

Synoptic CB: Porewater SO₄/Cl

May 2025 Samples

2025-10-15

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##Add Required Packages

0.1 Run Information

```
##### Run information - PLEASE CHANGE
Date_Run = "20250529" #Date that instrument was run
Run_by = "Melanie Giessner" #Instrument user
Script_run_by = "Zoe Read" #Code user
Project = "COMPASS"
run_notes = "Some sample IDs were entered incorrectly so they had to be fixed in code.
Samples 15 and 16 need to be diluted and rerun.
" #any notes from the run

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_id_dil = "Raw Data/2025May_H2S_Datasheets.xlsx"
Sheet = "Plate 1"
raw_file_name_data = "Raw Data/20250529_COMPASS_H2S_Plate1.xlsx"

#file path and name of processed data file
tidy_file_name = "Tidy Data/20250529_COMPASS_H2S_Plate1_tidy.csv"
processed_file_name = "Processed Data/COMPASS_H2S_20250529_Plate4.csv"
samples_need_dilution_name = "Processed Data/COMPASS_H2S_20250529_Plate4_SamplesNeedDilution.csv"
samples_high_cv_name = "Processed Data/COMPASS_H2S_20250529_Plate4_SamplesHighCV.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"
Raw_IDs = "Raw Data/20250529_COMPASS_H2S_IDs.xlsx"

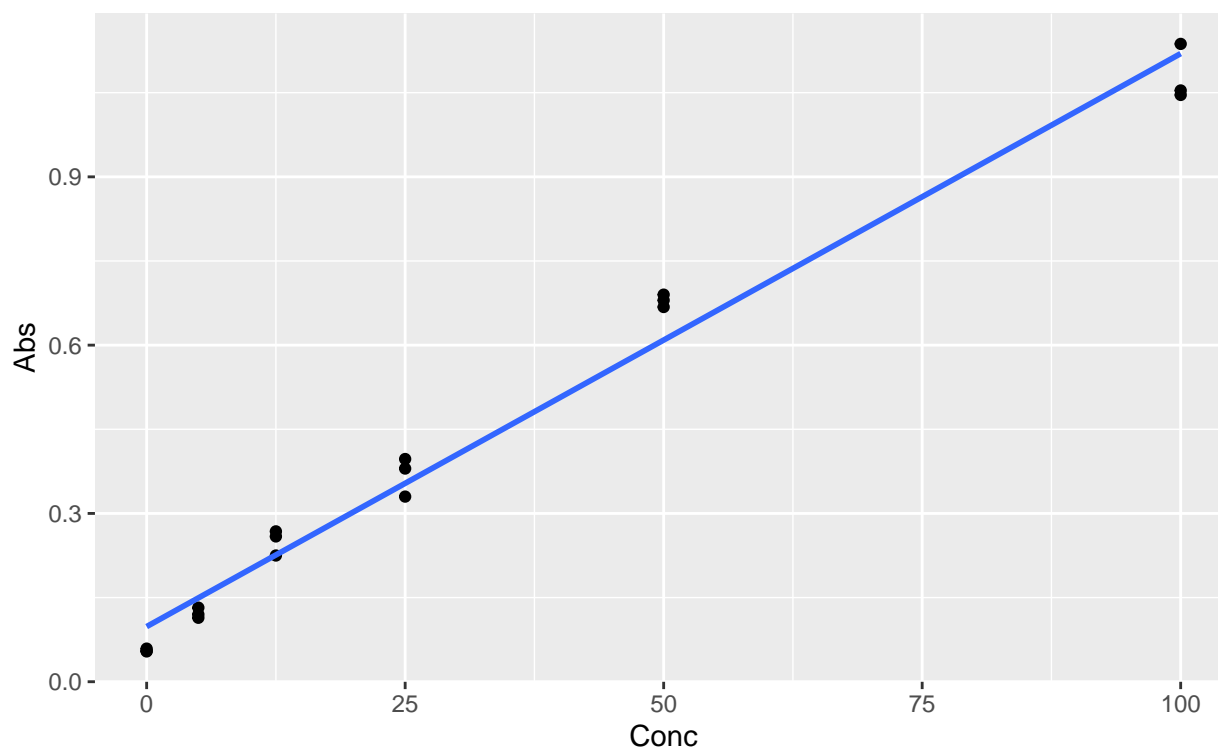
#qaqc log file path for this year
Log_path = "Raw Data/Sulfide_STD_QAQC.csv"
```

