

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
```

```
##Tidy data
```

```
##Read in tidy data
```

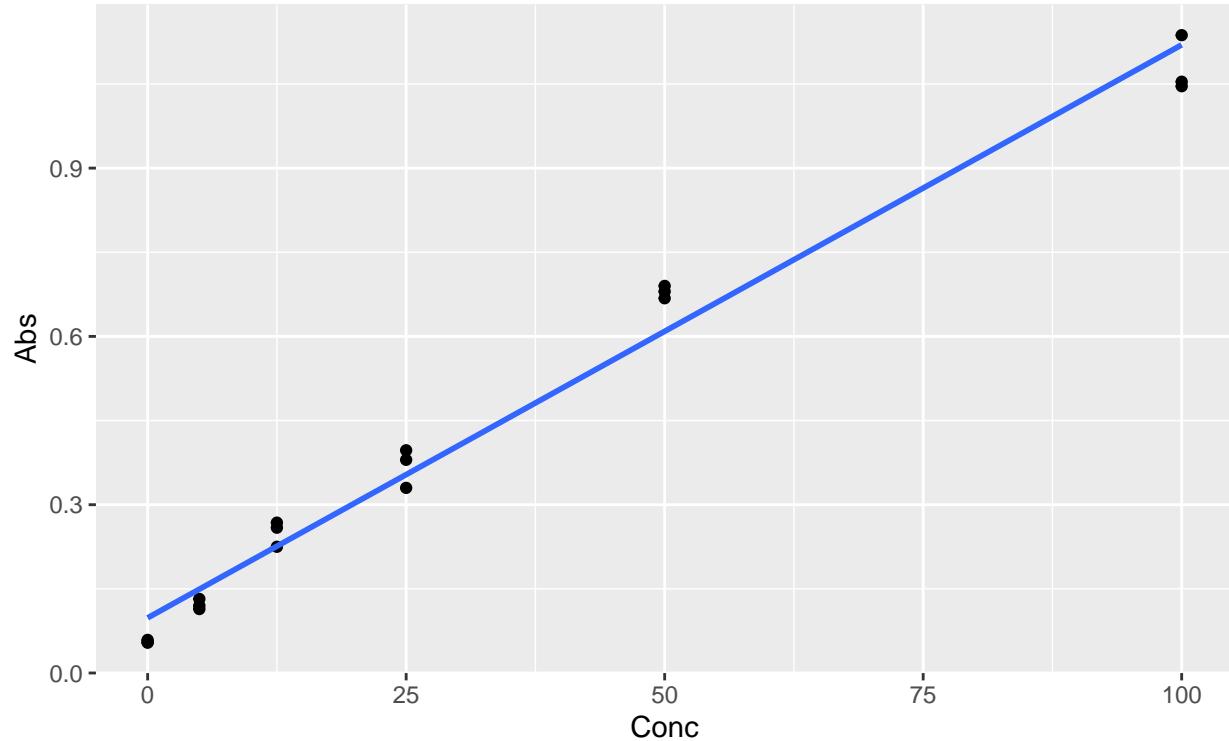
0.2 Fix data that was entered incorrectly

```
##Sample data entered incorrectly
dat$IDs[dat$IDs == "17 Dup"] <- "16 Dup"
dat$IDs[dat$IDs == "18 Dup"] <- "16 Dup"

