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Draft Final 2021 Unreclaimed Sites Investigation: XRF to Laboratory Correlation and Regression Analyses Procedure

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May 16, 2022

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RE: Draft Final 2021 Unreclaimed Sites Investigation: XRF to Laboratory Correlation and Regression Analyses Procedure

Agency Representatives:

I am writing to you on behalf of Atlantic Richfield Company to submit the 2021 Unreclaimed Sites Investigation: XRF to Laboratory Correlation and Regression Analyses Procedure. As described in the BPSOU Unreclaimed Sites Quality Assurance Project Plan (QAPP), XRF results and analytical laboratory sample results were compared to evaluate the relative strength of the relationship between the XRF and laboratory concentration results. The strength of the linear relationship between XRF and analytical data was evaluated to confirm whether the range of plus or minus 35% for the XRF results was appropriate to limit decision errors. Results from XRF analysis in this range were near the waste identification and action levels and confirmation analysis through analytical laboratory methods was appropriate.

Upon Agency approval, the memo will be attached to the BPSOU Unreclaimed Sites QAPP for reference.

The Procedure Report may be downloaded at the following link:

https://pioneertechnicalservices.sharepoint.com/:f:/s/submitted/ElGJXtYHP89PksuHmw47u74BLwOrs1XFdEFW0EyvWJA8Aw.

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If you have any questions or comments, please call me at (907) 355-3914.

Sincerely,

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SILVER BOW CREEK/BUTTE AREA NPL SITE
BUTTE PRIORITY SOILS OPERABLE UNIT

Draft Final

2021 Unreclaimed Sites Investigation: XRF to Laboratory Correlation and Regression Analyses Procedure

Atlantic Richfield Company

2022

SILVER BOW CREEK/BUTTE AREA NPL SITE
BUTTE PRIORITY SOILS OPERABLE UNIT

Draft Final

2021 Unreclaimed Sites Investigation: XRF to Laboratory Correlation and Regression Analyses Procedure

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2022

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ABBREVIATIONS AND ACRONYMS

Acronym	Definition	Acronym	Definition
b	y-intercept	**Pioneer**	Pioneer Technical Services, Inc.
BPSOU	Butte Priority Soils Operable Unit	**QAPP**	Quality Assurance Project Plan
CD	Consent Decree	**R**	Correlation Coefficients
COC	Containment of Concern	**R^2**	Coefficient of Determination
DVR	Data Validation Report	**RSS**	Residual Sum of Squares
***f(x)*-value**	Modeled Output	**TSS**	Total Sum of Squares
ICP	Inductively Coupled Plasma	**XRF**	X-Ray Fluorescence
m	Slope	**y-value**	Actual Output
mg/kg	Milligrams per kilogram		

1.0 INTRODUCTION

The BPSOU Consent Decree (CD) (EPA, 2020) defines remedial action construction activities for potential waste located within the Butte Priority Soils Operable Unit (BPSOU). Pioneer Technical Services, Inc. (Pioneer) collected soil samples from 14 Unreclaimed Sites and 112 sample stations during the 2018 and 2021 sampling events to determine the extent of the potential waste. Pioneer analyzed the samples for contaminants of concern (COCs) using an X-ray fluorescence (XRF) analyzer. Samples with XRF concentrations within plus or minus 35% of COC action levels and waste identification criteria were submitted for laboratory analysis. Additional details on the samples selected for XRF and/or laboratory analysis are included in Section 3.6.2.6 of the approved *2021 Final Unreclaimed Sites Quality Assurance Project Plan* (QAPP) (Atlantic Richfield Company, 2021) (referred to herein as the Unreclaimed Sites QAPP).

This report was prepared to evaluate the statistical relationship between XRF and laboratory concentrations for each COC per the requirements in Section 2.3 of the Unreclaimed Sites QAPP. The report will be updated annually to provide a compounding dataset collected under the Unreclaimed Sites QAPP.

2.0 METHODS

The first step in conducting a correlation and regression analysis is to define the purpose and application of the regression model to determine which variables are input variables and which are output variables when setting up the regression analysis. The regression analysis discussed in this report was used to determine if the laboratory concentration for any given XRF concentration was generally greater than or less than the action level concentrations, especially at XRF concentrations near the plus or minus 35% of the action level thresholds defined in the Unreclaimed Sites QAPP (Figure 1 through Figure 5 show the action levels in relation to the XRF and Inductively Coupled Plasma [ICP] data). This required that the XRF concentrations be designated as the input values and the laboratory concentrations be designated as the output values. After collecting additional data, the regression analysis will be updated and used to evaluate the variability in laboratory concentrations with respect to XRF concentrations to determine appropriate action level thresholds. Since the final objective of this analysis will be to determine the possible variations in laboratory concentrations at each XRF concentration, the XRF concentrations were used as input variables, and the ICP concentrations were used as output variables.

Comparing Two Methods

When applying the regression model, in this case a linear model with the format $y = f(x_i) = mx_i + b$, there is an input variable (x-value) and an output variable (*f(x)*-value). When setting up the regression analysis, the variables must be designated as an input variable (x-value) or an output variable (y-value and *f(x)*-value). Therefore, there are two instances when the variables can be designated as input or output variables: first, when conducting the regression analysis, and second, when applying the regression model.

Because there are two instances when the variables can be designated as input or output variables, there are two possible methods to employ when setting up a regression analysis and applying the regression model. These two possible methods are referred to as Method A and Method B. In Method A, the designation of input and output variables during the regression analysis is opposite to that of the final application of the regression model. In Method B, the designation of input and output variables during the regression analysis matches the final application of the regression model. In the analyses described in this document, the regression model application required that the laboratory concentrations be designated the output values. Therefore, in the final application of Method A and Method B, the XRF concentrations were the input values and the ICP concentrations were the output values. The key difference between Method A and Method B is that during the regression analysis, Method A designated the ICP concentrations as the input variables and the XRF concentrations as the output variables. The equation produced by the Method A regression analysis must be solved for the ICP concentration to use the equation in the final application of the regression model. In Method B, the regression model produced during the regression analysis does not need to be transformed and can be applied directly.

Method A

If Method A is used to conduct the regression analysis, the designation of variables must be opposite to that of the application of the regression model. Therefore, when setting up the regression analysis the laboratory concentration is designated as the input variable (x-value) and the XRF concentration as the output variable (y-value and *f(x)*-value). Note that in the following equations the laboratory concentration is denoted as "ICP." To apply the regression model produced by the Method A regression analysis ($XRF_i = f(ICP_i) = m_2 * ICP_i + b_2$) to determine the laboratory concentration at any given XRF concentration, the equation must be solved for the x-value (the laboratory concentrations) so that the regression model input is the XRF concentration, and the regression model output is the laboratory concentration. The revised formula is formatted as follows: $ICP_i = f(XRF_i) = \frac{1}{m_2} * XRF_i - \frac{b_2}{m_2} = m_3 * XRF_i + b_3$.

Method B

In Method B, the designation of input and output variables during the regression analysis matches the final application of the regression model. The formula produced during the Method B regression analysis ($ICP_i = f(XRF_i) = m_1 * XRF_i + b_1$) can be directly applied to adjust the XRF concentrations.

As discussed above, during the regression analysis Method A and Method B do not produce the same regression formulas. Method A produces an equation where the output is the XRF concentration ($XRF_i = m_2 * ICP_i + b_2$) and Method B produces an equation where the output is the laboratory concentration ($ICP_i = m_1 * XRF_i + b_1$). When Method A and Method B are applied, the Method A equation must be adjusted so that the output is the laboratory concentration. Once this adjustment is made, Method A has an equation ($ICP_i = m_3 * XRF_i + b_3$) that can directly compare with the equation from Method B, because both equations have the same output and input variables. The slope and y-intercept from Method A (m_3 and b_3) will not be equal to the slope and y-intercept from Method B (m_1 and b_1). The following sections describe how the regression models are created and why Method A and Method B produce different slope and y-intercept values.

How Regression Models are Created and How it Impacts the Regression Model Fit

When setting up a regression analysis, it is important that the variables are set as input (x-value) or output (y-value) in a way that matches the final application of the linear regression model that will be produced by the regression analysis. If the variables are assigned to axes in a manner that does not reflect the final application of the linear regression model, the final linear regression model will likely not fit the data. To explain why this happens, it is necessary to understand how the linear regression models are created.

Data analysis programs such as Excel Data Analysis ToolPak (used for this analysis) use the method of least squares to determine the slope and y-intercept for a given set of data (Microsoft 2022a and Microsoft 2022b). The formula for the method of least squares determines the slope and y-intercept values that correspond to the lowest Residual Sum of Squares (RSS) value (Montgomery and Runger, 2007). The RSS value is equal to the sum of the residuals, which is the difference between the modeled outputs (*f(x)*-values) and the y-values, squared:

$$RSS = \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$$

Where y_i is the actual y-value that corresponds to the x_i (actual input x-value), $f(x_i)$ is the modeled value of y_i, and n is the upper limit of summation (Montgomery and Runger, 2007). Figure 6 shows a visual representation of how the residuals are determined for each method (i.e., the residuals are equal to the vertical distance between the point and the regression line). The formula used by Excel Data Analysis ToolPak determines the regression coefficients that produce the lowest RSS value. The RSS value represents the unexplained variation between the actual dataset and the regression model. By finding the slope and y-intercept that correspond to the lowest RSS value, programs like Excel Data Analysis ToolPak produce a regression model that fits with the lowest variation between y-values and *f(x)*-values.

The RSS value is also used to evaluate how well the regression model fits with the data. The coefficient of determination (R^2) value is calculated by subtracting the quotient of the unexplained variation, RSS, and the total variation (total sum of squares [TSS]) from 1. The formula for determining R^2 is:

$$R^2 = 1 - \frac{RSS}{TSS} = 1 - \frac{\sum_{i=1}^{n}\left(y_i - f(x_i)\right)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Where y_i is the actual y-value that corresponds to x_i (the input x-value), $f(x_i)$ is the modeled value of y_i, $\bar{y}$ is the average of the y-values, and n is the upper limit of summation (Montgomery and Runger, 2007). A model with an R^2 value of 1 would have an RSS value of 0, meaning there is no unexplained variation between the modeled data and the actual data or, put another way, the actual data points (y-values) match up exactly with the modeled data points (*f(x)*-values). A model with an R^2 value of less than 0 indicates that there is more unexplained variation between

the actual data (y-values) and the model than the total variation in the actual data (*y*-values). In other words, the model does not adequately predict the y-values at each x-value.

Using Method A, Excel Data Analysis ToolPak uses the XRF concentrations to calculate the residuals, produce the regression coefficients (m_2 and b_2), and determine the R^2 value, because the XRF concentrations are set as the y-values and *f(x)*-values. However, when the regression model is applied, the laboratory concentrations are the y-values and *f(x)*-values. It is therefore necessary to recalculate the residuals and the R^2 value using laboratory values to determine how well the regression model with the m_3 and b_3 coefficients fits the data. The bottom left plot on Figure 6 shows how the residuals for Method A change when the equation is flipped from its original version, with the m_2 and b_2 coefficients (where the residuals are XRF concentrations), to the final version, with the m_3 and b_3 coefficients (where the residuals are ICP concentrations). When viewed on a plot set up for the regression analysis, with the XRF concentrations on the y-axis and the laboratory concentrations on the x-axis, the residuals with the m_2 and b_2 coefficients are equal to the vertical distance between the points and the regression line while the residuals with the m_3 and b_3 coefficients are equal to the horizontal distance between the data points and the regression line.

Figure 6 lists the two R^2 values for Method A, which were calculated first with the XRF concentrations, R^2 (XRF) during the regression analysis (using the m_2 and b_2 coefficients), and then with the laboratory concentrations, R^2 (ICP) after application of the regression model (using the m_3 and b_3 coefficients). Note that the R^2 values were calculated using a dataset from a different project (as an example) and an outlier analysis was performed using the same methodology described in Section 3.2.1. The outliers were removed before the R^2 values were calculated. These values are shown as an example of how the R^2 (XRF) and R^2 (ICP) values differ when using Method A. The R^2 (ICP) values are generally less than R^2 (XRF) values when applying Method A. The decrease in R^2 values is to be expected. During the regression analysis, Excel Data Analysis ToolPak selected the regression coefficients using the RSS values calculated using the actual XRF concentrations (y-values) and modeled XRF concentrations (*f(x)*-values). The outliers were selected from the standard residuals which were also calculated with the XRF concentrations. When the regression model is applied and the R^2 values are recalculated with the laboratory concentrations to determine the fit of the model with the m_3 and b_3 coefficients, it is likely that there will be greater unexplained variance between the actual laboratory concentrations (y-values) and the modeled laboratory concentrations (*f(x)*-values). The increase in unexplained variance will result in lower R^2 values. In some instances, the R^2 values can be less than 0, which indicates that the Method A coefficients m_3 and b_3 create more variance between the actual laboratory concentrations (y-values) and modeled laboratory concentrations (*f(x)*-values) than exists within the actual laboratory dataset. Therefore, the regression models produced using the Method A approach do not adequately predict the laboratory concentrations, which is why Method A is not the preferred approach to conducting a regression analysis.

Method A should always produce R^2 (ICP) values that are less than the Method B R^2 (ICP) values. Even when comparing Method A R^2 (XRF) values to the Method B R^2 (ICP) values, Method B will nearly always produce a linear model that is better able to predict the laboratory

concentrations, because the model was created using the variance between the actual laboratory data and the modeled laboratory data.

Using the Residuals to Predict the Range in ICP Concentrations for each XRF Concentration

As defined in the Unreclaimed Sites QAPP, the purpose of collecting soil samples and having them analyzed for COC concentrations is to determine if contaminants are present and, if they are, do the concentrations exceed appropriate action levels. Since the XRF unit allows for instantaneous results, it can be used by the field teams to adjust the location and number of samples in real time to better define waste extents. Since the data will be gathered with the XRF unit in the field, but the laboratory analysis is the preferred method for determining COC concentrations, it is important to know how much laboratory concentrations can vary with each XRF result to reduce the risk of false positive and false negative determinations when comparing the sample concentrations to the action levels. A false positive determination, shown on the lower right section of Figure 7, results in an XRF point that requires remedy, but the laboratory result does not require remedy. A false negative determination, shown on the upper left section of Figure 7, results in an XRF point that does not require remedy, but the laboratory results do require remedy. It is important to minimize false negative and positive points to reduce failing to remediate and over remediating sites.

Figure 7 shows a plot of the XRF and laboratory arsenic concentrations, outlining sections on the plot where XRF concentrations below the -35% of the action level threshold could be classified as passing the action level but would exceed the action level if they were sent for laboratory analysis (false negative section). The figure also shows the section on the plot where XRF concentrations above the +35% of the action level threshold would be classified as failing the action level but would pass if the sample was sent for laboratory analysis (false positive section). The Unreclaimed Sites QAPP set the plus or minus 35% XRF thresholds to reduce the probability of false negatives and false positives by requiring that samples with XRF concentrations less than +35% of the action level and greater than -35% of the action level be sent for laboratory confirmation sampling (confirmation section). The residuals produced in the regression analysis can be used to predict the variability of laboratory concentrations in future XRF samples. That variability can be used to fine tune the XRF concentration thresholds that determine the boundaries of the confirmation section shown on the plot on Figure 7.

The residuals produced in a regression analysis are typically normally distributed, which means that the risk of residuals exceeding a certain value can be determined. The average residual value should be 0, as represented by the regression line shown on the plot on Figure 7. Since the residuals are equal to the magnitude of the vertical distance between each data point and the regression line, the probability that a particular residual will occur can be represented by a parallel line offset from the regression line. The magnitude of the offset is equal to the product of the standard deviation of the residuals and a multiplier that corresponds to a desired probability (z-value). Overlaid on the plot on Figure 7 are lines that show the range of possible ICP concentrations that could occur in future samples based on the distribution of residuals produced by the regression analysis. For example, 95% of ICP concentrations should occur between the upper and lower 95% lines and there is only a 2.5% chance that the ICP concentrations will fall above the upper 95% line.

These probabilities can be used to adjust the XRF thresholds that define the confirmation section shown on Figure 7. For example, if it is determined that the risk of a false negative should not exceed 2.5%, then the XRF concentration at the intersection between the upper 95% line and the Residential Human Health Action Level line can be used as the lower XRF concentration threshold. Since the risk of false positives has fewer negative consequences, it may be determined that 5% or even 12.5% is an acceptable risk of false positives. In this case, the XRF concentration at the intersection between the lower 90% or lower 75% (not shown) lines and the Residential Human Health Action Level line can be used as the upper XRF concentration threshold (Figure 7). Further assessment is needed to determine the XRF concentration thresholds, and that assessment will be completed after additional data are collected and a new regression analysis is created with the additional data.

Since this analysis of using residuals to predict the variability in laboratory concentrations uses the laboratory residuals to predict the variations in laboratory concentrations, it is still important that the regression analysis be completed so that the laboratory concentrations are used to create the regression line. If Method A (Figure 6) is used for regression analysis, the XRF concentrations would be used to determine the slope and y-intercept of the regression line. To determine the variability in ICP concentrations, the modified equation $ICP_i = \frac{1}{m_2} * XRF_i - \frac{b_2}{m_2}$ would be used to compare the modeled laboratory concentrations (*f(x)-values*) to the actual laboratory values (y-values) to determine the laboratory residuals. Because the regression line was created using the XRF concentrations, the laboratory residuals may not have an average of 0, in which case the regression line will no longer represent the average laboratory concentration. Additionally, the laboratory residuals may no longer be normally distributed, which will make determining the probability of occurrence more difficult. In short, Method B (i.e., setting the regression analysis so that the regression output matches the final application output) should be applied when setting up the regression analysis.

3.0 DATA

The Unreclaimed Sites investigations began in October 2018. During the investigation activities conducted in 2018 through 2021, Pioneer analyzed 3,255 XRF data points (arsenic, cadmium, copper, mercury, lead, and zinc data points), 1,131 of which contained paired XRF and laboratory data. The soil samples were analyzed with the XRF unit (results referenced herein as "XRF data") on site or in the Pioneer field office located at 244 Anaconda Road in Butte, Montana. Two units were used for the 2021 Unreclaimed Sites XRF analysis: unit #92951 was used from 6/30/21 to 9/1/21 for 2 Unreclaimed Sites, and unit #98052 was used from 9/1/21 to 11/10/21 for 11 Unreclaimed Sites. Table 1 lists the total number of paired samples used in the analyses and all non-detect XRF results, Table 2 lists how the results were paired, and Table 3 lists the analytical criteria. Soil samples were sent for laboratory analysis, per the action levels and waste identification criteria in Table 3, if exceedances were detected in the XRF data. The samples analyzed with the XRF were sieved with a #10 sieve to remove pieces of aggregate greater than 2 millimeters in diameter. The data used to determine the regression relationship were first validated and deemed usable through Pioneer's data validation process; details about the data validation process are in the specific Data Validation Report (Section 4) for each site.

Paired Dataset

To facilitate the correlation between XRF analysis and laboratory concentrations, a subset of the data collected during the 2018 and 2021 Site Investigations included a "paired" dataset, where composite samples from the same location and depth interval were prepared and split for analysis. One sample was analyzed using XRF and the split sample was submitted for laboratory analysis. Table 1 lists the total number of paired samples used in the correlation and regression analyses and all non-detect XRF results. All paired data points with non-detect XRF results were excluded from the correlation and regression analyses. The 2018 and 2021 site investigation dataset included 787 paired sample results used in the final analysis. Table 2 lists how these results were paired. The XRF-to-laboratory correlation and regression analyses for arsenic, cadmium, copper, lead, and zinc were performed on the paired dataset. Refer to section 3.1 for further information on mercury.

3.1 Correlation Analysis

The paired COC (arsenic, cadmium, copper, lead, mercury, and zinc) datasets from the XRF and laboratory analyses were compared to determine the strength of the relationship between the XRF and laboratory concentration results. The correlations were set so the independent or input value (x-value) was the XRF concentration and the dependent or actual output value (y-value) was the laboratory result, as per the method described in *Field Portable XRF Analysis of Environmental Samples* (Kalnicky and Singhvi, 2001). This method is discussed in Section 2.0.

