

Synoptic CB: Porewater SO₄/Cl

August 2024 Samples

2025-09-04

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```
##Add Required Packages
```

0.1 Run Information

```
##### 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 S04 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

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_c1 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202408_C1.txt"
raw_file_name_s04 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202408_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_C1_S04_202408.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_C1_S04_QAAClog_2024.csv"
```

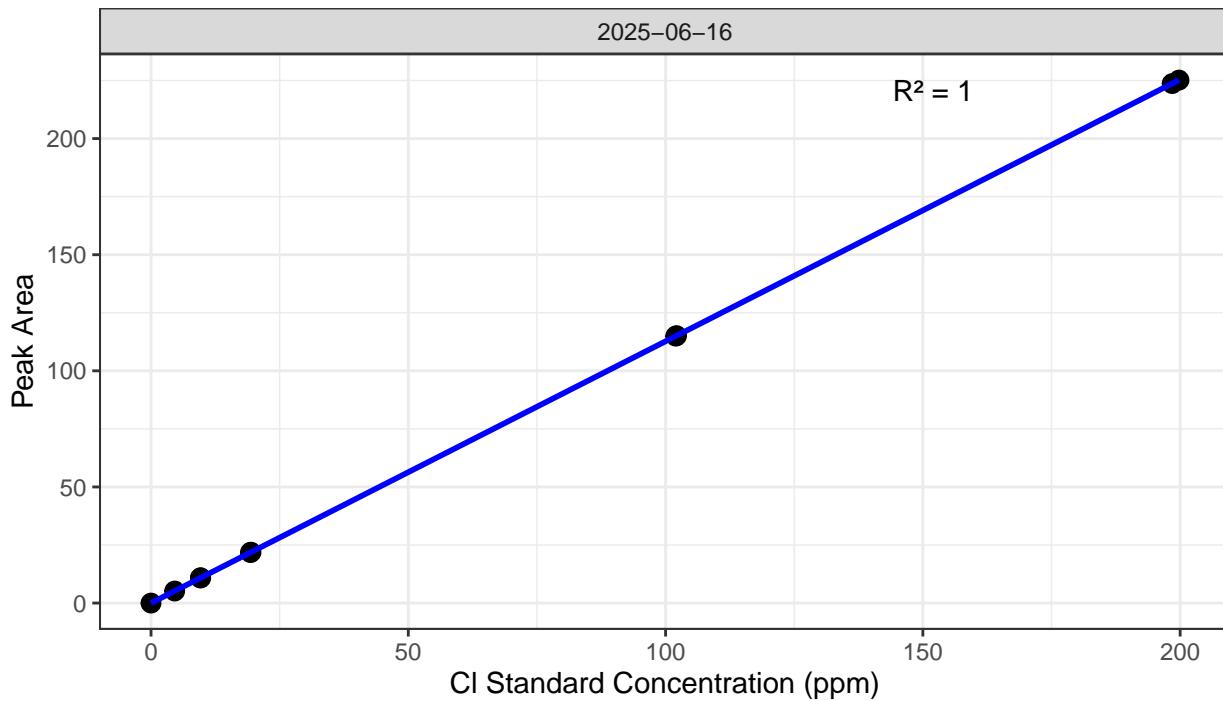
```
##Set Up Code - constants and QAQC cutoffs
```

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

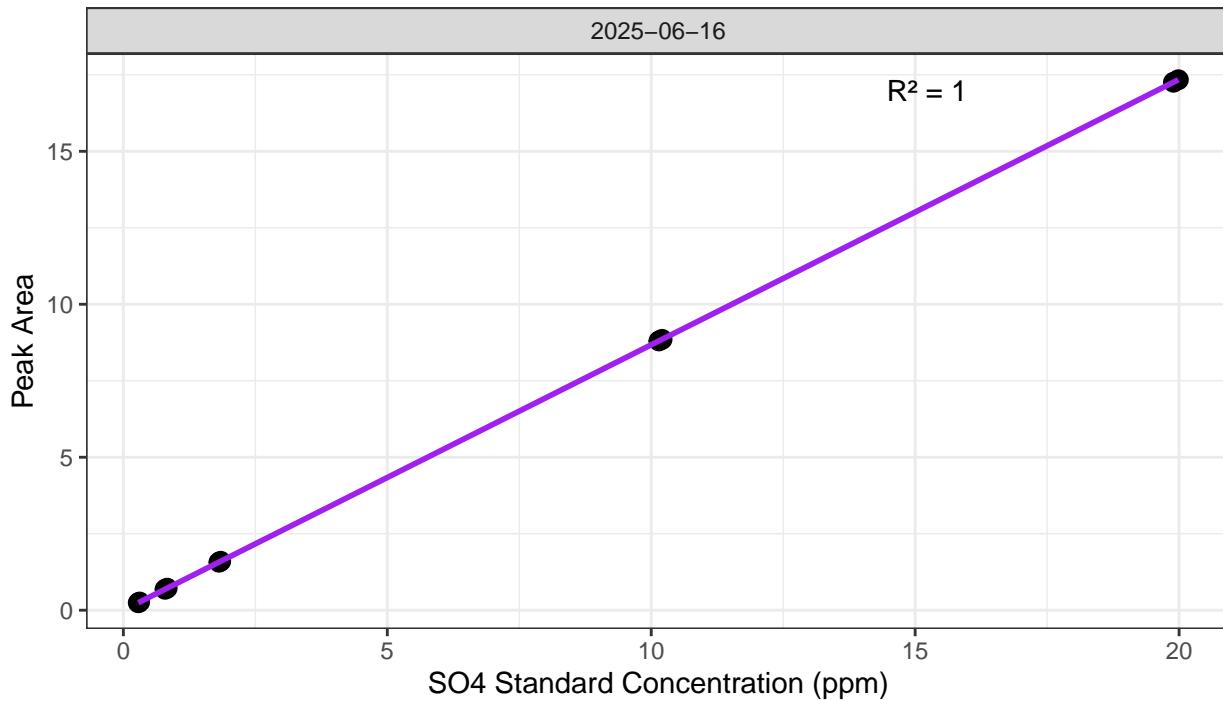
```
##Import Sample Data
```

0.2 Assess Standard Curves

Chloride Std Curve

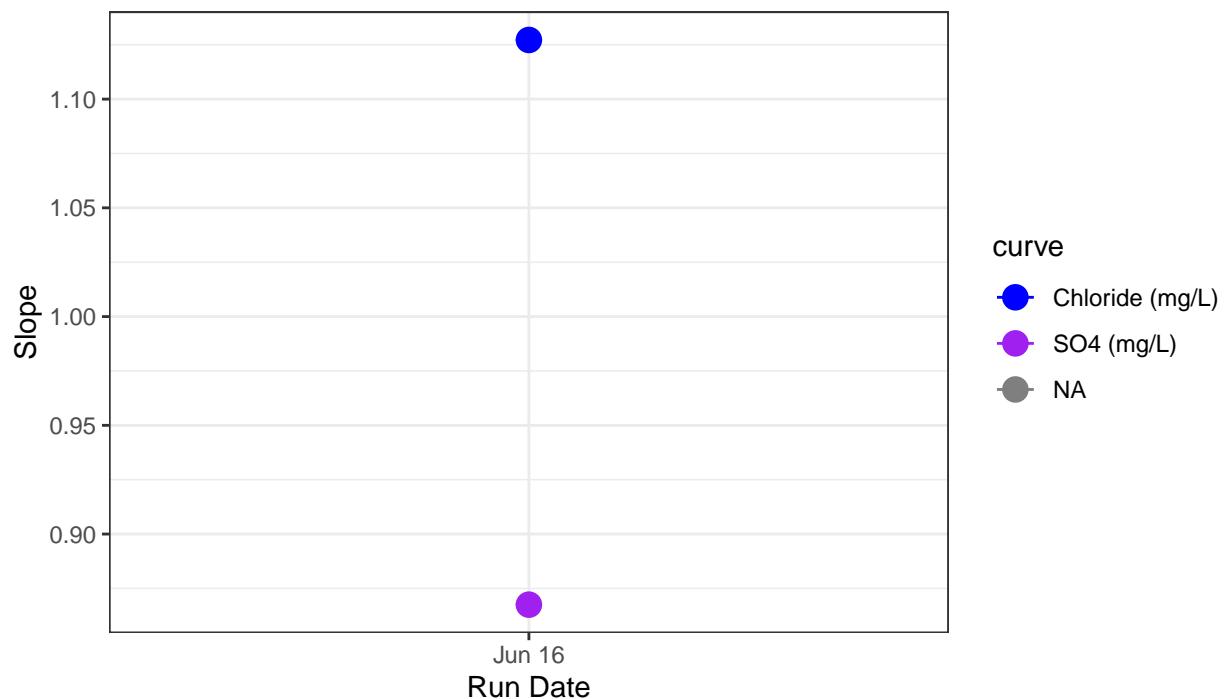