#Set Up Code - constants and QAQC cutoffs

0.2 Tidy data

0.3 Read in tidy data

0.4 Plot standards



```
##
## Call:
## lm(formula = H2S_stds$Abs ~ H2S_stds$Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.073720 -0.038309 -0.009167  0.039780  0.080994
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.0982916  0.0158802   6.19 1.30e-05 ***
## H2S_stds$Conc 0.0102143  0.0003372  30.29 1.47e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.04932 on 16 degrees of freedom
## Multiple R-squared:  0.9829, Adjusted R-squared:  0.9818
## F-statistic: 917.5 on 1 and 16 DF,  p-value: 1.474e-15

## Curve      R2      Slope Intercept
## 1    H2S 0.981789 0.01021429 0.0982916
```

```
## # A tibble: 6 x 5
##   IDs   H2S_mean_Abs H2S_sd H2S_cv Dilution
##   <chr>         <dbl>   <dbl> <dbl>   <int>
## 1 Std 0         0.056 0.00265  4.72     1
## 2 Std 1         0.122 0.00917  7.51     1
## 3 Std 2         0.251 0.0227   9.05     1
## 4 Std 3         0.369 0.0348   9.44     1
## 5 Std 4         0.679 0.0110   1.62     1
## 6 Std 5         1.08  0.0504   4.67     1

## # A tibble: 6 x 6
##   IDs   H2S_mean_Abs H2S_sd H2S_cv Dilution H2S_cv_flag
##   <chr>         <dbl>   <dbl> <dbl>   <int> <chr>
## 1 Std 0         0.056 0.00265  4.72     1 within range
## 2 Std 1         0.122 0.00917  7.51     1 within range
## 3 Std 2         0.251 0.0227   9.05     1 within range
## 4 Std 3         0.369 0.0348   9.44     1 within range
## 5 Std 4         0.679 0.0110   1.62     1 within range
## 6 Std 5         1.08  0.0504   4.67     1 within range

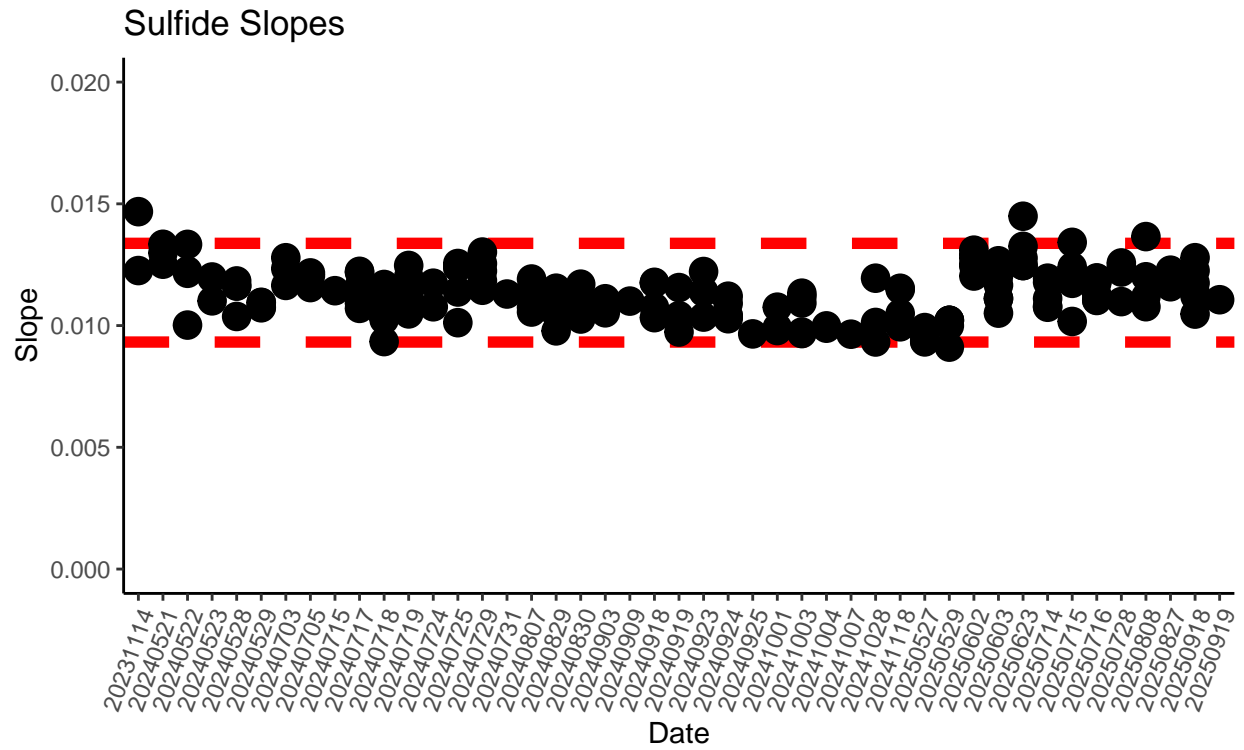
## [1] "Continue"
```

0.5 Assess Standard Curves

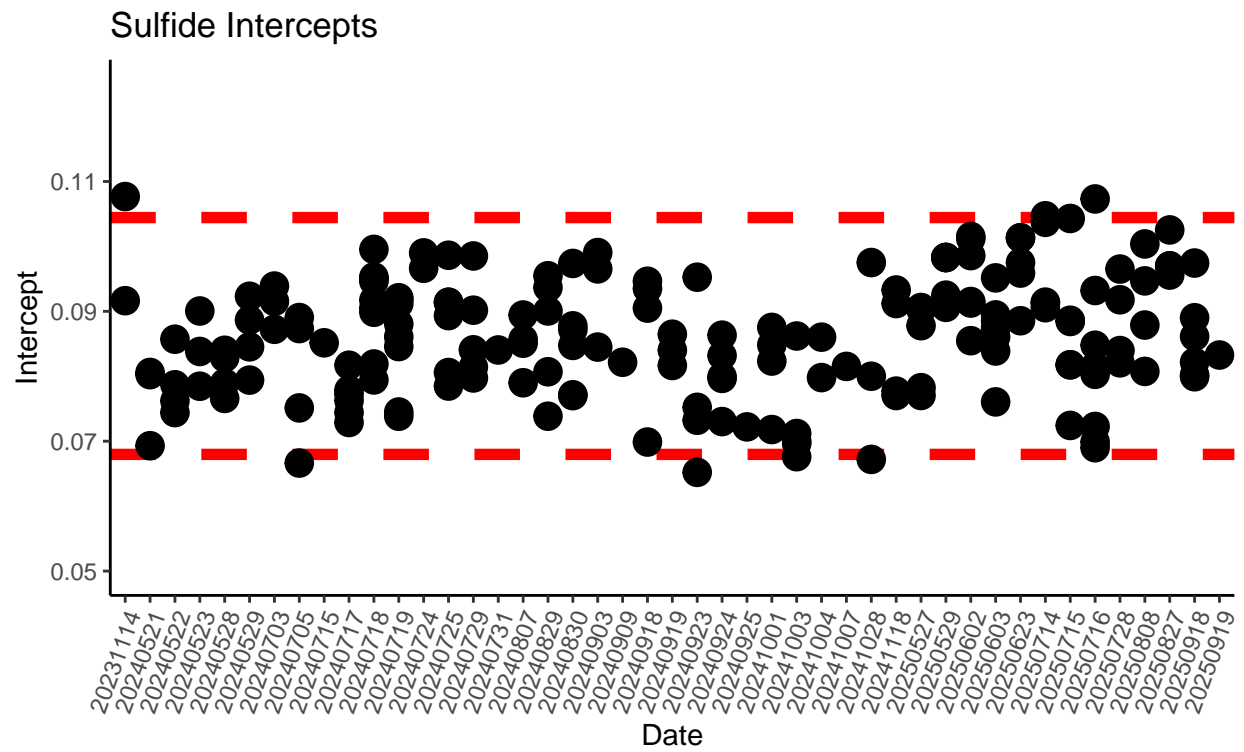
```
##       Date Project      R2      Slope Intercept Top_STD
## 1 20250529 COMPASS 0.9817890 0.01021429 0.09829160    100
## 2 20250529 COMPASS 0.9817890 0.01021429 0.09829160    100
## 3 20250919 LTREB 0.9928463 0.01106119 0.08327176    100
## 4 20250918 LTREB 0.9895866 0.01225734 0.08613143    100
## 5 20250918 LTREB 0.9940289 0.01136305 0.08901385    100
## 6 20250918 LTREB 0.9864830 0.01278678 0.07992404    100
```

```
##       Date Project      R2      Slope Intercept Top_STD
## 1 20250529 COMPASS 0.981789 0.01021429 0.0982916    100
```

