

Dionex_COMPASS_TEMPEST

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Daily Set up

Read in and Format the raw data - change wd & file names (Make sure files are UTF-8 encoded)

```
# SULFATE DATA:

## Read in raw data file from Dionex - copied and saved as a txt
Sdat <- read.table("Raw Data/COMPASS_TEMPEST_20230606_SO4a.txt",sep='\t' , header=T, skip=3)
head(Sdat)

##      X          X.1    IC.SO4 IC.SO4.1 IC.SO4.2 IC.SO4.3 IC.SO4.4
## 1 44 TEMPEST_C_C6_20230603 Unknown   n.a.     n.a.     n.a.     n.a.
## 2 45 TEMPEST_C_H6_20230603 Unknown   n.a.     n.a.     n.a.     n.a.
## 3 46 TEMPEST_C_I5_20230603 Unknown   n.a.     n.a.     n.a.     n.a.
## 4 47 TEMPEST_C_H6_20230605 Unknown 4.373    2.3894   0.47    0.0544   0.35
## 5 48 TEMPEST_FW_C3_20230603 Unknown 4.383    6.9627   0.69    0.1403   0.90
## 6 49 TEMPEST_FW_D5_20230603 Unknown   n.a.     n.a.     n.a.     n.a.
##      IC.SO4.5
## 1      n.a.
## 2      n.a.
## 3      n.a.
## 4      M
## 5      M
## 6      n.a.

## Only keep the columns that we need
Sdat <- Sdat[,c(2,5,7)] # dont need this here
head(Sdat)

##          X.1 IC.SO4.1 IC.SO4.3
## 1 TEMPEST_C_C6_20230603   n.a.     n.a.
## 2 TEMPEST_C_H6_20230603   n.a.     n.a.
## 3 TEMPEST_C_I5_20230603   n.a.     n.a.
## 4 TEMPEST_C_H6_20230605 2.3894   0.0544
## 5 TEMPEST_FW_C3_20230603 6.9627   0.1403
## 6 TEMPEST_FW_D5_20230603   n.a.     n.a.
```

```

## Name the columns correctly
colnames(Sdat) <- c( "Sample_ID", "S04_ppm", "S04_Area")
Sdat$Sample_ID <- as.factor(Sdat$Sample_ID)
Sdat$S04_ppm <- as.numeric(Sdat$S04_ppm)

## Warning: NAs introduced by coercion

Sdat$S04_Area <- as.numeric(Sdat$S04_Area)

## Warning: NAs introduced by coercion

Sdat <- as.data.frame(Sdat)
head(Sdat)

##             Sample_ID S04_ppm S04_Area
## 1  TEMPEST_C_C6_20230603      NA      NA
## 2  TEMPEST_C_H6_20230603      NA      NA
## 3  TEMPEST_C_I5_20230603      NA      NA
## 4  TEMPEST_C_H6_20230605  2.3894   0.0544
## 5 TEMPEST_FW_C3_20230603  6.9627   0.1403
## 6 TEMPEST_FW_D5_20230603      NA      NA

#Chloride data
## Read in raw data file from Dionex - copied and saved as a txt
Cldat <- read.table("Raw Data/COMPASS_TEMPEST_20230606_Cla.txt",sep='\t' , header=T, skip=3)
head(Cldat)

##      X          X.1      X.2 IC.Cl IC.Cl.1 IC.Cl.2 IC.Cl.3 IC.Cl.4
## 1 44 TEMPEST_C_C6_20230603 Unknown n.a.    n.a.    n.a.    n.a.    n.a.
## 2 45 TEMPEST_C_H6_20230603 Unknown n.a.    n.a.    n.a.    n.a.    n.a.
## 3 46 TEMPEST_C_I5_20230603 Unknown n.a.    n.a.    n.a.    n.a.    n.a.
## 4 47 TEMPEST_C_H6_20230605 Unknown n.a.    n.a.    n.a.    n.a.    n.a.
## 5 48 TEMPEST_FW_C3_20230603 Unknown n.a.    n.a.    n.a.    n.a.    n.a.
## 6 49 TEMPEST_FW_D5_20230603 Unknown n.a.    n.a.    n.a.    n.a.    n.a.

##      IC.Cl.5
## 1      n.a.
## 2      n.a.
## 3      n.a.
## 4      n.a.
## 5      n.a.
## 6      n.a.

## Only keep the columns that we need
Cldat <- Cldat[,c(2,5,7)]
head(Cldat)

##          X.1 IC.Cl.1 IC.Cl.3
## 1 TEMPEST_C_C6_20230603  n.a.    n.a.
## 2 TEMPEST_C_H6_20230603  n.a.    n.a.
## 3 TEMPEST_C_I5_20230603  n.a.    n.a.
## 4 TEMPEST_C_H6_20230605  n.a.    n.a.
## 5 TEMPEST_FW_C3_20230603  n.a.    n.a.
## 6 TEMPEST_FW_D5_20230603  n.a.    n.a.

```

```

## Name the columns correctly
colnames(Cldat) <- c( "Sample_ID", "Cl_ppm", "Cl_Area")
Cldat$Sample_ID <- as.factor(Cldat$Sample_ID)
Cldat$Cl_ppm <- as.numeric(Cldat$Cl_ppm)

```

```

## Warning: NAs introduced by coercion

```

```

Cldat$Cl_Area <- as.numeric(Cldat$Cl_Area)

```

```

## Warning: NAs introduced by coercion

```

```

Cldat <- as.data.frame(Cldat)
head(Cldat)

```

```

##             Sample_ID Cl_ppm Cl_Area
## 1  TEMPEST_C_C6_20230603     NA     NA
## 2  TEMPEST_C_H6_20230603     NA     NA
## 3  TEMPEST_C_I5_20230603     NA     NA
## 4  TEMPEST_C_H6_20230605     NA     NA
## 5 TEMPEST_FW_C3_20230603     NA     NA
## 6 TEMPEST_FW_D5_20230603     NA     NA

```

Bring the data back together:

```

all_dat <- merge(Sdat, Cldat, by="Sample_ID")
head(all_dat)

```

```

##   Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area
## 1       168.9031  23.3576 203.7164 279.6752
## 2       168.9031  23.3576  29.8315  32.6201
## 3       168.9031  23.3576   0.0014  0.0001
## 4       168.9031  23.3576  40.9777  53.7128
## 5       168.9031  23.3576      NA      NA
## 6       13.6022   2.4364 203.7164 279.6752

```

Remove empty lines

```

all_dat <- all_dat[!(is.na(all_dat$Sample_ID) | all_dat$Sample_ID=="") , ]
head(all_dat)

```

```

##   Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area
## 26 Lab Blank      NA      NA      NA      NA
## 27 Lab Blank      NA      NA  0.0079  0.0108
## 28 Lab Blank      NA      NA      NA      NA
## 29 Lab Blank      NA      NA      NA      NA
## 30 Lab Blank      NA      NA  0.0114  0.0156
## 31 Lab Blank      NA      NA      NA      NA

```

```

all_dat <- droplevels(all_dat[!all_dat$Sample_ID == 'Lab Blank',])
head(all_dat)

