

Synoptic_CB_Nutrients_202306

June 2023

2025-07-01

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##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 accomodate 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 and 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 one this 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

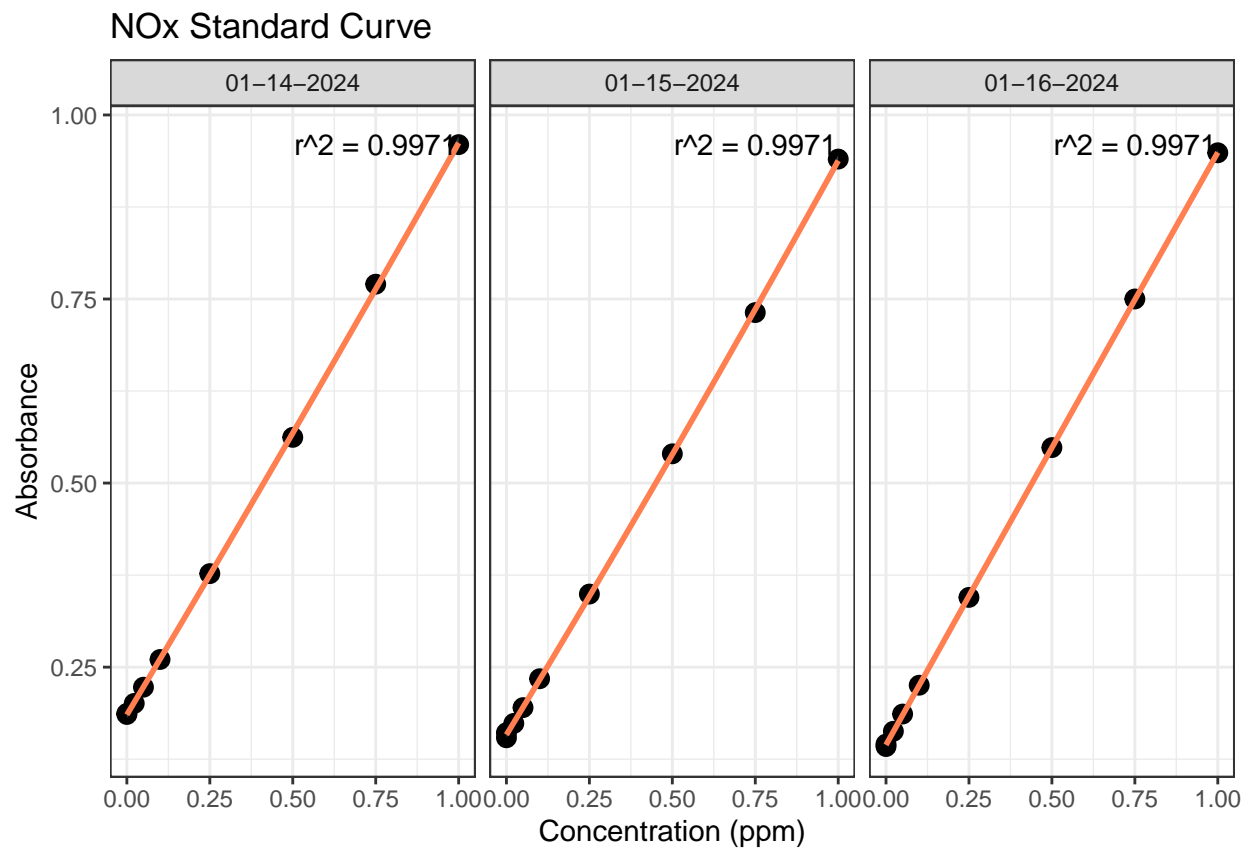
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

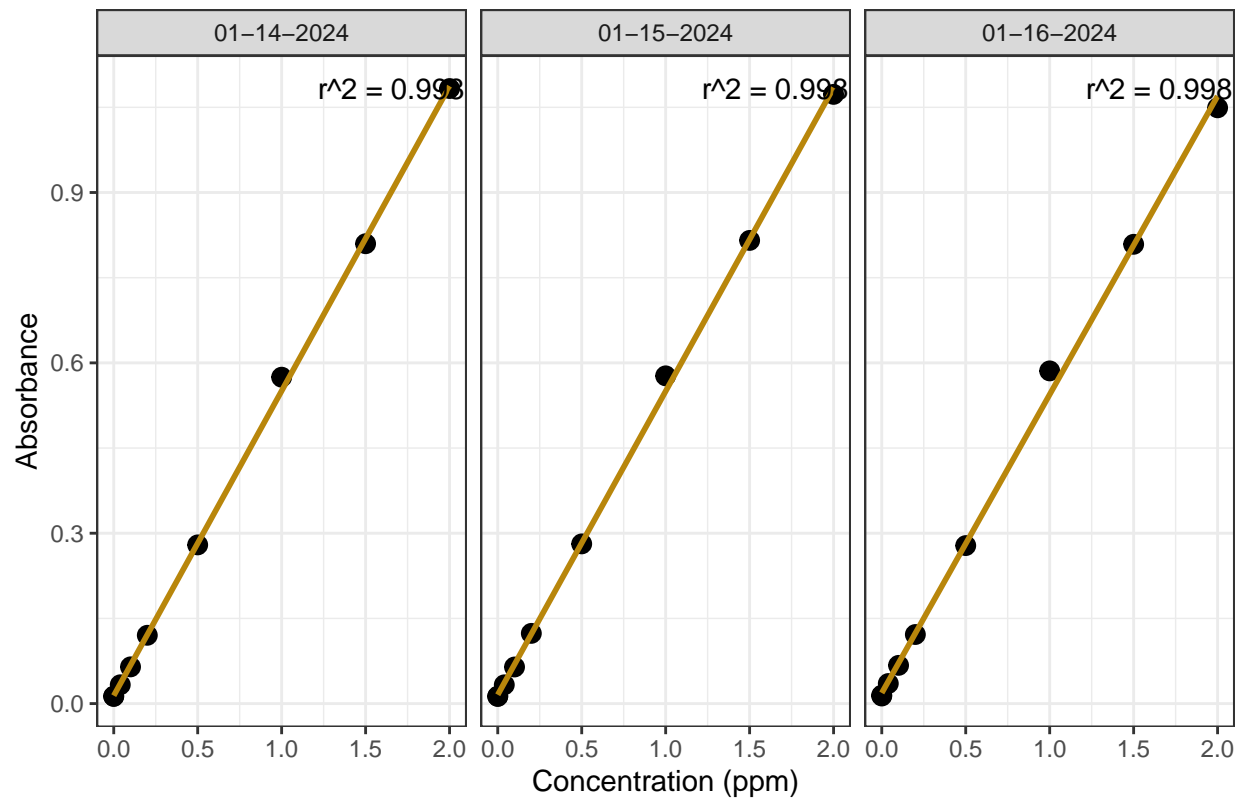
```
#Plot standards data
```

```
## Assess Standard Curves
```



