

# Los Alamos National Laboratory

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APR 4 1995

Date:  
Refer to: EM/ER:95-126

Ms. Barbara Driscoll  
RCRA Permit Branch  
US Environmental Protection Agency, Region 6  
1445 Ross Ave., Suite 1200  
Dallas, TX 75202-2733

Dear Ms. Driscoll:

**SUBJECT: STATISTICAL COMPARISONS TO BACKGROUND: PART 1**

Enclosed for your approval is the final version of the Los Alamos National Laboratory Environmental Restoration (ER) Assessment Council's position paper entitled, "Statistical Comparisons to Background: Part 1," dated March 28, 1995. This document now incorporates all comments received including your comments received during the March 2, 1995 phone call between you, Maria Martinez, Alison Dorries, and Randy Ryti. With your approval of this document, we will distribute the paper to ER personnel and adopt it as an ER policy.

If you have any questions regarding this document, please call Alison Dorries at (505) 665-4791. Thank you.

Sincerely,

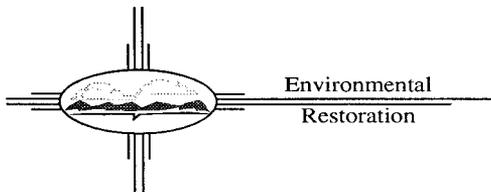
Jorg Jansen, Project Manager  
Environmental Restoration

JJ/TT/bp

Sincerely,

Theodore J. Taylor, Program Manager  
Los Alamos Area Office

Enclosure: Statistical Comparisons to Background: Part 1



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**DRAFT**

**Statistical Comparisons to Background**

**Part I**

**Los Alamos National Laboratory**

**Environmental Restoration Project  
Assessments Council**

**March 28, 1995**

## **INTRODUCTION**

The main purpose of this policy is to provide guidance to the Los Alamos National Laboratory (the Laboratory) Environmental Restoration (ER) personnel on recommended statistical comparisons between Potential Release Site (PRS) data and naturally occurring concentrations of metals (including radionuclides) in soils. Any background comparison approach consists of two components. The first is to assemble a defensible set of background data. This document describes comparisons to the Laboratory wide set of background data collected by Longmire (Longmire et al. 1994, 1142). The second is the selection of the statistical method(s) used to compare site data to background data. Two statistical methods are presented. In the first method, site concentration data are compared with a statistic representing the upper percentile of background concentrations, the upper tolerance limit (UTL). The UTL is used as a screening value, or extreme (hot) value, to determine if a significant release has occurred at the site. The second is a group of methods designed to detect a distributional shift between site data and background data. Although guidelines for the application of these methods are presented in this document, each data analysis report should briefly describe the statistical analysis method chosen and justify its application to the data in question. In PRS data, particular attention should be paid to background comparisons of beryllium and arsenic, because background concentrations of these elements exceed risk-based screening action values. Each data analysis report should also justify the use of Laboratory-wide background concentration data, or present the rationale for using site-specific background concentration data.

Comparisons of PRS data with background concentrations are needed as part of the Resource Conservation and Recovery Act (RCRA) corrective action process. The guidance on statistical comparisons between PRS data and naturally occurring concentrations of metals (including radionuclides) in soils provided by this document may also be applicable to background comparisons of certain anthropogenic compounds (e.g., radionuclides distributed from nuclear fallout or organic chemicals associated with urban activities). It should be emphasized that the approach presented in this document should be applied to naturally-occurring metals only.

## **REGULATORY LITERATURE REVIEW**

The Environmental Protection Agency (EPA) guidance documents supporting the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) and RCRA

programs provide specific information on how to design background studies and how to statistically compare site data with background data.

