COMPASS_SynopticCB_PW_SO4_Cl_202311_Template

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Contents

##Setup - Change things here & write any notes

```
#identify section
cat("Setup Information")
```

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "2023-09-05"  #Date that instrument was run
  Run_by = "Unknown"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "Samples missing from metadata: MSM_202311_UP_LYSC_45CM MSM_202311_WC_LYSB_45CM MSM_20231
MSM_202311_WC_RHZ_LYSC. 118_MSM_202311_TR_RHZ_SF_Tree_1 value above cal curve for SO4, but only slightly

  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/2023/Raw Data/COMPASS_Synoptic_CB_MonM
    # raw_file_name_so4 = "Porewater/Sulfate_Chloride/Synoptic_CB/2023/Raw Data/COMPASS_Synoptic_CB_Mon

    raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202311_Cl.txt"
    raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202311_SO4.txt"

#file path and name of processed data file
    # processed_file_name = "Porewater/Sulfate_Chloride/Synoptic_CB/2023/Processed Data/COMPASS_Synopti
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202311.csv"

###### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
  # Raw_Metadata = "Porewater/Sulfate_Chloride/Synoptic_CB/2023/Raw Data/COMPASS_SynopticCB_PW_SampleLo
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"

#qaqc log file path for this year
  # Log_path = "Porewater/Sulfate_Chloride/Synoptic_CB/2023/Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_20
  Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2023.csv"
```

##Add Required Packages

##Set Up Code

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

#Any coefficients / constants that are needed for calculations
  cl_mw <- 35.45     #molecular weight of Chloride: 35.45
  s_mw <- 32.06      #molecular weight of sulfur: 32.06

#Flags for Dionex
  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_dups = 10 #this is the maximum cv allowed for duplicates
  chks_flag = 0.80 #this is the percent of chks we want to have a CV less than the max allowable cv
  #blank_flag - calculated based on samples later in this code as lower 25% quantile of sample concentr

#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),
    Cl_std_conc = c(5, 10, 20, 100, 200))

#Spike concentration calc
  spk_std <- (250/s_mw)    # in mM
  spkvol <- 10             # in uL
  spkvol <- spkvol/1000000 # in L
  #spike for these samples was 10uL of the 250 µg/mL standard
  spk_Conc <- (spk_std)*spkvol # mmoles of SO4

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

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

#plot indicators
  site_order <- c('GCW', 'MSM', 'GWI', 'SWH')
  plot_order <- c('UP', 'SWAMP', 'TR', 'WC', 'SW')
  plot_colors <- c("#20063B", "darkgrey", "#FFBC42", "#419973", "#25ABE6" )
```

