

Synoptic CB: Porewater SO₄/Cl

July 2024 Samples

2025-09-18

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##Add Required Packages

0.1 Run Information

```
##### Run information - PLEASE CHANGE
Date_Run = "2024-08-08" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "<80% of Sulfate Check Standards are within range of expected concentration - REASSESS;
Check standards 1 and 2 are lower than the expected concentrations.
Some SWH samples had no SO4 (bdl).
Some sample IDs are missing from metadata: MSM_202407_UP_A_20CM
" #any notes from the run
samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names
samples_pattern <- paste(samples, collapse = "|")
#samples_pattern <- "GCW" #use this instead of the line above if you have only one site code

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202407_Cl.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202407_SO4.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202407.csv"

##### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"

#qaqc log file path for this year
Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv"
```

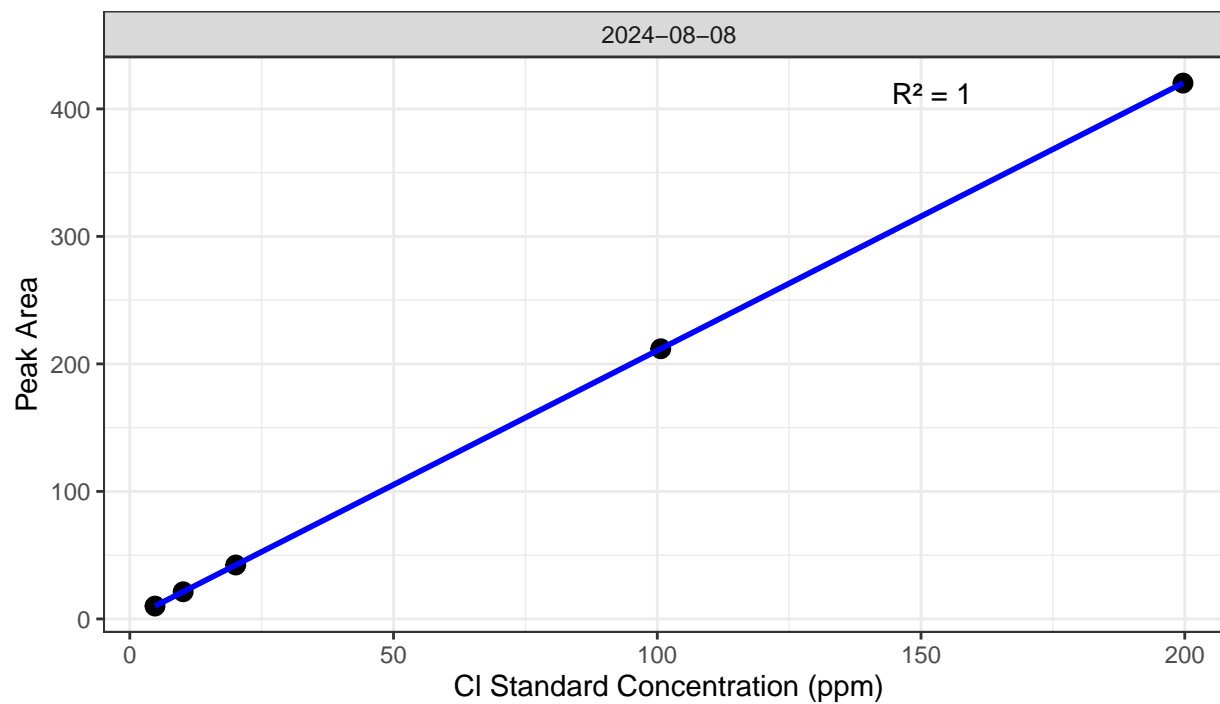
##Set Up Code - constants and QAQC cutoffs

