Peak area determination proficiency test

for the "Reference Database for Neutron Activation Analysis" CRP of the IAEA

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1. Introduction

At the first RCM on "Reference Database for Neutron Activation Analysis", it was decided to organize a proficiency test to establish the ability of the potential participants to determine peak areas. To this end, a test procedure was used much like the 1995 IAEA intercomparison for commercially available software [1].

A test spectrum was created in Delft and distributed amongst the participants, as shown in the Appendices. The participants returned the results to me and I processed them as described in this document.

2. Participants, programs and remarks

The following information was provided by the participants and was known before the actual proficiency test was performed.

Program	Participant	Name	Remarks by participant(s)
GAMANAL	María Arribére	arri	
Hypermet PC 5.01	Alessandro Borella	bor1	DT unknown
Hypermet PC 5.01	Borella and Blaauw	bor2	E-cal improved, DT unknown
Hyperlab 2002.3	Frans De Corte	corte1	
Hypermet PC 5.0	Frans De Corte	corte2	
k0-IAEA	Radojko Jacimovic	jacko1	
Hyperlab 2002.3	Radojko Jacimovic	jacko2	
Unknown	Sunday Jonah	Jonah	No DT correction
Hypermet PC	Zsolt Revay	revay	DT applied
k0-IAEA	Petra Rogan	rogan	

In addition, I found that Borella had misidentified the 121.8 as the 344 keV peak, so I recalculated his peak energies and created the Bor2 dataset (with myself as extra participant).

3. Experimental

A radioactive source containing ^{152}Eu and ^{22}Na was measured in a very large well-type detector (10 % absolute full-energy peak efficiency for the ^{60}Co lines) during 278 minutes and 14 minutes. The dead time was about 4%, as established with a 25 Hz pulser present in the spectra at channel 3555. The spectrum with the long acquisition time was analyzed with great care with two analysis programs: The in-house Apollo software named "SPECFIT" [2] and the "k0-IAEA" program [3]. Both programs were written by Menno Blaauw, but k0-IAEA allows for more interactive fitting. Both programs were previously validated using the IAEA 1995 test spectra [1,4,5]. The dead-time corrected analysis results were evaluated side by side. The overall χ_r^2 of the peak areas reported by the two programs was 1.7, mostly due to peaks not detected by k0-IAEA. Since these peaks are much too noisy to be detectable in the spectrum counted 20 times shorter, the programs are in good agreement for all practical purposes.

The SPECFIT program does not perform doublet deconvolutions. Since the purpose of the proficiency test was to see if the participants can reliably determine a singlet peak area - after all, single-element gamma-ray spectra are to be the topic of the CRP - total multiplet peak areas are listed as reference peak areas, but tagged with a '0' digit, meaning they are not be taken into account in the intercomparison. See the table below for a section of the reference file containing such a multiplet.

The test spectra contained an anomaly in that the 121.8 keV was off the energy calibration curve, relative to all the others. If all the other ^{152}Eu peaks were to come up with the right energy, the 121.8 keV came up with 120.6 keV. Some participants had only used the 121.8 and the 1408 for energy calibration purposes, resulting in mismatches for all or most peaks apart from the two mentioned. To correct for this mistake, a second reference peak area file was created based on the same energy calibration approach followed by these participants.

4. Data handling

The same procedures were applied as in the 1995 IAEA intercomparison [1]. Since it was not clear whether the various participants had corrected their peak areas for dead time, the peak areas were compared in terms of the weighted average of the peak area ratios. Ideally, this factor should be unity in the absence of bias, but in this test the values reflected the dead time correction.

5. Results

The results for the bias factors are shown in Table 1. The uncertainty in each factor is about 0.4 %.

Table 1: Bias factors for each participant, reflecting absence of dead time correction. Dead time as derived from RT/LT is 9.17 %, requiring a 1.101 correction factor.

Name	121.8 - 1408 Ecal	Area normalization factor
arri	no	1.085
bor1	not applicable	not applicable
bor2	no	1.090
corte1	yes	1.087
corte2	yes	1.088
jacko1	yes	1.095
jacko2	no	1.090
Jonah	no	1.092
revay	yes	1.092
rogan	yes	1.092

In Figure 1, Figure 2 and Figure 3, the results are shown in terms of statistical control for peak areas. In Figure 4, the same is shown for peak energies. In Figure 5, the numbers of detected small peaks, misses and false hits are shown. In Figure 6, the associated χ_r^2-values are plotted.

