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Intercomparison of gamma ray analysis software packages

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FOREWORD

With the advances in personal computers, software packages started to play a key role in the control, acquisition and validation of the data in nuclear experiments In particular, because of the wide range of applications of gamma ray spectrometry, gamma ray spectrum analysis software packages are among the most used software in any nuclear laboratory They are being used in such important applications as environmental studies, low level monitoring, neutron activation analysis, accelerator based nuclear analytical techniques, and a number of medical applications On the other hand such software packages are expensive Therefore, it would be of general common interest to have precise and specific information available on the present status and performance of advanced gamma ray spectrum analysis software

The IAEA undertook an intercomparison exercise to review available software This TECDOC describes the methods used in the intercomparison exercise, characterizes the software packages reviewed and presents the results obtained Only direct results are given without any recommendation for a particular software or method for gamma ray spectrum analysis

Since this report covers a wide selection of commercially and non-commercially available software and reports their performance under different circumstances, it reflects to some extent the present state of the art in the field of gamma ray spectrometry analysis software

This TECDOC will be useful to a wide range of persons, including university students, technical staff doing gamma ray spectrometry, software programmers, scientists interested in technical aspects of data analysis in gamma ray spectrometry, software operators and executive directors or project managers who might be involved in setting up a project in this field or involved in the process of purchasing equipment and software.

The IAEA is grateful to M Blaauw for his work on the drafting and editing of the manuscript S Fazinic and V Osorio of the Division of Physical and Chemical Sciences were the IAEA officers responsible for this publication

EDITORIAL NOTE

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CONTENTS

Symbols used

In this document a number of symbols are adopted in order to catch the attention and provide a fast guide to the reader. They are as follows

⇧ Advantages issues

⇩ Disadvantages

⊗ Improper performance or error encountered during the operation of the software. This is more known as a **Bug** in the program

Tips or Hints on a certain issue

☞ **For Notes**

The two first are purely based on the subjective opinion of the participants and authors of this report.

A companion diskette with the set of test spectra and the programs for processing the test results is attached.

CHAPTER 1: INTRODUCTION

With the advent of powerful computers and structured programming languages, the software has reached an important level as the "logical controller" at different stages; from a single instrument to an entire computer-controlled experiment. That is also the case for software packages in nuclear instruments and experiments.

Today, software in nuclear techniques and experiments controls the instrument's operation, performs the data acquisition, storage and their validation and analysis.

In particular, because of the wide range of applications of gamma ray spectrometry, software packages in this field are among the most used. There is a vast selection of commercial and open-domain software packages that has been designed for the efficient and correct analysis of high-resolution gamma ray spectra. It is the aim of this intercomparison to test and describe the abilities of 12 such software packages.

In the past, similar intercomparisons have been made and reported in the literature[1–6]. They all deal, in one way or the other, with topics like:

- precision of the programs finding peaks (large, small ones in low baseline, small ones on the Compton edge, etc.),
- precision finding multiplets,
- accuracy and correctness performing energy, FWHM and efficiency calibration,

and many others.

They all rely on different sets of test spectra [2, 3], which in many cases did not represent real measured spectra and lacked statistical correctness. On the other hand, the ANSI standard 42.12, section 8 [7], specifies methods to verify the performance of such software packages. The basic concepts of this standard were applied to selected programs by Koskelo [8–10].

After an Advisory Group meeting (AGM) organised by the IAEA it was recommended to perform an intercomparison of gamma ray spectrum analysis software based on a new set of test spectra [11].

This time, the main objective of the proposed intercomparison was to focus on aspects such as:

- the ability of the programs to determine the peak areas and the peak area uncertainties,
- the peak positions and the peak position uncertainties,
- and the statistical control and stability of reported results.

The idea is: "It is not so important how successful the program is in finding (or not) a small peak (in different situations), as much as how the found peak is reported and how stable is that finding." Meaning, if a program finds a small peak on a large baseline, it is very difficult to judge its existence, in this case it is more important to have it reported with corresponding large uncertainty. A program that missed such a small peak should not be "penalised" as much as in the previous intercomparisons; because such a peak is "doubtful" and the amount of information that it might carry can be poorly extracted.

The above-mentioned phrase also means that it is important that results are correctly reported in statistical meaning and that a program should operate and give stable results.

These were the syllabus and objectives of our task.

In this report, the task, methods and results of the intercomparison are presented in order to assist the potential users of such software and to stimulate the development of even better γ ray spectrum analysis software.

A companion diskette is attached to this TECDOC. It contains the set of test spectra and the software for processing the test results.

CHAPTER 2: THE TASK

2.1. Procedure for testing the spectrometry programs

The first stage of the intercomparison is the preparation of the test spectra. This is described in detail in the next chapter. However a short description of the spectra is relevant in this part of the report.

The list of test spectra is as follows:

CALIB ASC	calibration spectrum containing Co-57, Cs-137, Na-22, Mn-54 and Co-60.
STRAIGHT.ASC	Ra-226 + progeny spectrum, counted for 2000 s.
DISTORT ASC	same as above, but counted in the presence of a Am-241 source to induce high-energy tailing.
ADD1N1 ASC	Sum of two Ra-226 spectra, one of them shifted by 3 channels to the right.
ADD3N1 ASC	Sum of two Ra-226 spectra, one counted for 2000 s, one for 667 s, the second shifted to the right by 3 channels.
ADD1N3 ASC	Sum of two Ra-226 spectra, one counted for 2000 s, one for 667 s, the second shifted to the left by 3 channels.
ADD10N1.ASC	Sum of two Ra-226 spectra, one counted for 2000 s, one for 200 s, the second shifted to the right by 3 channels.
ADD1N100.ASC	Sum of two Ra-226 spectra, one counted for 2000 s, one for 20 s, the second shifted to the left by 3 channels.

The participants in the workshop[1] had the responsibility of testing either one or two programs each from the 12 programs that were available for the test[2] All the participants were considered experienced γ ray spectrometrists. They also represented a wide-range of users: from developed laboratories to spectrometrists from developing countries. Among the participants there were also experienced programmers and persons with experience in statistical analysis of data

All the programs were tested as received on original diskettes as provided by the manufacturers, together with protection keys (if there was any) and the full documentation as it is distributed on commercial basis or the documentation "as received" from the manufacturer for the participation in the intercomparison No "special made" software was accepted for the intercomparison.

Each participant was asked to spend at least 4 hours familiarising himself with the manuals before attempting to install the corresponding software in his assigned computer. The computer capabilities and configuration were also carefully done in order to match or exceed the requirements of the manufacturers

☞ **As a separate exercise, programs were tested in different hardware configurations or drivers: e.g. double-space drivers (like Stacker®) , running with many TSR programs in RAM, SCSI drivers, etc. This was done only with the purpose to test the stability of the operation of the programs.**

[1] See Contributors to Drafting and Review for complete list of participants.

[2] See Appendix II for complete list of tested software packages and their providers

After the programs were installed in the respective computers, first energy and shape calibration was performed using the spectrum CALIB and a reference list of peaks, as follows:

Channel	Energy (keV)
301	122.06
1281	511.00
1661	661.66
2097	834 84
2951	1173 24
3207	1274 54
3353	1332 50

The reference lists specify peak positions in terms of energy. To separate the problem of peak position determination from the simpler problem of energy calibration, the conversion from channel to energy was performed by a program that applied the same energy calibration to the output of all programs, allowing for different methods of numbering of channels: some programs start counting at channel # 1, others at # 0 Also, it was found that, for the added spectra, a slightly different energy calibration is optimal than for the "straight" and "distort" spectra For both groups, a quadratic energy calibration was applied. For the added spectra, the relation between peak position p and energy E used is given by

$$E = 2.78 + 0.396952p - 4\ 0x10^{-8} p^2$$

and for the "straight" and "distort" spectra

$$E = 2.78 + 0.396952p - 7.0x10^{\ 8} p^2$$

The same conversion program yielded output in a standard format similar to the format of the reference lists, containing peak positions in terms of energy and peak areas, both with their absolute 1 standard deviation uncertainties. This step was not entirely trivial, because only a few programs did report uncertainties in the peak positions, i.e. Gamma-W, Hypermet-PC and Sampo90 For all the other programs, which reported energies with two or more digits after the dot, implying uncertainties of less that 0.01 keV, these uncertainties were set to 0.01 keV Also, not all programs reported 1 standard deviation uncertainties The reported uncertainties were converted to one standard deviation absolute uncertainties according to the definitions given in the documentation of the programs

The second stage of the comparison was to analyse the STRAIGHT and multiplet (ADD*) spectra in what we called the **Automatic Mode**, using the calibration above-mentioned This means a non-interactive analysis based on the default parameters for spectrum analysis provided by the producer of each program or in the absence of default parameters the values suggested in the documentation of each program in the "Getting Started" or equivalent chapter. The idea was to run each of the programs in the same way that an inexperienced end-user or beginner would be expected to do so The results were saved as ASCII files and processed by the comparison program (described latter in this chapter)

The third stage was to analyse the same spectra again in non-interactive mode but this time using *the best possible set of parameters*[3] for analysis. The only restriction being that energy and shape calibration data should come from the test spectrum. This part of the test tries to emulate as much as possible the results that an expert user would get from a large set of spectra when an interactive analysis would not be possible The STRAIGHT spectrum was used to optimise the different analysis parameters by experimenting with different values and checking the results The same parameters were applied to the ADD* spectra. To chose the best possible set of parameters the documentation provided was, of course, heavily referred

[3] Up to the judgement of the experimenter or user

Finally, a fully interactive analysis was performed for the STRAIGHT spectrum, using as initial values of the parameters the optimum values found in the third step. During the interactive analysis all the possibilities for improving the results **in each region of interest** were used This depends very much on the program being tested as some programs allow to change many items (add or delete peaks, change the fitting regions, background models, etc) while other programs allow only to add or delete peaks Certainly, the quality of the results in this test are more subjective than others and also will depend on the flexibility of the program and the accuracy with which each program interprets the operator commands[4]

A last test was devised and applied to some of the programs. In this test the STRAIGHT spectrum was used and a list of all the peaks of a ^{226}Ra spectrum was provided to the operator This time the participants were asked to use the interactive features of the programs in order to reproduce the list of references as accurately as possible Due to the problems described above this last test was not considered successful as no significant improvement in the results could be achieved for the tested programs.

All the results for each type of test were correspondingly coded. The analysis and processing of the results were done only after all tests were performed.

CHAPTER 3: THE TEST SPECTRA

The so called "**Test Spectra**" are a set of *gamma ray* spectra that served as bases and common spectra analysed with the different software packages during the intercomparison.

They were acquired experimentally, following most of the recommendations made by an Advisory Group Meeting (AGM) held in Vienna, December 1994 at IAEA HQ, and reported in its Final Report [11] During this AGM the need for new reference spectra was emphasised, to be used for the intercomparison of different γ ray spectrum analysis software packages and for quality assurance and quality control purposes. It was stated that these new test or reference spectra should be **real and measured spectra** which should therefore contain no model dependent peculiarities nor any unphysical characteristics. A subsequent meeting would then have the task to generate such spectra to be used for a software intercomparison in another action

3.1. Definition of the task

It was agreed that the reference set of spectra are to be measured with a high-purity germanium detector which contains a p-type crystal The detector shall have a relative efficiency of not more than 20% in order to supply test spectra which do not significantly deviate from the spectra measured in many of the nuclear analytical and research laboratories. The resolution (FWHM at 1332 5 keV) of the detector should be good (around 1.8 to 2.0 keV) and the crystal should exhibit no major defects which might show up as peak shape distortions in the measured spectra

The measurements of spectra should be performed in a temperature-stabilised environment where major variations of electronic properties due to variations of the ambient temperature can be excluded The electronic components used should be commercially available units which are neither specially configured nor modified in any way The setting of the amplifier and ADC should be such that the energy range going up to ca 3000 keV is measured in an 8k (8192 channels) spectrum In

[4] Some tested software proved to be extremely reluctant to perform the fitting, the way the operator wanted

contrast to the recommendation of the former AGM the experts in this meeting have decided to measure 8k spectra rather than 16k spectra. The reason for this deviation from former proposals is that the commercial market mostly supplies ADCs with a conversion gain of 8k and only new units allow to digitise onto 14-bit numbers. In addition, many existing MCA units do not support 16k spectra. Displaying an energy range of ca. 30 keV to ca. 3000 keV on 8k channels, the resolution function (FWHM vs channel number) is expected to span the range from FWHM=2 channels at the low energy end to FWHM=6 channels at high energies. This would allow to test also the ability of codes to treat very narrow peaks in a correct way.

The following basic rules pertinent to this task are defined:

- Spectra must contain only real, measured data without any synthetic or model-dependent modifications.
- Peaks in the spectra must have peak areas which span the range from >50000 counts (very large) to below the detection limit.
- Manipulations of spectra must not modify the correct statistical nature of the counts per channel distribution, i.e.:

  Spectra must not be scaled,

  Spectra must not be subtracted,

  Spectra may be added.

- Manipulations of spectra must not modify intrinsic dependencies of the detector used, such as e g the resolution function or the Peak to Compton ratio (P/C) as a function of the peak energy
- Numbers to be quantified must be obtained in such a way that no system- or model-dependent properties will influence them.

For the generation of multiplet peaks with known ratios of the peak-areas, however, one has to violate some of the above restrictions. It was decided that multiplets should be generated through the adding of two spectra which were measured under absolutely identical conditions but with different real counting times Thus, *the ratio of the areas of the same peak is well known through the ratio of the counting times* The multiplet nature should be generated in such a way that one spectrum is shifted by a small number of channels before making the adding procedure. In this way, well characterised multiplets can be generated preserving at the same time the exact nature of the resolution function Most, if not all spectrum analysis programs, however, make a similar assumption that the variance of closely neighboring peak-shape functions is the same, i.e overlapping or closely neighboring peaks are analysed using the same FWHM value for the functions. This violation of the above restrictions is considered permissible as long as the shifts are small with respect to the FWHM of peaks at low energies in the spectrum It was decided to restrict these shifts to less than *twice the FWHM* values at low energy which is less than *4 channels*. This will lead to peak separations of ca. 1.5*FWHM at low energies and ca. 0.5*FWHM for peaks above 2 MeV It should be noted that the adding of a shifted spectrum will lead to unphysical distortions in the first and last channels of the resulting spectrum. These channels may not be used for any kind of determinations or quantification.

It was decided that several series of spectra should be measured out of which the reference spectra for the intercomparison are generated. The radioactive source or sources to be used should emit a complex photon spectrum which is measured as a gamma ray spectrum with many peaks It is desirable that the spectrum *a priori* contains clearly separated singlet peaks as well as multiplets Radioactive sources available for the measurement were

- 40 kBq of ^{243}Am which generates a spectrum with lines up to 334 keV,
- 70 kBq of ^{227}Ac which generates a spectrum with lines up to 1109 keV,
- 160 kBq of ^{226}Ra (and progeny) which generates a spectrum with lines up to 2448 keV

All sources are sealed sources which have passed the prescribed wipe tests The ^{226}Ra source was also tested for the emanation of radon and no significant outgassing has been found.

It is finally agreed that the test spectra should be measured from the ^{226}Ra source at a large distance between the source and the detector endcap

The spectrum measurement scheme was set up in the following way

- 20 spectra were measured for 2000 seconds real time each, from which was determined the stability of the measuring set-up The sum spectrum of these 20 was used to generate the set of known peak positions and relative peak-areas
- A "*calibration*" spectrum from commercially available radioactive standards sources was acquired which have a simple photon emission pattern This spectrum can be used for any kind of calibration purpose required from the analysis programs. The calibration spectrum was decided *not* cover the whole range of energies as found in the test spectra, to force the testing of the physical meaningfulness of any calibration curves determined and used by the analysis programs
- A set of spectra was measured for 2000 seconds real time each, which was used later to perform the summing of multiplets No spectrum was used twice in the summing procedure
- Several spectra for known real times of 667 seconds, 200 seconds, and 20 seconds were acquired, which were added with a 3 channel shift to one of the above 2000-seconds spectra This generated multiplets with known peak-area ratios of 3 1, 10:1 and 100 1 with respect to the peaks in the 2000-seconds spectrum
- A spectrum where the peak-shape is distorted through random coincidences with photons coming from another highly active ^{241}Am source has been measured as well This source completely distorted the spectrum in the low-energy regime but the only significant influence at higher energies was through random coincidences alone, resulting in high energy tailing of all peaks

3.2. The measuring set-up

The measurements were performed in room no. B09ZK92/1 in the B-building of the IAEA headquarters The room is situated in the centre of the building, it has no windows and the air-condition keeps its environment conditions very stable The following units were used for the test

Semiconductor Detector	p-type coaxial, one open end, closed end facing the window Canberra model number GC1318-7500 High voltage +5000 Volts Relative efficiency 12 6% Resolution at 1332 5 keV = 1 72 keV Resolution at 122 keV = 700 eV P/C = 47 3 30 litres dewar with vertical dipstick
Preamplifier	Canberra model 2001C
High Voltage BIAS	Canberra model 3125, operated at +4500 Volts
Linear Amplifier	Tennelec TC244 with the following settings Coarse gain *20 Fine gain *1 000 Peaking time 8 microseconds Pulse shape Gaussian

	BLR manually set, symmetric, using an oscilloscope for control Input polarity negative Output unipolar Pileup rejector off
ADC:	Canberra model 8077 with the following settings: Range and Gain 8K Offset 0 Peak detect AUTO PHA mode No coincidence condition
MCA:	Canberra S-100 plug-in card in PC with an Intel 25 MHz 80486 CPU

Resulting in a set of spectra as follows:

Table 1 Set of measured spectra and their specifications

Spectrum name	Real time in seconds	Remarks
SD0000.MCA through SD0019.MCA	2000	Automated counting with Canberra S100 software
SD0020.MCA	2000	For comparison, if needed. This spectrum was measured 6 hours after termination of the above automatic task
SD0021.MCA	667	
SD0022.MCA	200	
SD0023.MCA	20	
SD0024.MCA	2000	
SD0025.MCA through SD0029.MCA	2000	Another automatic task
SD0030.MCA	2000	Same set-up as before but 37 kBq of additional ^{60}Co on the endcap
SD0031.MCA	2000	Same as before but with several additional sources present
SD0032.MCA	6000	A set of 37 kBq each calibration sources measured at 169 mm distance from the endcap
SD0033.MCA	40000	The ^{226}Ra source at 178 mm distance from the endcap. High voltage turned down to +2500 Volts
SD0034.MCA	2000	The ^{226}Ra source at 178 mm distance from the endcap. High voltage at +4500 Volts. An additional ^{241}Am source with ca. 10 mCi at ca. 280 mm from the endcap.

The detector head was situated inside a small castle with 50 mm average lead thickness. The inside of the castle was covered completely with 0.5 mm of copper. The ^{226}Ra source was placed in an acrylic sample holder at 178 mm distance from the detector endcap. The set-up was closed with the 50 mm thick lead cover and no modifications to the system were allowed during all measurements with the ^{226}Ra source. Before starting the first measurement the components were set to reach thermal equilibrium for one hour with all voltages applied.

The spectra shown in the Table 1 were measured under the above conditions in the course of the following four days.

3.3. The measured spectra

The relevant characteristics of the measured spectra are displayed in the following figures.

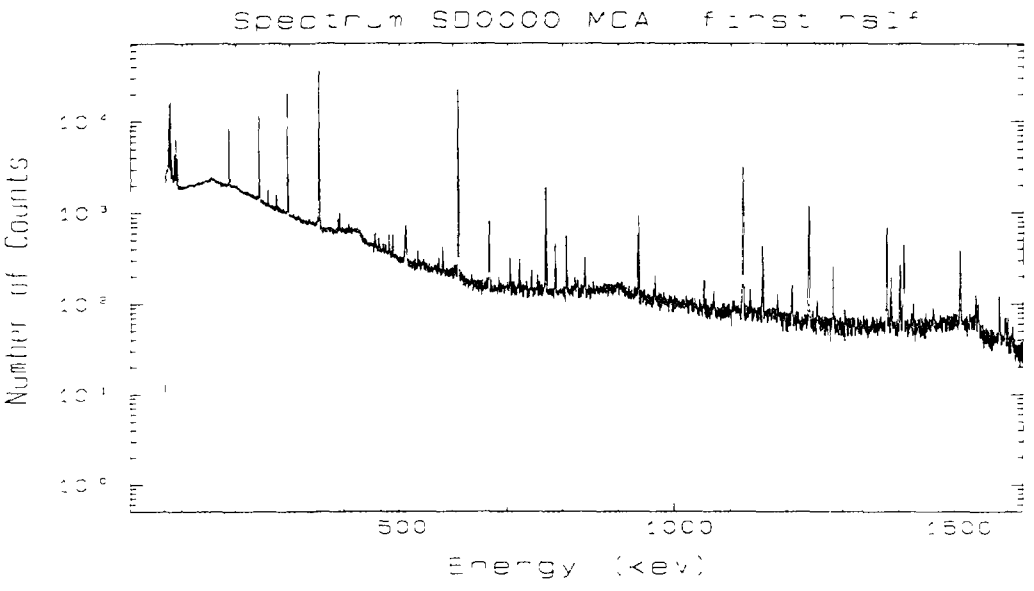


Figure 1. First half of spectrum SD0000.MCA.

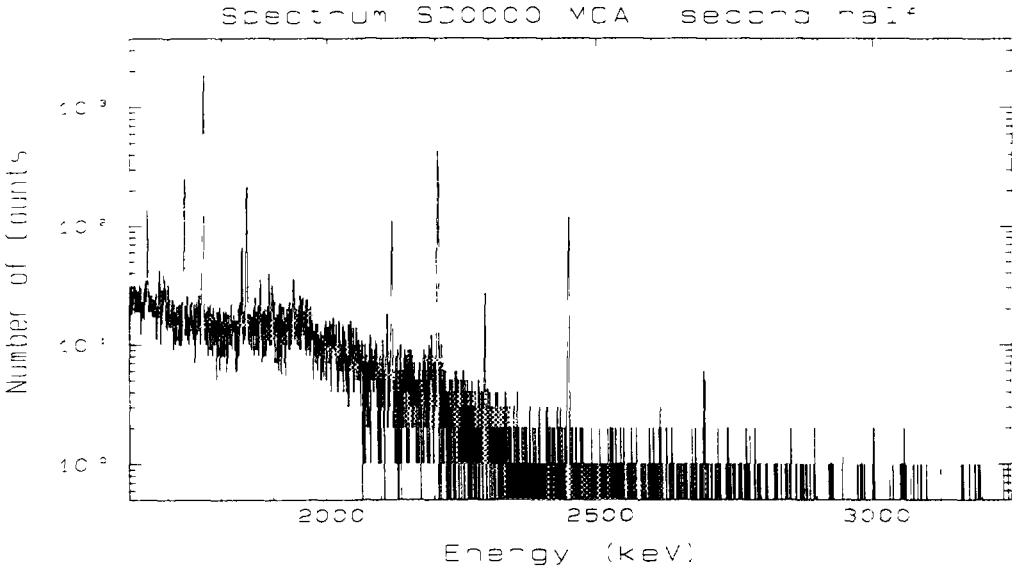


Figure 2. Second half of spectrum SD0000.

It is seen from Figs 1–4 that the spectrum contains a large number of peaks, most of which are clearly separated singlets and only a few small doublet peaks. The very closely situated peaks around channels number 3500 (see Figure 4) as well as other, smaller doublets are well suited to create complex quadruplets through adding of spectra after shifting them by a few channels.

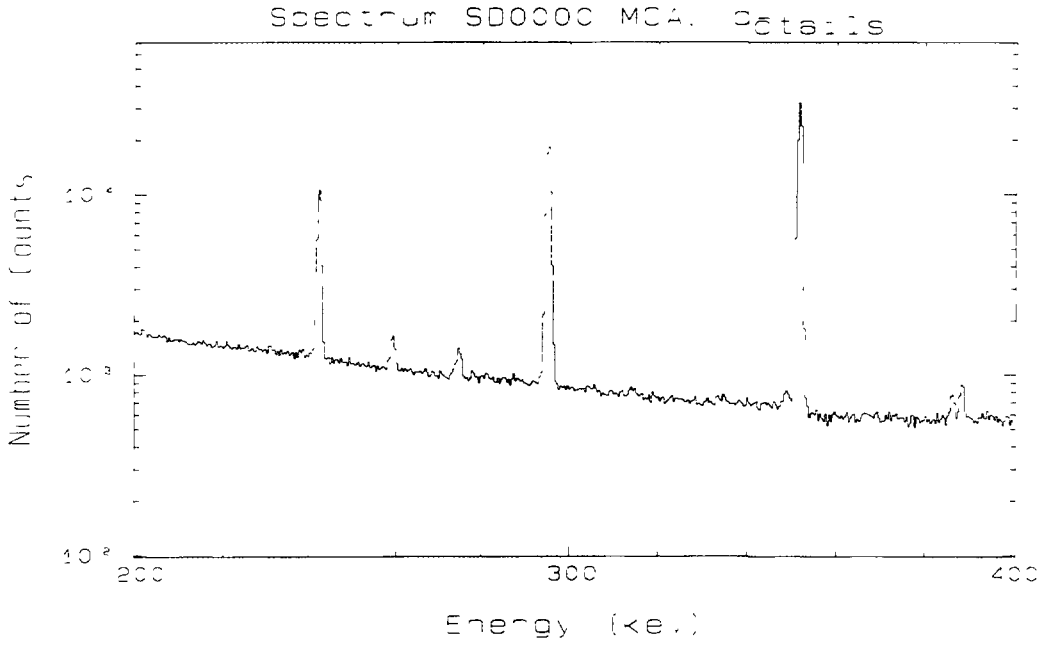


Figure 3. A detailed section of spectrum SD0000 containing singlet peaks.

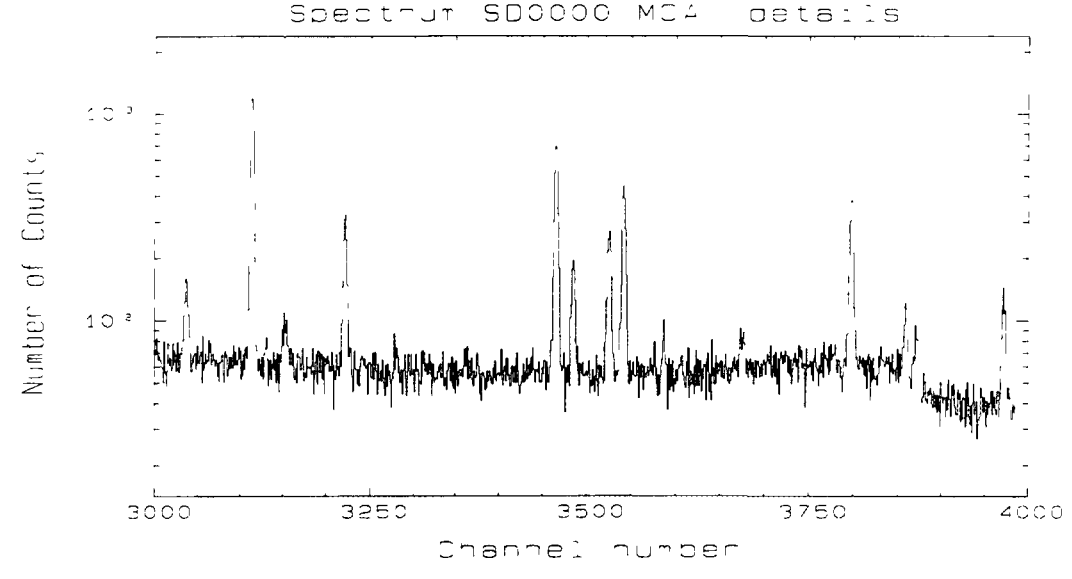


Figure 4. A detailed section of spectrum SD0000 containing a doublet peak.

All test spectra were generated from this same type of ^{226}Ra spectra as shown in Figure 1 to 4 through adding after shifting (see below). The only spectrum with different characteristics of the peaks is spectrum SD0034.MCA where a very strong source of ^{241}Am was added in order to deteriorate the peak-shapes of the ^{226}Ra peaks through random pileup. In Figure 5 the same section as in Figure 4 is shown from the distorted peak-shape spectrum SD0034.MCA for comparison.

