# COMPASS_Synoptic_SEAL_Data_Analysis_Nov2022

Stephanie J. Wilson

2023-03-03

## Information

```
##############################################################################################
####### COMPASS Synoptic
####### Chesapeake Bay Sites
####### Data Analysis Code: Porewater Nutrients
####### MONTH: November 2022
##############################################################################################


############################## Information ###################################
#Author: Stephanie J. Wilson
#Edited: 20220727

#Samples taken from Lysimeters & Sippers at CB Synoptic Sites
#Samples were filtered with 0.45 uM, kept on ice, frozen until analysis
#Field Protocol:
#Samples Analyzed on a SEAL discrete auto analyzer
#Lab Protocol: https://docs.google.com/document/d/1VaJT7Wb9AcdmM1tgsR_9ZtQ6kwcaoNmp/edit?usp=sharing&ou
#NOx method = https://drive.google.com/file/d/1sicqBFnzVxmDd5I2_pu8s8pj7iNOAuhF/view?usp=sharing
#NH4 method = https://drive.google.com/file/d/1ENGemUEvm_rffZqv3lz9BjDOpAMX5nzu/view?usp=sharing
#PO4 method = https://drive.google.com/file/d/1m3gXDZnJoIo_QmyhvZG4HRgGShCzm9Wq/view?usp=sharing
#Units from SEAL = mg/L and converted to uMoles/L
```

## QAQC on Slopes

```
library(ggplot2)
```

```
## Warning: package 'ggplot2' was built under R version 4.3.3
```

```
library(data.table)

#read in datafile with all the slopes
qlog <- read.csv("Raw Data/SERC_SEAL_STDs_Log.csv")
head(qlog)
```

```
##       Date             User   Machine Analysis  Slope Intercept     R2
```

```
## 1 20220513 Stephanie Wilson SERC SEAL      NH3 1.9370    -0.030 0.9995
## 2 20220513 Stephanie Wilson SERC SEAL      PO4 2.8690     0.002 0.9994
## 3 20220525 Stephanie Wilson SERC SEAL    V-Nox 1.0000     0.000 0.9990
## 4 20220614 Stephanie Wilson SERC SEAL      NH3 1.1487    -0.011 0.9999
## 5 20220614 Stephanie Wilson SERC SEAL      PO4 2.3950    -0.001 0.9998
## 6 20220615 Stephanie Wilson SERC SEAL    V-Nox 1.0000     0.000 0.9998
##   Nox_Red_Eff X
## 1           NA
## 2           NA
## 3           NA
## 4           NA
## 5           NA
## 6           NA
```

```
#pull out each method
qNH3 <- qlog[qlog$Analysis %like% "NH3", ]
head(qNH3)
```

```
##        Date             User   Machine Analysis  Slope Intercept     R2
## 1  20220513 Stephanie Wilson SERC SEAL      NH3 1.9370    -0.030 0.9995
## 4  20220614 Stephanie Wilson SERC SEAL      NH3 1.1487    -0.011 0.9999
## 7  20220615 Stephanie Wilson SERC SEAL      NH3 1.7070    -0.008 1.0000
## 10 20220718 Stephanie Wilson SERC SEAL      NH3 1.7080    -0.017 0.9995
## 12 20220718 Stephanie Wilson SERC SEAL      NH3 1.6590    -0.017 0.9997
## 14 20220719 Stephanie Wilson SERC SEAL      NH3 1.5560     0.000 0.9994
##    Nox_Red_Eff X
## 1            NA
## 4            NA
## 7            NA
## 10           NA
## 12           NA
## 14           NA
```

```
qPO4 <- qlog[qlog$Analysis %like% "PO4", ]
head(qPO4)
```

```
##        Date             User   Machine Analysis Slope Intercept     R2
## 2  20220513 Stephanie Wilson SERC SEAL      PO4 2.869     0.002 0.9994
## 5  20220614 Stephanie Wilson SERC SEAL      PO4 2.395    -0.001 0.9998
## 8  20220615 Stephanie Wilson SERC SEAL      PO4 2.349     0.000 0.9999
## 11 20220718 Stephanie Wilson SERC SEAL      PO4 2.445    -0.003 0.9993
## 13 20220718 Stephanie Wilson SERC SEAL      PO4 2.349    -0.004 0.9992
## 15 20220719 Stephanie Wilson SERC SEAL      PO4 2.271    -0.003 0.9993
##    Nox_Red_Eff X
## 2            NA
## 5            NA
## 8            NA
## 11           NA
## 13           NA
## 15           NA
```

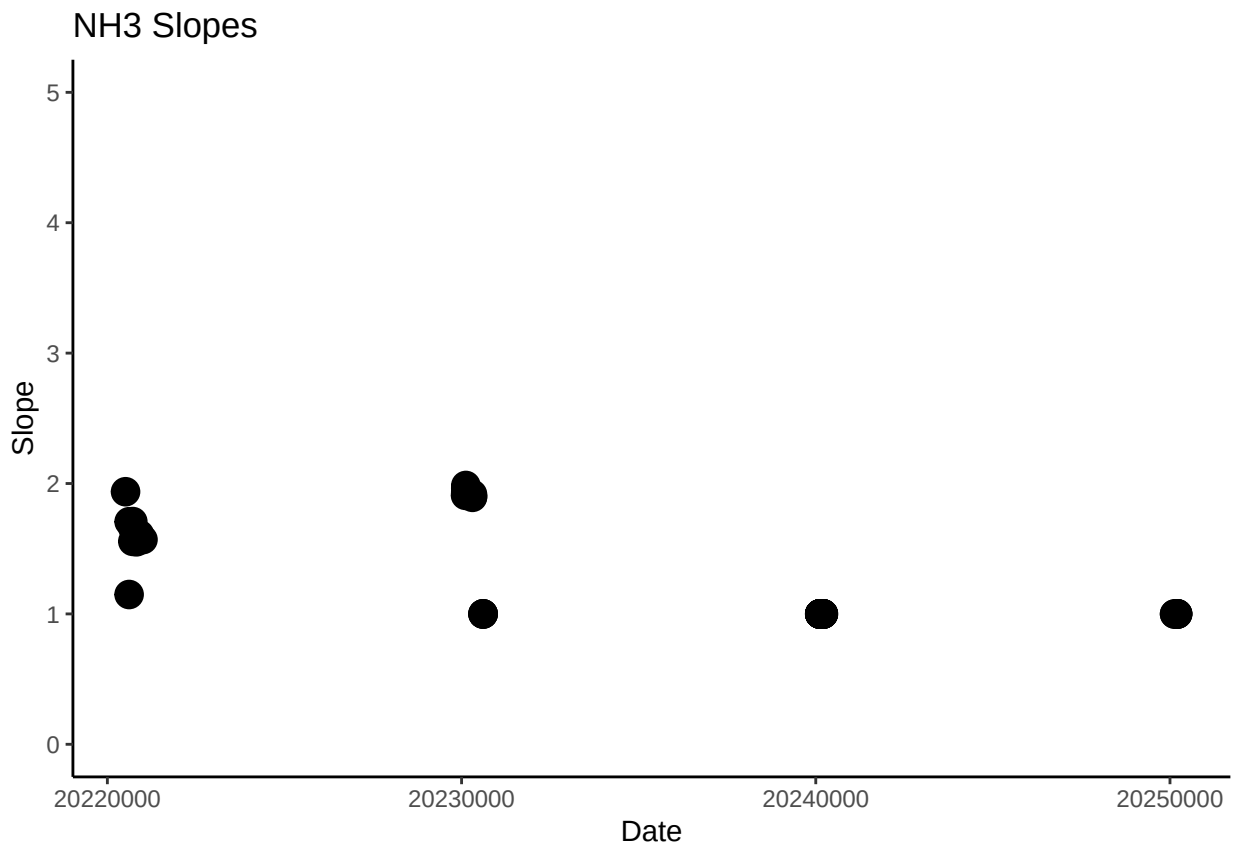
```
qNOx <- qlog[qlog$Analysis %like% "V-Nox", ]
head(qNOx)
```

```
##        Date             User   Machine Analysis Slope Intercept     R2
## 3  20220525 Stephanie Wilson SERC SEAL    V-Nox     1         0 0.9990
## 6  20220615 Stephanie Wilson SERC SEAL    V-Nox     1         0 0.9998
## 9  20220718 Stephanie Wilson SERC SEAL    V-Nox     1         0 0.9999
## 16 20220730 Stephanie Wilson SERC SEAL    V-Nox     1         0 1.0000
## 17 20220731 Stephanie Wilson SERC SEAL    V-Nox     1         0 1.0000
## 22 20220824 Stephanie Wilson SERC SEAL    V-Nox     1         0 0.9988
##    Nox_Red_Eff X
## 3           NA
## 6           NA
## 9           NA
## 16          NA
## 17          NA
## 22          NA
```

```
########### NH3
#plot the slopes to make sure there are no crazy outliers
slope1 <- ggplot(data=qNH3, aes(x=Date, y=Slope)) +
           #geom_line()+
            geom_point(aes(size=3)) +
            theme_classic() + ylim(0, 5) +
           theme(legend.position="none") +
           ggtitle("NH3 Slopes")

slope1
```