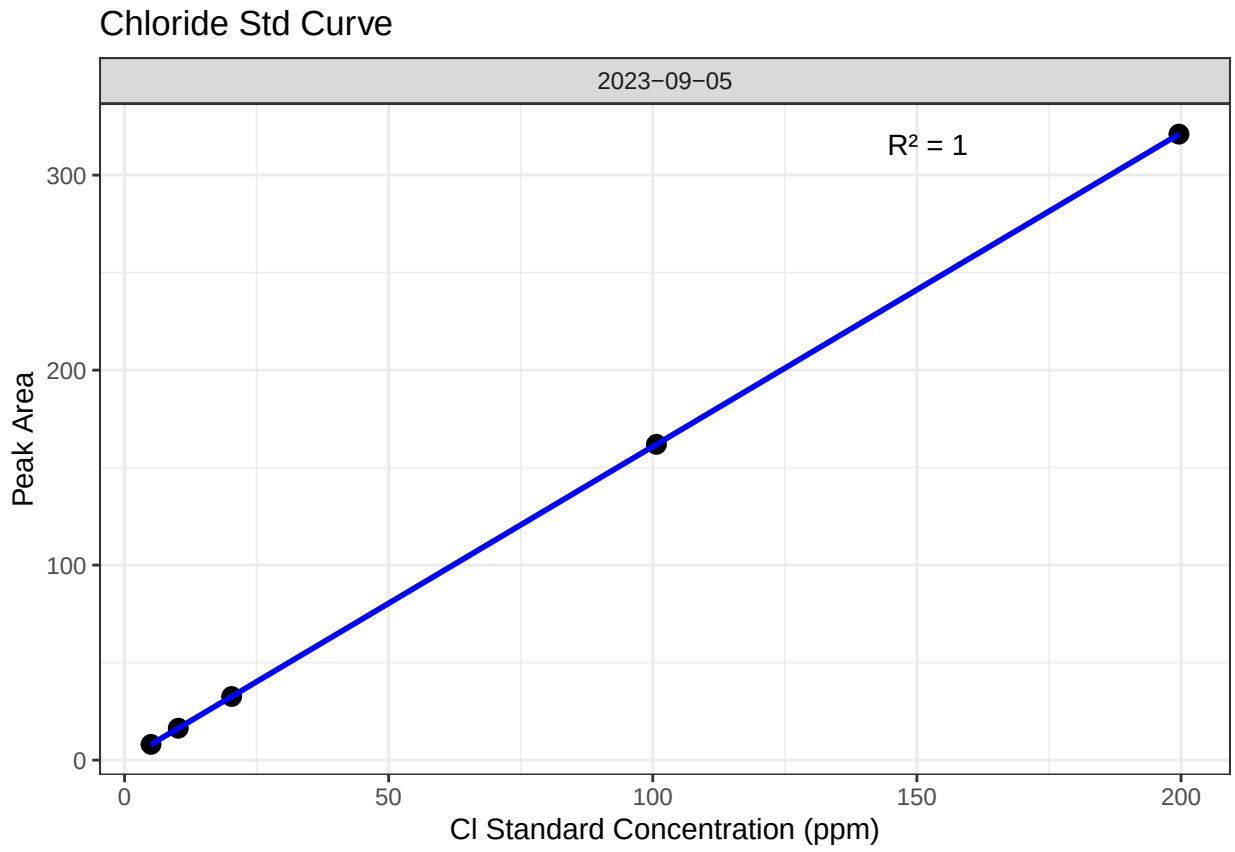
##Read in metadata and create similar sample IDs for matching to samples

