

# Synoptic CB: Porewater Nutrients

August 2023 Samples

2025-07-08

## 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 Rhizon Samples . . . . .	13
0.14	Check to see if samples run match metadata & merge info . . . . .	13
0.15	Visualize Data . . . . .	14
0.16	Export Processed Data . . . . .	16

##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 <- "01/22/2024"
sample_year <- 2023
sample_month <- 08
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_Aug2023_1.csv",
               "Raw Data/SEAL_COMPASS_Synoptic_NOx_Aug2023_2.csv",
               "Raw Data/SEAL_COMPASS_Synoptic_NOx_Aug2023_3.csv")
NH3_PO4_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Aug2023_1.csv",
                   "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Aug2023_2.csv",
                   "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Aug2023_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_202308.xlsx"

#record any notes about the run or anything other info here:
run_notes <- "NH3 peCheck is out of range, but other run metrics are good,
so we are accepting this run."

#Set up file path for metadata
#downloaded metadata csv - downloaded from Google drive as csv for this year
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"

cat(run_notes)
```

## NH3 peCheck is out of range, but other run metrics are good,  
## so we are accepting this run.

```
##Setup
```

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

## 0.1 Import Data & Clean

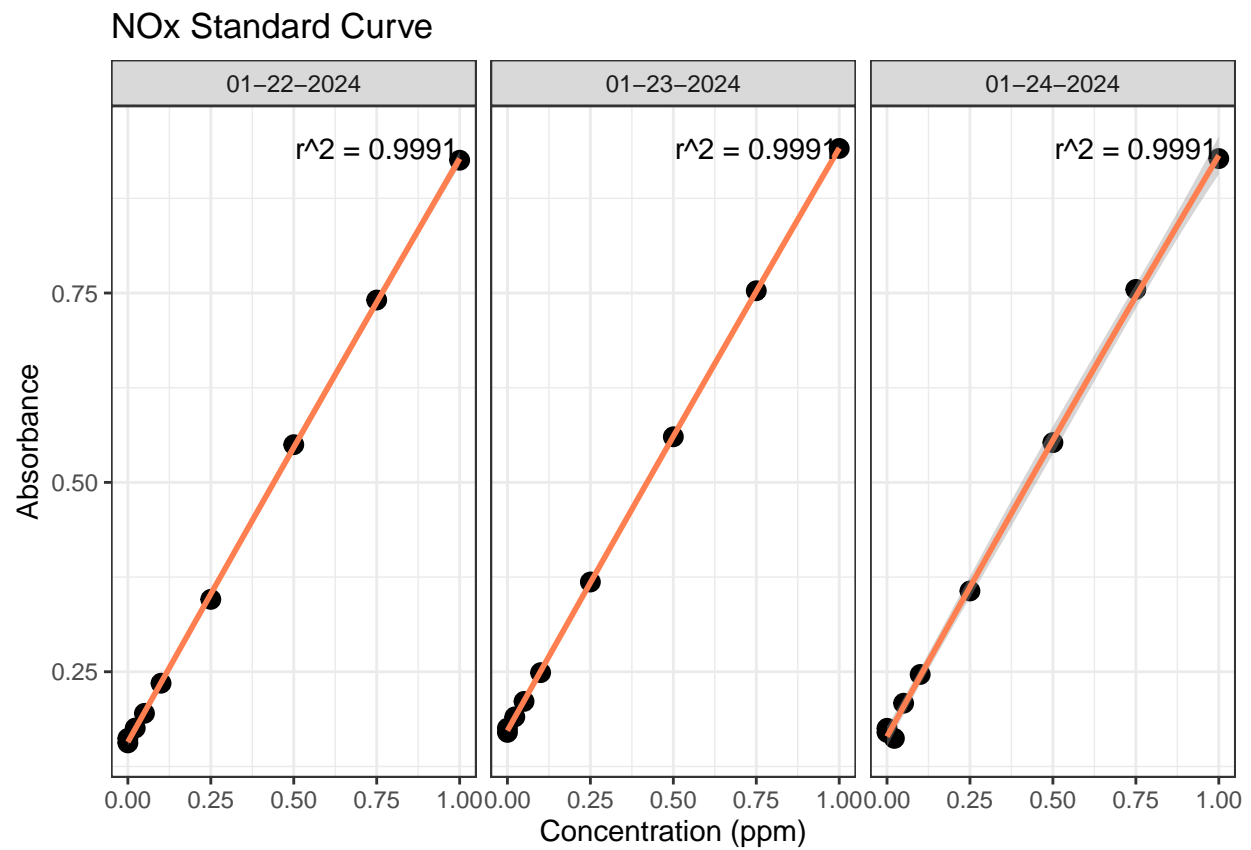
## 0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

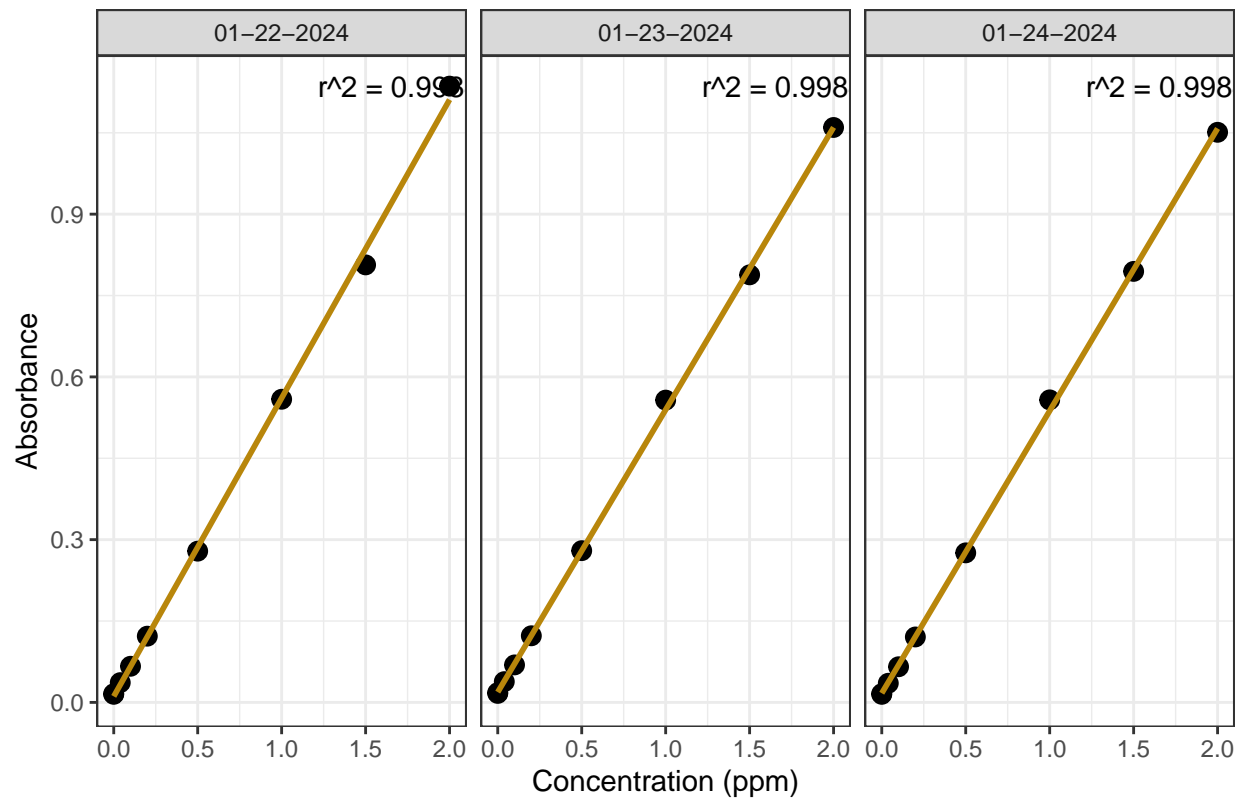
```
#Plot standards data
```