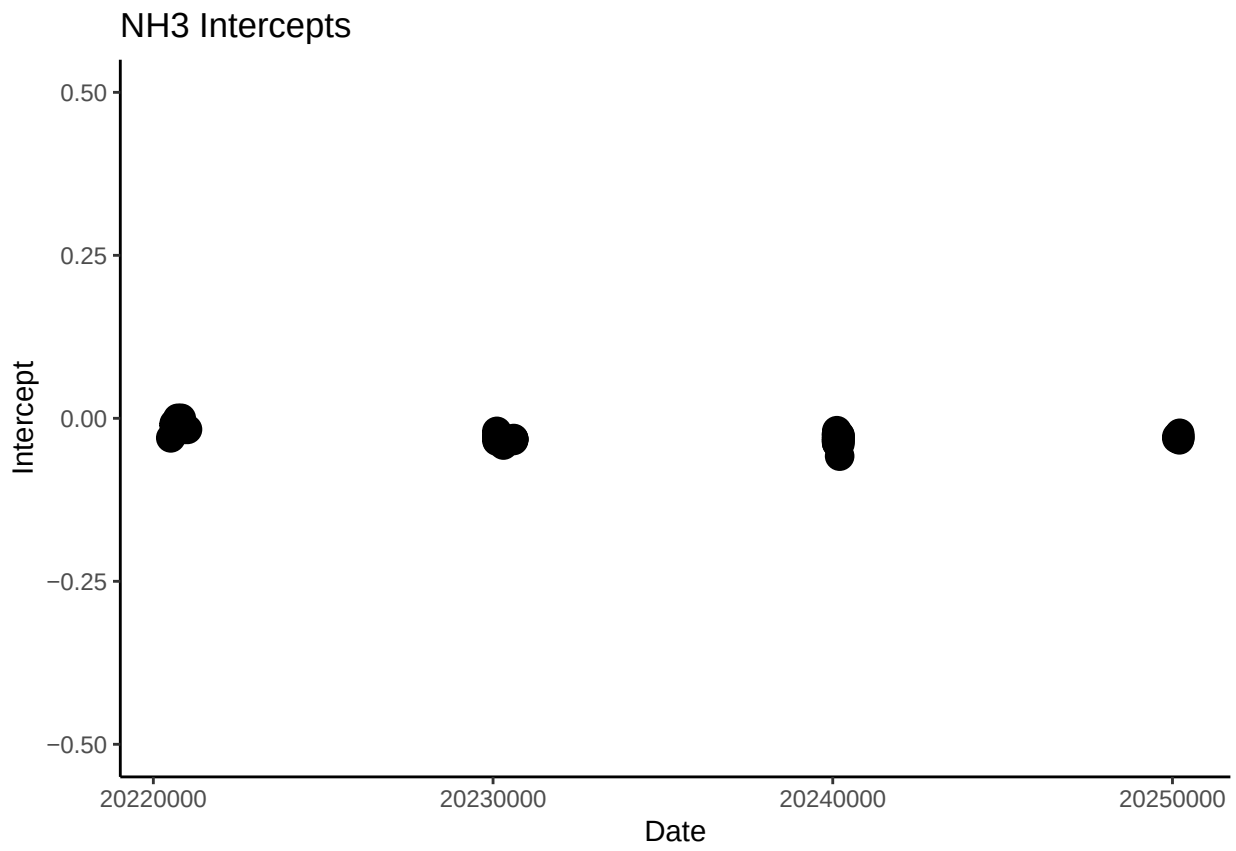
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#plot the intercepts to make sure there are no crazy outliers
int1 <- ggplot(data=qNH3, aes(x=Date, y=Intercept)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(-0.5,0.5) +
  theme(legend.position="none")+
  ggtitle("NH3 Intercepts")

int1
```

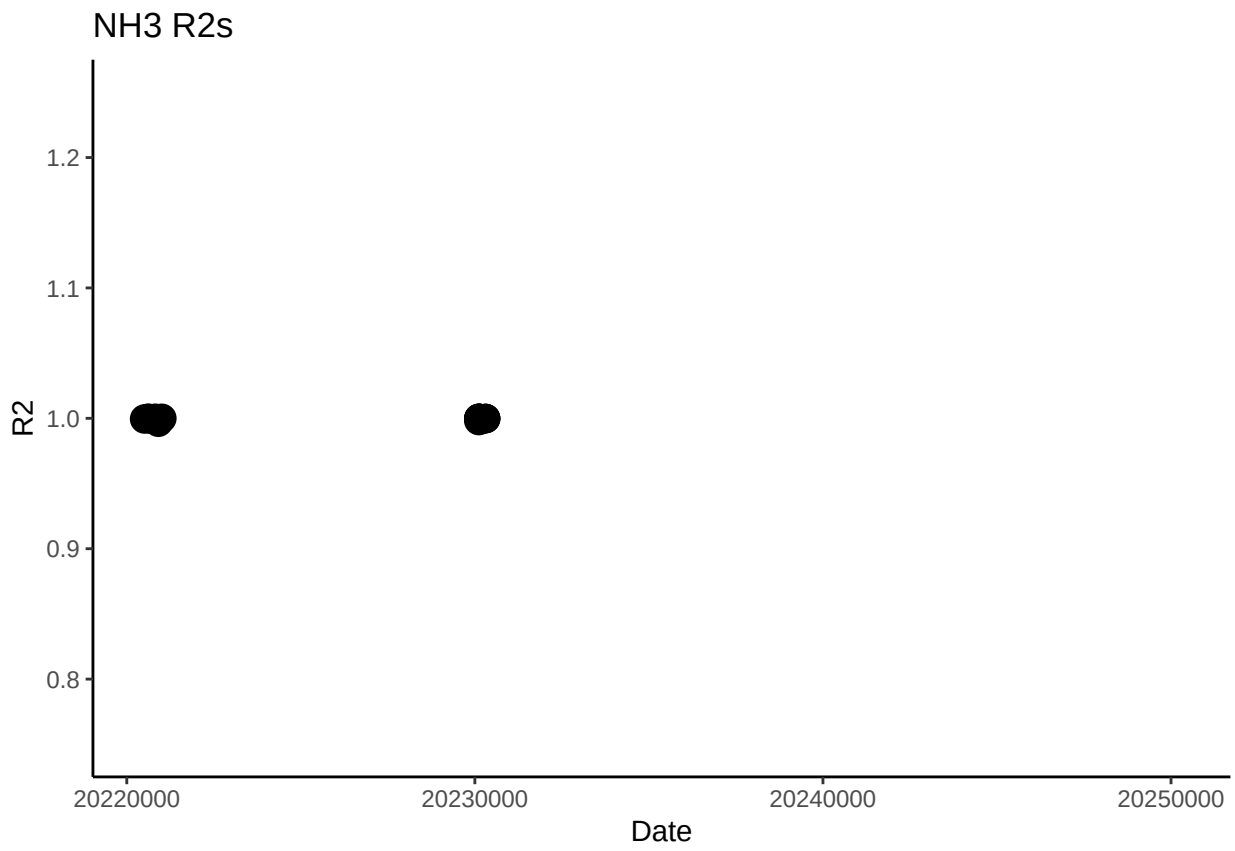
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#plot the R2s to make sure there are no crazy outliers
Rsq1 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NH3 R2s")

Rsq1
```

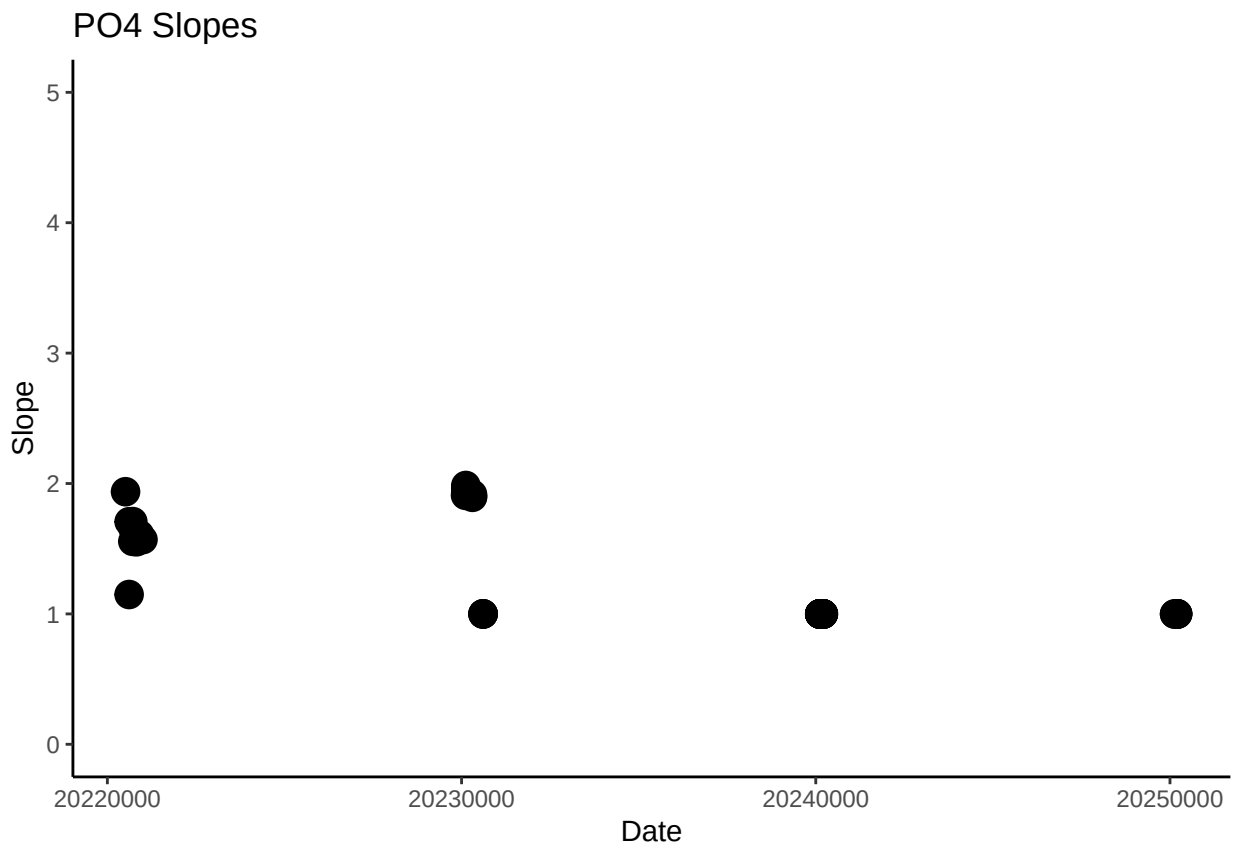
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




```
########### PO4
slope2 <- ggplot(data=qNH3, aes(x=Date, y=Slope)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0, 5) +
  theme(legend.position="none")+
  ggtitle("PO4 Slopes")

slope2
```

