

# Synoptic CB: Porewater SO<sub>4</sub>/Cl

July 2025 Samples

2025-10-23

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##Add Required Packages

## 0.1 Run Information

```
##### Run information - PLEASE CHANGE
Date_Run = "2025-10-02" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "Std 1 is lower than the expected concentration.
Some sample IDs are missing from metadata:
MSM_202507_UP_LYSB_20CM, MSM_202507_UP_LYSB_45CM, MSM_202507_UP_LYSC_10CM, GCW_202507_TR_LYSA_10CM,
9, 10, 88, 89 (test samples for Lucie)
" #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

##Fix samples that were entered incorrectly
samples_to_remove <- "GCW_202507_TR_LysA_10cm"
Old_ID_1 = NA
New_ID_1 = NA

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202507_C1.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202507_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_C1_S04_202507.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_2025.csv"

#qaqc log file path for this year
Log_path = "Raw Data/COMPASS_Synoptic_C1_S04_QAQClog_2024.csv"
```

##Set Up Code - constants and QAQC cutoffs

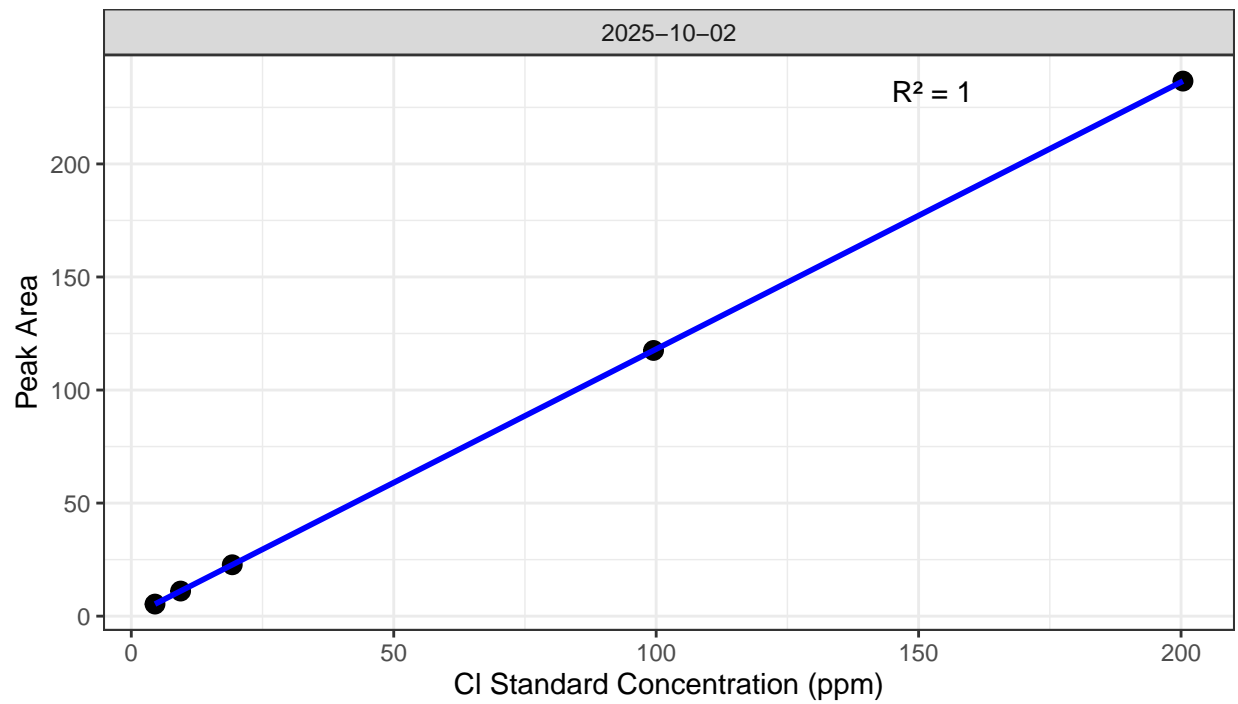
##Read in metadata and create similar sample IDs for matching to samples

