

Y-Spect: A Multi-Method Gamma Spectrometry Analysis Program

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ABSTRACT

To accomplish a more accurate, precise and correct interpretation and analysis of spectrum data collecting from a gamma spectrometry counting system, a fully interactive computer code, named Y-Spect, has been developed by using the Delphi 7.0 programming language. The code combines several popular methods for peak search, i.e.: Mariscotti, Phillips-Marlow, Robertson *et al.*, Routti-Prussin, Black, Sterlinski, Savitzky-Golay and Block *et al.* Any combinations of those methods can be chosen during a peak searching process, which can be performed in automatic or manual mode. Moving Window Average- and Savitzky-Golay-methods are available for spectrum data smoothing. Peak fitting is done by using a non-linear least square method of Levenberg-Marquardt for either a pure Gaussian peak shape or one with an additional Right/Left Tail function. Other than standard features, such as: peak identification and determination of: continuum, region of interest (ROI), and peak area, etc., Y-Spect has also a special feature which can predict the existence of escape- and/or sum peaks that belong to a certain radioisotope. Aside from displaying the complete spectrum graph, including: singlet or multiplet ROIs and peak identifications, Y-Spect can also display the first- or second-derivative of the spectrum data. Data evaluation is given as: isotope names, peak energy, Net-Count(-Rate), etc. Y-Spect is provided with a complete ENDF/B-VII.0 gamma-ray library file that contains of 16089 gamma energy lines from 1420 different radioisotopes. Other general specifications are: maximum number of: spectrum's channels = 16×1024 ; ROIs = 2×1024 ; ROI's width = 2×1024 channels; Overlapping peaks (multiplet) = 20; Identified isotopes = 3×1024 , and Isotope library's energy lines = 16×1024 .

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INTRODUCTION

Nowadays, many sophisticated gamma spectrometry analysis computer software are commercially available worldwide, such as Genie-2000, Sampo 90, Hypermet/HyperLabs, and Tennelec/ Nucleus-PCA. Those computer programs implement different methods of: peak searching, peak fitting as well as spectrum data smoothing. The methods, independently developed by individuals, groups or institutions, have been proven accurate and precise, and successfully implemented for handling almost any kind of gamma spectrometry problems. Experts have concluded that “*these methods have reached a high degree of maturity*” and that “*it is quite unlikely that spectacular new developments will emerge in the near future*” [1].

However, due to the statistical nature of gamma spectrum physics, as well as the imperfections occurring in the gamma counting systems, the quality of collected spectrum data will

always vary from cases to cases, so that none of the methods can be suitably applied to solve the problems found in all cases. One method will be superior in some cases, but the other method will do better to handle other situations.

Therefore, the main goal of the author is to combine all known and available methods of peak search and peak fitting into one fully interactive computer program, called Y-Spect. With this program, users will be able to accurately and precisely analyze a wide range of spectrum data files, without having to expend the great effort needed to master several different computer softwares.

The code combines several popular methods for peak search, i.e.: of Mariscotti (implemented in Genie-2000, Tennelec/Nucleus and Canberra S-100), Phillips-Marlow (implemented in Hypermet/ HyperLabs), Robertson *et al.* (implemented in Hypermet/HyperLabs), Routti-Prussin (implemented in Sampo 90), Black, Sterlinski, Savitzky-Golay and Block *et al.* Also, two other primitive methods are implemented in the code, namely, (First-) Derivative and Bare-Eyes methods.

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This paper will explore the peak search and peak fitting methods implemented in Y-Spect, general and special capabilities of Y-Spect, as well as show some results of the application of Y-Spect in analyzing gamma spectra emitted from some irradiated samples.

EXPERIMENTAL METHODS

Peak search methods

Consider an ideal gamma spectrum as shown on Fig. 1. The spectrum data as well as the resulted smoothed curve of the spectrum is so clear and clean that we can easily determine, by using only our naked eyes, where the peak is located and what the height of the peak is. Intuitively, we can locate the peak by tracing the spectrum data, beginning from the left side of the peak, until we find the highest value of spectrum data, which is signaled by the next spectrum data having a smaller value than the previous one.

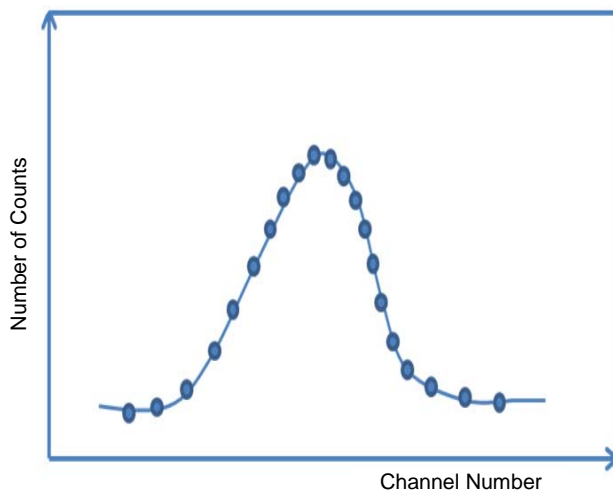


Fig. 1. Ideal gamma spectrum data and its smoothed curve.

