COMPASS_SynopticCB_PW_SO4_Cl_202408

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Contents

##Add Required Packages

##Keep the R Markdown output within the PDF margins

##Setup - Change things here & write any notes

```
###### Run information - PLEASE CHANGE
Date_Run = "2025-06-16"  #Date that instrument was run
Run_by = "Zoe Read"  #Instrument user
Script_run_by = "Zoe Read"  #Code user
run_notes = "All SO4 blanks were zero"  #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
chks_name = "Check Standard"  #what did you name your check standards?

###### File Names - PLEASE CHANGE file path and name for
###### raw summary data file raw_file_name_cl =
###### 'Porewater/Sulfate_Chloride/Synoptic_CB/2024/Raw
###### Data/COMPASS_Synoptic_CB_MonMon_202408_Cl.txt'
###### raw_file_name_so4 =
###### 'Porewater/Sulfate_Chloride/Synoptic_CB/2024/Raw
###### Data/COMPASS_Synoptic_CB_MonMon_202408_SO4.txt'

raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202408_Cl.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202408_SO4.txt"

# file path and name of processed data file
# processed_file_name =
# 'Porewater/Sulfate_Chloride/Synoptic_CB/2024/Processed
# Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202408.csv'
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202408.csv"

###### Log Files - PLEASE CHECK downloaded metadata csv -
###### downloaded from Google drive as csv for this year
###### Raw_Metadata =
###### 'Porewater/Sulfate_Chloride/Synoptic_CB/2024/Raw
###### Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv'
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"

# qaqc log file path for this year Log_path =
# 'Porewater/Sulfate_Chloride/Synoptic_CB/2024/Raw
# Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv'
Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv"
```

##Set Up Code

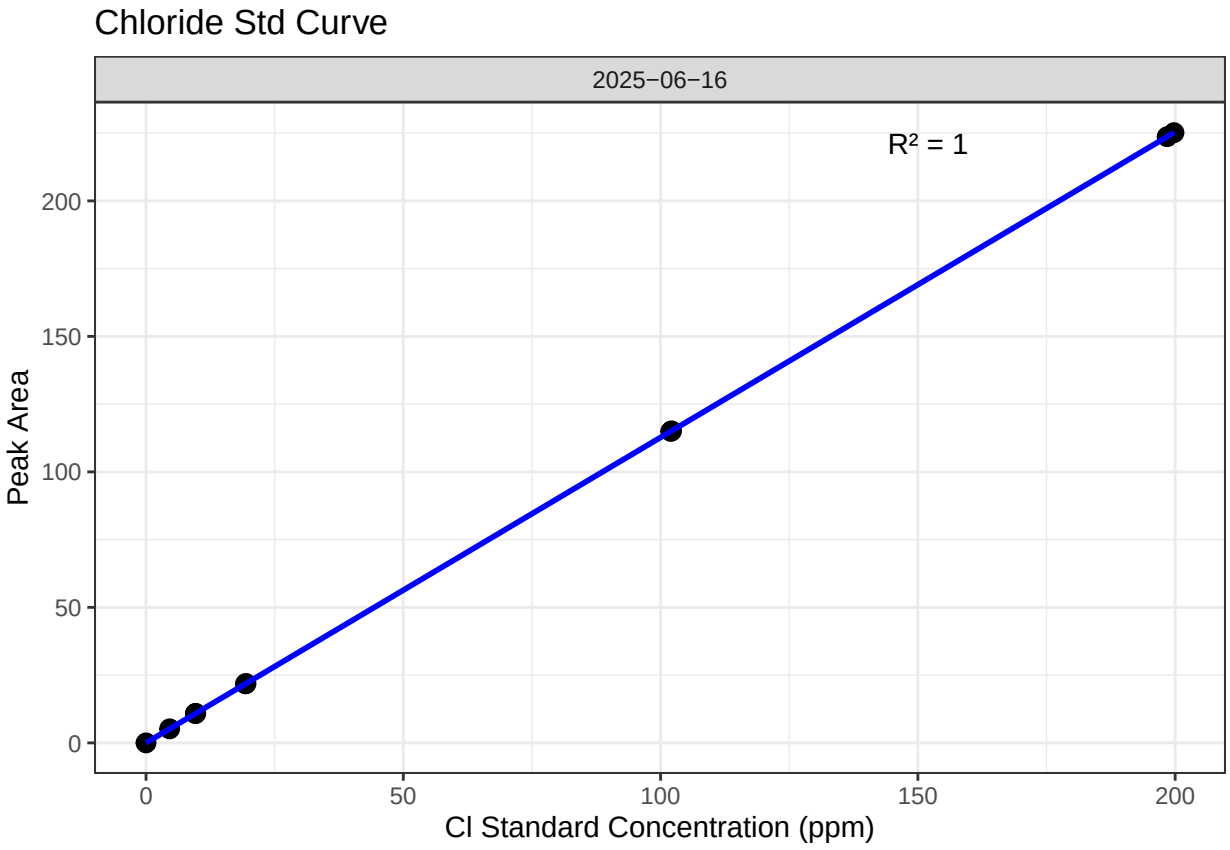
```
#Link to the protocol used for analysis
  #steph will add this soon

#Coefficients / constants that are needed for calculations
  cl_mw <- 35.45      #molecular weight of Chloride, g/mol
  s_mw <- 32.06       #molecular weight of sulfur, g/mol
  Con1 <- 1000000     #conversion factor value for spike volumes (uL -> L)
```