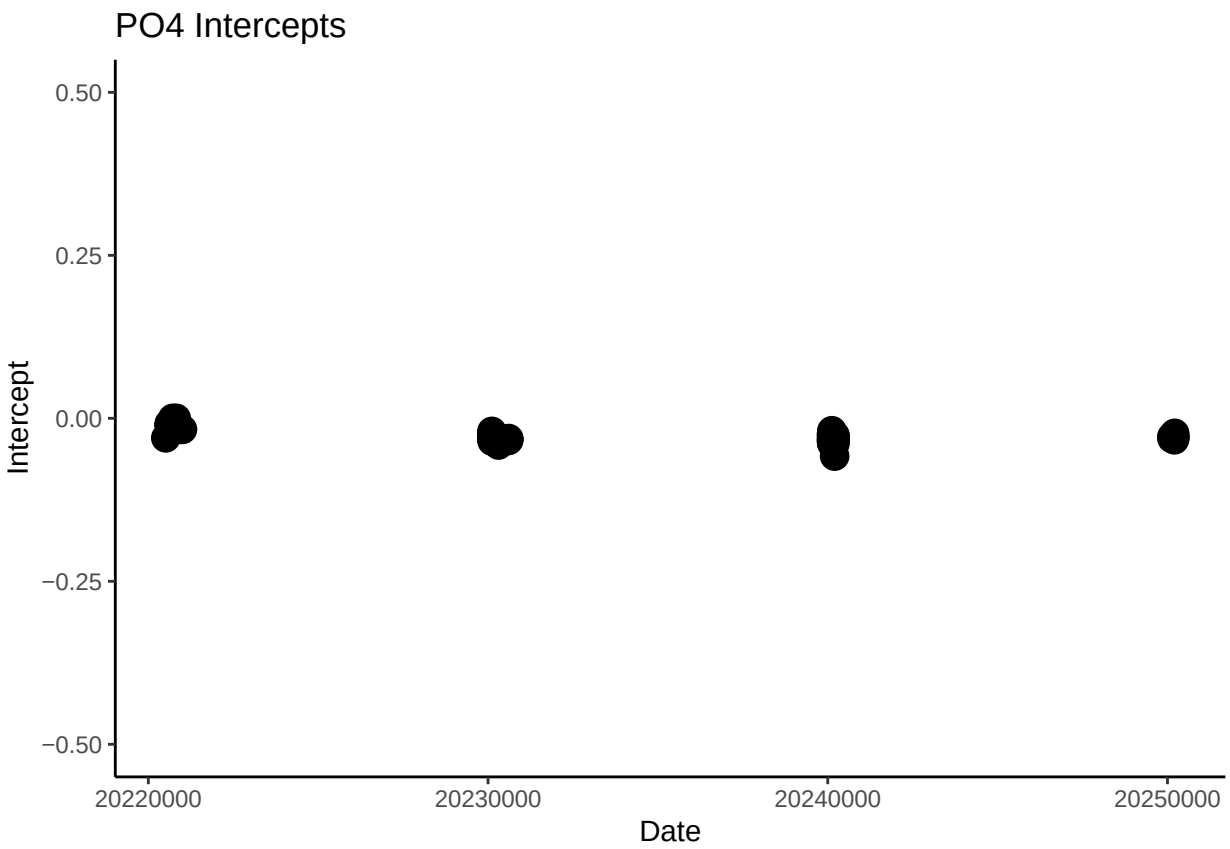
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#plot the intercepts to make sure there are no crazy outliers
int2 <- ggplot(data=qNH3, aes(x=Date, y=Intercept)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(-0.5,0.5) +
  theme(legend.position="none")+
  ggtitle("PO4 Intercepts")

int2
```

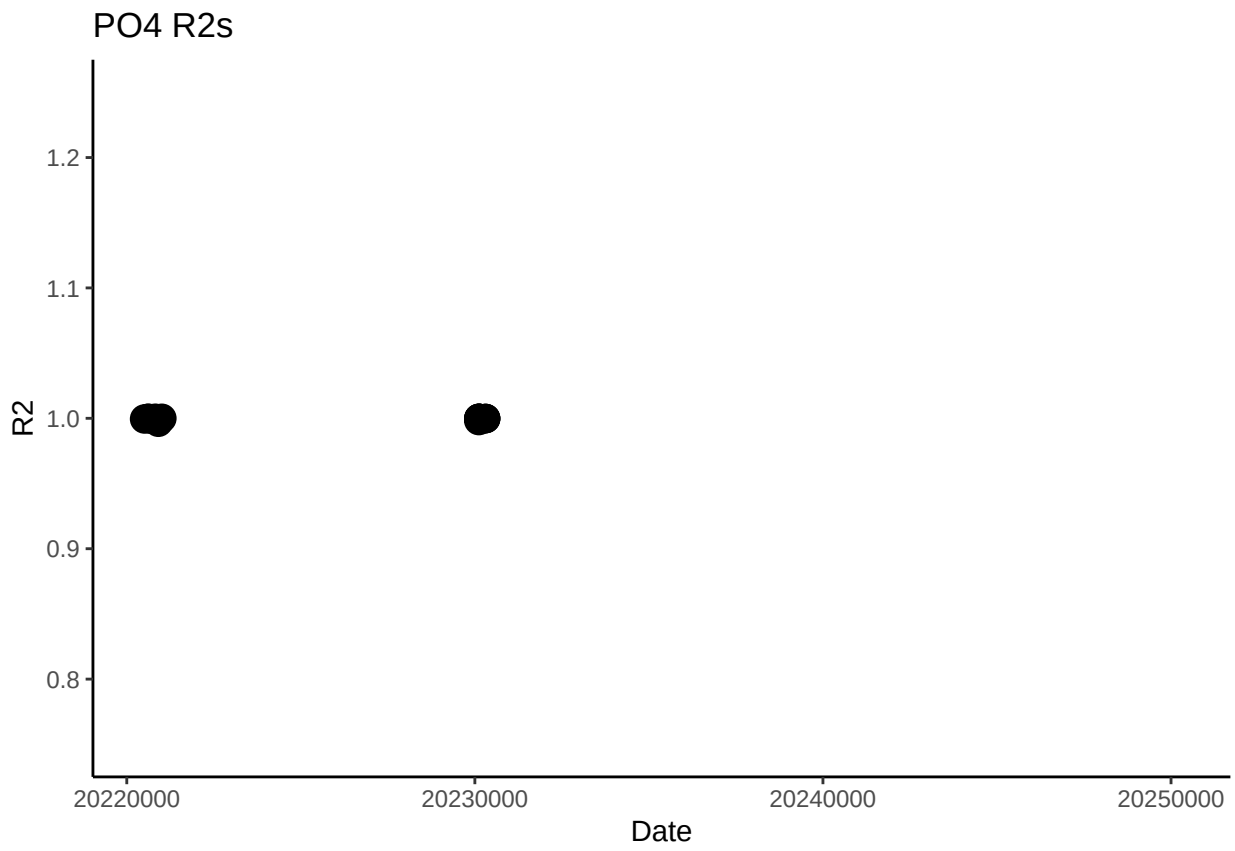
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




```
#plot the R2s to make sure there are no crazy outliers
Rsq2 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("PO4 R2s")

Rsq2
```

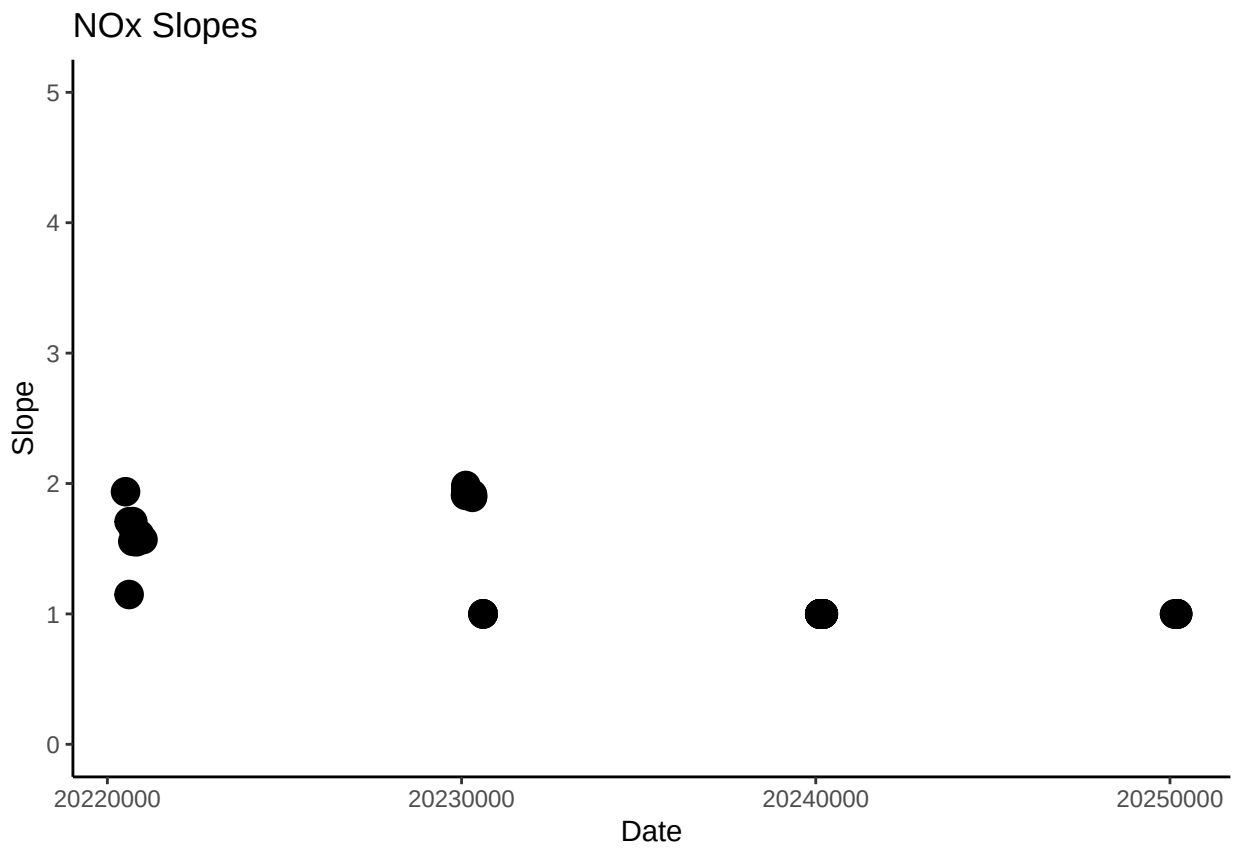
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




