

Synoptic CB: Porewater SO₄/Cl

November 2024 Samples

2025-09-05

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##Add Required Packages

0.1 Run Information

```
##### Run information - PLEASE CHANGE
Date_Run = "2025-06-23" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "Some sample IDs are missing from metadata: GCW_202411_TR_LYSC_45CM, MSM_202411_WC_LYSC_1
One Cl chk std and several S04 chk stds are lower than the expected concentration;
One S04 dup had high CV;
3 samples had S04 adl" #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_202411_Cl.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202411_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_S04_202411.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_S04_QAQClog_2024.csv"
```

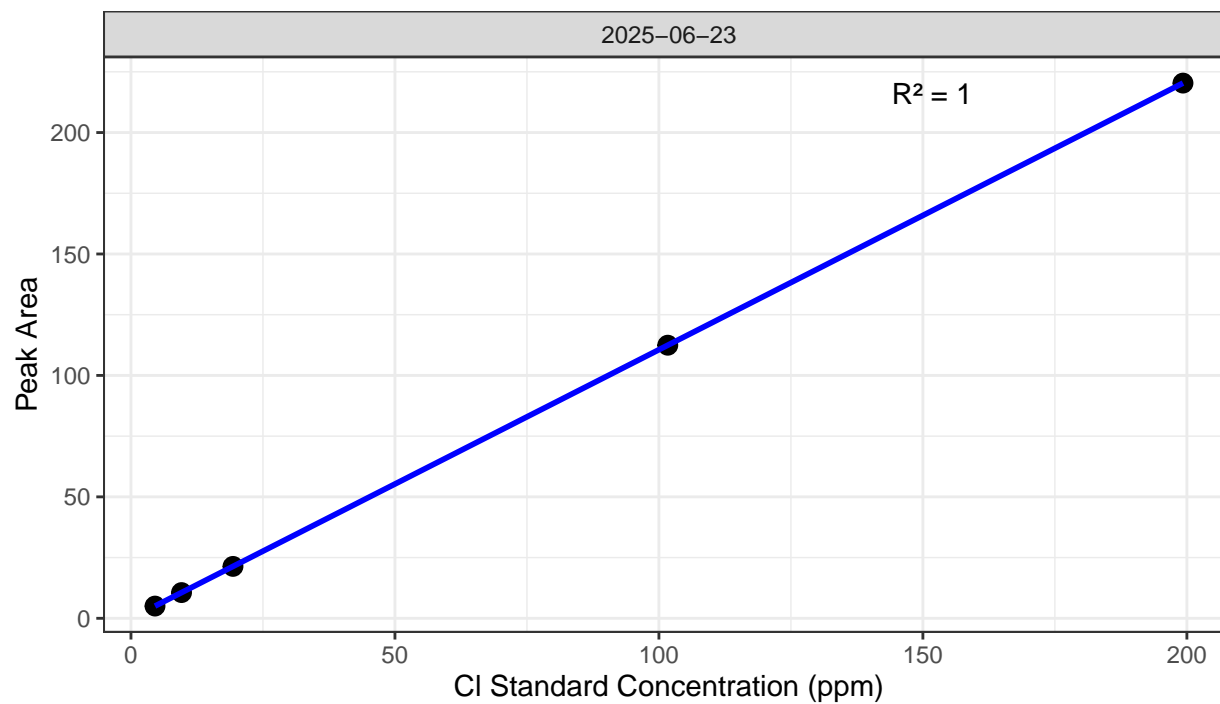
##Set Up Code - constants and QAQC cutoffs

