

# Synoptic\_CB\_Nutrients\_202306

June 2023

2025-07-01

## Contents

0.1	Import Data & Clean	3
0.2	Assessing standard Curves	3
0.3	Dilution Corrections - ensure the latest dilution is kept	7
0.4	Performance Check	7
0.5	Analyze the Check Standards	9
0.6	Analyze Blanks	10
0.7	Analyze Duplicates	11
0.8	Spikes	12
0.9	Matrix Effects	13
0.10	Unit Converted Data Column Added (mg/L to uM )	13
0.11	Sample Flagging - Within range of standard curve	13
0.12	Pull out sample id information	13
0.13	Pulling Out Rhizon Samples	13
0.14	Check to see if samples run match metadata & merge info	14
0.15	Visualize Data	15
0.16	Export Processed Data	17

```

##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_P04_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_June2023_1.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_June2023_2.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_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 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/1HCANO_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

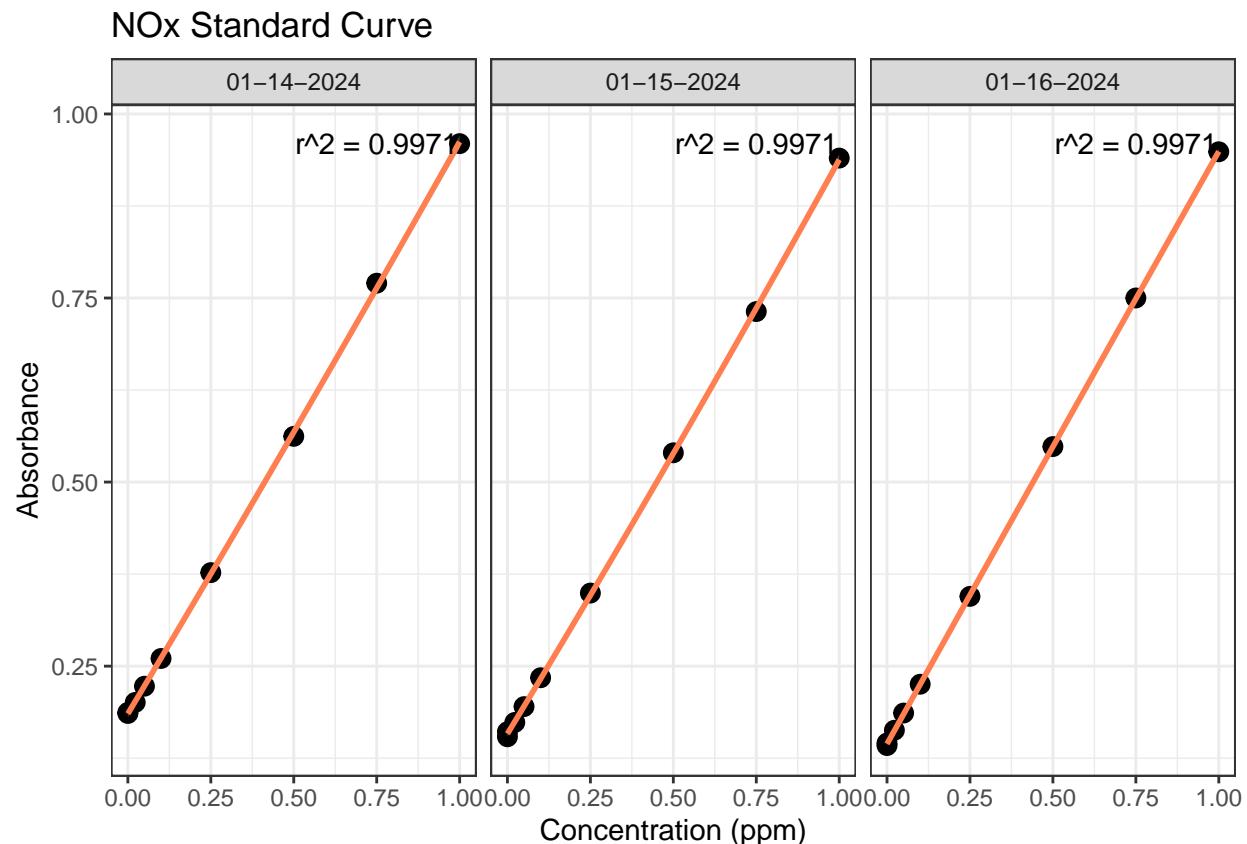
## 0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

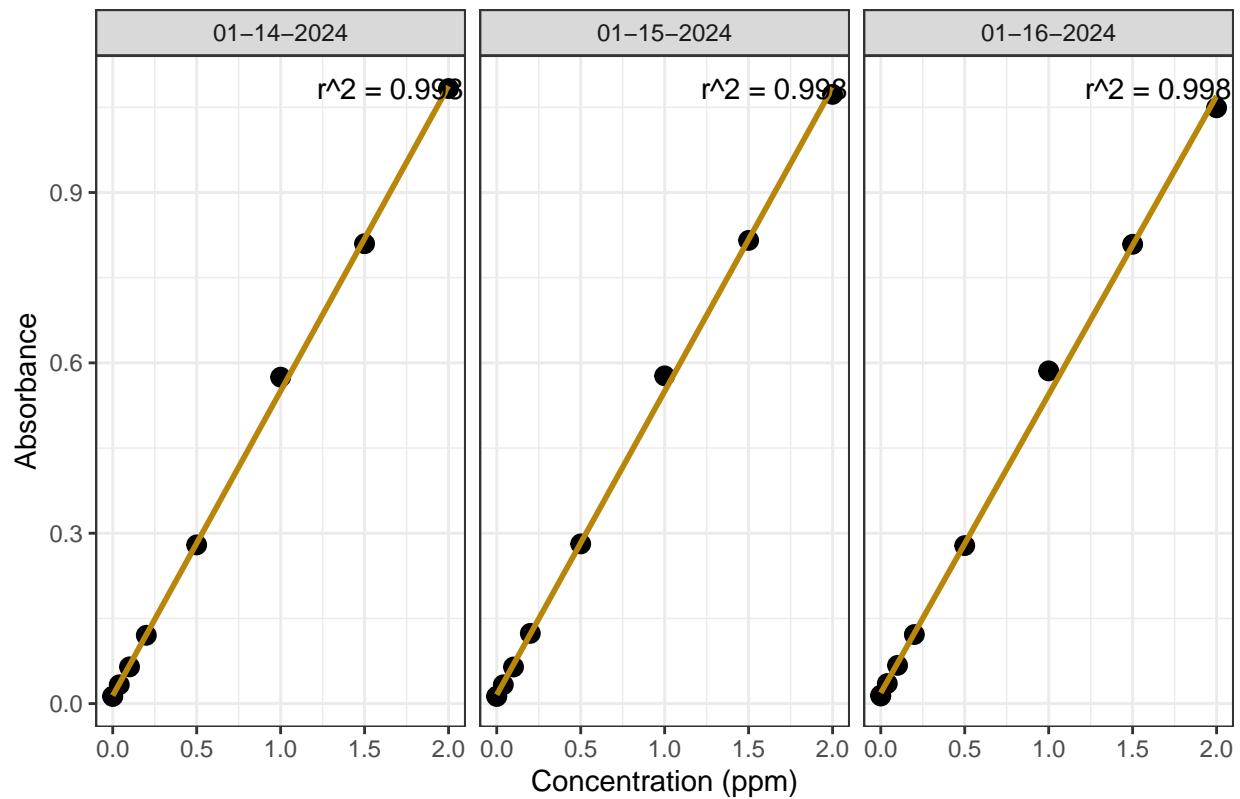
```
#Plot standards data
```

