



Gamma Spectra Evaluation Package - manual

Software package for processing and evaluation gamma spectra acquired from gamma spectrometric measurements

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Introduction

This manual provides detailed guidance on the installation, usage, and simplified theory behind the Gamma Spectra Evaluation Package. The software was developed by the Nuclear Group at the Faculty of Electrical Engineering and Communication, Brno University of Technology (BUT).

A brief list of available tools and features:

- Upload processed (fitted peaks) gamma spectra in `.prn` format from the Deimos32 program.
- Enter experimental, sample, and detector information for further analysis.
- Upload library values for gamma corrections.
- Calculate and apply gamma spectrometry corrections.
- Calculate reaction rates, yields, and similar values from original or corrected data.
- Statistically process results and export them.
- Additional features for library preparation:
 - Gamma peak efficiency evaluation for a selected detector and its geometry.
 - Preparation of non-linearity correction libraries for a selected detector.
 - Preparation of true coincidence summation libraries via the `Truecoinc` program automation.

1 Installation

The code is available in the GitHub repository Gamma Spectra Evaluation Package.

Users can install and run the program in two basic ways:

1. **Executable files:** Download compiled files from the latest release (usually available for Linux and Windows x64) and use them with a default Python ≥ 3.10 installation. All necessary packages are included in the compiled file.
2. **Source files:** Download the source files and install Python ≥ 3.10 along with the required libraries. A Python environment manager is highly recommended. Based on experience, Conda can create overly large environments without proper settings, making simpler tools like `virtualenv`, `venv`, or other managers preferable.

1.1 Executable files

This option offers the simplest way to use the Gamma Spectra Evaluation Package. Users need to download and install Python 3.10 or newer. The software is currently developed using Python version 3.12.

1.2 Source files

Users can run the source code if the packages listed below and their dependencies are installed:

- `Python` ≥ 3.10 ,
- `matplotlib`,
- `numpy`,
- `openpyxl`,

- `pandas`,
- `pathlib`,
- `pywin32`,
- `pywinauto`,
- `scipy`,
- `tkinter`,
- `ttkthemes`,
- `ttkwidgets`,
- `xlsxWriter`.

The program can be started by typing the following terminal command:

```
> python main_gamma_package.py
```

1.2.1 Program structure - source code

The directory structure of the program is as follows:

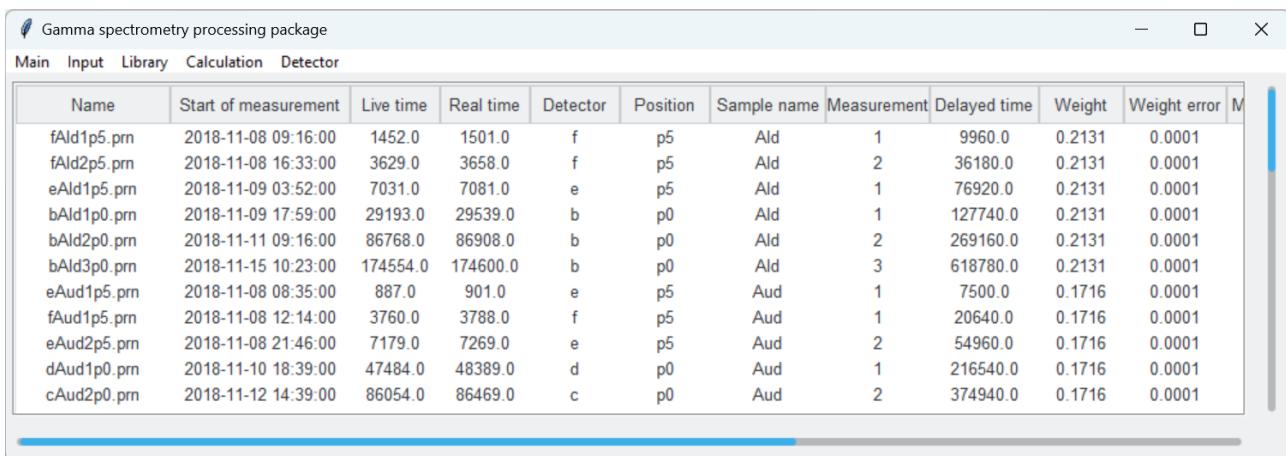
```
Program folder
  └── main_gsep.py
  └── README.md
  └── libraries
  └── modules
    ├── calc_coinc.py
    ├── calc_corr.py
    ├── calc_eff.py
    ├── calc_nonlin.py
    ├── calc_rr.py
    ├── corr_att.py
    ├── corr_bcg.py
    ├── corr_beam.py
    ├── corr_coinc.py
    ├── corr_eff.py
    ├── corr_nonlin.py
    ├── corr_sepdep.py
    ├── globals.py
    ├── inputs.py
    ├── settings.py
    └── utilities.py
```

2 Program description

When the program is launched, the user is presented with the **main window**, which includes a top menu bar with several options. Each menu option is described in detail in the following sections. The menu options are as follows:

- *Main* - load/change the working directory, show selected information connected to irradiation, display the content of the spectrum file, export selected spectrum, export all spectra or exit the program.
- *Input* - menu for entering information about the experiment, samples, detectors and non-point correction.
- *Library* - selection of library files.
- *Calculation* - opens a window for calculating spectrometric corrections or final results.
- *Detector* - allows processing spectra for preparing efficiency, nonlinearity, or coincidence correction libraries.

The purpose of main window is accessing Menu bar and show information about the loaded spectra in a table that is filling rest of the main window, as shown in Fig. 1.



The screenshot shows the main window of the Gamma spectrometry processing package. The window title is "Gamma spectrometry processing package". The menu bar includes "Main", "Input", "Library", "Calculation", and "Detector". Below the menu bar is a table with the following data:

Name	Start of measurement	Live time	Real time	Detector	Position	Sample name	Measurement	Delayed time	Weight	Weight error	M
fAld1p5.prm	2018-11-08 09:16:00	1452.0	1501.0	f	p5	Ald	1	9960.0	0.2131	0.0001	
fAld2p5.prm	2018-11-08 16:33:00	3629.0	3658.0	f	p5	Ald	2	36180.0	0.2131	0.0001	
eAld1p5.prm	2018-11-09 03:52:00	7031.0	7081.0	e	p5	Ald	1	76920.0	0.2131	0.0001	
bAld1p0.prm	2018-11-09 17:59:00	29193.0	29539.0	b	p0	Ald	1	127740.0	0.2131	0.0001	
bAld2p0.prm	2018-11-11 09:16:00	86768.0	86908.0	b	p0	Ald	2	269160.0	0.2131	0.0001	
bAld3p0.prm	2018-11-15 10:23:00	174554.0	174600.0	b	p0	Ald	3	618780.0	0.2131	0.0001	
eAud1p5.prm	2018-11-08 08:35:00	887.0	901.0	e	p5	Aud	1	7500.0	0.1716	0.0001	
fAud1p5.prm	2018-11-08 12:14:00	3760.0	3788.0	f	p5	Aud	1	20640.0	0.1716	0.0001	
eAud2p5.prm	2018-11-08 21:46:00	7179.0	7269.0	e	p5	Aud	2	54960.0	0.1716	0.0001	
dAud1p0.prm	2018-11-10 18:39:00	47484.0	48389.0	d	p0	Aud	1	216540.0	0.1716	0.0001	
cAud2p0.prm	2018-11-12 14:39:00	86054.0	86469.0	c	p0	Aud	2	374940.0	0.1716	0.0001	

Figure 1: Program main window with uploaded spectra

For each spectrum, the following information is displayed:

- *Name* - file name,
- *Start of measurement* - date and time when the measurement started,
- *Live time* - effective measurement time t_{live} (s),
- *Real time* - total measurement time t_{real} (s),
- *Detector* - detector designation,
- *Position* - position label of the detector measurement geometry,
- *Sample name* - sample name without information about detector, position and number of measurement,
- *Measurement number* - measurement number,
- *Weight* - sample weights (g),
- *Molar mass* - molar mass (g/mol),
- *Cal en_1* - calibration energy from the Deimos32 program (keV) - lower value,
- *Cal en_2* - calibration energy from the Deimos32 program (keV) - higher value,
- *Delayed time* - time between the end of irradiation and the start of measurement (s),

- *Element* - element(s) constituting the sample material,
- *Fraction by weight* - weight fraction (-) in case of more Elements,
- *Density* - density of the material (g/cm³),
- *Thickness* - sample thickness (mm),
- *Non-point* - non-point correction values.

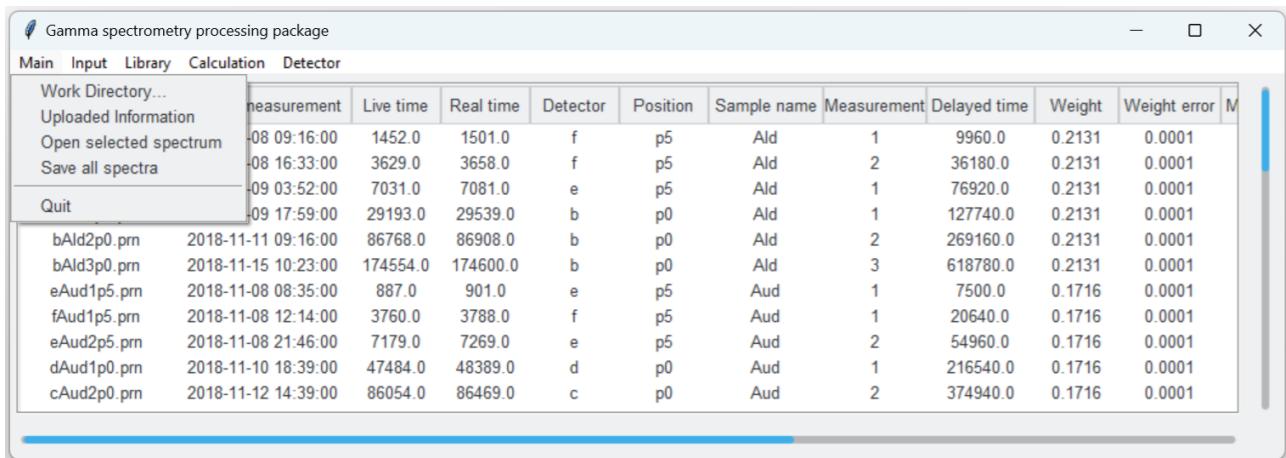
2.1 Common Features

Open spectrum - In most windows containing a treeview widget, the user can open the corresponding **spectrum** by double-clicking on the row with the spectrum name. This feature allows for easy comparison of spectrum values, including any calculated corrections, if available.

Sort treeview - Another available feature is the ability to sort the treeview table based on a specific column. This can be activated by clicking on the column header.

2.2 Main window menu - Main

The **Main** section in the menu (Fig. 2) is used for basic work with spectra. By selecting the option **Work Directory**, the user loads a folder with .prn spectrum files from the **Deimos32** program¹. In the selected folder, there may be files for calculating reaction rates as well as files for determining peak efficiency and detector nonlinearity correction.



The screenshot shows the main window of the Gamma spectrometry processing package. The title bar reads "Gamma spectrometry processing package". The menu bar includes "Main", "Input", "Library", "Calculation", and "Detector". The "Main" menu is currently active, displaying a list of options: "Work Directory...", "Uploaded Information", "Open selected spectrum", "Save all spectra", and "Quit". Below this menu is a table listing uploaded spectra. The columns are labeled: measurement, Live time, Real time, Detector, Position, Sample name, Measurement, Delayed time, Weight, and Weight error. The table contains 10 entries, each corresponding to a .prn file with its details.

	measurement	Live time	Real time	Detector	Position	Sample name	Measurement	Delayed time	Weight	Weight error	M
bAld2p0.prn	2018-11-11 09:16:00	86768.0	86908.0	b	p0	Ald	1	9960.0	0.2131	0.0001	
bAld3p0.prn	2018-11-15 10:23:00	174554.0	174600.0	b	p0	Ald	3	618780.0	0.2131	0.0001	
eAud1p5.prn	2018-11-08 08:35:00	887.0	901.0	e	p5	Aud	1	7500.0	0.1716	0.0001	
fAud1p5.prn	2018-11-08 12:14:00	3760.0	3788.0	f	p5	Aud	1	20640.0	0.1716	0.0001	
eAud2p5.prn	2018-11-08 21:46:00	7179.0	7269.0	e	p5	Aud	2	54960.0	0.1716	0.0001	
dAud1p0.prn	2018-11-10 18:39:00	47484.0	48389.0	d	p0	Aud	1	216540.0	0.1716	0.0001	
cAud2p0.prn	2018-11-12 14:39:00	86054.0	86469.0	c	p0	Aud	2	374940.0	0.1716	0.0001	

Figure 2: Menu Main - from main window

For the spectra upload process is important to follow a naming conventions described in Sec. 2.2.1. If the user fails to comply then files won't be loaded correctly into the program.

The designation of the detector and measuring position is important for gamma spectrometry corrections. The measurement number and file name are then used in the results processing.

The **Uploaded Information** option displays a window with information about the location of the working folder, irradiation duration, end of irradiation, and irradiation parameters (integral number of particles and corresponding uncertainty), see Fig. 3.

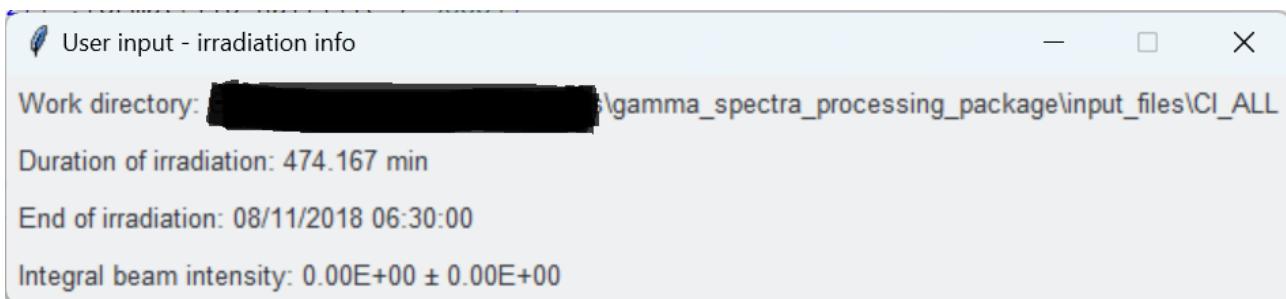


Figure 3: Main section - Uploaded Information

The initial window contains only general information about the uploaded spectra. By double-clicking with the left mouse button on a selected spectrum or by selecting the **Open selected spectrum** option in the menu **Main**, individual spectra can be opened in a new window. The user can compare uploaded content with .prn files. Furthermore, all calculated corrections are included to each spectrum file, see Fig. 4. From this window, it is also possible to save the spectrum content to a .xlsx file for later use.

¹The Deimos program was developed at the CAS NPI [1]

channel	cherr	energy	area	aer%	fwhm	chisq	isotope
785.206	0.486	159.662	3075.0	9.9	15.82	1.07	nan
1873.629	0.344	346.719	3577.2	7.3	15.0	1.03	nan
2831.281	0.166	511.302	13062.3	2.5	21.57	1.11	nan
4847.292	0.758	857.775	2049.4	12.6	19.34	0.94	nan
7819.827	0.012	1368.636	434497.4	0.2	17.45	1.55	nan
8356.133	0.325	1460.806	2482.8	6.2	17.53	1.07	nan
9933.36	0.04	1731.87	53420.6	0.7	18.66	1.89	nan
12902.956	0.067	2242.226	38802.3	0.9	23.6	1.08	nan
15724.673	0.13	2727.168	202458.4	0.4	16.79	3.64	nan

[Save to XLSX](#) [Close window](#)

Figure 4: Main section - Open selected spectrum

The option **Save all spectra** allows save all spectra to a single file `work directory/output/spectra/2024-10-25_all_spectra.xlsx` with corresponding date and time. Each spectrum is stored on its own sheet with the same name as the original file. Also, all spectra parameters information from the main window are saved into the file `work directory/output/2024-10-25_all_spectra_parameters.xlsx`. The export is performed to the output folder in the work directory.

The final option in this menu is **Quit**. This is one of two ways to exit the program. The other way is to simply click the "X" in the upper right corner of the main window.

2.2.1 Spectrum Files Naming Convention

The name of individual files have to follow this format (rules):

- name example: ***a5NaCl3p2***, where
 - *a* is the detector designation,
 - *5NaCl* is the sample name. The number can not follow NaCl because then it is in collision with the measurement number,
 - *3* is the measurement number,
 - *p2* is the detector position (geometry).
- the name might be modified to this format ***aNaCl5_3_p2***, where the sample name, measurement number, and measurement position are separated by underscores.