##Chk stds entered incorrectly
dat$IDs[dat$IDs == "ChkStd 1"] <- "ChkStd 0"
dat$IDs[dat$IDs == "ChkStd 2"] <- "ChkStd 0"
```

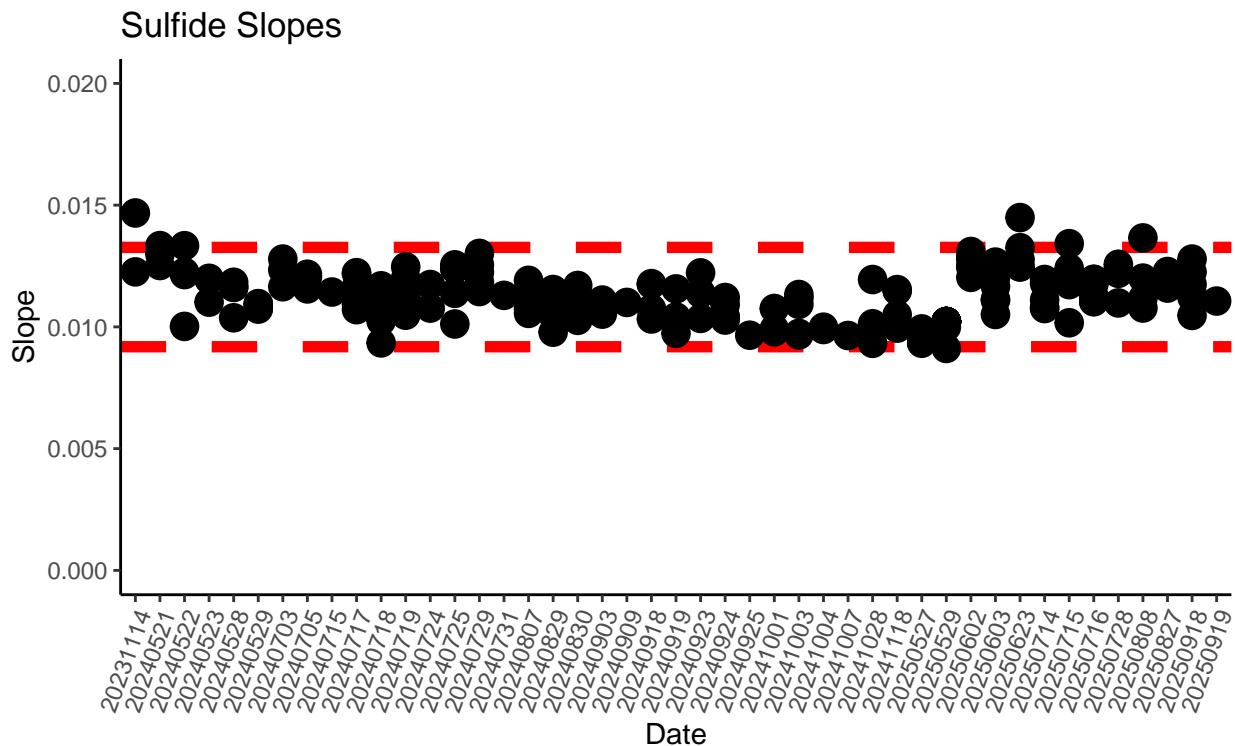
```
dat$IDs[dat$IDs == "ChkStd 5"] <- "ChkStd 4"  
dat$IDs[dat$IDs == "ChkStd 6"] <- "ChkStd 4"
```

0.3 Plot standards

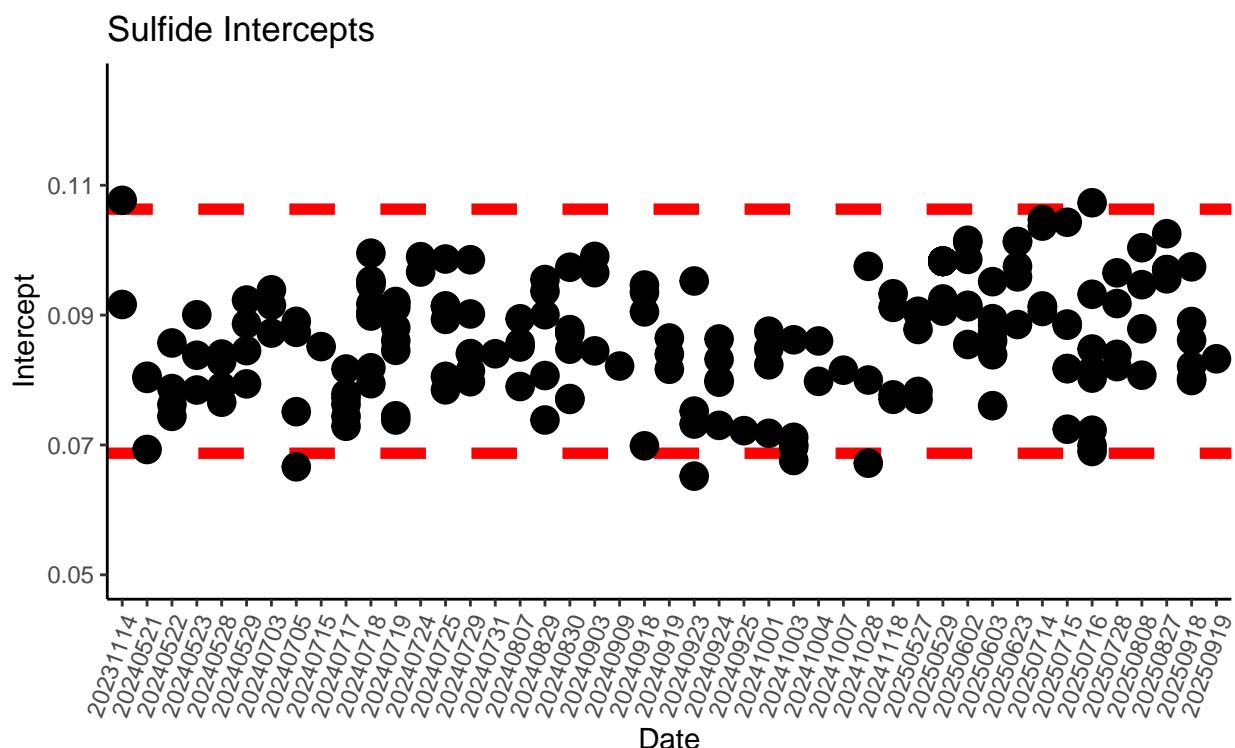


