Synoptic_CB_Nutrients_202308

August 2023

2025-07-01

Contents

Run Information

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

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

```r
#set the run date & user name
  run_date <- "20240114"
  sample_year <- 2023
  sample_month <- 08
  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_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.csv"

#record any notes about the run or anything other info here:
  run_notes <- "Duplicates are out of range because of detection limit, too small of values"

#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

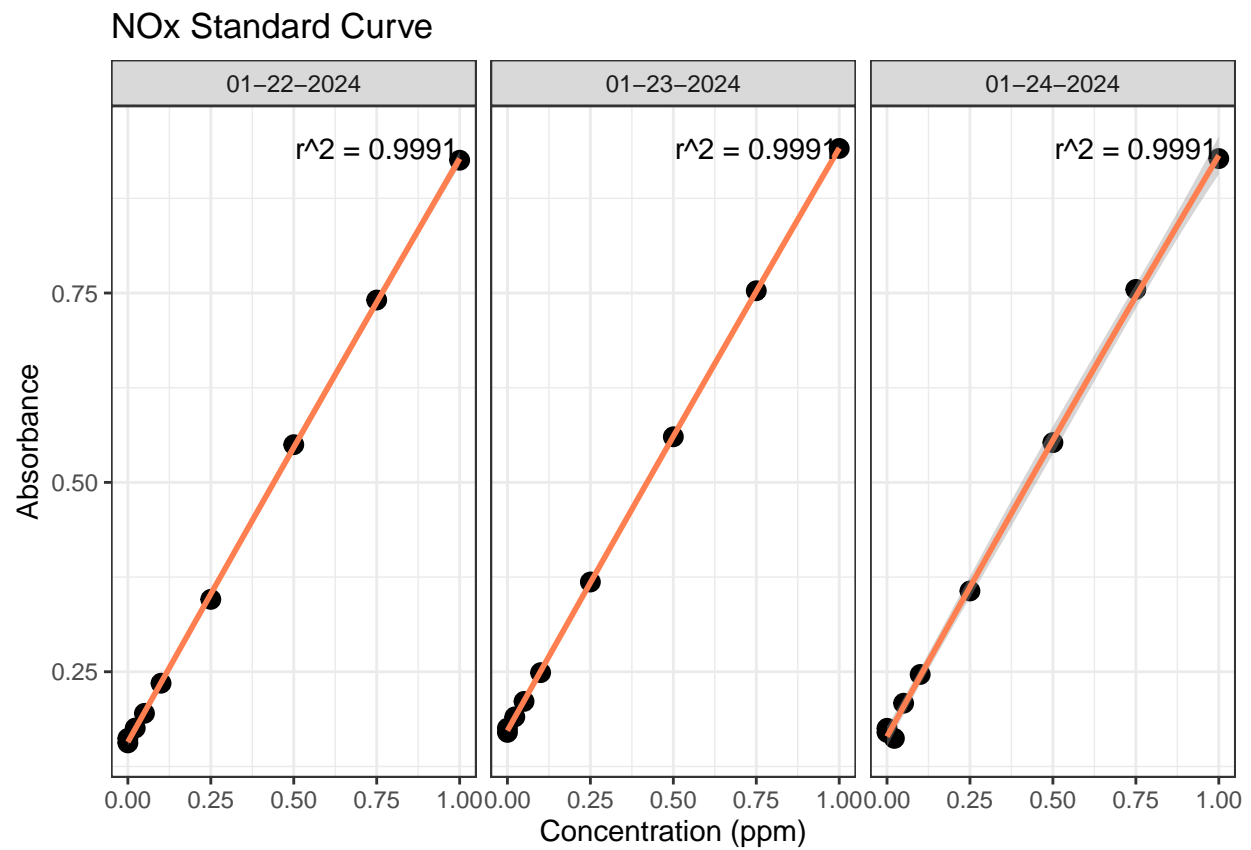## 0.2 Assessing standard Curves

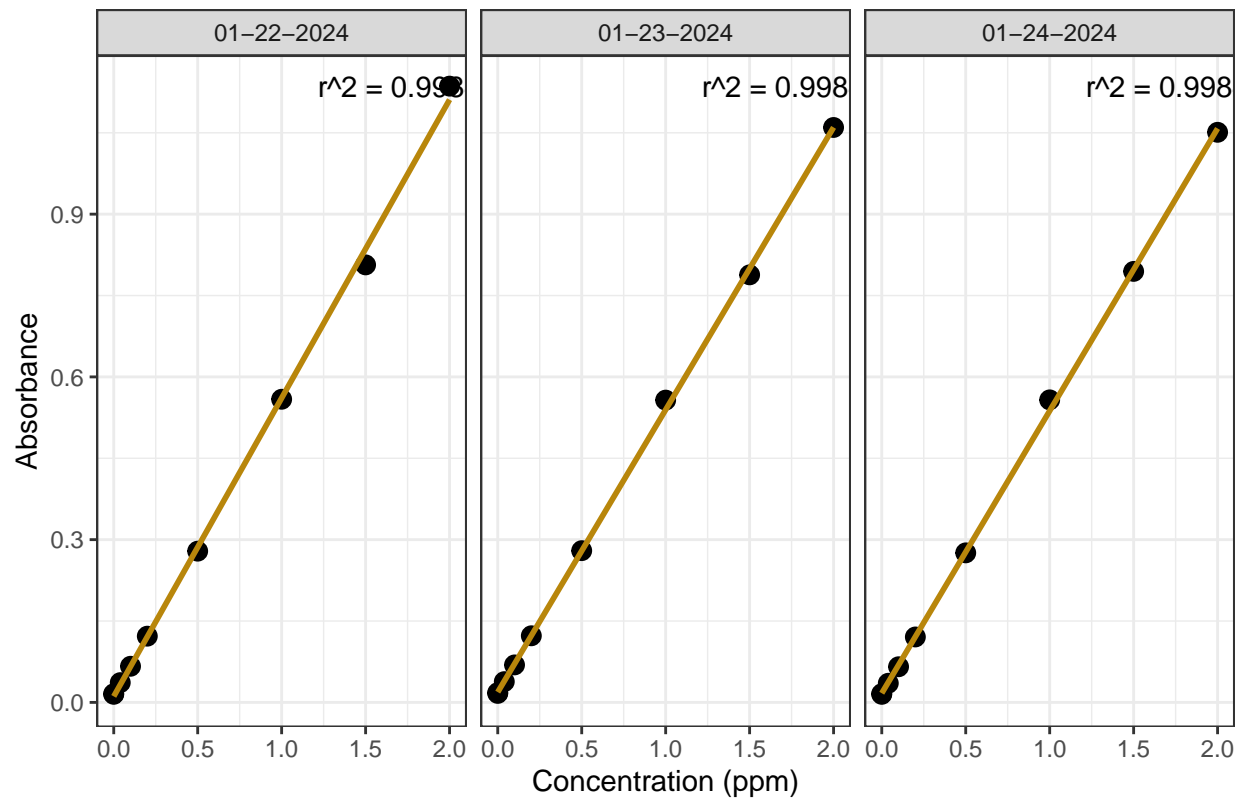#Pull out standards data