```
########### NOx
slope3 <- ggplot(data=qNH3, aes(x=Date, y=Slope)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0, 5) +
  theme(legend.position="none")+
  ggtitle("NOx Slopes")

slope3
```

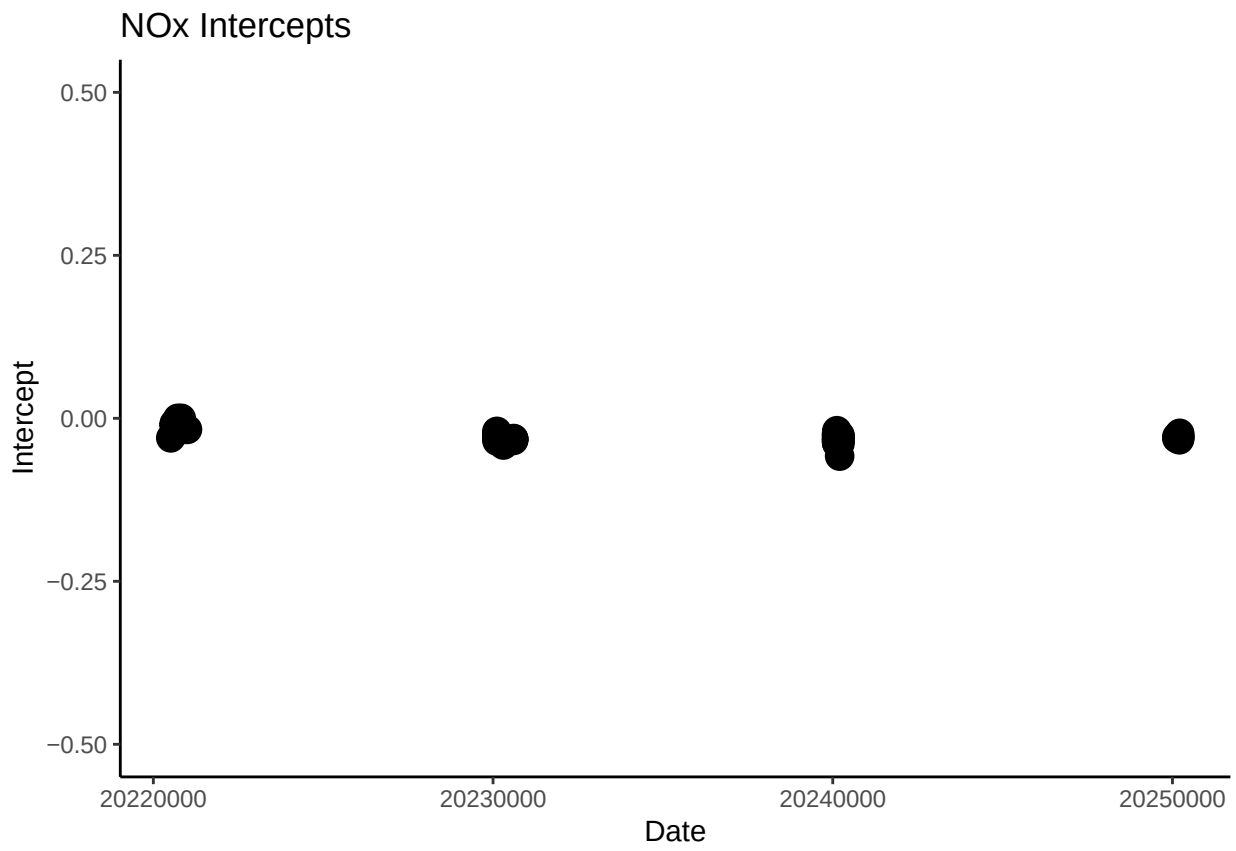
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#plot the intercepts to make sure there are no crazy outliers
int3 <- ggplot(data=qNH3, aes(x=Date, y=Intercept)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(-0.5,0.5) +
  theme(legend.position="none")+
  ggtitle("NOx Intercepts")

int3
```

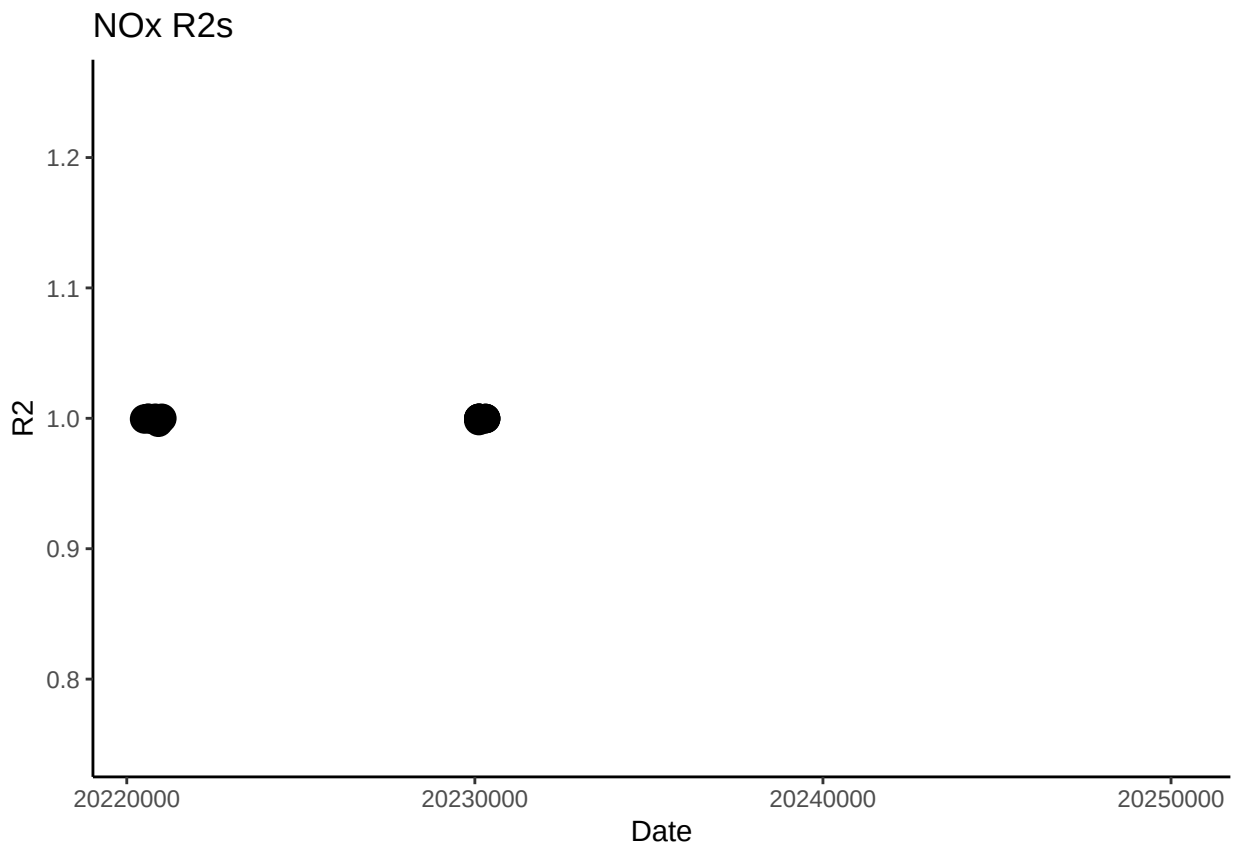
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




```
#plot the R2s to make sure there are no crazy outliers
Rsq3 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NOx R2s")

Rsq3
```

```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




### Code Set up

```
#packages:
library(ggplot2)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:data.table':
##
##     between, first, last

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(data.table)
library(matrixStats)
```

```
##
## Attaching package: 'matrixStats'
```

```
## The following object is masked from 'package:dplyr':
##
##     count
```

```
library(gridExtra)
```

```
##
## Attaching package: 'gridExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

```
library(ggpubr)
library(grid)
```

## Ammonia & Phosphate

```
#read in data
file1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202211_1.csv")
#Quick look at dataframe
head(file1)
```

```
##   RUNSTARTED X1674613599 X1.24.2023.21.26               X X.1      X.2      X.3
## 1     RESULT          -1               S1      Standard 1   0 0.015429 0.015429
## 2     RESULT          -2              S90  Standard .0389   1 0.033415 0.033415
## 3     RESULT          -2              S91  Standard .1000   2 0.064157 0.064157
## 4     RESULT          -2              S92  Standard .2000   3 0.116454 0.116454
## 5     RESULT          -2              S93  Standard .5000   4 0.269354 0.269354
## 6     RESULT          -2              S94 Standard 1.0000   5 0.543635 0.543635
##   X.4 X.5 X.6 X.7    X.8       X.9       X.10            X.11
## 1   0   0   0   0 mg N/L Ammonia 2 1674614837 1/24/2023 21:47
## 2   0   0   0   0 mg N/L Ammonia 2 1674614997 1/24/2023 21:49
## 3   0   0   0   0 mg N/L Ammonia 2 1674615157 1/24/2023 21:52
## 4   0   0   0   0 mg N/L Ammonia 2 1674615317 1/24/2023 21:55
## 5   0   0   0   0 mg N/L Ammonia 2 1674615477 1/24/2023 21:57
## 6   0   0   0   0 mg N/L Ammonia 2 1674615637 1/24/2023 22:00
```

```
#take out only the columns that we need
dat1 <- file1[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(dat1) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(dat1)
```

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.015429 0.015429 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.033415 0.033415 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.064157 0.064157 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.116454 0.116454 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.269354 0.269354 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.543635 0.543635 mg N/L Ammonia 2
```

```
#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202211_2.csv")
#Quick look at dataframe
head(file2)
```

```
##   RUNSTARTED X1678309436 X3.8.2023.16.03              X X.1      X.2      X.3
## 1     RESULT          -1              S1      Standard 1   0 0.016375 0.016375
## 2     RESULT          -2             S90  Standard .0389   1 0.036699 0.036699
## 3     RESULT          -2             S91  Standard .1000   2 0.068606 0.068606
## 4     RESULT          -2             S92  Standard .2000   3 0.120013 0.120013
## 5     RESULT          -2             S93  Standard .5000   4 0.278184 0.278184
## 6     RESULT          -2             S94 Standard 1.0000   5 0.562585 0.562585
##   X.4 X.5 X.6 X.7    X.8       X.9       X.10           X.11
## 1   0   0   0   0 mg N/L Ammonia 2 1678310875 3/8/2023 16:27
## 2   0   0   0   0 mg N/L Ammonia 2 1678311035 3/8/2023 16:30
## 3   0   0   0   0 mg N/L Ammonia 2 1678311195 3/8/2023 16:33
## 4   0   0   0   0 mg N/L Ammonia 2 1678311355 3/8/2023 16:35
## 5   0   0   0   0 mg N/L Ammonia 2 1678311515 3/8/2023 16:38
## 6   0   0   0   0 mg N/L Ammonia 2 1678311675 3/8/2023 16:41
```

