

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

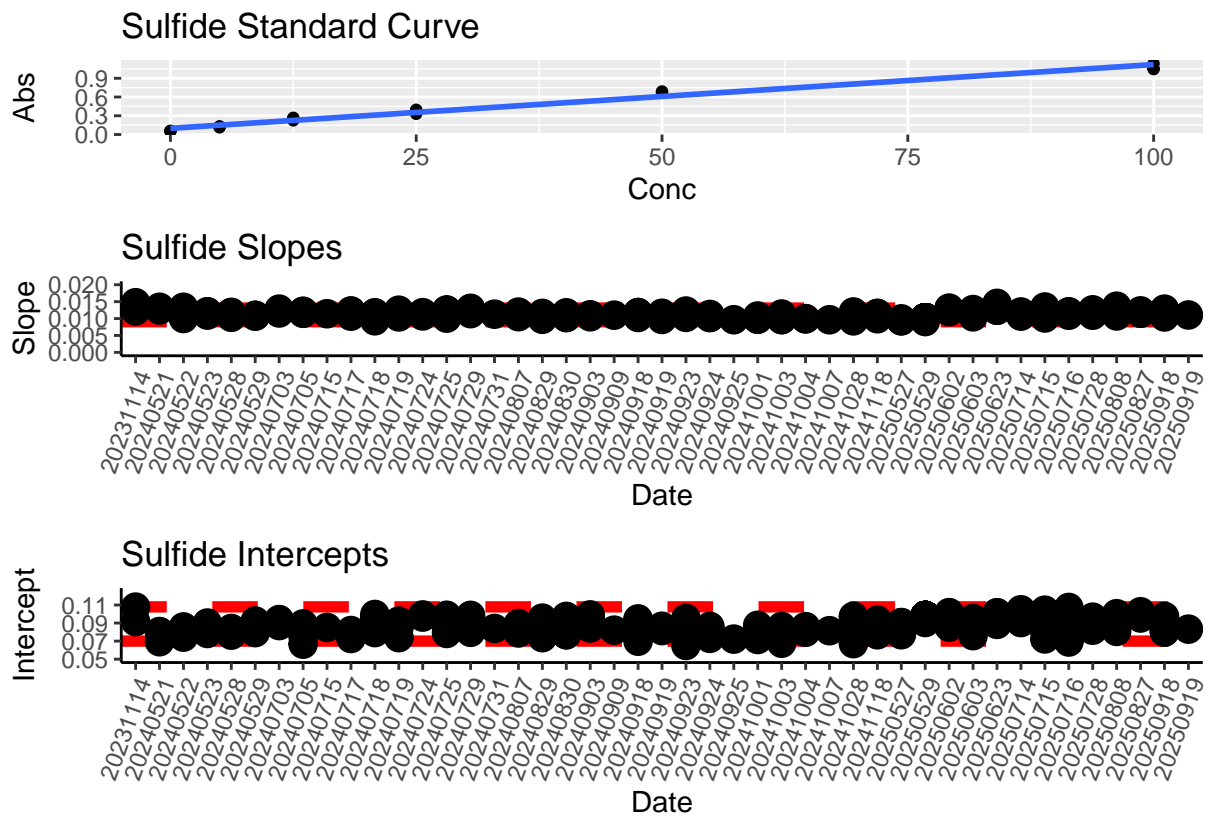
```
##Sample data entered incorrectly
dat$IDs[dat$IDs == "17 Dup"] <- "16 Dup"
dat$IDs[dat$IDs == "18 Dup"] <- "16 Dup"
##Chk stds entered incorrectly
dat$IDs[dat$IDs == "ChkStd 1"] <- "ChkStd 0"
dat$IDs[dat$IDs == "ChkStd 2"] <- "ChkStd 0"
dat$IDs[dat$IDs == "ChkStd 5"] <- "ChkStd 4"
dat$IDs[dat$IDs == "ChkStd 6"] <- "ChkStd 4"
```

```
##Plot standards
```

```
##Assess Standard Curves
```