2.2.2 Information on Peaks in Spectra

For each identified peak in the spectrum, the following data are loaded:

- *channel* - channel at the peak center (-),
- *cherr* - channel uncertainty (-),
- *energy* - energy (keV),
- *area* - area (-),

- *aerr%* - relative area uncertainty (%),
- *fwhm* - FWHM - full width at half maximum (-),
- *chisq* - χ^2 (chi-square) of the peak fit (-),
- *cor_en* - energy after detector non-linearity correction (keV),
- *en_diff* - size of the energy change after detector nonlinearity correction (keV),
- *cor_en_err* - error of the energy after detector nonlinearity correction (-),
- *bcg_diff* - size of the change after background correction (-),
- *bcg cor area* - area after background subtraction (-),
- *bcg cor area unc* - area error after background subtraction (-),
- *sep_dep_diff* - size of the are change after escape peaks correction (-),
- *SEP-DEP cor area* - area after subtraction of single and double escape peaks (-),
- *SEP-DEP cor area unc* - area error after subtraction of single and double escape peaks (-),
- *att cor* - self-absorption correction (-),
- *eff fep* - full-energy peak efficiency of the detector (-).

2.3 Main window menu - Input

The **Input** menu (in Fig. 5) is used to enter supplementary information describing experiment parameters and the characteristics of used detectors. Parameter for analysis strongly depends on applied corrections and results normalizations. Below is a description of each option.

	Irradiation	Sample	Start of measurement	Live time	Real time	Detector	Position	Sample name	Measurement	Delayed time	Weight	Weight error	M
f	Detector		2018-11-08 09:16:00	1452.0	1501.0	f	p5	Ald	1	9960.0	0.2131	0.0001	
f	Non-point		2018-11-08 16:33:00	3629.0	3658.0	f	p5	Ald	2	36180.0	0.2131	0.0001	
eAld1p5.prm			2018-11-09 03:52:00	7031.0	7081.0	e	p5	Ald	1	76920.0	0.2131	0.0001	
bAld1p0.prm			2018-11-09 17:59:00	29193.0	29539.0	b	p0	Ald	1	127740.0	0.2131	0.0001	
bAld2p0.prm			2018-11-11 09:16:00	86768.0	86908.0	b	p0	Ald	2	269160.0	0.2131	0.0001	
bAld3p0.prm			2018-11-15 10:23:00	174554.0	174600.0	b	p0	Ald	3	618780.0	0.2131	0.0001	
eAud1p5.prm			2018-11-08 08:35:00	887.0	901.0	e	p5	Aud	1	7500.0	0.1716	0.0001	
fAud1p5.prm			2018-11-08 12:14:00	3760.0	3788.0	f	p5	Aud	1	20640.0	0.1716	0.0001	
eAud2p5.prm			2018-11-08 21:46:00	7179.0	7269.0	e	p5	Aud	2	54960.0	0.1716	0.0001	
dAud1p0.prm			2018-11-10 18:39:00	47484.0	48389.0	d	p0	Aud	1	216540.0	0.1716	0.0001	
cAud2p0.prm			2018-11-12 14:39:00	86054.0	86469.0	c	p0	Aud	2	374940.0	0.1716	0.0001	

Figure 5: Main window - Input menu

Irradiation is used to collect information on the irradiation. This includes the date and time when the irradiation ended and its duration. The final parameter is the integral number of particles and its uncertainty. Input loaded through a separate window, as shown in Fig. 6. The date and time format is indicated in the window, and a period is used as the decimal separator.

User input - irradiation parameters

Date and time of irradiation end:
08/11/2018 06:30:00 (DD/MM/YYYY HH:MM:SS)

Duration of irradiation:
474.167 minutes

Integral number of particles and uncertainty:
0.00E+00 ± 0.00E+00

Save Quit

Figure 6: User input - irradiation parameters

Sample (see Fig. 7) allows the user to enter information about the masses of individual samples and the data required for self-absorption correction calculations. If the sample consists of a single element, the user must input the element symbol, proton number, and sample thickness. If the sample material is a compound, the **Material** field requires a list of all compound elements separated by slashes (see Fig. 8). The program permits spaces between slashes and values; however, these are automatically removed upon upload. It is generally not recommended to include spaces. The same rule applies to the mass fraction values, which must follow the same order as the respective elements and be separated by slashes. The program expects absolute values for these fractions.

The last two columns in the table correspond to the sample density and its thickness (measured perpendicular to the detector window). The density value is mandatory for compounds. If the density value is missing, the program will use default density values from the **attenuation** library.

	Sample parameters						
	Sample Weight (g)	Weight err (g)	Molar mass (-)	Material (-)	Frac. by weight (-)	Density (g/cm ³)	Thickness (mm)
Ald	0.2131	0.0001	26.9815	13Al	-	-	0.5
Aud	0.1716	0.0001	196.9666	79Au	-	-	0.06
Bid	0.7105	0.0001	208.9804	83Bi	-	-	0.5
Cod	0.7707	0.0001	58.9332	27Co	-	-	0.5
Cud	0.3684	0.0001	63.546	29Cu	-	-	0.25
Fed	0.2606	0.0001	55.845	26Fe	-	-	0.2
Ind	0.1177	0.0001	114.818	49In	-	-	0.1
Mnd	0.3733	0.0001	54.938	25Mn	-	-	0.2
Pbd	0.2175	0.0001	207.2	82Pb	-	-	0.125
Tad	0.313	0.0001	180.9479	73Ta	-	-	0.125
Vd	0.2355	0.0001	50.9415	23V	-	-	0.25
Yd	0.1607	0.0001	88.9059	39Y	-	-	0.25

Figure 7: User input - sample parameters - material from single element.

The **Non-point Source** option within the Sample window (Fig. 9) allows the user to input custom values for non-point source corrections for all sample positions for each detector. These parameters are not mandatory. Non-point correction compensates difference between the emission surface dimension and shape of reference standards used for spectrometer calibration and real samples.

Another option is **Detector** (see Fig. 10), which is used to enter information on calibration energies from the Deimos32 program, as shown in Fig. 11 in the lower left of the window. This calibration is used only if an additional energy calibration has been performed during peaks evaluation. In such cases, the Deimos32 program recalculates the calibration used during measurement to match the calibration used in evaluation.

The inputs described above are automatically saved in the `work directory/parameters.txt` file in the same folder as the original spectra. Every new program run of already processed spectra is automatically loaded, so the user doesn't need to re-enter them.

Sample parameters						
	Sample Weight (g)	Weight err (g)	Molar mass (-)	Material (-)	Frac. by weight (-)	Density (g/cm ³)
Ald	0.2131	0.0001	26.9815	1H/8O	0.11/0.89	0.9997
Aud	0.1716	0.0001	196.9666	79Au	-	-
Bid	0.7105	0.0001	208.9804	83Bi	-	-
Cod	0.7707	0.0001	58.9332	27Co	-	-
Cud	0.3684	0.0001	63.546	29Cu	-	-
Fed	0.2606	0.0001	55.845	26Fe	-	-
Ind	0.1177	0.0001	114.818	49In	-	-
Mnd	0.3733	0.0001	54.938	25Mn	-	-
Pbd	0.2175	0.0001	207.2	82Pb	-	-
Tad	0.313	0.0001	180.9479	73Ta	-	-
Vd	0.2355	0.0001	50.9415	23V	-	-
Yd	0.1607	0.0001	88.9059	39Y	-	-

Figure 8: User input - sample parameters - material composed of two elements (H_2O)

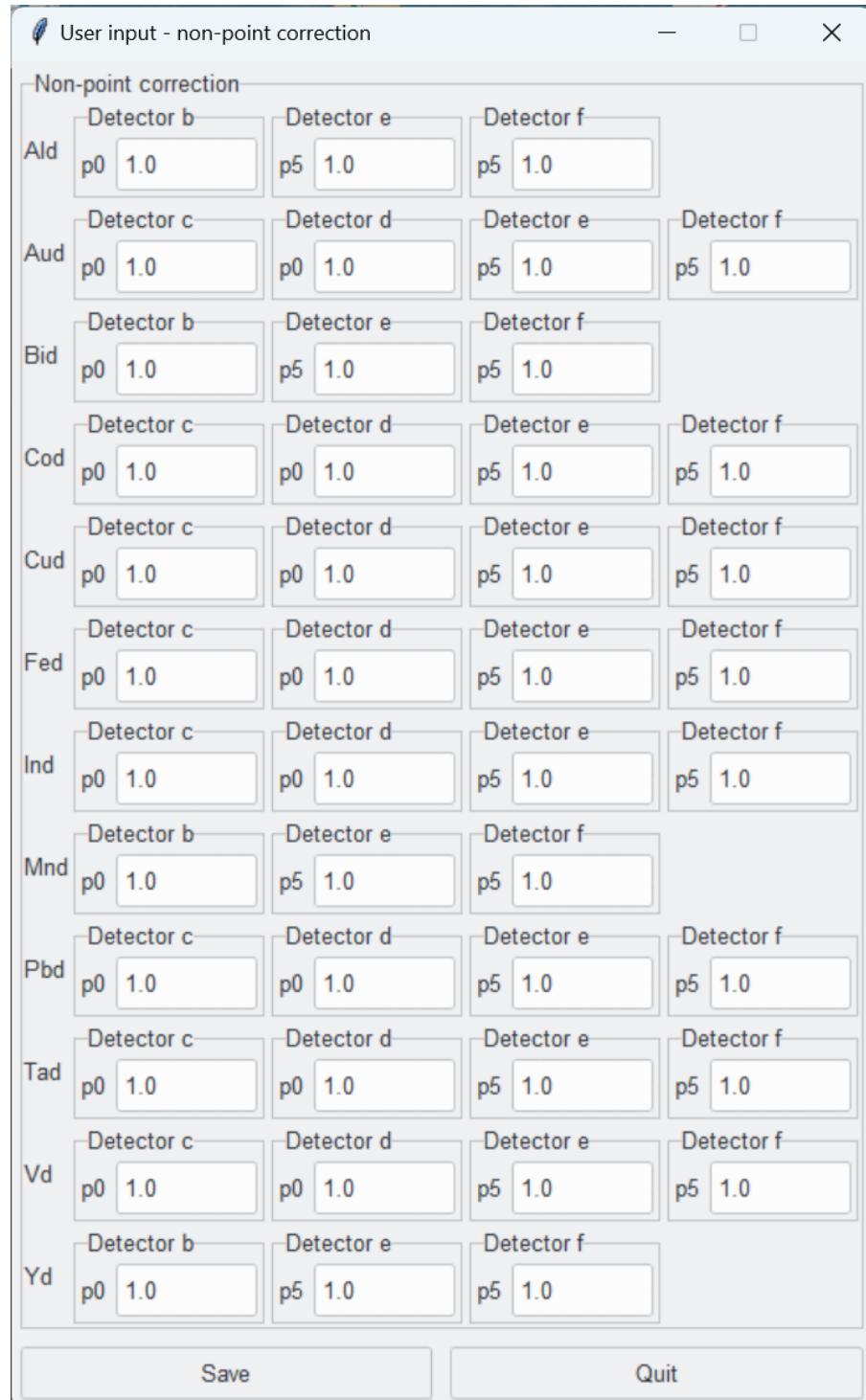


Figure 9: User input - non-point correction

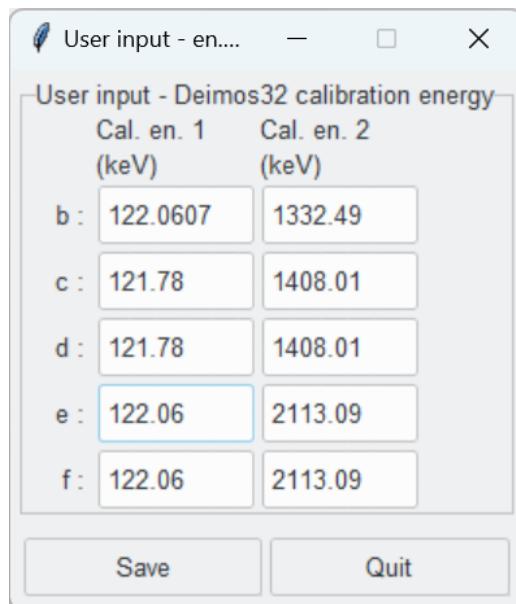


Figure 10: User input - detector calibration energies

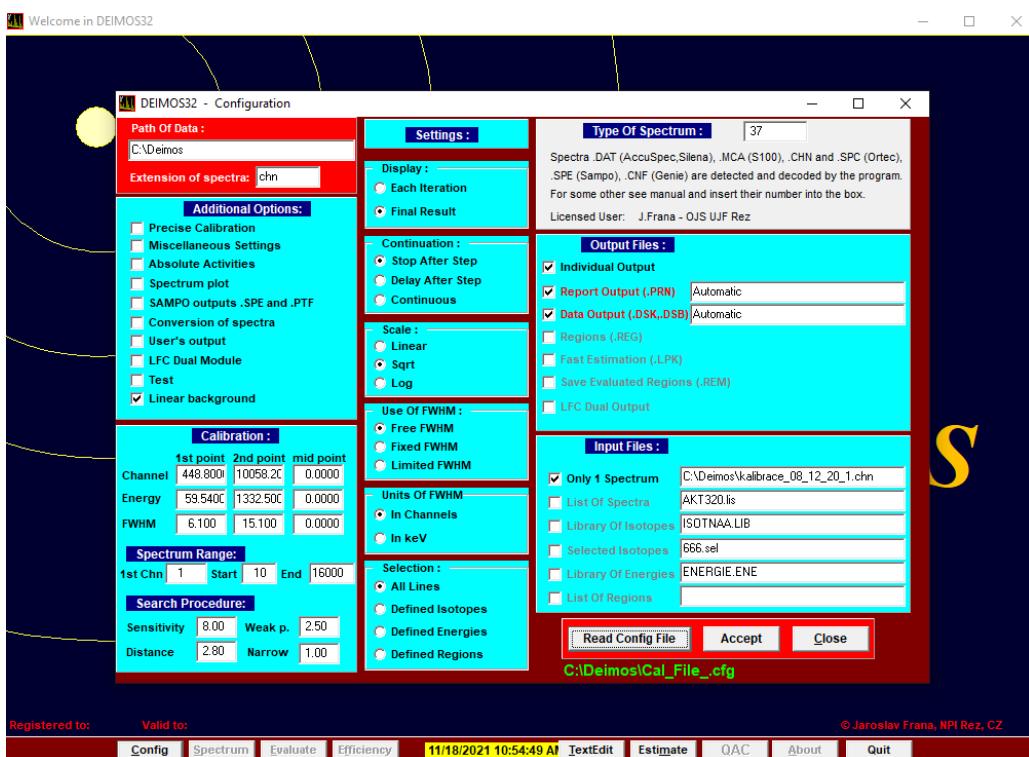


Figure 11: The Deimos32 configuration window

2.4 Main window menu - Library

The data necessary for calculating each correction are loaded from libraries stored in the ‘libraries’ folder, which is created alongside the main file. The **Libraries** menu (Fig. 12) allows the user to load custom libraries. The format of each library is described below. For all libraries, comments within the files are marked with a double hash symbol at the beginning of the line. The preferred file extension for libraries is ‘.lib’, and the recommended encoding is **UTF-8**.

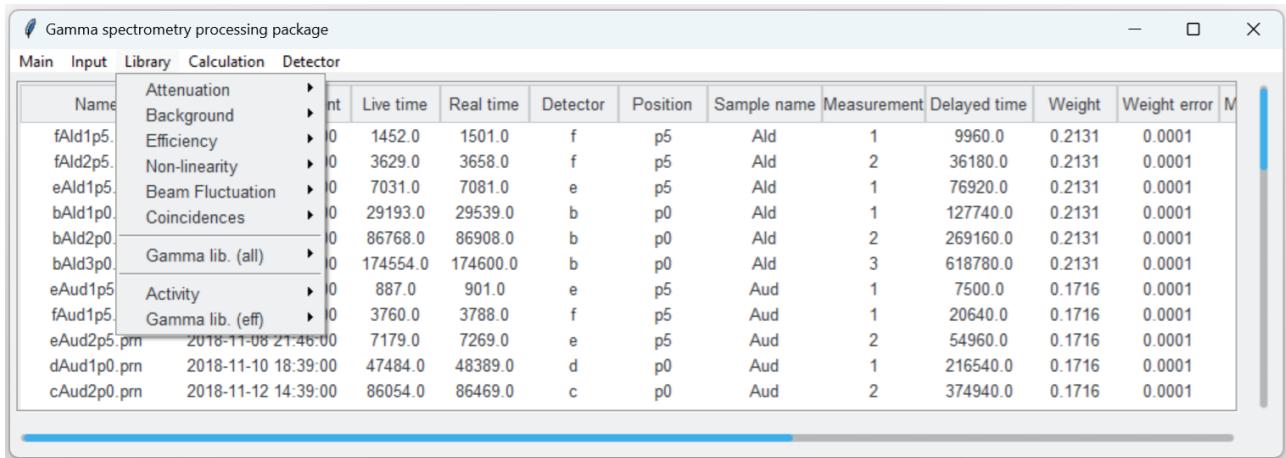


Figure 12: User Main window menu - Library selection

The program contains paths to default libraries stored in the **libraries** folder. Users can either create their own libraries, which can be uploaded during program run, or modify the default libraries. Below is a list of basic libraries with a brief description. The structure of each file is further detailed below. Library selection is made by hovering the mouse over the **Libraries** menu, where each type of library will be displayed. When hovering over each library option, the selected file and a button for uploading a new file appear. Some libraries contain internal menus, such as **Background** or **Coincidences**, with their number depending on the parameters of the loaded spectra².