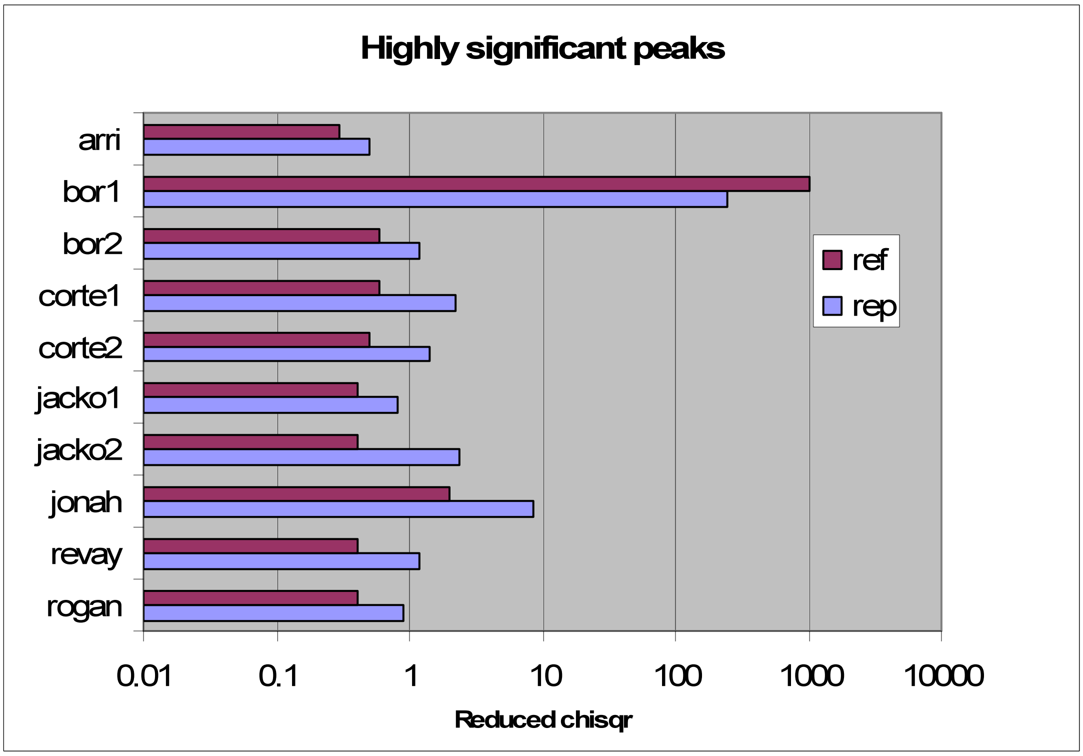

Figure 1: χ_r^2-Results for the areas of highly significant peaks

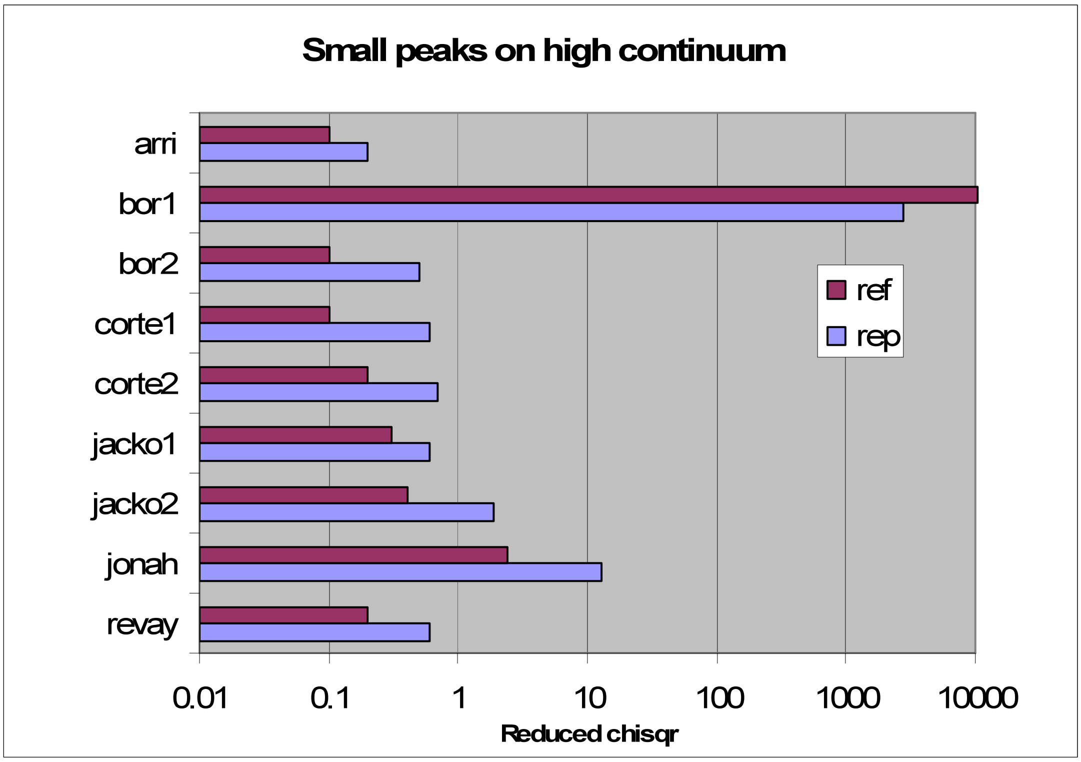

Figure 2: χ_r^2-Results for the areas of not-so significant peaks

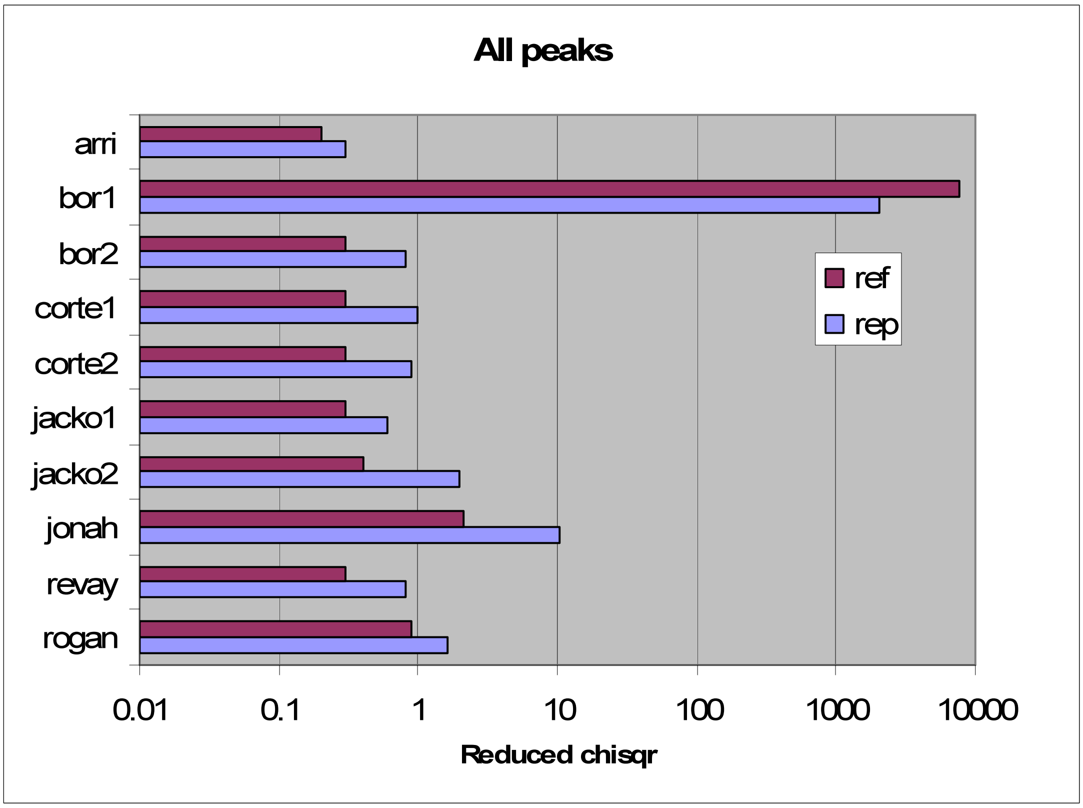

Figure 3: χ_r^2-Results for the areas of all matched peaks

