Synoptic CB: Porewater SO4/Cl

May 2025 Samples

2025-10-15

Contents

##Need to make sure that the QAQC_flag column makes it into the final processed data file!

##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_Plate1.csv"
  samples_need_dilution_name = "Processed Data/COMPASS_H2S_20250529_Plate1_SamplesNeedDilution.csv"
  samples_high_cv_name = "Processed Data/COMPASS_H2S_20250529_Plate1_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

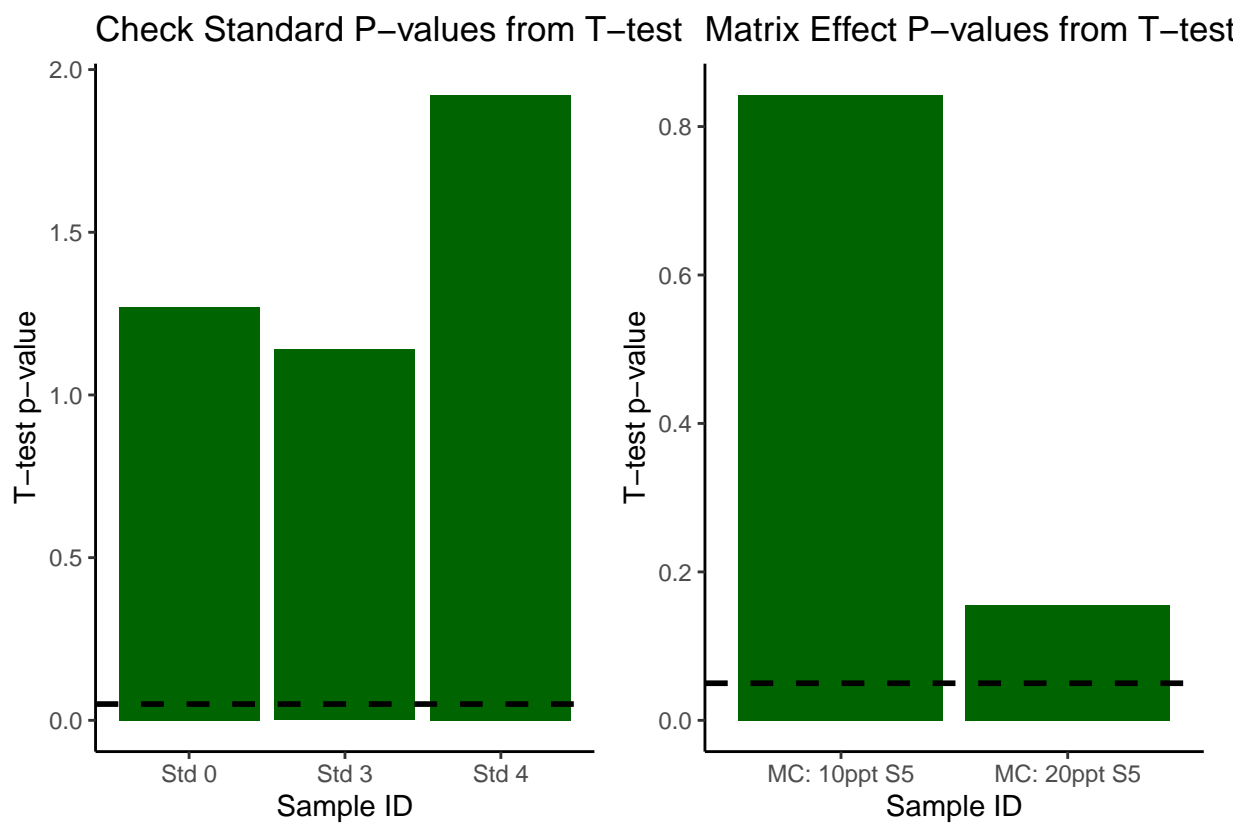## `geom_smooth()` using formula = 'y ~ x'
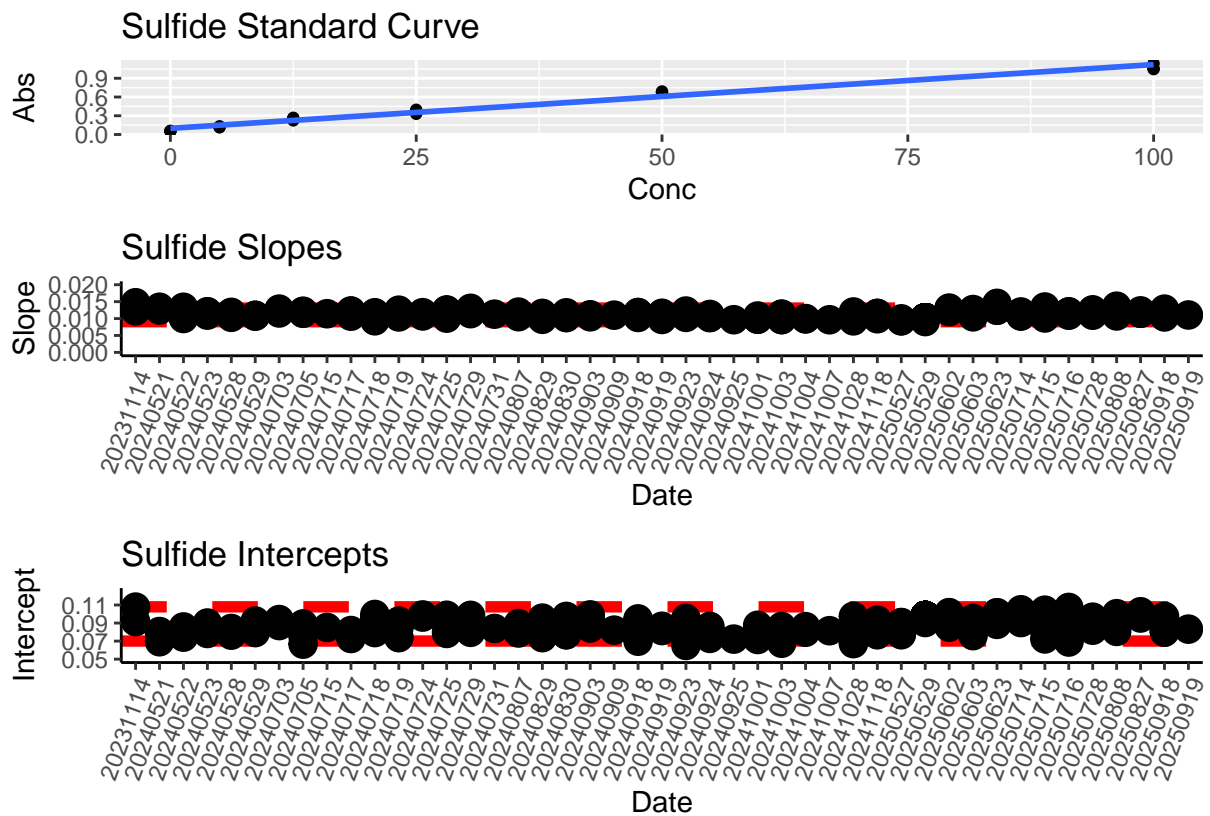
##Assess Check Standards