##Read in metadata and create similar sample IDs for matching to samples

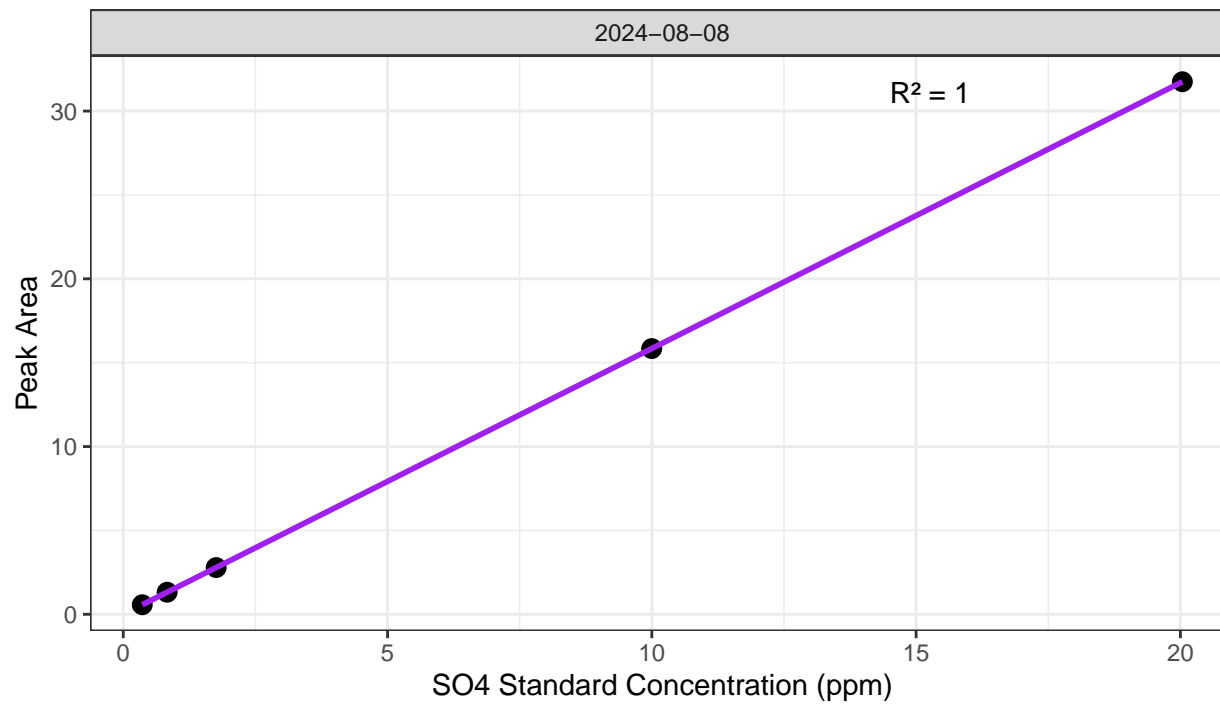
##Import Sample Data

0.2 Assess Standard Curves

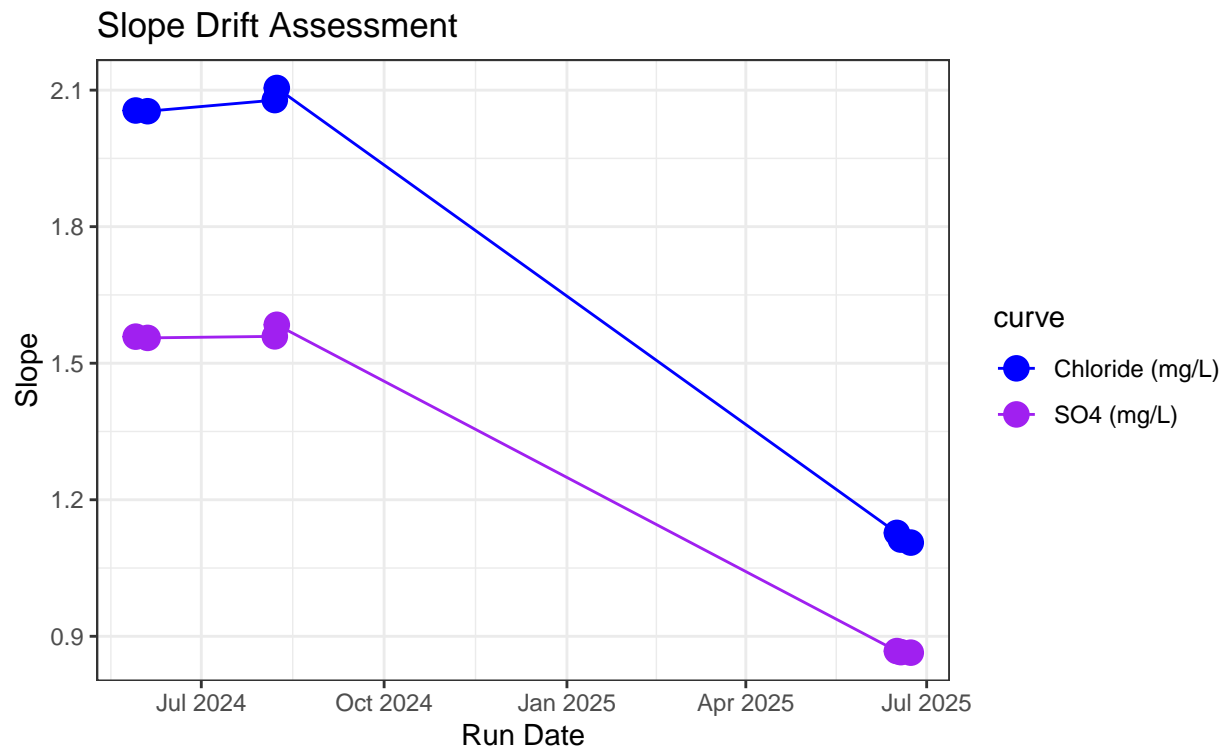
Chloride Std Curve



Sulfate Std Curve



```
## [1] "QAQC log file exists and has been read into the code."
```



```
## [1] "Cl Curve r2 GOOD"
```

```
## [1] "SO4 Curve r2 GOOD"
```

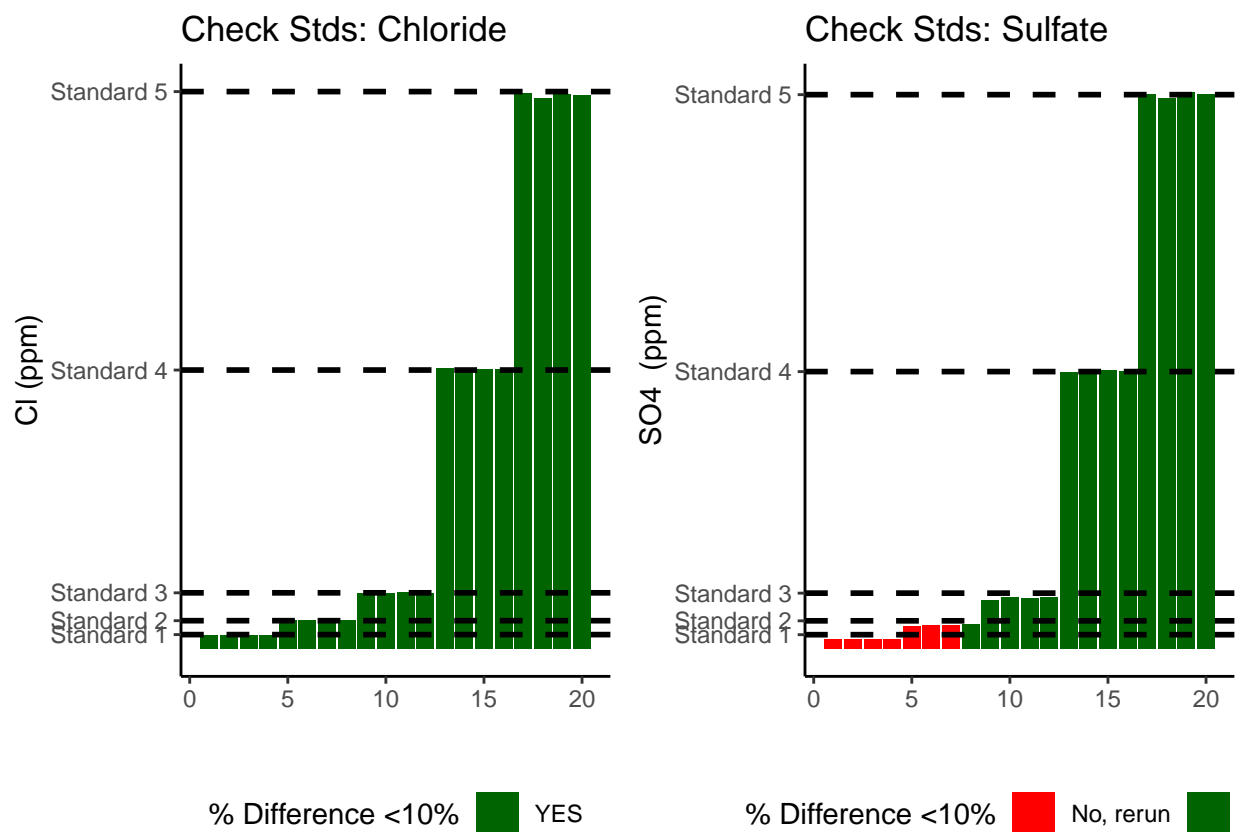
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID mean_Cl sd_Cl cv_Cl flag_Cl
##   <chr>      <dbl> <dbl> <dbl> <chr>
## 1 Standard 1 4.81 0.0324 0.00673 Chloride Check Standard RSD within Range - ~
## 2 Standard 2 10.1 0.0314 0.00309 Chloride Check Standard RSD within Range - ~
## 3 Standard 3 20.1 0.192 0.00954 Chloride Check Standard RSD within Range - ~
## 4 Standard 4 100. 0.385 0.00384 Chloride Check Standard RSD within Range - ~
## 5 Standard 5 199. 0.846 0.00426 Chloride Check Standard RSD within Range - ~
```