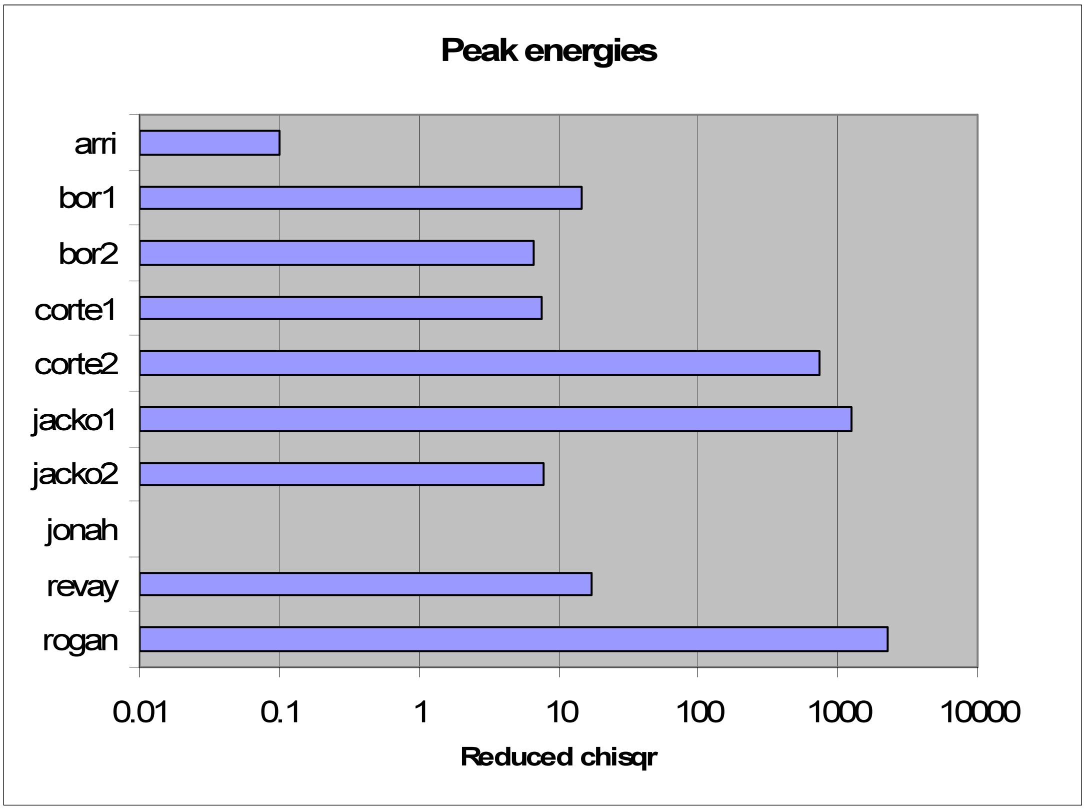

Figure 4: χ_r^2-Results for the energies of all matched peaks

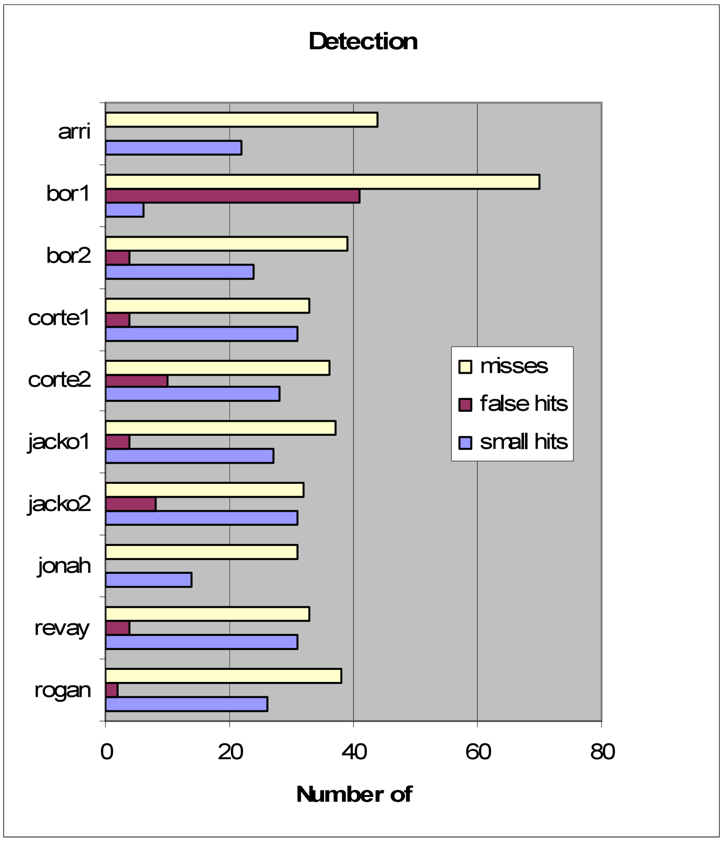

Figure 5: Detection of small peaks and the related occurrence of misses and false hits

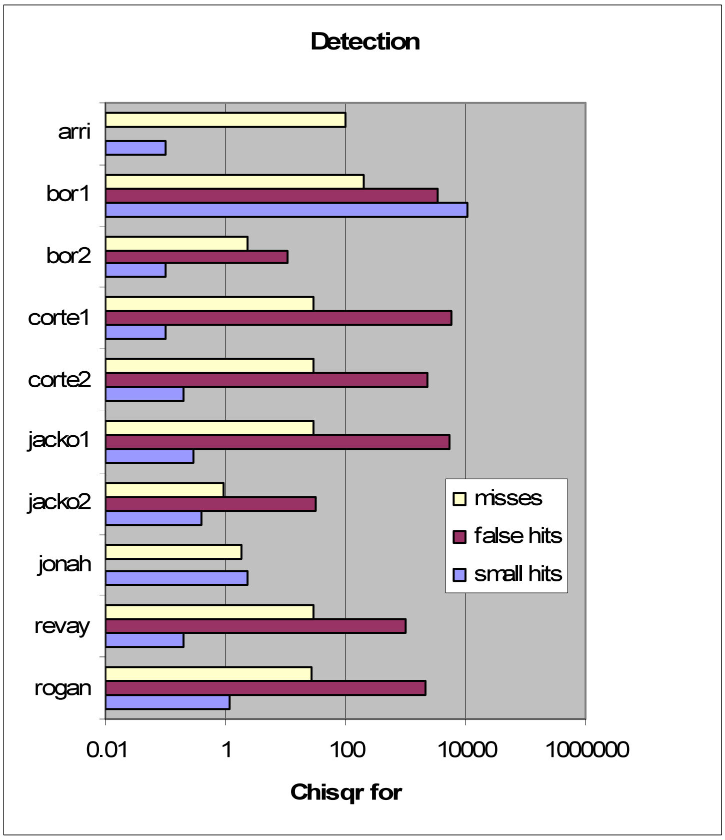

Figure 6: χ_r^2-values for detection of small peaks and the related misses and false hits

6. Discussion

The results for the bias factors as shown in Table 1 reflect the fact that no participants performed a dead-time correction, even though some stated they did and some stated they did not know whether they did or not.

