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INTEGRATION OF THE UNCERTAINTIES OF ANION AND TOC MEASUREMENTS INTO THE FLAMMABILITY CONTROL STRATEGY FOR SLUDGE BATCH 8 AT THE DWPF

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EXECUTIVE SUMMARY

The Savannah River National Laboratory (SRNL) has been working with the Savannah River Remediation (SRR) Defense Waste Processing Facility (DWPF) in the development and implementation of a flammability control strategy for DWPF's melter operation during the processing of Sludge Batch 8 (SB8). SRNL's support has been in response to technical task requests that have been made by SRR's Waste Solidification Engineering (WSE) organization. The flammability control strategy relies on measurements that are performed on Slurry Mix Evaporator (SME) samples by the DWPF Laboratory.

Measurements of nitrate, oxalate, formate, and total organic carbon (TOC) standards generated by the DWPF Laboratory are presented in this report, and an evaluation of the uncertainties of these measurements is provided. The impact of the uncertainties of these measurements on DWPF's strategy for controlling melter flammability also is evaluated. The strategy includes monitoring each SME batch for its nitrate content and its TOC content relative to the nitrate content and relative to the antifoam additions made during the preparation of the SME batch.

A linearized approach for monitoring the relationship between TOC and nitrate is developed, equations are provided that integrate the measurement uncertainties into the flammability control strategy, and sample calculations for these equations are shown to illustrate the impact of the uncertainties on the flammability control strategy.

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LIST OF ABBREVIATIONS

DWPF	Defense Waste Processing Facility
gal	gallons
IC	Ion Chromatography
JMP	Statistical software package from SAS Institute, Inc. [5]
Lab OPS	Laboratory Operations
LFL	Lower Flammability Limit
ppm	parts per million
SB8	Sludge Batch 8
SME	Slurry Mix Evaporator
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
TOC	Total Organic Carbon
TTQAP	Task Technical and Quality Assurance Plan
TTR	Technical Task Request
WSE	Waste Solidification Engineering
%RD	Percent Relative Difference
%RSD	Percent Relative Standard Deviation

1.0 Introduction

The Savannah River National Laboratory (SRNL) has been working with the Savannah River Remediation (SRR) Defense Waste Processing Facility (DWPF) in the development and implementation of the flammability control strategy for DWPF's melter operation during the processing of Sludge Batch 8 (SB8). The flammability control strategy relies on measurements that are performed on Slurry Mix Evaporator (SME) samples by the DWPF Laboratory. One of the SME analytes is nitrate, and the current Technical Safety Requirement (TSR) upper limit for the concentration of nitrate is 30,000 ppm for melter off gas (MOG) flammability.

Due to the potential acid demand of SB8, the limit of 30,000 ppm of nitrate in the SME product could be exceeded in DWPF, which under the current MOG flammability TSR would require remediation of the SME. To avoid the need for this remediation, the nitrate range for the MOG flammability calculation will need to be expanded. A technical task request (TTR) [1] was made by SRR's Waste Solidification Engineering (WSE) organization to SRNL requesting support in completing this expansion and the associated Type I calculation for SB8. This calculation has been completed and documented by Choi [2]. The resulting flammability control strategy relies on analytical measurements of SME samples that are performed by the DWPF Laboratory, and WSE has requested via a TTR [3] that SRNL provide an evaluation of the associated analytical error and error structure for these measurements. SRNL responded to this request by issuing a Task Technical and Quality Assurance Plan (TTQAP) [4] for the activities that are to be conducted in support of the completion of that task.

The sample data supporting the control strategy include measurements of total organic carbon (TOC) and measurements by Ion Chromatography (IC) of select anions: nitrate, oxalate, and formate. Specifically, SRNL is being requested to provide (1) an evaluation of the uncertainties associated with these measurements, (2) an approach for integrating the uncertainties of these measurements into the flammability control strategy, and (3) equations that may be used for facility implementation of the control strategy with uncertainties. JMP Version 9.0.0 was used to support the analyses presented in this report [5].

2.0 IC and TOC Measurements by the DWPF Laboratory

Measurements generated by the DWPF Laboratory for standards of the analytes of interest to this study were provided to SRNL by Laboratory Operations (Lab OPS) personnel. These data are presented and their uncertainties investigated in this section. For each analyte of interest, the goal of the investigation was to estimate (1) any potential bias in the measurement of the analyte and (2) the variation in the measurements due to day-to-day effects on the measurement process for that analyte. Both of these uncertainties are of interest since the average of the measurements from a set of SME samples for the given analyte may be biased by the influence of each of these two sources of uncertainty.

Table A1 in Appendix A provides IC and TOC measurements recently generated by the DWPF Laboratory. Included in the IC results are measurements for formate, nitrate, soluble oxalate, and total oxalate for standards at 2 parts per million (ppm) and 16 ppm for each of these anions. Table A1 also contains measurements for TOC standards at concentrations of 1 and 20 ppm. TOC measurements are typically collected in pairs: one pair (a measurement of the 1 ppm standard and a measurement of the 20 ppm standard) before and a similar pair after process samples are processed. The before pair is identified as TOC1 measurements and the after pair is labeled as TOC2 in Table A1.

The dates that the measurements were recorded are also provided as part of the information in Table A1. Also in this table are the differences between the measured and reference values as well as the percent relative differences (%RDs):

% Relative Difference = 100% × (Measurement – Reference Value) / (Reference Value),

The analyses conducted in this report utilize the values of these % relative differences.

Exhibit A1 in Appendix A provides variability plots of the DWPF Laboratory %RDs from Table A1 for the 2 ppm and 16 ppm standards for formate, nitrate, and oxalate (both soluble and total) and for the 1 ppm and 20 ppm standards for TOC. The values are arranged by date. Since some of the values in these plots appear to be potential outliers, a screening process was conducted for these data. Exhibit A2 of Appendix A provides boxplots for the results for each standard for each analyte of interest. These boxplots served as the basis for screening the data for potential outliers. An immediate concern, as one works with a data set, is the potential for the presence of one or more outliers in the data and the possible impact of such outliers on the conclusions being made about the data. Based on the boxplots, those values for an analyte that are beyond the distances given by:

upper quartile + 1.5*(interquartile range) and lower quartile - 1.5*(interquartile range),

(based upon the quartiles computed from the set of values with the interquartile range being the difference between the 1st quartile and 3rd quartile) are considered as questionable points (i.e., potential outliers). These are the points that fall beyond the "whiskers" (the lines extended from the boxes) of the boxplots, and they were excluded from the screened data. In the exhibit, each of the boxplots in the left column provides a display that includes all of the data while the corresponding plot in the right column shows the data after the screening process. For the analyses that follow, each investigation is conducted both with the full set of values and with the set of screened values. The objective of this approach is to select the outcome from the dual investigations that yields the more conservative (i.e., larger) estimated uncertainty.

In Exhibit A3 of Appendix A, the set of %RDs for each standard for each analyte (e.g., the measurements for the 2 ppm formate standard) is investigated using all of the measurements from Table A1 and using a random effects model to represent two sources of variation: between-day (or day-to-day) effects and within-day effects. Both sources of variation in the measurements of each analyte are of interest. The DWPF Lab measures samples from a given SME batch to determine the concentrations of the analytes of interest in evaluating the SME. Typically 4 measurements are obtained for each analyte with the average of the 4 measurements being computed and used to represent the content of that analyte in the SME. It should be noted that the variation in the 4 results for each analyte reflect not only the contributions to variability from the within-day effects on the measurement process but also sample-to-sample variation associated with the SME sampling process. However, since all four of the measurements are conducted on the same day, they are subject to a single random effect from the between-day or day-to-day source of variation, and this source of variation is be estimated from the measurements of the standards and subsequently accounted for as part of this uncertainty analysis.

Estimating this between-day variation is one of the goals of the analyses presented in Exhibit A3. The estimates of the two variance components of the random effects model for each set of values are provided in the tabulated portion of the exhibit under the heading "REML Variance Components Estimates." Exhibit 1 provides a closer look at the results for the 2 ppm standard for formate. The variance component for "Date" represents the estimated variance for the between-day random effect,

which has a value of 6.098 $(\%)^2$ in Exhibit 1. The square root of this value is the % relative standard deviation (%RSD) for these measurements with a value of 2.47%. The estimate of the within-day variance (in $\%^2$ units) is indicated in the "Residual" line of this table. For the 2 ppm standard for the formate data, this value is 5.892 $(\%)^2$. However, during the flammability control calculations, the estimate of this variance component for the SME samples will be determined directly from the measurements of those samples. The estimate of the between-day variance component for each of the standards for each analyte, which is of interest in this analysis, is presented in Exhibit A3 in the manner illustrated by Exhibit 1.

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.0348594	6.0978682	1.5359399	3.9321362	10.719743	50.857
Residual		5.8924604	0.8760424	4.4921277	8.0710572	49.143
Total		11.990329				100.000

Exhibit 1. REML Estimates of Variance Components

The results from the analyses in Exhibit A3 also provide an estimate of the bias associated with the set of %RDs of the measurements for each of the standards at one reference value for each analyte of interest. Since the %RDs are being utilized in these analyses, the bias information provided is in the form of a % relative bias. The estimate of the % relative bias is indicated in the exhibit as the "Intercept" under the "Parameter Estimates" table. If the p-value given in this table is 0.05 or smaller, the hypothesis of a zero bias is rejected at a significance level of 5%. Otherwise, the hypothesis cannot be rejected at this significance level. A 95% confidence interval for the bias is also provided in this table. If this bias is positive and statistically significant, the larger of the two endpoints for the confidence interval is a bound on the potential bias at more than 95% confidence. If the bias is negative and statistically significant, then the more negative value is a bound, with more than 95% confidence, on the potential negative bias affecting these measurements.

Exhibit 2 provides a closer look at the results for the 2 ppm standard for formate. The p-value is <0.0001, which indicates that the null hypothesis of a zero bias is rejected at the 5% significance level. The results indicate a positive bias, which may be bounded at a value of 2.997% with more than 95% confidence (as indicated in Exhibit 2).

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	2.3245102	0.337764	80.15	6.88	<.0001*	1.6523578	2.9966626

Exhibit 2. Estimate of % Relative Bias

Table 1 provides a summary of the vital information (i.e., the estimate of the between-day variance component and a bound on the bias, when statistically significant) for each standard and analyte from Exhibit A3. Once again, the analyses presented in Exhibit A3 utilized all of the data from Table A1.

**Table 1. Summary Information from Exhibit A3
Using All of the Measurements from Table A1**

Analyte	Reference Value (ppm)	Estimate of Day-to-Day Variance (%^{2})	Day-to-Day %RSD	% Bias Bound at Greater than 95% Confidence
Formate	2	6.098	2.47	3.00
	16	2.507	1.58	1.58
Nitrate	2	7.430	2.73	No significant bias
	16	2.383	1.54	No significant bias
Soluble Oxalate	2	9.060	3.01	4.30
	16	4.576	2.14	-1.27
Total Oxalate	2	21.143	4.60	5.41
	16	25.500	5.05	No significant bias
TOC	1	7.375	2.72	No significant bias
	20	4.010	2.00	No significant bias

Exhibit A4 in Appendix A provides the same analyses as Exhibit A3 except that only the screened data were used. Table 2 summarizes the vital information from the analyses of the screened data that is presented in Exhibit A4.

**Table 2. Summary Information from Exhibit A4
Using the Screened Measurements from Table A1**

Analyte	Reference Value (ppm)	Estimate of Day-to-Day Variance (%^{2})	Day-to-Day %RSD	% Bias Bound at Greater than 95% Confidence
Formate	2	2.858	1.69	3.03
	16	0.292	0.54	1.95
Nitrate	2	5.946	2.44	No significant bias
	16	0.730	0.85	0.76
Soluble Oxalate	2	7.092	2.66	4.53
	16	1.915	1.38	No significant bias
Total Oxalate	2	16.958	4.12	5.03
	16	4.686	2.16	No significant bias
TOC	1	6.342	2.52	No significant bias
	20	3.035	1.74	No significant bias

For each anion and for TOC, the between-day variance is a contributor to the uncertainty for the measurements of the samples from a given SME batch. This is a batch-to-batch variation affecting the measurements of a SME batch. Accounting for this variation as part of the uncertainty in the measurements of each of the anions and of TOC is addressed in the discussions that follow. In addition, for those analytes with a statistically significant bias, the effects of the biases on the flammability control strategy are to be conservatively accounted for. This is addressed below as part of subsequent discussions presented in this report.

3.0 The Maximum TOC versus NO_3 at 60% LFL

As stated in the Introduction, efforts are underway at SRNL to support WSE in the development of a melter flammability control strategy for SB8 [2]. The strategy relies on a SME batch satisfying a constraint on the TOC content of the SME based upon the nitrate content of the SME and tied to an estimate of the amount of antifoam used in the preparation of the SME batch. TOC versus nitrate constraints were developed by Choi [2] for three (3) different antifoam additions: 728, 894, and 1,017 gallons (gal). All three constraints were developed to be applicable for nitrate concentrations in the interval from 10,000 to 70,000 ppm. Before a SME batch is to be transferred to the melter, WSE must establish that the TOC concentration to the nitrate concentration satisfies the restrictions imposed by Choi's analysis [2]. WSE has requested that the efforts of this study address a conservative implementation of these constraints (i.e., one based on a linearized representation of the TOC to nitrate relationship) for flammability control (see Appendix B). Given that even this linearized implementation strategy relies on process measurements, WSE must account for the uncertainties of the measurements to confidently achieve a successful implementation of the flammability control strategy. The uncertainties of these measurements were investigated earlier in this report, and the purpose of this section is to establish the linearized approach, to provide a set of equations that integrate the measurement uncertainties into the flammability control strategy, and to provide sample calculations for these equations to illustrate their impact on the flammability control strategy.

The TOC constraints developed by Choi maintain the contributors to melter flammability to less than 60% of the lower flammability limit (LFL) [2]. The maximum allowable TOC was determined by Choi as a polynomial function of the nitrate concentration, and a different functional constraint on the TOC values was developed for each of three antifoam additions. Since all of these constraints were developed over the interval of nitrate concentrations from 10,000 ppm to 70,000 ppm, that interval of nitrate concentrations is the range of applicability for these functions. If the contents of a SME batch yield an average nitrate measurement outside of the interval from 10,000 to 70,000 ppm, then satisfying the TOC constraint may not be a reliable control for addressing melter flammability concerns for that SME batch. In the sections that follow, the impacts of the TOC and nitrate measurement uncertainties (that were determined in the previous section of this report) on the assessment of the nitrate content of the SME and for controlling melter flammability are investigated.

3.1 Assessing the Nitrate Content of the SME

To implement the melter flammability control strategy, there is a need to assure with high confidence that the nitrate (NO_3) content of the SME falls within the interval from 10,000 to 70,000 ppm. Demonstrating that this condition is met for a given SME batch will rely on the four nitrate measurements from that batch. The average of these measurements may be represented by $\overline{NO_3}$. The standard error, or the 1-sigma standard uncertainty, of this value may be represented by $se_{\overline{NO_3}}$, and its value is also computed from the four nitrate values: the standard error of the mean is the standard deviation computed from the four nitrate values divided by 2. In addition, from the discussion above, two other effects are to be accounted for in meeting this constraint: any bias in the measurements of the nitrate standards and the batch-to-batch 1-sigma relative uncertainty. For the nitrate results, there was a statistically significant bias in the measurements for the 16 ppm standards for the screened data. The mean of the measurements for the 16 ppm standards for the screened data was high relative to the nominal value for that standard, and it is not clear when the bias may become less significant for lower nitrate concentrations. Thus, the assumption being made in regard to nitrate measurements is

that the measured nitrate content of the SME may be slightly more than the actual amount (on average). Thus, in assessing if the nitrate content falls within the interval from 10,000 to 70,000 ppm, it is conservative to not adjust the nitrate content when it is compared to the upper limit (i.e., the 70,000 ppm limit) but to make the adjustment for a potentially high bias when the nitrate content is compared to the lower limit (i.e., the 10,000 ppm limit).

From the discussion above, a bound on the potentially high bias in the nitrate measurements, with more than 95% confidence, was determined to be 0.76% of the nominal 16 ppm value. In assessing the nitrate content of a SME batch against the 70,000 ppm lower limit, the average nitrate measurement will be adjusted for this potential bias, and that adjustment will be made by decreasing the amount of nitrate by 0.76% (i.e., by multiplying the average nitrate content by 0.9924).

In assessing the batch-to-batch variation affecting the nitrate measurements, the largest estimate of the between-day component of variance from Tables 1 and 2 yields a %RSD of 2.73% (determined from all of the measurements for the 2 ppm standard).

Following the guidelines and notational conventions presented in [6] (which may differ somewhat from the notation typically used in statistical models), an input term, δ_{NO_3}, representing the batch-to-batch random effect is to be added to the measurement equations for the NO_3 content in the SME.

If Low_{NO_3} is used to represent the difference between the estimated NO_3 content of the SME and the lower limit of 10,000 ppm, then the measurement equation for the measurand, Low_{NO_3}, may be written as:

Equation 1.

$$\text{Low}_{NO_3} = 0.9924 \cdot \left(\overline{NO_3} + \delta_{NO_3}\right) - 10000 > 0$$

where $\overline{NO_3}$ represents the average of the NO_3 concentration measurements for the 4 samples of the given SME batch. This average has a 1-sigma standard uncertainty of $se_{\overline{NO_3}}$,

0.9924 is the adjustment for a potentially high bias in the nitrate measurements, and

δ_{NO_3} represents the batch-to-batch source of variation affecting the nitrate measurements for a SME batch. For the evaluation of Low_{NO_3} by Equation 1, the value of δ_{NO_3} is zero. Its 1-sigma relative standard uncertainty is the batch-to-batch variation and is represented by $s_{\delta_{NO_3}}$, and based upon the discussion above, its value is given by 2.73% of the $\overline{NO_3}$ value.

The guidance provided in [6] relies on the use of a Taylor's series expansion of the measurement equation to approximate the variance of the measurand. The expression of this approximation is simplified if the errors associated with the inputs to the measurement equation are uncorrelated, which is the case for the errors associated with the two input terms of Equation 1[f]. For this simple

[f] The errors associated with the terms in the other measurement equations investigated as part of this study are also assumed to be uncorrelated.

measurement equation, the variance of Low_{NO_3} is equal to its Taylor's series expansion. However, for conservatism, the bias adjustment term (i.e., 0.9924) will not be included in the estimation of variance. The estimation of the variance of Low_{NO_3} is facilitated by estimating the standard deviations of $\overline{NO_3}$ and δ_{NO_3} by $se_{\overline{NO_3}}$ and $s_{\delta_{NO_3}}$, respectively, as indicated in Equation 2:

Equation 2.

$$\text{Est. Var}\left(Low_{NO_3}\right) = \left[\left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2\right]$$

where $\text{Est.Var}\left(Low_{NO_3}\right)$ represents the estimated variance of Low_{NO_3}, the estimated difference between the nitrate content of the SME and the lower limit of 10,000 ppm.

If $High_{NO_3}$ is used to represent the estimated difference between the upper limit of 70,000 ppm and the NO_3 content of the SME, then the measurement equation for the measurand, $High_{NO_3}$, may be written as:

Equation 3.

$$High_{NO_3} = 70000 - \left(\overline{NO_3} + \delta_{NO_3}\right) > 0$$

where $\overline{NO_3}$ represents the average of the NO_3 concentration measurements for the 4 samples of the given SME batch. This average has a 1-sigma standard uncertainty of $se_{\overline{NO_3}}$, and

δ_{NO_3} represents the batch-to-batch source of variation affecting the nitrate measurements for a SME batch. For the evaluation of $High_{NO_3}$ by Equation 3, the value of δ_{NO_3} is zero. Its 1-sigma relative standard uncertainty is represented by $s_{\delta_{NO_3}}$ and based upon the analyses summarized above, it has a value given by 2.73% of the $\overline{NO_3}$ value.

Once again, for this simple measurement equation, the variance of $High_{NO_3}$ is equal to its Taylor's series expansion, and the estimation of the variance of $High_{NO_3}$ is facilitated by estimating the standard deviations of $\overline{NO_3}$ and δ_{NO_3} by $se_{\overline{NO_3}}$ and $s_{\delta_{NO_3}}$, respectively, as indicated by:

Equation 4.

$$\text{Est. Var}\left(High_{NO_3}\right) = \left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2$$

where $\text{Est.Var}\left(High_{NO_3}\right)$ represents the estimated variance of $High_{NO_3}$.

To determine that the nitrate content of the SME is within the interval from 10,000 ppm to 70,000 ppm the inequalities of Equations 1 and 3 must be met after accounting for the uncertainties estimated in Equations 2 and 4. To determine the uncertainty at 95% confidence, the square roots of the estimates of the variances for Equations 1 and 3 must be multiplied by an appropriate Student's t statistic. Since a two-sided evaluation for the nitrate content is needed, a two-tailed t statistic may be used. For this situation, 3 degrees of freedom will be assumed for the estimated variances of Equations 1 and 3. For 3 degrees of freedom, the upper 2.5%-tail of the Student's t distribution is 3.182. That is,

Equation 5.

$$\mathrm{Low}_{NO_3} - t_{(0.025,3)} \cdot (\text{Est. var}(\mathrm{Low}_{NO_3}))^{0.5} > 0$$

and

Equation 6.

$$\mathrm{High}_{NO_3} - t_{(0.025,3)} \cdot (\text{Est. var}(\mathrm{High}_{NO_3}))^{0.5} > 0$$

Thus, the nitrate content of the SME is acceptable if

Equation 7.

$$\left(\overline{NO_3} \cdot 0.9924\right) - 10000 - 3.182 \cdot \sqrt{\left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2} > 0$$

and

Equation 8.

$$70000 - \overline{NO_3} - 3.182 \cdot \sqrt{\left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2} > 0$$

To illustrate these calculations, consider the four nitrate measurements (in ppm): 23700, 23604, 23229, and 23433. The sample mean of these values, $\overline{NO_3}$, is given by 23491.5, and the 1-sigma standard uncertainty of the sample mean is given by sample standard deviation divided by the square root of the sample size, or 206.928/2=103.464. The value of $s_{\delta_{NO_3}}$ is determined by 0.0273·23491.5=641.318.

The result for Equation 7 is

$$\left(\overline{NO_3} \cdot 0.9924\right) - 10000 - 3.182 \cdot \sqrt{\left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2}$$

$$= 23491.5 \cdot 0.9924 - 10000 - 3.182 \cdot 649.610$$

$$= 11245.9045 > 0$$

which shows acceptability, and the result for Equation 8 is

$$70000 - \overline{NO_3} - 3.182 \cdot \sqrt{\left(se_{\overline{NO_3}}\right)^2 + \left(s_{\delta_{NO_3}}\right)^2} = 70000 - 23491.5 - 2067.059$$

$$= 44441.441 > 0$$

which also shows acceptability.

3.2 Controlling Melter Flammability via the TOC to NO_3 Relationship

Each of the three functions (indexed by the level of antifoam addition) developed by Choi [2] relating TOC content to nitrate content may be expressed in the form of a 4th degree polynomial, as given by:

Equation 9.

$$TOC_i = a_i + b_i \cdot (NO_3) + c_i \cdot (NO_3)^2 + d_i \cdot (NO_3)^3 + e_i \cdot (NO_3)^4$$

where the TOC_i term on the left-hand side of the equation represents the maximum TOC allowed for a SME batch to maintain the DWPF melter system below the 60% LFL, while the NO_3 term on the right-hand side represents the nitrate content of the subsequent melter feed in ppm. The values of the a_i, b_i, c_i, d_i, and e_i coefficients are given in Table 3 for i=1, 2, and 3, and each value of the i index corresponds to one of the three additions of antifoam (in gal) for which Choi developed the associated TOC versus NO_3 relationship.

Table 3. Coefficients for Equations Relating TOC Content to NO_3 Content

i	Antifoam Addition (gal)	a_i	b_i	c_i	d_i	e_i
1	728	7557.6474	0.50526028	-9.2573423E-06	2.3456397E-10	-1.6391746E-15
2	894	9422.0849	0.07089545	9.1468028E-06	-6.620362E-11	5.7959687E-17
3	1,017	10556.47	-0.2167157	2.0961912E-05	-2.5179967E-10	1.0703826E-15

WSE requested that a linearized version of the TOC to NO_3 relationship be developed (see Appendix B) so that individual SME batches that are compliant with the linearized versions (see Equation 10) will be compliant with the family of Choi equations (given by Equation 9) when blended.

Equation 10.

$$TOC_i = f_i + g_i \cdot (NO_3)$$

where, once again, the term TOC_i term on the left-hand side of the equation represents the maximum TOC allowed to maintain the system below the 60% LFL based upon a linearized relationship between TOC and NO_3, while the NO_3 term on the right-hand side represents the nitrate content of the melter feed in ppm. The values of the f_i and g_i coefficients are given in Table 4 for i=1, 2, and 3, and each value of the i index corresponds to one of the three additions of antifoam (in gal) for which Choi developed an associated TOC versus NO_3 relationship. The f_i and g_i values were selected to help minimize the TOC margin lost in going to the linearized approach over the NO_3 interval of 10,000 to 30,000 ppm.

Table 4. Coefficients for the Linear Equations Relating TOC Content to NO_3 Content

i	Antifoam Addition (gal)	f_i	g_i
1	728	8140	0.37
2	894	6550	0.37
3	1,017	5300	0.37

Each of the linear approximations indicated in Table 4 was selected so that when the limit on the allowed TOC content is met for the linear equation, that outcome ensures that the limit imposed by the corresponding Choi equation is also being met. See Exhibit A5 in Appendix A for graphical comparisons between the Choi and linear equations which show that each Choi equation allows more TOC than the corresponding linear equation.

In the discussion above, no statistically significant bias was indicated for the TOC measurements; while for the nitrate measurements, there was a statistically significant high bias. Thus, to be conservative, an adjustment is made (in the manner of Equation 2) to the nitrate value in Equation 10 for this bias. The direct utilization of the family of equations given by Equation 10 for melter flammability control yields this acceptability equation for a given SME batch:

Equation 11.

$$D_i = f_i + g_i \cdot 0.9924 \cdot \overline{NO_3} - \overline{TOC} - other_C > 0$$

where D_i is the measurand, it represents the difference in ppm between the carbon allowed by Equation 10 and the carbon content of the SME, and its value must be positive,

f_i & g_i are the coefficients from Table 4 corresponding to the appropriate bound on the gallons of antifoam utilized in the preparation of the SME batch (indexed by i) as determined following the approach discussed in Section 4 below,

0.9924 is the adjustment for a potential high bias in the nitrate measurements, and

$\overline{NO_3}$ represents the average of the NO_3 concentration measurements in ppm for the samples of the given SME batch,

$\overline{TOC}$ represents the average of the TOC concentration measurements in ppm for the samples of the given SME batch, and

$other_C$ represents carbon that is present in the SME in a form that is not measured by the TOC analytical protocol. Note, however, that such carbon was included in the determination of the TOC relationship to nitrate given by Equation 9. Its value is associated with the amount of coal in the SME and is bounded in [2] by 240 ppm.

The form of Equation 11 is such that the value of D_i must be positive for acceptability. That is, the amount of TOC allowed by the use of Equation 10 must be greater than the TOC content of the given SME for the given level of antifoam addition (indexed by i), and this must be true with high confidence after accounting for the uncertainties in the measurements used to make this determination.

Following the approach and notational conventions of [6], Equation 11 is modified to make it a more complete measurement equation for the determination of D_i. Also in the discussion above, a batch-to-batch 1-sigma relative uncertainty of 2.73% was identified as affecting the nitrate measurements. For the TOC measurements, a review of the information in Tables 1 and 2 regarding the day-to-day variance components indicates that a conservative estimate of the batch-to-batch 1-sigma relative uncertainty is provided by 2.72%. If the errors for these sources of variation are represented as δ_{NO_3} and δ_{TOC}, respectively, they may be added to Equation 11 to obtain a more complete measurement equation for D_i (indexed by the value of the antifoam addition) as follows:

Equation 12.

$$D_i = f_i + g_i \cdot 0.9924 \cdot \left(\overline{NO_3} + \delta_{NO_3}\right) - \left(\overline{TOC} + \delta_{TOC}\right) - other_C > 0$$

The values of δ_{NO_3} and δ_{TOC} are zero in the determination of the value of D_i, but including these terms in the equation for D_i allows for their contributions to the variance of D_i to be included in the variance propagation for Equation 12.

A Taylor's series expansion approach is used to estimate the variance of D_i [6], and as above, for conservatism the bias adjustment term (0.9924) is not included in the estimation of variance. Assuming that the errors in Equation 12 are uncorrelated and that the value for $other_C$ is bounding and thus may be considered to be without error, the Taylor's series expansion approach yields:

Equation 13.

$$var(D_i) \approx \left(\frac{\partial D_i}{\partial \overline{NO_3}}\right)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + \left(\frac{\partial D_i}{\partial \delta_{NO_3}}\right)^2 \cdot \left(s_{\delta_{NO_3}}\right)^2 + \left(\frac{\partial D_i}{\partial \overline{TOC}}\right)^2 \cdot \left(se_{\overline{TOC}}\right)^2 + \left(\frac{\partial D_i}{\partial \delta_{TOC}}\right)^2 \cdot \left(s_{\delta_{TOC}}\right)^2$$

where $\frac{\partial D_i}{\partial \bullet}$ represents the partial derivative of D_i with respect to the variable (●), $se_{\overline{NO_3}}$ represents the 1-sigma standard uncertainty of the average nitrate measurement of the SME samples, $s_{\delta_{NO_3}}$ represents the 1-sigma relative standard uncertainty of the batch-to-batch variation in the nitrate measurements (i.e., 2.73% of the $\overline{NO_3}$ value), $se_{\overline{TOC}}$ represents the 1-sigma standard uncertainty of the average TOC measurement of the SME samples, and $s_{\delta_{TOC}}$ represents the 1-sigma relative standard uncertainty of the batch-to-batch variation in the TOC measurements (i.e., 2.72% of the $\overline{TOC}$ value). Once again, note that no error term is introduced in Equation 13 for the $other_C$ input of Equation 12.

Using this approach, the variance of D_i is estimated by:

Equation 14.

$$var(D_i) \approx (g_i)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + (g_i)^2 \cdot \left(s_{\delta_{NO_3}}\right)^2 + \left(se_{\overline{TOC}}\right)^2 + \left(s_{\delta_{TOC}}\right)^2$$

Note that since the value of g_i is 0.37 for each value of the index i (i= 1, 2, and 3), the equation for estimating the variance of D_i is the same for each value of i and it may be expressed as Equation 15.

$$\text{var}(D_1) = \text{var}(D_2) = \text{var}(D_3) \approx (0.37)^2 \cdot \left(se_{\overline{NO_3}} \right)^2 + (0.37)^2 \cdot \left(s_{\delta_{NO_3}} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + \left(s_{\delta_{TOC}} \right)^2$$

$$= 0.1368 \cdot \left(se_{\overline{NO_3}} \right)^2 + 0.1369 \cdot \left(s_{\delta_{NO_3}} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + \left(s_{\delta_{TOC}} \right)^2$$

Using the estimates of the batch-to-batch variations discussed above, Equation 15 may be expressed as:

Equation 16.

$$\text{var}(D_1) = \text{var}(D_2) = \text{var}(D_3) \approx 0.1369 \cdot \left(se_{\overline{NO_3}} \right)^2 + 0.1369 \cdot \left(s_{\delta_{NO_3}} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + \left(s_{\delta_{TOC}} \right)^2$$

$$= 0.1369 \cdot \left(se_{\overline{NO_3}} \right)^2 + 0.1369 \cdot \left(0.0273 \cdot \overline{NO_3} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + \left(0.0272 \cdot \overline{TOC} \right)^2$$

$$= 0.1369 \cdot \left(se_{\overline{NO_3}} \right)^2 + 0.00010203 \cdot \left(\overline{NO_3} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + 0.00073984 \cdot \left(\overline{TOC} \right)^2$$

3.3 Meeting the Constraint Imposed by the TOC to Nitrate Relationship

In meeting the constraint on TOC imposed by its relationship to nitrate, the value for the degrees of freedom for the estimate of the variance of D_i is taken to be 3. This is a conservative approach since it relies on only the degrees of freedom associated with the standard errors of the nitrate and TOC sample means. As indicated in Equation 12, the value of D_i must be positive for acceptability. To assure that the value of D_i is sufficiently positive, it must be larger than its estimated uncertainty at 95% confidence. To determine the uncertainty at 95% confidence, the square root of the estimate of the variance of D_i must be multiplied by an appropriate Student's t statistic. Since only a one-sided expression of the uncertainty of D_i is needed, a one-tailed t statistic may be used. For 3 degrees of freedom, the upper 5%-tail of the Student's t distribution is 2.353. Thus, the SME batch is acceptable from the perspective of its TOC content if:

Equation 17.

$$D_i - t_{(0.05,3)} \cdot (\text{Est. var}(D_i))^{0.5} = D_i - 2.353 \cdot (\text{Est. var}(D_i))^{0.5} > 0$$

where D_i is determined using Equation 12 (for the associated level of antifoam additions),

$t_{(0.05,3)}$ is the upper 5%-tail of the Student's t distribution (i.e., 2.353), and

Est. var(D_i) represents the estimate of the variance of D_i, which may be computed using Equation 16 regardless of the antifoam addition being considered.

3.4 Example Calculations in Meeting the TOC Constraint

To illustrate these calculations, they were performed for the nitrate and TOC values shown in Exhibit 3. In this exhibit four values (in ppm) are provided for TOC and nitrate. Also, in this exhibit the averages, standard deviations, and standard errors of the mean are shown. The averages are the simple arithmetic averages of the 4 values for each analyte, and the standard deviations are also computed using the traditional equation for this summary statistic. The standard error of the mean for each analyte is the value of its standard deviation divided by 2 (the square root of the number of observations used to determine the average).

	TOC (ppm)	Nitrate (ppm)
	12500	23700
	12750	23604
	12800	23229
	12666	23433
averages	12679.000	23491.500
standard deviations	131.5193	206.9275
standard error of the mean	65.75966	103.46376

Exhibit 3. Illustration of the Calculations for TOC to Nitrate Acceptability

With these values determined , Equations 11 and 16 can be used to compute the value for D_i and its estimated variance, respectively, for each of the antifoam additions (recall that the coefficients f_i and g_i are given in Table 4). Equation 18 provides the value for D_i (in ppm) for each of the antifoam additions.

Equation 18a (728 gal addition of antifoam).

$$D_1 = f_1 + g_1 \cdot 0.9924 \cdot \overline{NO_3} - \overline{TOC} - other_C$$

$$= 8140 + 0.37 \cdot 0.9924 \cdot 23491.500 - 12679.000 - 240$$

$$= 3846.797$$

$$> 0$$

Equation 18b (894 gal addition of antifoam).

$$D_2 = f_2 + g_2 \cdot 0.9924 \cdot \overline{NO_3} - \overline{TOC} - other_C$$

$$= 6550 + 0.37 \cdot 0.9924 \cdot 23491.500 - 12679.000 - 240$$

$$= 2256.797$$

$$> 0$$

Equation 18c (1,017 gal addition of antifoam).

$$D_3 = f_3 + g_3 \cdot 0.9924 \cdot \overline{NO_3} - \overline{TOC} - other_C$$

$$= 5300 + 0.37 \cdot 0.9924 \cdot 23491.500 - 12679.000 - 240$$

$$= 1006.797$$

$$> 0$$

The estimated variance for each of these D_i values is computed using the same equation (i.e., Equation 16) and the result is provided in Equation 19.

Equation 19.

$$\text{var}(D_1) = \text{var}(D_2) = \text{var}(D_3) \approx 0.1369 \cdot \left(se_{\overline{NO_3}} \right)^2 + \left(se_{\overline{TOC}} \right)^2 + 0.00010203 \cdot \left(\overline{NO_3} \right)^2 + 0.00073984 \cdot \left(\overline{TOC} \right)^2$$

$$= 0.1369 \cdot (103.46376)^2 + (65.75966)^2 + 0.00010203 \cdot (23491.500)^2 + 0.00073984 \cdot (12679.000)^2$$

$$= 181029.62$$

With these calculations in hand, the question of meeting the TOC constraint as defined by Equation 17 may be addressed for each candidate level of antifoam addition. Equation 20 provides the results (expressed in ppm of TOC) from these determinations.

Equation 20a (728 gal addition).

$$D_1 - t_{(0.05,3)} \cdot (\text{Est. var}(D_1))^{0.5} = 3846.797 - 2.353 \cdot (181029.62)^{0.5}$$

$$= 3846.797 - 2.353 \cdot 425.476$$

$$= 2845.65$$

$$> 0$$

Equation 20b (894 gal addition).

$$D_2 - t_{(0.05,3)} \cdot (\text{Est. var}(D_2))^{0.5} = 2256.797 - 2.353 \cdot (181029.62)^{0.5}$$

$$= 2256.797 - 2.353 \cdot 425.476$$

$$= 1255.65$$

$$> 0$$

Equation 20c (1,017 gal addition).

$$D_3 - t_{(0.05,3)} \cdot (\text{Est. var}(D_3))^{0.5} = 1006.797 - 2.353 \cdot (181029.62)^{0.5}$$

$$= 1006.797 - 2.353 \cdot 425.476$$

$$= 5.65$$

$$> 0$$

The results from the evaluations of Equation 20 indicate that the measured TOC content for this example is acceptable for antifoam additions of 728, 894, or 1,017 gal.

4.0 Estimation of the Antifoam Addition

As described above, the relationship between the maximum allowable TOC content and the NO_3 content of a SME batch was associated with the total amount of antifoam used to prepare the SME batch. Three levels for this total antifoam amount in gallons were established by Choi [2]: 728, 894, and 1,017 gal. As part of his study, Choi developed a relationship between the maximum amount of carbon that would be generated from each of these bounding amounts of antifoam and the NO_3 content of the SME. These relationships are given by:

Equation 21.

$$\left(\text{Antifoam}_{Ci}\right)^2 = h_i + j_i \cdot \left(NO_3\right) \Rightarrow \text{Antifoam}_C = \sqrt{h_i + j_i \cdot \left(NO_3\right)}$$

where Antifoam_{Ci} represents the maximum amount of carbon in ppm that would be generated from antifoam additions for three cases indexed by i: 1 corresponds to 728 gal, 2 to 894 gal, and finally, 3 to 1,017 gal of antifoam, and NO_3 represents the nitrate content of the SME in ppm. The h_i and j_i values, which are provided in Table 5, are from the models developed by Choi [2].

Table 5. Coefficients for the Equations Relating Maximum Carbon Content from Antifoam Additions to NO_3 Content

i	Antifoam Addition (gal)	h_i	j_i
1	728	5117745.1	-35.869438
2	894	7884790.5	-55.545316
3	1,017	10373798	-73.602487

Thus, DWPF's melter flammability control strategy requires that WSE confidently estimate an upper bound on the amount of carbon attributable to the antifoam added during the processing of each SME batch, and then use this result to confidently establish one of the three antifoam levels developed by Choi (i.e., for additions of no more than 728, 894, or 1,017 gal) as the upper bound on the gallons of antifoam added during the processing of the SME batch. The importance of this outcome is that it establishes the appropriate TOC to NO_3 relationship that must be used in satisfying Equation 17 as discussed in Section 3.

4.1 Bounding the Total Amount of Antifoam Additions Made to a SME Batch

Thus, there is a need to estimate the amount of antifoam that was added during DWPF's preparation of a given SME batch. From the previous section, there is a relationship between the nitrate content of the SME and the limit on the carbon generated by antifoam additions to that SME for three different levels of antifoam addition: 728, 894, and 1,017 gal. Thus, one may estimate the amount of antifoam added during the preparation of a SME batch by estimating an upper bound on the carbon content due to antifoam additions for the prepared SME. The estimation is conducted by backing out contributions to the measured TOC concentration in the SME from the oxalate and the formate concentrations that are measured in the SME. The resulting adjusted TOC value provides a basis for estimating the amount of carbon in the SME attributable to antifoam. When this estimate is bounded at 95% confidence by accounting for its uncertainty, the resulting bounded amount of carbon attributable to antifoam must be below the carbon allowed by the level of antifoam (i.e., one of the three values:728, 894, or 1,017 gal) that is selected to be appropriate for the given SME batch.

As the measured TOC concentration in the SME is adjusted for carbon contributions from oxalate and formate, these adjustments are to be modified in a conservative manner to handle the potential bias in the formate and in the oxalate results (as suggested by the analysis of the standards, the results from which were summarized in Tables 1 and 2). From the results of the formate standards, there was a consistently high bias for both the 2 and 16 ppm standards. Using the largest upper bound for this bias from Tables 1 and 2, a bound on this relative bias, with more than 95% confidence, is provided by 3.03%. The formate measurements will be adjusted for this potential bias, and that adjustment will be made by reducing the amount of carbon contributed by formate by 3.03% (i.e., by multiplying the average formate content by 0.9697).

In representing the oxalate content of the SME, either the soluble or total oxalate concentration measurements in ppm may be used. The analytical procedures used to measure soluble oxalate are more quickly completed than those used to measure the total oxalate. If the difference between the allowable amount of antifoam and the estimated amount is positive using the soluble oxalate value (after uncertainties have been accounted for), then the SME batch is acceptable in regards to its estimated amount of added antifoam. For the acceptability decision to be conservative, regardless of whether the soluble or total oxalate is used, the values bounding the bias and representing the batch-to-batch variability must cover the results for both forms of oxalate. From Tables 1 and 2, a conservative approach to bound the bias is to use the value of 5.41% (provided in the results from the 2 ppm standard for total oxalate in the Table 1, which utilized all of the measurements). The oxalate measurements will be adjusted for this potential bias, and that adjustment will be made by reducing the amount of carbon contributed by oxalate by 5.41% (i.e., by multiplying the average oxalate content by 0.9459). For the batch-to-batch variation, the conservative value of 5.05% (provided in the results from Table 1 for all of the measurements of the 16 ppm standard) is to be used. Once again, with this conservative approach, either soluble or total oxalate may be used to evaluate the acceptability of a SME batch in meeting the constraint imposed by Equation 21.

