

The 1995 IAEA intercomparison of γ -ray spectrum analysis software

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Abstract

In an intercomparison organized by the IAEA, 12 PC-based programs for γ -ray spectrum analysis were tested using seven reference spectra and a sum of squared differences method. It was found that all programs yield peak areas without bias, relative to each other. Most of the programs could analyze a spectrum containing only singlets in reasonable statistical control with respect to peak areas. Peak positions generally are reported with too small or absent uncertainties. Statistical control was found to be lacking in the analysis of doublet peak areas.

1. Introduction

Germanium semiconductor detectors have been available since the late 1960s. Quite a few fully developed software packages are available to perform the analysis of the spectra measured with these detectors. The last IAEA intercomparison of such packages, G-2, was performed in 1980 and dealt mostly with in-house software [1]. Test of commercial software were also performed [2–4]. The ANSI standard 42.12, section 8 [5], specifies methods to verify the performance of such software packages. The basic concepts of this standard were applied to selected programs by Koskela [6–8]. However, this standard method determines whether a program is good enough or not and is less suitable for an intercomparison, where one is looking for the best available program.

In November 1995 a consultant's meeting was called by the IAEA to perform an intercomparison of such programs for the analysis of γ -ray spectra, using reference spectra [9].

The reference spectra were analyzed in two different ways using 12 PC-based analysis programs. The results

were compared to the reference results using a reduced sum of squares methods, testing the ability of the programs to determine the peak areas, the peak area uncertainties, the peak positions and the peak position uncertainties. Since peak areas as determined by the different programs might be biased by differences in peak shape models, corresponding renormalization factors were determined prior to the statistical testing.

In this paper, the main methods and results of the intercomparison are presented in order to stimulate the development of even better γ -ray spectrum analysis software and assist the potential users of such software. Whenever possible, the relation between the test results presented here and the tests prescribed in the ANSI standard is made explicit. The intercomparison is described in greater detail in an IAEA Technical Document.

2. Method

2.1. The reference spectra

The reference spectra, as described in [9], are a calibration spectrum obtained from standard calibration sources containing ^{22}Na , ^{57}Co , ^{60}Co , ^{137}Cs and ^{54}Mn .

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and several ^{226}Ra with progeny spectra. Some of the latter have been manipulated by 3 channel shifts and subsequent additions to generate doublets with known but varying separation in terms of peak width and known peak area ratios. One of the spectra is distorted by pile-up due to the presence of an ^{241}Am source. The unmanipulated ^{226}Ra spectrum is called "straight", the distorted one "distort" and the added spectra are named according to the peak area ratios: "add1n1", "add1n3", "add3n1", "add10n1" and "add1n100". For each reference spectrum, reference data for expected peak areas and their uncertainties, obtained from an unmanipulated spectrum with a 20-fold longer counting time, are available.

2.2. The analysis programs

The programs tested were ActAn 2.5 (CEADEN, Cuba), GammaPlus 1.02.0 (Silenia SPA, Italy), Gamma-Trac 1.3.2 (Oxford Instruments Inc., USA), Gamma Vision 2.3 (EG&G Ortec, USA), Gamma-W 17.08 (Westmeier GmbH, Germany), Ganaas 3.2 (IAEA, Austria), GeniePC 2.2 (Canberra, USA), Hypermet PC 4.00 (KFKI, Hungary), InterWinner (Eurisys Mesures, France), OSQ/Professional 6.3 (Aptec Engineering Ltd., Canada), Sampo 90 (Helsinki University of Technology, Finland), and Span (Inst. of Nuclear Power, China). Two of the programs, i.e. ActAn and Ganaas, were developed under auspices of the IAEA. All programs ran under MS-DOS or Windows, except for GeniePC which runs under OS/2.

2.3. Analysis of spectra

Spectra were analyzed with each program by one user only. All team members were considered experienced γ -ray spectrometrists. Prior to the actual analysis of spectra, the manuals of the programs were studied for two hours. This amount of time was sufficient to read all of some manuals but not enough to read more than a fraction of others – the number of pages per manual varied from less than one hundred to several thousand.

The calibration spectrum was used to calibrate the programs with respect to peak shape and channel-energy relation. Using this calibration, each spectrum was analyzed twice. First with all parameters, such as peak search sensitivity and residual search sensitivity, set to the default values or, if available, to the values suggested in the manual of the program. Second, with the parameters set to the user's liking, attempting to optimize for the analysis of each spectrum. This optimization was performed using the information offered by the analysis program and its documentation. The statistical processing of the analysis results was performed only after all analysis runs had been completed.