```
#take out only the columns that we need
dat2 <- file2[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(dat2) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(dat2)
```

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.016375 0.016375 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.036699 0.036699 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.068606 0.068606 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.120013 0.120013 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.278184 0.278184 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.562585 0.562585 mg N/L Ammonia 2
```

```
#read in data
file3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202211_3.csv")
#Quick look at dataframe
head(file3)
```

```
##   RUNSTARTED X1678489492 X3.10.2023.18.04              X X.1      X.2      X.3
## 1     RESULT          -1              S1      Standard 1   0 0.014728 0.014728
## 2     RESULT          -2             S90  Standard .0389   1 0.035661 0.035661
## 3     RESULT          -2             S91  Standard .1000   2 0.068901 0.068901
## 4     RESULT          -2             S92  Standard .2000   3 0.121012 0.121012
```

```
## 5     RESULT          -2              S93  Standard .5000   4 0.281470 0.281470
## 6     RESULT          -2              S94 Standard 1.0000   5 0.557471 0.557471
##   X.4 X.5 X.6 X.7    X.8       X.9       X.10            X.11
## 1   0   0   0   0 mg N/L Ammonia 2 1678490736 3/10/2023 18:25
## 2   0   0   0   0 mg N/L Ammonia 2 1678490896 3/10/2023 18:28
## 3   0   0   0   0 mg N/L Ammonia 2 1678491056 3/10/2023 18:30
## 4   0   0   0   0 mg N/L Ammonia 2 1678491216 3/10/2023 18:33
## 5   0   0   0   0 mg N/L Ammonia 2 1678491376 3/10/2023 18:36
## 6   0   0   0   0 mg N/L Ammonia 2 1678491536 3/10/2023 18:38
```

```
#take out only the columns that we need
dat3 <- file3[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(dat3) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(dat3)
```

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.014728 0.014728 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.035661 0.035661 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.068901 0.068901 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.121012 0.121012 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.281470 0.281470 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.557471 0.557471 mg N/L Ammonia 2
```

```
alldat <- rbind(dat1, dat2, dat3)

#Pull out standards
stds <- alldat[alldat$Sample_Name %like% "Standard", ]
head(stds)
```

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.015429 0.015429 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.033415 0.033415 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.064157 0.064157 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.116454 0.116454 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.269354 0.269354 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.543635 0.543635 mg N/L Ammonia 2
```

```
#Pull out samples
alldat2 <- alldat[alldat$Sample_Name %like% "MSM_", ]
alldat2 <- rbind(alldat2, (alldat[alldat$Sample_Name %like% "GWI_", ]))
alldat2 <- rbind(alldat2, (alldat[alldat$Sample_Name %like% "GCrew_", ]))
head(alldat2)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units      Test
## 329   RESULT MSM_202211_UP_LysA_10cm 1.075965 0.585600 mg N/L Ammonia 2
## 330   RESULT MSM_202211_UP_LysA_20cm 1.957322 1.050864 mg N/L Ammonia 2
## 331   RESULT MSM_202211_UP_LysB_10cm 0.093142 0.066772 mg N/L Ammonia 2
## 338   RESULT MSM_202211_UP_LysB_20cm 0.376242 0.216219 mg N/L Ammonia 2
## 339   RESULT MSM_202211_UP_LysB_45cm 0.820627 0.450808 mg N/L Ammonia 2
## 340   RESULT MSM_202211_UP_LysC_10cm 0.525043 0.294770 mg N/L Ammonia 2
```

## NOx

```
#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202211_1.csv")
#Quick look at dataframe
head(Nfile1)
```

```
##   RUNSTARTED X1678209572 X3.7.2023.12.19           X X.1      X.2      X.3 X.4
## 1   RUNENDED  1678209575    PORT FAILURE              NA       NA       NA  NA
## 2 RUNSTARTED  1678209656  3/7/2023 12:20              NA       NA       NA  NA
## 3   RUNENDED  1678209658    PORT FAILURE              NA       NA       NA  NA
## 4 RUNSTARTED  1678283381   3/8/2023 8:49              NA       NA       NA  NA
## 5     RESULT          -1              S1  Standard 1   0 0.143925 0.143925   0
## 6     RESULT          -2             S90 Standard 90   1 0.162245 0.162245   0
##   X.5 X.6 X.7    X.8          X.9       X.10          X.11
## 1  NA  NA  NA                            NA
## 2  NA  NA  NA                            NA
## 3  NA  NA  NA                            NA
## 4  NA  NA  NA                            NA
## 5   0   0 512 mg N/L Vanadium NOx 1678285643 3/8/2023 9:27
## 6   0   0 512 mg N/L Vanadium NOx 1678285722 3/8/2023 9:28
```

```
#take out only the columns that we need
Ndat1 <- Nfile1[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(Ndat1) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat1)
```

```
##     Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RUNENDED                   NA       NA
## 2 RUNSTARTED                   NA       NA
## 3   RUNENDED                   NA       NA
## 4 RUNSTARTED                   NA       NA
## 5     RESULT  Standard 1 0.143925 0.143925 mg N/L Vanadium NOx
## 6     RESULT Standard 90 0.162245 0.162245 mg N/L Vanadium NOx
```

```
#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202211_2.csv")
#Quick look at dataframe
head(Nfile2)
```

```
##   RUNSTARTED X1678294819 X3.8.2023.12.00           X X.1      X.2      X.3 X.4
## 1     RESULT          -1              S1  Standard 1   0 0.158514 0.158514   0
## 2     RESULT          -2             S90 Standard 90   1 0.178012 0.178012   0
## 3     RESULT          -2             S91 Standard 91   2 0.201762 0.201762   0
## 4     RESULT          -2             S92 Standard 92   3 0.240047 0.240047   0
## 5     RESULT          -2             S93 Standard 93   4 0.358828 0.358828   0
## 6     RESULT          -2             S94 Standard 94   5 0.564456 0.564456   0
##   X.5 X.6 X.7    X.8          X.9       X.10          X.11
## 1   0   0   0 mg N/L Vanadium NOx 1678297042 3/8/2023 12:37
## 2   0   0   0 mg N/L Vanadium NOx 1678297121 3/8/2023 12:38
```

```
## 3   0   0   0 mg N/L Vanadium NOx 1678297202 3/8/2023 12:40
## 4   0   0   0 mg N/L Vanadium NOx 1678297281 3/8/2023 12:41
## 5   0   0   0 mg N/L Vanadium NOx 1678297362 3/8/2023 12:42
## 6   0   0   0 mg N/L Vanadium NOx 1678297441 3/8/2023 12:44
```

```
#take out only the columns that we need
Ndat2 <- Nfile2[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(Ndat2) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat2)
```

```
##   Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RESULT  Standard 1 0.158514 0.158514 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.178012 0.178012 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.201762 0.201762 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.240047 0.240047 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.358828 0.358828 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.564456 0.564456 mg N/L Vanadium NOx
```

```
#read in data
Nfile3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202211_3.csv")
#Quick look at dataframe
head(Nfile3)
```

```
##   RUNSTARTED X1678563859     X3.11.2023.14.44           X X.1      X.2      X.3
## 1   RUNENDED  1678563962 INSUFFICIENT REAGENT              NA       NA       NA
## 2 RUNSTARTED  1678565094      3/11/2023 15:04              NA       NA       NA
## 3     RESULT          -1                  S1  Standard 1   0 0.152308 0.152308
## 4     RESULT          -2                 S90 Standard 90   1 0.169833 0.169833
## 5     RESULT          -2                 S91 Standard 91   2 0.194393 0.194393
## 6     RESULT          -2                 S92 Standard 92   3 0.234361 0.234361
##   X.4 X.5 X.6 X.7    X.8          X.9       X.10            X.11
## 1  NA  NA  NA  NA                            NA
## 2  NA  NA  NA  NA                            NA
## 3   0   0   0 512 mg N/L Vanadium NOx 1678567272 3/11/2023 15:41
## 4   0   0   0 512 mg N/L Vanadium NOx 1678567351 3/11/2023 15:42
## 5   0   0   0 512 mg N/L Vanadium NOx 1678567432 3/11/2023 15:43
## 6   0   0   0 512 mg N/L Vanadium NOx 1678567511 3/11/2023 15:45
```

```
#take out only the columns that we need
Ndat3 <- Nfile3[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(Ndat3) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat3)
```

```
##     Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RUNENDED                   NA       NA
## 2 RUNSTARTED                   NA       NA
## 3     RESULT  Standard 1 0.152308 0.152308 mg N/L Vanadium NOx
## 4     RESULT Standard 90 0.169833 0.169833 mg N/L Vanadium NOx
## 5     RESULT Standard 91 0.194393 0.194393 mg N/L Vanadium NOx
## 6     RESULT Standard 92 0.234361 0.234361 mg N/L Vanadium NOx
```

```
Nalldat <- rbind(Ndat1, Ndat2, Ndat3)

#Pull out standards
Nstds <- Nalldat[Nalldat$Sample_Name %like% "Standard", ]
head(Nstds)
```

```
##    Run_Info Sample_Name     Conc      Abs  Units         Test
## 5    RESULT  Standard 1 0.143925 0.143925 mg N/L Vanadium NOx
## 6    RESULT Standard 90 0.162245 0.162245 mg N/L Vanadium NOx
## 7    RESULT Standard 91 0.186309 0.186309 mg N/L Vanadium NOx
## 8    RESULT Standard 92 0.225373 0.225373 mg N/L Vanadium NOx
## 9    RESULT Standard 93 0.345693 0.345693 mg N/L Vanadium NOx
## 10   RESULT Standard 94 0.533363 0.533363 mg N/L Vanadium NOx
```

```
#Pull out samples
Nalldat2 <- Nalldat[Nalldat$Sample_Name %like% "MSM_", ]
Nalldat2 <- rbind(Nalldat2, (Nalldat[Nalldat$Sample_Name %like% "GWI_", ]))
Nalldat2 <- rbind(Nalldat2, (Nalldat[Nalldat$Sample_Name %like% "GCrew_", ]))
head(Nalldat2)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units         Test
## 177   RESULT MSM_202211_UP_LysA_10cm 0.011350 0.169269 mg N/L Vanadium NOx
## 184   RESULT MSM_202211_UP_LysA_20cm 0.003121 0.162715 mg N/L Vanadium NOx
## 185   RESULT MSM_202211_UP_LysB_10cm 0.003154 0.162742 mg N/L Vanadium NOx
## 186   RESULT MSM_202211_UP_LysB_20cm 0.004066 0.163468 mg N/L Vanadium NOx
## 187   RESULT MSM_202211_UP_LysB_45cm 0.004513 0.163823 mg N/L Vanadium NOx
## 188   RESULT MSM_202211_UP_LysC_10cm 0.007430 0.166147 mg N/L Vanadium NOx
```

