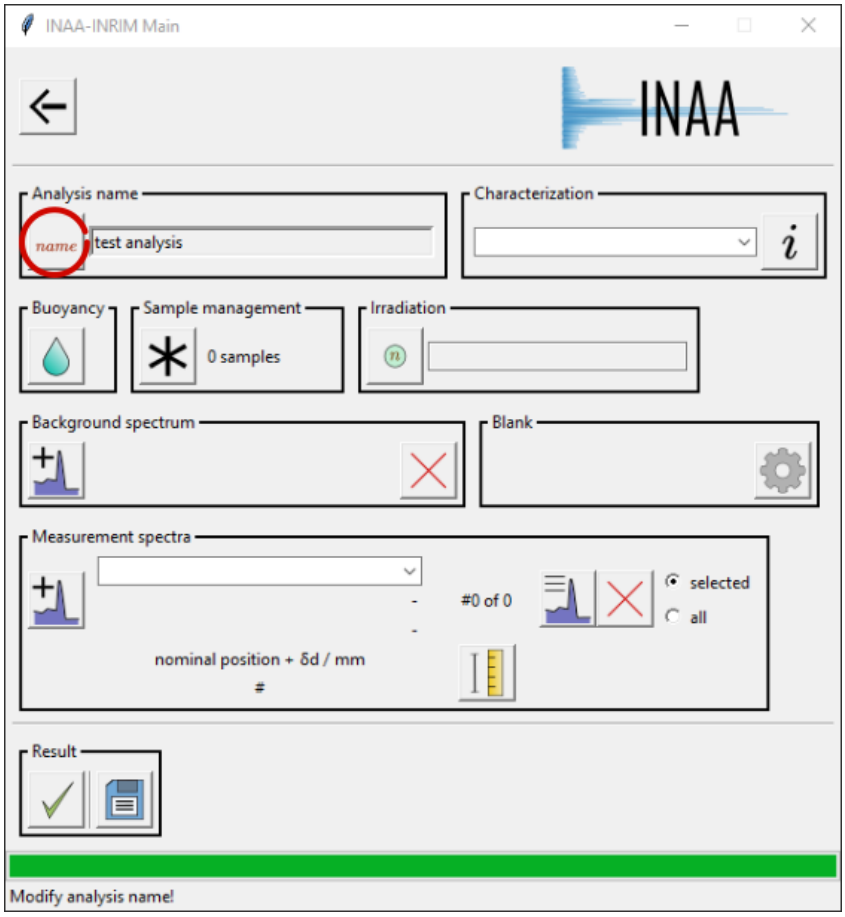


5. Perform test analysis

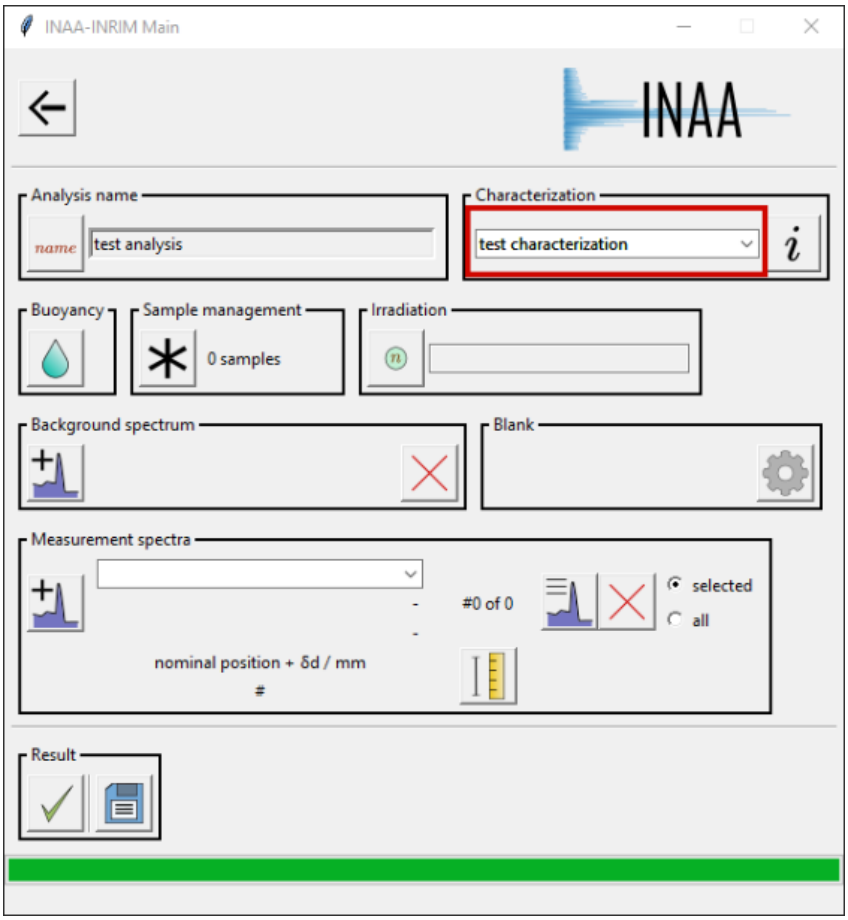
5.1. In the WELCOME window, check the box labeled “new analysis” (otherwise the previous analysis performed in the same instance is recalled) and click on the “INAA-INRIM analysis” button in the ***analysis*** section to access the INAA-INRIM MAIN window and start a new analysis



5.2. In the INAA-INRIM MAIN window, modify the analysis name through the “Modify analysis name!” button in the ***Analysis name*** section; press enter when the new name is inserted to confirm

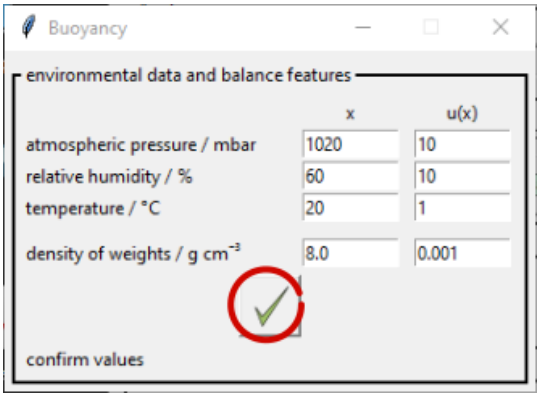


5.3. Select “test characterization” in the drop-down menu in the ***Characterization*** section

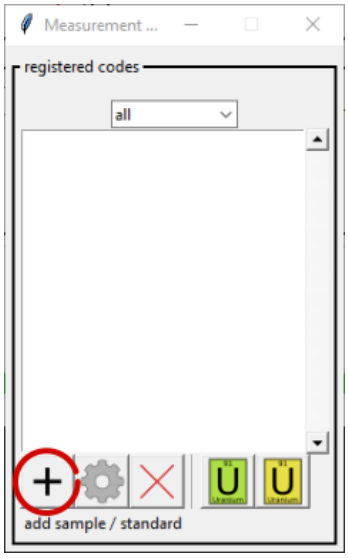


5.4. Click on the “Manage environmental conditions and balance features!” button in the ***Buoyancy*** section of the INAA-INRIM MAIN window to open the BUOYANCY window and fill the entries with the values reported in the following table; then click on the “confirm values” button in the BUOYANCY window to confirm

	x	u(x)
atmospheric pressure / mbar	1020	10
relative humidity / %	60	10
temperature / °C	20	1
density of weights / g cm^{-3}	8.0	0.001



5.5. Click on the “Manage measurement samples!” button in the ***Sample management*** section in the INAA-INRIM MAIN window to open the MEASUREMENT SAMPLES window and click on the “add sample/standard” button (the first from the left at the bottom of the MEASUREMENT SAMPLES window) to start adding information about samples and standards

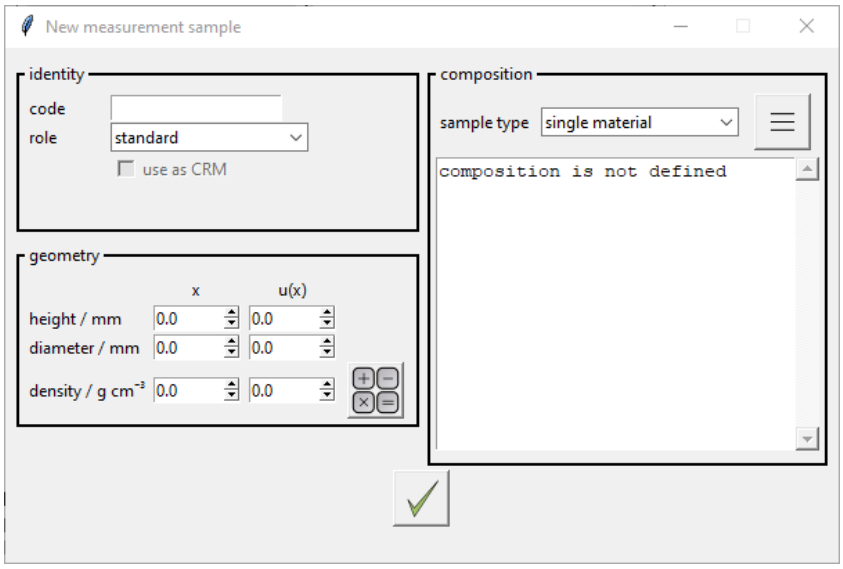


5.6. Create samples and standard to be analyzed following the information summarized in the following table, see 5.7-5.11 for details about how to correctly insert those data

code	role	use as CRM	height / mm	diameter / mm	density / g cm^{-3}	sample type	material	mass / g
A1	standard	no	0.15	6.0	1.0	pipetted solutions	Au_solution	0.01507
A2	sample	no	1.5	10.0	1.8	single material	unknown	0.21004