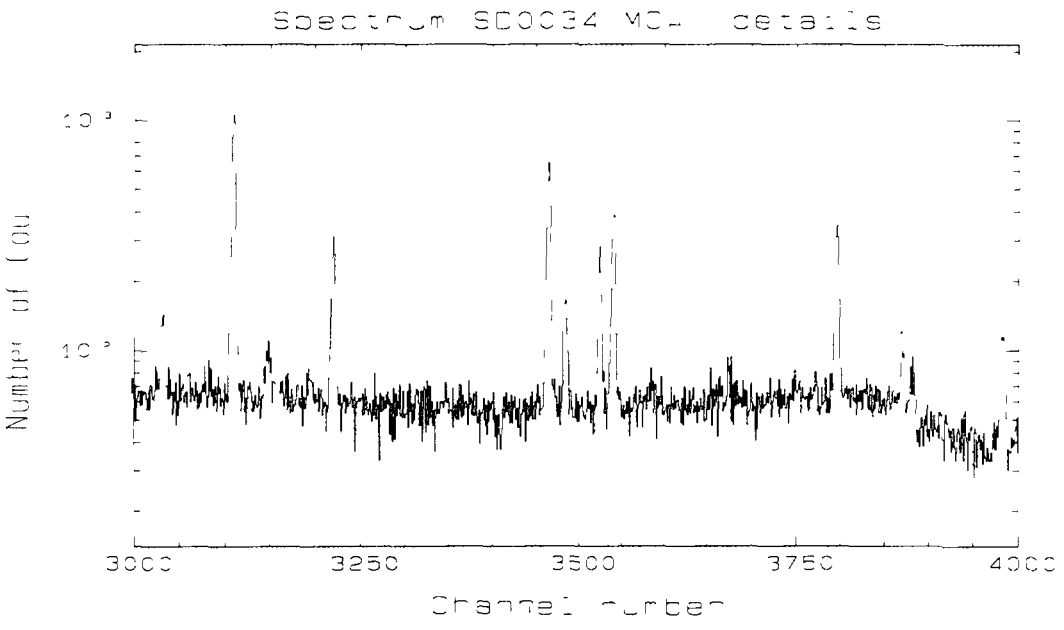


Figure 5. A detailed section of spectrum SD034 in which peak shapes are distorted due to random coincidences with low-energy photons.

3.4. Observed properties of the measured spectra

The first series of spectra (SD0000.MCA through SD0019.MCA) was measured in order to test the stability of the system and to generate reference data which may be used for later intercomparison. Several peaks out of the 20 spectra were evaluated and the peak positions as well as FWHM values were determined in order to test for the stability of the system. In Figure 6 we show the positions of a peak (ca. 1900 counts peak-area) in the 20 spectra, and Figure 7 displays the fitted FWHM values for the same peak. It is seen that the variation of the peak position is on the order of ± 0.1 keV whereas the resolution of this (small) peak varies quite considerably in the beginning of the experiment. Both quantities, the peak-position and the resolution become more stable towards the end of the experiment, which is about 16 hours after the measuring system was powered

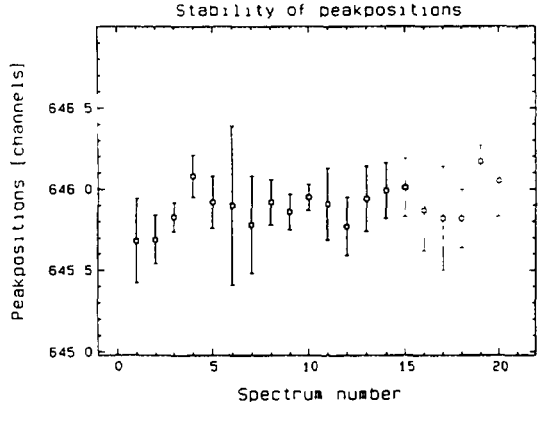


Figure 6. Positions of a peak in 20 successively measured spectra.

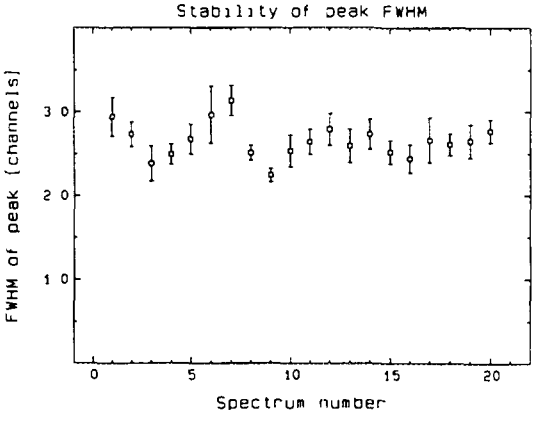


Figure 7. FWHM of a peak in 20 successively measured spectra.

3.5. Manipulations of the measured spectra

After considering the negligible instability of the measuring set-up as observed in the first spectra it was decided to sum up these 20 spectra in order to create a master spectrum which is used to extract reference data for the peak positions and peak areas. The position values were used in the intercomparison exercise for automatic analysis routines as **absolute reference values** The FWHM values are not recommended for use in any intercomparison because the values are dependent on the model used in the fitting process. The stability of the FWHM values, however, should not be dependent on the model and it can be used to determine the stability of the system Both the position and the FWHM values for the peaks are given in terms of channels which is a spectrometric quantity and does not require any secondary calibration. It is known that different computer programs define channels numbers differently, starting to count either from zero or one

For the generation of spectra with multiplets the following spectra were used

SD0024 MCA until SD0029.MCA 6 spectra measured for 2000 sec each

SD0021 MCA One spectrum measured for 667 sec

SD0022.MCA One spectrum measured for 200 sec

SD0023 MCA One spectrum measured for 20 sec

Doublet spectra were generated through shifting a spectrum by either +3 channels or -3 channels and adding it to another spectrum channel by channel. The following added spectra were generated

Table 2: Generated spectra

Operation	Characteristics	Result spectra
SD0024.MCA added to SD0024.MCA	with -3 channels shift	ADD1N1.ASC
SD0021.MCA added to SD0027.MCA	**with -3 channels shift**	ADD1N3.ASC
SD0021.MCA added to SD0026.MCA	with +3 channels shift	ADD3N1.ASC
SD0022.MCA added to SD0028.MCA	**with +3 channels shift**	ADD10N1.ASC
SD0023.MCA added to SD0029.MCA	with -3 channels shift	ADD1N100.ASC

The newly generated spectra were recorded in an ASCII format as one channel content per line The first channel of each spectrum contains a counting time which is the sum of live counting times of the two individual spectra which were summed together, the second channel contains the real time It should be noted that this counting time has limited spectrometric significance.

The final set of test spectra was conformed as follows:

CALIB.ASC: a calibration spectrum taken from weak point sources (ca. 37 kBq) of ^{57}Co, ^{22}Na, ^{137}Cs, ^{54}Mn and ^{60}Co Small contributions from other natural radionuclides are also detected in this spectrum.(originally measured as SD0031.MCA).

STRAIGHT.ASC a plain ^{226}Ra spectrum measured for 2000 sec real time This spectrum may be used for any kind of calibration needed by the software as well as for quantification purposes (originally measured as SD0020.MCA)

DISTORT.ASC. a ^{226}Ra spectrum measured for 2000 sec real time, distorted by the presence of the ^{241}Am source. The resulting peak shape distortion can be used to test the stability of analysis programs in circumstances where calibration and measurement do not agree (originally measured as SD0034.MCA)

ADD1N1.ASC a multiplet generated spectrum where the peak-area ratios are

	expected to be 1.1 within statistics
ADD1N3.ASC	a multiplet generated spectrum where the peak-area ratios are expected to be 1:3 within statistics
ADD3N1.ASC:	a multiplet generated spectrum where the peak-area ratios are expected to be 3:1 within statistics
ADD10N1.ASC	a multiplet generated spectrum where the peak-area ratios are expected to be 10.1 within statistics
ADD1N100.ASC:	a multiplet generated spectrum where the peak-area ratios are expected to be 1:100 within statistics

Due to the shift of either +3 or -3 channels the added spectra will exhibit a good separation of peaks at low energy (ca. 1.5*FWHM) whereas the separation at high energies is very poor (ca 0 5*FWHM) and many of the high-energy doublets may be indiscernible as such. The wide range of peak separations and peak-area ratios obtained allows for thorough tests of the ability of analysis programs to separate doublets automatically, with some user interference, or with methods of definition, whichever is possible or necessary.

3.6. Determination of reference peak positions and areas

As a result of the methods used to obtain the test spectra, no independent (and unbiased) method of sufficient precision and accuracy is available to determine the peak areas and positions in the test spectra It was decided that careful analysis of the summed spectrum, with a total counting time of 40,000 sec, by two experts, using two analysis programs in as interactive mode as possible, yields both positions and energies with the required precision and accuracy to compute good values for the expected positions and areas in the test spectra. The spectra measured at 40,000 sec have much worse statistics than the one measured at 2,000 sec and the proposed method is therefore valid. It was decided to use the programs GAMMA-W [13] and SAMPO 90 [14], because of previous expertise on them of the staff performing the task.

During analysis, logs were kept on each decision taken. In both programs, the shape and energy calibrations were made using the spectrum to be analysed itself and the gamma ray catalogue of Westmeier [15] The peaks used for this purpose were at 74 8 keV, 77.1 keV, 186 0 keV, 295 2 keV, 351 9 keV, 609 3 keV and 1120.3 keV. Second order energy calibration was used. GAMMA-W uses also second order fitting of the FWHM-channel dependency, SAMPO uses the linear relation between the square root of the peak width and the channel number. Knowledge of the gamma ray spectrum of ^{226}Ra and progeny were used in the determination of the peak areas and positions

With each analysis, a list was made of "*difficult*" peaks For GAMMA-W, these peaks are located at energies 275 keV, 280 keV, 295 keV, 352 keV, 511 keV, 543 keV, 703 keV, 741 keV, 786 keV, 1253 keV, 1694 keV and 1937 keV For SAMPO, these peaks are at channels 737, 785, 880, 1220, 1280, 1528, 1864, 1975, and 2074.

After these analysis runs, the lists of results were compared and matched. The results obtained for the clearly visible peaks, even the ones labeled as "difficult", were in good agreement within statistics, except for the doublet at 295 keV that is resolved differently by the two programs. This peak is therefore integrated for total area and labeled as **unresolvable** in the *reference list*. For all peaks where the agreement is good, the unweighted averages of the areas and positions reported by the two programs were taken as the reference values. As uncertainty of the reference values, the larger of the 1 standard deviation uncertainties reported by the two programs were taken Many noisy peaks were found by one program but not by the other. If these peaks have an uncertainty exceeding 20 %, they will be certainly be invisible in the test spectra with only 2000 seconds counting time and were therefore removed from the reference list In the cases where the uncertainty is less than 20 %, the spectrum was inspected visually for the presence of the peaks In all these

cases, the peak was observed visually and thus, not removed from the list. The area and uncertainty reported by the program that did detect the peak were taken as reference values

The last problem is the 511 keV peak: Its area was decided to be determined by integration

The resulting reference list was subsequently used to produce the corresponding reference lists for the test spectra by applying the identical shifts and dividing both areas and their absolute uncertainties by the ratio between the counting times of the test spectra and the reference spectrum

CHAPTER 4: THE METHOD

To evaluate the performance of the tested software and to represent the results within the scope of the objectives (explained in Chapter 1: Introduction) a **method** for processing of the results was adopted Here, it is explained in detail.

The aim of the tests for each program were.

- the quality of the peak area determination,
- the quality of the estimation of the uncertainty,
- the same for the peak position determination,
- the ability of the program to detect peaks and to properly weight them,
- and the ability to resolve multiplets.

All above for different type of gamma ray spectra.

4.1. Data handling

The overall intercomparison of the results was based on the statistical qualifier z-scores or standardized residuals This is, the differences of the magnitude reported against the one referred divided by their own uncertainties

$$z = \frac{Value_{rep} - Value_{ref}}{\sqrt{\sigma_{rep}^2 + \sigma_{ref}^2}} \qquad (1)$$

In such a way, "fair" scores will characterized the different tests, giving proper weight to misses, false hits, incorrectly quoted uncertainties, etc.

Therefore, for our specific case, the z-scores is the differences between reported values and reference values divided by their own uncertainties In those cases where both a reported area and a reference area were available ("hits"), two such z-scores could be computed:

1 A z-score related to the quality of area determination based on the uncertainties in the reference files, as

$$z_{ref} = \frac{A_{rep} - A_{ref}}{\sqrt{20\sigma_{ref}^2 + \sigma_{ref}^2}} \qquad (2)$$

2 and a z-score related to the statistical control of the analysis program based on both the reference uncertainty and the uncertainty reported by the analysis program

$$z_{rep} = \frac{A_{rep} - A_{ref}}{\sqrt{\sigma_{rep}^2 + \sigma_{ref}^2}} \qquad (3)$$

where A_{ref} and A_{rep} are the reference and reported peak area, and σ_{ref} and σ_{rep} their uncertainties, respectively Since, 20 is the ratio of the counting times of the reference spectrum and the test spectra (see Chapter 3), $\sqrt{20}\,\sigma_{ref}$ was considered the optimum uncertainty to be reported by the analysis programs Such z-scores are expected to be normally distributed with a zero mean and a unity standard deviation, i e z-scores higher than 2 or lower than -2 indicates that something is wrong at the $\alpha = 0\ 05$ level

In each comparison run

- the reference and reported[5] list of peaks were matched to begin with For each peak in the list of reference values, a partner in the list of reported values was looked for

> ☞ **The decision that a match[6] had been found was taken if the peak positions agreed to within their quadratically summed uncertainties, or if the distance between the peaks was less than 0.5 FWHM. The values for this refereed FWHM were taken from the commonly established calibration curve (see Chapter 2) as determined for the 40,000 seconds counting time spectrum**

- If no match was found in the reference list, the reported peak was considered to be a "false hit" and only the second z-score (3) could be computed, using zero both as the reference area and as its uncertainty
- If the reported area was missing, it was considered a "miss" and only the first z-score (2) could be computed

With such a method implemented, missing a noisy peak or reporting a false hit with a high uncertainty in the area do not result in high z-scores and grants a fear punctuation for the program

The same tests were designed for multiplets The added reference spectra contain doublets with separations varying from 0 4 to 1 2 x FWHM and with different area ratios

- For this test, if two peaks in the reference list matched one peak in the analysis program output, i e if both reference peaks were located within 0 5 x FWHM of the analysis result, the two reference peaks were merged before the computation of z-scores In such a way it is possible to test analysis programs determining the total area of doublets with small separation
- For test of peak positions, the same was also done if such two reference peaks were located within the position uncertainty reported by the analysis program
- Finally all the computed z-scores were squared, added and the total divided by the number of peaks in order to obtain reduced sums of squares as the final test results

For the implementation of above-described method a program "CMPSPEC" was written to perform these tasks As input, this program read two files: The file containing the reference data and the file containing the tested program's output To obtain the latter, the original output results of the different programs had to be converted to a uniform format, containing for each peak detected the peak position and absolute, one standard deviation uncertainty, the peak area and its absolute, one standard deviation uncertainty

---

[5] By the program

[6] In this report we are going to refer as a **hit** to an event when a reported value matched (within the expected deviation) a reference value A **miss** will be the opposite A **false** hit when a reported value is not in coincidence with the reference value

4.2. Peak area re-normalization

The first task performed by the CMPSPEC program was the determination of the normalization factors to be used for the correction of all peak areas for each program to compensate for possible bias in peak areas determination. This step was needed because of the of different methods for peak area determination, used by the programs. For this task the following steps were performed:

- The reference list and the measured list were matched.
- Then, using all "hits" for the case of the "straight" spectrum, a weighted average and its uncertainty of the ratios of reference peak areas and program output peak areas were determined. As its uncertainty, the internal standard uncertainty of the mean was taken. The weights used were the inversed squares of the uncertainties in the area ratios, computed from reference and reported uncertainty.
- Peak area ratios differing from unity by more than 0.1, assumed to be the results of incorrect deconvolutions, were excluded from the average.

Even though this uncertainty is the smallest that could have been taken within the rules of error propagation, the ratios found were all statistically unity, as can be seen in the Figure 27.

Since none of the re-normalization factors found for the "straight" spectrum deviated from unity significantly, as will be discussed later, the re-normalization factors were applied to the program output peak areas only in the case of the "distort" spectrum where the peak areas themselves were expected to be biased due to dead time. For this spectrum, a dead time relative to the straight spectrum of app. 9 % was thus established.

4.3. Computation of standardized residuals and reduced sums of squares

REFERENCE DATA				ANALYSIS PROGRAM OUTPUT				
E		A		E		A		z-scores
val	unc	val	unc	val	unc	val	unc	rep ref
2112.5	0.1	40	2	2112.5	0.1	0	10	-3.8
2120.0	0.1	593	6	2120.1	0.3	488	37	-2.8 -3.8
2121.2	0.1	593	6	2121.5	0.2	662	44	1.5 2.5
2194.1	0.1	16	2	2194.1	0.1	0	8	-1.7
2195.3	0.1	16	2	2195.3	0.1	0	8	-1.7
2205.6	0.1	2384	11	2205.8	0.2	1286	51	-20.8 -20.1
2206.8	0.1	2384	11	2206.5	0.1	2688	64	4.7 5.6
2207.3	0.2	0	0	2207.3	0.2	824	43	19.1 .

Figure 8. Section of z-score table, showing a "miss" at 2112.5 keV, a reasonable doublet fit at 2120.0 and 2121.2 keV, and an erroneous doublet fit at 2205.6 en 2206.8 keV, resulting in a "false hit" at 2207.3 keV.

Z-scores or standardized residuals were computed as described above for each peak in each test (for each type of spectra). A section from the comparison program (CMPSPEC) output is shown in Figure 8. From the Z-scores, reduced sums of squares χ^2 were computed for different categories of peaks.

If no re-normalization had been performed, the χ^2 for any category was computed as the sum of the squares of the z-scores in the corresponding category, divided by the number of peaks in that

category If re-normalization had been applied, the number of peaks in the category minus one was used in the division for the "hit" categories The categories and their definitions were:

1 Annihilation peak: Any peak closer than 3 keV to 511 keV.

2 High peaks. non-annihilation hits for which the ratio of reference peak area and reference peak uncertainty is larger than 10, i.e. $(A_{ref} / (\sqrt{20}\,\sigma_{ref})) > 10$

3 Small peaks on high continuum and small peaks on low continuum: Hits for which the peak area was less or more than $0.5b$, respectively, where b is the area of the continuum under the peak. Knowing that the reference uncertainties were determined from a spectrum with a counting time 20 times longer than the reference spectra, b was estimated from the reference peak area A_{ref} and its uncertainty σ_{ref} using

$$b = \frac{20\sigma_{ref}^2 - A_{ref}}{2} \qquad (4)$$

- Any match: All peaks belonging to the previous three categories, i.e high peaks, small peaks on high and small peaks on low continuum.
- Misses: Peaks, in the reference list not matched in the reported list of the programs for any of above categories.
- False hits: Peaks, in the reported list of the programs not matched in the reference list.
- Total All previous categories except for the annihilation peak.

A separate χ^2 was computed for a peak position from the differences between reference peak position and program output peak position and their uncertainties in terms of energy, analogous to the χ^2 for peak areas.

CHAPTER 5: WHAT DO THE NUMBERS MEAN?

Now that all the methodology has been explained and the tasks to be done were described, probably you got confused on the ocean of areas, uncertainties, z-scores and reduced χ^2.

So lets have a look to all of these using examples and some data.

Before anything, keep in mind the formulas described in the previous Chapter This are formulas (2) and (3) mainly. Take a piece of paper and write them and have them in front of you.

So, after processing the different test spectra we obtained a set of output files from the tested program. This set is processed by the program CMPSPEC, which gives an ASCII file illustrated in Figure 8 This output table contents:

- **Energy** and **uncertainty** for *Reference* as well as for *reported processed spectrum.*
- **Net Peak Area** and **uncertainty** for *Reference* as well as for *reported processed spectrum.*
- **Z-scores** calculated with *Reference* and *Reported uncertainties*

Let's take a look at some of the cases that may happen, just to explain the meaning of our results[7]. Here, a table of the CMPSPEC program's output is presented

[7] Here uncertainties in the energy column were omitted in order to simplify our discussion

Case No	Reference data En val	Reference data Area val	Reference data Area unc	Reported (measured) data En val	Reported (measured) data Area val	Reported (measured) data Area unc	Z-score rep	Z-score ref
1	106.7	101	24	106 7	0	109		-0 9
2	186 2	18035	36	186 1	17786	182	-1.3	-1 5
3	230 6	0	0	230.6	236	85	2.4	
4	609.2	0	0	609.2	34921	339	103.	
5	609 3	73073	437	609 6	37566	335	-64 4	-17 7

Case No. 1: The Area reported by the program is 0. That means, this peak at 106 7 keV was not detected by the program In this case the Z-score is calculated from the reference spectrum value alone (Z_{ref}) If the peak in the reference spectrum has a large uncertainty, therefore the contribution to the (Z_{ref}) will be small, as in this case. Meaning, this peak is not so important in terms of information that might be extracted from it. So "penalisation" for missing it should not be large In the opposite case, the program is substantially penalized with a high Z_{ref} value, because a significant peak has been missed And the case is counted for the **missed** peaks category

Case No. 2: Both areas are different from zero. In this case, the program found a true peak at 186 2 keV This category was classified as **Matches.** The Z-score is calculated using both the reported uncertainty (Z_{rep}) and the uncertainty from the reference spectrum (Z_{ref}). The fact that values for Z-scores are nonzero means that the reported and reference areas are not the same. As long as the difference between the reported area and the reference one are in statistical control, the calculated Z-scores should be low (average value 0, standard deviation 1). Otherwise, the program is penalised because of an **erroneous peak area calculation.**

Case No. 3 The area for this peak in the reference spectrum is 0 That means at 230.6 keV was considered not to be any peak in the reference spectrum This category was classified as **False Hits** If the reported uncertainty of the program for that false hit peak is large, then the contribution to the Z_{rep} will remain low. Illustrating one of the main ideas of the intercomparison (see Introduction Chapter), that is, "it is not as bad whether the programs detects or not a peak as much as it detects it with its corresponding uncertainties" That is telling to the user: "look there might be or not a peak, it is up to you to decide, and be careful extracting any information from it".

In the opposite case, the program that finds a "doubtful" peak and reports it with great conviction (small uncertainties) should be heavily penalised, because of such bad habit.

This case gives no contribution to the Z_{ref} value.

Cases No. 4 and 5: This is an interesting example where a *false hit* and bad area calculation are present It arises from wrong deconvolution of a very significant peak at 609 3 keV. In this case that peak has been wrongly splitted in two peaks: 609.2 and 609 3 keV Therefore the program was penalized twice, once for making a FALSE HIT at 609.2 keV and second because a wrong reported value for the area of highly significant peak at 609.3 has been calculated. In this case a significant contribution is made to both Z-scores.

The CMPSPEC program also reported the following statements after every table of analysis of the results:

```
TRUE MATCHES
      Number of matches for high peaks: 46
         related chisqr for areas and reported uncertainty:  0.8 *
         and for reported areas with reference uncertainty:  1.2
```

Let's have a quick look at their meanings

The total number of matches (reported peaks in coincidence with reference peaks, within permissible interval of variance) for peaks with high significance (A_{ref} / ($\sqrt{20}\sigma_{ref}$)) > 10 is reported Ideally, the chi-square (χ^2) value[8] of unity should be expected for the "reported uncertainty" case. In this example a value of 0.8 was obtained. The * mark notifies of a significant deviation of calculated χ^2 from the expected value (unity), according to the χ^2 distribution with 46 degrees of freedom The value of 1.2 was obtained when the Z-score values were calculated using the reference uncertainty. This difference (1.2-0.8) means that the program is slightly **overestimating** uncertainties for high significance peaks, that is the calculated uncertainty is higher than reference one, therefore a lower value of related chi-square is obtained.

Another case for a different category:

```
Number of matches for small peaks on high continuum: 7
        related chisqr for areas and reported uncertainty:  2.7 *
          and for reported areas with reference uncertainty: 2.4
```

The number of matches corresponding to **SMALL PEAKS** category lying on the high background (3 0*Net_Area < GROSS) are reported Again here, the * mark denotes that the deviation of the calculated chi-square from the expected value (unity) is significant according to the chi-square distribution The value of 2.4 was obtained when the Z-values were calculated using the reference uncertainty The difference between Chi-Squares (2.7-2 4) is small, thus meaning that in this case of small peaks on high background, the uncertainty calculation of the program is accurate.

```
Number of matches for small peaks on low continuum: 6
     related chisqr for areas and reported uncertainty: 2.2
and for reported areas with reference uncertainty: 2.1
```

The number of matches corresponding to **SMALL PEAKS** lying on the low background **(3.0*Net Area > GROSS)** are reported In this example a value of 2.2 was obtained for χ^2 reported by the program The value of 2 1 was obtained when the Z-score values were calculated using the reference uncertainty. The difference (2.2-2.1) is very small. Besides both chi-squared values lie inside the confidence interval for the number of degrees of freedom obtained (6 peaks) Therefore in the case of small peaks on low background the uncertainty calculation in the program is accurate

```
Number of non-511 matches all together: 59
       related chisqr for areas and reported uncertainty:  1.2
       and for reported areas with reference uncertainty:  1.4
        and the chisqr for their positions:  15.0 *
```

This is a summary of the chi-squares for all peaks (total of matches. 59) As can be seen the results are very good. The program resulting in this is certainly in very good statistical control. It calculates net peak area as well as uncertainties with very good accuracy for all cases (high peaks, small peaks in the low and in the high background)

```
FITTING THE 511 keV PEAK
        Number of peaks found there: 2
      related chisqr:                  160.3 *
```

This is the test for the treatment of the annihilation 511 keV peak. The above example is not the case of a good determination of this peak, because it has been splitted into two peaks

[8] This is the average of the squares of the Z-scores values in a category

```
MISSES AND FALSE HITS
   Number of misses: 110
      related chisqr:                9.9 *
```

The total number of missed peaks is evaluated for a program. A high value of χ^2 is reporting the fact that some significant peaks were missed.

```
   Number of false hits: 1
      related chisqr:               99.1 *
```

The total number of false hits is given, as well. A high value of χ^2 in this case is telling that some significant false peak was reported by the program. Usually this situation arises from the erroneous splitting of a significant peak during the analysis.

```
TOTALS
   Number of regarded peaks: 172
      related chisqr for areas:          9.2 *

CONSTANTS USED:
• Threshold energy: 100.00 keV.
• Criteria for energy matching:
          E1 - E2  <  2 * sqrt(sqr(dE1) + sqr(dE2)), or E1 - E2  <  0.5 * FWHM(E1).
• Criterion for high significance: A/ref_err > 10.
• Criterion for high continuum: 3.0 * net < gross.
• Criterion for annihilaton peak: |E - 511| < 3.0.
--------------------------------------------------------------------------------
```

As shown here, the analysis program CMPSPEC is also reporting the criteria and parameters used

Now lets gives some *Hints and Tips* for which qualifiers you should look at in order to find your *golden gamma ray spectrum analysis program.*

Looking for a general purpose gamma ray spectrum analysis program

A general purpose gamma ray spectrum analysis program should detect "normal" peaks in all possible types of gamma ray spectra and report them with the correct uncertainty Then in our test we should look for a program that would gives a χ^2 values in statistical control (meaning without an ugly * mark) for the following categories:

```
Number of non-511 matches all together: 59
   related chisqr for areas and reported uncertainty:  1.2
   and for reported areas with reference uncertainty:  1.4
```

This category includes all matches together: high peaks, small peaks, small on high and low baseline

If there is any problem (you find a * near the reported χ^2 value), then you should check for which type of category of peaks the code is given incorrect values. If this will not be your case, you can have that program in the list of favorites.

Looking for a program with outstanding peak search capabilities

Check the following values in the STRAIGHT spectra test

- ***Chi-squares of MISSES*** This value should be near to one. A high value means that significant peaks from the reference spectrum were missed.
- ***Chi-squares of FALSE HITS:*** This value should be also near to one. A high value of chi-square in this case means that some significant false peak was reported. Since, usually this situation arises from the wrong splitting of the significant peak, you should look carefully at it. If this is not the case, this qualifier can give you a hint for a good peak finder program
- ***The number of HIGH PEAKS MATCHES*** should be equal to 48 (8K STRAIGHT spectrum).

