APPENDIX C: CALCULATION OF TOTAL ANALYTICAL UNCERTAINTY

ASSAY RESULTS

In this sheet the results of two or three Assays are entered. Calibration dates are entered so Assays having the same calibration uncertainty may be treated correctly. (Assays having a common calibration share the same calibration uncertainty.)

Enter the results for up to three separate assays in chronological order below.

ASSAY 1

500 = estimated concentration
0.005 = 95% uncertainty (expressed as percentage of estimated concentration)
0.5 = portion of 95% uncertainty2 due to calibration
35551 = date of prior calibration

ASSAY 2

500 = estimated concentration
0.005 = 95% uncertainty (expressed as percentage of estimated concentration)
0.5 = portion of 95% uncertainty2 due to calibration
35582 = date of prior calibration

ASSAY 3 (if applicable)

500 = estimated concentration
0.005 = 95% uncertainty (expressed as percentage of estimated concentration)
0.5 = portion of 95% uncertainty2 due to calibration
35582 = date of prior calibration

Number of different calibrations represented by the above data:
N = 2 (If this value seems to be incorrect, check the dates entered for the three assays. The earliest data should be for Assay 1. Trailing spaces may cause N's formula to interpret identical dates as different.)

COMPARISONS

			Upper Confidence Limits			Variance Components	
Calibration	Assay	Lower Confidence Limits	Assay 1 502.5	Assay 2 502.5	Assay 3 502.5	Calibration	Imprecision
1	1	497.5	---	True	True	3.125	3.125
2	2	497.5	True	---	True	3.125	3.125
2	3	497.5	True	True	---	3.125	3.125

"FALSE" indicates an inconsistency such as an upper confidence limit for one assay that is lower than a lower confidence limit for another (non-overlapping intervals). "FALSE" will appear for Assay 3 if no data have been entered for Assay 3.

OVERALL ESTIMATE

Note: Calibration Case = 15

Case		Cal. No.	Cal. No.	Cal. No.
4*	=	1	1	---
6*	=	1	2	---
9	=	1	1	1
12	=	1	1	2
15	=	1	2	2
18	=	1	2	3

*4 and 6 are cases where there is no 3rd assay. In case 4, the two assays share a common calibration. In case 6, the two assays have different calibrations.

The standard error of the estimate produced in an assay is equal to approximately ½ of the "95% uncertainty." The inverse of the square of the standard error is the (raw) weighting factor used in producing an overall estimate of the concentration. The raw weights are adjusted (Adj. Wt.) so their sum is 1.00.

Calibration	Estimate	95% Uncert.	Raw Wt.	Adj. Wt.	Wt. *Conc.	Variance of Wt. *Est.
1	500	0.005	40000	0.4285714	214.28571	1.1479592

2	500	0.0043301	53333.333	0.5714286	285.71429	1.5306122
			0	0	0	0

500 = overall estimate of the candidate standard's concentration
1.6366342 = 95% uncertainty (concentration units)
0.0032733 = 95% relative uncertainty

The standard error and 95% uncertainty displayed above do not account for uncertainty in the reference standards used to calibrate the analytical instrument. In the space below, enter the 95% uncertainty (typically 2 times the standard error) of the reference standards. If different calibration standards had different uncertainties, enter the largest.

Example: If NIST SRMs were used in the calibration and their certified concentrations were 100 +/- 1 ppm, 200 +/- 1 ppm, 300 +/- 2 ppm, 400 +/- 3 ppm and 500 +/- 4 ppm, then the largest 95% uncertainty is for the 100 ppm standard: 1/100 = 0.01 or 1%. (SRM uncertainties are expressed as two-sigma limits which are 95% confidence intervals.)

0.005 = 95% uncertainty (2 times the standard error) of the reference standard

0.0059761 = 95% uncertainty of the candidate standard (including the contribution of the reference standard)