Beaker Labs

Calculation Algorithm Validation Worksheet

Summary of Analysis Parameters

for Ag Total ICP 200.7

on Water

by EPA 200.7

This document is a worksheet used to validate algorithms that are utilized in the LIMS system to obtain final analytical results from initial values entered into the system.

Laboratory Director: _____

SOP # _____

Document Control Number: _____

Beaker Labs

Calculation Algorithm Validation Worksheet

Analytical Method Information

Printed: 01/21/2015 4:38 pm

Ag Total ICP 200.7 in Water (EPA 200.7)

Preservation: Add HNO3 to pH<2

Container: Poly HNO3 - 500mL **Amount Required:** 500mL **Hold Time:** 180 days

Analyte	MDL	Reporting Limit	Surrogate %Rec	Duplicate RPD	----Matrix Spike---- %Rec	RPD	--Blank Spike / LCS-- %Rec	RPD
Silver	0.443	10.0 ug/L		20	75-125	20	80-120	20

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the final result (R_f) in final units:

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf} \quad \text{(Equation 1)}$$

where:

- R_f = Final result in final units, rounded to number of significant figures specified on the *Analysis Matrix* dialog.
- R_i = Initial result in initial data units from the *Data Entry* dialog.
- F_{Ri} = Unit conversion factor for initial result units.
- P_f = Preparation final amount from the *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- F_{Pf} = Unit conversion factor for final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_i = Preparation initial amount from the *Bench Sheet* Dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog.
- D = Dilution factor from *Data Entry* dialog. Defaults to 1.
- F_S = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected.
- F_{Rf} = Unit conversion factor for final result units. Note ... if special report units are used, this factor is "1".

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit, respectively.

$ppm \ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm \ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm \ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
R_f =		ug/L
R_i =		ug/L
F_{Ri} =	1,000.00	
P_f =	50.00	mL
F_{Pf} =	1.00	
F_{Pi} =	1.00	
P_i =	50.00	mL
S =	1	
D =	1.00	
F_S =	1	
F_{Rf} =	1,000.00	

Use the worksheet below to validate the algorithm used to determine the Final Results.

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

R_f = [ ] = [ ] / [ ] X [ ] / [ ] X [ ] / [ ] X [ ] / [ ] X [ ] X [ ] X [ ]

Approved By _____ Date _____

Beaker Labs

Calculation Algorithm Validation Worksheet

Pre-Prep Spike Concentration

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the Spike Concentration (C_f) in final units:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf} \qquad \text{(Equation 2)}$$

where:

- C_f = Spike level in final units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog.
- C_i = Initial concentration of target analyte in the spike mix (ppm).
- V = Volume of spike mix added to the sample during preparation, as indicated on the *Bench Sheet* dialog (uL). The 1000 factor is in the equation to convert uL to mL.
- F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_i = Preparation initial amount from the *Bench Sheet* Dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog.
- F_S = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected.
- F_{Rf} = Unit conversion factor for final result units.

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit, respectively.

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		ug/L
C_i =		ppm
V =		
F_{Pi} =	1.00	
P_i =	50.00	mL
S =	1	
F_S =	1	
F_{Rf} =	1,000.00	

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

$$C_f = \square = \frac{\square}{1000} \times \square \times \frac{\square}{\square} \times \frac{1}{\square} \times \square \times \square$$

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Post-Prep Spike Concentration

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the Spike Concentration (C_f) in final units:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pf}}{P_f} \times F_{Ri} \qquad \text{(Equation 3)}$$

where:

- C_f = Spike level in initial units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog.
- C_i = Initial concentration of target analyte in the spike mix (ppm).
- V = Volume of spike mix added to the sample during preparation, as indicated on the *Bench Sheet* dialog (uL). The 1000 factor is in the equation to convert uL to mL.
- F_{Pf} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_f = Preparation initial amount from the *Bench Sheet* dialog.
- F_{Ri} = Unit conversion factor for initial (instrument) result units.

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit, respectively.

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		ug/L
C_i =		ppm
V =		
F_{Pf} =	1.00	
P_f =	50.00	mL
F_{Ri} =	1,000.00	

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pf}}{P_f} \times F_{Ri}$$

C_f = [ ] = [ ] / 1000 x [ ] x [ ] / [ ] x [ ]

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Static Spike Concentration

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the Spike Concentration (C_f) in final units:

$$C_f = C_i \times F_{Rf} \times F_S \qquad \text{(Equation 4)}$$

where:

- C_f = Spike level in final units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog.
- C_i = Initial concentration of target analyte in the spike mix (ppm).
- F_{Rf} = Unit conversion factor for final result units.
- F_s = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected.

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit, respectively.

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		ug/L
C_i =		ppm
F_{Rf} =	1,000	
F_s =		

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

$$C_f = C_i \times F_{Rf} \times F_S$$

C_f = [ ] = [ ] X [ ] X [ ]

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Spike Recovery for Pre-Prep Spiking

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the final result % R:

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100 \qquad \text{(Equation 5)}$$

where:

$\%R$ = Percent Recovery.