- **Attenuation** - att.lib - this file contains information on the mass attenuation coefficient ($\text{m}^2 \cdot \text{kg}^{-1}$) and material density for various chemical elements. The library does not contain data for all elements of the periodic table. If data are missing or if the material density needs to be adjusted, they can be added by modifying the library.
- **Background** - library files names are single letters representing each detector. The original .prn extension has to be replaced with .bcg and the name changed to single letter detector designator (e.g. a.bcg).
- **Efficiency** - eff.lib - contains the parameters of functions used to fit the measurement data and evaluate the detector’s peak efficiency. Each detector and its measurement positions have unique values for these parameters.
- **Nonlinearity** - nonlin.lib - similar to the previous library, it contains parameters of functions that describe the deviations of the detectors used from a linear channel-energy relationship.

²Each detector used for spectrum measurements has its own file for true coincidence corrections and also requires its own file for background correction.

- **Beam Fluctuation** - `beam.lib` - an optional library containing information on irradiation progress (timestamp and beam power³).
- **Coincidences** - `Xname.clip` - provides information on true cascade coincidence corrections for individual detectors, measurement positions, and radionuclides. This correction must be calculated, for instance, using the TrueCinc program, based on knowledge of the detector's peak and total efficiency. The X is a detector designator and must be modified to agree with spectra's detectors.
- **Gamma Intensity (all)** - `gamma_all.llb` - serves as a database of gamma transitions, their intensities, and radionuclide half-lives.
- **Gamma Intensity (ref)** - `gamma_eff.llb` - similar to *Gamma Intensity (all)*, but contains only information on radionuclides used as calibration sources for determining detector efficiency or energy calibration.
- **Activity** - `activity.lib` - contains information on individual calibration sources, such as the reference date, reference activity, identifier, and radionuclide label, in the form of chemical symbol and nucleon number.

2.4.1 Attenuation (self-absorption)

The `att.lib` library is used to calculate the self-absorption correction, and its change is possible by selecting **Attenuation**. The library structure is illustrated in Fig. 13.

```

92UC 1 19.043 density[g/cm^3] 0.1156 dividing energy[MeV]
92U 2.17574E-02 9.222E+01
92U 3.00000E-02 4.128E+01
92U 4.00000E-02 1.983E+01
92U 5.00000E-02 1.121E+01
92U 6.00000E-02 7.035E+00
92U 8.00000E-02 3.395E+00
92U 1.00000E-01 1.954E+00
92U 1.15590E-01 1.378E+00
92U 1.15610E-01 4.893E+00
92U 1.50000E-01 2.591E+00
92U 2.00000E-01 1.298E+00
92U 3.00000E-01 5.192E-01
92U 4.00000E-01 2.922E-01
92U 5.00000E-01 1.976E-01
92U 6.00000E-01 1.490E-01
92U 8.00000E-01 1.016E-01
92U 1.00000E+00 7.896E-02
92U 1.25000E+00 6.370E-02
92U 1.50000E+00 5.587E-02
92U 2.00000E+00 4.878E-02
92U 2.50000E+00 4.628E-02
92U 3.00000E+00 4.447E-02
#####
90ThC 1 11.724 density[g/cm^3] 0.109605 dividing energy[MeV]
90Th 2.04721E-02 1.018E+02
90Th 3.00000E-02 3.892E+01

```

Figure 13: Library format for self-absorption correction calculation

The library includes data for individual elements that make up the sample material. Each record is separated by a line with a double hash symbol. The first data line for each element contains the element's name, composed of its atomic number and chemical symbol, followed by

³This can be provided as a relative or absolute value.

the letter C⁴. Next, it specifies whether the data in the library should be fitted with a single curve (0) or two curves (1). The fit is used to interpolate the value for the energies of peaks from the spectra⁵.

Following this is the material density in g/cm³ and the dividing energy in MeV (for single-curve fitting, the dividing energy is 0). Subsequent lines contain individual points of the μ/ρ function, which describe the attenuation of radiation intensity as it passes through the material. Each line provides the element name, energy in MeV, and the function value for this energy in cm²/g.

2.4.2 Background (background subtraction)

The `Background.fon` library was removed and its use is deprecated. The latest version works with background `.prn`, respectively `.bcg` spectrum files. The main advantage is no need of creating `.fon` file.

In principle, these are same files as regular `.prn` spectra. They are processed for non-lin and SEP/DEP corrections before their use for background correction.

All **background files** have to be stored in **work directory** together with other input spectra or they could be added manually through **Library** menu. The automated loading works only if the naming convention agrees (e.g. `b.bcg`).

2.4.3 Efficiency (detector efficiency)

Data for calculating the detector efficiency correction are contained in the `eff.lib` library, which can be modified by selecting **Efficiency**. The format of the library is shown in Fig. 14.

a	p9	210 keV	dubna	# Dubna detA		
7.038140887		-0.814772477	0.150901906		-0.138006147	
7.0480264165		-0.8634397265	0.0201645344	-0.1488655673	-0.0727182154	
a	p11	0 keV	dubna	# Dubna detA		
6.2795640479		-0.8318314844	0.0686881751	-0.1505625703	-0.1270915965	
b	p0	0 keV	keV	# Brno		
-640.377		509.867	-161.535	25.4162	-1.99059	

Figure 14: Library format for detector efficiency correction

The library contains data for each detector and each position where measurements were taken. The first line includes the detector designation, the measurement position label, the cutoff energy in keV, and information about the method used to derive the coefficients for the fitting functions. Currently, three methods are available for calculating efficiency or performing the fit.

- **keV** - The function describing efficiency was fitted for energies in **keV**. The function used for fitting is $\varepsilon_{FEP}(E_\gamma) = e^{\sum_{i=0}^n a_i \ln^i(E_\gamma)}$ (keV).

⁴This format is derived from an older non-GUI software that used this format. For compatibility purposes, it has not been modified.

⁵Values of the linear or mass attenuation coefficient are not continuous due to the electron shell structure and the nature of absorption of indirectly ionizing radiation such as X-rays and gamma rays.

- **MeV** - The function describing efficiency was fitted for energies in MeV. The function used for fitting is $\varepsilon_{FEP}(E_\gamma) = e^{\sum_{i=0}^n a_i \ln^i(E_\gamma)}$ (MeV).
- **dubna** - The efficiency function was fitted using the method employed by the research group at JINR in Dubna. The function used for fitting is $\varepsilon_{FEP}(E_\gamma) = e^{\sum_{i=0}^n a_i \ln^i(E_\gamma/1000)} \cdot 10^{-6}$ (keV).

Depending on whether the function fit uses one or two curves, one or two lines follow, each containing the polynomial coefficients from the exponent of the corresponding function. The maximum polynomial degree is theoretically unlimited, but in practice, polynomials up to the 8th degree are considered. Individual entries are separated by blank lines.

2.4.4 Non-linearity (detector non-linearity)

Data for calculating the detector nonlinearity correction are contained in the `nonlin.lib` library, which can be modified by selecting **Nonlinearity**. The library format is shown in Fig. 15.

The format is similar to that of the detector efficiency library. For each detector, the first line contains the detector identifier, followed by the cutoff energy in keV. Depending on whether the data are fitted with one or two curves, one or two lines of function coefficients follow. Individual entries are separated by a blank line.

```

a      350 keV      # Dubna detA
-9.27129300e-2  1.98558000e-3  -2.77439582e-6
1.99080790e-1  2.23723895e-4  -1.04598745e-7

b      2505 keV     # Brno
-0.00709756    0.00147105   -6.41296e-07
0.992073       0.0984365   -3.95087e-05

c      160 keV      # Vyskov Canberra
-2.95441        0.035025    -8.69507e-05
0.369525        0.000561377  -6.13674e-07

```

Figure 15: Library format for calculating detector nonlinearity correction

If it is necessary to evaluate nonlinearity for additional detectors, a dependence of the deviations between the measured and theoretical peak energies on the measured energy must be constructed. This should be followed by fitting the data with one or two quadratic functions, where the values input into the fit are in keV.

2.4.5 Beam fluctuation (particle beam intensity fluctuation)

Information for calculating the correction for particle beam intensity fluctuations, which affect the irradiated samples, is stored in the `beam.lib` file, which can be modified by selecting the **Beam Fluctuation** option. The file consists of three columns—date, time, and the particle count in the beam at the respective time—expressed in either absolute or relative values (see Fig. 16). The beam intensity fluctuation correction is applied during the determination of production or reaction rates, as one of the calculation inputs is the half-life, which cannot be determined until the evaluated radionuclide is known.

25.05.2018	15:20:06	0.56
25.05.2018	15:20:22	1.16
25.05.2018	15:20:39	1.85
25.05.2018	15:20:55	2.98
25.05.2018	15:21:12	3.06
25.05.2018	15:21:28	3.04
25.05.2018	15:21:45	2.96
25.05.2018	15:22:01	3.03
25.05.2018	15:22:18	3.03
25.05.2018	15:22:34	3.00
25.05.2018	15:22:51	2.99
25.05.2018	15:23:10	2.99
25.05.2018	15:23:26	2.98

Figure 16: Library format for calculating beam fluctuation correction

2.4.6 Coincidences (true cascade coincidences)

Library files are not automatically uploaded when the program starts and must be added manually through the **Library** menu. The program ensures that there is an entry for each detector used in the uploaded spectra.

The data required for calculating corrections for true cascade coincidences are divided into multiple files, each named **Xname.clib**, where X represents the detector identifier. In the **Coincidences** menu, an entry is created for each detector used in the measured spectra.

The library files contain information for the transition energies of individual isotopes, organized line by line (see Fig. 17). Each line includes the isotope identifier, energy, and coincidence correction values for specific positions. Corrections for true cascade coincidences must be applied whenever measurements are performed in close measurement geometries. It is also critical to determine these corrections for each specific peak efficiency or detector setting.

# Isotope	Energy	P2	P3	P4	P5	P6	P7	P8
100Rh	446.153	0.811	0.867	0.891	0.917	1.000	1.000	1.000
100Rh	539.512	0.878	0.918	0.932	0.948	1.000	1.000	1.000
100Rh	822.654	0.823	0.877	0.899	0.923	1.000	1.000	1.000
100Rh	1107.223	0.839	0.889	0.908	0.930	1.000	1.000	1.000
100Rh	1362.152	0.926	0.954	0.959	0.969	1.000	1.000	1.000
100Rh	1553.348	0.868	0.911	0.925	0.944	1.000	1.000	1.000
100Rh	1929.811	0.882	0.922	0.934	0.950	1.000	1.000	1.000
100Rh	2375.976	0.895	0.932	0.942	0.957	1.000	1.000	1.000
103Ru	497.080	1.000	1.000	1.000	1.000	1.000	1.000	1.000
105Rh	306.250	1.000	1.000	1.000	1.000	1.000	1.000	1.000
105Rh	319.140	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Figure 17: Library format for calculating coincidence correction

2.4.7 Gamma lib (all)

The **gamma_all.lib** library is used for calculating production or reaction rates, and it can be modified by selecting **Gamma Intensity (all)**. Each row contains the energy of the γ transition, the absolute uncertainty of this energy, the intensity, the absolute uncertainty of the gamma transition intensity, the isotope label, the half-life, and the absolute uncertainty of the half-life, followed by the time unit (see Fig. 18).

In isotope names, various additional symbols may appear. For instance, the letter **m** or **m2**, etc., indicates an isomer (a metastable state) of the given isotope, and this symbol is placed after the nucleon number. Another example is the letter **D**, which is appended to the standard chemical element symbol, e.g., **130LaD**. This symbol is used when ^{130}La is part of a decay chain where the parent isotope, which decays to ^{130}La , has a significantly longer half-life than ^{130}La . In such cases, the decay curve for ^{130}La is primarily determined by the longer half-life of the parent radionuclide.

The library **gamma_lib_ref.lib** follows the same format but contains data only for reference sources. This library can be modified by selecting **Gamma Intensity (ref)**.

250.332	0.001	0.4630000	0.0160000	39C1	T1/2 =	55.600	0.200	m
1517.508	0.001	0.3920000	0.0090000	39C1	T1/2 =	55.600	0.200	m
372.760	0.001	0.8700000	0.0100000	43K	T1/2 =	22.300	0.100	h
617.490	0.001	0.7920000	0.0060000	43K	T1/2 =	22.300	0.100	h
396.861	0.001	0.1185000	0.0008000	43K	T1/2 =	22.300	0.100	h
593.390	0.001	0.1126000	0.0008000	43K	T1/2 =	22.300	0.100	h
220.631	0.001	0.0480000	0.0006000	43K	T1/2 =	22.300	0.100	h
271.130	0.010	0.8670000	0.0030000	44mSc	T1/2 =	58.600	0.100	h

Figure 18: Format of the γ line energy library

2.4.8 Activity

The **activity.lib** library contains information about reference sources. This library can be modified by selecting **Activity**.

Each row contains information about one reference source, in the format shown in Fig. 19. The first entry is the isotope label, consisting of the nucleon number and chemical symbol. This is followed by an identification number, reference date, reference activity in Bq, and the uncertainty of the reference activity in %.

44Ti	5651	23-01-2017	108000	10
44Ti	6844	01-05-2013	11500	5
<hr/>				
55Fe	5884	23-01-2017	150500	10
55Fe	6844	01-05-2013	22700	5
<hr/>				
54Mn	5199	23-01-2017	116800	10
54Mn	6844	01-05-2013	40400	5

Figure 19: Format of the reference source activity library

2.4.9 Gamma lib. (eff.)

The **gamma_eff.llb** library has same structure as **gamma_all.llb**, but content of the file is focused on FEP efficiency evaluation. This means the radionuclides should correspond with information in **activity.lib**.

2.5 Main window menu - Calculation

The most important option from the top menu bar is **Calculation** with two sub options, shown in Fig. 21. The first option controls corrections calculation. Program opens a new window where user may select which corrections are calculated. The list of options is shown in Fig. 21. The second option opens window for final results evaluation.

Name	Corrections Calculation	Start	Live time	Real time	Detector	Position	Sample name	Measurement	Delayed time	Weight	Weight error	M
fAld1p5.prm	2018-11-08 09:16:00	1452.0	1501.0	f	p5	Ald	1	9960.0	0.2131	0.0001		
fAld2p5.prm	2018-11-08 16:33:00	3629.0	3658.0	f	p5	Ald	2	36180.0	0.2131	0.0001		
eAld1p5.prm	2018-11-09 03:52:00	7031.0	7081.0	e	p5	Ald	1	76920.0	0.2131	0.0001		
bAld1p0.prm	2018-11-09 17:59:00	29193.0	29539.0	b	p0	Ald	1	127740.0	0.2131	0.0001		
bAld2p0.prm	2018-11-11 09:16:00	86768.0	86908.0	b	p0	Ald	2	269160.0	0.2131	0.0001		
bAld3p0.prm	2018-11-15 10:23:00	174554.0	174600.0	b	p0	Ald	3	618780.0	0.2131	0.0001		
eAud1p5.prm	2018-11-08 08:35:00	887.0	901.0	e	p5	Aud	1	7500.0	0.1716	0.0001		
fAud1p5.prm	2018-11-08 12:14:00	3760.0	3788.0	f	p5	Aud	1	20640.0	0.1716	0.0001		
eAud2p5.prm	2018-11-08 21:46:00	7179.0	7269.0	e	p5	Aud	2	54960.0	0.1716	0.0001		
dAud1p0.prm	2018-11-10 18:39:00	47484.0	48389.0	d	p0	Aud	1	216540.0	0.1716	0.0001		
cAud2p0.prm	2018-11-12 14:39:00	86054.0	86469.0	c	p0	Aud	2	374940.0	0.1716	0.0001		

Figure 20: Main window - Calculation menu

A brief description of each correction:

- *Nonlinearity* recalculates the energy of individual peaks based on correction functions. This function is recommended, as the nonlinearity of some detection systems can range from a few keV to tens of keV in different parts of the spectrum. Incorrect energy determination can lead to inaccurate PR and RR evaluations.
- *Background* correction requires a processed spectrum file from the **Deimos32** program from the detector used in the sample-free measurement. The program automatically identifies which peaks need correction and calculates the necessary correction based on the measurement time.
- *Escape peaks* correction enables determination of contributions from escape peaks for peaks with energies above 1024 keV and subtracts them from peaks in spectra with which they may have interacted.
- *Attenuation* correction is primarily applied to samples with significant thickness and when measuring lower energies. For proper execution, library data on linear attenuation coefficients for the selected elements and the evaluated energy range are required.
- *Efficiency* is one of the most important corrections and must be applied to calculate PR or RR. This correction requires that parameters for all detectors and measurement positions used during the measurement are available in the libraries.
- *Non-point source* is an additional correction that considers the non-point nature of the measured sample. The program itself cannot calculate this correction value, but it can be obtained using Monte Carlo-based codes if the exact dimensions of the detector are known to create its model.