Note that to add conservatism to the implementation of Equation 21, the nitrate value in the equation will not be adjusted for the potential high bias in the nitrate measurements. Based upon this approach, the restriction imposed on the contents of the SME by Equation 21 may be expressed as:

Equation 22.

$$M_{Ci} = \sqrt{h_i + j_i \cdot \overline{NO_3}} - \overline{TOC} + f_C \cdot \overline{formate} \cdot 0.9697 + o_C \cdot \overline{oxalate} \cdot 0.9459 > 0$$

where

M_{Ci} is the measurand; it represents the difference between the allowable concentration in ppm of carbon from antifoam at a level indexed by i (where i=1 represents 728 gal, 2 represents 894 gal, and 3 represents 1,017 gal) and the estimated amount of carbon attributable to antifoam; and the difference must be positive,

i is used as an index for the level of antifoam addition in gallons, i = 1 (728 gal), 2 (894 gal), and 3 (1,017 gal).

h_i & j_i are the coefficients corresponding to the i^{th} level of antifoam (their values are provided in Table 5),

$\overline{NO_3}$ represents (as above) the average of the NO_3 concentration measurements in ppm for the samples of the given SME batch,

$\overline{TOC}$ is (as above) the average of the TOC measurements in ppm for the samples from the given SME batch,

$\overline{formate}$ is the average of the formate measurements in ppm for the samples from the SME batch[f],

$\overline{oxalate}$ is the average of the oxalate measurements in ppm for the samples from the SME batch,

0.9697 is included in the measurement equation to adjust (with a better than 95% confidence) for the potential bias in the formate measurement,

f_C is the conversion factor needed to determine the carbon contributed by the formate content of the SME in ppm,

o_C is the conversion factor needed to determine the carbon contributed by the oxalate content of the SME in ppm, and

0.9459 is included in the measurement equation to adjust (with a better than 95% confidence) for the potential bias in the oxalate measurement,

The conversion factor for formate is 0.26681 ppm carbon per ppm of formate as determined by:

Equation 23.

$$\frac{1\,\text{mg formate}}{\text{kg SME Slurry}} \times \frac{1\,\text{gram}}{1000\,\text{mg}} \times \frac{1\,\text{gmole formate}}{45.0177\,\text{g formate}} \times \frac{1\,\text{gmole carbon}}{1\,\text{gmole formate}} \times \frac{12.011\,\text{g carbon}}{1\,\text{gmole carbon}} \times \frac{1000\,\text{mg}}{1\,\text{gram}} = 0.266806 \frac{1\,\text{mg carbon}}{\text{kg SME Slurry}}$$

and for oxalate, the factor is 0.27292 ppm carbon per ppm of oxalate as determined by

[f] Note the multiplications by 0.9697 and 0.9459. This makes the adjustments for the potential biases in the measured formate and oxalate content, respectively, of the SME.

Equation 24.

$$\frac{1\,\text{mg oxalate}}{\text{kg SME Slurry}} \times \frac{1\,\text{gram}}{1000\,\text{mg}} \times \frac{1\,\text{gmole oxalate}}{88.019\,\text{g oxalate}} \times \frac{2\,\text{gmole carbon}}{1\,\text{gmole oxalate}} \times \frac{12.011\,\text{g carbon}}{1\,\text{gmole carbon}} \times \frac{1000\,\text{mg}}{1\,\text{gram}} = 0.27292 \frac{1\,\text{mg carbon}}{\text{kg SME Slurry}}$$

The uncertainty in meeting the constraint imposed by Equation 22 is now determined. To facilitate this process, the equation is modified using notational conventions suggested by [6] to develop a more complete measurement equation. This involves introducing terms for the batch-to-batch effects for NO_3, δ_{NO_3}, for formate, δ_{formate}, for oxalate, δ_{oxalate}, and for TOC, δ_{TOC}. The measurement equation resulting from these additions is given by:

Equation 25.

$$M_{Ci} = \sqrt{h_i + j_i \cdot \left(\overline{NO_3} + \delta_{NO_3}\right)} - \left(\overline{TOC} + \delta_{TOC}\right)$$

$$+ f_C \cdot \left(\overline{\text{formate}} + \delta_{\text{formate}}\right) \cdot 0.9697 + o_C \cdot \left(\overline{\text{oxalate}} + \delta_{\text{oxalate}}\right) \cdot 0.9459 > 0$$

where all of the terms in Equation 25 are as indicated above with the addition of the δ terms representing the batch-to-batch variations in the measurements of these analytes.

For the evaluation of Equation 25, the values of δ_{NO_3}, δ_{TOC}, δ_{formate}, and δ_{oxalate} are taken to be zero. The variance of M_{Ci}, the difference between the allowable carbon from antifoam and the estimated carbon from antifoam, will be estimated using a Taylor's series expansion approach as utilized above, and as above, for conservatism the bias adjustment terms (0.9697 and 0.9459) are not included in the estimation of variance. The resulting estimated variance is provided in the following equation:

Equation 26.

$$\text{var}\left(M_{Ci}\right) \approx \left(\frac{\partial M_{Ci}}{\partial \overline{NO_3}}\right)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + \left(\frac{\partial M_{Ci}}{\partial \delta_{NO_3}}\right)^2 \cdot \left(s_{\delta_{NO_3}}\right)^2$$

$$+ \left(\frac{\partial M_{Ci}}{\partial \overline{TOC}}\right)^2 \cdot \left(se_{\overline{TOC}}\right)^2 + \left(\frac{\partial M_{Ci}}{\partial \delta_{TOC}}\right)^2 \cdot \left(s_{\delta_{TOC}}\right)^2$$

$$+ \left(\frac{\partial M_{Ci}}{\partial \overline{\text{formate}}}\right)^2 \cdot \left(se_{\overline{\text{formate}}}\right)^2 + \left(\frac{\partial M_{Ci}}{\partial \delta_{\text{formate}}}\right)^2 \cdot \left(s_{\delta_{\text{formate}}}\right)^2$$

$$+ \left(\frac{\partial M_{Ci}}{\partial \overline{\text{oxalate}}}\right)^2 \cdot \left(se_{\overline{\text{oxalate}}}\right)^2 + \left(\frac{\partial M_{Ci}}{\partial \delta_{\text{oxalate}}}\right)^2 \cdot \left(s_{\delta_{\text{oxalate}}}\right)^2$$

where $var(M_{Ci})$ represents the estimate of the variance of the difference between the allowable carbon content from the i^{th} (i=1, 2, or 3) level of antifoam addition and the estimated carbon content from the addition; $\frac{\partial M_{Ci}}{\partial \bullet}$ represents the partial derivative of M_{Ci} with respect to the variable (●), $se_{\overline{NO_3}}$ represents the 1-sigma standard uncertainty of the average nitrate measurement of the SME samples, $s_{\delta_{NO_3}}$ represents the 1-sigma relative standard uncertainty of the batch-to-batch variation in the nitrate measurements (i.e., 2.73% of the $\overline{NO_3}$ value), $se_{\overline{TOC}}$ represents the 1-sigma standard uncertainty of the average TOC measurement of the SME samples, $s_{\delta_{TOC}}$ represents the 1-sigma relative standard uncertainty of the batch-to-batch variation in the TOC measurements (i.e., 2.72% of the $\overline{TOC}$ value), $se_{\overline{formate}}$ represents the 1-sigma standard uncertainty of the average formate measurement of the SME samples, $s_{\delta_{formate}}$ represents the 1-sigma standard uncertainty of the batch-to-batch variation in the formate measurements (based upon the results in Table 1 that value is given by 2.47% of the $\overline{formate}$ value), $se_{\overline{oxalate}}$ represents the 1-sigma standard uncertainty of the average oxalate measurement of the SME samples, where all oxalate values are above detection, and $s_{\delta_{oxalate}}$ represents the 1-sigma standard uncertainty of the batch-to-batch variation in the oxalate measurements (based upon the results in Table 1, that value is given by 3.01% of the $\overline{oxalate}$ value for the soluble oxalate and 5.05% of the $\overline{oxalate}$ value for the total oxalate). To be conservative in allowing either soluble or total oxalate to be used in this evaluation, the larger value, i.e., 5.05%, is utilized for the 1-sigma standard uncertainty of the batch-to-batch variation for oxalate.

Taking the partial derivatives and noting that the values of δ_{NO_3}, δ_{TOC}, $\delta_{formate}$, and $\delta_{oxalate}$ are taken to be zero lead to the following equation:

Equation 27.

$$var(M_{Ci}) \approx \left(0.5 \cdot j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + \left(0.5 \cdot j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(s_{\delta_{NO_3}}\right)^2$$
$$+ (-1)^2 \cdot \left(se_{\overline{TOC}}\right)^2 + (-1)^2 \cdot \left(s_{\delta_{TOC}}\right)^2$$
$$+ (f_C)^2 \cdot \left(se_{\overline{formate}}\right)^2 + (f_C)^2 \cdot \left(s_{\delta_{formate}}\right)^2$$
$$+ (o_C)^2 \cdot \left(se_{\overline{oxalate}}\right)^2 + (o_C)^2 \cdot \left(s_{\delta_{oxalate}}\right)^2$$

Substituting the values for the s_δ terms and for the f_C and o_C terms yields:

Equation 28.

$$\mathrm{var}(M_{Ci}) \approx \left(0.5 \cdot j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + \left(0.5 \cdot j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(0.0273 \cdot \overline{NO_3}\right)^2$$

$$+ (-1)^2 \cdot \left(se_{\overline{TOC}}\right)^2 + (-1)^2 \cdot \left(0.0272 \cdot \overline{TOC}\right)^2$$

$$+ (0.26681)^2 \cdot \left(se_{\overline{formate}}\right)^2 + (0.26681)^2 \cdot \left(0.0247 \cdot \overline{formate}\right)^2$$

$$+ (0.27292)^2 \cdot \left(se_{\overline{oxalate}}\right)^2 + (0.27292)^2 \cdot \left(0.0505 \cdot \overline{oxalate}\right)^2$$

This equation may be further simplified, for each level of antifoam addition (indexed by i) to

Equation 29.

$$\mathrm{var}(M_{Ci}) \approx 0.25 \cdot \left(j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(se_{\overline{NO_3}}\right)^2 + 0.000186323 \cdot \left(j_i \cdot \left(h_i + j_i \cdot \overline{NO_3}\right)^{-0.5}\right)^2 \cdot \left(\overline{NO_3}\right)^2$$

$$+ \left(se_{\overline{TOC}}\right)^2 + 0.00073984 \cdot \left(\overline{TOC}\right)^2 + 0.0711876 \cdot \left(se_{\overline{formate}}\right)^2 + 0.000043431 \cdot \left(\overline{formate}\right)^2$$

$$+ 0.0744853 \cdot \left(se_{\overline{oxalate}}\right)^2 + 0.000189956 \cdot \left(\overline{oxalate}\right)^2$$

4.2 Meeting the Constraint on the Antifoam Addition

The expanded uncertainty of the estimated difference, M_{Ci}, at 95% confidence is determined by multiplying the square root of the estimated variance of M_{Ci} by an appropriate Student's t statistic. In this case a one-sided confidence statement is needed; so, an upper 5%-tail of the Student's t distribution will be used. Again, utilizing a conservative 3 degrees of freedom for the estimated variance, the t value is 2.353. Thus, at 95% confidence the expanded uncertainty of the difference is 2.353 times the square root of the estimated variance of M_{Ci}. Thus, for the antifoam content of the SME to be acceptable (at 95% confidence), the following constraint must be met:

Equation 30.

$$M_{Ci} - 2.353 \cdot (\mathrm{Var}(M_{Ci}))^{0.5} > 0$$

where, for each level of antifoam indexed by i, M_{Ci} is determined from Equation 22 above, and $\mathrm{Var}(M_{Ci})$ is the estimate of the variance of M_{Ci} determined using Equation 29. The smallest of the three levels of antifoam that meets the constraint imposed by Equation 30 is used to select the appropriate TOC constraint that must also be met (as described in Section 3) for an acceptable SME decision.

4.3 Example Calculations in Meeting the Constraint on the Antifoam Addition

Sample calculations are given for the antifoam acceptability determination for the situation provided in Exhibit 4. In this exhibit four values (in ppm) are provided for TOC, formate, nitrate, and oxalate. Also, the averages, standard deviations, and standard errors of the mean are shown in this exhibit. The averages are the simple arithmetic averages of the 4 values for each analyte, and the standard deviations are also computed using the traditional equation for this summary statistic. The standard error of the mean for each analyte is the value of its standard deviation divided by 2 (the square root of the number of observations used to determine the average).

	TOC (ppm)	Formate (ppm)	Nitrate (ppm)	Oxalate (ppm)
	12500	42144	23700	4000
	12750	42827	23604	4150
	12800	41246	23229	3990
	12666	42783	23433	4125
averages	12679.000	42250.000	23491.500	4066.250
standard deviations	131.5193	738.5278	206.9275	83.0035
standard error of the mean	65.75966	369.26391	103.46376	41.50176

Exhibit 4. Inputs for the Illustration of Calculations for Antifoam Addition

With these values determined , Equations 22 and 29 can be used to compute the value for M_{Ci} and its estimated variance, respectively, for each of the antifoam additions (recall that the coefficients h_i and j_i are given in Table 5). Equation 31 provides the value for M_{Ci} for each of the antifoam additions.

Equation 31a (728 gal addition).

$$M_{C1} = \sqrt{h_1 + j_1 \cdot \overline{NO_3} - \overline{TOC} + f_C \cdot \overline{formate} \cdot 0.9697 + o_C \cdot \overline{oxalate} \cdot 0.9459}$$

$$= \sqrt{5117745.1 - 35.869438 \cdot 23491.500 - 12679.000 + 0.26681 \cdot 42250.000 \cdot 0.9697}$$

$$+ 0.27292 \cdot 4066.250 \cdot 0.9459$$

$$= 1369.5178$$

Equation 31b (894 gal addition).

$$M_{C2} = \sqrt{h_2 + j_2 \cdot \overline{NO_3} - \overline{TOC} + f_C \cdot \overline{formate} \cdot 0.9697 + o_C \cdot \overline{oxalate} \cdot 0.9459}$$

$$= \sqrt{7884790.5 - 55.545316 \cdot 23491.500 - 12679.000 + 0.26681 \cdot 42250.000 \cdot 0.9697}$$

$$+ 0.27292 \cdot 4066.250 \cdot 0.9459$$

$$= 1867.0228$$

Equation 31c (1,017 gal addition).

$$M_{C3} = \sqrt{h_3 + j_3 \cdot \overline{NO_3}} - \overline{TOC} + f_C \cdot \overline{formate} \cdot 0.9697 + o_C \cdot \overline{oxalate} \cdot 0.9459$$

$$= \sqrt{10373798 - 73.602487 \cdot 23491.500} - 12679.000 + 0.26681 \cdot 42250.000 \cdot 0.9697$$

$$+ 0.27292 \cdot 4066.250 \cdot 0.9459$$

$$= 2242.0800$$

Equation 32 provides the estimated variance for the M_{Ci} value for each antifoam addition.

Equation 32a (728 gal addition).

$$\mathrm{var}(M_{C1}) \approx 0.25 \cdot \left(j_1 \cdot \left(h_1 + j_1 \cdot \overline{NO_3}\right)^{-0.5} \right)^2 \cdot \left(se_{\overline{NO_3}} \right)^2$$

$$+ 0.000186323 \cdot \left(j_1 \cdot \left(h_1 + j_1 \cdot \overline{NO_3}\right)^{-0.5} \right)^2 \cdot \left(\overline{NO_3}\right)^2$$

$$+ \left(se_{\overline{TOC}}\right)^2 + 0.00073984 \cdot \left(\overline{TOC}\right)^2 + 0.0711876 \cdot \left(se_{\overline{formate}}\right)^2 + 0.000043431 \cdot \left(\overline{formate}\right)^2$$

$$+ 0.0744853 \cdot \left(se_{\overline{oxalate}} \right)^2 + 0.000189956 \cdot \left(\overline{oxalate}\right)^2$$

$$= 0.25 \cdot \left(-35.869438 \cdot \left(5117745.1 - 35.869438 \cdot 23491.500\right)^{-0.5} \right)^2 \cdot \left(103.46376\right)^2$$

$$+ 0.000186323 \cdot \left(-35.869438 \cdot \left(5117745.1 - 35.869438 \cdot 23491.500\right)^{-0.5} \right)^2 \cdot \left(23491.500\right)^2$$

$$+ \left(65.75966\right)^2 + 0.00073984 \cdot \left(12679.000\right)^2 + 0.0711876 \cdot \left(369.26391\right)^2 + 0.000043431 \cdot \left(42250.000\right)^2$$

$$+ 0.0744853 \cdot \left(41.50176\right)^2 + 0.000189956 \cdot \left(4066.250\right)^2$$

$$= 213793.566$$

Equation 32b (894 gal addition).

$$\mathrm{var}(M_{C2}) \approx 0.25 \cdot \left(j_2 \cdot \left(h_2 + j_2 \cdot \overline{NO_3} \right)^{-0.5} \right)^2 \cdot \left(se_{\overline{NO_3}} \right)^2$$

$$+ 0.000186323 \cdot \left(j_2 \cdot \left(h_2 + j_2 \cdot \overline{NO_3} \right)^{-0.5} \right)^2 \cdot \left(\overline{NO_3} \right)^2$$

$$+ \left(se_{\overline{TOC}} \right)^2 + 0.00073984 \cdot \left(\overline{TOC} \right)^2 + 0.0711876 \cdot \left(se_{\overline{formate}} \right)^2 + 0.000043431 \cdot \left(\overline{formate} \right)^2$$

$$+ 0.0744853 \cdot \left(se_{\overline{oxalate}} \right)^2 + 0.000189956 \cdot \left(\overline{oxalate} \right)^2$$

$$= 0.25 \cdot \left(- 55.545316 \cdot \left(7884790.5 - 55.545316 \cdot 23491.500 \right)^{-0.5} \right)^2 \cdot \left(103.46376 \right)^2$$

$$+ 0.000186323 \cdot \left(- 55.545316 \cdot \left(7884790.5 - 55.545316 \cdot 23491.500 \right)^{-0.5} \right)^2 \cdot \left(23491.500 \right)^2$$

$$+ \left(65.75966 \right)^2 + 0.00073984 \cdot \left(12679.000 \right)^2 + 0.0711876 \cdot \left(369.26391 \right)^2 + 0.000043431 \cdot \left(42250.000 \right)^2$$

$$+ 0.0744853 \cdot \left(41.50176 \right)^2 + 0.000189956 \cdot \left(4066.250 \right)^2$$

$$= 213811.284$$

Equation 32c (1,017 gal addition).

$$\begin{aligned}
\mathrm{var}(M_{C2}) \approx\ & 0.25 \cdot \left(j_3 \cdot \left(h_3 + j_3 \cdot \overline{NO_3}\right)^{-0.5} \right)^2 \cdot \left(se_{\overline{NO_3}} \right)^2 \\
& + 0.000186323 \cdot \left(j_3 \cdot \left(h_3 + j_3 \cdot \overline{NO_3}\right)^{-0.5} \right)^2 \cdot \left(\overline{NO_3}\right)^2 \\
& + \left(se_{\overline{TOC}}\right)^2 + 0.00073984 \cdot \left(\overline{TOC}\right)^2 + 0.0711876 \cdot \left(se_{\overline{formate}}\right)^2 + 0.000043431 \cdot \left(\overline{formate}\right)^2 \\
& + 0.0744853 \cdot \left(se_{\overline{oxalate}} \right)^2 + 0.000189956 \cdot \left(\overline{oxalate}\right)^2 \\
=\ & 0.25 \cdot \left(- 73.602487 \cdot \left(10373798 - 73.602487 \cdot 23491.500\right)^{-0.5} \right)^2 \cdot \left(103.46376\right)^2 \\
& + 0.000186323 \cdot \left(- 73.602487 \cdot \left(10373798 - 73.602487 \cdot 23491.500\right)^{-0.5} \right)^2 \cdot \left(23491.500\right)^2 \\
& + \left(65.75966\right)^2 + 0.00073984 \cdot \left(12679.000\right)^2 + 0.0711876 \cdot \left(369.26391\right)^2 + 0.000043431 \cdot \left(42250.000\right)^2 \\
& + 0.0744853 \cdot \left(41.50176\right)^2 + 0.000189956 \cdot \left(4066.250\right)^2 \\
=\ & 213827.928
\end{aligned}$$

With these calculations in hand, the question of meeting the antifoam constraint as defined by Equation 30 may be addressed for each candidate level of antifoam addition. Equation 33 provides the results from these determinations.

Equation 33a (728 gal addition).

$$\begin{aligned}
M_{C1} - 2.353 \cdot (\mathrm{Var}(M_{C1}))^{0.5} &= 1369.5178 - 2.353 \cdot (213793.566)^{0.5} \\
&= 1369.5178 - 2.353 \cdot 462.378 \\
&= 1369.5178 - 1087.975 \\
&= 281.54 \\
&> 0
\end{aligned}$$

Equation 33b (894 gal addition).

$$M_{C2} - 2.353 \cdot (Var(M_{C2}))^{0.5} = 1867.0228 - 2.353 \cdot (213811.284)^{0.5}$$

$$= 1867.0228 - 2.353 \cdot 462.397$$

$$= 1867.0228 - 1088.020$$

$$= 779.00$$

$$> 0$$

Equation 33c (1,017 gal addition).

$$M_{C3} - 2.353 \cdot (Var(M_{C3}))^{0.5} = 2242.0800 - 2.353 \cdot (213827.928)^{0.5}$$

$$= 2242.0800 - 2.353 \cdot 462.415$$

$$= 2242.0800 - 1088.062$$

$$= 1154.02$$

$$> 0$$

Note that the unit of measure for each of the Equation 33 results is ppm of carbon and since all of the results are positive, they indicate that the amount of carbon attributed to antifoam versus the amount allowed is acceptable for each of the antifoam additions considered in this example. Thus, the constraint imposed by TOC to NO_3 relationship for the smallest level of antifoam addition (i.e., 728 gal) would be the appropriate constraint to be used in evaluating the acceptability of the given SME batch.

5.0 Summary

Measurements of nitrate, oxalate, formate, and TOC standards generated by the DWPF Laboratory are presented in this report and an evaluation of the uncertainties of these measurements is provided. The impact of the uncertainties of these measurements on DWPF's strategy for controlling melter flammability is evaluated. The strategy includes monitoring each SME batch for its nitrate content and its TOC content relative to the nitrate content and relative to the antifoam additions made during the preparation of the SME batch.

A linearized approach for monitoring the relationship between TOC and nitrate is developed, equations are provided that integrate the measurement uncertainties into the flammability control strategy, and sample calculations for these equations are shown to illustrate the impact of the uncertainties on the flammability control strategy.

References

[1] Holtzscheiter, E.W. and J.P. Windham, "Technical Task Request: DWPF Melter Off-Gas Flammability Calculation for Sludge Batch 8," HLW-DWPF-TTR-2013-0009, December 4, 2012.

[2] Choi, A.S., "DWPF Melter Off-Gas Flammability Assessment (Sludge Batch 8)," Revision 8, X-CLC-S-00164, March 2013.

[3] Fellinger, T.L., "Technical Task Request: SB8 – Analytical Error Analysis for Melter Off Gas Flammability," HLW-DWPF-TTR-2013-0022, February 01, 2013.

[4] Edwards, T.B., "Task Technical and Quality Assurance Plan: SB8 – Analytical Error Analysis for Melter Off Gas Flammability," SRNL-RP-2013-00090, Revision 0, February 11, 2013.

[5] JMP Version 9.0.0, SAS Institute, Inc., Cary NC, 1989-2010.

[6] International Organization for Standardization (ISO), **Guide to the Expression of Uncertainty in Measurement**, ISO, Geneva, 1993, Corrected and reprinted, 1995.

Appendix A.

Measurement Data for Standards and Statistical Exhibits

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Total Oxalate	11/01/2012	2.05	2	0.05	2.5
Total Oxalate	11/03/2012	2.12	2	0.12	6
Total Oxalate	11/05/2012	2.08	2	0.08	4
Total Oxalate	11/07/2012	2.01	2	0.01	0.5
Total Oxalate	11/08/2012	2.04	2	0.04	2
Total Oxalate	11/09/2012	2.03	2	0.03	1.5
Total Oxalate	11/10/2012	2.04	2	0.04	2
Total Oxalate	11/13/2012	2.1	2	0.1	5
Total Oxalate	11/14/2012	2.1	2	0.1	5
Total Oxalate	11/15/2012	2.08	2	0.08	4
Total Oxalate	11/16/2012	2.09	2	0.09	4.5
Total Oxalate	11/16/2012	2.09	2	0.09	4.5
Total Oxalate	11/17/2012	2.1	2	0.1	5
Total Oxalate	11/18/2012	2.09	2	0.09	4.5
Total Oxalate	11/19/2012	2.06	2	0.06	3
Total Oxalate	11/20/2012	2.06	2	0.06	3
Total Oxalate	11/21/2012	2.07	2	0.07	3.5
Total Oxalate	11/21/2012	2.09	2	0.09	4.5
Total Oxalate	11/22/2012	2.09	2	0.09	4.5
Total Oxalate	11/24/2012	2.07	2	0.07	3.5
Total Oxalate	11/24/2012	2.1	2	0.1	5
Total Oxalate	11/24/2012	2.13	2	0.13	6.5
Total Oxalate	11/25/2012	2.09	2	0.09	4.5
Total Oxalate	11/26/2012	2.09	2	0.09	4.5
Total Oxalate	11/26/2012	2.09	2	0.09	4.5
Total Oxalate	11/27/2012	2.1	2	0.1	5
Total Oxalate	11/28/2012	2.06	2	0.06	3
Total Oxalate	11/28/2012	2.11	2	0.11	5.5
Total Oxalate	11/28/2012	2.11	2	0.11	5.5
Total Oxalate	11/29/2012	2.07	2	0.07	3.5
Total Oxalate	11/30/2012	2.09	2	0.09	4.5
Total Oxalate	12/02/2012	2.1	2	0.1	5
Total Oxalate	12/02/2012	2.15	2	0.15	7.5
Total Oxalate	12/03/2012	2.13	2	0.13	6.5
Total Oxalate	12/03/2012	2.14	2	0.14	7
Total Oxalate	12/04/2012	2.09	2	0.09	4.5
Total Oxalate	12/06/2012	2.09	2	0.09	4.5
Total Oxalate	12/06/2012	2.16	2	0.16	8
Total Oxalate	12/07/2012	2.13	2	0.13	6.5
Total Oxalate	12/08/2012	2.08	2	0.08	4
Total Oxalate	12/09/2012	2.07	2	0.07	3.5
Total Oxalate	12/10/2012	2.14	2	0.14	7
Total Oxalate	12/11/2012	2.07	2	0.07	3.5
Total Oxalate	12/12/2012	2.08	2	0.08	4
Total Oxalate	12/12/2012	2.11	2	0.11	5.5
Total Oxalate	12/13/2012	2.06	2	0.06	3
Total Oxalate	12/13/2012	2.07	2	0.07	3.5
Total Oxalate	12/14/2012	1.93	2	-0.07	-3.5
Total Oxalate	12/14/2012	1.94	2	-0.06	-3
Total Oxalate	12/14/2012	1.97	2	-0.03	-1.5
Total Oxalate	12/15/2012	1.95	2	-0.05	-2.5
Total Oxalate	12/15/2012	1.95	2	-0.05	-2.5
Total Oxalate	12/15/2012	1.97	2	-0.03	-1.5
Total Oxalate	12/16/2012	1.98	2	-0.02	-1
Total Oxalate	12/17/2012	1.99	2	-0.01	-0.5
Total Oxalate	12/20/2012	2.04	2	0.04	2
Total Oxalate	12/20/2012	2.05	2	0.05	2.5
Total Oxalate	12/21/2012	2.01	2	0.01	0.5
Total Oxalate	12/21/2012	2.05	2	0.05	2.5
Total Oxalate	12/23/2012	1.84	2	-0.16	-8
Total Oxalate	12/23/2012	1.96	2	-0.04	-2
Total Oxalate	12/23/2012	2.03	2	0.03	1.5
Total Oxalate	12/23/2012	2.03	2	0.03	1.5
Total Oxalate	12/24/2012	1.89	2	-0.11	-5.5
Total Oxalate	12/25/2012	1.91	2	-0.09	-4.5
Total Oxalate	12/27/2012	2.01	2	0.01	0.5
Total Oxalate	12/28/2012	2.02	2	0.02	1
Total Oxalate	12/29/2012	2.02	2	0.02	1
Total Oxalate	12/30/2012	2.02	2	0.02	1
Total Oxalate	12/31/2012	2.01	2	0.01	0.5
Total Oxalate	12/31/2012	2.02	2	0.02	1
Total Oxalate	01/01/2013	2.02	2	0.02	1
Total Oxalate	01/01/2013	2.02	2	0.02	1
Total Oxalate	01/02/2013	2.02	2	0.02	1
Total Oxalate	01/03/2013	1.98	2	-0.02	-1
Total Oxalate	01/03/2013	2	2	0	0
Total Oxalate	01/04/2013	2.01	2	0.01	0.5
Total Oxalate	01/05/2013	1.98	2	-0.02	-1
Total Oxalate	01/05/2013	1.99	2	-0.01	-0.5
Total Oxalate	01/06/2013	1.99	2	-0.01	-0.5
Total Oxalate	01/07/2013	1.99	2	-0.01	-0.5
Total Oxalate	01/08/2013	2.15	2	0.15	7.5
Total Oxalate	01/08/2013	2.21	2	0.21	10.5
Total Oxalate	01/09/2013	2.21	2	0.21	10.5
Total Oxalate	01/10/2013	2.23	2	0.23	11.5
Total Oxalate	01/11/2013	2.11	2	0.11	5.5
Total Oxalate	01/11/2013	2.18	2	0.18	9
Total Oxalate	01/12/2013	2.09	2	0.09	4.5
Total Oxalate	01/13/2013	2.15	2	0.15	7.5
Total Oxalate	01/13/2013	2.15	2	0.15	7.5
Total Oxalate	01/13/2013	2.15	2	0.15	7.5
Total Oxalate	01/14/2013	2.15	2	0.15	7.5
Total Oxalate	01/14/2013	2.18	2	0.18	9
Total Oxalate	01/14/2013	2.19	2	0.19	9.5
Total Oxalate	01/14/2013	2.24	2	0.24	12
Total Oxalate	01/15/2013	2.28	2	0.28	14
Total Oxalate	01/16/2013	2.27	2	0.27	13.5
Total Oxalate	01/16/2013	2.4	2	0.4	20
Total Oxalate	01/17/2013	2.26	2	0.26	13
Total Oxalate	01/17/2013	2.28	2	0.28	14
Total Oxalate	01/18/2013	2.4	2	0.4	20
Total Oxalate	01/19/2013	2.21	2	0.21	10.5
Total Oxalate	01/19/2013	2.3	2	0.3	15
Total Oxalate	01/20/2013	2.28	2	0.28	14
Total Oxalate	01/20/2013	2.31	2	0.31	15.5
Total Oxalate	01/21/2013	2.25	2	0.25	12.5
Total Oxalate	01/21/2013	2.32	2	0.32	16
Total Oxalate	01/22/2013	2.3	2	0.3	15
Total Oxalate	01/22/2013	2.3	2	0.3	15
Total Oxalate	01/23/2013	2.27	2	0.27	13.5
Total Oxalate	01/23/2013	2.36	2	0.36	18
Total Oxalate	01/24/2013	2.27	2	0.27	13.5
Total Oxalate	01/24/2013	2.29	2	0.29	14.5
Total Oxalate	01/25/2013	2.06	2	0.06	3
Total Oxalate	01/25/2013	2.06	2	0.06	3
Total Oxalate	01/26/2013	2	2	0	0
Total Oxalate	01/26/2013	2	2	0	0
Total Oxalate	01/26/2013	2	2	0	0
Total Oxalate	01/26/2013	2.01	2	0.01	0.5
Total Oxalate	01/26/2013	2.01	2	0.01	0.5
Total Oxalate	01/27/2013	2.01	2	0.01	0.5
Total Oxalate	01/28/2013	2.01	2	0.01	0.5
Total Oxalate	01/28/2013	2.01	2	0.01	0.5
Total Oxalate	01/28/2013	2.01	2	0.01	0.5
Total Oxalate	01/29/2013	2.08	2	0.08	4
Total Oxalate	01/30/2013	2.06	2	0.06	3
Total Oxalate	01/31/2013	2.01	2	0.01	0.5
Total Oxalate	02/01/2013	2.01	2	0.01	0.5
Total Oxalate	02/01/2013	2.02	2	0.02	1
Total Oxalate	02/01/2013	2.02	2	0.02	1
Total Oxalate	02/01/2013	2.03	2	0.03	1.5
Total Oxalate	02/02/2013	2.05	2	0.05	2.5
Total Oxalate	02/03/2013	2.06	2	0.06	3
Total Oxalate	02/04/2013	2.06	2	0.06	3
Total Oxalate	02/04/2013	2.08	2	0.08	4
Total Oxalate	02/05/2013	2.06	2	0.06	3
Total Oxalate	02/05/2013	2.09	2	0.09	4.5
Total Oxalate	02/06/2013	2.12	2	0.12	6
Total Oxalate	02/07/2013	2.09	2	0.09	4.5
Total Oxalate	02/07/2013	2.1	2	0.1	5
Total Oxalate	02/08/2013	2.02	2	0.02	1
Total Oxalate	02/09/2013	1.94	2	-0.06	-3
Total Oxalate	02/09/2013	2.01	2	0.01	0.5
Total Oxalate	02/09/2013	2.15	2	0.15	7.5
Total Oxalate	02/10/2013	2.07	2	0.07	3.5
Total Oxalate	11/01/2012	15.88	16	-0.12	-0.75
Total Oxalate	11/03/2012	15.89	16	-0.11	-0.6875
Total Oxalate	11/05/2012	15.96	16	-0.04	-0.25
Total Oxalate	11/07/2012	15.67	16	-0.33	-2.0625
Total Oxalate	11/08/2012	15.79	16	-0.21	-1.3125
Total Oxalate	11/09/2012	15.77	16	-0.23	-1.4375
Total Oxalate	11/10/2012	15.77	16	-0.23	-1.4375
Total Oxalate	11/13/2012	15.81	16	-0.19	-1.1875
Total Oxalate	11/14/2012	15.85	16	-0.15	-0.9375
Total Oxalate	11/15/2012	15.77	16	-0.23	-1.4375
Total Oxalate	11/16/2012	15.85	16	-0.15	-0.9375
Total Oxalate	11/16/2012	16.32	16	0.32	2
Total Oxalate	11/17/2012	16.33	16	0.33	2.0625
Total Oxalate	11/18/2012	15.92	16	-0.08	-0.5
Total Oxalate	11/19/2012	15.78	16	-0.22	-1.375
Total Oxalate	11/20/2012	16.44	16	0.44	2.75
Total Oxalate	11/21/2012	15.55	16	-0.45	-2.8125
Total Oxalate	11/21/2012	15.87	16	-0.13	-0.8125
Total Oxalate	11/22/2012	15.89	16	-0.11	-0.6875
Total Oxalate	11/24/2012	16.06	16	0.06	0.375
Total Oxalate	11/24/2012	16.1	16	0.1	0.625

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Total Oxalate	11/24/2012	16.51	16	0.51	3.1875
Total Oxalate	11/25/2012	16.45	16	0.45	2.8125
Total Oxalate	11/26/2012	15.54	16	-0.46	-2.875
Total Oxalate	11/26/2012	15.86	16	-0.14	-0.875
Total Oxalate	11/27/2012	16.05	16	0.05	0.3125
Total Oxalate	11/28/2012	15.8	16	-0.2	-1.25
Total Oxalate	11/28/2012	16.05	16	0.05	0.3125
Total Oxalate	11/28/2012	16.05	16	0.05	0.3125
Total Oxalate	11/29/2012	16.06	16	0.06	0.375
Total Oxalate	11/30/2012	15.4	16	-0.6	-3.75
Total Oxalate	12/02/2012	15.98	16	-0.02	-0.125
Total Oxalate	12/02/2012	16.07	16	0.07	0.4375
Total Oxalate	12/03/2012	16.14	16	0.14	0.875
Total Oxalate	12/03/2012	16.75	16	0.75	4.6875
Total Oxalate	12/04/2012	15.69	16	-0.31	-1.9375
Total Oxalate	12/06/2012	16.36	16	0.36	2.25
Total Oxalate	12/06/2012	16.41	16	0.41	2.5625
Total Oxalate	12/07/2012	16.05	16	0.05	0.3125
Total Oxalate	12/08/2012	15.82	16	-0.18	-1.125
Total Oxalate	12/09/2012	15.97	16	-0.03	-0.1875
Total Oxalate	12/10/2012	15.85	16	-0.15	-0.9375
Total Oxalate	12/11/2012	16	16	0	0
Total Oxalate	12/12/2012	15.91	16	-0.09	-0.5625
Total Oxalate	12/12/2012	16	16	0	0
Total Oxalate	12/13/2012	15.97	16	-0.03	-0.1875
Total Oxalate	12/13/2012	16.02	16	0.02	0.125
Total Oxalate	12/14/2012	15.73	16	-0.27	-1.6875
Total Oxalate	12/14/2012	15.94	16	-0.06	-0.375
Total Oxalate	12/14/2012	15.97	16	-0.03	-0.1875
Total Oxalate	12/15/2012	16	16	0	0
Total Oxalate	12/15/2012	16	16	0	0
Total Oxalate	12/15/2012	16.01	16	0.01	0.0625
Total Oxalate	12/16/2012	16.02	16	0.02	0.125
Total Oxalate	12/17/2012	16.02	16	0.02	0.125
Total Oxalate	12/20/2012	16.22	16	0.22	1.375
Total Oxalate	12/20/2012	16.38	16	0.38	2.375
Total Oxalate	12/21/2012	15.19	16	-0.81	-5.0625
Total Oxalate	12/21/2012	16.49	16	0.49	3.0625
Total Oxalate	12/23/2012	14.75	16	-1.25	-7.8125
Total Oxalate	12/23/2012	14.88	16	-1.12	-7
Total Oxalate	12/23/2012	15.74	16	-0.26	-1.625
Total Oxalate	12/23/2012	15.74	16	-0.26	-1.625
Total Oxalate	12/24/2012	14.66	16	-1.34	-8.375
Total Oxalate	12/25/2012	14.4	16	-1.6	-10
Total Oxalate	12/27/2012	15.99	16	-0.01	-0.0625
Total Oxalate	12/28/2012	16.03	16	0.03	0.1875
Total Oxalate	12/29/2012	16.04	16	0.04	0.25
Total Oxalate	12/30/2012	16.1	16	0.1	0.625
Total Oxalate	12/31/2012	16.07	16	0.07	0.4375
Total Oxalate	12/31/2012	16.08	16	0.08	0.5
Total Oxalate	01/01/2013	16.11	16	0.11	0.6875
Total Oxalate	01/01/2013	16.12	16	0.12	0.75
Total Oxalate	01/02/2013	16.13	16	0.13	0.8125
Total Oxalate	01/03/2013	15.67	16	-0.33	-2.0625
Total Oxalate	01/03/2013	15.97	16	-0.03	-0.1875
Total Oxalate	01/04/2013	15.72	16	-0.28	-1.75
Total Oxalate	01/05/2013	15.83	16	-0.17	-1.0625
Total Oxalate	01/05/2013	15.83	16	-0.17	-1.0625
Total Oxalate	01/06/2013	15.81	16	-0.19	-1.1875
Total Oxalate	01/07/2013	15.99	16	-0.01	-0.0625
Total Oxalate	01/08/2013	15.74	16	-0.26	-1.625
Total Oxalate	01/08/2013	16.18	16	0.18	1.125
Total Oxalate	01/09/2013	16.74	16	0.74	4.625
Total Oxalate	01/10/2013	15.91	16	-0.09	-0.5625
Total Oxalate	01/11/2013	15.9	16	-0.1	-0.625
Total Oxalate	01/11/2013	17	16	1	6.25
Total Oxalate	01/12/2013	16.77	16	0.77	4.8125
Total Oxalate	01/13/2013	16.04	16	0.04	0.25
Total Oxalate	01/13/2013	16.45	16	0.45	2.8125
Total Oxalate	01/13/2013	16.52	16	0.52	3.25
Total Oxalate	01/14/2013	16.45	16	0.45	2.8125
Total Oxalate	01/14/2013	16.7	16	0.7	4.375
Total Oxalate	01/14/2013	16.85	16	0.85	5.3125
Total Oxalate	01/14/2013	17.23	16	1.23	7.6875
Total Oxalate	01/15/2013	16.83	16	0.83	5.1875
Total Oxalate	01/16/2013	16.74	16	0.74	4.625
Total Oxalate	01/16/2013	16.75	16	0.75	4.6875
Total Oxalate	01/17/2013	16.85	16	0.85	5.3125
Total Oxalate	01/17/2013	16.88	16	0.88	5.5
Total Oxalate	01/18/2013	22.26	16	6.26	39.125
Total Oxalate	01/19/2013	16.87	16	0.87	5.4375
Total Oxalate	01/19/2013	17.79	16	1.79	11.1875
Total Oxalate	01/20/2013	17.19	16	1.19	7.4375
Total Oxalate	01/20/2013	17.58	16	1.58	9.875
Total Oxalate	01/21/2013	16.91	16	0.91	5.6875
Total Oxalate	01/21/2013	17.38	16	1.38	8.625
Total Oxalate	01/22/2013	17.12	16	1.12	7
Total Oxalate	01/22/2013	17.12	16	1.12	7
Total Oxalate	01/23/2013	17.17	16	1.17	7.3125
Total Oxalate	01/23/2013	17.27	16	1.27	7.9375
Total Oxalate	01/24/2013	17.43	16	1.43	8.9375
Total Oxalate	01/24/2013	17.56	16	1.56	9.75
Total Oxalate	01/25/2013	16.15	16	0.15	0.9375
Total Oxalate	01/25/2013	16.15	16	0.15	0.9375
Total Oxalate	01/26/2013	15.94	16	-0.06	-0.375
Total Oxalate	01/26/2013	15.97	16	-0.03	-0.1875
Total Oxalate	01/26/2013	15.98	16	-0.02	-0.125
Total Oxalate	01/26/2013	16	16	0	0
Total Oxalate	01/26/2013	16.02	16	0.02	0.125
Total Oxalate	01/27/2013	16.03	16	0.03	0.1875
Total Oxalate	01/28/2013	16.01	16	0.01	0.0625
Total Oxalate	01/28/2013	16.01	16	0.01	0.0625
Total Oxalate	01/28/2013	16.02	16	0.02	0.125
Total Oxalate	01/29/2013	15.52	16	-0.48	-3
Total Oxalate	01/30/2013	14.82	16	-1.18	-7.375
Total Oxalate	01/31/2013	15	16	-1	-6.25
Total Oxalate	02/01/2013	15.43	16	-0.57	-3.5625
Total Oxalate	02/01/2013	15.43	16	-0.57	-3.5625
Total Oxalate	02/01/2013	15.46	16	-0.54	-3.375
Total Oxalate	02/01/2013	15.53	16	-0.47	-2.9375
Total Oxalate	02/02/2013	15.14	16	-0.86	-5.375
Total Oxalate	02/03/2013	15.6	16	-0.4	-2.5
Total Oxalate	02/04/2013	15.62	16	-0.38	-2.375
Total Oxalate	02/04/2013	15.63	16	-0.37	-2.3125
Total Oxalate	02/05/2013	15.06	16	-0.94	-5.875
Total Oxalate	02/05/2013	15.73	16	-0.27	-1.6875
Total Oxalate	02/06/2013	15.14	16	-0.86	-5.375
Total Oxalate	02/07/2013	15.71	16	-0.29	-1.8125
Total Oxalate	02/07/2013	15.79	16	-0.21	-1.3125
Total Oxalate	02/08/2013	15.57	16	-0.43	-2.6875
Total Oxalate	02/09/2013	15.03	16	-0.97	-6.0625
Total Oxalate	02/09/2013	15.45	16	-0.55	-3.4375
Total Oxalate	02/09/2013	15.81	16	-0.19	-1.1875
Total Oxalate	02/10/2013	15.61	16	-0.39	-2.4375
Formate	11/09/2012	2.09	2	0.09	4.5
Formate	11/10/2012	2.05	2	0.05	2.5
Formate	11/11/2012	2.03	2	0.03	1.5
Formate	11/13/2012	2.03	2	0.03	1.5
Formate	11/13/2012	2.05	2	0.05	2.5
Formate	11/14/2012	2.02	2	0.02	1
Formate	11/16/2012	2.02	2	0.02	1
Formate	11/16/2012	2.07	2	0.07	3.5
Formate	11/17/2012	2.01	2	0.01	0.5
Formate	11/18/2012	2.02	2	0.02	1
Formate	11/19/2012	2.03	2	0.03	1.5
Formate	11/20/2012	2.03	2	0.03	1.5
Formate	11/21/2012	1.92	2	-0.08	-4
Formate	11/21/2012	2.06	2	0.06	3
Formate	11/21/2012	2.06	2	0.06	3
Formate	11/22/2012	1.95	2	-0.05	-2.5
Formate	11/24/2012	1.9	2	-0.1	-5
Formate	11/24/2012	1.96	2	-0.04	-2
Formate	11/24/2012	2.01	2	0.01	0.5
Formate	11/24/2012	2.01	2	0.01	0.5
Formate	11/25/2012	1.97	2	-0.03	-1.5
Formate	11/25/2012	1.99	2	-0.01	-0.5
Formate	11/25/2012	1.99	2	-0.01	-0.5
Formate	11/25/2012	2.2	2	0.2	10
Formate	11/26/2012	2.17	2	0.17	8.5
Formate	11/26/2012	2.17	2	0.17	8.5
Formate	11/27/2012	2.21	2	0.21	10.5
Formate	11/28/2012	2.19	2	0.19	9.5
Formate	11/28/2012	2.21	2	0.21	10.5
Formate	11/28/2012	2.21	2	0.21	10.5
Formate	11/29/2012	2.2	2	0.2	10
Formate	11/30/2012	2.13	2	0.13	6.5
Formate	12/02/2012	2.04	2	0.04	2
Formate	12/02/2012	2.06	2	0.06	3
Formate	12/03/2012	2.07	2	0.07	3.5
Formate	12/03/2012	2.07	2	0.07	3.5
Formate	12/04/2012	1.97	2	-0.03	-1.5
Formate	12/04/2012	2.06	2	0.06	3
Formate	12/06/2012	1.88	2	-0.12	-6
Formate	12/06/2012	2.06	2	0.06	3
Formate	12/07/2012	1.94	2	-0.06	-3
Formate	12/08/2012	2.07	2	0.07	3.5