2.4. Data handling

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 needed 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

$$E = 2.78 + 0.396952p - 4.0 \times 10^{-8}p^2$$

and for the "straight" and "distort" spectra

$$E = 2.78 + 0.396952p - 7.0 \times 10^{-8}p^2.$$

The same conversion program yielded output in a standard format similar to the format of the reference lists, containing peak positions and areas, both with their absolute one 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 Sampo 90. For all the other programs, which reported energies with two or more digits after the dot, implying uncertainties of less than 0.01 keV, these uncertainties were set to 0.01 keV. Also, not all programs reported one 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.

2.4.1. Principle of the test

A separate program, available with the reference spectra, was used to perform a statistical comparison based on standardized residuals or z -scores, i.e. 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. A z -score related to the quality of area determination based on the uncertainties in the reference files:

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

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:

$$Z_{\text{rep}} = \frac{A_{\text{rep}} - A_{\text{ref}}}{\sqrt{\sigma_{\text{rep}}^2 + \sigma_{\text{ref}}^2}},$$

where A_{ref} and A_{rep} are the reference and reported peak area, σ_{ref} and σ_{rep} their uncertainties, respectively. The ratio of the counting times of the reference spectrum and the test spectra is 20 and $\sqrt{20\sigma_{ref}}$ 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 indicate that something is wrong at the $\alpha = 0.05$ level.

If the reference area was missing, the reported peak was considered to be a "false hit" and only the second z -score 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 could be computed. Missing a noisy peak or reporting a false hit with a high uncertainty in the area do not result in high z -scores and are therefore "allowed" in this test.

The added reference spectra contain doublets with separations varying from 0.4 to $1.2 \times \text{FWHM}$. It was decided to allow for analysis programs determining the total area of doublets with small separation. To this end, if two peaks in the reference list matched one peak in the analysis program output, i.e. if both reference peaks were located within $0.5 \times \text{FWHM}$ of the analysis result, the two reference peaks were merged before the computation of z -scores. This was also done if such two reference peaks were located within the position uncertainty reported by the analysis program.

The 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.

2.4.2. Peak area renormalization

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. 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. Since none of the renormalization factors found for the "straight" spectrum deviated from unity significantly, as will be discussed later, the renormalization 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 approx. 9% was thus established.

2.4.3. Computation of standardized residuals and reduced sums of squares

Z -scores or standardized residuals were computed as described above. A section from the comparison program output is shown in Fig. 1. From the z -scores, reduced sums of squares X^2 were computed for different categories of peaks. If no renormalization had been performed, the X^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 the category. If renormalization 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:

- Annihilation peak: Any peak closer than 3 keV to 511 keV.
- High peaks: non-annihilation hits for which the ratio of reference peak area and reference peak uncertainty is larger than 10.
- 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

REFERENCE DATA				ANALYSIS PROGRAM OUTPUT				z-scores	
E	unc	A		E	unc	A	unc	rep	ref
val		val	unc	val		val			
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	

Fig. 1. 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 and 2206.8 keV, resulting in a "false hit" at 2207.3 keV.

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

$$b = (20\sigma_{\text{ref}}^2 - A_{\text{ref}})/2.$$

- 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.
- False hits.
- Total: All previous categories except for the annihilation peak.

A separate χ^2 was computed for 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.

3. Results and discussion

3.1. Tables of results

The number of peaks in each category and the χ^2 -results for the different programs are shown in Tables 1–11. 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. During the intercomparison, some analysis runs were not performed by mistake. These data are therefore missing from the tables. From the data presented, graphs were produced that are shown in this section.

3.2. 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 listed in the tables. These numbers are shown in Fig. 2. 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 Fig. 3, the difference between the numbers of detected small peaks on high background and the numbers of false hits are shown. It must be pointed out that

Table 1
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 Annihilation	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
	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 2
GammaTrac

		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 3
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 4
GammaVision

		Default settings							User settings						
		stra	dist	ln1	3nl	ln3	ln100	ln100	stra	dist	ln1	3nl	ln3	ln100	ln100
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	1.2×10^4	234.8	2.2	1.7	3.9	4.0	185.3	1.2×10^4	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 5
Gamma-W

		Default settings							User settings						
		stra	dist	ln1	3nl	ln3	ln100	ln100	stra	dist	ln1	3nl	ln3	ln100	ln100
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 6
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 7
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 8
HypermetPC

		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 9
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		12	3		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 10
Sampo90

		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	55660.0						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 11
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

Table 12
InterWinner

		Default settings							User settings						
		stra	dist	ln1	3nl	ln3	10nl	ln100	stra	dist	ln1	3nl	ln3	10nl	ln100
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

detection of a spurious peak is not necessarily a bad thing if the peak area is reported with a high uncertainty as indicated by the X^2 -value for the false hits. Also, spurious peaks can result from unavoidable imperfection of the peak search algorithm as well as from incorrect multiplet deconvolutions. Nevertheless, it is clear from the figures that a program like Gamma-W is performing better in this respect than e.g. InterWinner.