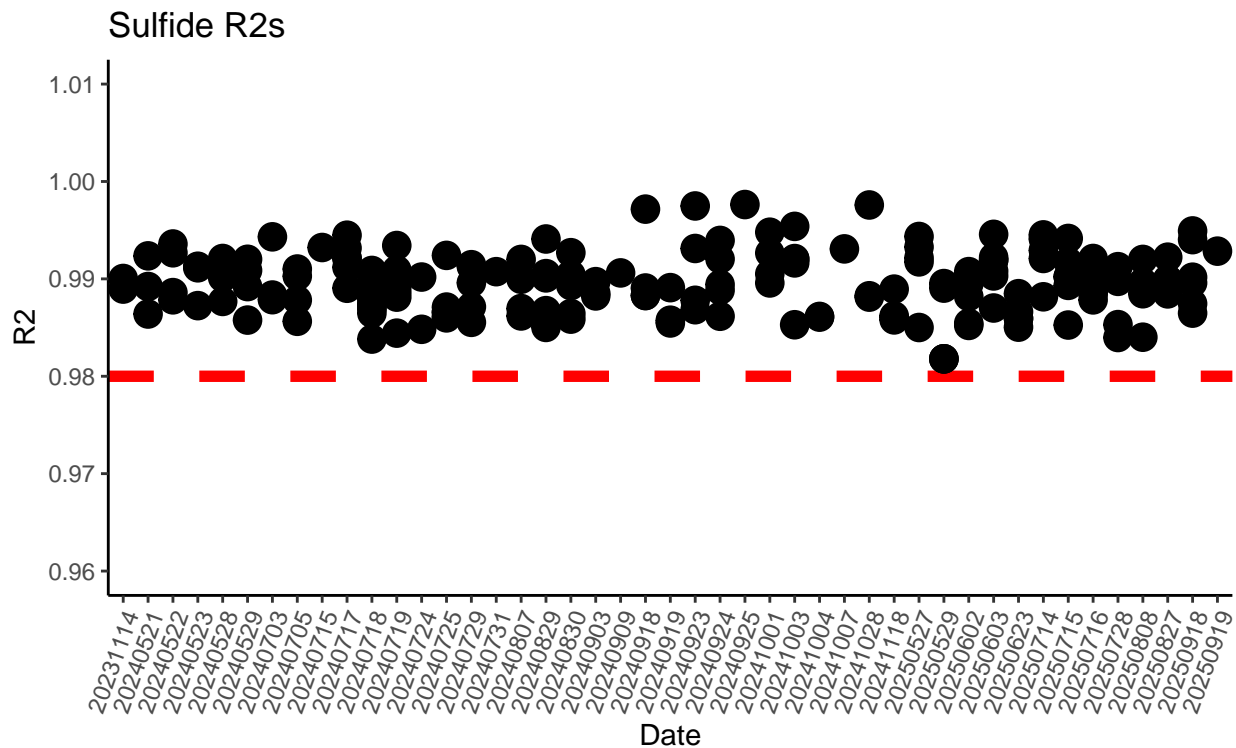
```
##       Date Project      R2      Slope Intercept Top_STD
## 1 20250529 COMPASS 0.9817890 0.01021429 0.09829160    100
## 2 20250529 COMPASS 0.9817890 0.01021429 0.09829160    100
## 3 20250529 COMPASS 0.9817890 0.01021429 0.09829160    100
## 4 20250919 LTREB 0.9928463 0.01106119 0.08327176    100
## 5 20250918 LTREB 0.9895866 0.01225734 0.08613143    100
## 6 20250918 LTREB 0.9940289 0.01136305 0.08901385    100
```



```
## [1] "continue"
```



```
## [1] "continue"
```



```
## [1] "continue"
```

0.6 Assess Check Standards

```
##
## Two Sample t-test
##
## data: std0$Abs and Chkstd0$Abs
## t = -0.85096, df = 7, p-value = 0.4229
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.005668144 0.002668144
## sample estimates:
## mean of x mean of y
## 0.0560 0.0575
```

```
## [1] "Continue"
```

```
##
## Two Sample t-test
##
## data: std3$Abs and Chkstd3$Abs
## t = -0.98443, df = 4, p-value = 0.3806
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.09805567 0.04672233
## sample estimates:
```

```
## mean of x mean of y
## 0.3690000 0.3946667

## [1] "Continue"

##
## Two Sample t-test
##
## data: std4$Abs and Chkstd4$Abs
## t = 0.50412, df = 4, p-value = 0.6407
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.04207049 0.06073716
## sample estimates:
## mean of x mean of y
## 0.6793333 0.6700000

## [1] "Continue"
```

0.7 Matrix Check QAQC

```
##
## Two Sample t-test
##
## data: std5$Abs and MC10$Abs
## t = 1.2457, df = 4, p-value = 0.2809
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.04997386 0.13130719
## sample estimates:
## mean of x mean of y
## 1.079000 1.038333

## [1] "Continue"

##
## Two Sample t-test
##
## data: std5$Abs and MC20$Abs
## t = 2.7402, df = 4, p-value = 0.0519
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.001713046 0.260379712
## sample estimates:
## mean of x mean of y
## 1.0790000 0.9496667

## [1] "Continue"
```

0.8 Flag sample data

```
## # A tibble: 6 x 4
##   Wells   Abs IDs   Dilution
##   <chr> <dbl> <chr>     <int>
## 1 A04    0.069 1         1
## 2 A05    0.071 1         1
## 3 A06    0.068 1         1
## 4 A07    0.063 9         1
## 5 A08    0.06  9         1
## 6 A09    0.056 9         1

## # A tibble: 6 x 5
##   Wells   Abs IDs   Dilution  Conc
##   <chr> <dbl> <chr>     <int> <dbl>
## 1 A04    0.069 1         1 -2.87
## 2 A05    0.071 1         1 -2.67
## 3 A06    0.068 1         1 -2.97
## 4 A07    0.063 9         1 -3.46
## 5 A08    0.06  9         1 -3.75
## 6 A09    0.056 9         1 -4.14

## # A tibble: 6 x 7
##   Wells   Abs IDs   Dilution  Conc H2S_Conc_Final H2S_info
##   <chr> <dbl> <chr>     <int> <dbl>         <dbl> <chr>
## 1 A04    0.069 1         1 -2.87           0 bdl
## 2 A05    0.071 1         1 -2.67           0 bdl
## 3 A06    0.068 1         1 -2.97           0 bdl
## 4 A07    0.063 9         1 -3.46           0 bdl
## 5 A08    0.06  9         1 -3.75           0 bdl
## 6 A09    0.056 9         1 -4.14           0 bdl
```