```
## # A tibble: 5 x 5
##   sample_ID mean_S04 sd_S04 cv_S04 flag_S04
##   <chr>      <dbl> <dbl> <dbl> <chr>
## 1 Standard 1 0.354 0.00886 0.0251 Sulfate Check Standard RSD within Range --
## 2 Standard 2 0.845 0.0166 0.0196 Sulfate Check Standard RSD within Range --
## 3 Standard 3 1.82 0.0414 0.0228 Sulfate Check Standard RSD within Range --
## 4 Standard 4 10.0 0.0390 0.00389 Sulfate Check Standard RSD within Range --
## 5 Standard 5 20.0 0.0978 0.00489 Sulfate Check Standard RSD within Range --
```

```
## [1] ">80% of Chloride Check Standards have RSD within range - PROCEED"
```

```
## [1] ">80% of Sulfate Check Standards have RSD within range - PROCEED"
```



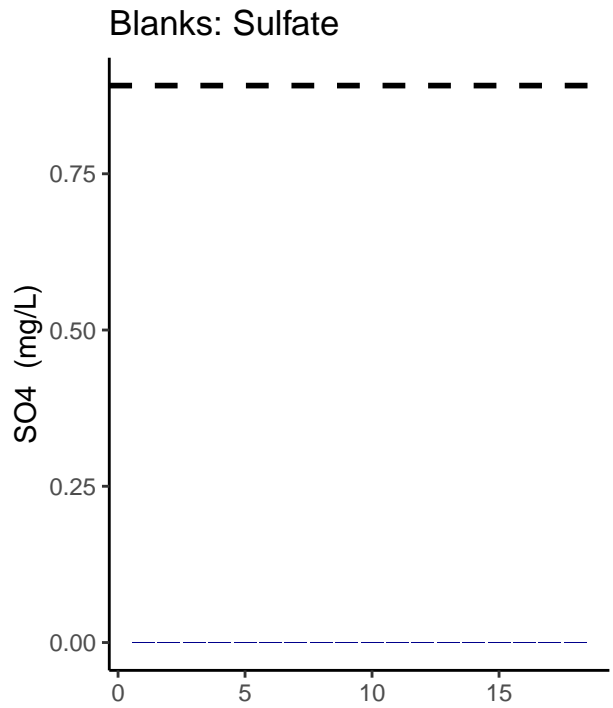
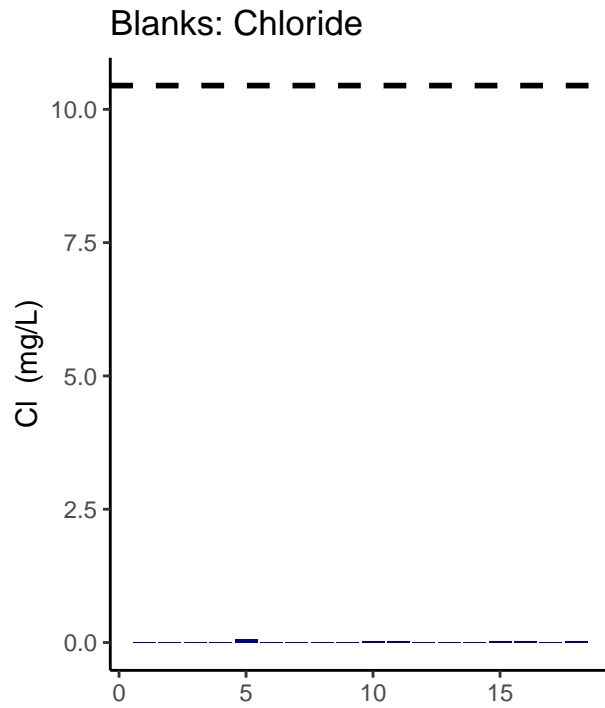
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [1] "<80% of Sulfate Check Standards are within range of expected concentration - REASSESS"
```

0.4 Assess Blanks

```
## [1] ">80% of Chloride Blank concentrations are lower 25% quartile of samples"
```

```
## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"
```