As Figure 1, Figure 2 and Figure 3 demonstrate, except for the bor1 entry, most participants prove to be able to determine a peak area reasonably well with the software used. Remarkably, the χ_r^2-values calculated with the reference uncertainties exclusively tend to be smaller than the χ_r^2-values calculated with the reported uncertainties. This means that the uncertainties in the reference peak areas are larger than the uncertainties reported by the participants - too much so, even, since the "ref" χ_r^2-values tend to be smaller than unity. This effect is more pronounced in the smallish peaks than in the determination of peak areas of highly significant peaks.

The peak energies are reported with underestimated uncertainties in most cases. The exceptions are the arri and jonah datasets. The jonah dataset specifies uncertainties in the order of 10 keV for most peaks, the arri dataset of 0.1-0.6 keV, typically.

The numbers of detected small peaks and false hits in Figure 5 show that an erroneous peak identification in the energy calibration step leads to disastrous result here, too. Also, the jonah data appear to have been obtained with a higher peak search threshold than the other participants', who present comparable results. It appears that in the arri dataset, no peaks above 1408 keV were detected, which results in a high χ_r^2-value for misses as shown in Figure 6, apart from the high number of misses also observed in Figure 5.

7. Conclusions and recommendations

Of all entries, two are outliers: bor1 and jonah. The first is the result of erroneous peak identification (and probably also of an energy calibration based on only two data points without checking the other peaks). Other datasets were also based on such two-point energy calibrations without regard for the majority of the peaks. It is to be hoped that more attention would be paid to gamma-ray spectra obtained with the aim of determining constants for NAA.

The jonah dataset contains fewer peaks than the others. The uncertainties in the reported peak energies are very large - typically 10 keV. These appears to be widths of ROIs rather than centroid uncertainties. The quality of the peak areas leaves room for improvement.

No participant corrected the peak areas for dead time, even though some thought they did. This reflects on software that does not make clear to the user what was corrections were applied. Such lack of clarity can have disastrous effects when nuclear constants are to be determined from combinations of flux monitor spectra and sample spectra, all obtained with different dead time percentages.

8. References

1. M. Blaauw, V. Osorio Fernandez, P .v. Espen, G. Bernasconi, R.Capote Noy, H. Manh Dung, N.I. Molla, "The 1995 IAEA intercomparison of commercially available γ-ray spectrum analysis software", Nucl.Instr.Meth. **A387** (1997) 416-432
2. M.Blaauw, "Multiplet Deconvolution as a Cause of Unstable Results in INAA", Nucl.Instr.Meth. A333 (1993) 548-552
3. Matthias Rossbach, Menno Blaauw, Marcio Bacchi, Xilei Lin, The K_0-IAEA program, *in press* J.Radioanal.Nucl.Chem. 271-3
4. M. Blaauw, "The Reference Peak Areas of the 1995 IAEA Test Spectra for Gamma-Ray Spectrum Analysis Programs are Absolute and Traceable", Nucl.Instr.Meth. A432 (1999) 74-76
5. M. Rossbach, M. Blaauw, "Progress in the k0-IAEA program", Nucl.Instr.Meth.A 564 (2006) 698-701

APPENDIX 1 - Description of the test spectrum as emailed to the participants

Description of the AC02-33 test spectrum

This spectrum contains peaks from two radionuclides: Eu-152 and Na-22. It was measured on a highly efficient well-type detector, so that the relative peak intensities are greatly affected by coincidence summing. The 121.8 keV is located near channel 138, the 1408.0 keV is located near channel 1696. There is a pulser peak near channel 3406.

You are requested to determine the peak areas and energies in this spectrum as well as you can. Here in Delft, we analyzed a spectrum from the same set-up, but counted 20 times longer, in order to determine what the "truth" is. In our analysis, we tried to deconvolute the doublets as well as we could, but if you prefer to report total areas of such doublets, that will be fine, too.

Please report peak energy, uncertainty in energy, area and uncertainty in area for each peak in the following format:

121.80 0.01 12000 110

where all the uncertainties are absolute, 1 standard deviation, and the energies are in keV. Report one peak per line in your report, please. Please state in the accompanying note to me if you corrected for dead time using the live time/dead time information in the spectrum.

The spectrum is supplied in two formats:
1/ The .k0s format that the k0-IAEA program can read, which is identical to the IAEA .spe format. It's really a text format so you can see what it is with a simple text editor
2/ The Ortec .chn format that most programs out there can read.

APPENDIX II - Header section of the test spectrum

```
$SPEC_ID:
ac_now11-AC02
$SPEC_REM:
DET# 0
DETDESC# now-ak0
AP# IRI Menno Blaauw Software
$DATE_MEA:
06/26/2006  14:28:31
$MEAS_TIM:
763 840
$DATA:
0 4095
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       1       1       1
       0       6       6     429     828     966     976     941     946     836
     811     770     840     862     886     868     904     997     908     880
     842     881     909     945    1023     942     909     888     947     876
     889     898     901     875     792     872     899     852     885     900
     903     971     879     895     942     882     923     974     922    1170
```

APPENDIX III - sample output

This report was generated by CMPSPEC (version Apr 20 2007, 15:02:47)