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

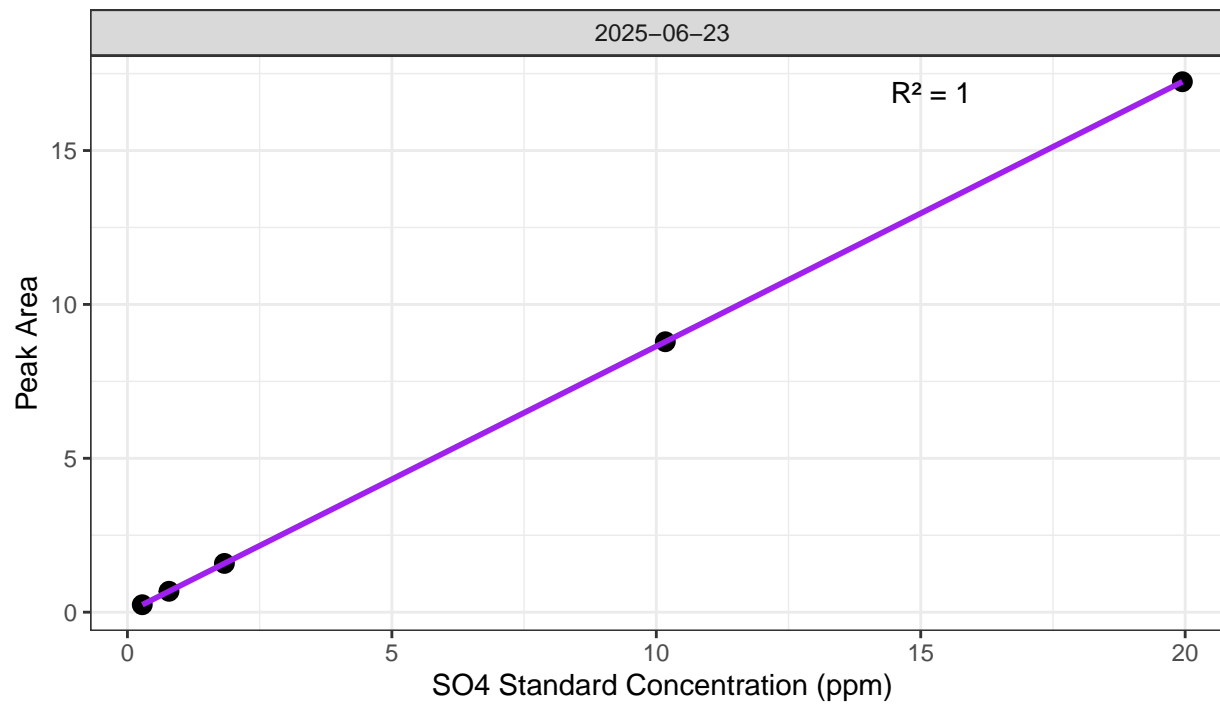
##Import Sample Data

0.2 Assess Standard Curves

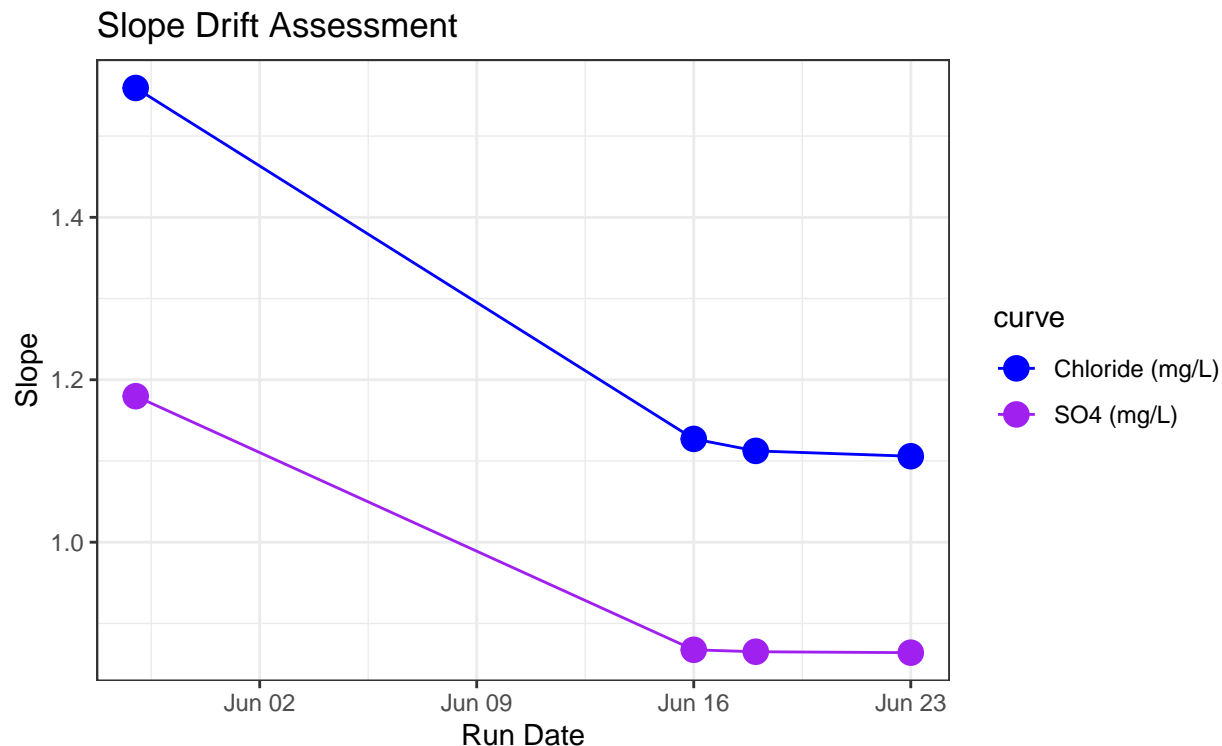
Chloride Std Curve



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"
```

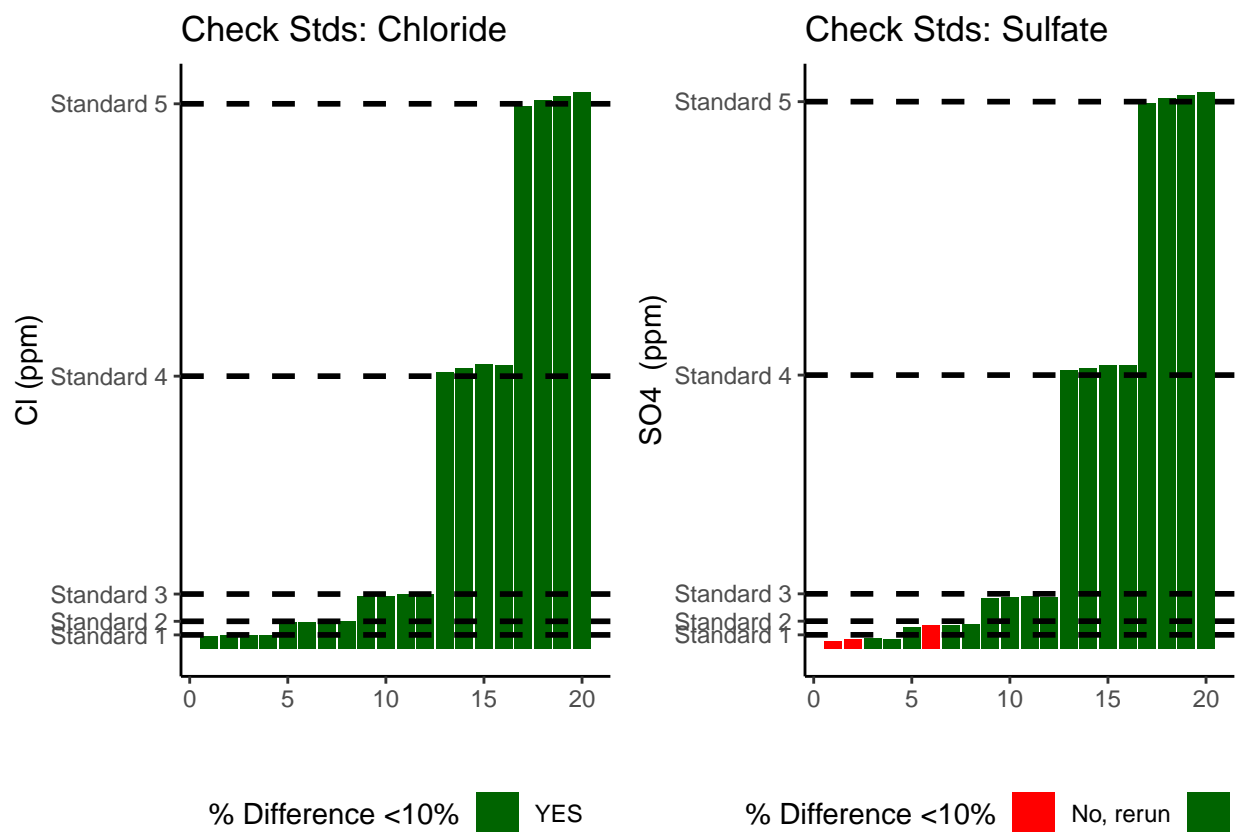
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID mean_Cl sd_Cl  cv_Cl flag_Cl
##   <chr>      <dbl> <dbl>  <dbl> <chr>
## 1 Standard 1    4.77 0.150 0.0314 Chloride Check Standard RSD within Range - PR~
## 2 Standard 2    9.84 0.187 0.0190 Chloride Check Standard RSD within Range - PR~
## 3 Standard 3   19.7 0.351 0.0178 Chloride Check Standard RSD within Range - PR~
## 4 Standard 4  103.  1.24 0.0120 Chloride Check Standard RSD within Range - PR~
## 5 Standard 5  202.  2.22 0.0110 Chloride Check Standard RSD within Range - PR~
```

```
## # A tibble: 5 x 5
##   sample_ID mean_S04 sd_S04  cv_S04 flag_S04
##   <chr>      <dbl> <dbl>  <dbl> <chr>
## 1 Standard 1    0.344 0.0428 0.124  Sulfate Check Standard RSD within Range - ~
## 2 Standard 2    0.851 0.0447 0.0525 Sulfate Check Standard RSD within Range - ~
## 3 Standard 3    1.88 0.0346 0.0184 Sulfate Check Standard RSD within Range - ~
## 4 Standard 4   10.3 0.0955 0.00927 Sulfate Check Standard RSD within Range - ~
## 5 Standard 5   20.2 0.179 0.00889 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"
```