Blank Conc <25% Quartile Samples ■ Y

Blank Conc <25% Quartile Samples ■ Y

```
## Chloride blanks mean ppm:
```

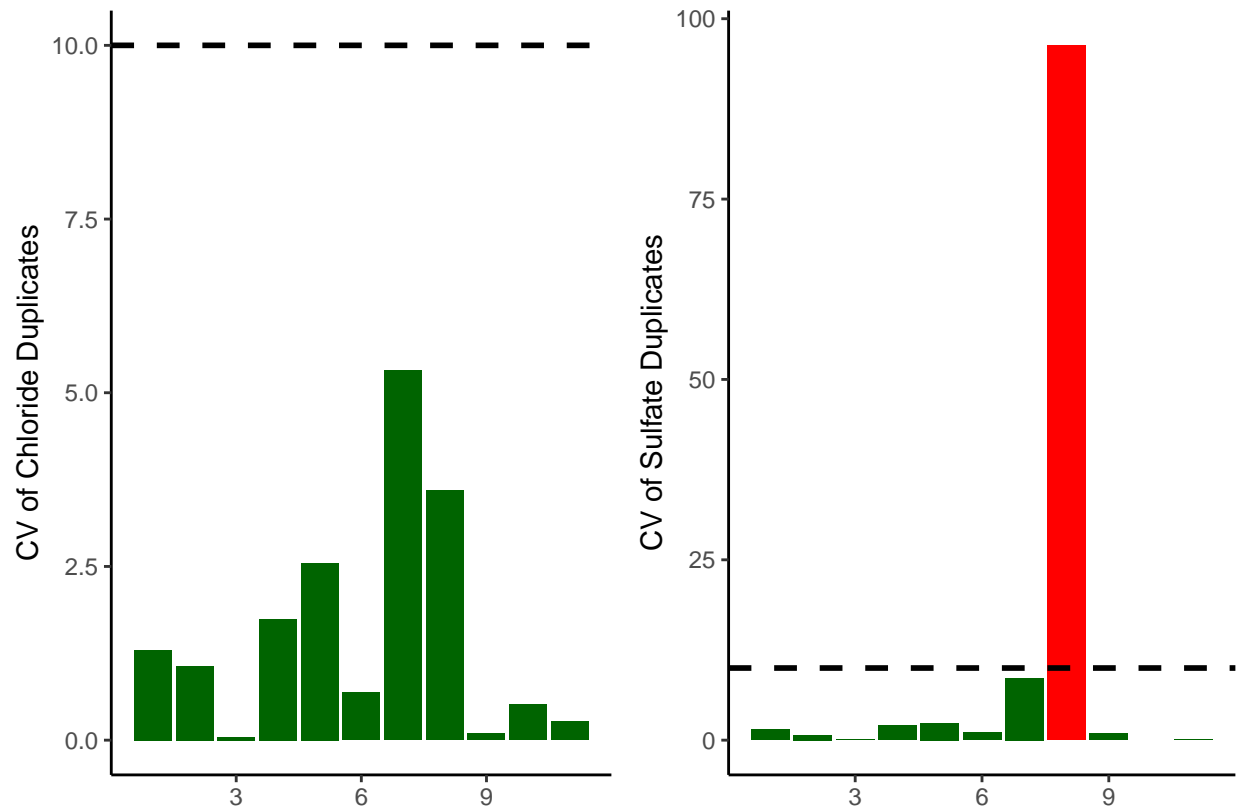
```
## [1] 0.01748333
```

```
## Sulfate blanks mean ppm:
```

```
## [1] 0
```