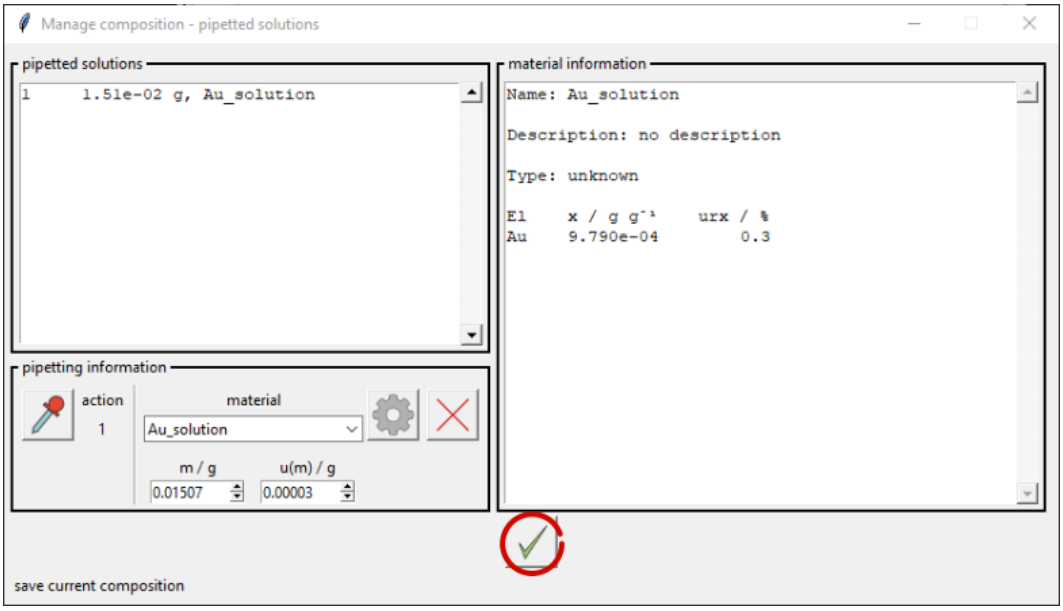
A3	standard	no	0.15	6.0	1.0	pipetted solutions	Au_solution	0.01512
A4	sample	no	1.5	10.0	1.8	single material	unknown	0.21093
A5	standard	no	0.15	6.0	1.0	pipetted solutions	Au_solution	0.01509

5.7. In the NEW/MODIFY MEASUREMENT SAMPLE window, insert the code (unique ID to identify the sample) in the entry labeled “code” and choose role (standard or sample) in the drop-down menu labeled “role” within the ***identity*** section. To use a sample as a CRM, check the corresponding checkbox (this is only available for samples)

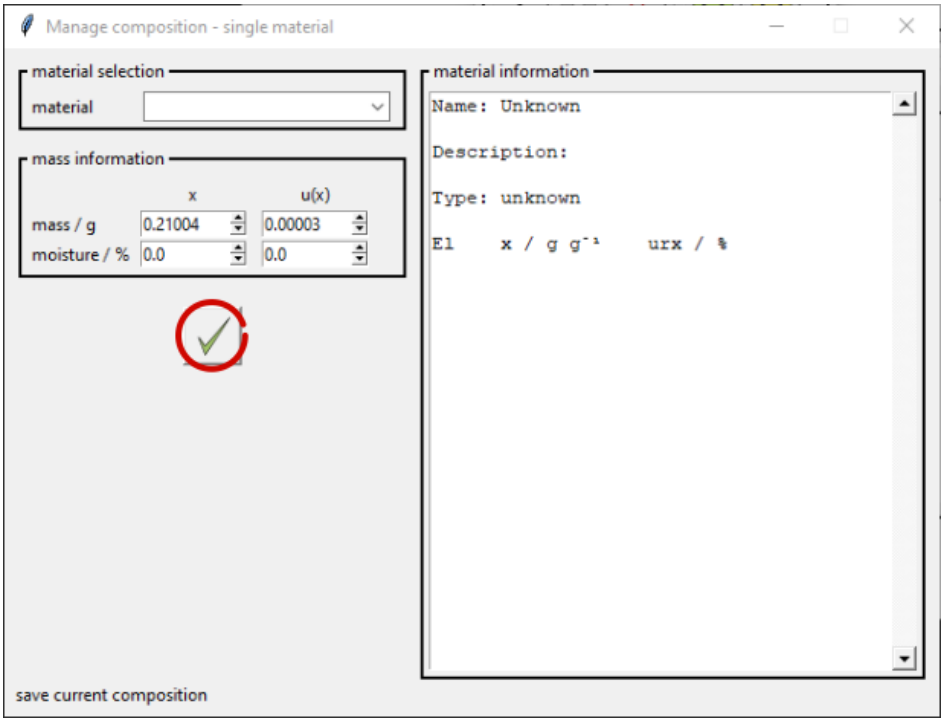


5.8. Select either “single material” or “pipetted solution” in the drop-down menu labeled “sample type” within the ***composition*** section of the NEW/MODIFY MEASUREMENT SAMPLE window and click on the icon next to it to choose the material included in the composition through the MANAGE COMPOSITION window

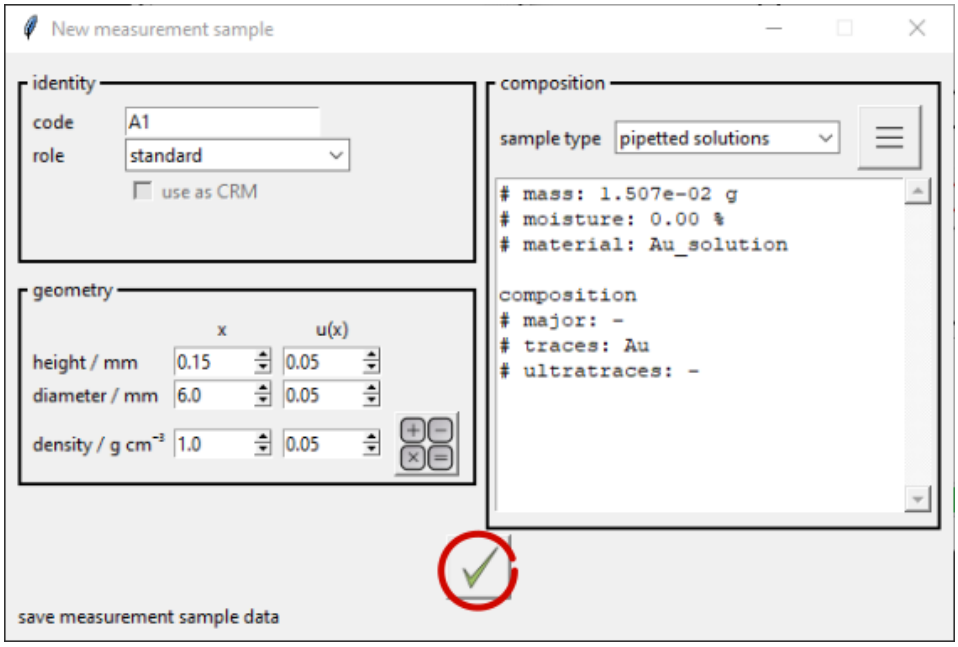
5.9. The MANAGE COMPOSITION window will differ according to the choice performed in the “sample type” drop-down menu of the previous window. If “pipetted solutions” is chosen, click on the “add new pipetting” button in the ***pipetting information*** section (at the bottom of the MANAGE COMPOSITION window) to increase the action count (each pipetting counts as an action); remaining in the ***pipetting information*** section, select the material from the drop-down menu labeled “material” and fill the boxes labeled “m / g” and “u(m) / g” with the value and uncertainty (put 0.00003 in the uncertainty box) of the weighted mass of the pipetted solution, respectively. Confirm the entered information by clicking on the “save/modify current datum” button and the corresponding line will appear ***pipetted solutions*** section. Save the sample composition by clicking on the “save current composition” button and close the MANAGE COMPOSITION window afterwards



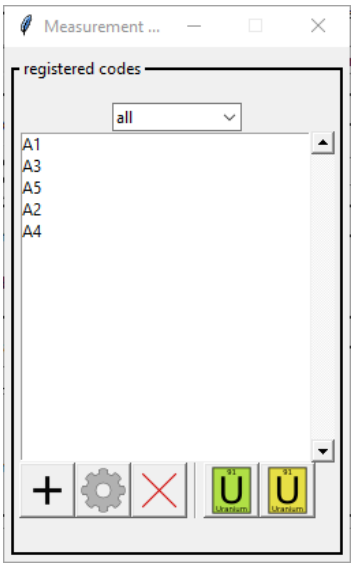
5.10. If “single material” is chosen, select the material from the drop-down menu labeled “material” in the ***material selection*** section of the MANAGE COMPOSITION window (selecting the empty option counts as if the sample is unknown) and fill the boxes labeled “mass / g” and “moisture / %” with the value and uncertainty (put 0.00003 and 0.0 in the uncertainty boxes, respectively) in the columns “x” and “u(x)” respectively. To confirm click on the “save current composition” button and close the MANAGE COMPOSITION window afterwards



5.11. Going back in the NEW/MODIFY MEASUREMENT SAMPLE window, in the ***geometry*** section fill the boxes labeled “height / mm”, “diameter / mm” and “density / g cm^{-3}” in both “x” and “u(x)” columns, with corresponding values and uncertainties, respectively. Adopt 0.05 for all uncertainty in this section. Once all is complete, click on the “save measurement sample data” button at the bottom of the window to save all information concerning the current sample. The code will appear in the list in the ***registered codes*** section of the MEASUREMENT SAMPLES window



5.12. Repeat the previous points until all samples are accounted for and appear in the ***registered codes*** section of the MEASUREMENT SAMPLES window

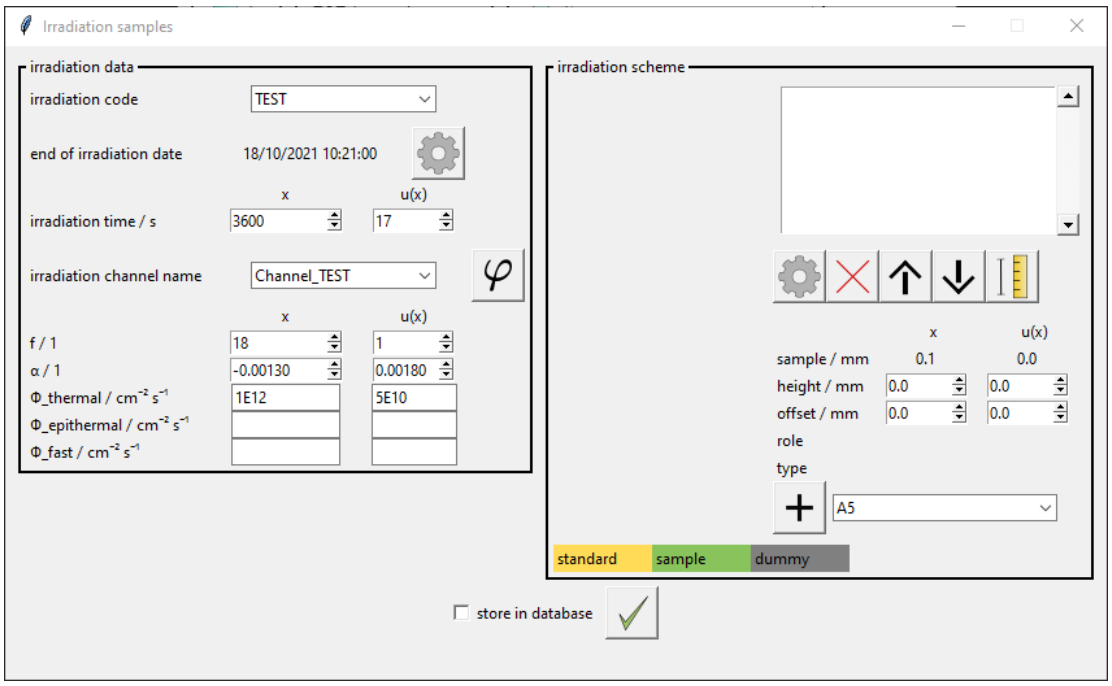


5.13. Back to the INAA-INRIM MAIN window, click on the "New irradiation!" button in the ***Irradiation*** section to open the IRRADIATION SAMPLES window and insert the information reported in the following tables, see 5.14-5.15 for details about how to correctly manage those data