```
## Assess Standard Curves
```



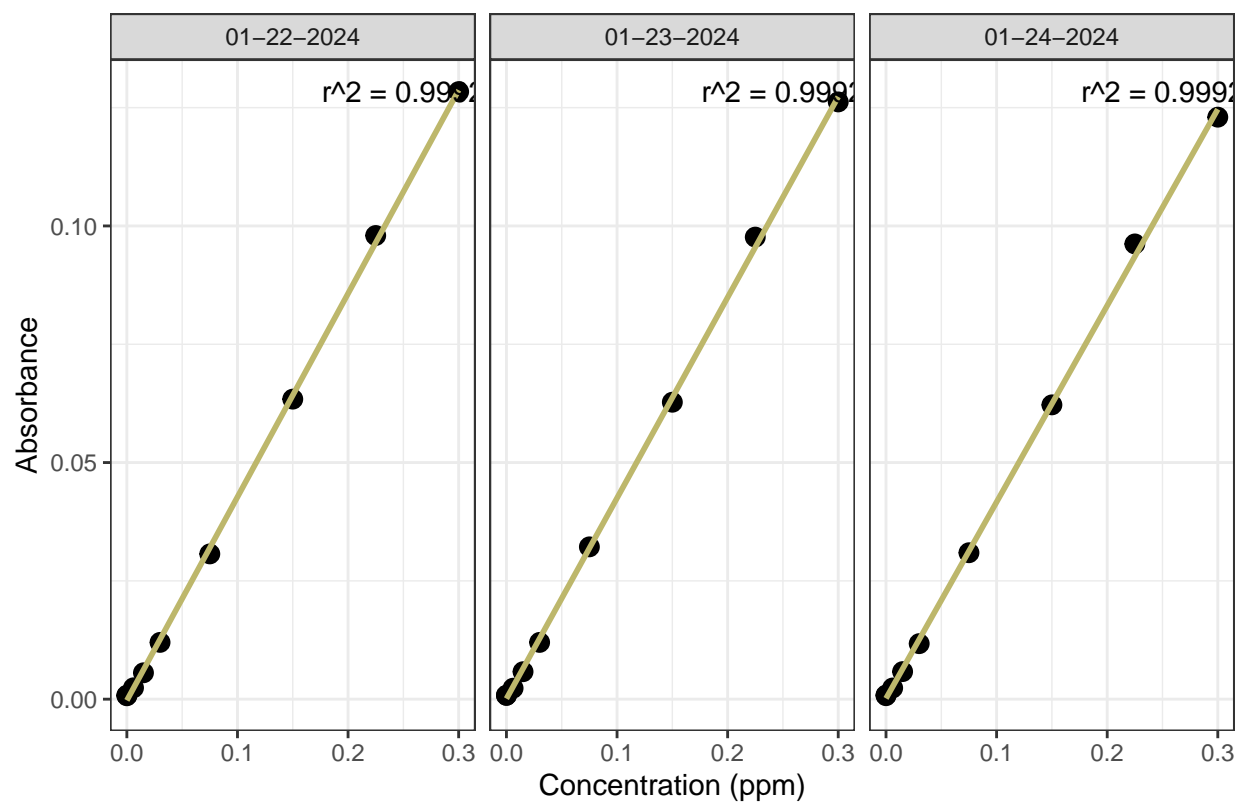
```
## 'geom_smooth()' using formula = 'y ~ x'
```

## 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."
```