0.3 Plot standard graphs

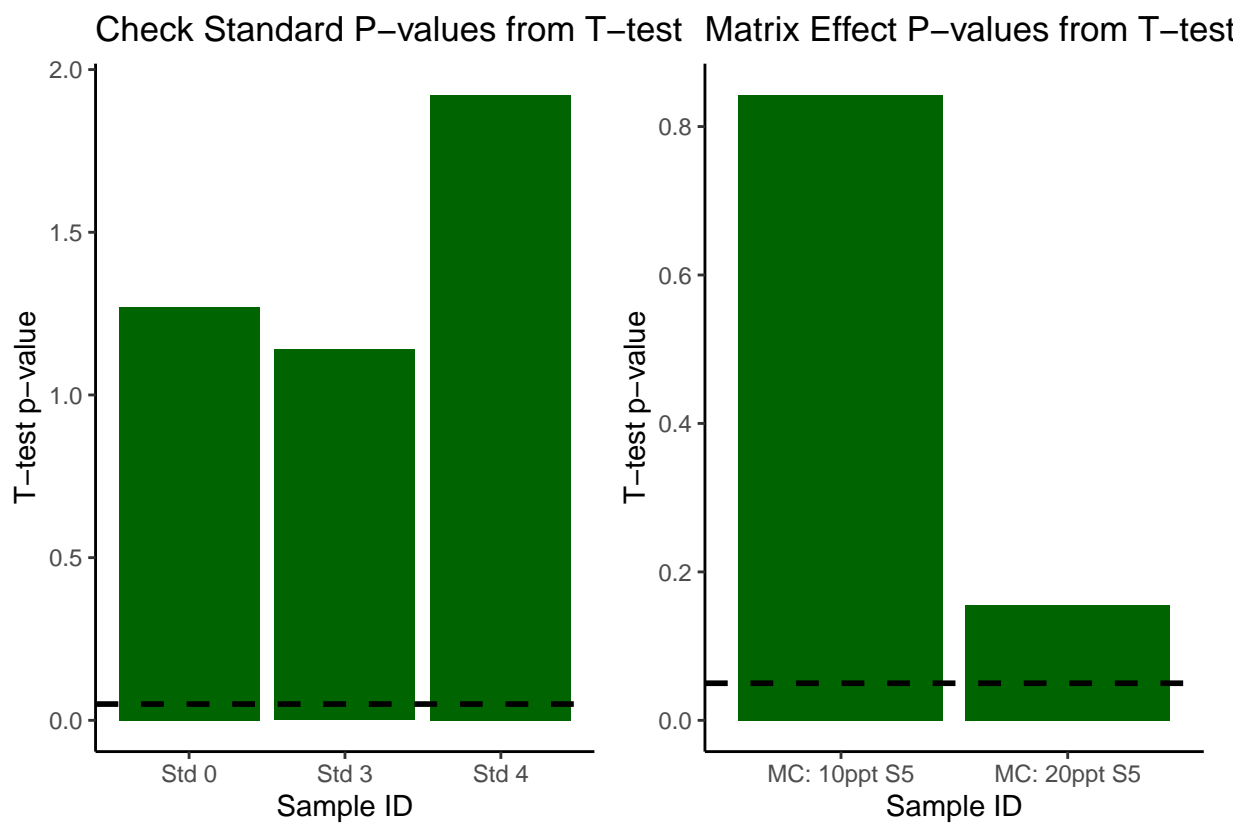
```
## 'geom_smooth()' using formula = 'y ~ x'
```



```
##Assess Check Standards
```

```
##Matrix Check QAQC
```

0.4 Plot check standards and matrix checks

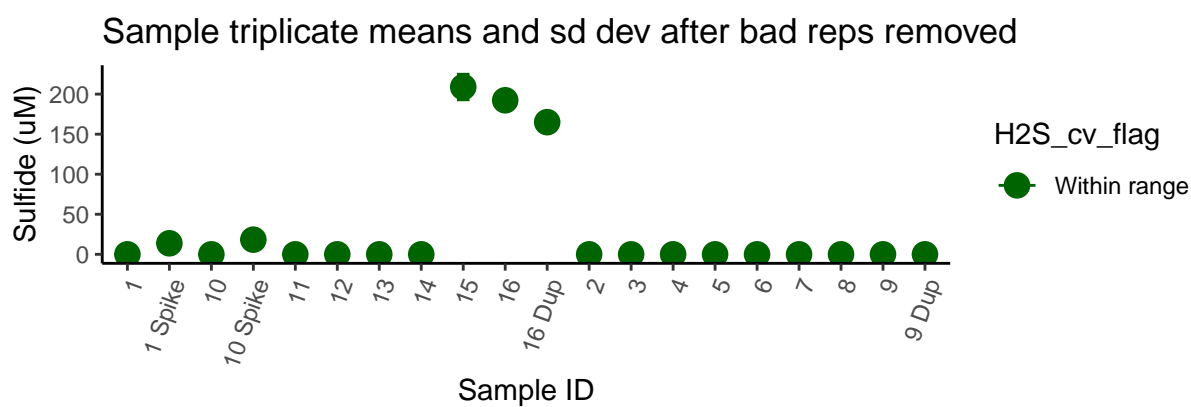
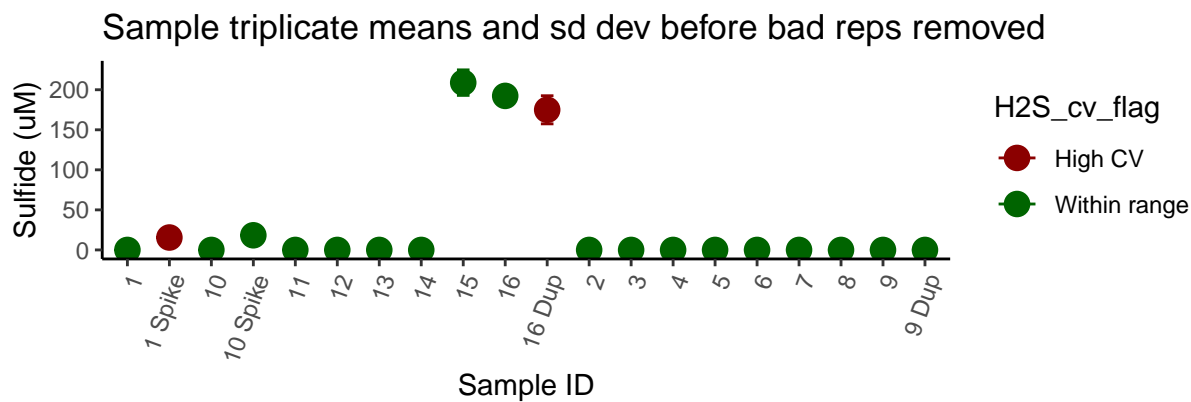