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Formate	12/09/2012	1.9	2	-0.1	-5
Formate	12/09/2012	2.04	2	0.04	2
Formate	12/09/2012	2.06	2	0.06	3
Formate	12/10/2012	2.06	2	0.06	3
Formate	12/11/2012	1.96	2	-0.04	-2
Formate	12/12/2012	1.91	2	-0.09	-4.5
Formate	12/12/2012	1.98	2	-0.02	-1
Formate	12/14/2012	2.07	2	0.07	3.5
Formate	12/14/2012	2.07	2	0.07	3.5
Formate	12/15/2012	2.01	2	0.01	0.5
Formate	12/15/2012	2.04	2	0.04	2
Formate	12/15/2012	2.04	2	0.04	2
Formate	12/16/2012	2.05	2	0.05	2.5
Formate	12/17/2012	1.94	2	-0.06	-3
Formate	12/17/2012	2.04	2	0.04	2
Formate	12/17/2012	2.05	2	0.05	2.5
Formate	12/18/2012	2.02	2	0.02	1
Formate	12/20/2012	2.06	2	0.06	3
Formate	12/20/2012	2.07	2	0.07	3.5
Formate	12/21/2012	2.03	2	0.03	1.5
Formate	12/21/2012	2.05	2	0.05	2.5
Formate	12/22/2012	2.05	2	0.05	2.5
Formate	12/23/2012	2.03	2	0.03	1.5
Formate	12/23/2012	2.04	2	0.04	2
Formate	12/23/2012	2.06	2	0.06	3
Formate	12/23/2012	2.06	2	0.06	3
Formate	12/24/2012	2	2	0	0
Formate	12/24/2012	2.07	2	0.07	3.5
Formate	12/25/2012	1.85	2	-0.15	-7.5
Formate	12/25/2012	1.85	2	-0.15	-7.5
Formate	12/27/2012	2.06	2	0.06	3
Formate	12/27/2012	2.06	2	0.06	3
Formate	12/27/2012	2.07	2	0.07	3.5
Formate	12/28/2012	1.91	2	-0.09	-4.5
Formate	12/28/2012	2.06	2	0.06	3
Formate	12/28/2012	2.06	2	0.06	3
Formate	12/29/2012	2.05	2	0.05	2.5
Formate	12/29/2012	2.05	2	0.05	2.5
Formate	12/29/2012	2.07	2	0.07	3.5
Formate	12/30/2012	2.06	2	0.06	3
Formate	12/31/2012	2.02	2	0.02	1
Formate	12/31/2012	2.06	2	0.06	3
Formate	01/01/2013	2.05	2	0.05	2.5
Formate	01/01/2013	2.07	2	0.07	3.5
Formate	01/02/2013	2.08	2	0.08	4
Formate	01/03/2013	2.04	2	0.04	2
Formate	01/03/2013	2.04	2	0.04	2
Formate	01/04/2013	2.02	2	0.02	1
Formate	01/05/2013	2.06	2	0.06	3
Formate	01/05/2013	2.06	2	0.06	3
Formate	01/06/2013	2	2	0	0
Formate	01/07/2013	1.83	2	-0.17	-8.5
Formate	01/08/2013	2.01	2	0.01	0.5
Formate	01/11/2013	1.89	2	-0.11	-5.5
Formate	01/11/2013	2.07	2	0.07	3.5
Formate	01/12/2013	1.88	2	-0.12	-6
Formate	01/12/2013	2	2	0	0
Formate	01/13/2013	1.98	2	-0.02	-1
Formate	01/13/2013	2.01	2	0.01	0.5
Formate	01/13/2013	2.06	2	0.06	3
Formate	01/14/2013	1.93	2	-0.07	-3.5
Formate	01/14/2013	1.93	2	-0.07	-3.5
Formate	01/14/2013	1.98	2	-0.02	-1
Formate	01/14/2013	2	2	0	0
Formate	01/14/2013	2.05	2	0.05	2.5
Formate	01/15/2013	2.07	2	0.07	3.5
Formate	01/16/2013	2.06	2	0.06	3
Formate	01/17/2013	2.1	2	0.1	5
Formate	01/18/2013	2.07	2	0.07	3.5
Formate	01/18/2013	2.07	2	0.07	3.5
Formate	01/18/2013	2.15	2	0.15	7.5
Formate	01/18/2013	2.15	2	0.15	7.5
Formate	01/18/2013	2.15	2	0.15	7.5
Formate	01/19/2013	2.05	2	0.05	2.5
Formate	01/19/2013	2.13	2	0.13	6.5
Formate	01/19/2013	2.14	2	0.14	7
Formate	01/20/2013	2.1	2	0.1	5
Formate	01/21/2013	2.06	2	0.06	3
Formate	01/21/2013	2.13	2	0.13	6.5
Formate	01/21/2013	2.13	2	0.13	6.5
Formate	01/22/2013	2.04	2	0.04	2
Formate	01/22/2013	2.07	2	0.07	3.5
Formate	01/22/2013	2.11	2	0.11	5.5

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Formate	01/23/2013	2.03	2	0.03	1.5
Formate	01/23/2013	2.03	2	0.03	1.5
Formate	01/23/2013	2.04	2	0.04	2
Formate	01/23/2013	2.05	2	0.05	2.5
Formate	01/24/2013	2.04	2	0.04	2
Formate	01/24/2013	2.06	2	0.06	3
Formate	01/25/2013	2.04	2	0.04	2
Formate	01/25/2013	2.09	2	0.09	4.5
Formate	01/25/2013	2.11	2	0.11	5.5
Formate	01/26/2013	2.12	2	0.12	6
Formate	01/26/2013	2.12	2	0.12	6
Formate	01/26/2013	2.12	2	0.12	6
Formate	01/26/2013	2.13	2	0.13	6.5
Formate	01/26/2013	2.14	2	0.14	7
Formate	01/27/2013	2.12	2	0.12	6
Formate	01/27/2013	2.13	2	0.13	6.5
Formate	01/28/2013	2.01	2	0.01	0.5
Formate	01/28/2013	2.12	2	0.12	6
Formate	01/28/2013	2.12	2	0.12	6
Formate	01/29/2013	2.08	2	0.08	4
Formate	01/29/2013	2.12	2	0.12	6
Formate	01/30/2013	2.08	2	0.08	4
Formate	01/31/2013	2.08	2	0.08	4
Formate	01/31/2013	2.1	2	0.1	5
Formate	01/31/2013	2.11	2	0.11	5.5
Formate	02/01/2013	1.97	2	-0.03	-1.5
Formate	02/01/2013	2	2	0	0
Formate	02/01/2013	2	2	0	0
Formate	02/01/2013	2.01	2	0.01	0.5
Formate	02/01/2013	2.08	2	0.08	4
Formate	02/01/2013	2.08	2	0.08	4
Formate	02/02/2013	2.09	2	0.09	4.5
Formate	02/03/2013	2.04	2	0.04	2
Formate	02/03/2013	2.04	2	0.04	2
Formate	02/03/2013	2.1	2	0.1	5
Formate	02/04/2013	1.98	2	-0.02	-1
Formate	02/04/2013	2.03	2	0.03	1.5
Formate	02/05/2013	1.99	2	-0.01	-0.5
Formate	02/05/2013	2	2	0	0
Formate	02/06/2013	2.06	2	0.06	3
Formate	02/07/2013	2.06	2	0.06	3
Formate	02/07/2013	2.09	2	0.09	4.5
Formate	02/08/2013	2.07	2	0.07	3.5
Formate	02/09/2013	2.06	2	0.06	3
Formate	02/09/2013	2.07	2	0.07	3.5
Formate	02/09/2013	2.09	2	0.09	4.5
Formate	02/10/2013	2.08	2	0.08	4
Formate	11/09/2012	16.47	16	0.47	2.9375
Formate	11/10/2012	16.09	16	0.09	0.5625
Formate	11/11/2012	16.02	16	0.02	0.125
Formate	11/13/2012	16.09	16	0.09	0.5625
Formate	11/13/2012	16.14	16	0.14	0.875
Formate	11/14/2012	15.94	16	-0.06	-0.375
Formate	11/16/2012	16.13	16	0.13	0.8125
Formate	11/16/2012	16.44	16	0.44	2.75
Formate	11/17/2012	16.38	16	0.38	2.375
Formate	11/18/2012	16.12	16	0.12	0.75
Formate	11/19/2012	16.25	16	0.25	1.5625
Formate	11/20/2012	16.22	16	0.22	1.375
Formate	11/21/2012	15.2	16	-0.8	-5
Formate	11/21/2012	16.23	16	0.23	1.4375
Formate	11/21/2012	16.39	16	0.39	2.4375
Formate	11/22/2012	15.64	16	-0.36	-2.25
Formate	11/24/2012	15.7	16	-0.3	-1.875
Formate	11/24/2012	16.16	16	0.16	1
Formate	11/24/2012	16.35	16	0.35	2.1875
Formate	11/24/2012	16.39	16	0.39	2.4375
Formate	11/25/2012	15.88	16	-0.12	-0.75
Formate	11/25/2012	15.88	16	-0.12	-0.75
Formate	11/25/2012	16.34	16	0.34	2.125
Formate	11/25/2012	16.5	16	0.5	3.125
Formate	11/26/2012	15.74	16	-0.26	-1.625
Formate	11/26/2012	16.16	16	0.16	1
Formate	11/27/2012	16.59	16	0.59	3.6875
Formate	11/28/2012	16.57	16	0.57	3.5625
Formate	11/28/2012	16.57	16	0.57	3.5625
Formate	11/28/2012	16.66	16	0.66	4.125
Formate	11/29/2012	16.57	16	0.57	3.5625
Formate	11/30/2012	15.86	16	-0.14	-0.875
Formate	12/02/2012	16.14	16	0.14	0.875
Formate	12/02/2012	16.27	16	0.27	1.6875
Formate	12/03/2012	15.84	16	-0.16	-1
Formate	12/03/2012	16.54	16	0.54	3.375

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Formate	12/04/2012	16.33	16	0.33	2.0625
Formate	12/04/2012	16.39	16	0.39	2.4375
Formate	12/06/2012	16.55	16	0.55	3.4375
Formate	12/06/2012	16.64	16	0.64	4
Formate	12/07/2012	14.91	16	-1.09	-6.8125
Formate	12/08/2012	16.11	16	0.11	0.6875
Formate	12/09/2012	16.22	16	0.22	1.375
Formate	12/09/2012	16.55	16	0.55	3.4375
Formate	12/09/2012	16.56	16	0.56	3.5
Formate	12/10/2012	16.53	16	0.53	3.3125
Formate	12/11/2012	15.9	16	-0.1	-0.625
Formate	12/12/2012	15.29	16	-0.71	-4.4375
Formate	12/12/2012	15.75	16	-0.25	-1.5625
Formate	12/14/2012	16.41	16	0.41	2.5625
Formate	12/14/2012	16.43	16	0.43	2.6875
Formate	12/15/2012	16.23	16	0.23	1.4375
Formate	12/15/2012	16.23	16	0.23	1.4375
Formate	12/15/2012	16.24	16	0.24	1.5
Formate	12/16/2012	16.34	16	0.34	2.125
Formate	12/17/2012	16.29	16	0.29	1.8125
Formate	12/17/2012	16.3	16	0.3	1.875
Formate	12/17/2012	16.43	16	0.43	2.6875
Formate	12/18/2012	16.24	16	0.24	1.5
Formate	12/20/2012	15.96	16	-0.04	-0.25
Formate	12/20/2012	16.1	16	0.1	0.625
Formate	12/21/2012	16.29	16	0.29	1.8125
Formate	12/21/2012	16.36	16	0.36	2.25
Formate	12/22/2012	16.24	16	0.24	1.5
Formate	12/23/2012	15.64	16	-0.36	-2.25
Formate	12/23/2012	16.26	16	0.26	1.625
Formate	12/23/2012	16.26	16	0.26	1.625
Formate	12/23/2012	16.36	16	0.36	2.25
Formate	12/24/2012	16.31	16	0.31	1.9375
Formate	12/24/2012	16.46	16	0.46	2.875
Formate	12/25/2012	16.18	16	0.18	1.125
Formate	12/25/2012	16.18	16	0.18	1.125
Formate	12/27/2012	16.41	16	0.41	2.5625
Formate	12/27/2012	16.41	16	0.41	2.5625
Formate	12/27/2012	16.48	16	0.48	3
Formate	12/28/2012	16	16	0	0
Formate	12/28/2012	16.43	16	0.43	2.6875
Formate	12/28/2012	16.43	16	0.43	2.6875
Formate	12/29/2012	16.17	16	0.17	1.0625
Formate	12/29/2012	16.38	16	0.38	2.375
Formate	12/29/2012	16.38	16	0.38	2.375
Formate	12/30/2012	16.42	16	0.42	2.625
Formate	12/31/2012	16.39	16	0.39	2.4375
Formate	12/31/2012	16.42	16	0.42	2.625
Formate	01/01/2013	16.32	16	0.32	2
Formate	01/01/2013	16.45	16	0.45	2.8125
Formate	01/02/2013	16.35	16	0.35	2.1875
Formate	01/03/2013	16.01	16	0.01	0.0625
Formate	01/03/2013	16.34	16	0.34	2.125
Formate	01/04/2013	16.02	16	0.02	0.125
Formate	01/05/2013	16	16	0	0
Formate	01/05/2013	16.27	16	0.27	1.6875
Formate	01/06/2013	15.77	16	-0.23	-1.4375
Formate	01/07/2013	15.67	16	-0.33	-2.0625
Formate	01/08/2013	15.92	16	-0.08	-0.5
Formate	01/11/2013	15.3	16	-0.7	-4.375
Formate	01/11/2013	16.43	16	0.43	2.6875
Formate	01/12/2013	15.11	16	-0.89	-5.5625
Formate	01/12/2013	15.55	16	-0.45	-2.8125
Formate	01/13/2013	15.01	16	-0.99	-6.1875
Formate	01/13/2013	15.19	16	-0.81	-5.0625
Formate	01/13/2013	16.07	16	0.07	0.4375
Formate	01/14/2013	15.09	16	-0.91	-5.6875
Formate	01/14/2013	15.09	16	-0.91	-5.6875
Formate	01/14/2013	15.24	16	-0.76	-4.75
Formate	01/14/2013	15.32	16	-0.68	-4.25
Formate	01/14/2013	15.37	16	-0.63	-3.9375
Formate	01/15/2013	15.27	16	-0.73	-4.5625
Formate	01/16/2013	16.2	16	0.2	1.25
Formate	01/17/2013	16.25	16	0.25	1.5625
Formate	01/18/2013	15.57	16	-0.43	-2.6875
Formate	01/18/2013	15.57	16	-0.43	-2.6875
Formate	01/18/2013	16.28	16	0.28	1.75
Formate	01/18/2013	16.28	16	0.28	1.75
Formate	01/18/2013	16.59	16	0.59	3.6875
Formate	01/19/2013	16.54	16	0.54	3.375
Formate	01/19/2013	16.57	16	0.57	3.5625
Formate	01/20/2013	16.32	16	0.32	2
Formate	01/20/2013	16.47	16	0.47	2.9375
Formate	01/21/2013	16.11	16	0.11	0.6875
Formate	01/21/2013	16.19	16	0.19	1.1875
Formate	01/21/2013	16.25	16	0.25	1.5625
Formate	01/22/2013	16.25	16	0.25	1.5625
Formate	01/22/2013	16.28	16	0.28	1.75
Formate	01/22/2013	16.36	16	0.36	2.25
Formate	01/23/2013	16.13	16	0.13	0.8125
Formate	01/23/2013	16.16	16	0.16	1
Formate	01/23/2013	16.35	16	0.35	2.1875
Formate	01/23/2013	16.35	16	0.35	2.1875
Formate	01/24/2013	16.51	16	0.51	3.1875
Formate	01/24/2013	16.52	16	0.52	3.25
Formate	01/25/2013	16.48	16	0.48	3
Formate	01/25/2013	16.55	16	0.55	3.4375
Formate	01/25/2013	16.55	16	0.55	3.4375
Formate	01/26/2013	16.27	16	0.27	1.6875
Formate	01/26/2013	16.47	16	0.47	2.9375
Formate	01/26/2013	16.48	16	0.48	3
Formate	01/26/2013	16.52	16	0.52	3.25
Formate	01/26/2013	16.53	16	0.53	3.3125
Formate	01/27/2013	16.5	16	0.5	3.125
Formate	01/27/2013	16.55	16	0.55	3.4375
Formate	01/28/2013	15.79	16	-0.21	-1.3125
Formate	01/28/2013	16.5	16	0.5	3.125
Formate	01/28/2013	16.5	16	0.5	3.125
Formate	01/29/2013	16.42	16	0.42	2.625
Formate	01/29/2013	16.44	16	0.44	2.75
Formate	01/30/2013	16.32	16	0.32	2
Formate	01/31/2013	15.96	16	-0.04	-0.25
Formate	01/31/2013	16.41	16	0.41	2.5625
Formate	01/31/2013	16.42	16	0.42	2.625
Formate	02/01/2013	15.78	16	-0.22	-1.375
Formate	02/01/2013	15.84	16	-0.16	-1
Formate	02/01/2013	16.47	16	0.47	2.9375
Formate	02/01/2013	16.47	16	0.47	2.9375
Formate	02/01/2013	16.47	16	0.47	2.9375
Formate	02/01/2013	16.47	16	0.47	2.9375
Formate	02/02/2013	16.49	16	0.49	3.0625
Formate	02/03/2013	16.46	16	0.46	2.875
Formate	02/03/2013	16.5	16	0.5	3.125
Formate	02/03/2013	16.5	16	0.5	3.125
Formate	02/04/2013	15.82	16	-0.18	-1.125
Formate	02/04/2013	16.45	16	0.45	2.8125
Formate	02/05/2013	15.24	16	-0.76	-4.75
Formate	02/05/2013	16.44	16	0.44	2.75
Formate	02/06/2013	16.18	16	0.18	1.125
Formate	02/07/2013	16.1	16	0.1	0.625
Formate	02/07/2013	16.4	16	0.4	2.5
Formate	02/08/2013	16.41	16	0.41	2.5625
Formate	02/09/2013	16.42	16	0.42	2.625
Formate	02/09/2013	16.42	16	0.42	2.625
Formate	02/09/2013	16.43	16	0.43	2.6875
Formate	02/10/2013	16.41	16	0.41	2.5625
Nitrate	11/09/2012	2.02	2	0.02	1
Nitrate	11/10/2012	1.99	2	-0.01	-0.5
Nitrate	11/11/2012	1.98	2	-0.02	-1
Nitrate	11/13/2012	1.95	2	-0.05	-2.5
Nitrate	11/13/2012	1.96	2	-0.04	-2
Nitrate	11/14/2012	1.95	2	-0.05	-2.5
Nitrate	11/16/2012	1.95	2	-0.05	-2.5
Nitrate	11/16/2012	2	2	0	0
Nitrate	11/17/2012	1.93	2	-0.07	-3.5
Nitrate	11/18/2012	1.96	2	-0.04	-2
Nitrate	11/19/2012	1.97	2	-0.03	-1.5
Nitrate	11/20/2012	1.96	2	-0.04	-2
Nitrate	11/21/2012	1.86	2	-0.14	-7
Nitrate	11/21/2012	2	2	0	0
Nitrate	11/21/2012	2	2	0	0
Nitrate	11/22/2012	1.9	2	-0.1	-5
Nitrate	11/24/2012	1.88	2	-0.12	-6
Nitrate	11/24/2012	1.94	2	-0.06	-3
Nitrate	11/24/2012	1.99	2	-0.01	-0.5
Nitrate	11/24/2012	2	2	0	0
Nitrate	11/25/2012	1.98	2	-0.02	-1
Nitrate	11/25/2012	2	2	0	0
Nitrate	11/25/2012	2	2	0	0
Nitrate	11/25/2012	2.11	2	0.11	5.5
Nitrate	11/26/2012	2.08	2	0.08	4
Nitrate	11/26/2012	2.1	2	0.1	5
Nitrate	11/27/2012	2.11	2	0.11	5.5
Nitrate	11/28/2012	2.07	2	0.07	3.5
Nitrate	11/28/2012	2.11	2	0.11	5.5
Nitrate	11/28/2012	2.11	2	0.11	5.5

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Nitrate	11/29/2012	2.1	2	0.1	5
Nitrate	11/30/2012	2.02	2	0.02	1
Nitrate	12/02/2012	1.97	2	-0.03	-1.5
Nitrate	12/02/2012	1.99	2	-0.01	-0.5
Nitrate	12/03/2012	1.99	2	-0.01	-0.5
Nitrate	12/03/2012	1.99	2	-0.01	-0.5
Nitrate	12/04/2012	1.87	2	-0.13	-6.5
Nitrate	12/06/2012	1.99	2	-0.01	-0.5
Nitrate	12/06/2012	1.99	2	-0.01	-0.5
Nitrate	12/07/2012	1.89	2	-0.11	-5.5
Nitrate	12/08/2012	1.97	2	-0.03	-1.5
Nitrate	12/09/2012	1.81	2	-0.19	-9.5
Nitrate	12/09/2012	1.93	2	-0.07	-3.5
Nitrate	12/09/2012	1.96	2	-0.04	-2
Nitrate	12/09/2012	1.97	2	-0.03	-1.5
Nitrate	12/09/2012	1.98	2	-0.02	-1
Nitrate	12/10/2012	1.97	2	-0.03	-1.5
Nitrate	12/11/2012	1.91	2	-0.09	-4.5
Nitrate	12/12/2012	1.87	2	-0.13	-6.5
Nitrate	12/12/2012	1.93	2	-0.07	-3.5
Nitrate	12/14/2012	1.98	2	-0.02	-1
Nitrate	12/14/2012	1.98	2	-0.02	-1
Nitrate	12/15/2012	1.93	2	-0.07	-3.5
Nitrate	12/15/2012	1.96	2	-0.04	-2
Nitrate	12/15/2012	1.96	2	-0.04	-2
Nitrate	12/16/2012	1.96	2	-0.04	-2
Nitrate	12/17/2012	1.83	2	-0.17	-8.5
Nitrate	12/17/2012	1.96	2	-0.04	-2
Nitrate	12/17/2012	1.96	2	-0.04	-2
Nitrate	12/18/2012	1.95	2	-0.05	-2.5
Nitrate	12/20/2012	1.98	2	-0.02	-1
Nitrate	12/20/2012	1.98	2	-0.02	-1
Nitrate	12/21/2012	1.95	2	-0.05	-2.5
Nitrate	12/21/2012	1.96	2	-0.04	-2
Nitrate	12/22/2012	1.97	2	-0.03	-1.5
Nitrate	12/23/2012	1.98	2	-0.02	-1
Nitrate	12/23/2012	1.98	2	-0.02	-1
Nitrate	12/23/2012	2	2	0	0
Nitrate	12/23/2012	2.03	2	0.03	1.5
Nitrate	12/24/2012	1.91	2	-0.09	-4.5
Nitrate	12/24/2012	1.99	2	-0.01	-0.5
Nitrate	12/25/2012	1.94	2	-0.06	-3
Nitrate	12/25/2012	1.94	2	-0.06	-3
Nitrate	12/27/2012	1.98	2	-0.02	-1
Nitrate	12/27/2012	1.98	2	-0.02	-1
Nitrate	12/27/2012	1.98	2	-0.02	-1
Nitrate	12/28/2012	1.84	2	-0.16	-8
Nitrate	12/28/2012	1.98	2	-0.02	-1
Nitrate	12/28/2012	1.98	2	-0.02	-1
Nitrate	12/29/2012	1.96	2	-0.04	-2
Nitrate	12/29/2012	1.96	2	-0.04	-2
Nitrate	12/29/2012	1.99	2	-0.01	-0.5
Nitrate	12/30/2012	1.98	2	-0.02	-1
Nitrate	12/31/2012	1.94	2	-0.06	-3
Nitrate	12/31/2012	1.98	2	-0.02	-1
Nitrate	01/01/2013	1.97	2	-0.03	-1.5
Nitrate	01/01/2013	1.98	2	-0.02	-1
Nitrate	01/02/2013	1.97	2	-0.03	-1.5
Nitrate	01/03/2013	1.94	2	-0.06	-3
Nitrate	01/03/2013	1.94	2	-0.06	-3
Nitrate	01/04/2013	1.92	2	-0.08	-4
Nitrate	01/05/2013	1.96	2	-0.04	-2
Nitrate	01/05/2013	1.97	2	-0.03	-1.5
Nitrate	01/06/2013	1.92	2	-0.08	-4
Nitrate	01/07/2013	1.77	2	-0.23	-11.5
Nitrate	01/08/2013	1.9	2	-0.1	-5
Nitrate	01/11/2013	1.78	2	-0.22	-11
Nitrate	01/11/2013	1.96	2	-0.04	-2
Nitrate	01/12/2013	1.77	2	-0.23	-11.5
Nitrate	01/12/2013	1.9	2	-0.1	-5
Nitrate	01/13/2013	1.91	2	-0.09	-4.5
Nitrate	01/13/2013	1.92	2	-0.08	-4
Nitrate	01/13/2013	1.94	2	-0.06	-3
Nitrate	01/14/2013	1.85	2	-0.15	-7.5
Nitrate	01/14/2013	1.85	2	-0.15	-7.5
Nitrate	01/14/2013	1.91	2	-0.09	-4.5
Nitrate	01/14/2013	1.93	2	-0.07	-3.5
Nitrate	01/14/2013	1.96	2	-0.04	-2
Nitrate	01/15/2013	2.01	2	0.01	0.5
Nitrate	01/16/2013	1.99	2	-0.01	-0.5
Nitrate	01/17/2013	1.99	2	-0.01	-0.5
Nitrate	01/18/2013	2.01	2	0.01	0.5
Nitrate	01/18/2013	2.01	2	0.01	0.5

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Nitrate	01/18/2013	2.08	2	0.08	4
Nitrate	01/18/2013	2.08	2	0.08	4
Nitrate	01/18/2013	2.1	2	0.1	5
Nitrate	01/19/2013	2.02	2	0.02	1
Nitrate	01/19/2013	2.08	2	0.08	4
Nitrate	01/19/2013	2.08	2	0.08	4
Nitrate	01/20/2013	2.05	2	0.05	2.5
Nitrate	01/21/2013	2.03	2	0.03	1.5
Nitrate	01/21/2013	2.08	2	0.08	4
Nitrate	01/21/2013	2.09	2	0.09	4.5
Nitrate	01/22/2013	2.02	2	0.02	1
Nitrate	01/22/2013	2.04	2	0.04	2
Nitrate	01/22/2013	2.08	2	0.08	4
Nitrate	01/23/2013	2.03	2	0.03	1.5
Nitrate	01/23/2013	2.03	2	0.03	1.5
Nitrate	01/23/2013	2.04	2	0.04	2
Nitrate	01/23/2013	2.05	2	0.05	2.5
Nitrate	01/24/2013	2.08	2	0.08	4
Nitrate	01/24/2013	2.09	2	0.09	4.5
Nitrate	01/25/2013	2.04	2	0.04	2
Nitrate	01/25/2013	2.06	2	0.06	3
Nitrate	01/25/2013	2.08	2	0.08	4
Nitrate	01/26/2013	2.07	2	0.07	3.5
Nitrate	01/26/2013	2.07	2	0.07	3.5
Nitrate	01/26/2013	2.07	2	0.07	3.5
Nitrate	01/26/2013	2.08	2	0.08	4
Nitrate	01/26/2013	2.08	2	0.08	4
Nitrate	01/27/2013	2.07	2	0.07	3.5
Nitrate	01/27/2013	2.07	2	0.07	3.5
Nitrate	01/28/2013	1.96	2	-0.04	-2
Nitrate	01/28/2013	2.07	2	0.07	3.5
Nitrate	01/28/2013	2.07	2	0.07	3.5
Nitrate	01/29/2013	2.04	2	0.04	2
Nitrate	01/29/2013	2.07	2	0.07	3.5
Nitrate	01/30/2013	2.05	2	0.05	2.5
Nitrate	01/31/2013	2.05	2	0.05	2.5
Nitrate	01/31/2013	2.07	2	0.07	3.5
Nitrate	02/01/2013	1.95	2	-0.05	-2.5
Nitrate	02/01/2013	1.99	2	-0.01	-0.5
Nitrate	02/01/2013	2.02	2	0.02	1
Nitrate	02/01/2013	2.02	2	0.02	1
Nitrate	02/01/2013	2.05	2	0.05	2.5
Nitrate	02/01/2013	2.05	2	0.05	2.5
Nitrate	02/02/2013	2.07	2	0.07	3.5
Nitrate	02/03/2013	2.01	2	0.01	0.5
Nitrate	02/03/2013	2.01	2	0.01	0.5
Nitrate	02/03/2013	2.07	2	0.07	3.5
Nitrate	02/04/2013	1.97	2	-0.03	-1.5
Nitrate	02/04/2013	2.02	2	0.02	1
Nitrate	02/05/2013	1.99	2	-0.01	-0.5
Nitrate	02/05/2013	2	2	0	0
Nitrate	02/06/2013	2.02	2	0.02	1
Nitrate	02/07/2013	2.03	2	0.03	1.5
Nitrate	02/07/2013	2.05	2	0.05	2.5
Nitrate	02/08/2013	2.04	2	0.04	2
Nitrate	02/09/2013	2.04	2	0.04	2
Nitrate	02/09/2013	2.04	2	0.04	2
Nitrate	02/09/2013	2.06	2	0.06	3
Nitrate	02/10/2013	2.06	2	0.06	3
Nitrate	11/09/2012	16.5	16	0.5	3.125
Nitrate	11/10/2012	16.21	16	0.21	1.3125
Nitrate	11/11/2012	16.12	16	0.12	0.75
Nitrate	11/13/2012	16.01	16	0.01	0.0625
Nitrate	11/13/2012	16.03	16	0.03	0.1875
Nitrate	11/14/2012	15.95	16	-0.05	-0.3125
Nitrate	11/16/2012	16.17	16	0.17	1.0625
Nitrate	11/16/2012	16.44	16	0.44	2.75
Nitrate	11/17/2012	16.36	16	0.36	2.25
Nitrate	11/18/2012	16.18	16	0.18	1.125
Nitrate	11/19/2012	16.24	16	0.24	1.5
Nitrate	11/20/2012	16.04	16	0.04	0.25
Nitrate	11/21/2012	15	16	-1	-6.25
Nitrate	11/21/2012	16.12	16	0.12	0.75
Nitrate	11/21/2012	16.28	16	0.28	1.75
Nitrate	11/22/2012	15.49	16	-0.51	-3.1875
Nitrate	11/24/2012	15.57	16	-0.43	-2.6875
Nitrate	11/24/2012	16.12	16	0.12	0.75
Nitrate	11/24/2012	16.25	16	0.25	1.5625
Nitrate	11/24/2012	16.3	16	0.3	1.875
Nitrate	11/25/2012	15.84	16	-0.16	-1
Nitrate	11/25/2012	15.84	16	-0.16	-1
Nitrate	11/25/2012	16.3	16	0.3	1.875
Nitrate	11/25/2012	16.39	16	0.39	2.4375

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Nitrate	11/26/2012	15.61	16	-0.39	-2.4375
Nitrate	11/26/2012	16.01	16	0.01	0.0625
Nitrate	11/27/2012	16.35	16	0.35	2.1875
Nitrate	11/28/2012	16.32	16	0.32	2
Nitrate	11/28/2012	16.37	16	0.37	2.3125
Nitrate	11/28/2012	16.37	16	0.37	2.3125
Nitrate	11/29/2012	16.38	16	0.38	2.375
Nitrate	11/30/2012	15.7	16	-0.3	-1.875
Nitrate	12/02/2012	15.94	16	-0.06	-0.375
Nitrate	12/02/2012	16.07	16	0.07	0.4375
Nitrate	12/03/2012	15.65	16	-0.35	-2.1875
Nitrate	12/03/2012	16.23	16	0.23	1.4375
Nitrate	12/04/2012	15.94	16	-0.06	-0.375
Nitrate	12/06/2012	16.24	16	0.24	1.5
Nitrate	12/06/2012	16.24	16	0.24	1.5
Nitrate	12/07/2012	14.74	16	-1.26	-7.875
Nitrate	12/08/2012	15.79	16	-0.21	-1.3125
Nitrate	12/09/2012	14.95	16	-1.05	-6.5625
Nitrate	12/09/2012	15.7	16	-0.3	-1.875
Nitrate	12/09/2012	15.91	16	-0.09	-0.5625
Nitrate	12/09/2012	16.19	16	0.19	1.1875
Nitrate	12/09/2012	16.26	16	0.26	1.625
Nitrate	12/10/2012	16.24	16	0.24	1.5
Nitrate	12/11/2012	15.7	16	-0.3	-1.875
Nitrate	12/12/2012	15	16	-1	-6.25
Nitrate	12/12/2012	15.47	16	-0.53	-3.3125
Nitrate	12/14/2012	16.28	16	0.28	1.75
Nitrate	12/14/2012	16.33	16	0.33	2.0625
Nitrate	12/15/2012	15.99	16	-0.01	-0.0625
Nitrate	12/15/2012	16.12	16	0.12	0.75
Nitrate	12/15/2012	16.12	16	0.12	0.75
Nitrate	12/16/2012	16.1	16	0.1	0.625
Nitrate	12/17/2012	16.07	16	0.07	0.4375
Nitrate	12/17/2012	16.08	16	0.08	0.5
Nitrate	12/17/2012	16.11	16	0.11	0.6875
Nitrate	12/18/2012	16.11	16	0.11	0.6875
Nitrate	12/20/2012	15.89	16	-0.11	-0.6875
Nitrate	12/20/2012	15.92	16	-0.08	-0.5
Nitrate	12/21/2012	16.21	16	0.21	1.3125
Nitrate	12/21/2012	16.23	16	0.23	1.4375
Nitrate	12/22/2012	16.23	16	0.23	1.4375
Nitrate	12/23/2012	15.67	16	-0.33	-2.0625
Nitrate	12/23/2012	16.2	16	0.2	1.25
Nitrate	12/23/2012	16.2	16	0.2	1.25
Nitrate	12/23/2012	16.26	16	0.26	1.625
Nitrate	12/24/2012	16.21	16	0.21	1.3125
Nitrate	12/24/2012	16.21	16	0.21	1.3125
Nitrate	12/25/2012	15.93	16	-0.07	-0.4375
Nitrate	12/25/2012	15.93	16	-0.07	-0.4375
Nitrate	12/27/2012	16.26	16	0.26	1.625
Nitrate	12/27/2012	16.32	16	0.32	2
Nitrate	12/27/2012	16.32	16	0.32	2
Nitrate	12/28/2012	15.82	16	-0.18	-1.125
Nitrate	12/28/2012	16.28	16	0.28	1.75
Nitrate	12/28/2012	16.28	16	0.28	1.75
Nitrate	12/29/2012	16.08	16	0.08	0.5
Nitrate	12/29/2012	16.17	16	0.17	1.0625
Nitrate	12/29/2012	16.17	16	0.17	1.0625
Nitrate	12/30/2012	16.29	16	0.29	1.8125
Nitrate	12/31/2012	16.25	16	0.25	1.5625
Nitrate	12/31/2012	16.27	16	0.27	1.6875
Nitrate	01/01/2013	16.12	16	0.12	0.75
Nitrate	01/01/2013	16.29	16	0.29	1.8125
Nitrate	01/02/2013	16.1	16	0.1	0.625
Nitrate	01/03/2013	16.11	16	0.11	0.6875
Nitrate	01/03/2013	16.24	16	0.24	1.5
Nitrate	01/04/2013	15.86	16	-0.14	-0.875
Nitrate	01/05/2013	15.85	16	-0.15	-0.9375
Nitrate	01/05/2013	16.15	16	0.15	0.9375
Nitrate	01/06/2013	15.68	16	-0.32	-2
Nitrate	01/07/2013	15.65	16	-0.35	-2.1875
Nitrate	01/08/2013	15.8	16	-0.2	-1.25
Nitrate	01/11/2013	15.02	16	-0.98	-6.125
Nitrate	01/11/2013	16.17	16	0.17	1.0625
Nitrate	01/12/2013	14.82	16	-1.18	-7.375
Nitrate	01/12/2013	15.14	16	-0.86	-5.375
Nitrate	01/13/2013	14.75	16	-1.25	-7.8125
Nitrate	01/13/2013	14.98	16	-1.02	-6.375
Nitrate	01/13/2013	15.93	16	-0.07	-0.4375
Nitrate	01/14/2013	14.96	16	-1.04	-6.5
Nitrate	01/14/2013	14.96	16	-1.04	-6.5
Nitrate	01/14/2013	15.06	16	-0.94	-5.875
Nitrate	01/14/2013	15.26	16	-0.74	-4.625
Nitrate	01/14/2013	15.35	16	-0.65	-4.0625
Nitrate	01/15/2013	15.32	16	-0.68	-4.25
Nitrate	01/16/2013	15.9	16	-0.1	-0.625
Nitrate	01/17/2013	15.9	16	-0.1	-0.625
Nitrate	01/18/2013	15.22	16	-0.78	-4.875
Nitrate	01/18/2013	15.22	16	-0.78	-4.875
Nitrate	01/18/2013	15.9	16	-0.1	-0.625
Nitrate	01/18/2013	15.9	16	-0.1	-0.625
Nitrate	01/18/2013	16.17	16	0.17	1.0625
Nitrate	01/19/2013	16.1	16	0.1	0.625
Nitrate	01/19/2013	16.2	16	0.2	1.25
Nitrate	01/19/2013	16.23	16	0.23	1.4375
Nitrate	01/20/2013	15.94	16	-0.06	-0.375
Nitrate	01/21/2013	15.83	16	-0.17	-1.0625
Nitrate	01/21/2013	15.83	16	-0.17	-1.0625
Nitrate	01/21/2013	15.97	16	-0.03	-0.1875
Nitrate	01/22/2013	15.96	16	-0.04	-0.25
Nitrate	01/22/2013	16.02	16	0.02	0.125
Nitrate	01/22/2013	16.03	16	0.03	0.1875
Nitrate	01/23/2013	15.84	16	-0.16	-1
Nitrate	01/23/2013	15.92	16	-0.08	-0.5
Nitrate	01/23/2013	16.06	16	0.06	0.375
Nitrate	01/23/2013	16.06	16	0.06	0.375
Nitrate	01/24/2013	16.32	16	0.32	2
Nitrate	01/24/2013	16.34	16	0.34	2.125
Nitrate	01/25/2013	16.23	16	0.23	1.4375
Nitrate	01/25/2013	16.27	16	0.27	1.6875
Nitrate	01/25/2013	16.3	16	0.3	1.875
Nitrate	01/26/2013	16.11	16	0.11	0.6875
Nitrate	01/26/2013	16.27	16	0.27	1.6875
Nitrate	01/26/2013	16.3	16	0.3	1.875
Nitrate	01/26/2013	16.31	16	0.31	1.9375
Nitrate	01/26/2013	16.33	16	0.33	2.0625
Nitrate	01/27/2013	16.34	16	0.34	2.125
Nitrate	01/27/2013	16.34	16	0.34	2.125
Nitrate	01/28/2013	15.59	16	-0.41	-2.5625
Nitrate	01/28/2013	16.28	16	0.28	1.75
Nitrate	01/28/2013	16.28	16	0.28	1.75
Nitrate	01/29/2013	16.23	16	0.23	1.4375
Nitrate	01/29/2013	16.24	16	0.24	1.5
Nitrate	01/30/2013	16.31	16	0.31	1.9375
Nitrate	01/31/2013	15.75	16	-0.25	-1.5625
Nitrate	01/31/2013	16.25	16	0.25	1.5625
Nitrate	02/01/2013	15.64	16	-0.36	-2.25
Nitrate	02/01/2013	15.66	16	-0.34	-2.125
Nitrate	02/01/2013	16.31	16	0.31	1.9375
Nitrate	02/01/2013	16.31	16	0.31	1.9375
Nitrate	02/01/2013	16.31	16	0.31	1.9375
Nitrate	02/01/2013	16.31	16	0.31	1.9375
Nitrate	02/02/2013	16.27	16	0.27	1.6875
Nitrate	02/03/2013	16.3	16	0.3	1.875
Nitrate	02/03/2013	16.3	16	0.3	1.875
Nitrate	02/03/2013	16.3	16	0.3	1.875
Nitrate	02/04/2013	15.65	16	-0.35	-2.1875
Nitrate	02/04/2013	16.28	16	0.28	1.75
Nitrate	02/05/2013	15.12	16	-0.88	-5.5
Nitrate	02/05/2013	16.21	16	0.21	1.3125
Nitrate	02/06/2013	15.95	16	-0.05	-0.3125
Nitrate	02/07/2013	15.93	16	-0.07	-0.4375
Nitrate	02/07/2013	16.16	16	0.16	1
Nitrate	02/08/2013	16.19	16	0.19	1.1875
Nitrate	02/09/2013	16.08	16	0.08	0.5
Nitrate	02/09/2013	16.15	16	0.15	0.9375
Nitrate	02/09/2013	16.18	16	0.18	1.125
Nitrate	02/10/2013	16.25	16	0.25	1.5625
Soluble Oxalate	11/09/2012	2.14	2	0.14	7
Soluble Oxalate	11/10/2012	2.11	2	0.11	5.5
Soluble Oxalate	11/11/2012	2.09	2	0.09	4.5
Soluble Oxalate	11/13/2012	2.05	2	0.05	2.5
Soluble Oxalate	11/13/2012	2.05	2	0.05	2.5
Soluble Oxalate	11/14/2012	2.05	2	0.05	2.5
Soluble Oxalate	11/16/2012	2.04	2	0.04	2
Soluble Oxalate	11/16/2012	2.08	2	0.08	4
Soluble Oxalate	11/17/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	11/18/2012	2.03	2	0.03	1.5
Soluble Oxalate	11/19/2012	2.04	2	0.04	2
Soluble Oxalate	11/20/2012	2.03	2	0.03	1.5
Soluble Oxalate	11/21/2012	1.9	2	-0.1	-5
Soluble Oxalate	11/21/2012	2.09	2	0.09	4.5
Soluble Oxalate	11/21/2012	2.09	2	0.09	4.5
Soluble Oxalate	11/22/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	11/24/2012	1.92	2	-0.08	-4
Soluble Oxalate	11/24/2012	1.92	2	-0.08	-4