R_{Spike} = Final result for the spiked sample in final units, unrounded.

R_{Source} = Final result for the source sample in final units, unrounded.

C_f = Final spike level in final units.

Note ... the final result for the spiked sample and the source sample are calculated using the **Final Results** (R_f) equation (see Equation 1).

Below is a calculation worksheet to validate the algorithm % Recovery:

First, use the following equation to determine the Final Result of the spiked sample and the source sample in final concentration units.

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

R_{Spike} = [ ] = [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ] X [ ] X [ ]

R_{Source} = [ ] = [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ] X [ ] X [ ]

Then, use the equation below to calculate the spike concentration used for the Matrix Spike.

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

C_f = [ ] = [ ]/1000 X [ ] X [ ]/[ ] X 1/[ ] X [ ] X [ ]

Finally, use the values that were determined from the equations above to determine the % recovery of the Matrix Spike.

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

$\%R$ = [ ] = ([ ] - [ ])/[ ] X 100

Approved By Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Spike Recovery for Post-Prep Spiking

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the final result % R:

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100 \qquad \text{(Equation 5)}$$

where:

- $\%R$ = Percent Recovery.
- R_{Spike} = Final result for the spiked sample in final units, unrounded.
- R_{Source} = Final result for the source sample in final units, unrounded.
- C_f = Final spike level in final units.

Note ... the final result for the spiked sample and the source sample are calculated using the **Final Results** (Rf) equation (see Equation 1).

Below is a calculation worksheet to validate the algorithm % Recovery:

First, use the following equations to determine the Final Result of the spiked sample and the source sample in initial concentration units.

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times D \times F_S \times F_{Rf}$$

R_f = [ ] = [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ] X [ ] X [ ]

$$R_{Source} = R_f \times \frac{P_{ispike}}{F_{PiSpike}} \times \frac{F_{PfSpike}}{P_{fSpike}} \times \frac{F_{Ri}}{F_{Rf}}$$

R_{Source} = [ ] = [ ] X [ ]/[ ] X [ ]/[ ] X [ ]/[ ]

where:

- R_{Source} = The amount of source in the matrix spike in initial concentration units.
- P_{iSpike} = Preparation initial amount of the matrix spike from *Bench Sheet* dialog.
- $F_{PiSpike}$ = Unit conversion factor for the initial preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- $F_{PfSpike}$ = Unit conversion factor for the final preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_{fSpike} = Preparation final amount of the matrix spike from *Bench Sheet* dialog.
- F_{Ri} = Unit conversion factor for the initial concentration units of the matrix spike.
- F_{Rf} = Unit conversion factor for the final concentration units of the matrix spike.

Continued on next page ...

Beaker Labs

Calculation Algorithm Validation Worksheet

Continued from previous page ...

$$R_{Spike} = R_i \times D$$

R_{Spike} = [ ] = [ ] X [ ]

Then, use the equation below to calculate the spike concentration used for the Matrix Spike.

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pf}}{P_f} \times F_S \times F_{Ri}$$

C_f = [ ] = $\frac{[\ ]}{1000}$ X [ ] X $\frac{[\ ]}{[\ ]}$ X [ ] X [ ]

Finally, use the values that were determined from the equations above to determine the % Recovery of the Matrix Spike.

$$\%\ R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

% R = [ ] = $\frac{[\ ] - [\ ]}{[\ ]}$ X [100]

Beaker Labs

Calculation Algorithm Validation Worksheet

Spike Recovery for Static Spiking

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the final result % R:

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100 \qquad \text{(Equation 5)}$$

where:

$\%R$ = Percent Recovery.

R_{Spike} = Final result for the spiked sample in final units, unrounded.

R_{Source} = Final result for the source sample in final units, unrounded.

C_f = Final spike level in final units.

Note ... the final result for the spiked sample and the source sample are calculated using the **Final Results** (Rf) equation (see Equation 1).

Below is a calculation worksheet to validate the algorithm % Recovery:

First, use the following equations to determine the Final Result of the spiked sample and the source sample in final concentration units.

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_s \times F_{Rf}$$

$R_f =$ [ ] = [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ]/[ ] X [ ] X [ ] X [ ]

$$R_{Source} = R_f \times \frac{P_{ispike}}{F_{PiSpike}} \times \frac{F_{PfSpike}}{P_{fSpike}}$$

$R_{Source} =$ [ ] = [ ] X [ ]/[ ] X [ ]/[ ]

where:

P_{iSpike} = Preparation initial amount of the matrix spike from *Bench Sheet* dialog.

$F_{PiSpike}$ = Unit conversion factor for the initial preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the

$F_{PfSpike}$ = Unit conversion factor for the final preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

P_{fSpike} = Preparation final amount of the matrix spike from *Bench Sheet* dialog.

