

Synoptic CB: Porewater SO₄/Cl

May 2025 Samples

2025-10-15

Contents

0.1	Run Information	2
0.2	Tidy data	3
0.3	Read in tidy data	3
0.4	Plot standards	3
0.5	Assess Standard Curves	4
0.6	Assess Check Standards	6
0.7	Matrix Check QAQC	7
0.8	Flag sample data	8
0.9	Calculate avg, std dev, and cv across wells	8
0.10	Remove bad reps	10
0.11	Check the dups for QAQC	15
0.12	Check the spks for QAQC	16
0.13	Export final data and samples to rerun	18

```
##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"

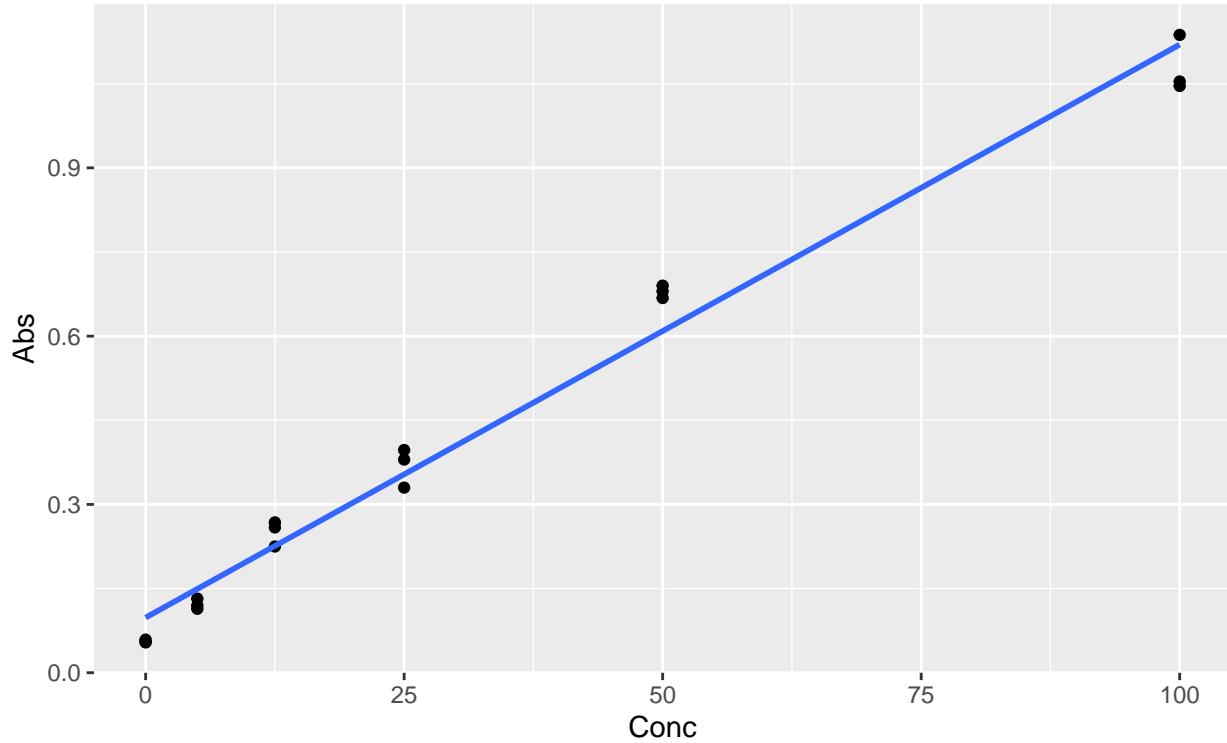
#qaqc log file path for this year
Log_path = "Raw Data/Sulfide_STD_QAQC.csv"
```

```
#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

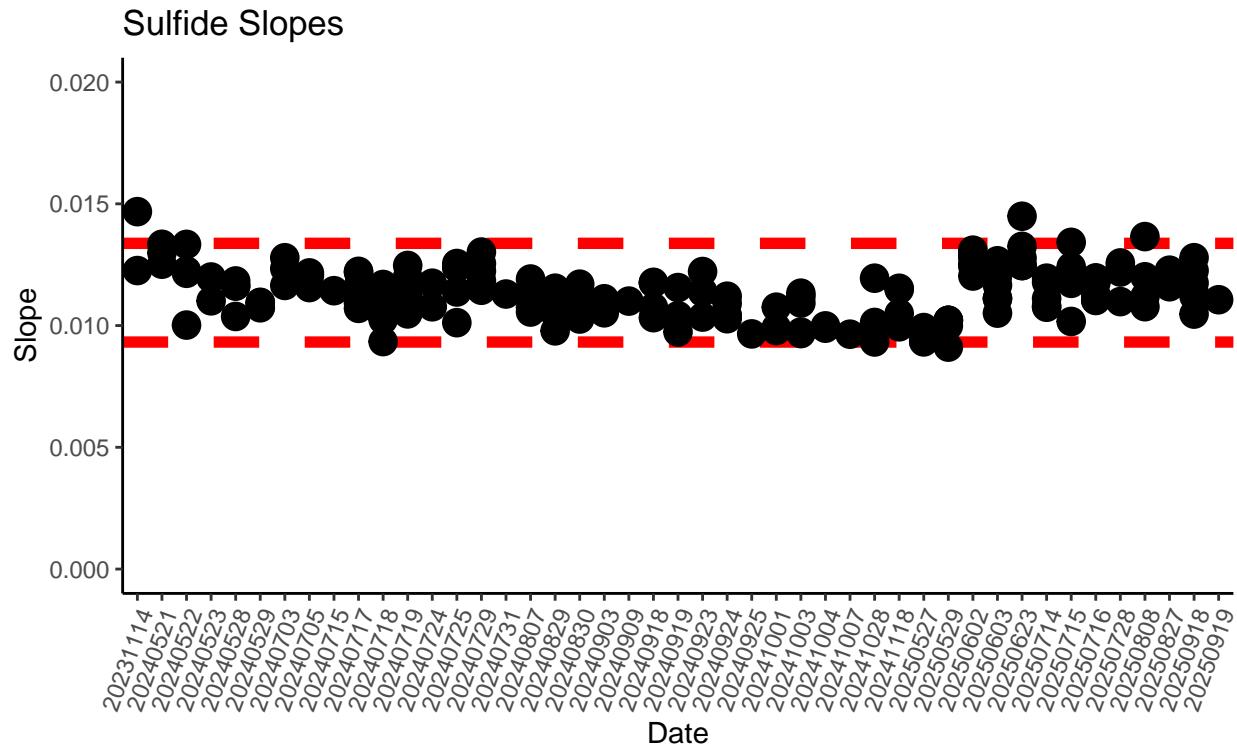
```