The CERCLA document, *Guidance on Data Useability in Risk Assessment (Part A)* (EPA 1992, 1166), recommends collecting background data prior to collecting site data. If the comparison of background data with site-derived data for a given constituent does not show a difference statistically, that constituent is eliminated from further analyses. The CERCLA guidance also suggests basing the number of background samples collected from a site on the "minimum detectable difference" procedure (EPA 1989, 0303). Data analysts unfamiliar with this approach should contact the statistical specialists designated by the Assessments Council Chair.

Background comparisons for groundwater monitoring data are addressed in the RCRA document, *The RFI Guidance* (EPA 1989, 0088). Methods for comparing data derived from upgradient wells with data from downgradient wells is presented in the RCRA groundwater statistical analysis document (EPA 1989, 1141), referenced in the EPA RCRA facility investigation (RFI) guidance (EPA 1989, 0088). These statistical methods are codified in 40 CFR Part 264, *Statistical Methods for Evaluating Ground-Water Monitoring from Hazardous Waste Facilities: Final Rule* Federal Register Tues. Oct. 11, 1988.

Statistical methods used for background comparisons of groundwater can be applied to background comparisons for data from other media as stated in the preface of EPA (1989, 1141):

**"This scenario can be applied to other non-RCRA situations involving the same spatial relationships and the same null hypothesis. The explicit null hypothesis for testing contrasts between means, or where appropriate between medians, is that the means between groups (here monitoring wells) are equal (i.e., no release has been detected), or that the group means are below a prespecified action level (e.g., the ground-water protection standard). Statistical methods that can be used to evaluate these conditions are described in Section 5.2 (Analysis of Variance), 5.3 (Tolerance Intervals), and 5.4 (Prediction Intervals)." Bold added for emphasis.**

The RCRA groundwater monitoring guidance suggests that the specific approach proposed by the owner/operator should be submitted to EPA for approval, especially where methods other than those presented in the guidance are used. Statistical methods presented below are consistent with those found in the analysis of variance and tolerance interval sections of the RCRA groundwater monitoring document (EPA 1989, 1141).

## **BACKGROUND COMPARISON APPROACHES AT OTHER DOE FACILITIES**

Based on information presented at the 1994 Technical Information Exchange (TIE) Workshop, most DOE facilities have funded a facility-wide background analysis of all potentially impacted media (soil, sediment, surface water, groundwater). Most have information on the soil horizon or other data that support a site-specific comparison with background. No single statistical test for comparing site data with background data is used throughout the DOE facilities studied.

Background comparison approaches at specific facilities include:

- 1) Hanford Site (Richland, WA): a background conceptual model has been developed. This model includes metals (including certain radionuclides) and considers transport between soil, sediment, surface water and groundwater.
- 2) Oak Ridge Reservation (Oak Ridge, TN): a statistically significant difference between site data and background data is required before including the constituent in a risk assessment.
- 3) Sandia National Laboratories (Albuquerque, NM): upper tolerance limits (UTL) of metals and radionuclides are calculated based on historical data collected within and outside of PRSs. UTL calculations are made if there is an adequate number of "detects" reported by the analytical laboratory. The UTL is calculated using a method dependent on the distributional properties of the analyte.

## **LABORATORY BACKGROUND DATA**

The strategy at the Laboratory has been to collect samples that are representative of Laboratory-wide background metal concentrations in soil and tuff (see Longmire et al. 1994, 1142) for comparison with PRS data. (Readers interested in more detail on the statistical distribution of naturally-occurring metals are referred to the Appendix of this paper.) Longmire's data, representing Laboratory-wide variation in soil and volcanic tuff, are used as the default background data for making comparisons in the initial RFI screening assessment process. The Laboratory-wide background data were collected from sites representing the range of soil conditions observed at the Laboratory. At present, Longmire has 47 soil samples (A, B or C soil horizon) analyzed by EPA SW 846 methods, and 50 soil (A, B or C soil horizon) and 38 tuff samples analyzed by Instrumental Neutron Activation Analysis (INAA). The INAA data represent

total elemental concentrations and are useful for background comparisons only at selected PRSs with data using a comparable method of analysis. Additional soil, sediment and volcanic tuff background analyses will be added to the Laboratory-wide background data base during 1995. The new data will be made available to ER Project personnel and other interested parties as soon as validated data are received.