```
## Assess Standard Curves
```



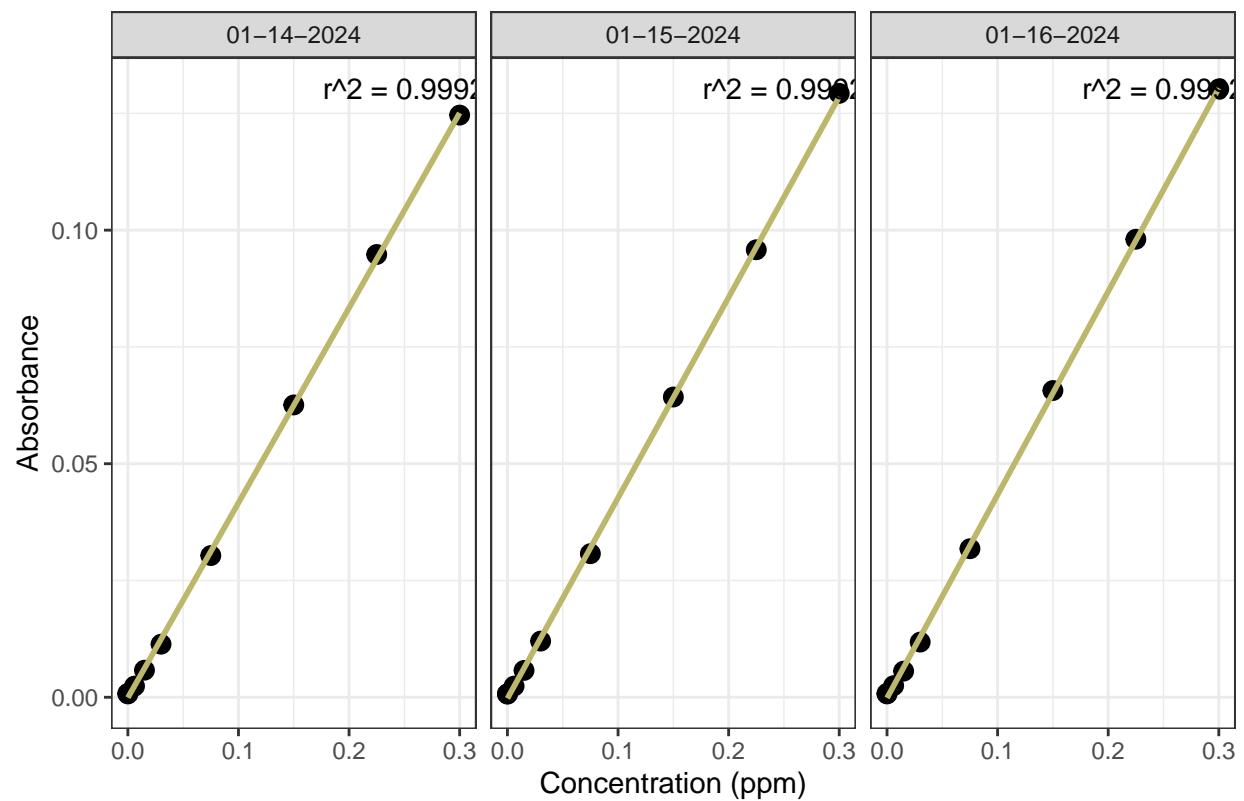
```
## `geom_smooth()` using formula = 'y ~ x'
```

## NH<sub>3</sub> 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."
```