```

```

##      Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area
## 107 Standard 1  0.4622   0.5264  5.2376  7.1905
## 108 Standard 1  0.4622   0.5264  5.1529  7.0742
## 109 Standard 1  0.4374   0.4982  5.2376  7.1905
## 110 Standard 1  0.4374   0.4982  5.1529  7.0742
## 111 Standard 2  1.0048   1.1446 11.4708 15.7479
## 112 Standard 2  1.0048   1.1446 11.3597 15.5954

```

```
all_dat[is.na(all_dat)] <- 0
```

Pull out standards - could do some checks here if we want

```

stds <- all_dat[grep("Standard", all_dat$Sample_ID),]
head(stds)

```

```

##      Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area
## 107 Standard 1  0.4622   0.5264  5.2376  7.1905
## 108 Standard 1  0.4622   0.5264  5.1529  7.0742
## 109 Standard 1  0.4374   0.4982  5.2376  7.1905
## 110 Standard 1  0.4374   0.4982  5.1529  7.0742
## 111 Standard 2  1.0048   1.1446 11.4708 15.7479
## 112 Standard 2  1.0048   1.1446 11.3597 15.5954

```

```

stds_chk_S <- stds %>%
  group_by(Sample_ID) %>%
  summarise(mean = mean(S04_ppm), sd = sd(S04_ppm))
stds_chk_S$cv <- (stds_chk_S$sd/stds_chk_S$mean)*100
stds_chk_S$flag <- ifelse(stds_chk_S$cv <2, 'YES', 'NO, rerun')
head(stds_chk_S)

```

```

## # A tibble: 5 x 5
##   Sample_ID     mean       sd     cv flag
##   <fct>        <dbl>     <dbl>  <dbl> <chr>
## 1 Standard 1  0.450    0.0143   3.18 NO, rerun
## 2 Standard 2  0.993    0.0138   1.39 YES
## 3 Standard 3  2.02     0.0309   1.53 YES
## 4 Standard 4  10.5     NA       NA     <NA>
## 5 Standard 5  20.5     NA       NA     <NA>

```

```

stds_chk_Cl <- stds %>%
  group_by(Sample_ID) %>%
  summarise(mean = mean(Cl_ppm), sd = sd(Cl_ppm))
stds_chk_Cl$cv <- (stds_chk_Cl$sd/stds_chk_Cl$mean)*100
stds_chk_Cl$flag <- ifelse(stds_chk_Cl$cv <2, 'YES', 'NO, rerun')
head(stds_chk_Cl)

```

```

## # A tibble: 5 x 5
##   Sample_ID     mean       sd     cv flag
##   <fct>        <dbl>     <dbl>  <dbl> <chr>
## 1 Standard 1  5.20     0.0489   0.941 YES

```

```

## 2 Standard 2 11.4 0.0641 0.562 YES
## 3 Standard 3 20.8 0.117 0.564 YES
## 4 Standard 4 103. NA NA <NA>
## 5 Standard 5 204. NA NA <NA>

```

```

lmS <- lm(stds$S04_Area ~ stds$S04_ppm)
S04_sum <- summary(lmS)
S04_Slope <- S04_sum$coefficients[2, 1]
S04_Int <- S04_sum$coefficients[1, 1]

lmCl <- lm(stds$Cl_Area ~ stds$Cl_ppm)
Cl_sum <- summary(lmCl)
Cl_Slope <- Cl_sum$coefficients[2, 1]
Cl_Int <- Cl_sum$coefficients[1, 1]

```

Calculate mmol/L concentrations

```

#remove standards from sample dataframe
sampledat <- all_dat[!grepl("Standard", all_dat$Sample_ID),]
head(sampledat)

##                               Sample_ID S04_ppm S04_Area   Cl_ppm Cl_Area
## 126 TEMPEST_C_C6_20230515  0.3224   0.3338 30.5616 38.1427
## 127 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000  0.0000
## 128 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000  0.0000
## 129 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000  0.0000
## 130 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000  0.0000
## 131 TEMPEST_C_F6_20230515  0.0000   0.0000 28.2531 35.2615

# Constants needed for calculations:
clmw <- 35.45      #molecular weight of Chloride: 35.45
smw <- 32.06        #molecular weight of sulfur: 32.06

# Convert ppm to mmol/L
sampledat$S04_mM <- (sampledat$S04_ppm / smw)
sampledat$Cl_mM <- (sampledat$Cl_ppm / clmw)

# 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
sampledat$salinity <- ((1.807 * sampledat$Cl_ppm) + 0.026) / 1000

head(sampledat)

##                               Sample_ID S04_ppm S04_Area   Cl_ppm Cl_Area      S04_mM      Cl_mM

```

```

## 126 TEMPEST_C_C6_20230515 0.3224 0.3338 30.5616 38.1427 0.01005614 0.8621044
## 127 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 128 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 129 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 130 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 131 TEMPEST_C_F6_20230515 0.0000 0.0000 28.2531 35.2615 0.00000000 0.7969845
##           salinity
## 126 0.05525081
## 127 0.00002600
## 128 0.00002600
## 129 0.00002600
## 130 0.00002600
## 131 0.05107935

```

Pull out dups and check with percent difference

```

#Show me the data that we have from the calculations
head(sampledat)

```

```

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM     Cl_mM
## 126 TEMPEST_C_C6_20230515 0.3224 0.3338 30.5616 38.1427 0.01005614 0.8621044
## 127 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 128 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 129 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 130 TEMPEST_C_C6_20230603 0.0000 0.0000 0.0000 0.0000 0.00000000 0.0000000
## 131 TEMPEST_C_F6_20230515 0.0000 0.0000 28.2531 35.2615 0.00000000 0.7969845
##           salinity
## 126 0.05525081
## 127 0.00002600
## 128 0.00002600
## 129 0.00002600
## 130 0.00002600
## 131 0.05107935

```

```

#pull out any rows that have "dup" in the SampleID column
dups <- sampledat %>%
  filter(str_detect(Sample_ID, "_dup"))      #have to change this to match data
head(dups)

```

```

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM
## 1 TEMPEST_C_I5_20230518_dup 4.1578 4.3055 25.5009 31.8266 0.12968808
## 2 TEMPEST_SW_H3_20230603_dup 0.0000 0.0000 0.0000 0.0000 0.00000000
## 3 TEMPEST_SW_H6_20230515_dup 0.4053 0.4197 36.6535 45.7458 0.01264192
##           Cl_mM   salinity
## 1 0.7193484 0.04610613
## 2 0.0000000 0.00002600
## 3 1.0339492 0.06625887

```

```

#remove these from sample dataframe in a new dataframe
sampledat2 <- sampledat %>%
  filter(!str_detect(Sample_ID, "_dup")) %>%