40 peaks in ARRI.TXT
168 peaks in COMBIREF.TXT
367.77 and 366.50 matched 366.81 so were merged
Ratio to multiply all measured peak areas with: 1.0854 +/- 0.434 %

	'TRUE' DATA COMBIREF.TXT				MEASURED DATA ARRI.TXT					
	E		A		E		A		Z-scores	
	val	unc	val	unc	val	unc	val	unc	rep	ref
*	37.6	0.5	291	54	37.6	0.5	0	261		0.0
*	43.2	0.1	359	50	43.2	0.1	0	244		0.0
*	44.1	0.5	480	57	44.1	0.5	0	276		0.0
*	44.7	0.2	86	26	44.7	0.2	0	127		0.0
*	55.5	0.0	31	15	55.5	0.0	0	71		0.0
*	65.2	0.0	4160	227	65.2	0.0	0	1100		0.0
*	67.1	0.0	8032	377	67.1	0.0	0	1827		0.0
*	76.3	0.0	3686	115	76.3	0.0	0	560		0.0
*	78.6	0.0	1035	50	78.6	0.0	0	242		0.0
*	96.8	0.1	36	19	96.8	0.1	0	93		0.0
	120.6	0.0	34597	179	120.8	0.7	34986	557	0.7	0.5
*	129.9	0.0	13	20	129.9	0.0	0	97		0.0
*	136.5	0.0	53	16	136.5	0.0	0	77		0.0
	147.4	0.1	75	16	147.4	0.1	0	79		-1.0
*	183.4	0.4	2178	78	183.4	0.4	0	381		0.0
*	188.5	0.2	80	34	188.5	0.2	0	163		0.0
	190.6	0.1	123	51	190.6	0.1	0	248		-0.5
*	195.1	0.0	58	24	195.1	0.0	0	116		0.0
*	205.6	0.0	1821	52	205.6	0.0	0	250		0.0
*	207.5	0.0	6	23	207.5	0.0	0	111		0.0
*	232.3	0.0	11	15	232.3	0.0	0	72		0.0
	244.7	0.0	14136	71	244.9	0.6	14383	226	1.0	0.8
	251.6	0.2	103	86	251.6	0.2	0	418		-0.3
	276.0	0.1	39	20	276.0	0.1	0	99		-0.4
*	282.2	0.4	901	43	282.2	0.4	0	207		0.0
	285.4	0.3	2	19	285.4	0.3	0	93		-0.0
	296.0	0.0	615	36	296.2	0.6	497	127	-0.9	-0.7
*	300.9	0.0	20	14	300.9	0.0	0	69		0.0
*	313.6	0.5	425	55	313.4	0.6	380	189	0.0	0.0
*	322.6	0.2	82	15	322.6	0.2	0	71		0.0
*	324.8	0.2	83	15	324.8	0.2	0	72		0.0
	329.6	0.1	146	103	329.6	0.1	0	499		-0.3
	334.0	0.3	54	14	334.0	0.3	0	67		-0.9
	344.4	0.0	57799	168	344.5	0.6	57870	661	0.1	0.1
*	353.8	0.0	-19	20	353.8	0.0	0	95		
*	366.5	0.0	2154	78	366.8	0.6	1968	153	0.0	0.0
	386.3	0.2	85	48	386.3	0.2	0	234		-0.4
*	411.2	0.0	1722	44	411.4	0.6	1737	169	0.0	0.0
*	412.8	0.2	104	26	412.8	0.2	0	127		0.0
	416.7	0.2	173	123	416.7	0.2	0	596		-0.3
*	423.5	0.4	390	113	423.5	0.4	0	548		0.0
	444.1	0.0	4045	31	444.2	0.6	3890	181	-0.8	-1.1
*	457.9	0.0	28	13	457.9	0.0	0	61		0.0
	488.8	0.1	384	69	488.7	0.5	334	110	-0.4	-0.2
A	510.9	3.3	86250	101	511.2	0.5	85450	988	-0.8	-1.7
*	521.8	0.4	229	31	521.8	0.4	0	151		0.0
	540.3	0.3	55	31	540.3	0.3	0	149		-0.4
*	564.2	0.1	552	34	564.7	0.5	990	256	0.0	0.0
*	566.1	0.1	372	26	566.1	0.1	0	124		0.0
	579.1	2.7	870	25	578.9	0.5	767	307	-0.3	-0.9
*	584.6	0.0	102	342	584.6	0.0	0	1657		0.0
*	586.8	0.0	377	1133	586.8	0.0	0	5496		0.0
	589.2	0.4	438	709	589.2	0.4	0	3439		-0.1