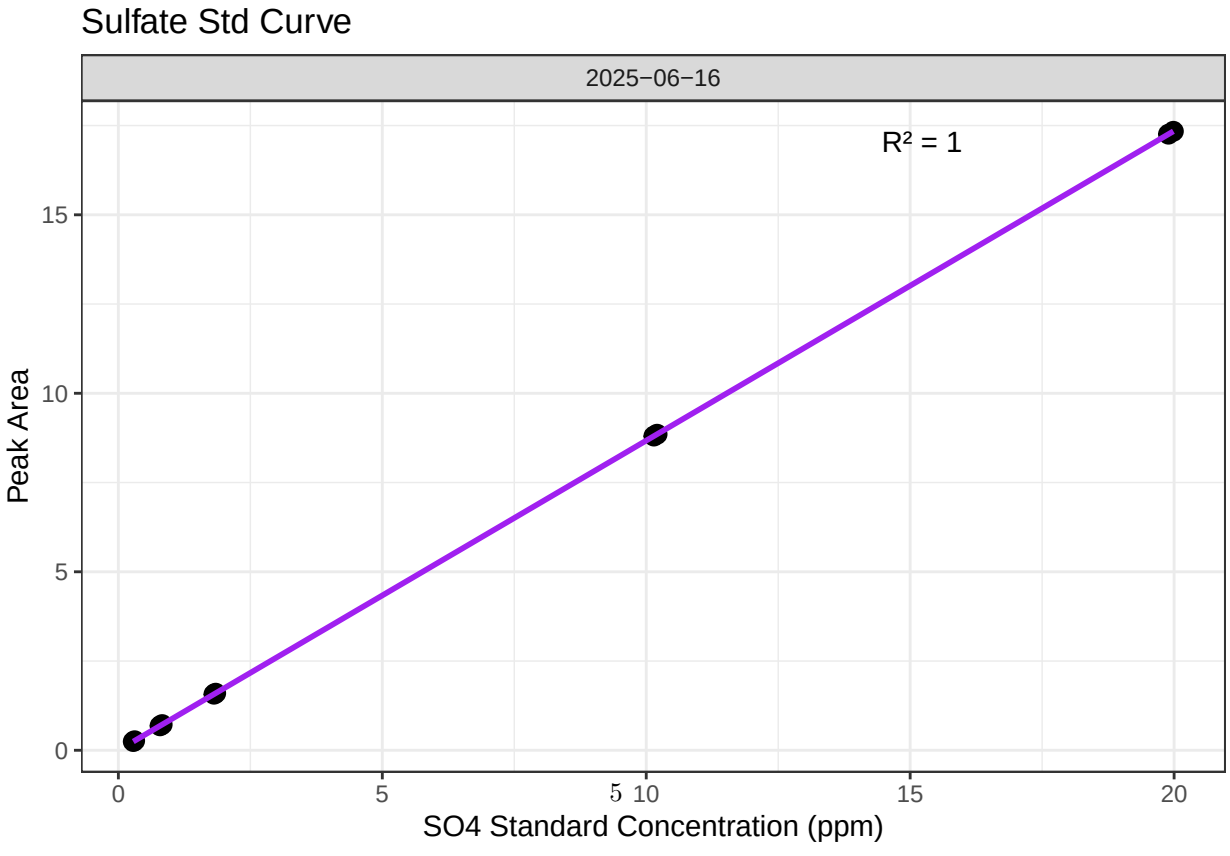
```
#Flag cutoffs
  r2_cutoff = 0.98            #this is the level below which we want to rerun or consider a curve
  chk_flag_std_s = 10         #this is the maximum cv allowed for sulfate check standards
  chk_flag_std_cl = 5         #this is the maximum cv allowed for chloride check standards
  chk_flag_std_perc = 15      #this is the maximum perc diff allowed for check standards
  chk_flag_dups = 10          #this is the maximum cv allowed for duplicates
  high_recovery_cutoff = 120  #this is the maximum percent recovery of SO4 allowed in spiked samples
  low_recovery_cutoff = 80    #this is the minimum percent recovery of SO4 allowed in spiked samples
  chks_flag = 0.80            #if less than this percent of samples pass a check, a flag is added

#Standard concentrations - Update if running different standard curve:
  standards <- tibble(
    sample_ID = c("Standard 1", "Standard 2", "Standard 3", "Standard 4", "Standard 5"),
    SO4_std_conc = c(0.5, 1.0, 2.0, 10, 20),  #ug/mL
    Cl_std_conc = c(5, 10, 20, 100, 200))     #ug/mL

#Spike concentration calc
  #spike for these samples was 10uL of the 250 µg/mL standard
  spk_std <- (250/s_mw)         # mM of SO4 calculated from 250 ug/mL SO4 spike solution
  spkvol <- 10                  # uL volume of spike added
  spkvol <- spkvol/Con1         # L volume of spike added
  spk_Conc <- (spk_std)*spkvol  # mmoles of SO4 added to each spiked sample

#Top standard Concentrations- Update if running different standard curve:
   top_std_cl = 200   #ug/mL
   top_std_so4 = 20   #ug/mL

#Set time zone
  common_tz = "Etc/GMT+5"
  Sys.setenv(TZ = "America/New_York")
```