##       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

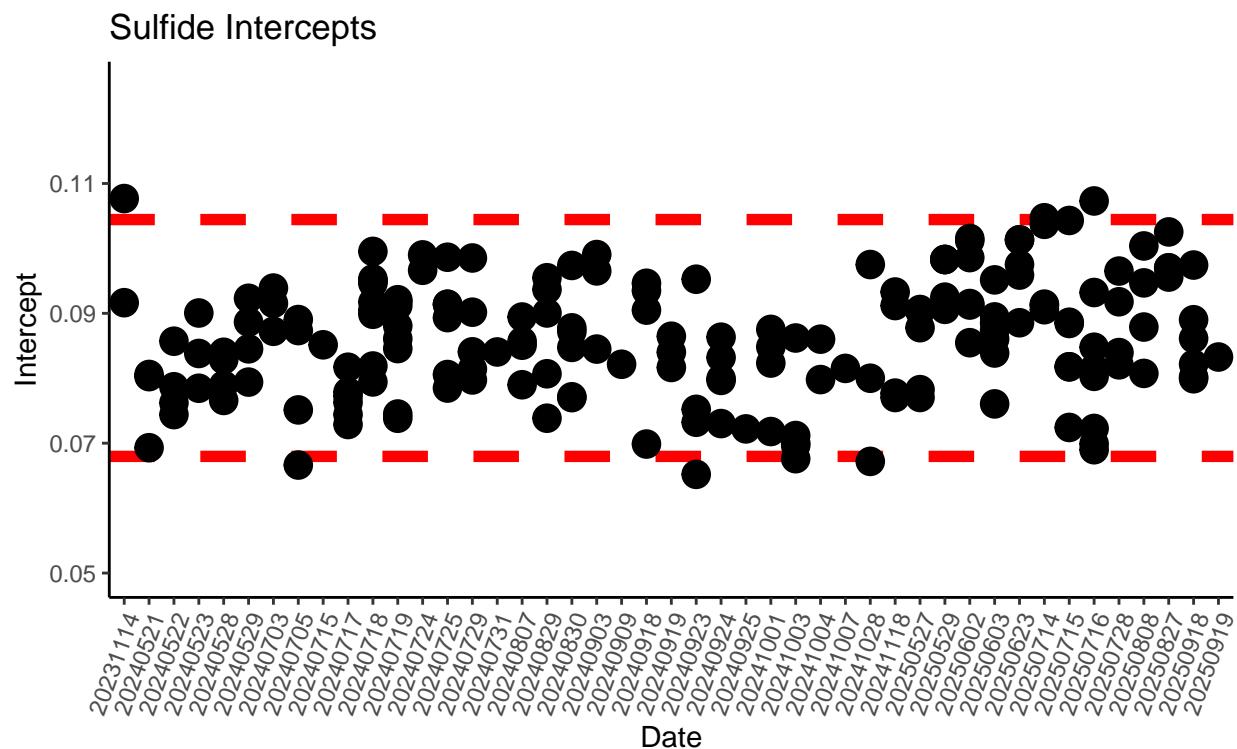
##       Date Project      R2      Slope Intercept Top_STD
## 1 20250529 COMPASS 0.981789 0.01021429 0.0982916    100