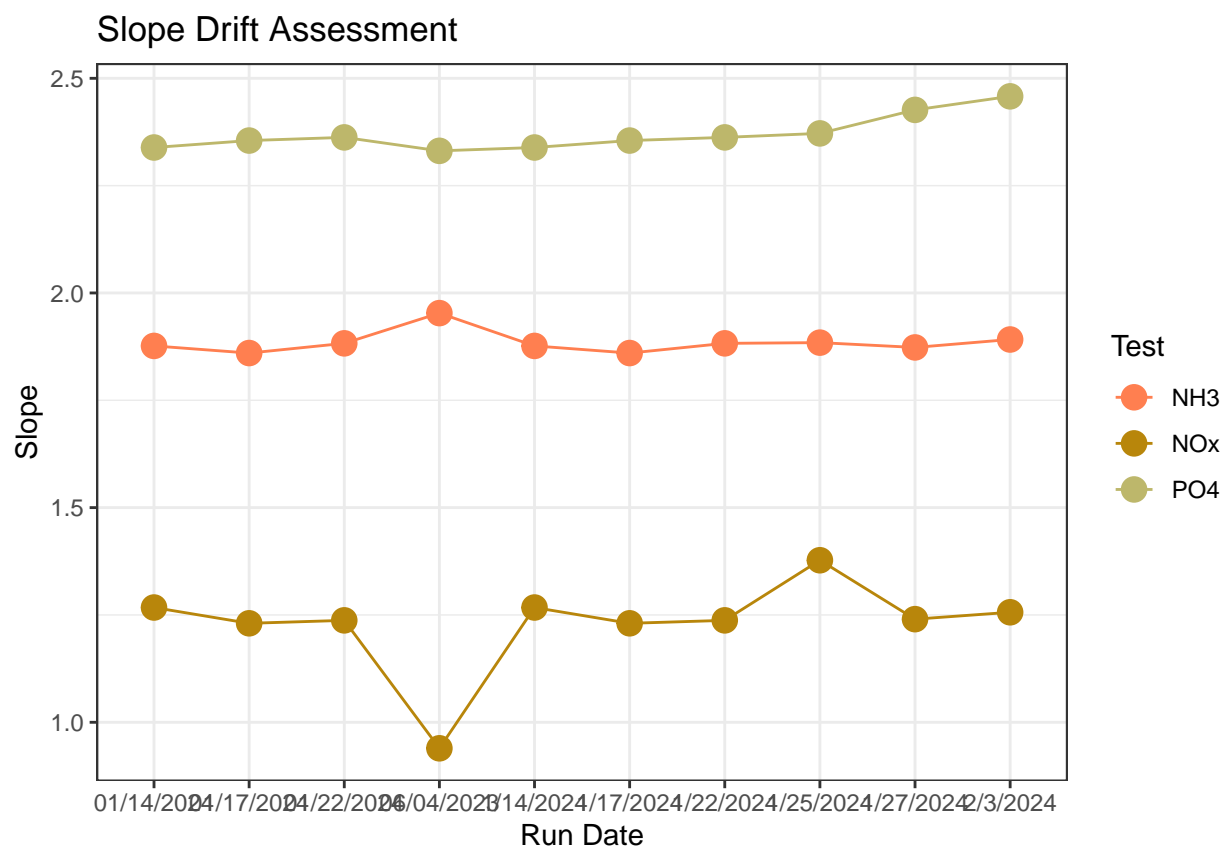


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.884
NOx	1.228
PO4	2.370

### 0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections
```

```
## Duplicated samples: GCW_202308_WC_LysA_45cm, MSM_202308_TR_LysA_20cm, MSM_202308_TR_LysB_20cm, MSM_202308_TR_LysC_20cm
```

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

### 0.4 Performance Check