```

```

filter(!str_detect(Sample_ID, "_spk"))
head(sampledat2)

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area     SO4_mM     Cl_mM
## 1 TEMPEST_C_C6_20230515 0.3224  0.3338 30.5616 38.1427 0.01005614 0.8621044
## 2 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 3 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 4 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 5 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 6 TEMPEST_C_F6_20230515 0.0000  0.0000 28.2531 35.2615 0.00000000 0.7969845
##   salinity
## 1 0.05525081
## 2 0.00002600
## 3 0.00002600
## 4 0.00002600
## 5 0.00002600
## 6 0.05107935

#remove the dup from these IDs so we will have duplicate sample names
dups$Sample_ID<-gsub("_dup","",as.character(dups$Sample_ID))
dups <- dups[, -c(2:5)]
colnames(dups) <- c('Sample_ID', 'SO4_mM_dup', "Cl_mM_dup", "salinity_dup")
head(dups)

##           Sample_ID SO4_mM_dup Cl_mM_dup salinity_dup
## 1 TEMPEST_C_I5_20230518 0.12968808 0.7193484  0.04610613
## 2 TEMPEST_SW_H3_20230603 0.00000000 0.0000000  0.00002600
## 3 TEMPEST_SW_H6_20230515 0.01264192 1.0339492  0.06625887

#put it back together with the old data set and look for duplicates
QAdups <- merge(sampledat2, dups)
head(QAdups)

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area     SO4_mM     Cl_mM
## 1 TEMPEST_C_I5_20230518 4.4207  4.5778 25.4606 31.7763 0.13788833 0.7182116
## 2 TEMPEST_SW_H3_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 3 TEMPEST_SW_H3_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 4 TEMPEST_SW_H3_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 5 TEMPEST_SW_H3_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 6 TEMPEST_SW_H6_20230515 0.3839  0.3975 28.1246 35.1012 0.01197442 0.7933597
##   salinity SO4_mM_dup Cl_mM_dup salinity_dup
## 1 0.04603330 0.12968808 0.7193484  0.04610613
## 2 0.00002600 0.00000000 0.0000000  0.00002600
## 3 0.00002600 0.00000000 0.0000000  0.00002600
## 4 0.00002600 0.00000000 0.0000000  0.00002600
## 5 0.00002600 0.00000000 0.0000000  0.00002600
## 6 0.05084715 0.01264192 1.0339492  0.06625887

QAdups$SO4_dups_chk <- ((abs(QAdups$SO4_mM-QAdups$SO4_mM_dup))/((QAdups$SO4_mM+QAdups$SO4_mM_dup)/2))*10
QAdups$SO4_dups_flag <- ifelse(QAdups$SO4_dups_chk <10, 'YES', 'NO, rerun')

```

```

QAdups$Cl_dups_chk <- ((abs(QAdups$Cl_mM-QAdups$Cl_mM_dup))/((QAdups$Cl_mM+QAdups$Cl_mM_dup)/2))*100
QAdups$Cl_dups_flag <- ifelse(QAdups$Cl_dups_chk <10, 'YES', 'NO, rerun')

head(QAdups)

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM     Cl_mM
## 1 TEMPEST_C_I5_20230518  4.4207  4.5778 25.4606 31.7763 0.13788833 0.7182116
## 2 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000 0.00000000 0.0000000
## 3 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000 0.00000000 0.0000000
## 4 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000 0.00000000 0.0000000
## 5 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000 0.00000000 0.0000000
## 6 TEMPEST_SW_H6_20230515  0.3839  0.3975 28.1246 35.1012 0.01197442 0.7933597
##   salinity S04_mM_dup Cl_mM_dup salinity_dup S04_dups_chk S04_dups_flag
## 1 0.04603330 0.12968808 0.7193484 0.04610613 6.129277      YES
## 2 0.00002600 0.00000000 0.0000000 0.00002600      NaN    <NA>
## 3 0.00002600 0.00000000 0.0000000 0.00002600      NaN    <NA>
## 4 0.00002600 0.00000000 0.0000000 0.00002600      NaN    <NA>
## 5 0.00002600 0.00000000 0.0000000 0.00002600      NaN    <NA>
## 6 0.05084715 0.01264192 1.0339492 0.06625887 5.423213      YES
##   Cl_dups_chk Cl_dups_flag
## 1      0.1581586      YES
## 2        NaN    <NA>
## 3        NaN    <NA>
## 4        NaN    <NA>
## 5        NaN    <NA>
## 6 26.3326649      NO, rerun

#plot dups output as a bar graph to easily check - want any over 10% to be red need to work on this
Sdupsbar <- ggplot(data = QAdups, aes(x = Sample_ID, y = S04_dups_chk, fill=S04_dups_chk)) +
  geom_bar(stat = 'identity') +
  scale_fill_gradient2(low='darkgreen', mid='darkgreen', high='darkgrey', space='Lab') +
  theme_classic() + labs(x= "Sample ID", y="Difference Between S04 Duplicates (%)") +
  theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed",
                                             color = "black", size=1)

## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.

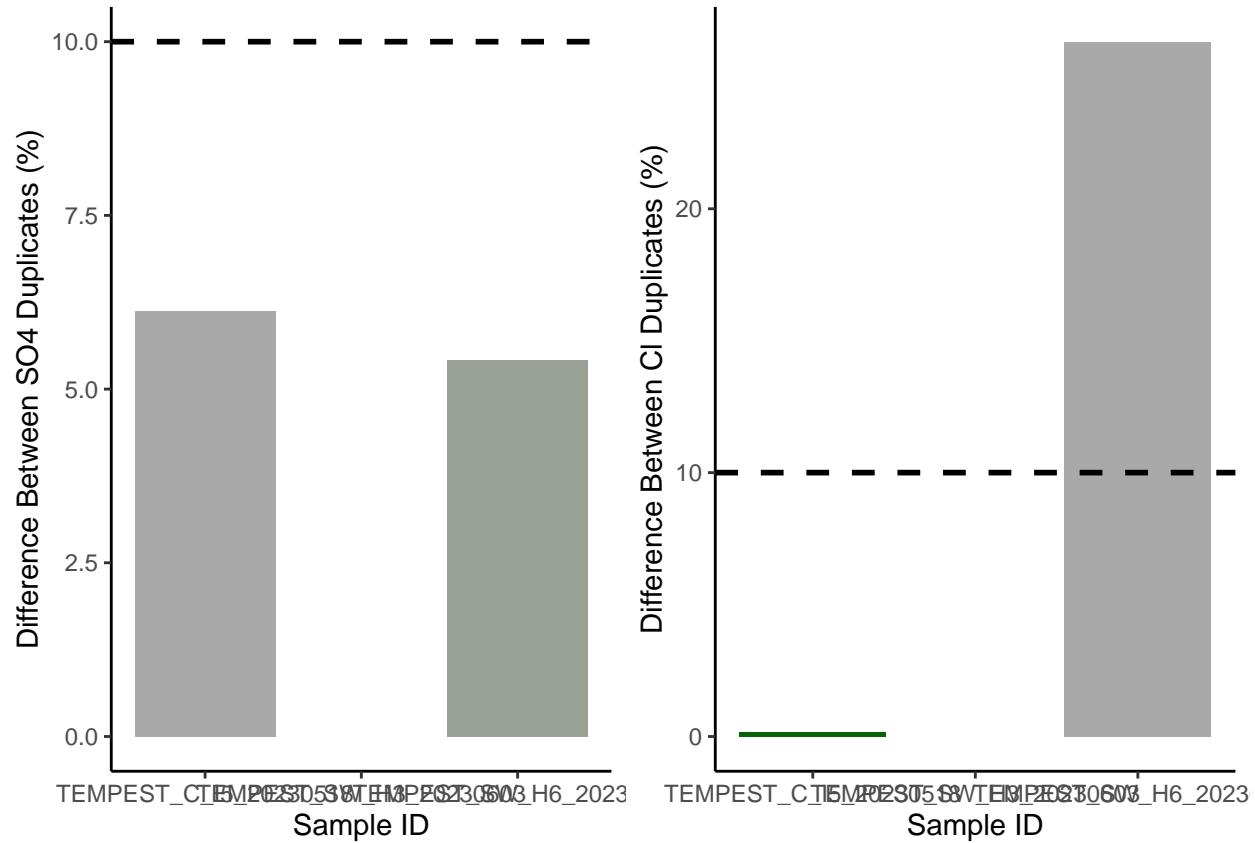
Cldupsbar <- ggplot(data = QAdups, aes(x = Sample_ID, y = Cl_dups_chk, fill=Cl_dups_chk)) +
  geom_bar(stat = 'identity') +
  scale_fill_gradient2(low='darkgreen', mid='darkgreen', high='darkgrey', space='Lab') +
  theme_classic() + labs(x= "Sample ID", y="Difference Between Cl Duplicates (%)") +
  theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed",
                                             color = "black", size=1)

ggarrange(Sdupsbar, Cldupsbar, ncol=2, nrow=1)

## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_bar()').