Bare-eyes peak search method

A slight modification of the above peak search process, known as the Bare-Eyes method, is implemented in Y-Spect. The method is as follows:

- Trace the spectrum data, beginning from the leftmost point, until the highest value is found;
- A data point is considered as a peak when at least N previous data points have successively increasing values and N next data points have successively decreasing values, where N is an integer number predetermined by the user. The greater N is, the more valid the peak is.

(First-) Derivative peak search method

In reality, it is hard to find ideal spectrum data as given in the previous example. Due to random behaviour of radiation emission and imperfections inherent to counting system, the spectrum data always tends to contain random and even wildly scattered values around the averaged values. Such values will cause the simple Bare-Eyes method to fail to find the correct peaks. However, the curve of the first derivative of spectrum data always has a smoother shape. In addition, successively increasing raw data values mathematically means that the first derivative values have positive values, and successively decreasing in raw data values will have negative values in the first derivatives. The data point that is located in a peak will then have a zero value of its first derivative.

The Derivative peak search method is applied in Y-Spect as follows:

- Calculate the first derivative values from the raw spectrum data;
- Trace the first derivative values from the leftmost point, until a zero value is met;
- A data point is considered as a peak when at least N previous data points have successively positive values and the next N data points have negative values.

Mariscotti's peak search method

When the spectrum data is getting more and more complex, such as having peaks that are closely separate in energy, i.e. forming a group of overlapping peaks (multiplet), the First Derivative method frequently fails to discover the existence of those multiplets. Fortunately, the curve of second derivative values of the raw spectrum data tends to have a smoother shape compared to the curve of the first derivative. From elementary calculus, we know that any (continuous-) function will reach the highest value(s) at the point(s) where the first derivative value(s) has/have zero value(s) and the second derivative value(s) is/are negative. For our case, this is the data point where the peak located is.

To calculate (negative) second derivative values of raw spectrum data, Mariscotti [2] used the second difference formula, as follows:

$$SD[i] = \sum_{k=-1}^1 c[k] * N[i+k] \quad (1)$$

$$c[-1] = -1.0; \quad c[0] = 2.0; \quad c[1] = -1.0 \quad (2)$$

Where:

$SD[i]$ is the second difference value at data point i and $N[i+k]$ is raw data value at data point $i+k$.

To take the smoothing effect into account, Mariscotti replaced the $SD[i]$ with the average (to be more exact, the sum) of m (=positive integer number) neighbour data's $SD[i]$, namely,

$$SD[i, m] = \sum_{k=-m}^m SD[i + k] \quad (3)$$

Furthermore, Mariscotti repeated the above averaging process five times. Now, we are ready to use Eq. 3 for determination of peak location, namely the data point i which has maximum value of $SD[i, m]$.

However, instead of using the Eq. (3) for determining the location of a peak, in Y-Spect the Mariscotti method is implemented in a slightly modified way as follows [3,4]:

- a. Calculate the standard deviation of the second difference $SSD[i]$ as well as $SSD[i, m]$, using smoothing and averaging process in the similar way to calculating $SD[i]$ and $SD[i, m]$, as follows:

$$SSD[i] = \sum_{k=-1}^1 c[k]^2 * N[i + k] \quad (4)$$

$$c[-1] = -1.0; \quad c[0] = 2.0; \quad c[1] = -1.0 \quad (2)$$

$$SSD[i, m] = \sqrt{\sum_{k=-m}^m SSD[i + k]} \quad (5)$$

- b. Calculate the ratio of $SD[i, m]$ and $SSD[i, m]$, i.e., $SS[i, m]$:

$$SS[i, m] = \frac{SD[i, m]}{SSD[i, m]} \quad (6)$$

The peak is then located at data point i , which has $SS[i, m] \geq$ threshold value. It is recommended that the threshold value is ≥ 3.5 [3]. The greater the $SS[i, m]$ value, the more qualified the peak is.

Phillips-Marlow's peak search method

Phillips and Marlow [3] proposed another method for calculating $SD[i, m]$ and $SSD[i, m]$ values. Their method can be regarded as an extension of Mariscotti method, but without the need to perform the repeated averaging process.

$$SD[i, m] = \sum_{k=-m}^m c[k] * N[i + k] \quad (7)$$

$$SSD[i, m] = \sqrt{\sum_{k=-m}^m c[k]^2 * N[i + k]} \quad (8)$$

Where:

$$m = 2 * w + 1;$$

w (positive integer number) = width;

$$c[k] = -1 \quad \text{for} \quad k = -m \text{ to } -(w+1) \text{ and} \\ k = (w+1) \text{ to } m;$$

$$= 2 \quad \text{for} \quad k = -w \text{ to } w. \quad (9)$$

Then, Eq. 6 is used again to determine the peak locations.