```
## [1] "NOx pe Check has a % Difference <25% - PROCEED"
```

```
## Run mean = 0.7147915
```

```
## Expected = 0.706
```

```
## [1] "NH3 pe Check has a % Difference >25% - REASSESS"
```

```
## Run mean = 1.421895
```

```
## Expected = 0.948
```

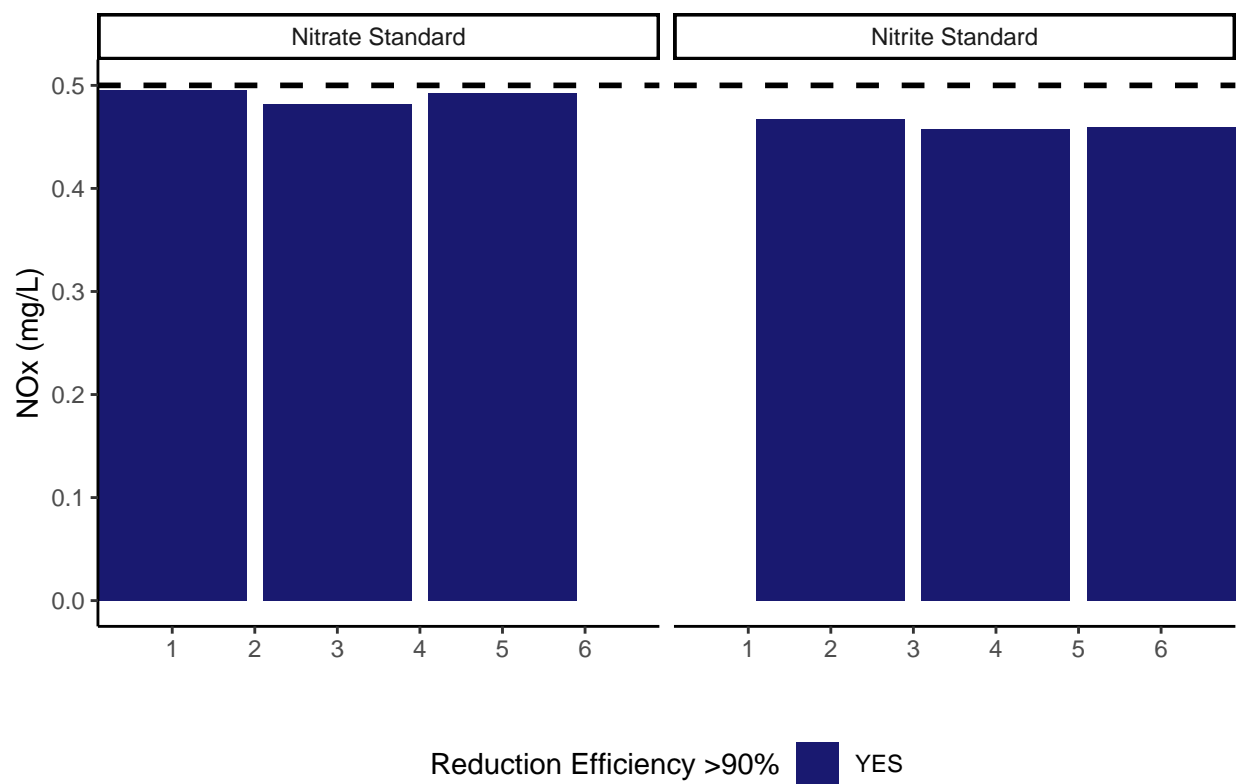
```
## [1] "PO4 pe Check has a % Difference <25% - PROCEED"
```

```
## Run mean = 0.849674
```

```
## Expected = 0.818
```

```
#Check NOx Reduction Efficiency
```

```
## Assess Reduction Efficiency
```



```
## [1] "Mean NOx Reduction Efficiency >95% - PROCEED"
```

```
## [1] 95.1625
```



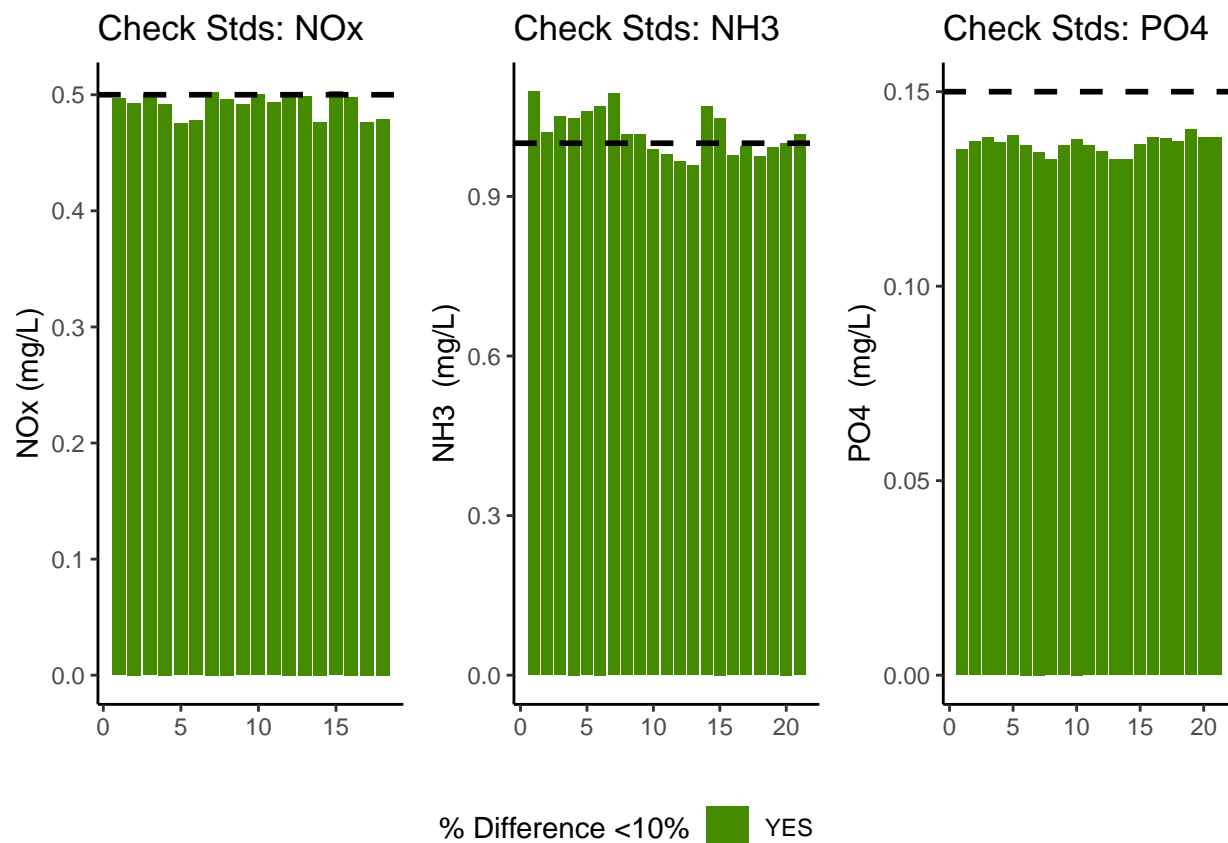
## 0.5 Analyze the Check Standards