## Constants

```
N_mw <- 14.0067   # molecular weight of N

P_mw <- 30.973762  # molecular weight of P

Con1 <- 1000       # conversion factor value

Con2 <- 1000000    # conversion factor value
```

## Convert Data from mg/L to uM

```
head(alldat2)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units      Test
## 329   RESULT MSM_202211_UP_LysA_10cm 1.075965 0.585600 mg N/L Ammonia 2
## 330   RESULT MSM_202211_UP_LysA_20cm 1.957322 1.050864 mg N/L Ammonia 2
## 331   RESULT MSM_202211_UP_LysB_10cm 0.093142 0.066772 mg N/L Ammonia 2
## 338   RESULT MSM_202211_UP_LysB_20cm 0.376242 0.216219 mg N/L Ammonia 2
## 339   RESULT MSM_202211_UP_LysB_45cm 0.820627 0.450808 mg N/L Ammonia 2
## 340   RESULT MSM_202211_UP_LysC_10cm 0.525043 0.294770 mg N/L Ammonia 2
```

```
head(Nalldat2)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units         Test
## 177   RESULT MSM_202211_UP_LysA_10cm 0.011350 0.169269 mg N/L Vanadium NOx
## 184   RESULT MSM_202211_UP_LysA_20cm 0.003121 0.162715 mg N/L Vanadium NOx
## 185   RESULT MSM_202211_UP_LysB_10cm 0.003154 0.162742 mg N/L Vanadium NOx
## 186   RESULT MSM_202211_UP_LysB_20cm 0.004066 0.163468 mg N/L Vanadium NOx
## 187   RESULT MSM_202211_UP_LysB_45cm 0.004513 0.163823 mg N/L Vanadium NOx
## 188   RESULT MSM_202211_UP_LysC_10cm 0.007430 0.166147 mg N/L Vanadium NOx
```

```
#subset by test
NH4samples <- subset(alldat2, Test == "Ammonia 2")
head(NH4samples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units      Test
## 329   RESULT MSM_202211_UP_LysA_10cm 1.075965 0.585600 mg N/L Ammonia 2
## 330   RESULT MSM_202211_UP_LysA_20cm 1.957322 1.050864 mg N/L Ammonia 2
## 331   RESULT MSM_202211_UP_LysB_10cm 0.093142 0.066772 mg N/L Ammonia 2
## 338   RESULT MSM_202211_UP_LysB_20cm 0.376242 0.216219 mg N/L Ammonia 2
## 339   RESULT MSM_202211_UP_LysB_45cm 0.820627 0.450808 mg N/L Ammonia 2
## 340   RESULT MSM_202211_UP_LysC_10cm 0.525043 0.294770 mg N/L Ammonia 2
```

```
PO4samples <- subset(alldat2, Test == "o-PHOS 0.3")
head(PO4samples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units       Test
## 474   RESULT MSM_202211_UP_LysA_10cm 0.010627 0.005675 mg P/L o-PHOS 0.3
## 475   RESULT MSM_202211_UP_LysA_20cm 0.005352 0.003417 mg P/L o-PHOS 0.3
## 476   RESULT MSM_202211_UP_LysB_10cm 0.001697 0.001852 mg P/L o-PHOS 0.3
## 484   RESULT MSM_202211_UP_LysB_20cm 0.002242 0.002085 mg P/L o-PHOS 0.3
## 485   RESULT MSM_202211_UP_LysB_45cm 0.009756 0.005302 mg P/L o-PHOS 0.3
## 486   RESULT MSM_202211_UP_LysC_10cm 0.002499 0.002195 mg P/L o-PHOS 0.3
```

```
NOXsamples <- subset(Nalldat2, Test == "Vanadium NOx")
head(NOXsamples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units         Test
## 177   RESULT MSM_202211_UP_LysA_10cm 0.011350 0.169269 mg N/L Vanadium NOx
## 184   RESULT MSM_202211_UP_LysA_20cm 0.003121 0.162715 mg N/L Vanadium NOx
## 185   RESULT MSM_202211_UP_LysB_10cm 0.003154 0.162742 mg N/L Vanadium NOx
## 186   RESULT MSM_202211_UP_LysB_20cm 0.004066 0.163468 mg N/L Vanadium NOx
## 187   RESULT MSM_202211_UP_LysB_45cm 0.004513 0.163823 mg N/L Vanadium NOx
## 188   RESULT MSM_202211_UP_LysC_10cm 0.007430 0.166147 mg N/L Vanadium NOx
```

```
NH4samples$Conc_uM <- (((as.numeric(NH4samples$Conc))/Con1)/N_mw)*Con2
head(NH4samples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units      Test
## 329   RESULT MSM_202211_UP_LysA_10cm 1.075965 0.585600 mg N/L Ammonia 2
## 330   RESULT MSM_202211_UP_LysA_20cm 1.957322 1.050864 mg N/L Ammonia 2
```

```
## 331   RESULT MSM_202211_UP_LysB_10cm 0.093142 0.066772 mg N/L Ammonia 2
## 338   RESULT MSM_202211_UP_LysB_20cm 0.376242 0.216219 mg N/L Ammonia 2
## 339   RESULT MSM_202211_UP_LysB_45cm 0.820627 0.450808 mg N/L Ammonia 2
## 340   RESULT MSM_202211_UP_LysC_10cm 0.525043 0.294770 mg N/L Ammonia 2
##        Conc_uM
## 329  76.817880
## 330 139.741838
## 331   6.649818
## 338  26.861573
## 339  58.588176
## 340  37.485132
```

```
PO4samples$Conc_uM <- (((as.numeric(PO4samples$Conc))/Con1)/N_mw)*Con2
head(PO4samples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units       Test
## 474   RESULT MSM_202211_UP_LysA_10cm 0.010627 0.005675 mg P/L o-PHOS 0.3
## 475   RESULT MSM_202211_UP_LysA_20cm 0.005352 0.003417 mg P/L o-PHOS 0.3
## 476   RESULT MSM_202211_UP_LysB_10cm 0.001697 0.001852 mg P/L o-PHOS 0.3
## 484   RESULT MSM_202211_UP_LysB_20cm 0.002242 0.002085 mg P/L o-PHOS 0.3
## 485   RESULT MSM_202211_UP_LysB_45cm 0.009756 0.005302 mg P/L o-PHOS 0.3
## 486   RESULT MSM_202211_UP_LysC_10cm 0.002499 0.002195 mg P/L o-PHOS 0.3
##       Conc_uM
## 474 0.7587083
## 475 0.3821029
## 476 0.1211563
## 484 0.1600663
## 485 0.6965238
## 486 0.1784146
```

```
NOXsamples$Conc_uM_raw <- (((as.numeric(NOXsamples$Conc))/Con1)/N_mw)*Con2
head(NOXsamples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units         Test
## 177   RESULT MSM_202211_UP_LysA_10cm 0.011350 0.169269 mg N/L Vanadium NOx
## 184   RESULT MSM_202211_UP_LysA_20cm 0.003121 0.162715 mg N/L Vanadium NOx
## 185   RESULT MSM_202211_UP_LysB_10cm 0.003154 0.162742 mg N/L Vanadium NOx
## 186   RESULT MSM_202211_UP_LysB_20cm 0.004066 0.163468 mg N/L Vanadium NOx
## 187   RESULT MSM_202211_UP_LysB_45cm 0.004513 0.163823 mg N/L Vanadium NOx
## 188   RESULT MSM_202211_UP_LysC_10cm 0.007430 0.166147 mg N/L Vanadium NOx
##     Conc_uM_raw
## 177   0.8103265
## 184   0.2228219
## 185   0.2251780
## 186   0.2902896
## 187   0.3222029
## 188   0.5304604
```

```
#add step to make negative values equal to bd (below detection) and replace with zeros
NOXsamples$Conc_uM <- ifelse(NOXsamples$Conc_uM_raw<0, 0, (NOXsamples$Conc_uM_raw) )
head(NOXsamples)
```

```
##     Run_Info             Sample_Name     Conc      Abs  Units         Test
## 177   RESULT MSM_202211_UP_LysA_10cm 0.011350 0.169269 mg N/L Vanadium NOx
## 184   RESULT MSM_202211_UP_LysA_20cm 0.003121 0.162715 mg N/L Vanadium NOx
## 185   RESULT MSM_202211_UP_LysB_10cm 0.003154 0.162742 mg N/L Vanadium NOx
## 186   RESULT MSM_202211_UP_LysB_20cm 0.004066 0.163468 mg N/L Vanadium NOx
## 187   RESULT MSM_202211_UP_LysB_45cm 0.004513 0.163823 mg N/L Vanadium NOx
## 188   RESULT MSM_202211_UP_LysC_10cm 0.007430 0.166147 mg N/L Vanadium NOx
##     Conc_uM_raw   Conc_uM
## 177   0.8103265 0.8103265
## 184   0.2228219 0.2228219
## 185   0.2251780 0.2251780
## 186   0.2902896 0.2902896
## 187   0.3222029 0.3222029
## 188   0.5304604 0.5304604
```