Correlation coefficients (R) can range from negative 1 (a strong negative linear relationship) to positive 1 (a strong positive linear relationship). A zero value indicates that the relationship is not linear, and a regression analysis would not be recommended for this dataset (Montgomery and Runger, 2007). Generally, an R value of 0.7 and greater or negative 0.7 and less indicates an acceptable correlation, and R values greater than 0.83 and less than negative 0.83 are preferred. However, additional analysis of the correlation is imperative to determine the strength of the linear relationship.

The R values are listed in Table 1. The data used in the analysis are listed in Table 2. The correlation analysis was performed on the paired dataset with detected XRF concentrations for each COC and then again after outliers were removed from the regression analysis to ensure that the modified data still had a linear relationship between the XRF and laboratory concentration results. The paired dataset with detected XRF concentrations for each COC was used to perform the initial correlation analysis. Outliers were then removed from the regression analysis, and the correlation analysis was repeated to ensure a linear relationship was maintained between the XRF and laboratory results from the modified data. Additional discussion related to outlier analysis is provided in Section 2.0. Both R values are shown in Table 1.

It was not possible to complete a correlation and regression analysis for the mercury dataset. Mercury analysis was performed on the samples collected in 2018 and 2021. The paired dataset included 196 samples; 193 of the XRF results were non-detect. Only 3 XRF data points were usable for the regression analysis. It is recommended that at least 10 points of data are available for linear regression analysis. Therefore, there was an inadequate number of mercury samples to complete an accurate and reliable regression analysis.

3.2 Regression Analysis

Regression models are defined by a slope (m) and a y-intercept (b) (referred to collectively as regression coefficients). The regression analysis produces an equation where the y-intercept (b) value is added to the product of the slope (m) and the x-value or input value to produce the modeled output value (*f(x)*). The equation has the following format: $y = f(x_i) = mx_i + b$ (note *i*=1 for all equations in this text). To differentiate between the two y-axis values discussed in this report, references to the actual data will be followed by (y-value) and references to the modeled output values will be followed by (*f(x)*-value).

Once it was determined that the XRF and laboratory concentration results had an acceptable linear relationship from the correlation analysis (Section 3.1), a regression analysis was conducted to produce a linear regression model and a coefficient of determination (R^2). The regression analyses were set so the independent or input value (x-value) was the XRF concentration result, and the dependent or actual output value (y-value) was the laboratory result. This method produces a linear regression model with an equation in the following format: $ICP_i = f(XRF_i) = m_1 * XRF_i + b_1$. This formula readily transforms the XRF concentration to laboratory concentration. Refer to Section 2.0 for details on setting the XRF value on the x-axis and the laboratory on the y-axis. Generally, R^2 values range from 0 to 1 and are used to determine the adequacy of the regression model. The R^2 value can be used loosely to describe how well the regression model accounts for the variability in the data. An R^2 model of 1 indicates a perfect model that accounts for 100% of the variability in the data (Montgomery and Runger, 2007). Generally, an R^2 value of 0.5 is considered acceptable, while an R^2 value of 0.7 and above is preferred. An R^2 value less than 0 indicates that the regression model does not fit the data and cannot predict the variability of the data (refer to Section 2.0). As with the correlation analysis, additional analysis is imperative to determining the adequacy of the regression model.

Table 1 lists a summary of the regression results and Table 2 lists the data used in the analysis. The regression results in Table 1 were produced with the dataset in which the non-detect XRF concentrations and outliers had been removed. The outlier analysis is discussed in Section 3.2.1.

3.2.1 Outlier Analysis

An outlier analysis was performed to remove any pairs of data that were not representative of the population for each COC. As with the correlation and regression analyses, the outlier analysis was completed with the XRF concentrations set as the input value (x-value) and the laboratory concentrations set as the actual output value (y-value). The analysis followed the methods recommended in *Field Portable XRF Analysis of Environmental Samples* (Kalnicky and Singhvi, 2001). The article describes the methods for conducting an XRF analysis of soil and other materials and includes recommendations on conducting an XRF-to-laboratory regression analysis. It recommends that the linear regression model between XRF and laboratory data is "*most meaningful, i.e., the one that omits outliers and retains data bracketing action level concentrations should be used for final evaluation of the XRF data.*"

Kalnicky and Singhvi (2001) recommend plotting the residuals, the differences between the modeled output values and the actual laboratory values, against the XRF concentration values to select outliers. On this plot, the residuals should appear as a random scattering of points around the zero residual line. Points that lie far outside of the group should be removed as outliers. To improve functionality of this method, a slightly different approach was applied, and the residuals were standardized by dividing each residual by the standard deviation of the residuals. Literature suggests that standardized residuals with values greater than 2 (outside of 95% of the population) or 3 (outside of 99.7% of the population) and less than negative 2 or 3 can be considered outliers (Montgomery and Runger, 2007; Penn State, 2018). Based on a review of the outlier summary plots (Figure 1 through Figure 5), using standardized residual threshold boundaries of positive and negative 2 were appropriate for all 5 COCs. Points outside these boundaries were scattered beyond the main clumping of data around the 0-standardized-residual line and were removed from the regression analysis.

For each regression analysis, Excel Data Analysis ToolPak was used to calculate the standardized residuals. Any point with a standardized residual value greater than 2 or less than negative 2 was deemed an outlier and removed from the dataset. The points removed from the dataset are indicated in Table 2. The outlier analysis removed 12 samples from the arsenic regression, 1 from the cadmium regression, 1 from the copper regression, 12 from the lead regression, and 1 from the zinc regression.

4.0 RESULTS AND DISCUSSION

The correlation analysis indicates that arsenic and lead XRF and laboratory concentration values have linear relationships before removing the outliers (R values ranged between 0.95 and 0.96). The strength of that relationship increases after the outliers are removed from the dataset (R values increased to between 0.96 and 0.97). The correlation analysis indicates that the relationship is not as strong before removing the outliers for cadmium, copper, and zinc (R values ranged between 0.22 and 0.59). The strength of the relationship increases after removing the outliers from the dataset (R values ranged between 0.81 and 0.95). The relationships between XRF and laboratory results do not indicate a non-linear (i.e., R value is approximately 0) relationship (Table 1).

The regression analyses indicate that the regression models for arsenic, copper, lead, and zinc adequately explain the variability in the data because the R^2 values for these 4 COCs were greater than 0.7 (Table 1). Even after removing the outliers, the R^2 for cadmium was 0.65; therefore, the regression model for this analysis can only explain approximately two-thirds of the variability in the data. The significance of the cadmium model is further discussed in the Regression Summary sections below.

4.1 Arsenic

Regression Summary

The regression analysis for arsenic indicated that the XRF analysis may overestimate the arsenic concentrations (m = 0.77). An initial offset to the data was indicated by the y-intercept, which is

equal to negative 5.2 milligrams per kilogram (mg/kg) (Table 1). The R^2 value can be interpreted to indicate that the model accounts for approximately 95% of the variability in the data (Table 1).

Figure 1 shows the five plots used to assess the regression analysis. The first plot (upper left-hand corner), *Arsenic XRF to Laboratory Correlation: Entire Data Set with Outliers*, shows the entire dataset, the outliers removed to calculate the regression, and the action levels for Human Health and storm water waste identification criteria. Along the regression lines are paired data points with the XRF/laboratory data.

The second plot (upper middle), *Arsenic XRF to Laboratory Regression View Near Commercial Human Health Action Level*, shows a zoomed-in view of the first plot and shows the points around the action level criteria of 500 mg/kg for commercial land use. The third plot (upper right-hand corner), *Arsenic XRF to Laboratory Regression View Near Storm Water Waste Identification Criteria*, shows a zoomed-in view of the first plot and shows the points around the storm water waste identification criteria of 200 mg/kg. The fifth plot (lower right-hand corner), *Arsenic XRF to Laboratory Regression View Near Residential Human Health Action Level*, shows a zoomed-in view of the first plot and shows the points around the action level criteria 250 mg/kg for residential land use (EPA, 2020). The points are generally densely grouped around the regression line for XRF concentrations ranging from 0 mg/kg to 200 mg/kg. They then are scattered above and below the regression line at higher XRF concentrations (Figure 1). Overall, the regression line provides a good balance between the points scattered above and those scattered below. This is reflected in the high R value (R = 0.97).

Outlier Summary

The fourth plot (lower left-hand corner), *Outlier Summary: Arsenic Standardized Residual Plot*, shows the standardized residuals of the entire dataset with respect to the XRF concentration values and the standardized residual threshold boundaries of positive and negative 2. Points that fall outside the positive and negative 2 standardized residual threshold boundary lines were considered outliers (Figure 1).

Conclusion

Overall, the regression model for arsenic appears to fit the data and falls in the center of the variability in the dataset. The negative y-intercept value indicates where the ICP concentration approaches non-detect or 0 mg/kg, the XRF unit overestimates the COC concentration and on average estimates them to be approximately 6.8 mg/kg. None (0) of the 164 arsenic results were determined to be false negative and 3 of the 164 results were determined to be false positives (0.0% and 1.8%, respectively) from the final regression analysis. Excluded from the count was 1 outlier result, determined to be a false negative, and 3 outlier results, determined to be false positives.

4.2 Cadmium

Regression Summary

The regression model for cadmium was not as strong as the regression models for the other 4 COCs; this may be attributed to fewer usable data pairs as 109 XRF results (58.2%) were non-detect. The correlation analysis indicates that the linear relationship between the XRF and

laboratory concentration results was not as strong as the relationships for the other 4 COCs (R value equaled 0.81 compared to R values ranging from 0.94 to 0.97). Additionally, the R^2 value was 0.65, indicating that the regression model can only account for 65% of the variability in the data (Table 1).

Figure 2 shows the two plots used to assess the regression analysis. The first plot, *Cadmium XRF to Laboratory Regression Entire Data Set with Removed Outliers*, shows the entire dataset, the outlier removed to calculate the regression, and the storm water waste identification criteria. The data points show a generally linear relationship, but there is far too much scattering in the points to indicate a strong linear relationship. The scattering supports the lower strength of the linear relationship and the lower R^2 value.

Outlier Summary

The second plot on Figure 2, *Outlier Summary: Cadmium Standardized Residual Plot*, identifies the outlier above the standardized residual threshold boundary value of 2. The location of the outlier on the first plot reinforces the designation as an outlier as the point sits well above the other points in the dataset (Figure 2).

Conclusion

The slope (m = 0.69) indicates that the regression model found the XRF concentration results to be overestimated. There is a small initial negative offset to the data indicated by the y-intercept equal to negative 4.5 mg/kg. When examining the plot of XRF-to-laboratory results (Figure 2), the regression appears to capture the midpoint of the scattered data. The centroid of the final regression dataset (the outlier was removed), where the XRF value is equal to the average XRF values in the regression dataset (12.4 mg/kg) and the laboratory value is equal to the average laboratory values (4.0 mg/kg), intersects the regression line. The predicted laboratory value (*f(x)*-value) where the XRF value equals 12.4 mg/kg is 4.0 mg/kg. None (0) of the 77 cadmium results were determined to be false negative or false positive (0.0% and 0.0%, respectively). Excluded from the count was 1 outlier result, determined to be a false negative. There were no false positive outlier results.

4.3 Copper

Regression Summary

The slope of the copper regression analysis (m) was 0.88, indicating that XRF analysis may overestimate the copper concentrations. A small initial negative offset to the data was indicated by the y-intercept (b = -28.1) (Table 1). The R^2 value can be interpreted to indicate that the model accounts for approximately 91% of the variability in the data (Table 1).

Figure 3 shows the 3 plots used to assess the regression analysis. The first plot, *Copper XRF to Laboratory Correlation Entire Data Set with Removed Outliers*, shows the entire dataset, with the 1 removed outlier, the storm water waste identification criteria, and the linear regression model. Note that the 1 outlier point has an ICP concentration over 10 times greater than the next highest ICP concentration, but the XRF concentration is just less than the 90^{th} percentile XRF concentration. The second plot, *Copper XRF to Laboratory Correlation View Near Storm Water Waste Identification Criteria*, shows a zoomed-in view of the first plot and shows the points near

the storm water waste identification criteria (1,000 mg/kg). The data points generally follow the regression lines with a few points scattered above and below the linear regression model.

Outlier Summary
The third plot on Figure 3, *Outlier Summary: Copper Standardized Residual Plot*, identifies the outlier above the standardized residual threshold boundary value of 2. The location of the outlier on the third plot reinforces the designation as an outlier as the point sits well above the other points in the dataset (Figure 3).

Conclusion
Overall, the regression model for copper appears to fit the data well and falls through the midpoint in the variability in the dataset. The negative y-intercept value indicates that where the ICP concentration approaches non-detect or 0 mg/kg, the XRF unit overestimates the COC concentration and on average estimates them to be approximately 32 mg/kg. None (0) of the 186 copper results used in the final regression analysis were determined to be false negative or false positive (0.0% and 0.0%, respectively). No outlier results were determined to be false negative or false positive.

4.4 Lead

Regression Summary
The regression analysis performed for lead indicated that the XRF analysis, on average, underestimates lead laboratory concentrations in the samples (m = 1.10). A small initial negative offset to the data was indicated by the y-intercept (b = -25.4). The R^2 value can be interpreted to indicate that the model accounts for approximately 92% of the variability in the data (Table 1).

Figure 4 shows the 5 plots used to assess the regression analysis. The first plot (upper left-hand corner), *Lead XRF to Laboratory Correlation Entire Data Set with Removed Outliers*, shows the entire dataset, the outliers removed to calculate the regression, and the linear regression model. The data points generally fall below the regression lines, meaning the regressions provide conservative estimates of the paired concentrations. The second plot (upper middle), *Lead XRF to Laboratory Regression: View Near Recreational and Commercial Human Health Action Level*, shows a zoomed-in view of the first plot and shows the points near the action level criteria 2,300 mg/kg for Recreational and Commercial land use (EPA, 2020). The third plot (upper right-hand corner), *Lead XRF to Laboratory Regression: View Near Storm Water Waste Identification Criteria*, shows a zoomed-in view of the first plot and shows the points near the storm water waste identification criteria 1,000 mg/kg. The fifth plot (lower middle), *Lead XRF to Laboratory Regression: View Near Residential Human Health Action Level*, shows a zoomed-in view of the first plot and shows the points near the action level criteria 1,200 mg/kg for residential land use (EPA, 2020) (Figure 4).

Outlier Summary
The fourth plot (lower left-hand corner), *Outlier Summary: Lead Standardized Residual Plot*, shows the standardized residuals of the entire dataset plotted against the XRF concentration values. The outlier points are scattered above and below other values, which generally fall well within the positive and negative standardized residual threshold boundary lines. The location of

the outliers on the first plot reinforces their designation as outliers: they sit above and below the other points in the dataset (Figure 4).

Conclusion
Overall, the regression model for lead appears, on average, to underestimate the laboratory concentrations and falls through the center of the variability in the dataset. The negative y-intercept value indicates that where the ICP concentration approaches non-detect or 0 mg/kg, the XRF unit overestimates the COC concentration and on average estimates them to be approximately 23.5 mg/kg. None (0) of the 174 lead results were determined to be false negative or false positive (0.0% and 0.0%, respectively) from the final regression analysis. Excluded from the count was 1 outlier result, determined to be a false negative, and 2 outlier results, determined to be false positives.

4.5 Zinc

Regression Analysis
The slope of the regression analysis for zinc indicated that the XRF analysis overestimates the zinc concentrations in the samples (m = 0.57). The y-intercept (b = 191.9) suggests that some points are pulling the regression line upward. The R^2 value can be interpreted to indicate that the model accounts for approximately 88% of the variability in the data (Table 1).

Figure 5 shows the 4 plots used to assess the regression analysis. The first plot, *Zinc XRF to Laboratory Correlation: Entire Data Set with Removed Outliers*, shows the entire dataset, the outliers removed to calculate the regression, and the linear regression model. The outlier is located well above and to the left of the dataset. The second plot, *Zinc XRF to Laboratory Correlation: Final Regression Analysis Dataset (Outlier not Included)*, shows a concentrated mass near the XRF and laboratory concentrations ranging from 0 mg/kg to 1,000 mg/kg, the storm water waste identification criteria. The cluster near the lower concentrations is also shown on the second plot. The third plot, *Zinc XRF to Laboratory Regression: View Near Storm Water Waste Identification Criteria*, shows a zoomed-in view of the first plot and shows the points near the storm water waste identification criteria, 1,000 mg/kg (EPA, 2020). The regression line overestimates concentrations near the waste criteria (1,000 mg/kg). Still, the scatter increases dramatically as the XRF concentration values increase above the storm water waste identification criteria (Figure 5).

Outlier Analysis
The fourth plot, *Outlier Summary: Zinc Standardized Residual Plot*, shows the standardized residuals of the entire dataset plotted against the XRF concentration values. One outlier point falls well above the standardized residual threshold boundary line (Figure 5).

Conclusion
The scattering of points at the higher XRF concentration values appears to shift the entire regression upward, resulting in a high y-intercept. This shift likely results in the regression line overestimating COC concentrations of the lower XRF concentrations (less than 500 mg/kg), which produces a more conservative model. At concentrations greater than the storm water waste identification criteria (1,000 mg/kg), the regression balances the scattering of points. None (0) of

the 186 zinc results were determined to be false negatives and 2 of the 186 results (0.0% and 1.1%, respectively) from the final regression analysis were determined to be false positives. There were no outlier results identified as false negative or false positive.

5.0 CONCLUSION

If the final output variable (ICP) is set on the x-axis during regression analysis, the resulting regression line will likely have a poorer fit when predicting the final output variable due to greater variance of typical XRF datasets, compared to typical ICP datasets. Therefore, all data have been presented with the final output variable (ICP) on the y-axis.

The objective of this approach is to identify a process for future correlation and regression analyses of XRF to laboratory ICP results to establish statistical confidence in field XRF measurements. Table 1 lists the results of the regression and correlation analyses and Table 2 lists all the data that were used and rejected during the analysis. In total, 313 non-detect XRF data points and 27 outliers were removed from the analysis. From the 2018 and 2021 sampling events, 787 paired data points were used in the final analysis.

Evaluation of the paired data set could be used to predict the output of a non-paired data set (using XRF concentrations only with no laboratory confirmation analyses). Of the 787 COC data points used in the final regression analysis, excluding non-detect and outlier data points:

- 0 of 787 (0%) results were determined to be false negatives (i.e., no results below action levels were miscategorized based on the XRF data).
- 5 of 787 (0.6%) results were determined to be false positives (i.e., results above action levels may have been miscategorized, resulting in additional potential remediation performed based on XRF data).

With outliers included, 2 of the 814 XRF results were determined to be false positives and 10 of the 814 XRF results were determined to be false negatives (0.2% and 1.2%, respectively).

Based on the nominal occurrence of false negative and false positive results the following key conclusions are drawn:

- Unreclaimed Sites confirmation thresholds (± 35% action levels) are adequate for waste identification.

Field XRF provides instantaneous and statistically defensible estimates for As, Cd, Cu, Pb, and Zn concentrations in soil and typically overestimates concentrations when compared to analytical laboratory concentrations. Based on the samples from this paired dataset, the overall percentage of miscategorization of XRF data resulting in false positives (over-remediation) is much higher than miscategorization of XRF data resulting in false negatives (under-remediation).