The respective correction calculations are performed by clicking the **Calculate** button in the bottom part of the window. If the corrections calculation finishes successfully then the program ask user to open **Calculation** option from menu.

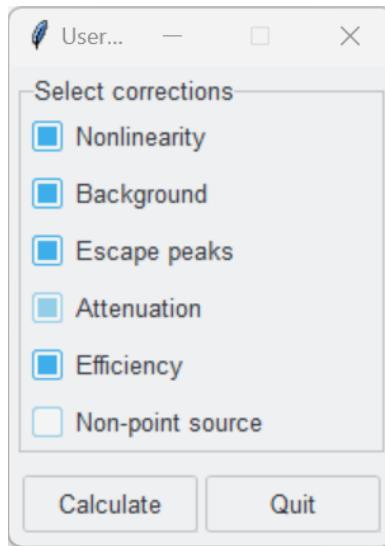


Figure 21: Spectrometric corrections calculation window

The resulting corrections can be viewed for each spectrum using the **Open selection** function mentioned above or by double-clicking on any spectrum. All corrected data are added into new columns.

2.5.1 Determinations of final results

After completing all mandatory steps, the user can proceed with calculating the final values. The control window, shown in Fig. 22, is divided into three sections: a results table, a graph displaying the decay function, and a control panel at the bottom.

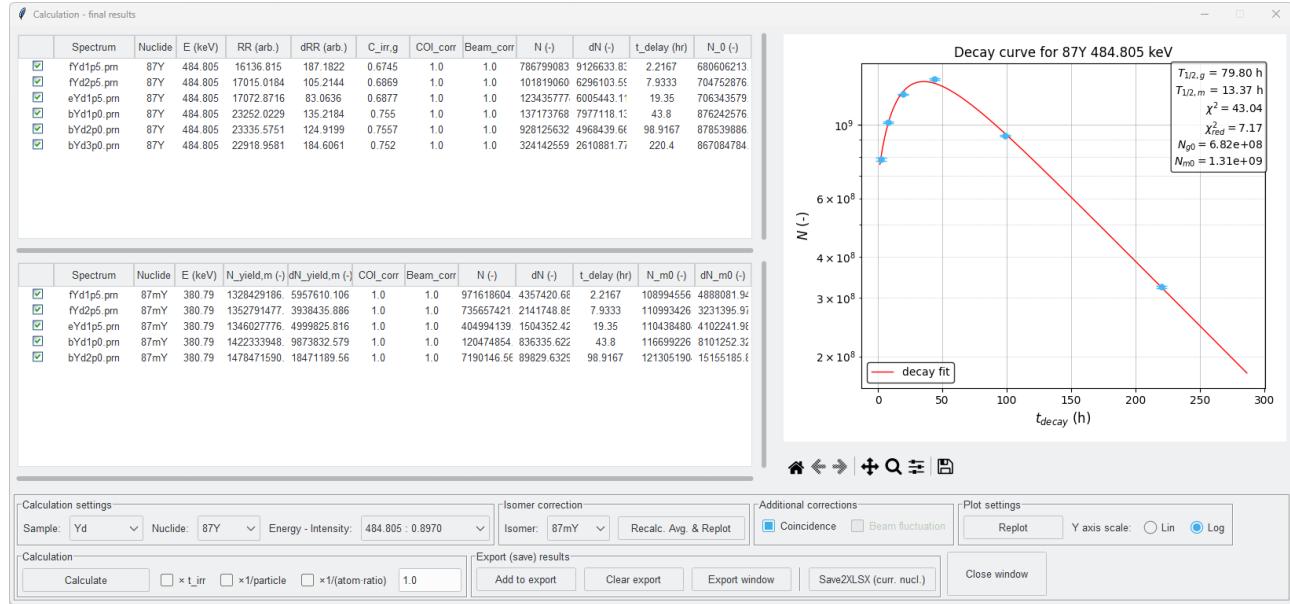


Figure 22: Calculation window during the evaluation process.

To perform the calculation, the user must select a specific sample from the list of all samples in the **Work directory**. Subsequently, the radionuclide and a single gamma line must be specified using the corresponding option menu. By clicking the **Calculate** button, the program processes all files and searches for the selected value. Even with non-linearity correction, small

residuals may remain between the library and the measured values. To address this, the search process applies conditions to ensure accurate identification of the correct peaks. More information might be found in the Sec. 3.2.

If the program fails to locate the peaks correctly (e.g., too many peaks are missed or incorrectly added), the rules can be adjusted by modifying coefficients in the `settings.py` file. Unfortunately, this option is currently available only for the uncompiled version of the program⁶.

The final dimension of the calculated values:

The resulting dimensions depend on the user-selected normalizations, which are available next to the **Calculate** button. By default, the output is the **production rate** (s^{-1}) if all normalization checkboxes are **unchecked**. If the irradiation time is applied, the result corresponds to the yield, where $[N_{yield}] = (-)$. Other normalization options include calculations per one atom of the sample or per one incident particle. Additionally, the user can refine the normalization per atom by selecting only a portion of the total atoms in the sample through the entry widget next to this option. This feature is particularly useful for samples containing multiple elements or isotopes of the same element. Finally, the result can also be recalculated to account for the total irradiation time.

Additional spectrometric corrections:

The control panel also includes two additional spectrometric corrections for **beam fluctuations** during irradiation and **true cascade coincidences**. These corrections depend on the selected radionuclide, specifically its half-life, and must be calculated individually for each radionuclide. They are applied during the evaluation process. Both corrections are available only if the corresponding libraries are uploaded.

Two step decay correction (Isomer correction): A specific type of correction is the **Isomer** option. This feature allows the user to select a radionuclide in an excited state, whose decay contributes to the activity increase of the primary selected radionuclide in its ground state, e.g. ^{76m}Y and ^{76}Y . Obviously, it doesn't work for different radionuclides.

The approach of this correction is different from regular evaluation. User has to set properly all three option menus in **Calculation settings**. Specifically, the first nuclide must be the daughter product of the isomer decay selected in the **Isomer correction** menu. If all prerequisites are met, the evaluation process proceeds in two steps:

1. Unlike standard calculations, the program does not search for a single energy value but instead attempts to locate all gamma lines from the **Gamma Library**. The normalization options do not affect the results, which are strictly represented as $N_{yield,m}$ (yield of the selected reaction). Additionally, N_{m0} denotes the number of activated nuclei in the sample at the end of irradiation. These results are displayed in the **bottom** treeview. The program calculates a weighted average of the aforementioned values, either from all detected results or from a subset manually selected by the user. The user can change the basis for the calculation by selecting values from the treeview. The results are updated after clicking the **Recalc. Avg. & Replot** button and are stored in the appropriate variable for future use. The average values are shown in the message window after each recalculation and are also displayed in the plot within a small text box in the top-right corner.

⁶In future updates, some settings will be moved from the code into `.json` files, which is the current standard for configuration options.

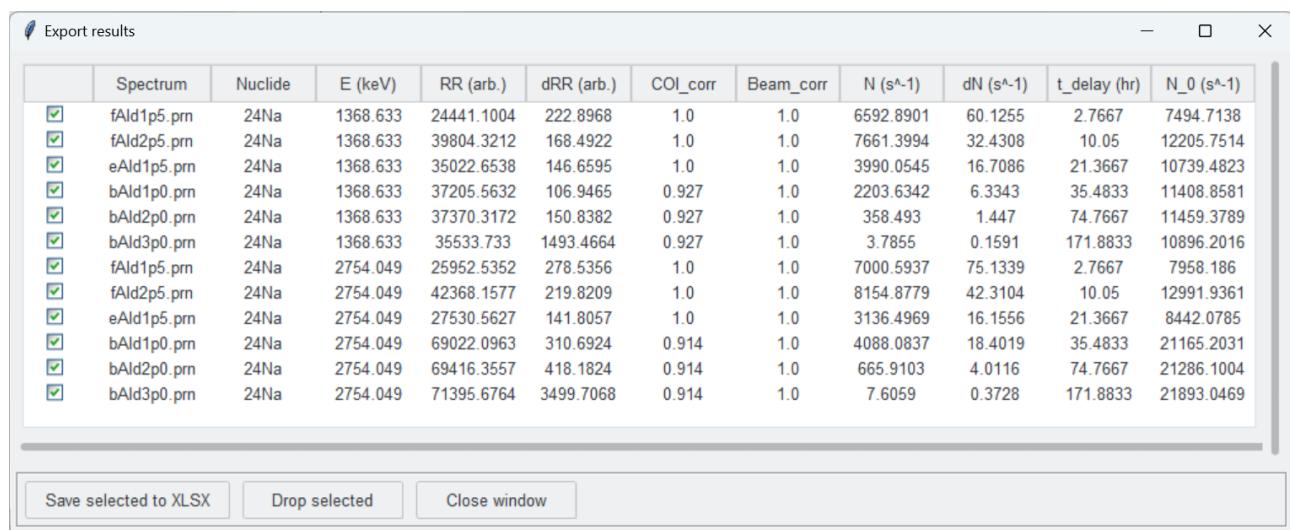
2. The evaluation can only proceed with the correction calculation if the average results from the first step are prepared and an isomeric nuclide is selected. The user needs to press the **Calculate** button for the second time while the bottom treeview remains populated. The program will then calculate the ground state values of the selected radionuclide. The resulting values are displayed in the **top** treeview. Unlike in the first step, the final results for a single energy are calculated using the average values obtained in the first step. At the end of this step, all selected normalizations are applied to the results.

Determination of Decay Curve:

The decay curve is a key method for verifying the accuracy of the calculated values. The program fits the number of nuclei normalized to the beginning of each measurement, N . For a simple calculation, the graph displays a comparison between the reference half-life value, $T_{1/2,\text{tab}}$, and the half-life value obtained from the fit, $T_{1/2,\text{fit}}$. Using the number of nuclei at the end of irradiation, N_0 , and the reference half-life, theoretical values at the beginning of each measurement, N_{teor} , are calculated. These values represent the idealized course of the decay curve.

In addition, the program calculates χ^2 and χ^2_{red} values to evaluate the goodness of fit and the agreement between the experimental data and the theoretical decay curve. These metrics are displayed directly on the plot, along with additional details presented in a text box.

Users can refine the fit by modifying the selection of data points included in the calculation. This is done via checkboxes at the beginning of each row in the results table's treeview. After adjusting the selection, clicking the **Replot** button recalculates the fit and updates the graph accordingly. Each time the graph is updated, it is automatically saved in the **work directory/output** folder. The filename includes a timestamp and metadata about the calculation, such as the sample, radionuclide, and energy.



The screenshot shows a window titled "Export results". Inside, there is a table with 16 rows of data. The columns are labeled: Spectrum, Nuclide, E (keV), RR (arb.), dRR (arb.), COI_corr, Beam_corr, N (s^-1), dN (s^-1), t_delay (hr), and N_0 (s^-1). Each row contains a checkbox in the first column followed by the corresponding values for each parameter. At the bottom of the window, there are three buttons: "Save selected to XLSX", "Drop selected", and "Close window".

	Spectrum	Nuclide	E (keV)	RR (arb.)	dRR (arb.)	COI_corr	Beam_corr	N (s^-1)	dN (s^-1)	t_delay (hr)	N_0 (s^-1)
<input checked="" type="checkbox"/>	fAld1p5.prm	24Na	1368.633	24441.1004	222.8968	1.0	1.0	6592.8901	60.1255	2.7667	7494.7138
<input checked="" type="checkbox"/>	fAld2p5.prm	24Na	1368.633	39804.3212	168.4922	1.0	1.0	7661.3994	32.4308	10.05	12205.7514
<input checked="" type="checkbox"/>	eAld1p5.prm	24Na	1368.633	35022.6538	146.6595	1.0	1.0	3990.0545	16.7086	21.3667	10739.4823
<input checked="" type="checkbox"/>	bAld1p0.prm	24Na	1368.633	37205.5632	106.9465	0.927	1.0	2203.6342	6.3343	35.4833	11408.8581
<input checked="" type="checkbox"/>	bAld2p0.prm	24Na	1368.633	37370.3172	150.8382	0.927	1.0	358.493	1.447	74.7667	11459.3789
<input checked="" type="checkbox"/>	bAld3p0.prm	24Na	1368.633	35533.733	1493.4664	0.927	1.0	3.7855	0.1591	171.8833	10896.2016
<input checked="" type="checkbox"/>	fAld1p5.prm	24Na	2754.049	25952.5352	278.5356	1.0	1.0	7000.5937	75.1339	2.7667	7958.186
<input checked="" type="checkbox"/>	fAld2p5.prm	24Na	2754.049	42368.1577	219.8209	1.0	1.0	8154.8779	42.3104	10.05	12991.9361
<input checked="" type="checkbox"/>	eAld1p5.prm	24Na	2754.049	27530.5627	141.8057	1.0	1.0	3136.4969	16.1556	21.3667	8442.0785
<input checked="" type="checkbox"/>	bAld1p0.prm	24Na	2754.049	69022.0963	310.6924	0.914	1.0	4088.0837	18.4019	35.4833	21165.2031
<input checked="" type="checkbox"/>	bAld2p0.prm	24Na	2754.049	69416.3557	418.1824	0.914	1.0	665.9103	4.0116	74.7667	21286.1004
<input checked="" type="checkbox"/>	bAld3p0.prm	24Na	2754.049	71395.6764	3499.7068	0.914	1.0	7.6059	0.3728	171.8833	21893.0469

Figure 23: Export results window with values for two gamma lines of a single radionuclide.

Final export: The program offers two options for exporting results. The user can save the current selection from the results table by clicking the **Save2XLSX (curr. nucl.)** button. Alternatively, the user can add the current selection to the database of final results by clicking the **Export window** button (see Fig. 23). The database content can be further modified as

needed.

When the **Save selected to XLSX** button is pressed, the current selection is exported to a **.xlsx** file. Simultaneously, the program calculates a weighted average for each group of measurements with the same energy and radionuclide. Finally, a weighted average is computed from these previously calculated values.

2.6 Main Window Menu - Detector (Additional Tools)

In addition to the functions described above, the program allows users to determine the detector's peak efficiency, assess detector nonlinearity, and automate true coincidence correction using the **TrueCinc** program [2].

Name	Start of mea	FEP efficiency	me	Detector	Position	Sample name	Measurement	Delayed time	Weight	Weight error	M
Non-linearity											
Coincidence (Truecoinc)											
fAld1p5.prm	2018-11-08 16:33:00	3629.0	3658.0	f	p5	Ald	1	9960.0	0.2131	0.0001	
fAld2p5.prm	2018-11-08 16:33:00	7081.0	7081.0	f	p5	Ald	2	36180.0	0.2131	0.0001	
eAld1p5.prm	2018-11-09 03:52:00	7031.0	29539.0	e	p5	Ald	1	76920.0	0.2131	0.0001	
bAld1p0.prm	2018-11-09 17:59:00	29193.0	29539.0	b	p0	Ald	1	127740.0	0.2131	0.0001	
bAld2p0.prm	2018-11-11 09:16:00	86768.0	86908.0	b	p0	Ald	2	269160.0	0.2131	0.0001	
bAld3p0.prm	2018-11-15 10:23:00	174554.0	174600.0	b	p0	Ald	3	618780.0	0.2131	0.0001	
eAud1p5.prm	2018-11-08 08:35:00	887.0	901.0	e	p5	Aud	1	7500.0	0.1716	0.0001	
fAud1p5.prm	2018-11-08 12:14:00	3760.0	3788.0	f	p5	Aud	1	20640.0	0.1716	0.0001	
eAud2p5.prm	2018-11-08 21:46:00	7179.0	7269.0	e	p5	Aud	2	54960.0	0.1716	0.0001	
dAud1p0.prm	2018-11-10 18:39:00	47484.0	48389.0	d	p0	Aud	1	216540.0	0.1716	0.0001	
cAud2p0.prm	2018-11-12 14:39:00	86054.0	86469.0	c	p0	Aud	2	374940.0	0.1716	0.0001	

Figure 24: Main window - Detector menu.

To calculate the detector's efficiency or nonlinearity, it is first necessary to load a folder containing gamma spectra. This process is similar to regular spectra processing, with the difference that these files do not need to be corrected. As outlined in the first chapter, this can be done by selecting **Work directory** in the **Main** menu. The file names must follow a specified format:

a152Eu1111p1 or **a152Eu_1111_p1** (program removes all underscores), where:

- **a** is the detector label,
- **152Eu** is the radionuclide of the reference source,
- **1111** is the reference source identification label. This number distinguishes sources with different activities and reference dates. The ID number must be larger than 1000, and
- **p1** is the position during measurement.

2.6.1 Detector menu - FEP Efficiency

The determination of detector peak efficiency is available by selecting **Efficiency** in the **Detector** menu. The program opens a new window without any data (see Fig. 25). Before using this option, the user must upload spectra from the work directory in the **Main window**.