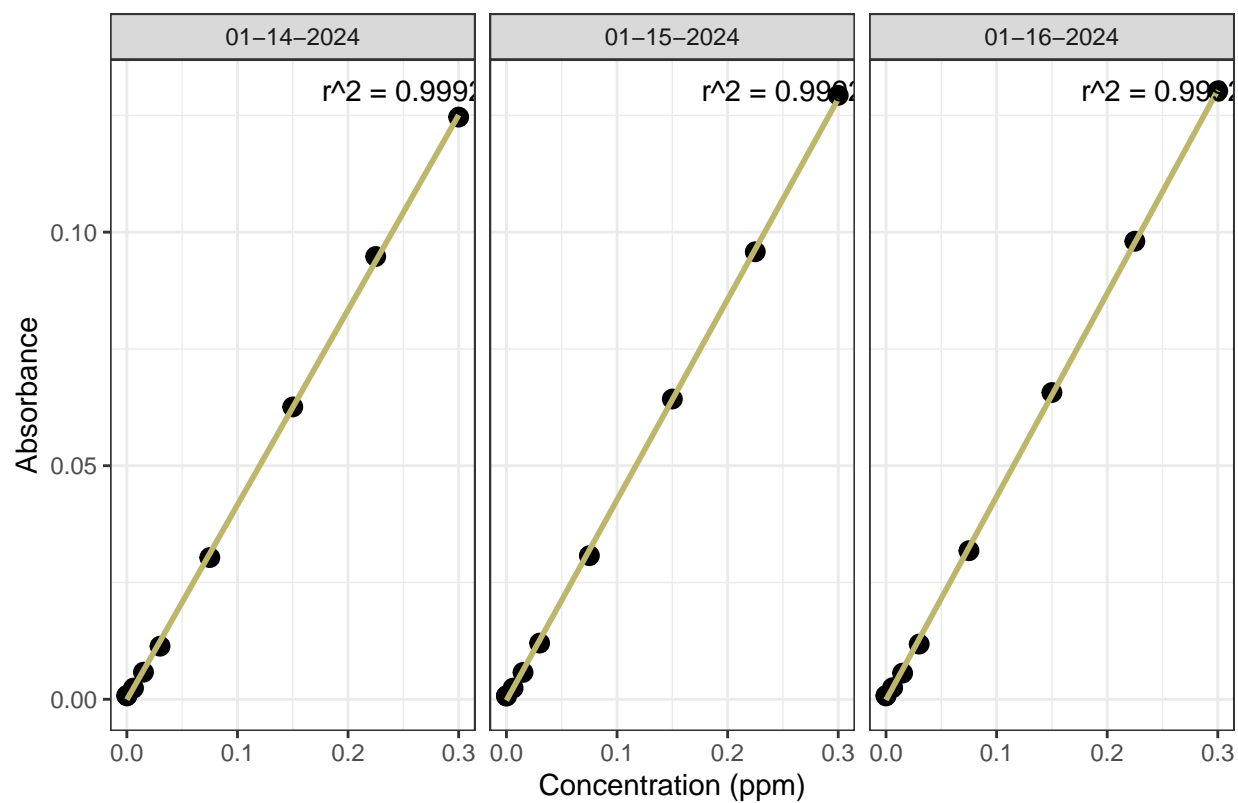
```
## 'geom_smooth()' using formula = 'y ~ x'
```

NH3 Standard Curve



```
## '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."
```