Irradiation code	TEST	
End of irradiation date	18/10/2021 10:21:00	
	x	u(x)
Irradiation time / s	3600	17
Irradiation channel name	Channel_TEST	
	x	u(x)
f / 1	18	1
A / 1	-0.00130	0.00180
ϕ_thermal / cm^{-2} s^{-1}	1E12	5E10

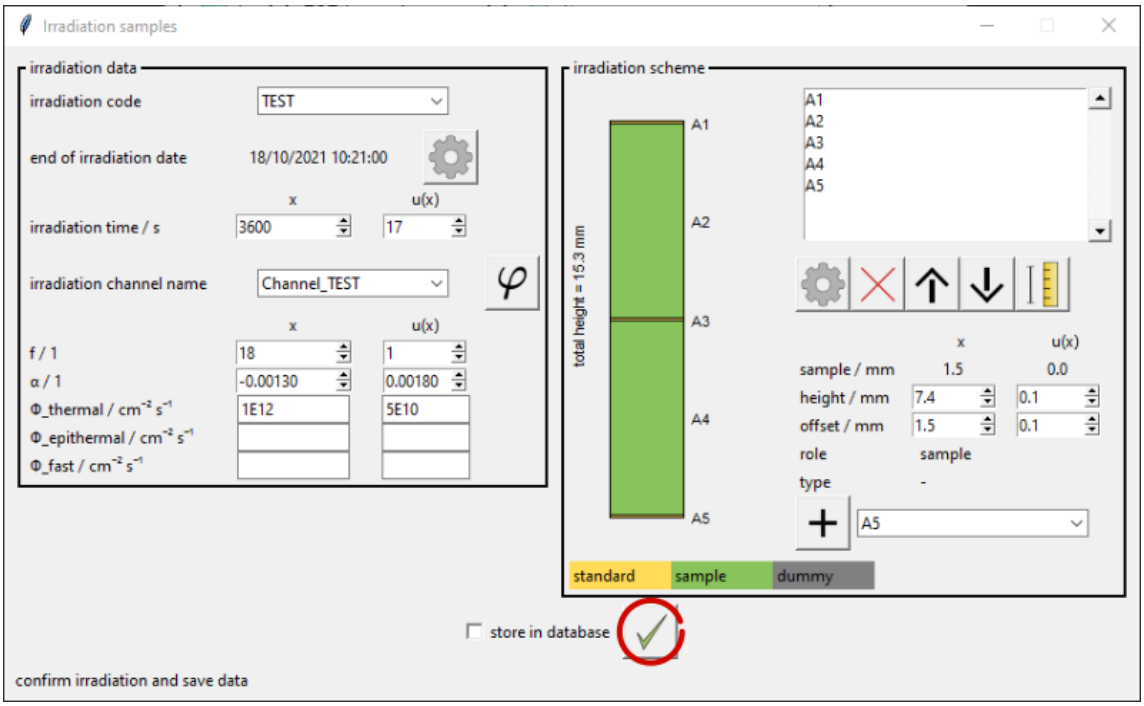
irradiation scheme	distances	x	u(x)
A1	height / mm	0.15	0.1
	offset / mm	0.0	0.0
A2	height / mm	7.4	0.1
	offset / mm	1.5	0.1
A3	height / mm	0.15	0.1
	offset / mm	0.0	0.0
A4	height / mm	7.4	0.1
	offset / mm	1.5	0.1
A5	height / mm	0.15	0.1
	offset / mm	0.0	0.0

5.14. In the ***irradiation data*** section of the IRRADIATION SAMPLES window insert the code of the irradiation in the drop-down menu labeled “irradiation code”, the end of irradiation date through the “change date” button on the same line with the label “end of irradiation date”, value and uncertainty of irradiation time in the boxed labeled as “irradiation time / s”, name of the channel used for irradiation in the drop-down menu labeled “irradiation channel name”, and values and uncertainty of *f* and α parameters and conventional thermal flux in the boxes labeled “f / 1”, “α / 1” and “ϕ_themal / cm^{-2} s^{-1}” in the columns “x” and “u(x)”

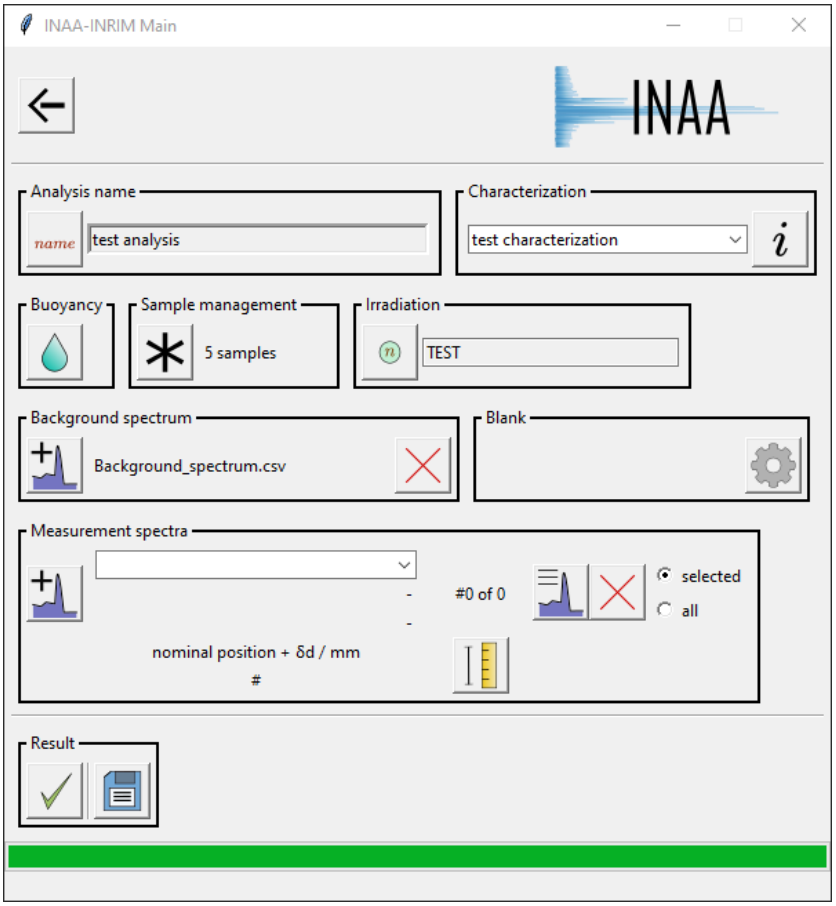


5.15. In the ***irradiation scheme*** section of IRRADIATION SAMPLES window select each one of the sample names from the drop-down menu and click on the “add item to irradiation scheme” button in the order reported in the second table at 5.13 (to mimic their position in the irradiation container). The list of names in the order will appear at the top right of the ***irradiation scheme*** section while a visual reference will appear on the left. Double click on each sample name from the list at the top right and fill in the boxes labeled “height / mm” and “offset / mm” for the columns “x” and “u(x)” (the sample height and role are sample features and cannot be modified from here), when the values are modified, click the “modify selected item” button to confirm the changes. Once all the data are inserted, click the “confirm irradiation and save data” button to save the irradiation information and close the IRRADIATION SAMPLES window; the irradiation code will appear in the

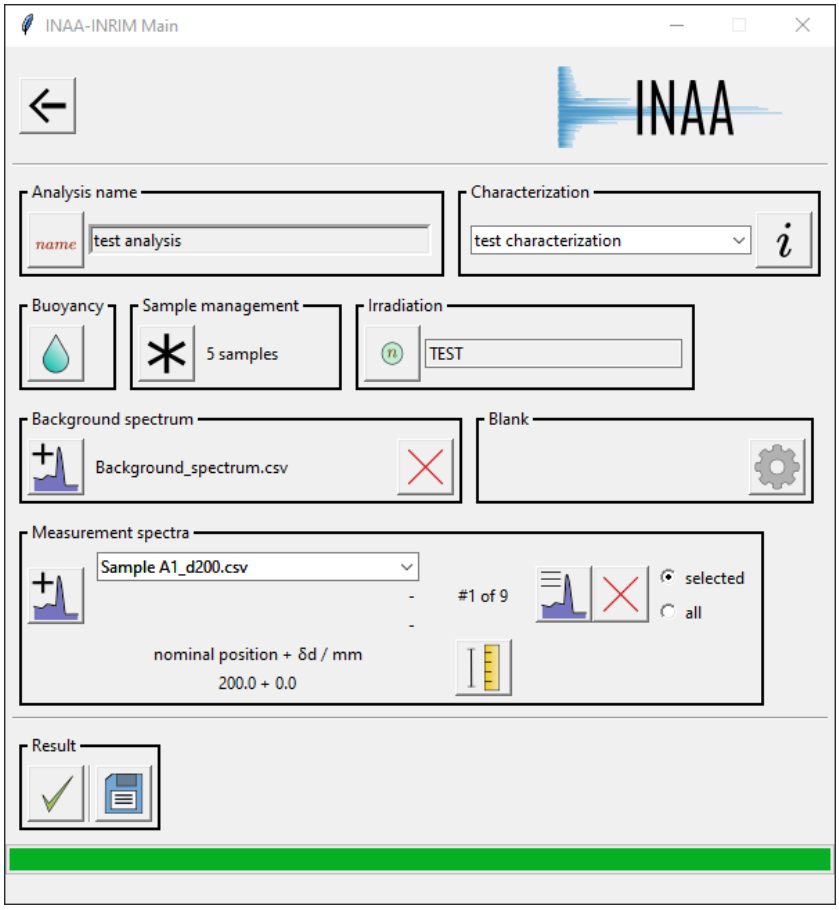
main window. If the “store in database” checkbox is checked, flux information are saved in an internal database (visible from the DATABASES window)