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

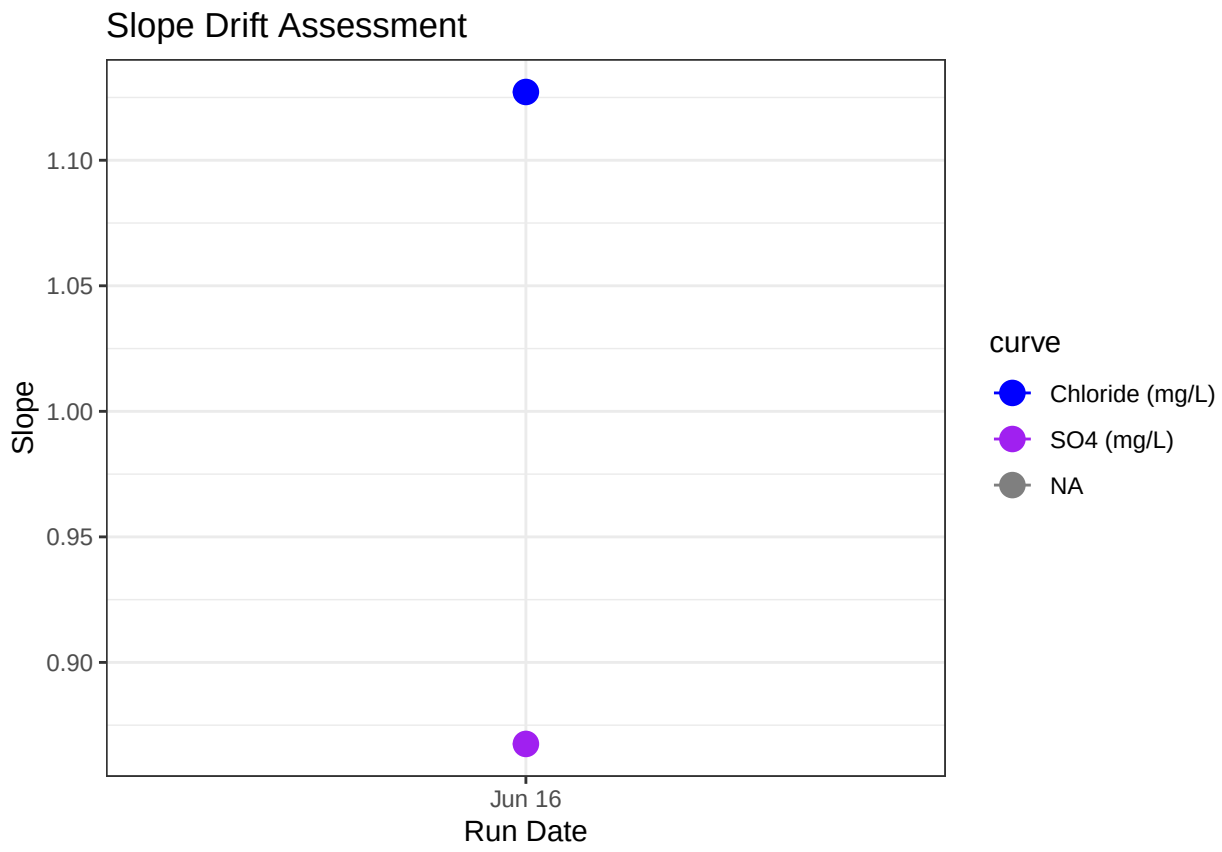
0.1 Import Sample Data

0.2 Assessing Standard Curves





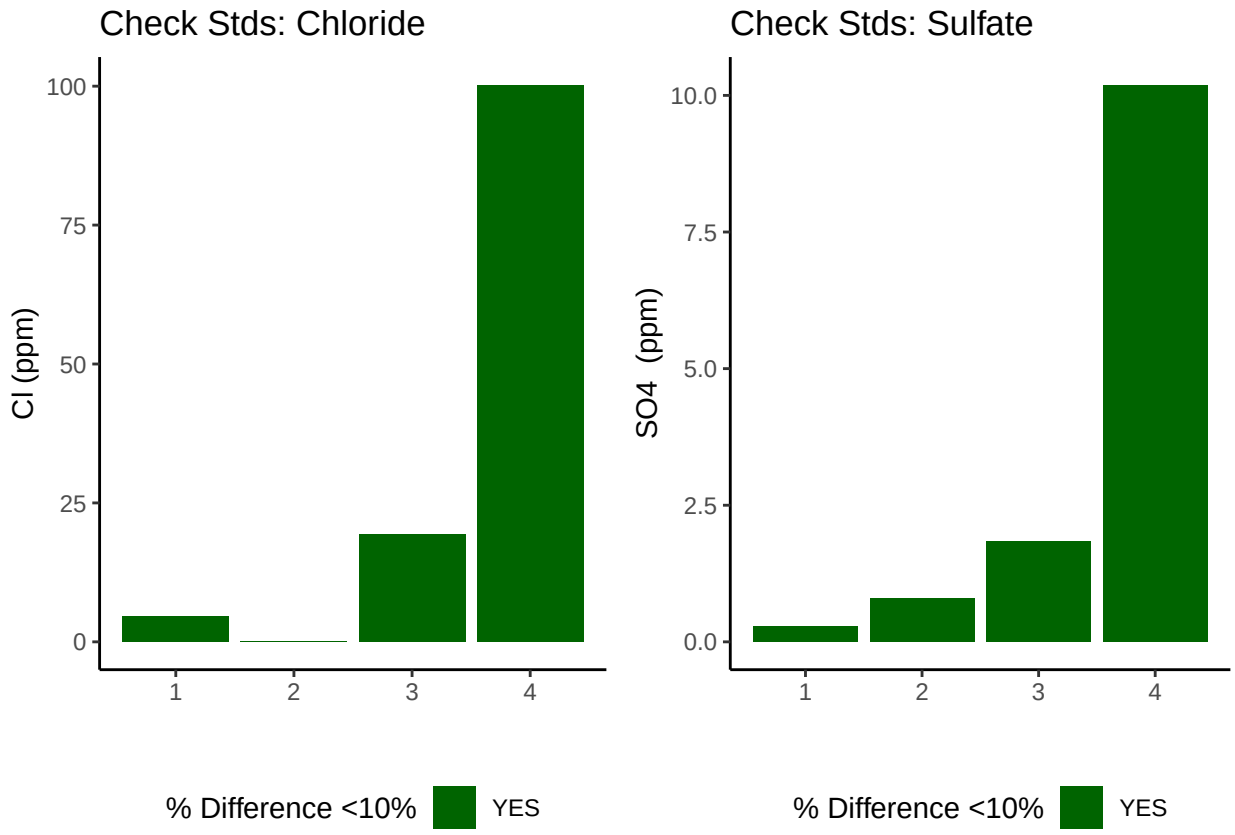
```
## [1] "QAQC log file exists and has been read into the code."
```