```
## Assess Standard Curves
```

#Plot standards data

```
## Assess Standard Curves
```
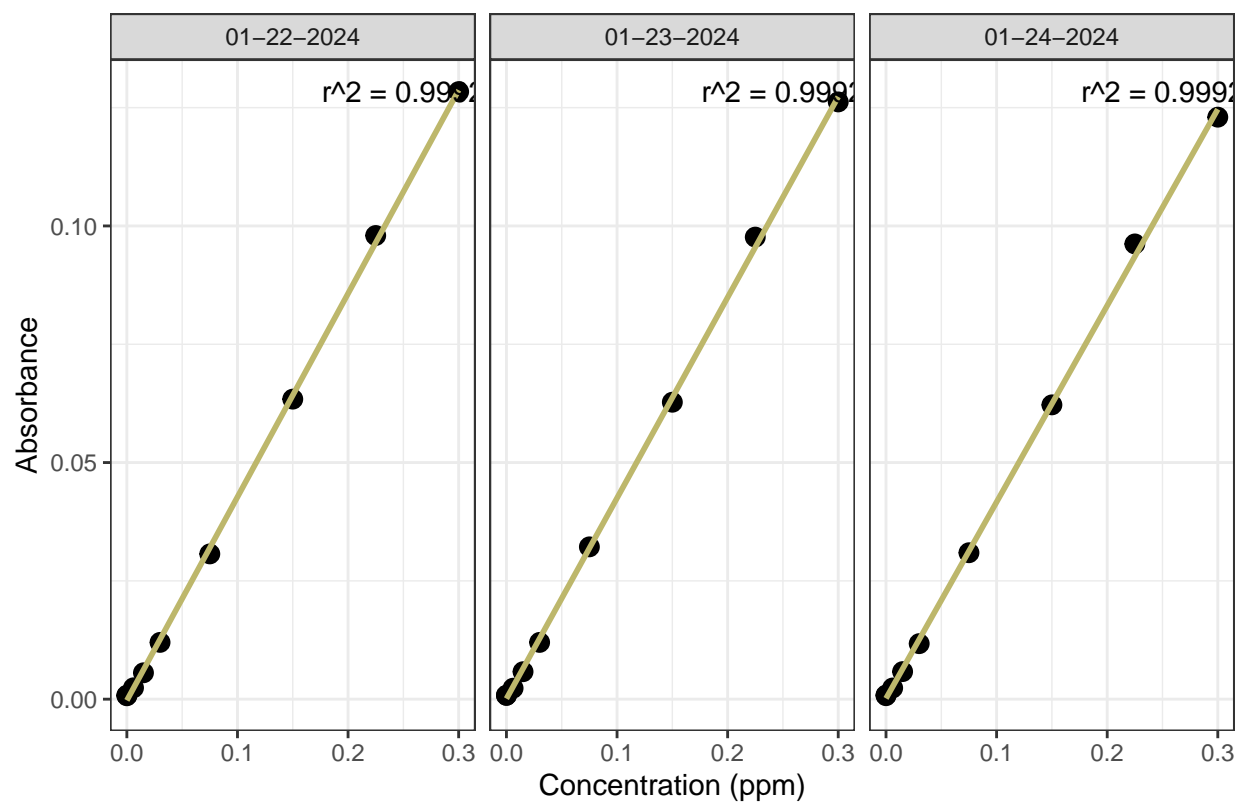

NOx Standard Curve