##       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

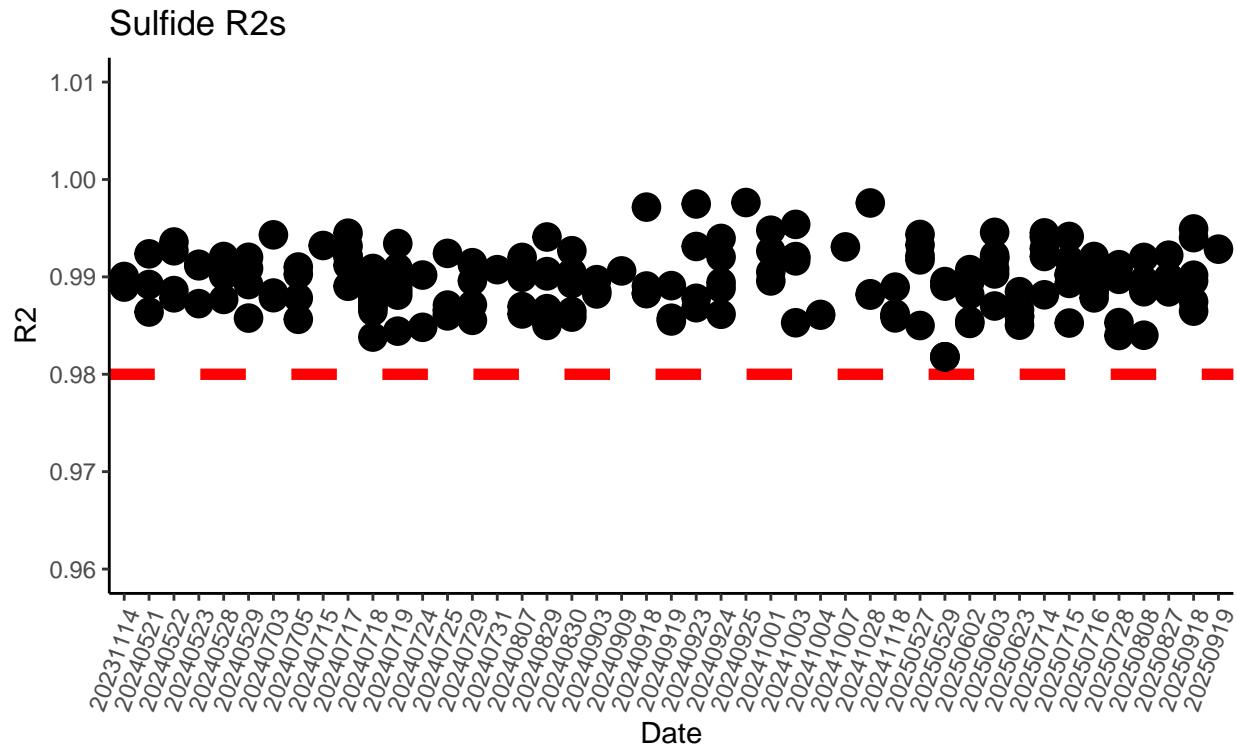
```



```
## [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

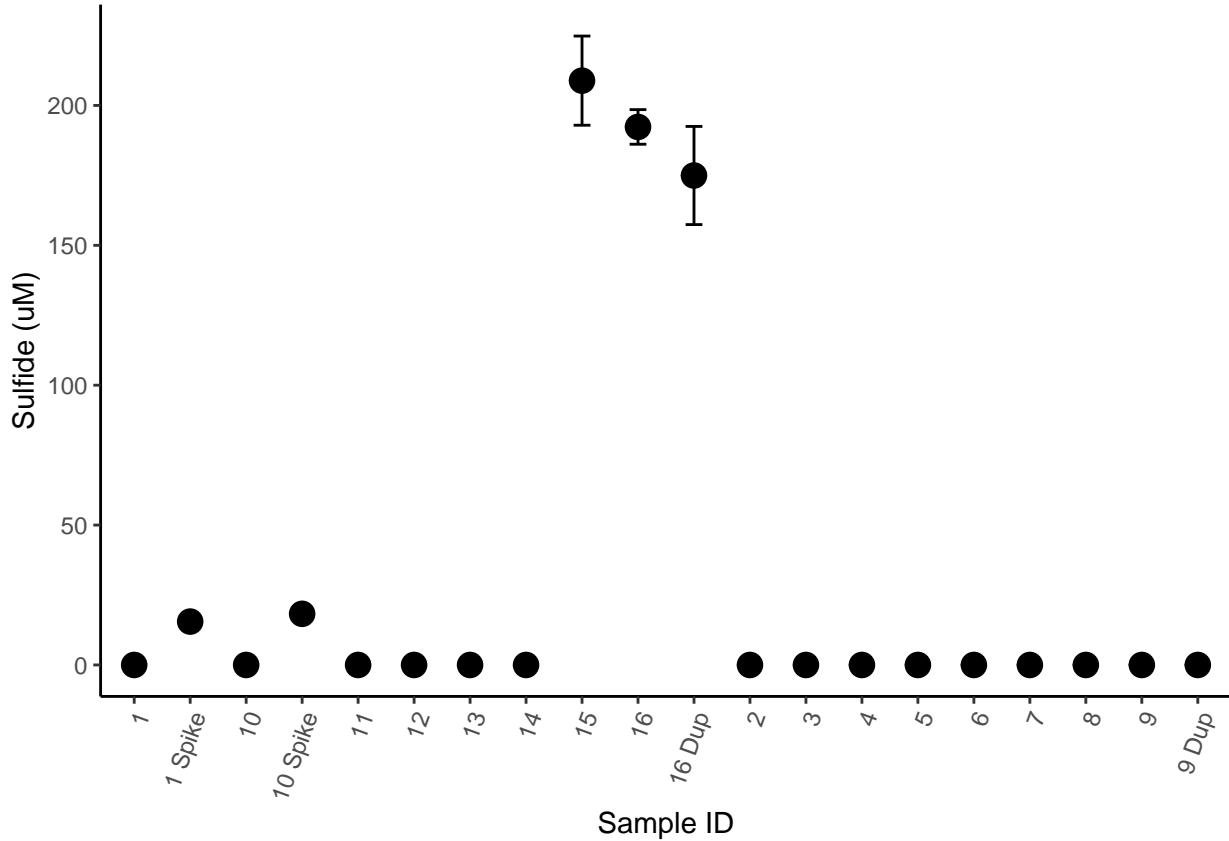
#Flag high cvs
dat1$H2S_cv_flag <- ifelse(dat1$H2S_cv > cv_flag_sample, 'High CV', 'within range')