```
## 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 Blanks are below the lower 25% quartile of samples or 1/2 detection limit - PROCEED"
```

```
## [1] ">60% of NH3 Blanks are below the lower 25% quartile of samples - PROCEED"
```

```
## [1] ">60% of PO4 Blanks are below the lower 25% quartile of samples- PROCEED"
```

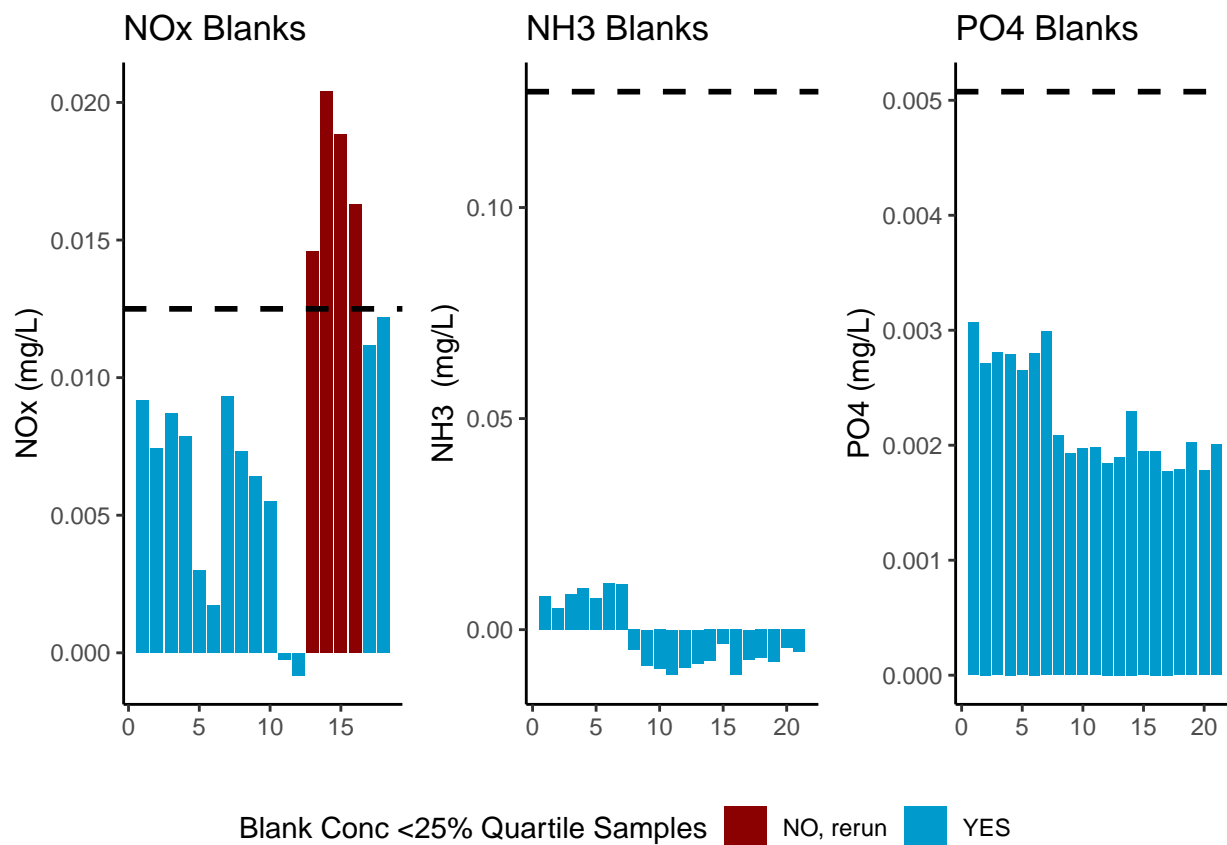


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0088
NH3	-0.0020
PO4	0.0022

## 0.7 Analyze Duplicates