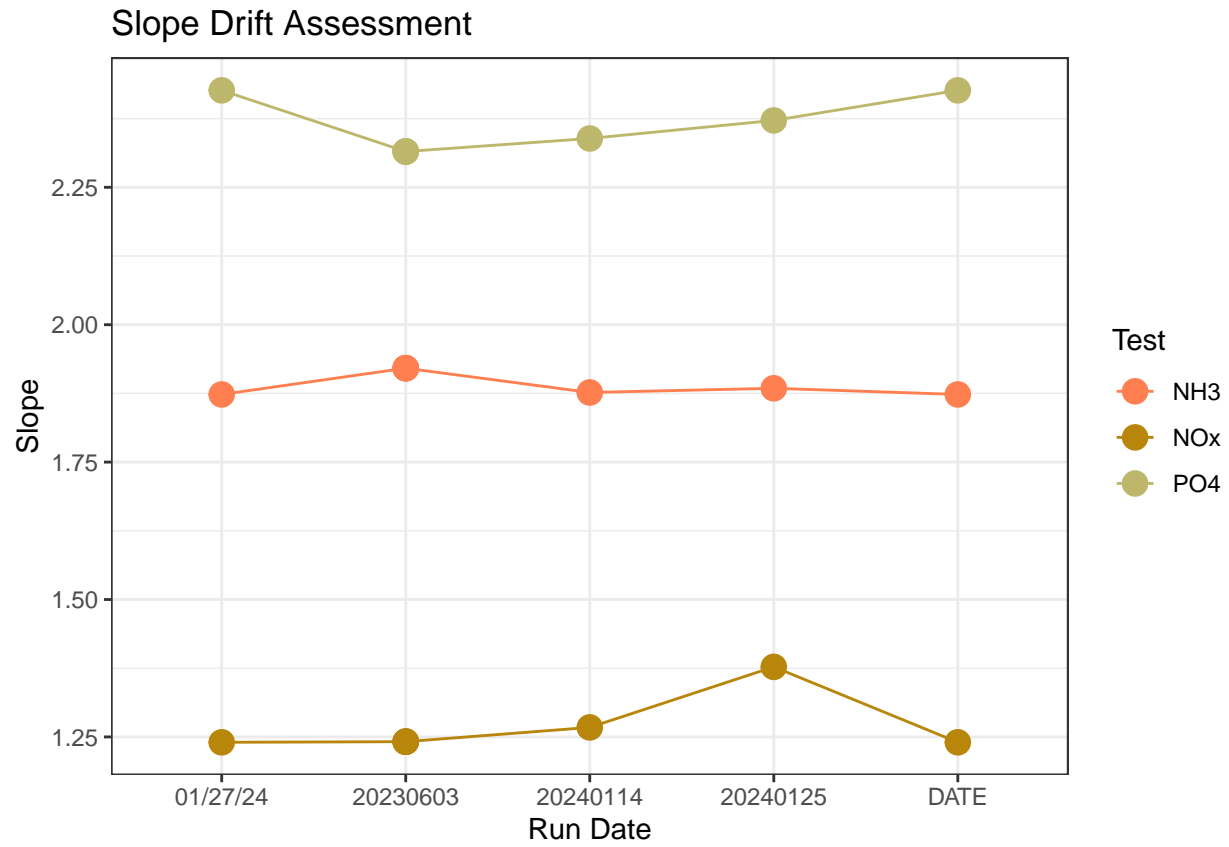


Table 1: Average Slope by Analyte

| Test | avg_slope |
|------|-----------|
| NH3 | 1.899 |
| NOx | 1.261 |
| PO4 | 2.353 |

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_202306_WC_LysA_45cm
```

```
## All duplicated samples have valid dilutions. No naming issues detected.
```

0.4 Performance Check

```
## [1] "NOx pe Check has a % Difference <10% - PROCEED"
```

```
## Run mean = 0.714342
```

```
## Expected = 0.706
```

```
## [1] "NH3 pe Check has a % Difference >10% - REASSESS"
```

```
## Run mean = 1.20727
```

```
## Expected = 0.948
```

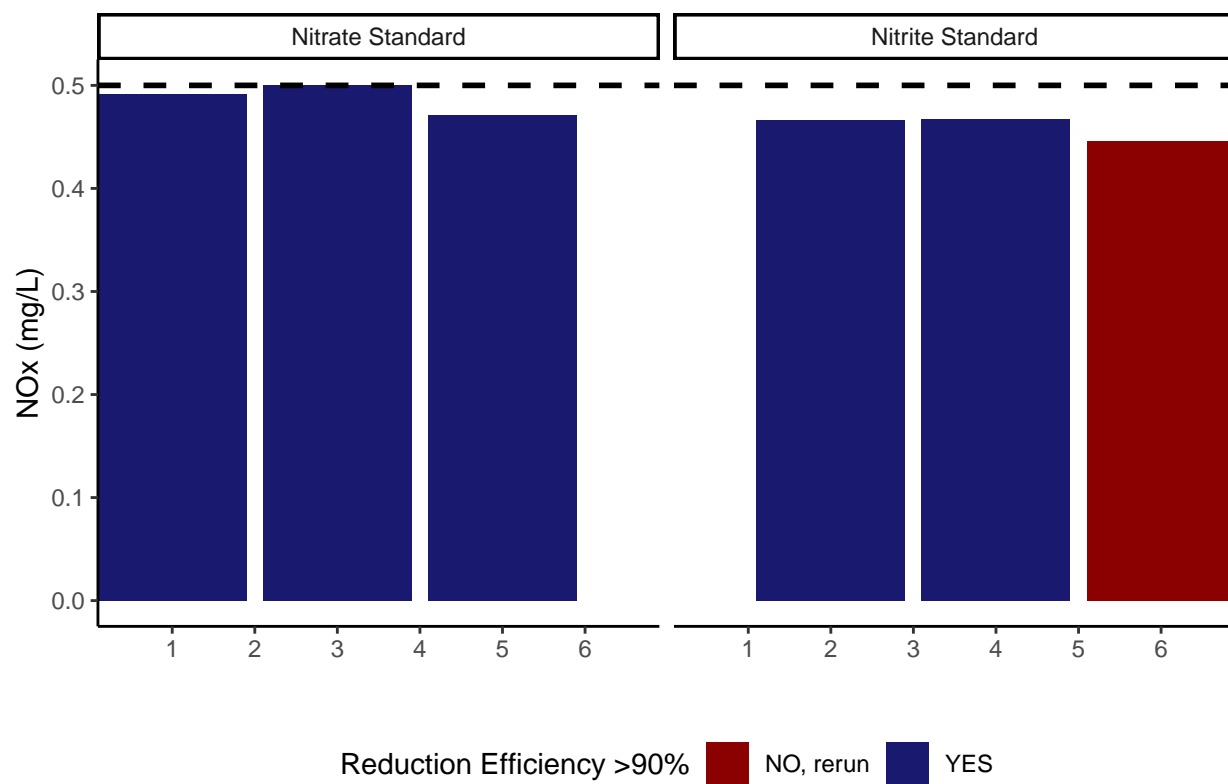
```
## [1] "PO4 pe Check has a % Difference >10% - REASSESS"
```