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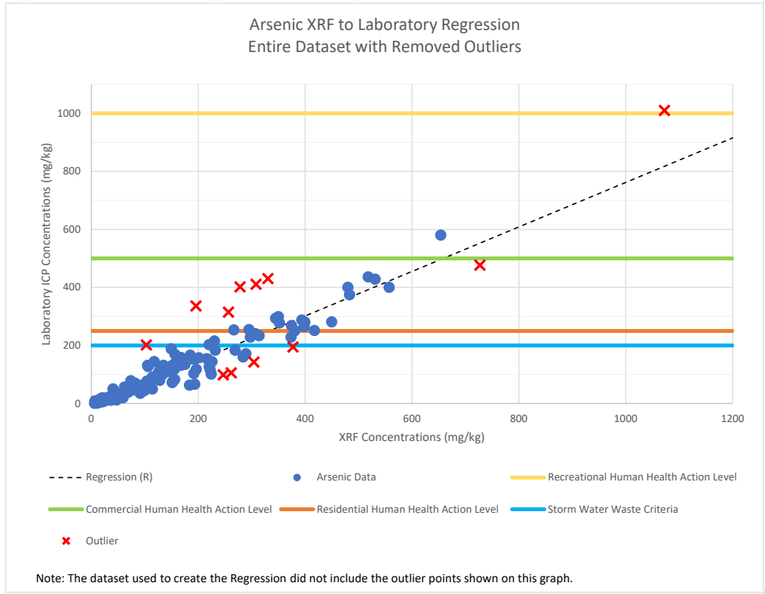
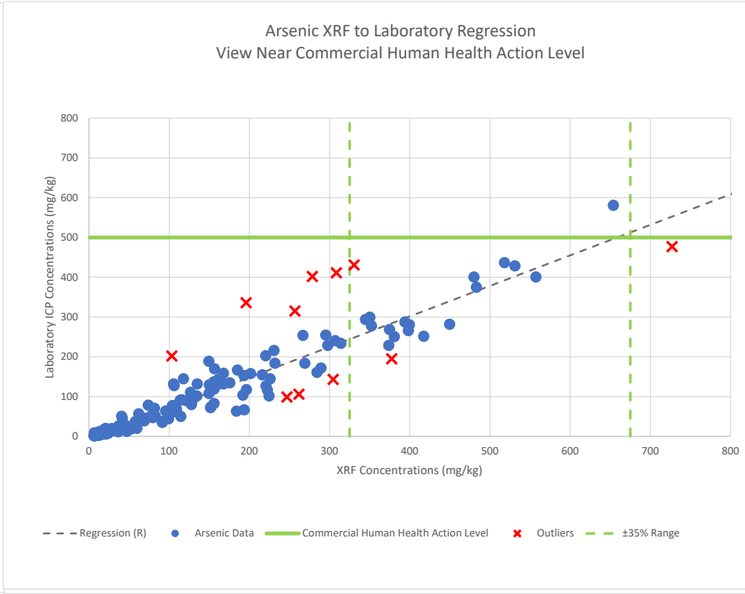
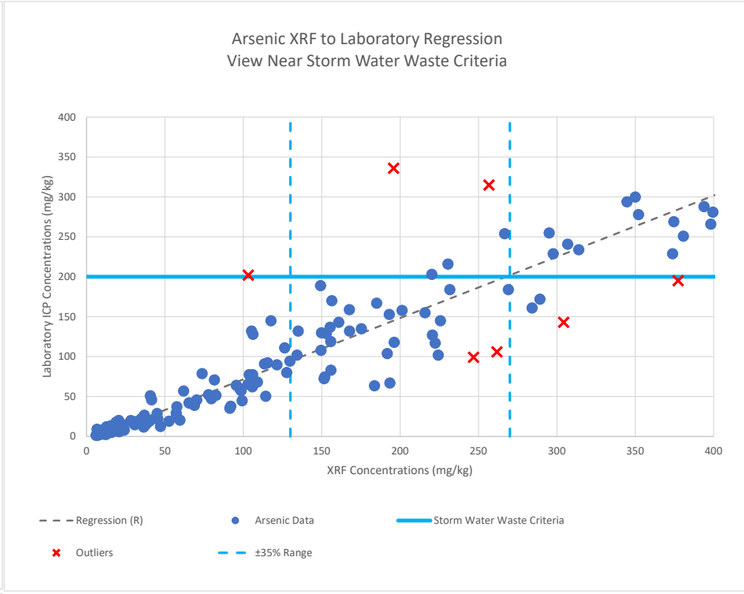
FIGURES

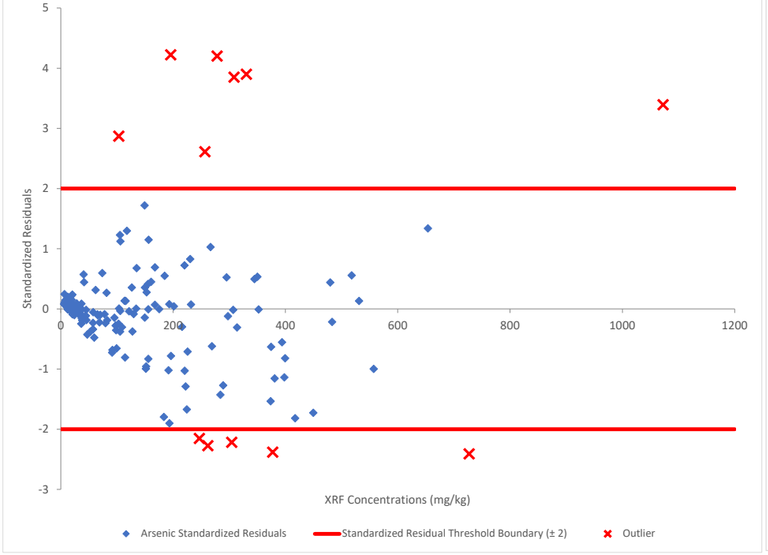
Figure 1. Arsenic Regression Analysis



Note: The dataset used to create the Regression did not include the outlier points shown on this graph.







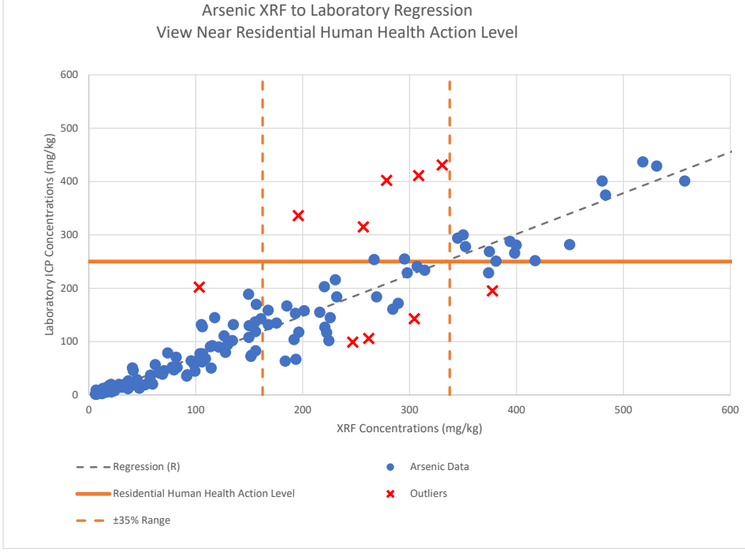
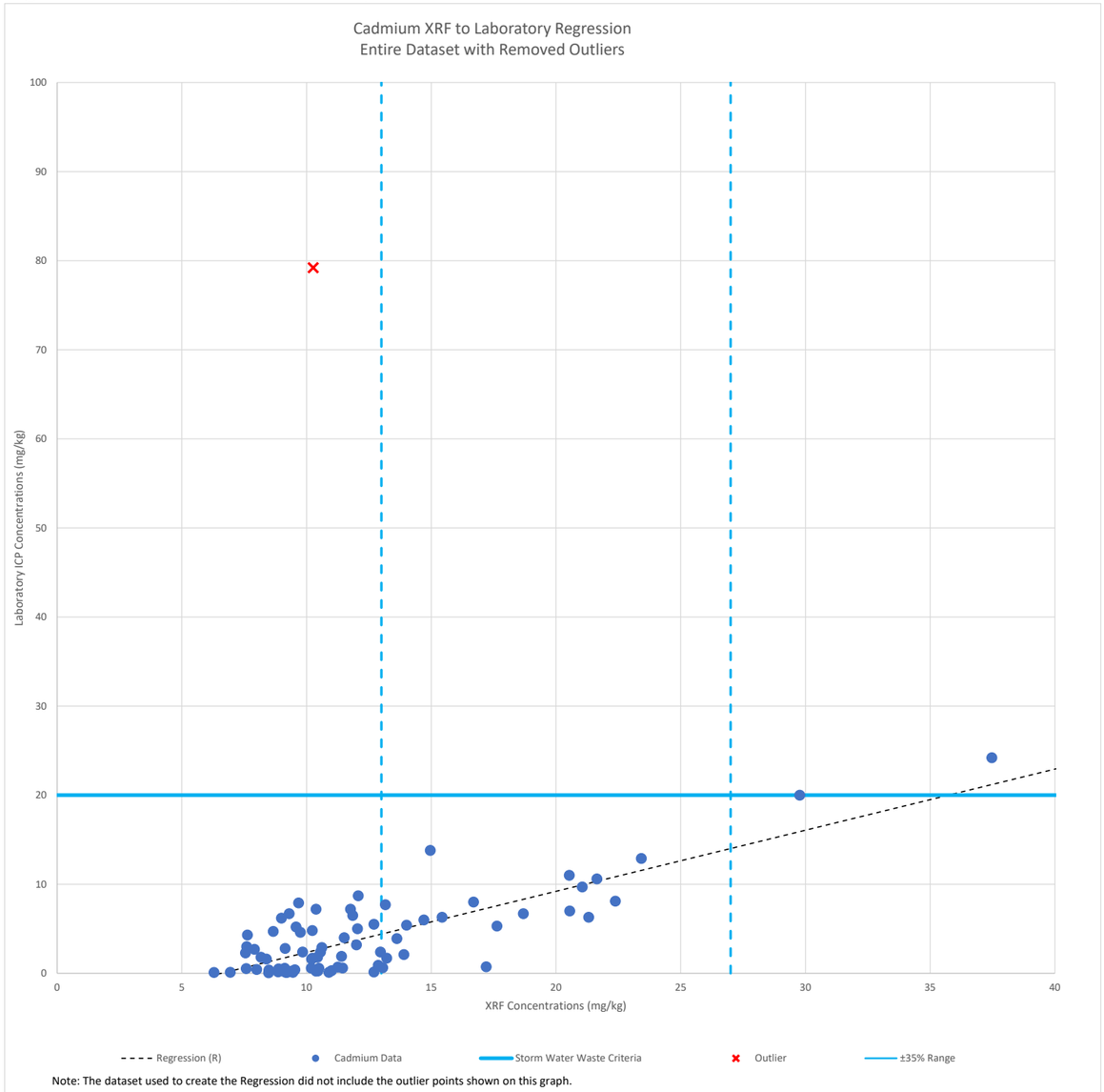


Figure 2. Cadmium Regression Analysis



Note: The dataset used to create the Regression did not include the outlier points shown on this graph.

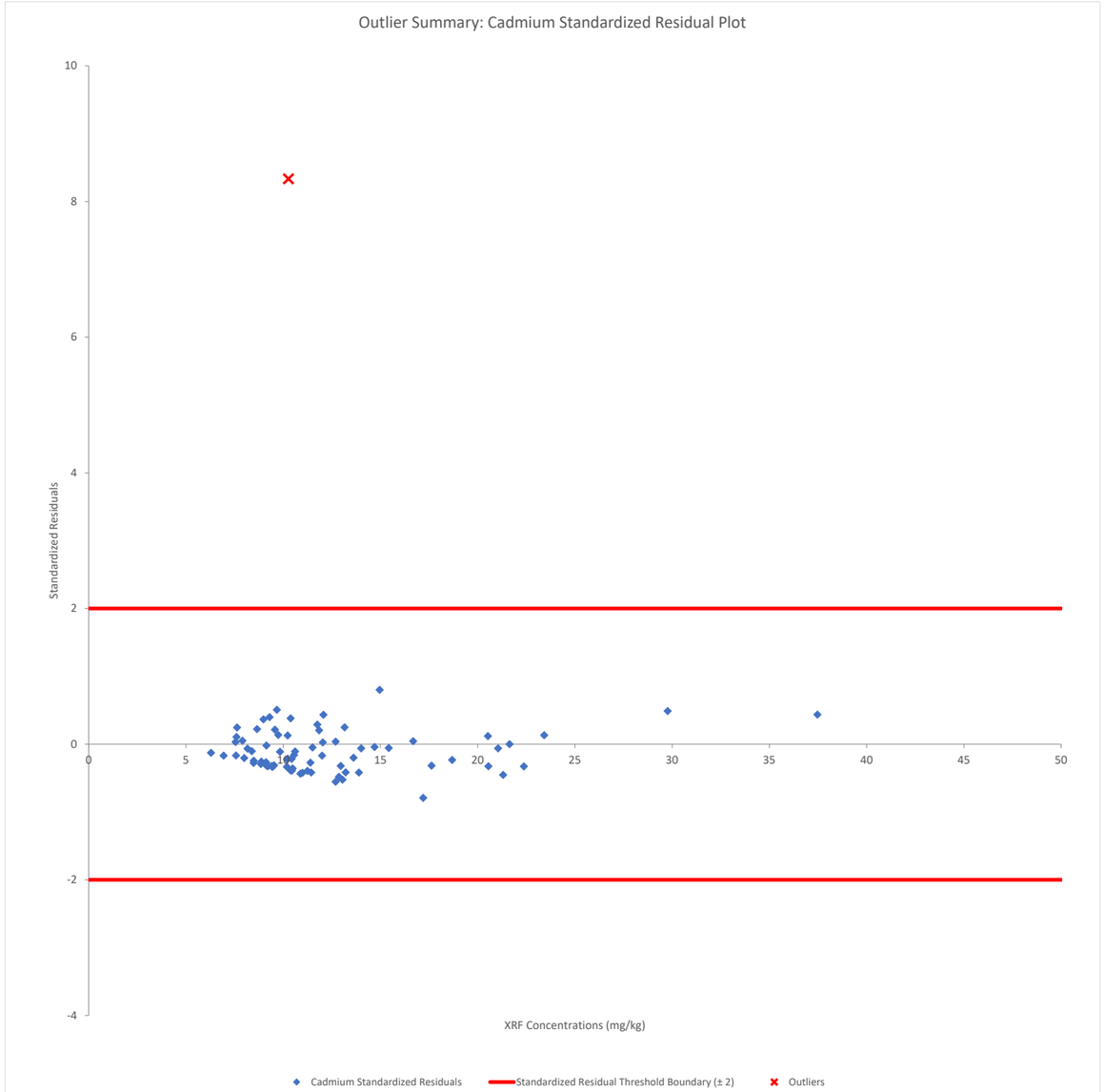
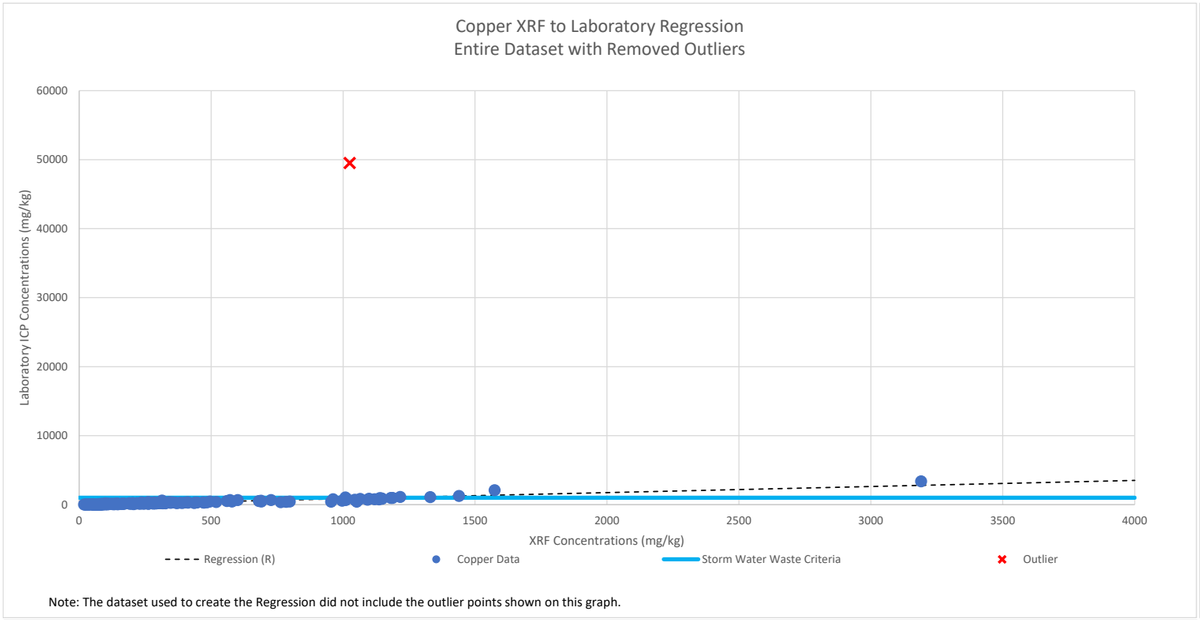
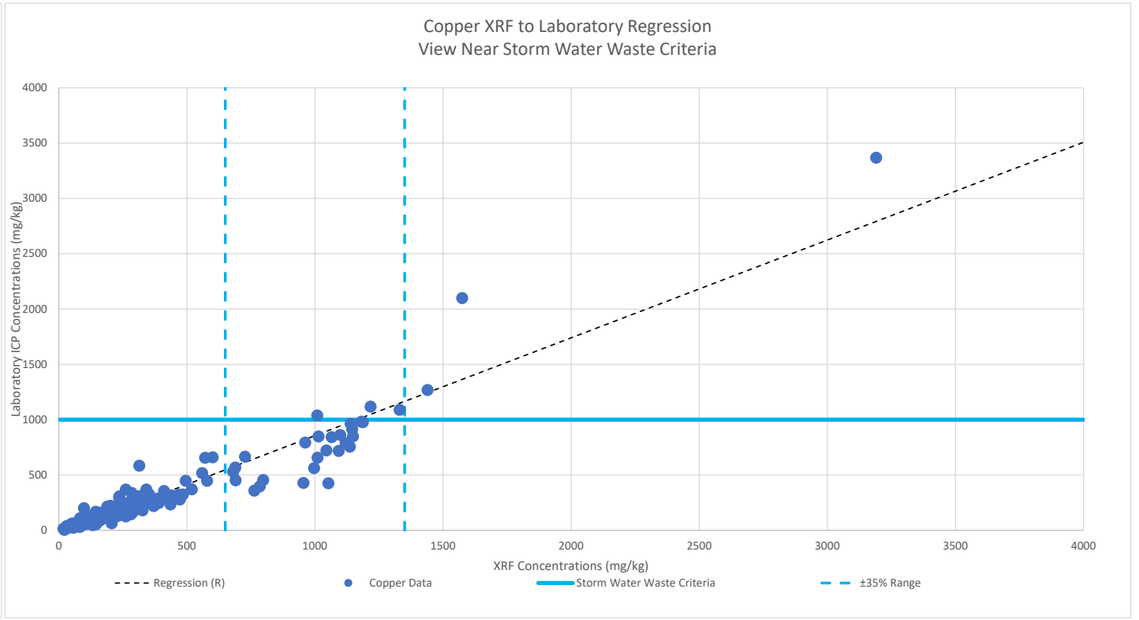


Figure 3. Copper Regression Analysis



Note: The dataset used to create the Regression did not include the outlier points shown on this graph.