```

```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_bar()').
```



```
#check for percent of no, reruns to see if it would warrant reruns
Perc_dups <- QAdups %>%
  group_by(S04_dups_flag) %>%
  summarise(S_no_rows = length(S04_dups_flag))
Perc_dups <- Perc_dups %>%
  filter(!is.na(S04_dups_flag))
Perc_dups1 <- QAdups %>%
  group_by(Cl_dups_flag) %>%
  summarise(Cl_no_rows = length(Cl_dups_flag))
Perc_dups1 <- Perc_dups1 %>%
  filter(!is.na(Cl_dups_flag))
colnames(Perc_dups) <- c("Flag", "S_no_rows")
colnames(Perc_dups1) <- c("Flag", "Cl_no_rows")
Perc_dups2 <- cbind(Perc_dups, Perc_dups1)

Perc_dups2$Total <- length(QAdups$S04_dups_flag)
Perc_dups2$S_Percent <- (Perc_dups2$S_no_rows / Perc_dups2$Total)*100
Perc_dups2$Cl_Percent <- (Perc_dups2$Cl_no_rows / Perc_dups2$Total)*100
head(Perc_dups2)
```

	Flag	S_no_rows	Flag	Cl_no_rows	Total	S_Percent	Cl_Percent
## 1	YES	2	NO, rerun	1	6	33.33333	16.66667
## 2	YES	2	YES	1	6	33.33333	16.66667

Pull out dups and check with cv

```
#the cv
# calculate the sd bewteen the two duplicates then divide by the mean and multiply by 100

df2 <- as.data.frame(QAdups$S04_mM)
df2$dups <- QAdups$S04_mM_dup

df2$sds <- apply(df2, 1, sd)

QAdups$S04_dups_cv <- (df2$sds)/((QAdups$S04_mM+QAdups$S04_mM_dup)/2) * 100
QAdups$S04_dups_cv_flag <- ifelse(QAdups$S04_dups_cv <11, 'YES', 'NO, rerun')

head(QAdups)

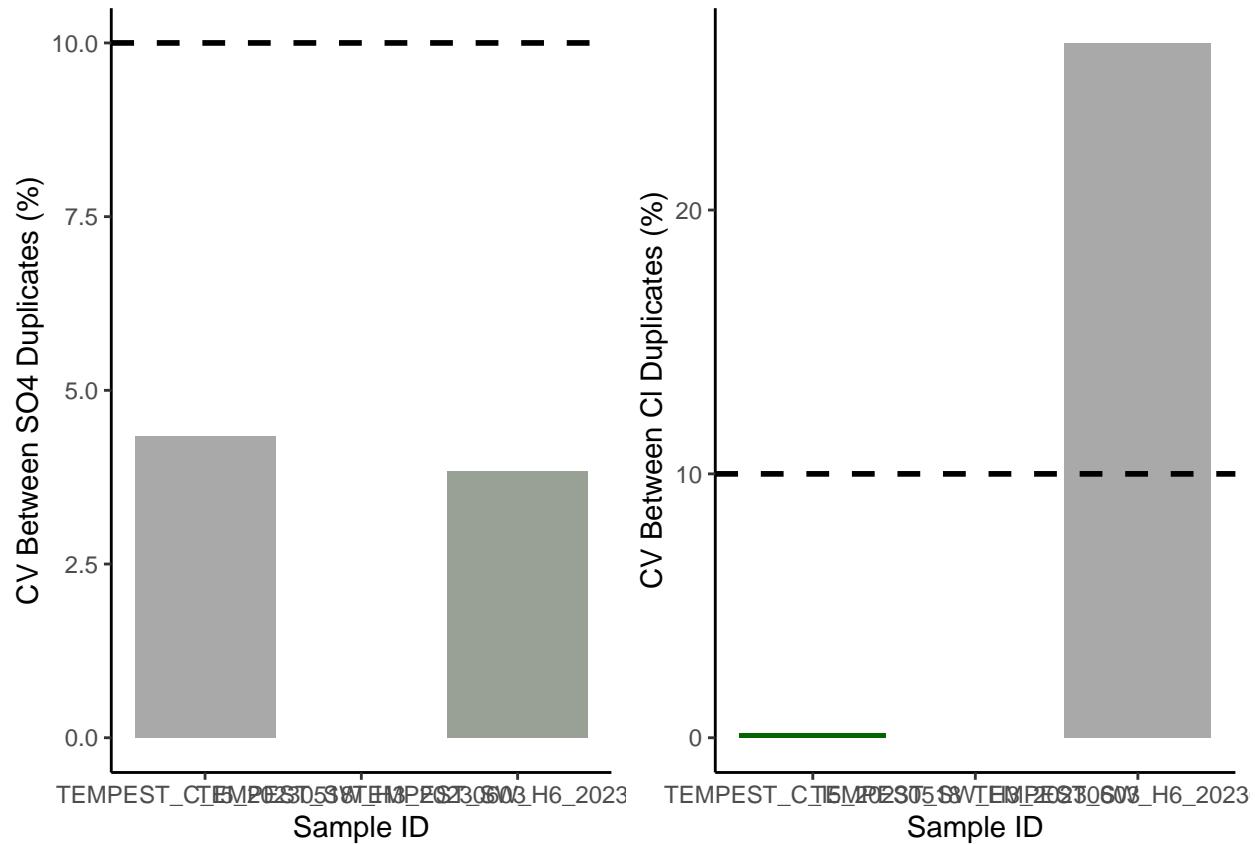
##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM     Cl_mM
## 1 TEMPEST_C_I5_20230518  4.4207  4.5778 25.4606 31.7763 0.13788833 0.7182116
## 2 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000  0.00000000 0.0000000
## 3 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000  0.00000000 0.0000000
## 4 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000  0.00000000 0.0000000
## 5 TEMPEST_SW_H3_20230603  0.0000  0.0000  0.0000  0.0000  0.00000000 0.0000000
## 6 TEMPEST_SW_H6_20230515  0.3839  0.3975 28.1246 35.1012 0.01197442 0.7933597
##   salinity S04_mM_dup Cl_mM_dup salinity_dup S04_dups_chk S04_dups_flag
## 1 0.04603330 0.12968808 0.7193484  0.04610613  6.129277      YES
## 2 0.00002600 0.00000000 0.0000000  0.00002600      NaN    <NA>
## 3 0.00002600 0.00000000 0.0000000  0.00002600      NaN    <NA>
## 4 0.00002600 0.00000000 0.0000000  0.00002600      NaN    <NA>
## 5 0.00002600 0.00000000 0.0000000  0.00002600      NaN    <NA>
## 6 0.05084715 0.01264192 1.0339492  0.06625887  5.423213      YES
##   Cl_dups_chk Cl_dups_flag S04_dups_cv S04_dups_cv_flag
## 1 0.1581586      YES     4.334053      YES
## 2      NaN    <NA>      NaN    <NA>
## 3      NaN    <NA>      NaN    <NA>
## 4      NaN    <NA>      NaN    <NA>
## 5      NaN    <NA>      NaN    <NA>
## 6 26.3326649    NO, rerun  3.834791      YES

#plot dups output as a bar graph to easily check - want any over 10% to be red need to work on this
Sdupsbar <- ggplot(data = QAdups, aes(x = Sample_ID, y = S04_dups_cv, fill=S04_dups_chk)) +
  geom_bar(stat = 'identity') +
  scale_fill_gradient2(low='darkgreen', mid='darkgreen', high='darkgrey', space='Lab') +
  theme_classic() + labs(x= "Sample ID", y="CV Between S04 Duplicates (%)") +
  theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed",
                                             color = "black", size=1)

Cldupsbar <- ggplot(data = QAdups, aes(x = Sample_ID, y = Cl_dups_chk, fill=Cl_dups_chk)) +
  geom_bar(stat = 'identity') +
  scale_fill_gradient2(low='darkgreen', mid='darkgreen', high='darkgrey', space='Lab') +
  theme_classic() + labs(x= "Sample ID", y="CV Between Cl Duplicates (%)") +
  theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed",
                                             color = "black", size=1)
```

```
ggarrange(Sdupsbar, Cldupsbar, ncol=2, nrow=1)
```

```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 4 rows containing missing values or values outside the scale range
## ('geom_bar()').
```



```
#check for percent of no, reruns to see if it would warrant reruns
Perc_dups <- QAdups %>%
  group_by(SO4_dups_flag) %>%
  summarise(S_no_rows = length(SO4_dups_flag))
Perc_dups <- Perc_dups %>%
  filter(!is.na(SO4_dups_flag))
Perc_dups1 <- QAdups %>%
  group_by(Cl_dups_flag) %>%
  summarise(Cl_no_rows = length(Cl_dups_flag))
Perc_dups1 <- Perc_dups1 %>%
  filter(!is.na(Cl_dups_flag))
colnames(Perc_dups) <- c("Flag", "S_no_rows")
colnames(Perc_dups1) <- c("Flag", "Cl_no_rows")
Perc_dups2 <- cbind(Perc_dups, Perc_dups1)

Perc_dups2$Total <- length(QAdups$SO4_dups_flag)
Perc_dups2$S_Percent <- (Perc_dups2$S_no_rows / Perc_dups2$Total)*100
```

```
Perc_dups2$Cl_Percent <- (Perc_dups2$Cl_no_rows / Perc_dups2$Total)*100
head(Perc_dups2)
```

```
##   Flag S_no_rows      Flag Cl_no_rows Total S_Percent Cl_Percent
## 1 YES        2 NO, rerun       1     6 33.33333 16.66667
## 2 YES        2      YES       1     6 33.33333 16.66667
```