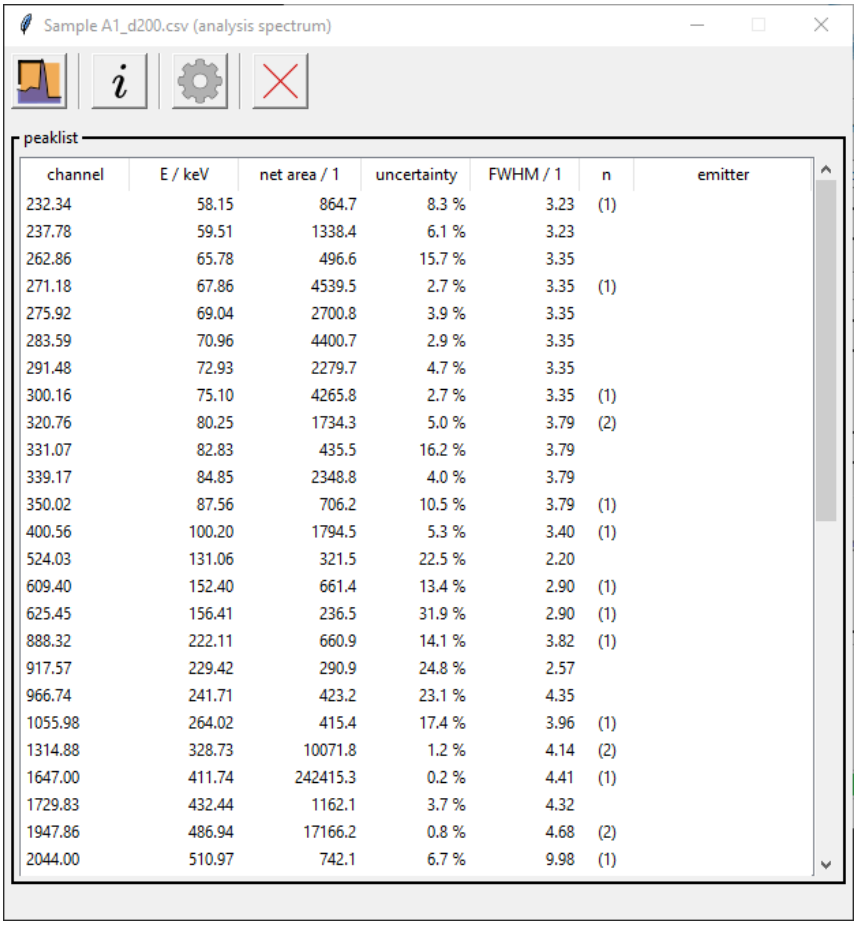
5.16. Back to the INAA-INRIM MAIN window, ***Background spectrum*** and ***Blank*** sections provide optional information that, if active, are used to apply the corresponding corrections to all measurement spectra in the analysis. Click the “Recall background spectrum!” button from the ***Background spectrum*** section and open the “background_spectrum.csv” file. The filename will be shown next to the button indicating the background correction is active



5.17. In the INAA-INRIM MAIN window, click on the “Recall spectra!” button in the ***Measurement spectra*** section and open all the γ-spectra related to the current analysis (meaning spectra acquired from the samples registered in *Sample management*, irradiated in the neutron irradiation in the ***Irradiation*** section and acquired on the detector used to perform the characterization recalled in the ***Characterization*** section). Recall the spectra “Sample A1_d200.csv”, “Sample A2_d20.csv”, “Sample A2_d60.csv”, “Sample A2_d100.csv”, “Sample A2_d200.csv”, “Sample A3_d200.csv”, “Sample A4_d60.csv”, “Sample A4_d200.csv” and ”Sample A5_d200.csv” (where the number following _d indicates the nominal distance of its acquisition). Once recalled their filenames will appear in the drop-down menu in the ***Measurement spectra*** section together with other relevant information related to the selected spectrum, such as a progressive number acting as an index and the counting position it was acquired at

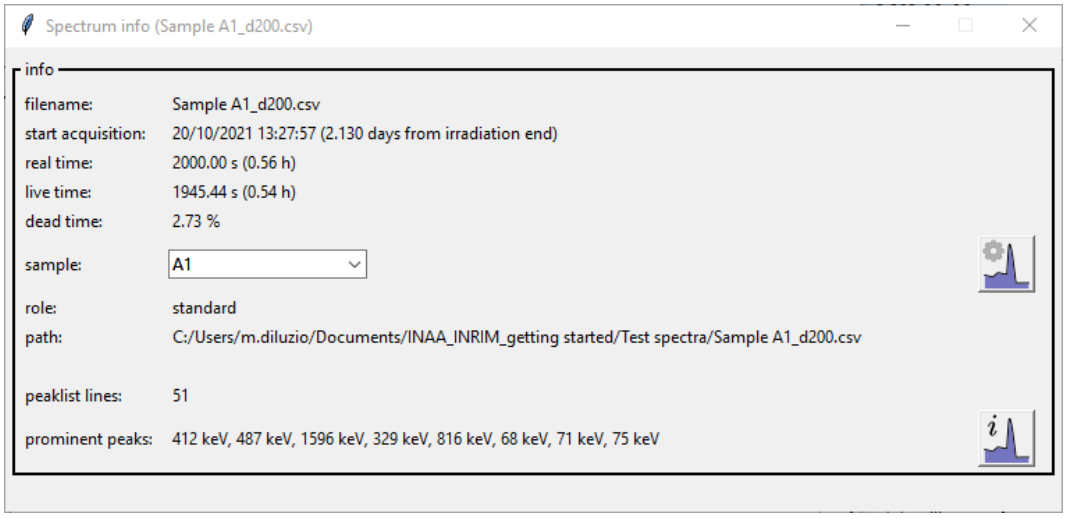


5.18. For any of the recalled spectra, select a spectrum from the drop-down menu in the ***Measurement spectra*** section of the INAA-INRIM MAIN window and click on the "Peaklist!" button (to the right, next to the spectrum counter) to access the PEAKLIST MANAGEMENT window containing a list of all peaks in the spectrum, and a few commands to identify the corresponding sample and emitters responsible for those peaks



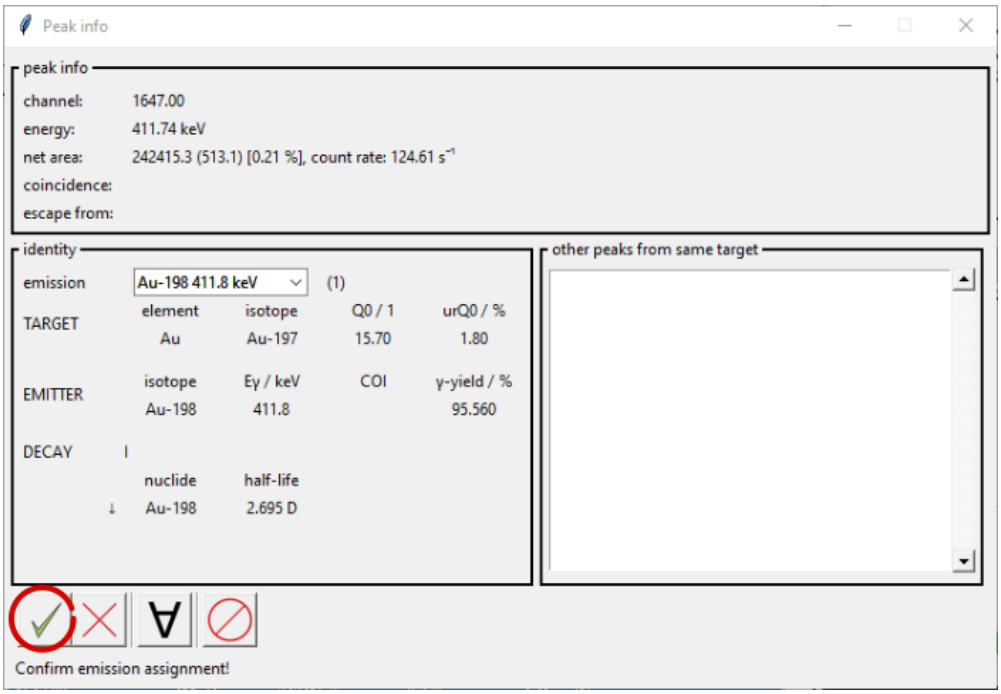
channel	E / keV	net area / 1	uncertainty	FWHM / 1	n	emitter
232.34	58.15	864.7	8.3 %	3.23	(1)	
237.78	59.51	1338.4	6.1 %	3.23		
262.86	65.78	496.6	15.7 %	3.35		
271.18	67.86	4539.5	2.7 %	3.35	(1)	
275.92	69.04	2700.8	3.9 %	3.35		
283.59	70.96	4400.7	2.9 %	3.35		
291.48	72.93	2279.7	4.7 %	3.35		
300.16	75.10	4265.8	2.7 %	3.35	(1)	
320.76	80.25	1734.3	5.0 %	3.79	(2)	
331.07	82.83	435.5	16.2 %	3.79		
339.17	84.85	2348.8	4.0 %	3.79		
350.02	87.56	706.2	10.5 %	3.79	(1)	
400.56	100.20	1794.5	5.3 %	3.40	(1)	
524.03	131.06	321.5	22.5 %	2.20		
609.40	152.40	661.4	13.4 %	2.90	(1)	
625.45	156.41	236.5	31.9 %	2.90	(1)	
888.32	222.11	660.9	14.1 %	3.82	(1)	
917.57	229.42	290.9	24.8 %	2.57		
966.74	241.71	423.2	23.1 %	4.35		
1055.98	264.02	415.4	17.4 %	3.96	(1)	
1314.88	328.73	10071.8	1.2 %	4.14	(2)	
1647.00	411.74	242415.3	0.2 %	4.41	(1)	
1729.83	432.44	1162.1	3.7 %	4.32		
1947.86	486.94	17166.2	0.8 %	4.68	(2)	
2044.00	510.97	742.1	6.7 %	9.98	(1)	

5.19. Click on the “general spectrum information” button (the second from the left at the top of the PEAKLIST MANAGEMENT window) and select, in the ***info*** section of the GENERAL SPECTRUM INFORMATION window that pops up, the corresponding sample from the drop-down menu labeled “sample”, this will identify the spectrum as an acquisition from the selected sample; once the sample is assigned it is possible to click on the “automatic peaks identification” button (to the right of the sample drop-down menu) to automatically assign emitters to peaks based on the composition of the selected sample, although manual peak identification (see 5.20) is always preferred