Variation in certain elements makes comparisons with Laboratory-wide background less valid than comparisons with site-specific background concentrations. For example, due to natural variability in element concentrations of Bandelier Tuff, background soils from Technical Areas (TAs) at the east and west ends of the Laboratory are likely to be enriched, or depleted, in certain elements relative to Laboratory-wide background values. Bandelier Tuff was derived from a zoned magma chamber in which some elements were concentrated at the top and others were concentrated at the bottom. During the eruption resulting in deposition of the Bandelier Tuff, magmas at the top of the chamber were erupted first. Consequently, those elements that were concentrated in the upper magmas are in higher abundance at TAs to the east of the Laboratory because the Bandelier Tuff subunit exposed in that region represents the earlier-erupted magmas. Thus, soils derived from tuff located to the east of the Laboratory are likely to have higher abundance of certain elements than Laboratory-wide background soils. For example, at TA-33 uranium in background soils is at higher levels than Laboratory-wide background because it is more abundant in the stratigraphically lowest units of the Tschirege Member of the Bandelier Tuff. Thus, it is important to develop site-specific background for some sites.

All users of background data must follow some simple guidelines to ensure that site data is being compared with Laboratory background data in a scientifically valid manner. A primary requirement is that PRS data and background data be collected from soil or tuff having the same physical properties. If PRS data are collected from sediments, background data should also come from sediments. For example, if site data were collected exclusively from a soil horizon naturally enriched in a metal, these data would appear to be greater than Laboratory background data. A second requirement is that PRS samples be assayed by the same analytical methods as used for background samples.

Each data analysis report should demonstrate that the above guidelines were considered before using Laboratory-wide background distributions. Failure to meet these guidelines may be an indication that site-specific background be collected or that a subset of Laboratory-wide background data be compared with PRS data. Lack of data for a particular analyte could be justification for the collection of site-specific background data. Before recommending the

collection of site-specific background for an analyte, data analysts should confirm whether the analyte in question could be present by looking at historical information. On the other hand, lack of defensible historical information might justify the collection of site-specific background data.

Should site-specific background data seem warranted, data analysts are encouraged to seek technical advice from the background specialists designated by the Laboratory ER Project Assessments and Earth Sciences Council Chairs. These specialists will be able to provide detailed guidance on the location and number of samples required for site-specific background comparisons.

## **PROPOSED STATISTICAL METHODS**

Because background comparisons are used to make decisions throughout the RCRA process from site screening to corrective measures implementation, data analysts must have statistical methods that can be applied over a broad range of decisions. This guidance defines two statistical methods for background comparisons. Both methods meet the requirements for RCRA decision-making. In the first method, the "hot measurement" test, site concentration data are compared with a statistic representing the upper percentile of background concentrations. In the second method, the "distributional shift test," the mean of site data is compared with the mean of background data to determine if the former is statistically greater than the latter. Used together, or separately, these tests help demonstrate if a release at a PRS occurred, and help define what risk consequence the release may have. Figure 1 illustrates the differences between site data and background data detected by the two methods.

The decision to be supported by the background comparison determines which test is more appropriate. In an initial RFI screening, when a single high value should trigger further analysis, the hot measurement test is typically more appropriate. When extensive data are collected to support a risk assessment and a change in the average concentration should lead to further action at the site, the distributional shift test may be more appropriate. A data analysis report should clearly indicate the rationale for selecting a statistical method that differs from those presented in this guidance document.

It is emphasized that the level of effort spent in evaluating potential differences between PRS data and background data should be related to the site-specific information available. For example, if historical information indicates that beryllium was released at a firing site, the potential

differences between the beryllium concentration data at the firing site and Laboratory or site-specific background data should be carefully evaluated and presented in the data analysis report.