##Import Sample Data

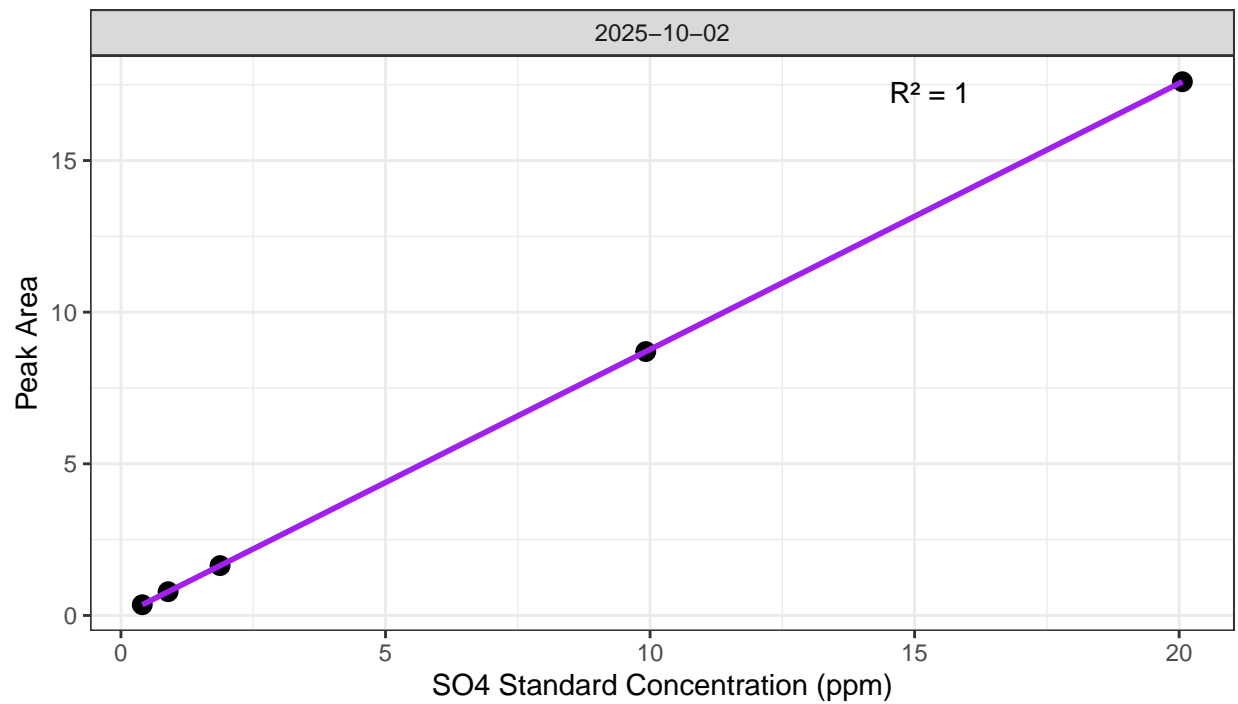
##Fix samples entered incorrectly

## 0.2 Assess Standard Curves

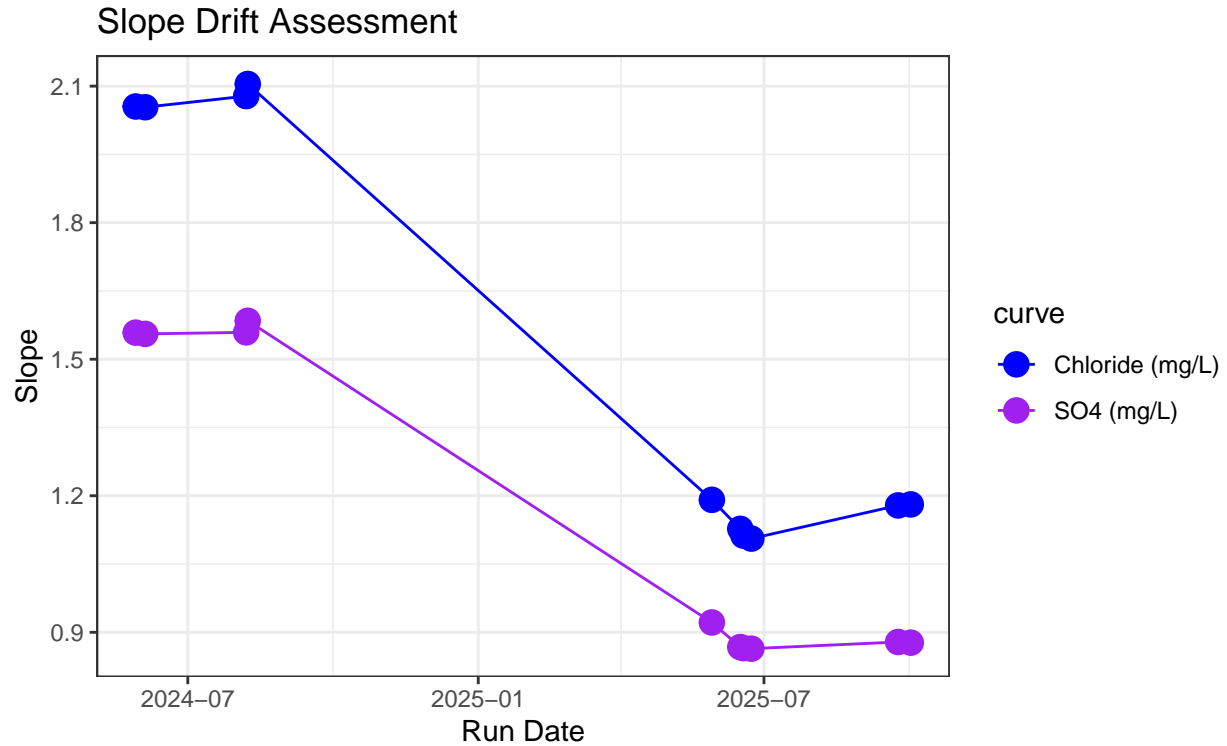
Chloride Std Curve



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"
```

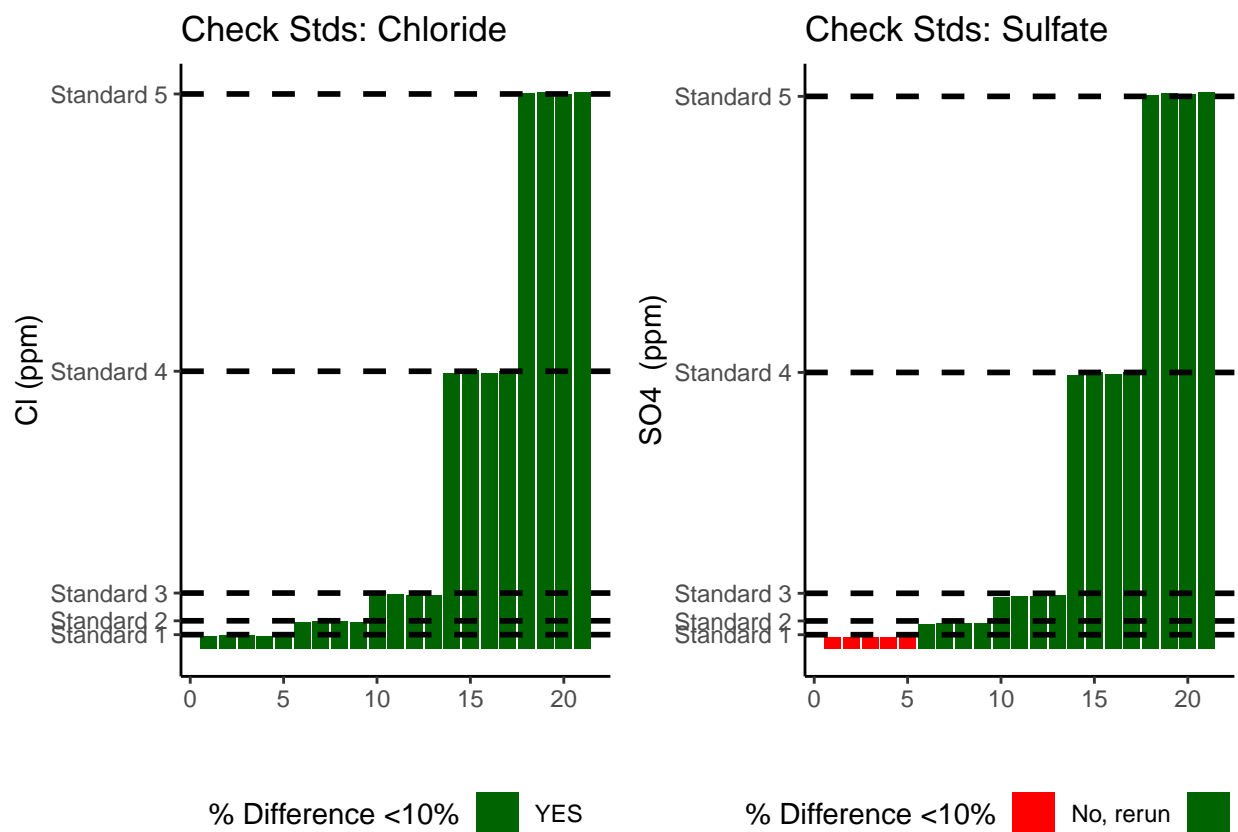
### 0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID mean_Cl sd_Cl   cv_Cl flag_Cl
##   <chr>      <dbl> <dbl>   <dbl> <chr>
## 1 Standard 1    4.66 0.133 0.0284 Chloride Check Standard RSD within Range - P~
## 2 Standard 2    9.63 0.218 0.0226 Chloride Check Standard RSD within Range - P~
## 3 Standard 3   19.3 0.206 0.0107 Chloride Check Standard RSD within Range - P~
## 4 Standard 4   99.8 0.526 0.00527 Chloride Check Standard RSD within Range - P~
## 5 Standard 5  201. 0.353 0.00176 Chloride Check Standard RSD within Range - P~
```

```
## # A tibble: 5 x 5
##   sample_ID mean_S04 sd_S04   cv_S04 flag_S04
##   <chr>      <dbl> <dbl>   <dbl> <chr>
## 1 Standard 1    0.419 0.0113 0.0269 Sulfate Check Standard RSD within Range - ~
## 2 Standard 2    0.914 0.0166 0.0182 Sulfate Check Standard RSD within Range - ~
## 3 Standard 3    1.91 0.0238 0.0125 Sulfate Check Standard RSD within Range - ~
## 4 Standard 4    9.98 0.0516 0.00517 Sulfate Check Standard RSD within Range - ~
## 5 Standard 5   20.1 0.0485 0.00241 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"
```



