

COMPASS_Synoptic_SEAL_Data_Analysis_Sept2022

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Information

```
#####
##### COMPASS Synoptic
##### Chesapeake Bay Sites
##### Data Analysis Code: Porewater Nutrients
##### MONTH: August 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_pu8s8pj7iNUAhF/view?usp=sharing
#NH4 method = https://drive.google.com/file/d/1ENGemUEvm_rffZqv3lz9BjD0pAMX5nzu/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      P04 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      P04 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

```

```

qP04 <- qlog[qlog$Analysis %like% "P04", ]
head(qP04)

```

```

##           Date      User Machine Analysis Slope Intercept     R2
## 2 20220513 Stephanie Wilson SERC SEAL      P04 2.869   0.002 0.9994
## 5 20220614 Stephanie Wilson SERC SEAL      P04 2.395 -0.001 0.9998
## 8 20220615 Stephanie Wilson SERC SEAL      P04 2.349   0.000 0.9999
## 11 20220718 Stephanie Wilson SERC SEAL      P04 2.445 -0.003 0.9993
## 13 20220718 Stephanie Wilson SERC SEAL      P04 2.349 -0.004 0.9992
## 15 20220719 Stephanie Wilson SERC SEAL      P04 2.271 -0.003 0.9993
##   Nox_Red_Eff X
## 2       NA
## 5       NA
## 8       NA
## 11      NA
## 13      NA
## 15      NA