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

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

0.3 Assess Check Standards



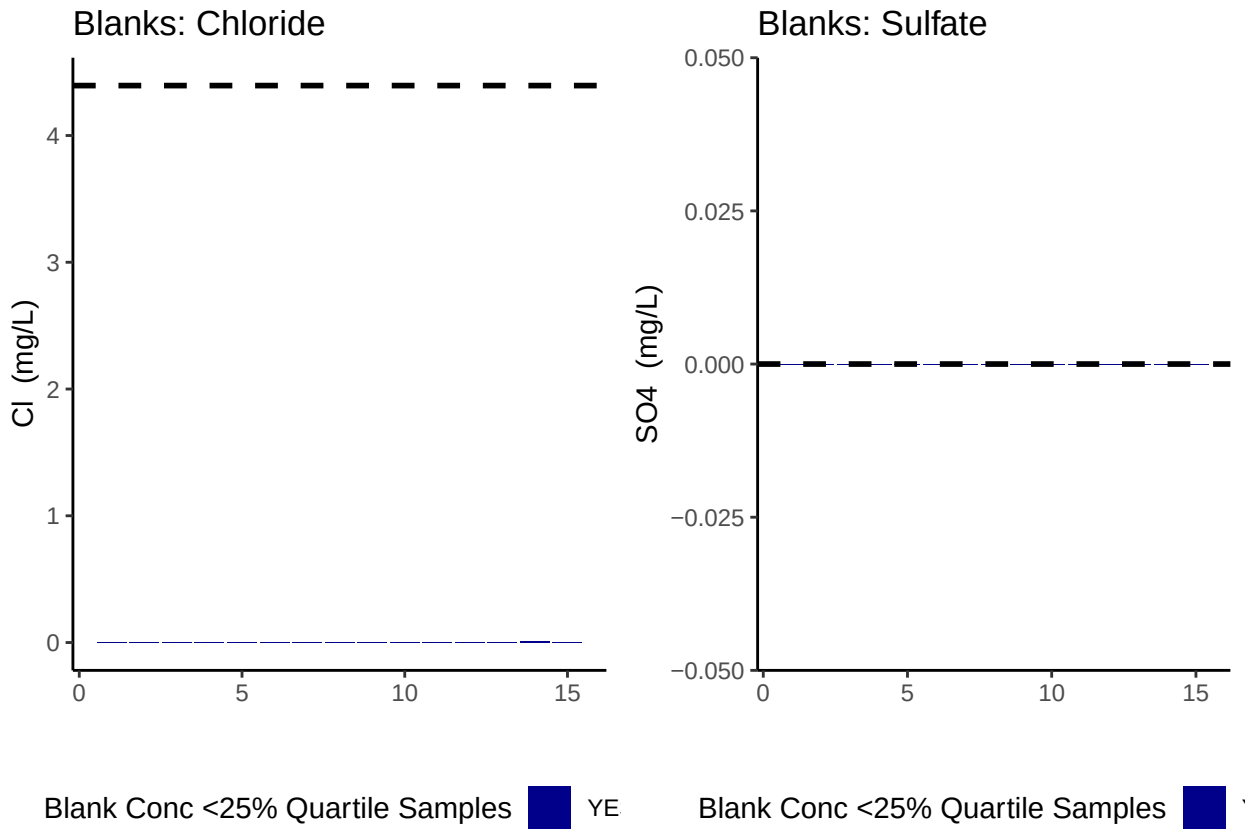

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration"
```

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

0.4 Assess Blanks

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

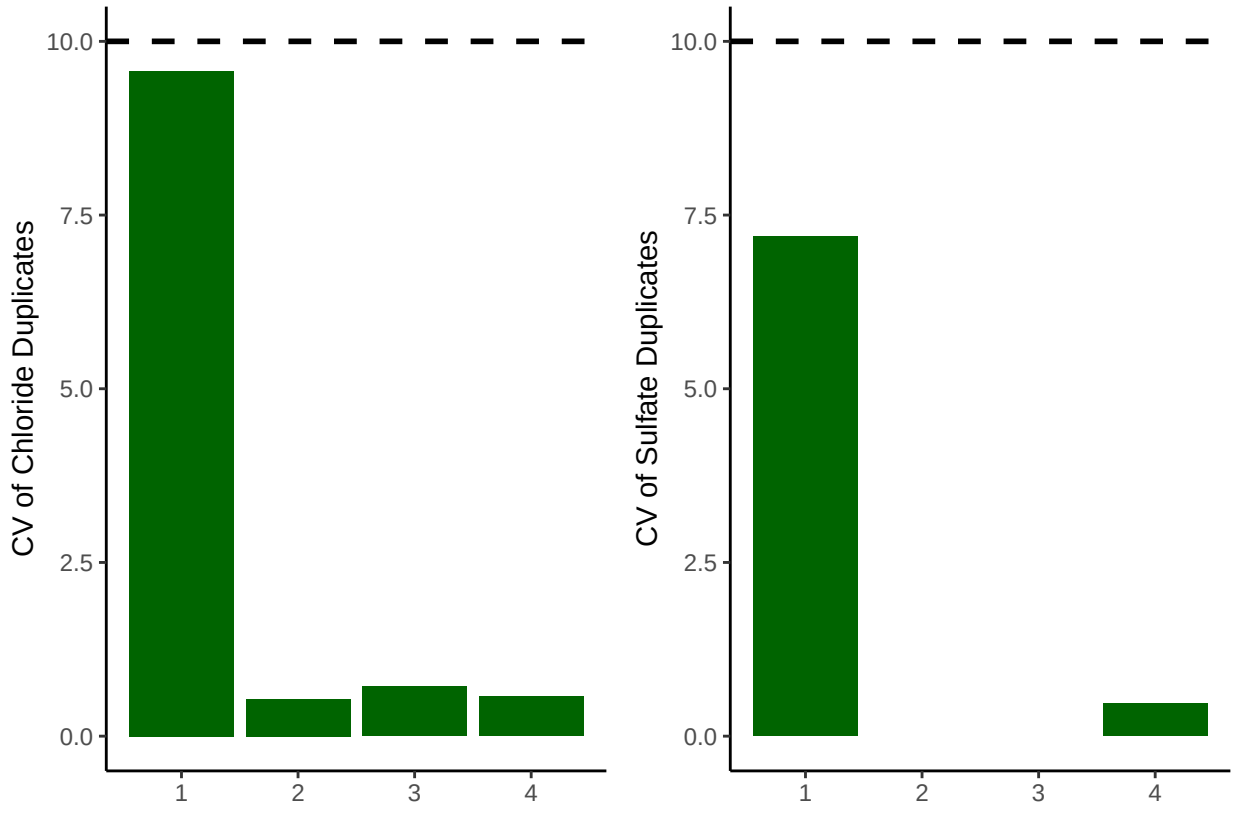
```
## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"
```




```
## Chloride blanks mean ppm:

## [1] 0.0008533333

## Sulfate blanks mean ppm:

## [1] 0
```

0.5 Assess Duplicates

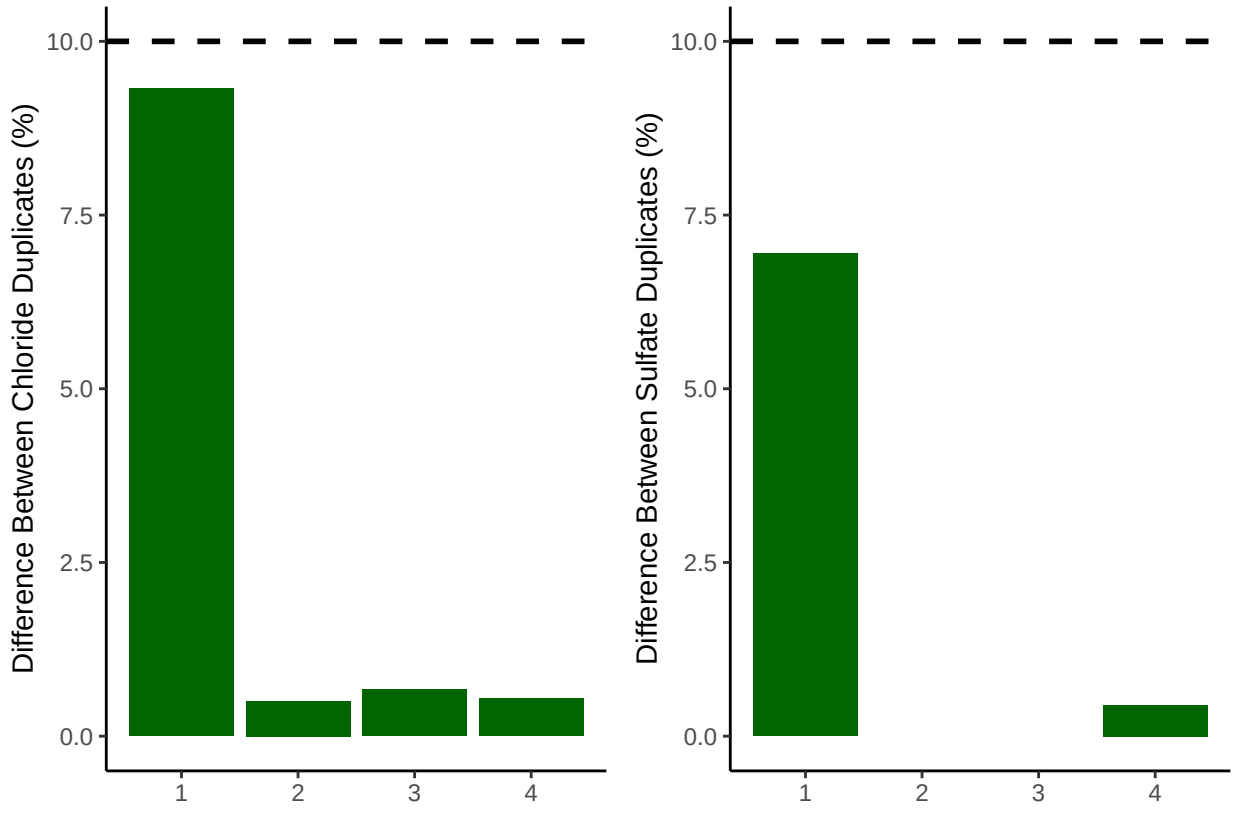
```
## Warning: Removed 2 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```




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

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