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Soluble Oxalate	11/24/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	11/24/2012	2.03	2	0.03	1.5
Soluble Oxalate	11/25/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	11/25/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	11/26/2012	2.19	2	0.19	9.5
Soluble Oxalate	11/26/2012	2.2	2	0.2	10
Soluble Oxalate	11/27/2012	2.22	2	0.22	11
Soluble Oxalate	11/28/2012	2.13	2	0.13	6.5
Soluble Oxalate	11/28/2012	2.22	2	0.22	11
Soluble Oxalate	11/29/2012	2.21	2	0.21	10.5
Soluble Oxalate	11/30/2012	2.11	2	0.11	5.5
Soluble Oxalate	12/02/2012	2.08	2	0.08	4
Soluble Oxalate	12/02/2012	2.12	2	0.12	6
Soluble Oxalate	12/03/2012	2.09	2	0.09	4.5
Soluble Oxalate	12/03/2012	2.11	2	0.11	5.5
Soluble Oxalate	12/04/2012	1.93	2	-0.07	-3.5
Soluble Oxalate	12/04/2012	2.03	2	0.03	1.5
Soluble Oxalate	12/06/2012	2.04	2	0.04	2
Soluble Oxalate	12/06/2012	2.09	2	0.09	4.5
Soluble Oxalate	12/07/2012	1.94	2	-0.06	-3
Soluble Oxalate	12/08/2012	2.05	2	0.05	2.5
Soluble Oxalate	12/09/2012	2.05	2	0.05	2.5
Soluble Oxalate	12/10/2012	2.07	2	0.07	3.5
Soluble Oxalate	12/11/2012	1.98	2	-0.02	-1
Soluble Oxalate	12/12/2012	1.9	2	-0.1	-5
Soluble Oxalate	12/12/2012	1.98	2	-0.02	-1
Soluble Oxalate	12/14/2012	2.07	2	0.07	3.5
Soluble Oxalate	12/14/2012	2.07	2	0.07	3.5
Soluble Oxalate	12/15/2012	1.99	2	-0.01	-0.5
Soluble Oxalate	12/15/2012	2.06	2	0.06	3
Soluble Oxalate	12/15/2012	2.06	2	0.06	3
Soluble Oxalate	12/16/2012	2.06	2	0.06	3
Soluble Oxalate	12/17/2012	2.06	2	0.06	3
Soluble Oxalate	12/18/2012	2.04	2	0.04	2
Soluble Oxalate	12/20/2012	2.08	2	0.08	4
Soluble Oxalate	12/20/2012	2.08	2	0.08	4
Soluble Oxalate	12/21/2012	2.06	2	0.06	3
Soluble Oxalate	12/21/2012	2.07	2	0.07	3.5
Soluble Oxalate	12/22/2012	2.1	2	0.1	5
Soluble Oxalate	12/23/2012	2.04	2	0.04	2
Soluble Oxalate	12/23/2012	2.06	2	0.06	3
Soluble Oxalate	12/23/2012	2.1	2	0.1	5
Soluble Oxalate	12/23/2012	2.1	2	0.1	5
Soluble Oxalate	12/24/2012	2	2	0	0
Soluble Oxalate	12/24/2012	2.09	2	0.09	4.5
Soluble Oxalate	12/25/2012	2.05	2	0.05	2.5
Soluble Oxalate	12/25/2012	2.05	2	0.05	2.5
Soluble Oxalate	12/27/2012	2.06	2	0.06	3
Soluble Oxalate	12/28/2012	2.09	2	0.09	4.5
Soluble Oxalate	12/28/2012	2.09	2	0.09	4.5
Soluble Oxalate	12/29/2012	2.04	2	0.04	2
Soluble Oxalate	12/29/2012	2.04	2	0.04	2
Soluble Oxalate	12/29/2012	2.1	2	0.1	5
Soluble Oxalate	12/30/2012	2.08	2	0.08	4
Soluble Oxalate	12/31/2012	2.03	2	0.03	1.5
Soluble Oxalate	12/31/2012	2.07	2	0.07	3.5
Soluble Oxalate	01/01/2013	2.07	2	0.07	3.5
Soluble Oxalate	01/01/2013	2.08	2	0.08	4
Soluble Oxalate	01/02/2013	2.07	2	0.07	3.5
Soluble Oxalate	01/03/2013	2.05	2	0.05	2.5
Soluble Oxalate	01/03/2013	2.05	2	0.05	2.5
Soluble Oxalate	01/04/2013	2.02	2	0.02	1
Soluble Oxalate	01/05/2013	2.04	2	0.04	2
Soluble Oxalate	01/05/2013	2.06	2	0.06	3
Soluble Oxalate	01/06/2013	2	2	0	0
Soluble Oxalate	01/07/2013	1.83	2	-0.17	-8.5
Soluble Oxalate	01/08/2013	1.97	2	-0.03	-1.5
Soluble Oxalate	01/11/2013	1.85	2	-0.15	-7.5
Soluble Oxalate	01/11/2013	2.04	2	0.04	2
Soluble Oxalate	01/12/2013	1.83	2	-0.17	-8.5
Soluble Oxalate	01/12/2013	1.93	2	-0.07	-3.5
Soluble Oxalate	01/13/2013	2.01	2	0.01	0.5
Soluble Oxalate	01/13/2013	2.02	2	0.02	1
Soluble Oxalate	01/13/2013	2.04	2	0.04	2
Soluble Oxalate	01/14/2013	2.02	2	0.02	1
Soluble Oxalate	01/14/2013	2.06	2	0.06	3
Soluble Oxalate	01/14/2013	2.07	2	0.07	3.5
Soluble Oxalate	01/15/2013	2.15	2	0.15	7.5
Soluble Oxalate	01/17/2013	2.15	2	0.15	7.5
Soluble Oxalate	01/18/2013	2.11	2	0.11	5.5
Soluble Oxalate	01/18/2013	2.18	2	0.18	9
Soluble Oxalate	01/18/2013	2.11	2	0.11	5.5
Soluble Oxalate	01/19/2013	2.12	2	0.12	6

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Soluble Oxalate	01/19/2013	2.19	2	0.19	9.5
Soluble Oxalate	01/20/2013	2.16	2	0.16	8
Soluble Oxalate	01/21/2013	2.12	2	0.12	6
Soluble Oxalate	01/22/2013	2.1	2	0.1	5
Soluble Oxalate	01/22/2013	2.13	2	0.13	6.5
Soluble Oxalate	01/23/2013	2.07	2	0.07	3.5
Soluble Oxalate	01/23/2013	2.07	2	0.07	3.5
Soluble Oxalate	01/23/2013	2.1	2	0.1	5
Soluble Oxalate	01/23/2013	2.1	2	0.1	5
Soluble Oxalate	01/24/2013	2.04	2	0.04	2
Soluble Oxalate	01/24/2013	2.09	2	0.09	4.5
Soluble Oxalate	01/25/2013	2.02	2	0.02	1
Soluble Oxalate	01/25/2013	2.13	2	0.13	6.5
Soluble Oxalate	01/25/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/26/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/26/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/26/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/26/2013	2.18	2	0.18	9
Soluble Oxalate	01/26/2013	2.18	2	0.18	9
Soluble Oxalate	01/27/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/27/2013	2.18	2	0.18	9
Soluble Oxalate	01/28/2013	2.05	2	0.05	2.5
Soluble Oxalate	01/28/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/28/2013	2.17	2	0.17	8.5
Soluble Oxalate	01/29/2013	2.15	2	0.15	7.5
Soluble Oxalate	01/30/2013	2.13	2	0.13	6.5
Soluble Oxalate	01/31/2013	2.13	2	0.13	6.5
Soluble Oxalate	01/31/2013	2.14	2	0.14	7
Soluble Oxalate	01/31/2013	2.15	2	0.15	7.5
Soluble Oxalate	02/01/2013	2.05	2	0.05	2.5
Soluble Oxalate	02/01/2013	2.01	2	0.01	0.5
Soluble Oxalate	02/01/2013	2.04	2	0.04	2
Soluble Oxalate	02/01/2013	2.05	2	0.05	2.5
Soluble Oxalate	02/03/2013	2.09	2	0.09	4.5
Soluble Oxalate	02/04/2013	2.04	2	0.04	2
Soluble Oxalate	02/04/2013	2.09	2	0.09	4.5
Soluble Oxalate	02/05/2013	2.06	2	0.06	3
Soluble Oxalate	02/05/2013	2.06	2	0.06	3
Soluble Oxalate	02/06/2013	2.12	2	0.12	6
Soluble Oxalate	02/07/2013	2.12	2	0.12	6
Soluble Oxalate	02/07/2013	2.15	2	0.15	7.5
Soluble Oxalate	02/08/2013	2.13	2	0.13	6.5
Soluble Oxalate	02/09/2013	2.11	2	0.11	5.5
Soluble Oxalate	02/09/2013	2.13	2	0.13	6.5
Soluble Oxalate	02/09/2013	2.15	2	0.15	7.5
Soluble Oxalate	02/10/2013	2.16	2	0.16	8
Soluble Oxalate	11/09/2012	16.27	16	0.27	1.6875
Soluble Oxalate	11/10/2012	15.99	16	-0.01	-0.0625
Soluble Oxalate	11/11/2012	15.89	16	-0.11	-0.6875
Soluble Oxalate	11/13/2012	15.69	16	-0.31	-1.9375
Soluble Oxalate	11/13/2012	15.7	16	-0.3	-1.875
Soluble Oxalate	11/14/2012	15.63	16	-0.37	-2.3125
Soluble Oxalate	11/16/2012	15.82	16	-0.18	-1.125
Soluble Oxalate	11/16/2012	16.08	16	0.08	0.5
Soluble Oxalate	11/17/2012	15.98	16	-0.02	-0.125
Soluble Oxalate	11/18/2012	15.81	16	-0.19	-1.1875
Soluble Oxalate	11/19/2012	15.89	16	-0.11	-0.6875
Soluble Oxalate	11/20/2012	15.82	16	-0.18	-1.125
Soluble Oxalate	11/21/2012	14.78	16	-1.22	-7.625
Soluble Oxalate	11/21/2012	15.95	16	-0.05	-0.3125
Soluble Oxalate	11/21/2012	16.11	16	0.11	0.6875
Soluble Oxalate	11/22/2012	15.3	16	-0.7	-4.375
Soluble Oxalate	11/24/2012	15.39	16	-0.61	-3.8125
Soluble Oxalate	11/24/2012	15.87	16	-0.13	-0.8125
Soluble Oxalate	11/24/2012	15.99	16	-0.01	-0.0625
Soluble Oxalate	11/24/2012	16.13	16	0.13	0.8125
Soluble Oxalate	11/25/2012	15.64	16	-0.36	-2.25
Soluble Oxalate	11/26/2012	15.44	16	-0.56	-3.5
Soluble Oxalate	11/26/2012	15.85	16	-0.15	-0.9375
Soluble Oxalate	11/27/2012	16.16	16	0.16	1
Soluble Oxalate	11/28/2012	16.05	16	0.05	0.3125
Soluble Oxalate	11/28/2012	16.17	16	0.17	1.0625
Soluble Oxalate	11/28/2012	16.17	16	0.17	1.0625
Soluble Oxalate	11/29/2012	16.2	16	0.2	1.25
Soluble Oxalate	11/30/2012	15.49	16	-0.51	-3.1875
Soluble Oxalate	12/02/2012	15.8	16	-0.2	-1.25
Soluble Oxalate	12/02/2012	15.92	16	-0.08	-0.5
Soluble Oxalate	12/03/2012	15.53	16	-0.47	-2.9375
Soluble Oxalate	12/03/2012	16.09	16	0.09	0.5625
Soluble Oxalate	12/04/2012	15.72	16	-0.28	-1.75
Soluble Oxalate	12/04/2012	16.13	16	0.13	0.8125
Soluble Oxalate	12/06/2012	16.05	16	0.05	0.3125
Soluble Oxalate	12/06/2012	16.1	16	0.1	0.625

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Soluble Oxalate	12/07/2012	14.62	16	-1.38	-8.625
Soluble Oxalate	12/08/2012	15.59	16	-0.41	-2.5625
Soluble Oxalate	12/09/2012	15.98	16	-0.02	-0.125
Soluble Oxalate	12/10/2012	16.11	16	0.11	0.6875
Soluble Oxalate	12/11/2012	15.6	16	-0.4	-2.5
Soluble Oxalate	12/12/2012	14.89	16	-1.11	-6.9375
Soluble Oxalate	12/12/2012	15.34	16	-0.66	-4.125
Soluble Oxalate	12/14/2012	15.98	16	-0.02	-0.125
Soluble Oxalate	12/14/2012	16.03	16	0.03	0.1875
Soluble Oxalate	12/15/2012	15.7	16	-0.3	-1.875
Soluble Oxalate	12/15/2012	15.83	16	-0.17	-1.0625
Soluble Oxalate	12/15/2012	15.83	16	-0.17	-1.0625
Soluble Oxalate	12/16/2012	15.85	16	-0.15	-0.9375
Soluble Oxalate	12/17/2012	15.82	16	-0.18	-1.125
Soluble Oxalate	12/18/2012	15.86	16	-0.14	-0.875
Soluble Oxalate	12/20/2012	15.67	16	-0.33	-2.0625
Soluble Oxalate	12/20/2012	15.68	16	-0.32	-2
Soluble Oxalate	12/21/2012	15.99	16	-0.01	-0.0625
Soluble Oxalate	12/21/2012	15.99	16	-0.01	-0.0625
Soluble Oxalate	12/22/2012	16.05	16	0.05	0.3125
Soluble Oxalate	12/23/2012	15.49	16	-0.51	-3.1875
Soluble Oxalate	12/23/2012	15.99	16	-0.01	-0.0625
Soluble Oxalate	12/23/2012	16.03	16	0.03	0.1875
Soluble Oxalate	12/23/2012	16.03	16	0.03	0.1875
Soluble Oxalate	12/24/2012	16	16	0	0
Soluble Oxalate	12/24/2012	16.04	16	0.04	0.25
Soluble Oxalate	12/25/2012	15.76	16	-0.24	-1.5
Soluble Oxalate	12/27/2012	16.08	16	0.08	0.5
Soluble Oxalate	12/28/2012	15.6	16	-0.4	-2.5
Soluble Oxalate	12/28/2012	16.02	16	0.02	0.125
Soluble Oxalate	12/28/2012	16.02	16	0.02	0.125
Soluble Oxalate	12/29/2012	15.93	16	-0.07	-0.4375
Soluble Oxalate	12/29/2012	15.93	16	-0.07	-0.4375
Soluble Oxalate	12/29/2012	16.04	16	0.04	0.25
Soluble Oxalate	12/30/2012	16.09	16	0.09	0.5625
Soluble Oxalate	12/31/2012	16.02	16	0.02	0.125
Soluble Oxalate	12/31/2012	16.08	16	0.08	0.5
Soluble Oxalate	01/01/2013	15.86	16	-0.14	-0.875
Soluble Oxalate	01/01/2013	16.08	16	0.08	0.5
Soluble Oxalate	01/02/2013	15.85	16	-0.15	-0.9375
Soluble Oxalate	01/03/2013	15.84	16	-0.16	-1
Soluble Oxalate	01/03/2013	15.84	16	-0.16	-1
Soluble Oxalate	01/04/2013	15.57	16	-0.43	-2.6875
Soluble Oxalate	01/05/2013	15.53	16	-0.47	-2.9375
Soluble Oxalate	01/05/2013	15.85	16	-0.15	-0.9375
Soluble Oxalate	01/06/2013	15.39	16	-0.61	-3.8125
Soluble Oxalate	01/07/2013	15.34	16	-0.66	-4.125
Soluble Oxalate	01/08/2013	15.46	16	-0.54	-3.375
Soluble Oxalate	01/11/2013	14.7	16	-1.3	-8.125
Soluble Oxalate	01/11/2013	15.81	16	-0.19	-1.1875
Soluble Oxalate	01/12/2013	14.44	16	-1.56	-9.75
Soluble Oxalate	01/12/2013	14.78	16	-1.22	-7.625
Soluble Oxalate	01/13/2013	14.43	16	-1.57	-9.8125
Soluble Oxalate	01/13/2013	14.67	16	-1.33	-8.3125
Soluble Oxalate	01/13/2013	15.65	16	-0.35	-2.1875
Soluble Oxalate	01/14/2013	14.65	16	-1.35	-8.4375
Soluble Oxalate	01/14/2013	14.65	16	-1.35	-8.4375
Soluble Oxalate	01/14/2013	15.17	16	-0.83	-5.1875
Soluble Oxalate	01/15/2013	15.15	16	-0.85	-5.3125
Soluble Oxalate	01/17/2013	16.2	16	0.2	1.25
Soluble Oxalate	01/18/2013	15.55	16	-0.45	-2.8125
Soluble Oxalate	01/18/2013	16.23	16	0.23	1.4375
Soluble Oxalate	01/18/2013	16.48	16	0.48	3
Soluble Oxalate	01/19/2013	16.45	16	0.45	2.8125
Soluble Oxalate	01/19/2013	16.5	16	0.5	3.125
Soluble Oxalate	01/20/2013	16.22	16	0.22	1.375
Soluble Oxalate	01/21/2013	16.11	16	0.11	0.6875
Soluble Oxalate	01/22/2013	16.25	16	0.25	1.5625
Soluble Oxalate	01/22/2013	16.31	16	0.31	1.9375
Soluble Oxalate	01/23/2013	16.16	16	0.16	1
Soluble Oxalate	01/23/2013	16.22	16	0.22	1.375
Soluble Oxalate	01/23/2013	16.33	16	0.33	2.0625
Soluble Oxalate	01/23/2013	16.33	16	0.33	2.0625
Soluble Oxalate	01/24/2013	16.54	16	0.54	3.375
Soluble Oxalate	01/24/2013	16.62	16	0.62	3.875
Soluble Oxalate	01/25/2013	16.45	16	0.45	2.8125
Soluble Oxalate	01/25/2013	16.47	16	0.47	2.9375
Soluble Oxalate	01/25/2013	16.55	16	0.55	3.4375
Soluble Oxalate	01/26/2013	16.28	16	0.28	1.75
Soluble Oxalate	01/26/2013	16.45	16	0.45	2.8125
Soluble Oxalate	01/26/2013	16.46	16	0.46	2.875
Soluble Oxalate	01/26/2013	16.48	16	0.48	3
Soluble Oxalate	01/26/2013	16.49	16	0.49	3.0625

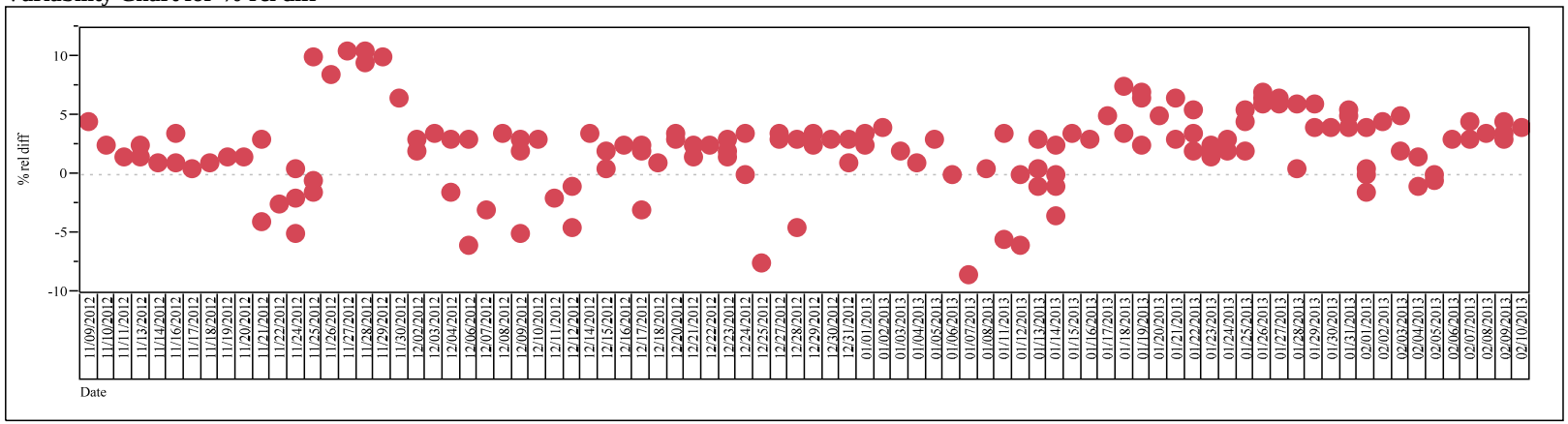
Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
Soluble Oxalate	01/27/2013	16.48	16	0.48	3
Soluble Oxalate	01/27/2013	16.48	16	0.48	3
Soluble Oxalate	01/28/2013	15.73	16	-0.27	-1.6875
Soluble Oxalate	01/28/2013	16.41	16	0.41	2.5625
Soluble Oxalate	01/28/2013	16.41	16	0.41	2.5625
Soluble Oxalate	01/29/2013	16.37	16	0.37	2.3125
Soluble Oxalate	01/30/2013	16.34	16	0.34	2.125
Soluble Oxalate	01/31/2013	15.81	16	-0.19	-1.1875
Soluble Oxalate	01/31/2013	16.32	16	0.32	2
Soluble Oxalate	01/31/2013	16.33	16	0.33	2.0625
Soluble Oxalate	02/01/2013	15.72	16	-0.28	-1.75
Soluble Oxalate	02/01/2013	15.72	16	-0.28	-1.75
Soluble Oxalate	02/01/2013	16.33	16	0.33	2.0625
Soluble Oxalate	02/01/2013	16.37	16	0.37	2.3125
Soluble Oxalate	02/03/2013	16.41	16	0.41	2.5625
Soluble Oxalate	02/04/2013	15.76	16	-0.24	-1.5
Soluble Oxalate	02/04/2013	16.38	16	0.38	2.375
Soluble Oxalate	02/05/2013	15.26	16	-0.74	-4.625
Soluble Oxalate	02/05/2013	16.43	16	0.43	2.6875
Soluble Oxalate	02/06/2013	16.09	16	0.09	0.5625
Soluble Oxalate	02/07/2013	16.07	16	0.07	0.4375
Soluble Oxalate	02/07/2013	16.31	16	0.31	1.9375
Soluble Oxalate	02/08/2013	16.34	16	0.34	2.125
Soluble Oxalate	02/09/2013	16.22	16	0.22	1.375
Soluble Oxalate	02/09/2013	16.29	16	0.29	1.8125
Soluble Oxalate	02/09/2013	16.32	16	0.32	2
Soluble Oxalate	02/10/2013	16.38	16	0.38	2.375
TOC 1	10/15/2012	0.97	1	-0.03	-3
TOC 2	10/15/2012	0.98	1	-0.02	-2
TOC 1	10/15/2012	1	1	0	0
TOC 2	10/15/2012	1.01	1	0.01	1
TOC 1	10/24/2012	0.96	1	-0.04	-4
TOC 1	10/24/2012	0.97	1	-0.03	-3
TOC 2	10/24/2012	0.97	1	-0.03	-3
TOC 2	10/24/2012	0.99	1	-0.01	-1
TOC 1	11/21/2012	0.96	1	-0.04	-4
TOC 2	11/21/2012	0.96	1	-0.04	-4
TOC 1	11/21/2012	0.96	1	-0.04	-4
TOC 2	11/21/2012	0.97	1	-0.03	-3
TOC 1	11/25/2012	0.99	1	-0.01	-1
TOC 1	11/25/2012	0.99	1	-0.01	-1
TOC 2	11/25/2012	1	1	0	0
TOC 2	11/25/2012	1.01	1	0.01	1
TOC 1	12/04/2012	1.04	1	0.04	4
TOC 2	12/04/2012	1.04	1	0.04	4
TOC 1	12/04/2012	1.05	1	0.05	5
TOC 2	12/04/2012	1.05	1	0.05	5
TOC 1	12/06/2012	1.01	1	0.01	1
TOC 1	12/06/2012	1.02	1	0.02	2
TOC 2	12/06/2012	1.02	1	0.02	2
TOC 2	12/06/2012	1.02	1	0.02	2
TOC 1	12/09/2012	0.98	1	-0.02	-2
TOC 2	12/09/2012	0.99	1	-0.01	-1
TOC 2	12/09/2012	0.99	1	-0.01	-1
TOC 1	12/09/2012	1.01	1	0.01	1
TOC 1	12/13/2012	0.98	1	-0.02	-2
TOC 1	12/13/2012	1	1	0	0
TOC 2	12/13/2012	1	1	0	0
TOC 2	12/13/2012	1.03	1	0.03	3
TOC 2	12/14/2012	0.9	1	-0.1	-10
TOC 1	12/14/2012	0.96	1	-0.04	-4
TOC 1	12/14/2012	1.06	1	0.06	6
TOC 2	12/14/2012	1.06	1	0.06	6
TOC 1	12/23/2012	0.96	1	-0.04	-4
TOC 2	12/23/2012	0.98	1	-0.02	-2
TOC 1	12/23/2012	0.99	1	-0.01	-1
TOC 2	12/23/2012	0.99	1	-0.01	-1
TOC 1	12/24/2012	0.98	1	-0.02	-2
TOC 1	12/24/2012	0.98	1	-0.02	-2
TOC 2	12/24/2012	0.99	1	-0.01	-1
TOC 2	12/24/2012	0.99	1	-0.01	-1
TOC 1	12/25/2012	1	1	0	0
TOC 1	12/25/2012	1	1	0	0
TOC 2	12/25/2012	1.04	1	0.04	4
TOC 2	12/25/2012	1.05	1	0.05	5
TOC 1	01/12/2013	0.96	1	-0.04	-4
TOC 2	01/12/2013	0.97	1	-0.03	-3
TOC 2	01/12/2013	0.97	1	-0.03	-3
TOC 1	01/12/2013	0.98	1	-0.02	-2
TOC 1	01/13/2013	0.96	1	-0.04	-4
TOC 2	01/13/2013	0.97	1	-0.03	-3
TOC 1	01/13/2013	0.97	1	-0.03	-3
TOC 2	01/13/2013	0.97	1	-0.03	-3

Table A1. DWPF Laboratory Measurements of Anion and TOC Standards

Analyte	Date	Measurement (ppm)	Reference Value (ppm)	diff	% rel diff
TOC 1	01/14/2013	0.96	1	-0.04	-4
TOC 1	01/14/2013	0.96	1	-0.04	-4
TOC 1	01/14/2013	0.96	1	-0.04	-4
TOC 2	01/14/2013	0.97	1	-0.03	-3
TOC 1	01/14/2013	0.97	1	-0.03	-3
TOC 2	01/14/2013	0.97	1	-0.03	-3
TOC 2	01/14/2013	0.98	1	-0.02	-2
TOC 2	01/14/2013	0.98	1	-0.02	-2
TOC 1	01/22/2013	1.03	1	0.03	3
TOC 2	01/22/2013	1.06	1	0.06	6
TOC 1	01/22/2013	1.06	1	0.06	6
TOC 2	01/22/2013	1.06	1	0.06	6
TOC 1	01/23/2013	0.97	1	-0.03	-3
TOC 2	01/23/2013	0.97	1	-0.03	-3
TOC 1	01/23/2013	0.97	1	-0.03	-3
TOC 2	01/23/2013	0.97	1	-0.03	-3
TOC 1	01/26/2013	0.99	1	-0.01	-1
TOC 2	01/26/2013	1	1	0	0
TOC 1	01/26/2013	1	1	0	0
TOC 2	01/26/2013	1.02	1	0.02	2
TOC 1	01/28/2013	0.99	1	-0.01	-1
TOC 2	01/28/2013	1	1	0	0
TOC 1	01/28/2013	1.01	1	0.01	1
TOC 2	01/28/2013	1.02	1	0.02	2
TOC 1	02/01/2013	0.95	1	-0.05	-5
TOC 2	02/01/2013	0.96	1	-0.04	-4
TOC 1	02/01/2013	0.96	1	-0.04	-4
TOC 2	02/01/2013	0.96	1	-0.04	-4
TOC 1	02/01/2013	1	1	0	0
TOC 2	02/01/2013	1.04	1	0.04	4
TOC 1	02/01/2013	1.04	1	0.04	4
TOC 2	02/01/2013	1.05	1	0.05	5
TOC 1	02/09/2013	1.03	1	0.03	3
TOC 2	02/09/2013	1.04	1	0.04	4
TOC 1	02/09/2013	1.11	1	0.11	11
TOC 2	02/09/2013	1.12	1	0.12	12
TOC 1	10/15/2012	18.98	20	-1.02	-5.1
TOC 2	10/15/2012	19	20	-1	-5
TOC 1	10/15/2012	19.23	20	-0.77	-3.85
TOC 2	10/15/2012	19.3	20	-0.7	-3.5
TOC 1	10/24/2012	18.89	20	-1.11	-5.55
TOC 1	10/24/2012	18.92	20	-1.08	-5.4
TOC 2	10/24/2012	18.97	20	-1.03	-5.15
TOC 2	10/24/2012	19.13	20	-0.87	-4.35
TOC 1	11/21/2012	19.74	20	-0.26	-1.3
TOC 2	11/21/2012	19.81	20	-0.19	-0.95
TOC 1	11/21/2012	19.87	20	-0.13	-0.65
TOC 2	11/21/2012	19.94	20	-0.06	-0.3
TOC 1	11/25/2012	19.72	20	-0.28	-1.4
TOC 1	11/25/2012	19.78	20	-0.22	-1.1
TOC 2	11/25/2012	19.86	20	-0.14	-0.7
TOC 2	11/25/2012	19.97	20	-0.03	-0.15
TOC 1	12/04/2012	20.09	20	0.09	0.45
TOC 2	12/04/2012	20.09	20	0.09	0.45
TOC 1	12/04/2012	20.09	20	0.09	0.45
TOC 2	12/04/2012	20.26	20	0.26	1.3
TOC 1	12/06/2012	20.18	20	0.18	0.9
TOC 1	12/06/2012	20.22	20	0.22	1.1
TOC 2	12/06/2012	20.38	20	0.38	1.9
TOC 2	12/06/2012	20.39	20	0.39	1.95
TOC 1	12/09/2012	19.88	20	-0.12	-0.6
TOC 2	12/09/2012	20.06	20	0.06	0.3
TOC 2	12/09/2012	20.07	20	0.07	0.35
TOC 1	12/09/2012	20.23	20	0.23	1.15
TOC 1	12/13/2012	19.69	20	-0.31	-1.55
TOC 1	12/13/2012	19.74	20	-0.26	-1.3
TOC 2	12/13/2012	19.93	20	-0.07	-0.35
TOC 2	12/13/2012	20	20	0	0
TOC 2	12/14/2012	19.66	20	-0.34	-1.7
TOC 1	12/14/2012	19.79	20	-0.21	-1.05
TOC 1	12/14/2012	19.96	20	-0.04	-0.2
TOC 2	12/14/2012	20.13	20	0.13	0.65
TOC 1	12/23/2012	19.9	20	-0.1	-0.5
TOC 2	12/23/2012	19.93	20	-0.07	-0.35
TOC 1	12/23/2012	20.05	20	0.05	0.25
TOC 2	12/23/2012	20.13	20	0.13	0.65
TOC 1	12/24/2012	19.88	20	-0.12	-0.6
TOC 1	12/24/2012	19.88	20	-0.12	-0.6
TOC 2	12/24/2012	19.89	20	-0.11	-0.55
TOC 2	12/24/2012	20.02	20	0.02	0.1
TOC 1	12/25/2012	19.64	20	-0.36	-1.8
TOC 1	12/25/2012	19.73	20	-0.27	-1.35
TOC 2	12/25/2012	19.73	20	-0.27	-1.35
TOC 2	12/25/2012	19.75	20	-0.25	-1.25
TOC 1	01/12/2013	20.09	20	0.09	0.45
TOC 2	01/12/2013	20.09	20	0.09	0.45
TOC 2	01/12/2013	20.3	20	0.3	1.5
TOC 1	01/12/2013	20.33	20	0.33	1.65
TOC 1	01/13/2013	20.27	20	0.27	1.35
TOC 2	01/13/2013	20.44	20	0.44	2.2
TOC 1	01/13/2013	20.65	20	0.65	3.25
TOC 2	01/13/2013	20.73	20	0.73	3.65
TOC 1	01/14/2013	20.27	20	0.27	1.35
TOC 1	01/14/2013	20.44	20	0.44	2.2
TOC 1	01/14/2013	20.57	20	0.57	2.85
TOC 2	01/14/2013	20.68	20	0.68	3.4
TOC 1	01/14/2013	20.72	20	0.72	3.6
TOC 2	01/14/2013	20.93	20	0.93	4.65
TOC 2	01/14/2013	20.94	20	0.94	4.7
TOC 2	01/14/2013	21.27	20	1.27	6.35
TOC 1	01/22/2013	19.83	20	-0.17	-0.85
TOC 2	01/22/2013	19.86	20	-0.14	-0.7
TOC 1	01/22/2013	19.86	20	-0.14	-0.7
TOC 2	01/22/2013	19.99	20	-0.01	-0.05
TOC 1	01/23/2013	20.15	20	0.15	0.75
TOC 2	01/23/2013	20.26	20	0.26	1.3
TOC 1	01/23/2013	20.3	20	0.3	1.5
TOC 2	01/23/2013	20.44	20	0.44	2.2
TOC 1	01/26/2013	19.81	20	-0.19	-0.95
TOC 2	01/26/2013	19.83	20	-0.17	-0.85
TOC 1	01/26/2013	20.02	20	0.02	0.1
TOC 2	01/26/2013	20.12	20	0.12	0.6
TOC 1	01/28/2013	19.31	20	-0.69	-3.45
TOC 2	01/28/2013	19.32	20	-0.68	-3.4
TOC 1	01/28/2013	19.65	20	-0.35	-1.75
TOC 2	01/28/2013	19.67	20	-0.33	-1.65
TOC 1	02/01/2013	19.97	20	-0.03	-0.15
TOC 2	02/01/2013	20.03	20	0.03	0.15
TOC 1	02/01/2013	20.11	20	0.11	0.55
TOC 2	02/01/2013	20.21	20	0.21	1.05
TOC 1	02/01/2013	20.31	20	0.31	1.55
TOC 2	02/01/2013	20.36	20	0.36	1.8
TOC 1	02/01/2013	20.43	20	0.43	2.15
TOC 2	02/01/2013	20.47	20	0.47	2.35
TOC 1	02/09/2013	19.88	20	-0.12	-0.6
TOC 2	02/09/2013	19.98	20	-0.02	-0.1
TOC 1	02/09/2013	20.31	20	0.31	1.55
TOC 2	02/09/2013	20.36	20	0.36	1.8

Exhibit A1. Measurements of Anion and TOC Standards by Date

Analyte=Formate, Analyte - Detail=Formate, Reference Value (ppm)=2
Variability Chart for % rel diff



Analyte=Formate, Analyte - Detail=Formate, Reference Value (ppm)=16
Variability Chart for % rel diff

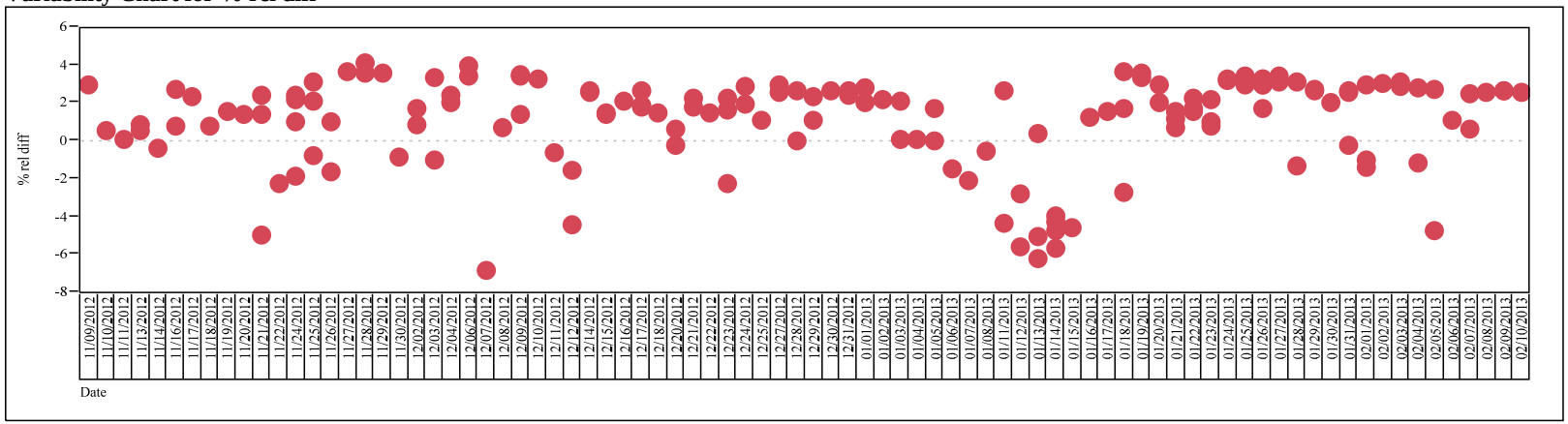
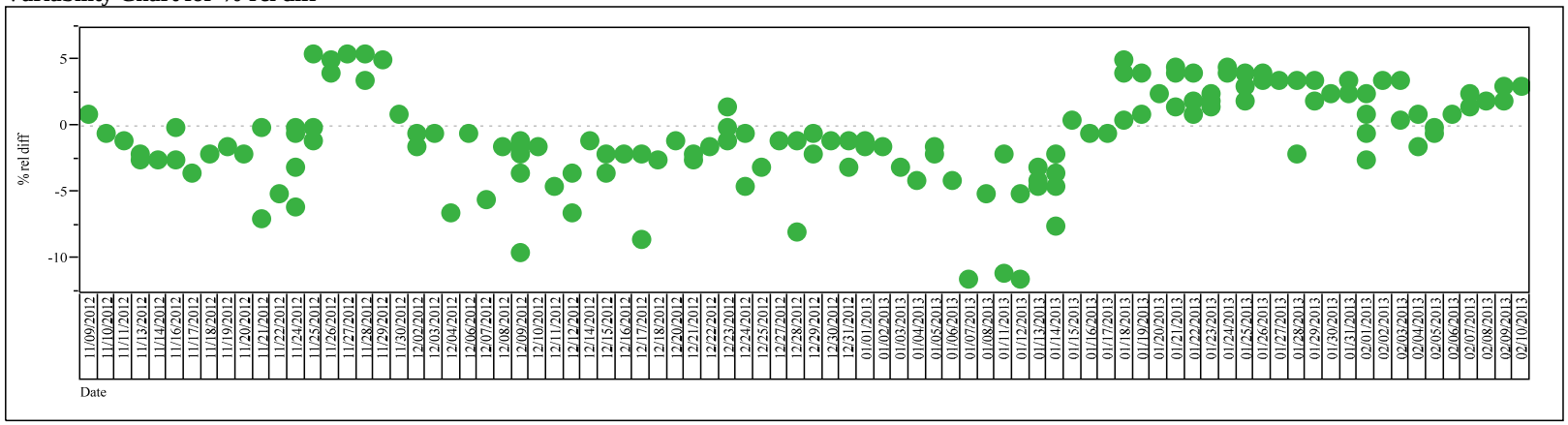


Exhibit A1. Measurements of Anion and TOC Standards by Date

Analyte=Nitrate, Analyte - Detail=Nitrate, Reference Value (ppm)=2
Variability Chart for % rel diff



Analyte=Nitrate, Analyte - Detail=Nitrate, Reference Value (ppm)=16
Variability Chart for % rel diff

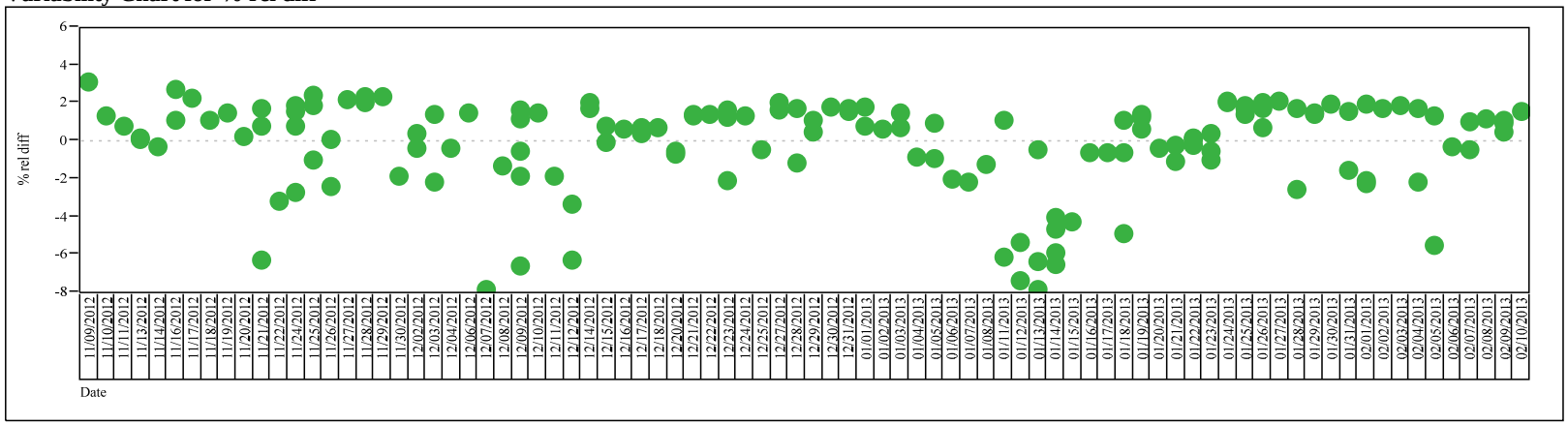
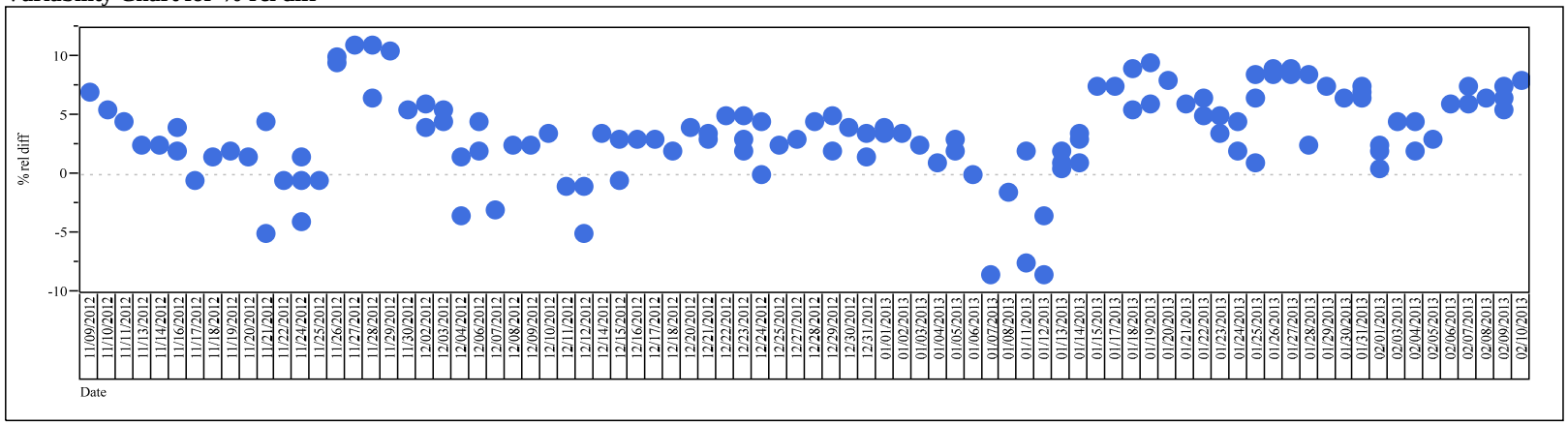