Sulfate Std Curve



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

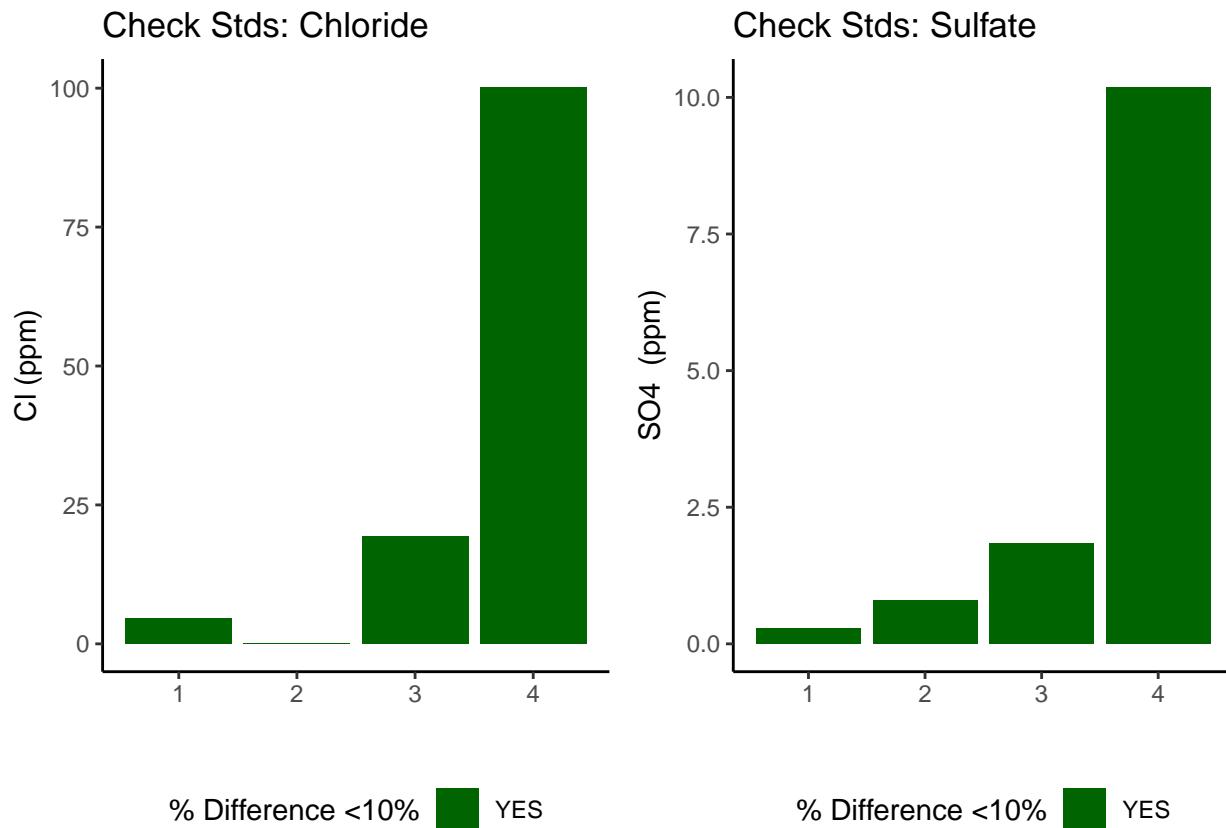
Slope Drift Assessment



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

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

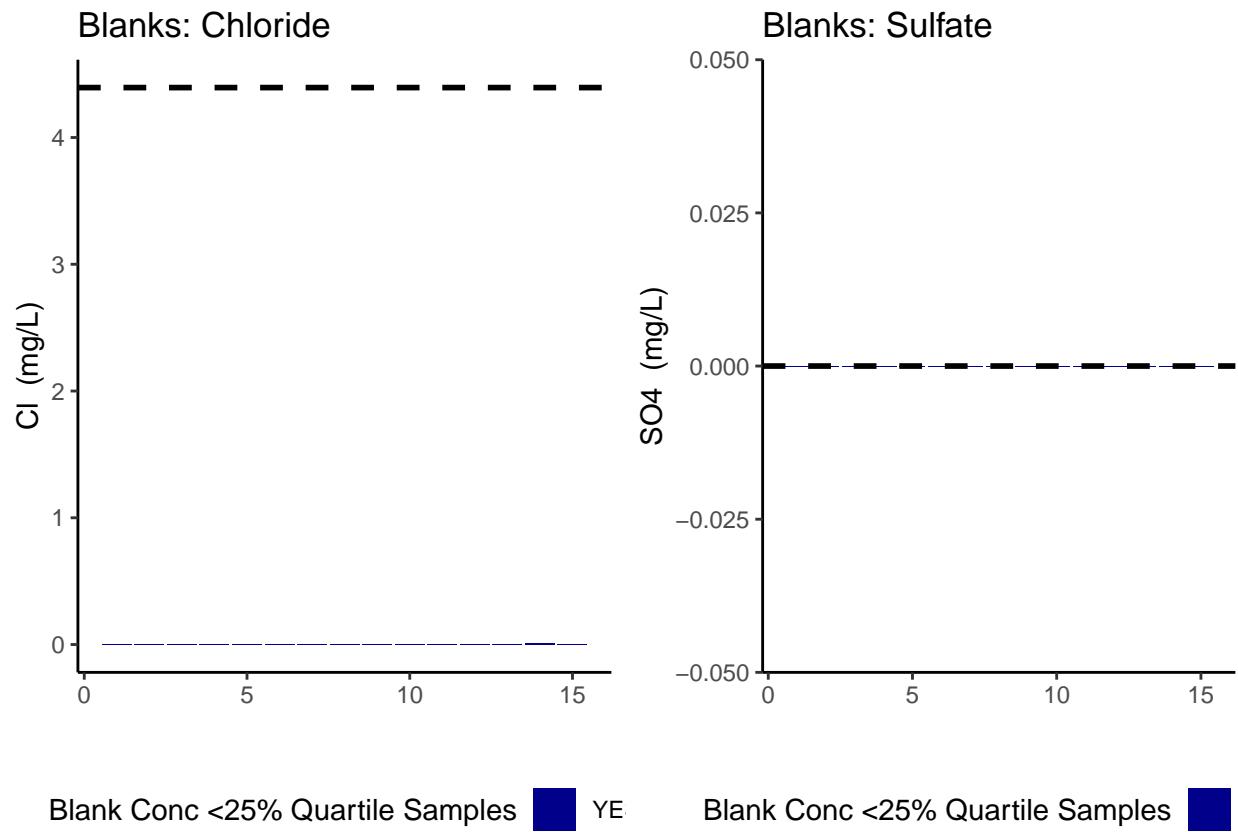