Pull out spikes and check with dionex output conc.

```
#Show me the data that we have from the calculations
head(sampledat)
```

```
##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area    SO4_mM    Cl_mM
## 126 TEMPEST_C_C6_20230515 0.3224  0.3338 30.5616 38.1427 0.01005614 0.8621044
## 127 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 128 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 129 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 130 TEMPEST_C_C6_20230603 0.0000  0.0000 0.0000 0.0000 0.00000000 0.0000000
## 131 TEMPEST_C_F6_20230515 0.0000  0.0000 28.2531 35.2615 0.00000000 0.7969845
##   salinity
## 126 0.05525081
## 127 0.00002600
## 128 0.00002600
## 129 0.00002600
## 130 0.00002600
## 131 0.05107935
```

```
#pull out any rows that have "spk" in the SampleID column
spks <- sampledat %>%
  filter(str_detect(Sample_ID, "spk"))      #have to change this to match data
head(spks)
```

```
##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area    SO4_mM    Cl_mM
## 1 TEMPEST_SW_H3_20230603_spk 168.9031  3.4046      0      0 5.268344      0
##   salinity
## 1 2.6e-05
```

```
#remove the dup from these IDs so we will have duplicate sample names
spks$Sample_ID <- gsub("_spk", "", as.character(spks$Sample_ID))
spks <- spks[ , -c(2, 3, 5, 6)]
colnames(spks) <- c('Sample_ID', 'SO4_mM_spk')
head(spks)
```

```
##           Sample_ID SO4_mM_spk NA      NA
## 1 TEMPEST_SW_H3_20230603          0  0 2.6e-05
```

```
#put it back together with the old data set and look for duplicates
QAspks <- merge(sampledat, spks)
head(QAspks)
```

```

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
##   SO4_mM_spk NA     NA.1
## 1          0 0 2.6e-05
## 2          0 0 2.6e-05
## 3          0 0 2.6e-05
## 4          0 0 2.6e-05

```

```

#now we need to calculate the spike concentration and calculate the spike recovery
spkconc <- (250/smw)      # in mM
spkvol <- 10               # in uL
spkvol <- spkvol/1000000
#spike for these samples was 10uL of the 250mM standard
QAspks$SO4_spk_Conc <- (spkconc)*spkvol      # mmoles of SO4
head(QAspks)

```

```

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0      0      0      0      0      0 2.6e-05
##   SO4_mM_spk NA     NA.1 SO4_spk_Conc
## 1          0 0 2.6e-05 7.797879e-05
## 2          0 0 2.6e-05 7.797879e-05
## 3          0 0 2.6e-05 7.797879e-05
## 4          0 0 2.6e-05 7.797879e-05

```

```

#need to determine dilution factors and initial amount of sample added
#if your samples are all the same dilution just use the first line
#for Steph / COMPASS this depends on the site so...
QAspks$Dilution <- 1
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_UP"), 50, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_TR"), 50, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_WC"), 100, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_UP"), 50, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_TR"), 50, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_WC"), 100, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_UP"), 100, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_TR"), 100, QAspks$Dilution)
QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_WC"), 200, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_UP"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_TR"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_WC"), 100, QAspks$Dilution)

#Set Sample volumes in uL
QAspks$SampleVol <- 1
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_UP"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_TR"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_WC"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_UP"), 1501, QAspks$SampleVol)