```
## '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."
```

Slope Drift Assessment
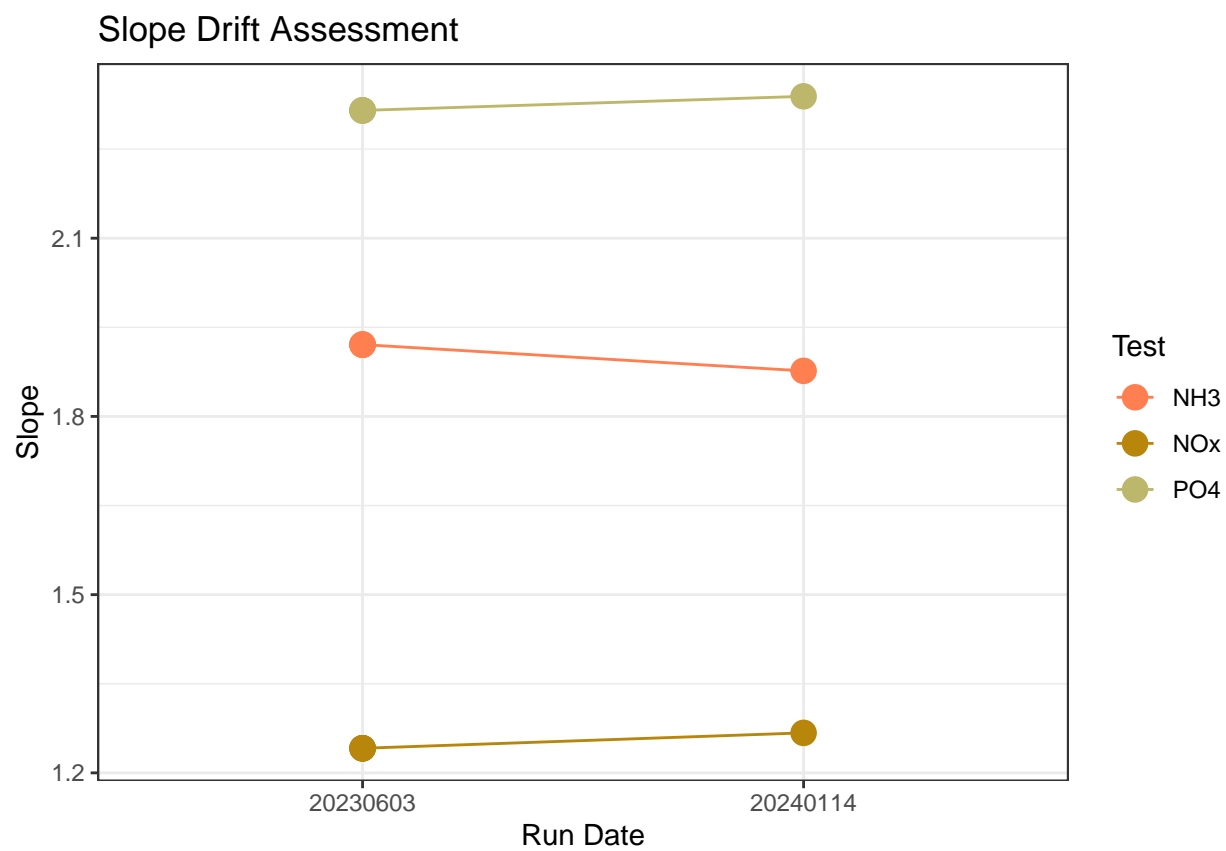

Table 1: Average Slope by Analyte

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: GCW_202308_WC_LysA_45cm, MSM_202308_TR_LysA_20cm, MSM_202308_TR_LysB_20cm, MSM_2C

## 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 = 0.7147915

## Expected  = 0.706

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

## Run mean = 1.421895

## Expected  = 0.948

## [1] "PO4 pe Check has a % Difference <10% - PROCEED"

## Run mean = 0.849674

## Expected  = 0.818
```
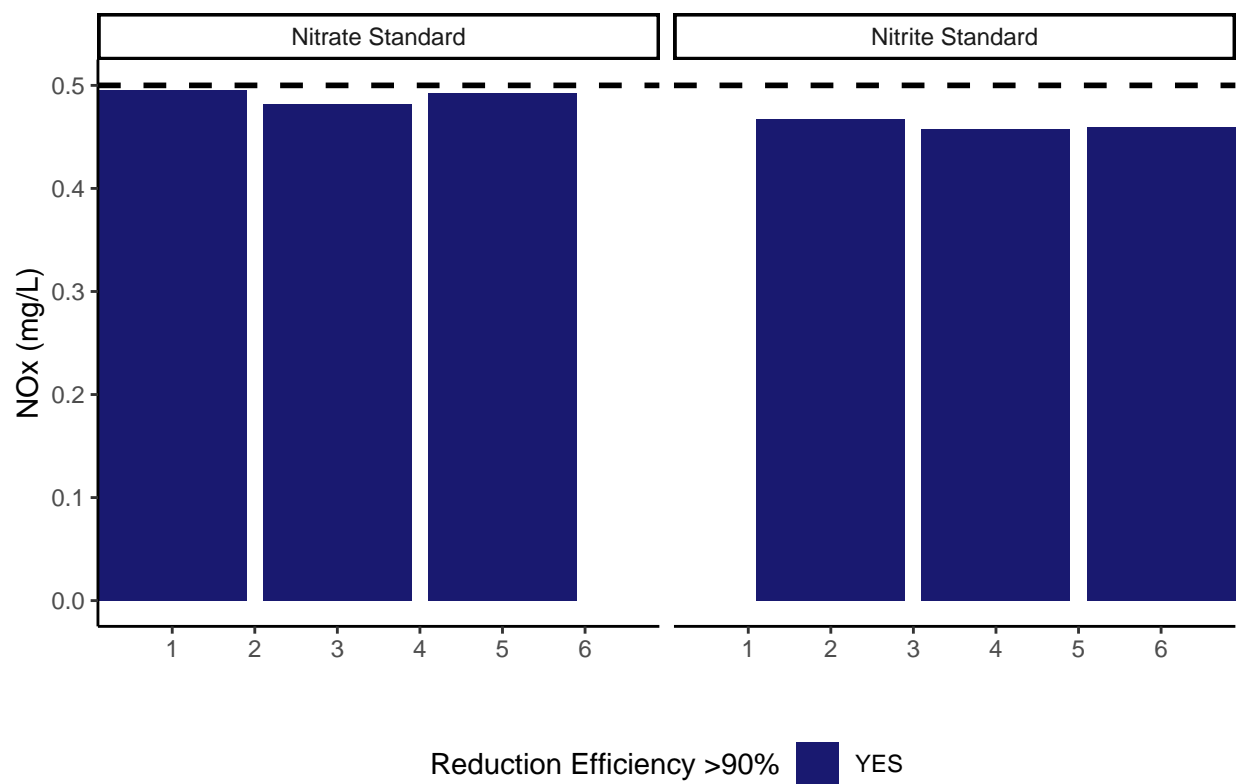
#Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```