Exhibit A1. Measurements of Anion and TOC Standards by Date

Analyte=Soluble Oxalate, Analyte - Detail=Soluble Oxalate, Reference Value (ppm)=2
Variability Chart for % rel diff



Analyte=Soluble Oxalate, Analyte - Detail=Soluble Oxalate, Reference Value (ppm)=16
Variability Chart for % rel diff

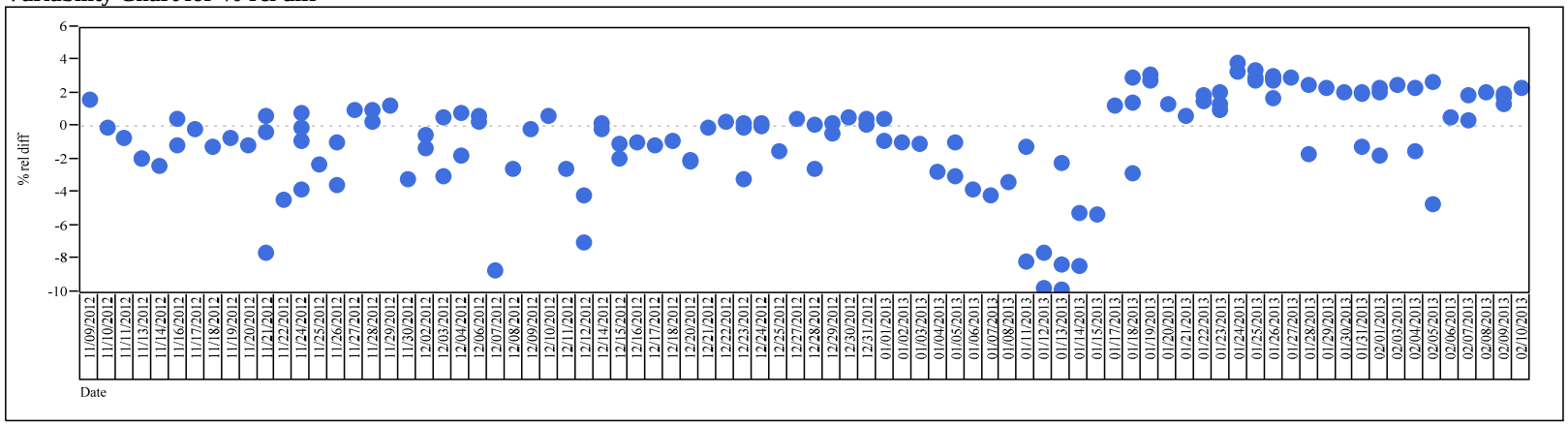
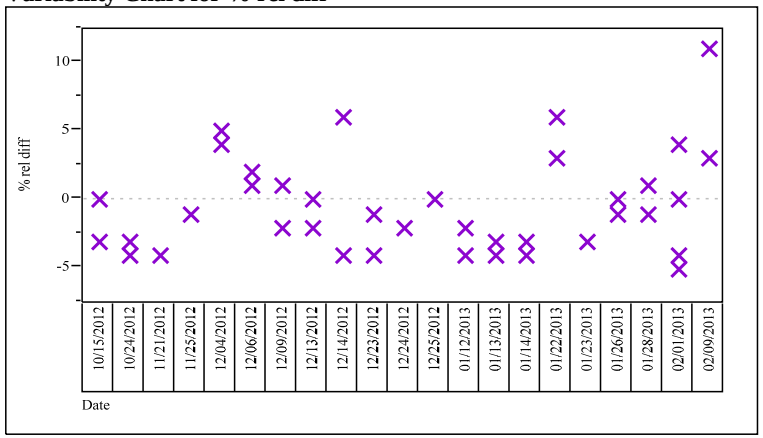
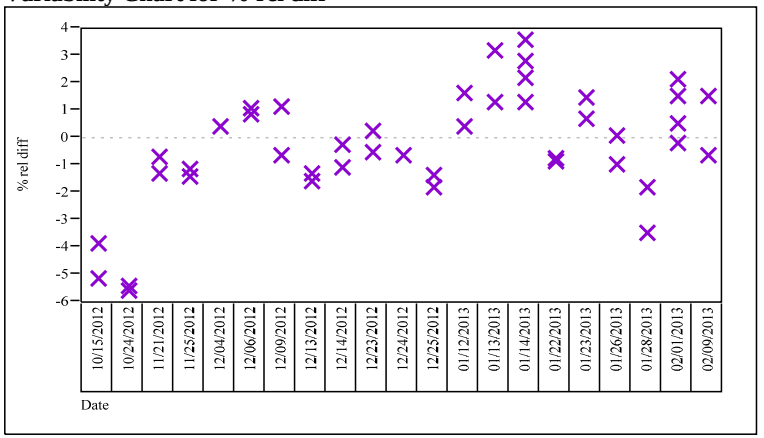


Exhibit A1. Measurements of Anion and TOC Standards by Date

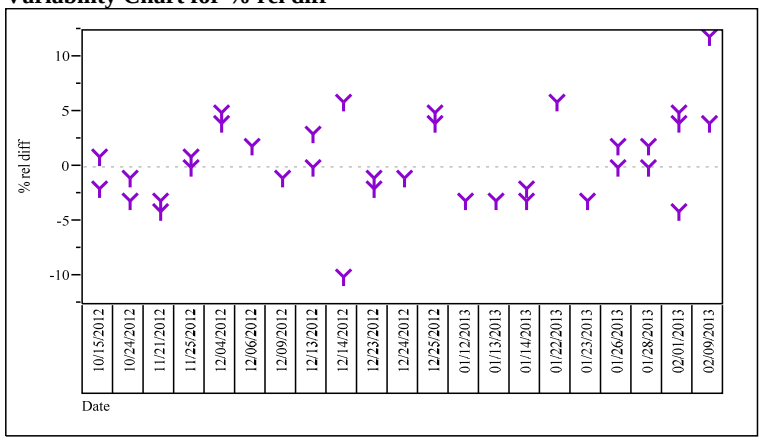
Analyte=TOC, Analyte - Detail=TOC 1, Reference Value (ppm)=1
Variability Chart for % rel diff



Analyte=TOC, Analyte - Detail=TOC 1, Reference Value (ppm)=20
Variability Chart for % rel diff



Analyte=TOC, Analyte - Detail=TOC 2,
Reference Value (ppm)=1
Variability Chart for % rel diff



Analyte=TOC, Analyte - Detail=TOC 2,
Reference Value (ppm)=20
Variability Chart for % rel diff

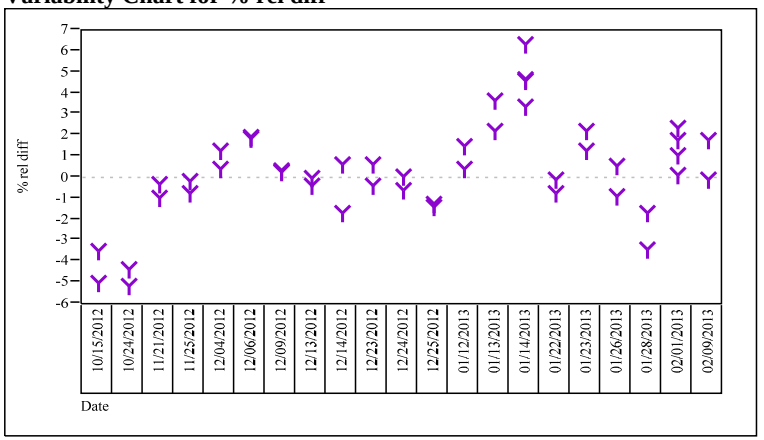
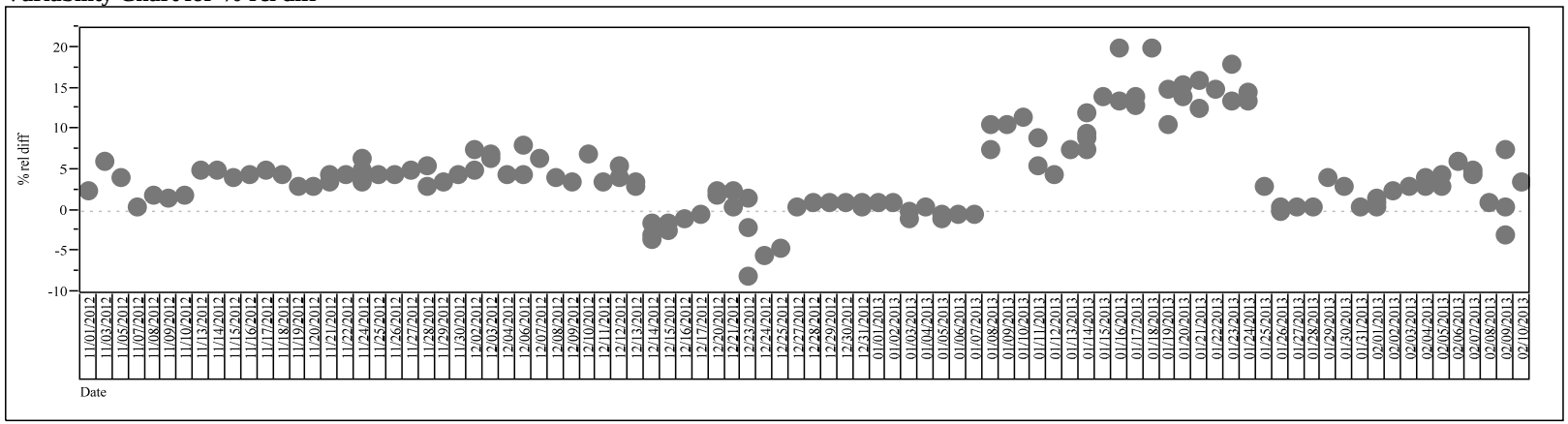


Exhibit A1. Measurements of Anion and TOC Standards by Date

Analyte=Total Oxalate, Analyte - Detail=Total Oxalate, Reference Value (ppm)=2
Variability Chart for % rel diff



Analyte=Total Oxalate, Analyte - Detail=Total Oxalate, Reference Value (ppm)=16
Variability Chart for % rel diff

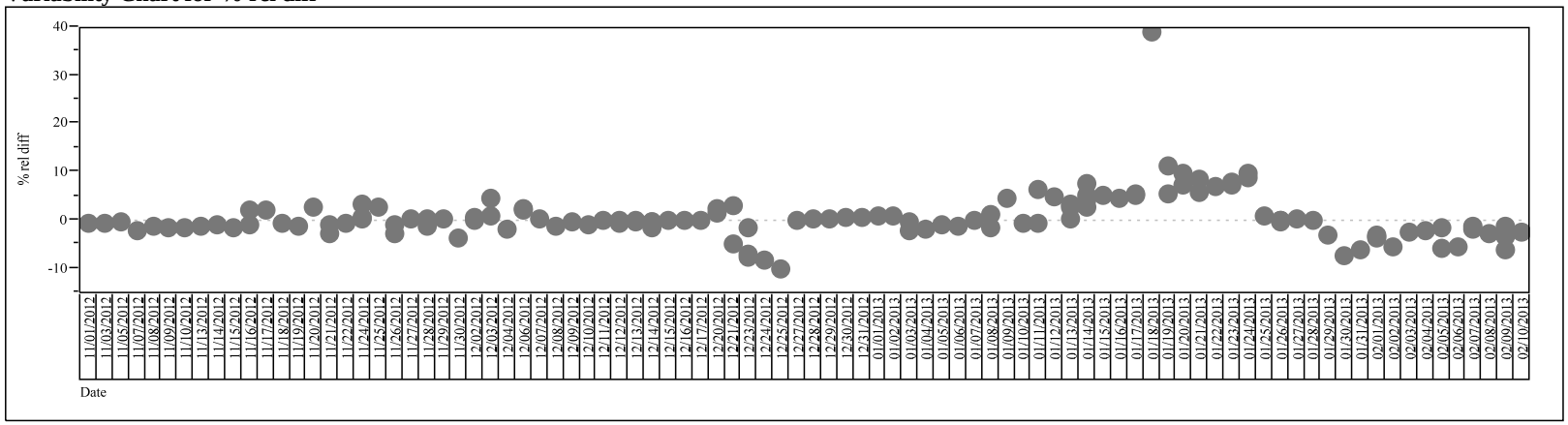


Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=Formate, Analyte - Detail=Formate, Nominal Value (ppm)=2
Variability Chart for Measurement (ppm)

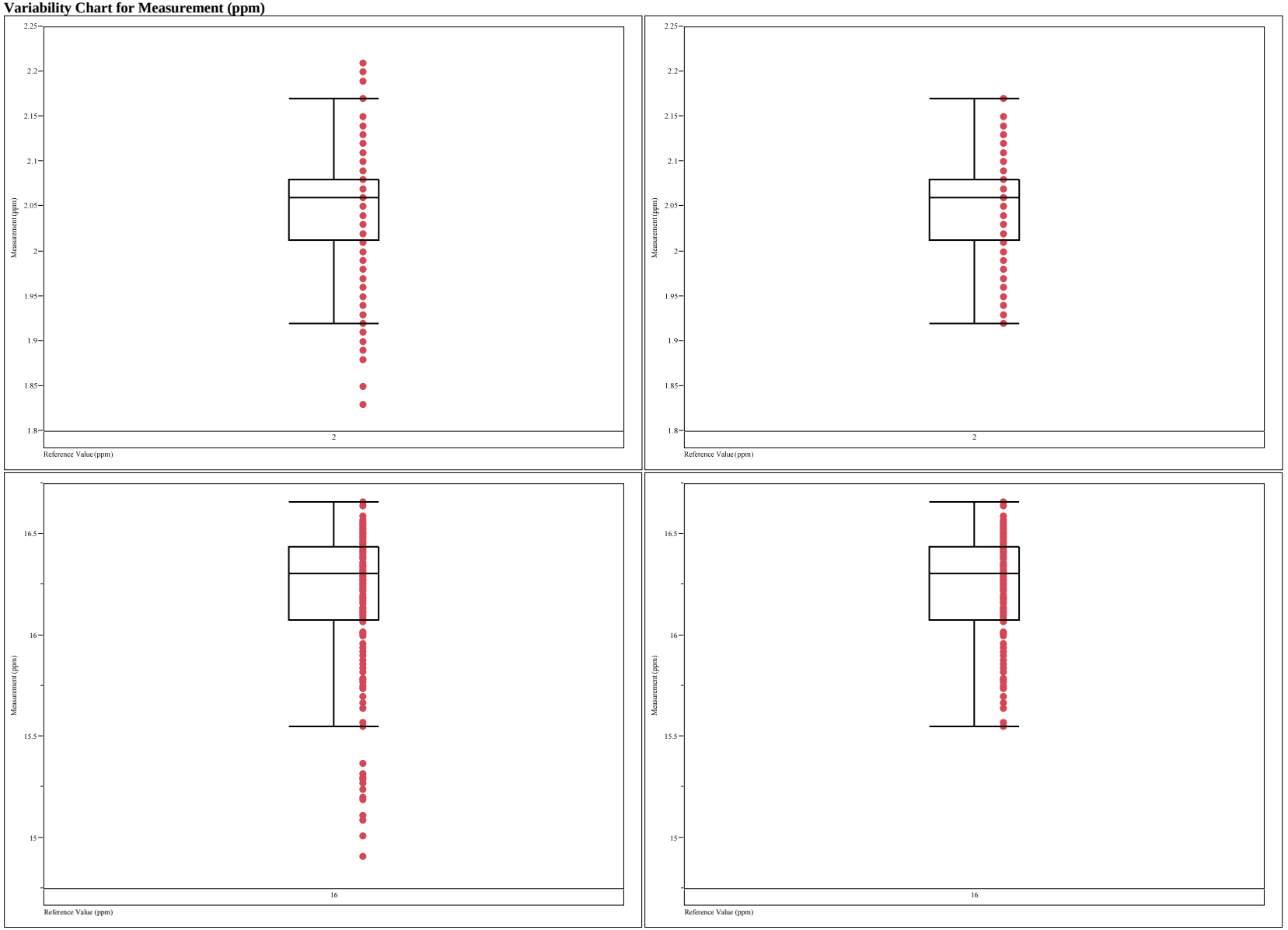


Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=Nitrate, Analyte - Detail=Nitrate, Nominal Value (ppm)=2
Variability Chart for Measurement (ppm)

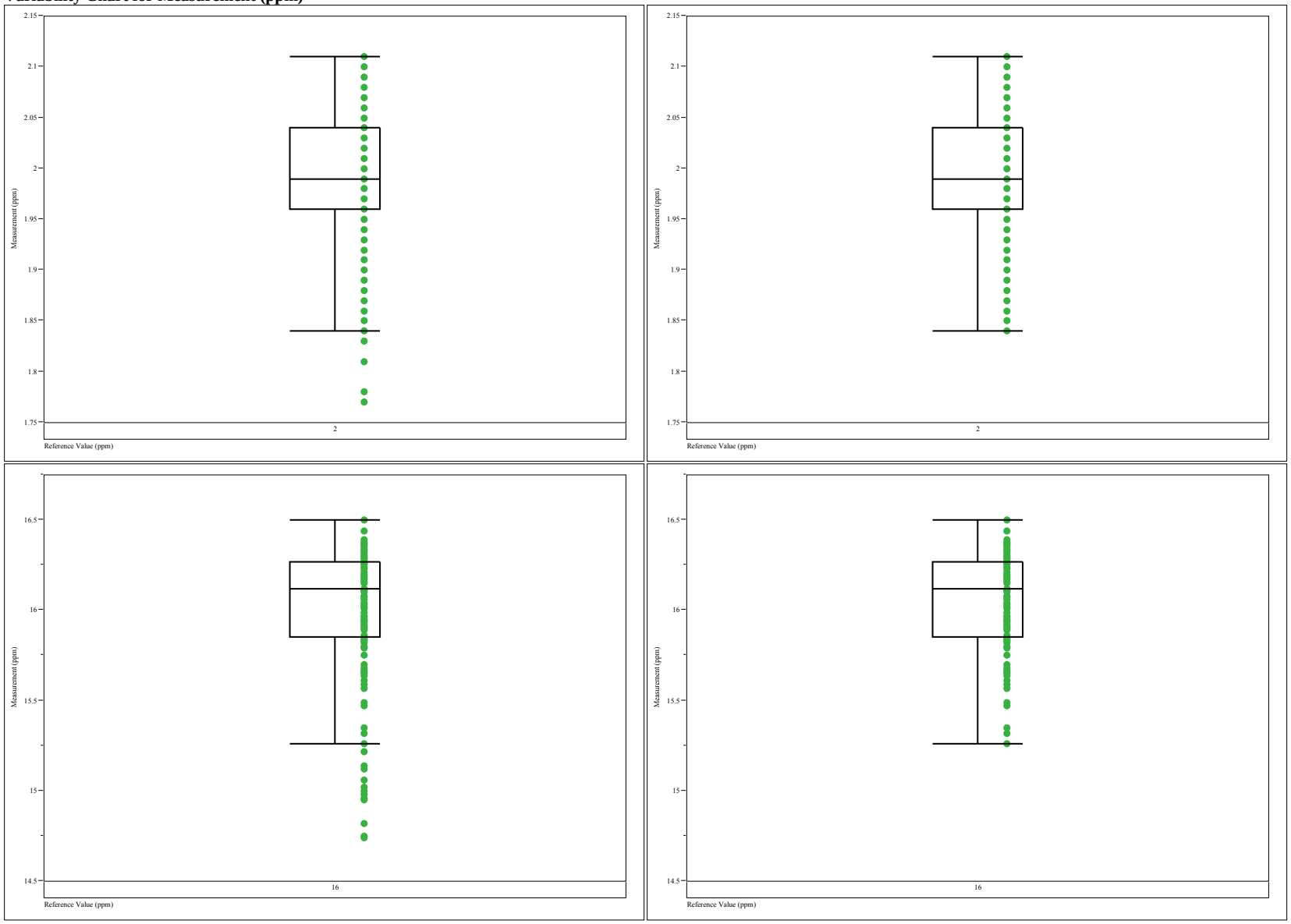


Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=Soluble Oxalate, Analyte - Detail=Soluble Oxalate, Nominal Value (ppm)=2
Variability Chart for Measurement (ppm)

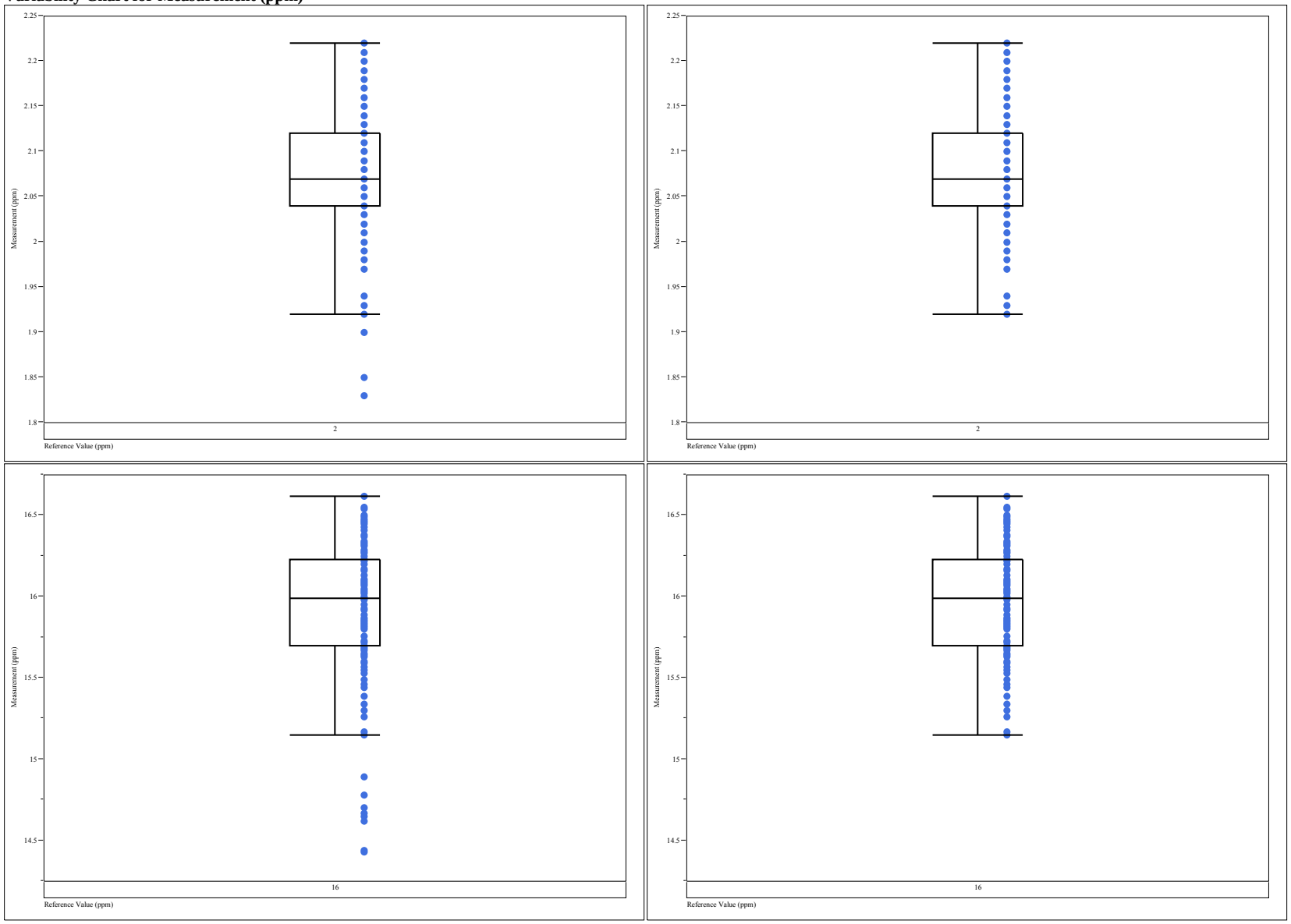


Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=TOC, Analyte - Detail=TOC 1, Nominal Value (ppm)=1
Variability Chart for Measurement (ppm)

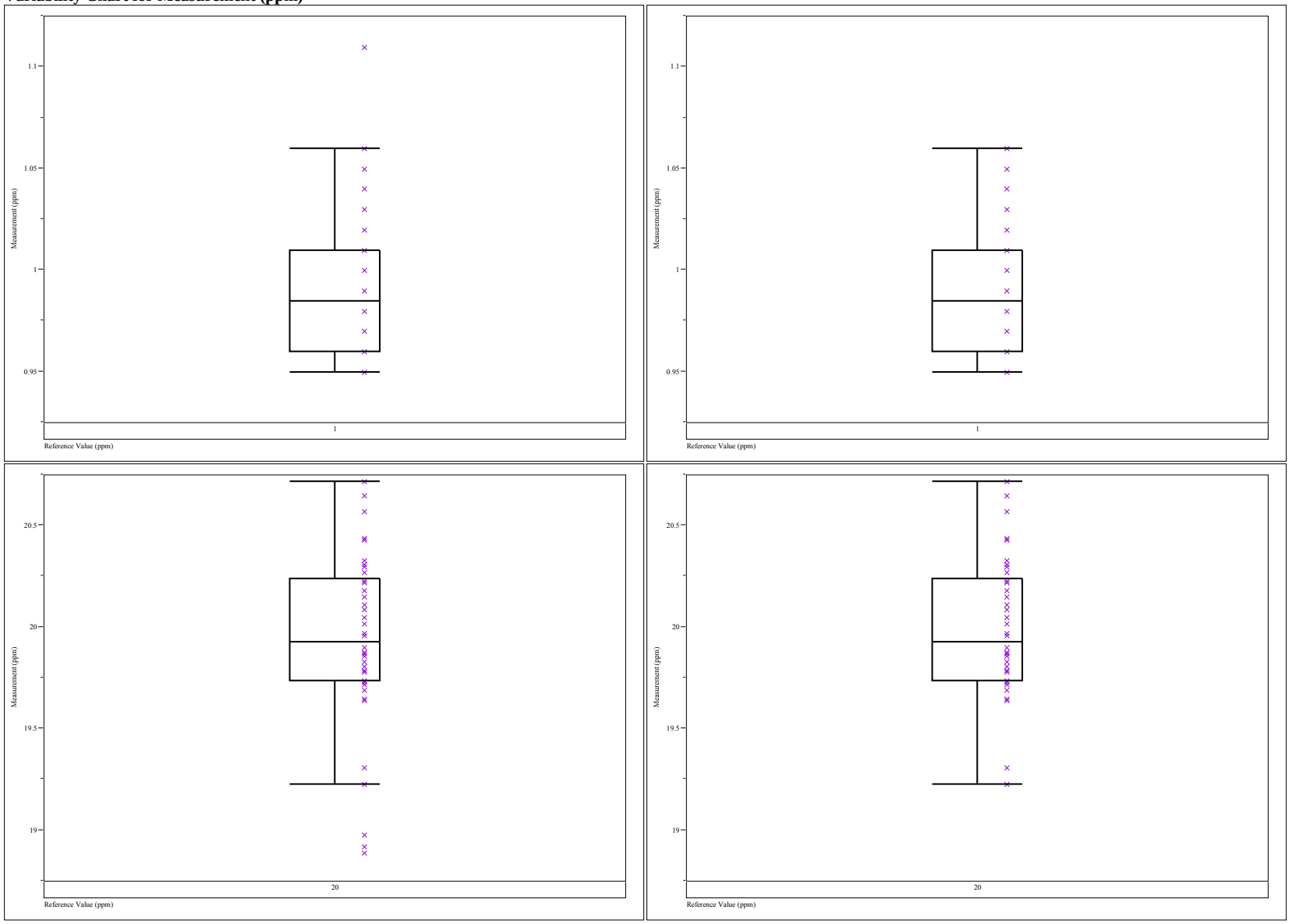


Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=TOC, Analyte - Detail=TOC 2, Nominal Value (ppm)=1
Variability Chart for Measurement (ppm)

Exhibit A2. Boxplots of the Measurements of Anion and TOC Standards

Variability Gauge Analyte=Total Oxalate, Analyte - Detail=Total Oxalate, Nominal Value (ppm)=2
Variability Chart for Measurement (ppm)

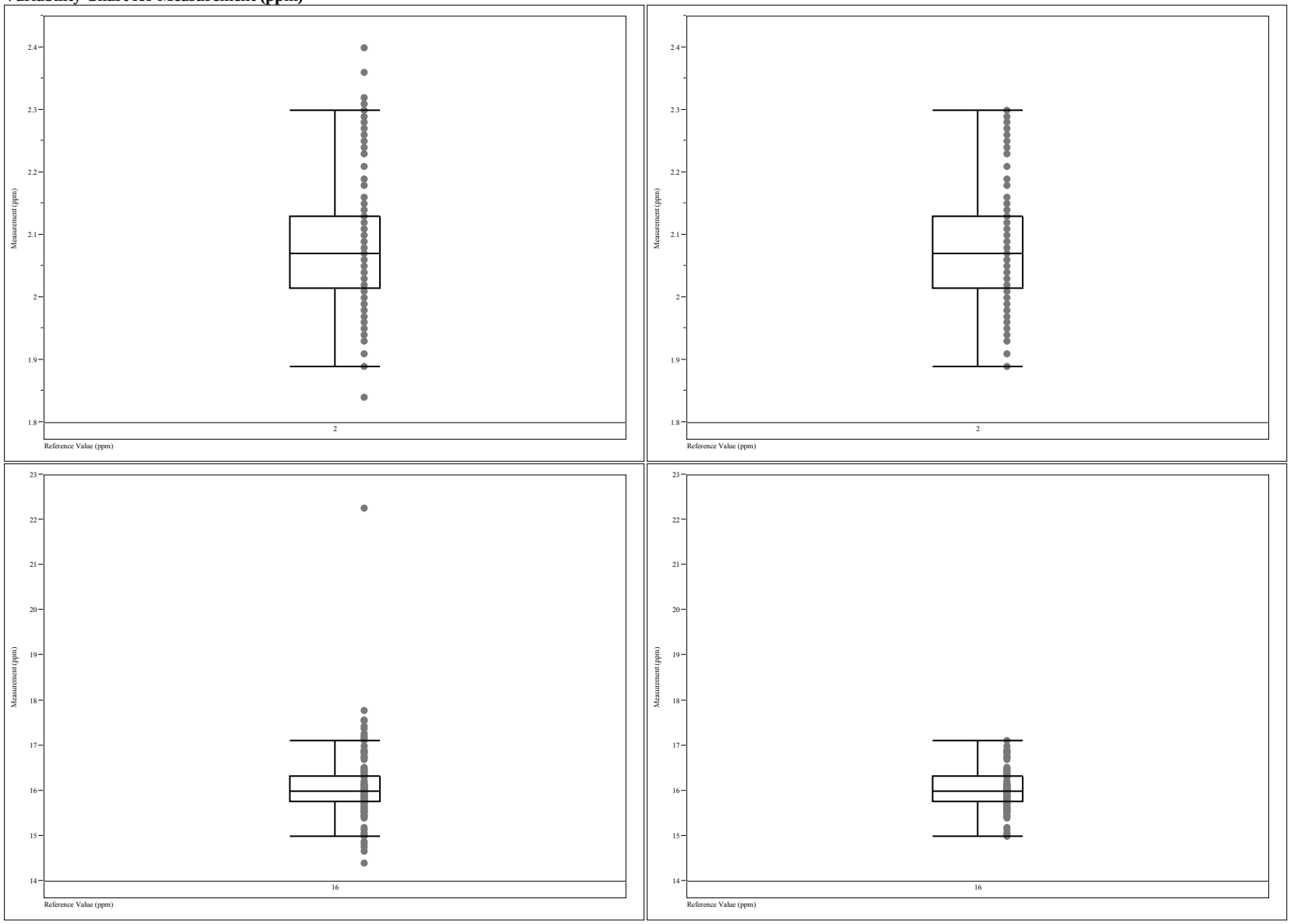


Exhibit A3. Analysis of Variance Results Utilizing All of the Measurements

Response % rel diff Analyte=Formate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.658674
RSquare Adj	0.658674
Root Mean Square Error	2.427439
Mean of Response	2.375
Observations (or Sum Wgts)	172

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	2.3245102	0.337764	80.15	6.88	<.0001*	1.6523578	2.9966626

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.0348594	6.0978682	1.5359399	3.9321362	10.719743	50.857
Residual		5.8924604	0.8760424	4.4921277	8.0710572	49.143
Total		11.990329				100.000

-2 LogLikelihood = 882.70672337

Response % rel diff Analyte=Nitrate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.757416
RSquare Adj	0.757416
Root Mean Square Error	2.115353
Mean of Response	-0.49419
Observations (or Sum Wgts)	172

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.707104	0.347836	81.79	-2.03	0.0453*	-1.399088	-0.01512

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.6603838	7.4297501	1.6033298	5.0707968	11.931278	62.411
Residual		4.4747186	0.6680637	3.4076856	6.1379086	37.589
Total		11.904469				100.000

-2 LogLikelihood = 862.23411341

Response % rel diff Analyte=Formate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.618141
RSquare Adj	0.618141
Root Mean Square Error	1.754986
Mean of Response	1.138808
Observations (or Sum Wgts)	172

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	1.1333337	0.22615	83.94	5.01	<.0001*	0.683605	1.5830624

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.8141134	2.5074494	0.6637224	1.5853073	4.5560093	44.877
Residual		3.0799757	0.4451162	2.3646863	4.1789794	55.123
Total		5.5874251				100.000

-2 LogLikelihood = 759.69980111

Response % rel diff Analyte=Nitrate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.582341
RSquare Adj	0.582341
Root Mean Square Error	1.836233
Mean of Response	-0.07086
Observations (or Sum Wgts)	172

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.023932	0.227543	84.69	-0.11	0.9165	-0.476373	0.4285092

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.7068575	2.3833469	0.6626396	1.4765914	4.4841349	41.413
Residual		3.37175	0.481439	2.5963721	4.5568816	58.587
Total		5.7550969				100.000

-2 LogLikelihood = 768.18030244

Exhibit A3. Analysis of Variance Results Utilizing All of the Measurements

Response % rel diff Analyte=Soluble Oxalate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.797124
RSquare Adj	0.797124
Root Mean Square Error	2.163915
Mean of Response	3.581633
Observations (or Sum Wgts)	147

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	3.535159	0.385417	78.83	9.17	<.0001*	2.7679806	4.3023374

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.9348062	9.0597823	1.9902095	6.1451578	14.68848	65.926
Residual		4.6825271	0.8221606	3.4120741	6.826564	34.074
Total		13.742309				100.000

-2 LogLikelihood = 760.21710755

Response % rel diff Analyte=TOC, Reference Value (ppm)=1
Summary of Fit

RSquare	0.59746
RSquare Adj	0.59746
Root Mean Square Error	2.572658
Mean of Response	-0.29348
Observations (or Sum Wgts)	92

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.16464	0.652668	19.8	-0.25	0.8034	-1.526949	1.1976697

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.114229	7.3746015	2.853044	3.9044395	18.835186	52.701
Residual		6.618569	1.1121052	4.8838163	9.4798986	47.299
Total		13.99317				100.000

-2 LogLikelihood = 469.79796611

Response % rel diff Analyte=Soluble Oxalate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.731589
RSquare Adj	0.731589
Root Mean Square Error	1.895452
Mean of Response	-0.59184
Observations (or Sum Wgts)	147

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.693349	0.291201	84.71	-2.38	0.0195*	-1.272364	-0.114334

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.2735472	4.5755218	1.0758887	3.0285176	7.7093779	56.016
Residual		3.5927383	0.5961297	2.6603953	5.1208071	43.984
Total		8.16826				100.000

-2 LogLikelihood = 697.40840142

Response % rel diff Analyte=TOC, Reference Value (ppm)=20
Summary of Fit

RSquare	0.882928
RSquare Adj	0.882928
Root Mean Square Error	0.854231
Mean of Response	0.002174
Observations (or Sum Wgts)	92

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.22151	0.446316	20.1	-0.50	0.6251	-1.152215	0.7091949

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	5.4946917	4.0095367	1.3197497	2.3031143	8.6664422	84.603
Residual		0.7297109	0.1223857	0.5387296	1.0444233	15.397
Total		4.7392476				100.000

-2 LogLikelihood = 298.03873621

Exhibit A3. Analysis of Variance Results Utilizing All of the Measurements

Response % rel diff Analyte=Total Oxalate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.933962
RSquare Adj	0.933962
Root Mean Square Error	1.962956
Mean of Response	4.417241
Observations (or Sum Wgts)	145

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	4.3860995	0.516632	90.93	8.49	<.0001*	3.3598629	5.4123361

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	5.4871174	21.142935	3.5770974	15.571163	30.365406	84.585
Residual		3.8531953	0.7196047	2.7564722	5.7680065	15.415
Total		24.99613				100.000

-2 LogLikelihood = 803.21154614

Response % rel diff Analyte=Total Oxalate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.937194
RSquare Adj	0.937194
Root Mean Square Error	1.850139
Mean of Response	0.568966
Observations (or Sum Wgts)	145

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	0.4386456	0.558451	85.96	0.79	0.4343	-0.671526	1.5488171

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	7.4496956	25.500415	4.3244038	18.767948	36.657437	88.165
Residual		3.4230144	0.6697995	2.4132885	5.2345602	11.835
Total		28.92343				100.000

-2 LogLikelihood = 810.52221003

Exhibit A4. Analysis of Variance Results Utilizing Screened Measurements

Response % rel diff Analyte=Formate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.669789
RSquare Adj	0.669789
Root Mean Square Error	1.708833
Mean of Response	2.612179
Observations (or Sum Wgts)	156

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	2.5431886	0.242491	81.16	10.49	<.0001*	2.0607226	3.0256545

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.9786265	2.8576978	0.7255778	1.8369995	5.0497658	49.460
Residual		2.9201108	0.4461764	2.210638	4.0376856	50.540
Total		5.7778086				100.000

-2 LogLikelihood = 689.97364933

Response % rel diff Analyte=Nitrate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.789642
RSquare Adj	0.789642
Root Mean Square Error	1.754211
Mean of Response	-0.1976
Observations (or Sum Wgts)	167

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.438369	0.307911	81.63	-1.42	0.1583	-1.050944	0.1742066

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.9321424	5.9456996	1.2407545	4.1045202	9.3831542	65.895
Residual		3.0772575	0.4693084	2.3307313	4.2521869	34.105
Total		9.0229571				100.000

-2 LogLikelihood = 785.14713632

Response % rel diff Analyte=Formate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.203092
RSquare Adj	0.203092
Root Mean Square Error	1.483219
Mean of Response	1.689478
Observations (or Sum Wgts)	158

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	1.6712851	0.136973	59.67	12.20	<.0001*	1.3972674	1.9453029

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.1328641	0.2922929	0.2881751	0.0802065	10.569505	11.728
Residual		2.1999397	0.3443145	1.6550114	3.0679984	88.272
Total		2.4922327				100.000

-2 LogLikelihood = 592.26669674

Response % rel diff Analyte=Nitrate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.436081
RSquare Adj	0.436081
Root Mean Square Error	1.303847
Mean of Response	0.521895
Observations (or Sum Wgts)	157

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	0.4696731	0.146369	57.75	3.21	0.0022*	0.1766569	0.7626893

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.4293125	0.7298385	0.3625152	0.3343649	2.6485938	30.036
Residual		1.700017	0.299423	1.2376456	2.4816236	69.964
Total		2.4298556				100.000

-2 LogLikelihood = 576.70975117

Exhibit A4. Analysis of Variance Results Utilizing Screened Measurements

Response % rel diff Analyte=Soluble Oxalate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.83463
RSquare Adj	0.83463
Root Mean Square Error	1.713166
Mean of Response	3.950704
Observations (or Sum Wgts)	142

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	3.8597184	0.335376	77.26	11.51	<.0001*	3.1919367	4.5275

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	2.4162829	7.0916436	1.5029649	4.8700815	11.280917	70.728
Residual		2.9349393	0.5370179	2.1126688	4.3541439	29.272
Total		10.026583				100.000

-2 LogLikelihood = 683.00153828

Response % rel diff Analyte=TOC, Reference Value (ppm)=1
Summary of Fit

RSquare	0.561156
RSquare Adj	0.561156
Root Mean Square Error	2.550307
Mean of Response	-0.41758
Observations (or Sum Wgts)	91

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.241309	0.613701	19.3	-0.39	0.6985	-1.524471	1.0418526

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.9750435	6.3417445	2.5604445	3.2809814	17.044239	49.368
Residual		6.5040635	1.1046477	4.7848418	9.3553786	50.632
Total		12.845808				100.000

-2 LogLikelihood = 461.10053743

Response % rel diff Analyte=Soluble Oxalate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.609615
RSquare Adj	0.609615
Root Mean Square Error	1.561006
Mean of Response	-0.02418
Observations (or Sum Wgts)	137

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.216472	0.211321	71.83	-1.02	0.3091	-0.637749	0.2048053

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	0.7857824	1.9147481	0.6457306	1.0870944	4.2337115	44.002
Residual		2.4367409	0.4575394	1.7402884	3.6564574	55.998
Total		4.351489				100.000

-2 LogLikelihood = 575.92543962

Response % rel diff Analyte=TOC, Reference Value (ppm)=20
Summary of Fit

RSquare	0.842579
RSquare Adj	0.842579
Root Mean Square Error	0.794719
Mean of Response	0.23314
Observations (or Sum Wgts)	86

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.13755	0.391172	18.91	-0.35	0.7290	-0.956539	0.6814389

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	4.8052691	3.0349036	1.0451216	1.7055548	6.8473579	82.774
Residual		0.6315783	0.1117264	0.4592145	0.9236298	17.226
Total		3.6664819				100.000

-2 LogLikelihood = 266.03182726

Exhibit A4. Analysis of Variance Results Utilizing Screened Measurements

Response % rel diff Analyte=Total Oxalate, Reference Value (ppm)=2
Summary of Fit

RSquare	0.945955
RSquare Adj	0.945955
Root Mean Square Error	1.58117
Mean of Response	4.021583
Observations (or Sum Wgts)	139

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	4.1162088	0.460629	88.37	8.94	<.0001*	3.2008592	5.0315584

REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	6.7831249	16.958481	2.858398	12.502644	24.3197	87.152
Residual		2.5000987	0.4969121	1.7538078	3.851688	12.848
Total		19.45858				100.000

-2 LogLikelihood = 730.3571031

Response % rel diff Analyte=Total Oxalate, Reference Value (ppm)=16
Summary of Fit

RSquare	0.81388
RSquare Adj	0.81388
Root Mean Square Error	1.564364
Mean of Response	0.039904
Observations (or Sum Wgts)	130

Parameter Estimates

Term	Estimate	Std Error	DFDen	t Ratio	Prob>|t|	Lower 95%	Upper 95%
Intercept	-0.014665	0.280109	81.82	-0.05	0.9584	-0.57191	0.54258

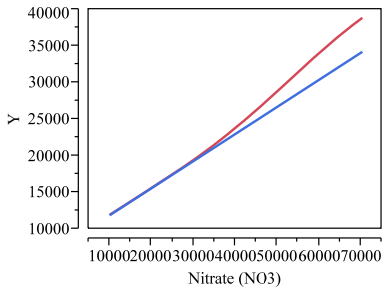
REML Variance Component Estimates

Random Effect	Var Ratio	Var Component	Std Error	95% Lower	95% Upper	Pct of Total
Date	1.9149787	4.6864004	1.0598033	3.1462399	7.7207174	65.694
Residual		2.4472337	0.495362	1.7065697	3.8037416	34.306
Total		7.1336341				100.000

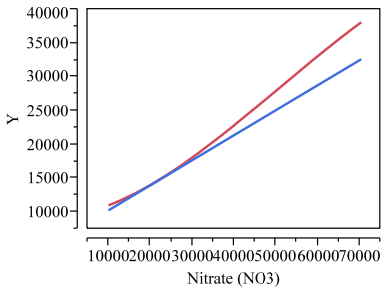
-2 LogLikelihood = 594.9843697

Exhibit A5. Graphical Comparisons of Choi versus Linear TOC to Nitrate Equations

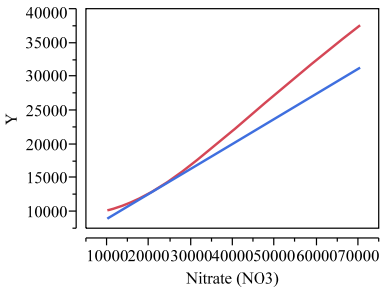
Overlay Plot Antifoam Addition=728

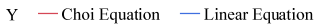


Overlay Plot Antifoam Addition=894

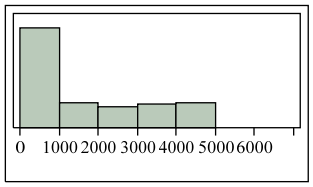


Overlay Plot Antifoam Addition=1017





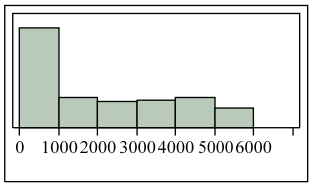
Distributions Antifoam Addition=728
Choi - Linear



Quantiles

100.0%	maximum	4637.78
99.5%		4630.99
97.5%		4576.59
90.0%		4194.18
75.0%	quartile	2933.73
50.0%	median	852.435
25.0%	quartile	77.31
10.0%		39.8599
2.5%		27.0165
0.5%		26.2181
0.0%	minimum	26.194

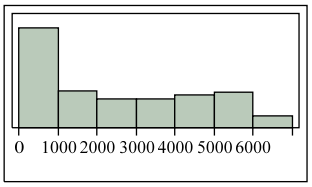
Distributions Antifoam Addition=894
Choi - Linear



Quantiles

100.0%	maximum	5472.49
99.5%		5455.04
97.5%		5345.68
90.0%		4864.13
75.0%	quartile	3656.75
50.0%	median	1480.14
25.0%	quartile	312.187
10.0%		68.862
2.5%		25.6118
0.5%		22.8802
0.0%	minimum	22.7897

Distributions Antifoam Addition=1017
Choi - Linear



Quantiles

100.0%	maximum	6278.3
99.5%		6254.99
97.5%		6115.04
90.0%		5571.57
75.0%	quartile	4349.47
50.0%	median	1983.07
25.0%	quartile	498.817
10.0%		127.222
2.5%		60.0232
0.5%		56.0008
0.0%	minimum	55.8958

Appendix B.