0.9 Calculate avg, std dev, and cv across wells

```
head(dat_flagged)
```

```
## # A tibble: 6 x 7
##   Wells   Abs IDs   Dilution  Conc H2S_Conc_Final H2S_info
##   <chr> <dbl> <chr>     <int> <dbl>         <dbl> <chr>
## 1 A04    0.069 1         1 -2.87           0 bdl
## 2 A05    0.071 1         1 -2.67           0 bdl
## 3 A06    0.068 1         1 -2.97           0 bdl
## 4 A07    0.063 9         1 -3.46           0 bdl
## 5 A08    0.06  9         1 -3.75           0 bdl
## 6 A09    0.056 9         1 -4.14           0 bdl
```

```
####Data entered incorrectly -- fix here####
dat_flagged$IDs[dat_flagged$IDs == "17 Dup"] <- "16 Dup"
dat_flagged$IDs[dat_flagged$IDs == "18 Dup"] <- "16 Dup"

#summarize by sampleID so that we can calculate the mean and std. dev. of the three wells
```



```

dat1 <- dat_flagged %>%
  group_by(IDs) %>%
  summarise(H2S_mean = mean(H2S_Conc_Final), H2S_sd = sd(H2S_Conc_Final), H2S_cv = cv(H2S_Conc_Final),
            H2S_flag = first(H2S_info),
            Dilution = first(Dilution))

```

```
head(dat1)
```

```

## # A tibble: 6 x 6
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int>
## 1 1          0      0      0    bdl          1
## 2 1 Spike    15.5   3.05  19.7 Within_Range 1
## 3 10         0      0      0    bdl          1
## 4 10 Spike    18.3   0.994  5.44 Within_Range 1
## 5 11         0      0      0    bdl          1
## 6 12         0      0      0    bdl          1

```

```
#Flag high cvs
```

```
dat1$H2S_cv_flag <- ifelse(dat1$H2S_cv > cv_flag_sample, 'High CV', 'within range')
```

```
head(dat1)
```

```

## # A tibble: 6 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1          0      0      0    bdl          1 within range
## 2 1 Spike    15.5   3.05  19.7 Within_Range 1 High CV
## 3 10         0      0      0    bdl          1 within range
## 4 10 Spike    18.3   0.994  5.44 Within_Range 1 within range
## 5 11         0      0      0    bdl          1 within range
## 6 12         0      0      0    bdl          1 within range

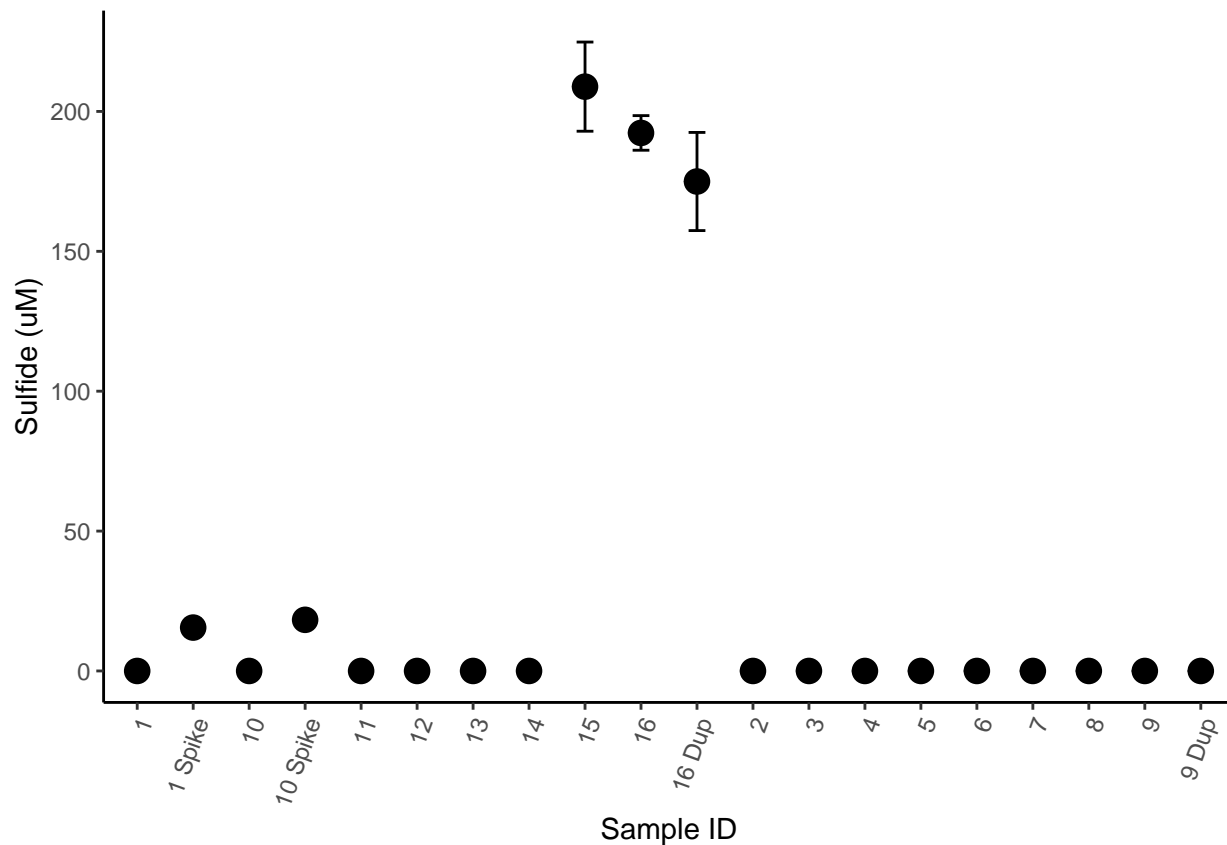
```

```
#plot data and sd's just to check and see what they look like - just a quick first look
```

```

H2S <- ggplot(dat1, aes(x=IDs, y=H2S_mean))+
  geom_point(size=4) + theme_classic() +
  labs(y="Sulfide (uM)", x="Sample ID") +
  geom_errorbar(aes(ymin=H2S_mean-H2S_sd,
                    ymax=H2S_mean+H2S_sd),width=0.3,position=position_dodge(.1))+
  guides(x = guide_axis(angle = 70))
H2S