```
## Warning: Removed 2 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```




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

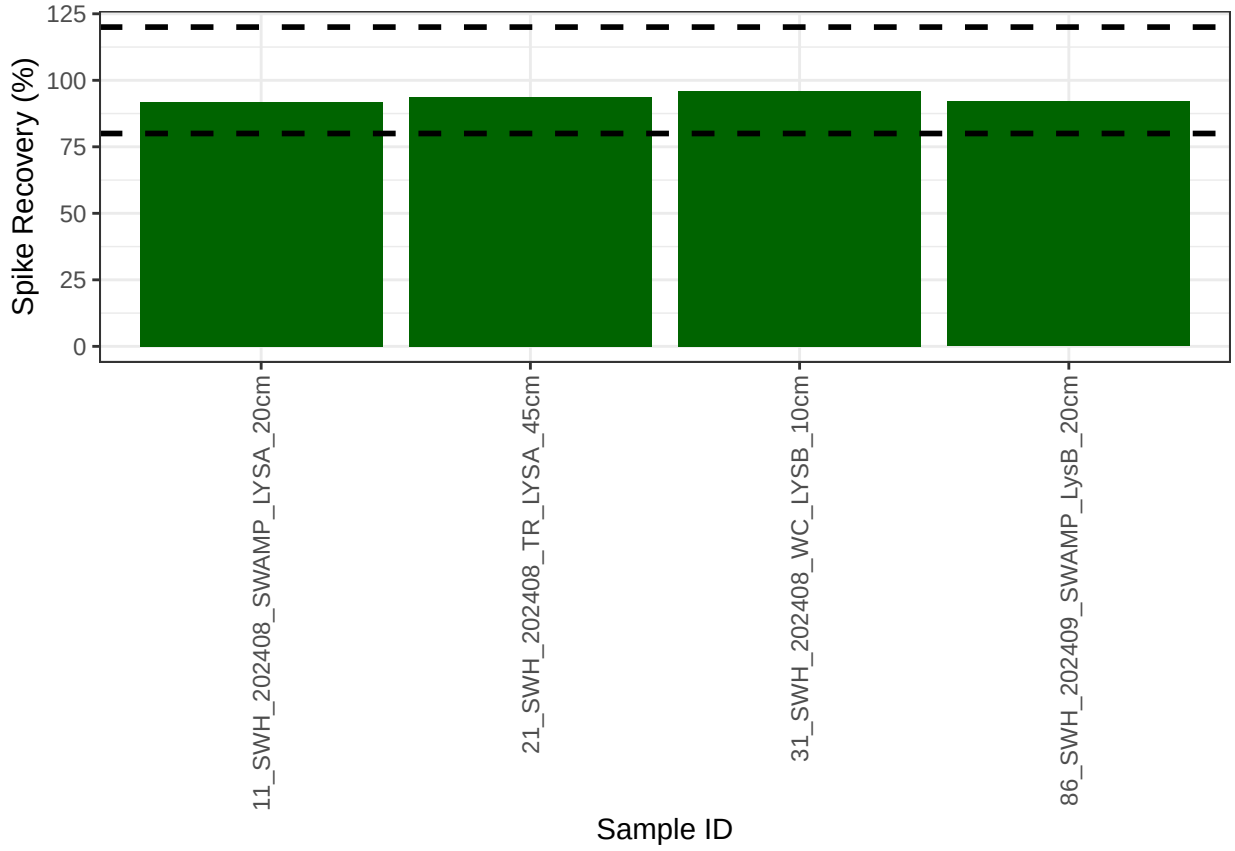
```
## [1] ">80% of Sulfate Duplicates have a percent difference <10%"
```

0.6 Calculate mmol/L concentrations & salinity, add dilutions