At the top of the window (Fig. 25), the user selects the detector and position for which the efficiency will be calculated. After clicking the **Calculate** button, the module computes efficiency values for each peak (energy) identified in the spectra.

The program requires additional libraries for successful evaluation. Specifically, users need to upload a gamma library containing efficiency calculation data for radionuclides used as reference sources. Another required library is the **Activity.lib** file, which contains the reference date and activity for a list of radionuclides with their identification numbers.

The resulting data is organized into a list (Fig. 26), where values can be selected using checkboxes. Additionally, the user can choose whether the data will be fitted with one or

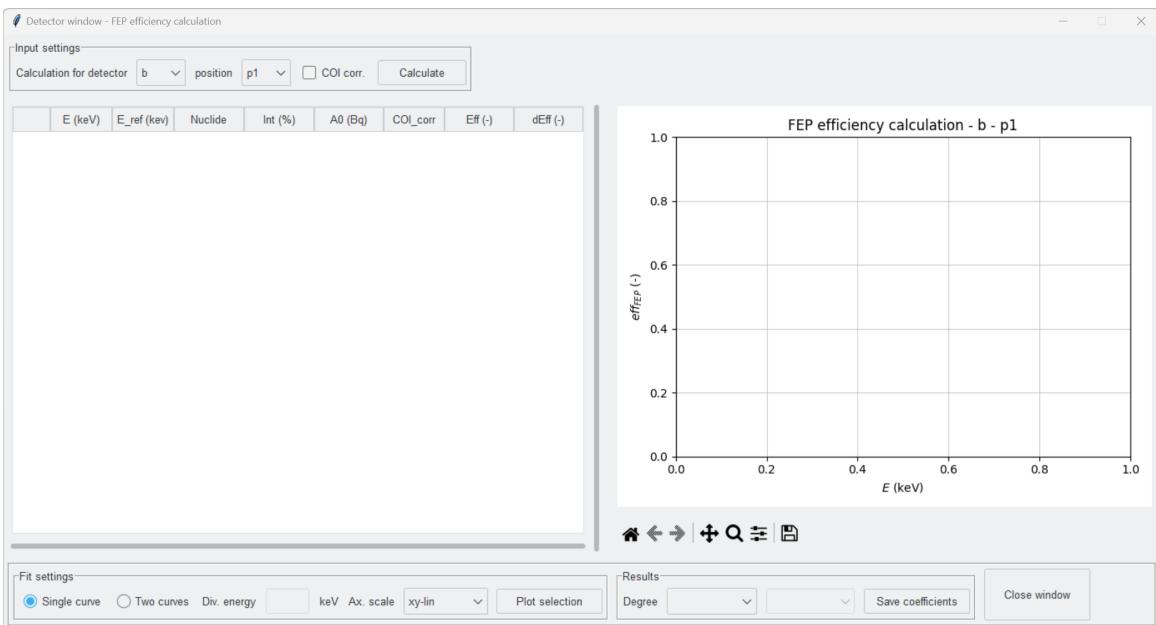


Figure 25: Efficiency preparation window - empty.

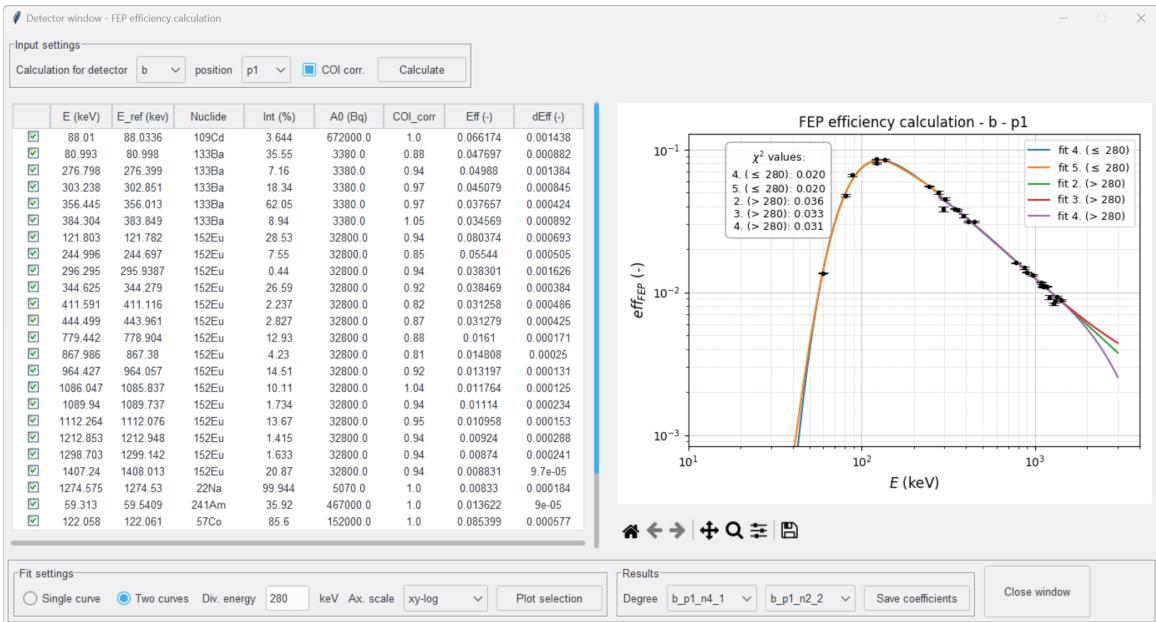


Figure 26: Efficiency preparation window - full, fit divided.

two curves. It can sometimes be challenging to achieve a good fit with a single curve. If two curves are selected, the dividing energy must also be specified. By selecting **Plot selection**, the dependency of the detector's peak efficiency on energy is plotted and displayed in linear, semi-logarithmic, and logarithmic formats. The measured data is fitted with curves described by the equation:

$$\varepsilon(E) = \exp \sum_{i=0}^n a_i \cdot \ln^i(E), \quad (1)$$

where $n = 2$ to 8 . For each function, the reduced chi-square χ^2_{red} is calculated. The button bar at the bottom of the window provides the same options for managing graph layouts as in the reaction rate calculation window.

The degree of the fit depends on whether a single or double curve option is chosen. In the current version of the code, users can change these values in `settings.py`.

The user selects the polynomial degree (or pair of degrees) that best fits the measured data. The chosen curve can be saved by clicking the **Save coefficients** button. The data is then added to the currently loaded `Efficiency.lib` library. If this file already contains efficiency data for the same detector and position, the program comments out the old values and appends the new coefficients beneath them. If the efficiency library does not exist, the program creates a new efficiency file containing the selected curves.

2.6.2 Detector menu - Non-linearity

The **Nonlinearity** option is used to calculate detector nonlinearity. The calculation window is shown in Fig. 27. The options in the window are similar to those for calculating peak efficiency, with some differences. When the new window opens, it is initially empty. The user selects the detector and position for which the calculation will be performed and presses the **Calculate** button. From the list of results, the user selects the values to include in the calculation (Fig. 28). Currently, the nonlinearity calculation is supported only for **efficiency spectra** and data from a **single position**, even though nonlinearity is geometry-independent⁷.

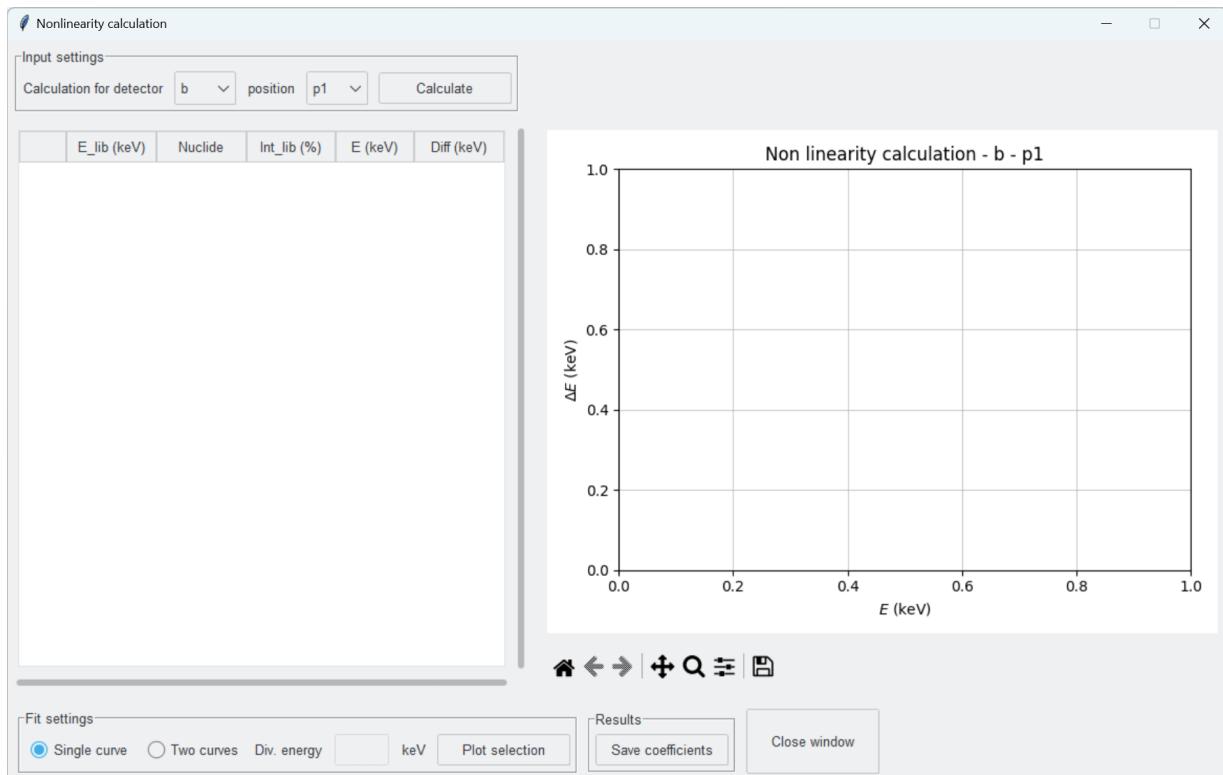


Figure 27: Nonlinearity preparation window - empty.

Additionally, the user can choose whether to fit the data with one or two curves. If two curves are selected, the **dividing energy** must be specified. The graph is plotted by clicking the **Plot selection** button. The coefficients of the fitted function can be saved by clicking the **Save coefficients** button. Unlike the **FEP Efficiency** results, these values are not saved in the primary nonlinearity library uploaded into the program. Instead, they are stored in a new file with the following naming convention: YYYY-MM-DD_HH-MM_nonlinearity.lib. This file is created in the **Work directory/output**.

The data is fitted using a **polynomial function of the second degree**. If the two-curve option is chosen, two second-degree polynomials are used. The program checks whether there are enough data points based on the specified dividing energy. This module doesn't work without **Gamma eff.** library.

⁷This will be improved in future versions to provide a broader solution with better error handling and statistical processing.

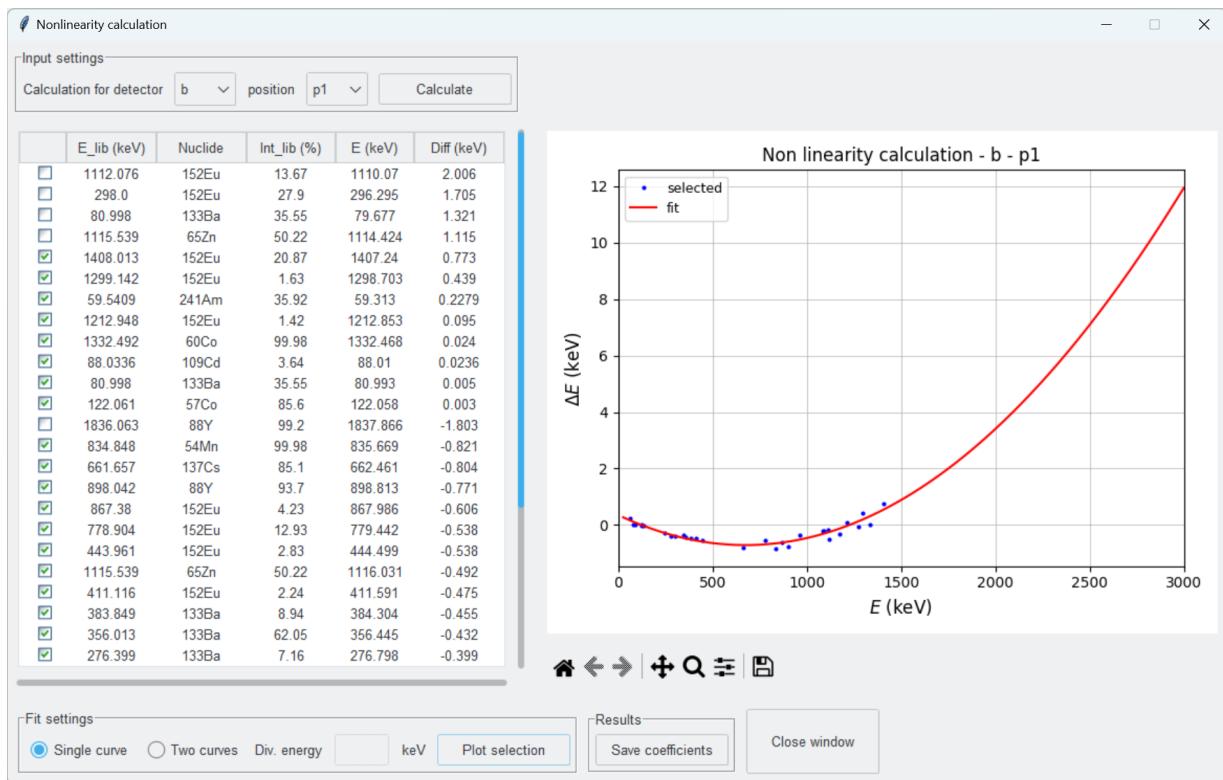


Figure 28: Nonlinearity preparation window - single fit.

2.6.3 Detector menu - Coincidence (TrueCoinc)

The **Coincidences** option is available only on the *MS Windows* operating system (developed and tested on Windows 11), as the **TrueCoinc** program does not support other platforms. The evaluation program verifies the operating system, and if the condition is not met, this option in the **Detector** menu is disabled. Furthermore, for the program to operate correctly, the **TrueCoinc** software [**sudar2002TrueCoinc**] must be installed, and the corresponding libraries must be organized in a specific folder structure (see the directory tree in Sec. 2.6.3). In particular, the folder names within the library must not be modified for the program to function properly.

Selecting **Coincidence (TrueCoinc)** in the **Detector** menu opens a new window, as shown in Fig. 29. The **TrueCoinc app** button allows the user to specify the path to the **TrueCoinc.exe** file, and the **TC folder** button allows the user to specify the path to the required library, which must contain the following three subfolders:

- **detector_efficiency**: Contains subfolders named after the detectors used for spectrum measurements (in uppercase). These subfolders store **.tcd** files, which include FEP and Total efficiency data for each position. File names follow a specific convention consisting of the detector and position labels (e.g., **A_P1.tcd** for detector A at position P1). These files must be created prior to running coincidence correction calculations.
- **endsf_data**: Contains the **pensdf2** directory with ENDSF datasets for each nuclide. These datasets are critical for coincidence calculations and are organized into subdirectories by mass number within the **pensdf2** folder. The data files are in the **.enx** format.
- **TrueCoinc_output**: Stores the output files generated by the **TrueCoinc** program. Results for each detector and position are saved in their corresponding directories.

After setting the paths, the user must specify the radionuclides for which corrections will

be prepared. A prerequisite for this step is a **Gamma Library** containing the necessary radionuclides. By clicking the **Get all nucl. from gamma lib.** button, the user can upload all radionuclides from the **Gamma Library** and modify the list (e.g., by adding or removing nuclides). The buttons on the right-hand side allow the user to clear the selection, such as by clicking **Delete all nucl..**

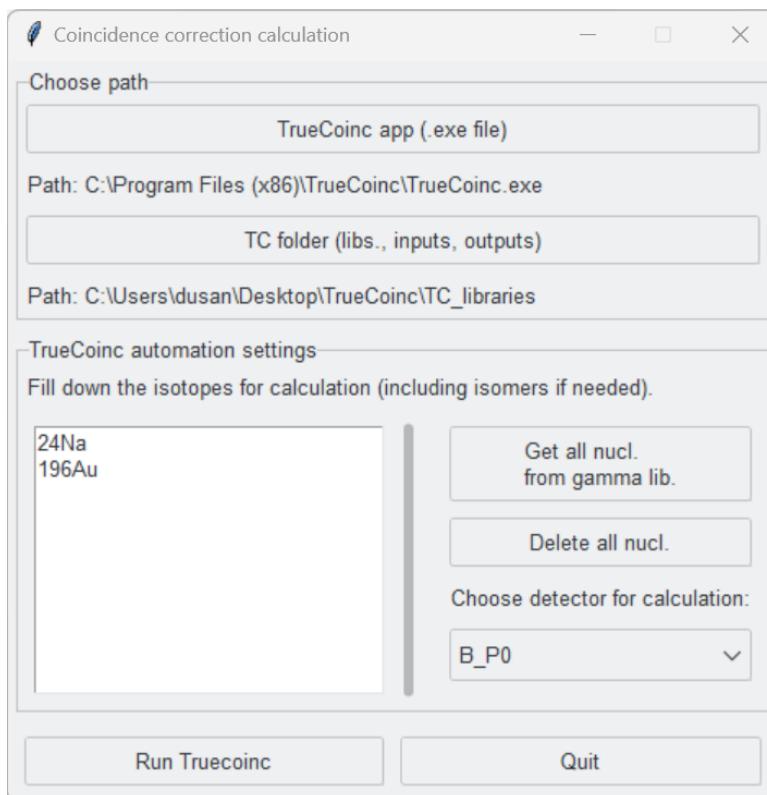


Figure 29: Coincidence preparation window - full view.