## COMMON DATA ANALYSIS PROCEDURES

Because certain methods depend on the statistical distributions of site and background data, analysts are encouraged to prepare graphical data displays to facilitate the communication of the results of data comparisons. Box plots (see Figure 1), in which background data and site data can be compared side-by-side, are most useful. Analysts should also consider using histograms and probability plots. These graphs provide tangible evidence of the similarity or differences between site data and background data.

## HOT MEASUREMENT TEST

The hot measurement test defines a threshold value that represents high background concentrations. No matter what parameters are chosen to define the threshold, there exists a probability that a background measurement will exceed the hot measurement threshold. The frequency of false positive results is minimized by using a threshold statistically related to higher background concentrations. The confidence limit on a percentile of the distribution, termed the tolerance limit, is such a value, and is one of the background comparison methods recommended by EPA (1989, 1141). The Laboratory has selected the 99th percentile for calculating the upper tolerance limit, based on the general guidance in the RCRA groundwater document. If the underlying distributional model is correct, the upper tolerance limit based on the 99th percentile is rarely exceeded. EPA recommends calculating an upper 95% confidence limit for the target percentile (EPA 1989, 1141). The Upper Tolerance Limit (UTL) for the 99th percentile at 95% confidence can be calculated using Equation (1).

$$UTL_{0.99,0.95} = \text{mean} + \text{standard deviation} * k_{0.99,0.95} \quad (1)$$

The "k-factor" depends on the number of background samples, and complete tables of k-factors are published in EPA (1989, 1141) and Gilbert (1987, 0312). Table 1 presents k-factors selected to represent the range of values used to compute UTLs for Laboratory background soil samples. To apply Equation (1), the background data must be normally distributed or transformed to normality (e.g., by using log-transformation). If data deviates sufficiently from normality, nonparametric methods for calculating tolerance limits should be considered (e.g., as described in

Gilbert [1987, 0312]). Alternatively, when appropriate, the data analyst may trim outliers from the distribution and calculate the UTL based on the trimmed mean and standard deviation.

The Laboratory soil background data were used to calculate the UTL values presented in Table 2. As discussed in section 4.0, use of the default is emphasized, or Laboratory-wide background data should be justified for the specific background comparison being performed. Table 2 UTL values should not be used without considering the guidelines discussed in section 4.0. A minimalist approach to data preparation was used for the initial UTL calculations. Because some soil concentration data were sufficiently skewed, a log-transformation was applied to improve the fit of these data to a normal distribution. (Readers interested in the details of these data distributions are referred to the Appendix of this policy paper.) The UTLs calculated for the lognormal distribution were backtransformed into original units to simplify comparisons with site data. No values were trimmed from the distributions used to calculate the mean and standard deviation. If four or fewer non-detects were reported for an analyte, values below the laboratory detection limit were replaced by one-half of the detection limit (EPA 1989, 1141). The UTL was not calculated for any analyte having more than four non-detect values (>10% non-detects).

The observed maximum concentration in the background data is an alternative to using the UTL as the hot measurement threshold. However, when few background samples are available, using the maximum will result in an underestimation of the upper background percentile. In general, the sample maximum (for "n" samples) is an estimate of the  $\left[ \frac{n-0.5}{n} \right]$ th percentile. Thus, if 10 samples are collected, the sample maximum is an estimate of the 95% percentile. As more Laboratory-wide background data become available, the maximum value will increase, but the UTL will typically not change. Because the maximum is extremely sensitive to background sample size, it is not recommended for use as a hot measurement threshold. Rarely detected analytes, which include: antimony, cadmium, mercury, selenium and thallium, are an exception to this general recommendation. For this limited subset of rarely detected analytes, the maximum detected background concentration can be used as the hot measurement threshold.