0.3 Assess Check Standards



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

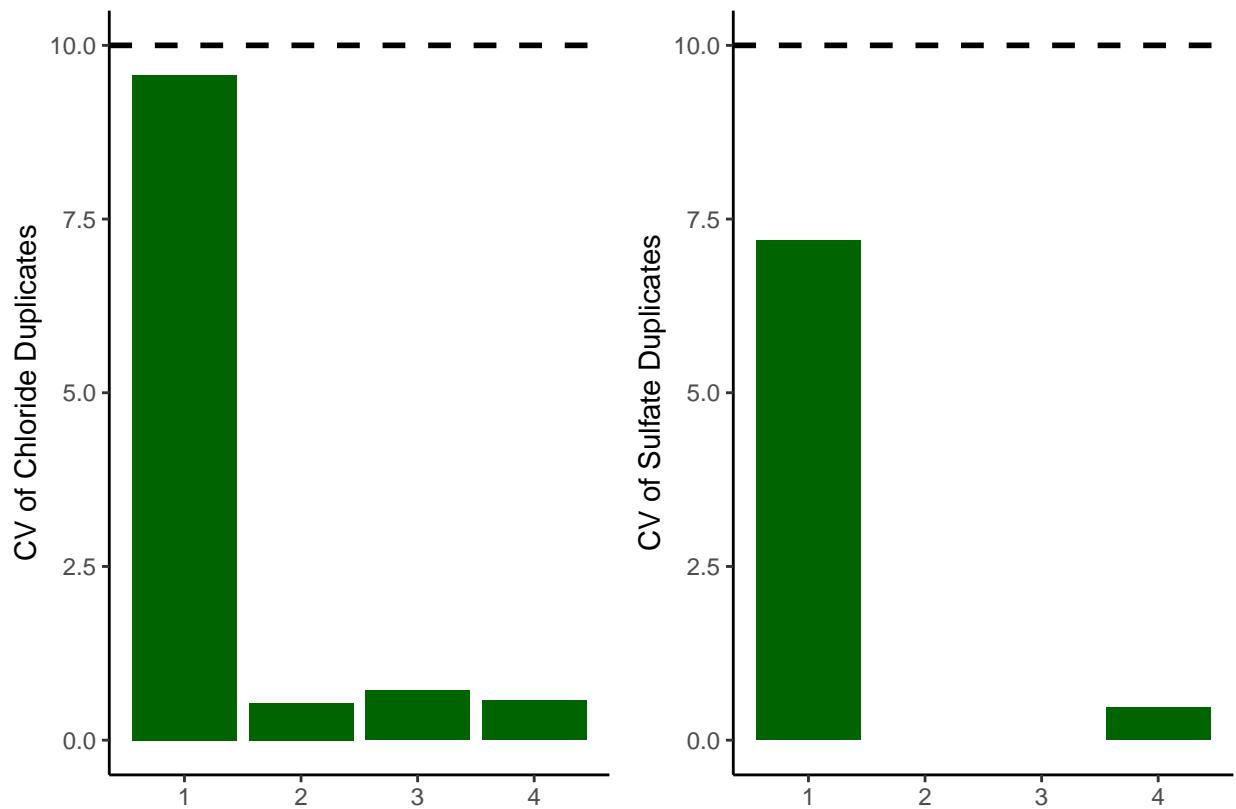
```
## [1] 0.0008533333
```

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

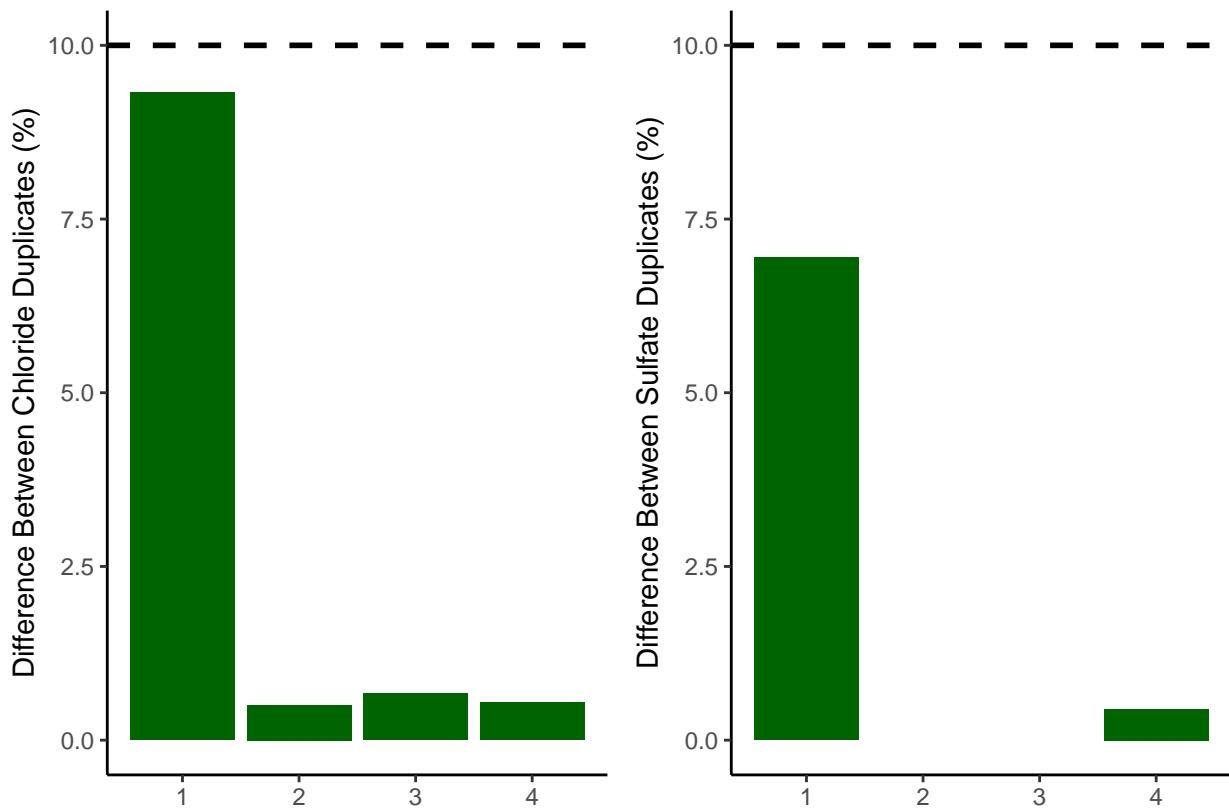
```
## [1] 0
```

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% - 