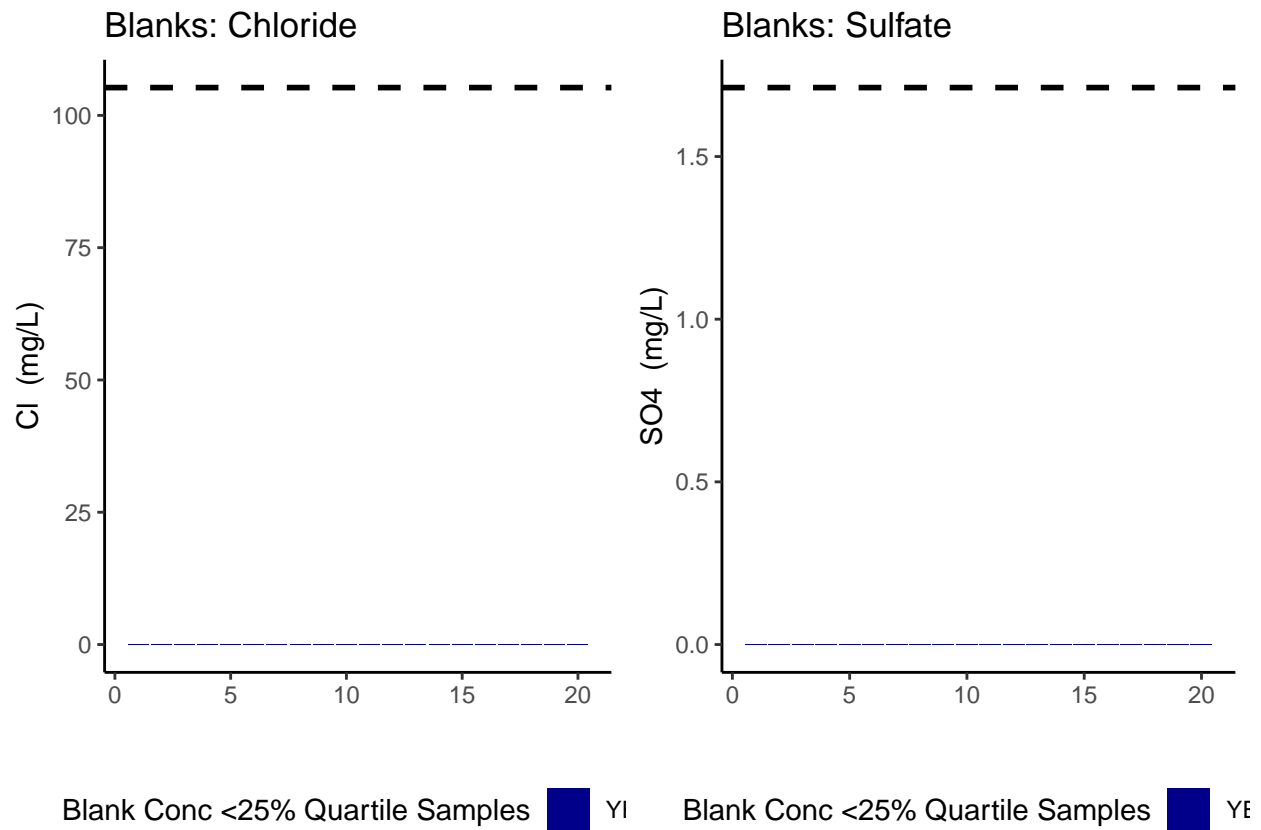
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