Exceeding the UTL does not prove that a release occurred at a PRS. Assuming the PRS is at background and the statistical model is correct, there is a 1% probability that the 99th percentile will be exceeded by each sample collected from the PRS. Furthermore, a typical metals suite requires comparison of 23 analytes to background. If the concentrations of the 23 metal analytes vary independently, the 1% probability that each PRS sample exceeds the 99th percentile increases to a 21% probability that at least one of the 23-99th percentiles will be exceeded in a

single sample. Additionally, given that the probability values for these multiple comparisons have not been adjusted, the overall level of confidence for 23 analytes will be substantially less than 95%. Consequently, the results of a hot measurement test must be carefully evaluated. The possibility of exceeding a UTL due to an unusual, but naturally occurring, soil matrix is a further consideration.

The results of the UTL comparison should also be evaluated relative to potential human health or ecological screening levels. Some analytes, arsenic and beryllium in particular, represent a special case. Because background levels at the Laboratory exceed risk-based screening levels, no screening action levels (SALs) for beryllium or arsenic have been calculated for the Laboratory ER Program. Seven metals (antimony, barium, chromium, lead, manganese, thallium, and vanadium) and one radionuclide (thorium-232) have background UTLs that appear close to their SAL values. The UTLs of this group represent a significant fraction of the SAL (8 to 50%). If, in a comparison similar to a multiple constituent test, each of these metals had a concentration equal to the SAL, the total of the metal UTLs divided by the corresponding SAL (in effect normalizing the UTL to SAL ratio) would equal 89%. Thus, the concentrations of most naturally-occurring metals are significantly lower than their respective SALs.

Both the multiple constituent evaluation and the UTL-to-SAL comparison will help determine what level of effort should be expended to evaluate deviations from background. For most naturally-occurring metals, when only a single statistical comparison to background is performed, the UTL will be adequate because probability levels are not compromised. Under this circumstance, the UTL is the simplest comparison and is functionally most similar to comparisons of site data to target risk levels or SALs.

### **DISTRIBUTIONAL SHIFT TEST**

The distributional shift test is used to determine if site data are systematically greater than background data. Several types of distributional shift tests are available. The Student t-test is a parametric, statistical, two-sample test that determines whether the mean concentration of site data is statistically greater than the mean concentration of background data. The Wilcoxon rank-sum test is the nonparametric equivalent to the t-test (Gilbert 1987, 0312; Gilbert and Simpson 1992, 0974). The Wilcoxon test pools site and background data into one aggregate set and determines if the average rank of site data is greater than that of the background data. The Wilcoxon test is recommended when site data consists of few samples or when non-detects are frequent. Another useful distributional shift test is the Quantile test (Gilbert and Simpson 1992,

0974). This test, which compares the upper quantile (e.g., 25%) of background data with that of PRS data, is more capable of detecting a difference when only a small number of PRS concentrations are elevated. The Quantile test is the most useful distributional shift test for PRSs at which samples from a release represent a small fraction of the overall data collected at the PRS because it does not artificially reduce statistical significance. For example, to detect contamination from historical spills at unknown locations, an RFI work plan may call for samples to be collected from a grid. Most sample results show no contamination, but those in or near spill locations show elevated concentrations.

Use of the distributional shift test is dependent on the number of samples available for comparison. In general, at least 10 sample concentrations for comparison with background data are needed to provide adequate confidence for detecting a shift. Frequently, in RFI Phase I, inadequate numbers of samples are collected to warrant a distributional shift comparison.

To infer a significant result in a distributional shift test, a 95% confidence level is recommended. Given that multiple comparisons will be performed with the distributional shift test, the same statistical interpretation issues cited above for the hot measurement test are also present. In addition, the human health and ecological consequences of a PRS concentration data above background must be considered along with differences in metal concentrations between soil horizons. In particular, multiple comparison tests with SALs must be performed and ecological SAL comparisons must be made.