```
## Run mean = 0.5901153
```

```
## Expected = 0.818
```

```
#Check NOx Reduction Efficiency
```

```
## Assess Reduction Efficiency
```



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

```
## [1] 94.7757
```

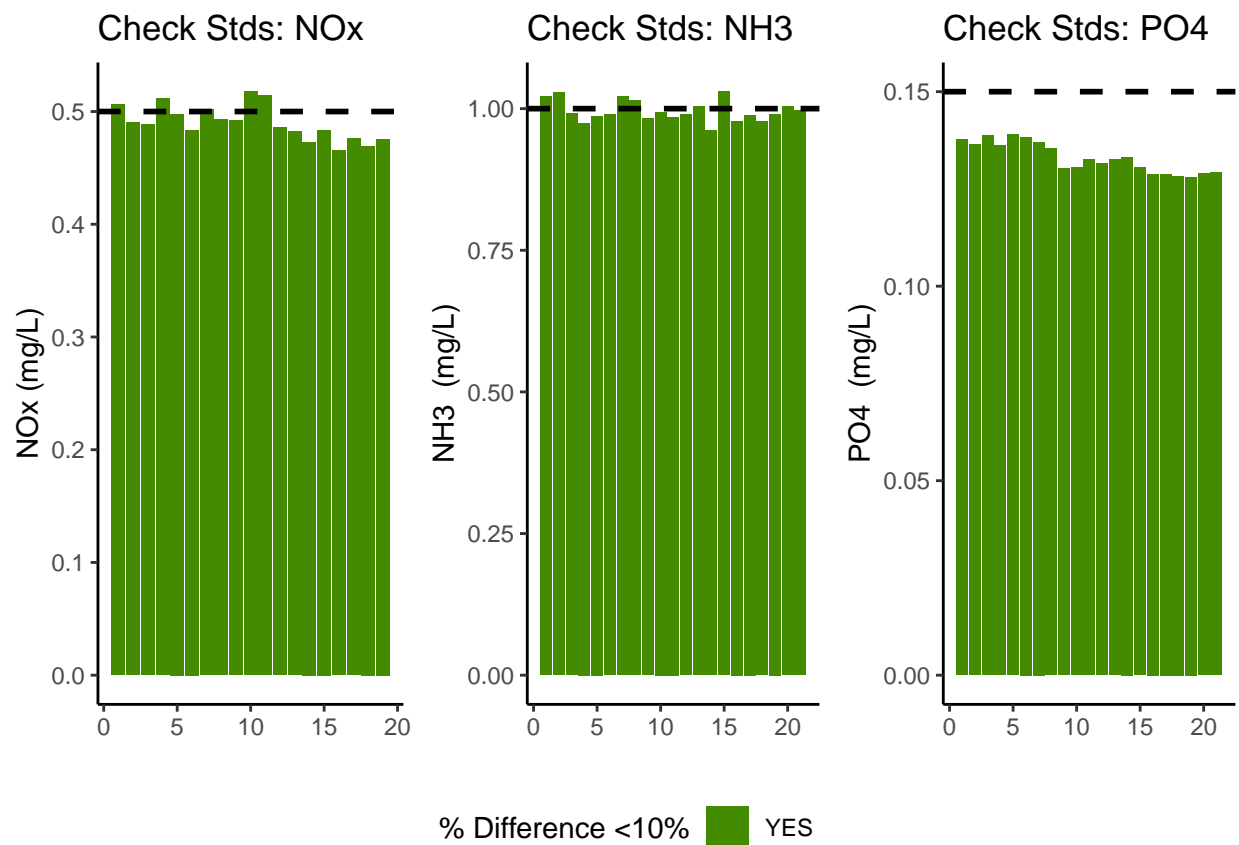

0.5 Analyze the Check Standards