## Slope Drift Assessment

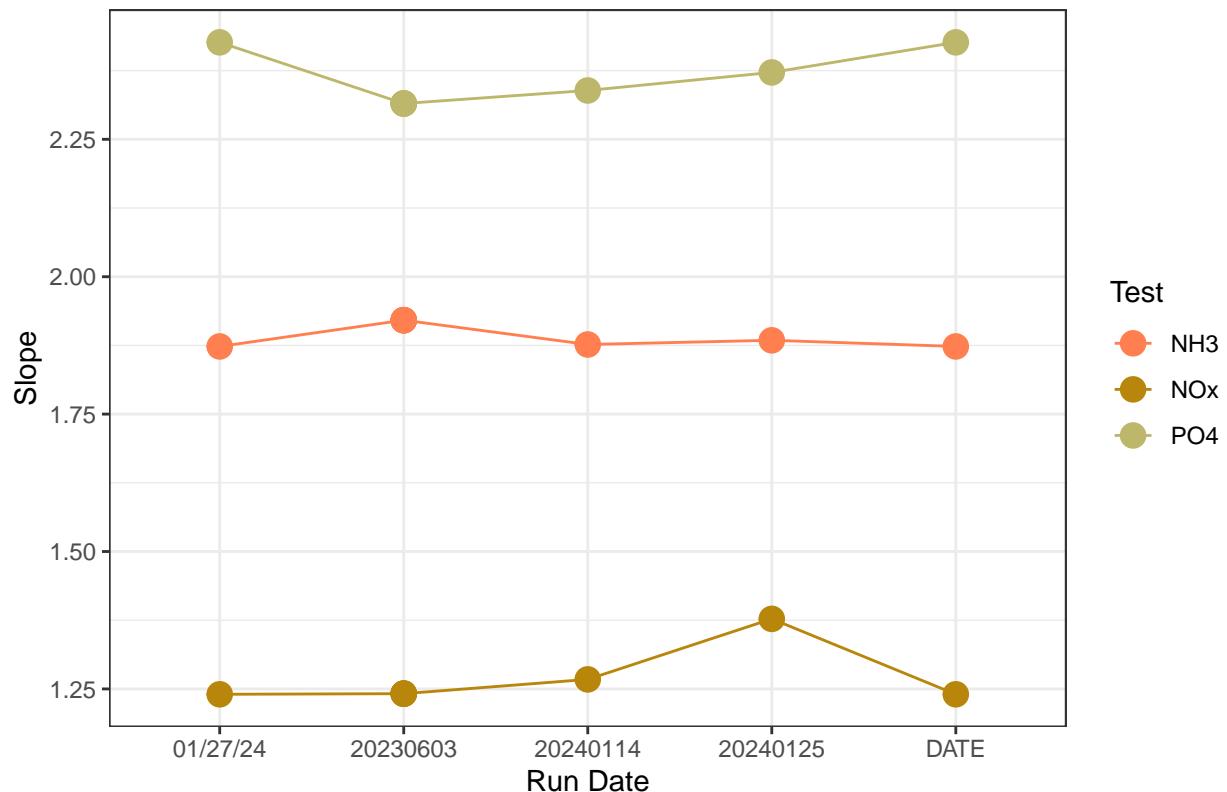


Table 1: Average Slope by Analyte

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_20cm

## 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

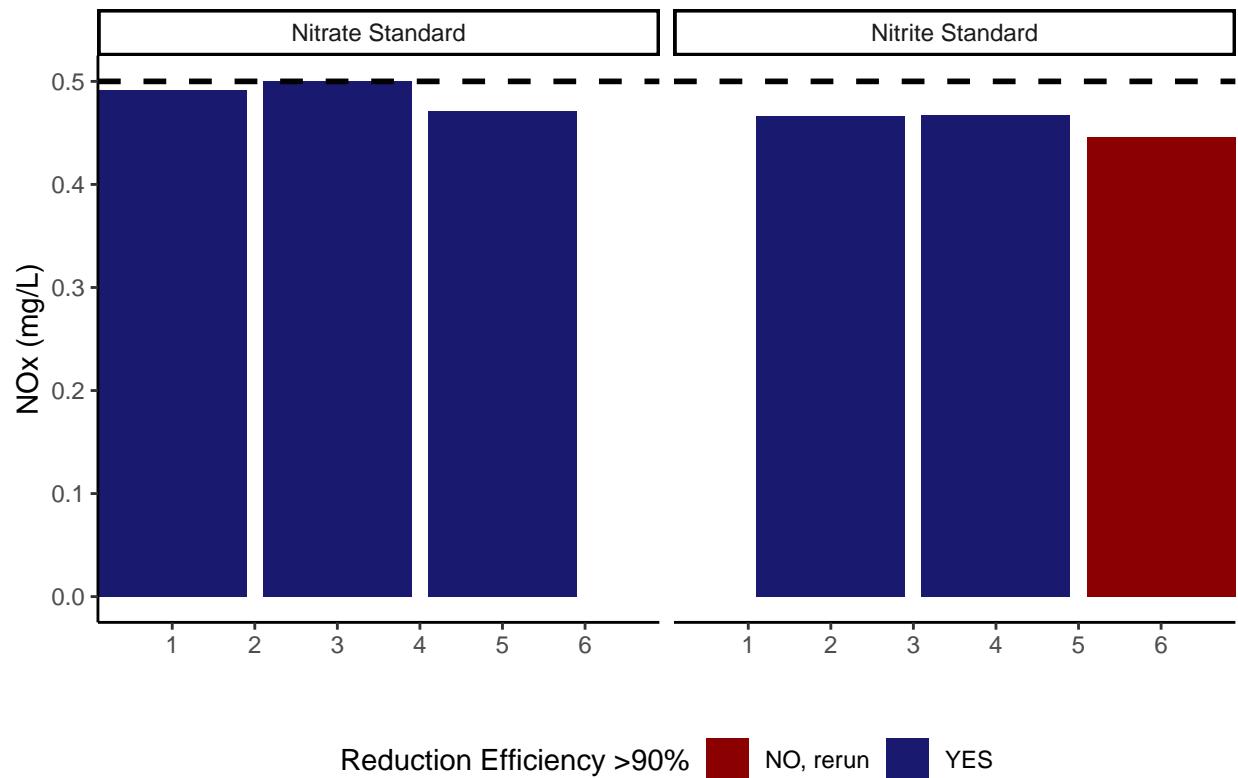
## [1] "PO4 pe Check has a % Difference >10% - REASSESS"

## Run mean = 