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

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"
```



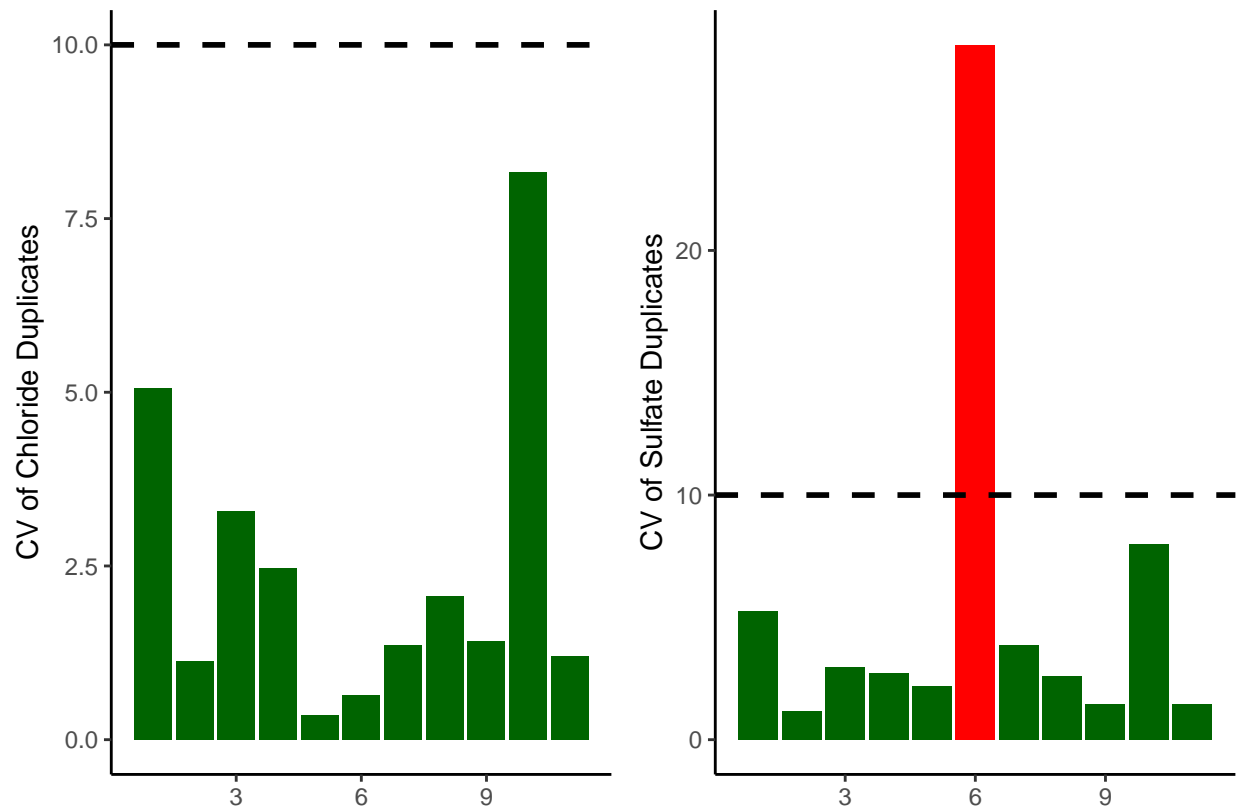
```
## Chloride blanks mean ppm:
```