Looking for a program with accurate peak area calculation in simple spectra

Look to following values in the STRAIGHT spectra test ·

- ***The number of HIGH PEAKS MATCHES*** should be equal to 48 (8K STRAIGHT spectrum), but with a value of ***chi-square for reference uncertainties*** near to one to be in statistical control A high value of ***chi-square for reference uncertainties*** in this case, would mean that area calculation of the singlet peaks is incorrect

O Looking for a program with outstanding accuracy in uncertainties calculation for simple spectra

Check the followings in the STRAIGHT spectra test:

- The ***chi-square of the HIGH PEAKS MATCHES*** for STRAIGHT spectra using ***reported and reference uncertainties*** should be approximately equal. If it is not the case then two cases are possible:

1 Overestimation of the reported errors by the program: $\chi^2_{rep} < \chi^2_{ref}$
2. Underestimation of the reported errors by the program: $\chi^2_{rep} > \chi^2_{ref}$

O Looking for a program with high multiplet resolving power

You should use ADD1N1, ADD1N3, ADD3N1 and ADD10N1 spectra for the test:

The complexity of spectra is growing from the ADD1N1 to ADD10N1 spectra, therefore you can trace the behavior of the program, as intensity ratios of the multiplet peaks are increasing

In this case a good performing program will result in a ***chi-square using reported uncertainty*** around **10** in the **HIGH PEAKS MATCHES** category . This value is obtained, because usually some doublets are not deconvoluted therefore a larger value of chi-square for **MISSED PEAKS** is obtained. The **SMALL PEAKS** chi-square value usually is in statistical control for these spectra.

O Test of my program for different capabilities on relatively simple spectra

Always use the STRAIGHT spectra test.

Many other examples can be brought, but the ones already given are sufficient for you to assemble the test of your choice. Now that everything has been explained, let us introduce our candidates.

CHAPTER 6: THE CANDIDATES

In this Chapter a short description of each program is given. For certain aspects of the operation of the programs more detail information is provided complementing the overview description presented in the Chapter 7. Advantages and inconveniences are also pointed out, whenever possible Faulty operations encountered during the intercomparison are reported as well For each program a picture of the fitted 186 keV peak is shown.

6.1. ActAn, version 2.5

by *Centre of Applied Studies for Nuclear Development, Havana Cuba.*

ActAn is a gamma spectrum and neutron activation analysis software developed at the Centre of Applied Studies for Nuclear Development, Havana, Cuba. The development of this program has been partially financed by an Agency Research Contract No. 5014.

The functions are high resolution gamma ray spectrum analysis and instrumental neutron activation analysis. A nuclear data library editor is also available.

The design goal was to have a program that could do a fair job on slow and small PC's, i e 286 PC's running DOS with no extra memory.

The package consists of one 3.25" HD installation floppy and a 20 page User's Manual.

Installation is done by running the batch file INSTALL.BAT that resides on the installation floppy with as argument the drive where the software needs to be installed, e.g.

A:>INSTALL C:

The batch file will create a directory \ACTAN and copy all files that make up the package. The next thing to do is to include the directory \ACTAN in the PATH and set the environment variable ACTAN to that directory, e.g.

PATH=...;C:\ACTAN

SET ACTAN=C:\ACTAN

The installation is very simple and primitive (do not allow to change target sub-directories, etc.) but it works fine.

When the program starts the "Main Screen" is displayed. From this main screen, functions can be accessed via menu's and sub-menu's. A number of functions are available trough the function keys.

The three main functions are:

- Gamma Spectrum Analysis,
- Instrumental Neutron Activation Analysis,
- Nuclear Data Library Editor.

⇧ The menu system can be used quite efficiently both with the mouse or the keyboard.

During spectrum analysis, or whenever ActAn displays graphical data, the so-called "Graphical User Interface" is used, which again can be operated by mouse or keyboard.

⇩ The documentation on the actual spectrum analysis procedures is rather limited. The parameters that affect the peak search and doublet resolution are briefly discussed in the user's manual.

The following parameters can be adjusted for peak search:

- Error limit to display peak search results. Peaks with a relative error in the peak area larger than this value will not be listed in the report
- Sensitivity for peak search, HW, range 2.7 - 7,
- Sensitivity for closed multiplets, Rmax, range 0 - 10,
- Maximum deviation of FWHM from calibration (DEV_FWHM),
- Maximum number of residual search iterations.

Initial peak search is based on a square wave correlator (parameter HW). Doublets are detected by comparing the fit with the measured spectrum (parameter Rmax). If the difference between FWHM of the peak and the calibration FWHM is less than DEV_FWHM, then the peak FWHM is used otherwise the FWHM from calibration is used, allowing for deconvolution of closed multiplets. The program can only add one peak per residual search iteration.

⇩ The actual peak area determination is not documented.

The baseline is removed from the spectrum using an iterative filter. A peak shape is calculated based on the peak shapes stored during the calibration step. This numerical function is fitted to the measured spectrum.

For this method to be valid, the peaks used for calculating the shape should have very good statistics, at least 10 times more counts than the spectra to analyse; otherwise the calculation of uncertainties in the fitted data will be biased. A consequence of using this method is that if the calibration spectrum is analysed, zero values for Chi-squares will be obtained.

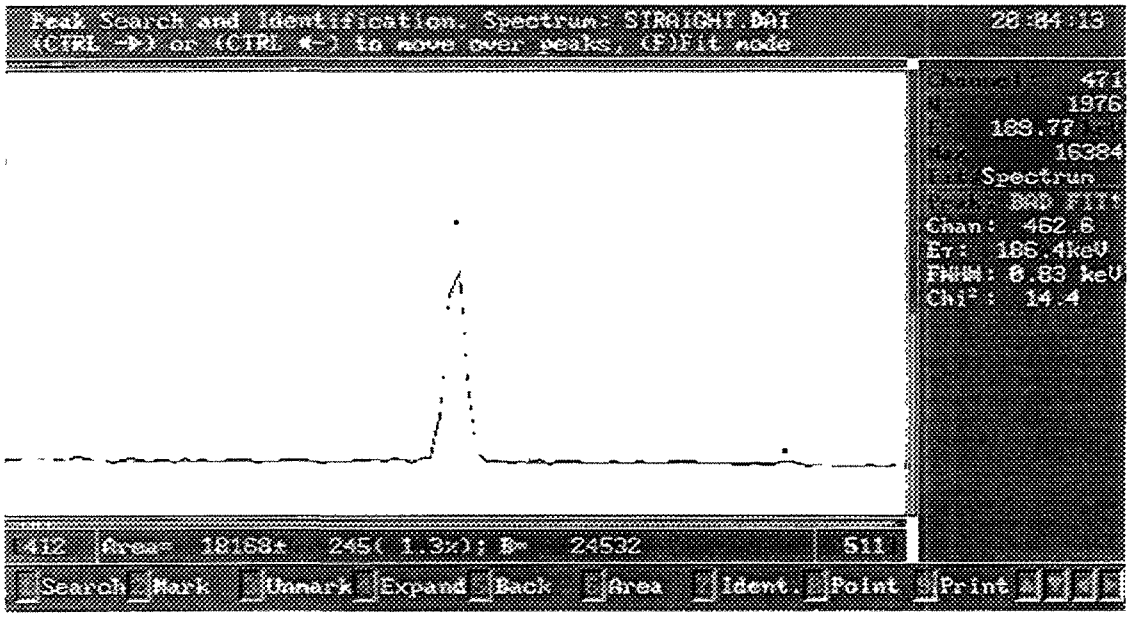


Figure 9. ActAn. Fitting of the 186 keV peak.

For each spectrum analysed a file with the same name and extension ".SRC" is created containing all information that can be displayed or listed. An ASCII file with extension ".SRP" contains the analysis results in a readable form. A typical example is shown below

```
ActAn v2.5 Peak Search and Area Calculation Report

Spectrum:                          C:\ACTAN\IAEA\STRAIGHT.DAT
Energy calibration:                C:\ACTAN\IAEA\CALIB1.CEN
Peak shape calibration:            C:\ACTAN\IAEA\CALIB2.SHP

Date of processing:12/11/95, 09:16:59

True time:   33.333m          Live time:   33.333m
Area error < 99.0 %
Background Iteration Cycles: 15
Sensitivity for peak search:  2.8
Sensitivity for closed multiplet search:  8
Maximum Deviation of FWHM from calibration: 20 %
Maximum iteration number for peak search in residuals:  1
Analysing from channel  256 to channel 8095

        Crit.Level = Net Area/sqrt(2*Background)

        Peak classification:
        Normal(-), Small(S), Residual(R), Bad fitted(F)
```

No	Centroid [Ch.]	Eγ [keV]	Net Area [counts]		Background [counts]	FWHM [keV]	Chi²	Crit. Level
1 F	462.6	186.45	18168±	245(1.3%)	24532	0.83	14.42	82.0
2 S	499.4	201.01	378±	175(46.3%)	15102	0.84	1.09	2.2
3 S	574.5	230.81	352±	157(44.5%)	12102	0.87	1.12	2.3
4 F	593.8	238.46	270±	154(56.9%)	11653	0.87	8.48	1.8
5 F	603.3	242.25	28303±	259(0.9%)	18394	0.88	8.48	147.6

⇧ The program properly keeps records of the job by listing all the files that were used for energy and shape calibration and all the parameters that were set for peak search.

For each peak quite complete information is given: the peak position in channels and keV, the net peak area and the standard deviation (also in percentage), the number of counts in the continuum under the peak, the FWHM and the χ^2 value. A qualification, "*Normal*", "*Small*", "*Residual*" or "*Bad fitted*" is given to each peak. "*Residual*" clearly indicates that peak was found during residual search.

⇩ The definitions of "*Small*", "*Normal*" or "*Bad*" are not given.

A parameter "Crit. Level" is calculated for each peak as explained in the listing, how this parameter should be used or interpreted is however not mentioned.

It was found usefull and nice capabilities built-in this software (e.g. library editor, among others) but they are not within the scope of this intercomparison.

6.2. GammaTrack, version 1.3 Release 2

by Oxford Instruments Inc., Tennessee USA

GammaTrack is a DOS gamma ray spectrum analysis program developed on the basis of a MCA emulation software. As a data acquisition device it works only with Oxford - Nucleus cards.

Hardware requirements are not stringent except for memory available to DOS. Running this program requires then that the computer is configured to get the maximum memory to DOS by placing the proper statements and devices in the CONFIG.SYS and AUTOEXEC.BAT files. On many systems the support for networking, sound cards or extra devices will have to be removed in order to successfully operate GammaTrack.

A hard-key (protection key type Sentinel) has to be connected before beginning the installation.

The installation program (INSTALL.EXE) is quite simple, although it lacks of some flexibility It prompts for a directory to install GammaTrack which is created if not existing. During the installation compressed files are extracted from the diskette using the LHA program. After installation is completed a browser displays a "readme" file, for updated information.

⇩ The install program is not able to create a sub-directory together with parents (e.g. c:\gamtests\gt).

The main program, can be started at the DOS command prompt as "gt", and it accepts pipeline options. Some of the pipeline parameters are essential for the proper operation of the program.

⇩ We have experience that this method for initialization is quite inconvenient as the user needs to remember the command line parameters, for example that typing *gt K* will allow erase of spectra during acquisition.

⇩ The program only accepts data formatted in the proprietary format types *.spt or *.spm . Even no ASCII formatted data can be read by the program.

⇧ The GammaTrack supports a very convenient and easy to operate energy calibration procedure. From the ROIs in the spectra the program automatically finds the tentatively standard energies. The calibration curve may be displayed together with the calibration coefficients. User-defied lines can be entered from the keyboard as well.

The FWHM calibration is performed simultaneously.

However, the program does not treat properly the 511 keV peak. If this peak is marked for calibration it results in an erroneous FWHM calibration. This could be corrected, only, by deleting the 511 keV peak from the list.

The drawback of this automated calibration is that it forces the user to use the calibration parameters and function that the program provides as the result of the calibration procedure. For instance, in this intercomparison exercise we needed a first order energy calibration function which will result in only two calibration parameters. In order to obtain that with GammaTrack, we were force to use only two experimental points. The dangerous in doing this, is that the FWHM and shape parameters had to be extracted from only two peaks !!!.

We have found out that calibration parameters can not be transferred from one spectrum to another. The problem arises from the fact that any calibration data in the header of the spectrum takes precedence over data in calibration files. The order of this precedence cannot be overridden.

⊗ Also a menu function called "*Merge calibration data*" does not work if the spectrum is not previously calibrated, and also fails if the calibration has been saved (reporting a division by 0 error).

The fitting procedure can be controlled by several parameters. The main sensitivity factor (and here higher numbers mean lower sensitivity), the number of peak insertion passes and the peak insertion sensitivity factor, "number of background channels" for the evaluation of the baseline under the peak.

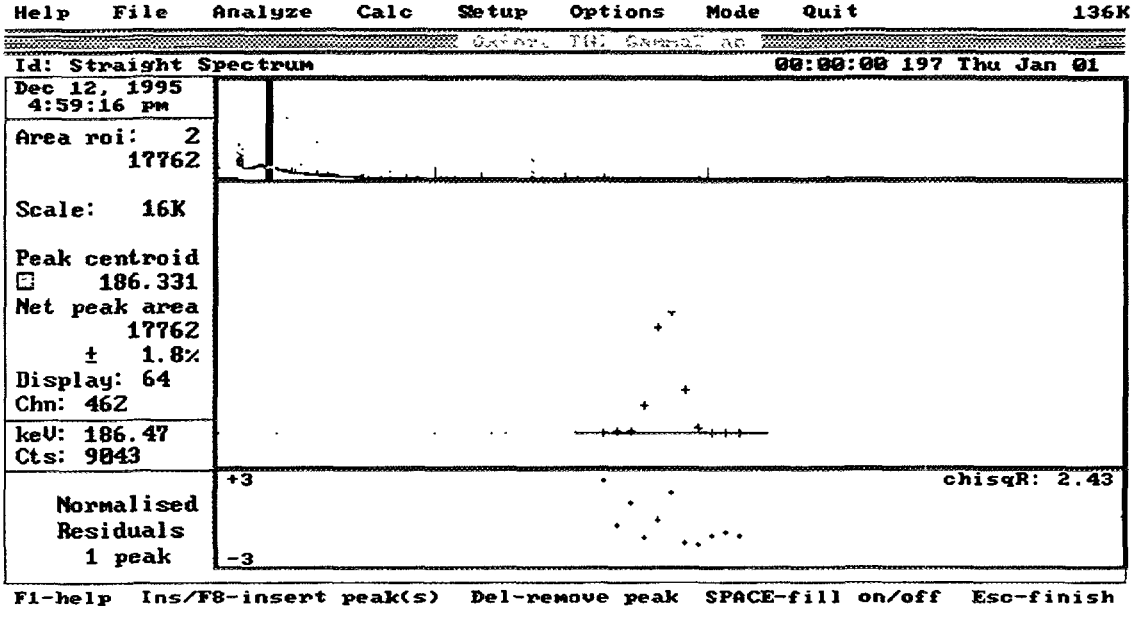


Figure 10. Oxford Gamma Track. Fitting of the 186 keV peak.

⇧ The fitting operation for a simple spectrum in the "default mode" (using default parameters) was found to be fast and effective, except for the region of 511 keV.

As seen from Figure 10 the splitted windows are properly used. The programs also display the residuals.

⊗ Another improper operation of GammaTrack was found during the intercomparison, and is related to the difficulty to save the analysis results in a file. The "Peak Search" menu has only the options to display on screen and print. If the unfortunate user chooses to print but no printer is connected he will be caught in a catch-22 situation between Retry and Ignore whose only door out is rebooting or killing the DOS session (if running under windows) with the loss of all the results.

⇩ The way to save the results into a file creates some confusion. The file name where results should be saved has to be set in the "Automatic analysis" parameters as report device, also the report template has to be set as "peakonly.tpl".

⇧ The implementation of the reports of the results, was found to be very flexible and powerful, through the template definitions of reports, but sometimes complicated.

The software complies with quality assurance and quality control rules.

The software comes with a 266-page Operation's Manual.

⇩ Most of the contents of the manual are duplicating the online help file. And it describes the operation of the version 1.2.

6.3. Gamma Plus, version 1.02.0

by Silena S.P.A., Italy

Gamma Plus is a DOS-based MCA emulation and gamma ray spectrum analysis software. As a data acquisition device it works only with Silena type of MCA acquisition add-on cards.

The installation should be quite simple (see comments below), through the install program. The software comes in one 3.5 " diskette and its operation is protected by the presence of a hard key in the parallel port.

Although, claimed to be simple the intercomparison exercise failed to install several times this software. Most of the problems were related to the type of drivers or hardware devices installed in our computers.

☞ **We found out that GammaPlus is not compatible with Quantum LPS540S SCSI hard disk drive. Problems on its operation were encountered in computers running compression drivers for hard disk, particularly Stacker® ver .4.00**

An incompatibility between GAMMAPLUS and EMM386 is noted. The following command line, must be present for proper operation of the software:

DEVICE=C:\DOS\EMM386.EXE FRAME=NONE

GammaPlus can read only spectra in Silena format, which is well documented in the Appendix B of the user's Manual.

⇧ The software has a nice and fast user interface implementation. It also properly uses the multiples windows facilities.

Energy calibration can be done automatically. In this case the software search the presence of standards peaks for calibration. The energy values are taken from the provided isotope data library. The user has also the possibility to enter or erase any peak from the automatic calibration. Energy values can be user-defined as well. The same goes for FWHM calibration. Peak shape calibration is done as an asymmetry calibration. All calibrations can be plotted.

⇧ The program detects and skips automatically the 511 keV from calibration procedures.

The spectrum analysis is done, first by peak search and then the peak areas are calculated by fitting the peaks.

The program uses the following formula for uncertainties:

$$\%\text{Error} = Z\,\sigma / \text{Area}$$

where Z is the confidence level and σ the standard deviation.

The analysis options in the software provides among others:

- Area Calculation: which is peak area calculation in a ROI using classical background subtraction
- Peak Location: which is peak search followed by fitting

Several parameters can be set in order to control the peak search and the fitting procedures, as for instance: Peak search criteria (number of times above σ of the baseline, for a peak to be accepted), Confidence level (the Z value to be used as described above), Gaussian filter, sensitivity for multiplets, search on residuals, etc.

⇧ The utility "Info-Peak", was found useful. It can be called from the main menu and performs a peak search around the current cursor position and then fits the peak(s) found and reports the position (or energy),the fitting region, the FWHM and the net peak area.

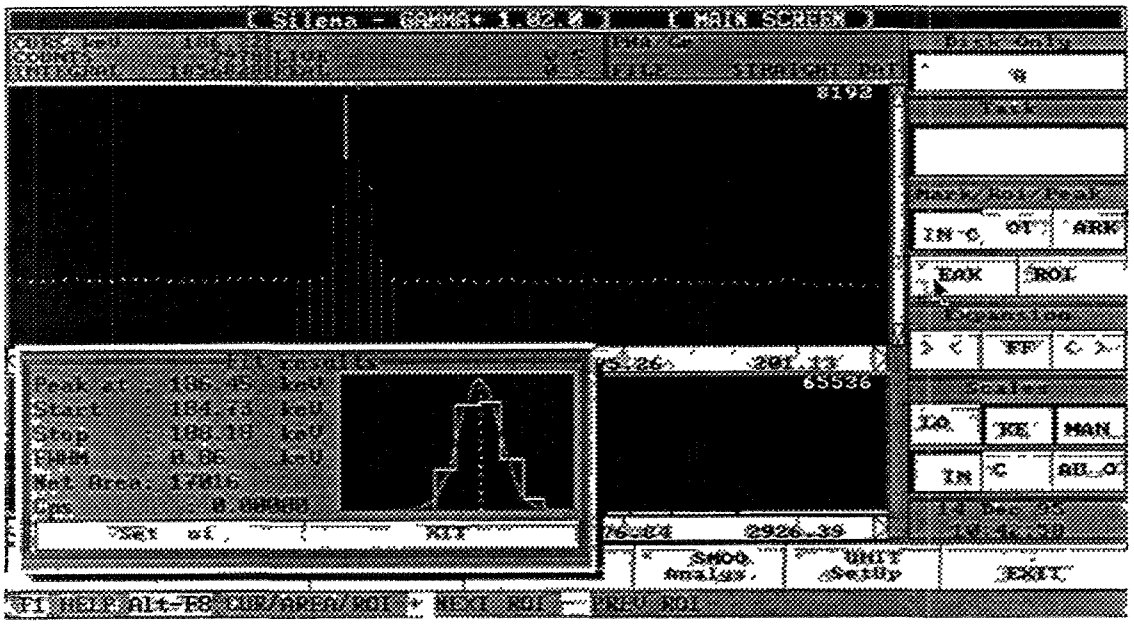


Figure 11. Silena GammaPlus. Fitting of the 186 keV peak. Overview of the graphical user interface.

The fit is shown graphically in a small window on a linear scale however without the possibility to change the y-axis

⇩ No uncertainties in any of the obtained values or any fit quality criteria such as chi-square, is reported The parameters that control the fit are the same as those used for the analysis function.

⇩ It is not possible to add or remove individual peaks.

The GammaPlus can perform some spectrum manipulation like: stripping, smoothing and normalization to factor

The user's manual contains quite a number of mistakes and misprints.

6.4. Gamma Vision, version 2.3

by EG&G Ortec, Oak Ridge, USA

The software GammaVision is an MCA emulation software together with a built-in environment for high-resolution gamma ray spectrum analysis software. It comes in a set of installation diskettes and two user's manuals. It has also a protection key through the parallel port.

This program operates under MS Windows 3.1 or later versions and had been designed under a powerful and "easy-to use" graphical user interface.

⇧ The software can be operated from a network.

⇧ The graphical capabilities and the powerful user interface provide extremely user-friendly and convenient way of operation, particularly for fitting and viewing the results and the residuals of the fits.

⇧ Calibrations are easy and efficiently implemented. It also includes an automatic peak detection for calibrations. In principle, only one data point is needed.

The efficiency calibration has built-in several mathematical functions for two intervals.

- above "the knee" point as interpolation, linear quadratic or polynomials of several user-defined degrees,
- bellow "the knee": interpolation, linear and quadratic functions

Polynomials are at most expressed in log(E).

The baseline function is calculated differently depending of the type of the peak. For singlets one of he following options can be chosen: automatic, average over five points, three points value or minimum For multiplets a choice between stepped or parabolic-type baseline functions

Gaussian peak shapes are used for fitting multiplets, while peak numerical integration is used for singlets

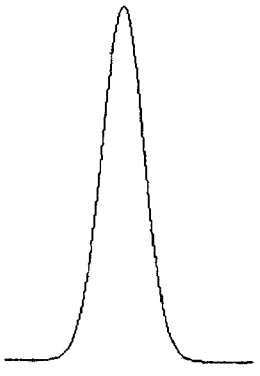


Figure 12. GammaVision. Fitting of the 186 keV peak.

It should be realized that the way GammaVision performs the spectrum analysis is unique and somehow different to the usual methods GammaVision will deconvolute multiplets when distinct centroids are determined either by the peak search or by the library In the case of overlapping peaks (multiplets), in which the peak routine cannot locate centroids in the spectral data, this reduces to using only constituent peaks that are in the gamma ray LIBRARY as deconvolution tools

In other words, GammaVision deconvolution operates in the following way:

Any peak region which has more one library entry or actual detected spectral peaks which would overlap is deconvoluted. If certain criteria are not met, the deconvolution may be aborted

Any peak envelope, for which no deconvolution is done, but which has a FWHM or FH25M which is in excess of 1 2 times the calibrated value, is flagged with a warning symbol

Obviously this method, has some advantages but also a number of disadvantages, and it is evident that such methodology requires a provision of good nuclear data libraries and relies on an accurate peak position routine

For creation of the specific libraries the GammaVision comes with a separate software package called: "Nuclide Navigator" a type of Visual Nuclear Data Base representing the chart of the nuclides and their most prominent characteristics Out of this software the user can make his own specific application nuclear data library It also can be edited through a provided library editor There is full compatibility between the gamma ray analysis software (nuclear data library manager and editor) and the application "Nuclide Navigator"

Detection limits are calculated, and can be chosen from 10 different types of formulas, some with doubtful physical meaning.

⇩ There is no on-line help provision in the software.

Activities and concentrations are calculated if all corresponding data exist.

⇧ The User's manuals are well written and organized.

However, the manual does not document the proprietary spectra format ".spc". Contrary to the old format ".chn" (fully documented).

6.5. Gamma-W, Version 17.08

by Dr. Westmeier, Westmeier GmbH, Molln, Germany

⇧ The software has a powerful conversion utility program that converts most available commercial spectra format into ASCII format, which is the default format for Gamma-W.

According to the manual, Gamma-W is a high sensitivity, high precision code for the analysis of gamma ray spectra from Ge(Li) and HPGe detectors. Peak areas are determined through the fitting of mathematical shape functions to experimental counts after the subtraction of the analytical background distribution. The figure below shows the graphical fit control on screen at 186 keV of STRAIGHT spectrum (in optimised automatic method).

Gamma-W is a DOS application. We have found that more than 512 Kbytes RAM provides sufficient space to operate the software properly.

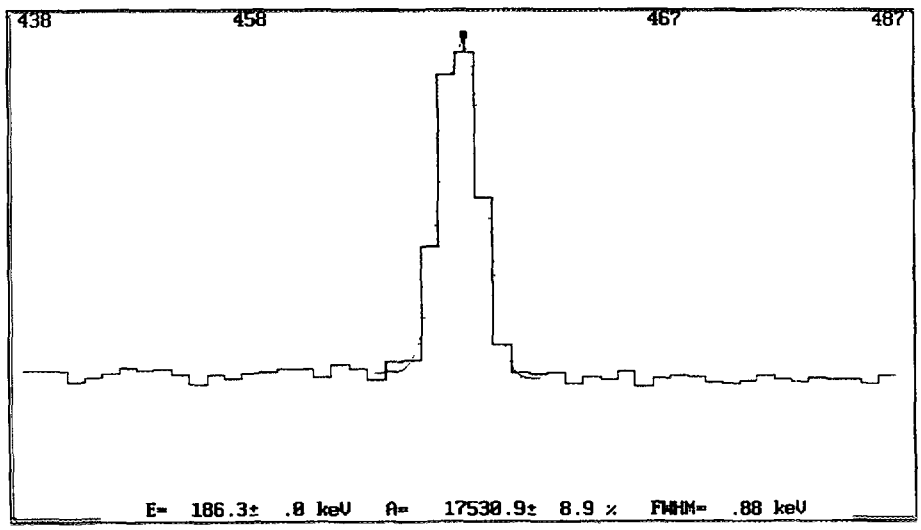


Figure 13. GammaW. Fitting of the 186 keV peak.

The spectrum can be displayed, the x-axis region controlled with functions keys, the y-axis with cursor keys. The latter can be logarithmic or linear, but the user has no control over the offset in the case of linear y-axis.

⇩ Some inconveniences in the graphical user interface were found. For example: the graph does not scroll horizontally if the cursor pushes against the left or right edge. The zooming in and out does not keep the cursor centered and can have a disorienting effect.

For the cursor position, channel number, energy and channel contents are displayed. The cursor is moved with the left and right cursor keys. As identification of the spectrum under study, the filename is shown on the screen. The user cannot set the colors used by the program.

⇧ Fit results, energy, shape and efficiency curves can all be shown graphically, with optional display of residuals, although the program does not use multiple windows.

Peak area determination is performed by first performing a peak search, then subtracting the background from the regions to fit and finally fitting the peaks.

One peak fitting function is available: A Gaussian with a low-energy tail

⇧ Three background functions can be used: Linear, linear with an error function under the peak and Bremmsstrahlung.

The error function is determined in the process of subtracting the background from the region to fit from the rest of the spectrum on the high-energy side of the spectrum. The fitting of the peak is done by a non-linear least-squares algorithm described by Slavic [16].

⇩ No exception is made for the 511 keV peak

The spectrum can be analysed in automated mode of the user's definition, using macros and/or batch mode. In interactive mode, the user can suggest peak positions and set the region to fit, but in the fitting process peaks may be dropped again by the program

The fitted peaks are reported with positions, energies, fitted areas and uncertainties There are two kinds of reports: The first is kind of log file that will contain everything computed in a session, the second a file containing only peak energies, areas and their uncertainties. The user has some control over the log-file output format. The log-file can be directed to a printer directly, or to a file All output files are plain ASCII.

The peak width calibration function is a second order polynomial, just like the energy calibration function

⇧ The program offers a vast selection of mathematical functions for efficiency calibration Among the most effective is a log-log polynomial with any number of parameters up to 10, or the Jaeckel & Westmeier curve as published in the literature [17].

⇧ The program can manipulate spectra and can run automatic analysis in a batch mode

The program can identify radionuclides and report the activities, once the efficiency calibration is performed. Activities are computed from each identified peak Also, concentrations can be computed from the activities for INAA, based on thermal and epithermal flux along with irradiation times.

6.6. GANAAS, Version 3.3

by Physics Section, IAEA. Vienna

The gamma ray and neutron activation analysis software (GANAAS) package has been developed by IAEA, Physics Section under auspices of its Technical Cooperation (TC) programme with the main objective to assist TC projects and nuclear analytical laboratories starting services based on nuclear analytical techniques, as well as to provide a common based and comprehensive software for several IAEA training courses and other training activities. The GANAAS software package is oriented towards the analysis of high-resolution gamma ray spectra, activities and element concentration calculations for Neutron Activation Analysis (NAA[9])

[9] Both, Thermal and Fast Neutron Activation Analysis

The Ganaas software is flexible and easily manageable. The program allows intensive dialogue with the operators. This is more applicable while doing calibrations.