```
## [1] "Std Curve r2 GOOD"
```

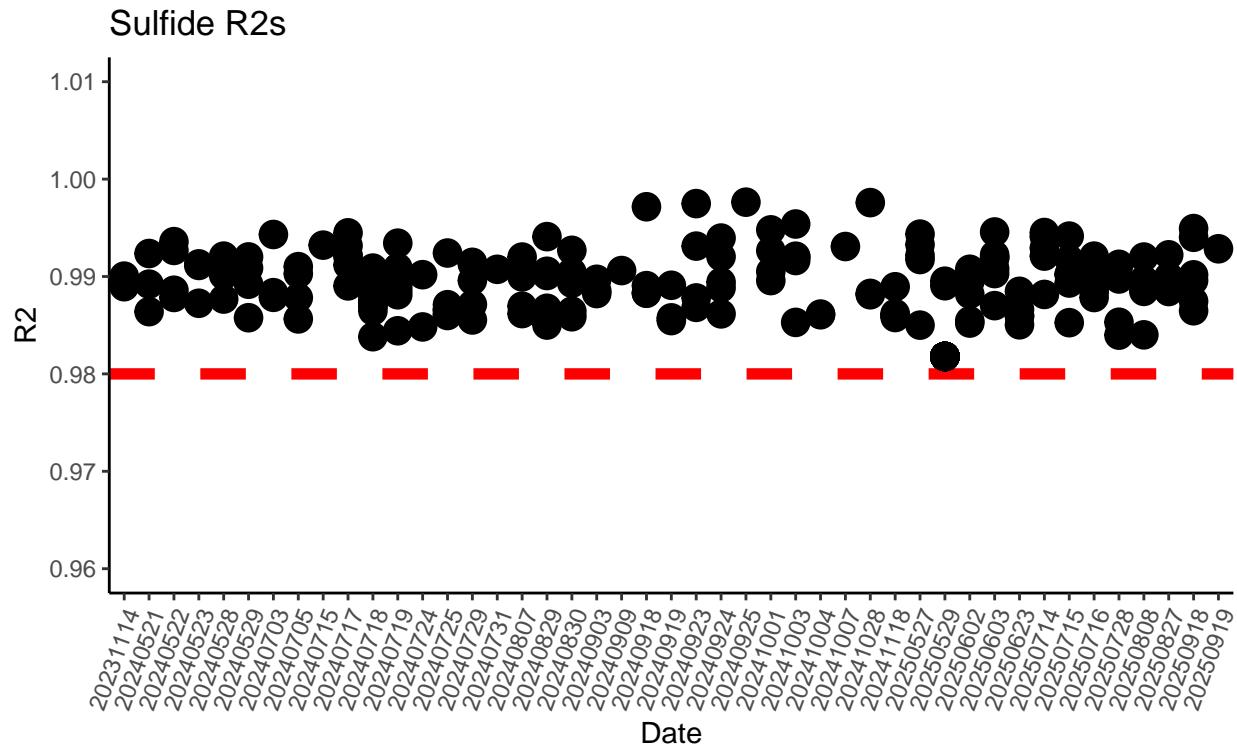
0.4 Assess Standard Curves