3.3. Peak shape model dependency of absolute peak area determination

In Fig. 4, the renormalization factors and their uncertainties for the peak areas determined by the analysis programs are shown.

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 Fig. 4, the programs tested yield unbiased peak areas, within the statistics of the test (the only outlier 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.)

3.4. Interpretation of the X^2 -values

The X^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

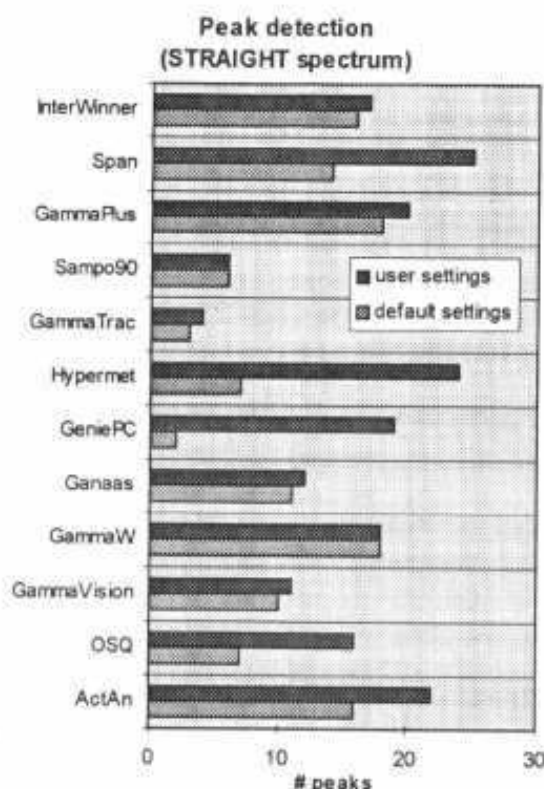


Fig. 2. Numbers of detected small peaks on high background.

underlying the X^2 -values, however, are not normally distributed: in those cases where incorrect deconvolution occurs, very high values can result. A high X^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.

Also, in this work two kinds of X^2 -values are defined: The first based on z -scores accounting for both the reference and the reported uncertainties, the second on the z -scores computed from reference uncertainties only. In this case, the first X^2 indicates the level of statistical control of the program as described above, the second indicates how well the peak areas themselves were determined regardless of the reported uncertainties.

3.5. 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

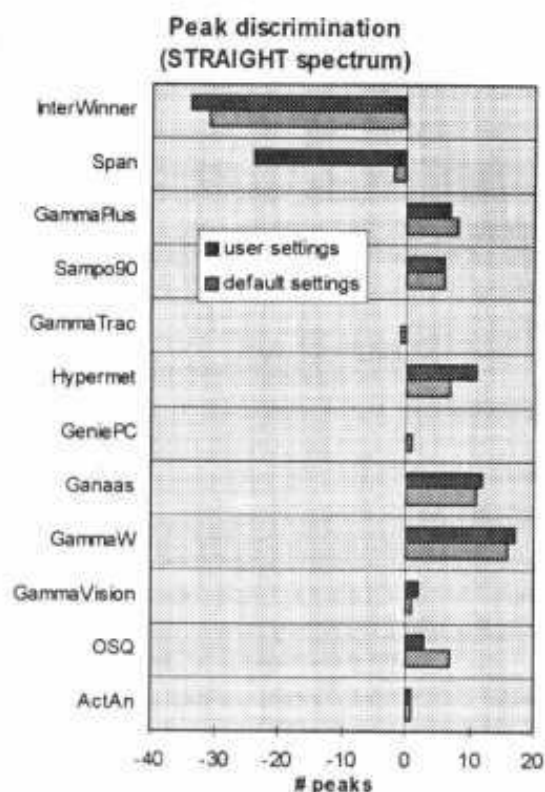


Fig. 3. Difference between number of detected small peaks on high background and number of false hits.

possible causes could be such a dependence. In Fig. 5, the X^2 -values based on the reference uncertainties are plotted for the programs in their different modes. It is clear 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 indicates that the information offered by the corresponding programs to judge the quality of the results can be improved.