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(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 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_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 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 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 Spike     13.8    0.831   6.03 Within_Range      1 within range
## 2 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 Spike     13.8    0.831   6.03 Within_Range      1 within range
## 2 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 Spike    18.3    0.994   5.44 Within_Range      1 within range
## 6 11       0        0        0        bdl         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_cv_flag)

####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))

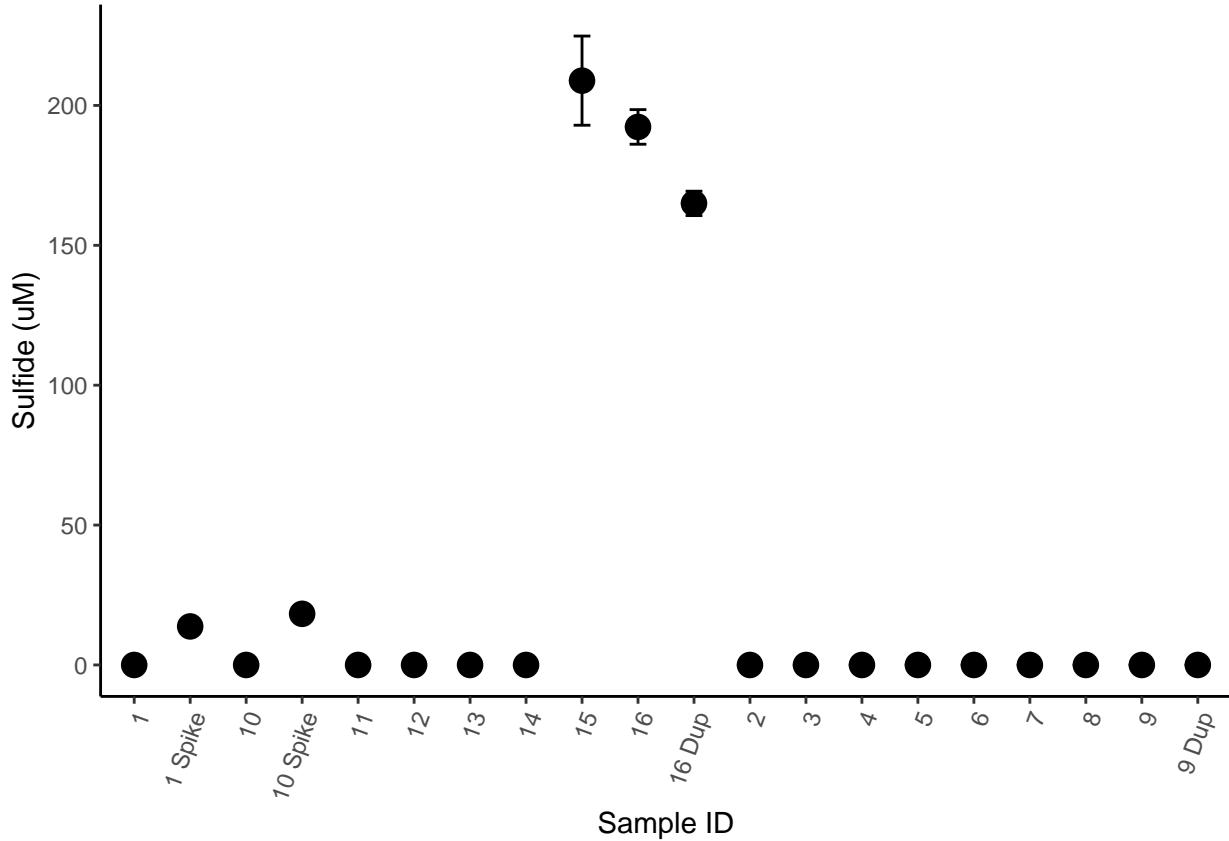
#head(dat1)