```



0.10 Remove bad reps

####This is a bit clunky but they figured out how to auto remove bad reps!####

```
# filter High CV Samples
dat1_HCV <- dat1 %>%
  filter(str_detect(H2S_cv_flag, "High CV"))
head(dat1_HCV)
```

```
## # A tibble: 2 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      15.5    3.05   19.7 Within_Range      1 High CV
## 2 16 Dup      175.    17.5   10.0 adl          1 High CV
```

```
dat_HCV <- subset(dat_flagged, (IDs %in% dat1_HCV$IDs ))
head(dat_HCV)
```

```
## # A tibble: 6 x 7
##   Wells Abs IDs      Dilution Conc H2S_Conc_Final H2S_info
##   <chr> <dbl> <chr>      <int> <dbl>      <dbl> <chr>
## 1 D10  0.292 1 Spike      1  19.0      19.0 Within_Range
## 2 D11  0.245 1 Spike      1  14.4      14.4 Within_Range
```

```
## 3 D12    0.233 1 Spike          1 13.2          13.2 Within_Range
## 4 G10    1.82 16 Dup           1 168.          168.  adl
## 5 G11    1.75 16 Dup           1 162.          162.  adl
## 6 G12    2.09 16 Dup           1 195.          195.  adl
```

```
#Columns 4 7 10
```

```
Column1= c("A04", "A07","A10", "B04","B10" ,"C04" , "C07", "C10",
"D04","D10", "E04","E07", "E10" ,"F04" , "F07" ,"G04","G07" ,"G10" ,"H01","H04","H07")
```

```
#Columns 5,8,11
```

```
Column2= c("A05", "A08","A11", "B05","B11" ,"C05" , "C08", "C11",
"D05","D11", "E05","E08", "E11" ,"F05" , "F08" ,"G05","G08" ,"G11" ,"H02","H05","H08")
```

```
#Columns 6,9,12
```

```
Column3= c("A06", "A09","A12", "B06" ,"B12" ,"C06" , "C09", "C12",
"D06","D12", "E06","E09", "E12" ,"F06" , "F09" ,"G06","G09" ,"G12" ,"H03","H06","H09")
```

```
#Delete Column one
```

```
dat_HCV1 <- subset(dat_HCV, !(Wells %in% Column1 ))
```

```
#Delete Column two
```

```
dat_HCV2 <- subset(dat_HCV, !(Wells %in% Column2 ))
```

```
#Delete Column three
```

```
dat_HCV3 <- subset(dat_HCV, !(Wells %in% Column3 ))
```

```
##Find CV for each data set with one column's data removed
```

```
#W/out column1
```

```
dat_HCV1 <- dat_HCV1 %>%
  group_by(IDs) %>%
  summarise(H2S_mean = mean(H2S_Conc_Final), H2S_sd = sd(H2S_Conc_Final), H2S_cv = cv(H2S_Conc_Final),
            H2S_flag = first(H2S_info),
            Dilution = first(Dilution))
dat_HCV1$H2S_cv_flag <- ifelse(dat_HCV1$H2S_cv > cv_flag_sample, 'High CV', 'within range')
```

```
#W/out column2
```

```
dat_HCV2 <- dat_HCV2 %>%
  group_by(IDs) %>%
  summarise(H2S_mean = mean(H2S_Conc_Final), H2S_sd = sd(H2S_Conc_Final), H2S_cv = cv(H2S_Conc_Final),
            H2S_flag = first(H2S_info),
            Dilution = first(Dilution))
dat_HCV2$H2S_cv_flag <- ifelse(dat_HCV2$H2S_cv > cv_flag_sample, 'High CV', 'within range')
```

```
#W/out column3
```

```
dat_HCV3 <- dat_HCV3 %>%
  group_by(IDs) %>%
  summarise(H2S_mean = mean(H2S_Conc_Final), H2S_sd = sd(H2S_Conc_Final), H2S_cv = cv(H2S_Conc_Final),
            H2S_flag = first(H2S_info),
            Dilution = first(Dilution))
dat_HCV3$H2S_cv_flag <- ifelse(dat_HCV3$H2S_cv > cv_flag_sample, 'High CV', 'within range')
```

```
#find lowest CVs
dat_HCV1_1 <- subset(dat_HCV1, dat_HCV1$H2S_cv < dat_HCV2$H2S_cv & dat_HCV1$H2S_cv < dat_HCV3$H2S_cv)
head(dat_HCV1_1)
```

```
## # A tibble: 1 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 within range
```

```
dat_HCV2_2 <- subset(dat_HCV2, dat_HCV2$H2S_cv < dat_HCV1$H2S_cv & dat_HCV2$H2S_cv < dat_HCV3$H2S_cv)
head(dat_HCV2_2)
```

```
## # A tibble: 1 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 within range
```

```
dat_HCV3_3 <- subset(dat_HCV3, dat_HCV3$H2S_cv < dat_HCV2$H2S_cv & dat_HCV3$H2S_cv < dat_HCV1$H2S_cv)
head(dat_HCV3_3)
```

```
## # A tibble: 1 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 16 Dup      165.   4.36   2.64 adl      1 within range
```

```
#recombine data frames
dat2_HCV <- rbind(dat_HCV1_1, dat_HCV2_2, dat_HCV3_3)
head(dat2_HCV)
```

```
## # A tibble: 2 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 within range
## 2 16 Dup      165.   4.36   2.64 adl      1 within range
```

```
dat1 <- subset(dat1, (!IDs %in% dat2_HCV$IDs ))
dat1 <- rbind(dat2_HCV, dat1)
head(dat1)
```

```
## # A tibble: 6 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 within range
## 2 16 Dup      165.   4.36   2.64 adl      1 within range
## 3 1          0      0      0 bd1      1 within range
## 4 10         0      0      0 bd1      1 within range
## 5 10 Spike     18.3  0.994  5.44 Within_Range      1 within range
## 6 11         0      0      0 bd1      1 within range
```

```

#dat1$H2S_mean <- ifelse(dat1$H2S_cv_flag == 'High CV', dat2_HCV$H2S_mean, dat1$H2S_mean)
#dat1$H2S_H2S_sd <- ifelse(dat1$H2S_cv_flag == 'High CV', dat2_HCV$H2S_H2S_sd, dat1$H2S_H2S_sd)
#dat1$H2S_H2S_cv <- ifelse(dat1$H2S_cv_flag == 'High CV', dat2_HCV$H2S_H2S_cv, dat1$H2S_H2S_cv)
#dat1$H2S_H2S_cv_flag <- ifelse(dat1$H2S_cv_flag == 'High CV', dat2_HCV$H2S_H2S_cv_flag, dat1$H2S_H2S_

###Manually Remove bad reps by row number in original dataframe
#dat <- dat[-c(10,13,16,21,28,31,37,40,48,52,60),]
#dat <- subset(dat, !(Wells %in% c("B04," )))

#rerun lines 231-253
#head(dat)

#summarize by sampleID so that we can calculate the mean and std. dev. of the three wells
#dat1 <- dat %>%
# group_by(IDs) %>%
# summarise(H2S_mean = mean(H2S_Conc_Final), H2S_sd = sd(H2S_Conc_Final), H2S_cv = cv(H2S_Conc_Final),
#           # H2S_flag = first(H2S_info),
#           # Dilution = first(Dilution))

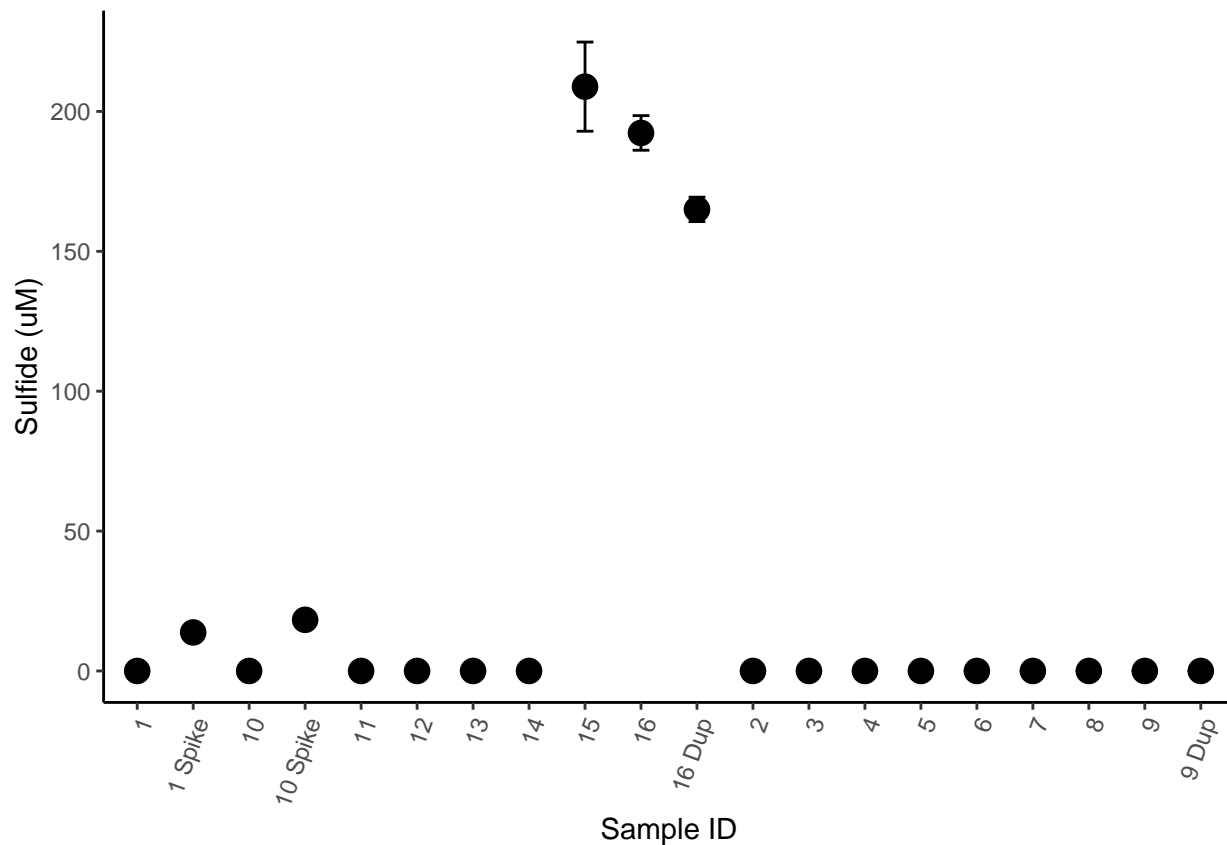
#head(dat1)

#Flag high cvs
#dat1$H2S_cv_flag <- ifelse(dat1$H2S_cv > 10, 'High CV rerun', 'within range')

#head(dat1)

#plot data and sd's just to check and see what they look like - just a quick first look
H2S <- ggplot(dat1, aes(x=IDs, y=H2S_mean))+
  geom_point(size=4) + theme_classic() +
  labs(y="Sulfide (uM)", x="Sample ID") +
  geom_errorbar(aes(ymin=H2S_mean-H2S_sd,
                    ymax=H2S_mean+H2S_sd),width=0.3,position=position_dodge(.1))+
  guides(x = guide_axis(angle = 70))
H2S