```
## 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"
```

0.6 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"

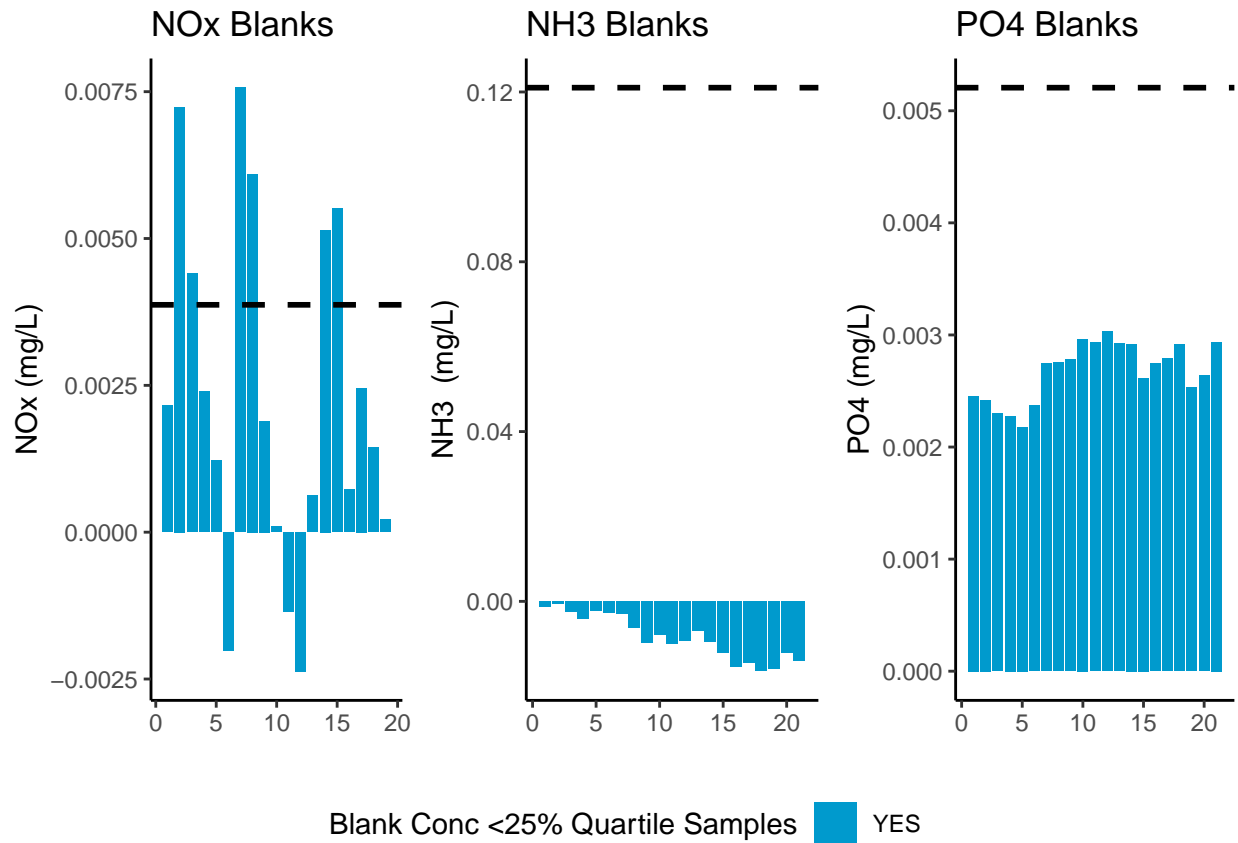


Table 2: Mean Concentration of Blanks

| Test | Blank_Mean_Conc |
|------|-----------------|
| NOx | 0.0023 |
| NH3 | -0.0084 |
| PO4 | 0.0027 |

0.7 Analyze Duplicates

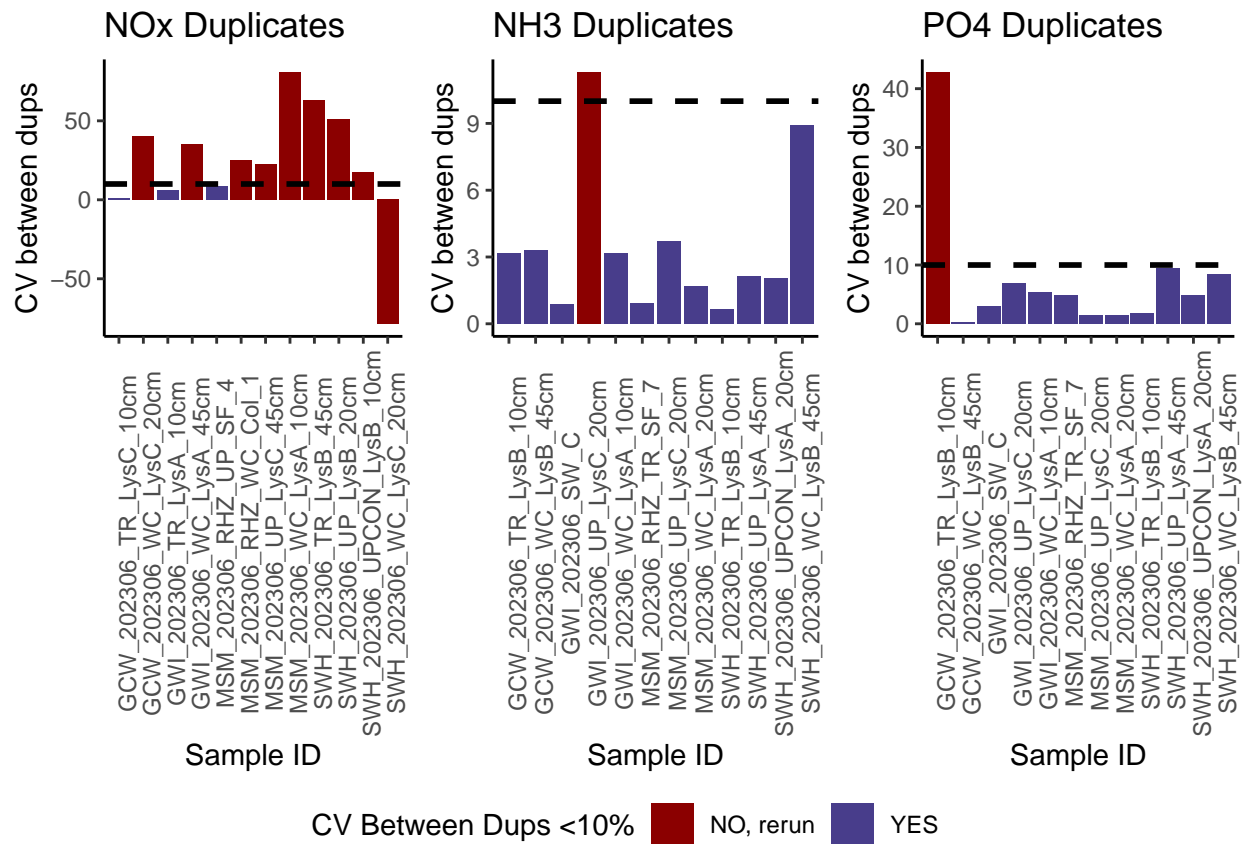
```
## Analyze Duplicates