⇧ The installation is quite simple and effective It is completely driven by a specialized installation program. This program allows to install the main software (called "essential module") and gives the user the opportunity to install only those modules that he will use If necessary it creates new sub-directories and file structure The installation package also offers a set of examples programs.

Although it works fine, the installation procedure lacks of some flexibility, e.g the name of the target sub-directory is fixed to "Ganaas" and can not be changed.

⇩ Although very simple to operate, the installation program is not documented. Only a brief explanation is provided in a text file included in the first installation diskette.

Ganaas is a DOS operated software It has an strong requirement on RAM available for proper operation. We have found that more than 600 Kbytes RAM provides sufficient space to operate properly the software.

⇩ This strong requirement on memory implies some limitations to DOS users, since many drivers and TSR programs have to be disabled from RAM, while working with Ganaas.

Ganaas is easy operated by its graphical user interface The software has been designed in a modular way It consists of the following modules:

- Set-up module- Organizes the different programs, their locations and sub-directories It also set-up the graphics and communication facilities.
- Parameter Setup- This program set and stores the parameters for the spectrum analysis It includes different calibration procedures and results in a file (*.PAR), which is called later for the fitting procedure
- Analysis Program- It allows the selection of the input parameter files, spectrum files and performs the spectral analysis and displays the results
- Activity Analysis- Calculates measured activities of the radioactive isotopes (* ACR)
- Concentration Determination- this module is used for NAA calculations. It can be done using fundamental parameters calculation or by the comparison method against samples corrections. It also includes a module for Fast Neutron activation analysis calculations with a solving routine for peak and reaction interference. Correction factors can be also taken into all above-mentioned stages
- Utilities Modules- include two libraries and the library manager and editor
- P-SPEDAC is a module used for reformatting the spectra from different formats to the required input format of the Ganaas program.

Ganaas needs about 3 Mbytes hard disk space for the installation of all the programs

After installation, the path has to be set to include the sub-directory C:\GANAAS\BIN

Spectral data from a source format is converted by the program P-SPEDAC to a target format, required as the input of the spectrum analysis program, in the following logical sequences

Select format of spectrum to be converted from - source,

Select format of spectrum to convert to - target,

Select directory of filenames of all source spectra,

Select directory of target spectra.

Once the source is selected , in the next stage the following sequences are executed

Read the spectrum in the source format,

Display the spectrum for visual inspection,

Save the spectrum in the target format,

STOP.

This procedure can be performed in a batch mode, for up to 12 spectra files.

⇧ Almost all commercially available formats are implemented in the file conversion module of the Ganaas.

Energy calibration, FWHM calibration is easy to perform in Ganaas. After it is done the table of points or the graphs with corresponding residuals can be seen.

The efficiency calibration is powerful in Ganaas. It can be done by entering the data points and then selecting a polynomial of different degrees (user-defined). Most of polynomials are based on the log(E)-log(E) functions.

⇧ As well as the usual method for efficiency calibration in Ganaas, there is a new feature in this package that make it unique compare to the others software. It is the provision of a possibility to calculate the efficiency of the detector based on only one experimental point and the characteristics of the detector itself (that the user has to enter before hand). Results of the efficiency calculated in such a way have been proven to be very effective and convenient in some cases were there is not sufficient data or time to measure the efficiency curve. The calculation method is based on information published by Gunnink [19].

The main spectrum analysis routine of Ganaas is based on a PC-adapted version of the well-known program GAMANAL [20].

In comparison with the other similar software, its most characteristic feature is the way Ganaas treats the continuum in the gamma ray spectrum. Instead of using a polynomial function together with the peak functions in a relatively narrow energy region, the Ganaas first determine the continuum background for the entire spectrum, identifying at the same time the non-peak regions. Then, when each peak is dealt with, the continuum beneath it is interpolated with a smoothed steep function. The peak shape function is a Gaussian with a tailing function on its low-energy side.

The Ganaas offers control for the spectrum analysis through several fitting and peak search parameters, that the user might select.

⇩ But these parameters are not well documented in the User's Manual.

⇧ The report of the spectrum analysis is very complete, it gives the peak positions in terms of channels and energy, the corresponding FWHM, calculated area and its uncertainty and the quality of the fit.

⇧ The results of the analysis can be seen in an ASCII scrolling table or visualized in the entire or individuals peaks. The spectrum data are presented in a histogram form in white. The fitted curves are displayed in red and the fitted backgrounds are in green colors. Each peak can be seen together with the residuals. The residual values appear below the fitted peaks providing impression about the goodness of the fit.

⇩ However color scheme of the program can not be user-defined or changed.

All the operational and calibration parameters, together with the spectral data and spectrum results are stored in different files. It would be more convenient, for tracebility purposes to have them all in one single file.

⇩ The program does not provide the option of manual insertion/deletion of peaks.

Ganaas provides a nuclear data library editor, with the use of which the user can extract his own library from the master library.

⇧ Ganaas suports a wide range of calculation modules and options. For example, it can calculate activities and concentrations as well, in an interactive or automated mode. Calculation of concentrations in terms of Neutron Activation Analysis, for both thermal and fast neutrons is provided. Peak interference is also implemented while working in this mode.

⇩ Ganaas software does not provide help on line and the user's manual was found to be not complete and not updated.

6.7. GeniePC, version 2.2

by Canberra Industries Inc., Meriden USA

GeniePC is a networking data acquisition and gamma spectroscopy system that runs under the IBM OS/2 operating system. The package has 2 different parts

- "Basic spectroscopy" for data collection, calibration of spectra and simple analysis which includes automatic peak deconvolution (3 diskettes).
- "Advanced options", this is provided in 2 additional diskettes titled "gamma analysis" and "interactive peak fit".

This design, in 2 parts has some drawbacks, particularly all the gamma analysis modules (with the exception of the interactive peak fit operate in a highly non-interactive way. Results are not updated in the spectrum display windows, unless the spectrum (data set) is manually reloaded. Even performing the energy calibration requires to run a new program which however, in this case allows to take the ROIs selected in the spectrum. No access to library energies is available during calibration

For the test we used a computer where OS/2 Warp version 3 was already installed. The installation of OS/2 will therefore not be discussed, however previous experience shows that installing OS/2 can be quite complicated, particularly if the computer is intended to operate in a network

⇧ The installation of Genie-PC and its additional components is quite simple and flexible.

The computer has to be rebooted after installing the "Spectroscopy Assistant". However it is not necessary to reboot the computer after installing the advanced options. In order to run any of the utilities that compose this package the user must run the "Virtual Data Manager (VDM)" first. This program stays resident and works as a virtual machine that performs I/O.

The program stores the spectral information in a proprietary binary format that takes the extension "cnf" and is called datasource.

A utility called FILECNVT converts spectra from various formats into GeniePC data-sources, also referred as CAM files in the manuals. This utility is implemented as a OS/2 command line program (has to be run from the OS/2 command box) and is cumbersome to use alone as for converting each spectra However it is convenient to use in batch files

The command to convert a spectrum is:

C >FILECNVT <INPUT FILE NAME> <OUTPUT FILE NAME> /QUALIFIER

The allowed qualifiers are:

/S100	Canberra S100 cards
/SPECTRAN	Canberra Spectran AT
/GAMMA	Canberra Gamma At

/TOOLKIT	Canberra Series 35 Toolkit
/SAMPO	Micro Sampo 90
/ORTEC	Ortec file type (chn or spe)
/ND6S	Nuclear Data 6 series MCAs
/NUCLEUS	Nucleus cards
/INTERTECH	Intertechnique (now Eurisys Meas) type format
/HELP	Provides a short help text

Unfortunately FILECNVT does not indicate plain ASCII which actually corresponds to the TOOLKIT option so the conversion of the test spectra to an intermediate format was performed

Finally a program to convert the spectra from ASCII format to *.cnf format was prepared using the OS/2 REXX batch language which provides a convenient way of transferring the data as file names can be selected from directory lists.

In summary, Genie-PC provides facilities to read other file formats but this facility is not conveniently implemented in the package.

⇧ The energy calibration procedure was found to be quite straight forward, effective and powerful Display capabilities and multiples windows are properly used, for the convenience of the user. It is also possible to load an already existing calibration parameters.

The "Markers" button loads the centroid of a peak between two markers. If the data set has been previously calibrated, it is possible to load the old data using the "Populate" button.

⇧ The Automatic mode of calibration was found to be quite convenient and efficient for simple and fast calibrations.

⇧ The user can select the degree of the polynomials.

The shape calibration is done in a similar way parallel to the energy calibration.

An additional parameter as " low Tail" is given and plotted, which illustrate the shape of the peaks in the whole range of spectrum energy

⇩ Note that the equations and data points are reported, but uncertainties in peak positions are shown only in graphical way. No uncertainty of the coefficients is reported. If the calibration report is produced (using the report utility together with the appropriate template and section) then the uncertainty in the channel position is reported but again not the uncertainty in coefficients or in calculated energies.

The analysis of a spectrum in GeniePC consist of various methods which run in a predefined order These methods can be selected by the user and are classified in groups like "Peak Search", "Area / Fit" and "Report" Other groups as "Acquisition", "Calibrate", "Area Correction" (baseline subtraction), "Nuclide Identification", etc. are also provided. All the procedures necessary for analysis can be set into an "Analysis Sequence" which may be prepared with the Analysis Sequence option of the "Edit" menu

The software provides full control of the analysis by setting several parameters, as shown in Figure 14 All settings of the parameters are well documented and logically accessible through screens and menu-options

⇧ GeniePC provides a flexible type of reports for the results The contains of the reports can be user-defined The type of the report can be chosen with the help of templates Although the report using the standard template is quite complete

⇧ GeniePC provides the possibility of an interactive peak fitting

The interactive peak fit is a separate procedure method that can be either associated to the "Peak Area" group or run after the "Sum/Peak Fit" algorithm The first option is recommended in the manual, but the second option allows to combine results from both methods The setup of this method allows to place filters so that not all the peaks have to be interactively analysed

⇧ The programs allows the manual insertion or removal of individual peaks

During the intercomparison, when the default fit was not satisfactory, the fit was modified either by adding peaks to the multiplets or changing the fitting region

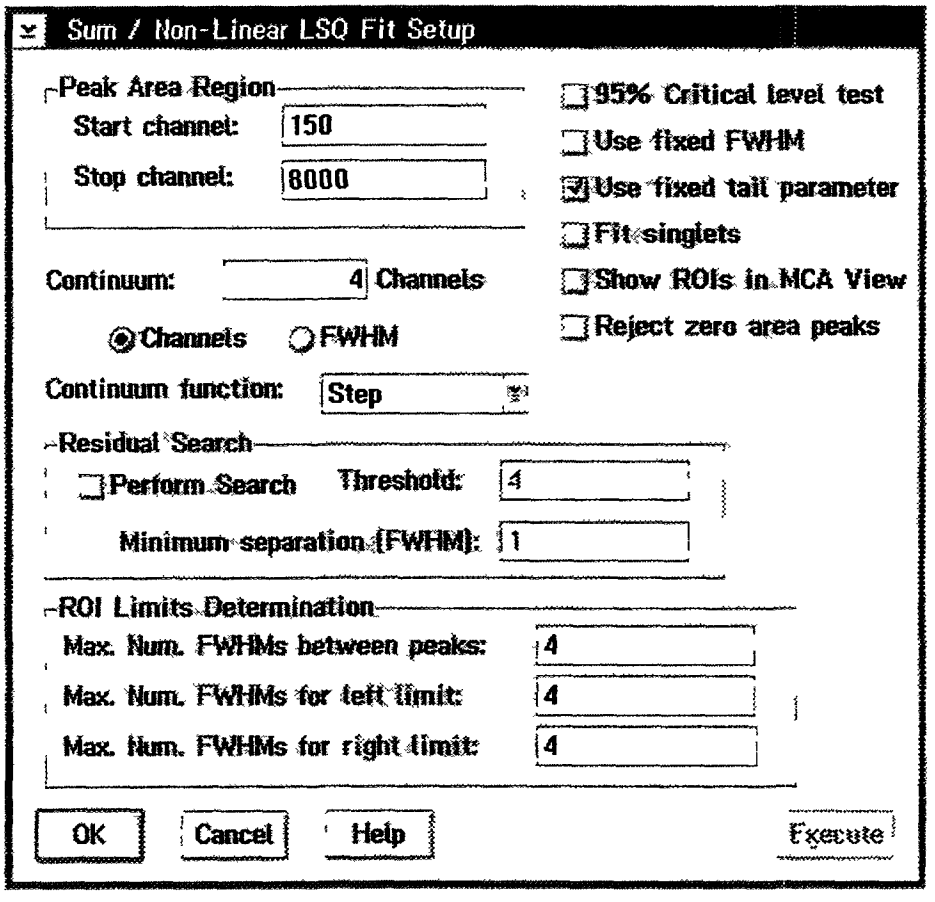
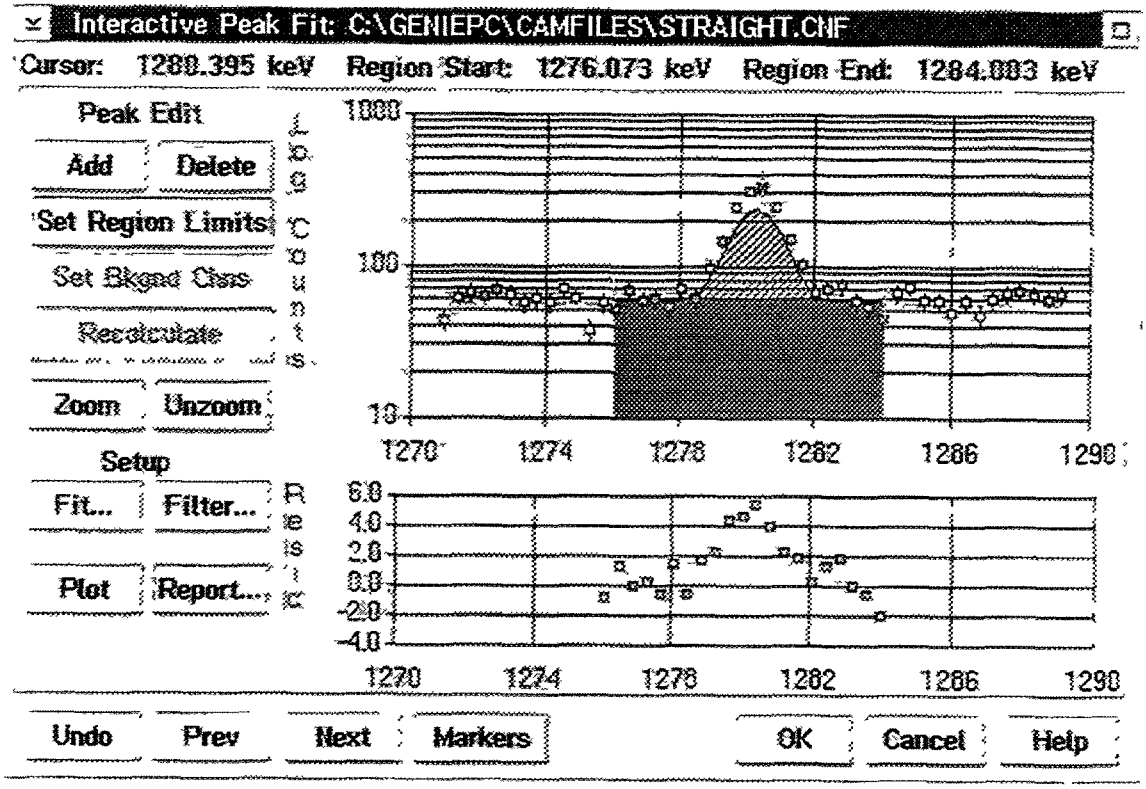


Figure 14. Canberra GeniePC. Parameters Set-up screen for fitting procedure.

⇧ The fitting parameters can be changed using the Peak function for each region A few other parameters can be changed to change the fitting region and number of peaks with their initial positions

When all the fits have been made for each region, then the results can be saved to the corresponding * cnf file A list of the results can be obtained using a Report procedure

⊗ It is interesting to point out that during the manual or interactive analysis of the STRAIGHT spectrum some peaks that appear to be incorrectly fitted independently of the values of the parameters (without changing the analysis algorithms) were found The images bellow illustrates these cases



In this case, a peak smaller than the reality was fitted (see residuals). Adding another peak next to the original one did not improve the situation. When it was attempted to fit this peak again individually by using the energy (1280 keV) as filter the program refused producing an error as seen in Figure 15.

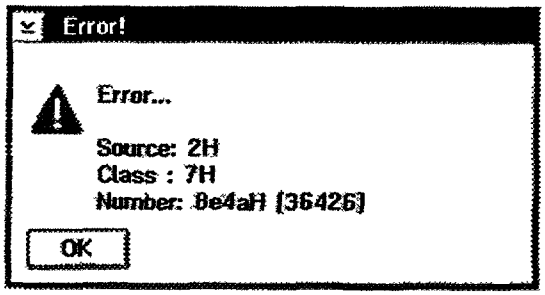


Figure 15: error code produced when trying to insert a manual peak.

After this errors it was necessary to reboot OS/2 in order to get normal operation again Apparently the interactive fit procedure remained active in the background making OS/2 unstable.

⇧ The programs of this package are well documented as well as the formulas used in the calculations.

The documentation of the programs that constitute Genie-PC is quite good although perhaps is too extensive, consisting of various thick manuals. Fortunately, due to the high quality of the user interface and the context sensitive online help available it is not strictly necessary to read the documentation for using the program.

6.8. Hypermet-PC , version 4.00

by Institute of Isotopes, Budapest Hungary

Hypermet-PC v4.0 is the PC version of the original HYPERMET code[18] developed by Philips & Marlow in 1976 at Naval Research Laboratory, Washington DC, USA; for automatic and efficient analysis of the complex gamma spectra

The current version has a short preliminary User's manual (29 pages), which is represents the minimum survival guide for operating the code in automatic mode. It includes the following chapters:

- Introduction,
- Starting HYPERMET,
- Initialisation of the Hypermet-PC parameters,
- Reading files, changing the display appearance,
- Fitting spectra and managing fit results,
- Additional options,
- The Nuclide ID option.

⇩ The User's Manual is really very preliminary and does not cover/explain all the possibilities of the software. For instance, there was found a very poor (almost none) explanation of fitting options (EXPERT MENU), which is extremely important for the orientation of the user.

Installation went smoothly, but it is "manually done". The user should copy himself the program files from floppy disks into the hard-disk, after creating the needed directories.

No peak shape calibration is needed. Shape parameters for peaks and background are found by a non-linear fit for each separate region in the spectrum using an initial first trial value for the peak width. Dynamic variations of the parameters throughout the spectrum are automatically adjusted.

⇧ As minimum input (using "*default*" parameters) this code requires only information for two peaks (approximate FWHM and exact energy). These two peaks should be selected as distant as possible This information is enough to carry out energy and automatic shape calibration

There is a LOG file for the whole fitting procedure, where all fitting operations and parameters are recorded and can be seen/analysed at any time. It is possible even to see the whole fitting sequence for each multiplet, for instance if you are doing three different fits in one region you can see graphically the results for each fit one after another.

⇧ The code has very easy and user-friendly way of adding/deleting peaks in any region of the spectra You can add or delete peaks using channel position or energy.

The program marks the BAD FITTED regions according to χ^2 criteria.

⇩ Although the HELP option appears in the main screen menu, no Help is available at all in this version (it might be implemented in the future).

⇩ The common graphical display of Energy vs. Channel and FWHM vs Channel are not implemented in the program.

⇩ The screen input for different parameters of fitting and logical operations is ugly and very inconvenient.

⊗ During the intercomparison a problem was found in relation to the capacity of the LOG file. It was seen that doing fitting for whole spectra which has many peaks, LOG file becomes too big. Once the file reaches the 64K capacity , the program hangs up.

⊗ During the intercomparison the program gave *Floating Point Errors* during its operation. It was found not very stable in operation yet.

There is no automatic recognition of the 511 keV peak, you can do only manual fit using variable FWHM (it is explicitly recommended in that way in the User's Manual).

There is an incorrect definition of the SIGMA_LIMIT parameter, which affects the criteria of goodness of fit [χ^2/(4*SIGMA_LIMIT)].

A linear sum of the Gaussian and a Gaussian with exponential tail on the left side is used as peak shape function. A step function folded with the Gaussian peak and a similarly folded "tail" function resembling a sharp Compton edge are added to the usual first or second degree polynomial baseline function.

Below are show some pictures illustrating some instances and performance of this program.

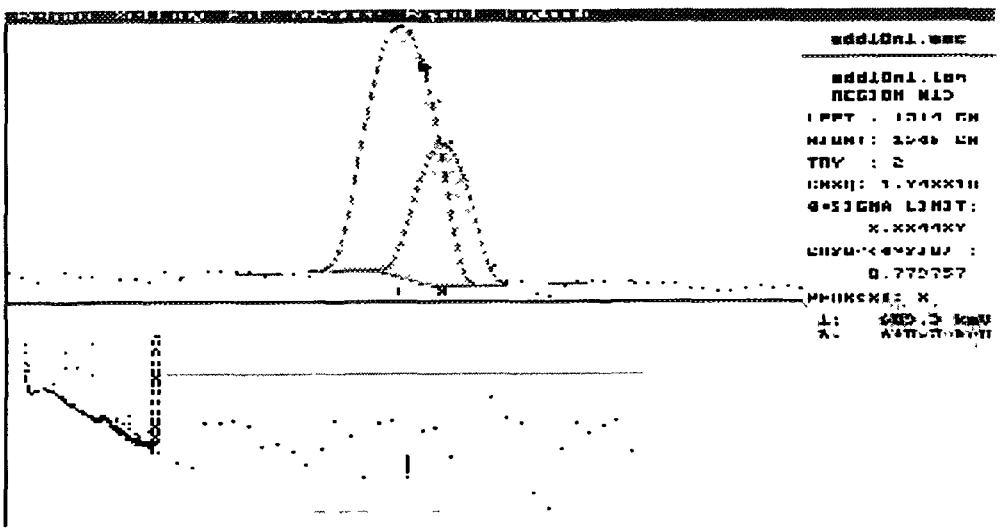


Figure 16. Perfect deconvolution of the multiplet in the spectrum *10n1* . High peak on the left side of a small peak with ratios 10 to 1).

In the following figure χ^2_r is equal to 1.74 but it is not understandable what is the meaning of the 4*SIGMA value.

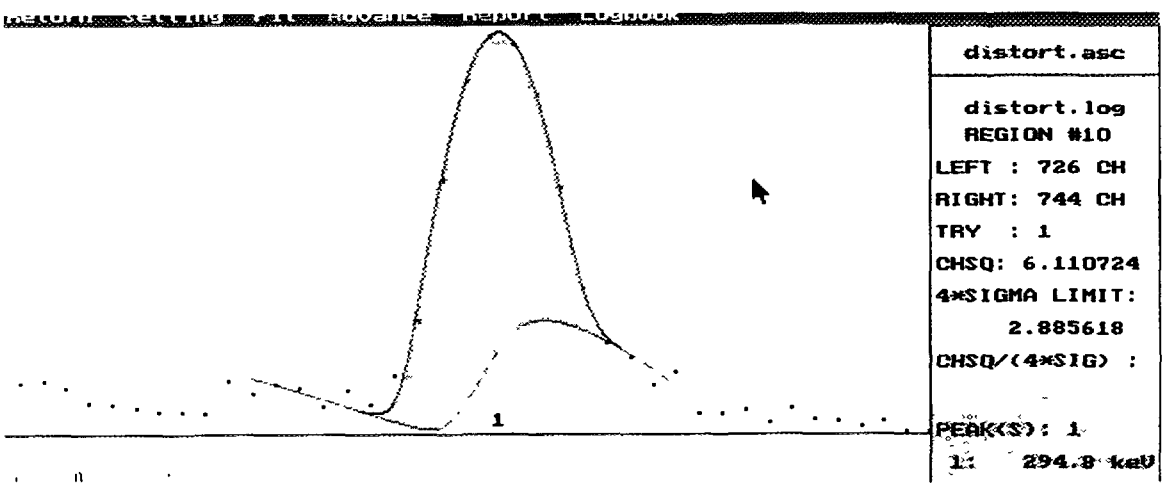


Figure 17. A bad background shape obtained during the automatic processing of the distorted spectrum.

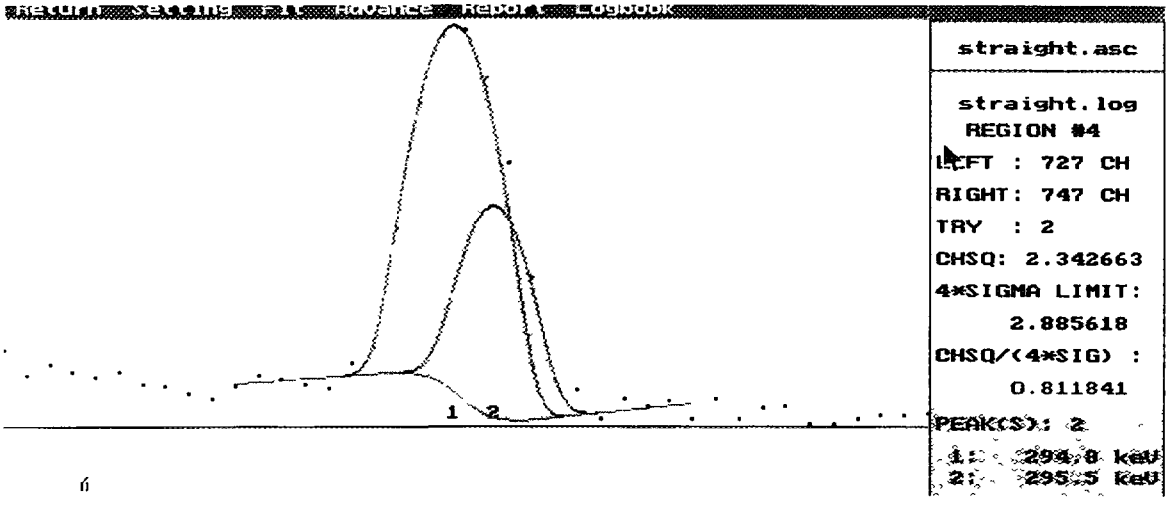


Figure 18. A very nice deconvolution of the closed doublet at 294-295 channels in the STRAIGHT spectra.

6.9. OSQ/Professional, version 6.3 release 1

by APTEC Engineering Ltd. , Canada

OSQ/Professional is a MS Windows based gamma ray spectrum analysis program developed on the basis of a MCA emulation software. As a data acquisition device it works only with Aptec cards.

It comes in a single 3.5" diskette and six different types of Manuals. Upon request a well-written and comprehensive Gamma ray Spectroscopy Workbook can be provided as well.

⇧ The installation is simple and efficient. It gives the choice of full or custom installation. It creates sub-directories if needed and it prompts for any replacement of a system or program files, for the user choice.

The software is eventually not protected, but it will print/save any spectrum analysis only with the presence of an APTEC MCA card. This might not be a nice option for a user (having purchased the package) who wants to analyse gamma ray spectra in a computer where an APTEC MCA is not installed.

⇧ It can import spectrum files from many commercial and non-commercial companies or type of formats (including VAX format !!!).

⊗ IAEA spectrum format conversion failed. In addition, IAEA type of format is listed with default file extension ".DAT" which is wrong.

⇧ The OSQ/Professional has an outstanding user interface. It is colorful, convenient and fast. Mouse operation is easy and most essential operations can be controlled by key-strokes.

Almost a wide spectrum information can be displayed, In addition to the spectrum ID, the preset time, true time, live time, dead time (as TT-LT/TT in %), gross count, counts/sec, start and stop times, start and stop dates and user's Id are displayed too.

⇩ Although the programs window can be splitted horizontally or vertically, for seeing another region of the spectra or a zoomed peak; full implementation of multiple windows is absent.

Meaning, several spectra or more than two parts of same spectra can not be viewed at the same time.

⇧ Any calibration is easy and efficiently done in OSQ/Professional. Energy and FWHM calibrations can be done in automated mode were peaks from the spectra are automatically identified and energy values are extracted from the provided nuclear data library (an specific one for calibration is provided, called "isotope.lib") Nevertheless, the user still has the option to change, delete or add any additional point or to change the reported calibration parameters

Efficiency calibration is also convenient and efficient. Functions like Polynomials of Ln(E), (1/E) and cubic spline are given for the choice of the operator. Polynomial's degrees can be chosen as well.