```



```
#If samples with cv >10 rerun those samples
H2S_HighCVRerun <- subset(dat1, H2S_cv_flag == "High CV")
H2S_DiluteRerun <- subset(dat1, H2S_flag == "ad1")
H2S_DiluteRerun$Top_STD <- Top_STD
H2S_bdl <- subset(dat1, H2S_flag == "bd1")
print(H2S_HighCVRerun)
```

```
## # A tibble: 0 x 7
## #   i 7 variables: IDs <chr>, H2S_mean <dbl>, H2S_sd <dbl>, H2S_cv <dbl>,
## #     H2S_flag <chr>, Dilution <int>, H2S_cv_flag <chr>
```

```
print(H2S_DiluteRerun)
```

```
## # A tibble: 3 x 8
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag Top_STD
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int>  <chr>      <dbl>
## 1 16 Dup      165.    4.36   2.64 ad1          1 within range    100
## 2 15          209.   15.9   7.63 ad1          1 within range    100
## 3 16          192.    6.19   3.22 ad1          1 within range    100
```

```
print(H2S_bdl)
```

```
## # A tibble: 15 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
```

```
##      <chr>      <dbl> <dbl> <dbl> <chr>      <int> <chr>
##  1 1          0      0      0 bdl          1 within range
##  2 10         0      0      0 bdl          1 within range
##  3 11         0      0      0 bdl          1 within range
##  4 12         0      0      0 bdl          1 within range
##  5 13         0      0      0 bdl          1 within range
##  6 14         0      0      0 bdl          1 within range
##  7 2          0      0      0 bdl          1 within range
##  8 3          0      0      0 bdl          1 within range
##  9 4          0      0      0 bdl          1 within range
## 10 5          0      0      0 bdl          1 within range
## 11 6          0      0      0 bdl          1 within range
## 12 7          0      0      0 bdl          1 within range
## 13 8          0      0      0 bdl          1 within range
## 14 9          0      0      0 bdl          1 within range
## 15 9 Dup      0      0      0 bdl          1 within range
```