0.5901153

## Expected = 0.818

#Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



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

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

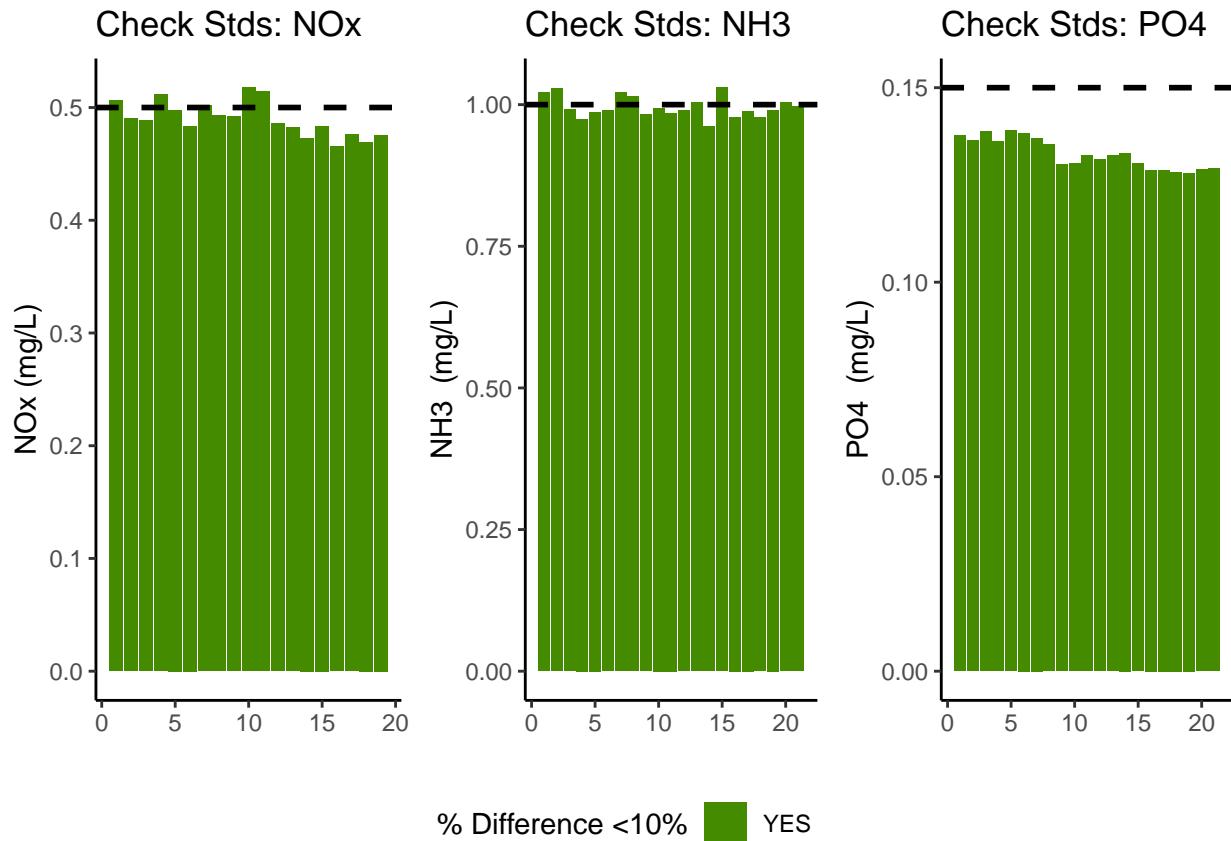
## 0.5 Analyze the Check Standards

```
## 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"
```