```
## Analyze Duplicates
```

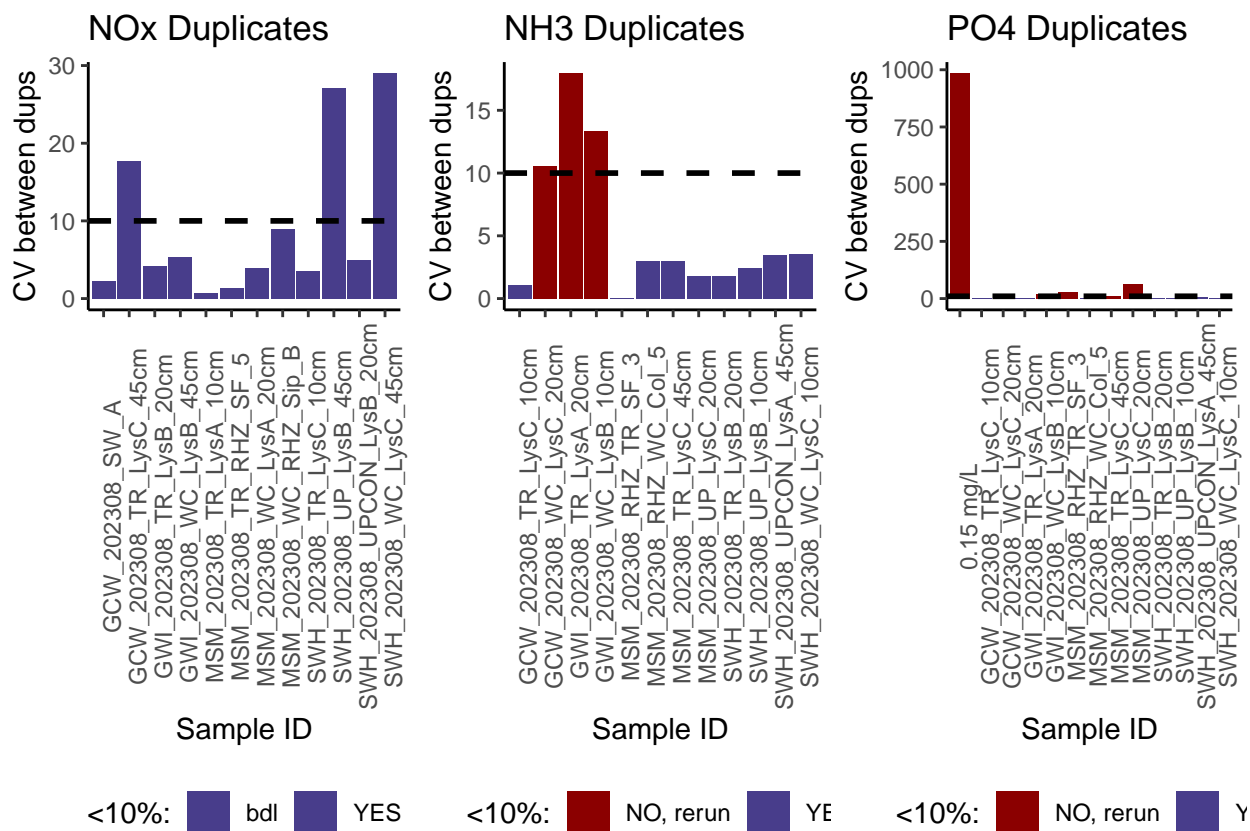
```
## Warning: Returning more (or less) than 1 row per 'summarise()' group was deprecated in
## dplyr 1.1.0.
## i Please use 'reframe()' instead.
## i When switching from 'summarise()' to 'reframe()', remember that 'reframe()'
## always returns an ungrouped data frame and adjust accordingly.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```

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

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

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

```
## 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.
```