0.5 Assess Duplicates

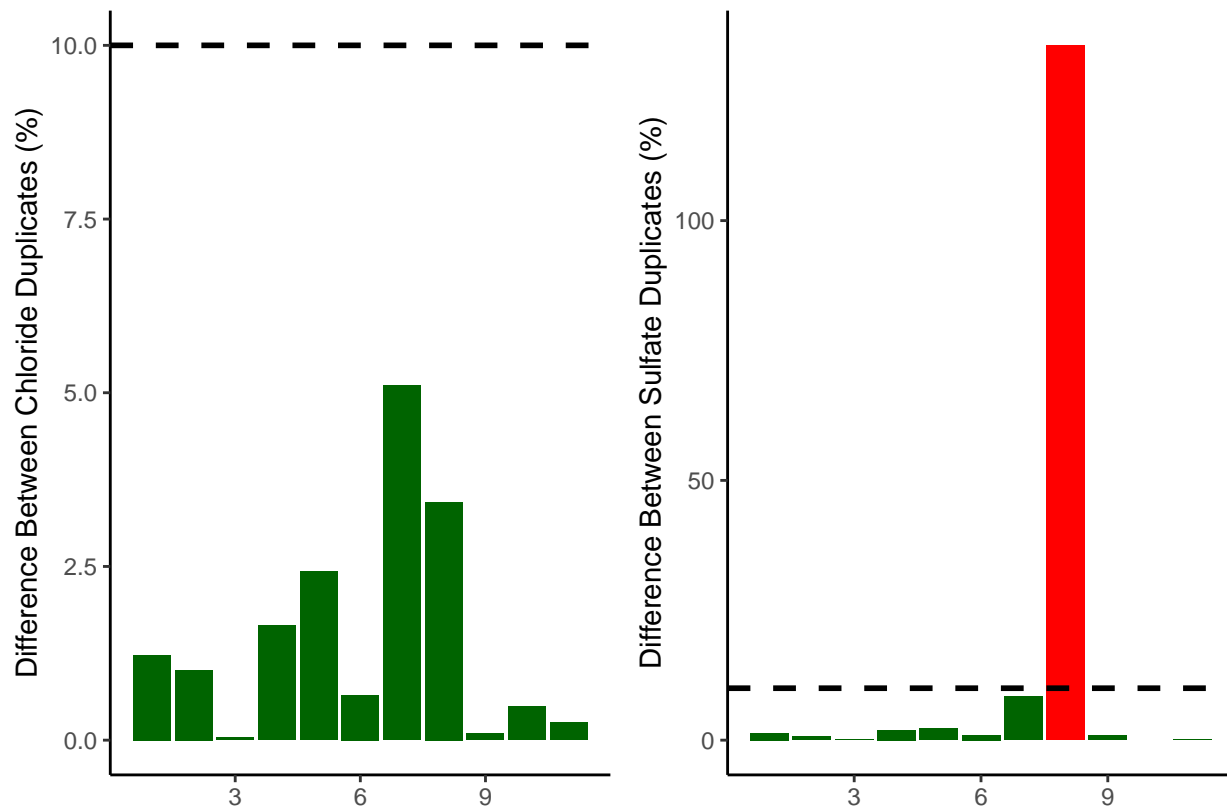
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
```



```
## [1] ">80% of Chloride Duplicates have a CV <10% - PROCEED"
```

```
## [1] ">80% of Sulfate Duplicates have a CV <10% - PROCEED"
```

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
```



```
## [1] ">80% of Chloride Duplicates have a percent difference <10% - PROCEED"
```

```
## [1] ">80% of Sulfate Duplicates have a percent difference <10% - PROCEED"
```

0.6 Calculate mmol/L concentrations & salinity, add dilutions

```
# Convert ppm to mmol/L
all_dat$S04_Conc_mM <- (all_dat$S04_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