## [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.
```

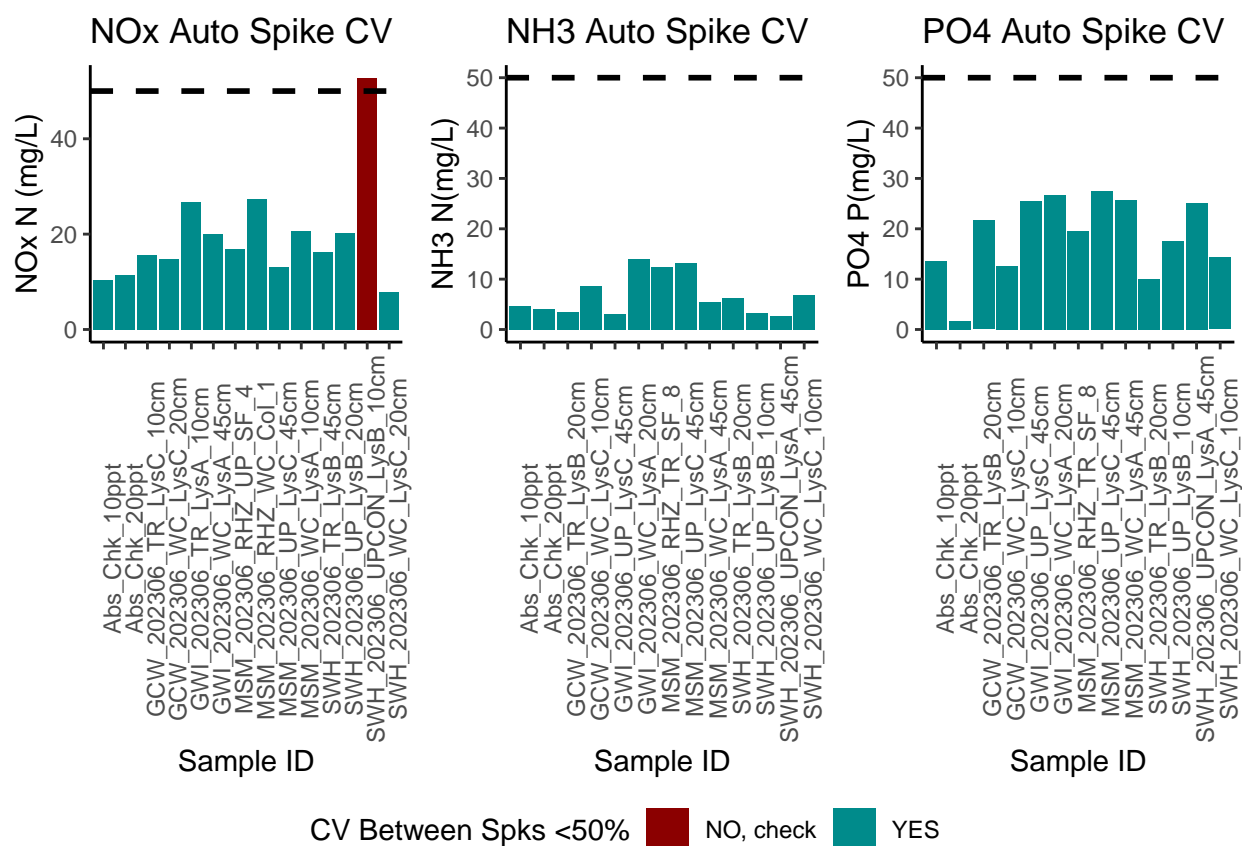


0.8 Spikes

[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"



0.9 Matrix Effects

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

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

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

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

0.11 Sample Flagging - Within range of standard curve

```
## Sample Flagging
```

0.12 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.
```

0.13 Pulling Out Rhizon Samples

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

```
## Check Sample IDs with Metadata
```

```
## Some sample IDs are missing from metadata.
```

