Synoptic_CB_Nutrients_202306

June 2023

2025-06-23

Contents

##Run Information

```
cat("Run Information: Input by User") #lets you know what section you're in
```

```
## Run Information: Input by User
```

```
#set the run date & user name
  run_date <- "20240114"
  sample_year <- 2023
  sample_month <- 06
  user <- "Stephanie Wilson"

#identify the files you want to read in
  #read in as a list to accommadate ultiple runs in a month
  NOx_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_1.csv",
               "Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_2.csv",
```

```
                "Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_3.csv")
  NH3_PO4_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_June2023_1.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_June2023_2.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_June2023_3.csv")

# Define the file path for QAQC log file - NO Need to change just check year
  file_path <- "Raw Data/SEAL_COMPASS_Synoptic_QAQC_Log_2023.csv"
  final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202306.csv"

#record any notes about the run or anything other info here:
  run_notes <- "There are two sample names we suspect were input incorrectly,
  they are listed below and have been checked against metadata. The metadata from Goodwin ans Sweethall

#duplicate sample names to be changed
  #list the sample iDs that are messed up and create a list
  #with run number as well so that we can change them below
  wrong_names <- c("GCW_202304_TR_LysC_45cm", "GCW_202304_TR_LysA_20cm_8",
                   "GWI_202304_UP_LysA_20cm", "GWI_202304_UP_LysA_20cm")
  wrong_nums <- c(20, 16, 46, 44)
  correct_names <- c("GCW_202304_TR_LysB_45cm", "GCW_202304_TR_LysA_20cm",
                     "GWI_202304_UP_LysA_10cm", "GWI_202304_UP_LysA_10cm")

  #can't determine from metadata - for now unsure
  remove_names <- c("GCW_202304_TR_LysA_20cm", "GCW_202304_TR_LysA_20cm",
                    "GCW_202304_TR_LysB_20cm_13", "GCW_202304_TR_LysB_20cm_13")
     #couldn't tell which onethis is from the metadata, no A_10cm which is what we thought
     #marked on the sheet, need to check sample vials in freezer
     #to see if we have a A_10cm from GCW_TR to be sure
  remove_nums <- c(15, 13, 21, 19 )

#Set up file path for metadata
  #downloaded metadata csv - downloaded from Google drive as csv for this year
  #https://docs.google.com/spreadsheets/d/1HCAN0_q6y17x0RUXVzID09hVal-RfwWc/edit?usp=sharing&ouid=10899.
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"
```