The peak search and fitting procedures are controlled by the user through a wide choice of parameters Figure 19, shows available parameters.

Possible peak centroids are located by filtering the spectrum with a third order derivative. A zero-crossing method together with criteria of statistical confidence are used to detect peaks and precisely locate peak positions.

⇩ However, residuals values are plotted only when multiplets are fitted.

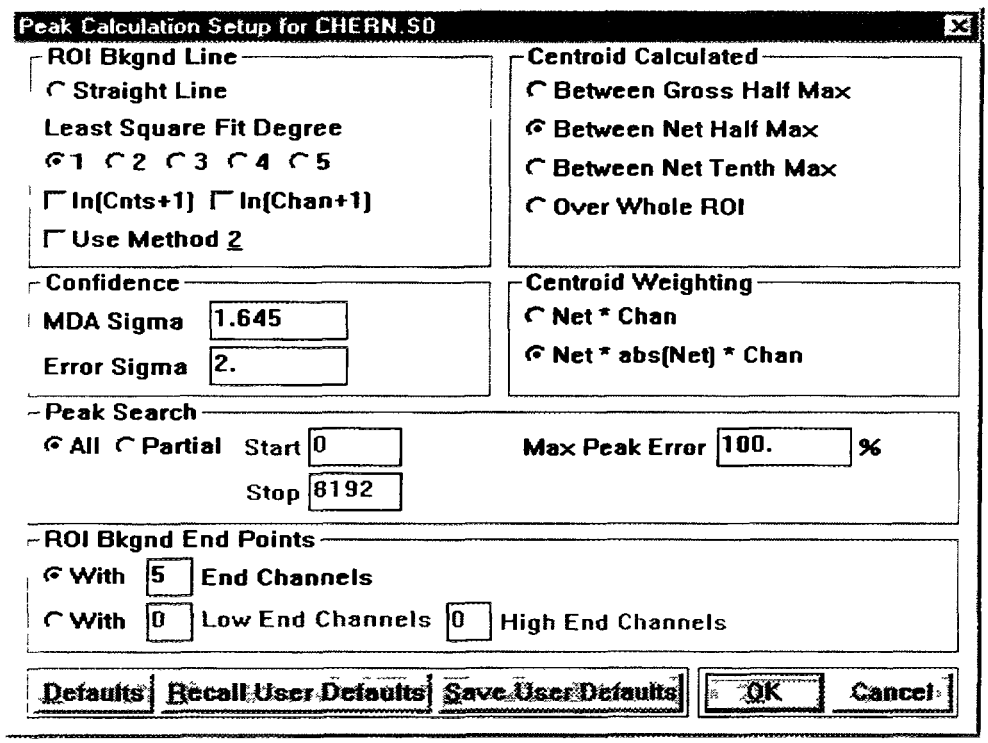


Figure 19. Aptec OSQ/Professional. Control parameters of the peak search.

The program can report activities and calculate Minimum Detectable Activities (MDA), for peaks which have not been found.

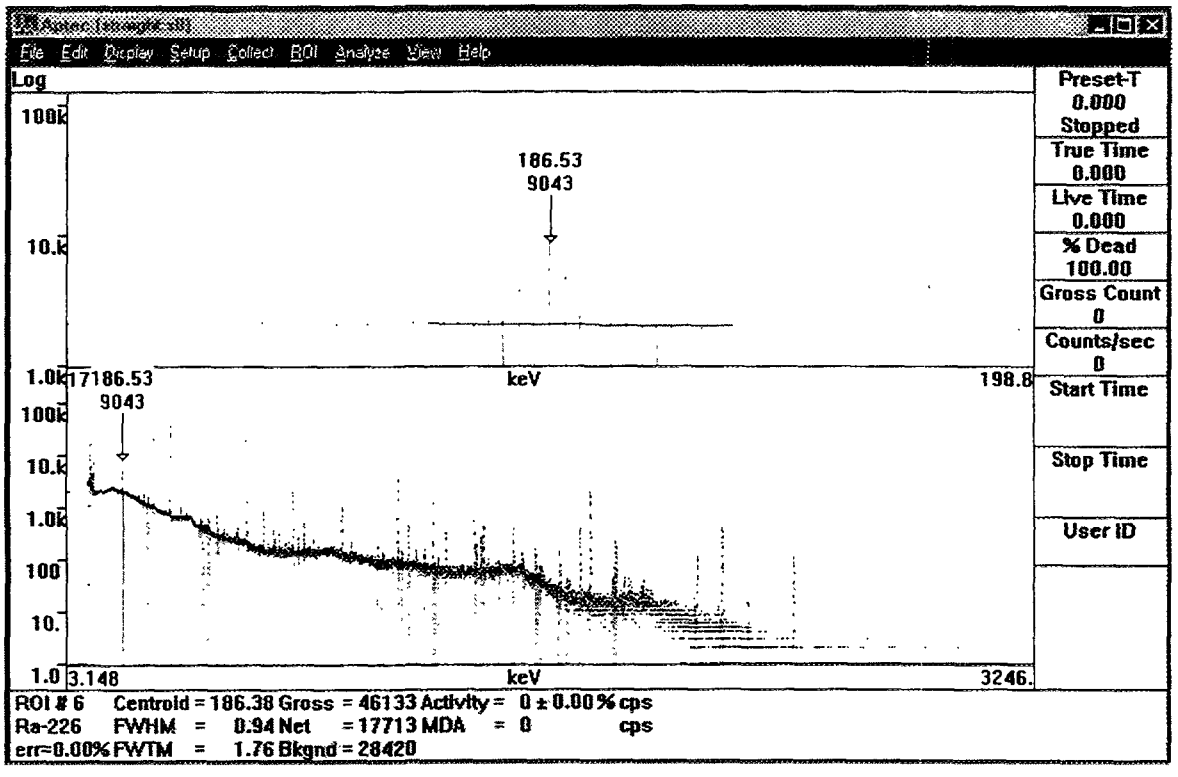


Figure 20. Aptec's OSQ/Professional. Fitting of the 186 keV peak.

OSQ/Professional provides a built-in utility for nuclear data library edition. It also provides some specific applications data libraries.

⇧ The user can define his report by selecting a number of options. Units in the reports can be standardised.

The help on-line is concise, although some times too short.

⇧ The manuals are excellent. Well written and edited with plenty of figures, examples, Tips and hints.

⇧ Aptec OSQ/Professional provide to the user many small but nice features, e.g. when the program starts it always loads the last analysed spectrum; or when looking at any particular region of the spectrum and you look (even load) into another spectrum, it will go to that region automatically (even expand it, if you were at expanded mode before).

6.10. Sampo 90, version 3.6

by Helsinki Univ. of Technology., Helsinki, Finland

The Sampo90 program is a well known gamma ray spectrum analysis program. It is a copyright of P. Aarnio et al., Helsinki Univ. of Technology, although several dealers are distributing it. The copy obtained for this intercomparison was operated under DOS ver. 3.3 or higher. It needs a 7 Mbytes disk space.

The installation is simple and effective using the restore command, but the user has to modify "config.sys" and "autoexec.bat" files by himself.

⇩ It has no mouse support, although it gives a full user operation through the keystrokes.

⇧ The Sampo90 software has a built-in a conversion utility from the Canberra S100, Accuspec, ORTEC ADCAM, The Nucleus' PCA spectrum formats. It has an extremely useful capability to import user-defined ASCII files.

⊗ Sampo90 does not accept all valid DOS filenames, e.g. filenames with '_' characters in them cannot be entered.

Sampo90's user interface is reasonably friendly and fast.

⇩ Input of numbers is a little cumbersome if cursor keys are used to select command: Even after using the program for days, the right moment to enter numbers was often missed. In some cases the same information has to be entered several times. Also, the different parts of the program are unaware of each other. For example if a 8192 ASCII spectrum is to be analyzed, the number has to be entered 3 times.

Graphs of peak fits, efficiency, shape and energy calibration are available. The shape calibration is the only one without a residual plot.

⇧ The energy plot has a unique and beautiful feature· It indicates increased uncertainty in energy when extrapolating outside the range of the calibration points.

⇧ For shape and energy calibration, the program can automatically find and fit suitable peaks for the shape calibration. The user can then modify the list to exclude "odd" peaks. An exception can be made for the 511 keV peak.

A very nice possibility of automatic shape calibration, where each peak the program proposes to use for the calibration, is shown to the user. The user can accept or reject the peak and if the peak is too close to others, the program offers the correct advice not to use the peak. The default significance level for the peaks in this procedure is only 4 - that should be a higher value, like 10-20.

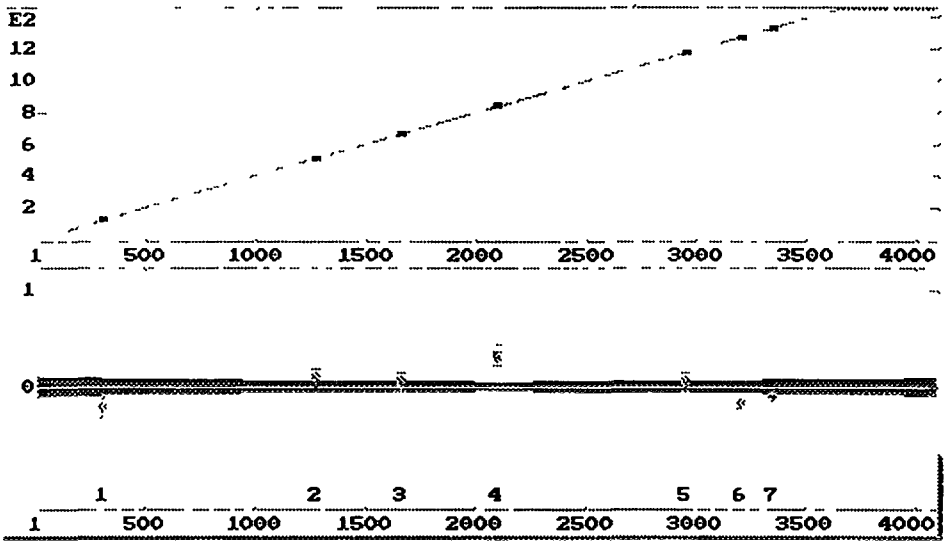


Figure 21. Sampo90. Energy calibration graph. In almost all Sampo90 graphs residuals are shown.

Spectrum analysis consists of peak search followed by a fitting procedure. The range of channels to be fitted can be indicated, but the search is not radionuclide-library oriented.

The peak-fitting function is the standard two-tailed Gaussian on a linear or parabolic background, without a Compton step under the peak. In the fitting procedure, the chi-square is minimized.

⇧ A separate peak shape can be used for the 511 keV peak, i.e a wider Gaussian

⇧ Spectrum analysis can be fully automatic, fully interactive or in between.

⇧ The significance thresholds for search and fit, as all parameters involved, are clearly defined in the manual and can be set by the user. Peaks can be inserted (or deleted) by the user even before fitting, should a peak be missed in the search, as well as during manual fitting.

Peak fit for singlets is linear by default: No uncertainty in peak position is determined. In the case of multiplets (or singlets if so desired), non-linear fitting is applied: Positions are varied as well as peak area, all other shape parameters are fixed. The user does not have the option to free the tail or width parameters.

Peaks are fitted together if separated by 4 or 6 FWHM (manual inconsistency). The fit area is determined automatically.

With a separate program not included in the standard package, concentrations in NAA can also be calculated using the comparative method.

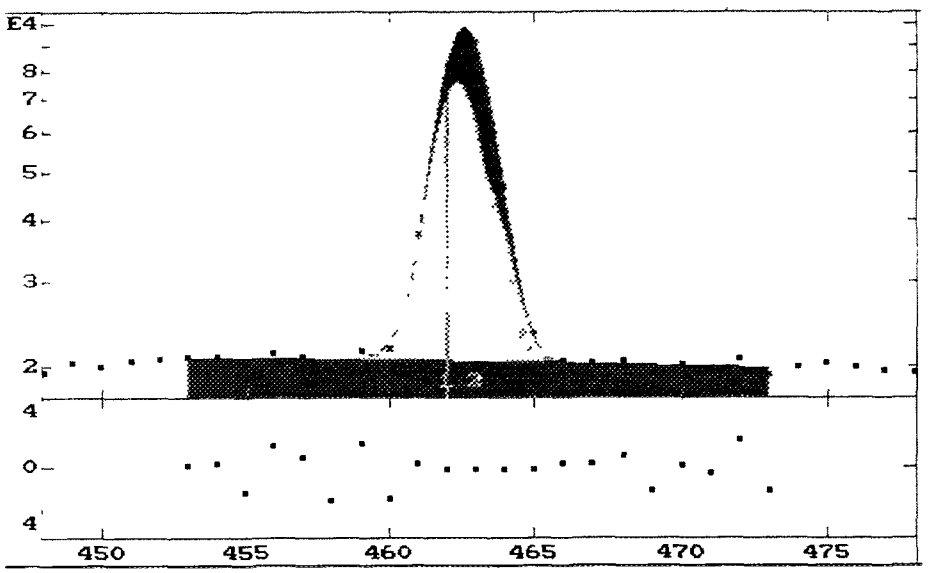


Figure 22. Sampo90. Fitting of the 186 keV peak, with the corresponding plot of the residuals.

⇧ Interference corrections when interpreting the spectrum are performed using least squares methods

⇧ There is context-sensitive help available in the program. Error messages are clear.

Peak positions, areas and their uncertainties can be reported in the end. The report can be user defined and can contain any parameter used in the program. It has an ASCII format and can be printed or written to file. The graphs can be sent to a printer directly. If the user wishes to create a report suited for it, QA-related information can be printed in the report.

⇧ The User's Manual (according to the authors not complete) was found to be well organized with excellent readability, containing tutorial section to start, 'procedures' section for more advanced operations, 'commands' section as reference. Algorithms are clearly explained and access to parameters pointed out. It just lacks an Index section to be an excellent manual.

6.11. Span, version 5.1

by Institute of Atomic Energy, Beijing, People's Republic of China

SPAN v5.1 is the multipurpose software package [21] used for gamma ray spectrum analysis and neutron activation analysis developed at the China Institute of Atomic Energy. The package consists of one 3.25" HD installation floppy and a 54 page user's manual.

The software was designed to run on a standard PC computer, under the DOS operating system.

⇩ Installation is difficult probably due to the disk protection scheme used by the code.

⊗ Moreover, automatic change of the "autoexec.bat" and "config.sys" files not always work.

☞ **We were not able to install the software in a notebook, COMPAQ 486DX-25 which used STACKER disk compression software. Installation was repeated three times before we finally got a working version of the code.**

⇧ The software can process the spectrum data produced by Nucleus, Ortec, Canberra or Silena data acquisition systems.

⊗ During the intercomparison Span program fail to read 8K spectra. It got wrong numbers after 4400 channels. This looks like a memory allocation problem.

⇩ The documentation on the spectrum analysis procedures is rather limited. The parameters that affect the peak search and doublet resolution are briefly discussed in the user's manual. The actual peak area determination is not documented.

The baseline is removed from the spectrum before the area calculation is done. A peak shape is calculated based on the peak shapes stored during the calibration step, after which an experimental peak shapes table is created; or using the Gaussian function (depending of the user choice).

The fitting procedure can be controlled by several parameters. Among others the following parameters can be adjusted for peak search:

1.-Peak Analysis Method: There are two approaches involved in the code the Total Peak Area (TPA) and Gaussian Function Fitting (GFF) methods. The limit of identification for closed doublet of equal intensities is about 0.5 times the FWHM of the components. User could select either the **TPA** method or **GFF** method for all peaks (both singlets and multiplets). These two methods can also be selected by computer automatically using the option **AUTO,** that means the TPA method is used for singlets and the GFF method for every multiplet.

2.- *Error Limit*: The user can limit the reported peaks by entering its error limit, that is, peaks with an relative error in the peak area larger than this value will not be listed in the report.

3.-Sensitivity factor for peak search: The less this value is, the more sensitive will a peak search. Only the optimum value of **5** is specified in the manual.

4.-Maximum peak number: This option sets the maximum peak number and allocates memory space for saving the parameters of the peaks. The maximum peak number should be between 200 and 512.

You can select to subtract the background contribution, calculated from the another spectra, from the results of the NAA calculation, for instance. This option was not used in this exercise.

The Integral Peak Technique which produces step background line was used. In this way the baseline can be subtracted from the raw spectral data before the nonlinear fit is done.

⊗ Residual fit is not shown on the screen, although there is a graphic region dedicated to this task.

⇩ There is not proper handling of the 511 peak.

The code usually combines Total Peak Area method for singlets with nonlinear squares fit to calculate net peak area and uncertainties for multiplets. The nonlinear fit can be done using either Gaussian shape or experimental peak shape previously stored in the calibration run.

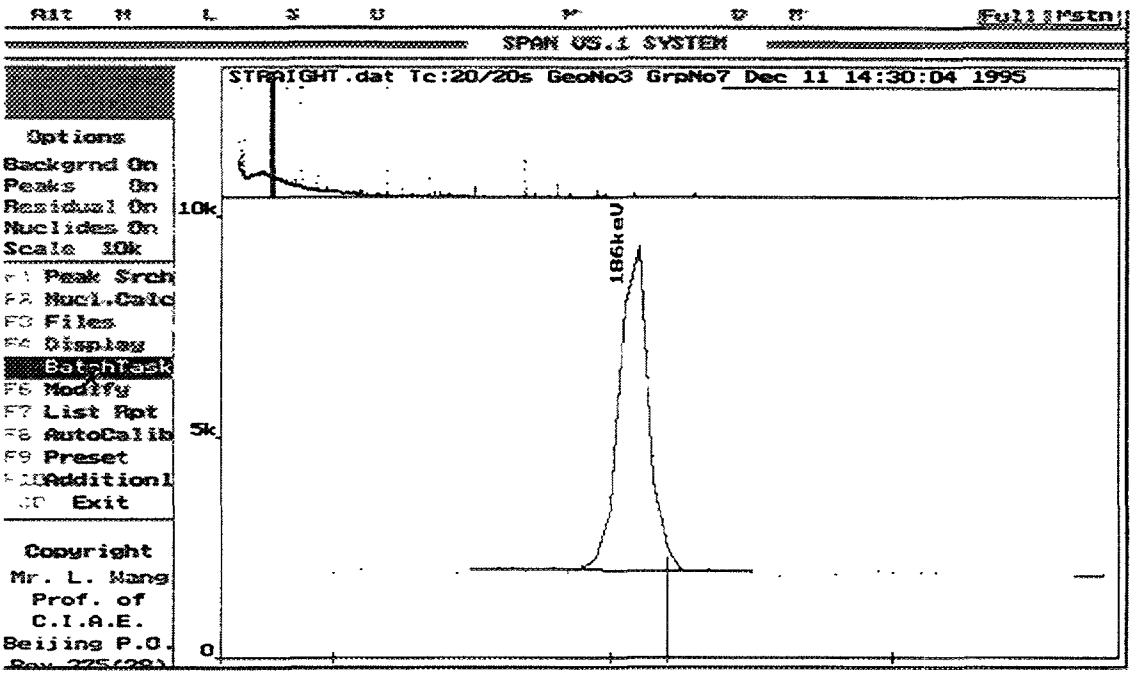


Figure 23. Span. Fitting of the 186 keV peak.

⇧ SPAN sports a batch processing capability as well as automatic energy re-calibration capability.

⇩ The output of the results are always written to the same file in the current directory named PEAKANAL.REP (undocumented feature).

⊗ There is no DOS ERROR trap capability build into the code. Every time when printer got out of paper, or operating system reported an error, the program reported nonsense.

The ***documentation*** is concise but gives complete information from the user's point of view. Detailed description of the used algorithms for area and uncertainties calculations is missing.

⇧ It has a very helpful flow diagram to show how user should proceed to use the software.

6.12. InterWinner/WinnerGamma, version 3.42

by Eurisys Mesures, France

The Winner/Gamma software package is a MS Windows (ver 3.1 or higher) based gamma ray spectrum analysis program developed on the basis of a MCA emulation software.

⇧ As a data acquisition device it can control and operates most of the commercially available MCA cards. It also has the built-in option for emulation of an acquisition system.

The installation is quite simple and requires the presence of the protection key as well as to operate the software. It also can be installed in three EU languages: English, French or German.

⇩ Although it operates most of the MCA cards, the software can not convert different spectrum formats. To read the IAEA ASCII format a special program was provided by the supplier, but it was not very flexible and efficient (e.g spectrum to be read must always have the same name and be in a fixed sub-directory).

Before running the program the Setup program should be started in order to configure the hardware in use and the software options

⇩ There is no provision for viewing the x-axis in channel numbers mode

⊗ The software seems to work only for 4K spectra, or it might be a problem in the conversion algorithm During the intercomparison, spectra with 8K were normally read until the 4098th channel, after which random data were stored into the next channels.

⇧ The Winner/Gamma software sports a nice and efficient interface, making use of all provisions of Windows operating system. Colors are user defined and it uses a multiple-window environment

⇩ However, the cursor in the spectra is misleading. Actually there is no provision of the cursor The often so-called cursor information (channel and channels content) is given while moving the mouse pointer over the spectrum, but even no marker is provided for exact visualization of the current position

The software provides an automatic mode of energy and resolution calibration In the resolution calibration the range of an interval (min and max) for the variation of the FWHM can be numerically entered and them the software on automatic mode will chose the proper function to fit the experimental points

⇧ A nice feature in this program is, while you are in the E-calibration, all the known calibration peaks are automatically identified and displayed, by clicking at the points in the display the user can chose to include it in the calibration and the available elements and their corresponding energy are displayed automatically besides the mouse pointer for the user selection.

Efficiency calibration is done using a ln(E) or (1/E) polynomials, with an user-defined degree The plot of the efficiency also reports uncertainties.

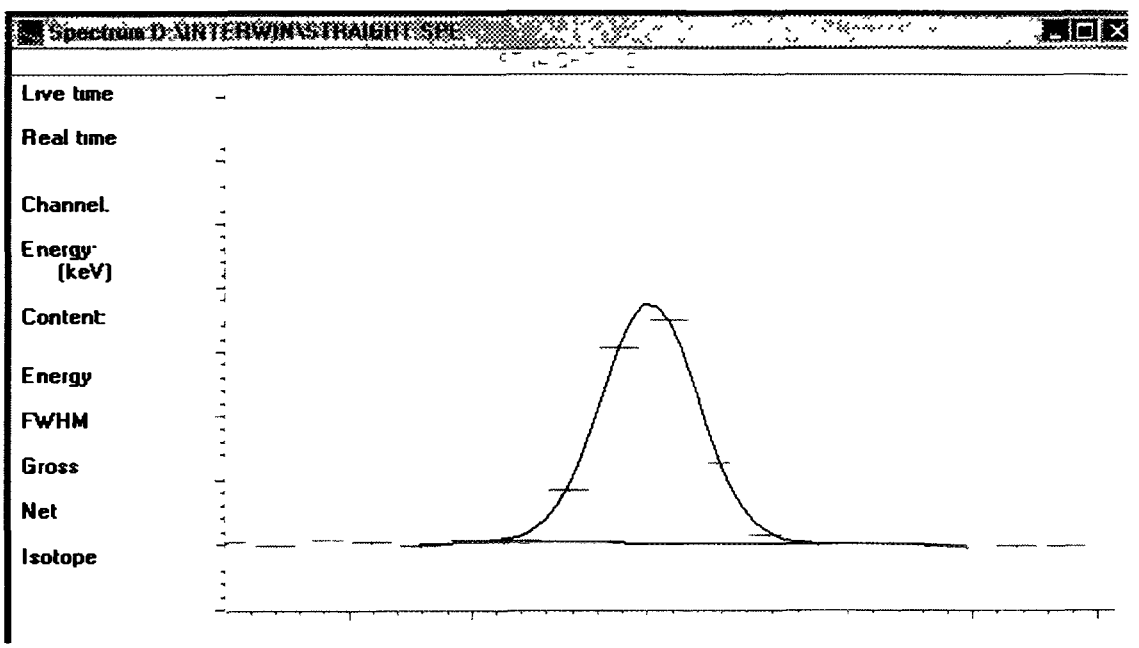


Figure 24. Eurisys Winner/Gamma. Fitting of the 186 keV peak.

The analysis of the spectra is based first on the peak search and then on the peak fit.

⇩ The peak search and fitting can be controlled by the operator, but is limited to the variation of the peak sensitivity factor only.

Activities can be also calculated and reported. Standard units can be user pre-defined for reporting activities.

⇩ Residuals of the fitting procedure are not displayed

The software allows the comparison of several spectra. It has implemented some spectrum manipulation features like: change of the contents for an specific channel (dangerous), smooth (with user-defined type of smooth polynom), strip, compress, multiply by a constant, add one or several spectra, subtract spectrum

The received User's manual was very limited. No information at all on specific issues like peak area determination and search, peak fitting, etc.

⇩ The software does not have any on-line help.

Routines analysis in batch mode are possible, even with pre-defined set of operational parameters for each batch.

A separate optional software WinnerScan can be provided, to work in conjunction with Winner/Gamma for automatic scanning of radioisotope activities (or peak areas) vs time.

CHAPTER 7: OVERVIEW

In this Chapter an overview of the possibilities and available options for each program are summarised. They are organised in areas of interest for different end-users. Some comments are given below each table. More detailed information on the particular aspects of each program is given in the previous Chapter.