#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 == "adl")
H2S_DiluteRerun$Top_STD <- Top_STD
H2S_bdl <- subset(dat1,H2S_flag == "bdl")
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  adl        1 within range    100
## 2 15        209.   15.9    7.63  adl        1 within range    100
## 3 16        192.    6.19   3.22  adl        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

```

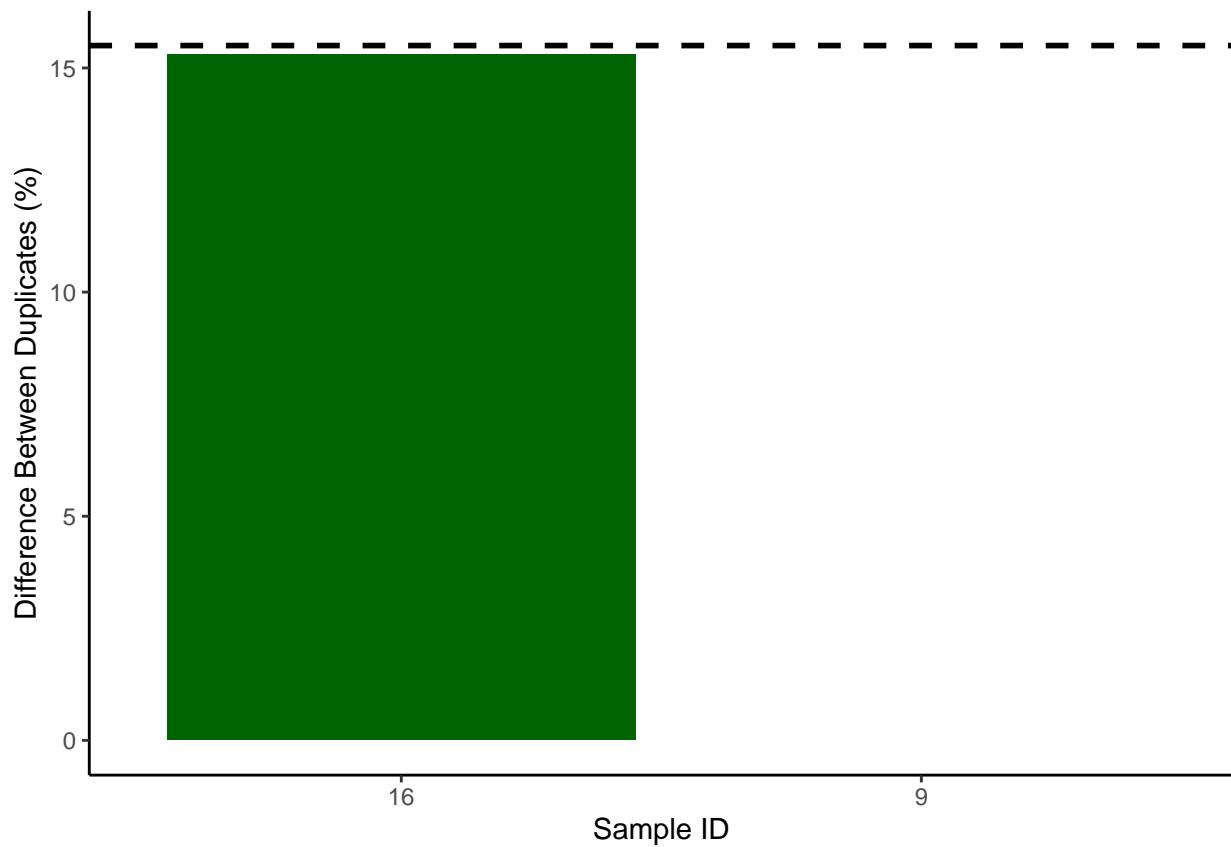
```

## 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 within range
## 2 10    Spike    18.3   0.994  5.44 Within_Range      1 within range