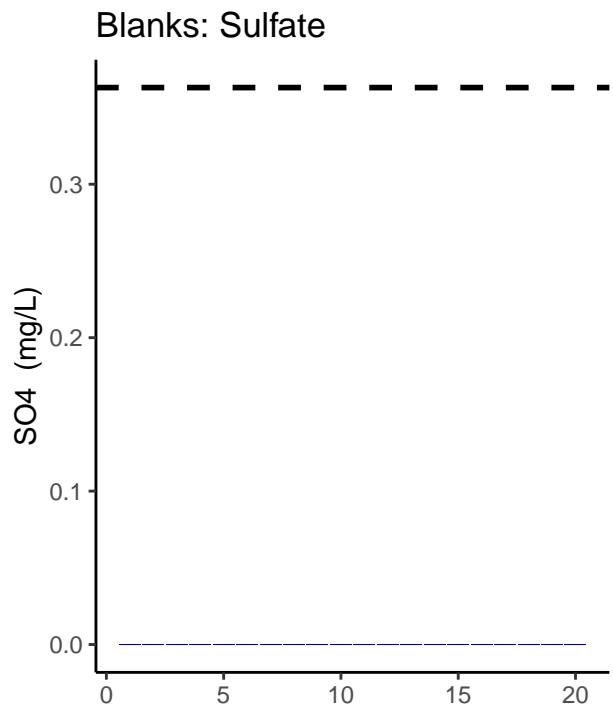
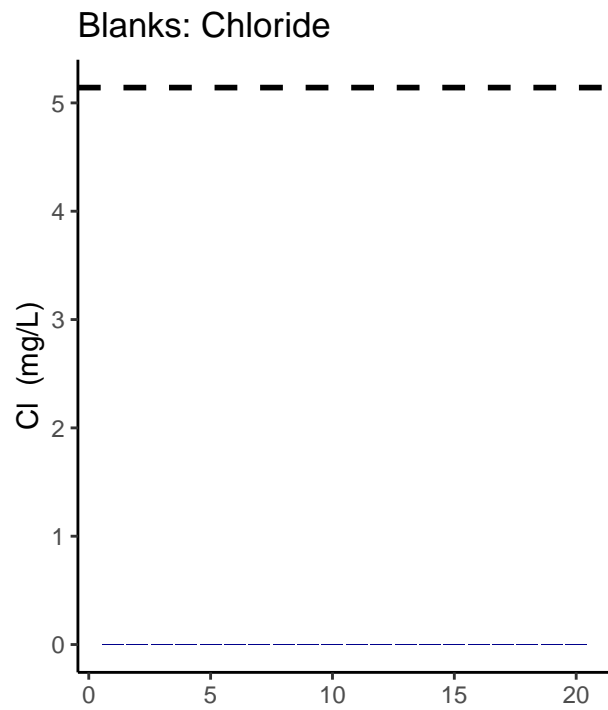
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [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 ■ YE