0.1 Import Sample Data

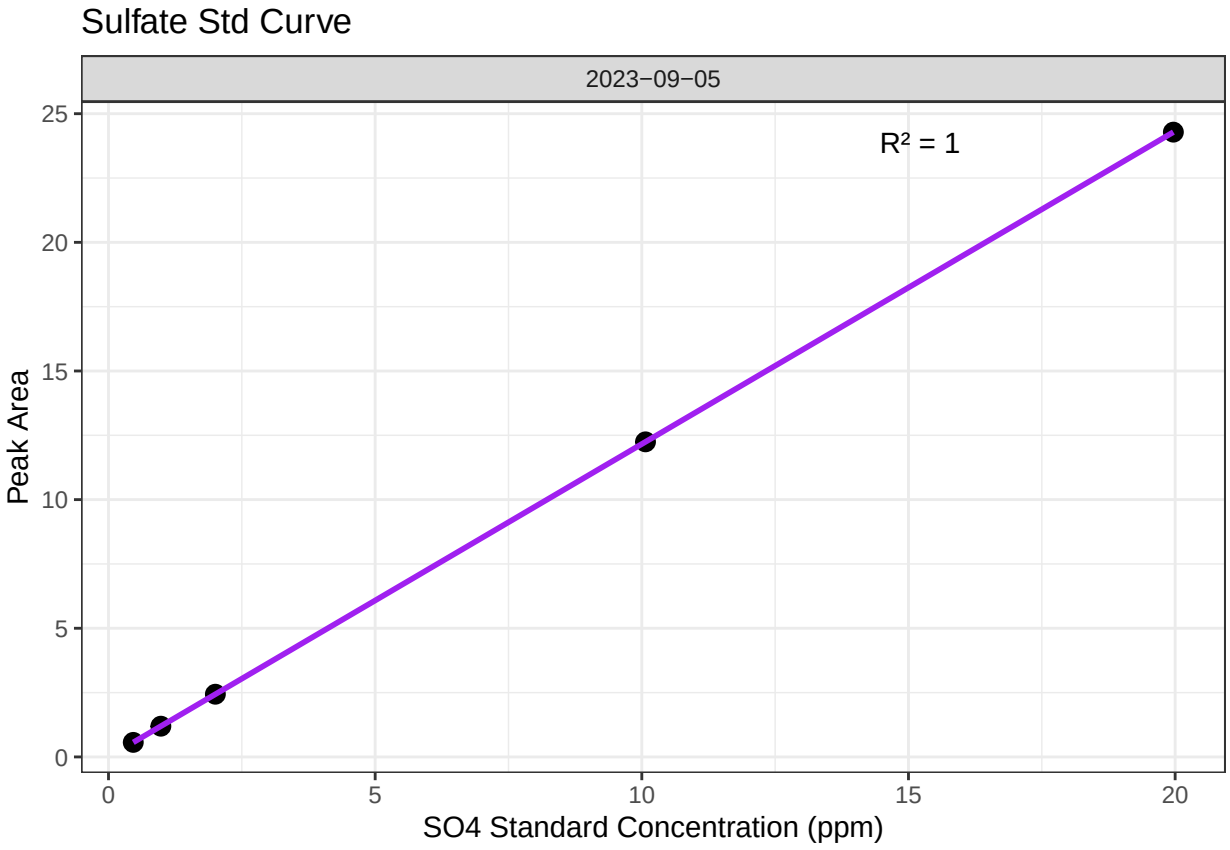
0.2 Assessing Standard Curves

```
## Assess the Standard Curves
```