```

```

QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_TR"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_WC"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_UP"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_TR"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_WC"), 1462, QAspks$SampleVol)
#QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_UP"), 100, QAspks$SampleVol)
#QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_TR"), 100, QAspks$SampleVol)
#QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_WC"), 100, QAspks$SampleVol)

#change sample volume to L
QAspks$SampleVol <- QAspks$SampleVol/1000000
head(QAspks)

##                               Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
##   SO4_mM_spk NA    NA.1 SO4_spk_Conc Dilution SampleVol
## 1          0 0 2.6e-05 7.797879e-05       1 1e-06
## 2          0 0 2.6e-05 7.797879e-05       1 1e-06
## 3          0 0 2.6e-05 7.797879e-05       1 1e-06
## 4          0 0 2.6e-05 7.797879e-05       1 1e-06

#gives us the total SO4 in the sample in mmoles
QAspks$SO4_Total_unspkd <- (QAspks$SO4_mM/QAspks$Dilution)*(QAspks$SampleVol)

##total SO4 in spiked sample in mmoles
QAspks$SO4_Total_spkd <- (QAspks$SO4_mM_spk/QAspks$Dilution)*(QAspks$SampleVol+spkvol)

QAspks$SO4_expctd_spkd <- (QAspks$SO4_Total_unspkd + QAspks$SO4_spk_Conc)
QAspks$spk_recovery <- (QAspks$SO4_Total_spkd/QAspks$SO4_expctd_spkd)*100
QAspks$SO4_spks_flag <- ifelse(QAspks$spk_recovery <=120 & QAspks$spk_recovery >=80 , 'YES', 'NO', rerun)

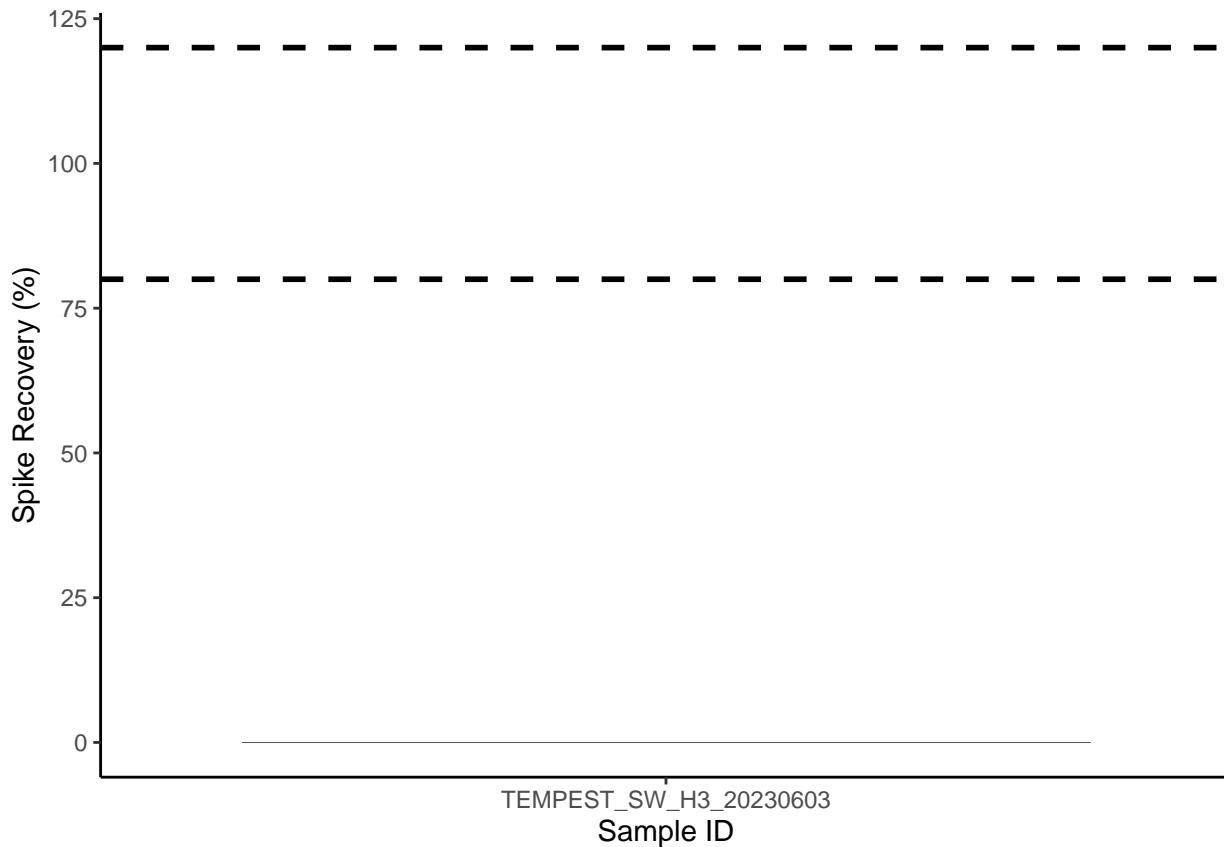
head(QAspks)

##                               Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0        0        0        0        0        0 2.6e-05
##   SO4_mM_spk NA    NA.1 SO4_spk_Conc Dilution SampleVol SO4_Total_unspkd
## 1          0 0 2.6e-05 7.797879e-05       1 1e-06          0
## 2          0 0 2.6e-05 7.797879e-05       1 1e-06          0
## 3          0 0 2.6e-05 7.797879e-05       1 1e-06          0
## 4          0 0 2.6e-05 7.797879e-05       1 1e-06          0
##   SO4_Total_spkd SO4_expctd_spkd spk_recovery SO4_spks_flag
## 1          0 7.797879e-05          0    NO, rerun
## 2          0 7.797879e-05          0    NO, rerun
## 3          0 7.797879e-05          0    NO, rerun
## 4          0 7.797879e-05          0    NO, rerun

```

```
#plot spk recoveries output as a bar graph to easily check - want any over 10% to be red need to work on this
spksbar <- ggplot(data = QAspks, aes(x = Sample_ID, y = spk_recovery)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("lightblue4")) +
  theme_classic() +
  labs(x= "Sample ID", y="Spike Recovery (%)") +
  theme(legend.position="none") +
  geom_hline(yintercept=80, linetype="dashed", color = "black", size=1) +
  geom_hline(yintercept=120, linetype="dashed", color = "black", size=1)

spksbar
```



```
#check for percent of no, reruns to see if it would warrant reruns
#Perc_spks <- QAspks %>%
#  group_by(SO4_spks_flag) %>%
#  summarise(no_rows = length(SO4_spks_flag))
#Perc_spks$Total <- length(QAspks$SO4_spks_flag)
#Perc_spks$Percent <- (Perc_spks$no_rows / Perc_spks$Total)*100
#head(Perc_spks)
```