In Fig. 6, the X^2 -values based on the uncertainties reported by the programs have been plotted. Even though most X^2 -values differ from unity significantly, 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

$$f = X_{rel}^2 / X_{rep}^2$$

The resulting values are shown in Fig. 7. Most programs turn out to overestimate the uncertainties they report, relative to the optimum uncertainties from the reference list. Relative to the actual discrepancies

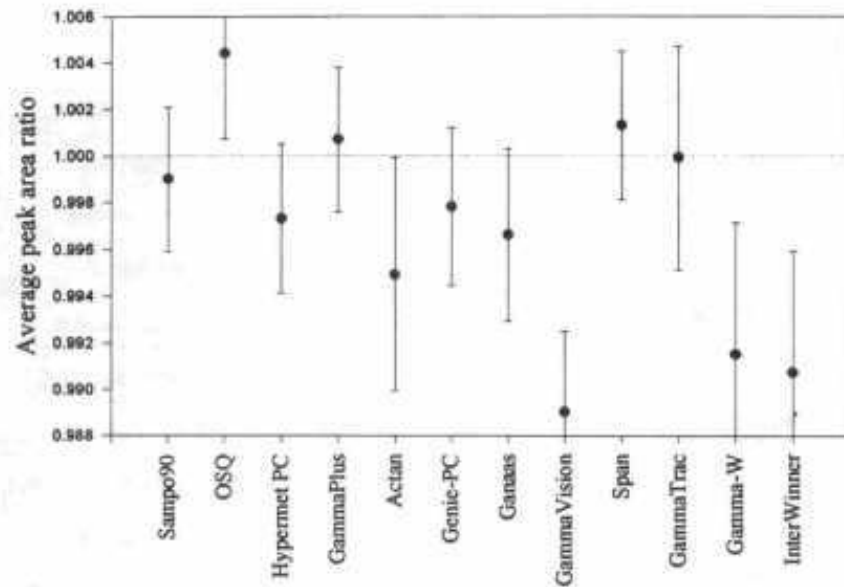
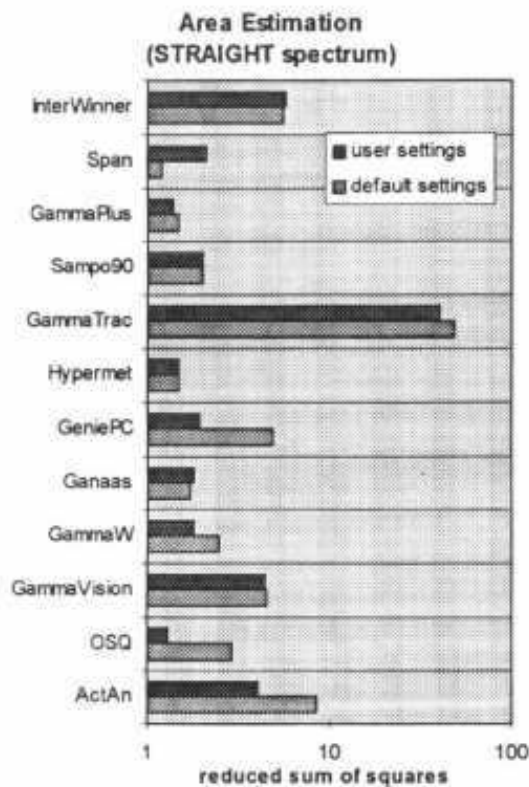
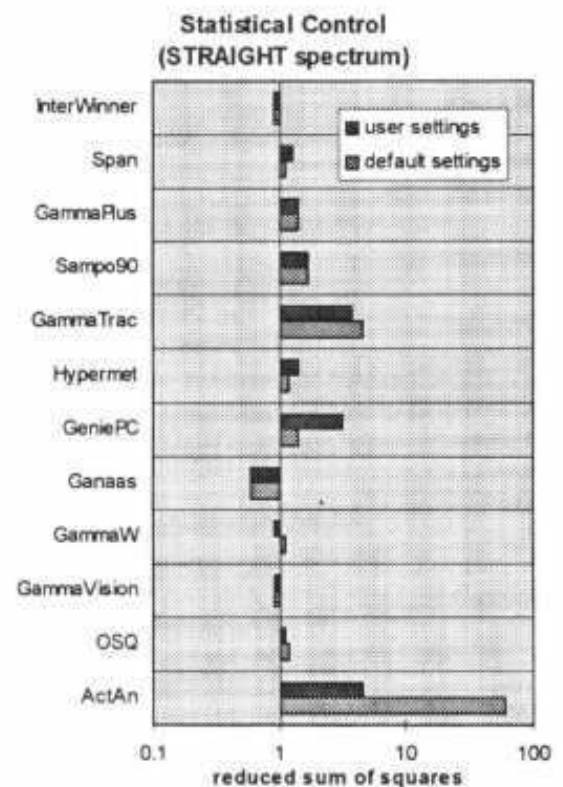