##Setup

##Read in metadata and create similar sample IDs for matching to samples

0.1 Import Data & Clean

0.2 Assessing standard Curves

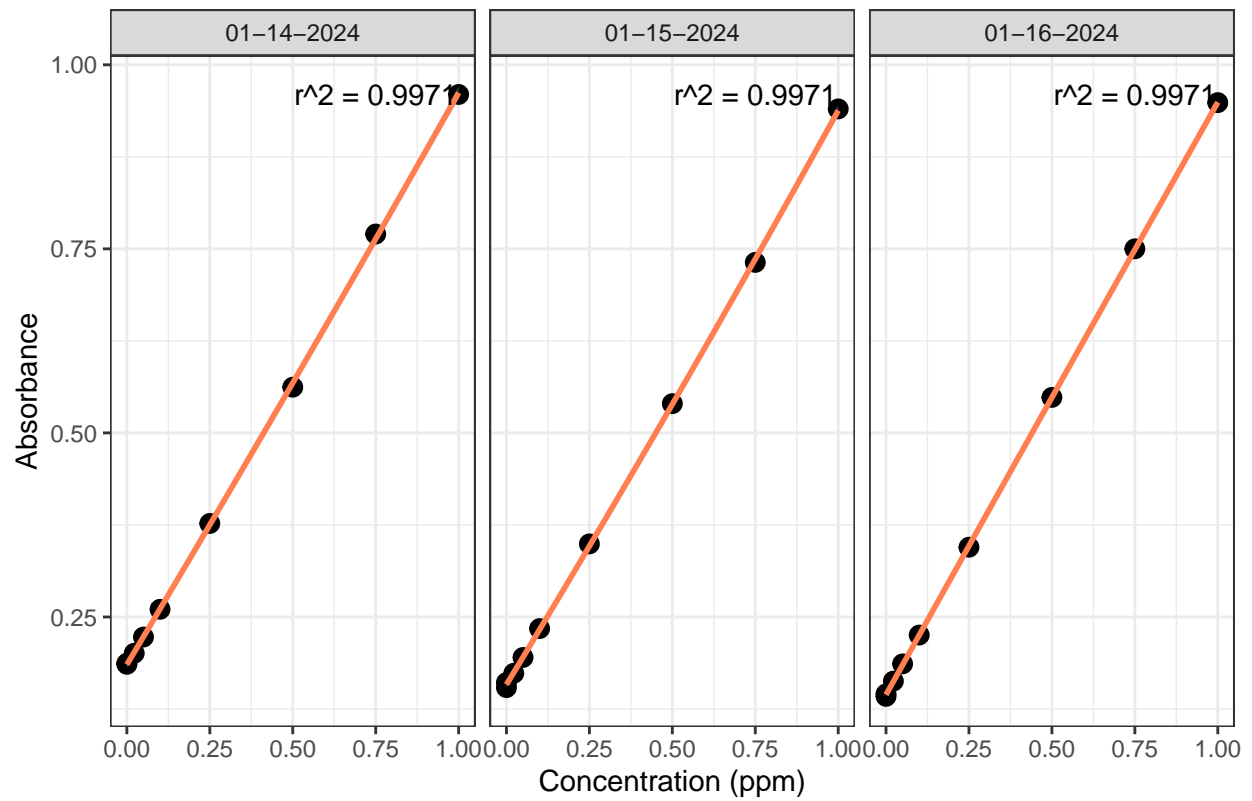#Pull out standards data

Assess Standard Curves

#Plot standards data

Assess Standard Curves
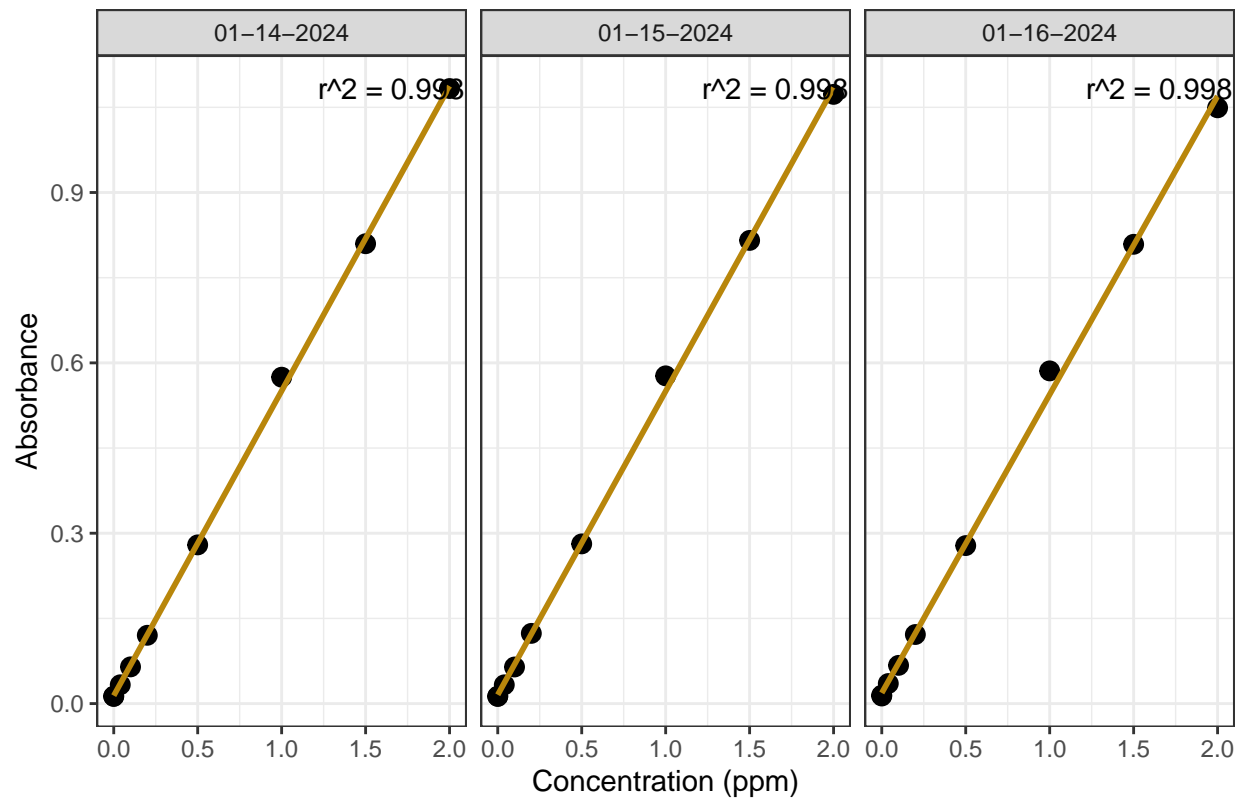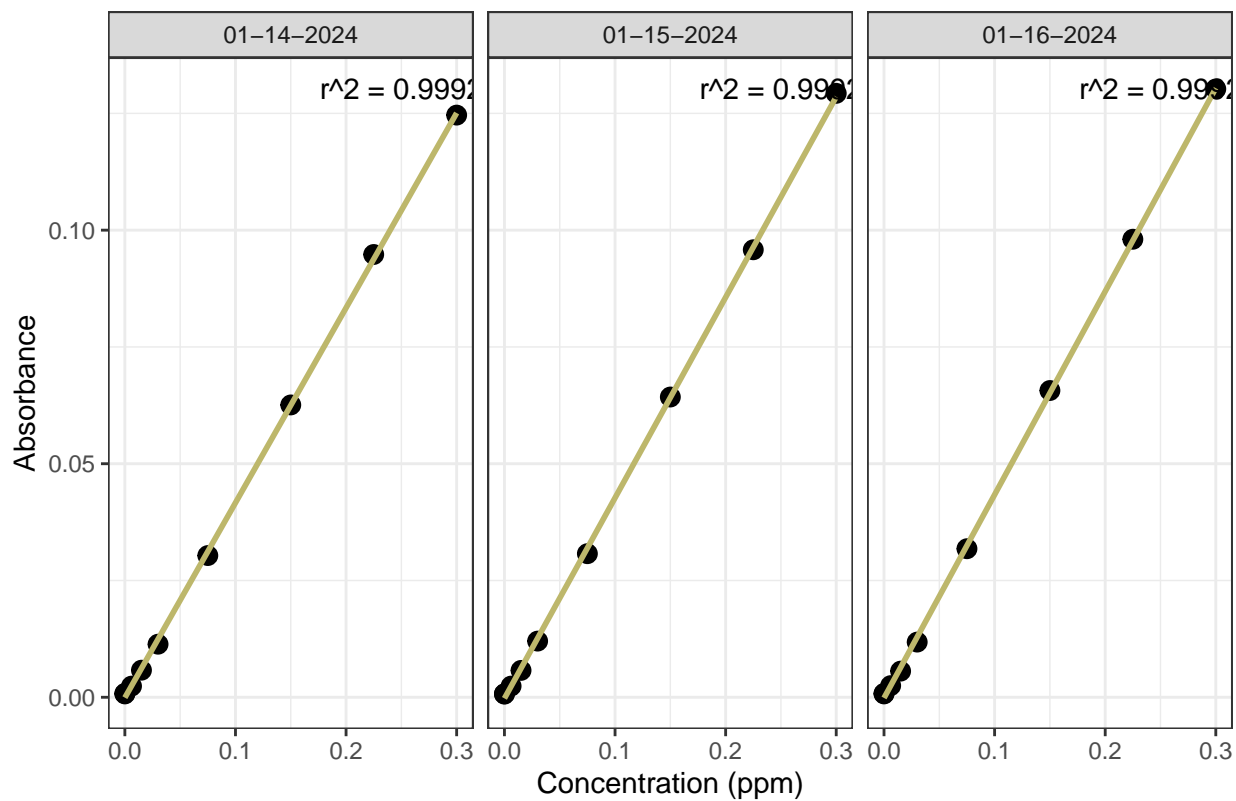
NOx Standard Curve

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

NH3 Standard Curve

01-14-2024	01-15-2024	01-16-2024
r^2 = 0.998	r^2 = 0.998	r^2 = 0.998

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

PO4 Standard Curve


```
## [1] "NOx Curve r2 GOOD - PROCEED"

## [1] "NH3 Curve r2 GOOD - PROCEED"

## [1] "PO4 Curve r2 GOOD - PROCEED"

## [1] "QAQC log file exists and has been read into the code."
```