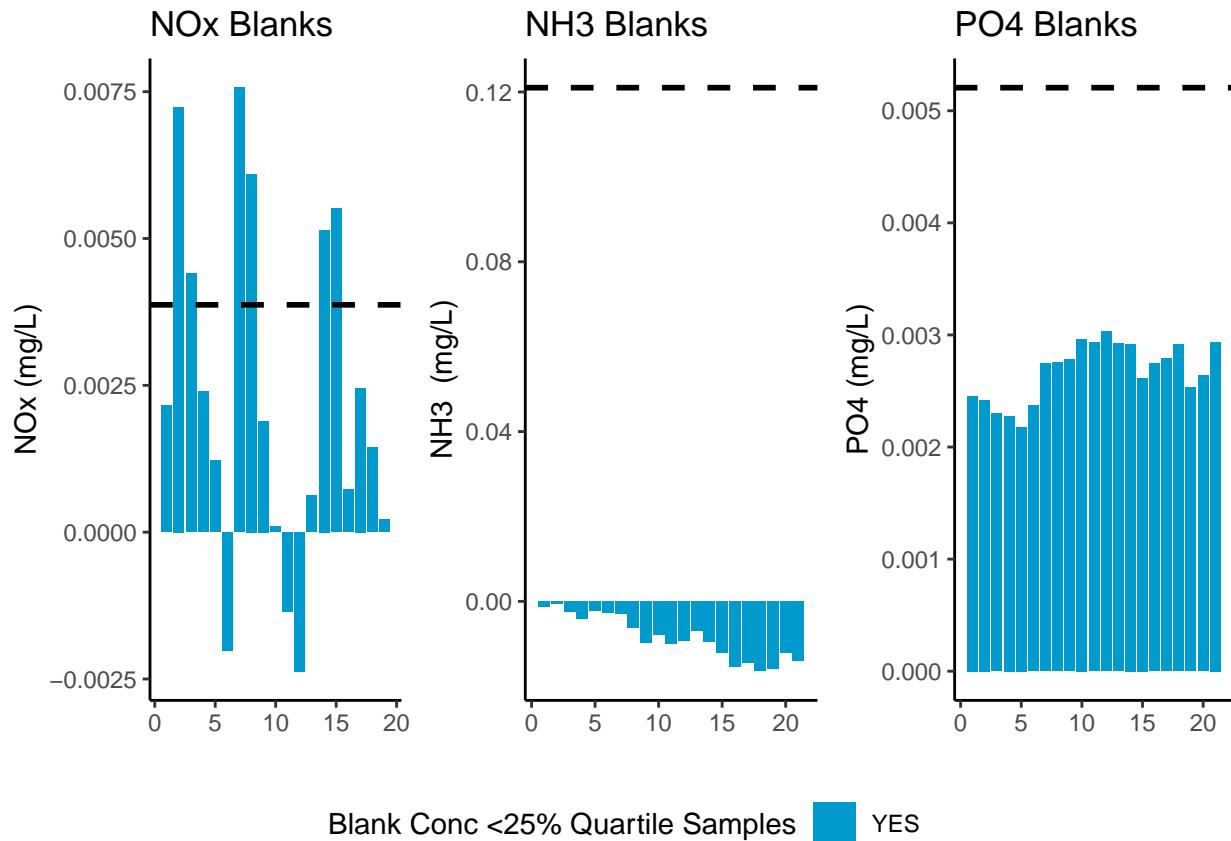


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0023
NH3	-0.0084
PO4	0.0027

## 0.7 Analyze Duplicates

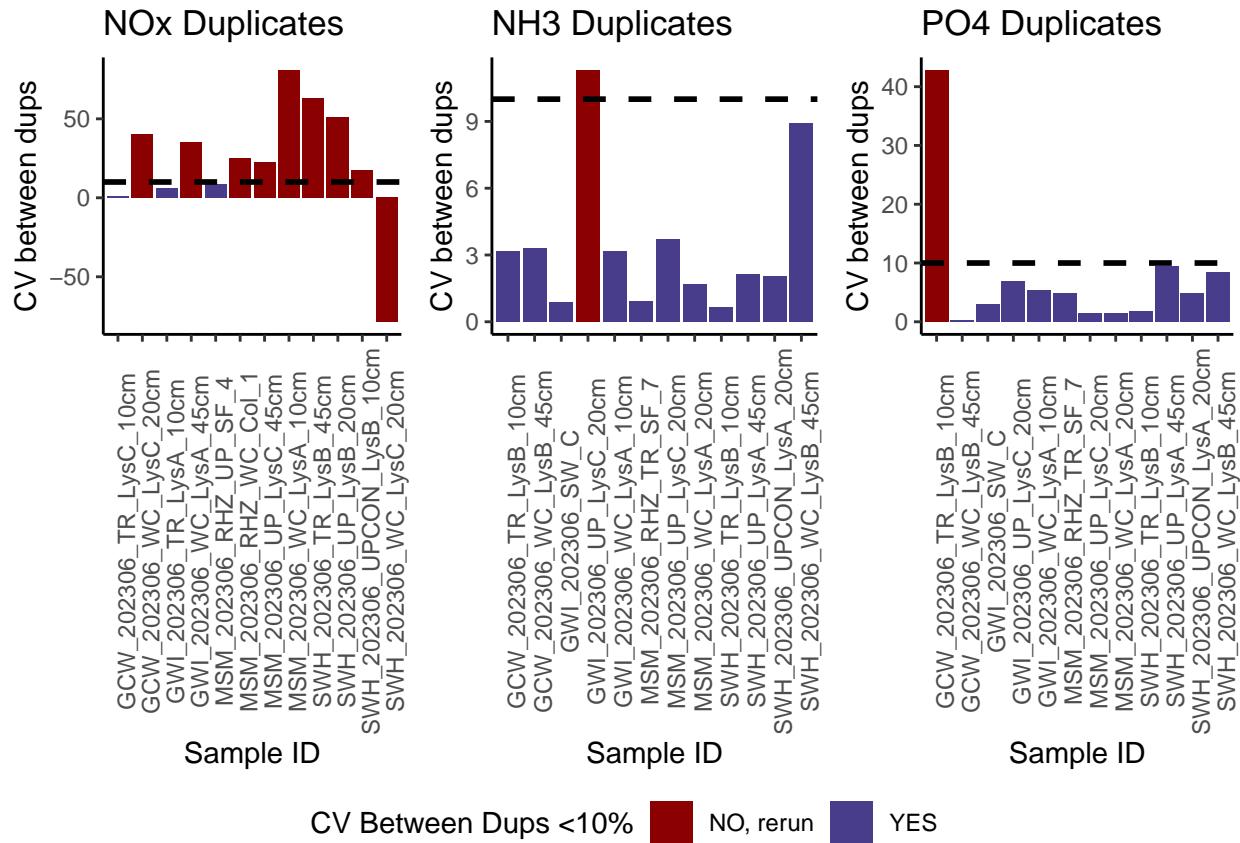
```
## Analyze Duplicates

## [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.
```