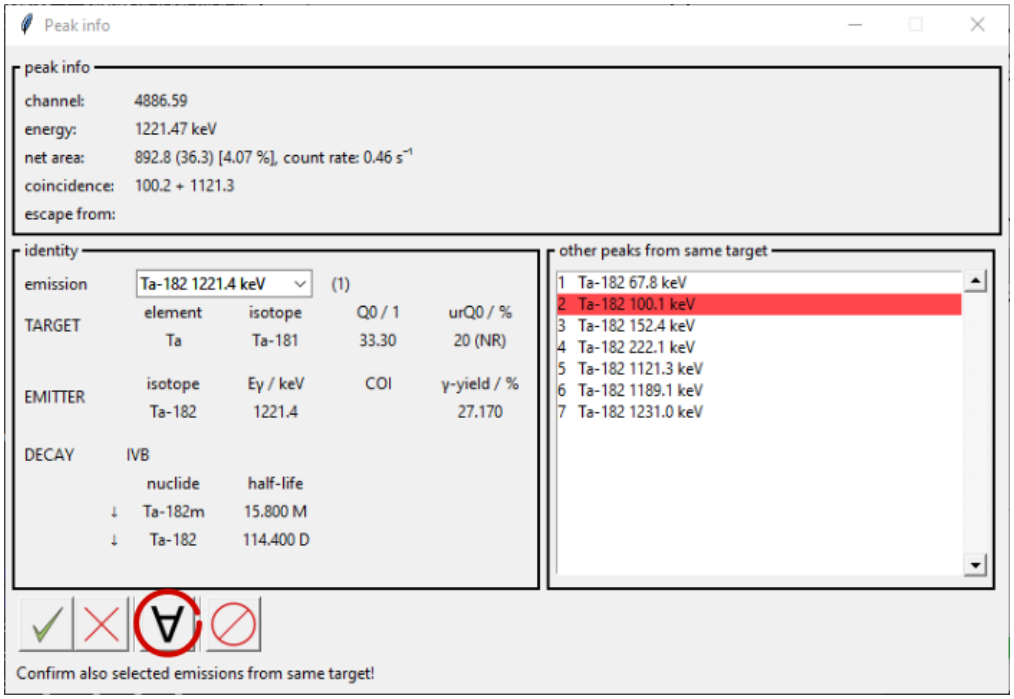


5.20. To manually assign a peak to the corresponding emitter, double click on the line in the ***peaklist*** section of the PEAKLIST MANAGEMENT window (alternatively press the “peak information” button, the third one from the left, after selecting a line from the ***peaklist*** section of the PEAKLIST

MANAGEMENT window). In the PEAK INFO window that pops up, general information can be found in the ***peak info*** section while selection among all suspect emitters is performed from the drop-down menu in the ***identity*** section, click the "confirm emission assignment!" button to confirm the choice

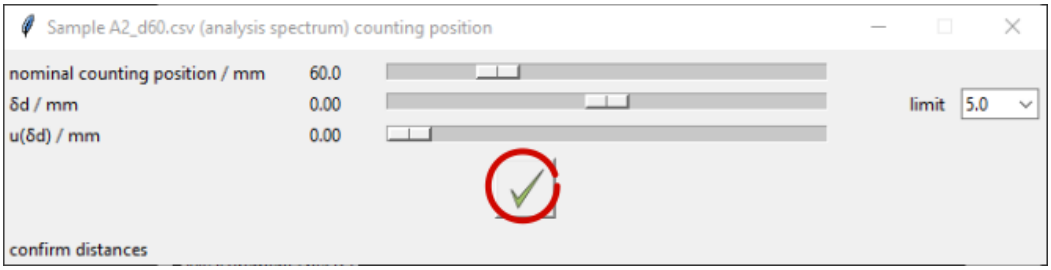


5.21. In case the selected emitter has multiple gamma emissions their corresponding peaks can be displayed in the list within the ***other peaks from same target*** section and selected by clicking the "Confirm also selected emissions from same target" button (the third from the left at the bottom of the PEAK INFO window); only white lines will be assigned, the lines highlighted in red are not affected from this automatic assignment; to change the status of a line, double click on it

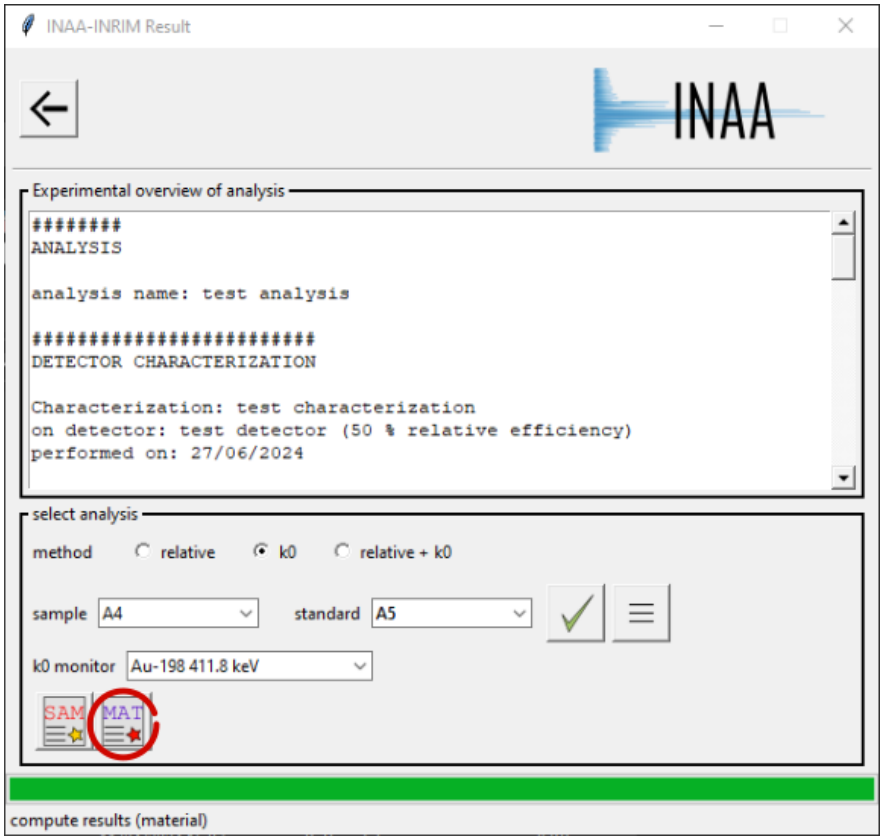


5.22. For each of the spectrum in the drop-down menu in ***Measurement spectra*** section in the INAA-INRIM MAIN window click the "Modify distances of counting position" button (at the bottom

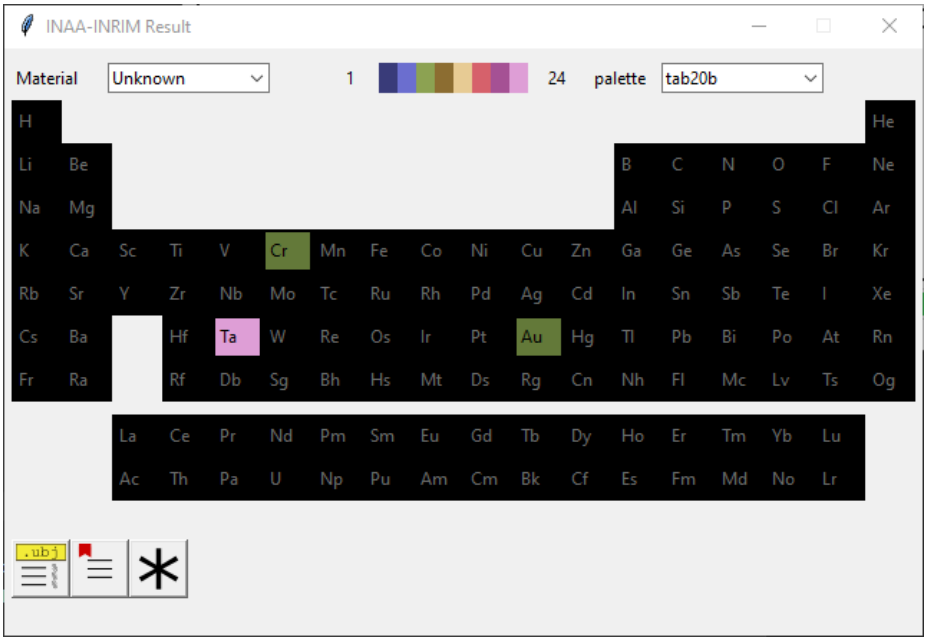
of the section) to assign a counting position. The accessed COUNTING POSITION window gives the option to select three values (two distances and an uncertainty) through sliders: (i) the nominal counting position, referred to the detector characterization ones, (ii) the offset of the actual counting position from the nominal counting position and (iii) the uncertainty of said offset. To confirm the entries, click on the “confirm distances” button



5.23. Once all the relevant information is introduced, return to the ***Results*** section in the INAA-INRIM MAIN window and click on the “Analysis overview!” button to proceed to the results or “Save analysis progress” button to save the information of the analysis in order to be recalled in future from the “load analysis” button found in the ***settings & data*** section from the WELCOME window. The analysis overview opens the INAA-INRIM RESULT window which summarizes all the relevant information about the analysis in the ***Experimental overview of analysis*** section; in the ***select analysis*** section the quantification method can be selected through the radiobutton among “relative”, “k0” or “relative + k0”: adopting direct comparator method, the single comparator method or a mix of the two, respectively. If one of the two options involving k_0 is selected, manual choice of monitor from the drop-down menu labeled “k0 monitor” becomes mandatory. In the second line within the ***select analysis*** section standard-sample pairs can be identified: for each sample in the drop-down menu labeled “sample” select a correspondence in the drop-down menu labeled “standard” (the pairings being A2 -> A3 and A4 -> A5); then click the “confirm pairing” button to confirm the selection noting that the complete list of pairings can be seen by clicking the “view all sample-standard pairings” button. To calculate and display the results click on one of the two buttons at the bottom of the window (the results are the same, it’s only the visualization that changes as they are discriminated by sample or by material)