# Calculate Salinity
# calculated using the Knudsen equation
# Salinity = 0.03 + 1.8050 * Chlorinity
# Ref: A Practical Handbook of Seawater Analysis by Strickland & Parsons (P. 11)
# = ((1.807 * Cl_ppm) + 0.026) / 1000
all_dat$salinity <- ((1.8070 * all_dat$Cl_ppm) + 0.026) / 1000

#Need to determine dilution factors for your samples
#for Steph / COMPASS this depends on the site so...
all_dat$Dilution <- 1
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "WC"),
```



```

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "SW"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "SW"),

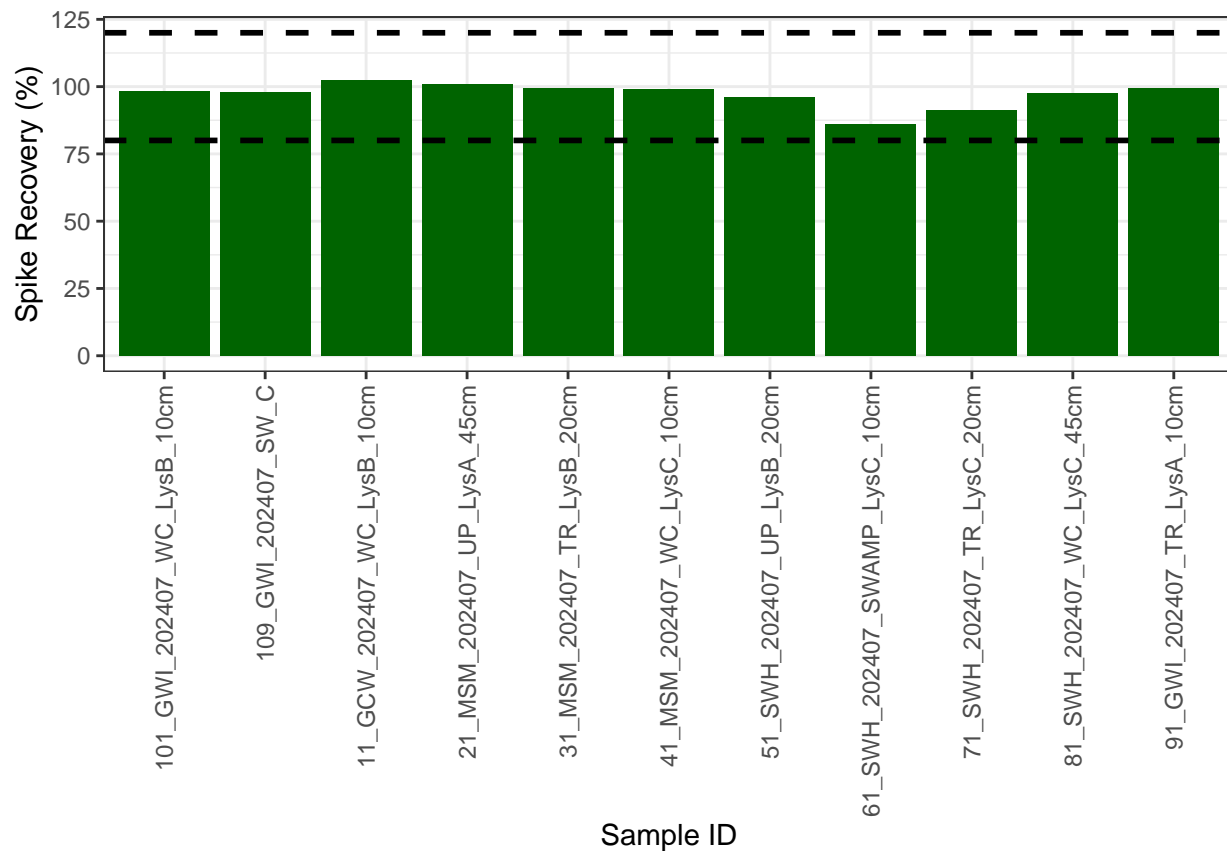
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "SW"),

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)

# head(all_dat)