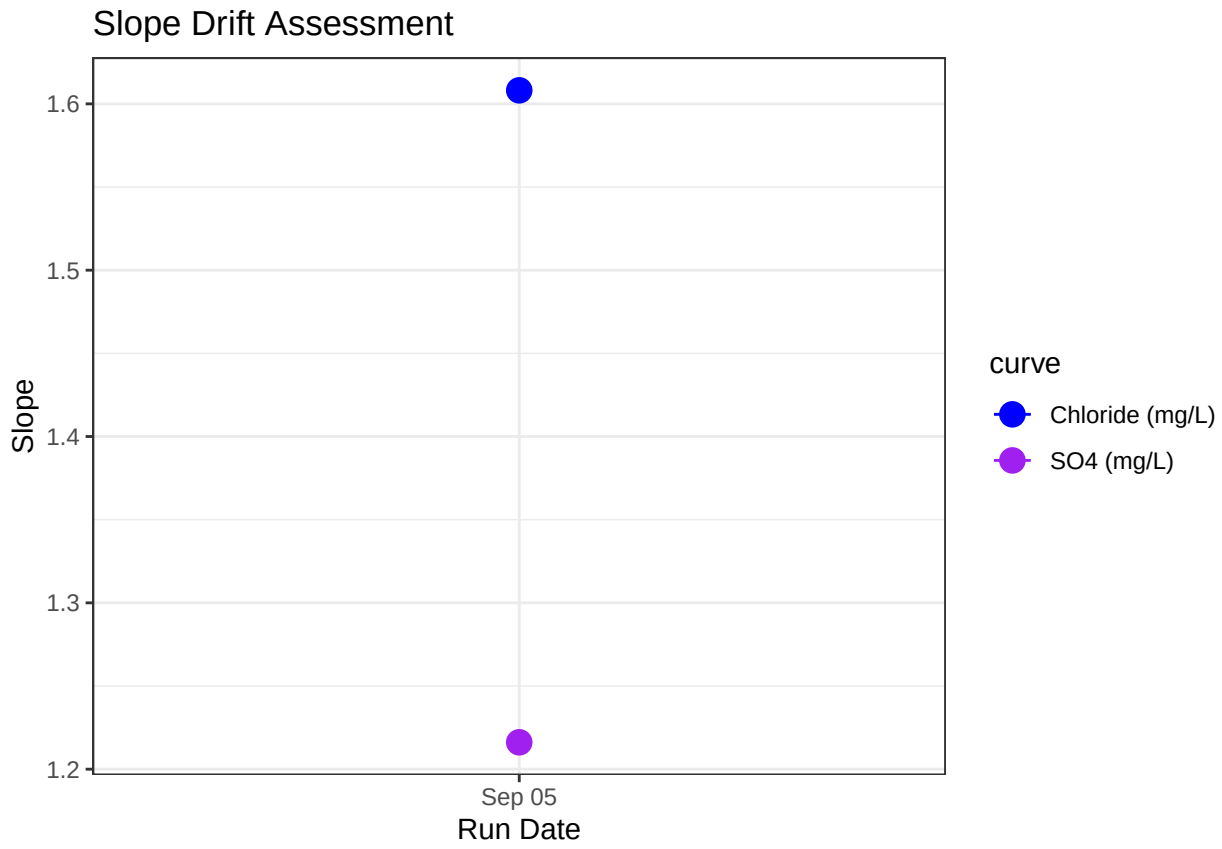
```
## `geom_smooth()` using formula = 'y ~ x'
```




```
## `geom_smooth()` using formula = 'y ~ x'
```




```
## `geom_line()`: Each group consists of only one observation.
## i Do you need to adjust the group aesthetic?
```