```
## [1] "Std curve slope is with 2 sd of previous slopes"
```



```
## [1] "Std curve intercept is with 2 sd of previous intercepts"
```



0.5 Assess Check Standards

Table 1: Two-Sample T-Test Comparing Chk Std 0 with Std 0

	Statistic	Value
t	t-statistic	-0.8509629
df	df	7.0000000
	p-value	0.4229409

```
## [1] "Chk Std 0 GOOD"
```

Table 2: Two-Sample T-Test Comparing Chk Std 3 with Std 3

	Statistic	Value
t	t-statistic	-0.9844326
df	df	4.0000000
	p-value	0.3806366

```
## [1] "Chk Std 3 GOOD"
```

Table 3: Two-Sample T-Test Comparing Chk Std 4 with Std 4

	Statistic	Value
t	t-statistic	0.5041160
df	df	4.0000000
	p-value	0.6406803

```
## [1] "Chk Std 4 GOOD"
```

0.6 Matrix Check QAQC

Table 4: Two-Sample T-Test Comparing MC10 with Std 5

	Statistic	Value
t	t-statistic	1.245676
df	df	4.000000
	p-value	0.280865

```
## [1] "Matrix Check 10 GOOD"
```

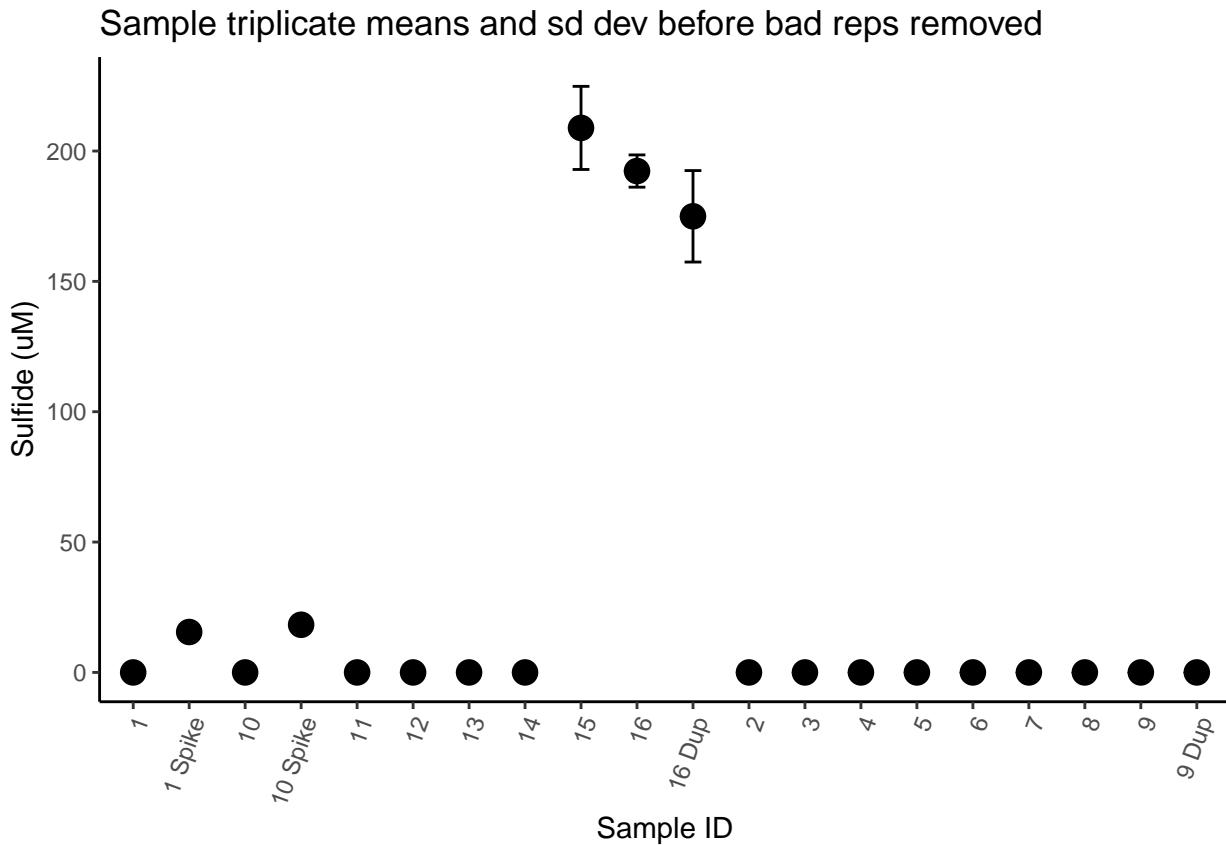
Table 5: Two-Sample T-Test Comparing MC20 with Std 5

	Statistic	Value
t	t-statistic	2.7401513
df	df	4.0000000
	p-value	0.0518974