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$salinity <- ((1.807 * all_dat$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"),
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"),  

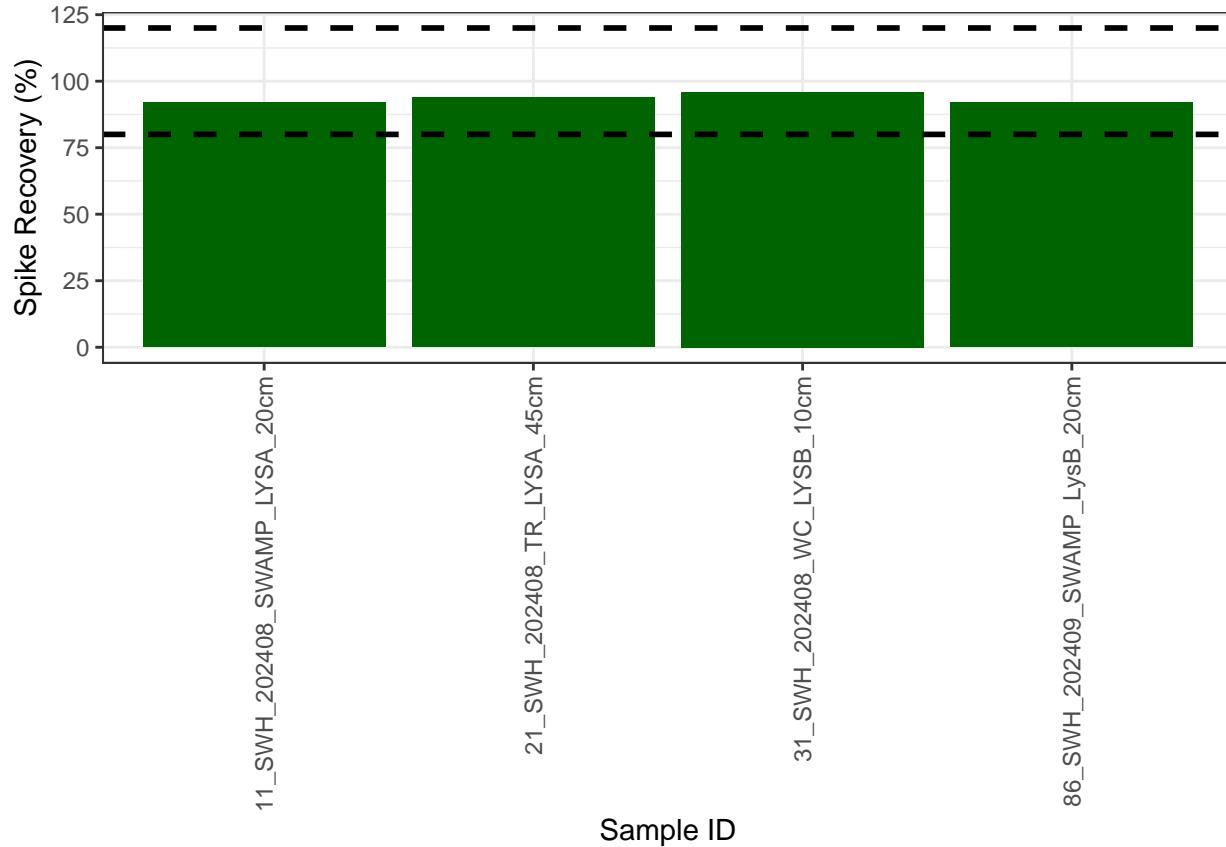
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)  

head(all_dat)