Hardware

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Minimum CPU required	80286	80286	80386	80386	8088	80286	80386	80386	80386	80286	80286	80386
Coprocessor required	Yes	Yes	Yes	Not	Not, but recommended	Not, but recommended	Yes	Yes	Yes	Yes	Yes	Not, but recommended
Minimum disk space	1 Mbyte	3 Mbytes + examples	2 33 Mbytes	5 Mbytes	2 Mbytes	3 Mbytes	Variable, depending on the options to be installed Basic Installation app 6 Mbytes	500 Kb programs , 300 Kb examples	2 13 Mb without samples spectra	7 Mbytes	500 Kb for the software 500 Kb for examples	2 Mbytes
Operating system required	DOS version 3 1 or later	DOS version 5 0 or later	DOS 4 0 or later	MS Windows 3 1 or later	DOS 2 00 or later	DOS 3 1 or later	OS/2 2 1 or later	DOS 3 1 or later	Windows 3 1 or later	DOS 3 3 or later	DOS 3 1 or later	Windows 3 1 or later
Minimum RAM	590 Kb	610 Kb **(strong requirement)**	4 Mbytes (8 Mbytes recommended)	4096 KB	512 KB	about 600 KB **(strong requirement)**	8 Mbytes 16 Mbytes recommended	300 Kb	8 Mbytes recommended if operating under Win 95	505 Kb	600 Kb (estimation)	8 Mb recommended
Graphics cards												
Minimum required	EGA	EGA	EGA	VGA	EGA	CGA	VGA	VGA	VGA	EGA	EGA	VGA
Modes that can be used effectively	CGA, EGA, VGA, SVGA	EGA, VGA and SVGA	CGA, EGA, VGA and LCD VGA	VGA and SVGA	EGA, VGA or better	CGA, EGA, VGA	Any driver supported by OS/2	VGA, SVGA	SVGA Graphics accelerator recommended	VGA, SVGA	EGA, VGA, SVGA	VGA, SVGA Graphics accelerator recommended
Color Monitor												
Required	Yes	Yes	Not, but recommended	Yes	Not, but recommended	Not, but recommended	Yes	Yes	Not, but recommended	Not, but recommended	Yes	Not, but recommended
Used	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Mouse support	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes
Keyboard operation only possible	Yes	Yes	Yes	Yes	Yes	Partially	No	No	Yes	Yes	Yes	Yes
Software protection	None	Parallel port key	Parallel port key	None	Parallel port key	None	Parallel Port Key, necessary only for network operation	Parallel port key	Software will operate normally without any protection but prints results	Parallel port key	Special format of the distribution diskette	Parallel port or PCMCIA key

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypernet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
									only with the presence of an Aptec MCA card		Maximum of three installations allowed	

Comments

Almost all the software packages do not strictly require a color monitor for their operations, but the fact that areas, fitting results, residuals and many other information are given in different colors, implies the requirement of color device for best performance and view

In the case of the software based on Windows OS the required amount of RAM is bounded to the requirements of the operating system itself Thus, here the recommended amount of RAM for a reasonable fast operation of the software is given

Some times the microprocessor requirements for a software are of those of its operating system E g the minimum microprocessor requirement for software packages running under MS Windows 3 1 are those minimum hardware requirements for the MS Windows itself, in this case microprocessor 386 is the minimum option

Programs running under DOS like GammaTrack and Ganaas have a strong requirement of free RAM available, the failure to meet that requirement will end in a non-operational software For those programs sometimes, it is compulsory to have DOS RAM free as much as possible, limiting the capabilities of running TSR programs

Graphical capabilities of the programs

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Plus	Sampo90	Span	Winner/ Gamma
Zoom Option available	Yes, ROI and fitted peaks	Yes As Expand facility ROIs, peak fits Zoom user defined but limited to 64 channels on X axis	Yes In expand mode the lower part screen shows entire spectrum, the upper part the expanded region	Yes ROIs, fitted peaks and residuals As Expand too	Yes (a little disorienting) ROI, fitted peaks and residuals	Yes ROI, fitted peaks and residuals	Yes As Expand facility ROIs, and any part of the spectra Zoom can be user defined It is not possible to display fits or residuals in the main program	Yes As expand option, controlled by the user	Yes User defined	Yes	Yes It can be defined by the user	Yes User defined
Y-scaling modes	Lin, Auto and Manual No Log and Sqrt	Lin, Log, Auto and Manual No Sqrt	Lin, Log, Auto and Manual No Sqrt	Lin, Log, Manual and Auto No Sqrt	Lin, Log,, Manual No Auto and Sqrt	Lin, Log, Sqrt Manual and Auto scaling	Lin, Log, Manual and Auto No Sqrt	Lin, Log, Sqrt, Auto, Manual	Lin, Log, Sqrt Auto and manual	Log and Auto only	Lin, Log, Auto and Manual No Sqrt	Lin, Log, Sqrt Manual and Auto scaling
User-defined colors	Yes	Yes	Yes	Yes	No	No Colors can be disable only	Yes	No	Yes	Yes	No	Yes
Menu												
Menu operation	Yes	Yes	Yes	Yes	Yes	Yes, also command operation	Yes	Yes	Yes	Yes	Yes	Yes
Can the menu options be user defined or changed	No	No	No	Yes	No	No	No	No	Yes But partially Choice between large and short type of menus	No	No	Yes
Graphical representation of												
spectra	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes, dotted and lines	Yes, full spectra or reduce representation	Yes	Yes	Yes, dotted or joined lines ROI as bars
fitted peaks	Yes (not documented how)	Yes	Yes Pressing "info peak" option	Yes, excellent	Yes, different ways Excellent representation	Yes Fitted and spectra points in diff colours	Yes Although requires to be in the interactive peak fitting mode Displays fits and residuals on a separate window	Yes, dotted only Fitted region presented as filled coloured	Yes As well as baseline under the peaks	Yes	Yes In the ROI mode peak fitting can be seen against spectra points	Yes Fitted peaks Doublets in different colors Continuum under the peaks

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Plus	Sampo90	Span	Winner/ Gamma
Residuals		Yes	No	Yes	Yes	Yes	Yes		Partially Residuals plotted only for mu,tiplets	Yes	Documented, but does not work	No
Energy calibration	Yes	Yes	Yes, but difference in eV Vs Energy	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes Can be superimposed over the spectrum
Resolution calibration	No	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes Can be superimposed over the spectrum
Efficiency calibration	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Multiple windows available	No Only split for zoom	Yes	Yes, but mainly for showing diff parts of spect Info The windows can not be resized	Yes	No	No	Yes	Yes	No Only split for zoom	Yes	No	Yes Each individual window can be configured independentl y
Additional information displayed	Yes	Yes Almost full header	Yes, Id, TT, LT	Yes Headers TT, LT, counts, energy, peak position	Yes Spectrum ID, I I, L I	headers TT, LT, counts, energy, peak position	Yes, very complete information of parameters and header provided	Yes Almost all information available in the header of the file	Yes, TT, LT, Ids, dates, gross counts Preset Time, etc	Yes, but very limited	Yes Almost all information available in the header of the file	Yes Channel, Counts/ch and energy TT and LT If ROI selected, info on ROI is displayed
Spectrum cursor												
Available	Yes, acceleration mode available Key and mouse controlled	Yes, slow and accelerated movement Key and mouse controlled	Yes, movement using arrow keys Accelerated movement provided mouse controlled as well	Yes, slow and accelerated movement Key and mouse controlled	Yes, good movement over spectra Key and mouse controlled	Yes, slow and accelerated movement Key and mouse controlled	Yes, using mouse	Yes	Yes, acceleration mode available Key and mouse controlled Keystrokes for fast movement provided	Yes	Yes, but can be moved using mouse only	Partially, a kind of cursor info is provided while moving the mouse

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Plus	Sampo90	Span	Winner/ Gamma
Which information it displays	channel or energy and counts at position	channel or energy and counts at position	channel or energy and counts at position	channel, energy and counts at position	channel, energy and counts at position	channel, energy and counts at position	Several Channel, energy, counts, markers, etc	channel, energy and counts at position	channel, energy and counts at position	channel, energy and channel content	channel, energy and counts at position	channel, energy and counts at position

Calibration Procedures

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Plus	Sampo90	Span	Winner/ Gamma
Minimum and Maximum number of parameters used for E-calibration	Min=2	Min=2	Min=1 Max=3 Automatic mode provided	Min=1 not limited for Max	Min=3 and Max=20	Min=2 and Max=11	Min=1	Linear calibration User defined polynomial E-calib also provided but as especial option	Min=1 Max=5 Automatic mode of calibration provided	User defined order Depending on the function	Min=2 Quadratic function using three exp points as Min	Min and Max=3 Automatic mode of calibration provided
Minimum and Maximum number of parameters used for Resolution-calibration	Min=2	Min=2	Min=1 Max=3 Automatic mode provided	Min=1 not limited for Max	Min=3 and Max=20	Min=2 and Max=11	Min=1 Only one parameter is used for shape calib , which is performed automatically	Resolution-cal performed automatic using two parameters	Min=1 Max=5 Automatic mode of calibration provided	User defined order Depending on the function	Three experimental peaks as Min to perform FWHM-calibration	Max and Min=3 A kind of automatic mode provided
Minimum and Maximum number of parameters used for Eff-calib	Min=2	Depending on the function	Min=1	Min=1 not limited for Max	Min=3 and Max=60	Min=1	Min=2 Maximum depending of available data points	Depending of type of function	Depending of type of function	User defined order Depending on the function	Depending of type of function	Min=1 Max=12, but depending on the exp data
Functions available for Eff-calibration	Several Polynomial function of Ln(E) or at (1/E)	Log of cubic polynomials and inverse exponential function		Divided in two regions interpolation, linear, quadratic and polynomial Bellow interpolation, linear and quadratic	Several Excellent choice and capabilities	Several Polynomials of Ln (e) and (1/E) of different degrees Parametrisation function is provided for calculation of eff using one exp point	Several Polynomials of Ln (e) and (1/E) of different degrees	Selectable degree of ortho-normalised polynomials to the data	Ln(E) polynomials of different degrees Polynomial of (1/E) at diff degrees Cubic Spline	Interpolation, diff Types polynomials, Ln(E) pol And SQRT pol	Selectable degree of ortho-normalised polynomials for three energy regions	Polynomial function of Ln(E) or of (1/E)

Spectrum analysis

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Is the spectrum analysis (peak-area determination) performed by peak search?	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Is the spectrum analysis (peak-area determination) possible by specific radionuclide determination?	No	Yes	Yes	Yes	No	No	Yes	No	Yes	No	No	Yes, but you have to buy the nuclides library option.
Fitting functions available	Parabolic interpolation of an experimental peak shape tables	Gaussian according to the manual	Gaussian with a tail.	Gaussian	Gaussian full energy distribution with a fifth power low energy tailing function	Gaussian with an exponential at low energy tail. Not described in the manual	Gaussian, when TAIL is set to none, and Gaussian with exponential tail on the left side	Linear sum of Gaussian and Gaussian with exponential tail on the left side	Gaussian with tail	Gaussian with two tailing on parabolic or linear continuous.	Gaussian or fitting based on experimental peak shape table	No information available
Are user-defined peak shape functions possible?	No	No	No. The asymmetry of peaks is fitted as polynomial, the degree of it can be changed	No	No	No	No. But alternative fitting functions are provided	No	No	No	No	No
Algorithm for fitting	Uses stored peak shapes from the calibration to fit the peaks	Non-linear fit (poss. Modified Marquardt)		Least square fitting	Least square fitting	Least square fitting	Non-linear fit using Marquardt algorithm	Non-linear Fit	Least square fitting	In case singlets, linear fit default Non-linear fit Chi-squares are minimised.	Non-linear fit	No information available
Baseline functions	A combination of iterative smoothing and a step	Parameter-less step function calculated from scaled	Not known. Not documented at all	For singlets automatic 5 or 3-points average For	In each region is calculated accordingly[10]	Smoothed Step-function. Not documented	Various options provided Default is a step function	Step-function folded with the Gaussian	Linear or Least square fit of up to 5 degrees	Linear or parabolic.	Total Peak Area Method based on a Step function Not well	No information available

[10] where the number of baseline counts in each channel is analytically determined from the experimental number of peak counts in all higher channels

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
	background	integral of the peak		multiplets stepped or parabolic functions			I inear and no function provided as well				documented	
Special treatment of the 511 keV peak	No	No	No	No	No	Yes	Yes	No But, it is possible to fit it manually outside the FWHM calibration	No	Yes	No	No
Automated mode of analysis with defaults parameters available	Yes	Yes, with reasonable good performance for simple spectra	Yes	Yes	Yes	Yes	Yes Very good performance at spectrum of singlets	Yes	Yes	Yes, very good performance	No	Yes
Threshold for peak search	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
User-selected threshold peak search parameter and well documented	Yes but not so well documented	Yes and well documented	Yes and well documented	Yes, effectively explained	Yes	Yes, but not well documented	Yes, well documented	Yes But input expert mode badly documented	Yes Very well documented	Yes Very well documented	Yes, but not documented No recommended value provided	Yes Not documented
Force (manual) peak insertion mode implementation	No	Yes	No	Yes	Yes	No	Yes	Yes	Partially, by inserting manually a ROI	Yes	No	No
Can a peak be added or removed manually in a multiplet ?	No	Yes	No	Yes	No	No	Yes, but extra software has to be requested	Yes	No	Yes	No	No
Peak area and standard deviation determination	Net area obtained from fitting It is not documented how the other values are obtained	Net peak area, and standard deviation reported in sigma in %	Net peak area, standard deviation reported in times sigma (1, 2or 3 σ in %)	Net peak area, standard deviation reported in sigma (1,2 or 3 σ in %)	Net peak area Relative uncertainty	Net peak area Relative uncertainty	The are is determine by fitting or integration Level of reported uncertainty can be chosen	Net peak area and relative uncertainty in % Method of uncertainty is not reported	Net, Gross, background peak area reported Uncertainty is relative and in %	User-defined Options are Net, Gross, background, relative or absolute uncertainties, etc	Net peak area Relative uncertainty How uncertainty is calculated is not documented	Net, Gross peak area reported Uncertainty is relative and in %

Peak identification

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Does the program performs radionuclide identification ?	Yes	Yes, including detection of possible interference	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Reports of the identification results	Printed and saved into a file ASCII, not to easy to import, since it contains special characters	Printed only or saved into a file (proprietary format only)	Printed and/or saved into a file ASCII format possible	Printed or saved into a file ASCII, easy to import	Printed and saved into a file ASCII, easy to import format	Printed or saved into ASCII file	Printed or saved into a file Both proprietary format (CAM files) of ASCII format files are provided Easy to export		Printed and saved into a file ASCII, easy to import	Printed or saved into ASCII file	**Printed ONLY** No save no ASCII format	Printed, or saved into a file ASCII format supported

Nuclear Data Libraries

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Is there any isotope nuclear data library available	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes, but very limited	Yes	Yes	Yes	Yes, but as optional item
Can the nuclear data library modified (edited) or created by the user ?	Yes An automated way of entering peak information is provided	Yes Library editor is integrated into the main program	Yes	Yes, see notes	Yes	Yes	Yes It has a very powerful library editor	Yes But no inside utility to perform it is provided Editions to the library should be done with an external ASCII editor	Yes	Yes	Yes	Yes An useful library editor is provided
Provision of specific application-oriented isotope library	Yes NAA	No	No	Yes	Yes	Yes, NAA	Yes, upon request	No	Yes, several	No	No	Yes, several

Reports

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Default report	Yes	Yes, many options	Yes	Yes	Yes	Yes	Yes	Yes	Yes, very complete	Yes, very complete	Yes	Yes
Can the user define the analysis report ?	No	Yes	No	Yes	No	No	Yes	No A Full or an Abbreviated type of reports are offered	Yes, with many different options (modules) But options are predefined and can not be changed	Yes	No	Yes, with many different options Even the units to be reported can be standardise
Possibilities on the output of the results	Print or ASCII	Print or saved into a file ASCII format is provided as well	Print or saving into a file ASCII format possible	Print or ASCII file An option for MS Word file type is also available	Print or ASCII file (easy to import)	Print and ASCII files Several ASCII files are kept as track-keepers	Printed or saved into a file Both proprietary format (CAM files) of ASCII format Easy to export	ASCII or Sampo90 format The short report is very suitable for importing into any spreadsheet	Print and/or save ASCII and ASCII separated by commas, ideally for importing them into spreadsheet	Print or saved into a file ASCII format also provided	Printed Only No save mode, no ASCII format	ASCII, Print to a file or to the screen only A creation of a database is possible as well

Others

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
Spectrum utilities												
spectrum format conversion	Only from ASCII	No Program might be requested from the supplier	Yes, several	Yes, major commercial formats	Yes, major commercial formats	Yes Vast choice, including major commercial formats	Yes, major commercial formats	Yes but limited	Yes, major commercial formats	Yes, major commercia l formats	Yes, major commercial formats	No But it can operate major commercial MCA cards
Can the program perform spectrum manipulation?	No	Yes Smooth and strip	Yes Smoothing, addition subtraction and multiplication	Yes Sum, strip and smooth	Yes	Partially Smooth using file format conversion option	Yes Smoothing and stripping	No		No	No	Yes Smoothing, add, subtract, multiply by const Add const
Calculations												
Activities calculations	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Can the program calculate concentrations?		Yes, but a template has to be programmed	Yes	No	No	Yes Two modules for Thermal and Fast NAA are included	Yes, but the report has to be programmed using the report language	Yes The isotope library is very limited	Yes	Yes	Yes	No
Report of detection limits	No	Yes LLD are calculated according to Curri's formula	Not known	several formulas provided including Curri's one		Partially, concentrations are reported as 3*sqr(sd(area)) when it is < LDL	MDA are calculated by the library driven peak search and area algorithms using peak erosion method		Yes, as Minimum Detectable Activity	Yes according to Curri's formulae or user defined	Not reported, but documented	Not reported Not documented
Quality Assurance and Quality Control												
How the program complies with Quality Assurance	Operational parameters are save into the file Results are compared with a cumulative distribution (T-factor)	Operational parameters are stored into the file Results of analysis are statistically controlled	Yes, to some extent Operational parameters are stored, not all	ANSI N13 30 and N42 14	N/A	Parameters files are kept for reproducibility of results, but program do not use them for QC	Has a complete and full QA and QC system built-in for reporting the results All parameters	Yes, parameters are stored into files	Operational parameters are stored into extensive headers Headers can be saved included into reports	Full track of operational parameters QA and QC is built	No info provided on peak search, identificatio n I ittle track of used parameters Almost no	Full track of operational parameters A database can be created QA and QC

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
							are stored into a file and a database is created		They can be viewed or changed any time	into the program	info on calibration used	is built into the program
How can all input data and calculations be traced	Menu and dialogue boxes Values are stored in files and can be re-called	Menu and dialogue boxes Most of the operational parameters are stored into the file	Some operational parameters are store in final file or report Menus and dialogues can change or display the different options	Menu and dialogue boxes Values are stored in files and re-called by software when requested	through menus and files	several parameters files are kept for reproducibility of results	A full set of all operational parameters are stored into a files and a comprehensive database corresponding to the experimental set-up is created	Menus and dialogue boxes Spectrum parameters are stored into results files	menu and dialogue boxes Extensive headers are provided and can be called at any time They can be included in reports	All parameters are kept and can be reported on the user's wish	See above	Menu and dialogue boxes Parameters values are stored in file and results report (if chosen option) A database can be created

Help and Documentation

	ActAn	Gamma Track	Gamma Plus	Gamma Vision	GammaW	Ganaas	GeniePC	Hypermet PC	OSQ/ Professional	Sampo90	Span	Winner/ Gamma
On-line help	Yes	Yes	Yes	No	Yes	No	Yes	No	Yes	Yes	Yes, but very limited	No
Availability of context sensitivity help	Yes but not complete	Yes	Yes, partially	No	No	No	Yes		Yes	Yes	No	No
Is there an updated and efficient User's Manual?	There is some documentatio n but not a User's Manual	Yes, some parts are inconsistent	Yes Manual is complete and update but not very well written Some guides are misleading or confuse	Yes	Yes, well updated	Yes User's Manual Not updated	Yes Very extensive and well presented	Yes	Yes, updated and well presented and written	Yes, well written and efficient	Yes Sometimes not very clear	Yes Poorly implemented
Is there any other type of documentation provided?	No	Examples files	No	Yes, the one describing Nuclide Navigator	No	Examples files	No	Yes The isotope library is very limited	Yes, samples files Different application specific data libraries A workbook on gamma spectrometry can be provided upon request	No	Yes, some example files	Yes, some example files
Telephone help-line or Internet address(including a WWW location) for help	E-mail	Not known	Not known	Yes Telephone help-line, WWW site	Yes Telephone help-line and E-mail	Yes E-mail and FTP address for exchange of info	Yes Telephone help-line, Internet E-mail and WWW site	Not known	Yes Telephone help line, E-mail and WWW site	Yes, but depending of the dealer	No	Not known

Comments

The Ganaas software provides an E-mail and FTP address for the exchange of information and user's help, but it is not documented in the User's Manual It is only mentioned in a README text file included in the first installation diskette.

CHAPTER 8: RESULTS AND DISCUSSIONS

In this Chapter the results of the intercomparison are presented and briefly discussed. Only the most relevant graphics has been shown here. The full report on the results is summarized through tables 1 to 12 in Appendix I to this report.

In these tables, "X1" and "X2" refer to the χ^2-values computed using the uncertainty reported by the program and the reference uncertainty, respectively. Doublets of the annihilation peak are unphysical and the corresponding results are therefore omitted from the tables.

Empty columns in these tables correspond to incomplete test or lack of reliable data. This might be the case of incomplete analysis runs, not performed by mistake during the intercomparison. These data are therefore missing from the tables.

8.1. Peak detection ability

The ability of the programs to detect singlet peaks, which is the first aspect to be tested according to the ANSI standard, can be judged from the number of detected small peaks on high background

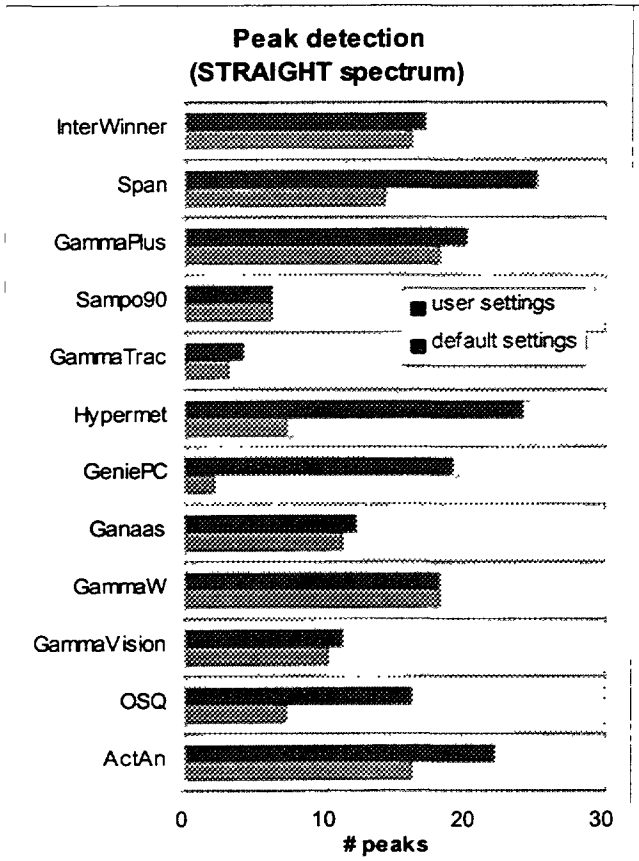


Figure 25. Numbers of detected small peaks on high background.

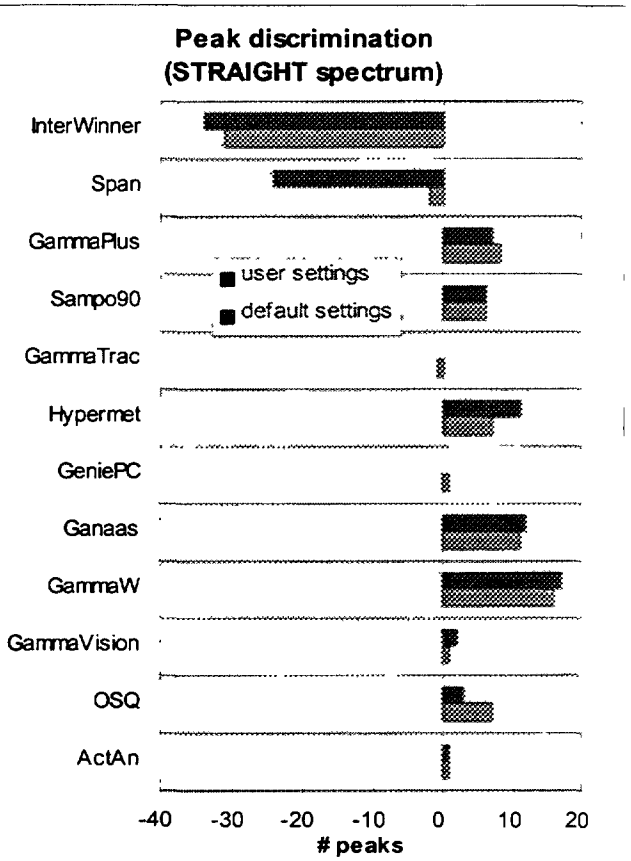


Figure 26. Difference between number of detected small peaks on high background and number of false hits.

listed in the tables. These numbers are shown in Figure 25. The number of misses and the related χ^2-value are also related to this ability, but less discriminating. Most programs allow the user to set a peak search sensitivity parameter directly influencing the detection ability and the data in this figure therefore mostly reflect the setting of this parameter.

In an intercomparison, a more interesting aspect of program performance is the ability to detect small peaks *and not to detect spurious peaks*, i.e. to have a small number of false hits. In Figure 26, the difference between the numbers of detected small peaks on high background and the numbers of false hits are shown. As we have stated in the "Introduction", a detection of a spurious peak is not necessarily a disadvantage of the program as long as its peak area is reported with a high uncertainty as indicated by the χ^2-value for the false hits. At the same time it should be pointed out that spurious peaks can result from unavoidable imperfection of the peak search algorithm as well as from incorrect multiplet deconvolutions. Taking this into consideration, it is clear form the figures that a program like Gamma-W is performing better in this respect than e.g. InterWinner (WinnerGamma).

8.2. Peak shape model dependency of absolute peak area determination

As described in Chapter 4 during the intercomparison a re-normalization factor has been calculated for each program in order to compensate any possible bias in the peak-area determination due to the different models employed in each program. In Figure 27, the re-normalization factors and their uncertainties for the peak areas determined by the analysis programs are shown.

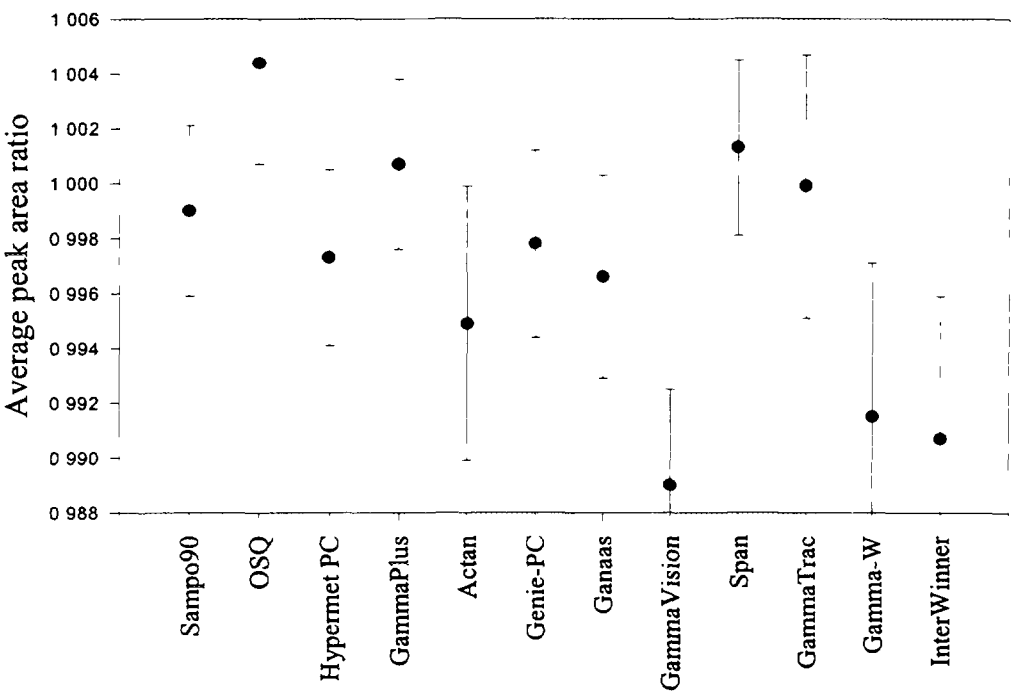


Figure 27. Renormalization factors and uncertainties for the analysis programs.

It has been said that peak areas in γ ray spectra can get defined differently when applying different peak shape models. This would mean that one analysis program could yield other areas than the next, as long it was self-consistent. The results from any determination would come out the same as long as the program was used both for calibration and measurement - a bias would cancel out. This is true as long as coincidence summing does not play a part.

A consistent bias in peak area determination would affect the apparent peak efficiency of a detector. But, where the peak area of a sum peak is given by the product of the photopeak efficiencies for the contributing photons, it would not be given by the product of the apparent photopeak efficiencies - the area determination bias factor would come in only once, not as many times as there are contributing photons.

As shown in Figure 27, the programs tested yield unbiased peak areas, within the statistics of the test (the only outliner at $\alpha = 0.01$ being GammaVision) as well as within a reasonable range of 1 %. No problems need therefore be expected when corrections for coincidence summing are to be computed from efficiency curves determined using one of these programs.

☞ **To ensure that GammaVision was not handicapped by its possible bias, in the remainder of the intercomparison, some of the statistical comparison runs were performed after peak area renormalization. It was found that the results only changed marginally.**

8.3. Interpretation of the χ^2 - values

The χ^2 -values computed in this intercomparison can be interpreted as reduced chi-squared values: A value of unity indicates statistical control, a value less than unity overestimation of uncertainties and a value larger than unity underestimation of uncertainties.

The z-scores underlying the χ^2 -values, however, are not normally distributed: in those cases where incorrect deconvolution occurs, very high values can result. Therefore, a high χ^2 - value can represent a group of nearly perfectly distributed z-scores, i.e. a mean value of 0 and a mean of squares of 1, containing such a single high z-score.

At the same time, as described in the Chapter 4, we are using two kinds of χ^2-values:

- the first, based on z-scores accounting for both the reference and the reported uncertainties (Z_{rep} defined in formulae (3) in Chapter 4),
- the second on z-scores computed from reference uncertainties only (Z_{ref} as defined in formulae (2), Chapter 4).

This two qualifiers can point out different meanings:

1. the first (χ^2_{rep}) indicates the level of statistical control of the program as described above
2. the second (χ^2_{ref}) indicates how well the peak areas themselves were determined regardless of the reported uncertainties.

8.4. Singlet peak area and uncertainty determination

Since only the "straight" and the "distort" spectra contain singlet peaks, the analysis results obtained from these spectra are relevant for the quality of singlet area determination of the programs.

The ANSI standard describes the testing of the independence of peak area determination from the baseline level. This aspect is not explicitly tested here. However, if a program performs well in the test described here, it follows that it satisfies the ANSI criterion. If it performs badly, one of the possible causes could be such a dependence.