```
## [1] 0.004165
```

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

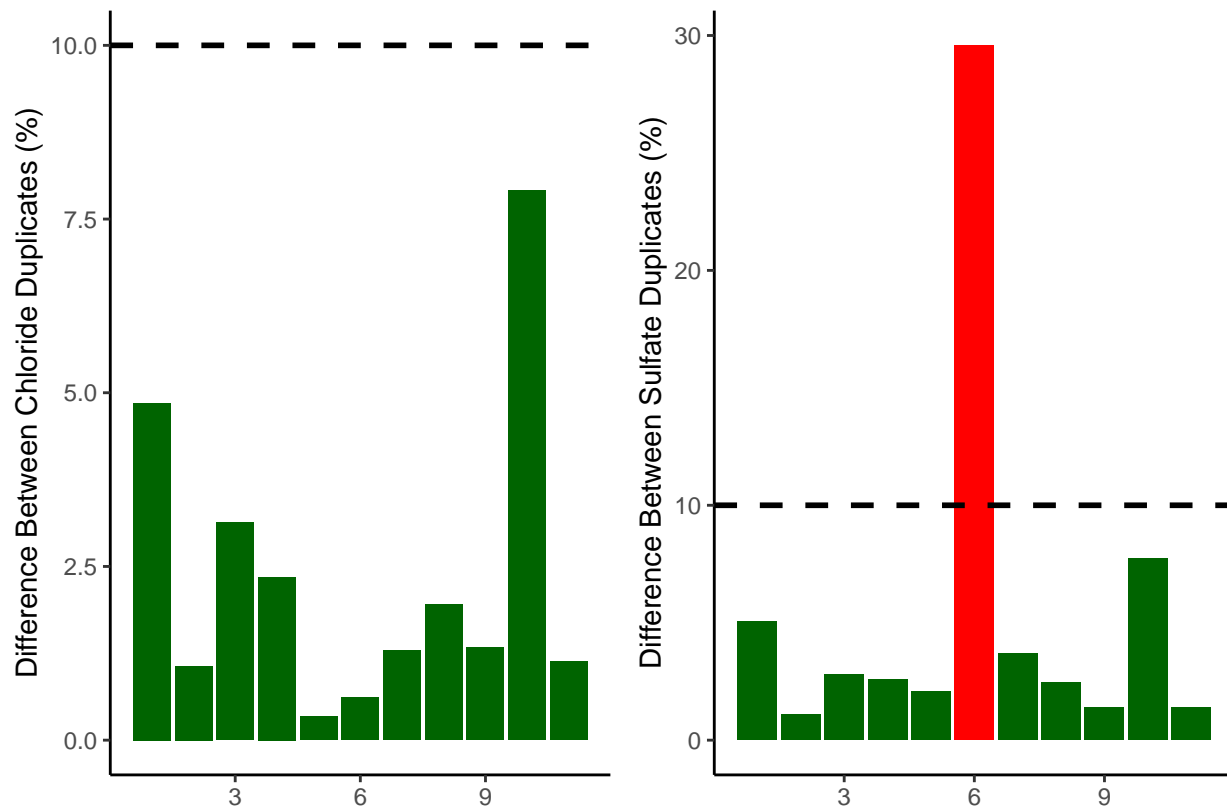
```
## [1] 0
```

0.5 Assess Duplicates



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

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



```
## [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$SO4_Conc_mM <- (all_dat$SO4_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"),