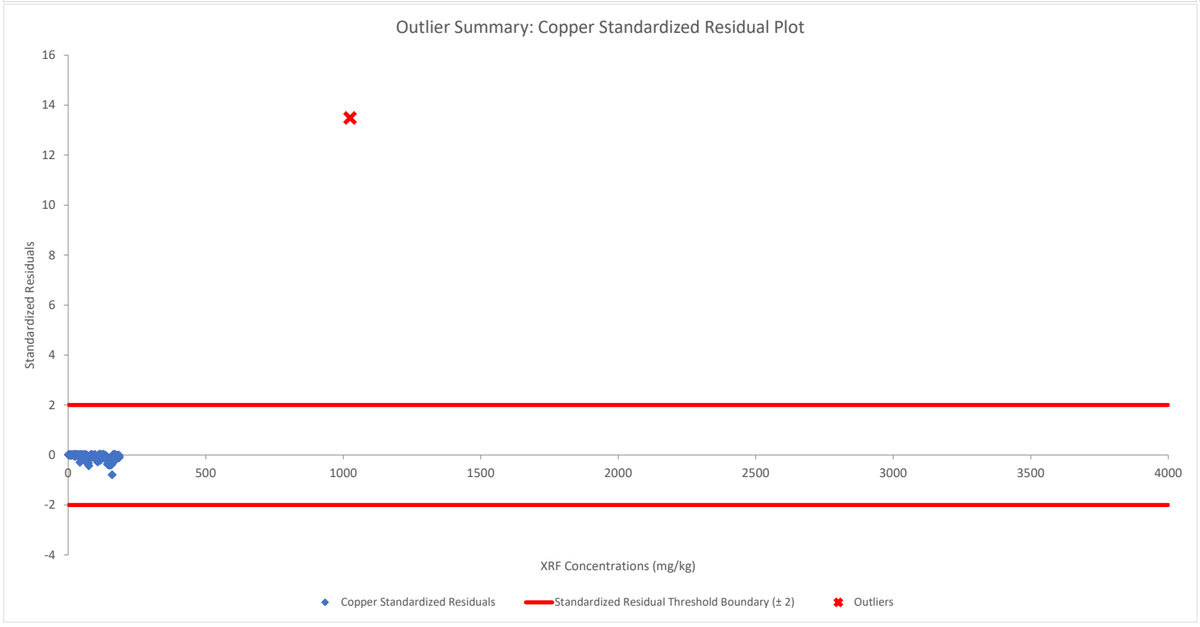
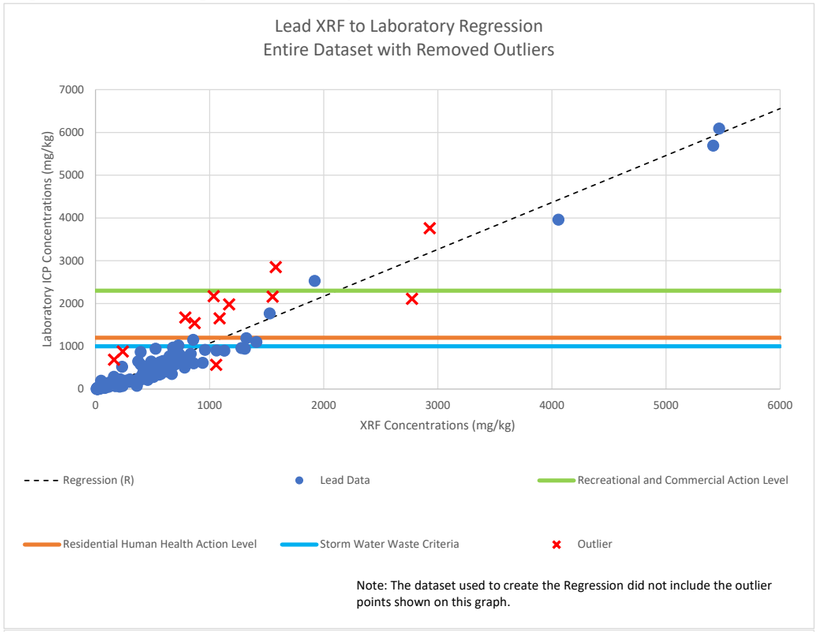
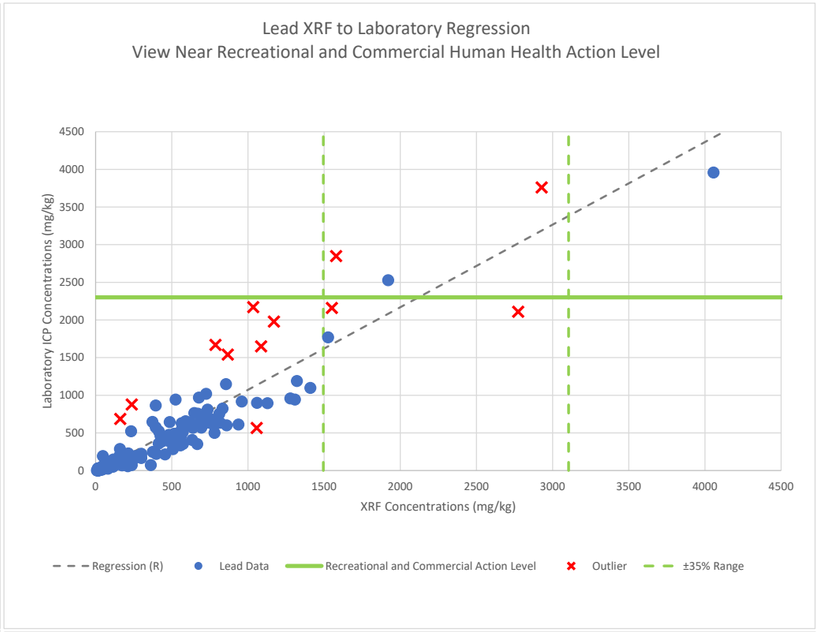
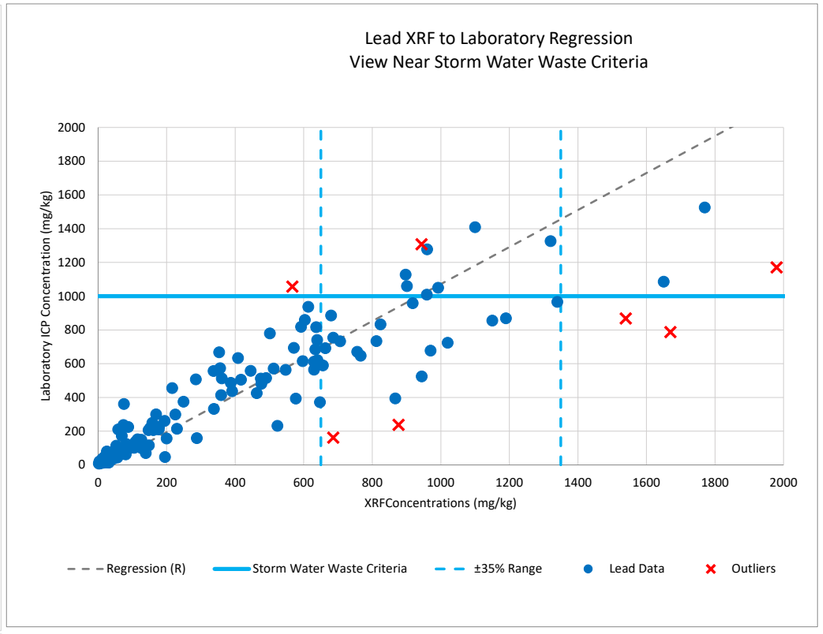
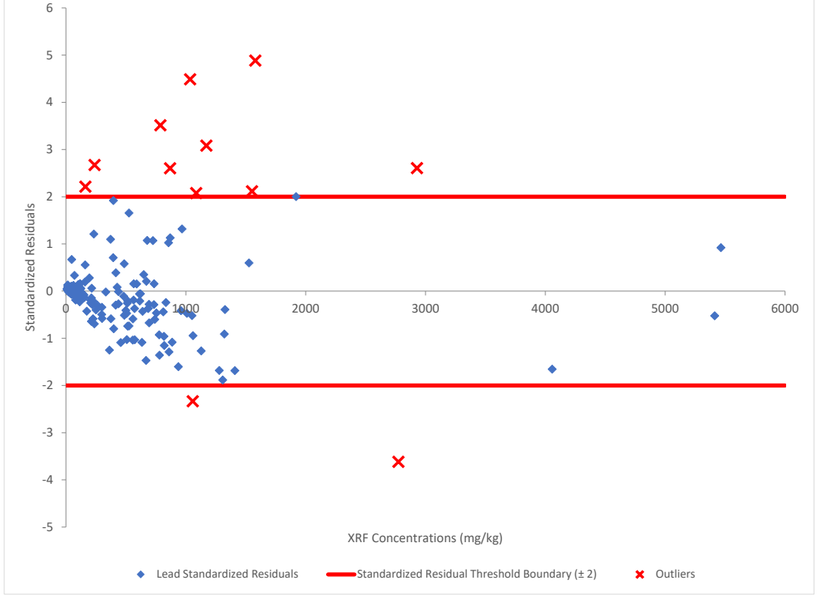


Figure 4. Lead Regression Analysis









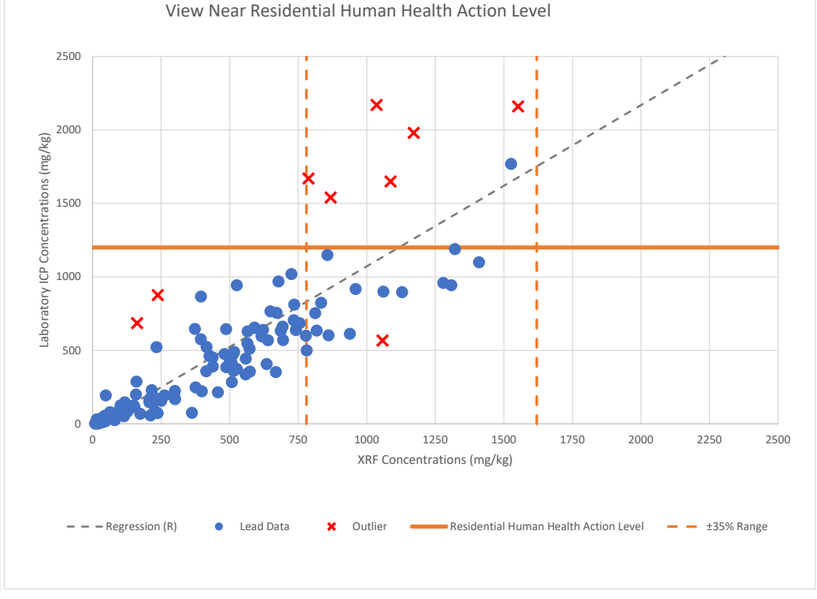
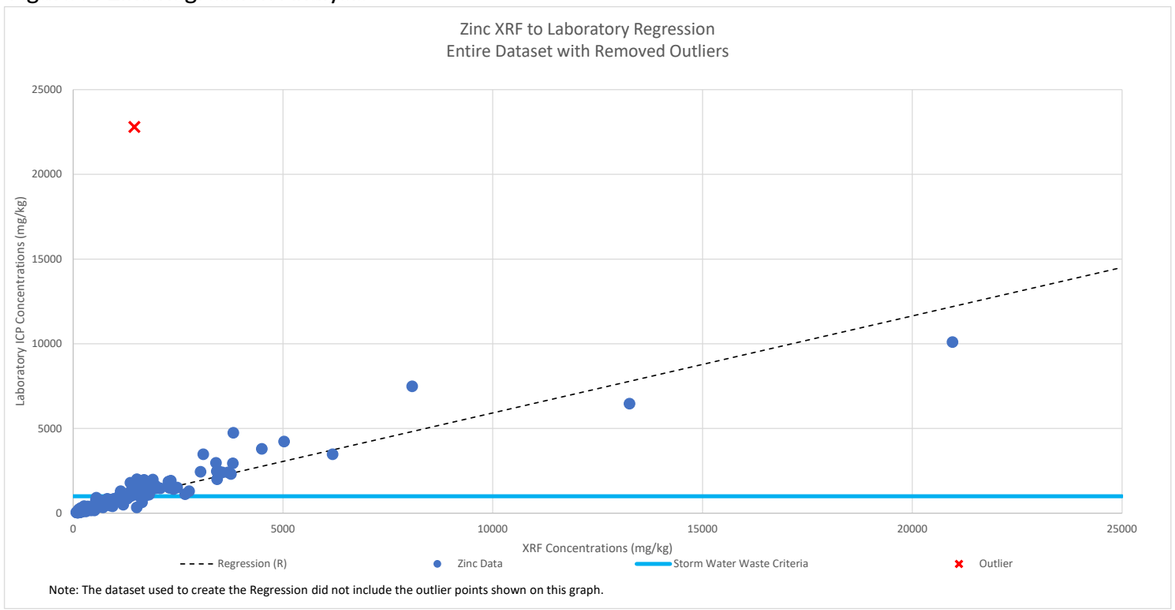
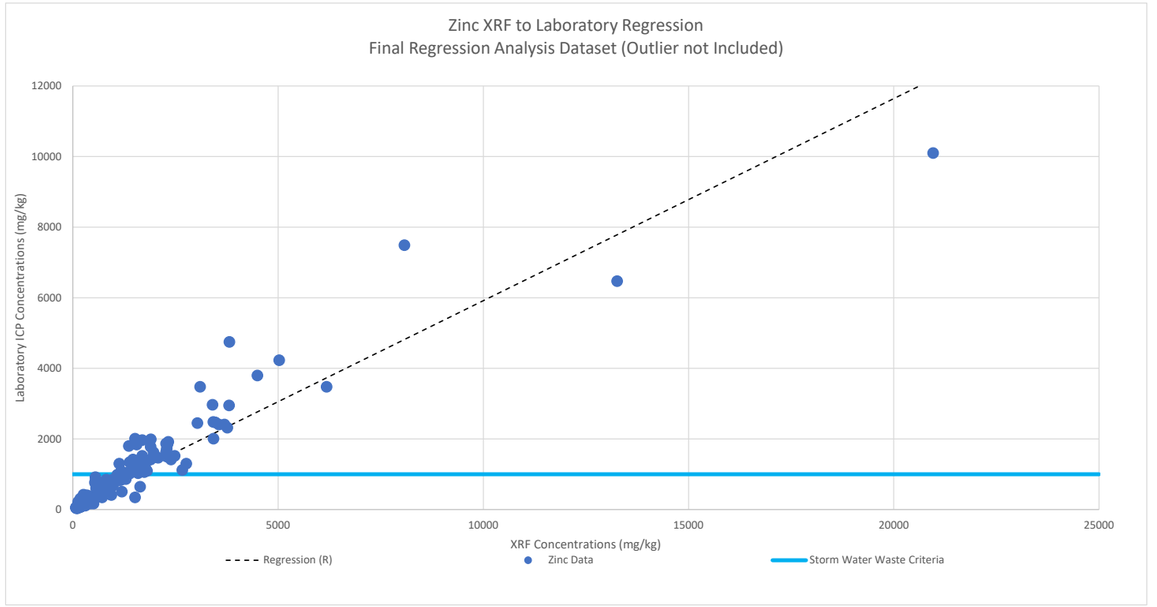
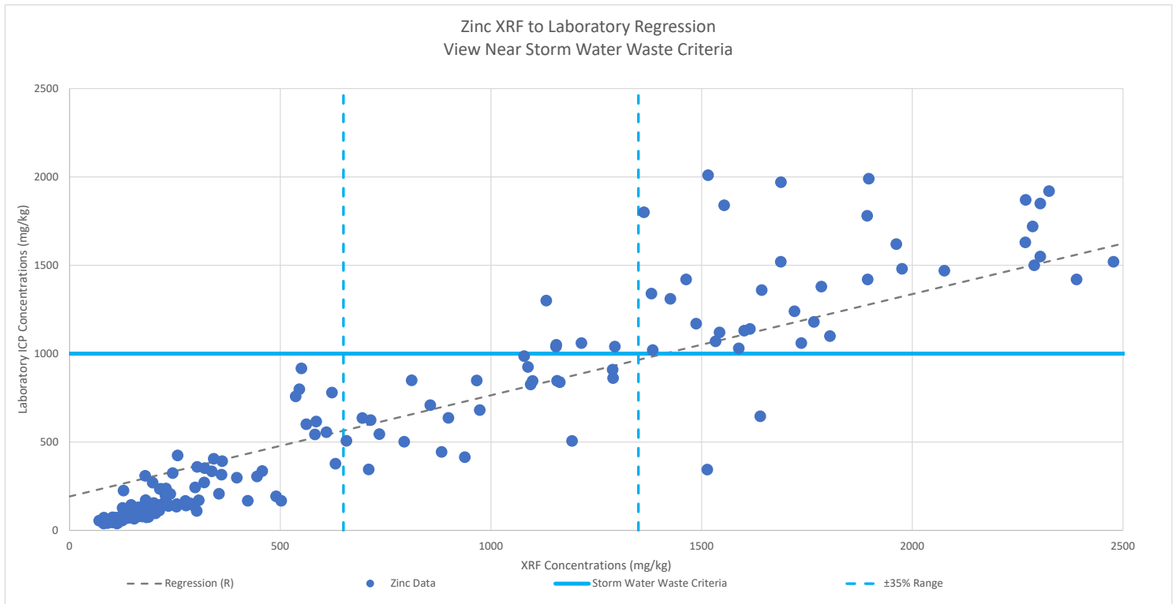


Figure 5. Zinc Regression Analysis



Note: The dataset used to create the Regression did not include the outlier points shown on this graph.