Slope Drift Assessment
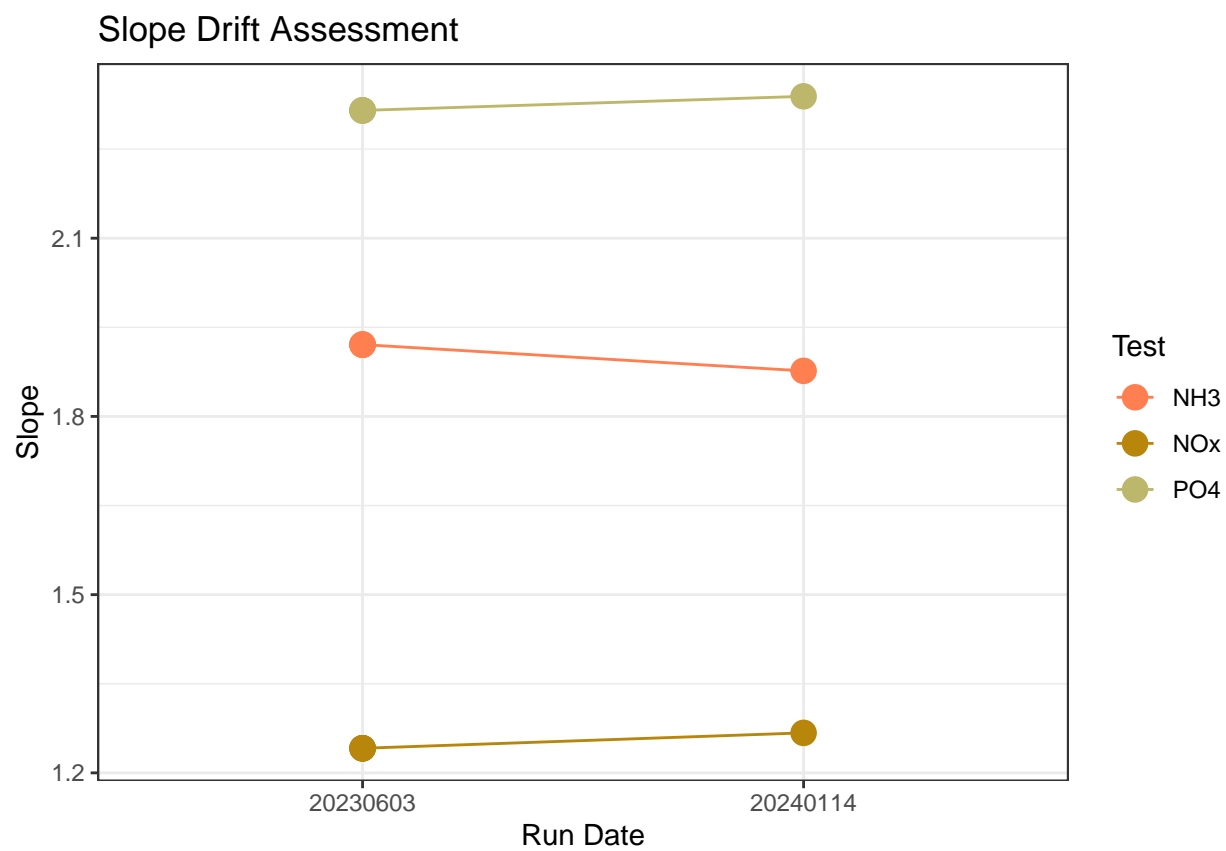

Table 1: Average Slope by Analyte

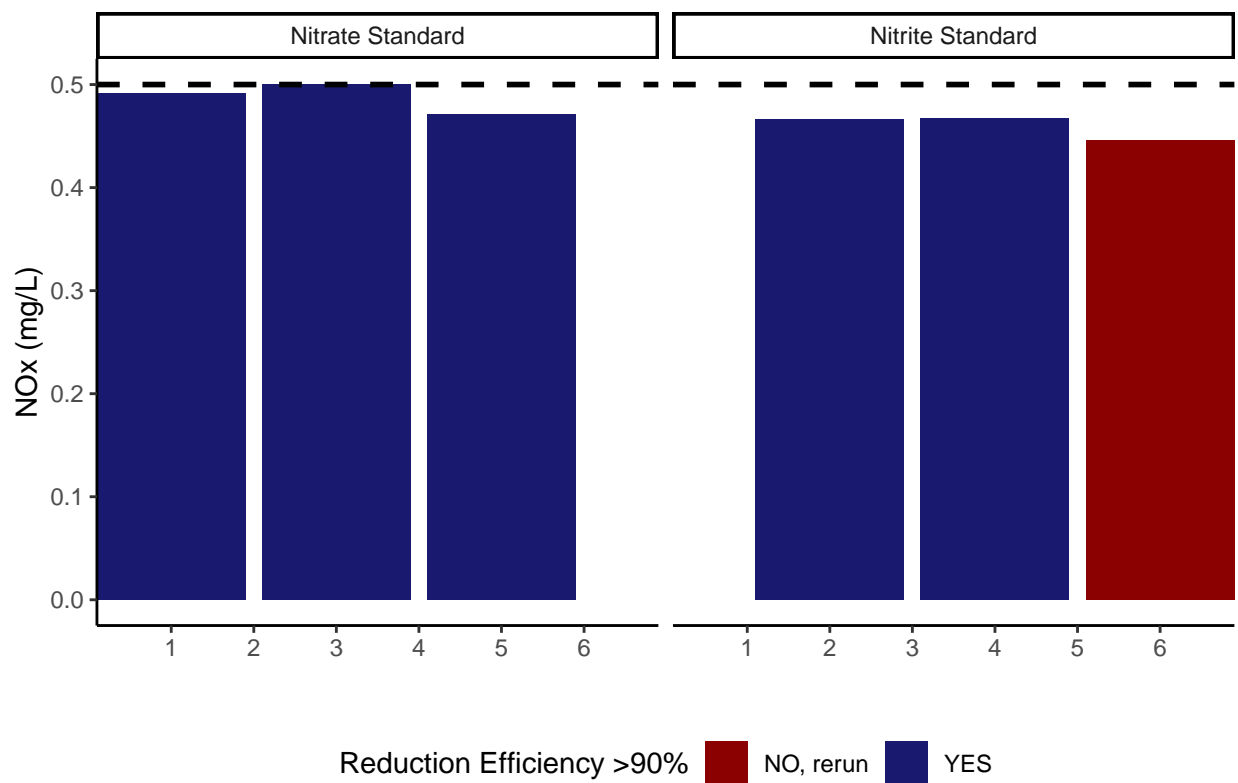| Test	avg_slope
NH3	1.912
NOx	1.247
PO4	2.320