*	590.3	0.4	485	39	590.3	0.4	0	191		0.0
*	591.1	0.0	131	420	591.1	0.0	0	2040		0.0
*	594.4	0.0	51	168	594.4	0.0	0	817		0.0
	610.8	0.1	65	20	610.8	0.1	0	99		-0.7
*	615.7	0.0	45	14	615.7	0.0	0	66		0.0
*	633.0	0.0	28	14	633.0	0.0	0	66		0.0
*	647.9	0.0	12	13	647.9	0.0	0	65		0.0
	656.6	0.2	110	60	656.6	0.2	0	291		-0.4
	675.2	0.1	51	18	675.2	0.1	0	88		-0.6
	678.7	0.1	128	33	678.7	0.1	0	159		-0.9
	688.8	0.0	1732	107	688.9	0.5	1954	266	0.8	0.5
*	707.9	0.4	39	23	707.9	0.4	0	113		0.0
	712.1	0.0	369	44	712.0	0.5	353	123	-0.1	-0.1
	719.6	0.1	199	20	719.6	0.1	0	95		-2.2
	723.4	0.1	138	15	723.4	0.1	0	74		-2.0
*	733.9	0.0	37	13	733.9	0.0	0	65		0.0
*	743.6	0.4	225	24	743.6	0.4	0	116		0.0
	755.5	0.0	1481	47	755.6	0.5	1551	153	0.4	0.3
	764.9	0.1	163	19	764.9	0.1	0	92		-1.9
	769.0	0.2	88	13	769.0	0.2	0	64		-1.5
	779.0	0.0	9560	89	779.1	0.5	9677	263	0.4	0.3
	810.5	0.0	741	72	810.7	0.5	713	138	-0.2	-0.1
	842.3	0.6	160	202	842.3	0.6	0	981		-0.2
*	846.0	0.0	113	69	846.0	0.0	0	334		0.0
*	848.0	0.0	177	90	848.0	0.0	0	435		0.0
*	856.2	0.0	28	18	856.2	0.0	0	90		0.0
	867.5	0.0	2554	112	867.5	0.5	2451	171	-0.5	-0.2
*	873.1	0.0	82	17	873.1	0.0	0	82		0.0
	897.4	0.2	73	15	897.4	0.2	0	72		-1.1
	901.2	0.1	232	36	901.3	0.5	228	100	-0.0	-0.0
	919.4	0.1	331	64	919.2	0.5	339	130	0.1	0.0
	926.4	0.1	152	16	926.4	0.1	0	79		-2.0
*	927.0	0.0	129	21	927.0	0.0	0	103		0.0
	930.6	0.0	322	30	930.6	0.5	228	96	-0.9	-0.7
	935.6	0.1	105	15	935.6	0.1	0	70		-1.6
	945.5	0.2	55	16	945.5	0.2	0	76		-0.8
	964.1	0.0	18547	130	964.1	0.5	18436	224	-0.4	-0.2
	989.1	0.1	329	36	989.0	0.5	316	123	-0.1	-0.1
	996.1	0.2	56	11	996.1	0.2	0	53		-1.1
	1005.1	0.1	558	49	1004.8	0.5	550	116	-0.1	-0.0
	1022.0	0.0	21388	125	1021.9	0.5	21066	216	-1.3	-0.6
	1032.0	2.7	508	19	1031.8	0.5	522	145	0.1	0.2
*	1041.7	0.1	161	28	1042.3	0.5	196	84	0.0	0.0
*	1044.1	0.4	36	13	1044.1	0.4	0	61		0.0
*	1057.0	0.0	59	11	1057.0	0.0	0	53		0.0
	1085.9	0.0	16211	6583	1085.8	0.5	16051	217	-0.0	-0.0
	1089.9	0.1	1191	2354	1089.5	0.5	1083	169	-0.0	-0.0
*	1096.7	0.0	26	26	1096.7	0.0	0	126		0.0
*	1100.8	0.0	0	26	1100.8	0.0	0	126		
	1112.1	0.0	18589	103	1112.0	0.5	18779	378	0.5	0.4
	1123.2	0.0	8192	70	1123.1	0.5	8444	288	0.9	0.8
	1163.0	0.1	33	20	1163.0	0.1	0	95		-0.4
	1170.6	0.5	259	66	1170.7	0.5	244	96	-0.1	-0.0
*	1178.7	0.1	140	21	1178.7	0.1	0	100		0.0
*	1180.7	0.1	310	34	1180.7	0.1	0	163		0.0
	1190.2	2.1	172	15	1190.2	2.1	0	72		-2.5
*	1200.0	0.0	-12	14	1200.0	0.0	0	66		
*	1205.8	0.0	21	11	1205.8	0.0	0	54		0.0
	1213.0	0.0	672	58	1212.9	0.6	654	94	-0.2	-0.1
*	1224.8	0.0	3	10	1224.8	0.0	0	51		0.0
	1233.8	0.0	2343	22	1233.7	0.6	2414	119	0.6	0.7
	1249.9	0.0	554	81	1249.7	0.6	641	107	0.7	0.2
*	1261.2	0.0	19	12	1261.2	0.0	0	57		0.0
	1274.6	0.0	24248	244	1274.3	0.6	24382	204	0.4	0.1
*	1281.9	0.0	70	29	1281.9	0.0	0	139		0.0
	1292.6	0.1	185	78	1292.8	0.6	233	91	0.4	0.1
	1299.2	0.0	773	38	1299.0	0.6	757	87	-0.2	-0.1
	1334.6	0.2	92	63	1334.6	0.2	0	308		-0.3