Based on the provided files, a list of available isotopes is generated, from which the user selects the radionuclides for which coincidence corrections will be calculated. It is highly recommended to prepare coincidence libraries iteratively rather than processing a large number of radionuclides in a single run, as the automation process may be interrupted, requiring a restart. Working incrementally ensures smoother operation and minimizes the risk of errors. The Fig. 30 shows how does look like the **TrueCoinc** in use.

Clicking the **Run TrueCoinc** button verifies that the necessary libraries and paths have been uploaded and warns the user not to use the computer during the automation process. After confirmation, the process begins. The program controls the **TrueCoinc** application via **pywinauto** and performs coincidence corrections for all radionuclides in the list.

The generated coincidence library file is saved in the **work directory/output** folder. The filename follows this format: `det_pos_YYYY-MM-DD_HH-MM_.clib`. The internal structure of this file is described in Sec. 2.4.6.

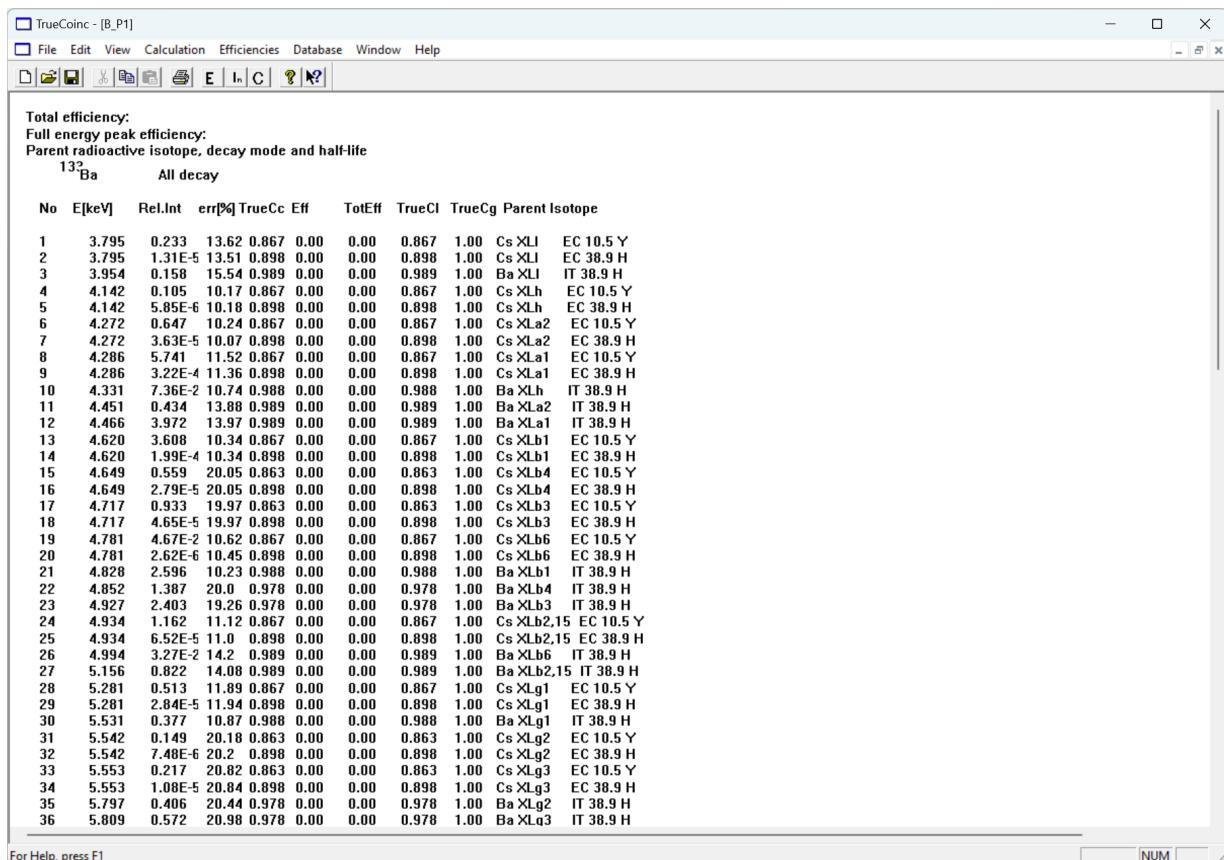
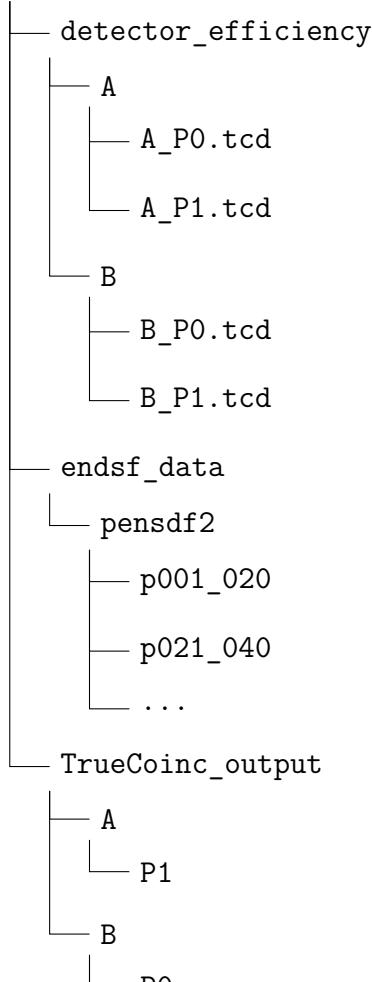


Figure 30: Coincidence preparation - TrueCoinc program window with calculated correction values

TrueCoinc Libraries File Structure

TC_libraries



3 Methodology description

This section provides a brief description of the gamma spectrometry corrections used in the software and other calculations, including the final results.

3.1 Gamma detector spectrometric corrections

The following describes the methodology of spectrometric corrections, including the necessary calibrations and corrections applied within this program.

3.1.1 Energy calibration and nonlinearity

Proper detector setup is crucial for the success of the experiment. If gamma spectra cannot be measured accurately after the activation phase, it may be necessary to repeat the measurement with a new set of samples, which is both time-consuming and expensive.

One of the fundamental calibrations involves setting the energy range and correctly assigning energy values to the measuring channels of the MCA (Multichannel Analyzer). This ensures that each recorded pulse is assigned the correct energy value. If necessary, this calibration can also be performed after the experiment, allowing for recalculation of data in the spectra.

While a linear channel-energy relationship is commonly used, it is often an approximation and not an exact representation of reality. The level of attention given to this issue depends on the user's requirements.

Linear fitting is generally applied in the detector control software. For calibration, it is standard to use gamma radiation sources with lines spanning the energy range. For example, ^{57}Co and ^{60}Co are often employed, though other sources with suitable lines may also be used.

3.1.2 Nonlinearity correction of used detectors

The evaluation package expects spectra processed by the **Deimos32** program as input. Simple linear calibration is not suitable for automated processing of complex spectra, where accurate energy determination is critical for identifying gamma lines from individual radionuclides. An example of nonlinearity curves is shown in Fig. 31, where the *x*-axis represents the energy range and the *y*-axis indicates the deviation from the linear energy-channel relationship.

The graph illustrates the nonlinearity fitted using two second-degree polynomials with a dividing point at 350 keV. The parameters of these curves, along with the dividing energy value, are stored in the library (see Chapter ??). Additional input includes the calibration energy values used in the **Deimos32** program. The correction itself is performed using the following polynomial:

$$\text{corF}(E_\gamma) = a_0 + a_1 E_\gamma + a_2 E_\gamma^2, \quad (2)$$

where a_i are the function parameters specific to each detector. The program calculates the deviation from the linear function used for detector calibration prior to the measurement. This requires knowing the calibration energy values $E_{\text{cal},1}$ and $E_{\text{cal},2}$, used in **Deimos32** for spectrum recalibration. The corrected energy is obtained from:

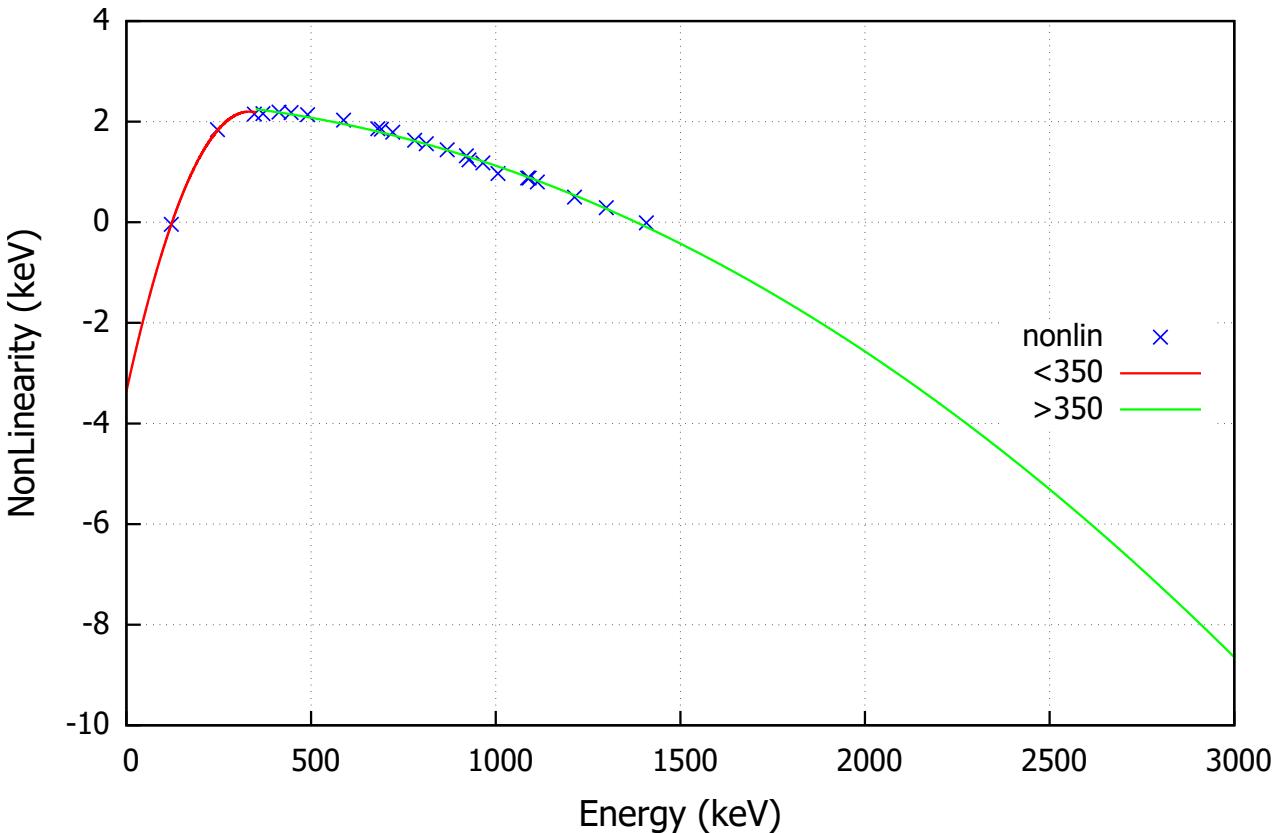


Figure 31: Nonlinearity of the Silena detector from UD.

$$E_{\gamma\text{cor}} = E_{\gamma} - [\text{corF}(E_{\gamma}) - (p_1 E_{\gamma} + q_1)], \quad (3)$$

where p_1 and q_1 are derived as follows:

$$p_1 = \frac{\text{corF}(E_{\text{cal},1}) - \text{corF}(E_{\text{cal},2})}{E_{\text{cal},1} - E_{\text{cal},2}}, \quad (4)$$

$$q_1 = \text{corF}(E_{\text{cal},1}) - E_{\text{cal},1} p_1. \quad (5)$$

3.1.3 Detector efficiency correction

This correction specifies the efficiency of gamma photon detection as a function of energy and the source's distance from the detector. Efficiency is defined as the probability that an incoming photon will deposit part of its energy within the detector's sensitive volume. It can be divided into two types: peak FEP efficiency and total efficiency.

The peak efficiency $\varepsilon_{\text{FEP}}^{\gamma}$ describes the relationship between energy and the number of photons detected in the full-energy peak at a given distance. In contrast, total efficiency includes all detected photons, making it particularly relevant for correcting True Cascade Coincidences (see Chapter 3.1.6). The program models efficiency using the following equation:

$$\varepsilon(E_{\gamma}) = e^{\sum_{i=0}^n a_i \cdot \ln^i(E_{\gamma})}, \quad (6)$$

where a_i are the function parameters derived by fitting experimentally measured values from calibration sources. However, achieving a high-quality fit is not always possible, as evaluated using χ^2 . In such cases, the fit is divided into two segments:

$$\varepsilon(E_\gamma) = \begin{cases} \sum_{i=0}^n a_i \cdot \ln^i(E_\gamma), & \text{if } E_\gamma < E_{\text{step}}, \\ \sum_{i=0}^N b_i \cdot \ln^i(E_\gamma), & \text{if } E_\gamma \geq E_{\text{step}}. \end{cases} \quad (7)$$

The next section briefly describes the calculation of total and peak efficiency using reference gamma sources.

3.1.4 Total efficiency

Total efficiency accounts for all detected photons, including those contributing to the Compton edge, backscatter peak, SEP/DEP peaks, and others. It is defined as:

$$\varepsilon_{\text{tot}} = \frac{P_{\text{total}}}{P_{\text{source}}}, \quad (8)$$

where P_{total} is the number of detected photons, and P_{source} is the number of photons emitted by the ionizing radiation source.

Total efficiency is determined using mono-energetic or quasi-mono-energetic (two-peak) calibration sources. Examples include ^{57}Co , ^{60}Co , ^{88}Y , ^{109}Cd , ^{137}Cs , and ^{241}Am . Pulses from the spectrum up to the end of the right edge of the FEP peak are included in the calculation. If the background spectrum significantly affects results, it should be subtracted. Total efficiency for a given energy is calculated using:

$$\varepsilon_{\text{tot}} = \frac{S_{\text{tot}} \lambda \frac{t_{\text{real}}}{t_{\text{live}}}}{A_0 I_\gamma(E_\gamma)} \frac{1}{e^{-\lambda t_0} (1 - e^{-\lambda t_{\text{real}}})}, \quad (9)$$

where:

- S_{tot} : total detected photons,
- λ : decay constant,
- t_{real} : total measurement time,
- t_{live} : live time, excluding dead time,
- A_0 : activity of the calibration source at the reference date,
- $I_\gamma(E_\gamma)$: gamma transition intensity,
- t_0 : time between the reference date and the start of the measurement.

The total efficiency values are point-specific and require fitting to enable further corrections. An example of the fit is shown in Fig. 32.