Email for Tommy Edwards

Additional Detail for Uncertainity for MOG Curves

Terri Fellinger to: Tommy Edwards 02/26/2013 12:07 PM

Cc: Jonathan Bricker, John Iaukea, David Sherburne, Damon Click, David Peeler

Tommy,

Based on recent discussions, Alex has generated three curves for TOC/NO3 vs. NO3 for varying amounts of antifoam and formic acid. Per HLW-DWPF-TTR-2013-0022, DWPF - Engineering is invoking the e-mail clause that states " Any additions or deletions to this Technical Task Request will be communicated via electronic mail from DWPF-E." Based on the three curves, please perform a linearization of each curve minimizing the TOC margin lost between 10,000 ppm and 30,000 ppm nitrate. If you have any questions, please call me.

Thanks,
Terri

Attachment 1

SAS CODE

```
Data Tommy;
Informat MDate Date7.0;
Input Analyte $ MDate Measurement RefValue;
Difference = Measurement - RefValue;
PctDiff = 100 * Difference/RefValue;
If Analyte = "TOC1" or Analyte = "TOC2" then Analyte = "TOC";
Cards;

{data}

PROC SORT Out=Tomsort; BY Analyte RefValue; RUN;
PROC MIXED ASYCOV NOBOUND  DATA=Tomsort ALPHA=0.05;
BY Analyte RefValue;
CLASS MDate;
MODEL  PctDiff =  / SOLUTION DDFM=KENWARDROGER;
RANDOM MDate / SOLUTION ; RUN;
```