```
## [1] "Matrix Check 20 GOOD"
```

```
##Flag sample data
```

0.7 Calculate CV across wells



0.8 Remove bad reps

Table 6: High CV Samples

IDs	H2S_mean	H2S_sd	H2S_cv	H2S_flag	Dilution	H2S_cv_flag
1 Spike	15.50525	3.052808	19.68887	Within_Range	1	High CV
16 Dup	174.95510	17.541237	10.02614	adl	1	High CV

Table 7: Samples that originally had high CVs

IDs	H2S_mean	H2S_sd	H2S_cv	H2S_flag	Dilution	H2S_cv_flag
1 Spike	13.77564	0.8307267	6.030401	Within_Range	1	within range
16 Dup	164.98540	4.3613151	2.643455	adl	1	within range

Sample triplicate means and sd dev after bad reps removed

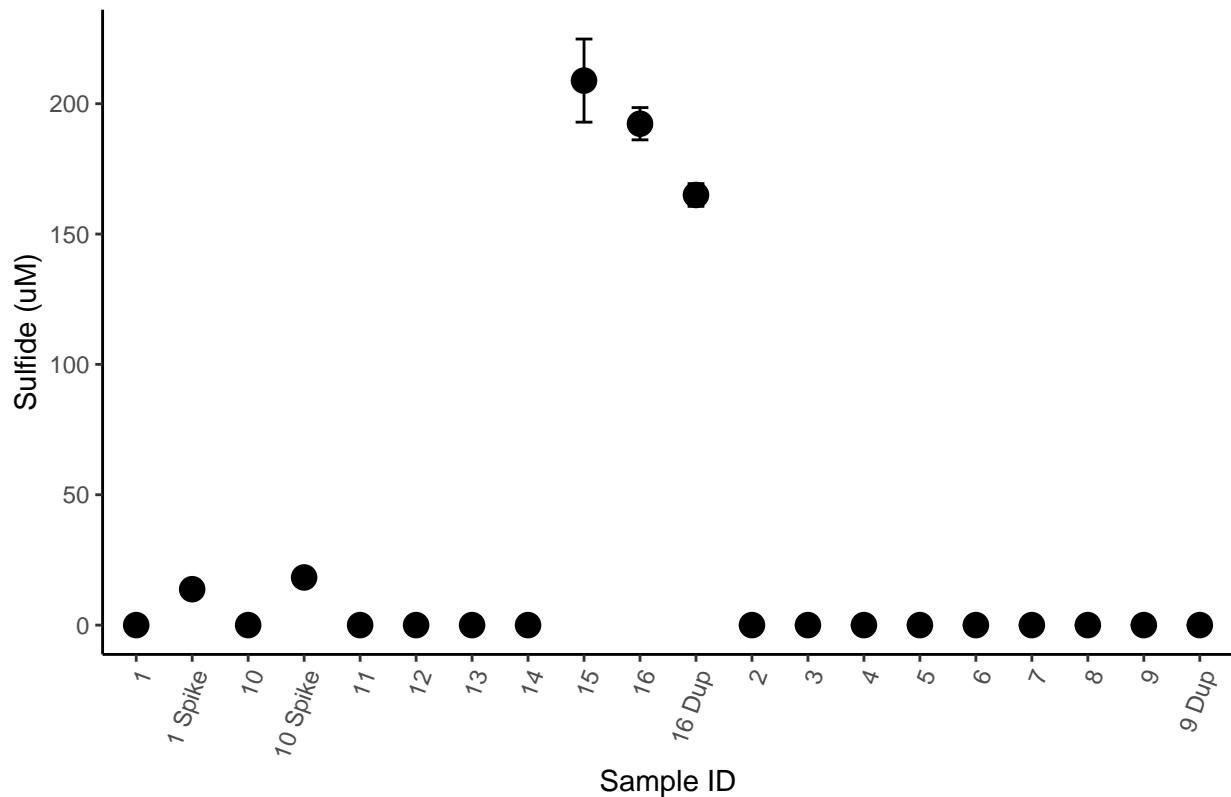


Table 8: Samples that still have High CVs

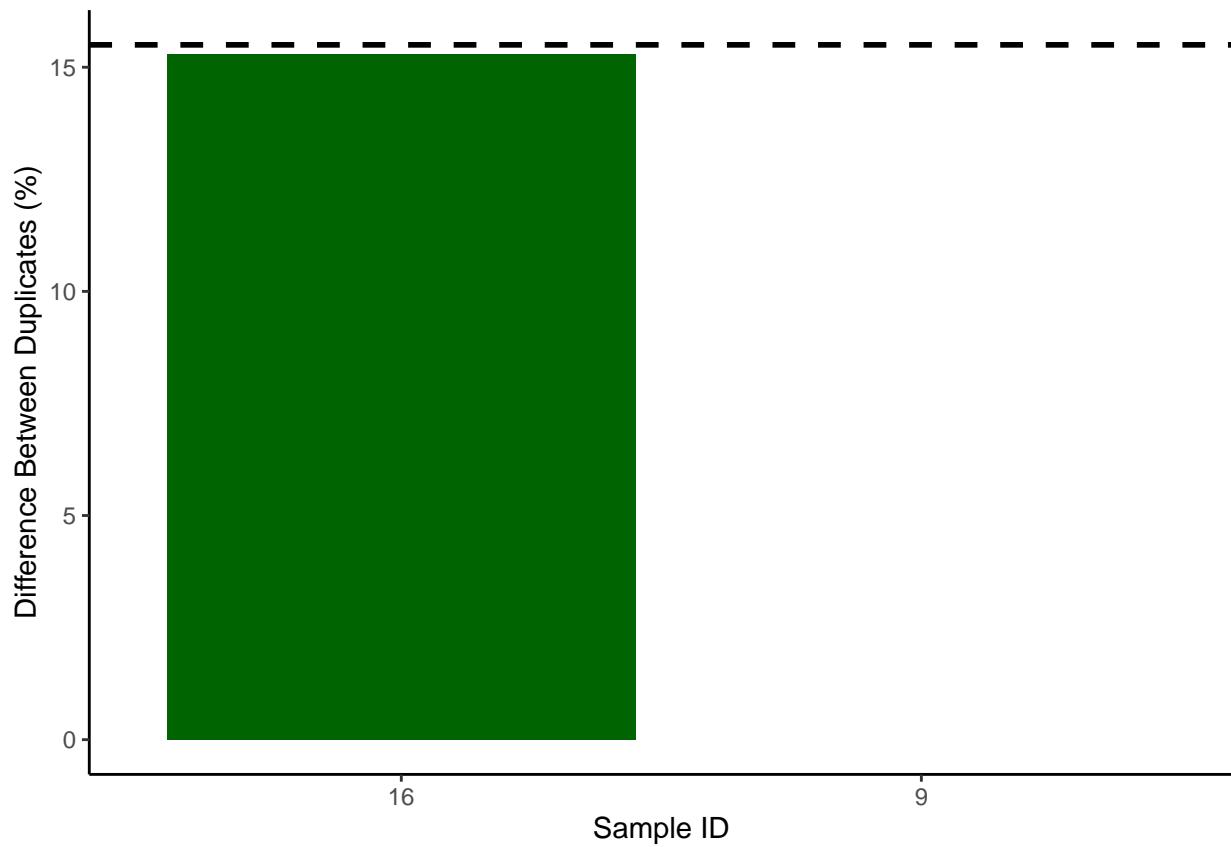
IDs	H2S_mean	H2S_sd	H2S_cv	H2S_flag	Dilution	H2S_cv_flag

Table 9: Samples that need to be diluted

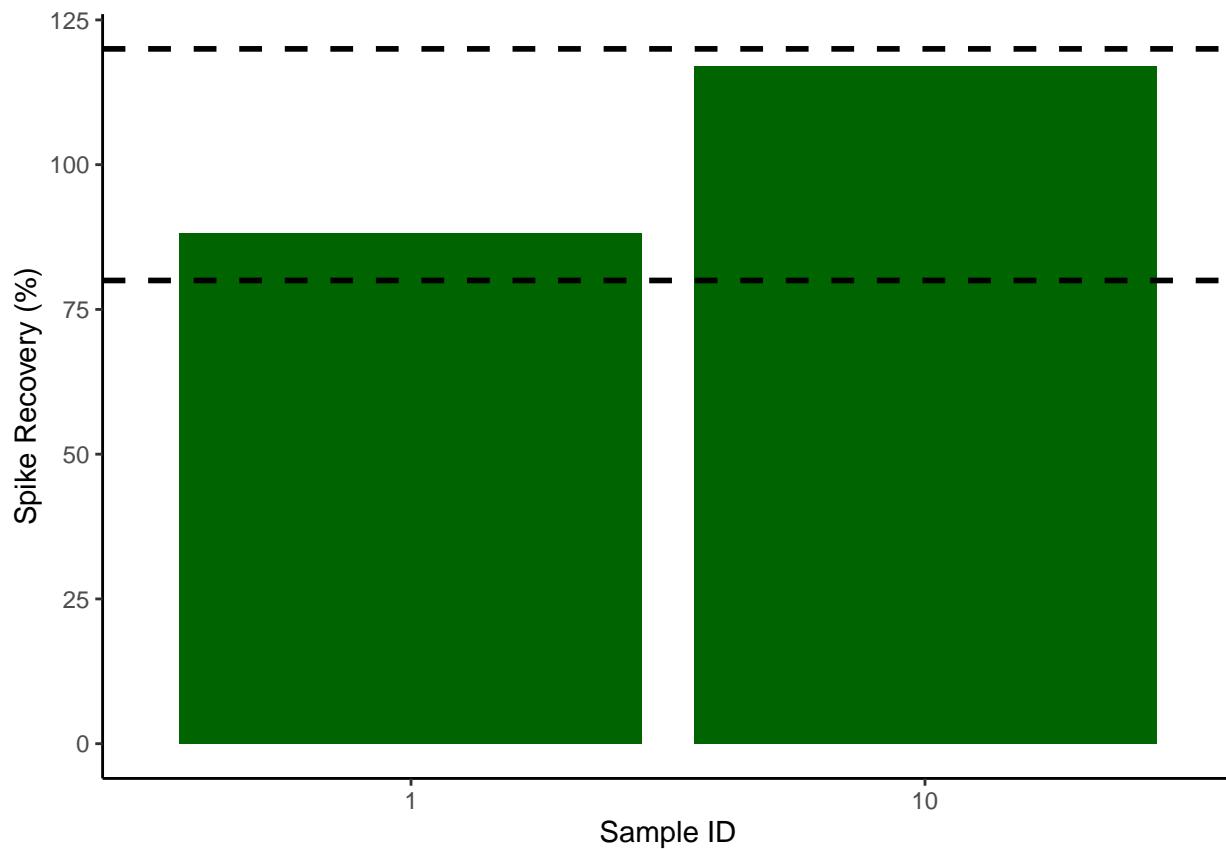
IDs	H2S_mean	H2S_sd	H2S_cv	H2S_flag	Dilution	H2S_cv_flag	Top_STD
16 Dup	164.9854	4.361315	2.643455	adl	1	within range	100
15	208.8619	15.938607	7.631172	adl	1	within range	100
16	192.3164	6.189032	3.218151	adl	1	within range	100

0.9 Check the dups for QAQC

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



0.10 Check the spks for QAQC



0.11 Export final data and samples to rerun

0.11.1 END