Fig. 4. Renormalization factors and uncertainties for the analysis programs.

Fig. 5. χ^2 -values based on reference uncertainties for each program in its two modes.

between reported areas and reference areas, however, the reported uncertainties are reasonable as Fig. 6 illustrates.

Even though most programs do not report peak position uncertainties but merely imply them to be 0.01 keV

Fig. 6. χ^2 -values based on the uncertainties reported by the programs in their two modes for the "straight" spectrum.

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

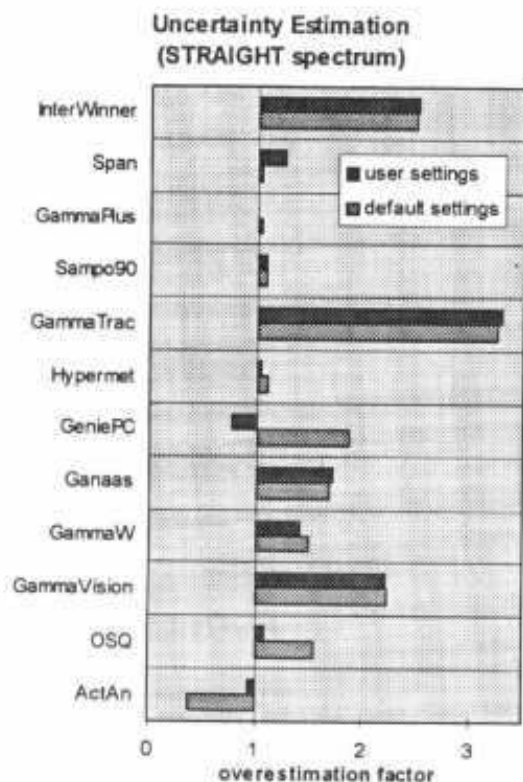


Fig. 7. Uncertainty overestimation factors.

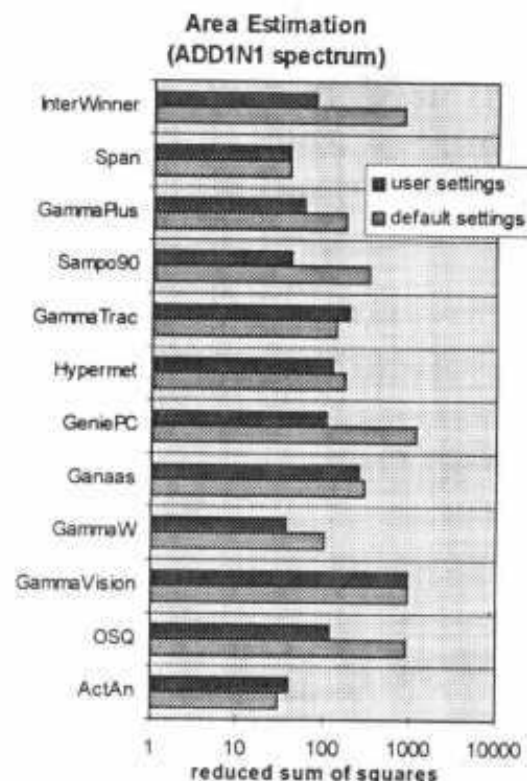
a 511 keV peak was present in the calibration spectrum.

The "distort" spectrum was analyzed well by GammaPlus, GammaVision 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.

3.6. 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 Figs. 8 and 9, in the same way as for the "straight" spectrum in Figs. 6 and 5.

As shown in Fig. 9, 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 uncertainty, with the user settings. In some cases, the user settings result in a change in X^2 -values of more than one order of magnitude. With the default settings, the

Fig. 8. X^2 -values based on the reference uncertainties for the programs in their two modes for the "add1n1" spectrum.