```

```

qN0x <- qlog[qlog$Analysis %like% "V-Nox", ]
head(qN0x)

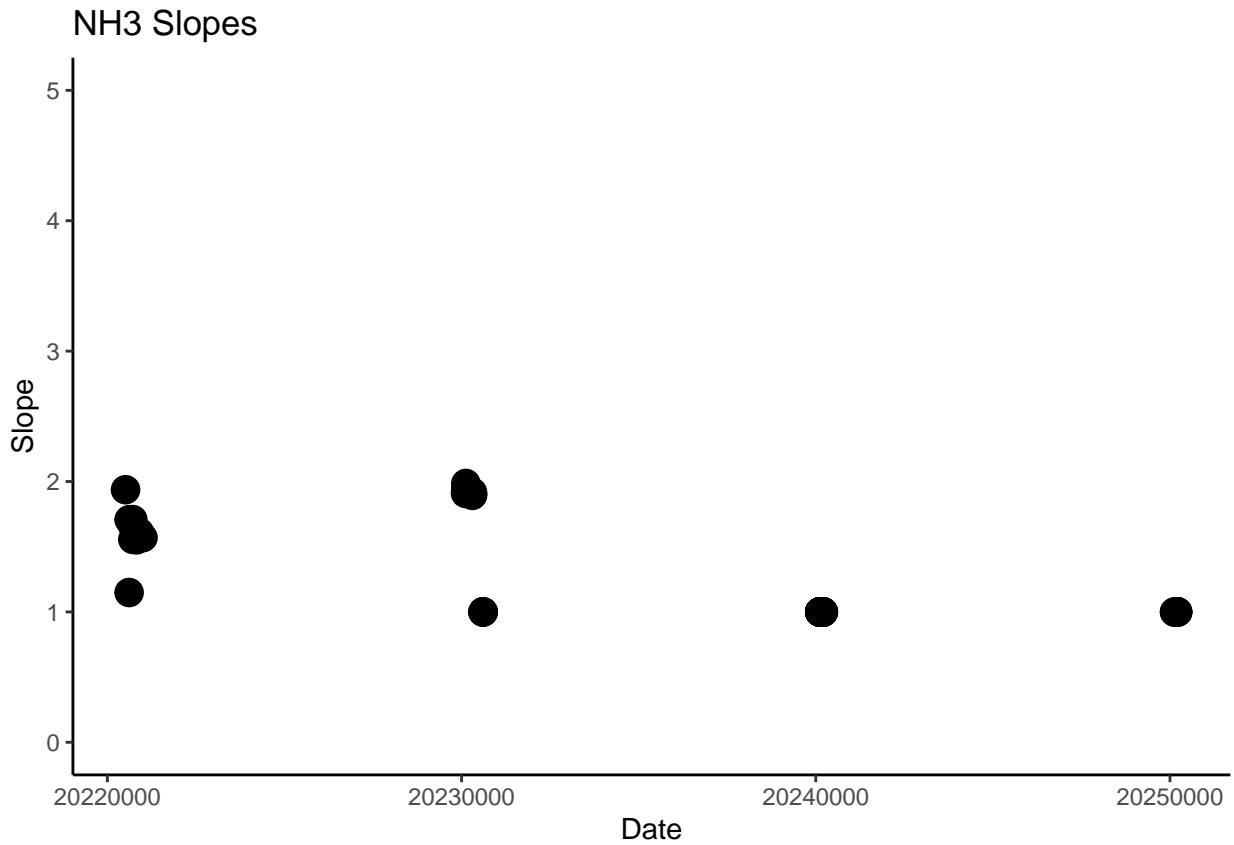
##           Date      User Machine Analysis Slope Intercept     R2
## 3 20220525 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9990
## 6 20220615 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9998
## 9 20220718 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9999
## 16 20220730 Stephanie Wilson 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()').

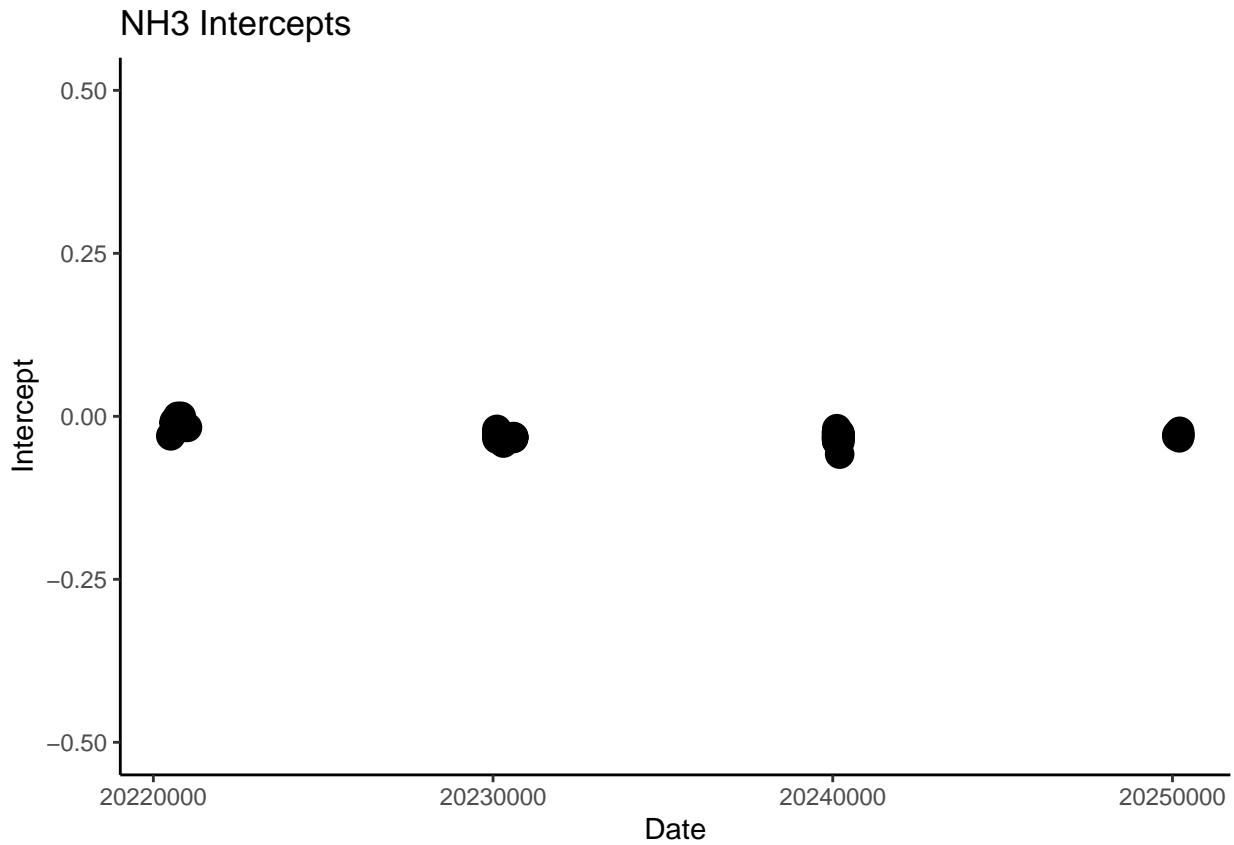
```



```
#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()').
```