Robertson et al's peak search method

Robertson *et al* [5] proposed exactly the same expressions of Eqs. 6, 7 and 8 in calculating $SS[i, m]$, $SD[i, m]$ and $SSD[i, m]$, but with different definitions of m and $c[k]$, as follows:

$$m = 5 * w + 1;$$

w (positive integer number) = width;

$$c[k] = -1 \quad \text{for} \quad k = -m \text{ to } -(w+1) \text{ and} \\ k = (w+1) \text{ to } m;$$

$$= 4 \quad \text{for} \quad k = -w \text{ to } w. \quad (10)$$

Routti-Prussin's peak search method

By assuming that a peak has a shape of pure Gaussian function, Routti and Prussin [4] introduced a more complicated but precise expression of $c[k]$ as follows:

$$c[k] = \frac{\sigma^2 - k^2}{\sigma^4} \exp\left(\frac{-k^2}{2\sigma^2}\right) \quad (11)$$

Where:

$$k = 0, \pm 1, \pm 2, \pm 3, \dots$$

σ is a constant corresponding to the standard deviation of the peak.

In Sampo 90 [6], the k value extends to a certain limit, i.e., $c[k+1] < 0.01 c[0]$.

Following the suggestion of Menno Blaauw [7], the implementation of Routti-Prussin method in Y-Spect is as follows:

- a. Let the k value extends until the condition $c[k+1] < 0.01 c[0]$ is satisfied;
- b. Sum up all the $c[k]$'s and divide it by $-(k+1)$, so we obtain:

$$r = \frac{-1}{k + 1} \sum_{i=-k}^k c[i] \quad (12)$$

- c. Let $c[k] = c[k]+r$;
- d. Set $m = k$;
- e. Then, the peak location is determined by using Eqs. 6, 7 and 8.

Black's peak search method

A similar but simpler approach in calculating the coefficient $c[k]$ was proposed by Black [7]:

$$c[k] = \exp\left(\frac{-k^2}{2\sigma^2}\right) \quad (13)$$

The implementation of Black method in Y-Spect is exactly the same as of Routti-Prussin previously mentioned.

Sterlinski's peak search method

A different approach in locating the peak position was proposed by Sterlinski [8,9], which is not based on second derivative values, but on the peak area and its standard deviation, as follows:

$$L[i, m] = mN[0] + \sum_{k=1}^{m-1} A[m, k] * B[i, k] - C[m] * D[i, m] \quad (14)$$

With: $A[m, k] = m - 2k + 0.5$;
 $B[i, k] = N[i - k] + N[i + k]$;
 $C[m] = m - 0.5$;
 $D[i, m] = N[i - m] + N[i + m]$.

$$S[i, m] = \sqrt{m^2N[0] + \sum_{k=1}^{m-1} A[m, k]^2 * B[i, k] - C[m]^2 * D[i, m]} \quad (15)$$

$$SS[i, m] = \frac{L[i, m]}{S[i, m]} \quad (16)$$

Where:
 $m =$ integer number = width;
 $L[i, m] =$ the peak area;
 $S[i, m] =$ the standard deviation of the peak area.

The peak is then located at data point i , which has $SS[i, m]$ value \geq threshold value.

Block's peak search method

Based on the statistical correlation between the shape of a peak in the spectrum and an assumed peak shape, Block [9,10] introduced the followings:

$$h[i, m] = \sum_{k=-m}^m g_k * \sum_{k=-m}^m g_k c_k N[i + k] - \sum_{k=-m}^m g_k c_k * \sum_{k=-m}^m g_k N[i + k] \quad (17)$$

$$\Delta h[i, m] = \sqrt{\sum_{k=-m}^m g_k * \left[\sum_{k=-m}^m g_k c_k^2 \sum_{k=-m}^m g_k - \left(\sum_{k=-m}^m g_k c_k \right)^2 \right]} \quad (18)$$

$$R[i, m] = \frac{h[i, m]}{\Delta h[i, m]} \quad (19)$$

$$c_k = \exp\left(-2.773 * \left(\frac{k}{FWHM}\right)^2\right) \quad (20)$$

$$g_k = \exp\left(-2.0 * \left(\frac{k}{FWHM}\right)^4\right) \quad (21)$$

Where:

$m =$ integer($1.1 * FWHM$);

$FWHM =$ a user supplied constant = full width at half maximum;

$h[i, m] =$ peak's height;

$\Delta h[i, m] =$ standard deviation of peak's height.