3.1.5 Full Energy Peak (FEP) efficiency

Peak efficiency considers only photons from the FEP peaks. A wide range of calibration standards can be used for its determination, significantly improving the accuracy of the calculation. The definition is based on the general formula:

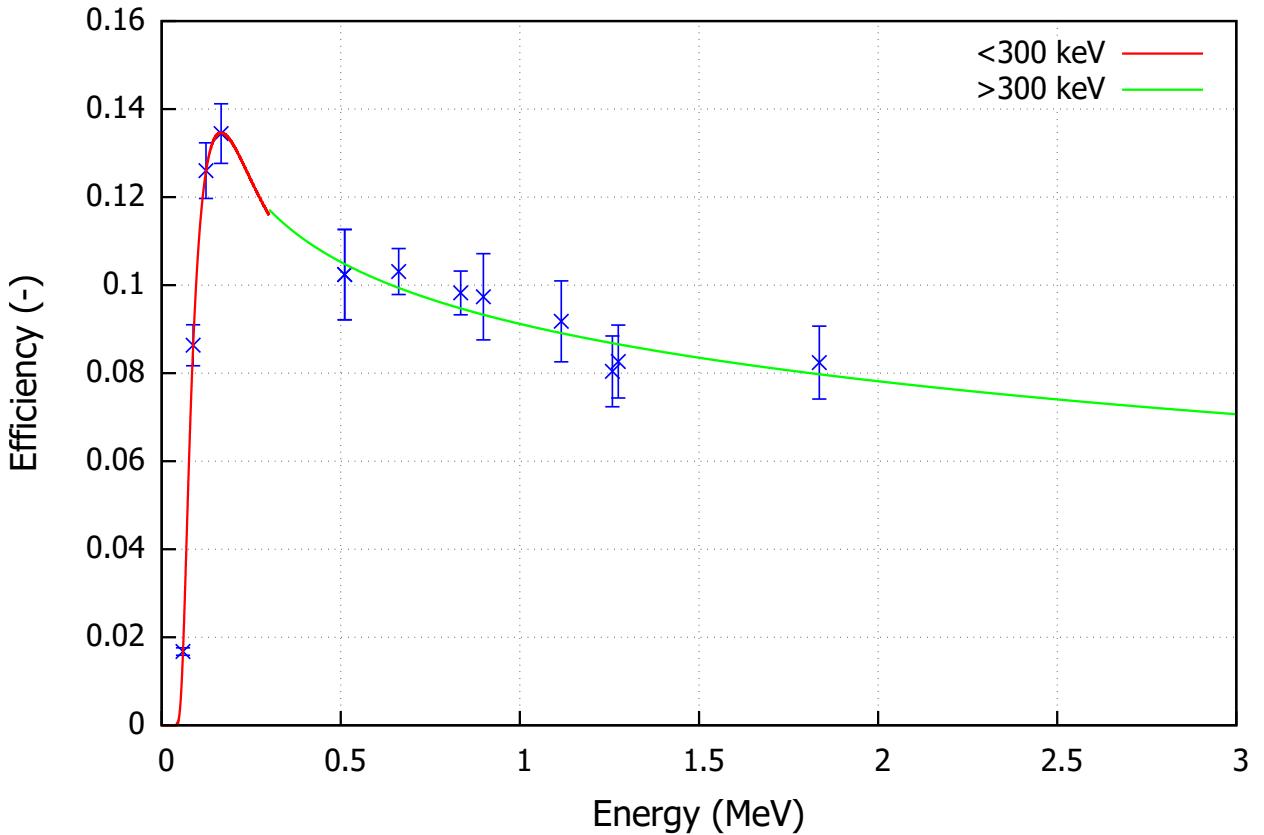


Figure 32: Total efficiency of the HPGe detector at FEEC, constructed from two curves for a distance of 5 mm between the standard and the detector.

$$\varepsilon_{\text{FEP}} = \frac{P_{\text{FEP}}}{P_{\text{source}}}, \quad (10)$$

where P_{FEP} is the number of pulses recorded in the FEP peak. The efficiency is then determined using a formula similar to Equation 9:

$$\varepsilon_{\text{FEP}} = \frac{S_{\text{FEP}}(E_\gamma) \lambda_{t_{\text{live}}}^{t_{\text{real}}}}{A_0 I_\gamma(E_\gamma)} \frac{1}{e^{-\lambda t_0} (1 - e^{-\lambda t_{\text{real}}})}, \quad (11)$$

where the difference lies in the use of the area S_{FEP} , which corresponds to the full-energy peak. For this correction, it is necessary to account for True Cascade Coincidences (see Chapter 3.1.6), as some calibration sources have non-trivial energy transition structures, e.g., ^{152}Eu . Initially, FEP efficiency values are calculated without corrections, based on spectra processed in the Deimos32 program and further analyzed in the software package, as described in Chapter 2.6.1.

True Cascade Coincidence corrections are determined using the `TrueCoinc` program [2], though alternative programs may also be used. Corrected values require a new fit, with the resulting parameters added to the program's libraries. The significance of this correction is illustrated in Fig. 33, highlighting differences, particularly below 500 keV.

The correction for FEP efficiency is one of the most important spectrometric corrections. Without it, comparing values obtained from different geometries or detectors is not possible.

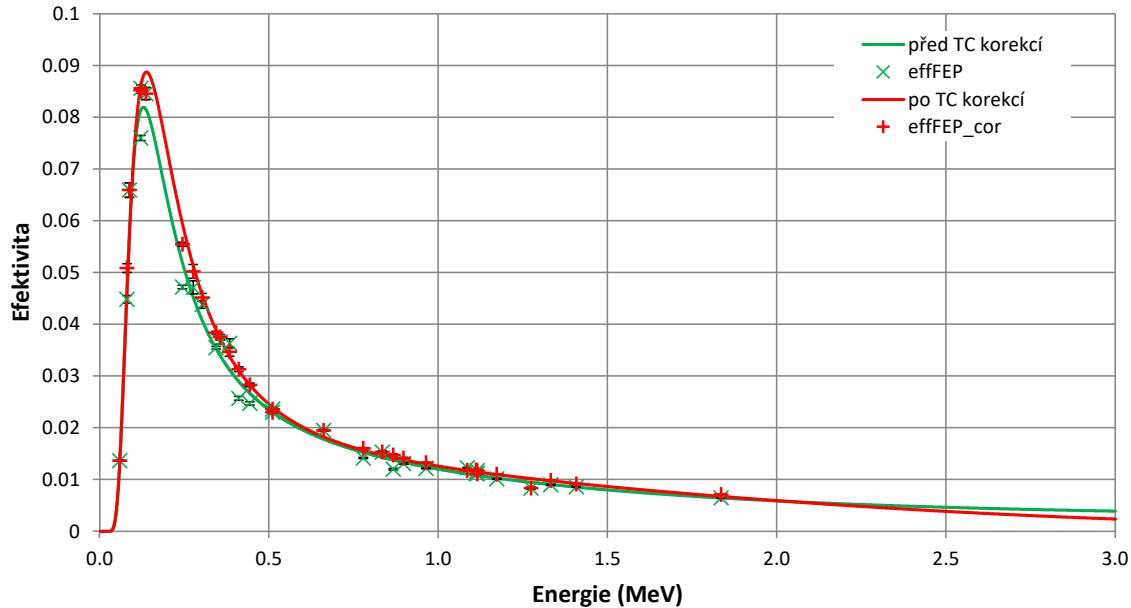


Figure 33: FEP efficiency of the HPGe detector before and after correction for True Cascade Coincidences.

3.1.6 True coincidence summing correction

As previously mentioned, cascade coincidences occur in radionuclides with complex energy transitions. Due to limitations in the speed of signal processing, multiple gamma photons may be recorded as a single photon with a summed energy. Coincidences can be categorized as true or random, depending on their source.

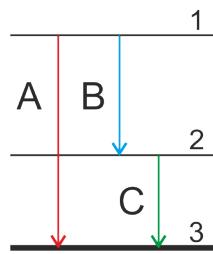


Figure 34: General cascade decay scheme.

True coincidences refer to those originating from the sum of photon energies emitted by a single radionuclide, while random coincidences may involve photons from different sources. Random coincidences cannot be easily eliminated. Fig. 34 shows a general decay scheme, illustrating that the nucleus can reach the ground state in two ways: by emitting a gamma photon with energy A or through a cascade emitting quanta B and C. For this simplified case,

two types of summing may occur:

1. Gamma quanta B and C are recorded simultaneously. The event is registered as a photon with an energy equal to the sum of energies B+C and is recorded as event A. The ratio between the number of events A and B+C is given by the following relation:

$$S(A) = S(B+C) = \frac{I_\gamma(B)}{I_\gamma(A)} a_{CC} c \frac{\varepsilon_{FEP}(C)}{\varepsilon_{FEP}(A)}, \quad (12)$$

where I_γ is the intensity of the gamma transition, a_C is the branching ratio of transition C, $c = \frac{1}{1+\alpha_t}$, and α_t is the total conversion coefficient.

2. If photon B is fully absorbed and photon C is partially absorbed, or vice versa, the event is recorded in a new peak that does not correspond to the FEP peaks of the mentioned transitions. For this type of event, coefficients must be determined to account for the reduction of peaks for transitions B and C:

$$L(B) = a_{CC} c \varepsilon_{tot}(C), \quad (13)$$

and similarly:

$$L(C) = \frac{I_\gamma(B)}{I_\gamma(C)} a_{CC} c \varepsilon_{tot}(B). \quad (14)$$

In practice, a single nucleus may involve one to dozens of transitions. The resulting coincidence correction for transition A is as follows:

$$\eta_{TC}(A) = [1 - L(A)] \cdot [1 + S(A)]. \quad (15)$$

Similar relationships can be derived for transitions B and C. However, in more complex cascades, the approach must be generalized.

The Nuclear Group at BUT uses the `TrueCoinc` program [2] to determine these corrections. The input for this program includes parameters of functions describing FEP and total efficiency.

To perform this correction accurately, it is necessary to identify the radionuclide and the energy of the specific transition. During the evaluation process, the program verifies that the target peak originates from the correct source, using a database of tabulated values stored within the program.

3.1.7 Self-absorption correction

For samples with significant thickness, this correction is recommended. Another important factor is the shielding properties of the sample materials. The physical description of the correction is as follows. If we consider a flat source with thickness t and activity N_0 homogeneously distributed throughout the sample volume, the number of emitted photons is given by:

$$N = \int_0^t N_0 e^{-\mu x} \frac{dx}{t} = N_0 \frac{1 - e^{-\mu t}}{\mu t}. \quad (16)$$

After simplification, the correction factor takes the following form:

$$\eta_A(E_\gamma) = \frac{N}{N_0} = 1 - \frac{1 - e^{-\mu(E_\gamma)t}}{\mu(E_\gamma)t}, \quad (17)$$

where $\mu(E_\gamma)$ is the linear attenuation coefficient. This correction strongly depends on the sample thickness and the linear attenuation coefficient, which accounts for gamma photon energy, sample material, and density. Tabulated values for attenuation coefficients are available in databases [3]. The evaluation program includes a library of mass attenuation coefficients for selected elements, which users can expand as needed (see Chapter 2.4.1).

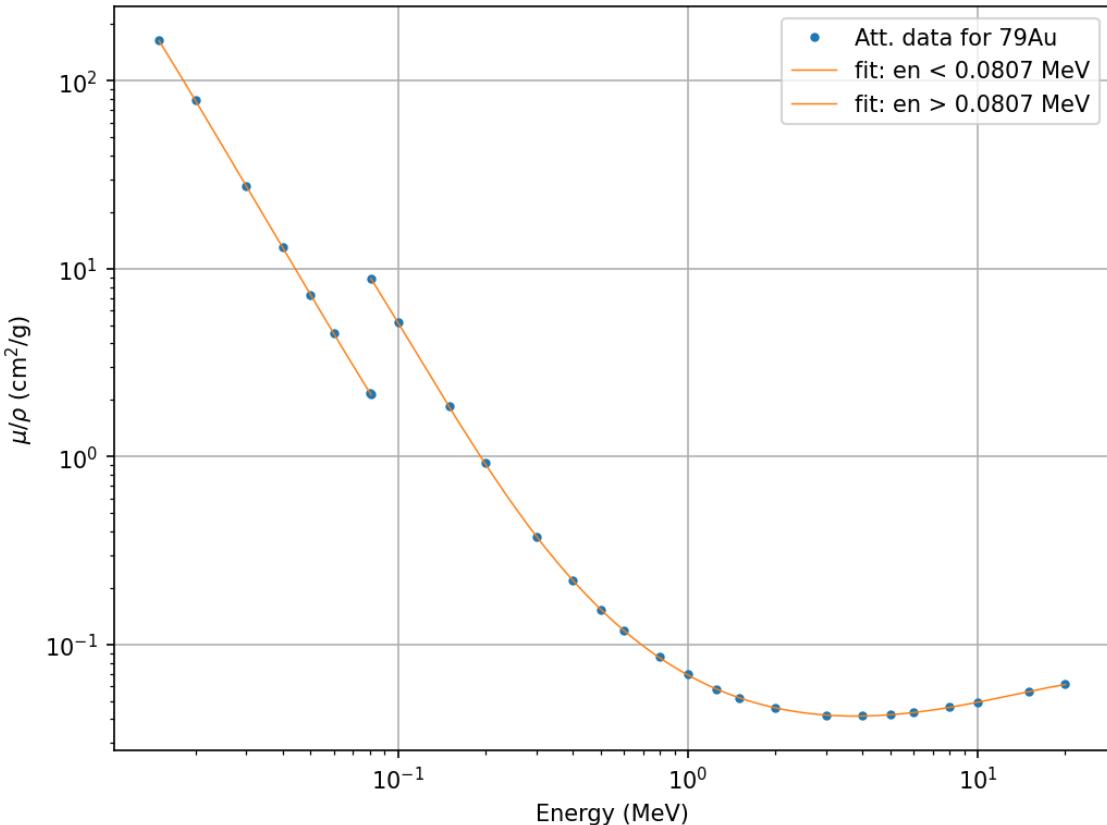


Figure 35: Fit of mass attenuation coefficient values for gold (Au) foils.

The tabulated data are point-specific values requiring interpolation to determine corrections for specific gamma energies. The evaluation program performs these fits, as shown in Fig. 35, using the following function⁸:

$$\eta_A(E_\gamma) = e^{\sum_{i=0}^n c_i \ln^i(E_\gamma)}, \quad (18)$$

where c_i are the fit parameters. The program applies this self-absorption correction to all peaks in the spectra, storing correction values for subsequent calculations. The source of the tabulated values is NIST [3].

⁸The fit is performed using a 7th-order polynomial.

3.1.8 Correction for beam intensity fluctuations

The calculation of final values assumes a constant level of activation during the irradiation period. However, beam intensity often fluctuates, and interruptions may occur. If information about the accelerator's power during irradiation is available, a correction factor can be calculated using:

$$\eta_{ba} = \frac{1 - e^{-\lambda t_{irr}}}{t_{irr} \sum_i^N \left[\frac{1}{t_p(i)} W(i) e^{-\lambda t_e(i)} (1 - e^{-\lambda t_p(i)}) \right]}, \quad (19)$$

where:

- t_{irr} : total irradiation time,
- $t_e(i)$: time between interval i and the end of irradiation,
- $t_p(i)$: length of the i -th interval,
- $W(i)$: ratio between the particles in the i -th interval and the total number of particles,
- λ : decay constant.

This correction, similar to cascade summing corrections, requires knowledge of the radionuclide's half-life. Input data, such as an accelerator log, should be in an appropriate format (see Chapter 2.4.5). This correction can be applied via the **Calculation** window (see Chapter 2.5.1).

3.1.9 Radiation background subtraction

During the measurement of target samples, background radiation is always present. Therefore, it is advisable to correct the spectra for background radiation. Background measurements are typically conducted once over a long period, lasting several hours or days, to ensure sufficient statistical quality.

The background spectrum, processed in the **Deimos32** program like other spectra, is stored in the evaluation package's library (see Chapter 2.4.2). Users can choose to include or exclude this correction. The program recalculates the size of background peaks based on the measurement duration for experimental samples and performs the subtraction as follows:

$$S'_{bcg}(E_\gamma) = \frac{t_{l,spec}}{t_{l,bcg}} S_{bcg}(E_\gamma), \quad (20)$$

where:

- $S'_{bcg}(E_\gamma)$: adjusted background area for a peak with energy E_γ ,
- $S_{bcg}(E_\gamma)$: total measured background peak area,
- $t_{l,spec}$: effective measurement time of the current spectrum,
- $t_{l,bcg}$: net measurement time of the background spectrum.

Equation 20 shows that the subtracted area is proportional to the net measurement times [1].

3.1.10 Correction for single and double escape peaks

At sufficiently high gamma-ray energies, the FEP peak is accompanied by the formation of SEP and DEP peaks. If multiple peaks in the spectrum could contribute to summing peaks, applying the appropriate correction is advisable.