```
cat("Unit Conversion and Salinity Calculation")

# Convert ppm to mmol/L
all_dat$SO4_mM <- (all_dat$SO4_ppm/s_mw)
all_dat$Cl_mM <- (all_dat$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$salinity <- ((1.807 * all_dat$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"), 50, all_dat$Dilution)
```

```
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") &
    str_detect(all_dat$sample_ID, "TR"), 50, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") &
    str_detect(all_dat$sample_ID, "WC"), 100, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") &
    str_detect(all_dat$sample_ID, "SW"), 100, all_dat$Dilution)

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") &
    str_detect(all_dat$sample_ID, "UP"), 50, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") &
    str_detect(all_dat$sample_ID, "TR"), 50, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") &
    str_detect(all_dat$sample_ID, "WC"), 100, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") &
    str_detect(all_dat$sample_ID, "SW"), 100, all_dat$Dilution)

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") &
    str_detect(all_dat$sample_ID, "UP"), 100, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") &
    str_detect(all_dat$sample_ID, "TR"), 100, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") &
    str_detect(all_dat$sample_ID, "WC"), 200, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") &
    str_detect(all_dat$sample_ID, "SW"), 200, all_dat$Dilution)

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

head(all_dat)
```

0.7 Assess Analytical Spikes

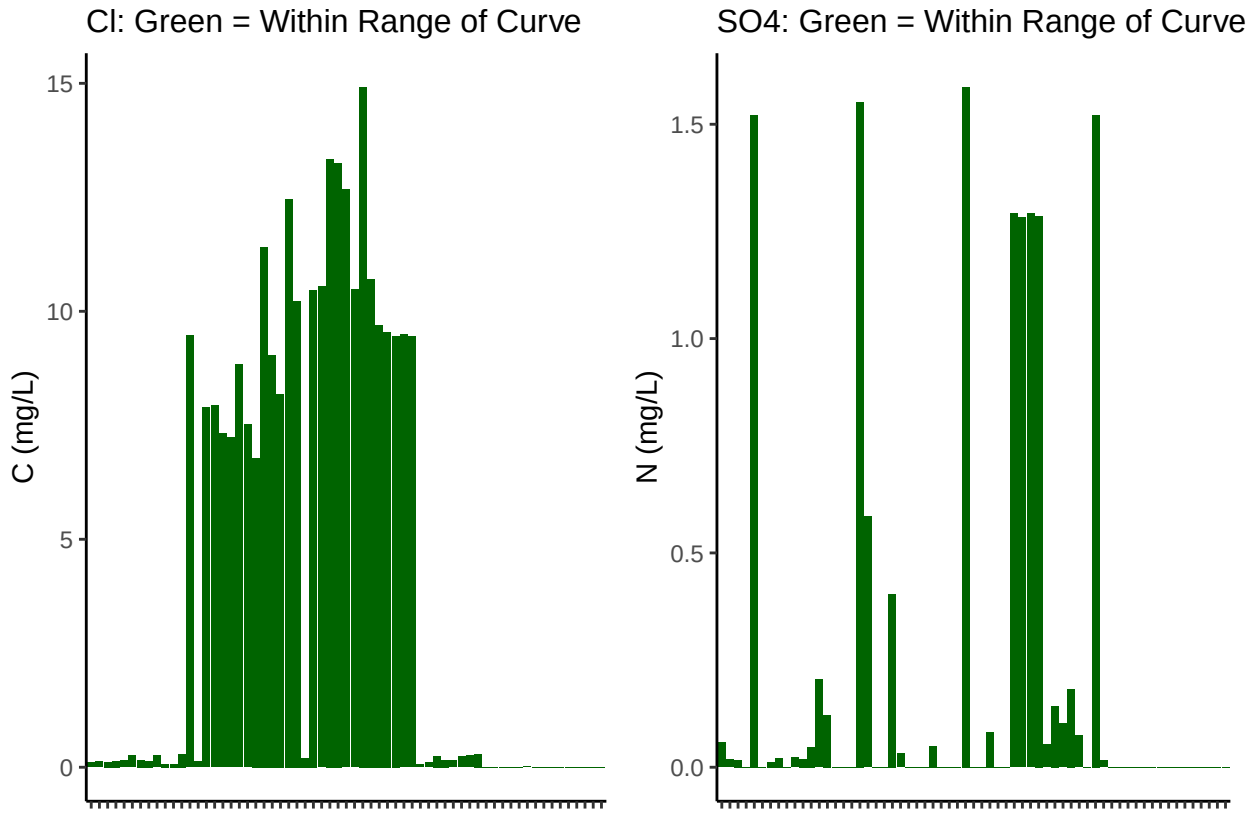