0.3 Dilution Corrections - ensure the latest dilution is kept

Dilution Corrections

Duplicated samples: MSM_202306_TR_LysB_20cm, GCW_202306_WC_LysA_45cm, SWH_202306_TR_LysB_45cm, SWH_20

Dilution Present, Need to Correct

#Check NOx Reduction Efficiency

Assess Reduction Efficiency

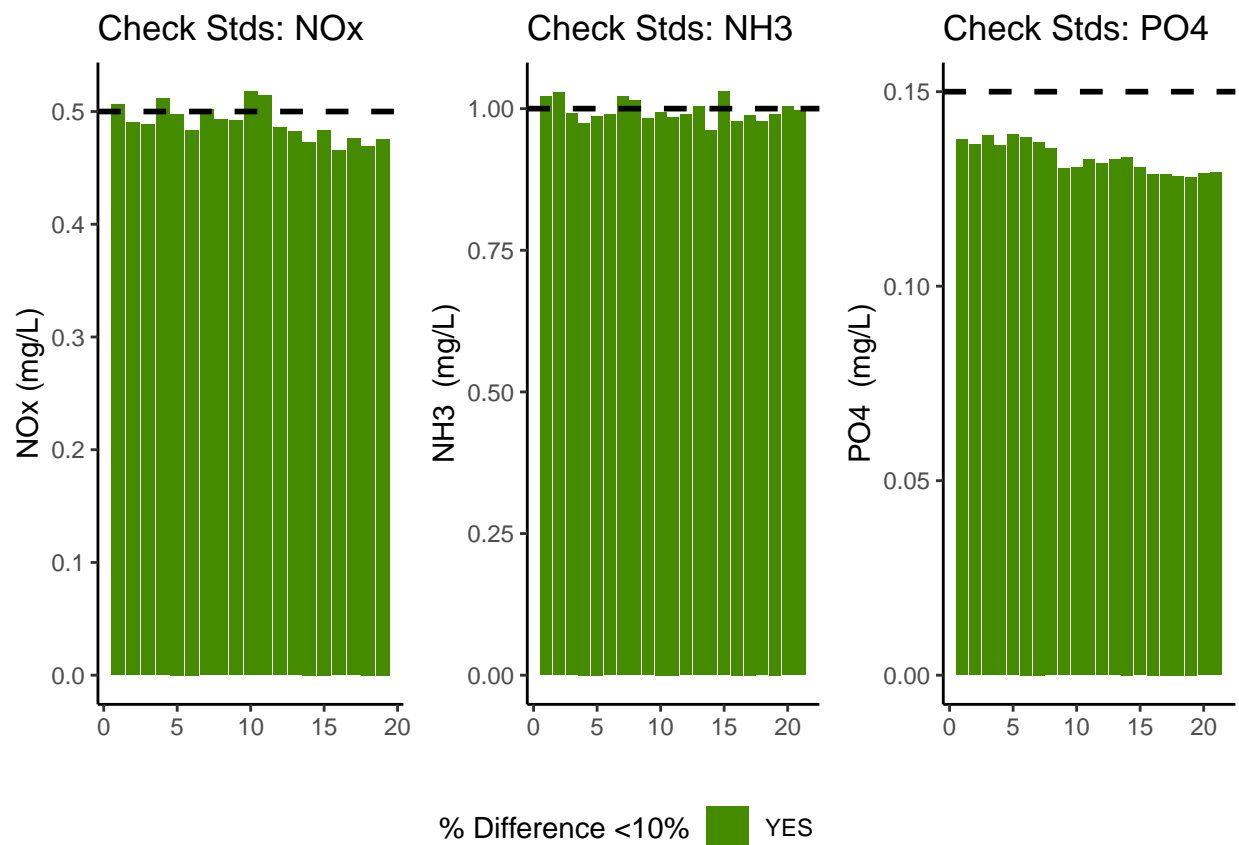## [1] "Mean NOx Reduction Efficiency <95% - REASSESS"

[1] 94.7757

0.4   Analyze the Check Standards

```
## Analyze Check Standards

## [1] "NOx Check Standard RSD within Range - PROCEED"

## [1] "NH3 Check Standard RSD within Range - PROCEED"

## [1] "PO4 Check Standard RSD within Range - PROCEED"
```



```
## [1] ">60% of NOx Check Standards are within range of expected concentration - PROCEED"

## [1] ">60% of NH3 Check Standards are within range of expected concentration - PROCEED"

## [1] ">60% of PO4 Check Standards are within range of expected concentration - PROCEED"
```