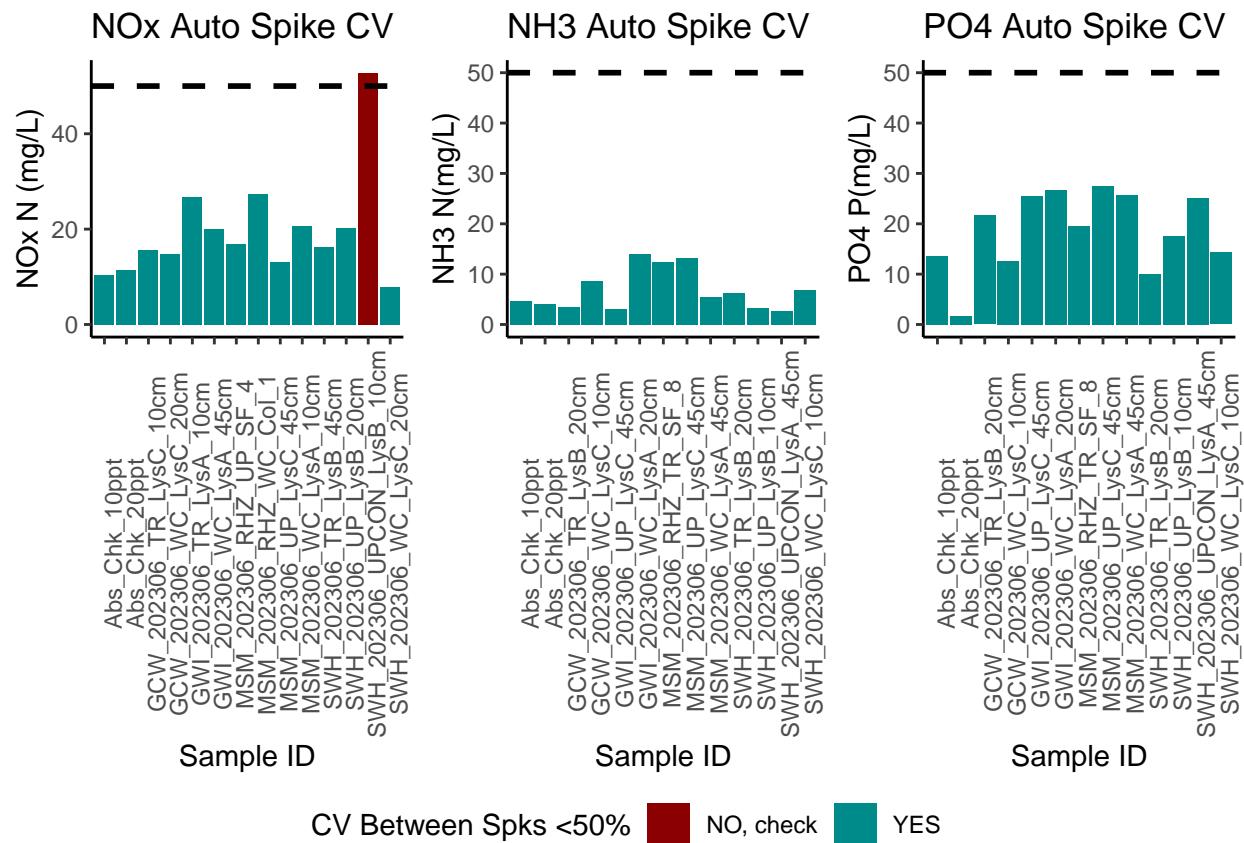


## 0.8 Spikes

```
## [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"

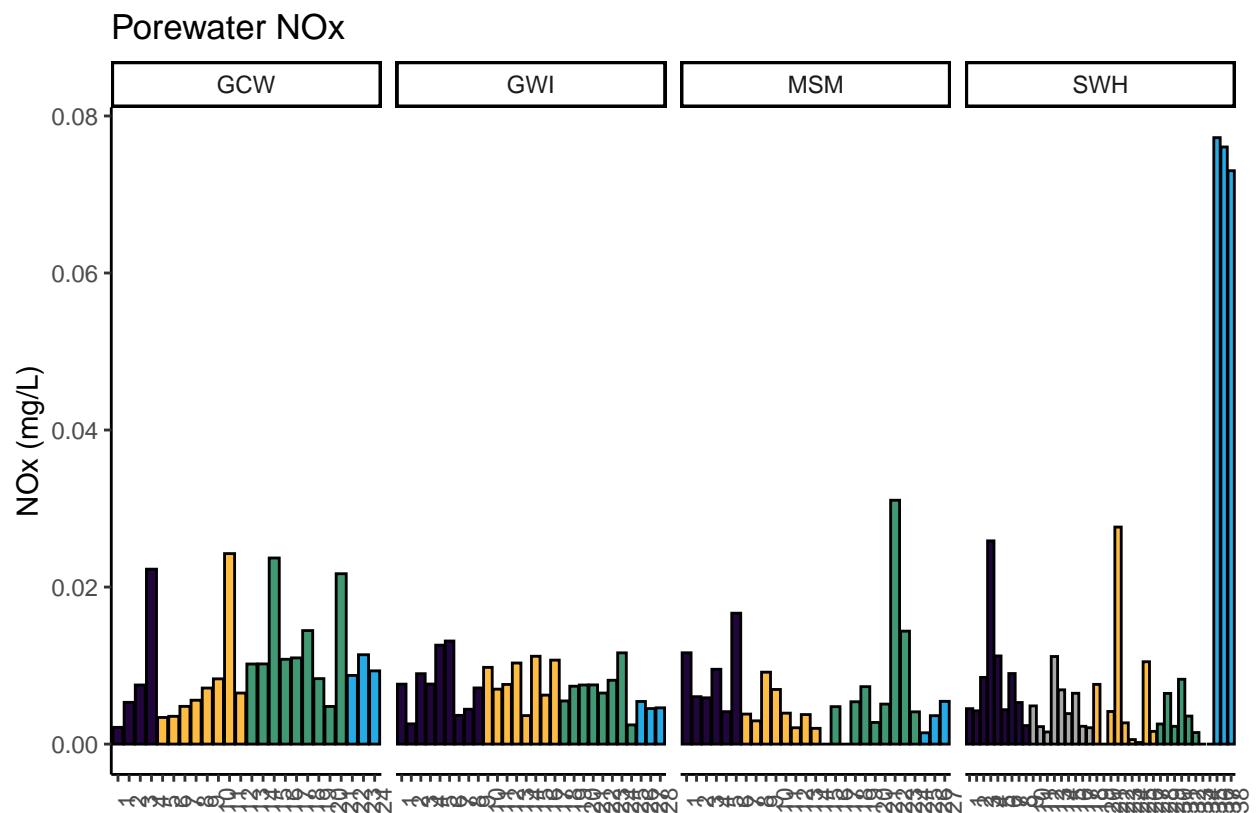
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,
## ...].
```