Continued on next page

Beaker Labs

Calculation Algorithm Validation Worksheet

Continued from previous page

$$R_{Spike} = R_i \times F_S \times F_{Rf}$$

R_{Spike} = [ ] = [ ] X [ ] X [ ]

Then, use the equation below to calculate the spike concentration used for the Matrix Spike.

$$C_f = C_i \times F_{Rf} \times F_S$$

C_f = [ ] = [ ] X [ ] X [ ]

Finally, use the values that were determined from the equations above to determine the % Recovery of the Matrix Spike.

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

$$\%R = [\ ] = \frac{[\ ] - [\ ]}{[\ ]} \text{ X } [100]$$

Beaker Labs

Calculation Algorithm Validation Worksheet

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to adjust Report Limits and Method Detection Limits for preparation variations:

$$RL_f = \frac{RL_i \times F_S \times D \times F_{Pi} \times F_{Pfd}}{PR \times S \times F_{Pf} \times F_{Pid}} \quad \text{(Equation 6)} \qquad PR = \frac{\frac{P_i}{P_f}}{\frac{P_{di}}{P_{df}}} \quad \text{(Equation 7)}$$

where:

- RL_f = Final MDL or MRL in final units, rounded to number of significant figures specified on the *Analysis Matrix* dialog.
- RL_i = Initial MDL or MRL in final data units from the *Analysis Matrix* dialog.
- F_S = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected.
- D = Dilution factor from *Data Entry* dialog. Defaults to 1.
- F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- F_{Pfd} = Unit conversion factor for default final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- PR = Preparation Ratio. Used to adjust the MDL and MRL whtn the actual preparation amounts differ from the default values upon which the normal MDL and MRL are based. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog, or if the percent PR is less than the default *Prep Ratio Threshold* specified in the *Lab Info* dialog.
- S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog.
- F_{Pf} = Unit conversion factor for final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- F_{Pid} = Unit conversion factor for default initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_i = Preparation initial amount from *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_f = Preparation final amount from *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.
- P_{di} = Default preparation initial amount from *Analysis Matrix* dialog. If no default is supplied, the actual Preparation Initial amount (P_i) is used.
- P_{df} = Default preparation final amount from *Analysis Matrix* dialog. If no default is supplied, the actual Preparation Final amount (P_f) is used.

Use the worksheet below to validate the algorithm used to determine the Final MDL or MRL:

$PR = \frac{\frac{P_i}{P_f}}{\frac{P_{di}}{P_{df}}}$ PR= [ ] / [ ]

$$RL_f = \frac{RL_i \times F_S \times D \times F_{Pi} \times F_{Pfd}}{PR \times S \times F_{Pf} \times F_{Pid}}$$

RLf = [ ] = [ ] X [ ] X [ ] X [ ] X [ ] / [ ] X [ ] X [ ] X [ ]

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate the Relative Percent Difference (RPD):

$$RPD = \left| \frac{R_1 - R_2}{R_1 + R_2} \right| \times 200 \qquad \text{(Equation 8)}$$

where:

RPD = Relative Percent Difference.

R_1 = Final concentration of the first sample, unrounded. If *Calculate RPD using %Recovery* is checked on the *Analysis Matrix* dialog, the final rounded percent recovery value is used when calculating the RPD between spiked samples.

R_2 = Final concentration of the second sample, unrounded. If *Calculate RPD using %Recovery* is checked on the *Analysis Matrix* dialog, the final rounded percent recovery value is used when calculating the RPD between spiked samples.

Use the worksheet below to validate the algorithm used to determine the RPD:

$$RPD = \left| \frac{R_1 - R_2}{R_1 + R_2} \right| \times 200$$

RPD = [ ] = | [ ] - [ ] / [ ] + [ ] | X [200]

Approved By

Date

Beaker Labs

Calculation Algorithm Validation Worksheet

Analysis: Ag Total ICP 200.7 **Matrix:** Water

The following is the equation used to calculate from Mass/Volume to Volume/Volume:

$$R_{v/v} = \frac{R_{m/v} \times F_A \times 1000}{MW} \qquad \text{(Equation 9)}$$

where:

- $R_{v/v}$ = Final result in volume/volume units, unrounded.
- $R_{m/v}$ = Final result in mass/volume units as calculated using the **Final Results** equation (Equation 1).
- F_A = Air Factor specified on the *Lab Info* dialog. Defaults to 24.11 L/Mol.
- MW = Molecular Weight of the analyte from the *Analyte* tab of the *Static Lists* dialog.

Use the worksheet below to validate the algorithm used to determine the Mass/Volume to Volume/Volume:

$$R_{v/v} = \frac{R_{m/v} \times F_A \times 1000}{MW}$$

$$R_{v/v} = \square = \frac{\square \text{ X } \square \text{ X } 1000}{\square}$$

Approved By

Date