The peak is then located at data point i , which has $R[i, m]$ value ≥ 2.0 [10].

Savitzky-Golay's peak search method

Savitzky and Golay [11,12] have developed an elegant general coefficient $c[k]$'s based on polynomials of order N . For calculation of second derivative values from raw spectrum data, the $c[k]$'s can be written in matrix form as follows:

$$c[k] = \sum_{n=0}^N \{(A^T \cdot A)^{-1}\}_{2n} k^n \quad (22)$$

Where:

A is matrix of element $A_{ij} = i^j$;

$i = -m$ to m ;

$j = 0, \dots, N$;

$m =$ integer number.

The algorithm developed by W. H. Press *et al* [12] for calculating $c[k]$'s from Eq. 22 is implemented in Y-Spect to calculate $SD[i, m]$, $SSD[i, m]$ and $SS[i, m]$ of Equations 7, 8 and 6, respectively. Then, the similar criterion for determination of valid peaks is applied, i.e., the data points which have $SS[i, m]$ values \geq threshold value.

Peak fitting

Any peaks found in the spectrum data, whether singlets or multiplets, are fitted to a summation of Gaussian-, Left- and Right-Tail- [13], and Background [13] functions, namely:

$$y(x) = \sum_{k=1}^K G_k(x) + L_k(x) + R_k(x) + BG_k(x) \quad (23)$$

$$G_k(x) = A_k \exp \left[- \left(\frac{x - B_k}{C_k} \right)^2 \right] \quad (24)$$

$$L(x) = D_k \exp \left(\frac{x - B_k}{C_k} \right) \operatorname{erfc} \left(\frac{x - B_k}{C_k} \right) \quad (25)$$

$$R(x) = E_k \exp \left(- \frac{x - B_k}{C_k} \right) \operatorname{erfc} \left(- \frac{x - B_k}{C_k} \right) \quad (26)$$

$$BG_k = P_{0k} + P_{1k}x + \dots + P_{Nk}x^N \quad (\text{polinomial}) \quad \text{or} \\ = S_{0k} + S_{1k} \operatorname{erfc}(x - S_{2k}) \quad (\text{step}) \quad (27)$$

Where:

$K=1$ for singlet and ≥ 2 for multiplet;
 $\operatorname{erfc}(x)$ is the complementary error function.

The non-linear least-square method of Levenberg-Marquardt [14] is applied to extract the best values of all fitting coefficients A, \dots, E , and P or S , using the algorithm developed by W. H. Press *et al* [12].

Peak Identification

Any peak with energy E is considered to have matched, within a tolerance $etol$, a gamma line of energy E_o , if it satisfies the inequality $E_o - etol \leq E \leq E_o + etol$.

Suppose we have N peaks in the spectrum data which match (within a tolerance $etol$) N gamma rays emitted by a certain radioisotope, which in total emits $M \geq N$ discrete gamma rays. Then, a confidence degree is associated to this as follows [6]:

$$f_i = \exp \left(\frac{-0.16(dE)^2}{etol} \right) \quad (28)$$

$$f = \frac{O}{T} \prod_{i=1}^N f_i \quad (29)$$

Where:

- f_i is the probability of peak i to belong to a certain radioisotope;
- f is the confidence degree, i.e., the probability of all N peaks to belong to the radioisotope, or in other words, the probability of the radioisotope is correctly identified;
- dE is the difference between peak's energy i and the matching gamma ray emitted by the radioisotope;
- O is the sum of N gamma ray yields, that have matching peaks' energies;

T is the sum of all (M) gamma ray yields, which are emitted by the radioisotope.

Peak parameter

Net peak area

In Y-Spect, for each peak found in a ROI, the net peak area is calculated by integrating the Eq. 23, but excluding the background term $BG_k(x)$, within the ROI's boundaries, by using Adaptive-Simpson [12] method.

Error of net peak area

Consider a ROI, in spectrum data, located from data point LB up to data point RB. To the left and right of the ROI there are M neighboring data points each, respectively. Then, for any peak k that resides in the ROI, the corresponding error of the net peak area, σ , is determined as follows:

$$\Delta N_b[i] = N[i] - BG_k(i)$$

$$\sigma_{bk} = \sqrt{\frac{1}{2M} \left(\sum_{i=LB-M}^{LB-1} (\Delta N_b[i])^2 + \sum_{i=RB+1}^{RB+M} (\Delta N_b[i])^2 \right)} \quad (30)$$

$$\sigma_{gpa} = \sqrt{\sum_{i=LB}^{RB} G_k(i) + L_k(i) + R_k(i) + BG_k(i)} \quad (31)$$

$$\sigma = k \sqrt{\sigma_{gpa}^2 + \sigma_{bk}^2} \quad (32)$$

Where:

- $N[i]$ is the value of data point i ;
- σ_{bk} is the standard error of the background;
- σ_{gpa} is the standard error of the gross peak area;
- σ is the error of the net peak area;
- k is a user supplied constant, that corresponds to the statistical confidence level.