Blank Conc <25% Quartile Samples ■ YE

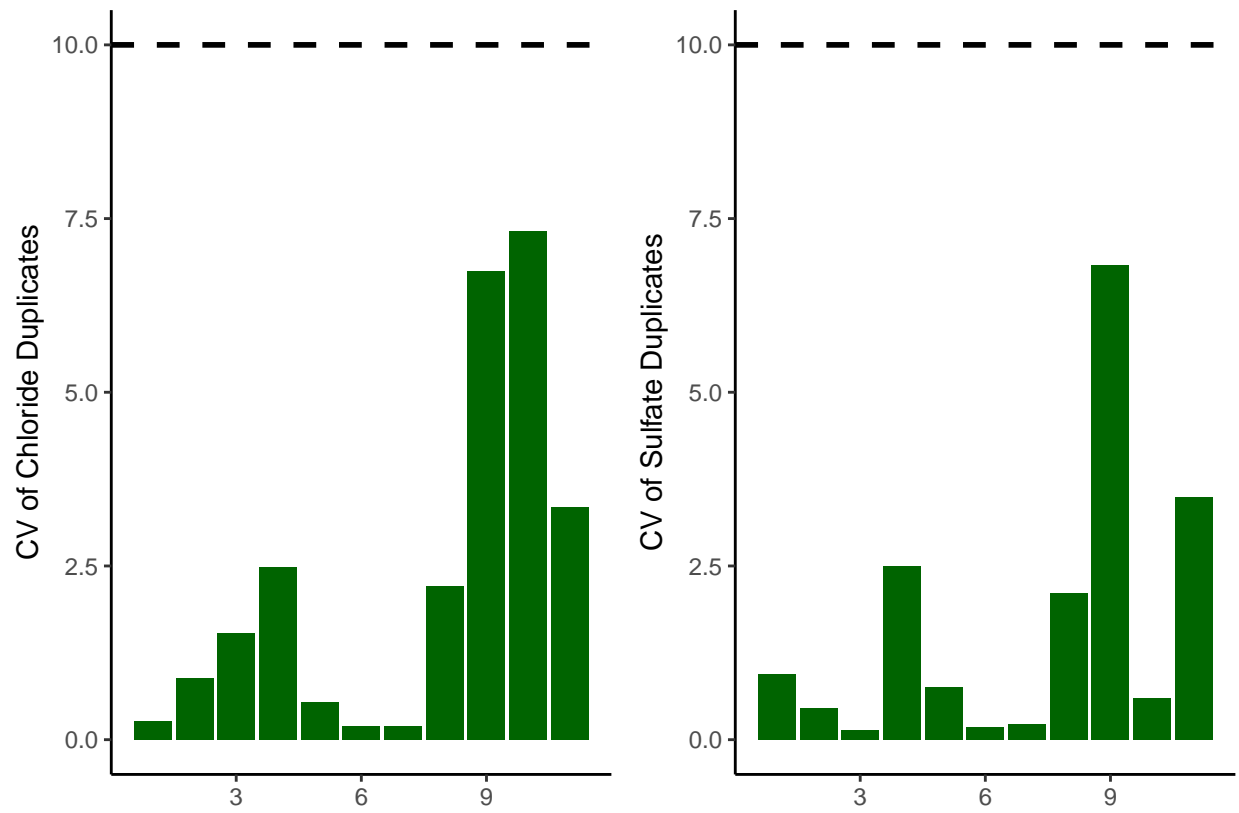
```
## Chloride blanks mean ppm:
```

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

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