Pull out spikes and check with area calc

```
#Show me the data that we have from the calculations
head(sampledat)
```

```

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM     Cl_mM
## 126 TEMPEST_C_C6_20230515 0.3224   0.3338 30.5616 38.1427 0.01005614 0.8621044
## 127 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 128 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 129 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 130 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 131 TEMPEST_C_F6_20230515 0.0000   0.0000 28.2531 35.2615 0.00000000 0.7969845
##           salinity
## 126 0.05525081
## 127 0.00002600
## 128 0.00002600
## 129 0.00002600
## 130 0.00002600
## 131 0.05107935

#now use area of all samples and calculate undilution corrected concentrations in ug/mL
sampledat$S04_ugmL <- ((sampledat$S04_Area-S04_Int)/S04_Slope
sampledat$Cl_ugmL <- (sampledat$Cl_Area-Cl_Int)/Cl_Slope
head(sampledat)

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM     Cl_mM
## 126 TEMPEST_C_C6_20230515 0.3224   0.3338 30.5616 38.1427 0.01005614 0.8621044
## 127 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 128 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 129 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 130 TEMPEST_C_C6_20230603 0.0000   0.0000 0.0000 0.0000 0.00000000 0.0000000
## 131 TEMPEST_C_F6_20230515 0.0000   0.0000 28.2531 35.2615 0.00000000 0.7969845
##           salinity     S04_ugmL     Cl_ugmL
## 126 0.05525081 2.93060e-01 2.778329e+01
## 127 0.00002600 1.61704e-05 7.223654e-06
## 128 0.00002600 1.61704e-05 7.223654e-06
## 129 0.00002600 1.61704e-05 7.223654e-06
## 130 0.00002600 1.61704e-05 7.223654e-06
## 131 0.05107935 1.61704e-05 2.568461e+01

#pull out any rows that have "spk" in the SampleID column
spks <- sampledat %>%
  filter(str_detect(Sample_ID, "spk"))      #have to change this to match data
head(spks)

##           Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area     S04_mM Cl_mM
## 1 TEMPEST_SW_H3_20230603_spk 168.9031   3.4046      0      0 5.268344      0
##           salinity S04_ugmL     Cl_ugmL
## 1 2.6e-05 2.988922 7.223654e-06

## Only keep the columns that we need
spks <- spks[ ,c(1,9,10)] # dont need this here
head(spks)

##           Sample_ID S04_ugmL     Cl_ugmL
## 1 TEMPEST_SW_H3_20230603_spk 2.988922 7.223654e-06

```

```

#remove the spk from these IDs so we will have duplicate sample names
spks$Sample_ID<-gsub("_spk","",as.character(spks$Sample_ID))
spks <- spks[,c(1,2)]
colnames(spks) <- c('Sample_ID', 'SO4_ugmL_spk')
head(spks)

##           Sample_ID SO4_ugmL_spk
## 1 TEMPEST_SW_H3_20230603      2.988922

#put it back together with the old data set and look for duplicates
QAspks <- merge(sampledat, spks)
head(QAspks)

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
##           SO4_ugmL   Cl_ugmL SO4_ugmL_spk
## 1 1.61704e-05 7.223654e-06      2.988922
## 2 1.61704e-05 7.223654e-06      2.988922
## 3 1.61704e-05 7.223654e-06      2.988922
## 4 1.61704e-05 7.223654e-06      2.988922

#now we need to calculate the spike concentration and calculate the spike recovery
spkconc <- (250)      # in ug
spkvol <- 10          # in uL
spkvol <- spkvol/1000
#spike for these samples was 10uL of the 250mM standard
QAspks$SO4_spk_Conc <- (spkconc)*spkvol      # mmoles of SO4
head(QAspks)

##           Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0       0     0       0     0       0 2.6e-05
##           SO4_ugmL   Cl_ugmL SO4_ugmL_spk SO4_spk_Conc
## 1 1.61704e-05 7.223654e-06      2.988922      2.5
## 2 1.61704e-05 7.223654e-06      2.988922      2.5
## 3 1.61704e-05 7.223654e-06      2.988922      2.5
## 4 1.61704e-05 7.223654e-06      2.988922      2.5

#need to determine dilution factors and initial amount of sample added
#if your samples are all the same dilution just use the first line
#for Steph / COMPASS this depends on the site so...
#QAspks$Dilution <- 1
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_UP"), 50, QAspks$Dilution)
#$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_TR"), 50, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "MSM_WC"), 100, QAspks$Dilution)
#$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_UP"), 50, QAspks$Dilution)

```

```

#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_TR"), 50, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_WC"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_UP"), 100, QAspks$Dilution)
##Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_TR"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "GWI_WC"), 200, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_UP"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_TR"), 100, QAspks$Dilution)
#QAspks$Dilution <- ifelse(str_detect(QAspks$Sample_ID, "SWH_WC"), 100, QAspks$Dilution)

#Set Sample volumes in uL
QAspks$SampleVol <- 1
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_UP"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_TR"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_WC"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_PPR_UP"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_PPR_TR"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "MSM_PPR_WC"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_UP"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_TR"), 1501, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GCrew_WC"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_UP"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_TR"), 1475, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "GWI_WC"), 1462, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_UP"), 100, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_TR"), 100, QAspks$SampleVol)
QAspks$SampleVol <- ifelse(str_detect(QAspks$Sample_ID, "SWH_WC"), 100, QAspks$SampleVol)

#change sample volume to L
QAspks$SampleVol <- QAspks$SampleVol/1000
head(QAspks)

```

```

##          Sample_ID SO4_ppm SO4_Area Cl_ppm Cl_Area SO4_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
##          SO4_ugmL     Cl_ugmL SO4_ugmL_spk SO4_spk_Conc SampleVol
## 1 1.61704e-05 7.223654e-06    2.988922        2.5   0.001
## 2 1.61704e-05 7.223654e-06    2.988922        2.5   0.001
## 3 1.61704e-05 7.223654e-06    2.988922        2.5   0.001
## 4 1.61704e-05 7.223654e-06    2.988922        2.5   0.001

#gives us the total SO4 in the sample in mmoles
QAspks$SO4_Total_unspkd <- QAspks$SO4_ugmL*QAspks$SampleVol

##total SO4 in spiked sample in mmoles
QAspks$SO4_Total_spkd <- (QAspks$SO4_ugmL_spk)*(QAspks$SampleVol+spkvol)

QAspks$SO4_expctd_spkd <- (QAspks$SO4_Total_unspkd + QAspks$SO4_spk_Conc)
QAspks$spk_recovery <- (QAspks$SO4_Total_spkd/QAspks$SO4_expctd_spkd)*100
QAspks$SO4_spks_flag <- ifelse(QAspks$spk_recovery <=120 & QAspks$spk_recovery >=80 , 'YES' , 'NO', rerun)

head(QAspks)