All Measurements

```
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---------------------------------- Analyte=Formate RefValue=2 ----------------------------------

                                The Mixed Procedure

                                 Model Information

Data Set                     WORK.TOMSORT
Dependent Variable           PctDiff
Covariance Structure         Variance Components
Estimation Method            REML
Residual Variance Method     Profile
Fixed Effects SE Method      Prasad-Rao-Jeske-
                             Kackar-Harville
Degrees of Freedom Method    Kenward-Roger


                Class Level Information

  Class    Levels    Values

  MDate        84    19306 19307 19308 19310 19311
                     19313 19314 19315 19316 19317
                     19318 19319 19321 19322 19323
                     19324 19325 19326 19327 19329
                     19330 19331 19333 19334 19335
                     19336 19337 19338 19339 19341
                     19342 19343 19344 19345 19347
                     19348 19349 19350 19351 19352
                     19354 19355 19356 19357 19358
                     19359 19360 19361 19362 19363
                     19364 19365 19366 19369 19370
                     19371 19372 19373 19374 19375
                     19376 19377 19378 19379 19380
                     19381 19382 19383 19384 19385
                     19386 19387 19388 19389 19390
                     19391 19392 19393 19394 19395
                     19396 19397 19398 19399


                          Dimensions

          Covariance Parameters            2
          Columns in X                     1
          Columns in Z                    84
          Subjects                         1
          Max Obs Per Subject            172
          Observations Used              172
          Observations Not Used            0
          Total Observations             172

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```

---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	914.17808926	
1	2	882.70672337	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	6.0979	0.05	3.0875	9.1082
Residual	5.8925	0.05	4.4921	8.0711

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	2.3591	-0.4136
2	Residual	-0.4136	0.7675

Fit Statistics

-2 Res Log Likelihood	882.7
AIC (smaller is better)	886.7
AICC (smaller is better)	886.8
BIC (smaller is better)	891.6

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	31.47	<.0001

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	2.3245	0.3378	80.1	6.88	<.0001

---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	1.1064	1.7850	127	0.62	0.5365
MDate	19307	0.08925	1.7850	127	0.05	0.9602
MDate	19308	-0.4193	1.7850	127	-0.23	0.8147
MDate	19310	-0.2188	1.4601	168	-0.15	0.8811
MDate	19311	-0.6736	1.7850	127	-0.38	0.7065
MDate	19313	-0.05024	1.4601	168	-0.03	0.9726
MDate	19314	-0.9279	1.7850	127	-0.52	0.6041
MDate	19315	-0.6736	1.7850	127	-0.38	0.7065
MDate	19316	-0.4193	1.7850	127	-0.23	0.8147
MDate	19317	-0.4193	1.7850	127	-0.23	0.8147
MDate	19318	-1.2539	1.2689	170	-0.99	0.3245
MDate	19319	-2.4536	1.7850	127	-1.37	0.1717
MDate	19321	-3.0804	1.1407	165	-2.70	0.0076
MDate	19322	-0.3620	1.1407	165	-0.32	0.7513
MDate	19323	4.1637	1.4601	168	2.85	0.0049
MDate	19324	4.1578	1.7850	127	2.33	0.0214
MDate	19325	5.9316	1.2689	170	4.67	<.0001
MDate	19326	3.9035	1.7850	127	2.19	0.0306
MDate	19327	2.1235	1.7850	127	1.19	0.2364
MDate	19329	0.1183	1.4601	168	0.08	0.9355
MDate	19330	0.7926	1.4601	168	0.54	0.5880
MDate	19331	-1.0616	1.4601	168	-0.73	0.4682
MDate	19333	-2.5786	1.4601	168	-1.77	0.0792
MDate	19334	-2.7079	1.7850	127	-1.52	0.1318
MDate	19335	0.5978	1.7850	127	0.33	0.7383
MDate	19336	-1.7582	1.2689	170	-1.39	0.1677
MDate	19337	0.3435	1.7850	127	0.19	0.8477
MDate	19338	-2.1993	1.7850	127	-1.23	0.2202
MDate	19339	-3.4214	1.4601	168	-2.34	0.0203
MDate	19341	0.7926	1.4601	168	0.54	0.5880
MDate	19342	-0.6236	1.2689	170	-0.49	0.6237
MDate	19343	0.08925	1.7850	127	0.05	0.9602
MDate	19344	-1.3800	1.2689	170	-1.09	0.2783
MDate	19345	-0.6736	1.7850	127	-0.38	0.7065
MDate	19347	0.6240	1.4601	168	0.43	0.6697
MDate	19348	-0.2188	1.4601	168	-0.15	0.8811
MDate	19349	0.08925	1.7850	127	0.05	0.9602
MDate	19350	0.04067	1.1407	165	0.04	0.9716
MDate	19351	-0.3874	1.4601	168	-0.27	0.7911
MDate	19352	-6.6240	1.4601	168	-4.54	<.0001
MDate	19354	0.6370	1.2689	170	0.50	0.6163
MDate	19355	-1.3800	1.2689	170	-1.09	0.2783
MDate	19356	0.3849	1.2689	170	0.30	0.7620
MDate	19357	0.3435	1.7850	127	0.19	0.8477

---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19358	-0.2188	1.4601	168	-0.15	0.8811
MDate	19359	0.4554	1.4601	168	0.31	0.7555
MDate	19360	0.8521	1.7850	127	0.48	0.6339
MDate	19361	-0.2188	1.4601	168	-0.15	0.8811
MDate	19362	-0.6736	1.7850	127	-0.38	0.7065
MDate	19363	0.4554	1.4601	168	0.31	0.7555
MDate	19364	-1.1822	1.7850	127	-0.66	0.5090
MDate	19365	-5.5050	1.7850	127	-3.08	0.0025
MDate	19366	-0.9279	1.7850	127	-0.52	0.6041
MDate	19369	-2.2415	1.4601	168	-1.54	0.1266
MDate	19370	-3.5900	1.4601	168	-2.46	0.0150
MDate	19371	-1.1279	1.2689	170	-0.89	0.3753
MDate	19372	-2.8699	1.0476	160	-2.74	0.0069
MDate	19373	0.5978	1.7850	127	0.33	0.7383
MDate	19374	0.3435	1.7850	127	0.19	0.8477
MDate	19375	1.3607	1.7850	127	0.76	0.4473
MDate	19376	2.9964	1.0476	160	2.86	0.0048
MDate	19377	2.2758	1.2689	170	1.79	0.0747
MDate	19378	1.3607	1.7850	127	0.76	0.4473
MDate	19379	2.2758	1.2689	170	1.79	0.0747
MDate	19380	1.0152	1.2689	170	0.80	0.4248
MDate	19381	-0.3620	1.1407	165	-0.32	0.7513
MDate	19382	0.1183	1.4601	168	0.08	0.9355
MDate	19383	1.2673	1.2689	170	1.00	0.3194
MDate	19384	3.3316	1.0476	160	3.18	0.0018
MDate	19385	2.6467	1.4601	168	1.81	0.0717
MDate	19386	1.3934	1.2689	170	1.10	0.2737
MDate	19387	1.8039	1.4601	168	1.24	0.2184
MDate	19388	0.8521	1.7850	127	0.48	0.6339
MDate	19389	1.8976	1.2689	170	1.50	0.1367
MDate	19390	-0.9972	0.9763	157	-1.02	0.3086
MDate	19391	1.1064	1.7850	127	0.62	0.5365
MDate	19392	0.5109	1.2689	170	0.40	0.6877
MDate	19393	-1.3987	1.4601	168	-0.96	0.3395
MDate	19394	-1.7358	1.4601	168	-1.19	0.2362
MDate	19395	0.3435	1.7850	127	0.19	0.8477
MDate	19396	0.9611	1.4601	168	0.66	0.5113
MDate	19397	0.5978	1.7850	127	0.33	0.7383
MDate	19398	1.0152	1.2689	170	0.80	0.4248
MDate	19399	0.8521	1.7850	127	0.48	0.6339

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff

Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	84	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	84
Subjects	1
Max Obs Per Subject	172
Observations Used	172
Observations Not Used	0
Total Observations	172

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	790.26409505	
1	2	763.50834622	0.01131333
2	1	760.38165140	0.00253792
3	1	759.73680056	0.00015864
4	1	759.69996176	0.00000072

5	1	759.69980112	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	2.5074	0.05	1.2066	3.8083
Residual	3.0800	0.05	2.3647	4.1790

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.4405	-0.08854
2	Residual	-0.08854	0.1981

Fit Statistics

-2 Res Log Likelihood	759.7
AIC (smaller is better)	763.7
AICC (smaller is better)	763.8
BIC (smaller is better)	768.6

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	30.56	<.0001

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---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	1.1333	0.2261	83.9	5.01	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|

MDate	19306	0.8096	1.2121	98.3	0.67	0.5057
MDate	19307	-0.2562	1.2121	98.3	-0.21	0.8331
MDate	19308	-0.4525	1.2121	98.3	-0.37	0.7097
MDate	19310	-0.2568	1.0121	151	-0.25	0.8000
MDate	19311	-0.6769	1.2121	98.3	-0.56	0.5778
MDate	19313	0.4014	1.0121	151	0.40	0.6922
MDate	19314	0.5572	1.2121	98.3	0.46	0.6467
MDate	19315	-0.1720	1.2121	98.3	-0.14	0.8874
MDate	19316	0.1926	1.2121	98.3	0.16	0.8741
MDate	19317	0.1085	1.2121	98.3	0.09	0.9289
MDate	19318	-1.0702	0.8878	169	-1.21	0.2297
MDate	19319	-1.5183	1.2121	98.3	-1.25	0.2133
MDate	19321	-0.1498	0.8020	171	-0.19	0.8520
MDate	19322	-0.1498	0.8020	171	-0.19	0.8520
MDate	19323	-0.8957	1.0121	151	-0.89	0.3775
MDate	19324	1.1462	1.2121	98.3	0.95	0.3467
MDate	19325	1.8565	0.8878	169	2.09	0.0380
MDate	19326	1.0901	1.2121	98.3	0.90	0.3707
MDate	19327	-0.9013	1.2121	98.3	-0.74	0.4589
MDate	19329	0.09164	1.0121	151	0.09	0.9280
MDate	19330	0.03356	1.0121	151	0.03	0.9736
MDate	19331	0.6918	1.0121	151	0.68	0.4953
MDate	19333	1.6017	1.0121	151	1.58	0.1156
MDate	19334	-3.5658	1.2121	98.3	-2.94	0.0041
MDate	19335	-0.2001	1.2121	98.3	-0.17	0.8692
MDate	19336	1.1618	0.8878	169	1.31	0.1924
MDate	19337	0.9779	1.2121	98.3	0.81	0.4217
MDate	19338	-0.7891	1.2121	98.3	-0.65	0.5166
MDate	19339	-2.5606	1.0121	151	-2.53	0.0124
MDate	19341	0.9241	1.0121	151	0.91	0.3627
MDate	19342	0.2306	0.8878	169	0.26	0.7954
MDate	19343	0.4450	1.2121	98.3	0.37	0.7143
MDate	19344	0.7036	0.8878	169	0.79	0.4292
MDate	19345	0.1645	1.2121	98.3	0.14	0.8923
MDate	19347	-0.5860	1.0121	151	-0.58	0.5635
MDate	19348	0.5563	1.0121	151	0.55	0.5834

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	0.1645	1.2121	98.3	0.14	0.8923
MDate	19350	-0.2455	0.8020	171	-0.31	0.7599
MDate	19351	0.7886	1.0121	151	0.78	0.4371
MDate	19352	-0.00516	1.0121	151	-0.01	0.9959
MDate	19354	1.1175	0.8878	169	1.26	0.2099
MDate	19355	0.4671	0.8878	169	0.53	0.5995
MDate	19356	0.5706	0.8878	169	0.64	0.5213
MDate	19357	0.6694	1.2121	98.3	0.55	0.5820
MDate	19358	0.8660	1.0121	151	0.86	0.3935

MDate	19359	0.7886	1.0121	151	0.78	0.4371
MDate	19360	0.4731	1.2121	98.3	0.39	0.6972
MDate	19361	-0.02452	1.0121	151	-0.02	0.9807
MDate	19362	-0.4525	1.2121	98.3	-0.37	0.7097
MDate	19363	-0.1794	1.0121	151	-0.18	0.8595
MDate	19364	-1.1537	1.2121	98.3	-0.95	0.3435
MDate	19365	-1.4342	1.2121	98.3	-1.18	0.2396
MDate	19366	-0.7330	1.2121	98.3	-0.60	0.5468
MDate	19369	-1.2248	1.0121	151	-1.21	0.2281
MDate	19370	-3.2963	1.0121	151	-3.26	0.0014
MDate	19371	-3.3612	0.8878	169	-3.79	0.0002
MDate	19372	-4.8133	0.7386	169	-6.52	<.0001
MDate	19373	-2.5561	1.2121	98.3	-2.11	0.0375
MDate	19374	0.05236	1.2121	98.3	0.04	0.9656
MDate	19375	0.1926	1.2121	98.3	0.16	0.8741
MDate	19376	-0.6188	0.7386	169	-0.84	0.4033
MDate	19377	1.4468	1.0121	151	1.43	0.1549
MDate	19378	0.8273	1.0121	151	0.82	0.4150
MDate	19379	0.008868	0.8878	169	0.01	0.9920
MDate	19380	0.5114	0.8878	169	0.58	0.5653
MDate	19381	0.3164	0.8020	171	0.39	0.6937
MDate	19382	1.2919	1.0121	151	1.28	0.2037
MDate	19383	1.5313	0.8878	169	1.72	0.0864
MDate	19384	1.3681	0.7386	169	1.85	0.0657
MDate	19385	1.3307	1.0121	151	1.31	0.1906
MDate	19386	0.3636	0.8878	169	0.41	0.6826
MDate	19387	0.9628	1.0121	151	0.95	0.3429
MDate	19388	0.3889	1.2121	98.3	0.32	0.7490
MDate	19389	0.3636	0.8878	169	0.41	0.6826
MDate	19390	0.3562	0.6895	166	0.52	0.6061
MDate	19391	0.8657	1.2121	98.3	0.71	0.4768
MDate	19392	1.3540	0.8878	169	1.53	0.1291
MDate	19393	-0.1794	1.0121	151	-0.18	0.8595
MDate	19394	-1.3216	1.0121	151	-1.31	0.1936
MDate	19395	-0.00374	1.2121	98.3	-0.00	0.9975

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19396	0.2659	1.0121	151	0.26	0.7931
MDate	19397	0.6414	1.2121	98.3	0.53	0.5979
MDate	19398	1.0731	0.8878	169	1.21	0.2285
MDate	19399	0.6414	1.2121	98.3	0.53	0.5979

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	84	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	84
Subjects	1
Max Obs Per Subject	172
Observations Used	172
Observations Not Used	0
Total Observations	172

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion

0	1	913.79436280	
1	2	862.23505060	0.00000340
2	1	862.23411352	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	7.4293	0.05	4.2871	10.5715
Residual	4.4749	0.05	3.4078	6.1381

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	2.5703	-0.2501
2	Residual	-0.2501	0.4463

Fit Statistics

-2 Res Log Likelihood	862.2
AIC (smaller is better)	866.2
AICC (smaller is better)	866.3
BIC (smaller is better)	871.1

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	51.56	<.0001

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---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.7071	0.3478	81.8	-2.03	0.0453

Solution for Random Effects

Std Err

Effect	MDate	Estimate	Pred	DF	t Value	Pr > |t|
MDate	19306	1.0654	1.7170	169	0.62	0.5358
MDate	19307	0.1292	1.7170	169	0.08	0.9401
MDate	19308	-0.1828	1.7170	169	-0.11	0.9153
MDate	19310	-1.1858	1.3571	163	-0.87	0.3836
MDate	19311	-1.1189	1.7170	169	-0.65	0.5155
MDate	19313	-0.4172	1.3571	163	-0.31	0.7589
MDate	19314	-1.7430	1.7170	169	-1.02	0.3115
MDate	19315	-0.8069	1.7170	169	-0.47	0.6390
MDate	19316	-0.4948	1.7170	169	-0.29	0.7735
MDate	19317	-0.8069	1.7170	169	-0.47	0.6390
MDate	19318	-1.3543	1.1641	152	-1.16	0.2465
MDate	19319	-2.6792	1.7170	169	-1.56	0.1205
MDate	19321	-1.4496	1.0404	147	-1.39	0.1656
MDate	19322	1.5923	1.0404	147	1.53	0.1280
MDate	19323	4.0019	1.3571	163	2.95	0.0037
MDate	19324	3.8738	1.7170	169	2.26	0.0253
MDate	19325	4.6140	1.1641	152	3.96	0.0001
MDate	19326	3.5618	1.7170	169	2.07	0.0396
MDate	19327	1.0654	1.7170	169	0.62	0.5358
MDate	19329	-0.2251	1.3571	163	-0.17	0.8685
MDate	19330	0.1592	1.3571	163	0.12	0.9068
MDate	19331	-3.6153	1.7170	169	-2.11	0.0367
MDate	19333	0.1592	1.3571	163	0.12	0.9068
MDate	19334	-2.9912	1.7170	169	-1.74	0.0833
MDate	19335	-0.4948	1.7170	169	-0.29	0.7735
MDate	19336	-2.4926	0.9531	146	-2.62	0.0099
MDate	19337	-0.4948	1.7170	169	-0.29	0.7735
MDate	19338	-2.3671	1.7170	169	-1.38	0.1698
MDate	19339	-3.2993	1.3571	163	-2.43	0.0161
MDate	19341	-0.2251	1.3571	163	-0.17	0.8685
MDate	19342	-1.4931	1.1641	152	-1.28	0.2016
MDate	19343	-0.8069	1.7170	169	-0.47	0.6390
MDate	19344	-2.8811	1.1641	152	-2.47	0.0144
MDate	19345	-1.1189	1.7170	169	-0.65	0.5155
MDate	19347	-0.2251	1.3571	163	-0.17	0.8685
MDate	19348	-1.1858	1.3571	163	-0.87	0.3836

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	-0.4948	1.7170	169	-0.29	0.7735
MDate	19350	0.5059	1.0404	147	0.49	0.6275
MDate	19351	-1.3779	1.3571	163	-1.02	0.3115
MDate	19352	-1.7622	1.3571	163	-1.30	0.1960
MDate	19354	-0.2439	1.1641	152	-0.21	0.8343
MDate	19355	-2.1871	1.1641	152	-1.88	0.0622
MDate	19356	-0.6603	1.1641	152	-0.57	0.5714

MDate	19357	-0.1828	1.7170	169	-0.11	0.9153
MDate	19358	-0.9936	1.3571	163	-0.73	0.4651
MDate	19359	-0.4172	1.3571	163	-0.31	0.7589
MDate	19360	-0.4948	1.7170	169	-0.29	0.7735
MDate	19361	-1.7622	1.3571	163	-1.30	0.1960
MDate	19362	-2.0551	1.7170	169	-1.20	0.2330
MDate	19363	-0.8015	1.3571	163	-0.59	0.5556
MDate	19364	-2.0551	1.7170	169	-1.20	0.2330
MDate	19365	-6.7358	1.7170	169	-3.92	0.0001
MDate	19366	-2.6792	1.7170	169	-1.56	0.1205
MDate	19369	-4.4521	1.3571	163	-3.28	0.0013
MDate	19370	-5.7970	1.3571	163	-4.27	<.0001
MDate	19371	-2.6035	1.1641	152	-2.24	0.0268
MDate	19372	-3.8314	0.9531	146	-4.02	<.0001
MDate	19373	0.7533	1.7170	169	0.44	0.6614
MDate	19374	0.1292	1.7170	169	0.08	0.9401
MDate	19375	0.1292	1.7170	169	0.08	0.9401
MDate	19376	3.1300	0.9531	146	3.28	0.0013
MDate	19377	3.0873	1.1641	152	2.65	0.0088
MDate	19378	2.0015	1.7170	169	1.17	0.2454
MDate	19379	3.3649	1.1641	152	2.89	0.0044
MDate	19380	2.5321	1.1641	152	2.18	0.0312
MDate	19381	2.2442	1.0404	147	2.16	0.0326
MDate	19382	3.8097	1.3571	163	2.81	0.0056
MDate	19383	3.0873	1.1641	152	2.65	0.0088
MDate	19384	3.9333	0.9531	146	4.13	<.0001
MDate	19385	3.2333	1.3571	163	2.38	0.0184
MDate	19386	1.9769	1.1641	152	1.70	0.0915
MDate	19387	2.6569	1.3571	163	1.96	0.0520
MDate	19388	2.0015	1.7170	169	1.17	0.2454
MDate	19389	2.8491	1.3571	163	2.10	0.0373
MDate	19390	1.2484	0.8874	145	1.41	0.1616
MDate	19391	2.6256	1.7170	169	1.53	0.1281
MDate	19392	1.8381	1.1641	152	1.58	0.1164
MDate	19393	0.3513	1.3571	163	0.26	0.7961
MDate	19394	0.3513	1.3571	163	0.26	0.7961
MDate	19395	1.0654	1.7170	169	0.62	0.5358

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19396	2.0805	1.3571	163	1.53	0.1272
MDate	19397	1.6895	1.7170	169	0.98	0.3265
MDate	19398	2.5321	1.1641	152	2.18	0.0312
MDate	19399	2.3136	1.7170	169	1.35	0.1796

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	84	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	84
Subjects	1
Max Obs Per Subject	172
Observations Used	172
Observations Not Used	0
Total Observations	172

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	794.48041355	
1	3	768.22269281	0.00017777
2	1	768.18051210	0.00000092
3	1	768.18030245	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	2.3833	0.05	1.0846	3.6820
Residual	3.3718	0.05	2.5964	4.5569

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.4391	-0.09791
2	Residual	-0.09791	0.2318

Fit Statistics

-2 Res Log Likelihood	768.2
AIC (smaller is better)	772.2
AICC (smaller is better)	772.3
BIC (smaller is better)	777.0

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	26.30	<.0001

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.02393	0.2275	84.7	-0.11	0.9165

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	1.3040	1.2193	81	1.07	0.2880
MDate	19307	0.5534	1.2193	81	0.45	0.6511
MDate	19308	0.3205	1.2193	81	0.26	0.7933
MDate	19310	0.08723	1.0310	133	0.08	0.9327
MDate	19311	-0.1195	1.2193	81	-0.10	0.9222
MDate	19313	1.1305	1.0310	133	1.10	0.2748
MDate	19314	0.9417	1.2193	81	0.77	0.4422
MDate	19315	0.4758	1.2193	81	0.39	0.6974
MDate	19316	0.6311	1.2193	81	0.52	0.6062
MDate	19317	0.1134	1.2193	81	0.09	0.9261
MDate	19318	-0.8332	0.9100	160	-0.92	0.3613
MDate	19319	-1.3101	1.2193	81	-1.07	0.2858
MDate	19321	0.2947	0.8249	169	0.36	0.7213
MDate	19322	0.4448	0.8249	169	0.54	0.5905
MDate	19323	-0.6815	1.0310	133	-0.66	0.5097
MDate	19324	0.9158	1.2193	81	0.75	0.4548
MDate	19325	1.5169	0.9100	160	1.67	0.0975
MDate	19326	0.9934	1.2193	81	0.81	0.4176
MDate	19327	-0.7666	1.2193	81	-0.63	0.5313
MDate	19329	0.03232	1.0310	133	0.03	0.9750
MDate	19330	-0.2056	1.0310	133	-0.20	0.8422
MDate	19331	-0.1454	1.2193	81	-0.12	0.9054
MDate	19333	0.8926	1.0310	133	0.87	0.3882
MDate	19334	-3.2513	1.2193	81	-2.67	0.0093
MDate	19335	-0.5336	1.2193	81	-0.44	0.6628
MDate	19336	-0.9459	0.7612	171	-1.24	0.2157
MDate	19337	0.6311	1.2193	81	0.52	0.6062
MDate	19338	-0.7666	1.2193	81	-0.63	0.5313
MDate	19339	-2.7863	1.0310	133	-2.70	0.0078
MDate	19341	1.1305	1.0310	133	1.10	0.2748
MDate	19342	0.3419	0.9100	160	0.38	0.7076
MDate	19343	0.2687	1.2193	81	0.22	0.8261
MDate	19344	0.3843	0.9100	160	0.42	0.6733
MDate	19345	0.2946	1.2193	81	0.24	0.8097
MDate	19347	-0.3337	1.0310	133	-0.32	0.7467
MDate	19348	0.8193	1.0310	133	0.79	0.4282

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	0.6052	1.2193	81	0.50	0.6210
MDate	19350	0.3986	0.8249	169	0.48	0.6296
MDate	19351	0.7827	1.0310	133	0.76	0.4491
MDate	19352	-0.2422	1.0310	133	-0.23	0.8146

MDate	19354	1.2904	0.9100	160	1.42	0.1581
MDate	19355	0.5542	0.9100	160	0.61	0.5433
MDate	19356	0.6109	0.9100	160	0.67	0.5030
MDate	19357	0.7605	1.2193	81	0.62	0.5346
MDate	19358	0.9658	1.0310	133	0.94	0.3506
MDate	19359	0.7644	1.0310	133	0.74	0.4597
MDate	19360	0.2687	1.2193	81	0.22	0.8261
MDate	19361	0.6546	1.0310	133	0.63	0.5266
MDate	19362	-0.3524	1.2193	81	-0.29	0.7733
MDate	19363	0.01402	1.0310	133	0.01	0.9892
MDate	19364	-0.8183	1.2193	81	-0.67	0.5040
MDate	19365	-0.8960	1.2193	81	-0.73	0.4646
MDate	19366	-0.5077	1.2193	81	-0.42	0.6782
MDate	19369	-1.4685	1.0310	133	-1.42	0.1567
MDate	19370	-3.7198	1.0310	133	-3.61	0.0004
MDate	19371	-3.2965	0.9100	160	-3.62	0.0004
MDate	19372	-4.2781	0.7612	171	-5.62	<.0001
MDate	19373	-1.7501	1.2193	81	-1.44	0.1550
MDate	19374	-0.2489	1.2193	81	-0.20	0.8388
MDate	19375	-0.2489	1.2193	81	-0.20	0.8388
MDate	19376	-1.5305	0.7612	171	-2.01	0.0459
MDate	19377	0.7666	0.9100	160	0.84	0.4008
MDate	19378	-0.1454	1.2193	81	-0.12	0.9054
MDate	19379	-0.5075	0.9100	160	-0.56	0.5778
MDate	19380	0.03042	0.9100	160	0.03	0.9734
MDate	19381	-0.1208	0.8249	169	-0.15	0.8837
MDate	19382	1.2220	1.0310	133	1.19	0.2380
MDate	19383	1.1488	0.9100	160	1.26	0.2086
MDate	19384	1.3048	0.7612	171	1.71	0.0883
MDate	19385	1.2586	1.0310	133	1.22	0.2243
MDate	19386	0.2286	0.9100	160	0.25	0.8020
MDate	19387	0.8743	1.0310	133	0.85	0.3980
MDate	19388	0.8123	1.2193	81	0.67	0.5072
MDate	19389	0.01402	1.0310	133	0.01	0.9892
MDate	19390	0.4745	0.7115	170	0.67	0.5057
MDate	19391	0.7087	1.2193	81	0.58	0.5627
MDate	19392	1.2904	0.9100	160	1.42	0.1581
MDate	19393	-0.1141	1.0310	133	-0.11	0.9120
MDate	19394	-1.2123	1.0310	133	-1.18	0.2418
MDate	19395	-0.1195	1.2193	81	-0.10	0.9222

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19396	0.1787	1.0310	133	0.17	0.8626
MDate	19397	0.5017	1.2193	81	0.41	0.6818
MDate	19398	0.5967	0.9100	160	0.66	0.5129
MDate	19399	0.6570	1.2193	81	0.54	0.5915

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---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	82	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19372 19373 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	82
Subjects	1
Max Obs Per Subject	147
Observations Used	147
Observations Not Used	0
Total Observations	147

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---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	799.79537440	
1	2	760.21718347	0.00000031
2	1	760.21710755	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	9.0597	0.05	5.1590	12.9605
Residual	4.6825	0.05	3.4121	6.8266

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	3.9609	-0.4510
2	Residual	-0.4510	0.6760

Fit Statistics

-2 Res Log Likelihood	760.2
AIC (smaller is better)	764.2
AICC (smaller is better)	764.3
BIC (smaller is better)	769.0

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	39.58	<.0001

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---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	3.5352	0.3854	78.8	9.17	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	2.2842	1.8134	143	1.26	0.2098
MDate	19307	1.2953	1.8134	143	0.71	0.4762
MDate	19308	0.6361	1.8134	143	0.35	0.7263
MDate	19310	-0.8226	1.4194	123	-0.58	0.5633
MDate	19311	-0.6824	1.8134	143	-0.38	0.7072
MDate	19313	-0.4253	1.4194	123	-0.30	0.7650
MDate	19314	-2.6602	1.8134	143	-1.47	0.1446
MDate	19315	-1.3417	1.8134	143	-0.74	0.4606
MDate	19316	-1.0121	1.8134	143	-0.56	0.5776
MDate	19317	-1.3417	1.8134	143	-0.74	0.4606
MDate	19318	-1.8782	1.2138	113	-1.55	0.1245
MDate	19319	-2.6602	1.8134	143	-1.47	0.1446
MDate	19321	-4.6804	1.0838	110	-4.32	<.0001
MDate	19322	-3.2065	1.4194	123	-2.26	0.0256
MDate	19323	4.9386	1.4194	123	3.48	0.0007
MDate	19324	4.9213	1.8134	143	2.71	0.0075
MDate	19325	4.1439	1.4194	123	2.92	0.0042
MDate	19326	4.5916	1.8134	143	2.53	0.0124
MDate	19327	1.2953	1.8134	143	0.71	0.4762
MDate	19329	1.1640	1.4194	123	0.82	0.4138
MDate	19330	1.1640	1.4194	123	0.82	0.4138
MDate	19331	-3.6038	1.4194	123	-2.54	0.0124
MDate	19333	-0.2266	1.4194	123	-0.16	0.8734
MDate	19334	-4.3084	1.8134	143	-2.38	0.0188
MDate	19335	-0.6824	1.8134	143	-0.38	0.7072
MDate	19336	-0.6824	1.8134	143	-0.38	0.7072
MDate	19337	-0.02318	1.8134	143	-0.01	0.9898
MDate	19338	-2.9898	1.8134	143	-1.65	0.1014
MDate	19339	-5.1931	1.4194	123	-3.66	0.0004
MDate	19341	-0.02794	1.4194	123	-0.02	0.9843
MDate	19342	-1.4517	1.2138	113	-1.20	0.2342
MDate	19343	-0.3528	1.8134	143	-0.19	0.8460
MDate	19344	-0.3528	1.8134	143	-0.19	0.8460
MDate	19345	-1.0121	1.8134	143	-0.56	0.5776
MDate	19347	0.3694	1.4194	123	0.26	0.7951
MDate	19348	-0.2266	1.4194	123	-0.16	0.8734

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---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	0.9657	1.8134	143	0.53	0.5952
MDate	19350	0.1903	1.0838	110	0.18	0.8610

MDate	19351	-1.0212	1.4194	123	-0.72	0.4732
MDate	19352	-0.8226	1.4194	123	-0.58	0.5633
MDate	19354	-0.3528	1.8134	143	-0.19	0.8460
MDate	19355	0.7667	1.4194	123	0.54	0.5901
MDate	19356	-0.4565	1.2138	113	-0.38	0.7075
MDate	19357	0.3065	1.8134	143	0.17	0.8660
MDate	19358	-0.8226	1.4194	123	-0.58	0.5633
MDate	19359	0.1707	1.4194	123	0.12	0.9045
MDate	19360	-0.02318	1.8134	143	-0.01	0.9898
MDate	19361	-0.8226	1.4194	123	-0.58	0.5633
MDate	19362	-1.6713	1.8134	143	-0.92	0.3583
MDate	19363	-0.8226	1.4194	123	-0.58	0.5633
MDate	19364	-2.3306	1.8134	143	-1.29	0.2008
MDate	19365	-7.9343	1.8134	143	-4.38	<.0001
MDate	19366	-3.3195	1.8134	143	-1.83	0.0692
MDate	19369	-4.9945	1.4194	123	-3.52	0.0006
MDate	19370	-7.5771	1.4194	123	-5.34	<.0001
MDate	19371	-2.0204	1.2138	113	-1.66	0.0988
MDate	19372	-0.8830	1.2138	113	-0.73	0.4684
MDate	19373	2.6139	1.8134	143	1.44	0.1516
MDate	19375	2.6139	1.8134	143	1.44	0.1516
MDate	19376	2.6713	1.2138	113	2.20	0.0298
MDate	19377	3.3493	1.4194	123	2.36	0.0199
MDate	19378	2.9435	1.8134	143	1.62	0.1067
MDate	19379	1.6250	1.8134	143	0.90	0.3717
MDate	19380	1.7600	1.4194	123	1.24	0.2174
MDate	19381	0.6330	1.0838	110	0.58	0.5604
MDate	19382	-0.2266	1.4194	123	-0.16	0.8734
MDate	19383	1.5339	1.2138	113	1.26	0.2089
MDate	19384	4.6810	0.9928	110	4.71	<.0001
MDate	19385	4.1439	1.4194	123	2.92	0.0042
MDate	19386	2.5291	1.2138	113	2.08	0.0394
MDate	19387	2.6139	1.8134	143	1.44	0.1516
MDate	19388	1.9546	1.8134	143	1.08	0.2829
MDate	19389	2.9556	1.2138	113	2.44	0.0164
MDate	19390	-1.4702	1.0838	110	-1.36	0.1777
MDate	19392	0.6361	1.8134	143	0.35	0.7263
MDate	19393	-0.2266	1.4194	123	-0.16	0.8734
MDate	19394	-0.4253	1.4194	123	-0.30	0.7650
MDate	19395	1.6250	1.8134	143	0.90	0.3717
MDate	19396	2.5547	1.4194	123	1.80	0.0744
MDate	19397	1.9546	1.8134	143	1.08	0.2829

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19398	2.5291	1.2138	113	2.08	0.0394
MDate	19399	2.9435	1.8134	143	1.62	0.1067

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---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	82	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19372 19373 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	82
Subjects	1
Max Obs Per Subject	147
Observations Used	147
Observations Not Used	0
Total Observations	147

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---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	731.58740679	
1	3	697.43670832	0.00012685
2	1	697.40849212	0.00000042
3	1	697.40840142	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	4.5755	0.05	2.4668	6.6842
Residual	3.5928	0.05	2.6604	5.1208

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	1.1575	-0.1691
2	Residual	-0.1691	0.3554

Fit Statistics

-2 Res Log Likelihood	697.4
AIC (smaller is better)	701.4
AICC (smaller is better)	701.5
BIC (smaller is better)	706.2

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	34.18	<.0001

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|

Intercept		-0.6933	0.2912	84.7	-2.38	0.0195

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	1.3336	1.4629	138	0.91	0.3635
MDate	19307	0.3534	1.4629	138	0.24	0.8095
MDate	19308	0.003276	1.4629	138	0.00	0.9982
MDate	19310	-0.8710	1.1778	143	-0.74	0.4608
MDate	19311	-0.9070	1.4629	138	-0.62	0.5363
MDate	19313	0.2735	1.1778	143	0.23	0.8167
MDate	19314	0.3184	1.4629	138	0.22	0.8280
MDate	19315	-0.2768	1.4629	138	-0.19	0.8502
MDate	19316	0.003276	1.4629	138	0.00	0.9982
MDate	19317	-0.2418	1.4629	138	-0.17	0.8690
MDate	19318	-1.3658	1.0172	133	-1.34	0.1816
MDate	19319	-2.0623	1.4629	138	-1.41	0.1609
MDate	19321	-0.2302	0.9120	127	-0.25	0.8011
MDate	19322	-0.8720	1.4629	138	-0.60	0.5521
MDate	19323	-1.0954	1.1778	143	-0.93	0.3539
MDate	19324	0.9485	1.4629	138	0.65	0.5178
MDate	19325	1.1935	1.0172	133	1.17	0.2428
MDate	19326	1.0886	1.4629	138	0.74	0.4581
MDate	19327	-1.3971	1.4629	138	-0.96	0.3412
MDate	19329	-0.1304	1.1778	143	-0.11	0.9120
MDate	19330	-0.3548	1.1778	143	-0.30	0.7636
MDate	19331	0.1613	1.1778	143	0.14	0.8913
MDate	19333	0.8345	1.1778	143	0.71	0.4798
MDate	19334	-4.4430	1.4629	138	-3.04	0.0029
MDate	19335	-1.0470	1.4629	138	-0.72	0.4754
MDate	19336	0.3184	1.4629	138	0.22	0.8280
MDate	19337	0.7735	1.4629	138	0.53	0.5978
MDate	19338	-1.0120	1.4629	138	-0.69	0.4902
MDate	19339	-3.4740	1.1778	143	-2.95	0.0037
MDate	19341	0.5203	1.1778	143	0.44	0.6593
MDate	19342	-0.5072	1.0172	133	-0.50	0.6189
MDate	19343	-0.1368	1.4629	138	-0.09	0.9257
MDate	19344	-0.2418	1.4629	138	-0.17	0.8690
MDate	19345	-0.1018	1.4629	138	-0.07	0.9446
MDate	19347	-0.9607	1.1778	143	-0.82	0.4160
MDate	19348	0.4530	1.1778	143	0.38	0.7011

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	0.5634	1.4629	138	0.39	0.7007

MDate	19350	-0.02123	0.9120	127	-0.02	0.9815
MDate	19351	0.5876	1.1778	143	0.50	0.6186
MDate	19352	-0.4519	1.4629	138	-0.31	0.7579
MDate	19354	0.6685	1.4629	138	0.46	0.6484
MDate	19355	-0.04490	1.0172	133	-0.04	0.9649
MDate	19356	0.3844	1.0172	133	0.38	0.7061
MDate	19357	0.7035	1.4629	138	0.48	0.6314
MDate	19358	0.7223	1.1778	143	0.61	0.5407
MDate	19359	0.3632	1.1778	143	0.31	0.7582
MDate	19360	-0.1368	1.4629	138	-0.09	0.9257
MDate	19361	-0.2202	1.1778	143	-0.19	0.8520
MDate	19362	-1.1170	1.4629	138	-0.76	0.4464
MDate	19363	-0.8934	1.1778	143	-0.76	0.4494
MDate	19364	-1.7472	1.4629	138	-1.19	0.2344
MDate	19365	-1.9223	1.4629	138	-1.31	0.1910
MDate	19366	-1.5021	1.4629	138	-1.03	0.3063
MDate	19369	-2.8457	1.1778	143	-2.42	0.0169
MDate	19370	-5.7404	1.1778	143	-4.87	<.0001
MDate	19371	-4.8168	1.0172	133	-4.74	<.0001
MDate	19372	-5.2791	1.0172	133	-5.19	<.0001
MDate	19373	-2.5874	1.4629	138	-1.77	0.0792
MDate	19375	1.0886	1.4629	138	0.74	0.4581
MDate	19376	0.9788	1.0172	133	0.96	0.3377
MDate	19377	2.6297	1.1778	143	2.23	0.0271
MDate	19378	1.1586	1.4629	138	0.79	0.4297
MDate	19379	0.7735	1.4629	138	0.53	0.5978
MDate	19380	1.7545	1.1778	143	1.49	0.1385
MDate	19381	1.9379	0.9120	127	2.13	0.0355
MDate	19382	3.1009	1.1778	143	2.63	0.0094
MDate	19383	2.9767	1.0172	133	2.93	0.0040
MDate	19384	2.9328	0.8366	124	3.51	0.0006
MDate	19385	2.6521	1.1778	143	2.25	0.0259
MDate	19386	1.4577	1.0172	133	1.43	0.1542
MDate	19387	1.6837	1.4629	138	1.15	0.2517
MDate	19388	1.5787	1.4629	138	1.08	0.2824
MDate	19389	1.3091	1.0172	133	1.29	0.2004
MDate	19390	0.7624	0.9120	127	0.84	0.4047
MDate	19392	1.8238	1.4629	138	1.25	0.2146
MDate	19393	0.8120	1.1778	143	0.69	0.4916
MDate	19394	-0.1978	1.1778	143	-0.17	0.8669
MDate	19395	0.7035	1.4629	138	0.48	0.6314
MDate	19396	1.3506	1.1778	143	1.15	0.2534
MDate	19397	1.5787	1.4629	138	1.08	0.2824

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19398	1.9200	1.0172	133	1.89	0.0613
MDate	19399	1.7188	1.4629	138	1.17	0.2421

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---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	21	19281 19290 19318 19322 19331 19333 19336 19340 19341 19350 19351 19352 19370 19371 19372 19380 19381 19384 19386 19390 19398

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	21
Subjects	1
Max Obs Per Subject	92
Observations Used	92
Observations Not Used	0
Total Observations	92

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	499.35938572	
1	2	469.80798070	0.00006352
2	1	469.79800150	0.00000023
3	1	469.79796611	0.00000000

Convergence criteria met.

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---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	7.3745	0.05	1.7828	12.9663
Residual	6.6186	0.05	4.8838	9.4799

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	8.1397	-0.3067
2	Residual	-0.3067	1.2368

Fit Statistics

-2 Res Log Likelihood	469.8
AIC (smaller is better)	473.8
AICC (smaller is better)	473.9
BIC (smaller is better)	475.9

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	29.56	<.0001

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.1646	0.6527	19.8	-0.25	0.8034

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19281	-0.6823	1.3072	71.5	-0.52	0.6033
MDate	19290	-2.1116	1.3072	71.5	-1.62	0.1106
MDate	19318	-2.9283	1.3072	71.5	-2.24	0.0282
MDate	19322	-0.06972	1.3072	71.5	-0.05	0.9576
MDate	19331	3.8098	1.3072	71.5	2.91	0.0048

---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19333	1.5638	1.3072	71.5	1.20	0.2355
MDate	19336	-0.4781	1.3072	71.5	-0.37	0.7156
MDate	19340	0.3387	1.3072	71.5	0.26	0.7963
MDate	19341	-0.2739	1.3072	71.5	-0.21	0.8346
MDate	19350	-1.4990	1.3072	71.5	-1.15	0.2553
MDate	19351	-1.0906	1.3072	71.5	-0.83	0.4069
MDate	19352	1.9721	1.3072	71.5	1.51	0.1358
MDate	19370	-2.3158	1.3072	71.5	-1.77	0.0807
MDate	19371	-2.5200	1.3072	71.5	-1.93	0.0578
MDate	19372	-2.6617	1.0557	65.4	-2.52	0.0141
MDate	19380	4.4224	1.3072	71.5	3.38	0.0012
MDate	19381	-2.3158	1.3072	71.5	-1.77	0.0807
MDate	19384	0.3387	1.3072	71.5	0.26	0.7963
MDate	19386	0.5428	1.3072	71.5	0.42	0.6792
MDate	19390	-0.3015	1.0557	65.4	-0.29	0.7761
MDate	19398	6.2601	1.3072	71.5	4.79	<.0001

---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	21	19281 19290 19318 19322 19331 19333 19336 19340 19341 19350 19351 19352 19370 19371 19372 19380 19381 19384 19386 19390 19398

Dimensions

Covariance Parameters	2
Columns in X	1

Columns in Z	21
Subjects	1
Max Obs Per Subject	92
Observations Used	92
Observations Not Used	0
Total Observations	92

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	407.75857326	
1	2	311.16743392	0.00223033
2	1	298.09650757	0.00098587
3	1	298.04074351	0.00003012
4	1	298.03873775	0.00000002
5	1	298.03873621	0.00000000

---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	4.0095	0.05	1.4229	6.5962
Residual	0.7297	0.05	0.5387	1.0444

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	1.7417	-0.00313
2	Residual	-0.00313	0.01498

Fit Statistics

-2 Res Log Likelihood	298.0
AIC (smaller is better)	302.0
AICC (smaller is better)	302.2
BIC (smaller is better)	304.1

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	109.72	<.0001

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.2215	0.4463	20.1	-0.50	0.6251

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19281	-3.9608	0.5989	52	-6.61	<.0001
MDate	19290	-4.6781	0.5989	52	-7.81	<.0001

---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19318	-0.5533	0.5989	52	-0.92	0.3598
MDate	19322	-0.5892	0.5989	52	-0.98	0.3297
MDate	19331	0.8455	0.5989	52	1.41	0.1639
MDate	19333	1.6107	0.5989	52	2.69	0.0096
MDate	19336	0.4988	0.5989	52	0.83	0.4087
MDate	19340	-0.5533	0.5989	52	-0.92	0.3598
MDate	19341	-0.3381	0.5989	52	-0.56	0.5748
MDate	19350	0.2238	0.5989	52	0.37	0.7101
MDate	19351	-0.1827	0.5989	52	-0.31	0.7616
MDate	19352	-1.1631	0.5989	52	-1.94	0.0575
MDate	19370	1.1803	0.5989	52	1.97	0.0541
MDate	19371	2.7107	0.5989	52	4.53	<.0001
MDate	19372	3.7732	0.5293	37.1	7.13	<.0001
MDate	19380	-0.3381	0.5989	52	-0.56	0.5748
MDate	19381	1.5868	0.5989	52	2.65	0.0106
MDate	19384	-0.05116	0.5989	52	-0.09	0.9322
MDate	19386	-2.2391	0.5989	52	-3.74	0.0005
MDate	19390	1.3716	0.5293	37.1	2.59	0.0136
MDate	19398	0.8455	0.5989	52	1.41	0.1639

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	90	19298 19300 19302 19304 19305 19306 19307 19310 19311 19312 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19340 19341 19342 19343 19344 19347 19348 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19367 19368 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	90
Subjects	1
Max Obs Per Subject	145
Observations Used	145
Observations Not Used	0
Total Observations	145

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	886.08626499	
1	2	803.45367835	0.00101122

2	1	803.22140282	0.00003580
3	1	803.21155644	0.00000004
4	1	803.21154614	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	21.1429	0.05	14.1319	28.1539
Residual	3.8532	0.05	2.7565	5.7680

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	12.7956	-0.3012
2	Residual	-0.3012	0.5178

Fit Statistics

-2 Res Log Likelihood	803.2
AIC (smaller is better)	807.2
AICC (smaller is better)	807.3
BIC (smaller is better)	812.2

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	82.87	<.0001

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---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	4.3861	0.5166	90.9	8.49	<.0001

Solution for Random Effects

Std Err

Effect	MDate	Estimate	Pred	DF	t Value	Pr > |t|
MDate	19298	-1.5954	1.8734	92	-0.85	0.3966
MDate	19300	1.3651	1.8734	92	0.73	0.4680
MDate	19302	-0.3266	1.8734	92	-0.17	0.8620
MDate	19304	-3.2871	1.8734	92	-1.75	0.0827
MDate	19305	-2.0183	1.8734	92	-1.08	0.2841
MDate	19306	-2.4412	1.8734	92	-1.30	0.1958
MDate	19307	-2.0183	1.8734	92	-1.08	0.2841
MDate	19310	0.5193	1.8734	92	0.28	0.7823
MDate	19311	0.5193	1.8734	92	0.28	0.7823
MDate	19312	-0.3266	1.8734	92	-0.17	0.8620
MDate	19313	0.1044	1.4174	88.2	0.07	0.9415
MDate	19314	0.5193	1.8734	92	0.28	0.7823
MDate	19315	0.09634	1.8734	92	0.05	0.9591
MDate	19316	-1.1724	1.8734	92	-0.63	0.5330
MDate	19317	-1.1724	1.8734	92	-0.63	0.5330
MDate	19318	-0.3539	1.4174	88.2	-0.25	0.8034
MDate	19319	0.09634	1.8734	92	0.05	0.9591
MDate	19321	0.5787	1.2072	92	0.48	0.6328
MDate	19322	0.09634	1.8734	92	0.05	0.9591
MDate	19323	0.1044	1.4174	88.2	0.07	0.9415
MDate	19324	0.5193	1.8734	92	0.28	0.7823
MDate	19325	0.2645	1.2072	92	0.22	0.8271
MDate	19326	-0.7495	1.8734	92	-0.40	0.6900
MDate	19327	0.09634	1.8734	92	0.05	0.9591
MDate	19329	1.7082	1.4174	88.2	1.21	0.2313
MDate	19330	2.1665	1.4174	88.2	1.53	0.1300
MDate	19331	0.09634	1.8734	92	0.05	0.9591
MDate	19333	1.7082	1.4174	88.2	1.21	0.2313
MDate	19334	1.7880	1.8734	92	0.95	0.3424
MDate	19335	-0.3266	1.8734	92	-0.17	0.8620
MDate	19336	-0.7495	1.8734	92	-0.40	0.6900
MDate	19337	2.2110	1.8734	92	1.18	0.2410
MDate	19338	-0.7495	1.8734	92	-0.40	0.6900
MDate	19339	0.3335	1.4174	88.2	0.24	0.8145
MDate	19340	-1.0412	1.4174	88.2	-0.73	0.4645
MDate	19341	-6.6489	1.2072	92	-5.51	<.0001

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19342	-6.1775	1.2072	92	-5.12	<.0001
MDate	19343	-4.5558	1.8734	92	-2.43	0.0170
MDate	19344	-4.1329	1.8734	92	-2.21	0.0299
MDate	19347	-1.9577	1.4174	88.2	-1.38	0.1707
MDate	19348	-2.6451	1.4174	88.2	-1.87	0.0653
MDate	19350	-5.8687	1.0822	97.3	-5.42	<.0001
MDate	19351	-8.3621	1.8734	92	-4.46	<.0001

MDate	19352	-7.5163	1.8734	92	-4.01	0.0001
MDate	19354	-3.2871	1.8734	92	-1.75	0.0827
MDate	19355	-2.8641	1.8734	92	-1.53	0.1297
MDate	19356	-2.8641	1.8734	92	-1.53	0.1297
MDate	19357	-2.8641	1.8734	92	-1.53	0.1297
MDate	19358	-3.3324	1.4174	88.2	-2.35	0.0209
MDate	19359	-3.1033	1.4174	88.2	-2.19	0.0312
MDate	19360	-2.8641	1.8734	92	-1.53	0.1297
MDate	19361	-4.4780	1.4174	88.2	-3.16	0.0022
MDate	19362	-3.2871	1.8734	92	-1.75	0.0827
MDate	19363	-4.7072	1.4174	88.2	-3.32	0.0013
MDate	19364	-4.1329	1.8734	92	-2.21	0.0299
MDate	19365	-4.1329	1.8734	92	-2.21	0.0299
MDate	19366	4.2286	1.4174	88.2	2.98	0.0037
MDate	19367	5.1714	1.8734	92	2.76	0.0070
MDate	19368	6.0173	1.8734	92	3.21	0.0018
MDate	19369	2.6247	1.4174	88.2	1.85	0.0674
MDate	19370	0.09634	1.8734	92	0.05	0.9591
MDate	19371	2.9356	1.2072	92	2.43	0.0170
MDate	19372	4.8911	1.0822	97.3	4.52	<.0001
MDate	19373	8.1319	1.8734	92	4.34	<.0001
MDate	19374	11.3314	1.4174	88.2	7.99	<.0001
MDate	19375	8.3528	1.4174	88.2	5.89	<.0001
MDate	19376	13.2070	1.8734	92	7.05	<.0001
MDate	19377	7.6654	1.4174	88.2	5.41	<.0001
MDate	19378	9.4984	1.4174	88.2	6.70	<.0001
MDate	19379	9.0401	1.4174	88.2	6.38	<.0001
MDate	19380	9.7275	1.4174	88.2	6.86	<.0001
MDate	19381	10.4149	1.4174	88.2	7.35	<.0001
MDate	19382	8.8110	1.4174	88.2	6.22	<.0001
MDate	19383	-1.2703	1.4174	88.2	-0.90	0.3726
MDate	19384	-4.0389	0.9979	103	-4.05	0.0001
MDate	19385	-3.2871	1.8734	92	-1.75	0.0827
MDate	19386	-3.6635	1.2072	92	-3.03	0.0031
MDate	19387	-0.3266	1.8734	92	-0.17	0.8620
MDate	19388	-1.1724	1.8734	92	-0.63	0.5330
MDate	19389	-3.2871	1.8734	92	-1.75	0.0827

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19390	-3.2385	1.0822	97.3	-2.99	0.0035
MDate	19391	-1.5954	1.8734	92	-0.85	0.3966
MDate	19392	-1.1724	1.8734	92	-0.63	0.5330
MDate	19393	-0.8121	1.4174	88.2	-0.57	0.5681
MDate	19394	-0.5830	1.4174	88.2	-0.41	0.6818
MDate	19395	1.3651	1.8734	92	0.73	0.4680
MDate	19396	0.3335	1.4174	88.2	0.24	0.8145
MDate	19397	-2.8641	1.8734	92	-1.53	0.1297

MDate	19398	-2.5637	1.2072	92	-2.12	0.0364
MDate	19399	-0.7495	1.8734	92	-0.40	0.6900

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---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	90	19298 19300 19302 19304 19305 19306 19307 19310 19311 19312 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19340 19341 19342 19343 19344 19347 19348 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19367 19368 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	90
Subjects	1
Max Obs Per Subject	145
Observations Used	145
Observations Not Used	0
Total Observations	145

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---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	870.62961936	
1	2	826.08398746	0.02872588
2	1	815.67595604	0.01239290
3	1	811.46988795	0.00284906
4	1	810.57843749	0.00019563
5	1	810.52251294	0.00000111
6	1	810.52221004	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	25.5001	0.05	17.0246	33.9756
Residual	3.4231	0.05	2.4133	5.2346

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	18.6997	-0.4503
2	Residual	-0.4503	0.4486

Fit Statistics

-2 Res Log Likelihood	810.5
AIC (smaller is better)	814.5
AICC (smaller is better)	814.6
BIC (smaller is better)	819.5

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	60.11	<.0001

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	0.4386	0.5584	86	0.79	0.4343

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19298	-1.0480	1.8189	82.3	-0.58	0.5661
MDate	19300	-0.9929	1.8189	82.3	-0.55	0.5866
MDate	19302	-0.6071	1.8189	82.3	-0.33	0.7394
MDate	19304	-2.2051	1.8189	82.3	-1.21	0.2288
MDate	19305	-1.5439	1.8189	82.3	-0.85	0.3984
MDate	19306	-1.6541	1.8189	82.3	-0.91	0.3658
MDate	19307	-1.6541	1.8189	82.3	-0.91	0.3658
MDate	19310	-1.4337	1.8189	82.3	-0.79	0.4328
MDate	19311	-1.2133	1.8189	82.3	-0.67	0.5066
MDate	19312	-1.6541	1.8189	82.3	-0.91	0.3658
MDate	19313	0.08678	1.3756	84.2	0.06	0.9498
MDate	19314	1.4317	1.8189	82.3	0.79	0.4335
MDate	19315	-0.8276	1.8189	82.3	-0.45	0.6503
MDate	19316	-1.5990	1.8189	82.3	-0.88	0.3819
MDate	19317	2.0378	1.8189	82.3	1.12	0.2658
MDate	19318	-2.1096	1.3756	84.2	-1.53	0.1289
MDate	19319	-0.9929	1.8189	82.3	-0.55	0.5866
MDate	19321	0.9162	1.1768	91.4	0.78	0.4383
MDate	19322	2.0929	1.8189	82.3	1.15	0.2532
MDate	19323	-2.1681	1.3756	84.2	-1.58	0.1188
MDate	19324	-0.1112	1.8189	82.3	-0.06	0.9514
MDate	19325	-0.6193	1.1768	91.4	-0.53	0.6000
MDate	19326	-0.05611	1.8189	82.3	-0.03	0.9755
MDate	19327	-3.6929	1.8189	82.3	-2.03	0.0456
MDate	19329	-0.2646	1.3756	84.2	-0.19	0.8479
MDate	19330	2.1953	1.3756	84.2	1.60	0.1143
MDate	19331	-2.0949	1.8189	82.3	-1.15	0.2527
MDate	19333	1.8438	1.3756	84.2	1.34	0.1837
MDate	19334	-0.1112	1.8189	82.3	-0.06	0.9514
MDate	19335	-1.3786	1.8189	82.3	-0.76	0.4507
MDate	19336	-0.5520	1.8189	82.3	-0.30	0.7623
MDate	19337	-1.2133	1.8189	82.3	-0.67	0.5066
MDate	19338	-0.3867	1.8189	82.3	-0.21	0.8321
MDate	19339	-0.6746	1.3756	84.2	-0.49	0.6251
MDate	19340	-0.4403	1.3756	84.2	-0.32	0.7497
MDate	19341	-1.1377	1.1768	91.4	-0.97	0.3362

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19342	-0.3999	1.1768	91.4	-0.34	0.7348
MDate	19343	-0.2765	1.8189	82.3	-0.15	0.8795
MDate	19344	-0.2765	1.8189	82.3	-0.15	0.8795
MDate	19347	1.3460	1.3756	84.2	0.98	0.3306
MDate	19348	-1.3482	1.3756	84.2	-0.98	0.3299
MDate	19350	-4.7934	1.0602	99.5	-4.52	<.0001
MDate	19351	-7.7705	1.8189	82.3	-4.27	<.0001
MDate	19352	-9.2032	1.8189	82.3	-5.06	<.0001
MDate	19354	-0.4418	1.8189	82.3	-0.24	0.8087
MDate	19355	-0.2214	1.8189	82.3	-0.12	0.9034
MDate	19356	-0.1663	1.8189	82.3	-0.09	0.9274
MDate	19357	0.1643	1.8189	82.3	0.09	0.9282
MDate	19358	0.02821	1.3756	84.2	0.02	0.9837
MDate	19359	0.2625	1.3756	84.2	0.19	0.8491
MDate	19360	0.3296	1.8189	82.3	0.18	0.8566
MDate	19361	-1.4653	1.3756	84.2	-1.07	0.2898
MDate	19362	-1.9296	1.8189	82.3	-1.06	0.2918
MDate	19363	-1.4067	1.3756	84.2	-1.02	0.3094
MDate	19364	-1.4337	1.8189	82.3	-0.79	0.4328
MDate	19365	-0.4418	1.8189	82.3	-0.24	0.8087
MDate	19366	-0.6453	1.3756	84.2	-0.47	0.6402
MDate	19367	3.6909	1.8189	82.3	2.03	0.0457
MDate	19368	-0.8827	1.8189	82.3	-0.49	0.6288
MDate	19369	2.2245	1.3756	84.2	1.62	0.1096
MDate	19370	3.8562	1.8189	82.3	2.12	0.0370
MDate	19371	1.5942	1.1768	91.4	1.35	0.1789
MDate	19372	4.4586	1.0602	99.5	4.21	<.0001
MDate	19373	4.1868	1.8189	82.3	2.30	0.0239
MDate	19374	3.9523	1.3756	84.2	2.87	0.0051
MDate	19375	4.6552	1.3756	84.2	3.38	0.0011
MDate	19376	34.1078	1.8189	82.3	18.75	<.0001
MDate	19377	7.3786	1.3756	84.2	5.36	<.0001
MDate	19378	7.7007	1.3756	84.2	5.60	<.0001
MDate	19379	6.2951	1.3756	84.2	4.58	<.0001
MDate	19380	6.1487	1.3756	84.2	4.47	<.0001
MDate	19381	6.7344	1.3756	84.2	4.90	<.0001
MDate	19382	8.3450	1.3756	84.2	6.07	<.0001
MDate	19383	0.4675	1.3756	84.2	0.34	0.7348
MDate	19384	-0.5367	0.9825	107	-0.55	0.5860
MDate	19385	-0.2214	1.8189	82.3	-0.12	0.9034
MDate	19386	-0.3401	1.1768	91.4	-0.29	0.7732
MDate	19387	-3.0317	1.8189	82.3	-1.67	0.0994
MDate	19388	-6.8889	1.8189	82.3	-3.79	0.0003
MDate	19389	-5.8970	1.8189	82.3	-3.24	0.0017

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19390	-3.6747	1.0602	99.5	-3.47	0.0008
MDate	19391	-5.1256	1.8189	82.3	-2.82	0.0060
MDate	19392	-2.5909	1.8189	82.3	-1.42	0.1581
MDate	19393	-2.6074	1.3756	84.2	-1.90	0.0615
MDate	19394	-3.9545	1.3756	84.2	-2.87	0.0051
MDate	19395	-5.1256	1.8189	82.3	-2.82	0.0060
MDate	19396	-1.8753	1.3756	84.2	-1.36	0.1764
MDate	19397	-2.7562	1.8189	82.3	-1.52	0.1335
MDate	19398	-3.8298	1.1768	91.4	-3.25	0.0016
MDate	19399	-2.5358	1.8189	82.3	-1.39	0.1670

Screened Measurements

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                                  The SAS System        09:55 Thursday, March 14, 2013   1

---------------------------------- Analyte=Formate RefValue=2 ----------------------------------

                                The Mixed Procedure

                                 Model Information

Data Set                     WORK.TOMSORT
Dependent Variable           PctDiff
Covariance Structure         Variance Components
Estimation Method            REML
Residual Variance Method     Profile
Fixed Effects SE Method      Prasad-Rao-Jeske-
                             Kackar-Harville
Degrees of Freedom Method    Kenward-Roger


                Class Level Information

  Class    Levels    Values