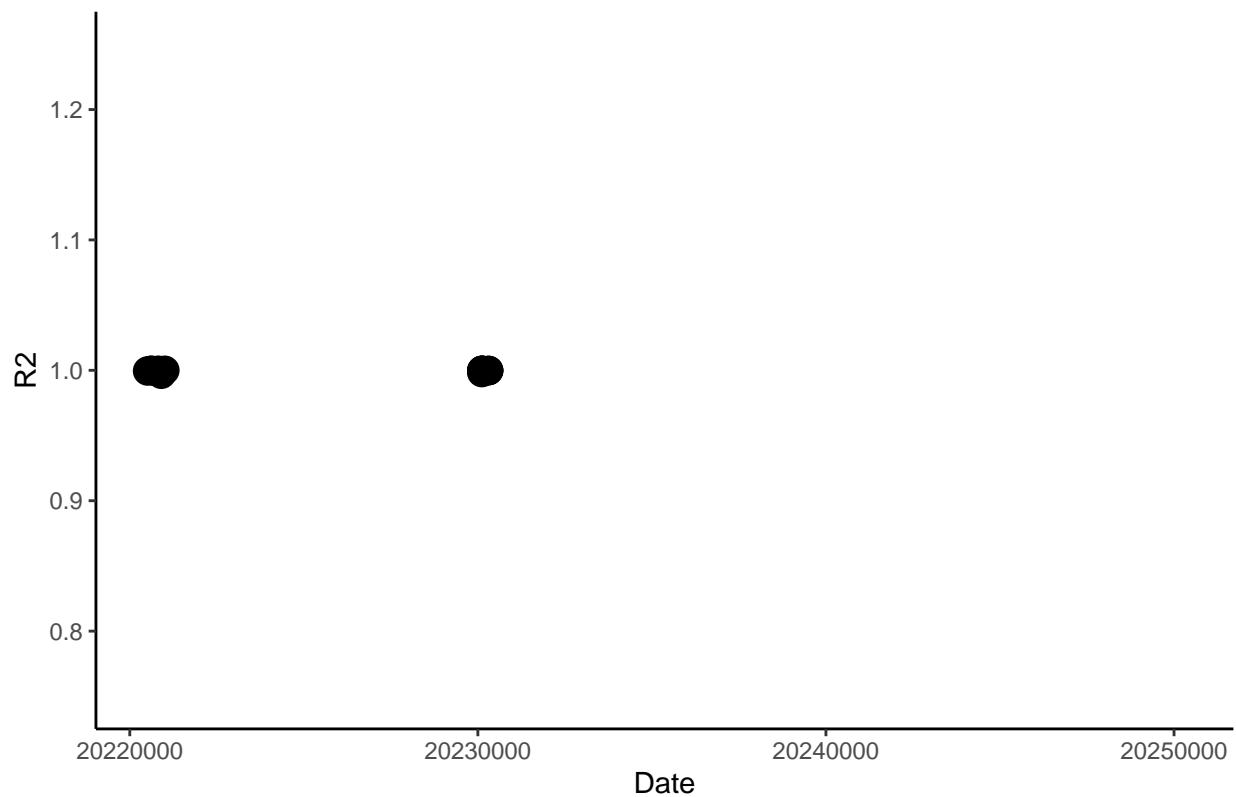


```
#plot the R2s to make sure there are no crazy outliers
Rsq1 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NH3 R2s")
```

```
Rsq1
```