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

## [1] 95.1625
```
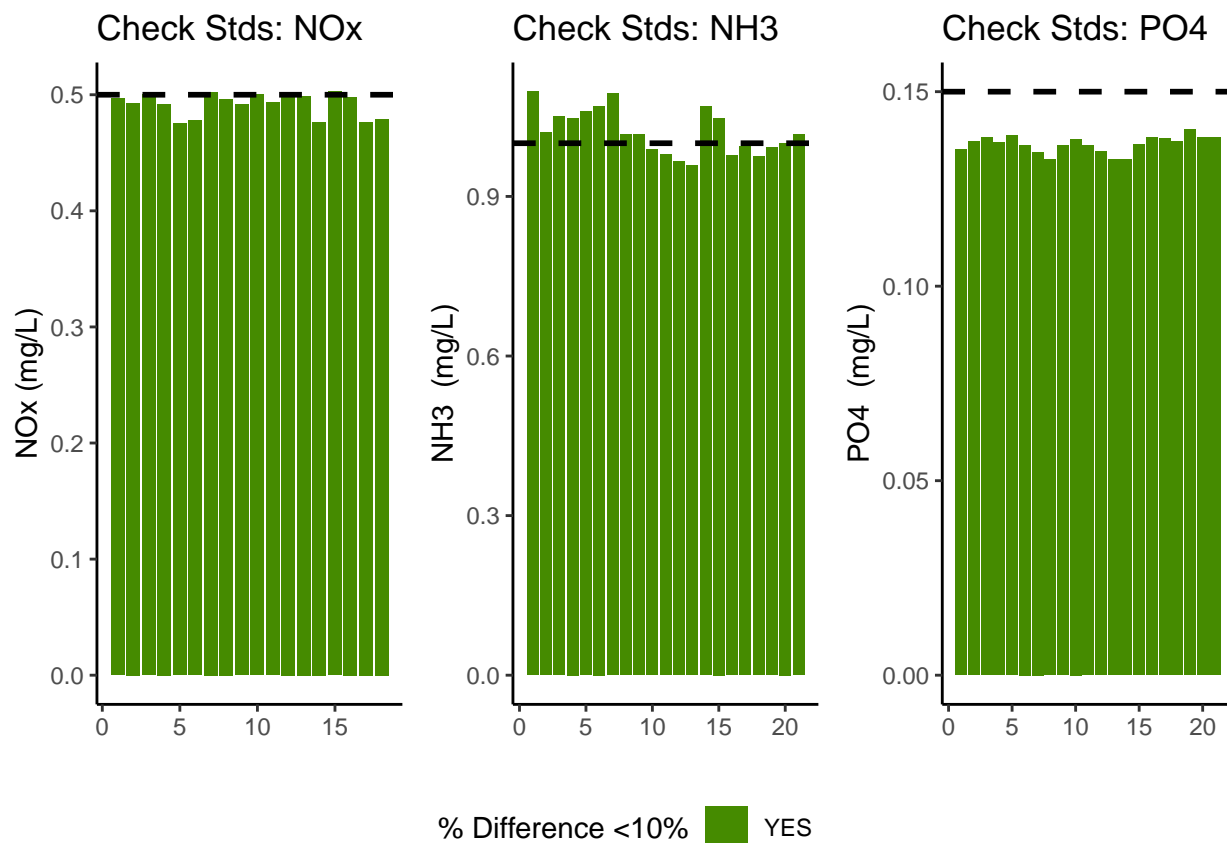
0.5 Analyze the Check Standards

```
## 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 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"
```
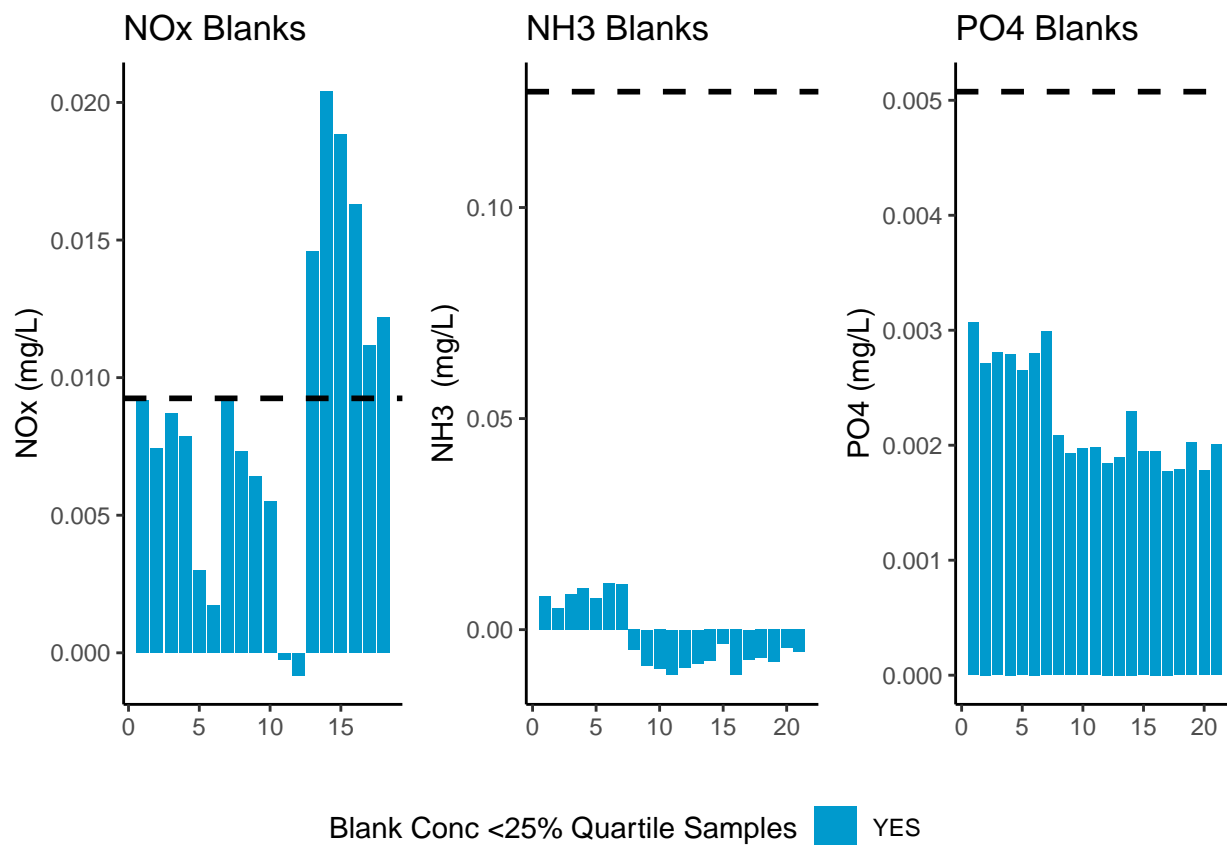

Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0088
NH3	-0.0020
PO4	0.0022

0.7 Analyze Duplicates