  MDate        79    19306 19307 19308 19310 19311
                     19313 19314 19315 19316 19317
                     19318 19319 19321 19322 19323
                     19327 19329 19330 19331 19333
                     19334 19335 19336 19337 19338
                     19339 19341 19342 19343 19344
                     19345 19347 19348 19349 19350
                     19351 19354 19355 19356 19357
                     19358 19359 19360 19361 19362
                     19363 19364 19366 19369 19370
                     19371 19372 19373 19374 19375
                     19376 19377 19378 19379 19380
                     19381 19382 19383 19384 19385
                     19386 19387 19388 19389 19390
                     19391 19392 19393 19394 19395
                     19396 19397 19398 19399


                          Dimensions

          Covariance Parameters            2
          Columns in X                     1
          Columns in Z                    79
          Subjects                         1
          Max Obs Per Subject            156
          Observations Used              156
          Observations Not Used            0
          Total Observations             156


                                  The SAS System        09:55 Thursday, March 14, 2013   2
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---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	725.17061574	
1	3	691.56933896	0.01146317
2	2	690.01983597	0.00024085
3	1	689.97400134	0.00000173
4	1	689.97364935	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	2.8576	0.05	1.4356	4.2797
Residual	2.9201	0.05	2.2107	4.0377

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.5264	-0.08596
2	Residual	-0.08596	0.1991

Fit Statistics

-2 Res Log Likelihood	690.0
AIC (smaller is better)	694.0
AICC (smaller is better)	694.1
BIC (smaller is better)	698.7

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	35.20	<.0001

---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	2.5432	0.2425	81.2	10.49	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	0.9678	1.2392	114	0.78	0.4364
MDate	19307	-0.02136	1.2392	114	-0.02	0.9863
MDate	19308	-0.5159	1.2392	114	-0.42	0.6779
MDate	19310	-0.3595	1.0190	151	-0.35	0.7247
MDate	19311	-0.7632	1.2392	114	-0.62	0.5392
MDate	19313	-0.1940	1.0190	151	-0.19	0.8492
MDate	19314	-1.0105	1.2392	114	-0.82	0.4165
MDate	19315	-0.7632	1.2392	114	-0.62	0.5392
MDate	19316	-0.5159	1.2392	114	-0.42	0.6779
MDate	19317	-0.5159	1.2392	114	-0.42	0.6779
MDate	19318	-1.3997	0.8880	155	-1.58	0.1170
MDate	19319	-2.4943	1.2392	114	-2.01	0.0465
MDate	19321	-2.1457	0.8880	155	-2.42	0.0168
MDate	19322	-2.5186	0.8880	155	-2.84	0.0052
MDate	19323	3.9424	1.0190	151	3.87	0.0002
MDate	19327	1.9570	1.2392	114	1.58	0.1171
MDate	19329	-0.02858	1.0190	151	-0.03	0.9777
MDate	19330	0.6333	1.0190	151	0.62	0.5353
MDate	19331	-1.1868	1.0190	151	-1.16	0.2460
MDate	19333	0.2259	1.2392	114	0.18	0.8557
MDate	19334	-2.7416	1.2392	114	-2.21	0.0289
MDate	19335	0.4732	1.2392	114	0.38	0.7033
MDate	19336	-0.02858	1.0190	151	-0.03	0.9777
MDate	19337	0.2259	1.2392	114	0.18	0.8557
MDate	19338	-2.2470	1.2392	114	-1.81	0.0724
MDate	19339	-1.7524	1.2392	114	-1.41	0.1600
MDate	19341	0.6333	1.0190	151	0.62	0.5353
MDate	19342	-0.7781	0.8880	155	-0.88	0.3822
MDate	19343	-0.02136	1.2392	114	-0.02	0.9863
MDate	19344	-1.5241	0.8880	155	-1.72	0.0881
MDate	19345	-0.7632	1.2392	114	-0.62	0.5392
MDate	19347	0.4678	1.0190	151	0.46	0.6469
MDate	19348	-0.3595	1.0190	151	-0.35	0.7247
MDate	19349	-0.02136	1.2392	114	-0.02	0.9863
MDate	19350	-0.1340	0.7996	151	-0.17	0.8672
MDate	19351	-0.5250	1.0190	151	-0.52	0.6072

---------- Analyte=Formate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19354	0.4651	0.8880	155	0.52	0.6012
MDate	19355	0.3023	1.0190	151	0.30	0.7671
MDate	19356	0.2164	0.8880	155	0.24	0.8078
MDate	19357	0.2259	1.2392	114	0.18	0.8557
MDate	19358	-0.3595	1.0190	151	-0.35	0.7247
MDate	19359	0.3023	1.0190	151	0.30	0.7671
MDate	19360	0.7205	1.2392	114	0.58	0.5621
MDate	19361	-0.3595	1.0190	151	-0.35	0.7247
MDate	19362	-0.7632	1.2392	114	-0.62	0.5392
MDate	19363	0.3023	1.0190	151	0.30	0.7671
MDate	19364	-1.2578	1.2392	114	-1.02	0.3122
MDate	19366	-1.0105	1.2392	114	-0.82	0.4165
MDate	19369	0.4732	1.2392	114	0.38	0.7033
MDate	19370	-1.2578	1.2392	114	-1.02	0.3122
MDate	19371	-1.2754	0.8880	155	-1.44	0.1529
MDate	19372	-3.0250	0.7352	147	-4.11	<.0001
MDate	19373	0.4732	1.2392	114	0.38	0.7033
MDate	19374	0.2259	1.2392	114	0.18	0.8557
MDate	19375	1.2151	1.2392	114	0.98	0.3289
MDate	19376	2.7872	0.7352	147	3.79	0.0002
MDate	19377	2.0812	0.8880	155	2.34	0.0204
MDate	19378	1.2151	1.2392	114	0.98	0.3289
MDate	19379	2.0812	0.8880	155	2.34	0.0204
MDate	19380	0.8380	0.8880	155	0.94	0.3468
MDate	19381	-0.5322	0.7996	151	-0.67	0.5067
MDate	19382	-0.02858	1.0190	151	-0.03	0.9777
MDate	19383	1.0867	0.8880	155	1.22	0.2229
MDate	19384	3.1193	0.7352	147	4.24	<.0001
MDate	19385	2.4533	1.0190	151	2.41	0.0173
MDate	19386	1.2110	0.8880	155	1.36	0.1746
MDate	19387	1.6260	1.0190	151	1.60	0.1127
MDate	19388	0.7205	1.2392	114	0.58	0.5621
MDate	19389	1.7083	0.8880	155	1.92	0.0562
MDate	19390	-1.1762	0.6859	145	-1.71	0.0885
MDate	19391	0.9678	1.2392	114	0.78	0.4364
MDate	19392	0.3407	0.8880	155	0.38	0.7017
MDate	19393	-1.5177	1.0190	151	-1.49	0.1385
MDate	19394	-1.8486	1.0190	151	-1.81	0.0716
MDate	19395	0.2259	1.2392	114	0.18	0.8557
MDate	19396	0.7987	1.0190	151	0.78	0.4344
MDate	19397	0.4732	1.2392	114	0.38	0.7033
MDate	19398	0.8380	0.8880	155	0.94	0.3468
MDate	19399	0.7205	1.2392	114	0.58	0.5621

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT

Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	81	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19370 19371 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	81
Subjects	1
Max Obs Per Subject	158
Observations Used	158
Observations Not Used	0
Total Observations	158

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	593.54995695	
1	2	592.26684550	0.00000098
2	1	592.26669674	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	0.2923	0.05	-0.2725	0.8571
Residual	2.2000	0.05	1.6550	3.0680

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.08304	-0.06010
2	Residual	-0.06010	0.1186

Fit Statistics

-2 Res Log Likelihood	592.3
AIC (smaller is better)	596.3
AICC (smaller is better)	596.3
BIC (smaller is better)	601.1

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	1.28	0.2573

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	1.6713	0.1370	59.7	12.20	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	0.1485	0.5665	2.7	0.26	0.8119
MDate	19307	-0.1300	0.5665	2.7	-0.23	0.8347

MDate	19308	-0.1813	0.5665	2.7	-0.32	0.7720
MDate	19310	-0.2000	0.5667	3.43	-0.35	0.7448
MDate	19311	-0.2400	0.5665	2.7	-0.42	0.7033
MDate	19313	0.02308	0.5667	3.43	0.04	0.9698
MDate	19314	0.08253	0.5665	2.7	0.15	0.8944
MDate	19315	-0.1080	0.5665	2.7	-0.19	0.8622
MDate	19316	-0.01276	0.5665	2.7	-0.02	0.9836
MDate	19317	-0.03475	0.5665	2.7	-0.06	0.9553
MDate	19318	0.05589	0.5667	3.43	0.10	0.9269
MDate	19319	-0.4599	0.5665	2.7	-0.81	0.4823
MDate	19321	-0.2546	0.5422	5.15	-0.47	0.6579
MDate	19322	-0.2546	0.5422	5.15	-0.47	0.6579
MDate	19323	-0.4164	0.5667	3.43	-0.73	0.5094
MDate	19324	0.2364	0.5665	2.7	0.42	0.7073
MDate	19325	0.5924	0.5566	4.25	1.06	0.3439
MDate	19326	0.2218	0.5665	2.7	0.39	0.7242
MDate	19327	-0.2986	0.5665	2.7	-0.53	0.6383
MDate	19329	-0.08188	0.5667	3.43	-0.14	0.8932
MDate	19330	-0.1016	0.5667	3.43	-0.18	0.8678
MDate	19331	0.1215	0.5667	3.43	0.21	0.8424
MDate	19333	0.4298	0.5667	3.43	0.76	0.4969
MDate	19335	-0.1154	0.5665	2.7	-0.20	0.8530
MDate	19336	0.3133	0.5566	4.25	0.56	0.6018
MDate	19337	0.1925	0.5665	2.7	0.34	0.7587
MDate	19338	-0.2693	0.5665	2.7	-0.48	0.6703
MDate	19339	-0.3792	0.5665	2.7	-0.67	0.5559
MDate	19341	0.2002	0.5667	3.43	0.35	0.7445
MDate	19342	-0.06069	0.5566	4.25	-0.11	0.9181
MDate	19343	0.05321	0.5665	2.7	0.09	0.9317
MDate	19344	0.1293	0.5566	4.25	0.23	0.8271
MDate	19345	-0.02009	0.5665	2.7	-0.04	0.9742
MDate	19347	-0.3115	0.5667	3.43	-0.55	0.6163
MDate	19348	0.07557	0.5667	3.43	0.13	0.9014
MDate	19349	-0.02009	0.5665	2.7	-0.04	0.9742

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19350	-0.2980	0.5422	5.15	-0.55	0.6056
MDate	19351	0.1543	0.5667	3.43	0.27	0.8010
MDate	19352	-0.1147	0.5667	3.43	-0.20	0.8510
MDate	19354	0.2955	0.5566	4.25	0.53	0.6220
MDate	19355	0.03431	0.5566	4.25	0.06	0.9536
MDate	19356	0.07586	0.5566	4.25	0.14	0.8978
MDate	19357	0.1118	0.5665	2.7	0.20	0.8574
MDate	19358	0.1805	0.5667	3.43	0.32	0.7685
MDate	19359	0.1543	0.5667	3.43	0.27	0.8010
MDate	19360	0.06054	0.5665	2.7	0.11	0.9223
MDate	19361	-0.1212	0.5667	3.43	-0.21	0.8427

MDate	19362	-0.1813	0.5665	2.7	-0.32	0.7720
MDate	19363	-0.1737	0.5667	3.43	-0.31	0.7769
MDate	19364	-0.3646	0.5665	2.7	-0.64	0.5703
MDate	19365	-0.4379	0.5665	2.7	-0.77	0.5015
MDate	19366	-0.2546	0.5665	2.7	-0.45	0.6867
MDate	19369	0.1192	0.5665	2.7	0.21	0.8482
MDate	19370	-0.5258	0.5665	2.7	-0.93	0.4285
MDate	19371	-0.1447	0.5665	2.7	-0.26	0.8166
MDate	19374	-0.04941	0.5665	2.7	-0.09	0.9366
MDate	19375	-0.01276	0.5665	2.7	-0.02	0.9836
MDate	19376	-0.5224	0.5265	6.13	-0.99	0.3587
MDate	19377	0.3773	0.5667	3.43	0.67	0.5476
MDate	19378	0.1674	0.5667	3.43	0.30	0.7847
MDate	19379	-0.1497	0.5566	4.25	-0.27	0.8005
MDate	19380	0.05212	0.5566	4.25	0.09	0.9296
MDate	19381	-0.04317	0.5422	5.15	-0.08	0.9395
MDate	19382	0.3249	0.5667	3.43	0.57	0.6019
MDate	19383	0.4618	0.5566	4.25	0.83	0.4508
MDate	19384	0.4655	0.5265	6.13	0.88	0.4100
MDate	19385	0.3380	0.5667	3.43	0.60	0.5880
MDate	19386	-0.00725	0.5566	4.25	-0.01	0.9902
MDate	19387	0.2133	0.5667	3.43	0.38	0.7287
MDate	19388	0.03855	0.5665	2.7	0.07	0.9505
MDate	19389	-0.00725	0.5566	4.25	-0.01	0.9902
MDate	19390	-0.04825	0.5106	7.18	-0.09	0.9273
MDate	19391	0.1632	0.5665	2.7	0.29	0.7940
MDate	19392	0.3905	0.5566	4.25	0.70	0.5194
MDate	19393	-0.1737	0.5667	3.43	-0.31	0.7769
MDate	19394	0.1265	0.5665	2.7	0.22	0.8391
MDate	19395	-0.06406	0.5665	2.7	-0.11	0.9178
MDate	19396	-0.02284	0.5667	3.43	-0.04	0.9701
MDate	19397	0.1045	0.5665	2.7	0.18	0.8666
MDate	19398	0.2777	0.5566	4.25	0.50	0.6425

---------- Analyte=Formate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19399	0.1045	0.5665	2.7	0.18	0.8666

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff

Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	83	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19366 19369 19370 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	83
Subjects	1
Max Obs Per Subject	167
Observations Used	167
Observations Not Used	0
Total Observations	167

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	843.91579313	
1	2	786.10905211	0.00326664
2	1	785.20726673	0.00023715
3	1	785.14749809	0.00000150
4	1	785.14713633	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	5.9456	0.05	3.5138	8.3773
Residual	3.0773	0.05	2.3308	4.2522

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	1.5394	-0.1234
2	Residual	-0.1234	0.2203

Fit Statistics

-2 Res Log Likelihood	785.1
AIC (smaller is better)	789.1
AICC (smaller is better)	789.2
BIC (smaller is better)	794.0

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	58.77	<.0001

The SAS System 09:55 Thursday, March 14, 2013 12

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.4384	0.3079	81.6	-1.42	0.1583

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	0.9478	1.4632	166	0.65	0.5180

MDate	19307	-0.04061	1.4632	166	-0.03	0.9779
MDate	19308	-0.3701	1.4632	166	-0.25	0.8006
MDate	19310	-1.4392	1.1463	151	-1.26	0.2112
MDate	19311	-1.3585	1.4632	166	-0.93	0.3545
MDate	19313	-0.6448	1.1463	151	-0.56	0.5746
MDate	19314	-2.0174	1.4632	166	-1.38	0.1698
MDate	19315	-1.0290	1.4632	166	-0.70	0.4829
MDate	19316	-0.6996	1.4632	166	-0.48	0.6332
MDate	19317	-1.0290	1.4632	166	-0.70	0.4829
MDate	19318	-1.6161	0.9805	142	-1.65	0.1015
MDate	19319	-3.0059	1.4632	166	-2.05	0.0415
MDate	19321	-1.7148	0.8757	139	-1.96	0.0522
MDate	19322	1.3843	0.8757	139	1.58	0.1162
MDate	19323	3.9231	1.1463	151	3.42	0.0008
MDate	19324	3.9131	1.4632	166	2.67	0.0082
MDate	19325	4.4960	0.9805	142	4.59	<.0001
MDate	19326	3.5836	1.4632	166	2.45	0.0154
MDate	19327	0.9478	1.4632	166	0.65	0.5180
MDate	19329	-0.4462	1.1463	151	-0.39	0.6976
MDate	19330	-0.04896	1.1463	151	-0.04	0.9660
MDate	19331	-3.9943	1.4632	166	-2.73	0.0070
MDate	19333	-0.04896	1.1463	151	-0.04	0.9660
MDate	19334	-3.3353	1.4632	166	-2.28	0.0239
MDate	19335	-0.6996	1.4632	166	-0.48	0.6332
MDate	19336	-1.3827	0.8757	139	-1.58	0.1166
MDate	19337	-0.6996	1.4632	166	-0.48	0.6332
MDate	19338	-2.6764	1.4632	166	-1.83	0.0692
MDate	19339	-3.6238	1.1463	151	-3.16	0.0019
MDate	19341	-0.4462	1.1463	151	-0.39	0.6976
MDate	19342	-1.7583	0.9805	142	-1.79	0.0751
MDate	19343	-1.0290	1.4632	166	-0.70	0.4829
MDate	19344	-1.2406	1.1463	151	-1.08	0.2809
MDate	19345	-1.3585	1.4632	166	-0.93	0.3545
MDate	19347	-0.4462	1.1463	151	-0.39	0.6976
MDate	19348	-1.4392	1.1463	151	-1.26	0.2112

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	-0.6996	1.4632	166	-0.48	0.6332
MDate	19350	0.2775	0.8757	139	0.32	0.7518
MDate	19351	-1.6378	1.1463	151	-1.43	0.1551
MDate	19352	-2.0350	1.1463	151	-1.78	0.0779
MDate	19354	-0.4790	0.9805	142	-0.49	0.6260
MDate	19355	-2.4690	0.9805	142	-2.52	0.0129
MDate	19356	-0.9054	0.9805	142	-0.92	0.3574
MDate	19357	-0.3701	1.4632	166	-0.25	0.8006
MDate	19358	-1.2406	1.1463	151	-1.08	0.2809
MDate	19359	-0.6448	1.1463	151	-0.56	0.5746

MDate	19360	-0.6996	1.4632	166	-0.48	0.6332
MDate	19361	-2.0350	1.1463	151	-1.78	0.0779
MDate	19362	-2.3469	1.4632	166	-1.60	0.1106
MDate	19363	-1.0420	1.1463	151	-0.91	0.3648
MDate	19364	-2.3469	1.4632	166	-1.60	0.1106
MDate	19366	-3.0059	1.4632	166	-2.05	0.0415
MDate	19369	-1.0290	1.4632	166	-0.70	0.4829
MDate	19370	-3.0059	1.4632	166	-2.05	0.0415
MDate	19371	-2.8954	0.9805	142	-2.95	0.0037
MDate	19372	-4.1337	0.8021	138	-5.15	<.0001
MDate	19373	0.6183	1.4632	166	0.42	0.6731
MDate	19374	-0.04061	1.4632	166	-0.03	0.9779
MDate	19375	-0.04061	1.4632	166	-0.03	0.9779
MDate	19376	2.9346	0.8021	138	3.66	0.0004
MDate	19377	2.9324	0.9805	142	2.99	0.0033
MDate	19378	1.9362	1.4632	166	1.32	0.1876
MDate	19379	3.2167	0.9805	142	3.28	0.0013
MDate	19380	2.3639	0.9805	142	2.41	0.0172
MDate	19381	2.0483	0.8757	139	2.34	0.0208
MDate	19382	3.7245	1.1463	151	3.25	0.0014
MDate	19383	2.9324	0.9805	142	2.99	0.0033
MDate	19384	3.7502	0.8021	138	4.68	<.0001
MDate	19385	3.1287	1.1463	151	2.73	0.0071
MDate	19386	1.7953	0.9805	142	1.83	0.0692
MDate	19387	2.5329	1.1463	151	2.21	0.0286
MDate	19388	1.9362	1.4632	166	1.32	0.1876
MDate	19389	2.7315	1.1463	151	2.38	0.0184
MDate	19390	1.0173	0.7472	139	1.36	0.1756
MDate	19391	2.5952	1.4632	166	1.77	0.0780
MDate	19392	1.6532	0.9805	142	1.69	0.0940
MDate	19393	0.1496	1.1463	151	0.13	0.8963
MDate	19394	0.1496	1.1463	151	0.13	0.8963
MDate	19395	0.9478	1.4632	166	0.65	0.5180
MDate	19396	1.9371	1.1463	151	1.69	0.0931

---------- Analyte=Nitrate RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19397	1.6067	1.4632	166	1.10	0.2737
MDate	19398	2.3639	0.9805	142	2.41	0.0172
MDate	19399	2.2657	1.4632	166	1.55	0.1234

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	82	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19371 19372 19373 19374 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	82
Subjects	1
Max Obs Per Subject	157
Observations Used	157
Observations Not Used	0
Total Observations	157

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	581.52544054	
1	2	576.87668549	0.00103196

2	1	576.71330748	0.00002413
3	1	576.70975318	0.00000001
4	1	576.70975117	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	0.7298	0.05	0.01932	1.4404
Residual	1.7000	0.05	1.2376	2.4816

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.1314	-0.06505
2	Residual	-0.06505	0.08965

Fit Statistics

-2 Res Log Likelihood	576.7
AIC (smaller is better)	580.7
AICC (smaller is better)	580.8
BIC (smaller is better)	585.5

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	4.82	0.0282

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	0.4697	0.1464	57.7	3.21	0.0022

Solution for Random Effects

Std Err

Effect	MDate	Estimate	Pred	DF	t Value	Pr > |t|
MDate	19306	0.7976	0.7705	19.4	1.04	0.3133
MDate	19307	0.2532	0.7705	19.4	0.33	0.7460
MDate	19308	0.08420	0.7705	19.4	0.11	0.9141
MDate	19310	-0.1592	0.6863	36.5	-0.23	0.8178
MDate	19311	-0.2349	0.7705	19.4	-0.30	0.7637
MDate	19313	0.6637	0.6863	36.5	0.97	0.3399
MDate	19314	0.5347	0.7705	19.4	0.69	0.4959
MDate	19315	0.1968	0.7705	19.4	0.26	0.8010
MDate	19316	0.3095	0.7705	19.4	0.40	0.6923
MDate	19317	-0.06598	0.7705	19.4	-0.09	0.9326
MDate	19318	0.3605	0.6863	36.5	0.53	0.6026
MDate	19319	-1.0985	0.7705	19.4	-1.43	0.1698
MDate	19321	-0.05983	0.5700	81.5	-0.10	0.9167
MDate	19322	0.06854	0.5700	81.5	0.12	0.9046
MDate	19323	-0.7656	0.6863	36.5	-1.12	0.2719
MDate	19324	0.5160	0.7705	19.4	0.67	0.5110
MDate	19325	0.9787	0.6208	58.2	1.58	0.1203
MDate	19326	0.5723	0.7705	19.4	0.74	0.4665
MDate	19327	-0.7043	0.7705	19.4	-0.91	0.3719
MDate	19329	-0.2025	0.6863	36.5	-0.30	0.7696
MDate	19330	-0.3902	0.6863	36.5	-0.57	0.5731
MDate	19331	-0.2537	0.7705	19.4	-0.33	0.7455
MDate	19333	0.4760	0.6863	36.5	0.69	0.4923
MDate	19335	-0.5353	0.7705	19.4	-0.69	0.4954
MDate	19336	-0.2376	0.5700	81.5	-0.42	0.6779
MDate	19337	0.3095	0.7705	19.4	0.40	0.6923
MDate	19338	-0.7043	0.7705	19.4	-0.91	0.3719
MDate	19339	-1.1360	0.7705	19.4	-1.47	0.1564
MDate	19341	0.6637	0.6863	36.5	0.97	0.3399
MDate	19342	0.005344	0.6208	58.2	0.01	0.9932
MDate	19343	0.04665	0.7705	19.4	0.06	0.9523
MDate	19344	0.04053	0.6208	58.2	0.07	0.9482
MDate	19345	0.06543	0.7705	19.4	0.08	0.9332
MDate	19347	-0.4913	0.6863	36.5	-0.72	0.4786
MDate	19348	0.4182	0.6863	36.5	0.61	0.5460
MDate	19349	0.2907	0.7705	19.4	0.38	0.7100

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19350	0.02904	0.5700	81.5	0.05	0.9595
MDate	19351	0.3894	0.6863	36.5	0.57	0.5739
MDate	19352	-0.4191	0.6863	36.5	-0.61	0.5452
MDate	19354	0.7911	0.6208	58.2	1.27	0.2076
MDate	19355	0.1813	0.6208	58.2	0.29	0.7713
MDate	19356	0.2282	0.6208	58.2	0.37	0.7145
MDate	19357	0.4033	0.7705	19.4	0.52	0.6066

MDate	19358	0.5337	0.6863	36.5	0.78	0.4417
MDate	19359	0.3749	0.6863	36.5	0.55	0.5882
MDate	19360	0.04665	0.7705	19.4	0.06	0.9523
MDate	19361	0.2883	0.6863	36.5	0.42	0.6769
MDate	19362	-0.4039	0.7705	19.4	-0.52	0.6061
MDate	19363	-0.2170	0.6863	36.5	-0.32	0.7537
MDate	19364	-0.7418	0.7705	19.4	-0.96	0.3475
MDate	19365	-0.7981	0.7705	19.4	-1.04	0.3130
MDate	19366	-0.5165	0.7705	19.4	-0.67	0.5105
MDate	19369	0.1781	0.7705	19.4	0.23	0.8197
MDate	19371	-0.2725	0.7705	19.4	-0.35	0.7274
MDate	19372	-2.2236	0.6863	36.5	-3.24	0.0025
MDate	19373	-1.4176	0.7705	19.4	-1.84	0.0811
MDate	19374	-0.3288	0.7705	19.4	-0.43	0.6743
MDate	19375	-0.3288	0.7705	19.4	-0.43	0.6743
MDate	19376	-0.2996	0.6208	58.2	-0.48	0.6312
MDate	19377	0.3572	0.6208	58.2	0.58	0.5672
MDate	19378	-0.2537	0.7705	19.4	-0.33	0.7455
MDate	19379	-0.6983	0.6208	58.2	-1.12	0.2652
MDate	19380	-0.2527	0.6208	58.2	-0.41	0.6855
MDate	19381	-0.4153	0.5700	81.5	-0.73	0.4683
MDate	19382	0.7358	0.6863	36.5	1.07	0.2907
MDate	19383	0.6738	0.6208	58.2	1.09	0.2822
MDate	19384	0.8052	0.5298	103	1.52	0.1316
MDate	19385	0.7647	0.6863	36.5	1.11	0.2724
MDate	19386	-0.08848	0.6208	58.2	-0.14	0.8872
MDate	19387	0.4615	0.6863	36.5	0.67	0.5055
MDate	19388	0.4409	0.7705	19.4	0.57	0.5737
MDate	19389	-0.2170	0.6863	36.5	-0.32	0.7537
MDate	19390	0.06687	0.4973	121	0.13	0.8933
MDate	19391	0.3658	0.7705	19.4	0.47	0.6403
MDate	19392	0.7911	0.6208	58.2	1.27	0.2076
MDate	19393	-0.3180	0.6863	36.5	-0.46	0.6458
MDate	19394	0.2532	0.7705	19.4	0.33	0.7460
MDate	19395	-0.2349	0.7705	19.4	-0.30	0.7637
MDate	19396	-0.08705	0.6863	36.5	-0.13	0.8998
MDate	19397	0.2156	0.7705	19.4	0.28	0.7826

---------- Analyte=Nitrate RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19398	0.2164	0.6208	58.2	0.35	0.7286
MDate	19399	0.3282	0.7705	19.4	0.43	0.6748

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	81	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19366 19369 19370 19371 19372 19373 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	81
Subjects	1
Max Obs Per Subject	142
Observations Used	142
Observations Not Used	0
Total Observations	142

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion

0	1	728.36964229	
1	3	683.02847649	0.00013228
2	1	683.00164361	0.00000050
3	1	683.00153828	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	7.0916	0.05	4.1459	10.0373
Residual	2.9350	0.05	2.1127	4.3542

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	2.2589	-0.2116
2	Residual	-0.2116	0.2884

Fit Statistics

-2 Res Log Likelihood	683.0
AIC (smaller is better)	687.0
AICC (smaller is better)	687.1
BIC (smaller is better)	691.8

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	45.37	<.0001

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	3.8597	0.3354	77.3	11.51	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	2.2211	1.4885	128	1.49	0.1381
MDate	19307	1.1601	1.4885	128	0.78	0.4372
MDate	19308	0.4529	1.4885	128	0.30	0.7614
MDate	19310	-1.1266	1.1519	107	-0.98	0.3303
MDate	19311	-0.9617	1.4885	128	-0.65	0.5194
MDate	19313	-0.7123	1.1519	107	-0.62	0.5376
MDate	19314	-3.0835	1.4885	128	-2.07	0.0403
MDate	19315	-1.6690	1.4885	128	-1.12	0.2643
MDate	19316	-1.3153	1.4885	128	-0.88	0.3785
MDate	19317	-1.6690	1.4885	128	-1.12	0.2643
MDate	19318	0.5305	1.1519	107	0.46	0.6461
MDate	19319	-3.0835	1.4885	128	-2.07	0.0403
MDate	19321	-5.0837	0.8768	100	-5.80	<.0001
MDate	19322	-3.6122	1.1519	107	-3.14	0.0022
MDate	19323	4.8804	1.1519	107	4.24	<.0001
MDate	19324	5.0502	1.4885	128	3.39	0.0009
MDate	19325	4.0518	1.1519	107	3.52	0.0006
MDate	19326	4.6966	1.4885	128	3.16	0.0020
MDate	19327	1.1601	1.4885	128	0.78	0.4372
MDate	19329	0.9448	1.1519	107	0.82	0.4139
MDate	19330	0.9448	1.1519	107	0.82	0.4139
MDate	19331	-4.0265	1.1519	107	-3.50	0.0007
MDate	19333	-0.5052	1.1519	107	-0.44	0.6619
MDate	19334	-4.8518	1.4885	128	-3.26	0.0014
MDate	19335	-0.9617	1.4885	128	-0.65	0.5194
MDate	19336	-0.9617	1.4885	128	-0.65	0.5194
MDate	19337	-0.2544	1.4885	128	-0.17	0.8645
MDate	19338	-3.4372	1.4885	128	-2.31	0.0225
MDate	19339	-3.4372	1.4885	128	-2.31	0.0225
MDate	19341	-0.2980	1.1519	107	-0.26	0.7963
MDate	19342	-1.7807	0.9822	101	-1.81	0.0728
MDate	19343	-0.6081	1.4885	128	-0.41	0.6836
MDate	19344	-0.6081	1.4885	128	-0.41	0.6836
MDate	19345	-1.3153	1.4885	128	-0.88	0.3785
MDate	19347	0.1162	1.1519	107	0.10	0.9198
MDate	19348	-0.5052	1.1519	107	-0.44	0.6619

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19349	0.8065	1.4885	128	0.54	0.5889
MDate	19350	-0.09943	0.8768	100	-0.11	0.9099
MDate	19351	-1.3337	1.1519	107	-1.16	0.2495
MDate	19352	-1.1266	1.1519	107	-0.98	0.3303
MDate	19354	-0.6081	1.4885	128	-0.41	0.6836
MDate	19355	0.5305	1.1519	107	0.46	0.6461

MDate	19356	-0.7555	0.9822	101	-0.77	0.4436
MDate	19357	0.09922	1.4885	128	0.07	0.9470
MDate	19358	-1.1266	1.1519	107	-0.98	0.3303
MDate	19359	-0.09091	1.1519	107	-0.08	0.9372
MDate	19360	-0.2544	1.4885	128	-0.17	0.8645
MDate	19361	-1.1266	1.1519	107	-0.98	0.3303
MDate	19362	-2.0226	1.4885	128	-1.36	0.1766
MDate	19363	-1.1266	1.1519	107	-0.98	0.3303
MDate	19364	-2.7299	1.4885	128	-1.83	0.0690
MDate	19366	-3.7908	1.4885	128	-2.55	0.0121
MDate	19369	-1.3153	1.4885	128	-0.88	0.3785
MDate	19370	-5.2054	1.4885	128	-3.50	0.0006
MDate	19371	-2.3666	0.9822	101	-2.41	0.0178
MDate	19372	-1.1949	0.9822	101	-1.22	0.2266
MDate	19373	2.5747	1.4885	128	1.73	0.0861
MDate	19375	2.5747	1.4885	128	1.73	0.0861
MDate	19376	2.4667	0.9822	101	2.51	0.0136
MDate	19377	3.2233	1.1519	107	2.80	0.0061
MDate	19378	2.9283	1.4885	128	1.97	0.0513
MDate	19379	1.5138	1.4885	128	1.02	0.3111
MDate	19380	1.5662	1.1519	107	1.36	0.1768
MDate	19381	0.3537	0.8768	100	0.40	0.6875
MDate	19382	-0.5052	1.1519	107	-0.44	0.6619
MDate	19383	1.2950	0.9822	101	1.32	0.1904
MDate	19384	4.4703	0.8037	102	5.56	<.0001
MDate	19385	4.0518	1.1519	107	3.52	0.0006
MDate	19386	2.3202	0.9822	101	2.36	0.0201
MDate	19387	2.5747	1.4885	128	1.73	0.0861
MDate	19388	1.8674	1.4885	128	1.25	0.2119
MDate	19389	2.7596	0.9822	101	2.81	0.0060
MDate	19390	-1.7986	0.8768	100	-2.05	0.0428
MDate	19392	0.4529	1.4885	128	0.30	0.7614
MDate	19393	-0.5052	1.1519	107	-0.44	0.6619
MDate	19394	-0.7123	1.1519	107	-0.62	0.5376
MDate	19395	1.5138	1.4885	128	1.02	0.3111
MDate	19396	2.3947	1.1519	107	2.08	0.0400
MDate	19397	1.8674	1.4885	128	1.25	0.2119
MDate	19398	2.3202	0.9822	101	2.36	0.0201

---------- Analyte=SolOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19399	2.9283	1.4885	128	1.97	0.0513

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	80	19306 19307 19308 19310 19311 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19335 19336 19337 19338 19339 19341 19342 19343 19344 19345 19347 19348 19349 19350 19351 19352 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19369 19371 19372 19373 19375 19376 19377 19378 19379 19380 19381 19382 19383 19384 19385 19386 19387 19388 19389 19390 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	80
Subjects	1
Max Obs Per Subject	137
Observations Used	137
Observations Not Used	0
Total Observations	137

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion

0	1	588.87330476	
1	2	575.92581417	0.00000229
2	1	575.92543964	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	1.9147	0.05	0.6491	3.1802
Residual	2.4368	0.05	1.7403	3.6565

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	0.4169	-0.1419
2	Residual	-0.1419	0.2093

Fit Statistics

-2 Res Log Likelihood	575.9
AIC (smaller is better)	579.9
AICC (smaller is better)	580.0
BIC (smaller is better)	584.7

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	12.95	0.0003

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---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.2165	0.2113	71.8	-1.02	0.3091

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19306	0.8378	1.0909	70.3	0.77	0.4451
MDate	19307	0.06775	1.0909	70.3	0.06	0.9507
MDate	19308	-0.2073	1.0909	70.3	-0.19	0.8499
MDate	19310	-1.0327	0.9136	120	-1.13	0.2606
MDate	19311	-0.9223	1.0909	70.3	-0.85	0.4007
MDate	19313	-0.05869	0.9136	120	-0.06	0.9489
MDate	19314	0.04025	1.0909	70.3	0.04	0.9707
MDate	19315	-0.4273	1.0909	70.3	-0.39	0.6965
MDate	19316	-0.2073	1.0909	70.3	-0.19	0.8499
MDate	19317	-0.3998	1.0909	70.3	-0.37	0.7151
MDate	19318	0.2469	0.9136	120	0.27	0.7875
MDate	19319	-1.8298	1.0909	70.3	-1.68	0.0979
MDate	19321	-0.5707	0.7237	134	-0.79	0.4317
MDate	19322	-0.8948	1.0909	70.3	-0.82	0.4149
MDate	19323	-1.2236	0.9136	120	-1.34	0.1830
MDate	19324	0.5353	1.0909	70.3	0.49	0.6252
MDate	19325	0.7225	0.8015	135	0.90	0.3689
MDate	19326	0.6453	1.0909	70.3	0.59	0.5561
MDate	19327	-1.3073	1.0909	70.3	-1.20	0.2348
MDate	19329	-0.4024	0.9136	120	-0.44	0.6604
MDate	19330	-0.5934	0.9136	120	-0.65	0.5172
MDate	19331	-0.1542	0.9136	120	-0.17	0.8663
MDate	19333	0.4187	0.9136	120	0.46	0.6475
MDate	19335	-1.0323	1.0909	70.3	-0.95	0.3473
MDate	19336	0.04025	1.0909	70.3	0.04	0.9707
MDate	19337	0.3977	1.0909	70.3	0.36	0.7165
MDate	19338	-1.0048	1.0909	70.3	-0.92	0.3602
MDate	19339	-1.7198	1.0909	70.3	-1.58	0.1194
MDate	19341	0.1514	0.9136	120	0.17	0.8687
MDate	19342	-0.7842	0.8015	135	-0.98	0.3296
MDate	19343	-0.3173	1.0909	70.3	-0.29	0.7720
MDate	19344	-0.3998	1.0909	70.3	-0.37	0.7151
MDate	19345	-0.2898	1.0909	70.3	-0.27	0.7913
MDate	19347	-1.1090	0.9136	120	-1.21	0.2272
MDate	19348	0.09409	0.9136	120	0.10	0.9181
MDate	19349	0.2327	1.0909	70.3	0.21	0.8317

---------- Analyte=SolOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19350	-0.3810	0.7237	134	-0.53	0.5994
MDate	19351	0.2087	0.9136	120	0.23	0.8197
MDate	19352	-0.5648	1.0909	70.3	-0.52	0.6063
MDate	19354	0.3152	1.0909	70.3	0.29	0.7734
MDate	19355	-0.3746	0.8015	135	-0.47	0.6410
MDate	19356	0.005711	0.8015	135	0.01	0.9943

MDate	19357	0.3427	1.0909	70.3	0.31	0.7543
MDate	19358	0.3233	0.9136	120	0.35	0.7241
MDate	19359	0.01770	0.9136	120	0.02	0.9846
MDate	19360	-0.3173	1.0909	70.3	-0.29	0.7720
MDate	19361	-0.4788	0.9136	120	-0.52	0.6012
MDate	19362	-1.0873	1.0909	70.3	-1.00	0.3223
MDate	19363	-1.0517	0.9136	120	-1.15	0.2519
MDate	19364	-1.5823	1.0909	70.3	-1.45	0.1514
MDate	19365	-1.7198	1.0909	70.3	-1.58	0.1194
MDate	19366	-1.3898	1.0909	70.3	-1.27	0.2069
MDate	19369	-0.4273	1.0909	70.3	-0.39	0.6965
MDate	19371	-0.8673	1.0909	70.3	-0.79	0.4293
MDate	19372	-2.1873	1.0909	70.3	-2.01	0.0488
MDate	19373	-2.2423	1.0909	70.3	-2.06	0.0436
MDate	19375	0.6453	1.0909	70.3	0.59	0.5561
MDate	19376	0.5323	0.8015	135	0.66	0.5077
MDate	19377	1.9465	0.9136	120	2.13	0.0352
MDate	19378	0.7003	1.0909	70.3	0.64	0.5230
MDate	19379	0.3977	1.0909	70.3	0.36	0.7165
MDate	19380	1.2017	0.9136	120	1.32	0.1909
MDate	19381	1.3970	0.7237	134	1.93	0.0557
MDate	19382	2.3476	0.9136	120	2.57	0.0114
MDate	19383	2.3023	0.8015	135	2.87	0.0047
MDate	19384	2.3247	0.6662	130	3.49	0.0007
MDate	19385	1.9656	0.9136	120	2.15	0.0334
MDate	19386	0.9565	0.8015	135	1.19	0.2348
MDate	19387	1.1128	1.0909	70.3	1.02	0.3112
MDate	19388	1.0303	1.0909	70.3	0.94	0.3482
MDate	19389	0.8249	0.8015	135	1.03	0.3052
MDate	19390	0.3302	0.7237	134	0.46	0.6490
MDate	19392	1.2228	1.0909	70.3	1.12	0.2662
MDate	19393	0.3996	0.9136	120	0.44	0.6626
MDate	19394	-0.4597	0.9136	120	-0.50	0.6158
MDate	19395	0.3427	1.0909	70.3	0.31	0.7543
MDate	19396	0.8580	0.9136	120	0.94	0.3496
MDate	19397	1.0303	1.0909	70.3	0.94	0.3482
MDate	19398	1.3661	0.8015	135	1.70	0.0906
MDate	19399	1.1403	1.0909	70.3	1.05	0.2995

---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	21	19281 19290 19318 19322 19331 19333 19336 19340 19341 19350 19351 19352 19370 19371 19372 19380 19381 19384 19386 19390 19398

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	21
Subjects	1
Max Obs Per Subject	91
Observations Used	91
Observations Not Used	0
Total Observations	91

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	484.89577517	
1	2	461.14220600	0.00025960
2	1	461.10107368	0.00000359
3	1	461.10053755	0.00000000

Convergence criteria met.

---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	6.3409	0.05	1.3235	11.3584
Residual	6.5042	0.05	4.7850	9.3556

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	6.5534	-0.3428
2	Residual	-0.3428	1.2203

Fit Statistics

-2 Res Log Likelihood	461.1
AIC (smaller is better)	465.1
AICC (smaller is better)	465.2
BIC (smaller is better)	467.2

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	23.80	<.0001

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.2413	0.6137	19.3	-0.39	0.6985

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19281	-0.6038	1.2712	68.6	-0.48	0.6363
MDate	19290	-1.9967	1.2712	68.6	-1.57	0.1209
MDate	19318	-2.7926	1.2712	68.6	-2.20	0.0314
MDate	19322	-0.00691	1.2712	68.6	-0.01	0.9957
MDate	19331	3.7736	1.2712	68.6	2.97	0.0041

---------- Analyte=TOC RefValue=1 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19333	1.5849	1.2712	68.6	1.25	0.2167
MDate	19336	-0.4049	1.2712	68.6	-0.32	0.7511
MDate	19340	0.3910	1.2712	68.6	0.31	0.7593
MDate	19341	-0.2059	1.2712	68.6	-0.16	0.8718
MDate	19350	-1.3997	1.2712	68.6	-1.10	0.2747
MDate	19351	-1.0018	1.2712	68.6	-0.79	0.4334
MDate	19352	1.9828	1.2712	68.6	1.56	0.1234
MDate	19370	-2.1956	1.2712	68.6	-1.73	0.0886
MDate	19371	-2.3946	1.2712	68.6	-1.88	0.0638
MDate	19372	-2.5560	1.0235	65.1	-2.50	0.0151
MDate	19380	4.3705	1.2712	68.6	3.44	0.0010
MDate	19381	-2.1956	1.2712	68.6	-1.73	0.0886

MDate	19384	0.3910	1.2712	68.6	0.31	0.7593
MDate	19386	0.5900	1.2712	68.6	0.46	0.6440
MDate	19390	-0.2293	1.0235	65.1	-0.22	0.8234
MDate	19398	4.8994	1.3944	65.8	3.51	0.0008

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---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	21	19281 19290 19318 19322 19331 19333 19336 19340 19341 19350 19351 19352 19370 19371 19372 19380 19381 19384 19386 19390 19398

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	21
Subjects	1
Max Obs Per Subject	86
Observations Used	86
Observations Not Used	0
Total Observations	86

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	342.39709134	
1	2	266.04482118	0.00022572
2	1	266.03188650	0.00000108
3	1	266.03182726	0.00000000

Convergence criteria met.

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---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	3.0349	0.05	0.9865	5.0832
Residual	0.6316	0.05	0.4592	0.9236

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	1.0922	-0.00697
2	Residual	-0.00697	0.01248

Fit Statistics

-2 Res Log Likelihood	266.0
AIC (smaller is better)	270.0
AICC (smaller is better)	270.2
BIC (smaller is better)	272.1

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	76.37	<.0001

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.1375	0.3912	18.9	-0.35	0.7290

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19281	-3.2041	0.6470	68.6	-4.95	<.0001
MDate	19290	-3.4868	0.8054	75.6	-4.33	<.0001
MDate	19318	-0.6297	0.5390	52.5	-1.17	0.2479
MDate	19322	-0.6653	0.5390	52.5	-1.23	0.2225
MDate	19331	0.7605	0.5390	52.5	1.41	0.1641

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---------- Analyte=TOC RefValue=20 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19333	1.5209	0.5390	52.5	2.82	0.0067
MDate	19336	0.4159	0.5390	52.5	0.77	0.4438
MDate	19340	-0.6297	0.5390	52.5	-1.17	0.2479
MDate	19341	-0.4158	0.5390	52.5	-0.77	0.4439
MDate	19350	0.1426	0.5390	52.5	0.26	0.7923
MDate	19351	-0.2614	0.5390	52.5	-0.48	0.6297
MDate	19352	-1.2357	0.5390	52.5	-2.29	0.0259
MDate	19370	1.0932	0.5390	52.5	2.03	0.0476
MDate	19371	2.6140	0.5390	52.5	4.85	<.0001
MDate	19372	3.2897	0.4824	39.7	6.82	<.0001
MDate	19380	-0.4158	0.5390	52.5	-0.77	0.4439
MDate	19381	1.4972	0.5390	52.5	2.78	0.0076
MDate	19384	-0.1307	0.5390	52.5	-0.24	0.8094
MDate	19386	-2.3050	0.5390	52.5	-4.28	<.0001
MDate	19390	1.2854	0.4722	37.3	2.72	0.0098
MDate	19398	0.7605	0.5390	52.5	1.41	0.1641

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---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	89	19298 19300 19302 19304 19305 19306 19307 19310 19311 19312 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19340

19341 19342 19343 19344 19347
19348 19350 19351 19352 19354
19355 19356 19357 19358 19359
19360 19361 19362 19363 19364
19365 19366 19367 19368 19369
19370 19371 19372 19373 19374
19375 19377 19378 19379 19380
19381 19382 19383 19384 19385
19386 19387 19388 19389 19390
19391 19392 19393 19394 19395
19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	89
Subjects	1
Max Obs Per Subject	139
Observations Used	139
Observations Not Used	0
Total Observations	139

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	808.33464356	
1	2	730.92958405	0.00204489
2	1	730.38112210	0.00009731
3	1	730.35716408	0.00000026
4	1	730.35710310	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	16.9584	0.05	11.3561	22.5608
Residual	2.5001	0.05	1.7538	3.8517

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	8.1704	-0.1766

2	Residual	-0.1766	0.2469

Fit Statistics

-2 Res Log Likelihood	730.4
AIC (smaller is better)	734.4
AICC (smaller is better)	734.4
BIC (smaller is better)	739.3

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	77.98	<.0001

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	4.1162	0.4606	88.4	8.94	<.0001

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19298	-1.4086	1.5416	79.6	-0.91	0.3637
MDate	19300	1.6418	1.5416	79.6	1.06	0.2901
MDate	19302	-0.1013	1.5416	79.6	-0.07	0.9478
MDate	19304	-3.1516	1.5416	79.6	-2.04	0.0442
MDate	19305	-1.8443	1.5416	79.6	-1.20	0.2351
MDate	19306	-2.2801	1.5416	79.6	-1.48	0.1431
MDate	19307	-1.8443	1.5416	79.6	-1.20	0.2351
MDate	19310	0.7702	1.5416	79.6	0.50	0.6187
MDate	19311	0.7702	1.5416	79.6	0.50	0.6187
MDate	19312	-0.1013	1.5416	79.6	-0.07	0.9478
MDate	19313	0.3574	1.1660	79.9	0.31	0.7600
MDate	19314	0.7702	1.5416	79.6	0.50	0.6187
MDate	19315	0.3345	1.5416	79.6	0.22	0.8288
MDate	19316	-0.9728	1.5416	79.6	-0.63	0.5298
MDate	19317	-0.9728	1.5416	79.6	-0.63	0.5298
MDate	19318	-0.1082	1.1660	79.9	-0.09	0.9263
MDate	19319	0.3345	1.5416	79.6	0.22	0.8288
MDate	19321	0.8424	0.9963	85.6	0.85	0.4002
MDate	19322	0.3345	1.5416	79.6	0.22	0.8288

MDate	19323	0.3574	1.1660	79.9	0.31	0.7600
MDate	19324	0.7702	1.5416	79.6	0.50	0.6187
MDate	19325	0.5247	0.9963	85.6	0.53	0.5998
MDate	19326	-0.5370	1.5416	79.6	-0.35	0.7285
MDate	19327	0.3345	1.5416	79.6	0.22	0.8288
MDate	19329	1.9873	1.1660	79.9	1.70	0.0922
MDate	19330	2.4530	1.1660	79.9	2.10	0.0386
MDate	19331	0.3345	1.5416	79.6	0.22	0.8288
MDate	19333	1.9873	1.1660	79.9	1.70	0.0922
MDate	19334	2.0775	1.5416	79.6	1.35	0.1816
MDate	19335	-0.1013	1.5416	79.6	-0.07	0.9478
MDate	19336	-0.5370	1.5416	79.6	-0.35	0.7285
MDate	19337	2.5133	1.5416	79.6	1.63	0.1070
MDate	19338	-0.5370	1.5416	79.6	-0.35	0.7285
MDate	19339	0.5903	1.1660	79.9	0.51	0.6141
MDate	19340	-0.8067	1.1660	79.9	-0.69	0.4910
MDate	19341	-6.4652	0.9963	85.6	-6.49	<.0001

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19342	-5.9886	0.9963	85.6	-6.01	<.0001
MDate	19343	-4.4589	1.5416	79.6	-2.89	0.0049
MDate	19344	-4.0231	1.5416	79.6	-2.61	0.0108
MDate	19347	-1.7381	1.1660	79.9	-1.49	0.1400
MDate	19348	-2.4366	1.1660	79.9	-2.09	0.0398
MDate	19350	-3.6057	0.9963	85.6	-3.62	0.0005
MDate	19351	-8.3807	1.5416	79.6	-5.44	<.0001
MDate	19352	-7.5092	1.5416	79.6	-4.87	<.0001
MDate	19354	-3.1516	1.5416	79.6	-2.04	0.0442
MDate	19355	-2.7158	1.5416	79.6	-1.76	0.0820
MDate	19356	-2.7158	1.5416	79.6	-1.76	0.0820
MDate	19357	-2.7158	1.5416	79.6	-1.76	0.0820
MDate	19358	-3.1351	1.1660	79.9	-2.69	0.0087
MDate	19359	-2.9023	1.1660	79.9	-2.49	0.0149
MDate	19360	-2.7158	1.5416	79.6	-1.76	0.0820
MDate	19361	-4.2993	1.1660	79.9	-3.69	0.0004
MDate	19362	-3.1516	1.5416	79.6	-2.04	0.0442
MDate	19363	-4.5321	1.1660	79.9	-3.89	0.0002
MDate	19364	-4.0231	1.5416	79.6	-2.61	0.0108
MDate	19365	-4.0231	1.5416	79.6	-2.61	0.0108
MDate	19366	4.5485	1.1660	79.9	3.90	0.0002
MDate	19367	5.5636	1.5416	79.6	3.61	0.0005
MDate	19368	6.4351	1.5416	79.6	4.17	<.0001
MDate	19369	2.9186	1.1660	79.9	2.50	0.0144
MDate	19370	0.3345	1.5416	79.6	0.22	0.8288
MDate	19371	3.2253	0.9963	85.6	3.24	0.0017
MDate	19372	5.1924	0.8963	92.3	5.79	<.0001
MDate	19373	8.6139	1.5416	79.6	5.59	<.0001

MDate	19374	8.1781	1.5416	79.6	5.30	<.0001
MDate	19375	8.7396	1.1660	79.9	7.50	<.0001
MDate	19377	8.0411	1.1660	79.9	6.90	<.0001
MDate	19378	8.6139	1.5416	79.6	5.59	<.0001
MDate	19379	7.3066	1.5416	79.6	4.74	<.0001
MDate	19380	10.1366	1.1660	79.9	8.69	<.0001
MDate	19381	8.1781	1.5416	79.6	5.30	<.0001
MDate	19382	9.2052	1.1660	79.9	7.89	<.0001
MDate	19383	-1.0396	1.1660	79.9	-0.89	0.3753
MDate	19384	-3.8040	0.8295	99.1	-4.59	<.0001
MDate	19385	-3.1516	1.5416	79.6	-2.04	0.0442
MDate	19386	-3.4468	0.9963	85.6	-3.46	0.0008
MDate	19387	-0.1013	1.5416	79.6	-0.07	0.9478
MDate	19388	-0.9728	1.5416	79.6	-0.63	0.5298
MDate	19389	-3.1516	1.5416	79.6	-2.04	0.0442
MDate	19390	-3.0054	0.8963	92.3	-3.35	0.0012

---------- Analyte=TotOx RefValue=2 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19391	-1.4086	1.5416	79.6	-0.91	0.3637
MDate	19392	-0.9728	1.5416	79.6	-0.63	0.5298
MDate	19393	-0.5739	1.1660	79.9	-0.49	0.6239
MDate	19394	-0.3411	1.1660	79.9	-0.29	0.7707
MDate	19395	1.6418	1.5416	79.6	1.06	0.2901
MDate	19396	0.5903	1.1660	79.9	0.51	0.6141
MDate	19397	-2.7158	1.5416	79.6	-1.76	0.0820
MDate	19398	-2.3348	0.9963	85.6	-2.34	0.0214
MDate	19399	-0.5370	1.5416	79.6	-0.35	0.7285

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Model Information

Data Set	WORK.TOMSORT
Dependent Variable	PctDiff
Covariance Structure	Variance Components
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Prasad-Rao-Jeske-Kackar-Harville
Degrees of Freedom Method	Kenward-Roger

Class Level Information

Class	Levels	Values
MDate	83	19298 19300 19302 19304 19305 19306 19307 19310 19311 19312 19313 19314 19315 19316 19317 19318 19319 19321 19322 19323 19324 19325 19326 19327 19329 19330 19331 19333 19334 19335 19336 19337 19338 19339 19340 19341 19342 19343 19344 19347 19348 19350 19354 19355 19356 19357 19358 19359 19360 19361 19362 19363 19364 19365 19366 19367 19368 19369 19370 19371 19372 19373 19374 19375 19377 19379 19380 19383 19384 19385 19386 19387 19389 19390 19391 19392 19393 19394 19395 19396 19397 19398 19399

Dimensions

Covariance Parameters	2
Columns in X	1
Columns in Z	83
Subjects	1
Max Obs Per Subject	130
Observations Used	130
Observations Not Used	0
Total Observations	130

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	624.26262434	
1	2	594.98459651	0.00000126
2	1	594.98436971	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Estimate	Alpha	Lower	Upper
MDate	4.6863	0.05	2.6092	6.7635
Residual	2.4473	0.05	1.7066	3.8038

Asymptotic Covariance Matrix of Estimates

Row	Cov Parm	CovP1	CovP2
1	MDate	1.1231	-0.1677
2	Residual	-0.1677	0.2454

Fit Statistics

-2 Res Log Likelihood	595.0
AIC (smaller is better)	599.0
AICC (smaller is better)	599.1
BIC (smaller is better)	603.8

Null Model Likelihood Ratio Test

DF	Chi-Square	Pr > ChiSq
1	29.28	<.0001

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.01466	0.2801	81.8	-0.05	0.9584

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19298	-0.4831	1.3146	121	-0.37	0.7139
MDate	19300	-0.4420	1.3146	121	-0.34	0.7373
MDate	19302	-0.1546	1.3146	121	-0.12	0.9066
MDate	19304	-1.3453	1.3146	121	-1.02	0.3082
MDate	19305	-0.8526	1.3146	121	-0.65	0.5178
MDate	19306	-0.9347	1.3146	121	-0.71	0.4784
MDate	19307	-0.9347	1.3146	121	-0.71	0.4784
MDate	19310	-0.7705	1.3146	121	-0.59	0.5589
MDate	19311	-0.6062	1.3146	121	-0.46	0.6455
MDate	19312	-0.9347	1.3146	121	-0.71	0.4784
MDate	19313	0.4329	1.0286	96.9	0.42	0.6748
MDate	19314	1.3646	1.3146	121	1.04	0.3013

MDate	19315	-0.3188	1.3146	121	-0.24	0.8088
MDate	19316	-0.8937	1.3146	121	-0.68	0.4979
MDate	19317	1.8162	1.3146	121	1.38	0.1696
MDate	19318	-1.4256	1.0286	96.9	-1.39	0.1690
MDate	19319	-0.4420	1.3146	121	-0.34	0.7373
MDate	19321	1.2014	0.8793	88.1	1.37	0.1753
MDate	19322	1.8573	1.3146	121	1.41	0.1603
MDate	19323	-1.4752	1.0286	96.9	-1.43	0.1548
MDate	19324	0.2149	1.3146	121	0.16	0.8704
MDate	19325	-0.1650	0.8793	88.1	-0.19	0.8516
MDate	19326	0.2560	1.3146	121	0.19	0.8459
MDate	19327	-2.4539	1.3146	121	-1.87	0.0644
MDate	19329	0.1355	1.0286	96.9	0.13	0.8955
MDate	19330	2.2170	1.0286	96.9	2.16	0.0336
MDate	19331	-1.2632	1.3146	121	-0.96	0.3385
MDate	19333	1.9197	1.0286	96.9	1.87	0.0650
MDate	19334	0.2149	1.3146	121	0.16	0.8704
MDate	19335	-0.7294	1.3146	121	-0.55	0.5800
MDate	19336	-0.1135	1.3146	121	-0.09	0.9313
MDate	19337	-0.6062	1.3146	121	-0.46	0.6455
MDate	19338	0.009634	1.3146	121	0.01	0.9942
MDate	19339	-0.2114	1.0286	96.9	-0.21	0.8376
MDate	19340	-0.01315	1.0286	96.9	-0.01	0.9898
MDate	19341	-0.6263	0.8793	88.1	-0.71	0.4782

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19342	0.03023	0.8793	88.1	0.03	0.9726
MDate	19343	0.09175	1.3146	121	0.07	0.9445
MDate	19344	0.09175	1.3146	121	0.07	0.9445
MDate	19347	1.4984	1.0286	96.9	1.46	0.1484
MDate	19348	-0.7813	1.0286	96.9	-0.76	0.4494
MDate	19350	-1.2769	1.0286	96.9	-1.24	0.2175
MDate	19354	-0.03143	1.3146	121	-0.02	0.9810
MDate	19355	0.1328	1.3146	121	0.10	0.9197
MDate	19356	0.1739	1.3146	121	0.13	0.8950
MDate	19357	0.4202	1.3146	121	0.32	0.7498
MDate	19358	0.3833	1.0286	96.9	0.37	0.7102
MDate	19359	0.5816	1.0286	96.9	0.57	0.5731
MDate	19360	0.5434	1.3146	121	0.41	0.6801
MDate	19361	-0.8804	1.0286	96.9	-0.86	0.3941
MDate	19362	-1.1400	1.3146	121	-0.87	0.3876
MDate	19363	-0.8309	1.0286	96.9	-0.81	0.4212
MDate	19364	-0.7705	1.3146	121	-0.59	0.5589
MDate	19365	-0.03143	1.3146	121	-0.02	0.9810
MDate	19366	-0.1866	1.0286	96.9	-0.18	0.8564
MDate	19367	3.0480	1.3146	121	2.32	0.0221
MDate	19368	-0.3599	1.3146	121	-0.27	0.7847

MDate	19369	2.2418	1.0286	96.9	2.18	0.0317
MDate	19370	3.1711	1.3146	121	2.41	0.0174
MDate	19371	1.8047	0.8793	88.1	2.05	0.0431
MDate	19372	3.5614	0.8793	88.1	4.05	0.0001
MDate	19373	3.4175	1.3146	121	2.60	0.0105
MDate	19374	3.7038	1.0286	96.9	3.60	0.0005
MDate	19375	4.2985	1.0286	96.9	4.18	<.0001
MDate	19377	3.5817	1.3146	121	2.72	0.0074
MDate	19379	3.7460	1.3146	121	2.85	0.0051
MDate	19380	5.5623	1.0286	96.9	5.41	<.0001
MDate	19383	0.7550	1.0286	96.9	0.73	0.4647
MDate	19384	-0.08858	0.7191	84.5	-0.12	0.9022
MDate	19385	0.1328	1.3146	121	0.10	0.9197
MDate	19386	0.08347	0.8793	88.1	0.09	0.9246
MDate	19387	-1.9612	1.3146	121	-1.49	0.1383
MDate	19389	-4.0962	1.3146	121	-3.12	0.0023
MDate	19390	-2.9585	0.7850	85.1	-3.77	0.0003
MDate	19391	-3.5214	1.3146	121	-2.68	0.0084
MDate	19392	-1.6327	1.3146	121	-1.24	0.2166
MDate	19393	-1.8469	1.0286	96.9	-1.80	0.0757
MDate	19394	-2.9867	1.0286	96.9	-2.90	0.0046
MDate	19395	-3.5214	1.3146	121	-2.68	0.0084
MDate	19396	-1.2274	1.0286	96.9	-1.19	0.2357

---------- Analyte=TotOx RefValue=16 ----------

The Mixed Procedure

Solution for Random Effects

Effect	MDate	Estimate	Std Err Pred	DF	t Value	Pr > |t|
MDate	19397	-1.7559	1.3146	121	-1.34	0.1842
MDate	19398	-3.0218	0.8793	88.1	-3.44	0.0009
MDate	19399	-1.5917	1.3146	121	-1.21	0.2283

Distribution:

Name:	Location:
Sharon Marra	773-A
Connie Herman	999-W
Charles J. Coleman	773-A
Clint Gregory	773-A
Mark Barnes	773-A
Patricia Lee	703-41A
Gene Shine	703-41A
Damon R. Click	999-W
Boyd Wiedenman	773-A
Tom White	773-A
Michael Stone	999-W
David Peeler	999-W
Tommy Edwards	999-W
Alex Choi	999-W
Gene Daniel	999-W
Frank Smith	703-41A
Shawn Tester	704-27S
John Schwenker	766-H
David Best	999-W
Eric Freed	704-S
Jonathan Bricker	704-27S

Name:	Location:
Dave Sherburne	704-S
John Iaukea	704-30S
Aaron Staub	704-27S
Jeff Ray	704-S
Robert Hinds	704-S
Perry Bovan	704-27S
Terri Fellinger	704-26S
Ryan McNew	704-S
Michael J. Hart	210-S
Roger N. Mahannah	704-28S
Michael T. Feller	704-28S
Omar Cardona-Quiles	704-24S
Amanda Shafer	704-27S
Mason Clark	704-27S
Helen Pittman	704-27S
Hank Elder	704-24S
Bill Holtzscheiter	704-15S
John Windham	704-30S
Pat Vaughan	773-41A