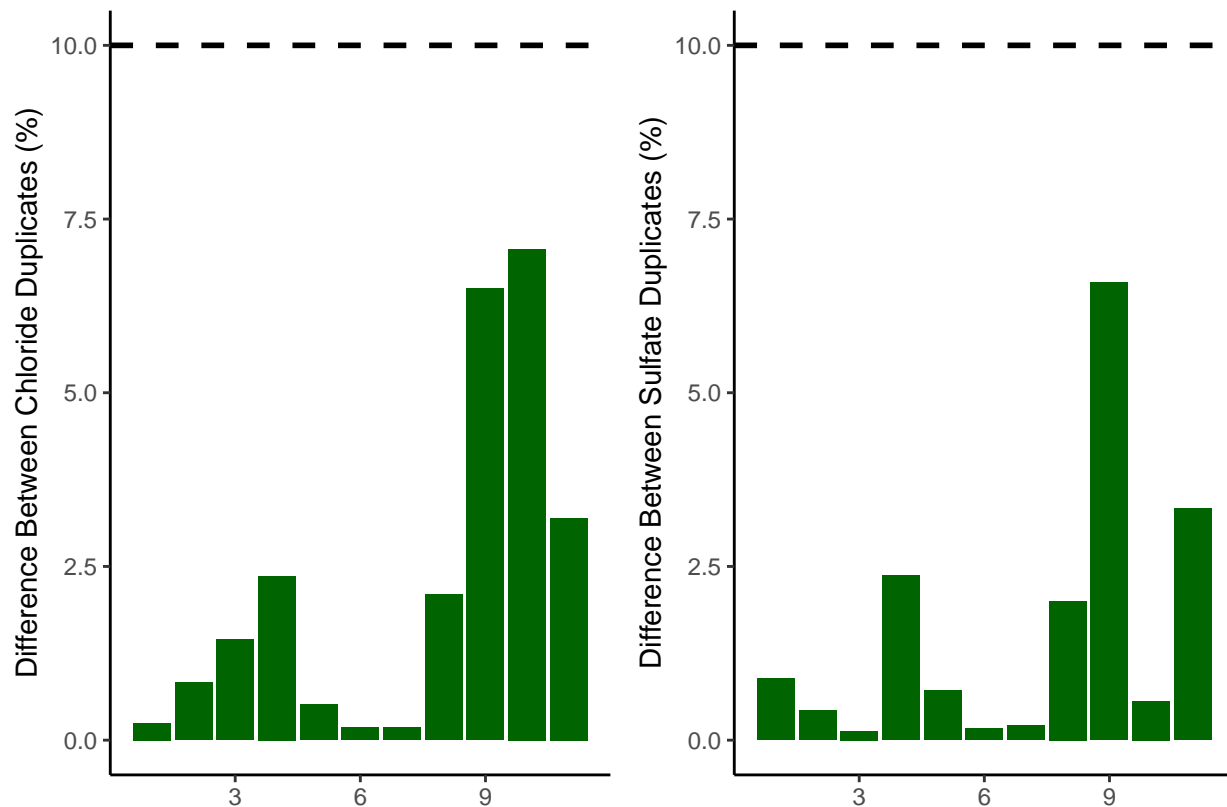
```
## [1] 0
```

## 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"),

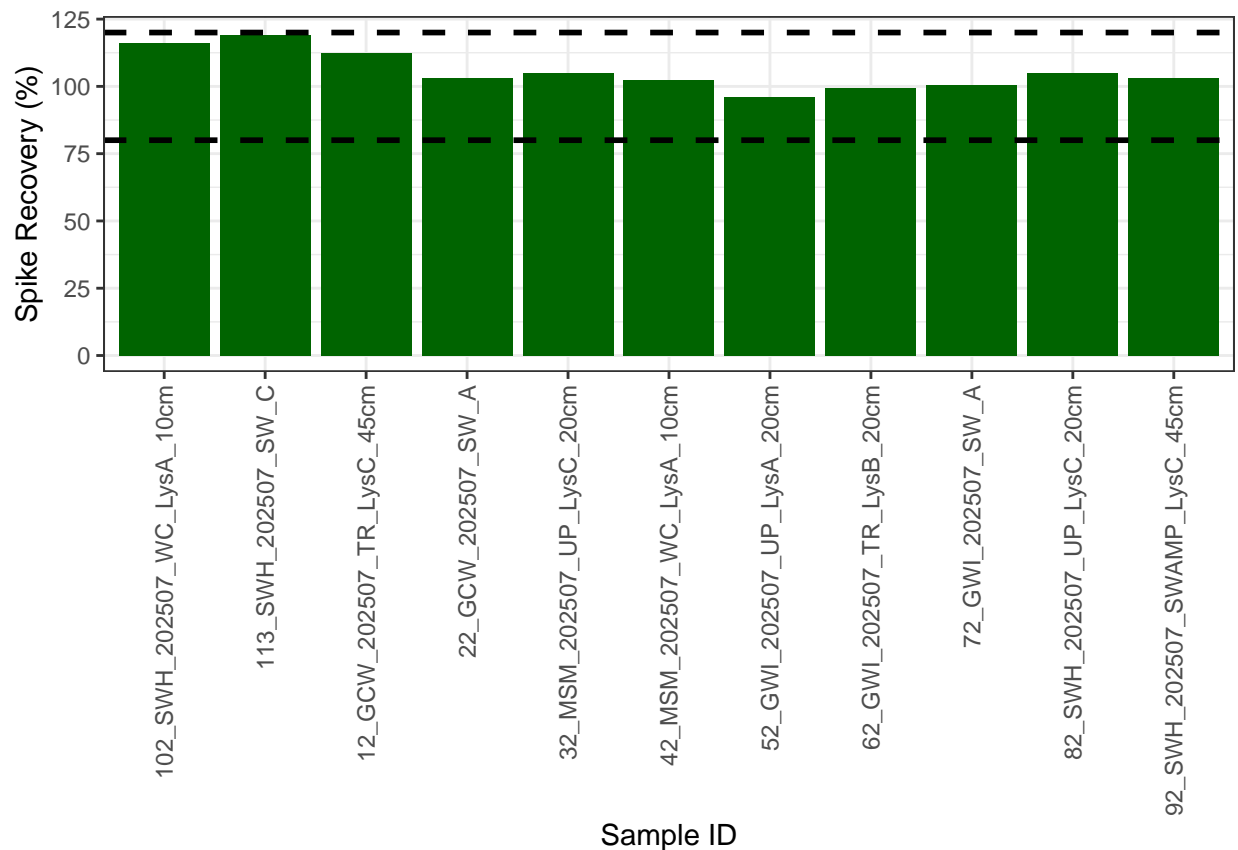
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)