```

0.7 Assess Analytical Spikes



```

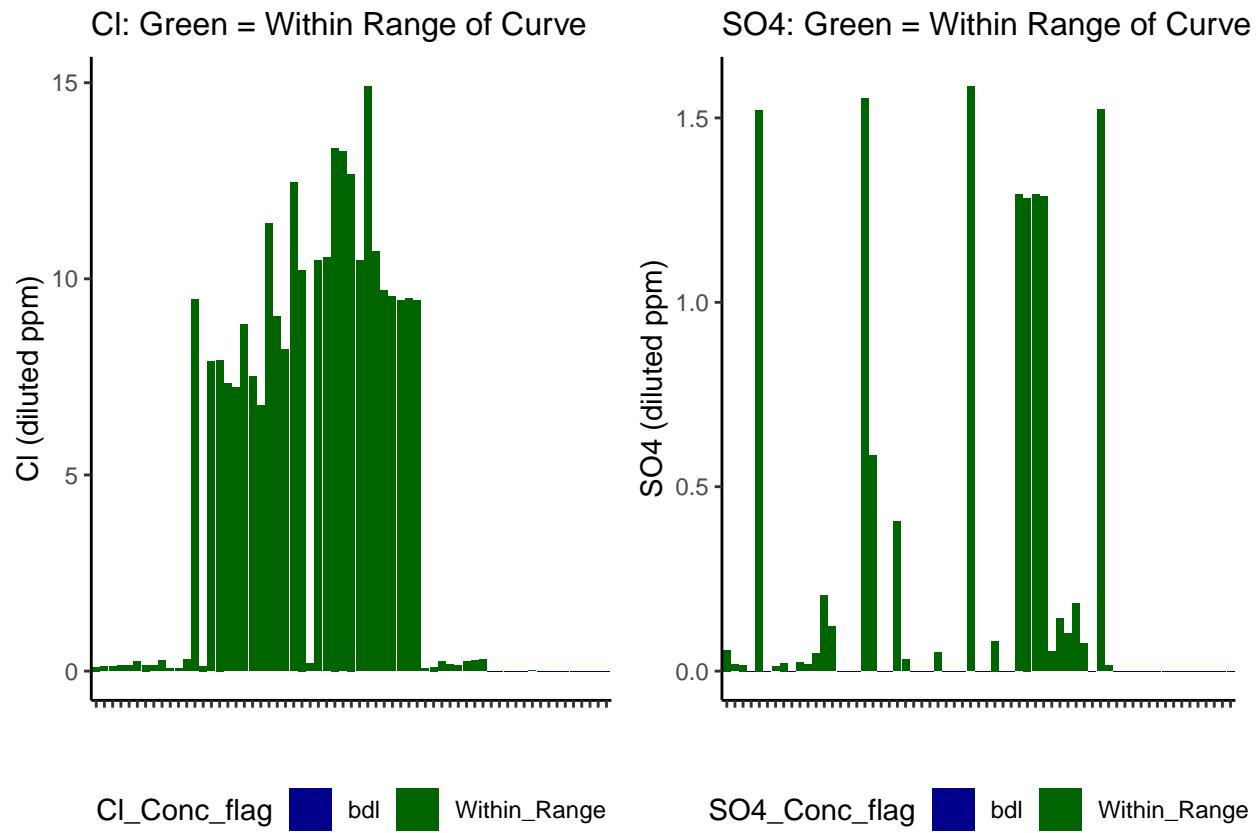
## # A tibble: 1 x 4
##   S04_spks_flag no_rows Total Percent
##   <chr>          <int> <int>    <dbl>
## 1 Yes             4      4     100
  

## [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
```