**REFERENCES**

EPA (US Environmental Protection Agency) 1989. "Ecological Assessment of Hazardous Waste Sites: A Field and Laboratory Reference," EPA/600 3-89/013, Environmental Research Laboratory, Corvallis, OR. (EPA 1989, 0303)

EPA (US Environmental Protection Agency) 1989. "Interim Final RCRA Facility Investigation (RFI) Guidance, Volume I of IV, Development of an RFI Work Plan and General Considerations for RCRA Facility Investigations," EPA/530-SW-89-031, OSWER General Directive 9502.00-6D, Office of Solid Waste, Washington, DC. (EPA 1989, 0088)

EPA (US Environmental Protection Agency) 1989. "Statistical Analysis of Ground-Water Monitoring Data at RCRA Facilities. Interim Final Guidance," Office of Solid Waste, Waste Management Division, US Environmental Protection Agency, Washington DC. April 1989. (EPA 1989, 1141)

EPA (US Environmental Protection Agency) 1992. "Guidance for Data Useability in Risk Assessment (Part A)," Office of Emergency Remedial Response, US Environmental Protection Agency, Washington DC. April 1992. (EPA 1992, 1166)

Gilbert, R.O. 1987. Statistical Methods for Environmental Pollution Monitoring. Von Nostrand Reinhold Company Inc. New York. 320 pp. (Gilbert 1987, 0312)

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Longmire, P., S. Reneau, P. Watt, J. Gardner, and C. Duffy. 1994. Geomorphology, Pedogenesis, and Geochemistry of Background Bandelier Tuff and Selected Soil Profiles, Los Alamos, New Mexico, 1994. (Longmire et al. 1994, 1142)

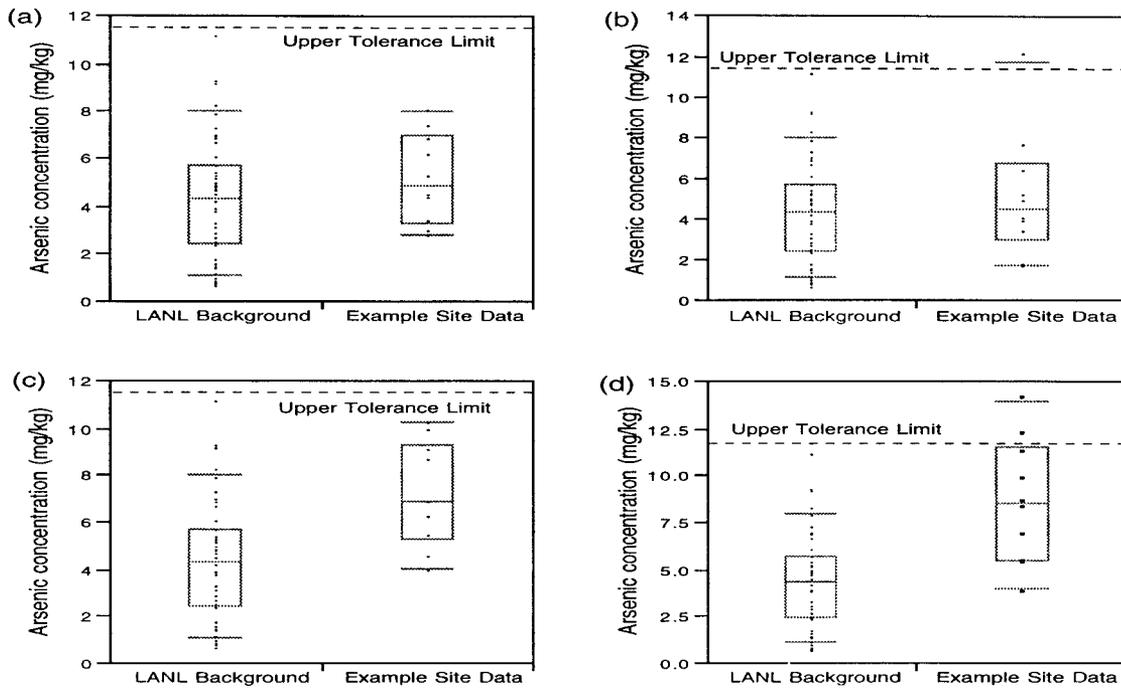


Figure 1. Box plot comparisons of example site data to Laboratory background data.