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 only if the constituent peaks are in its gamma-ray library or initially 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 Espen [10].

The remaining programs that yield more or less equally good results with default and user settings always fit and deconvolute peaks, but the user may exert some control over the process by setting parameters such as a residual peak search threshold.

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 $0.5 \times \text{FWHM}$ or the reported position uncertainty, as illustrated in Fig. 10. This is most likely to happen on the low-energy side of

the spectrum, where the doublet separation is $1.2 \times \text{FWHM}$. Additional runs of the comparison program were performed where the criterion for a match in peak position was varied from $0.2 \times \text{FWHM}$ to $1.2 \times \text{FWHM}$, covering the range of the doublet separations in the spectrum. From Fig. 11, where some results for one of the analysis programs are shown, it is clear how crucial this criterion is, even though it is 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 Section 2.4.1, these components are merged so that total doublet areas are compared.

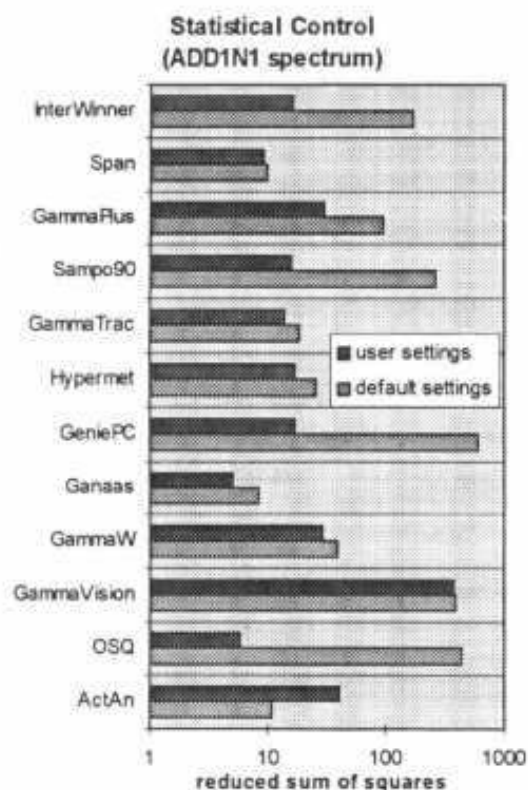


Fig. 9. X^2 -values based on the uncertainties reported by the programs in their two modes for the "add1n1" spectrum.

To establish how well the analysis programs could distinguish doublets from singlets, their resolving power was defined as the number of high peak in the add1n1 spectrum divided by the same in the straight spectrum. For this ratio, 2 would be a perfect score. The X^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 $1.0 \times \text{FWHM}$ matching criterion. The results are shown in Figs. 12 and 13.

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 clear that the threshold was set too 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 [8] and implemented earlier at IRI [11,12], 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 do not, search windows of 1 keV or $1 \times \text{FWHM}$ are common practice, unnecessarily complicating the interpretation process.

To establish the quality of the total area determination, the results from the $1 \times \text{FWHM}$ match criterion statistical comparison runs were used for Figs. 14 and 15, otherwise identical to Figs. 8 and 9. These figures indicate that the total areas of the doublets mistaken for singlets, as well as constituent 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.

REFERENCE DATA				ANALYSIS PROGRAM OUTPUT				z-scores
E	unc	A	unc	E	unc	A	unc	
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

Fig. 10. 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.