```
## Analyze Duplicates

## [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% - 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.
```
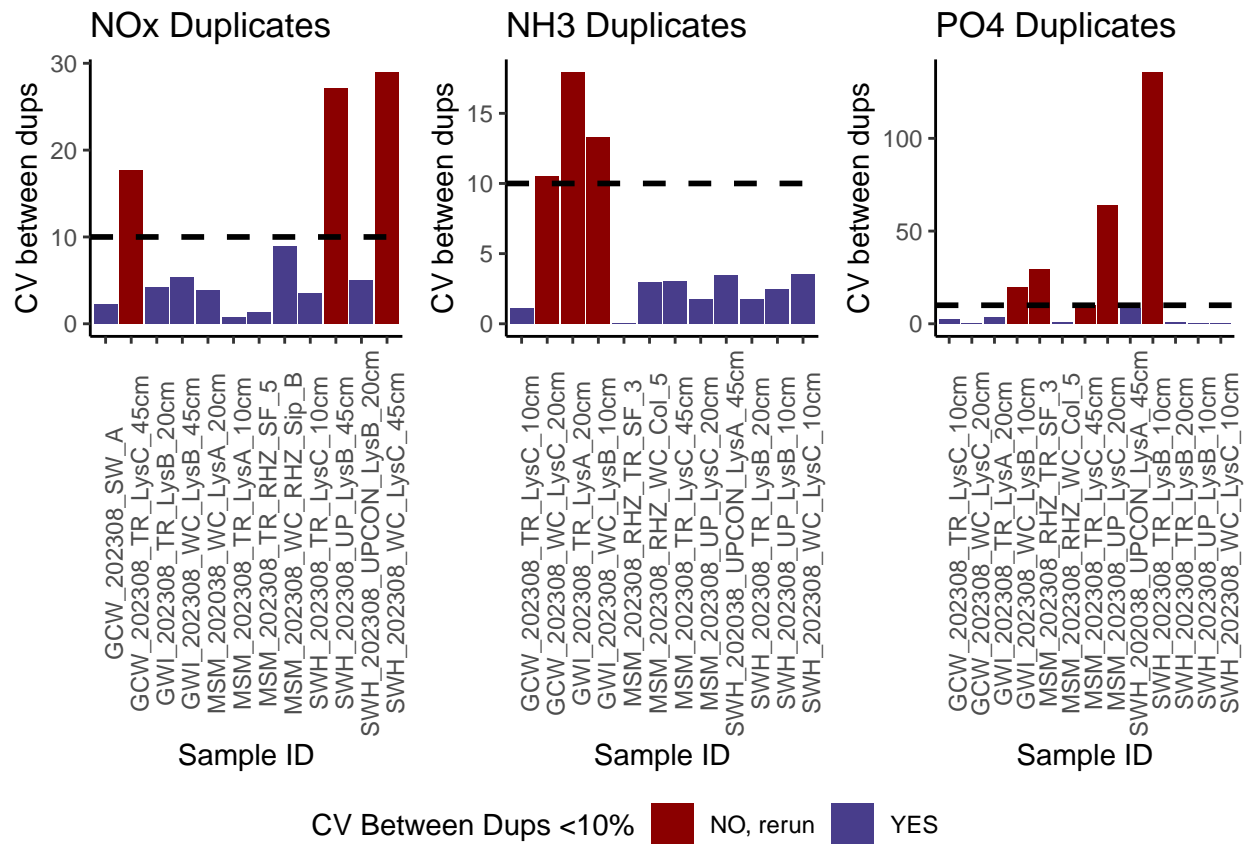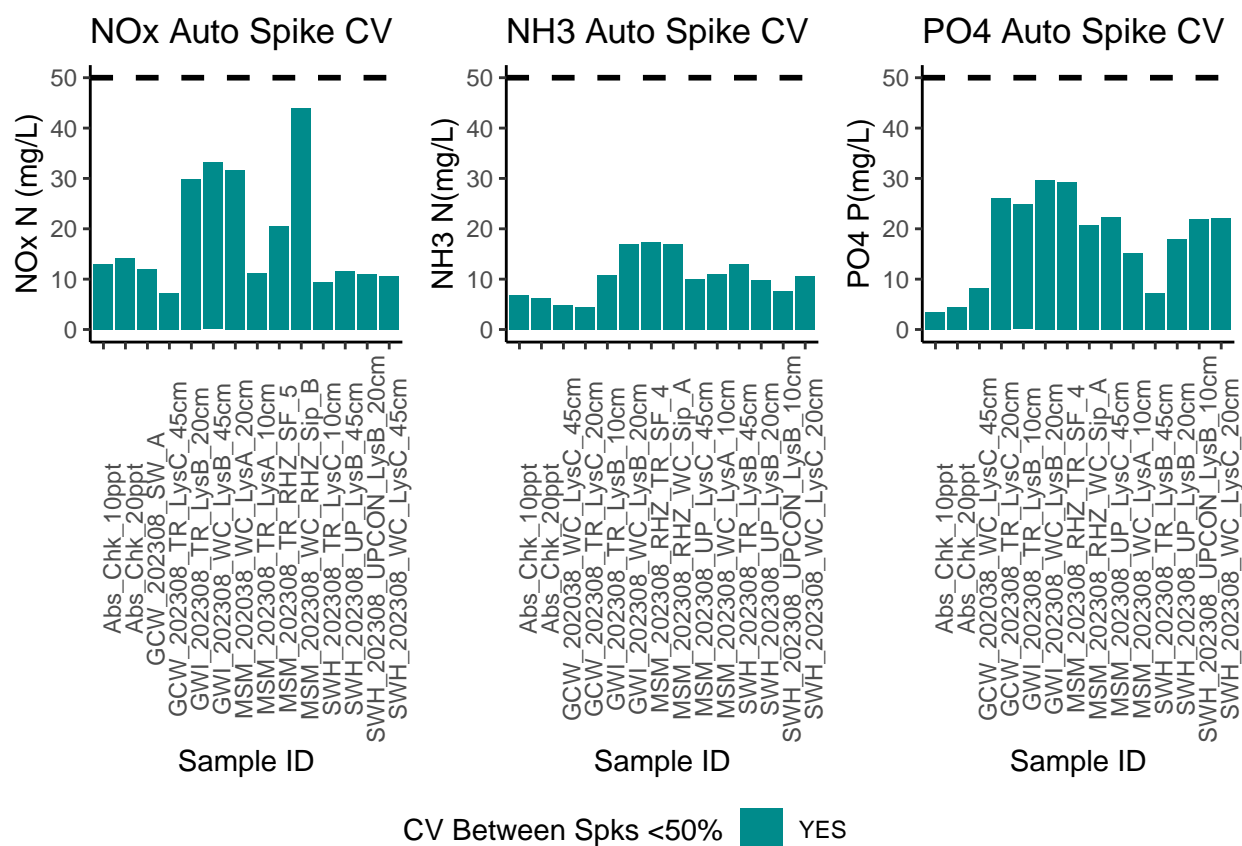
0.8   Spikes

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

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

0.13 Pulling 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.
```
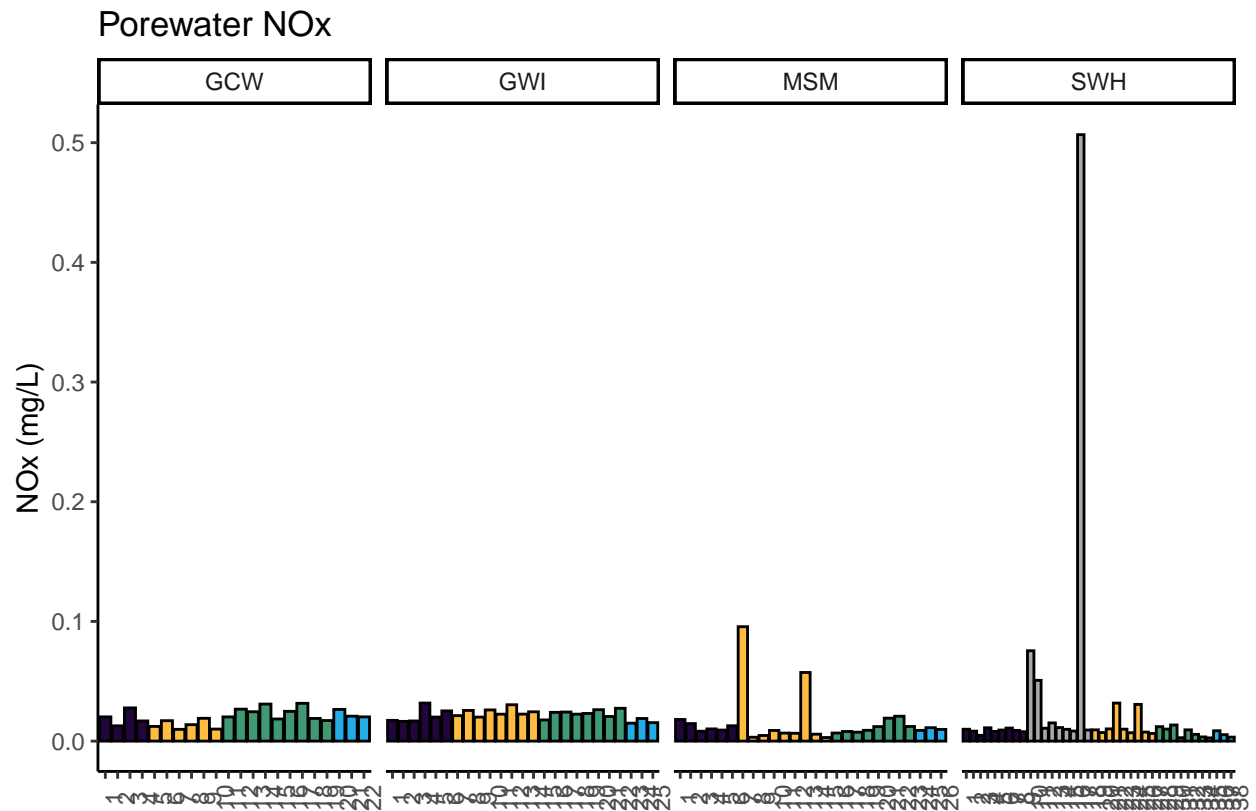
```
##  [1] "GCW_202308_UP_LysA_20cm"    "GCW_202308_UP_LysB_10cm"
##  [3] "GCW_202308_UP_LysB_20cm"    "GCW_202308_UP_LysC_10cm"
##  [5] "MSM_202038_TR_LysB_20cm"    "MSM_202038_WC_LysA_10cm"
##  [7] "MSM_202038_WC_LysA_20cm"    "SWH_202308_UPCON_LysA_10cm"
##  [9] "SWH_202308_UPCON_LysA_20cm" "SWH_202308_UPCON_LysA_45cm"
## [11] "SWH_202308_UPCON_LysB_10cm" "SWH_202308_UPCON_LysB_20cm"
## [13] "SWH_202308_UPCON_LysB_45cm" "SWH_202308_UPCON_LysC_10cm"
## [15] "SWH_202308_UPCON_LysC_20cm" "SWH_202308_UPCON_LysC_45cm"
## [17] "SWH_202308_WC_LysB_20cm"    "SWH_202308_WC_LysC_20cm"
## [19] "GCW_202038_WC_LysB_10cm"    "GCW_202038_WC_LysC_45cm"
## [21] "SWH_202038_UPCON_LysA_45cm"
```