```

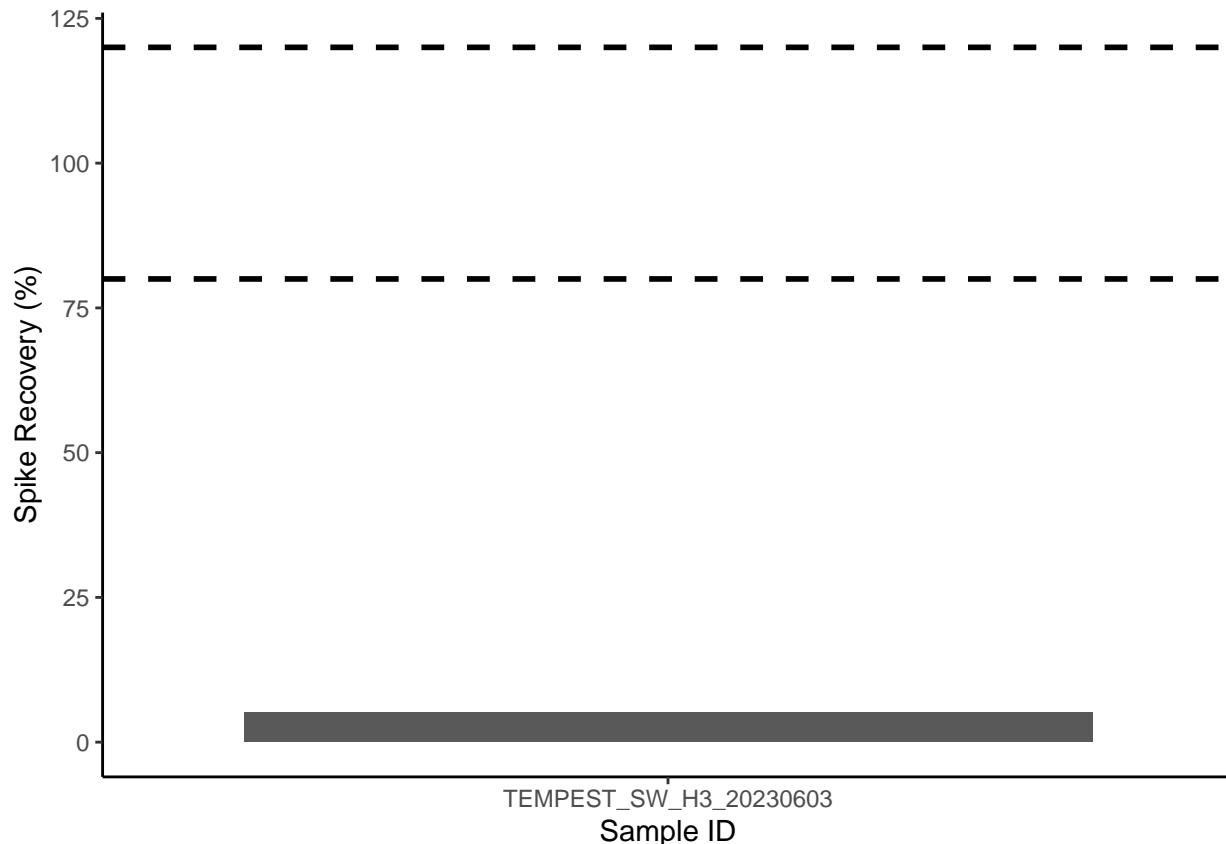
```

##          Sample_ID S04_ppm S04_Area Cl_ppm Cl_Area S04_mM Cl_mM salinity
## 1 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 2 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 3 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
## 4 TEMPEST_SW_H3_20230603      0       0       0       0       0       0 2.6e-05
##          S04_ugmL     Cl_ugmL S04_ugmL_spk S04_spk_Conc SampleVol S04_Total_unspkd
## 1 1.61704e-05 7.223654e-06    2.988922        2.5     0.001 1.61704e-08
## 2 1.61704e-05 7.223654e-06    2.988922        2.5     0.001 1.61704e-08
## 3 1.61704e-05 7.223654e-06    2.988922        2.5     0.001 1.61704e-08
## 4 1.61704e-05 7.223654e-06    2.988922        2.5     0.001 1.61704e-08
##          S04_Total_spkd S04_expctd_spkd spk_recovery S04_spks_flag
## 1      0.03287815            2.5     1.315126    NO, rerun
## 2      0.03287815            2.5     1.315126    NO, rerun
## 3      0.03287815            2.5     1.315126    NO, rerun
## 4      0.03287815            2.5     1.315126    NO, rerun

#plot spk recoveries output as a bar graph to easily check - want any over 10% to be red need to work on
spksbar <- ggplot(data = QAspks, aes(x = Sample_ID, y = spk_recovery)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("lightblue4")) +
  theme_classic() + labs(x= "Sample ID", y="Spike Recovery (%)") +
  theme(legend.position="none") +
  geom_hline(yintercept=80, linetype="dashed", color = "black", size=1) +
  geom_hline(yintercept=120, linetype="dashed", color = "black", size=1)

```

spksbar



```

#check for percent of no, reruns to see if it would warrant reruns
Perc_spks <- QAspks %>%
  group_by(S04_spks_flag) %>%
  summarise(no_rows = length(S04_spks_flag))
Perc_spks$Total <- length(QAspks$S04_spks_flag)
Perc_spks$Percent <- (Perc_spks$no_rows / Perc_spks$Total)*100
head(Perc_spks)

```

```

## # A tibble: 1 x 4
##   S04_spks_flag no_rows Total Percent
##   <chr>          <int>   <int>    <dbl>
## 1 NO, rerun      4        4     100

```

Make final dataframe with IDs

```

#for steph <- pull out identifiers of the sample names
#pull the sample ID and separate it by the underscores
IDs <- data.frame(do.call('rbind', strsplit(as.character(sampledat2$Sample_ID), '_', fixed=TRUE)))
colnames(IDs) <- c("Project" , "Plot","Grid", "Date")
head(IDs)

```

```

##   Project Plot Grid      Date
## 1 TEMPEST   C   C6 20230515
## 2 TEMPEST   C   C6 20230603
## 3 TEMPEST   C   C6 20230603
## 4 TEMPEST   C   C6 20230603
## 5 TEMPEST   C   C6 20230603
## 6 TEMPEST   C   F6 20230515

```

```

#rejoin them to the dataframe
alldat <- cbind(IDs, sampledat2)
head(alldat)

```

```

##   Project Plot Grid      Date      Sample_ID S04_ppm S04_Area Cl_ppm
## 1 TEMPEST   C   C6 20230515 TEMPEST_C_C6_20230515  0.3224   0.3338 30.5616
## 2 TEMPEST   C   C6 20230603 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000
## 3 TEMPEST   C   C6 20230603 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000
## 4 TEMPEST   C   C6 20230603 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000
## 5 TEMPEST   C   C6 20230603 TEMPEST_C_C6_20230603  0.0000   0.0000  0.0000
## 6 TEMPEST   C   F6 20230515 TEMPEST_C_F6_20230515  0.0000   0.0000 28.2531
##   Cl_Area   S04_mM   Cl_mM salinity
## 1 38.1427 0.01005614 0.8621044 0.05525081
## 2 0.0000 0.00000000 0.0000000 0.00002600
## 3 0.0000 0.00000000 0.0000000 0.00002600
## 4 0.0000 0.00000000 0.0000000 0.00002600
## 5 0.0000 0.00000000 0.0000000 0.00002600
## 6 35.2615 0.00000000 0.7969845 0.05107935

```

Make final dataframe with IDs

```
write.csv(alldat, file="Processed Data/COMPASS_TEMPEST_Dionex_ClSo4_Final_20230606.csv") #Chas
```

END