0.5 Analyze Blanks

```
## Assess Blanks

## [1] ">60% of NOx Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"

## [1] ">60% of NH3 Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"

## [1] ">60% of PO4 Blank concentrations are lower than the lower 25% quartile of samples- PROCEED"
```
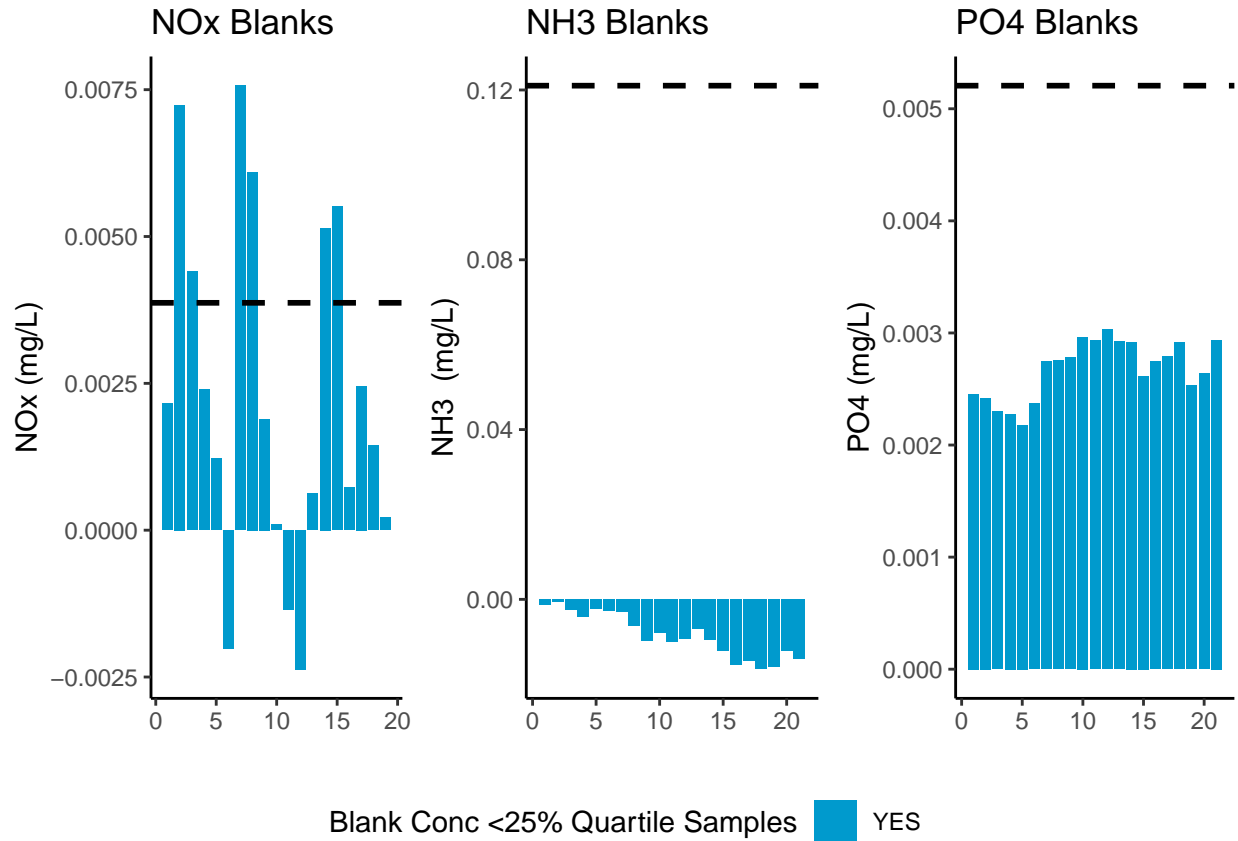

Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0023
NH3	-0.0084
PO4	0.0027

0.6 Analyze Duplicates

```
## Analyze Duplicates

## [1] "<60% of NOx Duplicates have a CV <10% - REASSESS"

## [1] ">60% of NH3 Duplicates have a CV <10% - PROCEED"

## [1] ">60% of PO4 Duplicates have a CV <10% - PROCEED"

## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```
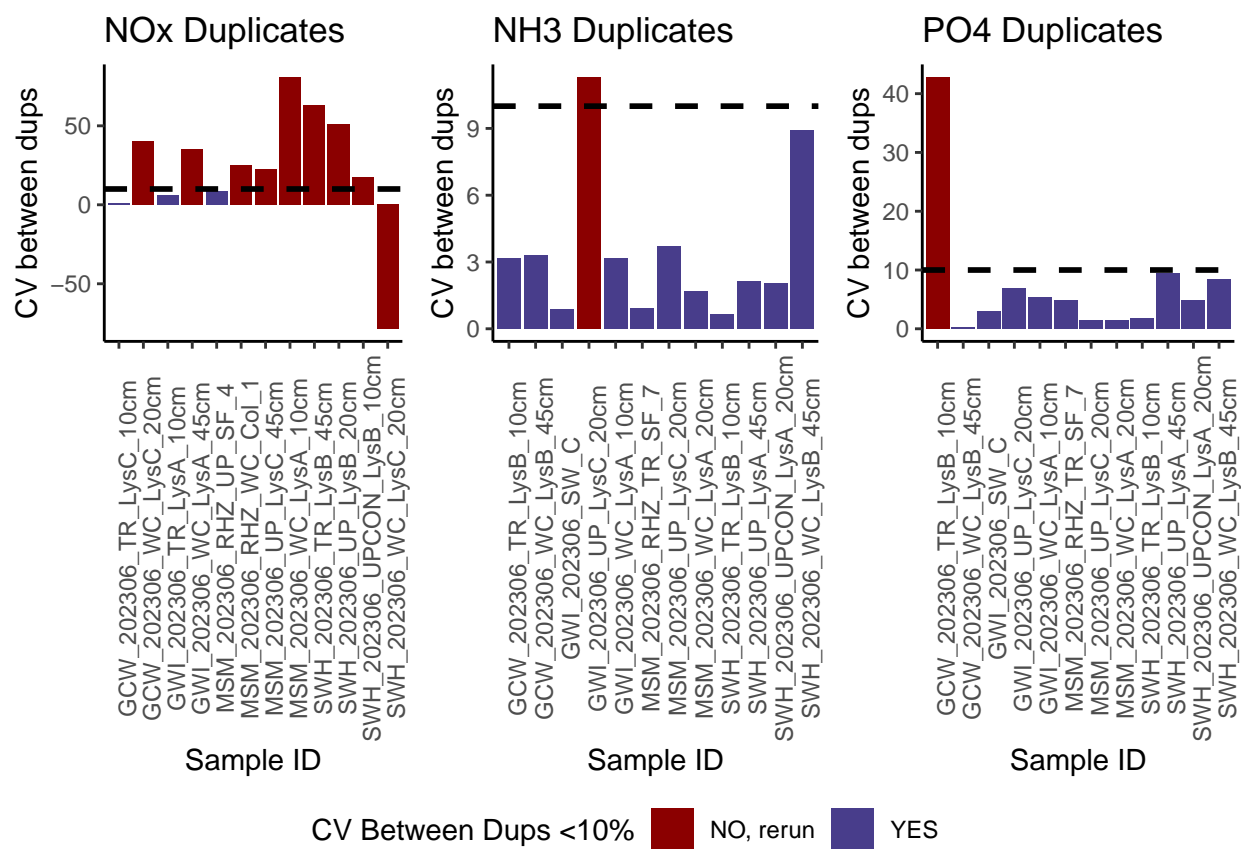
0.7 Spikes

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```
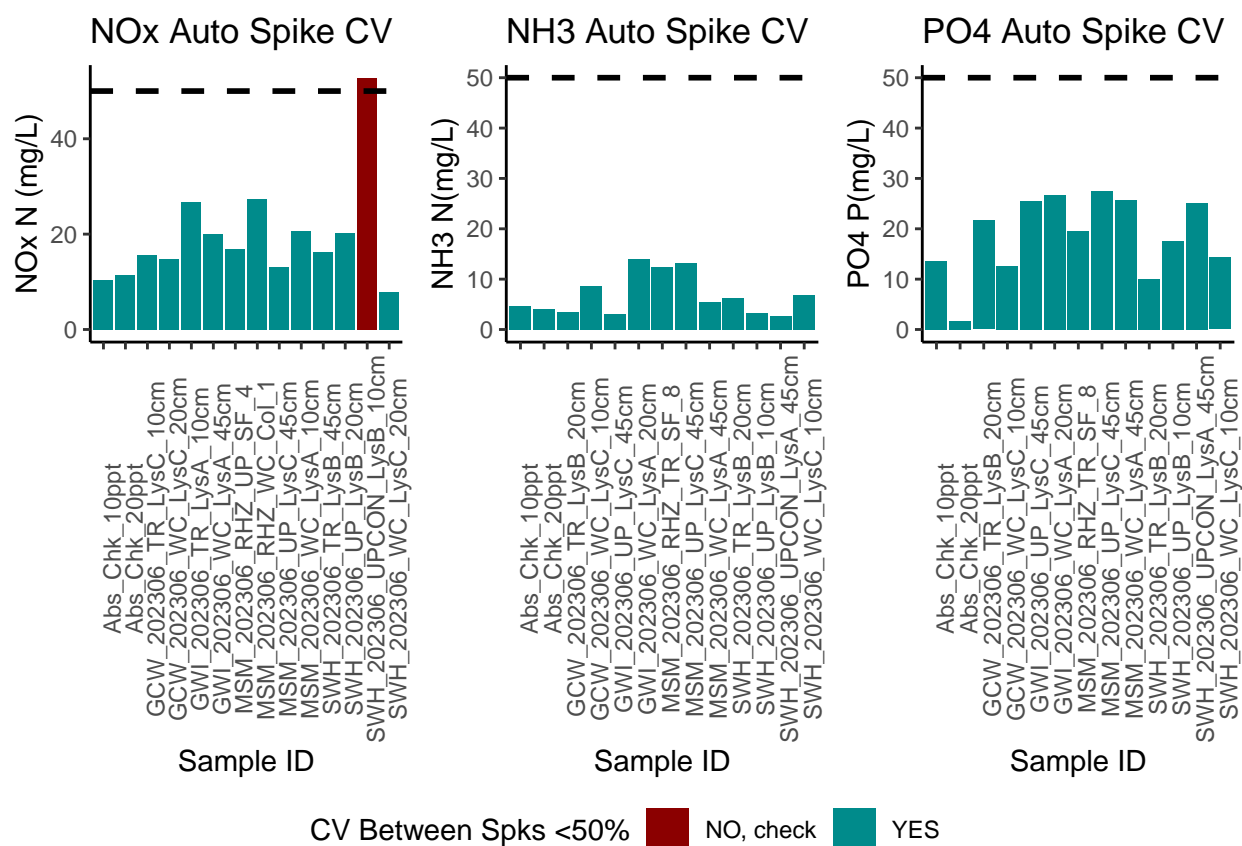
```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