	1342.4	2.9	350	15	1342.3	0.6	313	93	-0.4	-0.5
	1352.5	3.2	164	16	1352.5	3.2	0	78		-2.2
	1362.9	0.0	26	19	1362.9	0.0	0	93		-0.3
	1367.9	0.0	25	17	1367.9	0.0	0	80		-0.3
	1371.6	0.0	74	34	1371.6	0.0	0	167		-0.5
*	1397.6	0.0	30	19	1397.6	0.0	0	93		0.0
	1407.6	5.4	21996	55	1407.7	0.6	21985	250	-0.0	-0.0
	1434.0	0.0	979	52	1434.0	0.0	0	255		-4.1
	1457.7	0.0	1089	55	1457.7	0.0	0	265		-4.4
	1476.0	3.1	587	16	1476.0	3.1	0	76		-8.2
*	1486.0	0.1	190	22	1486.0	0.1	0	106		0.0
*	1488.4	0.3	41	10	1488.4	0.3	0	49		0.0
	1528.8	6.2	3747	45	1528.8	6.2	0	220		-18.0
*	1549.8	0.0	10	8	1549.8	0.0	0	40		0.0
*	1558.0	0.0	15	8	1558.0	0.0	0	39		0.0
	1579.6	0.1	163	33	1579.6	0.1	0	160		-1.1
	1596.6	0.3	53	60	1596.6	0.3	0	293		-0.2
	1643.6	0.0	712	31	1643.6	0.0	0	149		-5.1
	1649.9	0.1	124	16	1649.9	0.1	0	77		-1.7
*	1682.9	0.0	0	7	1682.9	0.0	0	35		0.0
*	1686.6	0.0	9	7	1686.6	0.0	0	34		0.0
	1719.5	0.4	35	35	1719.5	0.4	0	168		-0.2
	1785.9	7.9	16623	61	1785.9	7.9	0	294		-59.8
*	1853.6	0.2	104	19	1853.6	0.2	0	91		0.0
*	1855.9	0.2	44	10	1855.9	0.2	0	49		0.0
*	1864.5	0.0	35	7	1864.5	0.0	0	33		0.0
	1878.8	0.2	13	12	1878.8	0.2	0	59		-0.2
*	1896.3	0.0	10	5	1896.3	0.0	0	25		0.0
*	2003.0	0.0	4	5	2003.0	0.0	0	23		0.0
*	2006.3	0.0	9	5	2006.3	0.0	0	23		0.0
*	2159.4	0.0	0	3	2159.4	0.0	0	17		0.0
*	2206.9	0.0	1	3	2206.9	0.0	0	14		0.0
*	2261.9	0.0	6	3	2261.9	0.0	0	14		0.0
	2297.4	0.0	4062	26	2297.4	0.0	0	128		-33.6
*	2325.7	0.0	3	2	2325.7	0.0	0	7		0.0
*	2391.0	0.0	1	1	2391.0	0.0	0	6		0.0
*	2570.6	0.0	1	1	2570.6	0.0	0	5		0.0
*	2574.7	0.0	2	1	2574.7	0.0	0	5		0.0
*	2592.1	0.0	1	1	2592.1	0.0	0	5		0.0
*	2597.1	0.0	1	1	2597.1	0.0	0	5		0.0
*	2616.5	0.0	4	1	2616.5	0.0	0	6		0.0
*	2699.7	0.0	-0	1	2699.7	0.0	0	4		
*	2723.7	0.0	0	1	2723.7	0.0	0	5		0.0
*	2756.8	0.0	1	1	2756.8	0.0	0	5		0.0
*	2822.0	1.0	20865	31	2822.0	1.0	0	150		0.0
*	2876.8	0.0	2	1	2876.8	0.0	0	6		0.0

```
COMPARISON RESULTS FOR COMBIREF.TXT AND ARRI.TXT

TRUE MATCHES
    Number of matches for high peaks: 12
      related chisqr for areas and reported uncertainty:  0.5 *
      and for reported areas with reference uncertainty:  0.3 *
    Number of matches for small peaks on high continuum: 22
      related chisqr for areas and reported uncertainty:  0.2 *
      and for reported areas with reference uncertainty:  0.1 *
    Number of matches for small peaks on low continuum: 0
  Number of non-511 matches all together: 34
    related chisqr for areas and reported uncertainty:  0.3 *
    and for reported areas with reference uncertainty:  0.2 *
    and the chisqr for their positions:   0.1 *

FITTING THE 511 keV PEAK
  Number of peaks found there: 1
    related chisqr:                    0.7

MISSES AND FALSE HITS
```

```
  Number of misses: 44
    related chisqr:                   101.1 *
  Number of false hits: 0


TOTALS
  Number of considered peaks (ex 511): 78
    related chisqr for areas:         57.9 *


CONSTANTS USED:
  Second spectrum was counted 20.0 times shorter than the first.
  Threshold energy: 100.00 keV.
  Criteria for energy matching:
     E1 - E2  <  2 * sqrt(sqr(dE1) + sqr(dE2)) or
              <  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.
```