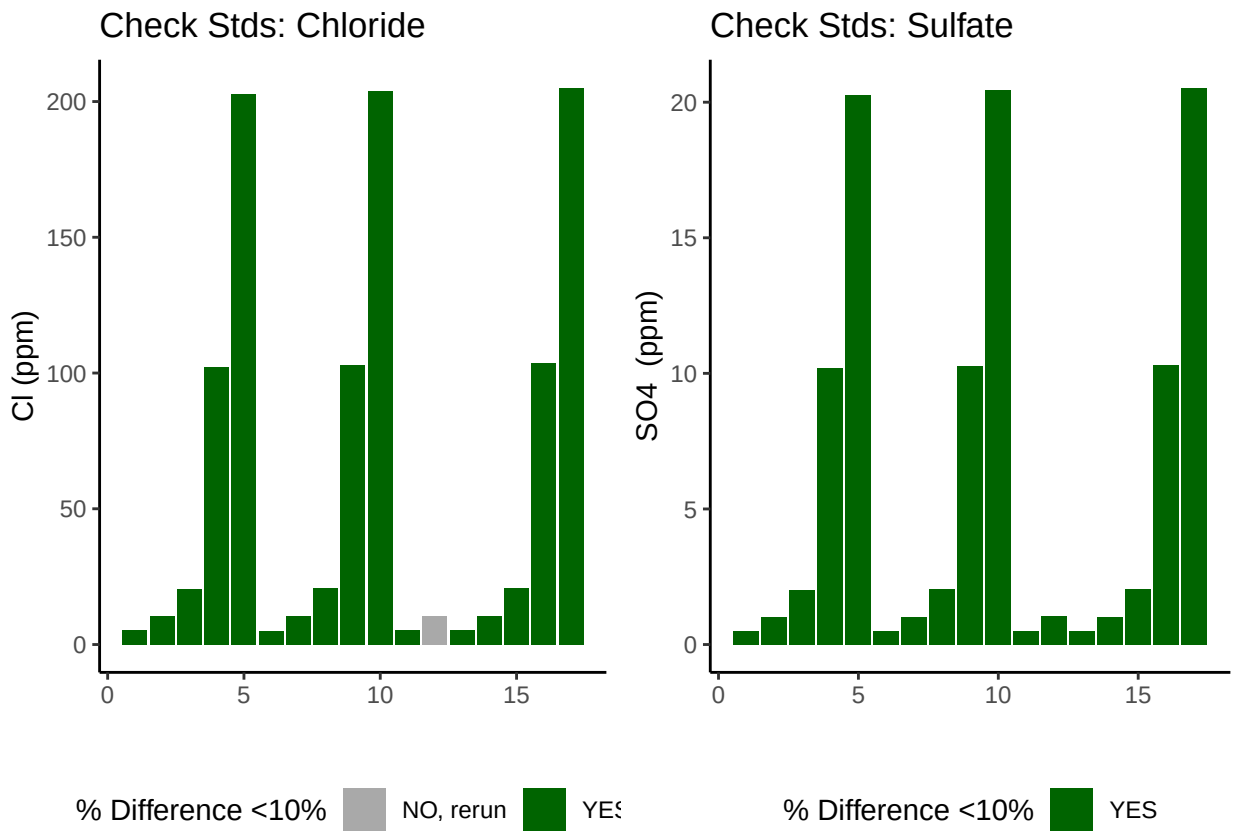



```
## [1] "Cl Curve r2 GOOD"
```

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

0.3 Assess Check Standards

```
## Assess the Check Standards
```




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

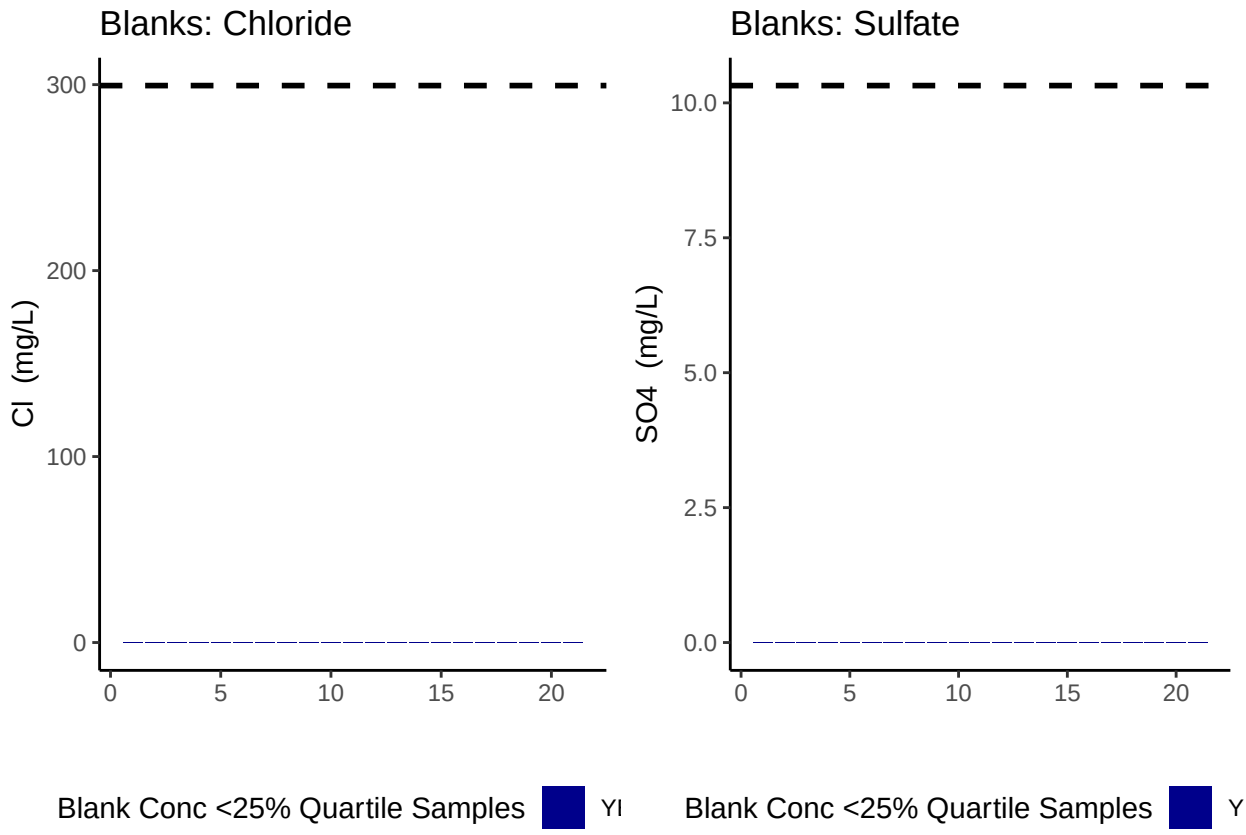
```
## [1] ">80% of Sulfate Check Standards are within range of expected concentration"
```