0.8 Matrix Effects

```
## [1] "NO NOx Matrix Effect, PROCEED"
```

```
## [1] "NO NH3 Matrix Effect, PROCEED"
```

```
## [1] "NO PO4 Matrix Effect, PROCEED"
```

0.9 Unit Converted Data Column Added (mg/L to uM)

0.10 Sample Flagging - Within range of standard curve

```
## Sample Flagging
```

0.11 Pull out sample id information

```
## Sample Processing
```

```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,
## ...].
```

```
## Warning: There was 1 warning in 'mutate()'.
## i In argument: 'Samp_Time = ym(Samp_Time)'.
## Caused by warning:
## !  2 failed to parse.
```

0.12 Pulling Rhizon Samples

```r
# Filter rhizon and peeper samples
df_rhizon <- df_all %>%
  filter(str_detect(Sample_Name, "RHZ"))
df_peep <- df_all %>%
  filter(str_detect(Sample_Name, "PPR"))

# Timestamp for backups
timestamp <- format(Sys.time(), "%Y-%m-%d_%H%M")

# Paths
folder_path <- file.path("Raw Data", "Rhizon+Peeper")
dir.create(folder_path, recursive = TRUE, showWarnings = FALSE)

rhizon_main <- file.path(folder_path, "rhizon_data.csv")
peeper_main <- file.path(folder_path, "peeper_data.csv")

rhizon_backup <- file.path(folder_path, paste0("rhizon_data_", timestamp, ".csv"))
peeper_backup <- file.path(folder_path, paste0("peeper_data_", timestamp, ".csv"))

# Write timestamped backups
```

```r
write.csv(df_rhizon, rhizon_backup, row.names = FALSE)
write.csv(df_peep, peeper_backup, row.names = FALSE)

# Overwrite the main files with latest data
write.csv(df_rhizon, rhizon_main, row.names = FALSE)
write.csv(df_peep, peeper_main, row.names = FALSE)

## ^^ I think there is a cleaner way to write this out, but this should work for now ^^
```