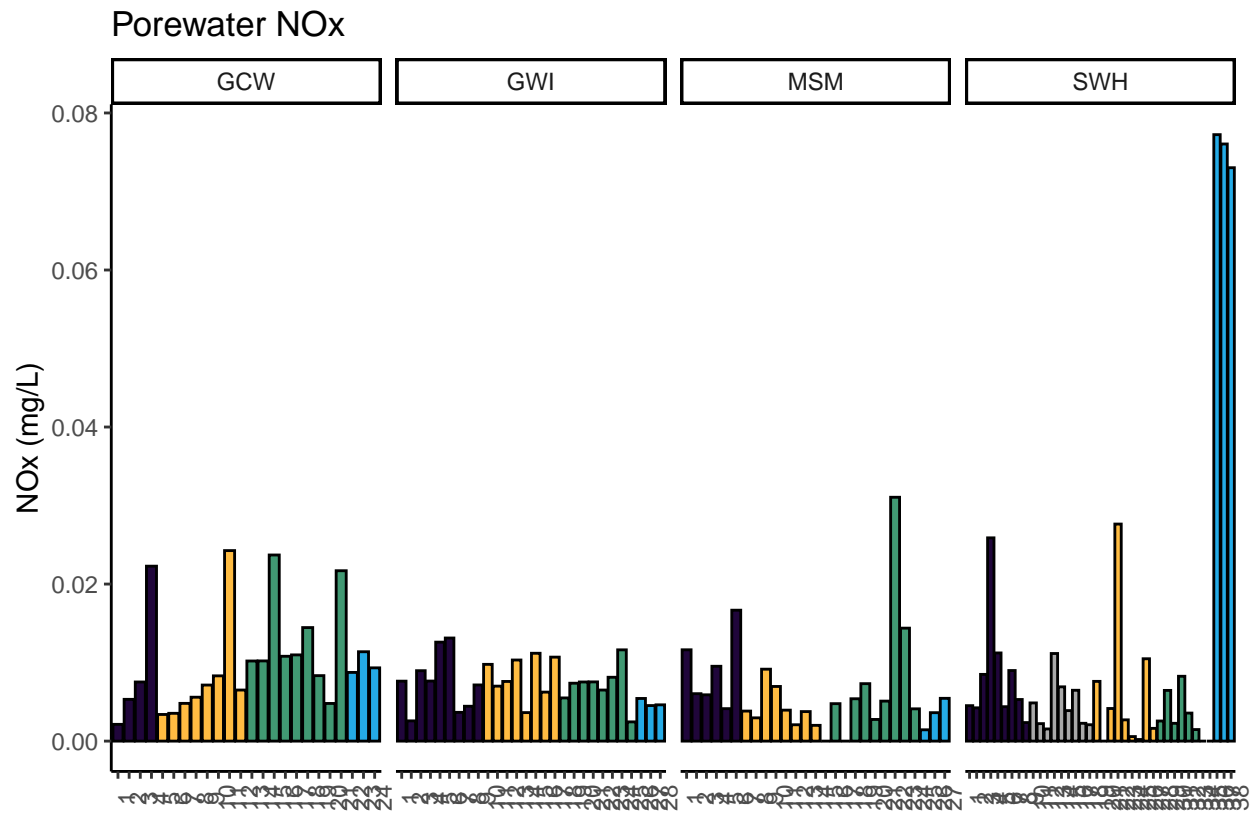
```
## [1] "MSM_202306_UP_LysA_45cm" "MSM_202306_UP_LysC_20cm"
## [3] "MSM_202306_UP_LysC_45cm" "MSM_202306_TR_LysA_45cm"
## [5] "SWH_202306_UPCON_LysA_10cm" "SWH_202306_UPCON_LysA_20cm"
## [7] "SWH_202306_UPCON_LysA_45cm" "SWH_202306_UPCON_LysB_10cm"
## [9] "SWH_202306_UPCON_LysB_20cm" "SWH_202306_UPCON_LysB_45cm"
## [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,
## ...].
```