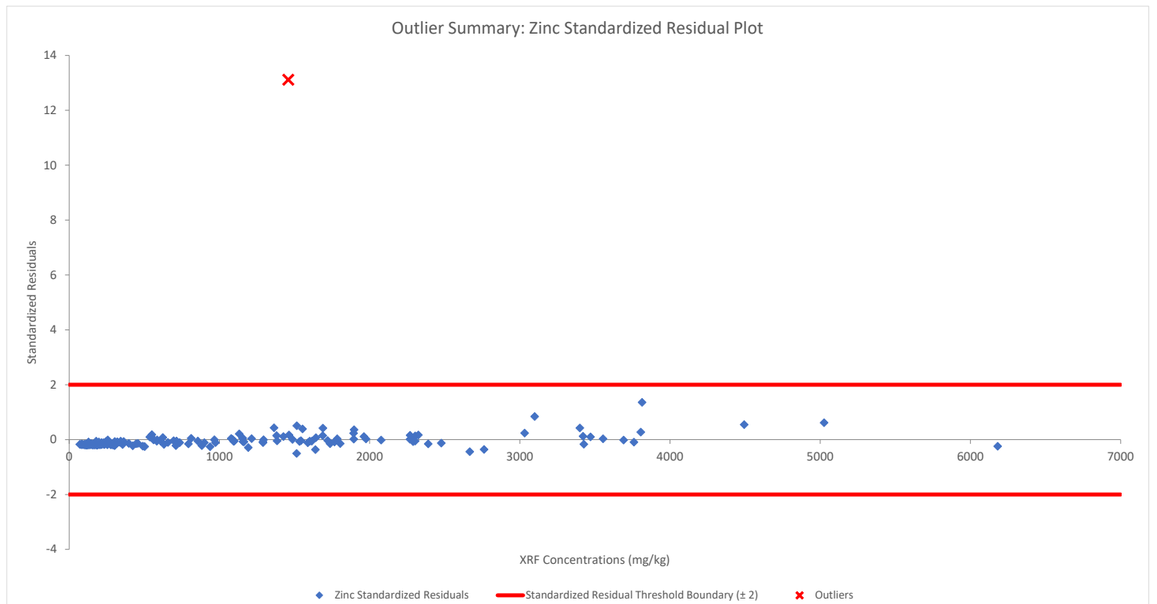
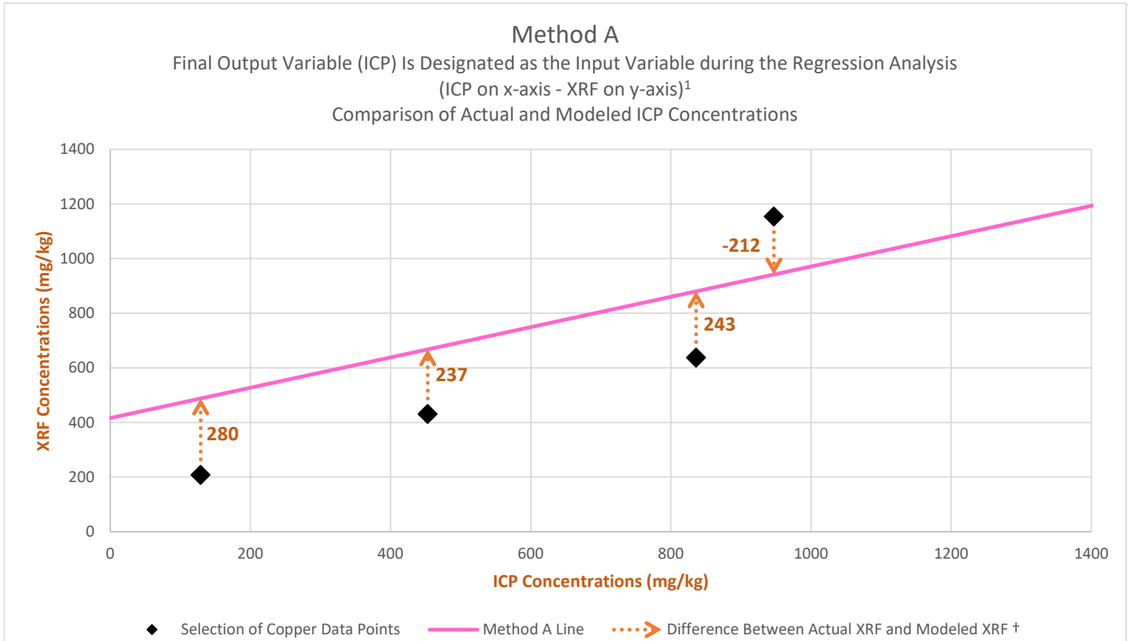
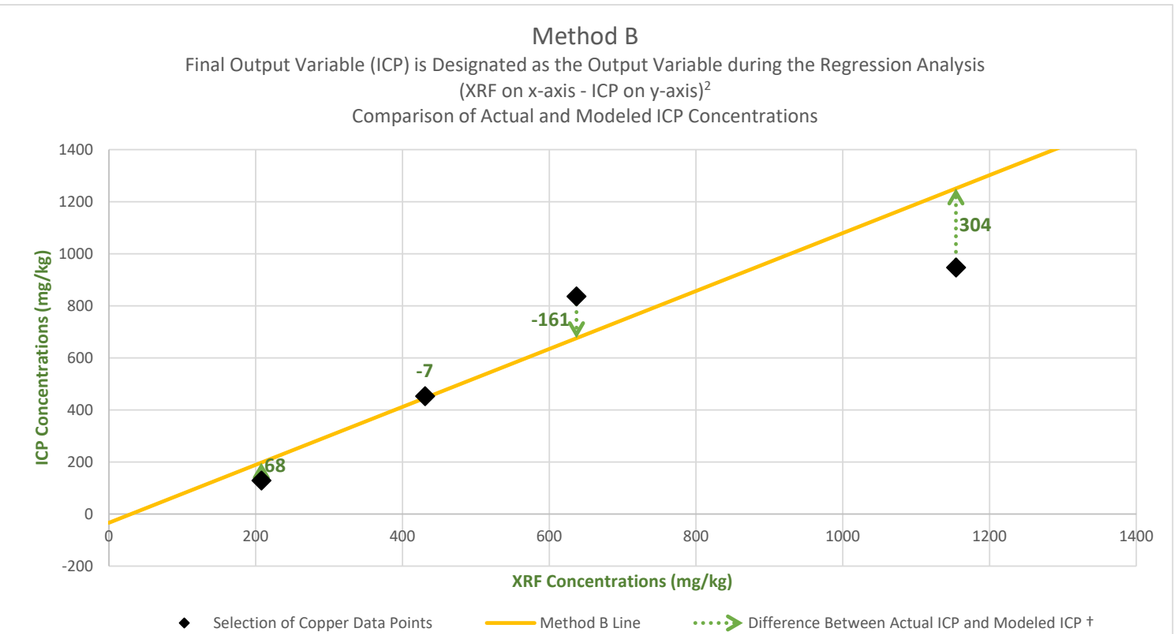
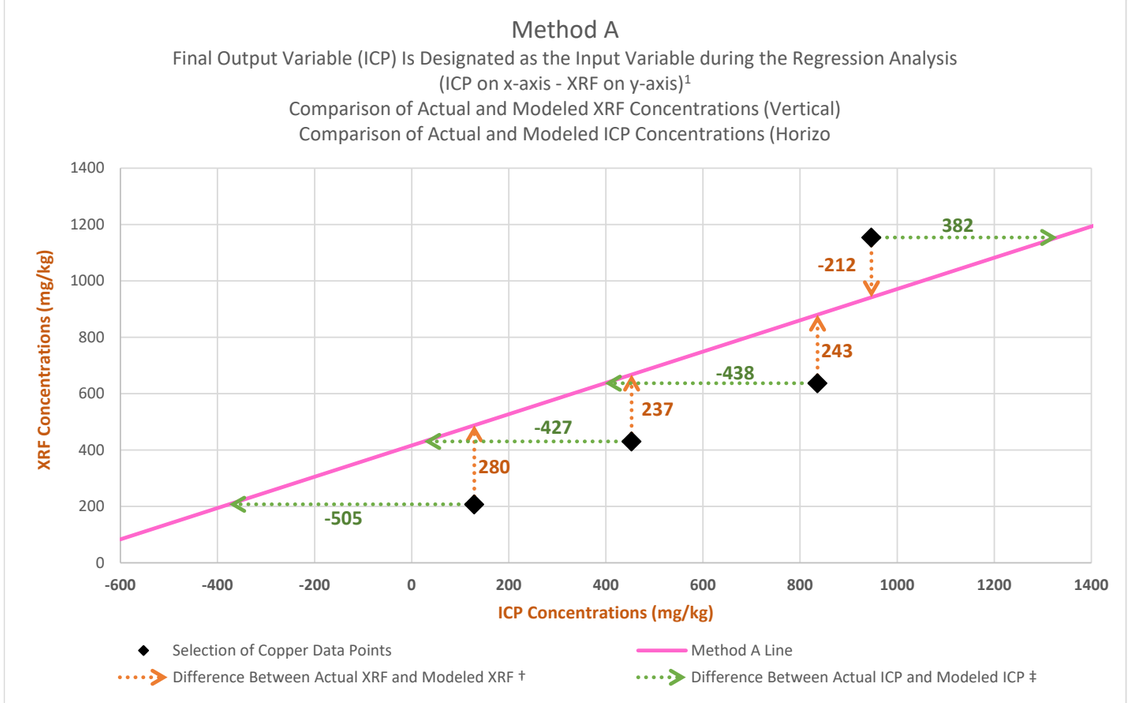


Figure 6. Visualization of the fit of a Regression Model and How R^2 Values are Calculated

Introduction: The first step in conducting any regression analysis is to determine how the regression model will be used and to determine the final output variable. In this example, the regression analysis was completed to determine predict ICP concentrations at particular XRF concentrations. The final output variable is the ICP concentration. This figure shows how placing the final output variable (ICP concentrations in this example) on the x-axis when conducting the regression analysis will result in a lower R^2 value (i.e., a model with a poorer fit) when the actual ICP concentrations are compared to the modeled ICP concentrations.







Regression Models

Method A[1]		**Method B[2]**	
m_2	b_2	m_1	b_1
0.56	416	1.11	-33.5
Goodness of Fit of the Copper Regression Models			
Method A[1]		**Method B[2]**	
R^2 (XRF)†	**R^2 (ICP)‡**	**R^2 (ICP)†**	
0.86	**0.33**	**0.88**	

Notes:

Four data points from a copper regression analysis conducted for a different project were selected for these graphs to demonstrate how the R^2 values, which indicate the goodness of fit of the regression model, are calculated. The same 4 datapoints were used in all three graphs. The points were selected so that the XRF and ICP values covered a range between 100 and 1200 mg/kg and the difference between the XRF and ICP concentrations were relatively small (between approximately 0 and 200 mg/kg). The criteria for selecting the points are based entirely on ease of visualization. The slope (m_1 and m_2), y-intercept (b_1 and b_2), and R^2(XRF) and R^2(ICP) values were the final values from the regression analysis where Method A and Method B were compared.

[1] For Method A, the regression analysis is completed with the ICP concentrations placed on the x-axis and XRF concentrations placed on the y-axis. The regression model creates an equation XRF = m_2*ICP+b_2. In this format the ICP value is the model input and the XRF value is the model output. To use this formula to adjust the XRF values to predict the corresponding ICP values (i.e., the XRF concentrations need to be the input values and the ICP concentrations need to be the output values), the equation has to be solved for the ICP concentration so that the equation reads: ICP = m_3*XRF+b_3 or ICP = $(1/m_2)$*XRF - (b_2/m_2).

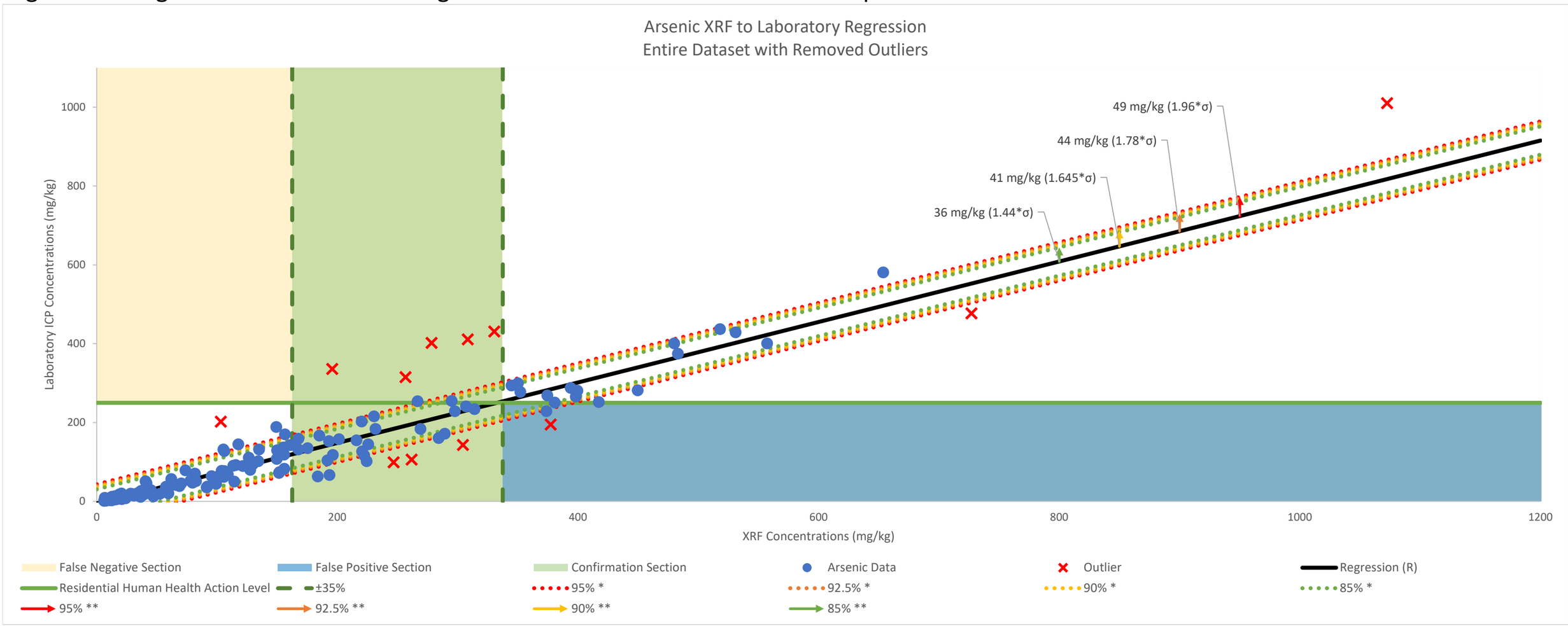
[2] For Method B, the regression analysis is completed with the XRF concentrations placed on the x-axis and the ICP concentrations placed on the y-axis. The regression model creates an equation ICP = m_1*XRF+b_1. This equation does not need to be altered to predict the ICP values at particular XRF concentrations.

† The values next to the datapoints are equal to the magnitude of the vertical distance between the data point and the regression line or the difference between the modeled output and the actual datapoint (this value is called the Residual). The sum of the squared Residuals is called the Residual Sum of Squares, which represents the unexplained variation between the actual data and the modeled outputs, and that value is used to calculate the R^2 value. The Method A R^2 (XRF) value is calculated using the actual XRF concentrations and the modeled XRF concentrations. The Method A R^2 (ICP) and Method B R^2 (ICP) values are calculated using the difference between the actual ICP concentrations and the modeled ICP concentrations.

‡ The values next to the datapoints in the chart are equal to the magnitude of the horizontal distance between the data point and the regression line. This horizontal difference represents the difference between the modeled data and the actual data when the Method A Equation XRF = m_2*ICP+b_2 has been adjusted to ICP = m_3*XRF+b_3 or ICP = $(1/m_2)$*XRF - (b_2/m_2). The R^2(ICP) value is calculated using the difference between the actual ICP concentrations and the modeled ICP concentrations.

Conclusion: If the final output variable is set on the x-axis during the regression analysis, the resulting regression line will most probably have a poorer fit (R^2 of 0.33 compared to 0.86 in this example) when predicting the final output variable than if the model output is set on the y-axis during the regression analysis. A quick rule of thumb: if the formula, y=mx+b has to be modified to solve for x when the regression equation is applied to the data, the regression analysis will need to be redone with the variables set on the other axes.

Figure 7. Using Residuals to Predict Range of ICP Concentrations in Future Samples



Notes:

False Negative Section - Using the ± 35% XRF concentrations to determine which points to send to the lab, points that fall in this area will be considered below the action level, but they would exceed the action level if sent for laboratory analysis. It is important to minimize false negative points to reduce the occurrence of inadvertently failing to remediate areas with COC concentrations that exceed action levels.

False Positive Section - Using the ± 35% XRF concentrations to determine which points to send to the lab, points that fall in this area will be considered above the action level, but they would have laboratory concentrations less than the action level if sent for laboratory analysis. It is important to minimize false positive points to reduce the occurrence of inadvertently remediating areas that do not require remediation.

Confirmation Section - This section was set by the Unreclaimed Sites QAPP as XRF concentrations between +35% and -35% of the action level. In this area, XRF samples will be sent to the laboratory to confirm the ICP concentration. There is a high degree of uncertainty in this section as to whether the sample would fall above or below the action level, which is why samples are sent for laboratory confirmation.

Regression - The Regression line represents the average laboratory concentration at each XRF concentration. It is also where the residual values, the difference between the modeled value and the actual value, are equal to 0.

* The percentages indicate the probability that the ICP concentration at any XRF concentration will fall between the upper and lower lines. For example, the probability that a laboratory concentration will fall between the upper and lower dotted red lines is 99.9%.

** The dotted lines were created by adding various multiples (z-values) of the standard deviation (σ) of the residuals to the y-intercept of the regression line (the slope remains the same). Residuals are typically normally distributed with an average of close to 0. The residuals can be used to predict the variability in laboratory concentrations with respect to the regression line. The regression line represents the average residual value or where the residuals are equal to 0. Points will be normally distributed above and below the regression line. For example, at any XRF concentration 49.95% of points will have a laboratory concentration that is less than or equal to 82 plus the regression model value at that XRF concentration. While 42.5% will have laboratory concentrations less than or equal to 49 plus the regression model value.

TABLES

Table 1: Summary of XRF and Laboratory Correlation and Regression Analyses

2018 to 2021 Unreclaimed Sampling

	Number of Samples	Number of Non-Detect XRF Results[1]	Number of Outliers Removed from Final Analysis	Number of Samples in Final Analysis	Correlation Coefficient		Coefficient of Determination[2]	Regression[2]		Outliers Removed	
					All Data	Outliers Removed		Slope	y-Intercept	Slope	y-Intercept
					R		R-Squared	m	b	m	b
Arsenic	187	11	12	164	0.95	0.97	0.95	0.81	-6.9	0.77	-5.2
Cadmium	187	109	1	77	0.34	0.81	0.65	0.61	-2.6	0.69	-4.5
Copper	187	0	1	186	0.22	0.95	0.91	1.97	-133.2	0.88	-28.1
Lead	187	0	12	174	0.96	0.96	0.92	1.08	-16.0	1.10	-25.4
Zinc	187	0	1	186	0.59	0.94	0.88	0.58	299.9	0.57	191.9
Mercury	196	193	Insufficient number of Mercury data points for correlation analysis								

[1] For the analysis, the non-detect XRF results were removed before performing the outlier analysis and were not used in the Final Analysis.

[2] The Coefficient of Determination and Regression were all generated using the dataset with the Non-Detect XRF Results and Outliers removed. The number of samples in the *Number of Samples in Final Analysis* column indicates the number of samples used to generate the linear models. Table 2 indicates which samples were used for these analyses.

Table 2. Sample Results Used in the XRF to Laboratory Correlation and Regression Analyses

Color Coding in the Station Name Column

Sample is a Field Duplicate collected for QA/QC.

Color Coding in the Analyte Result Columns

Mercury was re-collected and analyzed due to temperature exceedance upon arrival at the Pace Lab.

There was only Mercury XRF and lab result for this sample. Therefore this point was only used in the Mercury regression.

The XRF Results are Non-Detect. This sample pair was not used in the XRF to lab Regression Analysis. The non-detect XRF concentrations listed in this table are the XRF confidence interval values.

These points were identified as outliers and were not used in the final regression analyses.