## Pull all data back together and add flags

```
#pull out the columns we want from each dataframe
NH4_pull <- NH4samples[ ,c(2,3,7) ]
head(NH4_pull)
```

```
##                 Sample_Name     Conc    Conc_uM
## 329 MSM_202211_UP_LysA_10cm 1.075965  76.817880
## 330 MSM_202211_UP_LysA_20cm 1.957322 139.741838
## 331 MSM_202211_UP_LysB_10cm 0.093142   6.649818
## 338 MSM_202211_UP_LysB_20cm 0.376242  26.861573
## 339 MSM_202211_UP_LysB_45cm 0.820627  58.588176
## 340 MSM_202211_UP_LysC_10cm 0.525043  37.485132
```

```
PO4_pull <- PO4samples[ ,c(2,3,7) ]
head(PO4_pull)
```

```
##                 Sample_Name     Conc   Conc_uM
## 474 MSM_202211_UP_LysA_10cm 0.010627 0.7587083
## 475 MSM_202211_UP_LysA_20cm 0.005352 0.3821029
## 476 MSM_202211_UP_LysB_10cm 0.001697 0.1211563
## 484 MSM_202211_UP_LysB_20cm 0.002242 0.1600663
## 485 MSM_202211_UP_LysB_45cm 0.009756 0.6965238
## 486 MSM_202211_UP_LysC_10cm 0.002499 0.1784146
```

```
NOX_pull <- NOXsamples[ ,c(2,3,8) ]
head(NOX_pull)
```

```
##                 Sample_Name     Conc   Conc_uM
## 177 MSM_202211_UP_LysA_10cm 0.011350 0.8103265
## 184 MSM_202211_UP_LysA_20cm 0.003121 0.2228219
## 185 MSM_202211_UP_LysB_10cm 0.003154 0.2251780
## 186 MSM_202211_UP_LysB_20cm 0.004066 0.2902896
## 187 MSM_202211_UP_LysB_45cm 0.004513 0.3222029
## 188 MSM_202211_UP_LysC_10cm 0.007430 0.5304604
```

```r
#Bring all this data back together:
all_data <- merge(NH4_pull, PO4_pull, by="Sample_Name", all.x=TRUE)
all_data <- merge(all_data, NOX_pull, by="Sample_Name", all.x=TRUE)
head(all_data)
```

```
##                 Sample_Name   Conc.x Conc_uM.x   Conc.y Conc_uM.y     Conc
## 1         GCrew_202211_SW_A 0.033250  2.373864 0.027932 1.9941885 0.019116
## 2         GCrew_202211_SW_B 0.037850  2.702278 0.038704 2.7632490 0.016344
## 3         GCrew_202211_SW_C 0.031361  2.239000 0.032659 2.3316698 0.021298
## 4 GCrew_202211_TR_LysA_20cm 0.330395 23.588354 0.002721 0.1942642 0.015823
## 5 GCrew_202211_TR_LysA_45cm 0.073731  5.263981 0.003378 0.2411703 0.023454
## 6 GCrew_202211_TR_LysB_10cm 0.095799  6.839513 0.011660 0.8324588 0.011468
##    Conc_uM
## 1 1.364775
## 2 1.166870
## 3 1.520558
## 4 1.129674
## 5 1.674484
## 6 0.818751
```

```r
colnames(all_data) <- c("Sample_Name", "NH3_mgL", "NH3_uM", "PO4_mgL", "PO4_uM", "NOx_mgL", "NOx_uM")
head(all_data)
```

```
##                 Sample_Name  NH3_mgL    NH3_uM  PO4_mgL    PO4_uM  NOx_mgL
## 1         GCrew_202211_SW_A 0.033250  2.373864 0.027932 1.9941885 0.019116
## 2         GCrew_202211_SW_B 0.037850  2.702278 0.038704 2.7632490 0.016344
## 3         GCrew_202211_SW_C 0.031361  2.239000 0.032659 2.3316698 0.021298
## 4 GCrew_202211_TR_LysA_20cm 0.330395 23.588354 0.002721 0.1942642 0.015823
## 5 GCrew_202211_TR_LysA_45cm 0.073731  5.263981 0.003378 0.2411703 0.023454
## 6 GCrew_202211_TR_LysB_10cm 0.095799  6.839513 0.011660 0.8324588 0.011468
##     NOx_uM
## 1 1.364775
## 2 1.166870
## 3 1.520558
## 4 1.129674
## 5 1.674484
## 6 0.818751
```

```r
#add in an if then statement that tells us if they are within the range of the test - check this after
all_data$NH3_range <- ifelse(all_data$NH3_mgL<0.02, "bdl",  ifelse(all_data$NH3_mgL>2, "adl", "Within_Ra
all_data$PO4_range <- ifelse(all_data$PO4_mgL<0.003, "bdl",  ifelse(all_data$PO4_mgL>3, "adl", "Within_
all_data$NOx_range <- ifelse(all_data$NOx_mgL<0.025, "bdl",  ifelse(all_data$NOx_mgL>1, "adl", "Within_
head(all_data)
```

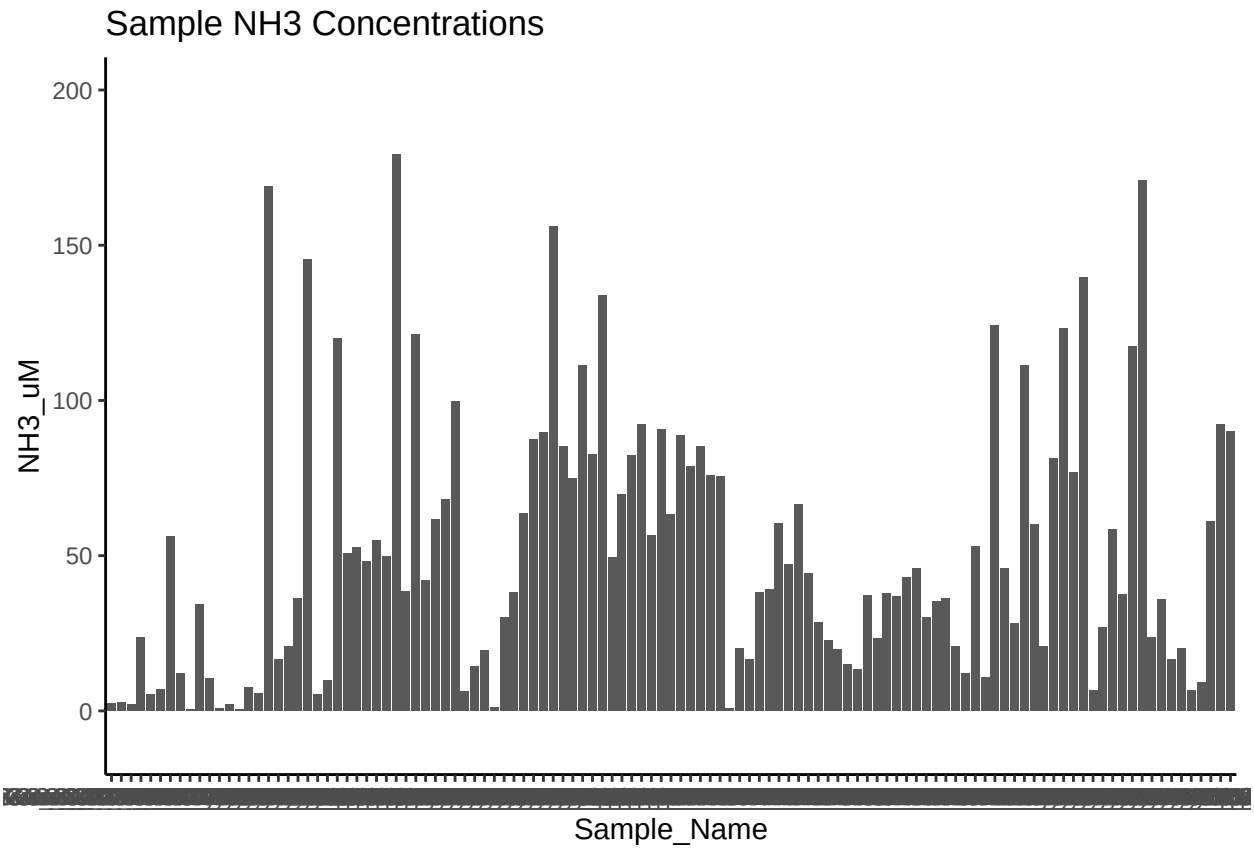
```
##                 Sample_Name  NH3_mgL    NH3_uM  PO4_mgL    PO4_uM  NOx_mgL
## 1         GCrew_202211_SW_A 0.033250  2.373864 0.027932 1.9941885 0.019116
## 2         GCrew_202211_SW_B 0.037850  2.702278 0.038704 2.7632490 0.016344
## 3         GCrew_202211_SW_C 0.031361  2.239000 0.032659 2.3316698 0.021298
## 4 GCrew_202211_TR_LysA_20cm 0.330395 23.588354 0.002721 0.1942642 0.015823
## 5 GCrew_202211_TR_LysA_45cm 0.073731  5.263981 0.003378 0.2411703 0.023454
## 6 GCrew_202211_TR_LysB_10cm 0.095799  6.839513 0.011660 0.8324588 0.011468
##     NOx_uM    NH3_range    PO4_range NOx_range
```

```
## 1 1.364775 Within_Range Within_Range       bdl
## 2 1.166870 Within_Range Within_Range       bdl
## 3 1.520558 Within_Range Within_Range       bdl
## 4 1.129674 Within_Range          bdl       bdl
## 5 1.674484 Within_Range Within_Range       bdl
## 6 0.818751 Within_Range Within_Range       bdl
```

### Take an initial look at concentrations

```
#plot data to get a sense of any outliers
NH3look <- ggplot(data=all_data, aes(x=Sample_Name, y=NH3_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-10, 200) +
  theme(legend.position="none") +
  ggtitle("Sample NH3 Concentrations")
NH3look
```