0.11 Check the dups for QAQC

```
## # A tibble: 6 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
##   <chr>      <dbl> <dbl> <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 within range
## 2 16 Dup      165.   4.36  2.64 adl          1 within range
## 3 1          0      0      0 bdl          1 within range
## 4 10         0      0      0 bdl          1 within range
## 5 10 Spike      18.3  0.994  5.44 Within_Range      1 within range
## 6 11         0      0      0 bdl          1 within range
```

```
## # A tibble: 2 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
##   <chr>      <dbl> <dbl> <dbl> <chr>      <int> <chr>
## 1 16 Dup      165.   4.36  2.64 adl          1 within range
## 2 9 Dup        0      0      0 bdl          1 within range
```

```
## # A tibble: 6 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
##   <chr>      <dbl> <dbl> <dbl> <chr>      <int> <chr>
## 1 1          0      0      0 bdl          1 within range
## 2 10         0      0      0 bdl          1 within range
## 3 11         0      0      0 bdl          1 within range
## 4 12         0      0      0 bdl          1 within range
## 5 13         0      0      0 bdl          1 within range
## 6 14         0      0      0 bdl          1 within range
```

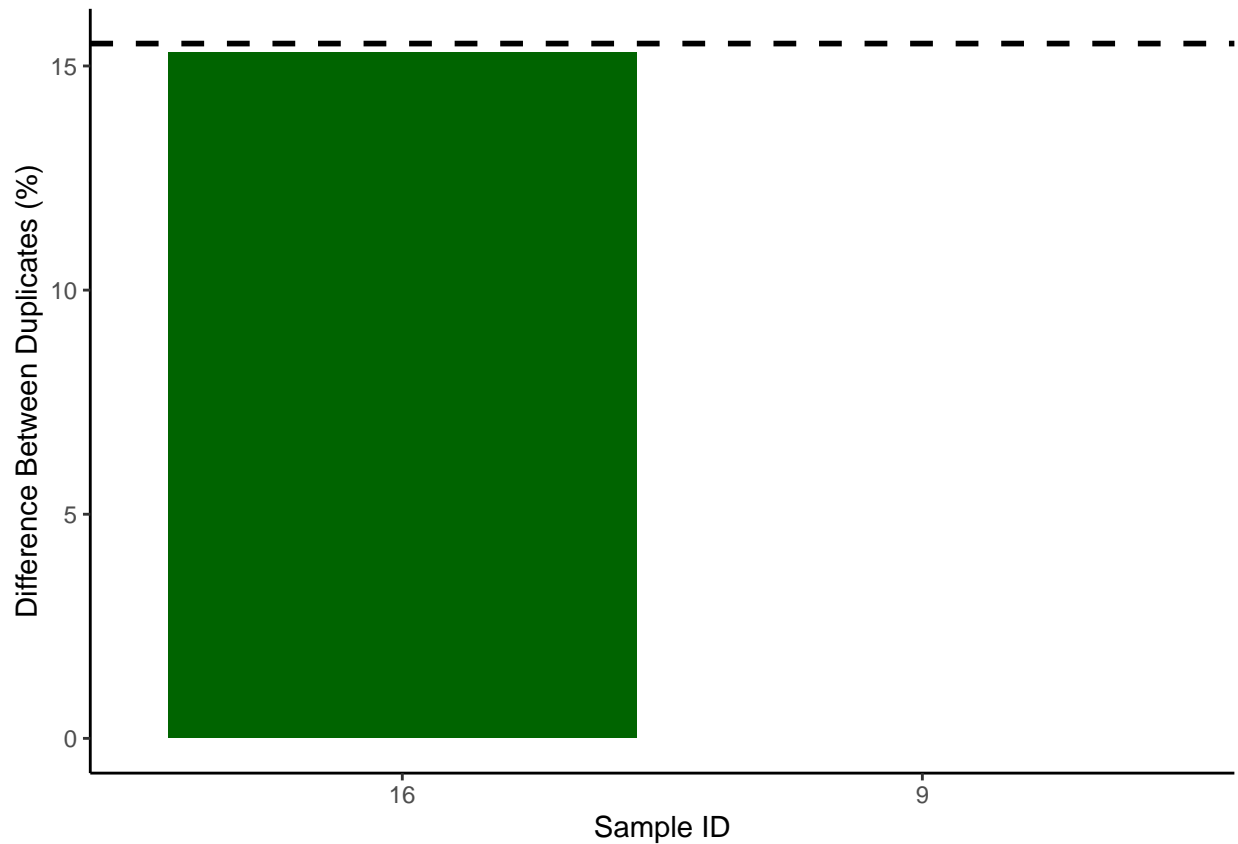
```
## # A tibble: 2 x 7
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
##   <chr>      <dbl> <dbl> <dbl> <chr>      <int> <chr>
## 1 16      165.   4.36  2.64 adl          1 within range
## 2 9         0      0      0 bdl          1 within range
```

```
##   IDs H2S_mean  H2S_sd  H2S_cv H2S_flag Dilution  H2S_cv_flag mean_dup
```

```
## 1 16 192.3164 6.189032 3.218151 adl 1 within range 164.9854
## 2 9 0.0000 0.000000 0.000000 bdl 1 within range 0.0000
## NA NA.1 NA.2 NA.3 NA.4
## 1 4.361315 2.643455 adl 1 within range
## 2 0.000000 0.000000 bdl 1 within range
```

```
## IDs H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag mean_dup
## 1 16 192.3164 6.189032 3.218151 adl 1 within range 164.9854
## 2 9 0.0000 0.000000 0.000000 bdl 1 within range 0.0000
## NA NA.1 NA.2 NA.3 NA.4 dups_chk dups_flag
## 1 4.361315 2.643455 adl 1 within range 15.29855 OK
## 2 0.000000 0.000000 bdl 1 within range NaN <NA>
```