##Flag sample data

##Calculate CV across wells

##Remove bad reps

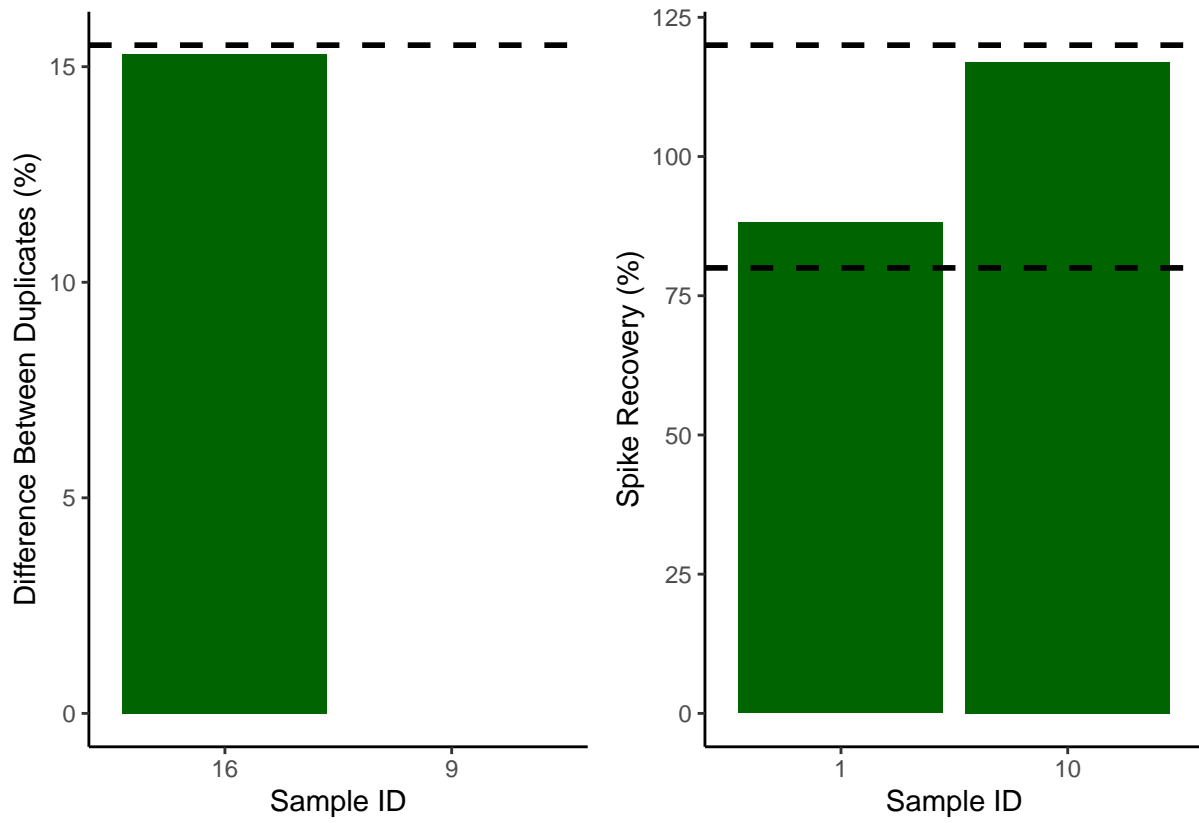
0.5 Plot samples before and after removing bad replicates



##Assess Duplicates

##Assess Analytical Spikes

0.6 Plot duplicates and spikes



##Export final data and samples to rerun

0.6.1 END