Site	Station Name	Field Sample ID (XRF)*	Lab (ICP)	Arsenic (ICP)	Arsenic (ICP) Detect	Arsenic (XRF)	Arsenic (XRF) Detect	Cadmium (ICP)	Cadmium (ICP) Detect	Cadmium (XRF)	Cadmium (XRF) Detect	Copper (ICP)	Copper (ICP) Detect	Copper (XRF)	Copper (XRF) Detect	Lead (ICP)	Lead (ICP) Detect	Lead (XRF)	Lead (XRF) Detect	Mercury (ICP)	Mercury (ICP) Detect	Mercury (XRF)	Mercury (XRF) Detect	Zinc (ICP)	Zinc (ICP) Detect	Zinc (XRF)	Zinc (XRF) Detect	Units
UR-01	UR-01-SS-01	BPSOU-UR01SS01-110321-2	PACE	4.7	Y	10.58	Y	0.19	Y	7.59	N	40.1	Y	50.41	Y	22.7	Y	30.97	Y	0.0081	N	6.78	N	70.3	Y	138.68	Y	mg/kg
UR-01	UR-01-SS-01	BPSOU-UR01SS01-110321-3	PACE	3.4	Y	9.86	Y	0.16	Y	7.88	N	42.1	Y	79.01	Y	24.7	Y	26.26	Y	0.0098	Y	7.09	N	75.5	Y	187.34	Y	mg/kg
UR-01	UR-01-SS-01	BPSOU-UR01SS01-110321-3-FD	PACE	3.1	Y	7.94	Y	0.18	Y	7.63	N	45.4	Y	73.98	Y	20.2	Y	21.84	Y	0.018	Y	6.79	N	76.9	Y	138.27	Y	mg/kg
UR-01	UR-01-SS-02	BPSOU-UR01SS02-110321-2	PACE	2.4	Y	5.5	N	0.11	Y	10.89	Y	41.5	Y	55.18	Y	6.1	Y	13.06	Y	0.01	Y	7.26	N	46.1	Y	101.97	Y	mg/kg
UR-01	UR-01-SS-02	BPSOU-UR01SS02-110321-2-FD	PACE	2.3	Y	6.64	Y	0.14	Y	9.14	Y	42.2	Y	65.49	Y	31	Y	14.51	Y	0.008	N	6.87	N	53.1	Y	100.34	Y	mg/kg
UR-01	UR-01-SS-03	BPSOU-UR01SS03-110321-1	PACE	3.7	Y	10.51	Y	0.23	Y	7.71	N	68.6	Y	107.65	Y	13.8	Y	13.88	Y	0.01	N	6.91	N	71.7	Y	135.54	Y	mg/kg
UR-01	UR-01-SS-03	BPSOU-UR01SS03-110321-2	PACE	9.2	Y	6.62	Y	0.24	Y	7.73	N	63.1	Y	73.47	Y	10.7	Y	21.28	Y	0.0088	N	6.89	N	92	Y	165.35	Y	mg/kg
UR-01	UR-01-SS-03	BPSOU-UR01SS03-110321-3	PACE	2.3	Y	7.66	Y	0.18	Y	7.83	N	39.5	Y	81.1	Y	8.3	Y	26.12	Y	0.0088	N	6.81	N	65.7	Y	153.01	Y	mg/kg
UR-01	UR-01-SS-04	BPSOU-UR01SS04-110321-1	PACE	2.8	Y	6.35	N	0.18	Y	7.58	N	49.7	Y	77.83	Y	16.9	Y	22.86	Y	0.0088	N	7.48	N	73.6	Y	182.68	Y	mg/kg
UR-01	UR-01-SS-04	BPSOU-UR01SS04-110321-2	PACE	3	Y	10.43	Y	0.13	Y	7.89	N	61.4	Y	85.53	Y	13.5	Y	16.84	Y	0.0084	N	6.73	N	59	Y	120.67	Y	mg/kg
UR-01	UR-01-SS-04	BPSOU-UR01SS04-110321-3	PACE	1.7	Y	6.06	Y	0.065	Y	8.48	Y	35.9	Y	62.84	Y	3.9	Y	11.53	Y	0.009	N	6.96	N	42.8	Y	114.34	Y	mg/kg
UR-01	UR-01-SS-05	BPSOU-UR01SS05-110321-1	PACE	5.2	Y	15.77	Y	0.56	Y	7.52	N	41.8	Y	74.76	Y	56.2	Y	44.23	Y	0.24	Y	6.69	N	158	Y	225.69	Y	mg/kg
UR-01	UR-01-SS-05	BPSOU-UR01SS05-110321-2	PACE	4.3	Y	14.42	N	0.4	Y	7.84	N	42.1	Y	78.79	Y	58.7	Y	211.17	Y	0.35	Y	7.21	N	152	Y	287.4	Y	mg/kg
UR-01	UR-01-SS-05	BPSOU-UR01SS05-110321-3	PACE	4.4	Y	13.15	Y	0.52	Y	7.64	N	37.8	Y	82.37	Y	40.6	Y	60.6	Y	0.84	Y	7.21	N	141	Y	276.32	Y	mg/kg
UR-01	UR-01-SS-06	BPSOU-UR01SS06-110321-1	PACE	3.2	Y	8.01	Y	0.14	Y	7.31	N	40	Y	65.65	Y	22.4	Y	15.37	Y	0.016	Y	6.64	N	53.5	Y	108.76	Y	mg/kg
UR-01	UR-01-SS-06	BPSOU-UR01SS06-110321-1-FD	PACE	3.2	Y	6.61	Y	0.13	Y	9.23	Y	42.8	Y	66.37	Y	18.6	Y	19.58	Y	0.017	Y	7.03	N	55.5	Y	112.3	Y	mg/kg
UR-01	UR-01-SS-06	BPSOU-UR01SS06-110321-2	PACE	3.4	Y	7.51	Y	0.18	Y	8.13	N	38.2	Y	50.27	Y	9.1	Y	13.98	Y	0.022	Y	7.69	N	49.9	Y	110.24	Y	mg/kg
UR-01	UR-01-SS-07	BPSOU-UR01SS07-110321-1	PACE	2	Y	7.57	Y	0.17	Y	7.5	N	31.2	Y	63.66	Y	9.2	Y	17.71	Y	0.013	Y	6.55	N	55.5	Y	123.77	Y	mg/kg
UR-01	UR-01-SS-07	BPSOU-UR01SS07-110321-2	PACE	1.5	Y	6.36	Y	0.18	Y	7.85	N	29.5	Y	55.93	Y	5.8	Y	9.67	Y	0.0084	N	7.24	N	46.6	Y	100.93	Y	mg/kg
UR-01	UR-01-SS-07	BPSOU-UR01SS07-110321-3	PACE	2.3	Y	7.3	Y	0.093	Y	9.19	Y	25.9	Y	58.12	Y	4.3	Y	17.27	Y	0.0083	N	6.87	N	38.6	Y	112.12	Y	mg/kg
UR-01	UR-01-SS-08	BPSOU-UR01SS08-110221-1	PACE	3.5	Y	10.37	Y	0.12	Y	7.46	N	41.7	Y	76.26	Y	18.9	Y	19.95	Y	0.019	Y	6.81	N	58.9	Y	120.96	Y	mg/kg
UR-01	UR-01-SS-08	BPSOU-UR01SS08-110221-2	PACE	4.2	Y	9.96	Y	0.14	Y	7.76	N	32.6	Y	63.45	Y	11.7	Y	24.03	Y	0.025	Y	6.93	N	51.6	Y	113.87	Y	mg/kg
UR-01	UR-01-SS-08	BPSOU-UR01SS08-110221-3	PACE	4.1	Y	7.41	N	0.4	Y	9.53	Y	40.1	Y	31.49	Y	12.1	Y	28.02	Y	0.012	Y	8.86	N	73.9	Y	101.85	Y	mg/kg
UR-01	UR-01-SS-10	BPSOU-UR01SS10-110221-2	PACE	4.9	Y	13.61	Y	0.33	Y	7.12	N	47.4	Y	131.6	Y	15	Y	28.89	Y	0.23	Y	6.61	N	78.5	Y	172.46	Y	mg/kg
UR-01	UR-01-SS-10	BPSOU-UR01SS10-110221-3	PACE	4.3	Y	11.09	Y	0.43	Y	6.78	N	64.8	Y	205.84	Y	17.7	Y	46.71	Y	0.55	Y	6.57	N	110	Y	301.58	Y	mg/kg
UR-01	UR-01-SS-11	BPSOU-UR01SS11-110221-2	PACE	4.7	Y	10.55	Y	0.26	Y	10.45	Y	44.6	Y	49.91	Y	26.7	Y	17.07	Y	0.02	Y	7.11	N	83.1	Y	161.57	Y	mg/kg
UR-01	UR-01-SS-11	BPSOU-UR01SS11-110221-3	PACE	7.3	Y	18.42	Y	0.58	Y	7.76	N	61.8	Y	100.03	Y	88.7	Y	95.7	Y	0.097	Y	7.11	N	167	Y	274.76	Y	mg/kg
UR-01	UR-01-SS-12	BPSOU-UR01SS12-110221-2	PACE	18	Y	18.87	Y	0.3	Y	7.68	N	35	Y	37.83	Y	20.6	Y	18.3	Y	0.014	Y	6.81	N	144	Y	145.94	Y	mg/kg
UR-01	UR-01-SS-13	BPSOU-UR01SS13-110221-1	PACE	9.4	Y	11.47	Y	0.3	Y	11	Y	59.2	Y	49.11	Y	25.5	Y	22.52	Y	0.032	Y	7.93	N	113	Y	128.92	Y	mg/kg
UR-01	UR-01-SS-13	BPSOU-UR01SS13-110221-2	PACE	4.9	Y	7.23	N	0.14	Y	12.7	Y	48.8	Y	57.81	Y	12.1	Y	36.74	Y	0.01	Y	7.23	N	78.3	Y	129.28	Y	mg/kg
UR-01	UR-01-SS-13	BPSOU-UR01SS13-110221-3	PACE	2.7	Y	12.29	Y	0.24	Y	9.41	Y	45.9	Y	74.15	Y	7.8	Y	17.39	Y	0.012	Y	6.51	N	79.3	Y	132.37	Y	mg/kg
UR-01	UR-01-SS-15	BPSOU-UR01SS15-110221-1	PACE	8.1	Y	23.97	Y	0.53	Y	7.58	Y	73.2	Y	101.97	Y	75.5	Y	361.91	Y	0.61	Y	6.67	N	168	Y	502.2	Y	mg/kg
UR-01	UR-01-SS-15	BPSOU-UR01SS15-110221-2	PACE	12.2	Y	17.05	Y	1.7	Y	10.24	Y	71.4	Y	103.46	Y	200	Y	157.75	Y	0.23	Y	6.95	N	315	Y	360.53	Y	mg/kg
UR-01	UR-01-SS-15	BPSOU-UR01SS15-110221-3	PACE	8.1	Y	10.2	Y	0.9	Y	12.87	Y	82	Y	91.28	Y	195	Y	47.54	Y	0.15	Y	6.88	N	243	Y	297.98	Y	mg/kg
UR-01	UR-01-SS-16	BPSOU-UR01SS16-110221-2	PACE	11.8	Y	23.77	Y	0.55	Y	7.19	N	46.7	Y	84.12	Y	43.5	Y	71.65	Y	0.11	Y	6.9	N	134	Y	253.47	Y	mg/kg
UR-01	UR-01-SS-16	BPSOU-UR01SS16-110221-3	PACE	6	Y	20.82	Y	0.46	Y	7.3	N	58.9	Y	106.88	Y	55.4	Y	86.25	Y	0.21	Y	6.96	N	138	Y	295.75	Y	mg/kg
UR-01	UR-01-SS-18	BPSOU-UR01SS18-110221-1	PACE	7.2	Y	11.8	Y	0.66	Y	7.24	N	54.7	Y	58.96	Y	80.7	Y	63.03	Y	0.12	Y	6.63	N	200	Y	227.03	Y	mg/kg
UR-01	UR-01-SS-18	BPSOU-UR01SS18-110221-2	PACE	5.1	Y	12.29	Y	0.21	Y	7.63	N	39.4	Y	69.63	Y	26.5	Y	34.61	Y	0.11	Y	6.78	N	79.4	Y	162.58	Y	mg/kg
UR-01	UR-01-SS-18	BPSOU-UR01SS18-110221-3	PACE	5	Y	8.71	Y	0.24	Y	7.69	N	39.4	Y	62.46	Y	23.8	Y	39.53	Y	0.082	Y	7.06	N	76.3	Y	138.98	Y	mg/kg
UR-01	UR-01-SS-19	BPSOU-UR01SS19-110221-1	PACE	5	Y	8.8	Y	0.33	Y	7.6	N	49.9	Y	71.01	Y	39.4	Y	60.56	Y	0.051	Y	7.01	N	114	Y	195.93	Y	mg/kg
UR-01	UR-01-SS-19	BPSOU-UR01SS19-110221-2	PACE	5	Y	12.81	Y	0.3	Y	8.64	N	50.2	Y	53.9	Y	39.1	Y	50.53	Y	0.057	Y	7.8	N	97.2	Y	149.59	Y	mg/kg
UR-01	UR-01-SS-19	BPSOU-UR01SS19-110221-3	PACE	4	Y	9.07	N	0.24	Y	10.38	Y	39.9	Y	48.57	Y	37.2	Y	49.16	Y	0.065	Y	8.57	N	102	Y	179.44	Y	mg/kg
UR-01	UR-01-SS-21	BPSOU-UR01SS21-110221-1	PACE	195	Y	377.35	Y	0.82	Y	7.59	N	398	Y	783.88	Y	119	Y	111.01	Y	0.25	Y	7.2	N	271	Y	319.24	Y	mg/kg
UR-01	UR-01-SS-21	BPSOU-UR01SS21-110221-2	PACE	158	Y	201.24	Y	0.25	Y	7.57	N	224	Y	248.5	Y	35.6	Y	44.26	Y	0.27	Y	6.67	N	96.3	Y	203.76	Y	mg/kg
UR-01	UR-01-SS-21	BPSOU-UR01SS21-110221-3	PACE	167	Y	184.97	Y	0.14	Y	7.71	N	241	Y	273.34	Y	18.2	Y	25.09	Y	0.062	Y	7.08	N	60	Y	103.75	Y	mg/kg
UR-01	UR-01-SS-22	BPSOU-UR01SS22-110221-2	PACE	22.2	Y	34.8	Y	0.49	Y	7.81	N	30.4	Y	42.46	Y	12.7	Y	21.66	Y	0.029	Y	6.79	N	42	Y	90.44	Y	mg/kg
UR-01	UR-01-SS-23	BPSOU-UR01SS23-110221-1	PACE	31.3	Y	21.81	N	9.4	Y	7.37	N	180	Y	218.46	Y	656	Y	590.29	Y	0.61	Y	7.28	N	2010	Y	1515.18	Y	mg/kg
UR-01	UR-01-SS-23	BPSOU-UR01SS23-110221-2	PACE	60.1	Y	97.64	Y	79.2	Y	10.27	Y	569	Y	688.3	Y	2850	Y	1579.49	Y	2.4	Y	8.15	N	22800	Y	1458.42	Y	mg/kg
UR-01	UR-01-SS-23	BPSOU-UR01SS23-110221-3	PACE	51.7	Y	82.46	Y	6	Y	7.46	N	285	Y	381.88	Y	1340	Y	967.11	Y	1.2	Y	7.77	N	1310	Y	1425.47	Y	mg/kg
UR-01	UR-01-SS-24	BPSOU-UR01SS24-110221-1	PACE	6.4	Y	10.09	Y	0.5	Y	6.8	N	49.5	Y	90.55	Y	47.3	Y	55.76	Y	0.069	Y	6.03	N	147	Y	217.63	Y	mg/kg
UR-01	UR-01-SS-25	BPSOU-UR01SS25-110221-1	PACE	7.1	Y	12.45	Y	0.49	Y	6.93	N	55.4	Y	76.37	Y	54.2	Y	63.1	Y	0.052	Y	6.35	N	155	Y	199.71	Y	mg/kg
UR-01	UR-01-SS-25	BPSOU-UR01SS25-110221-1-FD	PACE	4.8	Y	12.85	Y	0.33	Y	6.5	N	42.3	Y	87.31	Y	54.7	Y	51.22	Y	0.033	Y	5.88	N	113	Y	213.02	Y	mg/kg
UR-01	UR-01-SS-25	BPSOU-UR01SS25-110221-2	PACE	6.9	Y	17.74	Y	0.44	Y	7.08	N	55.5	Y	98.84	Y	58.9	Y	72.18	Y	0.042	Y	6.58	N	149	Y	233.38	Y	mg/kg
UR-01	UR-01-SS-26	BPSOU-UR01SS26-110221-2	PACE	14.8	Y	23	Y	2.8	Y	9.14	Y	77.7	Y	84.51	Y	148	Y	116.97	Y	0.092	Y	6.83	N	334	Y	337.29	Y	mg/kg
UR-01	UR-01-SS-26	BPSOU-UR01SS26-110221-3	PACE	15.5	Y	19.56	Y	1.9	Y	7.59	N	92.5	Y	105.37	Y	288	Y	159.78	Y	0.21	Y	6.81	N	405	Y	341.91	Y	mg/kg
UR-01	UR-01-SS-27	BPSOU-UR01SS27-110221-3	PACE	6.1	Y	9.93	Y	0.35	Y	7.66	N	64.5	Y	93.76	Y	25.3	Y	37.26	Y	0.034	Y	6.61	N	98.6	Y	148.24	Y	mg/kg
UR-03	UR-03-SS-01	BPSOU-UR03SS01-102821-1	PACE	255	Y	295.01	Y	1.7	Y	7.68	N	199	Y	228.15	Y	177	Y	211.3	Y	0.47	Y	7.36	Y	270	Y	196.94	Y	mg/kg
UR-03	UR-03-SS-01	BPSOU-UR03SS01-102821-1-FD	PACE	229	Y	297.61	Y	0.44	Y	8	Y	161	Y	164.93	Y	161	Y	206.76	Y	0.38	Y	7.08	N	171	Y	180.56	Y	mg/kg
UR-03	UR-03-SS-01	BPSOU-UR03SS01-102821-2	PACE	294	Y	344.7	Y	2.4	Y	7.42	N	223	Y	201.86	Y	230	Y	215.04	Y	0.32	Y	7.37	N	352	Y	320.45	Y	mg/kg
UR-03	UR-03-SS-01	BPSOU-UR03SS01-102821-3	PACE	216	Y	230.44	Y	1.2	Y	7.8	N	170	Y	144.15	Y	523	Y	232.66	Y	0.51	Y	7.08	N	359	Y	302.84	Y	mg/kg
UR-03	UR-03-SS-02	BPSOU-UR03SS02-102821-1	PACE	184	Y	231.66	Y	0.25	Y	7.29	N	45.7	Y	81.27	Y	70.1	Y	97.75	Y	0.12	Y	6.61	N	114	Y	180.5	Y	mg/kg
UR-03	UR-03-SS-02	BPSOU-UR03SS02-102821-3	PACE	118	Y	196.23	Y	0.4	Y	7.28	N	127	Y	111.65	Y	126	Y	101.49	Y	0.1	Y	6.63	N	211	Y	227.12	Y	mg/kg

Table 2. Sample Results Used in the XRF to Laboratory Correlation and Regression Analyses

Color Coding in the Station Name Column

Sample is a Field Duplicate collected for QA/QC.

Color Coding in the Analyte Result Columns

Mercury was re-collected and analyzed due to temperature exceedance upon arrival at the Pace Lab.

There was only Mercury XRF and lab result for this sample. Therefore this point was only used in the Mercury regression.

The XRF Results are Non-Detect. This sample pair was not used in the XRF to lab Regression Analysis. The non-detect XRF concentrations listed in this table are the XRF confidence interval values.

These points were identified as outliers and were not used in the final regression analyses.