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

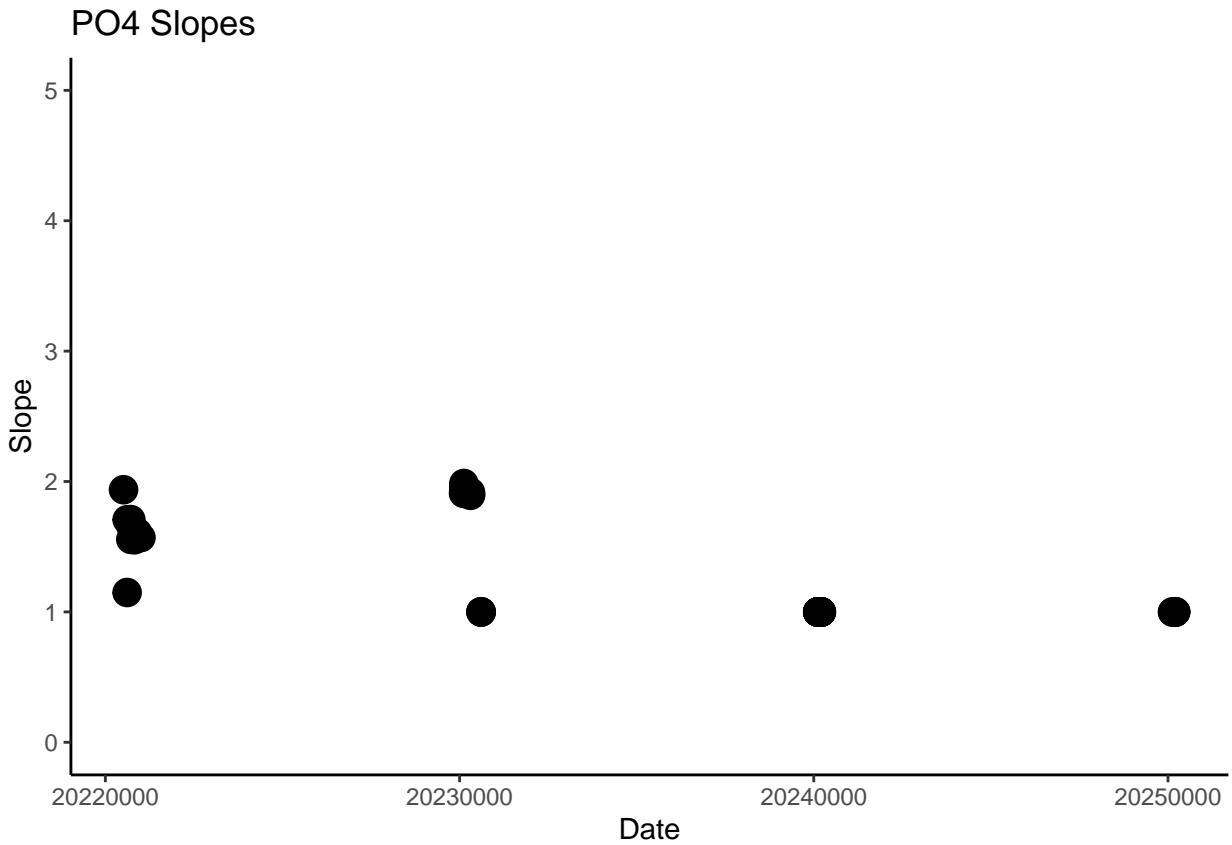
NH3 R2s



```
##### P04
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("P04 Slopes")

slope2
```

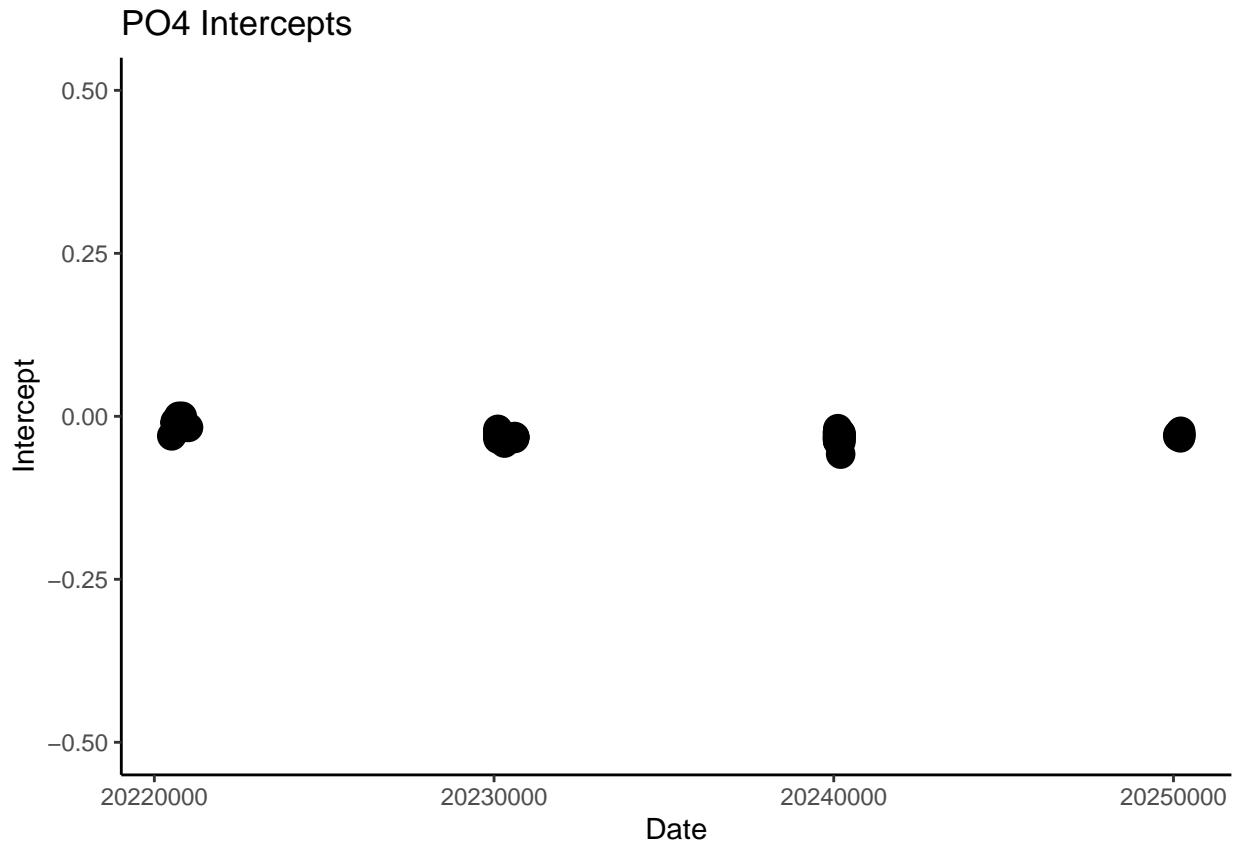
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#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("P04 Intercepts")