Minimum detectable activity

The expression of Currie's minimum detectable activity MDA is applied in Y-Spect as follows:

$$MDA = k^2 + 2k \sqrt{2 \sum_{i=LB}^{RB} BG_k(i)} \quad (33)$$

Programming

Y-Spect is designed to be a fully interactive program, with which users just have to click, click and drag, press a key, or type a value to activate a particular feature. Therefore, due to its superiority and complete programming routines, Delphi 7.0 compiler is chosen in building Y-Spect. Figure 2 shows diagrammatically several among dozens of tasks which are performed by Y-Spect.

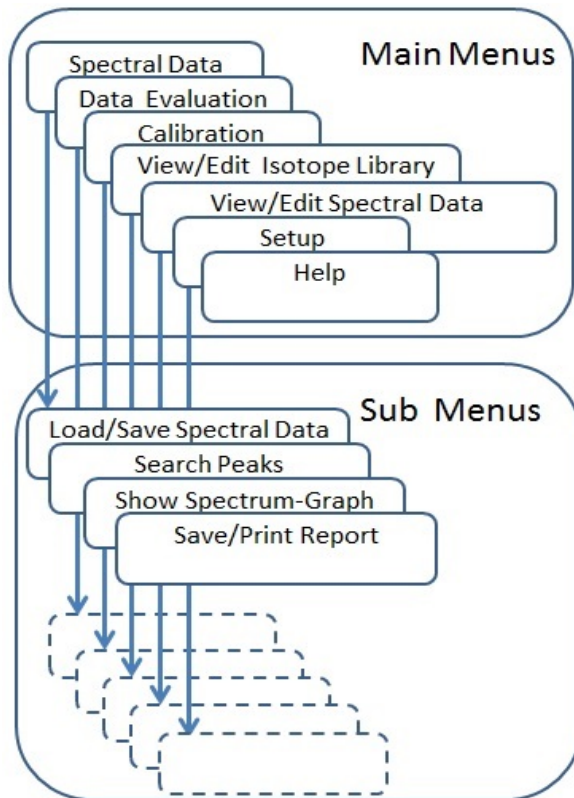


Fig. 2. Various tasks performed by Y-Spect.

Peak search process

To combine all the peak search methods mentioned above, the following programming strategies are applied in Y-Spect:

- Let the first user's chosen method search and recover the peaks in the spectrum data;
- Let the next chosen method seek and locate the peaks in the spectrum data;
- Compare all the peaks' locations found in step a) and b), respectively. New (additional) peaks are then found, when the peaks extracted in step b) have at least 2-channel separation from any peaks recovered in step a). When this is the case, the total number of recovered peaks is added accordingly;
- Repeat step b) and c) for the remaining user's chosen methods.

Region of interest determination

Even though it is theoretically possible to fit all the spectrum data with one single fitting function, the spectrum data is commonly divided into some numbers of regions of interest (ROIs). A ROI is a region/part of spectrum data that consists of successive number of data points, in which one or more peaks may contain. Y-Spect performs the following algorithm to determine ROIs in a spectrum data:

- Locate peaks with any combination of peak search methods above;
- Calculate the first derivative values of the spectrum raw data;
- For any peak found in step a), trace the first derivative values to the left side, beginning from the peak's location until a zero or negative value is reached. This is the left boundary of the ROI;
- Similarly, rightward trace the first derivative values until a zero or positive value is reached. Then the right boundary of the ROI is determined;
- If any two successively located peaks have a common right- and left-boundary, then the two peaks will have a common ROI, which its left boundary is the left boundary of the left/previous peak, and its right boundary is the right boundary of the right/next peak. This is the case, where a ROI contains two overlapping peaks (multiplet);
- If any, extend the step e) in determining a ROI with three or more overlapping peaks.

Continuum determination

The continuum is defined as the area under the peak curve or background, which is not regarded as a part of the peak. There are two continuum determination algorithms implemented in Y-Spect. Firstly, the continuum is extracted directly from the peak fitting function Eq. 23, namely, the $BG_k(x)$. Second, the continuum is reconstructed from N (specified by user) neighbour data points which reside beyond the left- and right boundary of a ROI, respectively. The continuum is then calculated by fitting Eq. 27 on those neighbour data points. Therefore, when doing this, any raw data within a ROI is automatically reduced with its corresponding continuum, and exclude the $BG_k(x)$ from Eq. 23, before performing the peak fitting process.