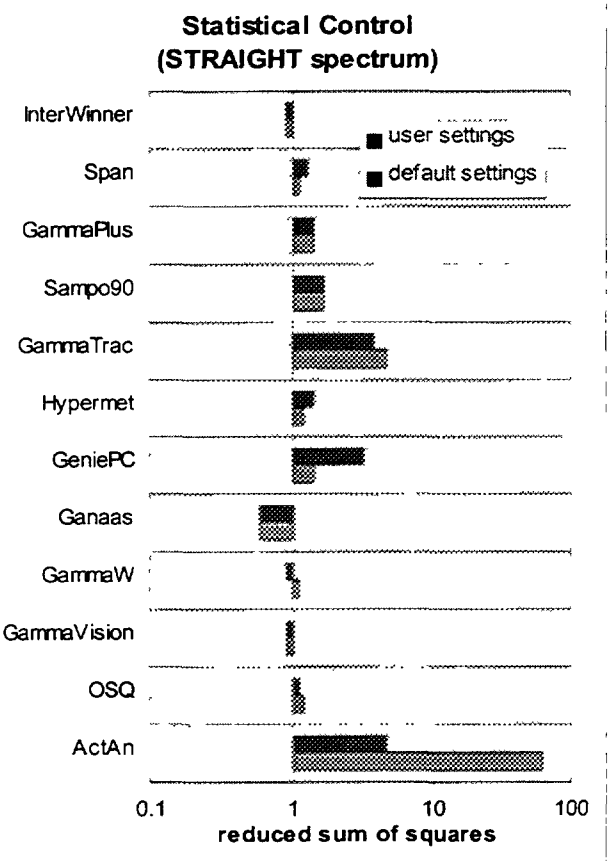


Figure 28. χ^2-values based on the uncertainties reported by the programs in their two modes for the "straight" spectrum.

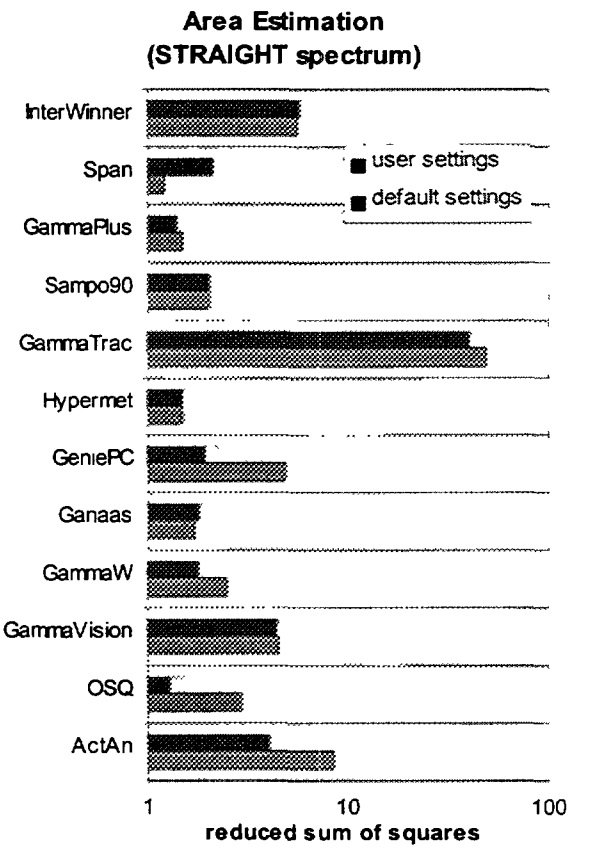


Figure 29. χ^2- values based on reference uncertainties for each program in its two modes.

In Figure 29, the χ^2-values based on the reference uncertainties are plotted for the programs in their different modes. It can be seen from the graph that the performance of most programs remained more or less the same when the change from default to user settings was made. In most cases, the user settings lead to slightly better results. This implies that the default settings of the analysis programs are suitable for the analysis of singlet peaks.

☞ **The fact that user settings do not always lead to better result might indicate that the information offered by the corresponding programs to judge the quality of the results can be improved.**

In Figure 28, the χ^2-values based on the uncertainties reported by the programs have been plotted. Although it can be seen that most χ^2-values differ from unity significantly (implying that more strengthening and development is needed in this aspect in the future); however, it also can be concluded that all programs, except one, demonstrate to be in reasonable statistical control, influenced to some degree by the user settings.

From the statistical control and the quality of the area determinations, an uncertainty overestimation factor f can be computed using

$$f = X^2_{ref} / X^2_{rep} \qquad (5)$$

The resulting values are shown in Figure 30. Most programs turn out to overestimate the uncertainties they report, relative to the optimum uncertainties from the reference list. Relative to the actual discrepancies between reported areas and reference areas, however, the reported uncertainties are reasonable as Figure 28 illustrates.

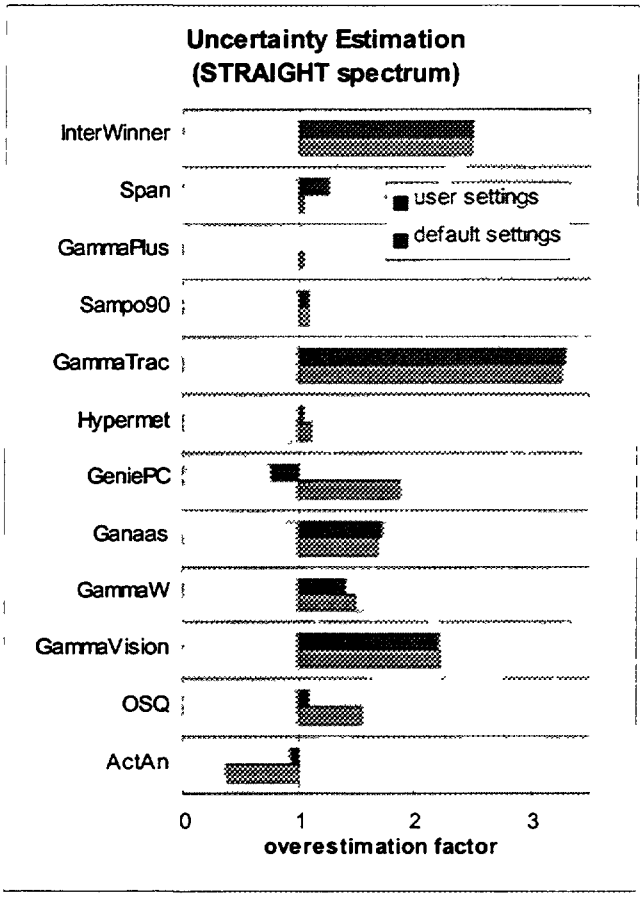


Figure 30. Uncertainty overestimation factors (*f*).

Even though most programs do not report peak position uncertainties but merely imply them to be 0.01 keV with two digits after the dot, the statistical control in this respect is quite good, as can be seen in the tables.

The 511 keV peak area is determined correctly only by Ganaas, GeniePC and InterWinner, even though a 511 keV peak was present in the calibration spectrum.

The "distort" spectrum was analysed well by GammaPlus, Gamma Vision and Gamma-W. None of the other programs, apparently more sensitive to the change in peak shape, reported to the user that such a change had occurred. In principle, this feature could be built in, since high-energy tailing distorts all peaks in the same way.

8.5. Doublet peak area and uncertainty determination

The programs cannot be expected to determine the peak areas in a spectrum containing only doublets as well as in the "straight" spectrum. Nevertheless, they should be in statistical control under all circumstances.

The quality of the area and its uncertainty estimation for the case of the "add1n1" spectrum is shown in Figure 31 and Figure 32, in the same way as for the "straight" spectrum in Figure 29 and Figure 28.

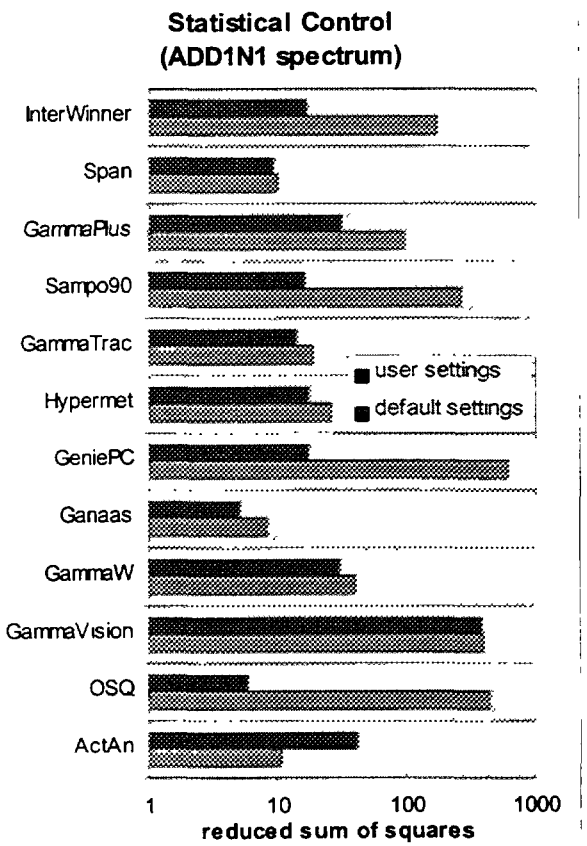


Figure 31. X^2-values based on the uncertainties reported by the programs in their two modes for the "add1n1" spectrum.

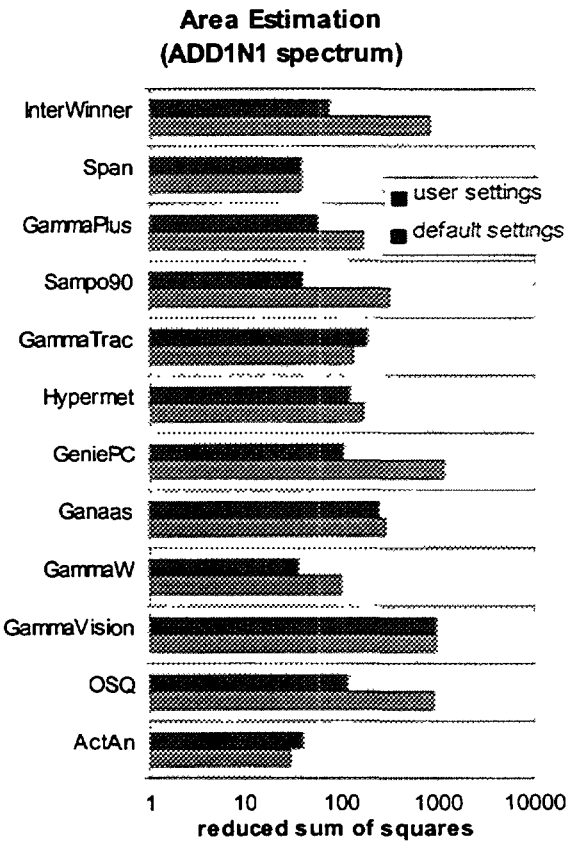


Figure 32. χ^2-values based on the reference uncertainties for the programs in their two modes for the "add1n1" spectrum.

As shown in Figure 31, none of the programs prove to be in statistical control. All programs underestimate the uncertainties in the peak areas they report. However, some programs are less over-confident than others. Most programs perform better, both with respect to peak area and to uncertainty, with the user settings. In some cases, the user settings result in a change in χ^2-values of more than one order of magnitude. With the default settings, the corresponding programs only

integrate peaks (e.g. GeniePC, OSQ/Professional) or do not perform a residual search (e.g. Sampo 90, GammaVision).

The reason that the GammaVision results do not improve with user settings is that this program will deconvolute multiplets if (first) the constituent peaks are in its gamma ray library (see Chapter 6) or (second) detected by the peak search algorithm. It was decided that supplying this library to the program would give it an unfair advantage over the other programs. Such library based multiplet deconvolution potentially could yield very stable results, as shown in the past for X ray spectrum analysis by v.Espen[22].

The remaining programs that yield more or less equally good results with default and user settings

REFERENCE DATA				ANALYSIS PROGRAM OUTPUT				
E		A		E		A		z-scores
val	unc	val	unc	val	unc	val	unc	rep ref
352.3	0.1	98593	492	352.3	0.1	0	2200	-43.7
352.8	0.0	0	0	352.8	0.01	199000	563	353.3
353.5	0.1	98593	492	353.5	0.1	0	2200	-43.7

Figure 33. Section of z-score table, showing a doublet mistaken for a singlet, reported with such a position uncertainty that the reported singlet matches neither of the doublet components.

always fit and deconvolute peaks, but the user may extert some control over the process by setting parameters such as a residual peak search threshold.

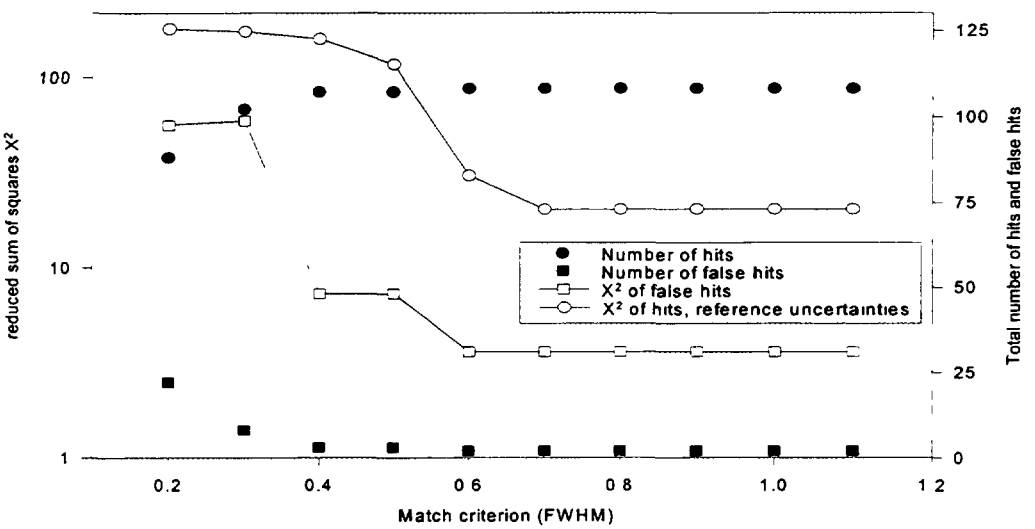


Figure 34. χ^2 based on reference uncertainties and the total number of matches as a function of the peak position match criterion in terms of FWHM. Lines were drawn to guide the eye.

To investigate the problems with the "add1n1" spectrum, the output of the statistical comparison program was studied and it was found that, in those cases where a doublet has been mistaken for a singlet, most of the programs report a singlet that does not match either of the doublet components to within 0 5 x FWHM or the reported position uncertainty, as illustrated in Figure 33 This is most likely to happen on the low-energy side of the spectrum, where the doublet separation is 1 2 x FWHM Additional runs of the comparison program were performed where the criterion for a

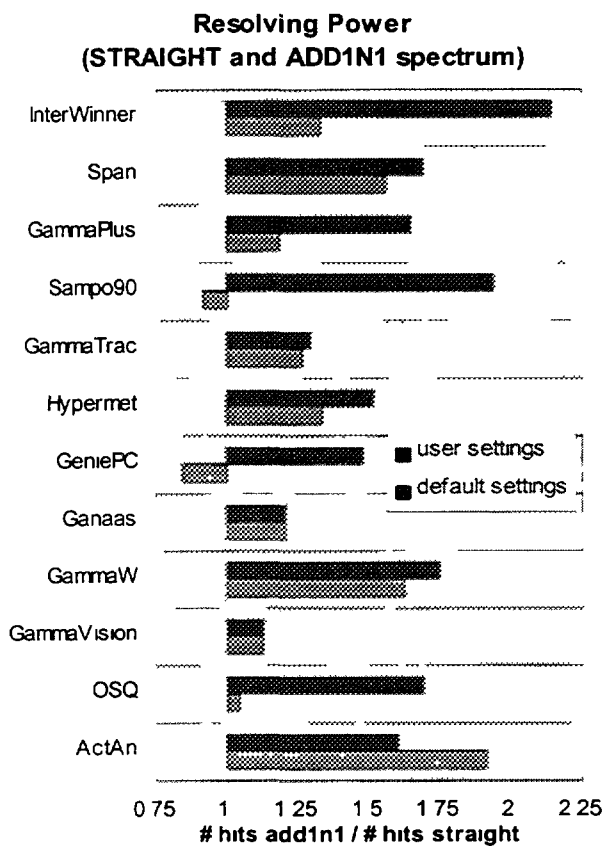


Figure 35. Resolving power of the analysis programs.

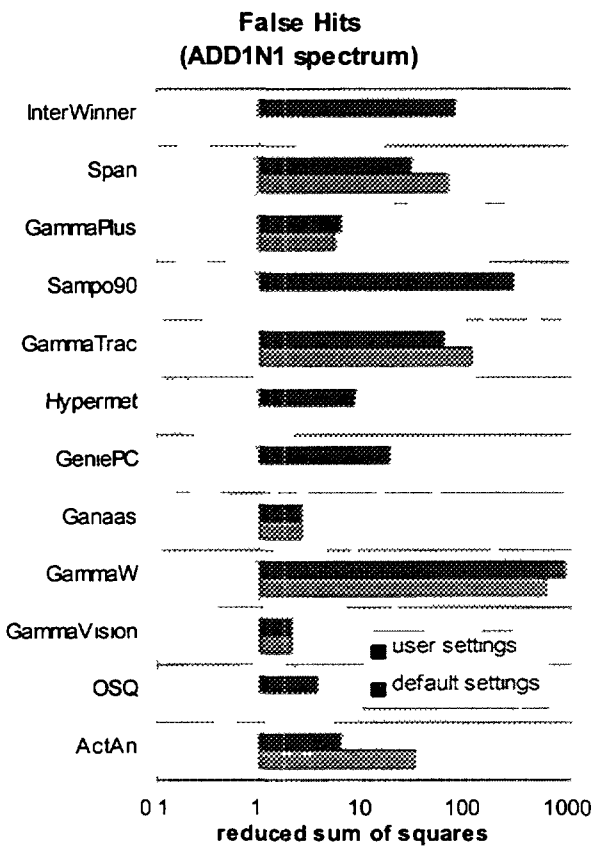


Figure 36. X^2-values related to false hits, indicating deconvolution correctness.

match in peak position was extended from 0 2 x FWHM to 1 2 x FWHM, covering the range of the doublet separations in the spectrum

From Figure 34, where some results for one of the analysis programs are shown, it is clear how crucial this criterion is, even though it's an extreme case At high values, the peak position uncertainties reported by the analysis program are no longer relevant, unrecognized doublets match both components in the reference list and, as described in Chapter 4, these components are merged so that total doublet areas are compared.

To establish how well the analysis programs could distinguish doublets from singlets, their resolving power was defined as the number of high peak hits in the add1n1 spectrum divided by the same in the straight spectrum. For this ratio, 2 would be a perfect score The χ^2-value for false hits in the "add1n1" spectrum indicates that doublets are being mistaken for multiplets To eliminate the effect of too small reported position uncertainties, the data were determined using a 1 0 x FWHM matching criterion The results are shown in Figure 35 and Figure 36

An analysis program that performs residual searches in the fitting process may miss multiplet components or detect spurious multiplet components The lower the residual search threshold, the less components will be missed but the more spurious components will be found From the graphs, it is seen that the threshold was set to low for Sampo 90 and InterWinner by the user - the

deconvolution power is very large, but so is the X^2-value for false hits. The trade-off between the two aspects turns out not to be the same for all analysis programs. For example, the trade-off has turned out less favorable for Gamma-W than for InterWinner.

As shown by Koskelo[10] and implemented earlier at IRI[23,24], an alternative for multiplet deconvolution is the determination of total area, followed by the determination of the constituent peak areas in the interpretation stage. This method can only work well if the total areas of the doublets in this test can be determined correctly by the analysis programs. Also, the programs should report a peak position uncertainty (maybe "multiplet range" would be a better term) in these cases that can be used as a search window in the γ ray catalogue. Since they don't, search windows of 1 keV or 1 x FWHM are common practice, unnecessarily complicating the interpretation process.

To establish the quality of the total area determination, the results from the 1 x FWHM match criterion statistical comparison runs were used for Figure 37 and Figure 38, otherwise identical to Figure 31 and Figure 32.

These figures indicate that the total areas of the doublets mistaken for singlets, as well as constituent

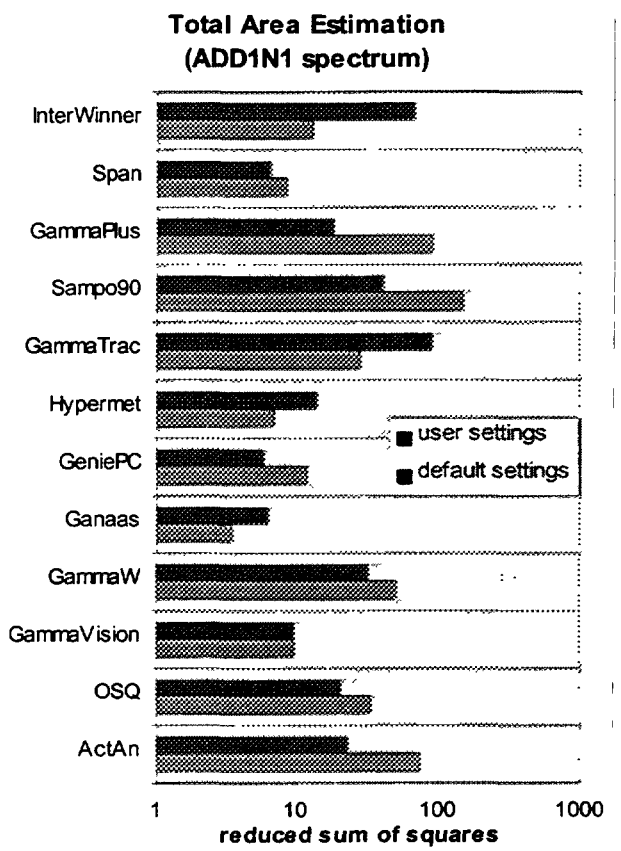


Figure 37. X^2-values based on the reference uncertainties for the programs in their two modes for the "add1n1" spectrum, determined with a 1 x FWHM match criterion.

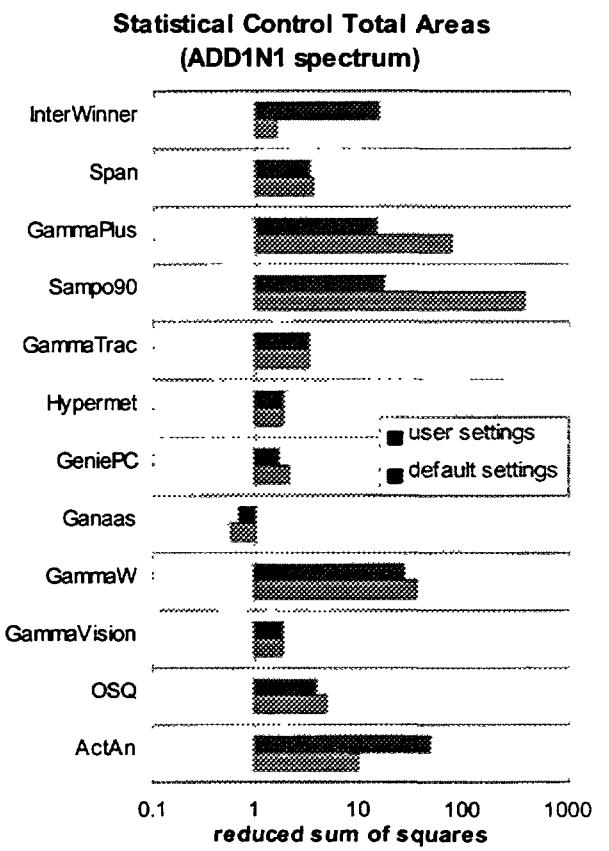


Figure 38. X^2-values based on the uncertainties reported by the programs in their two modes for the "add1n1" spectrum, determined with a 1 x FWHM match criterion.

areas of correctly recognized doublets, are determined well by Ganaas, Hypermet-PC, GammaVision, GeniePC and Span. These programs also demonstrate to be in reasonable statistical control in this respect.

CHAPTER 9: CONCLUSIONS

First of all, after this intercomparison exercise we can conclude that most of the gamma ray spectrum analysis programs are designed using advanced and powerful graphical and user interfaces. Many provide keyboard shortcuts, mouse operation and graphical capabilities, which leads to a more efficient operation and control of the spectrum analysis. Outstanding user interfaces were found in GeniePC, GammaVision and OSQ/Professional.

Most of the programs incorporate utility modules (e.g. spectrum format conversion) which extends their usefulness and applicability.

Some of the programs have built-in scripts, macros, application-oriented libraries and other features that were found very useful for predefined tasks, routine analyses, etc. Example of this is the batch analysis script provided by Sampo 90 and GeniePC among others.

Almost all the programs provide "easy-to-use" and powerful methods for energy, peak shape and efficiency calibration.

It was found that most of the programs integrate into their basic spectrum analysis routines a number of calculation programs or modules, which leads to more precise and correct calculations for element's concentration. Examples are: nuclear data libraries and library editors, efficiency calculations and extrapolations, geometry corrections, peak interference solvers, etc.

All the programs made good use of present capabilities of modern PC's. Spectrum deconvolution and calculations are done rapidly, and the user can inspect the results over the spectra using powerful graphical capabilities.

During the intercomparison it was found that all the tested programs reported almost the same peak areas (within 1%) independently of their used peak shape. **The expected peak shape model dependency was not found in practice.**

In the applied tests, singlet peak areas are determined quite well by all programs except GammaTrack and all programs are in reasonable statistical control with respect to the peak areas, positions and their uncertainties. Very good results were obtained with Span, GammaPlus, Hypermet-PC, Ganaas, OSQ/Professional, Sampo90 and Gamma-W (in no particular order).

Doublets at separations below 1.2 x FWHM often are mistaken for a singlet by all programs and reported with much too small peak position uncertainties, even if the settings of the program allow it to perform residual searches and add multiplet components in the fitting procedure. With respect to resolving power as defined in this test and quality of area determination, ActAn, Gamma-W and Sampo90 yielded the least bad results. Only after the consequences of peak position uncertainty underestimation were removed by a change in the test procedure, Ganaas, Hypermet-PC, GammaVision, GeniePC and Span proved to determine the constituent peak areas (or the total peak areas in case of an unrecognized doublet) quite well and also proved to be in statistical control.

The results obtained with user defined settings are usually better than the results obtained with the default settings. In those instances where this is not the case, the analysis program apparently can be improved with respect to the information offered to the user to judge the quality of the results, e.g. plots of residual patterns.

The report of the analysis results has been improved by almost all the programs. Many of them had implemented the multiple choices or "user-defined" type of reports. Excellent implementations were found in GeniePC, Sampo90, OSQ/Professional and GammaVision.

Even though some of the programs obviously need more improvement than others, no program emerges as *the* best from this intercomparison. The user may select the program that is the most suitable for the specific γ ray spectra to be analyzed, or the most flexible if different kinds of spectra are to be analyzed.