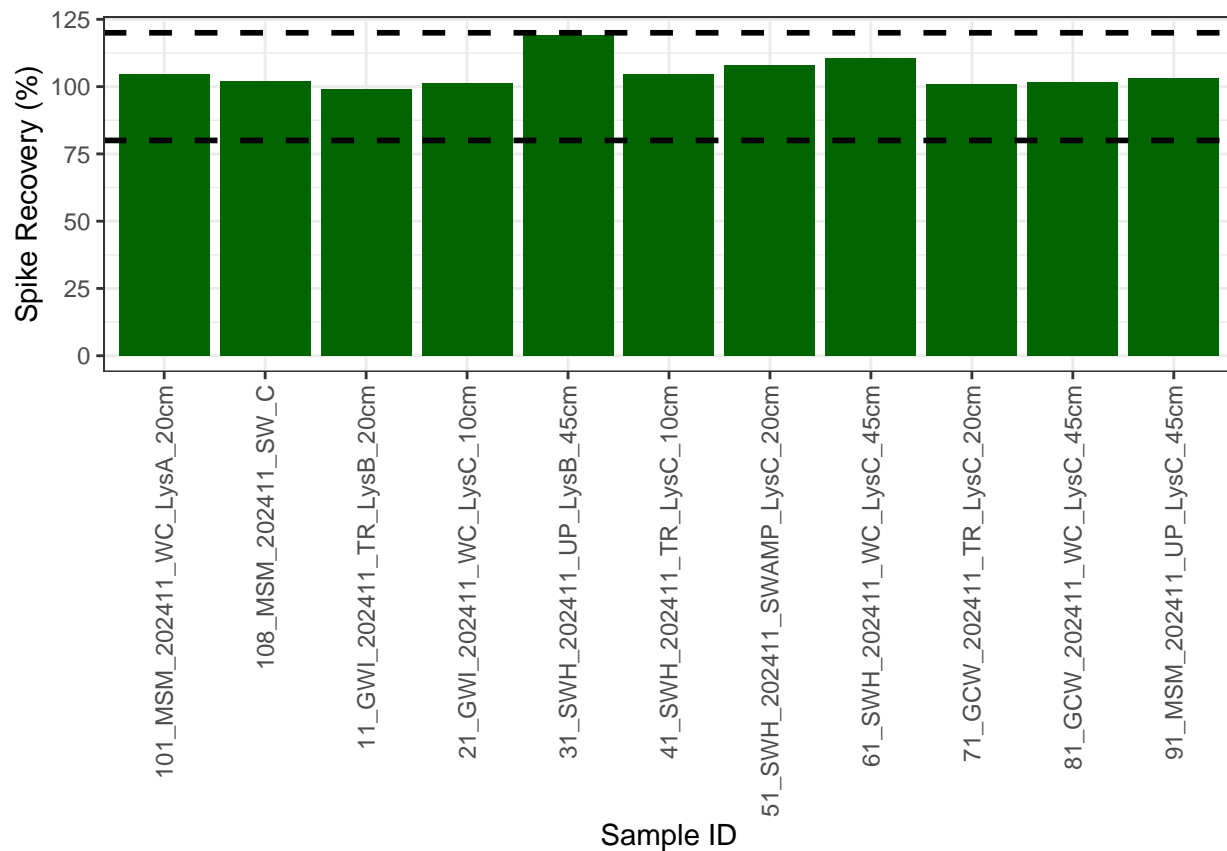
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID,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