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
```



0.12 Check the spks for QAQC

```
## # A tibble: 6 x 7
## IDs H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
## <chr> <dbl> <dbl> <dbl> <chr> <int> <chr>
## 1 1 Spike 13.8 0.831 6.03 Within_Range 1 within range
## 2 16 Dup 165. 4.36 2.64 adl 1 within range
## 3 1 0 0 0 bdl 1 within range
```



```
## 4 10      0      0      0      bdl      1 within range
## 5 10 Spike 18.3  0.994  5.44 Within_Range 1 within range
## 6 11      0      0      0      bdl      1 within range
```

```
## # A tibble: 2 x 7
```

```
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1 Spike      13.8  0.831  6.03 Within_Range      1 1 within range
## 2 10 Spike     18.3  0.994  5.44 Within_Range      1 1 within range
```

```
## # A tibble: 6 x 7
```

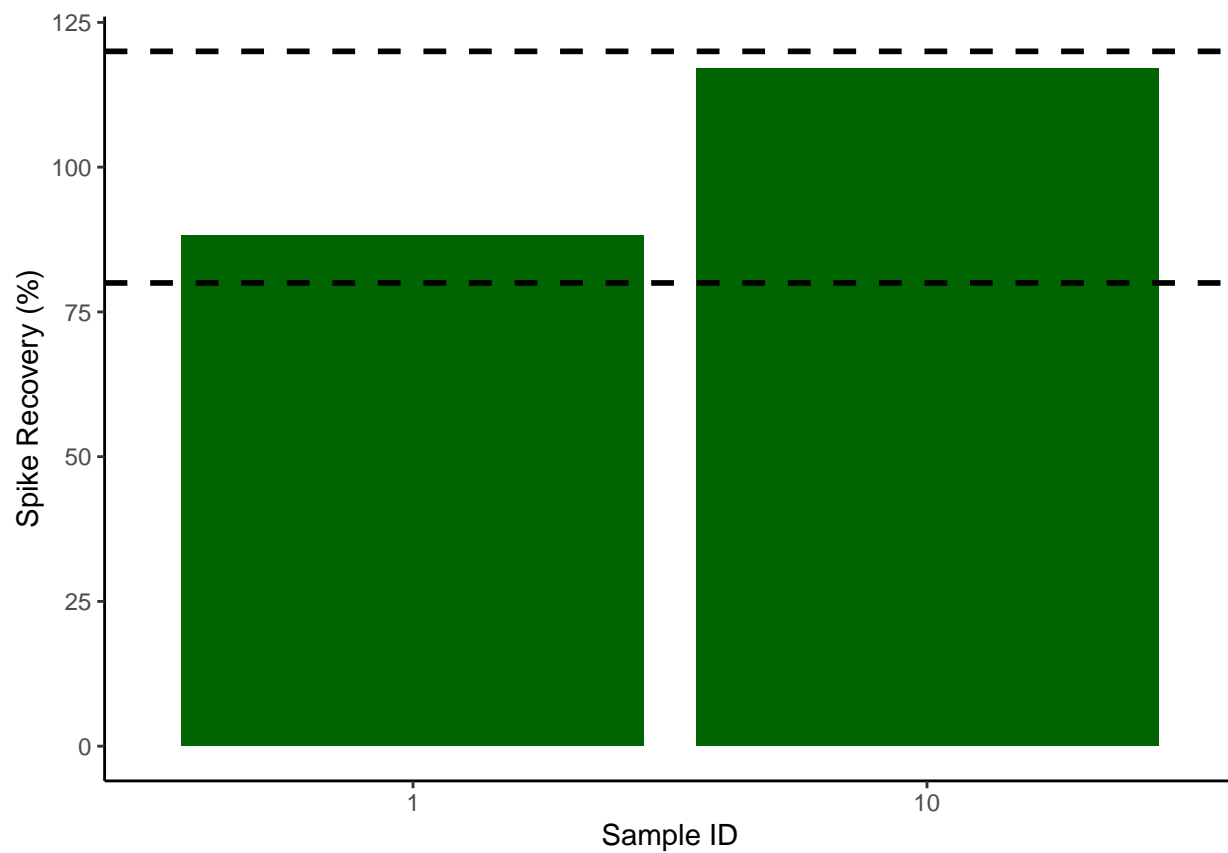
```
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1      0      0      0 bdl      1 1 within range
## 2 10     0      0      0 bdl      1 1 within range
## 3 11     0      0      0 bdl      1 1 within range
## 4 12     0      0      0 bdl      1 1 within range
## 5 13     0      0      0 bdl      1 1 within range
## 6 14     0      0      0 bdl      1 1 within range
```

```
## # A tibble: 2 x 7
```

```
##   IDs      H2S_mean H2S_sd H2S_cv H2S_flag      Dilution H2S_cv_flag
##   <chr>      <dbl>  <dbl>  <dbl> <chr>      <int> <chr>
## 1 1      13.8  0.831  6.03 Within_Range      1 1 within range
## 2 10     18.3  0.994  5.44 Within_Range      1 1 within range
```

```
##   IDs H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag mean_spk      NA
## 1 1      0      0      0      bdl      1 within range 13.77564 0.8307267
## 2 10     0      0      0      bdl      1 within range 18.27914 0.9935976
##   NA.1      NA.2 NA.3      NA.4
## 1 6.030401 Within_Range 1 within range
## 2 5.435691 Within_Range 1 within range
```

```
##   IDs H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag mean_spk      NA
## 1 1      0      0      0      bdl      1 within range 13.77564 0.8307267
## 2 10     0      0      0      bdl      1 within range 18.27914 0.9935976
##   NA.1      NA.2 NA.3      NA.4 unspkd      spkd expctd_spkd
## 1 6.030401 Within_Range 1 within range 0 0.004408206 0.005
## 2 5.435691 Within_Range 1 within range 0 0.005849325 0.005
##   spk_recovery spks_flag
## 1      88.16413      OK
## 2     116.98650      OK
```



0.13 Export final data and samples to rerun

0.13.1 END