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APPENDIX I: TABLES OF RESULTS

Table 3: ActAn

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	47	47	87	68	67	55	46	48	47	73	67	66	55	46
	X1	93.2	14.1	12.2	78.5	52.5	8.8	3.1	6.0	104.1	54.0	41.8	6.8	9.5	3.5
	X2	10.4	16.4	35.2	222.8	17.7	42.0	5.6	3.7	41.2	51.5	151.1	20.8	24.2	5.7
small on high	N	16	12	12	17	16	18	16	22	14	17	17	22	21	19
	X1	2.8	4.1	2.7	4.9	1.4	1.4	1.2	2.9	3.2	2.5	2.2	1.6	1.9	2.4
	X2	4.7	18.6	2.8	14.5	3.3	18.5	1.7	4.5	18.5	9.2	10.4	3.5	9.9	3.0
small on low	N	10	8	9	15	15	18	10	14	12	9	19	16	19	18
	X1	2.3	4.8	6.4	5.6	3.4	15.2	2.1	1.8	4.7	6.4	5.3	4.1	12.4	3.6
	X2	4.5	10.0	16.9	44.7	15.1	289.7	77.5	4.0	10.1	16.6	37.5	18.0	170.3	400.3
all matches	N	73	67	108	100	98	91	72	84	73	99	103	104	95	83
	X1	60.9	11.0	10.7	55.1	36.6	8.6	2.5	4.5	67.8	40.8	28.5	5.3	8.4	3.3
	X2	8.4	15.6	30.1	160.7	14.9	86.4	14.7	4.0	31.2	41.1	106.9	16.7	50.3	90.7
position	X	3.6	17.6	7.6	11.5	7.7	12.7	10.8	4.0	17.6	7.6	11.8	7.8	12.5	12.6
annihilation	N	1	1						1	1					
	X	25.2	29.6						25.2	28.1					
misses	N	97	103	212	207	228	206	178	86	97	214	200	221	199	167
	X	8.1	7.0	10.6	8.5	13.2	6.8	8.8	5.5	5.9	39.0	8.0	15.5	6.7	8.2
false hits	N	15	35	9	14	11	11	15	21	39	6	19	18	10	28
	X	717.5	144.0	26.1	82.9	609.9	31.8	1162.6	132.3	243.4	6.4	8.0	12.3	18.7	25.3
total	N	185	205	329	321	337	308	265	191	209	319	322	343	304	278
	X	86.4	31.8	11.0	26.2	39.5	8.2	72.4	19.0	71.9	38.9	14.6	12.2	7.6	8.5

Table 4: GammaPlus

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	48	47	50	51	49	47	47	48	47	74	62	65	54	47
	X1	1.4	1.4	142.2	16.4	24.8	4.3	1.4	1.3	1.7	42.0	41.4	31.4	2.9	1.4
	X2	1.7	2.4	265.1	13.6	24.0	4.7	1.7	1.5	2.7	78.3	13.0	12.0	3.9	1.6
small on high	N	18	15	11	13	16	16	15	20	16	17	17	22	19	18
	X1	1.9	6.3	8.8	2.6	3.8	2.2	2.1	2.0	6.9	3.1	2.2	3.9	2.0	1.6
	X2	1.4	16.6	4.5	1.4	3.3	9.8	1.4	1.4	16.1	3.3	1.3	3.3	7.3	1.2
small on low	N	15	14	14	16	12	15	15	14	14	14	17	14	16	15
	X1	1.1	1.2	2.4	2.1	1.1	2.2	0.9	0.7	1.2	2.8	2.0	1.2	2.3	0.9
	X2	1.2	2.2	5.2	4.4	2.5	3.3	1.1	0.9	2.2	5.4	4.1	3.5	3.6	1.0
all matches	N	81	76	75	80	77	78	77	82	77	105	96	101	89	80
	X1	1.4	2.3	96.6	11.3	16.8	3.5	1.4	1.4	2.6	30.5	27.5	21.2	2.6	1.4
	X2	1.5	5.0	178.4	9.8	16.4	5.5	1.5	1.4	5.2	56.5	9.3	9.0	4.6	1.4
position	X	1.9	18.3	9.3	16.0	3.2	12.0	9.4	1.7	18.4	8.2	14.1	5.5	11.1	9.5
annihilation	N	1	1						1	1					
	X	4.6	0.3						1.7	1.4					
misses	N	88	94	236	205	251	209	172	87	93	211	190	226	199	167
	X	5.6	5.5	199.1	41.8	81.7	27.6	7.8	5.6	5.5	71.7	12.7	23.3	8.8	7.7
false hits	N	10	15	8	4	9	5	7	13	20	12	7	10	4	10
	X	7.0	1223.7	16.7	6.2	4.3	2.8	5.4	6.3	952.8	6.2	4.5	4.1	2.4	5.0
total	N	179	185	319	289	337	292	256	182	190	328	293	337	292	257
	X	3.8	103.5	170.4	32.9	64.8	20.7	5.8	3.7	104.6	56.1	17.4	22.1	6.9	5.6

Table 5: GammaTrack

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	45		55	52	55	49	45	47	46	58	57	56	51	47
	X1	5.0		20.2	8.0	13.7	4.8	2.9	4.4	75.6	15.7	51.7	12.3	4.0	3.1
	X2	55.9		156.3	25.5	59.7	45.3	24.5	49.1	101.9	219.9	64.7	62.2	41.5	22.0
small on high	N	3		5	2	7	2	7	4	7	6	6	9	5	8
	X1	3.9		5.6	12.1	7.3	0.7	4.9	0.7	1.1	1.9	5.0	6.6	0.3	2.7
	X2	5.5		19.2	6.1	4.9	1.0	11.8	2.5	11.2	10.2	10.5	7.9	0.7	7.8
small on low	N	4		3	3	1	2	5	7	5	4	5	4	7	5
	X1	0.2		6.9	1.2	4.0	1.4	1.0	0.6	1.0	6.6	0.5	2.6	0.6	1.4
	X2	0.8		43.6	3.3	21.3	5.6	3.1	2.0	9.8	61.4	4.6	14.7	4.3	6.1
all matches	N	52		63	57	63	53	57	58	58	68	68	69	63	60
	X1	4.6		18.4	7.8	12.8	4.5	3.0	3.7	59.9	14.0	43.8	11.0	3.3	2.9
	X2	48.7		140.1	23.7	53.0	42.1	21.1	40.2	82.3	192.1	55.5	52.4	34.1	18.8
position	X	2.9		8.2	11.8	2.2	8.0	6.1	2.9	26.8	8.3	12.4	2.8	8.7	7.0
annihilation	N	3							3	3					
	X	254.7							234.5	553.2					
misses	N	118		258	254	268	251	196	111	111	251	234	260	235	192
	X	11.8		47.9	14.6	29.9	17.5	10.8	8.6	8.7	45.6	11.2	29.3	16.6	9.3
false hits	N	4		4	4	3	3	3	4	13	8	4	4	3	3
	X	48.8		111.0	137.3	53.4	35.3	25.0	47.8	691.5	60.4	237.6	38.2	34.2	31.4
total	N	174		325	315	334	307	256	173	182	327	306	333	301	255
	X	10.5		43.0	14.9	26.9	15.5	9.3	7.9	73.9	39.4	21.4	25.6	14.0	8.0

Table 6: Gamma Vision

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	47	44	47	45	45	44	46	47	44	47	45	45	44	46
	X1	0.8	0.9	473.5	45.5	149.4	6.8	0.8	0.8	0.9	471.7	45.6	149.5	6.8	0.8
	X2	4.0	6.8	1170.2	58.2	197.4	13.2	4.3	4.0	6.8	1170.2	58.2	197.4	13.2	4.3
small on high	N	10	14	6	10	14	10	11	11	14	6	10	14	10	11
	X1	1.7	2.4	17.6	2.5	4.3	2.7	1.7	1.5	2.4	17.6	2.5	4.3	2.7	1.7
	X2	8.2	40.8	55.3	11.4	31.8	138.2	20.3	7.5	40.8	55.3	11.4	31.8	138.2	20.3
small on low	N	8	6	5	6	5	8	7	8	6	5	6	5	8	7
	X1	0.5	0.8	2.9	1.8	2.1	3.8	0.2	0.5	0.8	2.9	1.8	2.1	3.8	0.2
	X2	2.4	5.8	33.5	55.6	21.6	134.6	1.9	2.4	5.8	33.5	55.6	21.6	134.6	1.9
all matches	N	65	64	58	61	64	62	64	66	64	58	61	64	62	64
	X1	0.9	1.2	385.8	34.1	106.1	5.7	0.9	0.9	1.2	384.3	34.2	106.2	5.7	0.9
	X2	4.5	13.5	956.9	50.3	147.5	49.0	6.8	4.4	13.5	956.9	50.3	147.5	49.0	6.8
position	X	2.2	17.6	8.8	17.6	3.5	11.4	8.3	2.1	17.6	8.8	17.6	3.5	11.4	8.3
annihilation	N	1	1						1	1					
	X	65.6	42.0						65.6	42.0					
misses	N	105	105	269	239	267	235	188	104	105	269	239	267	235	188
	X	9.6	10.4	237.5	119.0	110.8	27.1	9.0	9.7	10.4	237.5	119.0	110.8	27.1	9.0
false hits	N	9	24	11	17	11	11	15	9	24	11	18	11	12	15
	X	4.0	185.4	$1.2x10^4$	234.8	2.2	1.7	3.9	4.0	185.3	$1.2x10^4$	222.7	2.2	1.6	3.9
total	N	179	193	338	317	342	308	267	179	193	338	318	342	309	267
	X	6.2	29.2	646.5	108.9	106.5	21.9	6.8	6.1	29.2	641.5	108.6	106.5	21.8	6.8

Table 7: Gamma-W

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	48	47	75	56	64	51	45	48	46	81	64	67	52	45
	X1	0.7	1.2	50.5	17.1	15.2	7.3	0.9	0.7	9.2	37.6	7.5	3.5	2.2	2.1
	X2	2.1	5.1	134.7	46.2	28.8	22.6	3.1	1.9	11.9	42.4	12.8	8.7	6.2	2.5
small on high	N	18	14	19	18	18	14	10	18	14	18	18	16	14	13
	X1	1.8	6.7	5.8	3.2	4.9	2.2	3.3	1.5	7.3	3.4	2.2	3.2	2.0	2.8
	X2	2.6	42.6	11.6	7.7	7.8	2.9	5.4	1.7	33.2	12.9	5.5	7.1	2.5	2.0
small on low	N	8	7	6	14	9	9	10	7	7	6	12	9	9	10
	X1	1.8	1.8	6.3	52.1	1.4	2.0	1.0	0.9	1.4	5.6	2.3	0.9	2.3	0.9
	X2	4.5	6.1	23.9	6822.7	6.0	5.9	4.6	1.9	3.6	25.0	9.5	2.4	12.2	3.0
all matches	N	74	68	100	88	91	74	65	73	67	105	94	92	75	68
	X1	1.1	2.3	39.3	19.9	11.8	5.7	1.3	0.9	7.8	29.9	5.8	3.2	2.2	2.1
	X2	2.5	12.3	104.6	1116.4	22.4	16.8	3.7	1.8	15.0	36.4	11.0	7.8	6.3	2.5
position	X	0.5	5.9	1.9	122.3	1.4	3.3	3.3	0.5	5.6	2.3	3.5	1.9	3.1	3.2
annihilation	N	3	3						3	3					
	X	158.0	176.8						158.0	176.2					
misses	N	92	101	211	193	232	211	185	94	102	210	196	234	214	180
	X	6.1	8.7	39.7	35.0	20.6	14.5	9.8	6.5	9.4	13.7	7.7	14.3	8.7	9.7
false hits	N	2	28	14	4	4		1	1	27	13	2	3		1
	X	49.8	70.7	556.7	533.5	402.1		14.0	29.6	220.0	880.4	279.2	81.9		87.9
total	N	168	197	325	285	327	285	251	168	196	328	292	329	289	249
	X	4.4	15.4	61.9	37.4	22.8	12.2	7.6	4.2	38.0	53.2	9.0	11.8	7.0	7.9

Table 8: Ganaas

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	48	47	53	52	52	51	47	48	47	53	52	52	51	47
	X1	0.4	0.5	8.6	10.7	4.6	2.8	0.6	0.5	0.6	5.1	10.2	4.7	2.8	0.6
	X2	1.5	3.5	376.2	100.3	60.9	9.6	2.5	1.6	4.5	338.6	100.0	62.7	10.4	2.6
small on high	N	11	10	10	10	12	9	13	12	10	11	10	11	9	13
	X1	1.4	4.0	9.8	3.7	5.5	0.7	1.6	1.3	3.6	6.6	3.4	5.4	1.5	1.4
	X2	3.0	19.6	17.2	13.0	11.2	1.7	4.1	2.8	19.4	18.9	12.2	10.9	5.5	3.9
small on low	N	9	7	5	10	9	7	7	9	7	5	10	8	8	7
	X1	0.3	1.0	1.1	0.4	1.7	0.6	0.4	0.3	0.9	1.0	0.4	0.5	0.7	0.5
	X2	1.4	7.6	9.1	3.8	40.3	3.1	1.4	1.6	8.2	7.8	3.6	4.4	3.9	1.7
all matches	N	68	64	68	72	73	67	67	69	64	69	72	71	68	67
	X1	0.6	1.1	8.3	8.3	4.4	2.3	0.8	0.6	1.0	5.0	7.9	4.3	2.4	0.8
	X2	1.7	6.1	296.4	74.7	50.2	7.8	2.7	1.8	6.8	263.6	74.4	48.1	9.0	2.7
position	X	1.9	18.0	16.9	5.1	12.1	5.5	9.1	1.8	18.1	16.9	5.2	12.2	5.1	9.1
annihilation	N	1	1						1	1					
	X	1.2	0.2						1.2	0.2					
misses	N	101	105	231	250	239	247	184	100	105	230	250	241	247	184
	X	5.9	6.5	88.2	67.4	49.9	26.8	8.2	5.9	6.5	88.9	67.4	49.6	26.8	8.2
false hits	N	0	15	2	0	1	0	2	0	15	2	0	2	0	2
	X		584.4	8.9		2.9		4.2		583.6	14.2		7.9		3.8
total	N	169	184	301	322	313	314	253	169	184	301	322	314	315	253
	X	3.8	52.0	69.6	54.2	39.1	21.6	6.2	3.7	51.9	69.2	54.1	39.1	21.5	6.2

Table 9: GeniePC

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	45	42	35	43	39	45	43	48	47	65	59	61	56	47
	X1	1.3	1.6	629.6	126.0	183.0	14.9	1.3	4.0	1.1	20.4	1.7	4.4	4.2	0.9
	X2	5.1	6.1	1225.1	92.8	225.0	16.4	3.9	2.1	3.0	134.7	6.5	17.8	179.2	2.0
small on high	N	2	1	1	2	1	2	3	19	18	9	15	21	16	18
	X1	4.0	3.6	67.2	6.3	23.2	3.5	3.4	2.9	8.8	7.8	11.1	6.0	2.5	1.9
	X2	3.9	47.8	86.8	11.5	21.1	4.3	3.9	1.7	13.2	9.9	7.5	6.9	7.4	2.2
small on low	N	2	2	1	2	1	1	2	14	11	9	15	11	12	12
	X1	0.8	3.0	11.6	2.2	0.4	0.2	4.3	0.6	11.1	3.5	0.7	3.7	3.1	0.8
	X2	3.0	10.2	55.9	5.0	1.4	0.5	12.2	1.5	5.2	17.9	2.3	4.9	5.6	2.6
all matches	N	49	45	37	47	41	48	48	81	76	83	89	93	84	77
	X1	1.4	1.6	597.7	115.6	174.6	14.1	1.5	3.2	4.1	17.2	3.1	4.7	3.7	1.1
	X2	4.9	6.0	1162.7	85.6	214.6	15.6	4.2	1.9	5.5	108.5	6.0	13.8	121.7	2.2
position	X	2.6	18.5	9.8	19.4	2.8	15.0	8.9	3.3	17.5	8.1	13.1	4.9	10.0	9.7
annihilation	N	1	1						1	2					
	X	0.2	0.1						0.6	5476.9					
misses	N	121	125	292	260	292	252	204	87	93	237	198	234	208	174
	X	13.0	14.4	187.0	52.9	94.3	26.5	12.7	5.7	5.5	46.4	8.0	22.9	10.6	8.0
false hits	N	1	9	1	0	0	0	0	19	40	20	22	17	15	24
	X	33.7	1301.9	1.2×10^5					70.9	314.0	19.4	19.5	6.0	3.8	3.9
total	N	171	179	330	307	333	300	252	187	209	340	309	344	307	275
	X	9.8	76.3	610.8	62.5	104.2	24.5	10.6	11.2	64.3	37.7	7.4	17.1	8.4	5.7

Table 10: Hypermet-PC

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	47	47	59	54	55	52	46	48		69	55	56	53	47
	X1	0.8	1.3	28.1	2.2	16.5	1.8	1.0	0.7		24.9	2.4	17.1	1.8	1.1
	X2	1.2	2.6	199.9	7.8	44.1	4.8	1.5	1.1		188.4	8.6	44.2	4.6	1.7
small on high	N	7	9	6	9	8	9	8	24		24	25	23	23	21
	X1	3.1	8.4	8.8	7.4	6.9	4.3	7.4	2.3		4.1	3.7	5.2	2.7	4.1
	X2	2.8	26.7	10.3	8.5	6.3	4.5	5.4	2.0		8.5	5.3	7.1	3.6	194.7
small on low	N	6	5	4	6	7	7	8	15		17	22	14	13	16
	X1	2.2	0.5	11.0	1.0	3.1	2.3	1.0	2.1		5.5	2.8	3.7	5.2	0.9
	X2	2.1	0.8	36.6	1.3	5.8	5.4	1.3	1.8		11.6	8.7	7.1	116.9	2.1
all matches	N	60	61	69	69	70	68	62	87		110	102	93	89	84
	X1	1.2	2.1	25.4	2.8	14.1	2.2	1.8	1.4		17.3	2.8	12.2	2.6	1.8
	X2	1.5	5.6	173.9	7.3	35.9	4.8	1.9	1.5		121.8	7.8	29.4	20.8	50.0
position	X	0.8	11.7	4.1	10.7	2.3	7.9	6.9	1.0		3.1	8.1	2.2	6.7	6.0
annihilation	N	2	2						2						
	X	160.3	269.0						160.3						
misses	N	110	109	257	226	258	227	189	80		196	176	229	195	163
	X	8.9	7.6	56.9	10.5	33.3	9.5	8.9	5.3		63.3	9.3	35.6	9.5	7.8
false hits	N	0	15	1	0	1	0	1	13		12	11	15	11	15
	X		520.9	60.8		34.7		13.1	6.1		10.0	4.9	6.5	5.4	7.2
total	N	170	185	327	295	329	295	252	180		318	289	337	295	262
	X	6.2	47.6	50.3	8.7	29.2	7.8	7.2	3.5		45.4	6.9	27.9	7.3	5.9

Table 11: InterWinner/WinnerGamma

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	36	36	41	38	38	37	38	36	36	73	53	53	46	38
	X1	0.5	0.6	241.5	72.3	85.2	9.4	1.0	0.6	0.6	20.9	3.1	2.7	1.8	1.0
	X2	3.5	5.2	1175.1	135.3	233.7	23.4	10.6	3.8	5.2	87.6	18.1	18.5	15.3	9.8
small on high	N	16	13	13	21	16	15	19	17	13	17	25	22	16	17
	X1	1.6	3.3	9.3	1.7	4.9	2.2	1.2	1.3	3.3	1.7	2.2	1.5	1.6	1.9
	X2	5.5	219.3	47.1	24.0	32.3	66.2	37.9	5.1	219.3	23.3	33.9	13.2	36.7	23.1
small on low	N	5	8	5	7	6	6	8	6	8	5	14	14	11	10
	X1	1.4	1.4	1.0	1.9	1.5	2.0	1.2	1.2	1.4	3.8	1.6	1.0	2.2	1.4
	X2	21.3	23.3	19.0	78.4	22.8	22.7	161.5	19.1	23.3	66.3	54.3	23.0	110.3	425.8
all matches	N	57	57	59	66	60	58	65	59	57	95	92	89	73	65
	X1	0.9	1.2	169.9	42.4	55.4	6.8	1.1	0.9	1.2	16.5	2.6	2.2	1.8	1.3
	X2	5.6	53.2	828.6	93.8	158.9	34.4	37.1	5.7	53.2	75.0	27.9	17.9	34.3	77.3
position	X	4.6	12.9	9.8	14.8	6.3	10.9	10.1	4.3	12.9	8.1	10.2	7.0	8.2	9.5
annihilation	N	1	1						1	1					
	X	0.9	0.1						0.9	0.1					
misses	N	68	67	176	155	187	169	129	66	67	141	142	151	156	127
	X	49.5	10.8	263.2	180.0	133.2	32.7	9.1	50.6	10.8	9.5	11.0	10.9	9.4	8.9
false hits	N	47	66	42	58	35	48	44	51	66	39	38	40	25	32
	X	10.1	54.5	3.9	32.3	1.6	1.5	2.0	9.4	54.5	67.6	2.6	6.9	2.0	2.1
total	N	172	190	277	279	282	275	238	176	190	275	272	280	254	224
	X	22.7	23.2	204.1	116.7	100.3	21.8	5.6	22.0	23.2	20.2	7.0	7.6	6.5	5.7

Table 12: OSQ/Professional

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	47	43	43	47	45	45	46	48	47	77	52	61		47
	X1	1.2	2.1	601.8	129.4	138.5	15.9	1.3	1.0	2.7	6.4	3.9	3.3		1.3
	X2	3.2	5.1	1219.9	103.5	175.6	13.9	3.1	1.0	4.0	159.3	13.9	35.5		1.6
small on high	N	7	4	11	8	7	5	6	16	12	22	12	21		13
	X1	1.5	10.2	20.1	8.2	13.0	4.4	5.3	2.0	10.5	3.3	2.9	3.2		4.3
	X2	1.7	14.7	118.3	10.8	11.0	3.0	7.6	3.0	40.9	7.6	4.0	13.2		311.2
small on low	N	6	3	5	5	6	8	5	14	9	8	18	15		15
	X1	0.9	0.9	4.3	1.5	1.2	2.0	0.8	0.5	2.7	7.3	3.7	0.8		1.3
	X2	1.9	2.1	12.4	3.2	2.5	2.8	1.5	0.5	6.8	9.0	20.9	1.5		28.0
all matches	N	60	50	59	60	58	58	57	78	68	107	82	97		75
	X1	1.2	2.4	442.7	102.6	109.2	13.0	1.7	1.1	3.9	5.8	3.7	2.9		1.8
	X2	2.9	5.4	912.2	82.7	137.8	11.4	3.5	1.3	10.3	116.9	14.0	25.4		60.5
position	X	2.0	20.6	11.6	15.8	5.0	12.4	8.9	2.0	19.5	5.7	14.8	5.0		9.2
annihilation	N	1	2						4	2					
	X	4.5	1641.9						143.7	381.3					
misses	N	110	120	255	239	272	235	194	91	102	209	208	228		172
	X	8.9	12.9	343.3	74.3	110.0	32.2	10.0	6.1	7.6	122.5	25.5	68.9		7.9
false hits	N	0	12	3	0	0	0	0	13	26	3	11	11		5
	X		414.8	5.8×10^4					12.3	82.9	7.3	14.1	8.3		8.2
total	N	170	182	317	299	330	293	251	182	196	319	301	336		252
	X	6.2	36.7	906.1	79.9	109.8	28.4	8.1	4.4	16.4	82.3	19.2	47.9		6.1

Table 13: Sampo 90

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	47	46	38	48	46	46	46	47	46	86	67	69	56	47
	X1	1.8	1.8	299.0	20.2	27.0	5.3	1.8	1.8	1.8	20.0	5.4	7.5	6.2	10.9
	X2	2.3	3.0	364.9	15.7	22.6	5.9	2.1	2.3	3.0	53.2	39.1	23.3	379.1	37.5
small on high	N	6	4	2	4	4	5	5	6	4	20	25	29	27	28
	X1	1.4	12.8	22.7	2.2	4.5	0.4	4.3	1.4	12.8	4.5	7.5	7.4	4.7	4.1
	X2	1.4	47.9	5.0	1.1	5.0	0.3	3.5	1.4	47.9	4.6	16.2	18.5	20.6	1.7
small on low	N	4	5	3	3	3	5	5	4	5	14	24	19	18	18
	X1	0.5	0.9	9.8	0.9	1.6	1.7	1.8	0.5	0.9	9.2	6.3	3.5	48.3	2.2
	X2	0.6	1.5	14.4	1.2	3.4	3.2	1.6	0.6	1.5	7.6	13.8	7.6	31.3	2.7
all matches	N	57	55	43	55	53	56	56	57	55	120	116	117	101	93
	X1	1.7	2.3	266.0	17.8	23.9	4.5	2.0	1.7	2.3	16.2	6.0	6.8	13.3	7.2
	X2	2.0	5.3	323.7	13.9	20.2	5.1	2.2	2.0	5.3	39.8	29.0	19.5	221.3	20.0
position	X	0.6	10.1	5.3	9.1	1.7	6.5	5.2	0.6	10.1	3.2	4.6	3.1	4.8	4.3
annihilation	N	1	1						1	1					
	X	1074.3	877.4						1074.3	877.4					
misses	N	113	115	284	248	280	244	196	113	115	193	175	208	188	154
	X	9.7	8.1	197.9	56.0	92.8	30.5	9.5	9.7	8.1	12.3	98.8	12.9	8.1	7.7
false hits	N	0	7	2	0	0	0	0	0	7	40	42	35	44	40
	X		922.5	55660						922.5	288.9	28.7	36.5	17.1	26.6
total	N	170	177	329	303	333	300	252	170	177	353	333	360	333	287
	X	7.0	42.7	544.0	49.0	81 8	25.7	7.8	7.0	42.7	44.9	57.7	13.2	10.9	10.2

Table 14: Span

		Default settings							User settings						
		stra	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**	**stra**	**dist**	**1n1**	**3n1**	**1n3**	**10n1**	**1n100**
high peak	N	41		63	51	51	43	41	41		67	52	53	44	41
	X1	0.7		10.9	4.1	6.7	3.0	1.9	1.1		10.6	4.2	6.3	2.8	1.4
	X2	1.0		44.3	10.2	17.9	7.1	2.8	2.0		46.2	11.5	20.0	5.9	3.1
small on high	N	14		9	17	15	17	11	25		15	28	24	27	23
	X1	2.4		4.3	6.5	13.8	4.0	3.5	1.9		3.5	3.6	8.8	2.3	2.2
	X2	1.8		3.4	4.8	10.7	38.6	3.5	2.0		3.8	6.2	9.4	15.3	1.8
small on low	N	6		3	8	5	8	5	11		5	12	12	11	10
	X1	0.6		6.0	1.9	2.3	2.5	1.2	0.7		7.5	1.2	1.4	2.7	1.4
	X2	1.1		21.3	18.3	6.5	14.4	2.4	2.4		30.8	11.4	5.1	33.4	129.9
all matches	N	61		75	76	71	68	57	77		87	92	89	82	74
	X1	1.1		9.9	4.4	7.9	3.2	2.1	1.3		9.2	3.6	6.3	2.6	1.6
	X2	1.2		38.5	9.9	15.6	15.8	2.9	2.1		38.0	9.9	15.2	12.7	19.8
position	X	3.3		8.4	11.7	5.0	8.9	9.7	2.7		9.7	12.2	5.4	9.3	9.2
annihilation	N	1							1						
	X	1327.5							1327.5						
misses	N	70		175	156	184	166	146	54		163	134	165	150	128
	X	7.6		27.9	12.4	23.6	18.2	8.0	5.6		26.4	12.7	22.6	17.3	7.9
false hits	N	16		9	18	15	25	25	49		30	43	51	68	68
	X	2.6		14.5	3.3	5.3	3.4	4.2	3.1		5.4	2.9	3.1	3.2	3.4
total	N	147		259	250	270	259	228	180		280	269	305	300	270
	X	4.3		22.2	9.3	18.5	12.8	6.1	3.1		18.8	8.0	14.6	10.1	5.0

APPENDIX II: LIST OF TESTED SOFTWARE PACKAGES AND THEIR PRODUCERS

Software	Version	Producer
ActAn	2.5 (1995)	Centro de Estudios Aplicados al Desarrollo Nuclear (CEADEN) Calle 30 No. 502 e/ 5ta y 7ma. Miramar Playa Havana, CUBA Fax: (++ 53 7) Phone: (++53 7) 22 14 22 E-mail: ceaden@cenia.ac.cu
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Ganaas	3.3 (1995)	Physics Section, RIPC, IAEA Wagramerst. 5, P.O. Box 100 Vienna AUSTRIA Fax: (++43-1) 20607 Phone: (++43-1) 206021706 E-mail: T.Dolan@iaea.org WWW: http//www.iaea.or.at
GeniePC	2.2 (1995)	Canberra Industries, Inc. 800 Research Parkway, Meriden, CT 06450 USA Fax: (++203) 235-1347 Phone: (++203) 238-2351 E-mail: mmoslinger@canberra.com WWW: http//www.canberra.com
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Sampo90	3.6	Helsinki University of Technology Department of Technical Physics Rakentajanaukio 2 FIN-02 150 Espoo FINLAND Fax: (++358-0) 451 3195 Phone: (++358-0) 451 3191 E-mail: aarnio@hut.fi
Span	5.1	China Institute of Atomic Energy P.O.Box. 275 (29) Beijing, China 102413 Fax: +86-10 9357102 Phone: +86-10 9357102

CONTRIBUTORS TO DRAFTING AND REVIEW

BERNASCONI, G.	Seibersdorf Laboratories, International Atomic Energy Agency, Seibersdorf, Austria
BLAAUW, M.	Interfaculty Reactor Institute, University of Technology, Delft, Netherlands
CAPOTE Noy, R.	Centro de Estudios Aplicados al Desarrollo Nuclear (CEADEN) Havana, Cuba
van ESPEN, P.	Micro and Trace Analysis Center (MiTAC), University of Antwerp, Antwerp, Belgium
FAZINIC, S.	International Atomic Energy Agency
MANH, D.H.	Nuclear Physics Institute, Dalat, Viet Nam
MOLLA, N. Islam	Institute of Nuclear Science and Technology, Bangladesh Atomic Energy Commission, Dhaka, Bangladesh
OSORIO, V.	International Atomic Energy Agency
WESTMEIER, W.	Dr. Westmeier GmbH, Gesellschaft für Kernspektrometrie, Mölln, Germany