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

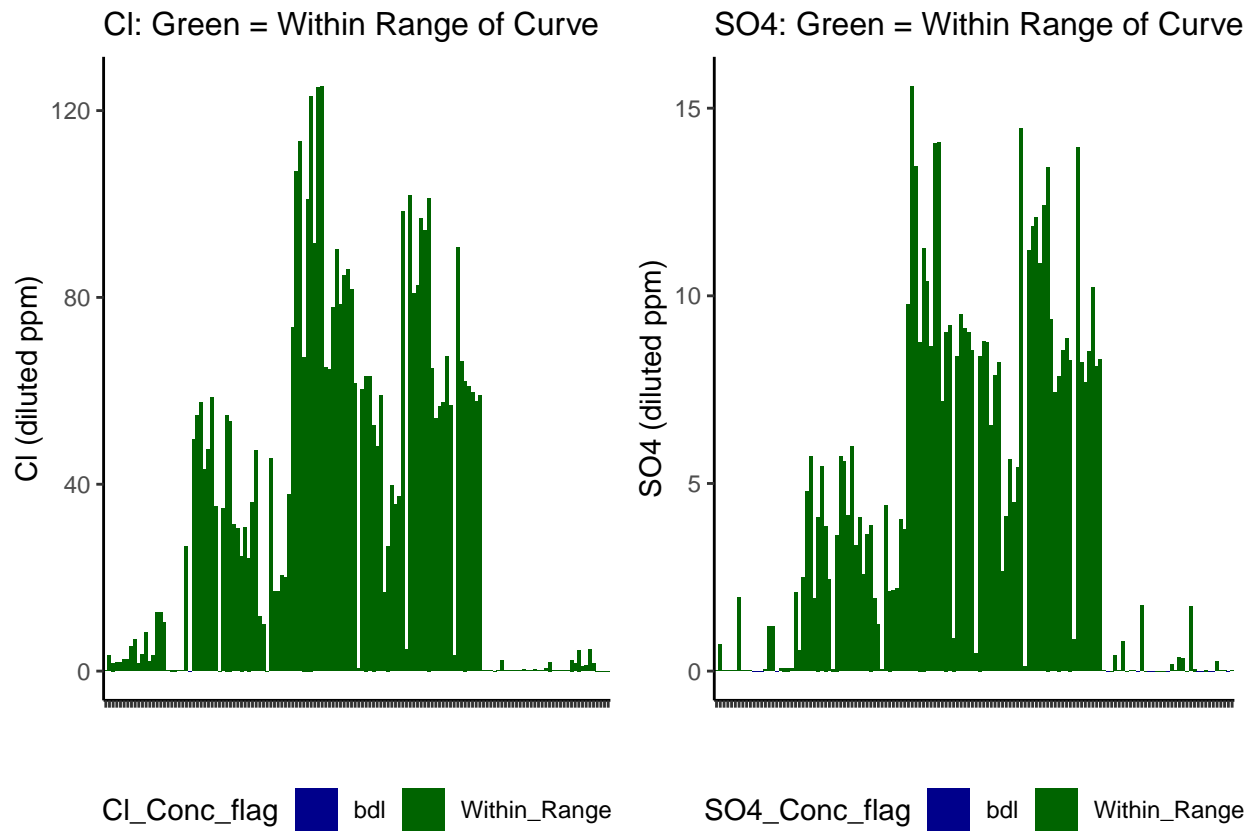


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	89.85507
bdl	10.14493

Table 2: Cl samples

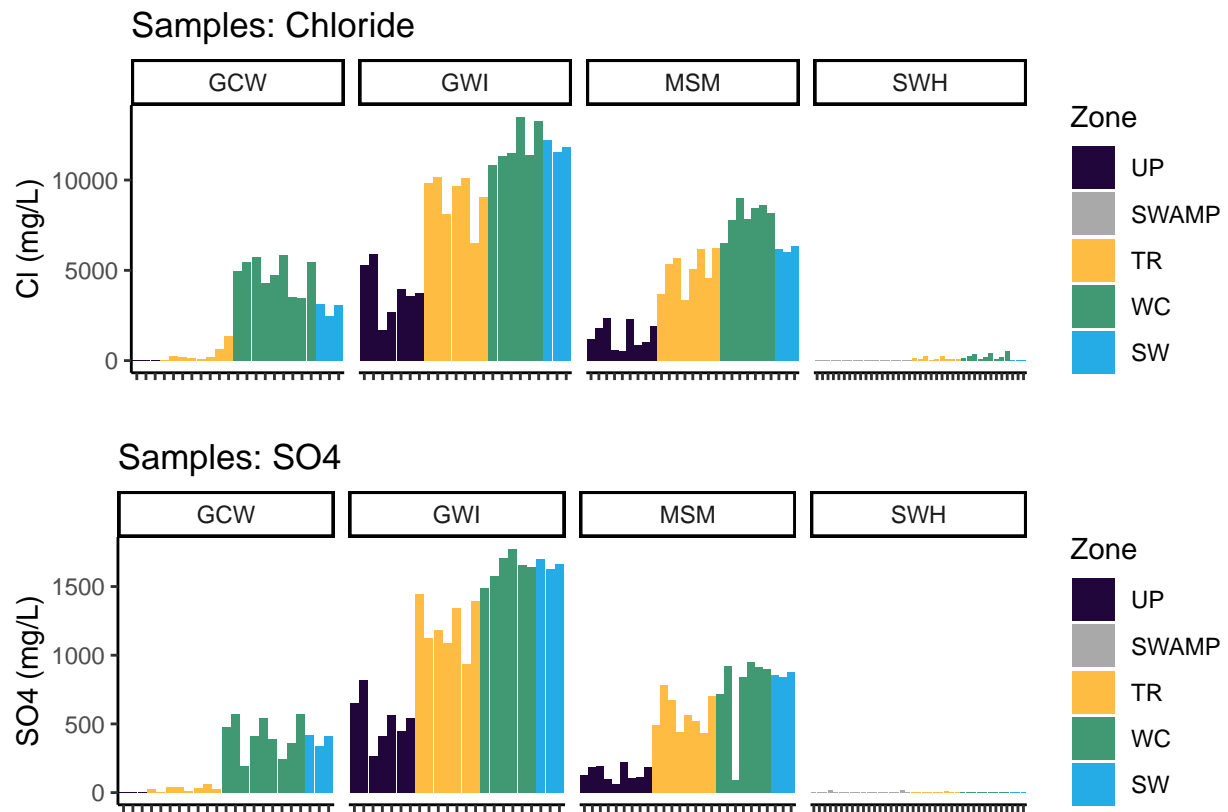
Cl_Conc_flag	Percent_samples
Within_Range	99.2753623
bdl	0.7246377

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

## Some sample IDs are missing from metadata.

## [1] "9" "10" "88" "89"

## 0.10 Visualize Data by Plot



## 0.11 Export Processed Data

#end