##Matrix Check QAQC
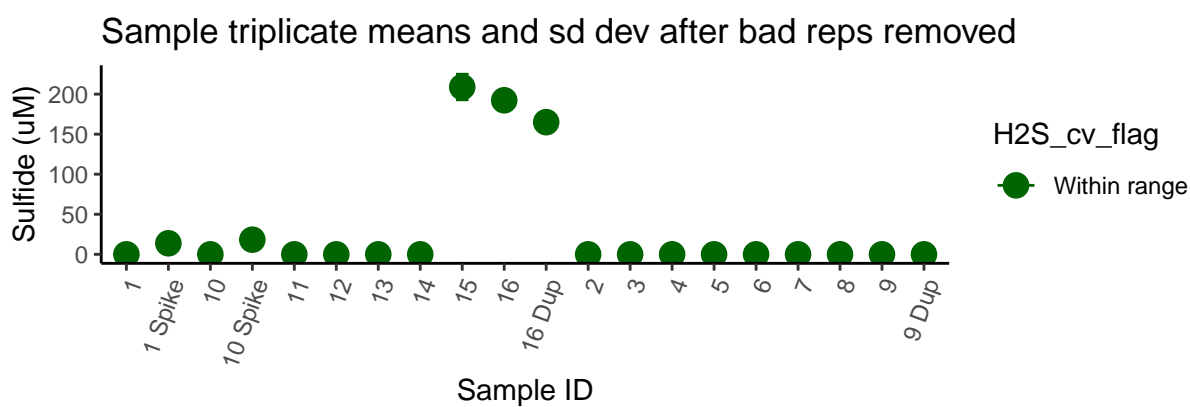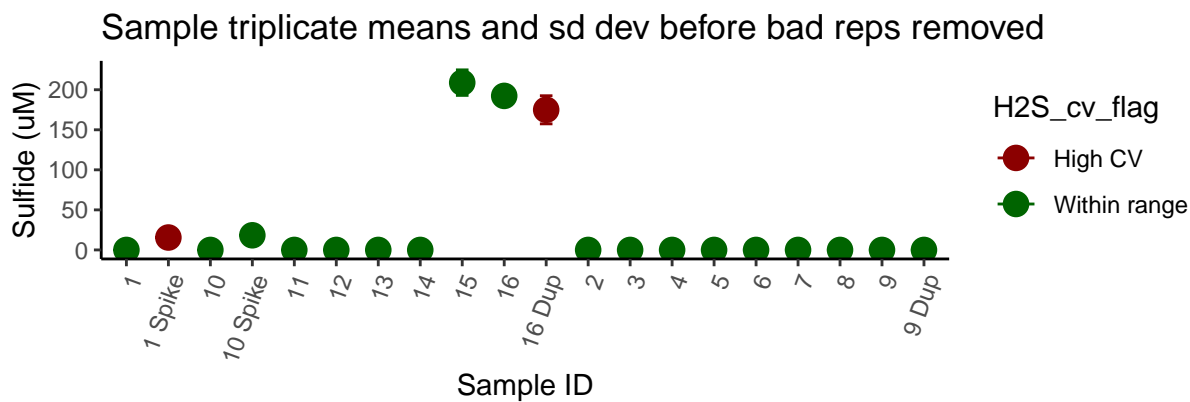
0.4 Plot check standards and matrix checks