Site	Station Name	Field Sample ID (XRF)*	Lab (ICP)	Arsenic (ICP)	Arsenic (ICP) Detect	Arsenic (XRF)	Arsenic (XRF) Detect	Cadmium (ICP)	Cadmium (ICP) Detect	Cadmium (XRF)	Cadmium (XRF) Detect	Copper (ICP)	Copper (ICP) Detect	Copper (XRF)	Copper (XRF) Detect	Lead (ICP)	Lead (ICP) Detect	Lead (XRF)	Lead (XRF) Detect	Mercury (ICP)	Mercury (ICP) Detect	Mercury (XRF)	Mercury (XRF) Detect	Zinc (ICP)	Zinc (ICP) Detect	Zinc (XRF)	Zinc (XRF) Detect	Units
UR-03	UR-03-SS-03	BPSOU-UR03SS03-102821-1	PACE	159	Y	167.61	Y	0.22	Y	7.03	N	135	Y	102.08	Y	127	Y	122.31	Y	0.19	Y	6.36	N	72.4	Y	81.28	Y	mg/kg
UR-03	UR-03-SS-03	BPSOU-UR03SS03-102821-2	PACE	184	Y	269.03	Y	0.15	Y	7.09	N	97.5	Y	115.28	Y	126	Y	149.69	Y	0.16	Y	6.41	N	54.3	Y	82.62	Y	mg/kg
UR-03	UR-03-SS-03	BPSOU-UR03SS03-102821-3	PACE	172	Y	289.15	Y	0.16	Y	8.86	Y	100	Y	136.46	Y	147	Y	206.85	Y	0.21	Y	6.89	N	82.5	Y	123.73	Y	mg/kg
UR-03	UR-03-SS-04	BPSOU-UR03SS04-102821-1	PACE	229	Y	373.71	Y	0.12	Y	9.45	Y	81.3	Y	112.52	Y	225	Y	299.8	Y	0.075	Y	6.73	N	55	Y	91.98	Y	mg/kg
UR-03	UR-03-SS-04	BPSOU-UR03SS04-102821-2	PACE	266	Y	398.11	Y	0.15	Y	7.44	N	95	Y	119.28	Y	361	Y	513.93	Y	0.098	Y	7	N	72.2	Y	110.38	Y	mg/kg
UR-03	UR-03-SS-04	BPSOU-UR03SS04-102821-3	PACE	288	Y	393.78	Y	0.37	Y	8.49	Y	110	Y	135.99	Y	634	Y	685.56	Y	0.22	Y	6.9	N	127	Y	125.58	Y	mg/kg
UR-05	UR-05-SS-02	BPSOU-UR05SS02-110421-1	PACE	161	Y	284.08	Y	4.7	Y	7.88	N	359	Y	763.22	Y	636	Y	816.97	Y	0.25	Y	9.27	N	1520	Y	2477.02	Y	mg/kg
UR-05	UR-05-SS-02	BPSOU-UR05SS02-110421-1-FD	PACE	203	Y	220.14	Y	4.6	Y	9.75	Y	519	Y	559.1	Y	630	Y	565.05	Y	0.2	Y	8.69	N	1720	Y	2285.46	Y	mg/kg
UR-05	UR-05-SS-02	BPSOU-UR05SS02-110421-2	PACE	145	Y	225.63	Y	3.6	Y	7.78	N	658	Y	1009.67	Y	639	Y	740.92	Y	0.31	Y	8.43	N	1380	Y	1784.01	Y	mg/kg
UR-05	UR-05-SS-02	BPSOU-UR05SS02-110421-3	PACE	62.3	Y	105.68	Y	3.8	Y	7.96	N	235	Y	435.64	Y	756	Y	671.16	Y	0.26	Y	9.01	N	1500	Y	2289	Y	mg/kg
UR-05	UR-05-SS-03	BPSOU-UR05SS03-110421-1	PACE	234	Y	313.89	Y	8.7	Y	12.07	Y	1120	Y	1216.2	Y	1980	Y	1170.94	Y	0.8	Y	9.79	N	2450	Y	3031.58	Y	mg/kg
UR-05	UR-05-SS-03	BPSOU-UR05SS03-110421-2	PACE	145	Y	117.58	Y	5.3	Y	17.63	Y	49500	Y	1024.87	Y	1190	Y	869.47	Y	0.45	Y	10.28	N	1840	Y	1553.31	Y	mg/kg
UR-05	UR-05-SS-03	BPSOU-UR05SS03-110421-3	PACE	117	Y	222.28	Y	4	Y	11.51	Y	426	Y	1051.54	Y	944	Y	1308.11	Y	0.65	Y	8.74	N	1630	Y	2267.83	Y	mg/kg
UR-05	UR-05-SS-04	BPSOU-UR05SS04-110421-1	PACE	37.9	Y	91.92	Y	1.6	Y	7.45	N	248	Y	390.21	Y	216	Y	456.39	Y	0.15	Y	7.64	N	506	Y	1192.12	Y	mg/kg
UR-05	UR-05-SS-04	BPSOU-UR05SS04-110421-2	PACE	35.5	Y	91.33	Y	1.6	Y	10.2	Y	250	Y	345.69	Y	571	Y	694.04	Y	0.16	Y	8.1	N	646	Y	1638.76	Y	mg/kg
UR-05	UR-05-SS-04	BPSOU-UR05SS04-110421-3	PACE	47.3	Y	79.55	Y	3.3	Y	8.02	N	238	Y	305.56	Y	812	Y	734.69	Y	0.26	Y	8.42	N	1180	Y	1765.97	Y	mg/kg
UR-05	UR-05-SS-05	BPSOU-UR05SS05-110421-1	PACE	12.2	Y	12.78	Y	0.68	Y	7.73	N	214	Y	219.27	Y	43.2	Y	46.79	Y	0.029	Y	6.81	N	206	Y	239	Y	mg/kg
UR-05	UR-05-SS-05	BPSOU-UR05SS05-110421-2	PACE	9.3	Y	19.68	Y	0.27	Y	7.33	N	151	Y	240.93	Y	26.6	Y	27.23	Y	0.038	Y	6.69	N	58.3	Y	126.44	Y	mg/kg
UR-05	UR-05-SS-05	BPSOU-UR05SS05-110421-3	PACE	19.9	Y	28.13	Y	0.32	Y	7.69	N	146	Y	196.23	Y	28.3	Y	39.26	Y	0.068	Y	6.99	N	85	Y	167.24	Y	mg/kg
UR-09	UR-09-SS-01	BPSOU-UR09-110118-0-2-01	PACE	402	Y	278.39	Y	0.1	N	6.29	Y	110	Y	82.61	Y	686	Y	162.09	Y	0.99	Y	6.34	N	324	Y	244.57	Y	mg/kg
UR-09	UR-09-SS-01	BPSOU-UR09-110118-2-6-01	PACE	411	Y	308.4	Y	0.099	N	5.98	N	63.2	Y	52.95	Y	139	Y	70.42	Y	0.43	Y	6.19	N	225	Y	127.89	Y	mg/kg
UR-09	UR-09-SS-04	BPSOU-UR09-110118-6-12-04	PACE	336	Y	195.81	Y	1.1	Y	6.19	N	130	Y	125.96	Y	353	Y	667.72	Y	0.27	Y	6.89	N	392	Y	361.82	Y	mg/kg
UR-09	UR-09-SS-07	BPSOU-UR09-103118-0-2-07	PACE	51	Y	40.59	Y	7.9	Y	9.68	Y	370	Y	341.07	Y	944	Y	525.39	Y	0.33	Y	7.57	N	1800	Y	1362.85	Y	mg/kg
UR-09	UR-09-SS-07	BPSOU-UR09-103118-2-6-07	PACE	70.9	Y	81.54	Y	7.2	Y	10.38	Y	357	Y	410.22	Y	897	Y	1128.37	Y	1	Y	8.37	N	1870	Y	2268.8	Y	mg/kg
UR-09	UR-09-SS-07	BPSOU-UR09-103118-6-12-07	PACE	46.1	Y	41.39	Y	2.3	Y	7.55	Y	139	Y	171.89	Y	547	Y	564.31	Y	0.61	Y	7.45	N	925	Y	1087.51	Y	mg/kg
UR-09	UR-09-SS-08	BPSOU-UR09-103118-6-12-08	PACE	78.8	Y	73.68	Y	3.6	Y	6.79	N	66.8	Y	92.72	Y	597	Y	615.78	Y	0.33	Y	8.49	N	1340	Y	1380.49	Y	mg/kg
UR-09	UR-09-SS-12	BPSOU-UR09-103118-0-2-12	PACE	8.8	Y	21.49	Y	0.88	Y	6.26	N	55.2	Y	145.52	Y	73.7	Y	236.79	Y	0.026	Y	7.06	N	344	Y	1513.32	Y	mg/kg
UR-24	UR-24-OP-01	BPSOU-UR24OP01-090121-2	PACE	102	Y	224.29	Y	1.4	Y	7.4	N	64.7	Y	125.84	Y	169	Y	300.07	Y	0.075	Y	7.28	N	502	Y	793.79	Y	mg/kg
UR-24	UR-24-SS-01	BPSOU-UR24SS01-090121-2	PACE	72.5	Y	151.44	Y	0.7	Y	11.25	Y	55	Y	86.74	Y	158	Y	249.75	Y	0.065	Y	6.89	N	207	Y	354.56	Y	mg/kg
UR-24	UR-24-SS-03	BPSOU-UR24SS03-090121-1	PACE	83.1	Y	155.83	Y	2.4	Y	9.84	Y	118	Y	162.49	Y	152	Y	219.58	Y	0.12	Y	7.56	N	847	Y	1156.59	Y	mg/kg
UR-24	UR-24-SS-03	BPSOU-UR24SS03-090121-2	PACE	104	Y	191.72	Y	2.7	Y	7.1	N	167	Y	289.25	Y	194	Y	261.81	Y	0.17	Y	7.2	N	1070	Y	1532.8	Y	mg/kg
UR-24	UR-24-SS-03	BPSOU-UR24SS03-090121-3	PACE	269	Y	374.51	Y	4.2	Y	7.11	N	258	Y	314.4	Y	512	Y	572.12	Y	0.23	Y	8.61	N	1620	Y	1961.57	Y	mg/kg
UR-24	UR-24-SS-03	BPSOU-UR24SS03-090121-3-FD	PACE	251	Y	380.58	Y	4.1	Y	7.23	N	230	Y	262.67	Y	475	Y	512.2	Y	0.31	Y	7.63	N	1420	Y	1463.02	Y	mg/kg
UR-30	UR-30-OP-01	BPSOU-UR30OP01-110821-2	PACE	20.1	Y	20.53	Y	0.6	Y	11.44	Y	76.5	Y	84.32	Y	66.1	Y	64.05	Y	0.028	Y	6.3	N	234	Y	213.93	Y	mg/kg
UR-30	UR-30-OP-01	BPSOU-UR30OP01-110821-2-FD	PACE	18.7	Y	30.98	Y	0.59	Y	10.19	Y	68.1	Y	69.46	Y	62.1	Y	72.09	Y	0.029	Y	5.81	N	237	Y	228.56	Y	mg/kg
UR-30	UR-30-OP-02	BPSOU-UR30OP02-110821-2	PACE	28.9	Y	44.97	Y	1.3	Y	6.9	N	206	Y	288.51	Y	178	Y	227.33	Y	0.11	Y	6.75	N	305	Y	444.84	Y	mg/kg
UR-30	UR-30-OP-02	BPSOU-UR30OP02-110821-3	PACE	37.3	Y	57.49	Y	1.2	Y	7.31	N	194	Y	273.53	Y	115	Y	152.28	Y	0.078	Y	6.58	N	336	Y	457.1	Y	mg/kg
UR-30	UR-30-SS-01	BPSOU-UR30SS01-110821-1	PACE	19.2	Y	39.87	Y	1.2	Y	7.88	N	316	Y	439.68	Y	81.5	Y	125.36	Y	0.099	Y	7.59	N	758	Y	536.52	Y	mg/kg
UR-30	UR-30-SS-01	BPSOU-UR30SS01-110821-2	PACE	19	Y	37.6	Y	0.63	Y	13.05	Y	326	Y	484.21	Y	40.7	Y	46.78	Y	0.05	Y	7.83	N	424	Y	256.37	Y	mg/kg
UR-30	UR-30-SS-01	BPSOU-UR30SS01-110821-3	PACE	16.4	Y	37.09	Y	0.41	Y	7.85	N	323	Y	469.15	Y	36.7	Y	66.89	Y	0.056	Y	7.75	N	193	Y	489.81	Y	mg/kg
UR-30	UR-30-SS-01	BPSOU-UR30SS01-110821-3-FD	PACE	11.8	Y	36.38	Y	0.39	Y	7.85	N	290	Y	411.7	Y	25.4	Y	80.78	Y	0.049	Y	7.04	N	170	Y	306.34	Y	mg/kg
UR-30	UR-30-SS-02	BPSOU-UR30SS02-110821-1	PACE	24.4	Y	44.76	Y	0.52	Y	7.59	N	180	Y	247.04	Y	47.6	Y	68.54	Y	0.042	Y	6.81	N	105	Y	147.28	Y	mg/kg
UR-30	UR-30-SS-02	BPSOU-UR30SS02-110821-2	PACE	14.8	Y	30.74	Y	0.15	Y	8.15	N	656	Y	570.93	Y	5.6	Y	18.4	Y	0.01	Y	7.39	N	54.8	Y	70.05	Y	mg/kg
UR-30	UR-30-SS-02	BPSOU-UR30SS02-110821-3	PACE	15.7	Y	38.04	Y	0.036	N	8.37	N	456	Y	797.32	Y	2	Y	8.58	Y	0.0087	N	7.83	N	39.2	Y	80.71	Y	mg/kg
UR-30	UR-30-SS-03	BPSOU-UR30SS03-110821-1	PACE	16.4	Y	30.92	Y	0.55	Y	7.46	N	251	Y	293.36	Y	66.2	Y	70.76	Y	0.039	Y	7.13	N	235	Y	217.41	Y	mg/kg
UR-30	UR-30-SS-03	BPSOU-UR30SS03-110821-2	PACE	18.6	Y	33.69	Y	0.57	Y	10.49	Y	216	Y	189.09	Y	69.1	Y	173.17	Y	0.053	Y	7.48	N	149	Y	254.37	Y	mg/kg
UR-30	UR-30-SS-03	BPSOU-UR30SS03-110821-3	PACE	19.7	Y	40.47	Y	0.63	Y	7.54	N	225	Y	304.52	Y	131	Y	123.33	Y	0.041	Y	7.19	N	138	Y	234.65	Y	mg/kg
UR-30	UR-30-SS-04	BPSOU-UR30SS04-110821-1	PACE	41.8	Y	65.82	Y	1.7	Y	7.42	N	198	Y	294.32	Y	119	Y	138.71	Y	0.084	Y	6.77	N	636	Y	694.55	Y	mg/kg
UR-30	UR-30-SS-04	BPSOU-UR30SS04-110821-2	PACE	24.8	Y	57.35	Y	2.7	Y	7.91	Y	146	Y	281.05	Y	109	Y	137.11	Y	0.076	Y	6.81	N	624	Y	714.41	Y	mg/kg
UR-30	UR-30-SS-04	BPSOU-UR30SS04-110821-3	PACE	21.9	Y	45.47	Y	1.6	Y	8.39	Y	130	Y	228.92	Y	87.8	Y	225.85	Y	0.083	Y	6.77	N	444	Y	882.5	Y	mg/kg
UR-30	UR-30-SS-05	BPSOU-UR30SS05-110821-1	PACE	13.2	Y	9.34	N	0.73	Y	17.2	Y	201	Y	97.59	Y	73.5	Y	66.06	Y	0.044	Y	7.84	N	309	Y	179.16	Y	mg/kg
UR-32	UR-32-OP-01	BPSOU-UR32OP01-110921-2	PACE	42.1	Y	65.34	Y	2.8	Y	6.9	N	306	Y	446.79	Y	663	Y	692.14	Y	18.2	Y	8.01	N	849	Y	811.54	Y	mg/kg
UR-32	UR-32-SS-01	BPSOU-UR32-063021-0-2-01	PACE	45.8	Y	70.25	Y	1.7	Y	13.21	Y	453	Y	689.91	Y	490	Y	515.89	Y	1.7	Y	7.25	N	556	Y	609.13	Y	mg/kg
UR-32	UR-32-SS-01	BPSOU-UR32SS01-082621-1	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	3.2	Y	7.25	N	NA	NA	NA	NA	mg/kg
UR-32	UR-32-SS-01	BPSOU-UR32-063021-2-6-02	PACE	155	Y	215.84	Y	4.6	Y	6.48	N	667	Y	726.68	Y	1770	Y	1525.93	Y	31.7	Y	22.57	Y	1040	Y	1154.06	Y	mg/kg
UR-32	UR-32-SS-01	BPSOU-UR32SS01-082621-2	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	7.9	Y	22.57	Y	NA	NA	NA	NA	mg/kg
UR-32	UR-32-SS-02	BPSOU-UR32-063021-0-2-04	PACE	29.4	Y	57.17	Y	2.4	Y	12.96	Y	153	Y	247.18	Y	2160	Y	1551.84	Y	1.8	Y	8.35	N	1050	Y	1154.92	Y	mg/kg
UR-32	UR-32-SS-02	BPSOU-UR32SS02-082621-1	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1.9	Y	8.35	N	NA	NA	NA	NA	mg/kg
UR-32	UR-32-SS-03	BPSOU-UR32-063021-6-12-09	PACE	4.7	Y	10.59	Y	0.16	Y	6.92	N	585	Y	313.73	Y	30.9	Y	57.99	Y	0.13	Y	6.64	N	93.5	Y	145.67	Y	mg/kg
UR-32	UR-32-SS-03	BPSOU-UR32SS03-082621-3	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1.9	Y	6.64	N	NA	NA	NA	NA	mg/kg
UR-32	UR-32-SS-03	BPSOU-UR32SS03-082621-3-FD	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2.1	Y	5.64	N	NA	NA	NA	NA	mg/kg
UR-32	UR-32-SS-03	BPSOU-UR32-063021-6-12-09-FD	PACE	6.2	Y	8.3	Y	0.17	Y	4.7	N	370	Y	261	Y	44.3	Y	36.47	Y	0.25	Y	5.64	N	104	Y	170.17	Y	mg/kg

Table 2. Sample Results Used in the XRF to Laboratory Correlation and Regression Analyses

Color Coding in the Station Name Column

Sample is a Field Duplicate collected for QA/QC.

Color Coding in the Analyte Result Columns

Mercury was re-collected and analyzed due to temperature exceedance upon arrival at the Pace Lab.

There was only Mercury XRF and lab result for this sample. Therefore this point was only used in the Mercury regression.

The XRF Results are Non-Detect. This sample pair was not used in the XRF to lab Regression Analysis. The non-detect XRF concentrations listed in this table are the XRF confidence interval values.

These points were identified as outliers and were not used in the final regression analyses.