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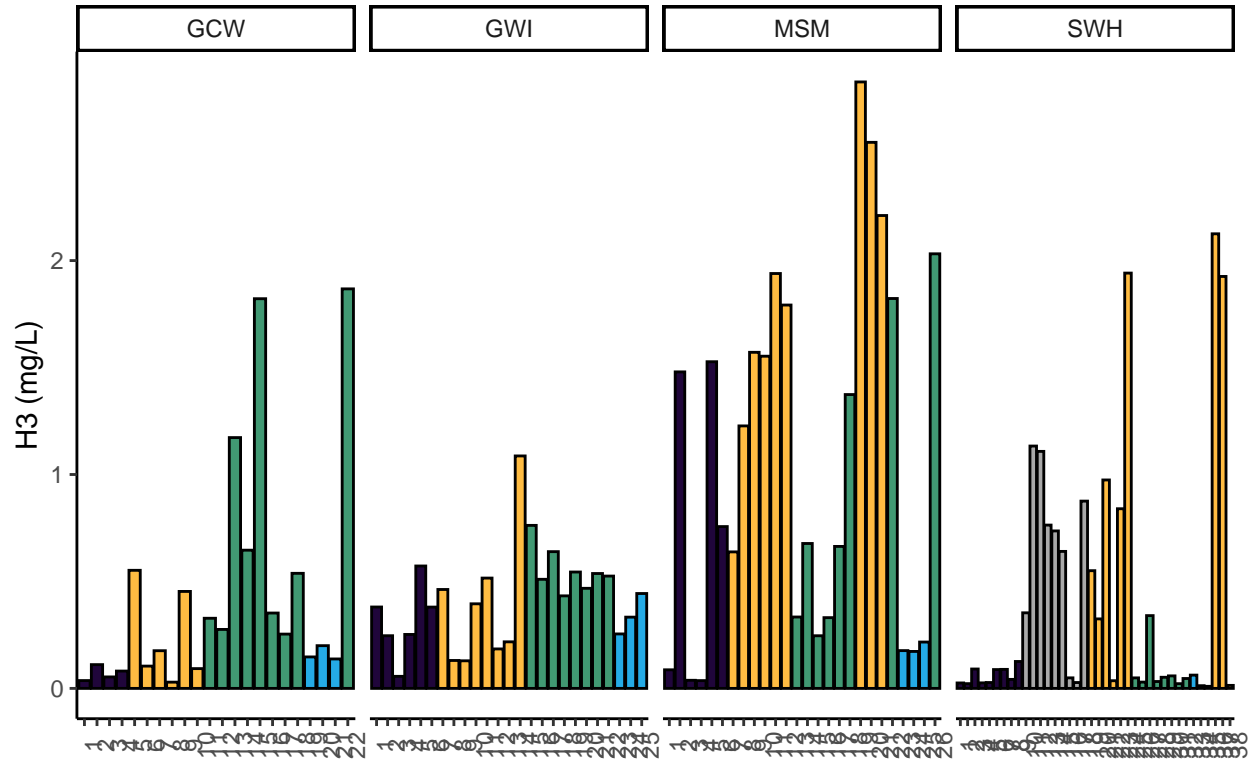
```
## Warning: There was 1 warning in 'mutate()'.
## i In argument: 'Samp_Time = ym(Samp_Time)'.
## Caused by warning:
## !  9 failed to parse.
```
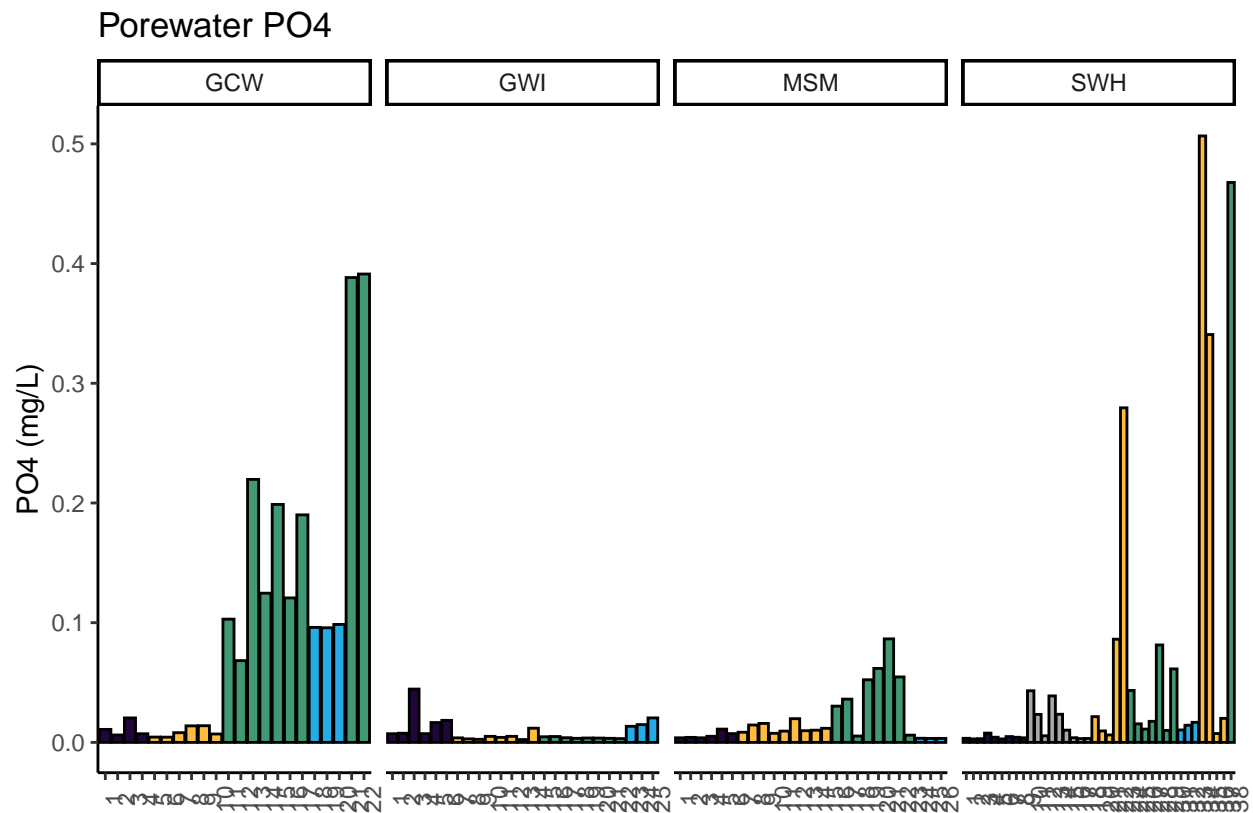
0.15 Visualize Data

```
## Visualize Data
```

Porewater NOx

Porewater NH3

Porewater PO4

0.16 Export Processed Data

#end