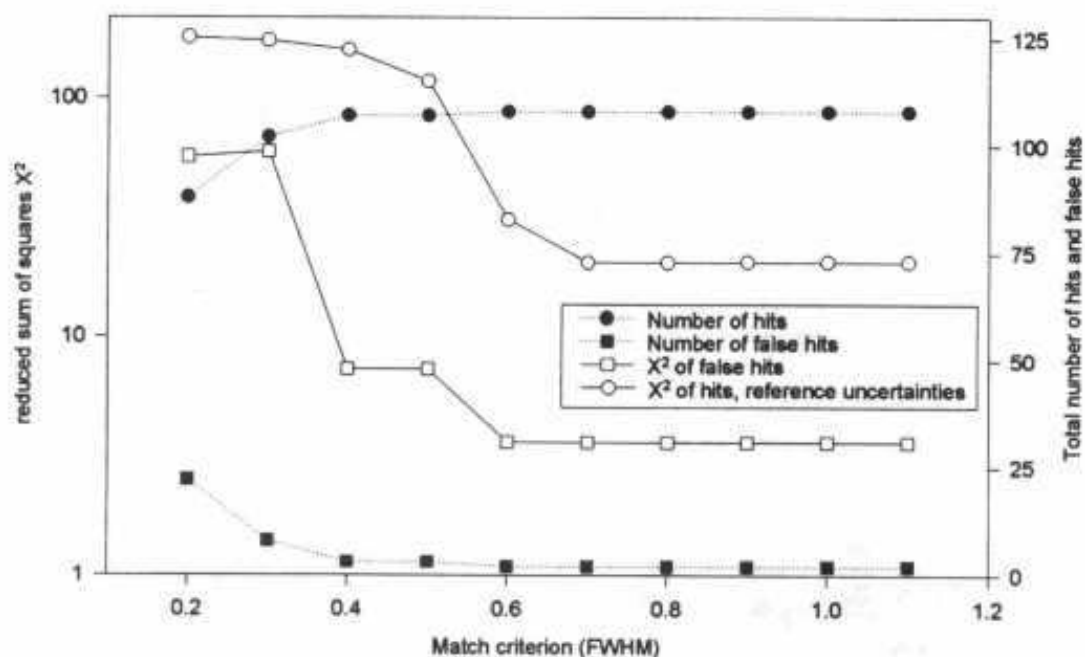


Fig. 11. χ^2 based on reference uncertainties and the total number of matches as a function of the peak position match criterion in terms of FWHM. Lines were drawn to guide the eye.

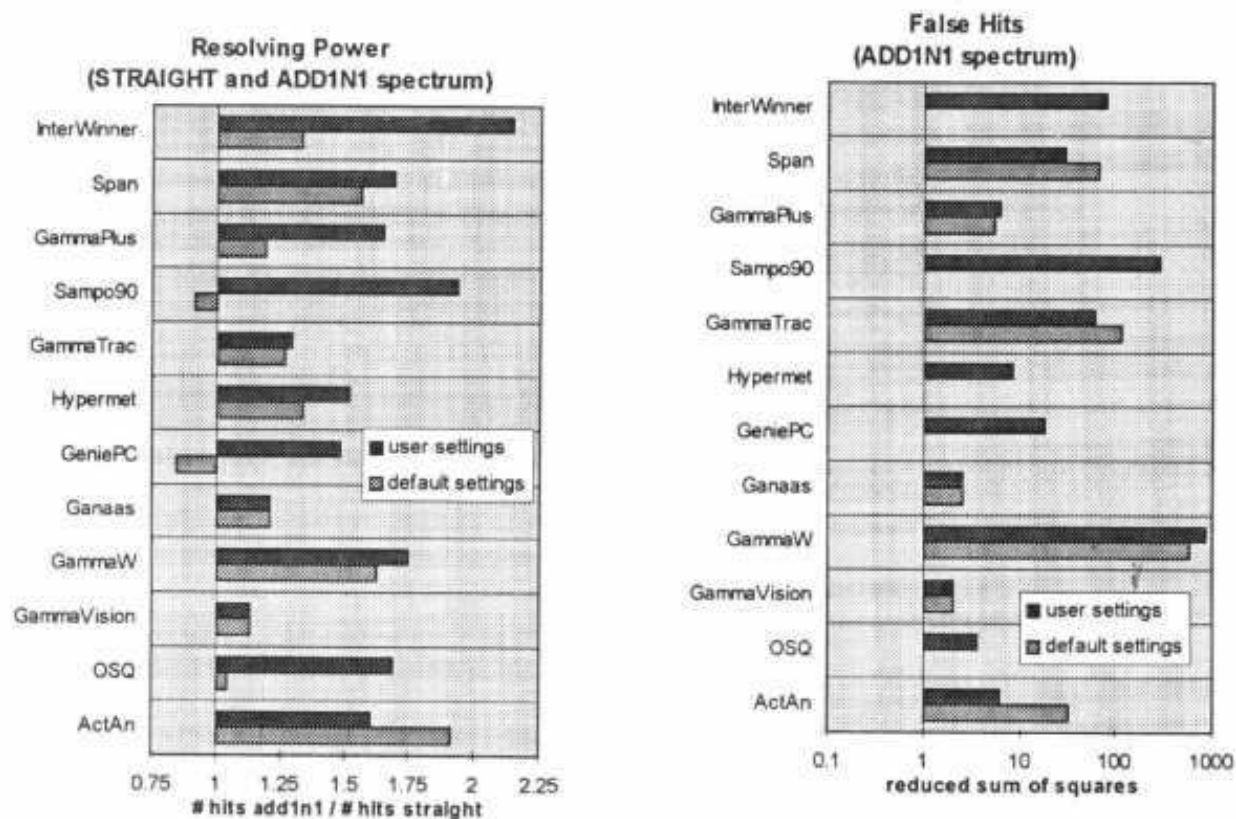


Fig. 12. Resolving power of the analysis programs.