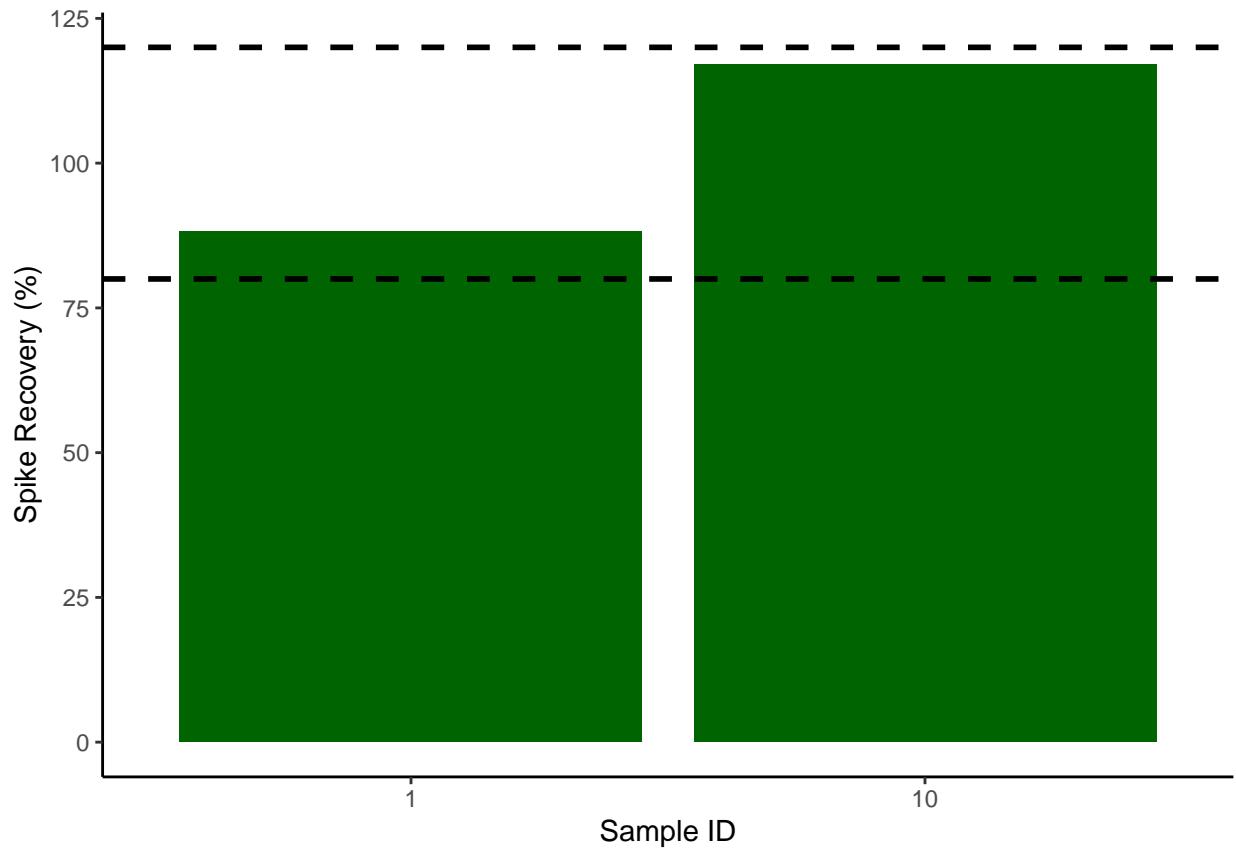
## # A tibble: 6 x 7
##   IDs     H2S_mean H2S_sd H2S_cv H2S_flag Dilution H2S_cv_flag
##   <chr>    <dbl>   <dbl>   <dbl> <chr>       <int> <chr>
## 1 1     1           0   0   0   bdl           1 within range
## 2 10    10          0   0   0   bdl           1 within range
## 3 11    11          0   0   0   bdl           1 within range
## 4 12    12          0   0   0   bdl           1 within range
## 5 13    13          0   0   0   bdl           1 within range
## 6 14    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 1     1           13.8  0.831  6.03 Within_Range      1 within range
## 2 10    10          18.3  0.994  5.44 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
## 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