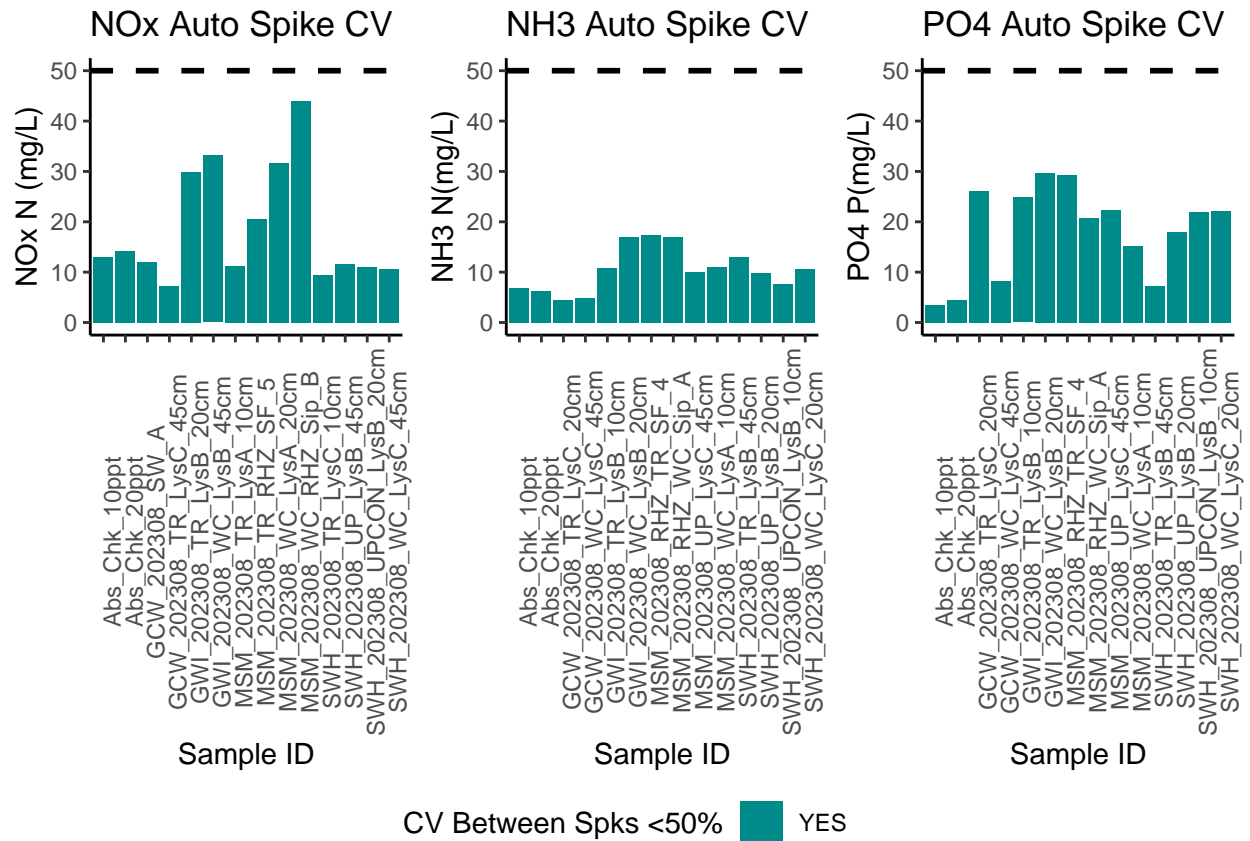


## 0.8 Spikes

## [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 [20, 21, 22, 46,  
## 47, 48, 84, 85, 86, 109, 110, 111, 130, 131, 132, 168, 169, 170, 199, 200,  
## ...].
```

## 0.13 Pulling Rhizon Samples

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

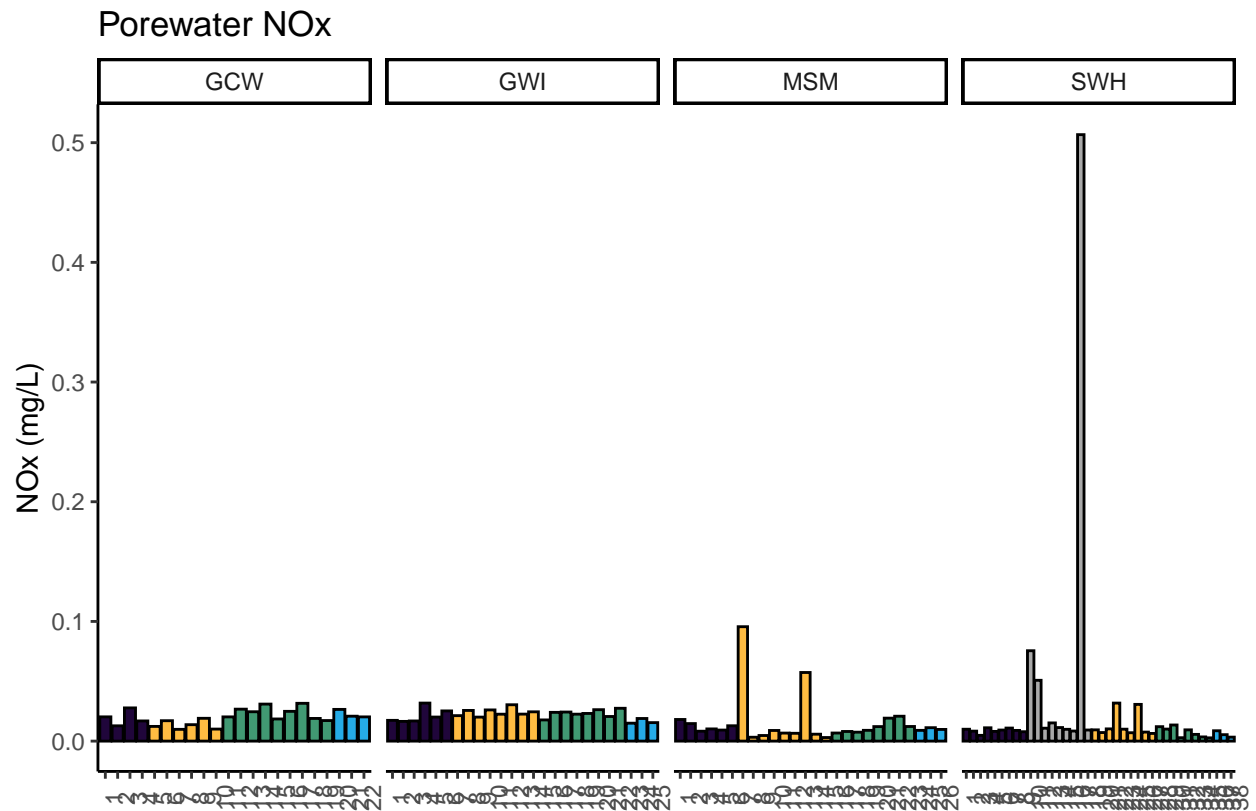
```
## Check Sample IDs with Metadata
```