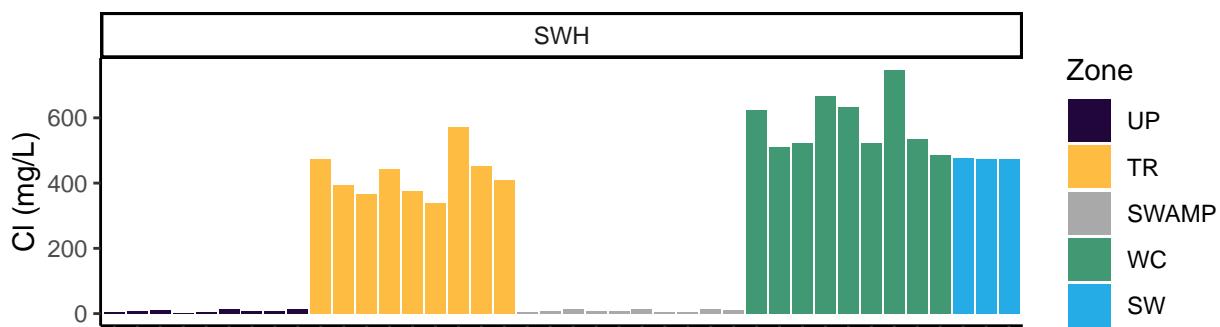


0.9 Check to see if samples run match metadata & merge info

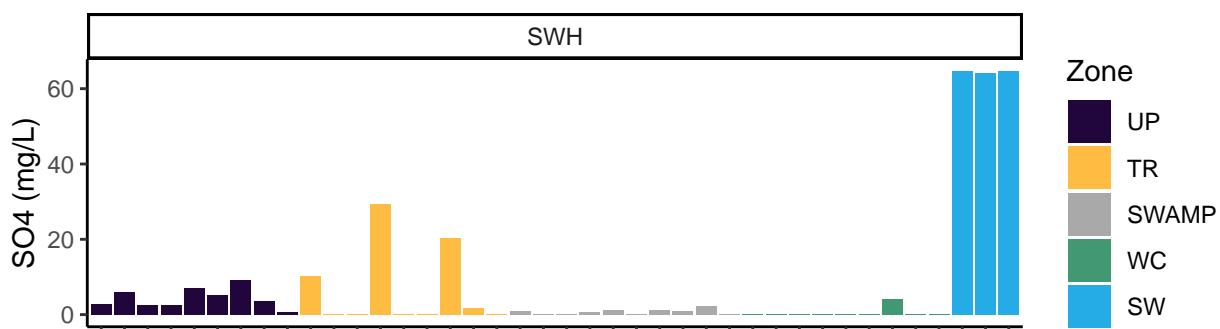
```
## All sample IDs are present in metadata.
```

0.10 Visualize Data by Plot

Samples: Chloride



Samples: SO4



0.11 Export Processed Data

#end