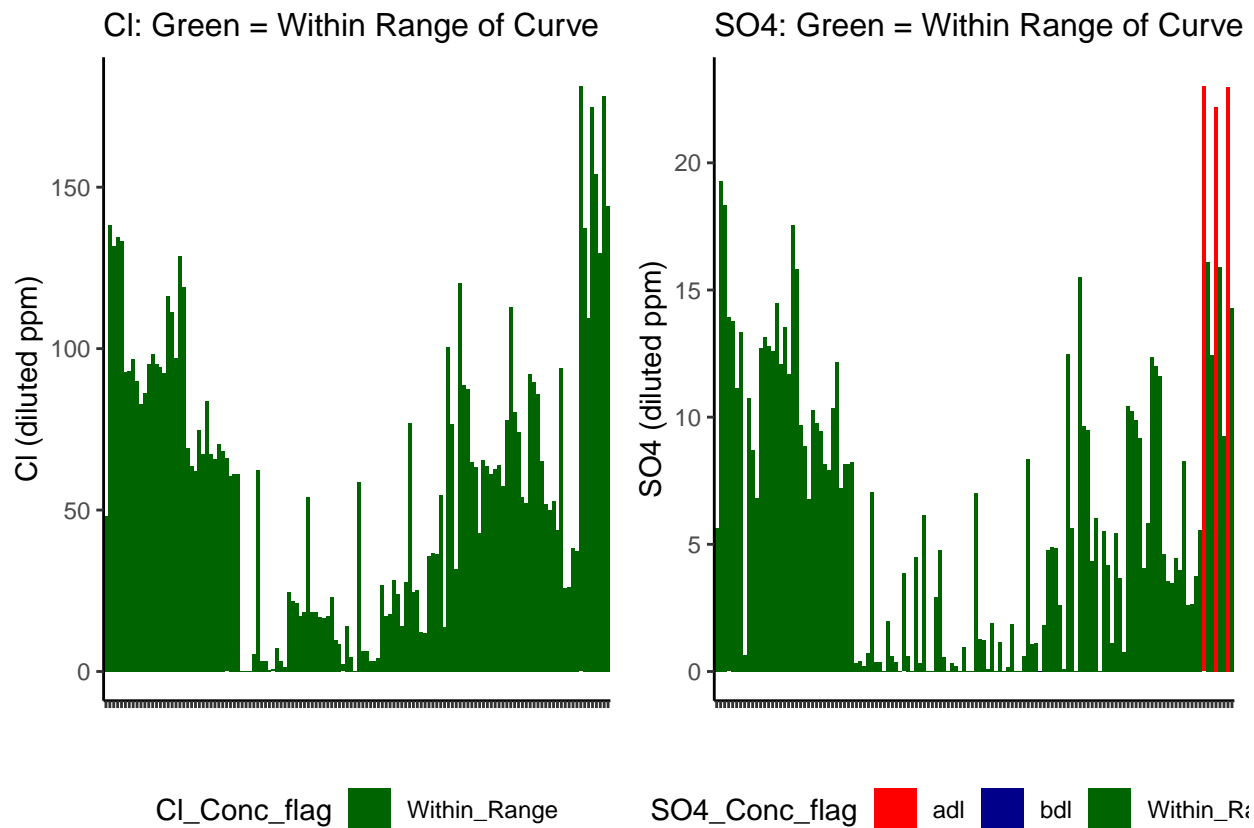


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	96.9230769
adl	2.3076923
bdl	0.7692308

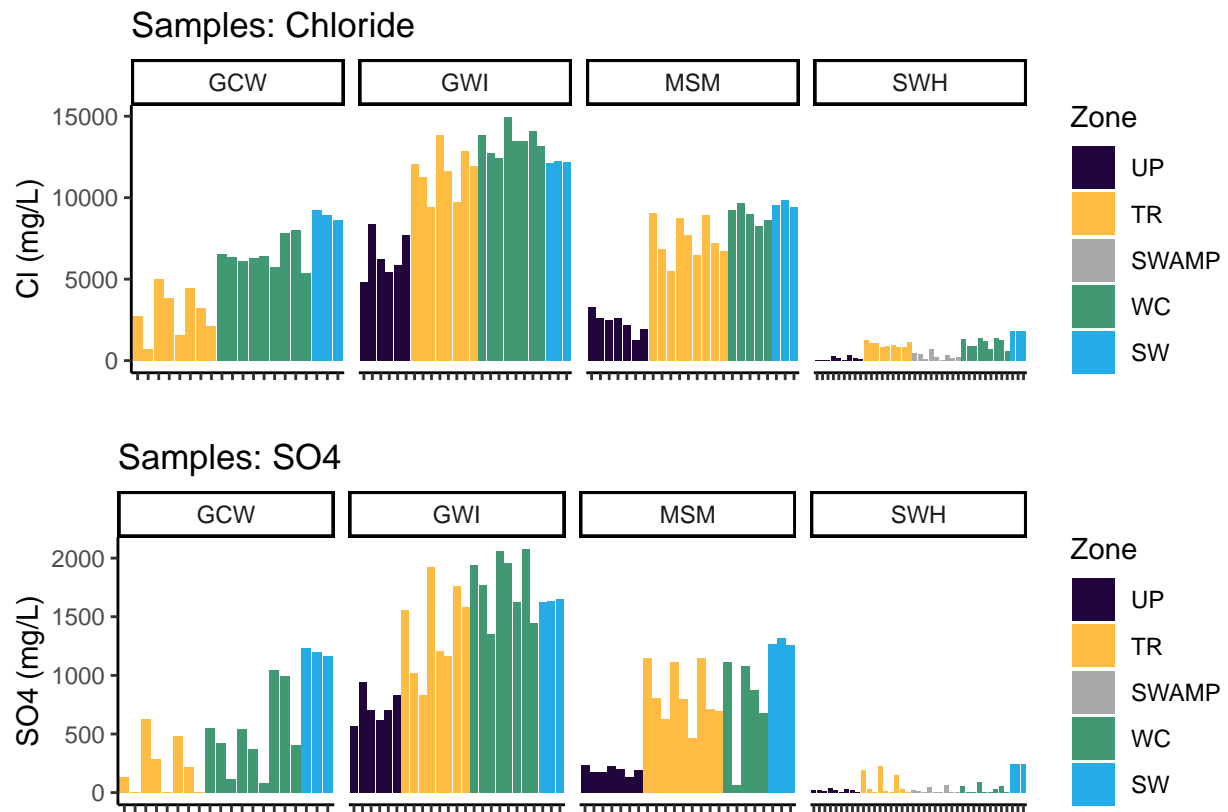
Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	100

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

```
## All sample IDs are present in metadata.
```

0.10 Visualize Data by Plot



0.11 Export Processed Data

#end