```
## All sample IDs are present in metadata.
```

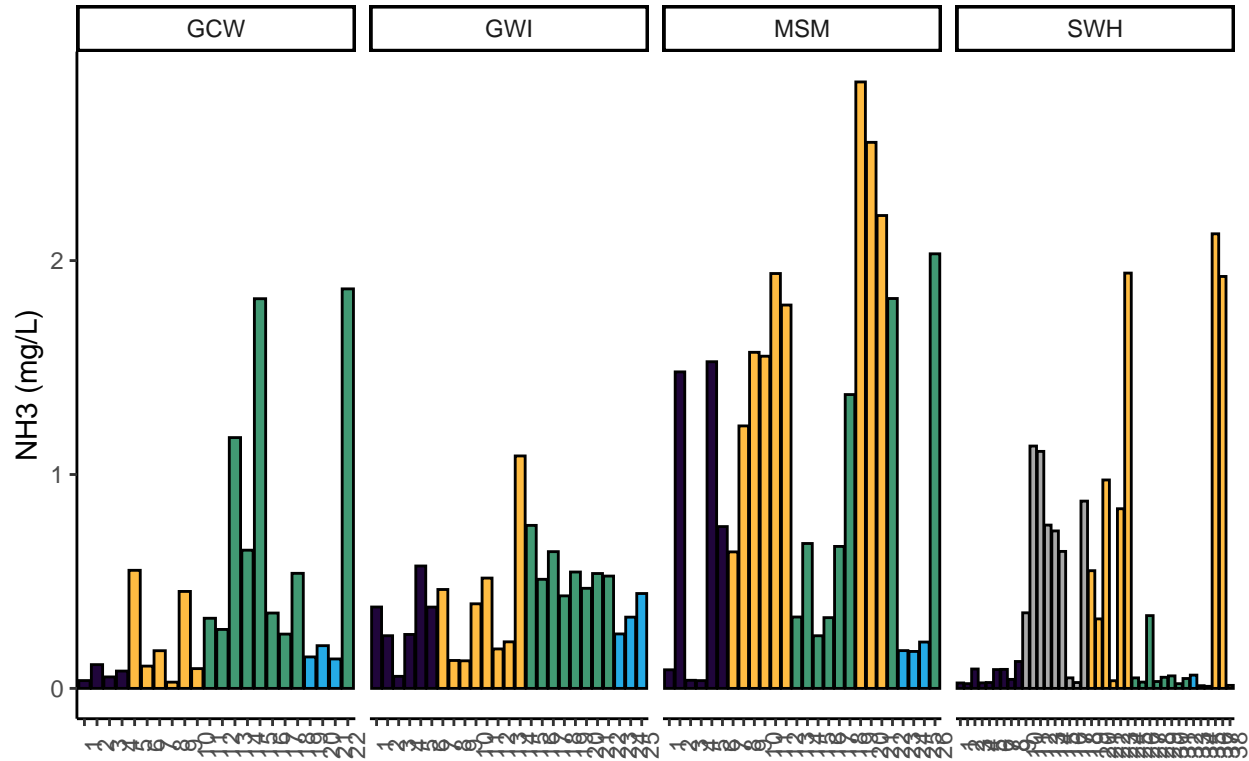
```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [20, 21, 22, 46,  
## 47, 48, 84, 85, 86, 109, 110, 111, 130, 131, 132, 168, 169, 170, 199, 200,  
## ...].
```

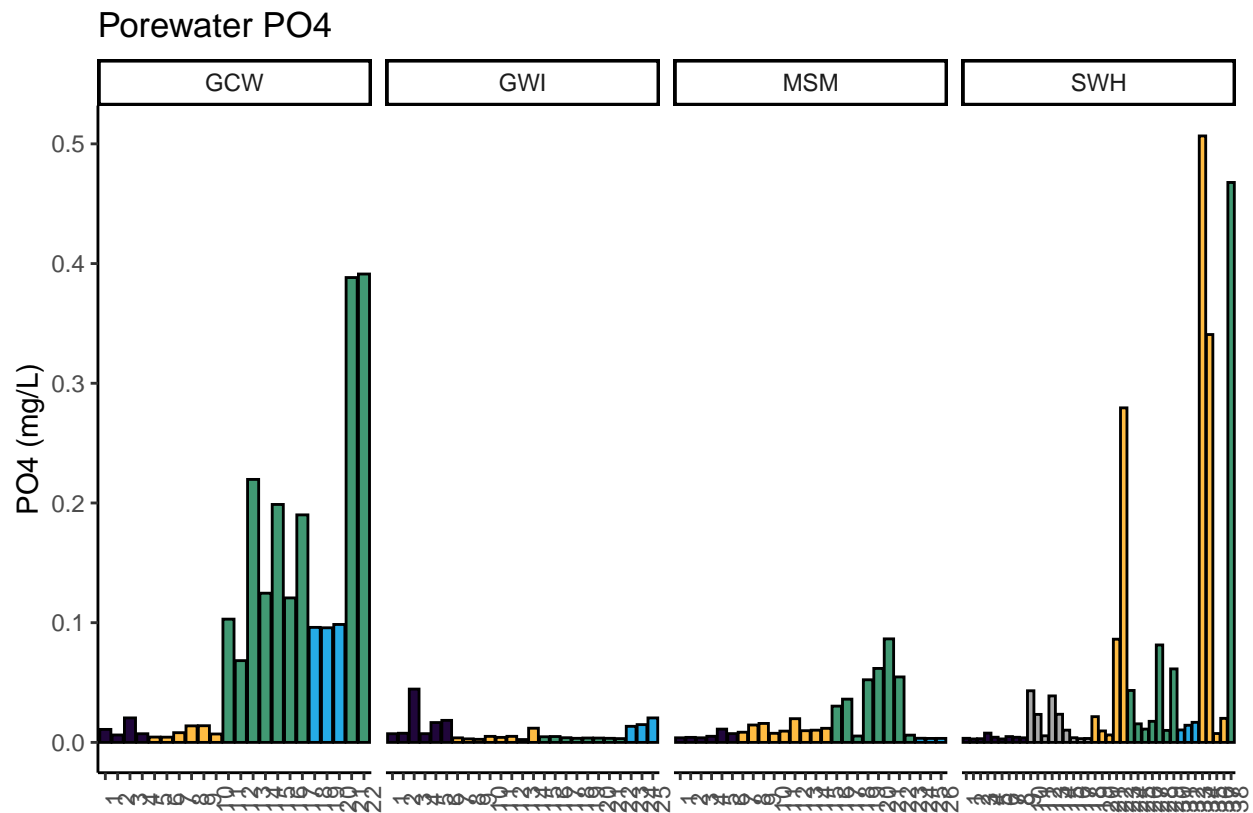
## 0.15 Visualize Data

## Visualize Data



Porewater NH3





## 0.16 Export Processed Data

#end