Peak rejection

All the peaks found from the previous Peak Search Process section are still classified as guessed peaks which are subject to rejection under some certain conditions. The rejection algorithm in Y-Spect is as follows:

- a. In any ROIs are found in the previous Region of Interest Determination section, perform the peak fitting using Eq. 23 on any (guessed) peaks found in the ROIs;
- b. For any peak resulting from the fitting process we get, calculate the followings: standard deviation (σ), peak location (μ), peak's height (H), minimum detectable activity (MDA) and full width at half maximum (FWHM);
- c. Any peak is considered as a qualified peak when all the conditions below are satisfied:
 - c.1) $\sigma > 0.0$;
 - c.2) ROI-left-boundary $< \mu <$ ROI-right-boundary;
 - c.3) $H > 0.0$;
 - c.4) MDA $>$ minimum MDA (specified by user);
 - c.5) FWHM $>$ minimum FWHM (specified by user);
- d. Any rejected peaks are deleted and the number of peaks in the corresponding ROIs is reduced accordingly;
- e. Repeat steps a) to d), until no peak is rejected.

Peak Identification

The following algorithm is followed during the peak identification process:

- a. Let us suppose that we already have a gamma ray library that consists of energy lines of different radioisotopes, increasingly sorted by energy only;
- b. Let the energy tolerance *etol* be a value specified by user;
- c. Then, only a part of the library will be considered during the peak identification process, namely the part beginning from the energy line which has a value of first peak energy minus *etol* and ending with the energy line which has a value of last peak energy plus *etol*;
- d. Among the considered energy lines in the library, find all the energy lines that have matching (within the tolerance *etol*) the peaks' energies found in the spectrum data, and their corresponding radioisotope IDs as well;
- e. For any matching radioisotope, calculate the confidence degree *f* using Eqs. 28 and 29;

- f. All those peaks are then labeled with its matching radioisotopes that have confidence degree $f \geq$ user specified confidence limit. All other peaks, which have no matching radioisotope, are labeled as unknown.

For accurate and precise peak identification, Y-Spect is provided with a complete gamma library, which consists of 16089 gamma energy lines from 1420 different radioisotopes. The library is generated from ENDF/B-VII.0 by using a special code for converting from ENDF-6 format to Y-Spect library format.

Escape- and sum peak identification

When the escape peak identification feature is activated, the peak identification process is extended to including all escape- and sum peaks that might exist in a radioisotope. This special feature is introduced for the first time ever in Y-Spect using the following simple algorithm:

- a. For each energy line which belongs to the identified radioisotope above, do the followings:
 - a.1) Create two new energy lines, which have the values of energy line minus 511 keV and of energy line minus 1022 keV; those two lines are the escape peaks.
 - a.2) Check whether there exist one or two of the existing peaks in the spectrum data which matches either one of the two escape peaks;
 - a.3) If such a peaks are found, then label the peaks as the escape peaks of the corresponding radioisotope;
- b. For each radioisotope which has been identified above, do the followings:
 - b.1) One by one, sum up any of the radioisotope's energy line with its corresponding higher energy lines, to create sum peaks;
 - b.2) Check whether there is one peak in the spectrum data which matches one of the sum peaks;
 - b.3) If such a peak is found, then tag the peak as the sum peak of the radioisotope.

RESULTS AND DISCUSSION

General features

By exploiting many sophisticated programming routines available in Delphi 7.0

compiler, Y-Spect has been developed as a fully interactive program which has a variety of features such as:

- a. Automatic and manual peak search and fitting;
- b. Automatic and manual ROI and continuum determination;
- c. Peak identification;
- d. Display of raw spectrum data, smoothed spectrum data, and first- and second-derivative;
- e. Spectrum data smoothing: moving window average and Savitzky-Golay;
- f. Readable spectrum data format: Aptec MCA v. 5.4 & 6.3, Tennelec/Nucleus PCA I, II & III, Canberra S-100 MCA (Single and Dual spectrum), ASCII data file, ToolKit TKA, IEC-1455/ IEEE-Std-1214-1992, ORTEC (CHN/SPC/UFO) and IAEA ASCII SPE;
- g. Calibration: energy, resolution and detector efficiency;
- h. Data evaluation: centroid, identified radioisotope, confidence degree, net peak area, standard error, and minimum detectable activity (MDA);
- i. View/Edit radioisotope/gamma library;
- j. View/Edit spectrum data;
- k. Setup: graphic/text appearance, peak search method, spectrum data smoothing, etc.;
- l. Online help;
- m. Limitations: Spectrums channels = 16×1024 ; ROIs = 2×1024 ; ROI's width = 2×1024 channels; Overlapping peaks in a ROI (multiplet) = 20; Identified isotopes = 3×1024 , and Isotope library's energy lines = 16×1024 .

The results of implementation of all methods and algorithms discussed in the previous sections are depicted on the following Fig. 3 through Fig. 9.