```
## # A tibble: 1 x 4
##   SO4_spks_flag no_rows Total Percent
##   <chr>           <int> <int>   <dbl>
## 1 Yes                 4     4     100
```

```
## [1] ">80% of SO4 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
```




```
## # A tibble: 1 x 4
##   Cl_flag no_rows Total Percent
##   <chr>     <int> <int>   <dbl>
## 1 ""           63    63     100
```

```
## [1] "All chloride samples are within the range of the standard curve - PROCEED"
```

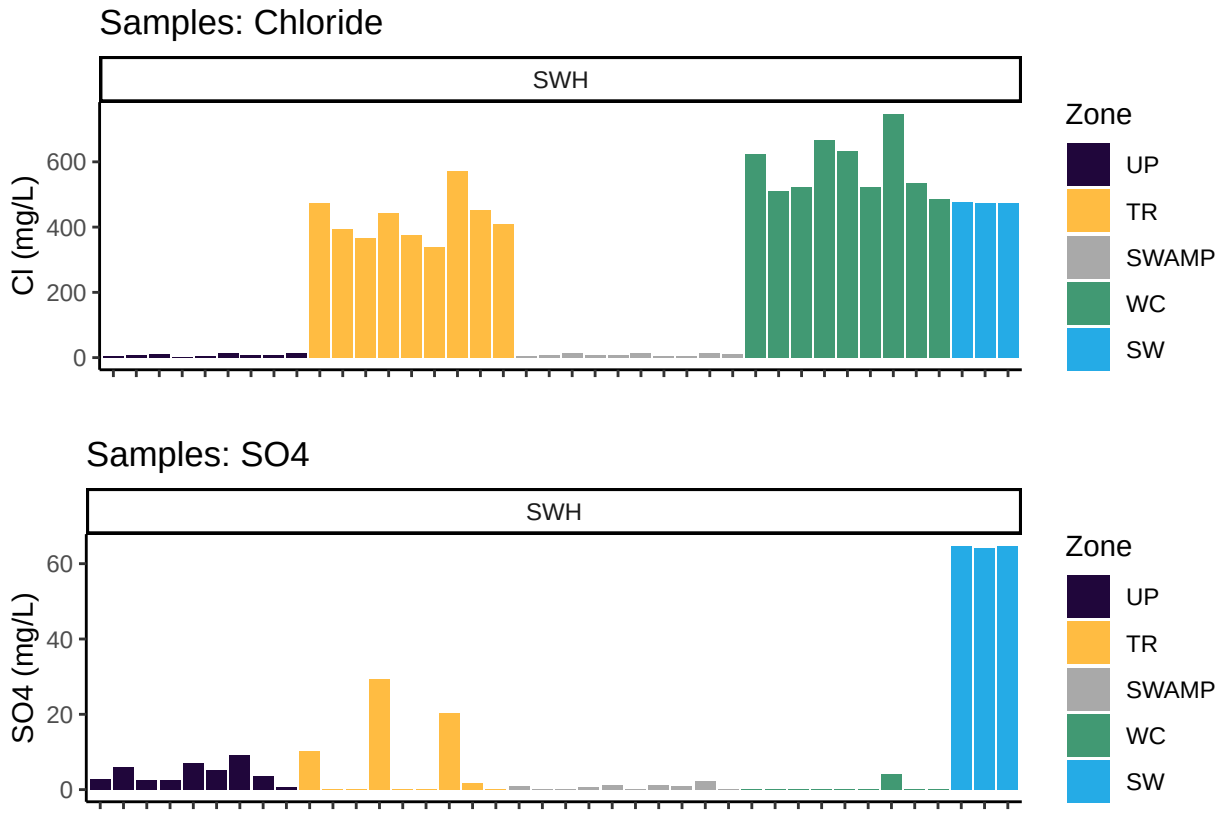
```
## # A tibble: 1 x 4
##   SO4_flag no_rows Total Percent
##   <chr>      <int> <int>   <dbl>
## 1 ""            63    63     100
```

```
## [1] "All chloride samples are within the range of the standard curve - PROCEED"
```

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