0.4 Assess Blanks

```
## Assess Blanks
```

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

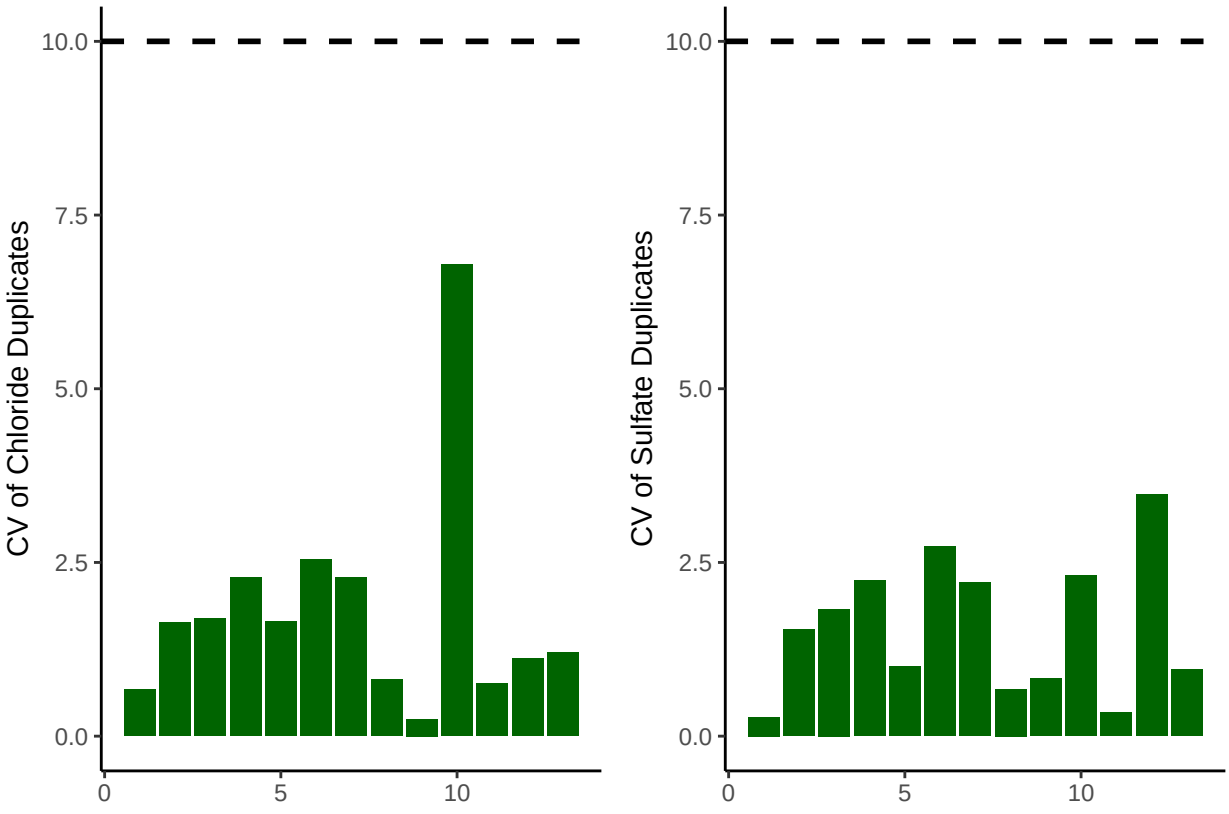
```
## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"
```




```
## Chloride blanks mean ppm:

## [1] 0.01699524

## Sulfate blanks mean ppm:

## [1] 0.004957143
```

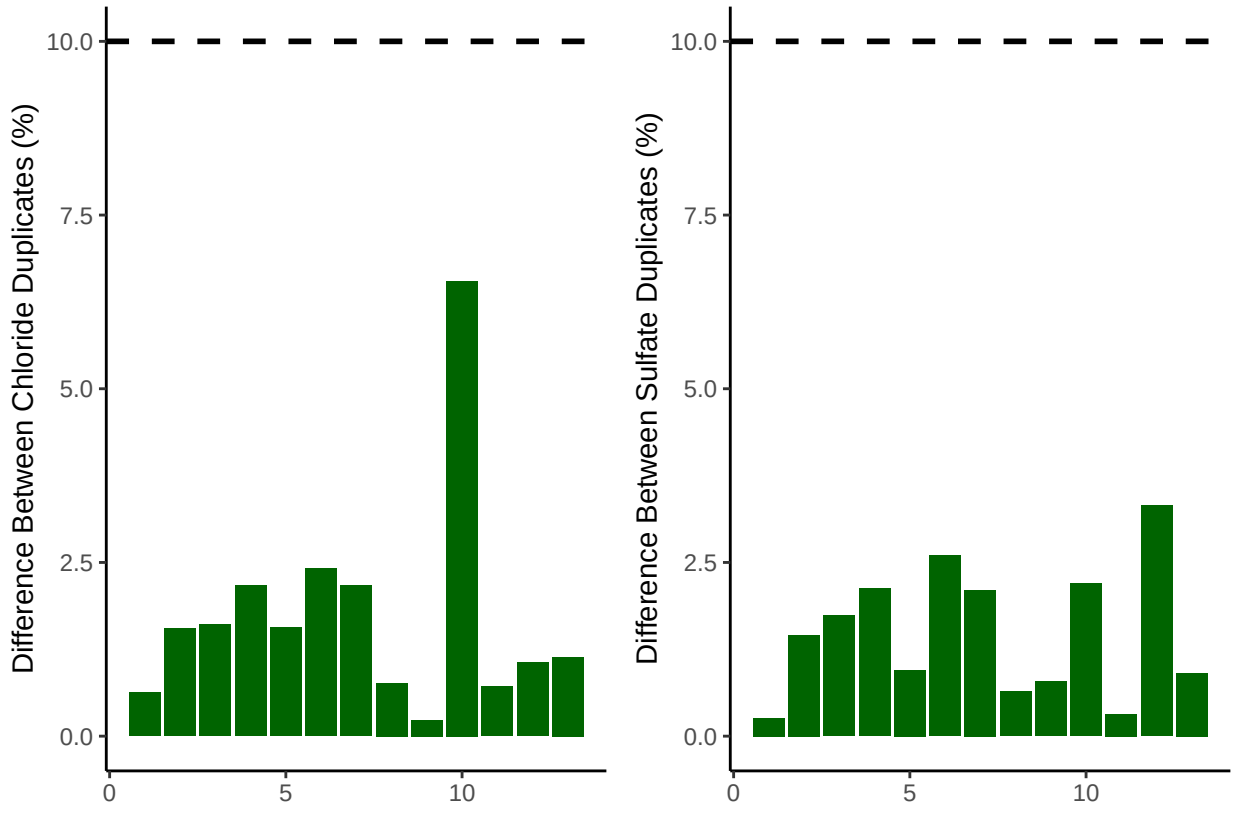
0.5 Assess Duplicates

```
## Assess Duplicates
```