Automatic peak search and fitting

Figure 3 shows the result of Y-Spect peak search and fitting on a spectrum data of irradiated soil sample. The peak IDs are hidden for graphic clarity purpose only. In this process, the peak search and fitting is performed in automatic mode. Five peak search methods are activated to work simultaneously, i.e., Mariscotti, Phillips-Marlow, Robertson, Routti-Prussin and Savitzky-Golay. In total, 101 peaks are recovered from the spectrum data.

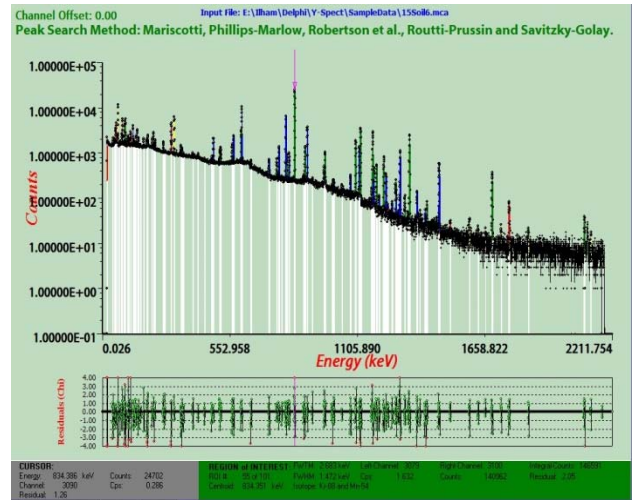


Fig. 3. Peak fitting on spectrum data of an irradiated oil sample.

Manual peak search and fitting

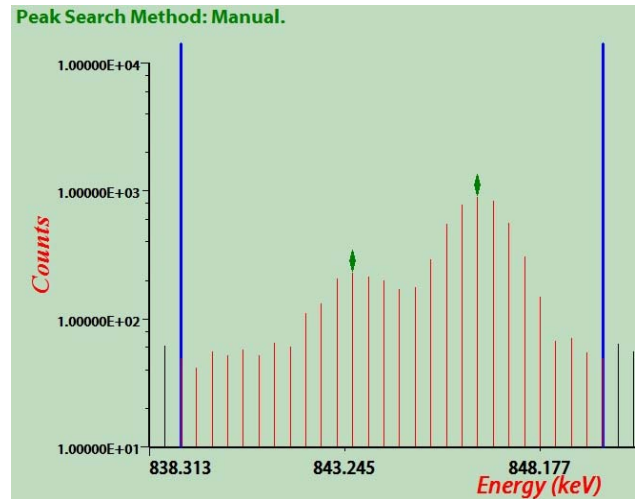


Fig. 4. Setting up the manual peak search and fitting.

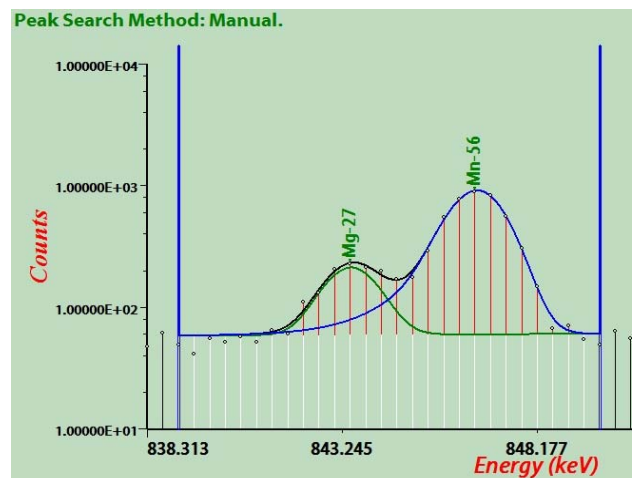


Fig. 5. After executing the manual peak search and fitting.

Figure 4 above shows how a user performs the manual peak search and fitting. Interactively, put and click the cursor on or near to any data point that

will be regarded as the left boundary and press the “L” key on the keyboard. The vertical line should appear, symbolizing the left boundary of a ROI. Next, similarly determine the right boundary, but press “R” key to set the right boundary of the ROI. The right vertical line will appear. Then, put and click the cursor on any data point, where the peak supposes to be. Pressing the “Y” key will mark a diamond symbol on the tip of that data point. Do the same action for the second peak. Finally, press the “X” key and manual peak search and fitting will be executed, as depicted on Fig. 5.

Tail function

The success of Y-Spect in implementing the Tail-function is shown on Fig. 7 which corrects the peak area of Al-28 significantly compared to one without Tail-function (see Fig. 6).