- (a) Site data are within the range of background: no distributional shift or hot measurements (i.e., values greater than the UTL).
- (b) Site data fail hot measurement test: one of 11 site arsenic concentration values exceeds the UTL of 11.6 mg/kg.
- (c) Site data show a distributional shift: the Wilcoxon rank sum test shows that site data tends to be greater than the background data.
- (d) Site data show a distributional shift and fail the hot measurement test: two of 10 site arsenic concentrations exceed the UTL of 11.6 mg/kg and the site data tend to be greater than the background data.

Table 1 - Selected "k-factors" used to calculate UTLs (\* reprinted from Gilbert 1987, 0312).

<b>Number of background samples</b>	<b><math>k_{0.99,0.95}</math></b>
45	2.897 *
46	2.8902
47	2.8834
48	2.8766
49	2.8698
50	2.863 *

Table 2 - List of UTLs for LABORATORY soil background data.

Analyte	SAL (mg/kg)	Mean (mg/kg)	Standard deviation (mg/kg)	UTL <sub>99%,0.95</sub> (mg/kg)	N	N > DL *
Aluminum (LT)		19000	13800	123000	47	47
Antimony	32	2.45	0.36	2.5 (MAX)	46	2
Arsenic		4.4	2.5	11.6	46	46
Barium (LT)	5,600	161	129	1140	47	47
Beryllium		1.15	0.75	3.31	47	47
Cadmium	80	0.39	0.54	2.7 (MAX)	47	5
Calcium (LT)		5790	12500	54400	47	47
Chromium (Total) †		11.7	7.8	34.2	47	47
Cobalt (LT)		15.2	7.6	51.1	47	47
Copper	3,000	5.3	3.6	15.7	47	45
Iron		14500	7320	35600	47	47
Lead	400	15.0	8.3	39.0	47	44
Magnesium (LT)		2920	2150	16100	47	47
Manganese	11,000	343	238	1030	47	47
Mercury	24	0.05	0.01	0.1 (MAX)	48	4
Molybdenum	400	NA	NA	NA	NA	NA
Nickel	1,600	9.7	5.9	26.7	47	45
Potassium		2420	1304	6180	47	47
Selenium	400	0.43	0.41	1.7 (MAX)	46	23
Silver	400	NA	NA	NA	NA	NA
Sodium (LT)		577	453	3320	47	47
Strontium	48,000	NA	NA	NA	NA	NA
Thallium	6.4	0.27	0.24	0.9 (MAX)	45	21
Vanadium	560	25	14	66	47	47
Zinc	24,000	41	21	101	47	47
<sup>40</sup> Potassium (1)		21.6	5.07	36.1	50	50
<sup>232</sup> Thorium (1)	5	1.71	0.34	2.68	50	50
<sup>234</sup> Uranium (1)	86	1.21	0.29	2.03	50	50
<sup>235</sup> Uranium (1)	18	0.052	0.012	0.088	50	50
<sup>238</sup> Uranium (1)	59	1.14	0.27	1.90	50	50

\* Concentration values < detection limit (DL) were replaced by 1/2 of the DL

† - SAL for Chromium-III is 80,000 mg/kg and for Chromium-VI is 400 mg/kg

LT - UTL is based on log transformed data

NA - data not available for Laboratory background

MAX - Maximum value is reported, rather than the UTL

(1) - Data are converted from elemental concentrations reported in the Laboratory background report. Units are in pCi/g.