```

0.7 Assess Analytical Spikes



```
## [1] ">80% of S04 spikes have a recovery between the high and low cutoff - PROCEED"
```

0.8 Check if samples within the range of the standard curve

```
## Sample Flagging
```

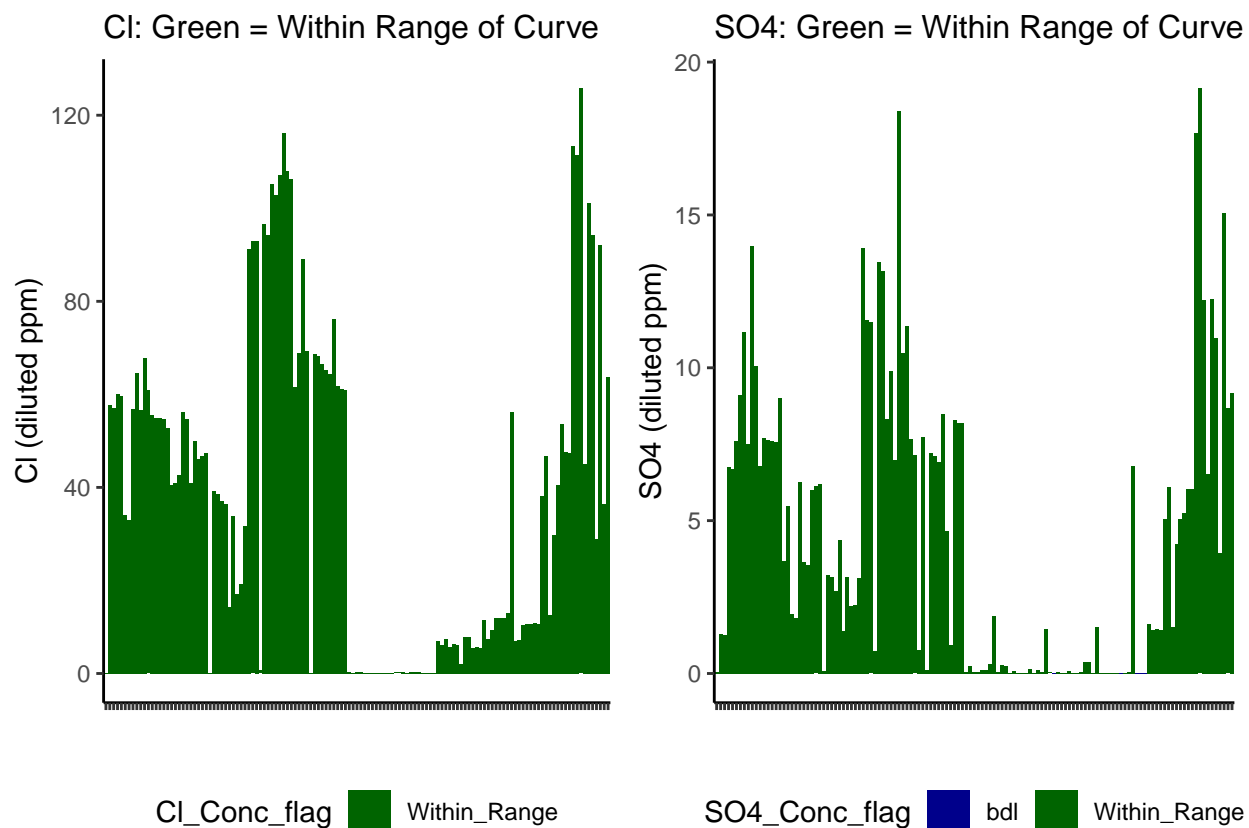


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	96.183206
bdl	3.816794

Table 2: Cl samples

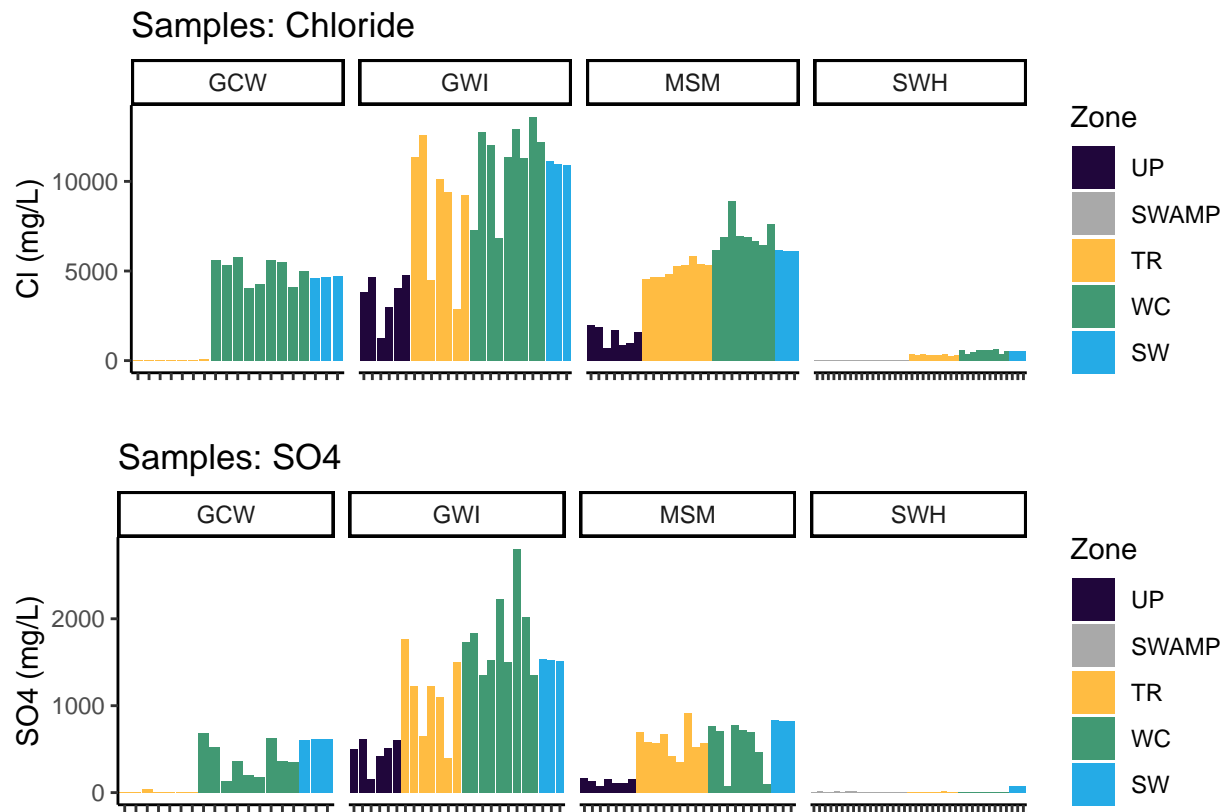
Cl_Conc_flag	Percent_samples
Within_Range	100

0.9 Check to see if samples run match metadata & merge info

```
## Some sample IDs are missing from metadata.
```

```
## [1] "MSM_202407_UP_A_20CM"
```

0.10 Visualize Data by Plot



0.11 Export Processed Data

#end