0.13 Check to see if samples run match metadata & merge info

```
## Check Sample IDs with Metadata

## Some sample IDs are missing from metadata.

##  [1] "MSM_202306_UP_LysA_45cm"     "MSM_202306_UP_LysC_20cm"
##  [3] "MSM_202306_UP_LysC_45cm"     "MSM_202306_TR_LysA_45cm"
##  [5] "SWH_202306_UPCON_LysA_10cm"  "SWH_202306_UPCON_LysA_20cm"
##  [7] "SWH_202306_UPCON_LysA_45cm"  "SWH_202306_UPCON_LysB_10cm"
##  [9] "SWH_202306_UPCON_LysB_20cm"  "SWH_202306_UPCON_LysB_45cm"
## [11] "SWH_202306_UPCON_LysC_10cm"  "SWH_202306_UPCON_LysC_20cm"
## [13] "SWH_202306_UPCON_LysC_45cm"  "SWH_202306_UP_LysA_10cm"
## [15] "SWH_202306_UP_LysA_20cm"     "SWH_202306_UP_LysA_45cm"
## [17] "SWH_202306_UP_LysB_10cm"     "SWH_202306_UP_LysB_20cm"
## [19] "SWH_202306_UP_LysB_45cm"     "SWH_202306_UP_LysC_10cm"
## [21] "SWH_202306_UP_LysC_20cm"     "SWH_202306_UP_LysC_45cm"
## [23] "SWH_202306_TR_LysA_10cm"     "SWH_202306_TR_LysA_20cm"
## [25] "SWH_202306_TR_LysA_45cm"     "SWH_202306_TR_LysB_10cm"
## [27] "SWH_202306_TR_LysB_20cm"     "SWH_202306_TR_LysB_45cm"
## [29] "SWH_202306_TR_LysC_10cm"     "SWH_202306_TR_LysC_20cm"
## [31] "SWH_202306_TR_LysC_45cm"     "SWH_202306_WC_LysA_10cm"
## [33] "SWH_202306_WC_LysA_45cm"     "SWH_202306_WC_LysB_10cm"
## [35] "SWH_202306_WC_LysB_20cm"     "SWH_202306_WC_LysB_45cm"
## [37] "SWH_202306_WC_LysC_10cm"     "SWH_202306_WC_LysC_20cm"
## [39] "SWH_202306_WC_LysC_45cm"     "SWH_202306_SW_A"