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

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




```
## [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

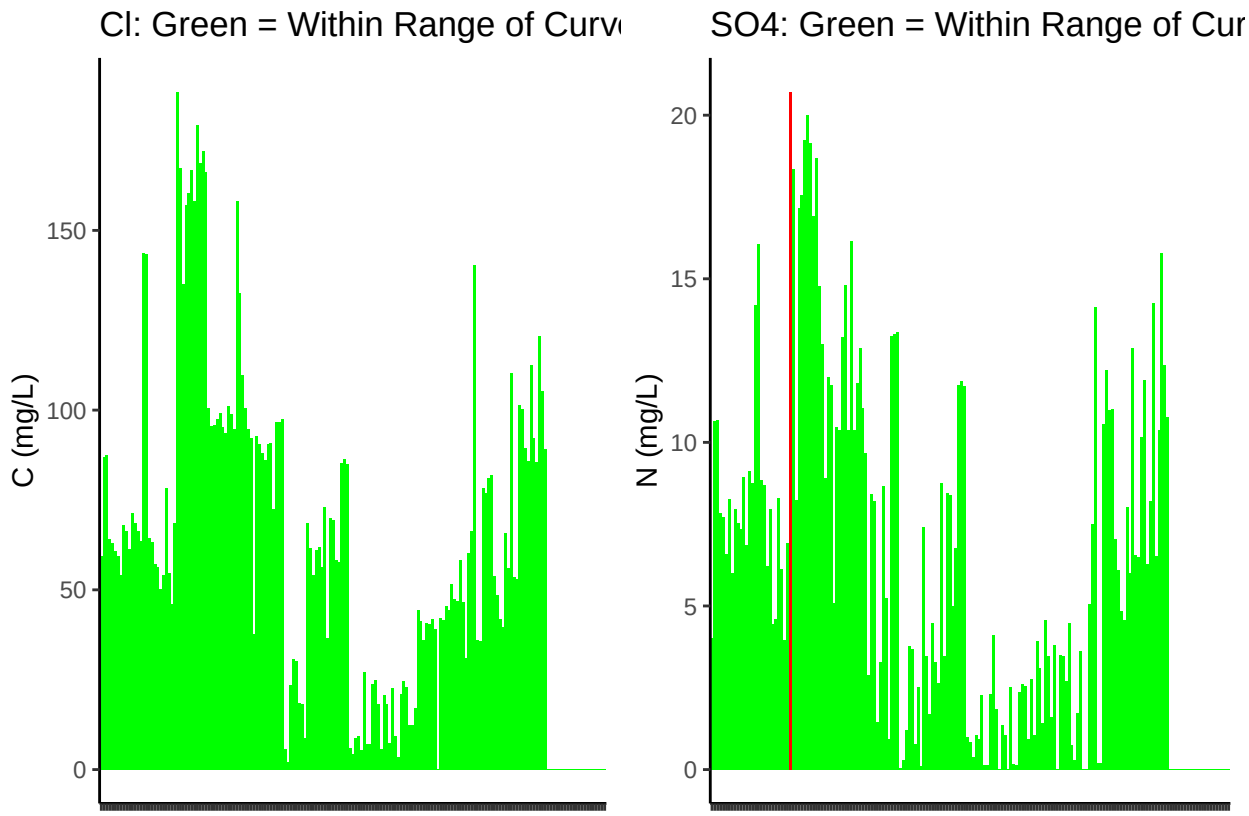
```
cat("Unit Conversion and Salinity Calculation")