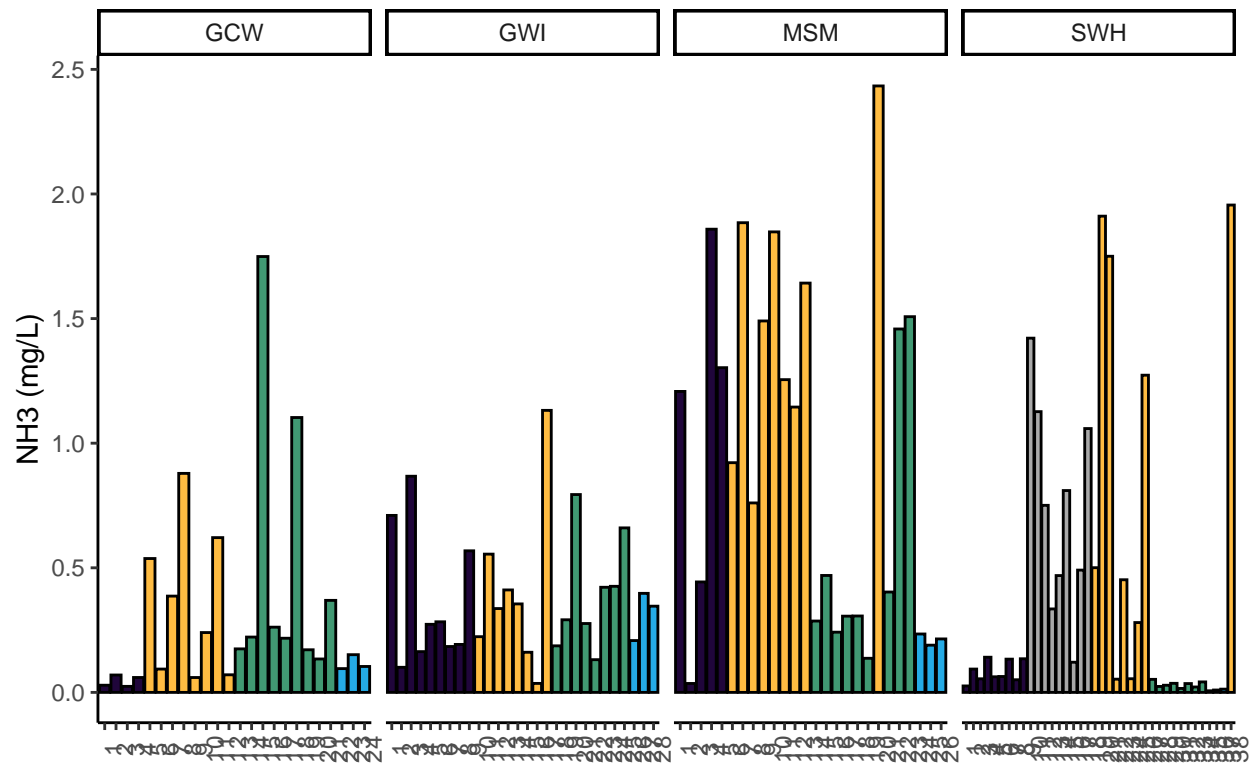
```
## Warning: There was 1 warning in 'mutate()'.
## i In argument: 'Samp_Time = ym(Samp_Time)'.
## Caused by warning:
## ! 2 failed to parse.
```

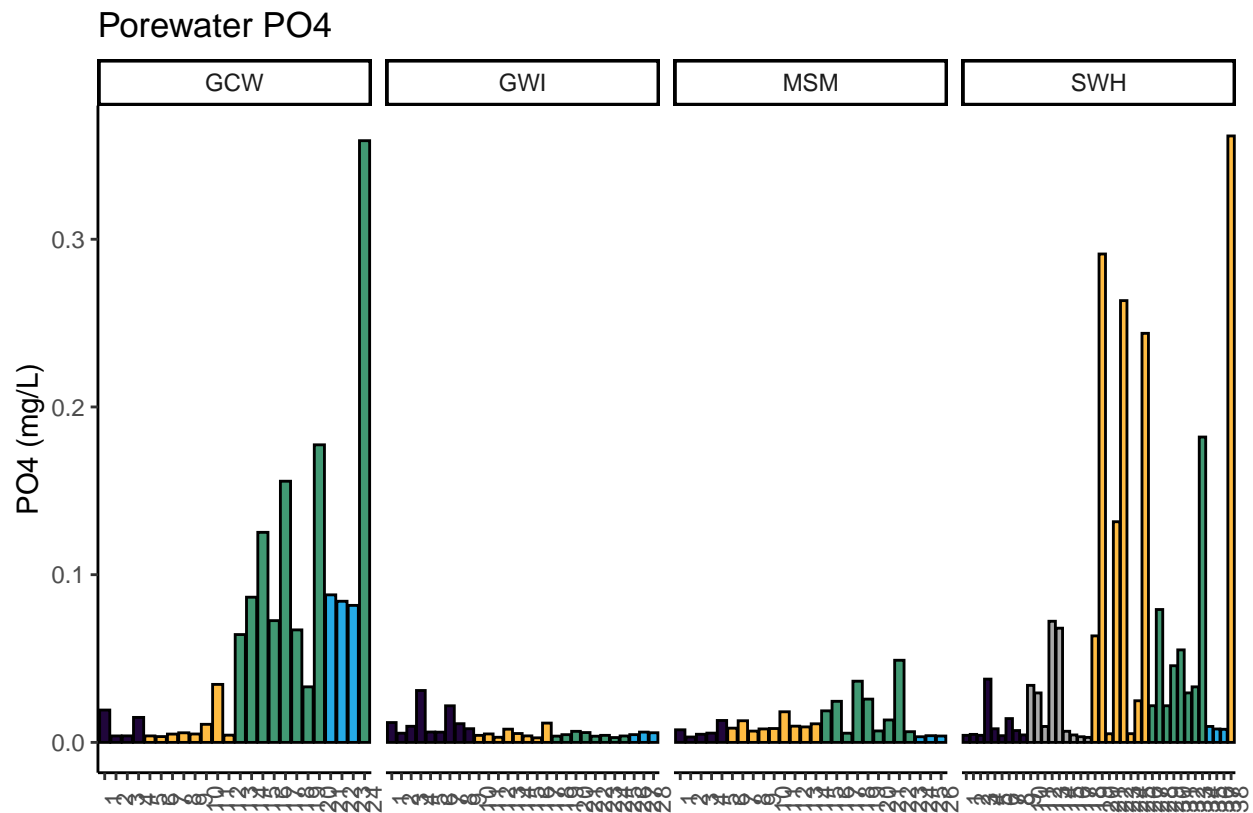
0.15 Visualize Data

Visualize Data



Porewater NH3





0.16 Export Processed Data

#end