## [41] "SWH_202306_SW_B"             "SWH_202306_SW_C"
## [43] "GWI_202306_UP_LysA_10cm"     "GWI_202306_UP_LysA_20cm"
## [45] "GWI_202306_UP_LysA_45cm"     "GWI_202306_UP_LysB_10cm"
## [47] "GWI_202306_UP_LysB_20cm"     "GWI_202306_UP_LysB_45cm"
## [49] "GWI_202306_UP_LysC_10cm"     "GWI_202306_UP_LysC_20cm"
## [51] "GWI_202306_UP_LysC_45cm"     "GWI_202306_TR_LysA_10cm"
## [53] "GWI_202306_TR_LysA_20cm"     "GWI_202306_TR_LysB_10cm"
## [55] "GWI_202306_TR_LysB_20cm"     "GWI_202306_TR_LysB_45cm"
## [57] "GWI_202306_TR_LysC_10cm"     "GWI_202306_TR_LysC_20cm"
## [59] "GWI_202306_TR_LysC_45cm"     "GWI_202306_WC_LysA_10cm"
## [61] "GWI_202306_WC_LysA_20cm"     "GWI_202306_WC_LysA_45cm"
## [63] "GWI_202306_WC_LysB_10cm"     "GWI_202306_WC_LysB_20cm"
## [65] "GWI_202306_WC_LysC_10cm"     "GWI_202306_WC_LysC_20cm"
## [67] "GWI_202306_WC_LysB_45cm"     "GWI_202306_SW_A"
## [69] "GWI_202306_SW_B"             "GWI_202306_SW_C"
## [71] "MSM_202036_WC_LysB_10cm"     "GWI_202306_WC_LysC_45cm"
```
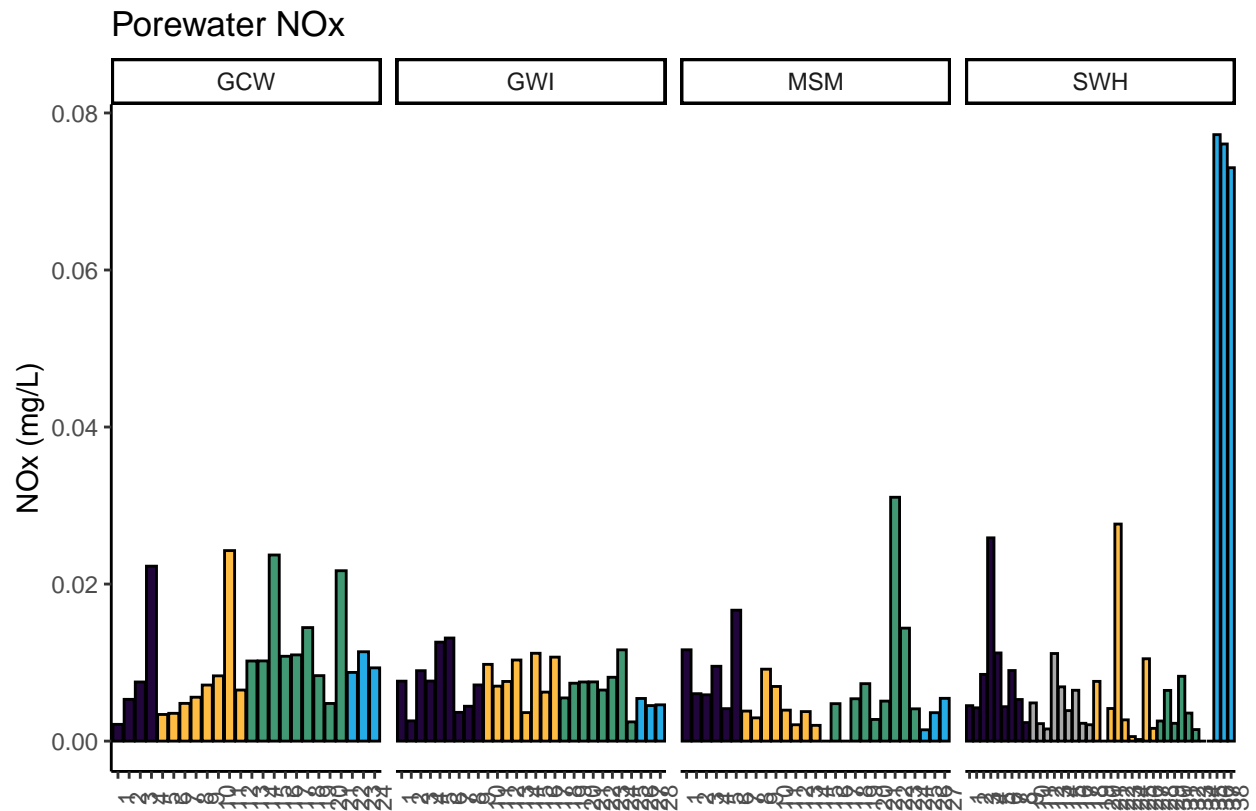
```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,
## ...].


## Warning: There was 1 warning in 'mutate()'.
## i In argument: 'Samp_Time = ym(Samp_Time)'.
## Caused by warning:
## !  2 failed to parse.
```
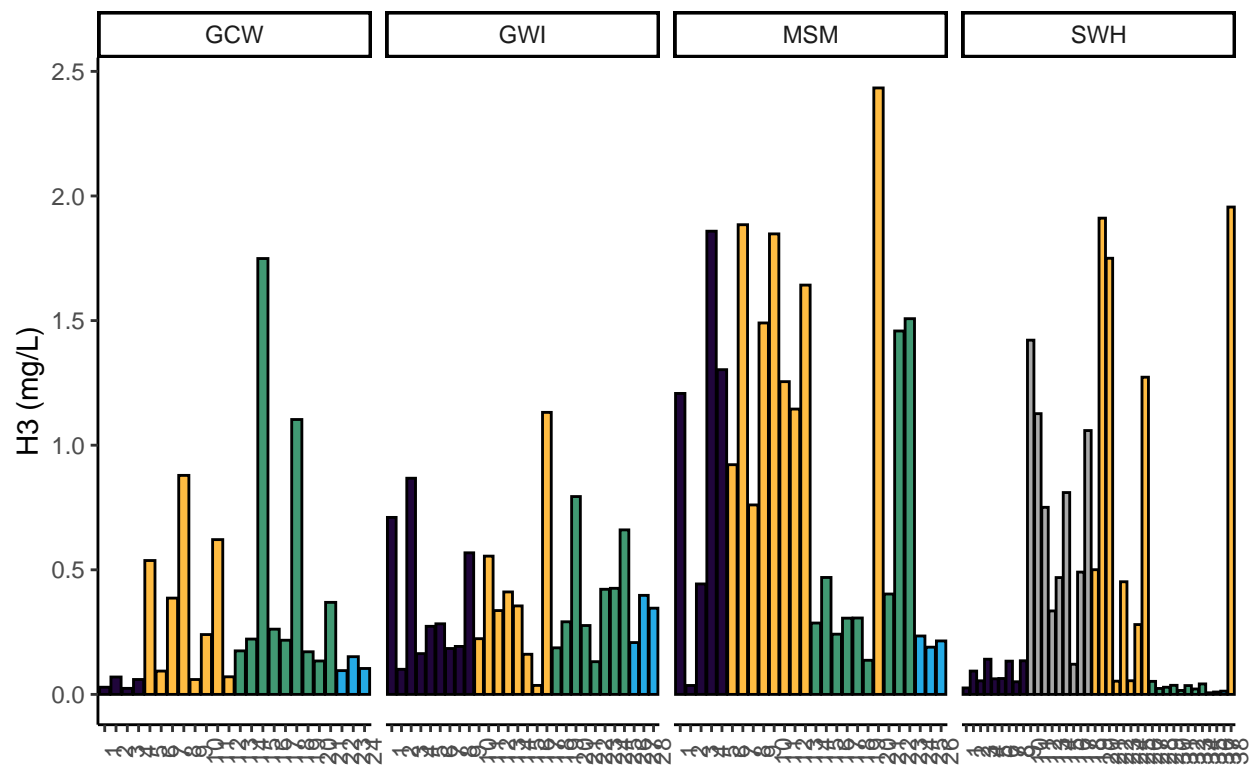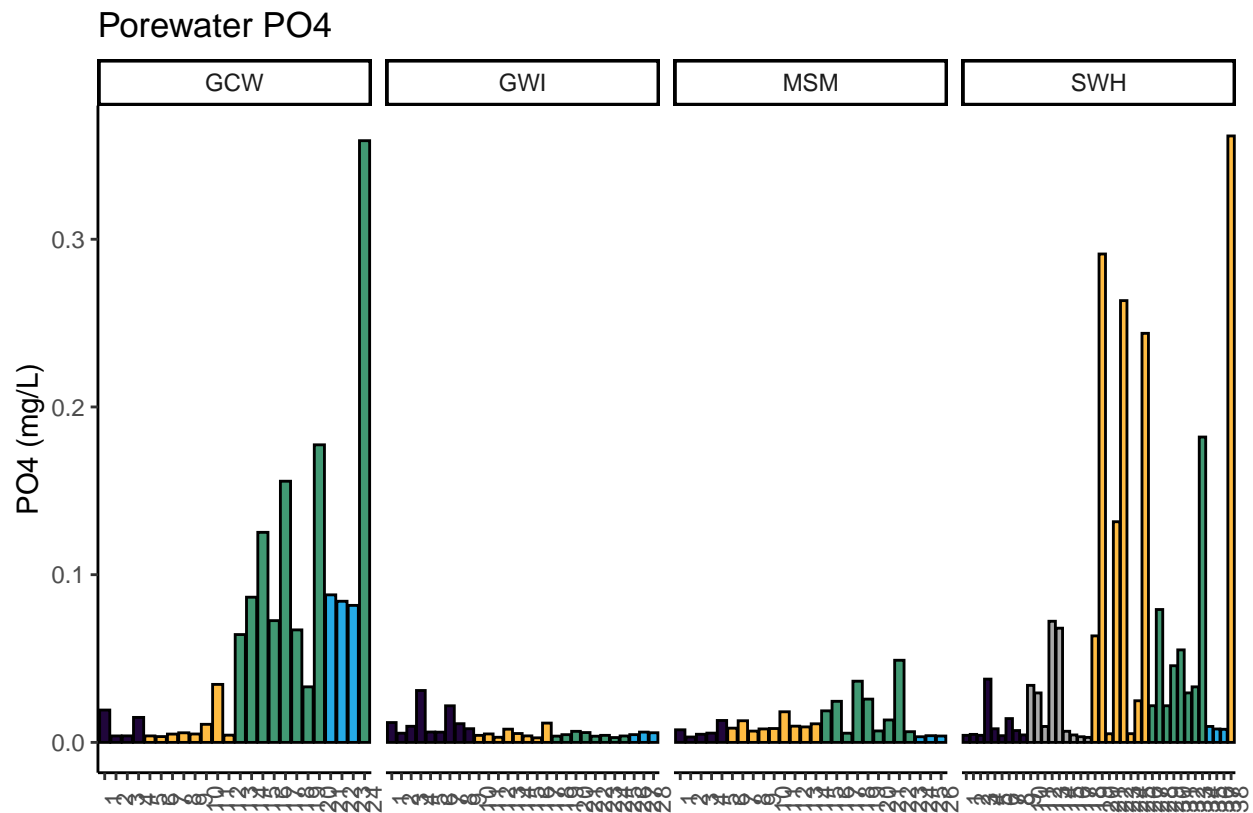
0.14 Visualize Data

Porewater NOx

Porewater NH3

Porewater PO4

0.15 Export Processed Data

#end