Fig. 13. χ^2 -values related to false hits, indicating deconvolution correctness.

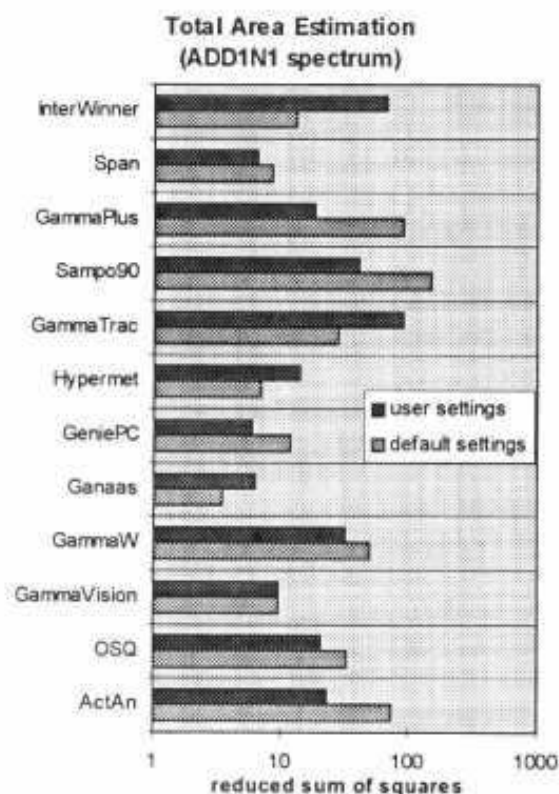


Fig. 14. χ^2 -values based on the reference uncertainties for the programs in their two modes for the “add1n1” spectrum, determined with a $1 \times \text{FWHM}$ match criterion.

4. Conclusions

All programs tested yield unbiased peak areas to within 1%. The expected peak shape model dependence was not found in practice. To avoid coincidence correction problems, any program developed in the future should be required to also yield unbiased peak areas.

In the applied tests, singlet peak areas are determined quite well by all programs except GammaTrac 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, Hypernet PC, Ganaas, OSQ/Professional, Sampo 90 and Gamma-W (in no particular order).

Doublets at separations below $1.2 \times \text{FWHM}$ 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 Sampo 90 yielded the least bad results. Only after the consequences of peak position uncertainty underestimation were removed by a change in the test

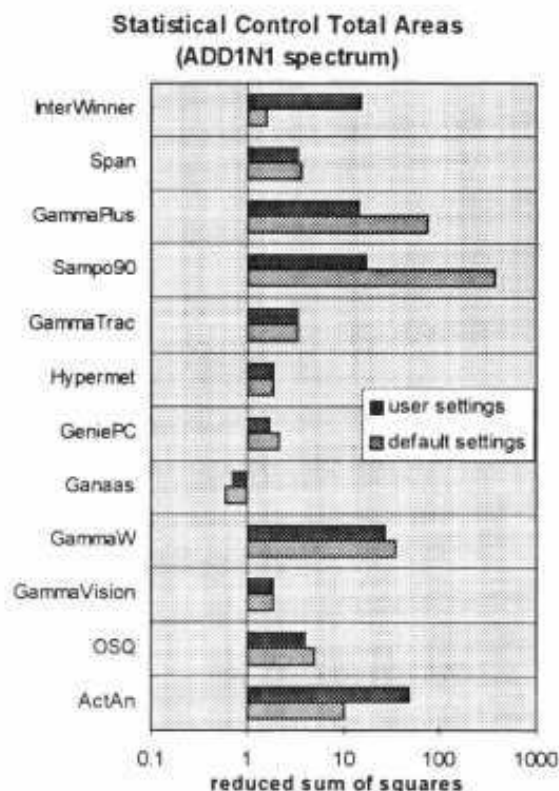


Fig. 15. χ^2 -values based on the uncertainties reported by the programs in their two modes for the “add1n1” spectrum, determined with a $1 \times \text{FWHM}$ match criterion.

procedure, Ganaas, Hypermet PC, Gamma Vision, 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.

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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