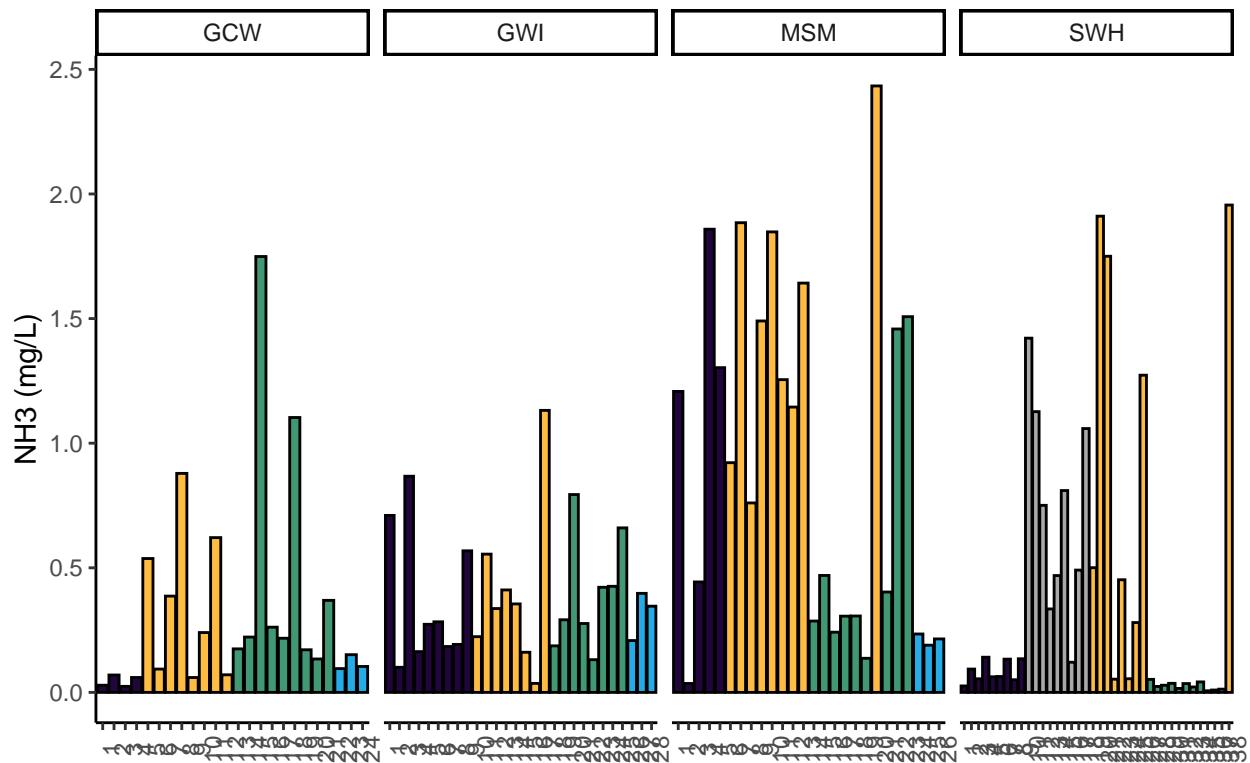
```
## Warning: There was 1 warning in 'mutate()' .
## i In argument: 'Samp_Time = ym(Samp_Time)' .
## Caused by warning:
## ! 2 failed to parse.
```

## 0.15 Visualize Data

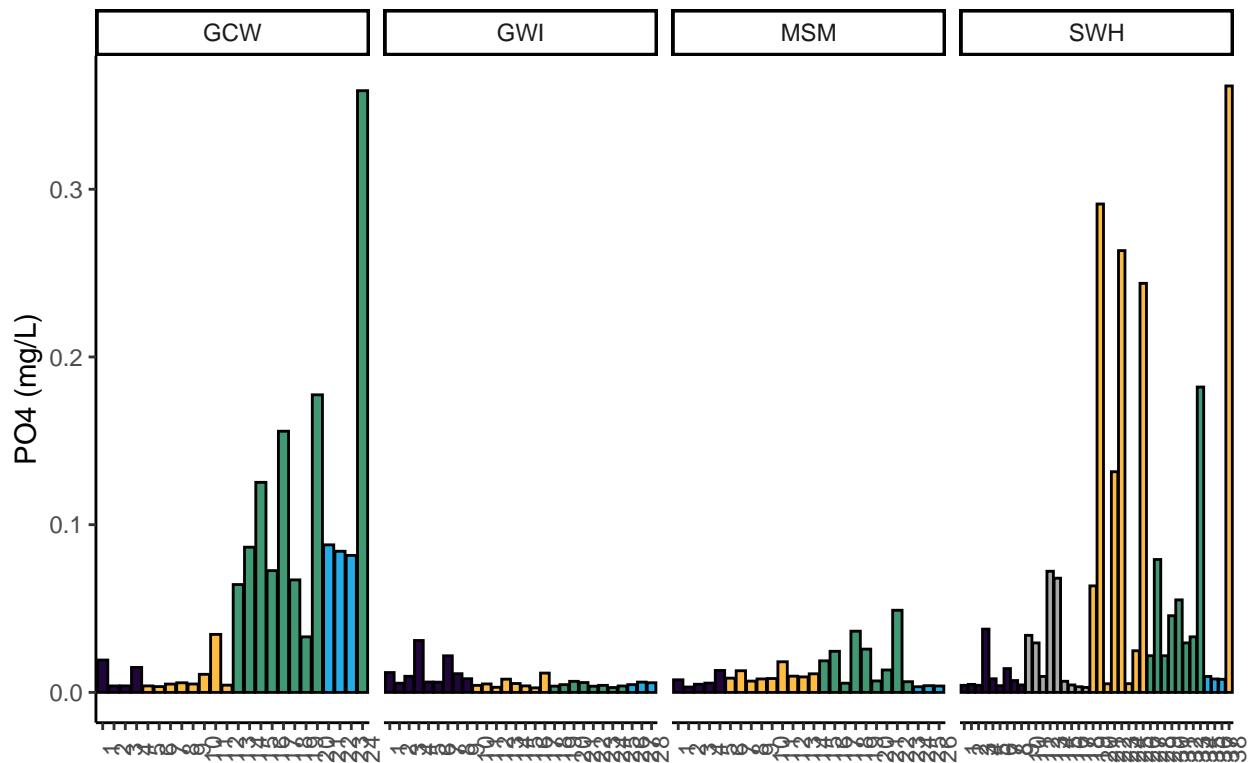
```
## Visualize Data
```



### Porewater NH<sub>3</sub>



## Porewater PO4



## 0.16 Export Processed Data

```
#end
```