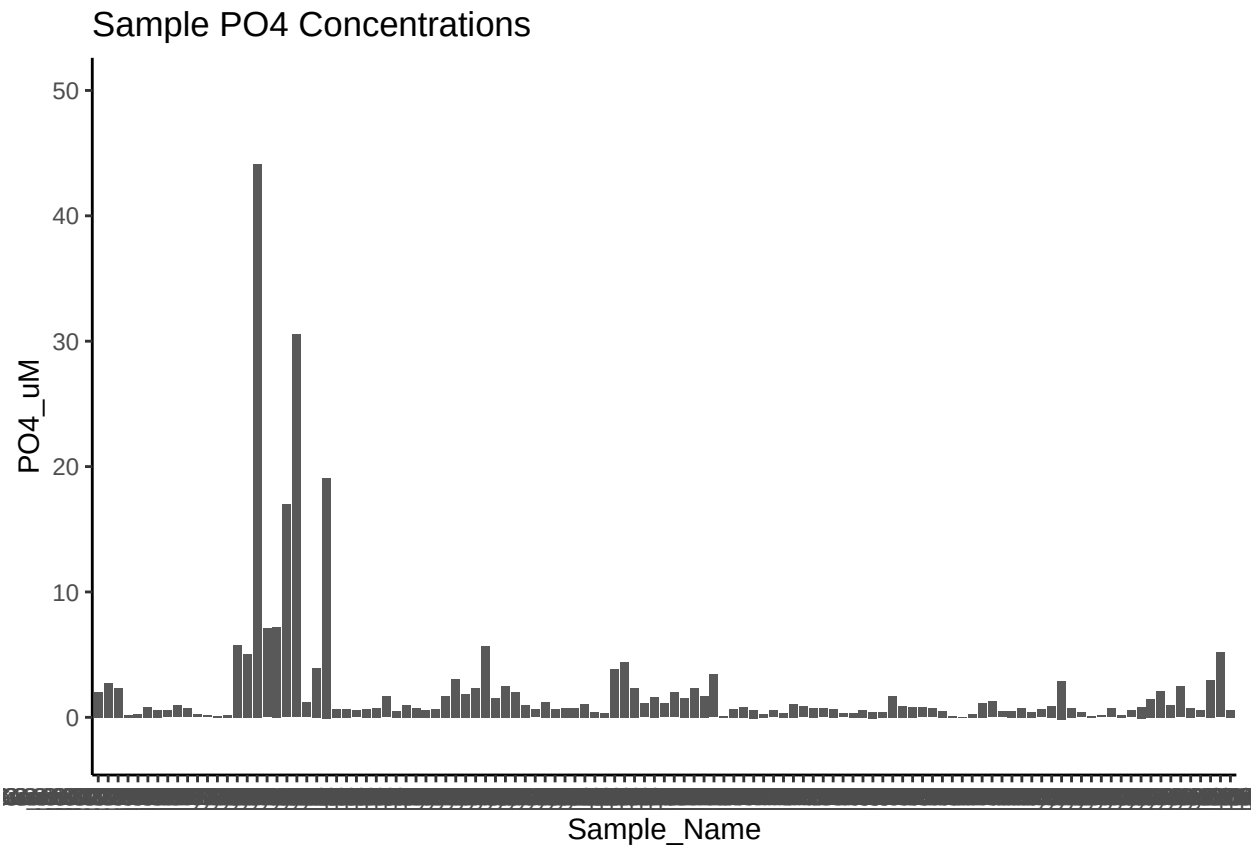
```
## Warning: Removed 5 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```




```
PO4look <- ggplot(data=all_data, aes(x=Sample_Name, y=PO4_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 50) +
```

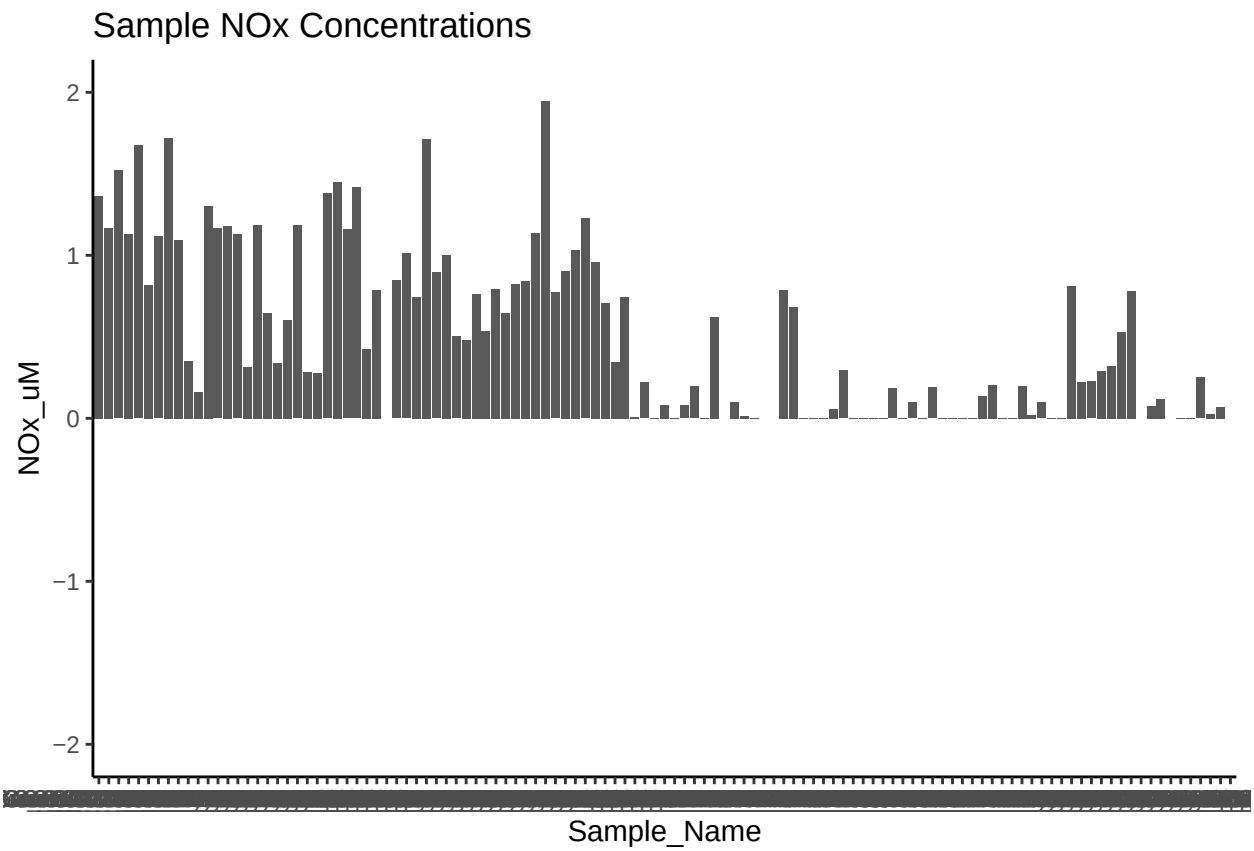
```
  theme(legend.position="none") +
  ggtitle("Sample PO4 Concentrations")
PO4look
```

```
## Warning: Removed 3 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```




```
NOXlook <- ggplot(data=all_data, aes(x=Sample_Name, y=NOx_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 2) +
  theme(legend.position="none") +
  ggtitle("Sample NOx Concentrations")
NOXlook
```

```
## Warning: Removed 14 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```




### Pull out data you need, make IDs

```
head(all_data)
```

```
##                 Sample_Name  NH3_mgL    NH3_uM  PO4_mgL    PO4_uM  NOx_mgL
## 1         GCrew_202211_SW_A 0.033250  2.373864 0.027932 1.9941885 0.019116
## 2         GCrew_202211_SW_B 0.037850  2.702278 0.038704 2.7632490 0.016344
## 3         GCrew_202211_SW_C 0.031361  2.239000 0.032659 2.3316698 0.021298
## 4 GCrew_202211_TR_LysA_20cm 0.330395 23.588354 0.002721 0.1942642 0.015823
## 5 GCrew_202211_TR_LysA_45cm 0.073731  5.263981 0.003378 0.2411703 0.023454
## 6 GCrew_202211_TR_LysB_10cm 0.095799  6.839513 0.011660 0.8324588 0.011468
##     NOx_uM    NH3_range    PO4_range NOx_range
## 1 1.364775 Within_Range Within_Range       bdl
## 2 1.166870 Within_Range Within_Range       bdl
## 3 1.520558 Within_Range Within_Range       bdl
## 4 1.129674 Within_Range          bdl       bdl
## 5 1.674484 Within_Range Within_Range       bdl
## 6 0.818751 Within_Range Within_Range       bdl
```

```
out <- all_data[ ,c(1,3,5,7,8,9,10)]
head(out)
```

```
##                 Sample_Name    NH3_uM    PO4_uM   NOx_uM    NH3_range
```

```
## 1         GCrew_202211_SW_A  2.373864 1.9941885 1.364775 Within_Range
## 2         GCrew_202211_SW_B  2.702278 2.7632490 1.166870 Within_Range
## 3         GCrew_202211_SW_C  2.239000 2.3316698 1.520558 Within_Range
## 4 GCrew_202211_TR_LysA_20cm 23.588354 0.1942642 1.129674 Within_Range
## 5 GCrew_202211_TR_LysA_45cm  5.263981 0.2411703 1.674484 Within_Range
## 6 GCrew_202211_TR_LysB_10cm  6.839513 0.8324588 0.818751 Within_Range
##      PO4_range NOx_range
## 1 Within_Range       bdl
## 2 Within_Range       bdl
## 3 Within_Range       bdl
## 4          bdl       bdl
## 5 Within_Range       bdl
## 6 Within_Range       bdl
```

```
#for steph <- pull out identifiers of the sample names
#pull the sample ID and separate it by the underscores
IDs <- data.frame(do.call('rbind', strsplit(as.character(out$Sample_Name),'_',fixed=TRUE)))
```

```
## Warning in rbind(c("GCrew", "202211", "SW", "A"), c("GCrew", "202211", "SW", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
colnames(IDs) <- c("Site" , "Date","Zone", "Replicate", "Depth")
IDs$Month <- "November"
head(IDs)
```

```
##    Site   Date Zone Replicate Depth    Month
## 1 GCrew 202211   SW         A GCrew November
## 2 GCrew 202211   SW         B GCrew November
## 3 GCrew 202211   SW         C GCrew November
## 4 GCrew 202211   TR      LysA  20cm November
## 5 GCrew 202211   TR      LysA  45cm November
## 6 GCrew 202211   TR      LysB  10cm November
```

```
#rejoin them to the dataframe
alldat <- cbind(IDs, out)
head(alldat)
```

```
##    Site   Date Zone Replicate Depth    Month               Sample_Name
## 1 GCrew 202211   SW         A GCrew November         GCrew_202211_SW_A
## 2 GCrew 202211   SW         B GCrew November         GCrew_202211_SW_B
## 3 GCrew 202211   SW         C GCrew November         GCrew_202211_SW_C
## 4 GCrew 202211   TR      LysA  20cm November GCrew_202211_TR_LysA_20cm
## 5 GCrew 202211   TR      LysA  45cm November GCrew_202211_TR_LysA_45cm
## 6 GCrew 202211   TR      LysB  10cm November GCrew_202211_TR_LysB_10cm
##      NH3_uM    PO4_uM   NOx_uM    NH3_range    PO4_range NOx_range
## 1  2.373864 1.9941885 1.364775 Within_Range Within_Range       bdl
## 2  2.702278 2.7632490 1.166870 Within_Range Within_Range       bdl
## 3  2.239000 2.3316698 1.520558 Within_Range Within_Range       bdl
## 4 23.588354 0.1942642 1.129674 Within_Range          bdl       bdl
## 5  5.263981 0.2411703 1.674484 Within_Range Within_Range       bdl
## 6  6.839513 0.8324588 0.818751 Within_Range Within_Range       bdl
```

### Export final data with flags

```
#Export Data

write.csv(alldat, file="Processed Data/COMPASS_Synoptic_CB_SEAL_NUTR_202211.csv")
```