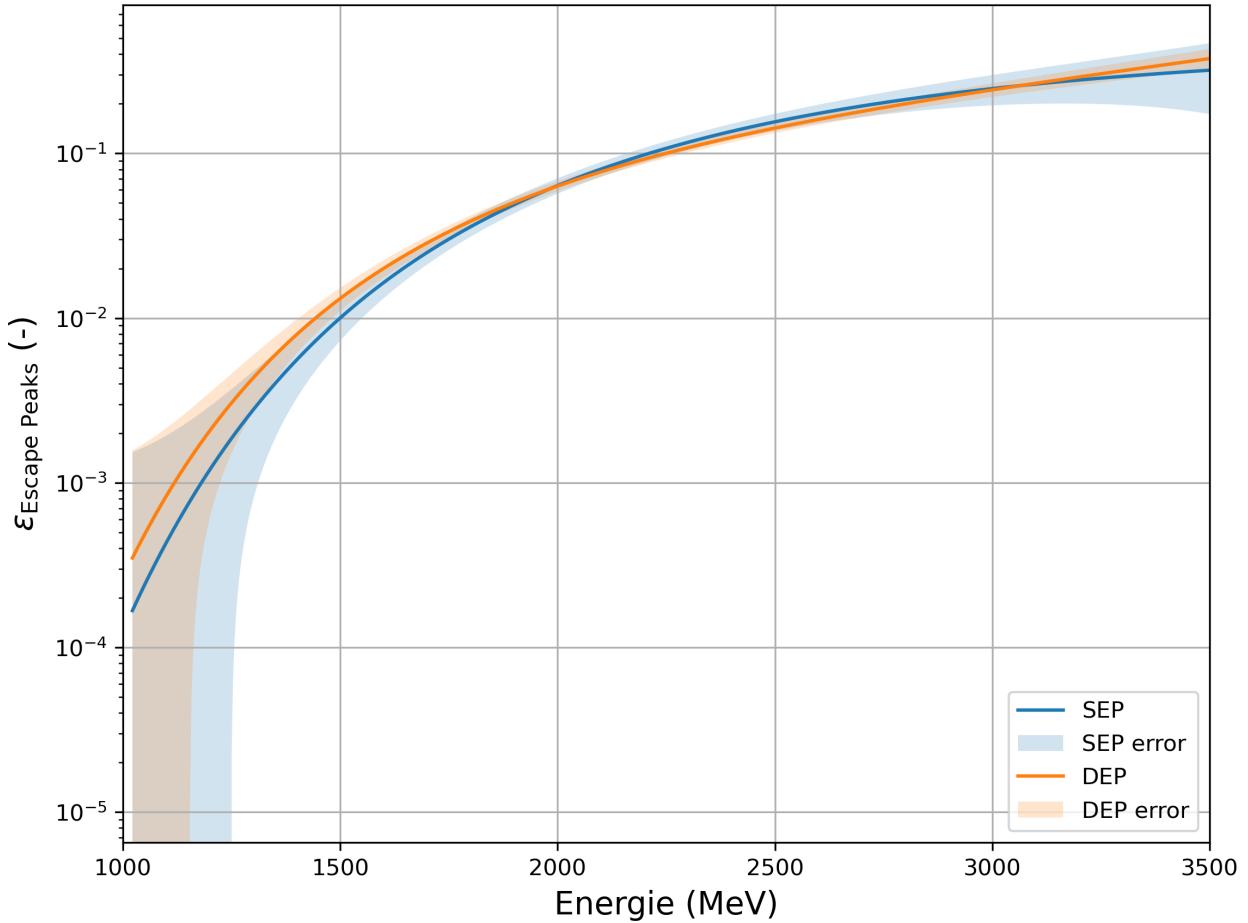


Figure 36: Relationship between escape peak formation and the energy of the FEP peak in the spectrum [4].

The evaluation program automatically identifies peaks with energy greater than 1022 keV and calculates their theoretical size and position for the SEP and DEP. It then compares these values with all peaks in the spectrum to identify matches. If matching peaks are found, the program applies an area subtraction using the formula:

$$S_{\text{cor}}(E_\gamma) = S_{E_{\text{FEP}}} \cdot \varepsilon_{\text{SEP/DEP}}(E_{\text{FEP}}), \quad (21)$$

where $S_{E_{\text{FEP}}}$ is the area of the FEP peak, and $\varepsilon_{\text{SEP}}(E_{\text{FEP}})$ or $\varepsilon_{\text{DEP}}(E_{\text{FEP}})$ represent the efficiencies indicating the ratio of the sizes of the SEP and DEP peaks [1].

To perform this correction, it is necessary to understand the relationship between the production of SEP and DEP peaks and the energy of the FEP peak. The evaluation program incorporates an experimentally determined relationship (see Fig. 36) from [4]. Studies have shown that this effect is independent of both the sample's distance from the detector and the detector type. The production of single and double escape peaks is described by the following equation:

$$\varepsilon_{\text{SEP/DEP}}(E_\gamma) = e^{(a_0 + a_1 \ln(E_\gamma) + a_2 \ln^2(E_\gamma) + a_3 \ln^3(E_\gamma))}. \quad (22)$$

The program includes curves for escape peak production, and users have the option to

update these parameters. The coefficients for this relationship are listed in Table 1.

Table 1: Parameters describing the relationship between escape peak formation and FEP peak energy [4].

Term	a_{SEP}	$a_{\text{SEP-err}}$	a_{DEP}	$a_{\text{DEP-err}}$
0	-2.0866	0.2860	-1.3273	0.1814
1	13.8833	1.1100	12.8054	0.8384
2	-8.2292	1.3993	-8.9129	1.1473
3	1.7179	0.5676	2.6471	0.4847

3.1.11 Correction for non-point source and non-trivial sample shape

FEP efficiency is typically determined using point sources, whereas real samples often have dimensions ranging from millimeters to centimeters. The magnitude of this correction strongly depends on the sample's dimensions, the energy of the emitted photons, the distance from the detector, and the detector's size. The largest errors occur in close or near-zero geometries, where deviations can reach tens of percent. Conversely, at greater distances from the detector, the sample can often be approximated as a point source, provided it is relatively small or sufficiently far away.

This correction can be determined experimentally if planar standards of various sizes are available, although this approach is often impractical. Alternatively, Monte Carlo simulations can be used, requiring detailed knowledge of the HPGe detector's dimensions and internal structure. However, obtaining this information is typically very challenging. The general formula for this correction is:

$$\eta_{\text{area}} = \frac{\varepsilon_p^{\text{area}}}{\varepsilon_p^{\text{point}}}, \quad (23)$$

where $\varepsilon_p^{\text{area}}$ is the simulated efficiency for the actual sample dimensions, and $\varepsilon_p^{\text{point}}$ is the simulated efficiency for an equivalent point source.

Alternatively, the correction can be determined mathematically, based on the sample's dimensions, the detector's size, and their relative positions. However, this method becomes increasingly complex for irregularly shaped samples.

While the evaluation software does not calculate this correction directly, users can input pre-determined correction values, which will be applied during the final calculation.

3.2 Conditions for applying selected spectrometric corrections

The appearance of a gamma spectrum depends on several factors, including the energy and type of primary particles, the irradiation duration, and the composition of the samples. For samples with complex compositions and sufficient primary particle energy, numerous reactions can occur, leading to the formation of multiple radionuclides and the emission of various gamma photons. This can result in closely spaced peaks, complicating the automation of the evaluation process. Specific conditions were therefore established to determine when certain corrections should be applied.

- **Background subtraction correction:** This correction is applied to peaks in the spectrum according to the following rules, adapted from [5]:

1. $|E_\gamma - E_\gamma^{\text{bcg}}| < n \cdot \sqrt{a^2 + (\Delta E_\gamma)^2 + (\Delta E_\gamma^{\text{bcg}})^2}$

where E_γ is the energy of the peak in the evaluated spectrum, E_γ^{bcg} is the energy of the corresponding peak in the background file, ΔE_γ and $\Delta E_\gamma^{\text{bcg}}$ are their respective uncertainties, and n is a user-adjustable sensitivity parameter. Typically, $n \approx 2$, and a is a correction factor accounting for nonlinearity effects, with an experimentally determined value of $a = 0.15$ keV.

2. $|E_\gamma - E_\gamma^{\text{bcg}}| < m \cdot \text{FWHM}(E_\gamma)$

where m is a correction factor accounting for the non-Gaussian nature of the fitted gamma peak. Typically, $m = 2$, a value determined empirically.

- **Conditions for single escape (SEP) and double escape (DEP) peaks:** These conditions are as follows:

1. $|E_\gamma - E'_\gamma| < n \cdot \sqrt{a^2 + (\Delta E_\gamma)^2 + (\Delta E'_\gamma)^2}$

where E_γ is the energy in the gamma spectrum, E'_γ is the energy of the SEP or DEP peak, ΔE_γ and $\Delta E'_\gamma$ are their uncertainties, n is a user-adjustable parameter (default $n = 1$), and a is a correction factor for nonlinearity effects, typically $a = 0.15$ keV.

2. $|E_\gamma - E'_\gamma| < m \cdot \text{FWHM}(E_\gamma) \cdot \frac{E_\gamma}{N_{\text{chn}}(E_\gamma)}$

where m is a correction factor for the non-Gaussian nature of the fitted gamma peak. The default value is $m = 1$, and N_{chn} is the centroid channel of the peak.

- **Gamma energy matching:** This condition is used to identify gamma energies in the input spectra and is not strictly a correction. It is applied as follows:

1. $|E_\gamma - E_\gamma^{\text{lib}}| < n \cdot \sqrt{A^2 + (\Delta E_\gamma^{\text{lib}})^2 + (\Delta E_\gamma)^2}$

where E_γ^{lib} is the gamma line energy from the **gamma line library**.

3.3 Summary of correction factors in the calculation of the R-Factor for individual energies

The following formula provides an example for calculating the R-factor, incorporating the corrections described above along with additional normalizations:

$$R_{\text{factor}} = S(E_\gamma) \frac{M}{N_A m} \frac{t_{\text{irr}}}{I_P} \frac{1}{t_{\text{live}}} \frac{1}{1 - e^{-\lambda t_{\text{irr}}}} \frac{1}{e^{-\lambda t_{\text{decay}}}} \frac{\lambda t_{\text{real}}}{1 - e^{-\lambda t_{\text{real}}}} \frac{1}{I_\gamma(E_\gamma)} \frac{1}{\varepsilon_{\text{FEP}}(E_\gamma)} \frac{1}{\eta_A \cdot \eta_{\text{TC}} \cdot \eta_{\text{area}}} \quad (24)$$

where:

- t_{real} : total measurement time on the detector,
- t_{live} : live time (excluding dead time),
- t_{decay} : time between the start of measurement and the end of activation,
- λ : decay constant,
- t_{irr} : irradiation duration,
- I_γ : gamma line intensity,
- $S(E_\gamma)$: area of the gamma line,
- $\varepsilon_{\text{FEP}}(E_\gamma)$: FEP efficiency for the given gamma line,
- N_A : Avogadro's constant,

- m : sample mass,
- M : molar mass of the sample,
- I_P : total number of particles to which the sample is exposed during activation,
- η : various spectrometric corrections.

A breakdown of the correction terms is as follows:

- $\frac{1}{t_{\text{live}}}$ correction for detector dead time,
- $\frac{1}{1 - e^{-\lambda t_{\text{irr}}}}$ correction for decay during irradiation,
- $\frac{1}{e^{-\lambda t_{\text{delay}}}}$ correction for decay during transport or between measurements,
- $\frac{\lambda t_{\text{real}}}{1 - e^{-\lambda t_{\text{real}}}}$ correction for decay during measurement,
- $\frac{1}{I_\gamma(E_\gamma)}$ correction for gamma line intensity,
- $\frac{1}{\varepsilon_{\text{FEP}}(E_\gamma)}$ correction for detector efficiency,
- η_A correction for self-absorption,
- η_{TC} correction for coincidence summing,
- η_{ba} correction for beam intensity fluctuations,
- η_{area} correction for non-point source and sample shape,
- $\frac{M}{N_A m}$ normalization per atom in the sample,
- $\frac{1}{I_P}$ normalization per particle,
- t_{irr} normalization to yield over the entire irradiation period.

The evaluation is performed in a semi-automatic mode, where the user selects which values are saved for further processing or directly exported. The calculation of activity for constructing the decay curve is performed using the following formula:

$$N = \frac{S(E_\gamma)}{I_\gamma(E_\gamma) \varepsilon_{\text{FEP}}(E_\gamma)} \frac{t_{\text{real}}}{t_{\text{live}}} \frac{\lambda}{1 - e^{-\lambda t_{\text{real}}}} \frac{\eta_{\text{ba}}}{\eta_A \cdot \eta_{\text{TC}} \cdot \eta_{\text{area}}}, \quad (25)$$

where N corresponds to the activity normalized to the start of the measurement for the respective spectrum. These activities are plotted and fitted to a decay curve. Based on the fit's agreement with individual activities, the user can assess whether the identified peaks in the spectrum correspond to the selected radionuclide. The goodness of fit is tested using χ^2 or the reduced χ^2 .

The final result for individual measurements is determined as the weighted average of individual results. If the selected radionuclide contains multiple gamma lines, the program calculates the overall weighted average of the final value using the following formulas:

Uncertainty of activity for a single measurement

$$A_{\text{err}} = \sqrt{\left[0.03 \left(\frac{t_{\text{real}}}{t_{\text{live}}} - 1\right)\right]^2 + (t_{\text{decay}})^2 \lambda^2 \left(T_{1/2}^{\text{err}}\right)^2 + S_{\text{err}}^2 + \left(I_\gamma^{\text{err}}\right)^2}, \quad (26)$$

where $T_{1/2}^{\text{err}}$ is the uncertainty of the half-life, S_{err} is the peak area uncertainty, and I_γ^{err} is the

uncertainty of the transition intensity.

Weights and weighted average

The weights w_i are calculated using the uncertainties:

$$w_i = \left(\frac{1}{\Delta x_i} \right)^2. \quad (27)$$

The weighted average \bar{X} for a group of results is calculated as:

$$\bar{X} = \frac{\sum_{i=1}^n w_i x_i}{\sum_{i=1}^n w_i}. \quad (28)$$

Uncertainty of the weighted result

The internal error $\Delta \bar{X}_{\text{int}}$ is determined as:

$$\Delta \bar{X}_{\text{int}} = \left(\sum_{i=1}^n w_i \right)^{-1}. \quad (29)$$

The external error $\Delta \bar{X}_{\text{ext}}$ is calculated as:

$$\Delta \bar{X}_{\text{ext}} = \sqrt{\frac{\sum_{i=1}^n w_i (x_i - \bar{X})^2}{(n-1) \sum_{i=1}^n w_i}}. \quad (30)$$

3.3.1 Correction of two-step decay

In the activation of most isotopes, radionuclides are produced in their ground state, or the lifetimes of excited states are very short, so all nuclei are in the ground state by the time of measurement. However, in certain cases, isomeric states with long half-lives may form. Examples include radionuclides like ^{87}Y , ^{196}Au , and others.

The equations provided earlier are defined only for simple exponential decay. However, for isotopes such as ^{196}Au , the following decay paths can occur: $^{196m1}\text{Au}$ or $^{196m2}\text{Au}$ to ^{196}Au . The first excited state does not require consideration, as its half-life is only 8.1 s, meaning all nuclei in this metastable state will decay to the ground state before the measurement begins. In contrast, the second metastable state has a half-life of 9.6 h. During the decay of ^{196}Au in the ground state, its activity increases due to the decay of $^{196m2}\text{Au}$, necessitating an appropriate correction.

To determine the correction during the cooling and measurement phases, we begin with the following differential equation:

$$dN_g = -\lambda_g N_g dt + \lambda_m N_m dt, \quad (31)$$

where the index g represents the ground state, and m represents the metastable or isomeric state. After rearrangement and simplification, the number of radionuclides in the ground state

can be expressed as:

$$N_{g0} = S(E_\gamma) \frac{1}{t_{\text{live}} \varepsilon_{\text{FEP}}(E_\gamma) I_\gamma(E_\gamma)} \frac{1}{e^{-\lambda_g t_{\text{decay}}}} \frac{t_{\text{real}}}{1 - e^{-\lambda_g t_{\text{real}}}} + \frac{\lambda_m N_{m0}}{\lambda_g - \lambda_m} \left(1 - e^{(\lambda_g - \lambda_m)t_{\text{decay}}}\right), \quad (32)$$

where N_{g0} and N_{m0} are the numbers of nuclei at the end of irradiation in the ground and metastable states, respectively. To account for the formation of isomeric states during irradiation, we start from Equation 32 and introduce a production term P_g :

$$dN_g = P_g - \lambda_g N_g dt + \lambda_m N_m dt, \quad (33)$$

The resulting correction for two-step decay during irradiation is as follows:

$$C_{\text{irr},g} = \frac{P_g \cdot t_{\text{irr}}}{N_{g0}} = \frac{\lambda_g t_{\text{irr}}}{1 - e^{-\lambda_g t_{\text{irr}}}} - \frac{N_{\text{yield},m}}{N_{g0}(1 - e^{-\lambda_g t_{\text{irr}}})} \left(1 - \frac{\lambda_m e^{-\lambda_g t_{\text{irr}}} - \lambda_g e^{-\lambda_m t_{\text{irr}}}}{\lambda_m - \lambda_g}\right), \quad (34)$$

The yield of the radionuclide in the ground state can then be determined using:

$$N_{\text{yield},g} = N_{g0} \cdot C_{\text{irr},g}. \quad (35)$$

A simple conversion relates the yield to the R-factor:

$$R_{\text{factor},g} = N_{g0} \cdot C_{\text{irr},g} \cdot \frac{M}{N_A m} \cdot \frac{1}{I_P} = \frac{N_{\text{yield},g}}{N_{\text{atoms}} \cdot I_P}, \quad (36)$$

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List of Acronyms

HPGe High Purity Germanium

SEP Single Escape Peak

FEP Full Energy Peak

DEP Double Escape Peak

FEEC Faculty of Electrical Engineering and Communication

BUT Brno University of Technology

MCA Multichannel Analyzer

UD University of Defense