Site	Station Name	Field Sample ID (XRF)*	Lab (ICP)	Arsenic (ICP)	Arsenic (ICP) Detect	Arsenic (XRF)	Arsenic (XRF) Detect	Cadmium (ICP)	Cadmium (ICP) Detect	Cadmium (XRF)	Cadmium (XRF) Detect	Copper (ICP)	Copper (ICP) Detect	Copper (XRF)	Copper (XRF) Detect	Lead (ICP)	Lead (ICP) Detect	Lead (XRF)	Lead (XRF) Detect	Mercury (ICP)	Mercury (ICP) Detect	Mercury (XRF)	Mercury (XRF) Detect	Zinc (ICP)	Zinc (ICP) Detect	Zinc (XRF)	Zinc (XRF) Detect	Units
UR-33	UR-33-SS-03	BPSOU-UR33SS03-090921-2	PACE	1.2	Y	4.77	N	0.11	Y	6.94	Y	4.8	Y	21.67	Y	7.1	Y	15.7	Y	0.0092	N	5.45	N	51.8	Y	80.89	Y	mg/kg
UR-33	UR-33-SS-05	BPSOU-UR33SS05-090921-3	PACE	6.4	Y	10.62	Y	0.73	Y	7.1	N	15.5	Y	17.84	Y	4	Y	19.67	Y	0.0093	N	5.91	N	121	Y	165.9	Y	mg/kg
UR-33	UR-33-SS-05	BPSOU-UR33SS05-090921-3-FD	PACE	6.3	Y	13.69	Y	0.79	Y	7.06	N	15.2	Y	26.8	Y	3.7	Y	21.67	Y	0.0096	N	5.67	N	131	Y	162.87	Y	mg/kg
UR-34	UR-34-OP-01	BPSOU-UR34OP01-111021-1	PACE	13.5	Y	15.38	Y	6	Y	14.7	Y	57.2	Y	78.27	Y	63.3	Y	69.11	Y	0.043	Y	6.97	N	1970	Y	1688.12	Y	mg/kg
UR-34	UR-34-OP-01	BPSOU-UR34OP01-111021-2	PACE	26.7	Y	36.83	Y	6.2	Y	8.99	Y	69.7	Y	94.47	Y	105	Y	101.54	Y	0.041	Y	7.35	N	1920	Y	2324.14	Y	mg/kg
UR-34	UR-34-OP-01	BPSOU-UR34OP01-111021-3	PACE	20.6	Y	34.63	Y	5	Y	7.3	N	99.3	Y	108.08	Y	48	Y	67.34	Y	0.039	Y	7.56	N	1850	Y	2303.24	Y	mg/kg
UR-34	UR-34-SS-01	BPSOU-UR34SS01-111021-1	PACE	64.1	Y	95.48	Y	3.4	Y	7.44	N	303	Y	401.33	Y	391	Y	437.79	Y	0.14	Y	7.73	N	1360	Y	1642.28	Y	mg/kg
UR-34	UR-34-SS-01	BPSOU-UR34SS01-111021-2	PACE	57.5	Y	98.55	Y	3.8	Y	7.7	N	220	Y	370.24	Y	359	Y	413.82	Y	0.13	Y	7.81	N	1170	Y	1486.68	Y	mg/kg
UR-34	UR-34-SS-01	BPSOU-UR34SS01-111021-3	PACE	52.3	Y	77.77	Y	3.2	Y	7.8	N	118	Y	191.71	Y	356	Y	573.52	Y	0.18	Y	7.97	N	1130	Y	1600.67	Y	mg/kg
UR-34	UR-34-SS-02	BPSOU-UR34SS02-111021-1	PACE	77.5	Y	103.71	Y	5.4	Y	14.01	Y	132	Y	164.63	Y	337	Y	557.46	Y	0.18	Y	8.13	N	1480	Y	1975.29	Y	mg/kg
UR-34	UR-34-SS-02	BPSOU-UR34SS02-111021-2	PACE	94.5	Y	129.7	Y	5.5	Y	12.7	Y	107	Y	144.14	Y	970	Y	677.54	Y	0.19	Y	7.9	N	1520	Y	1687.58	Y	mg/kg
UR-34	UR-34-SS-02	BPSOU-UR34SS02-111021-3	PACE	77.4	Y	105.87	Y	12.9	Y	23.42	Y	96.3	Y	148.09	Y	630	Y	613.1	Y	0.21	Y	9.12	N	2480	Y	3420.79	Y	mg/kg
UR-34	UR-34-SS-03	BPSOU-UR34SS03-111021-1	PACE	44.8	Y	99.18	Y	6.3	Y	15.43	Y	280	Y	472.2	Y	501	Y	780.14	Y	0.77	Y	9.32	N	2410	Y	3554.17	Y	mg/kg
UR-34	UR-34-SS-03	BPSOU-UR34SS03-111021-2	PACE	50.5	Y	114.25	Y	6.5	Y	11.85	Y	181	Y	326.3	Y	567	Y	1057.32	Y	0.65	Y	9.73	N	2320	Y	3759.53	Y	mg/kg
UR-34	UR-34-SS-03	BPSOU-UR34SS03-111021-2-FD	PACE	65.8	Y	102.92	Y	7.2	Y	11.76	Y	197	Y	316.5	Y	680	Y	885.87	Y	0.61	Y	9.73	N	2470	Y	3470.28	Y	mg/kg
UR-34	UR-34-SS-03	BPSOU-UR34SS03-111021-3	PACE	39.1	Y	68.77	Y	5	Y	12.04	Y	138	Y	262.7	Y	417	Y	505.99	Y	0.17	Y	8.95	N	2010	Y	3426.09	Y	mg/kg
UR-35	UR-35-OP-01	BPSOU-UR35OP01-090821-3	PACE	67	Y	193.47	Y	20	Y	29.77	Y	449	Y	578.65	Y	5690	Y	5412.23	Y	1	Y	16	N	6470	Y	13258.8	Y	mg/kg
UR-35	UR-35-SS-02	BPSOU-UR35SS02-090821-1	PACE	57	Y	61.91	Y	7	Y	7.72	N	563	Y	996.15	Y	1100	Y	1409.22	Y	0.3	Y	9.88	N	2410	Y	3690.9	Y	mg/kg
UR-35	UR-35-SS-02	BPSOU-UR35SS02-090821-2	PACE	129	Y	152.84	Y	13.8	Y	14.96	Y	983	Y	1180.62	Y	3760	Y	2928.28	Y	0.8	Y	11.05	N	4230	Y	5025.02	Y	mg/kg
UR-35	UR-35-SS-02	BPSOU-UR35SS02-090821-2-FD	PACE	99.1	Y	246.79	Y	10.6	Y	21.64	Y	758	Y	1135.88	Y	3960	Y	4056.24	Y	1	Y	12.69	N	3480	Y	6180.56	Y	mg/kg
UR-35	UR-35-SS-03	BPSOU-UR35SS03-090821-2	PACE	111	Y	126.35	Y	24.2	Y	37.47	Y	430	Y	954.51	Y	6090	Y	5464.07	Y	0.67	Y	18.97	N	10100	Y	20954.91	Y	mg/kg
UR-36	UR-36-OP-01	BPSOU-UR36OP01-090821-1	PACE	143	Y	160.81	Y	2.9	Y	7.71	N	850	Y	1013.44	Y	647	Y	372.53	Y	0.18	Y	8.8	N	1780	Y	1892.72	Y	mg/kg
UR-36	UR-36-OP-01	BPSOU-UR36OP01-090821-2	PACE	189	Y	149.22	Y	2.9	Y	10.61	Y	915	Y	1145.04	Y	867	Y	395.1	Y	0.21	Y	9.02	N	1550	Y	2303.35	Y	mg/kg
UR-36	UR-36-OP-01	BPSOU-UR36OP01-090821-3	PACE	130	Y	149.84	Y	2.3	Y	7.67	N	790	Y	1118.86	Y	285	Y	507.25	Y	0.17	Y	8.49	N	1020	Y	1383.73	Y	mg/kg
UR-36	UR-36-SS-01	BPSOU-UR36SS01-090721-1	PACE	437	Y	517.92	Y	3.2	Y	7.96	N	1270	Y	1438.59	Y	686	Y	754.74	Y	0.17	Y	9.41	N	1120	Y	1542.2	Y	mg/kg
UR-36	UR-36-SS-01	BPSOU-UR36SS01-090721-2	PACE	401	Y	479.85	Y	1.8	Y	8.17	Y	843	Y	1064.5699	Y	824	Y	833.41	Y	0.31	Y	8.71	N	637	Y	898.93	Y	mg/kg
UR-36	UR-36-SS-02	BPSOU-UR36SS02-090721-1	PACE	153	Y	193.07	Y	0.5	Y	8.88	Y	719	Y	1092.45	Y	249	Y	375.35	Y	0.13	Y	7.89	N	345	Y	709.82	Y	mg/kg
UR-36	UR-36-SS-04	BPSOU-UR36SS04-090721-1	PACE	90.9	Y	113.47	Y	2.4	Y	7.79	N	963	Y	1139.16	Y	445	Y	558.21	Y	0.13	Y	8.83	N	1420	Y	2389.68	Y	mg/kg
UR-36	UR-36-SS-04	BPSOU-UR36SS04-090721-1-FD	PACE	80.2	Y	127.6	Y	2.2	Y	7.75	N	863	Y	1098.22	Y	387	Y	487.25	Y	0.22	Y	9.17	N	1300	Y	2761.23	Y	mg/kg
UR-36	UR-36-SS-04	BPSOU-UR36SS04-090721-2	PACE	89.8	Y	121.38	Y	1.9	Y	11.4	Y	794	Y	961.81	Y	463	Y	426.31	Y	0.12	Y	9	N	1120	Y	2666.43	Y	mg/kg
UR-36	UR-36-SS-04	BPSOU-UR36SS04-090721-3	PACE	202	Y	103.2	Y	4.7	Y	8.66	Y	1090	Y	1329.67	Y	476	Y	481.01	Y	0.17	Y	8.24	N	1100	Y	1804.24	Y	mg/kg
UR-36	UR-36-SS-05	BPSOU-UR36SS05-090821-1	PACE	106	Y	261.77	Y	2.1	Y	13.9	Y	723	Y	1044.04	Y	613	Y	938.06	Y	0.15	Y	8.79	N	1140	Y	1614.46	Y	mg/kg
UR-36	UR-36-SS-05	BPSOU-UR36SS05-090821-2	PACE	119	Y	155.72	Y	5.2	Y	9.58	Y	978	Y	1186.5601	Y	1020	Y	724.99	Y	0.45	Y	8.72	N	1990	Y	1896.49	Y	mg/kg
UR-36	UR-36-SS-05	BPSOU-UR36SS05-090821-3	PACE	108	Y	149.53	Y	7.7	Y	13.16	Y	851	Y	1147.78	Y	766	Y	648.18	Y	0.61	Y	9.27	N	2970	Y	3399.43	Y	mg/kg
UR-36	UR-36-SS-06	BPSOU-UR36SS06-090821-1	PACE	135	Y	175.3	Y	3.9	Y	13.62	Y	3370	Y	3190.03	Y	960	Y	1278.4	Y	0.058	Y	20.59	N	7490	Y	8077.37	Y	mg/kg
UR-36	UR-36-SS-06	BPSOU-UR36SS06-090821-2	PACE	92.4	Y	115.46	Y	3.9	Y	8.69	N	2100	Y	1573.74	Y	1540	Y	868.37	Y	0.18	Y	12.87	N	4750	Y	3812.93	Y	mg/kg
UR-36	UR-36-SS-06	BPSOU-UR36SS06-090821-3	PACE	68.2	Y	108.95	Y	4.1	Y	8.01	N	1040	Y	1008.49	Y	992	Y	1050.87	Y	0.34	Y	11.05	N	3480	Y	3098.76	Y	mg/kg
UR-38	UR-38-SS-01	BPSOU-UR38SS01-090921-1	PACE	241	Y	306.87	Y	6.7	Y	18.69	Y	119	Y	136.69	Y	2170	Y	1035.67	Y	0.51	Y	8.3	N	1300	Y	1131.11	Y	mg/kg
UR-38	UR-38-SS-01	BPSOU-UR38SS01-090921-2	PACE	281	Y	399.46	Y	4.9	Y	7.76	N	56.8	Y	69.17	Y	959	Y	1009.33	Y	0.52	Y	7.49	N	917	Y	550.05	Y	mg/kg
UR-38	UR-38-SS-01	BPSOU-UR38SS01-090921-3	PACE	278	Y	352.06	Y	4.8	Y	10.23	Y	72.7	Y	74.14	Y	1650	Y	1086.89	Y	0.52	Y	7.92	N	780	Y	622.61	Y	mg/kg
UR-38	UR-38-SS-02	BPSOU-UR38SS02-090921-1	PACE	132	Y	134.94	Y	4.9	Y	7.85	N	27.1	Y	36.12	Y	592	Y	819.41	Y	0.55	Y	8.14	N	986	Y	1078.59	Y	mg/kg
UR-38	UR-38-SS-02	BPSOU-UR38SS02-090921-2	PACE	132	Y	167.68	Y	6.7	Y	9.3	Y	38.4	Y	72.24	Y	918	Y	959	Y	0.66	Y	8.47	N	1060	Y	1736.28	Y	mg/kg
UR-38	UR-38-SS-02	BPSOU-UR38SS02-090921-3	PACE	137	Y	155.34	Y	8.1	Y	22.38	Y	26.6	Y	51.52	Y	2530	Y	1920.31	Y	0.62	Y	8.91	N	862	Y	1289.69	Y	mg/kg
UR-38	UR-38-SS-03	BPSOU-UR38SS03-090921-2	PACE	132	Y	105.23	Y	1.7	Y	7.41	N	19.2	Y	26.24	Y	877	Y	237.9	Y	0.16	Y	6.94	N	377	Y	630.8	Y	mg/kg
UR-38	UR-38-SS-03	BPSOU-UR38SS03-090921-2-FD	PACE	170	Y	156.42	Y	2.4	Y	10.56	Y	22.3	Y	33.85	Y	338	Y	332.64	Y	0.14	Y	7.32	N	543	Y	582.25	Y	mg/kg
UR-38	UR-38-SS-04	BPSOU-UR38SS04-090921-1	PACE	128	Y	106.05	Y	3.4	Y	7.95	N	372	Y	518.66	Y	1670	Y	787.26	Y	0.3	Y	8.4	N	910	Y	1288.71	Y	mg/kg
UR-38	UR-38-SS-04	BPSOU-UR38SS04-090921-3	PACE	102	Y	134.19	Y	1.8	Y	10.44	Y	92.7	Y	96.52	Y	1320	Y	1326.79	Y	0.37	Y	8.32	N	545	Y	735.12	Y	mg/kg
UR-39	UR-39-OP-02	BPSOU-UR39OP02-082621-1	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1.1	Y	10.59	N	NA	NA	NA	NA	mg/kg
UR-39	UR-39-OP-02	BPSOU-UR39-070121-0-2-19	PACE	63.5	Y	183.61	Y	11	Y	20.53	Y	530	Y	680.36	Y	2110	Y	2773.99	Y	1.4	Y	10.59	N	2950	Y	3804.95	Y	mg/kg
UR-39	UR-39-SS-01	BPSOU-UR39SS01-110921-1	PACE	12.6	Y	15.35	N	9.7	Y	21.05	Y	88.8	Y	160.03	Y	261	Y	195.29	Y	0.11	Y	8.8	N	3800	Y	4493.76	Y	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39-070121-0-2-07	PACE	19.8	Y	34.66	N	7	Y	20.55	Y	272	Y	294.11	Y	901	Y	1059.87	Y	0.36	Y	8.48	N	1470	Y	2075.9	Y	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39SS03-082621-1	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.75	Y	8.48	N	NA	NA	NA	NA	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39-070121-0-2-07-FD	PACE	20.5	Y	59.48	Y	6.3	Y	21.31	Y	310	Y	316.06	Y	1150	Y	855.72	Y	0.37	Y	8.62	N	1420	Y	1893.74	Y	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39SS03-082621-1-FD	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.7	Y	8.62	N	NA	NA	NA	NA	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39-070121-6-12-09	PACE	19.2	Y	52.5	Y	8	Y	16.69	Y	198	Y	214.49	Y	706	Y	733.37	Y	0.67	Y	8.23	N	1240	Y	1720.09	Y	mg/kg
UR-39	UR-39-SS-03	BPSOU-UR39SS03-082621-3	PACE	12.7	Y	47.14	Y	0.56	Y	9.12	Y	32.2	Y	81.54	Y	52.6	Y	114.35	Y	0.24	Y	8.23	N	168	Y	422.92	Y	mg/kg
UR-40	UR-40-OP-01	BPSOU-UR40OP01-090721-3	PACE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.066	Y	6.48	N	NA	NA	NA	NA	mg/kg
UR-40	UR-40-OP-02	BPSOU-UR40OP02-090721-1	PACE	282	Y	449.57	Y	2.6	Y	7.38	N	276	Y	364.12	Y	408	Y	634.22	Y	0.19	Y	8.54	N	838	Y	1163.14	Y	mg/kg
UR-40	UR-40-OP-03	BPSOU-UR40OP03-090721-1	PACE	375	Y	483.03	Y	2.5	Y	7.24	N	661	Y	600.03	Y	640	Y	621.29	Y	0.2	Y	8.12	N	709	Y	855.83	Y	mg/kg
UR-40	UR-40-OP-04	BPSOU-UR40OP04-090721-1	PACE	401	Y	557.19	Y	3	Y	7.6	Y	448	Y	494.91	Y	603	Y	860	Y	0.5	Y	8.85	N	1060	Y	1214.35	Y	mg/kg
UR-40	UR-40-OP-04	BPSOU-UR40OP04-101821-2	PACE	300	Y	350.01	Y	2.3	Y	7.18	N	307	Y	236.44	Y	577	Y	394.07	Y	0.37	Y	7.37	N	799	Y	545.17	Y	mg/kg
UR-40	UR-40-OP-04	BPSOU-UR40OP04-090721-3	PACE	143	Y	304.35	Y	1.3	Y	7.18	N	126	Y	260.93	Y	222	Y	397.95	Y	0.16	Y	7.66	N	414	Y	937.59	Y	mg/kg

Table 2. Sample Results Used in the XRF to Laboratory Correlation and Regression Analyses

Color Coding in the Station Name Column

Sample is a Field Duplicate collected for QA/QC.

Color Coding in the Analyte Result Columns

Mercury was re-collected and analyzed due to temperature exceedance upon arrival at the Pace Lab.

There was only Mercury XRF and lab result for this sample. Therefore this point was only used in the Mercury regression.

The XRF Results are Non-Detect. This sample pair was not used in the XRF to lab Regression Analysis. The non-detect XRF concentrations listed in this table are the XRF confidence interval values.

These points were identified as outliers and were not used in the final regression analyses.

Site	Station Name	Field Sample ID (XRF)*	Lab (ICP)	Arsenic (ICP)	Arsenic (ICP) Detect	Arsenic (XRF)	Arsenic (XRF) Detect	Cadmium (ICP)	Cadmium (ICP) Detect	Cadmium (XRF)	Cadmium (XRF) Detect	Copper (ICP)	Copper (ICP) Detect	Copper (XRF)	Copper (XRF) Detect	Lead (ICP)	Lead (ICP) Detect	Lead (XRF)	Lead (XRF) Detect	Mercury (ICP)	Mercury (ICP) Detect	Mercury (XRF)	Mercury (XRF) Detect	Zinc (ICP)	Zinc (ICP) Detect	Zinc (XRF)	Zinc (XRF) Detect	Units
UR-40	UR-40-SS-01	BPSOU-UR40SS01-090221-1	PACE	429	Y	530.91	Y	3.1	Y	6.98	N	327	Y	352.44	Y	570	Y	639.25	Y	0.37	Y	8.94	N	1040	Y	1293.85	Y	mg/kg
UR-40	UR-40-SS-03	BPSOU-UR40SS03-090221-1	PACE	431	Y	330.5	Y	2.3	Y	7	N	210	Y	201.85	Y	646	Y	486.23	Y	0.36	Y	8.05	N	848	Y	966.26	Y	mg/kg
UR-40	UR-40-SS-03	BPSOU-UR40SS03-090221-2	PACE	315	Y	256.66	Y	1.8	Y	6.7	N	299	Y	235.16	Y	524	Y	415.33	Y	0.3	Y	7.21	N	616	Y	584.94	Y	mg/kg
UR-40	UR-40-SS-03	BPSOU-UR40SS03-090221-2-FD	PACE	254	Y	266.68	Y	1.9	Y	6.79	N	339	Y	284	Y	452	Y	437.33	Y	0.3	Y	7.5	N	601	Y	561.8	Y	mg/kg
UR-40	UR-40-SS-07	BPSOU-UR40SS07-090221-2	PACE	127	Y	220.59	Y	4.3	Y	7.63	Y	198	Y	245.21	Y	425	Y	499.51	Y	0.29	Y	7.23	N	507	Y	656.94	Y	mg/kg
UR-40	UR-40-SS-07	BPSOU-UR40SS07-090221-3	PACE	74.5	Y	151.91	Y	2.4	Y	7.68	N	100	Y	165.95	Y	186	Y	297.56	Y	0.16	Y	7.67	N	681	Y	973.23	Y	mg/kg
UR-40	UR-40-SS-08	BPSOU-UR40SS08-090221-1	PACE	252	Y	417.27	Y	2.4	Y	7.37	N	155	Y	215.06	Y	374	Y	525.25	Y	0.23	Y	8.79	N	826	Y	1094.01	Y	mg/kg
UR-40	UR-40-SS-08	BPSOU-UR40SS08-090221-3	PACE	581	Y	653.64	Y	0.69	Y	7.1	N	104	Y	124.13	Y	754	Y	811.77	Y	0.33	Y	7.99	N	298	Y	396.58	Y	mg/kg
UR-40	UR-40-SS-09	BPSOU-UR40SS09-090221-1	PACE	1010	Y	1072.47	Y	3.2	Y	12	Y	261	Y	278.79	Y	1190	Y	1320.88	Y	0.43	Y	9.72	N	1030	Y	1588.03	Y	mg/kg
UR-40	UR-40-SS-11	BPSOU-UR40SS11-090721-1	PACE	477	Y	727.04	Y	2.4	Y	7.62	N	187	Y	236.55	Y	601	Y	777.54	Y	0.25	Y	8.8	N	846	Y	1098.48	Y	mg/kg

Table 3: Action Levels and Waste Identification Criteria

Parameter	Land Use	Human Health Action Level	Units
Arsenic	Recreational	1000	mg/kg
Arsenic	Commercial	500	mg/kg
Arsenic	Residential	250	mg/kg
Mercury	Residential	147	mg/kg
Lead	Recreational	2300	mg/kg
Lead	Commercial	2300	mg/kg
Lead	Residential	1200	mg/kg

Parameter	Criteria	Storm Water Waste Criteria	
Arsenic	Storm Water	200	mg/kg
Cadmium	Storm Water	20	mg/kg
Copper	Storm Water	1000	mg/kg
Lead	Storm Water	1000	mg/kg
Mercury	Storm Water	10	mg/kg
Zinc	Storm Water	1000	mg/kg