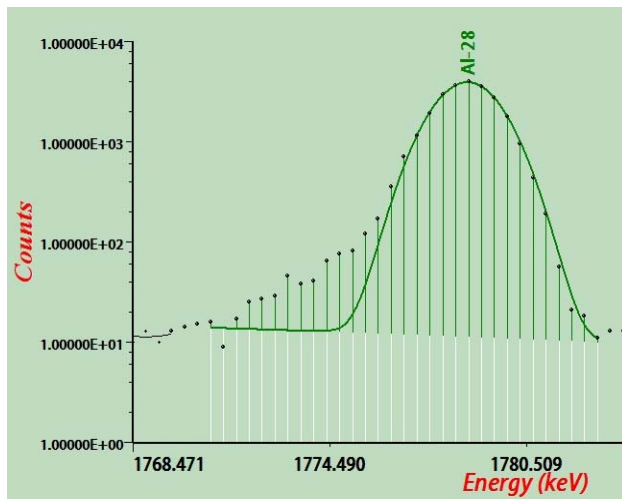


Fig. 6. Peak fitting without Tail-function.

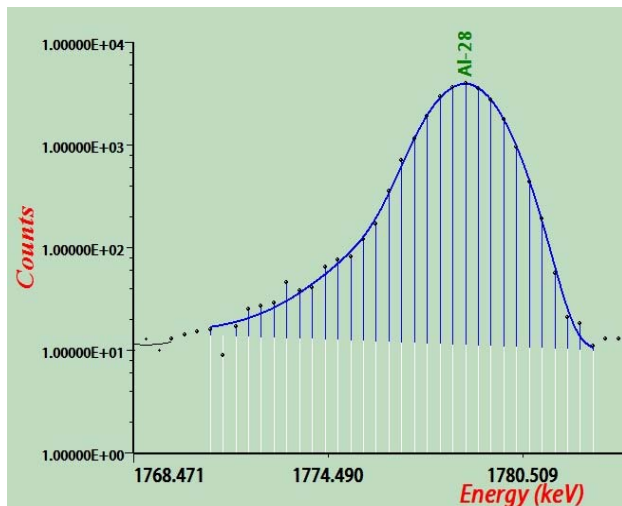


Fig. 7. Peak fitting with Left-Tail-function.

Escape- and sum peak identification

Figure 8 shows the result of automatic peak search and fitting on a spectrum data that was collected from a Co-60 standard source. The counting system setup was intentionally set improperly with the source being put too close to the HP-detector so that some spurious peaks appeared. Two tiny peaks were identified as unknowns. However, when the escape-/sum peak feature of Y-Spect is activated, Fig. 9 clearly shows that the tiny peaks are really true peaks, i.e. the escape peaks of Co-60. Further, the rightmost peak, which previously identified as 2505 keV Co-60, is now also labeled as Co-60S, namely the sum peak of Co-60. This is more reasonable, as the true yield of 2505 keV Co-60 is in fact much smaller.

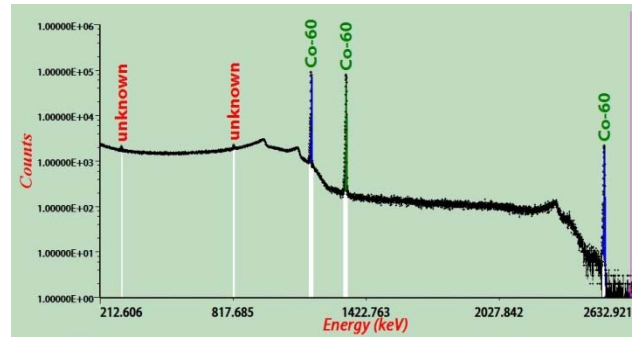


Fig. 8. Peak identification without activating escape-/sum peak feature.

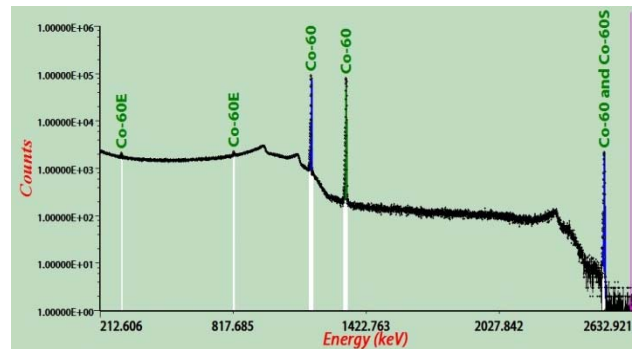


Fig. 9. Peak identification with escape-/sum peak feature activated.

CONCLUSION

Eight popular peak search methods, namely, Mariscotti, Phillips-Marlow, Robertson, Routti-Prussin, Black, Sterlinski, Savitzky-Golay and Block, as well as two basic methods, namely, Bare-Eyes and First Derivative, have been successfully implemented in a single fully interactive gamma spectrometry analysis program named Y-Spect. The peak fitting has been shown to work smoothly both in automatic and manual modes. The peak identification in Y-Spect, especially its escape-/sum

peak feature, has been proven useful to recover the significant unknown peaks as escape- or sum-peaks of some certain radioisotopes.

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