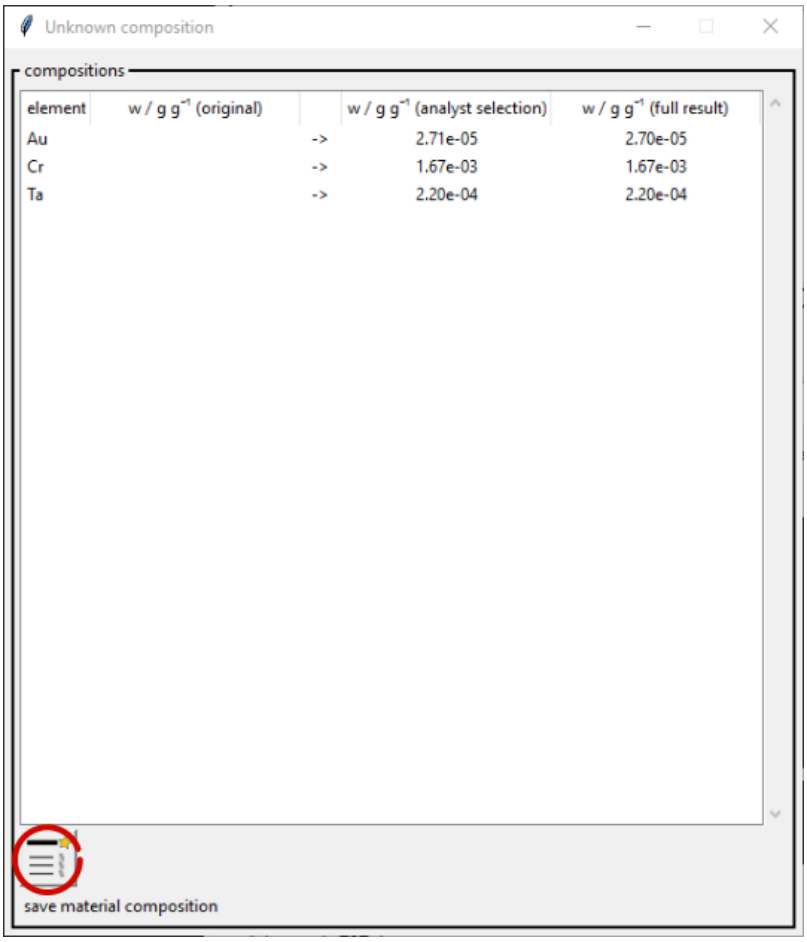


5.24. The results are displayed in a periodic table scheme with cells colored depending on how many budgets were produced for a certain element. At the top left of the window the material (or sample if the other visualization is chosen) can be selected and the visualization updates accordingly



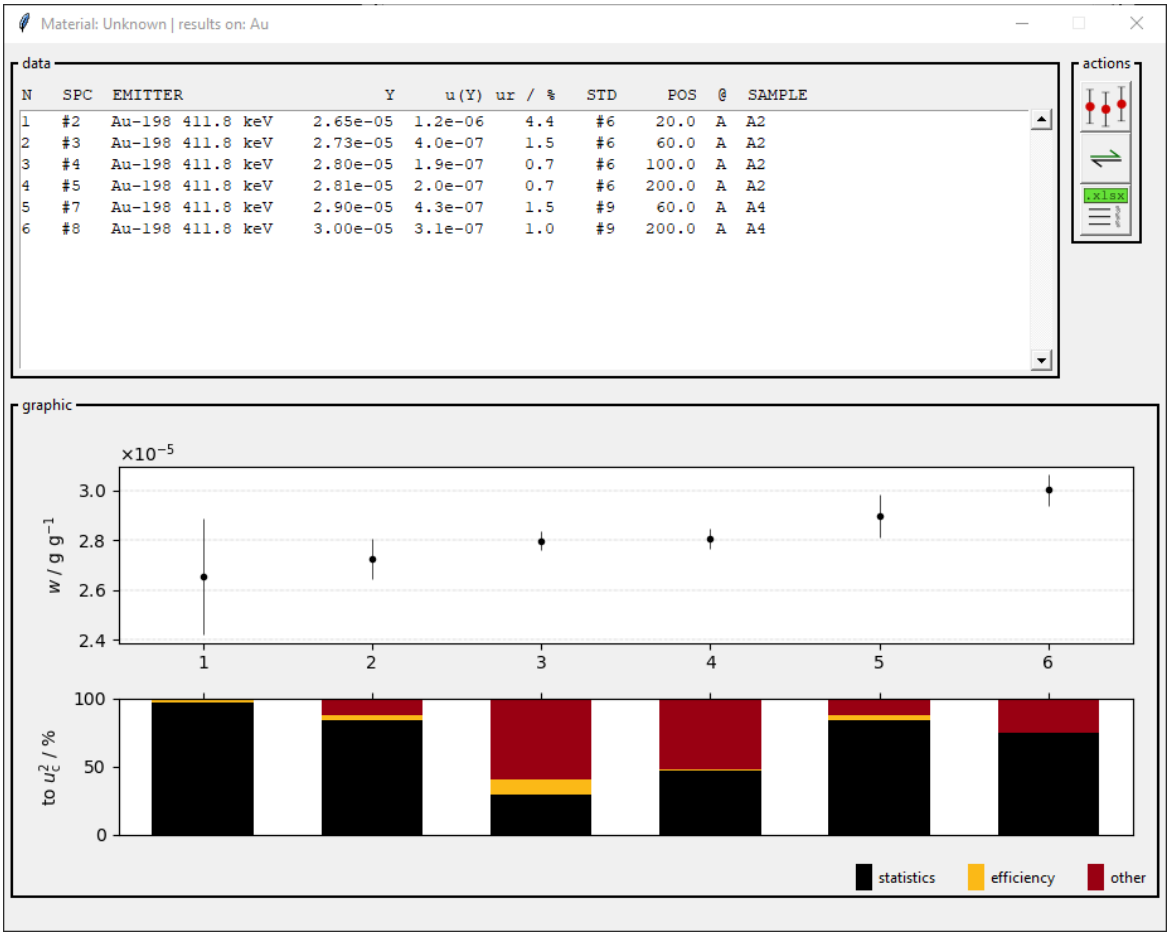
5.25. The buttons at the bottom of the INAA-INRIM RESULT periodic table window allows to save the results ("save results as Budgets Objects" button) to be recalled in the future from the ***manage results*** section in the main menu and display a richer overview of the whole analysis ("display analysis" button). Depending on the selected visualization method and sample options a few additional buttons could appear: the "display CRM validation" button shows a bar graph depicting z-scores for the certified elements in the selected CRM (if any), the "composition of material" button

opens a COMPOSITION window that displays and allows to optionally save the composition resulted from the analysis as a material file to be recalled for future analysis.

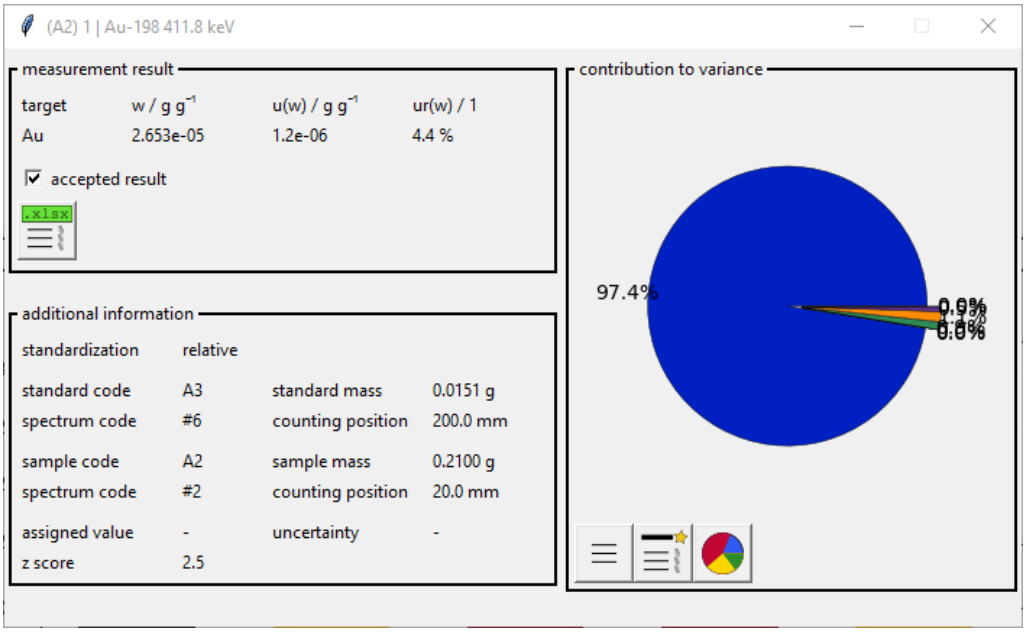


By clicking on the “save material composition” button at the bottom of the COMPOSITION window, one of two versions of the composition can be saved (one only accounting the results selected by the user or one including every result) and the filename can be modified too

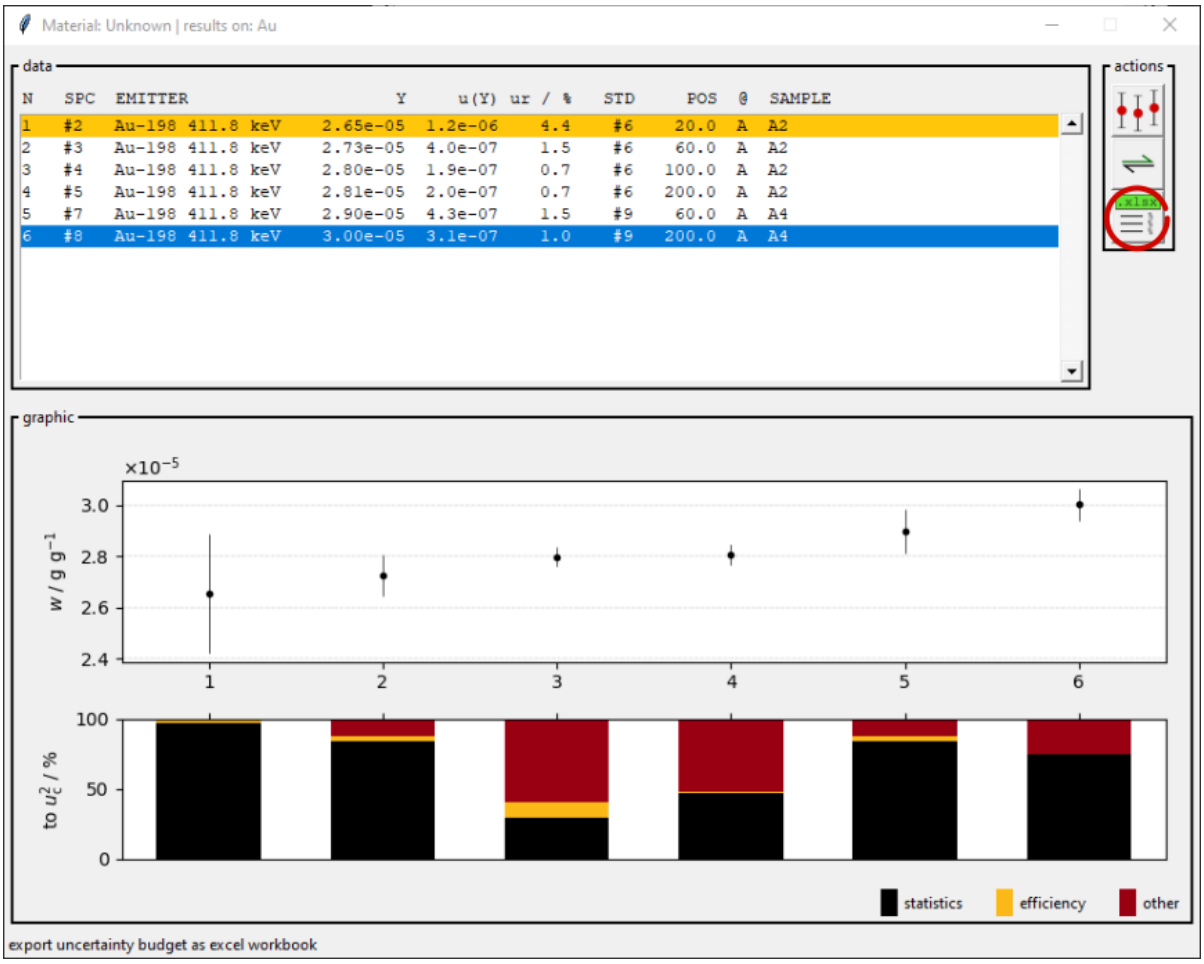
5.26. Single elements can be inspected by clicking on the corresponding symbol cell in the INAA-INRIM RESULT periodic table window to open an ELEMENT RESULTS window including all the information about the results related to the selected element. An overview of the results is listed in the ***data*** section while graphics depicting the mass fraction of the results and, for each, macro-contributors to the combined uncertainty (statistics, efficiency, other) are displayed in the ***graphic*** section. Access specific information concerning a single result by double clicking on a line of the list in ***data*** section to open the UNCERTAINTY BUDGET window