# 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$salinity <- ((1.8070 * all_dat$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"),
```

```r
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

0.8 Check if samples Within the range of the standard curve

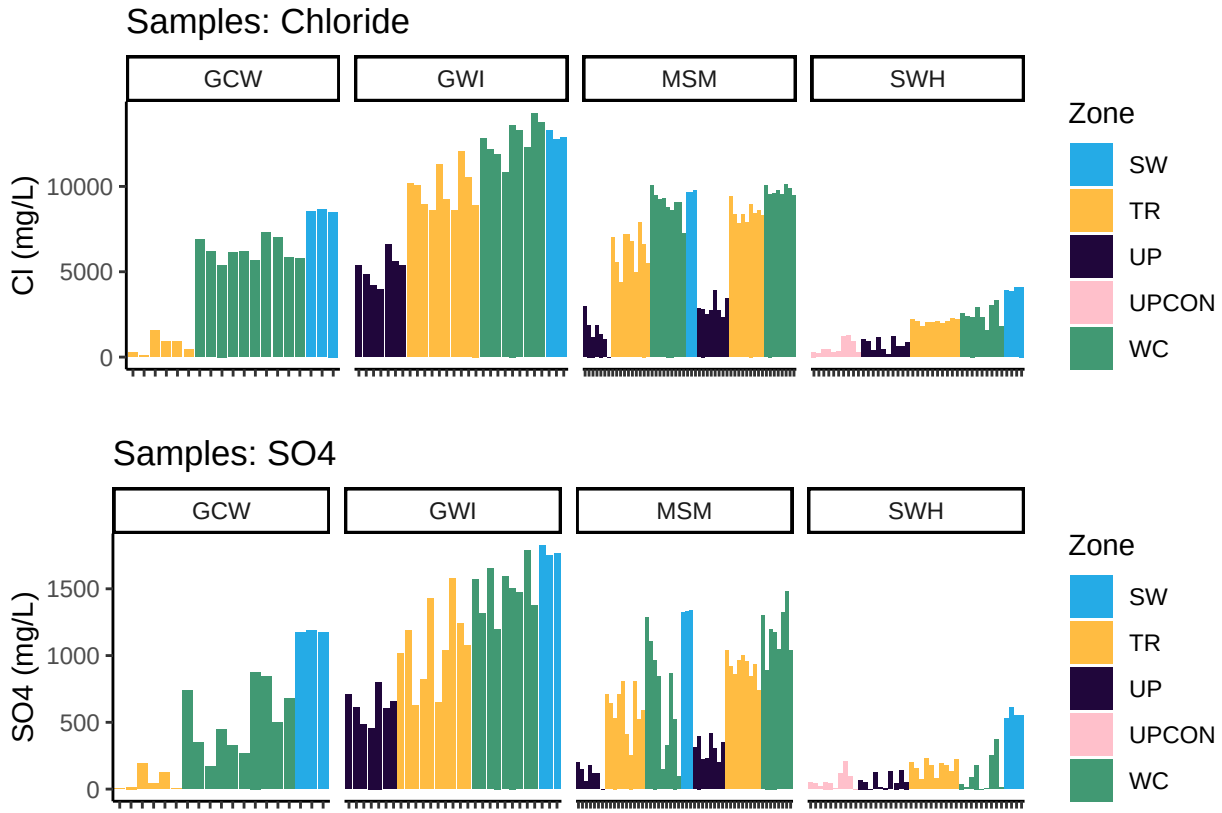
```
## Sample Flagging
```



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

0.10 Visualize Data by Plot

```
## Visualize Data
```



0.11 Export Processed Data

#end