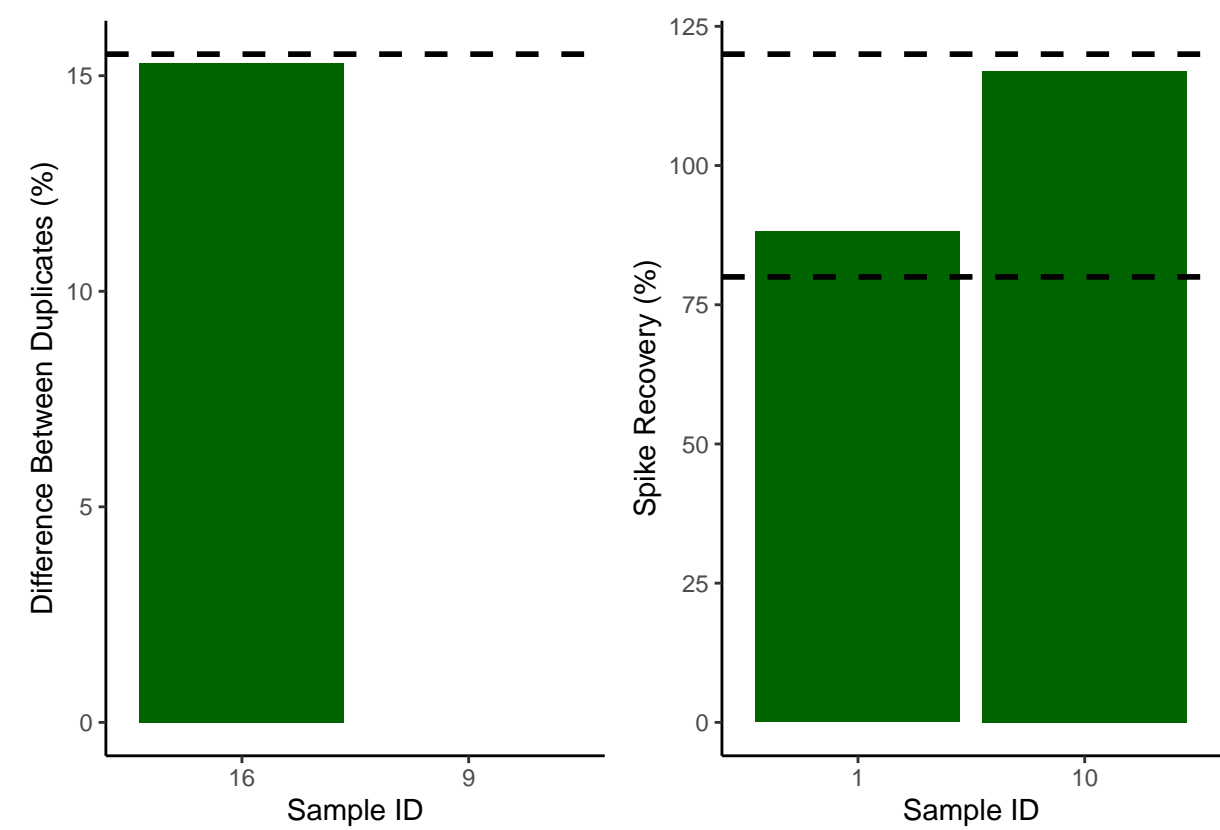##Flag sample data

##Calculate CV across wells

##Remove bad reps

0.5 Plot samples before and after removing bad replicates

Sample triplicate means and sd dev before bad reps removed

Sample triplicate means and sd dev after bad reps removed

##Assess Duplicates

##Assess Analytical Spikes

0.6 Plot duplicates and spikes

##Export final data and samples to rerun

0.6.1 END