5.27. After accessing the UNCERTAINTY BUDGET window, main and additional information concerning the selected datum are visible in the ***measurement result*** and ***additional information*** sections, the pie graph in the right section represents a more detailed contributor's impact with respect of the bar-chart in the previous ELEMENT RESULTS window. In ***measurement result*** section there is the option to exclude the current datum by disabling the checkbox labeled "accepted result" (excluded data will appear highlighted in yellow in the ***data*** section of the ELEMENT RESULTS window and won't be considered when exporting the results in excel format) or export an excel uncertainty budget by clicking on the "export uncertainty budget as excel workbook" button

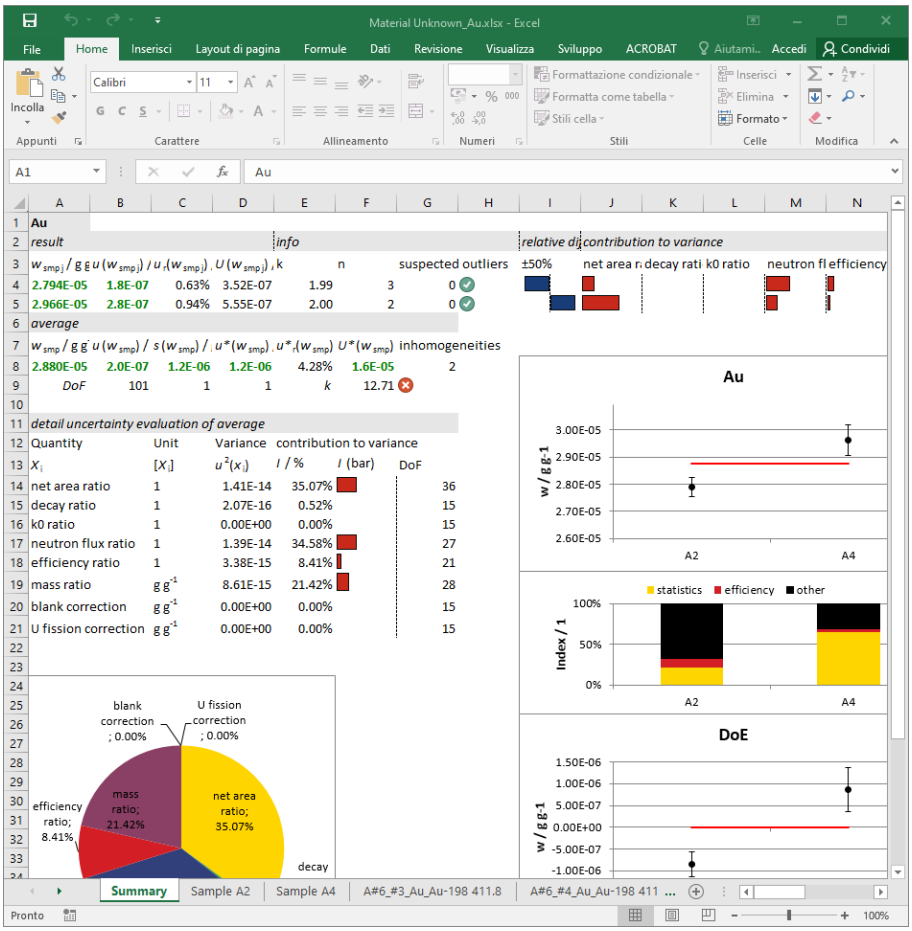


5.28. To save the selected data from the ELEMENT RESULTS window in an excel uncertainty budget per element, click on the "export uncertainty budget as excel workbook" button within the ***actions*** section at the right of the ELEMENT RESULTS window and select a filename and a path. A confirmation message will display if no errors occurred



6. Output overview

6.1. The output spreadsheet uncertainty budget encloses all the information related to the selected element and material. If multiple data from different sample are present, the first worksheet is a summary listing averaged mass fractions on a sample per sample basis and reporting the overall result of the analysis; following worksheets display results for single samples down to budgets related to single measurements. Most of the cells (and formulae) are locked but the user can still have access to the input cells of the single measurement budgets

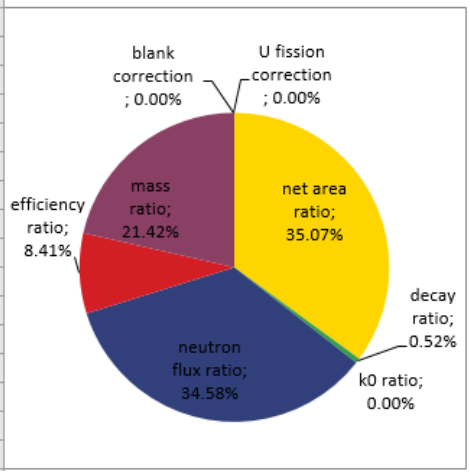


6.2. In detail, at the top left of the "Summary" worksheet results for the indicated element are listed (under the "result" label): for each one value and uncertainties are reported together with *k* value, number of data and how many suspected outliers are present in the dataset; the overall result is calculated as the arithmetic average of the listed data while the combined uncertainty is evaluated taking into account the uncertainty of the average and the experimental standard deviation of the data; the resulting standard (u^*) and expanded uncertainty (U^*) are reported together with number of possible inhomogeneities estimated with degree of equivalence approach, degrees of freedom for all three standard uncertainties and *k* value of the expanded uncertainty

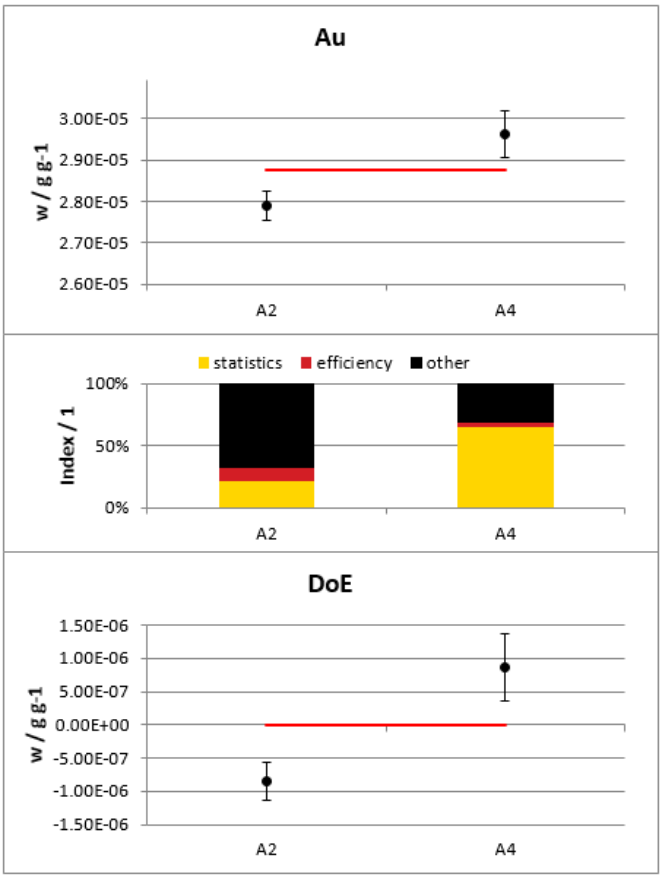
	A	B	C	D	E	F	G	H
1	**Au**							
2	*result*				*info*			
3	$w_{smp\,j}$ / g g^{-1}	$u(w_{smp\,j})$ / g g^{-1}	$u_r(w_{smp\,j})$	$U(w_{smp\,j})$ / g g^{-1}	k		n	suspected outliers
4	2.794E-05	1.8E-07	0.63%	3.52E-07	1.99		3	0
5	2.966E-05	2.8E-07	0.94%	5.55E-07	2.00		2	0
6	*average*							
7	w_{smp} / g g^{-1}	$u(w_{smp})$ / g g^{-1}	$s(w_{smp})$ / g g^{-1}	$u^*(w_{smp})$ / g g^{-1}	$u^*_r(w_{smp})$	$U^*(w_{smp})$		inhomogeneities
8	2.880E-05	2.0E-07	1.2E-06	1.2E-06	4.28%	1.6E-05		2
9	*DoF*	101	1	1	*k*	12.71		
10								

6.3. The combined uncertainty of the average is evaluated in the uncertainty budget reported just below the row “detail uncertainty evaluation of average” and takes into account the contributions of the 8 macro-parameters (net area ratio, decay ratio, k0 ratio, neutron flux ratio, efficiency ratio, mass ratio, blank correction and U fission correction) identified in the measurement model adopted by the software. Additionally, a pie graph depicting the contribution of each of the 8 macro-parameters is also provided

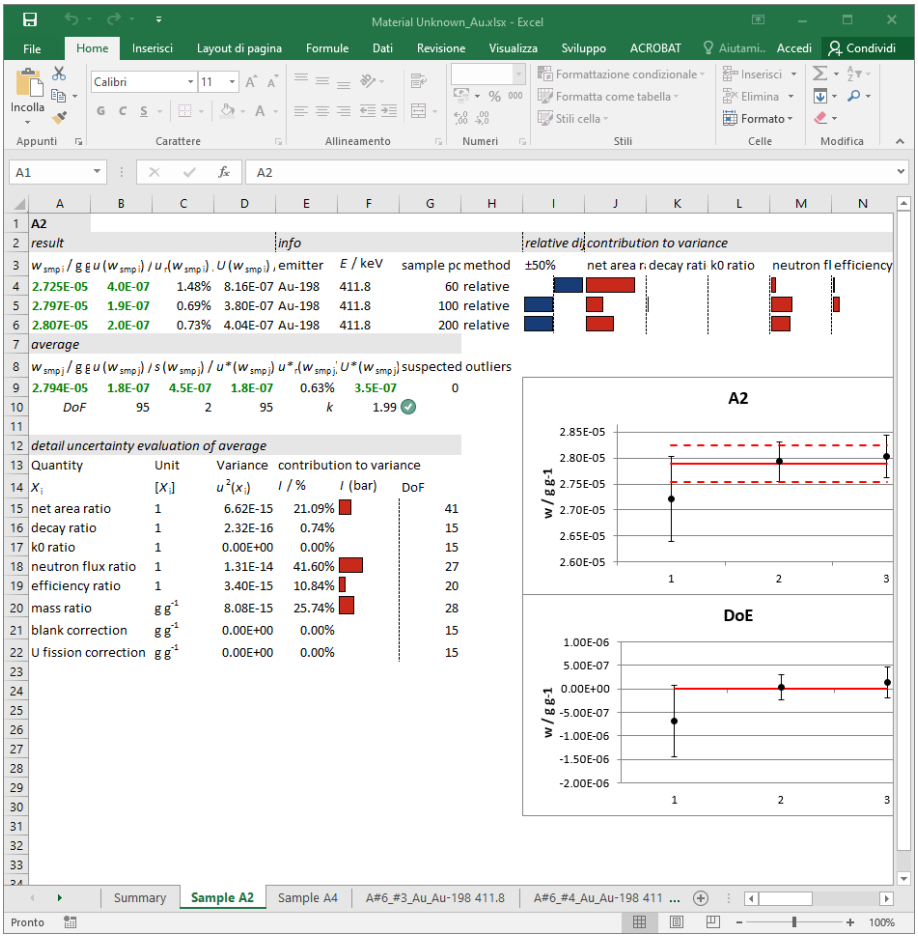
11	*detail uncertainty evaluation of average*					
12	Quantity	Unit	Variance	contribution to variance		
13	X_i	[X_i]	$u^2(x_i)$	I / %	I (bar)	DoF
14	net area ratio	1	1.41E-14	35.07%		36
15	decay ratio	1	2.07E-16	0.52%		15
16	k0 ratio	1	0.00E+00	0.00%		15
17	neutron flux ratio	1	1.39E-14	34.58%		27
18	efficiency ratio	1	3.38E-15	8.41%		21
19	mass ratio	g g^{-1}	8.61E-15	21.42%		28
20	blank correction	g g^{-1}	0.00E+00	0.00%		15
21	U fission correction	g g^{-1}	0.00E+00	0.00%		15



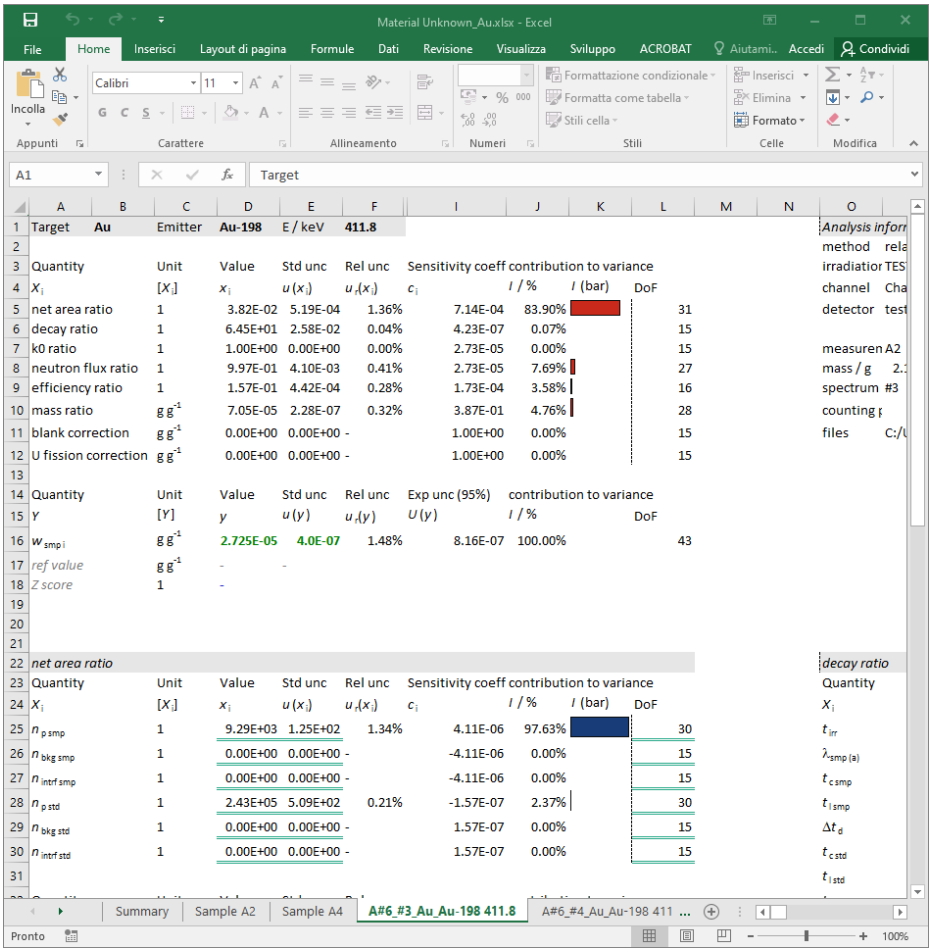
6.4. To graphically summarize the information provided in the “Summary” worksheet, three figures are also available, depicting for each of the investigated samples: (i) mass fraction results, (ii) contributors to the combined uncertainty (condensed to “statistics”, “efficiency” and “other” instead of the canonical 8 macro-parameters) and (iii) degrees of equivalence. In the mass fraction results plot the average and expanded uncertainty of the average are reported as red line and dashed red line, respectively

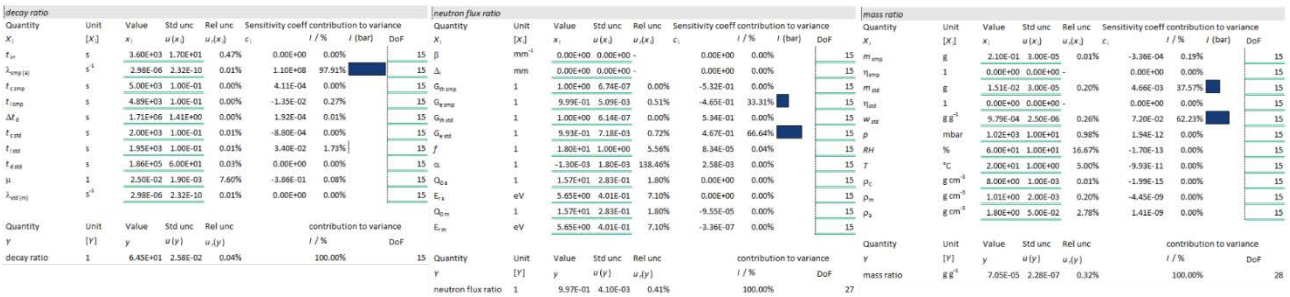


6.5. All information related to a specific sample can be viewed in its corresponding “Sample {sample code}” worksheet accessible from the internal link found in the column S (”link to budget”) of the “Summary” worksheet, next to the sample code. The “Sample” worksheet looks similar to the “Summary” worksheet with a few differences concerning the information provided: the data listed in results are related to the same sample thus information such as *k*, *n* and suspected outliers are replaced by emitter, gamma energy, counting position and quantification method. A weighted average is evaluated to get the result assigned to the corresponding sample and some graphic is not reported, aside from these differences the overall scheme of the worksheet is maintained



6.6. All information related to a specific measurement can be viewed in its corresponding Uncertainty Budget worksheet having a specific code composed of: “{analysis index}{standard spectrum counter}{sample spectrum counter}_{target element}_{emitter} {energy}”. The uncertainty budget worksheet is accessible from the internal link found in the column S (”link to budget”) of the “Sample” worksheet. In this worksheet, multiple uncertainty budgets are reported: the main one (top left of the page, including the 8 macro-parameters) and 8 additional budgets where each macro-parameter is dissected into atomic input parameters. If the input parameters cells are underlined with a green double line the value can be modified by the user otherwise they are blocked; this behavior can be changed from the *output* tab of the SETTINGS window. Aside from the input parameters, all other cells including formulae and graphics in all worksheets are locked and no user interaction is allowed





Related literature

1 D'Agostino et al; "Development and application of a comprehensive measurement equation for the direct comparator standardization method of Instrumental Neutron Activation Analysis"; Submitted to: Spectrochimica Acta Part B (2024).

2 Di Luzio et al; "Developments of the k0-NAA measurement model implemented in k0-INRIM software"; Journal of Radioanalytical and Nuclear Chemistry (2022). DOI: 10.1007/s10967-022-08476-x

3 Di Luzio et al; "A method to deal with correlations affecting γ counting efficiencies in analytical chemistry measurements performed by k0-NAA"; Measurement Science and Technology (2020). DOI: 10.1088/1361-6501/ab7ca8

4 D'Agostino et al; "An uncertainty spreadsheet for the k0-standardisation method in Neutron Activation Analysis"; Journal of Radioanalytical and Nuclear Chemistry (2018). DOI: 10.1007/s10967-018-6094-8

5 Di Luzio et al; "Validation of detection efficiency-based corrections implemented in the k0-INRIM software"; Journal of Radioanalytical and Nuclear Chemistry (2024). DOI: 10.1007/s10967-023-09223-6

6 Blaauw et al; "The 2021 IAEA software intercomparison for k0-INAA"; Journal of Radioanalytical and Nuclear Chemistry (2023). DOI: 10.1007/s10967-022-08626-1

7 Di Luzio et al; "The k0-INRIM software version 2.0: presentation and an analysis vademecum"; Journal of Radioanalytical and Nuclear Chemistry (2023). DOI: 10.1007/s10967-022-08622-5

8 D'Agostino et al; "Erratum: The k0-INRIM software: A tool to compile uncertainty budgets in neutron activation analysis based on k0-standardisation"; Measurement Science and Technology (2020). DOI: 10.1088/1361-6501/ab57c8