int2

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

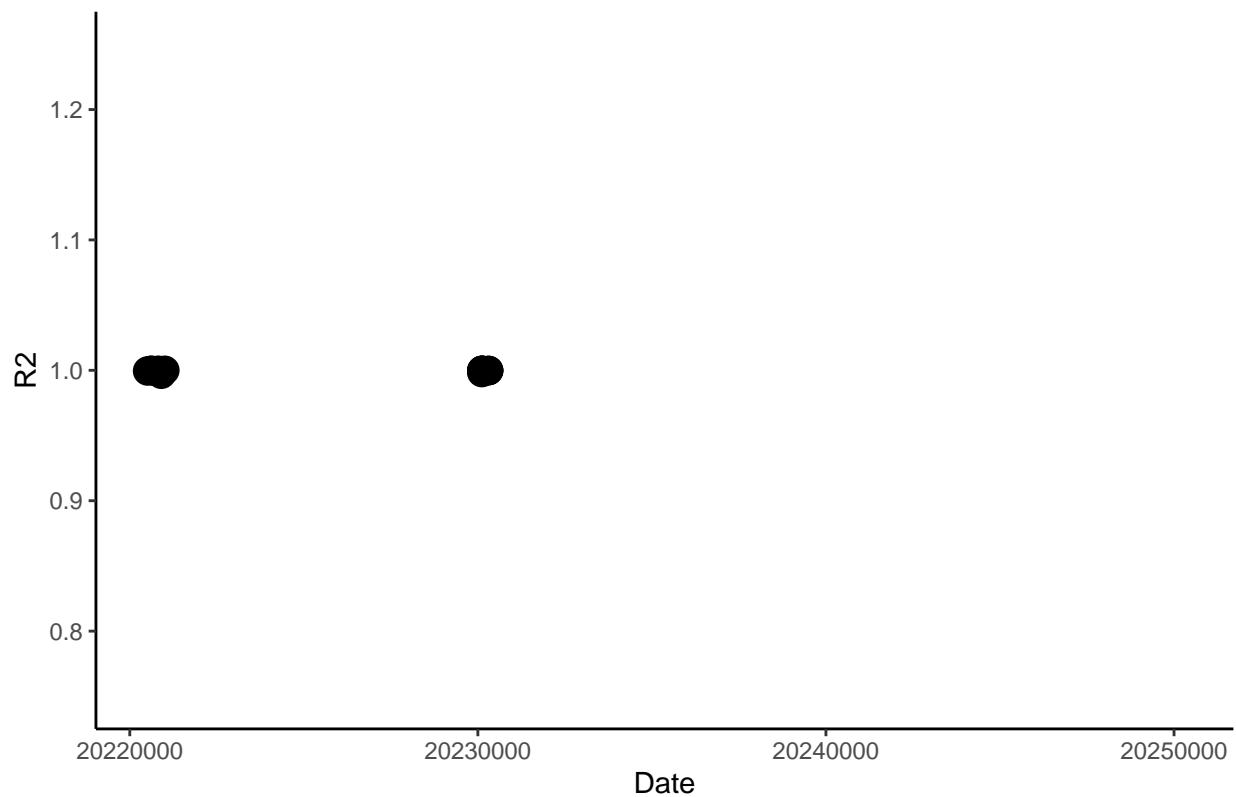


```
#plot the R2s to make sure there are no crazy outliers
Rsq2 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("P04 R2s")
```

```
Rsq2
```

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

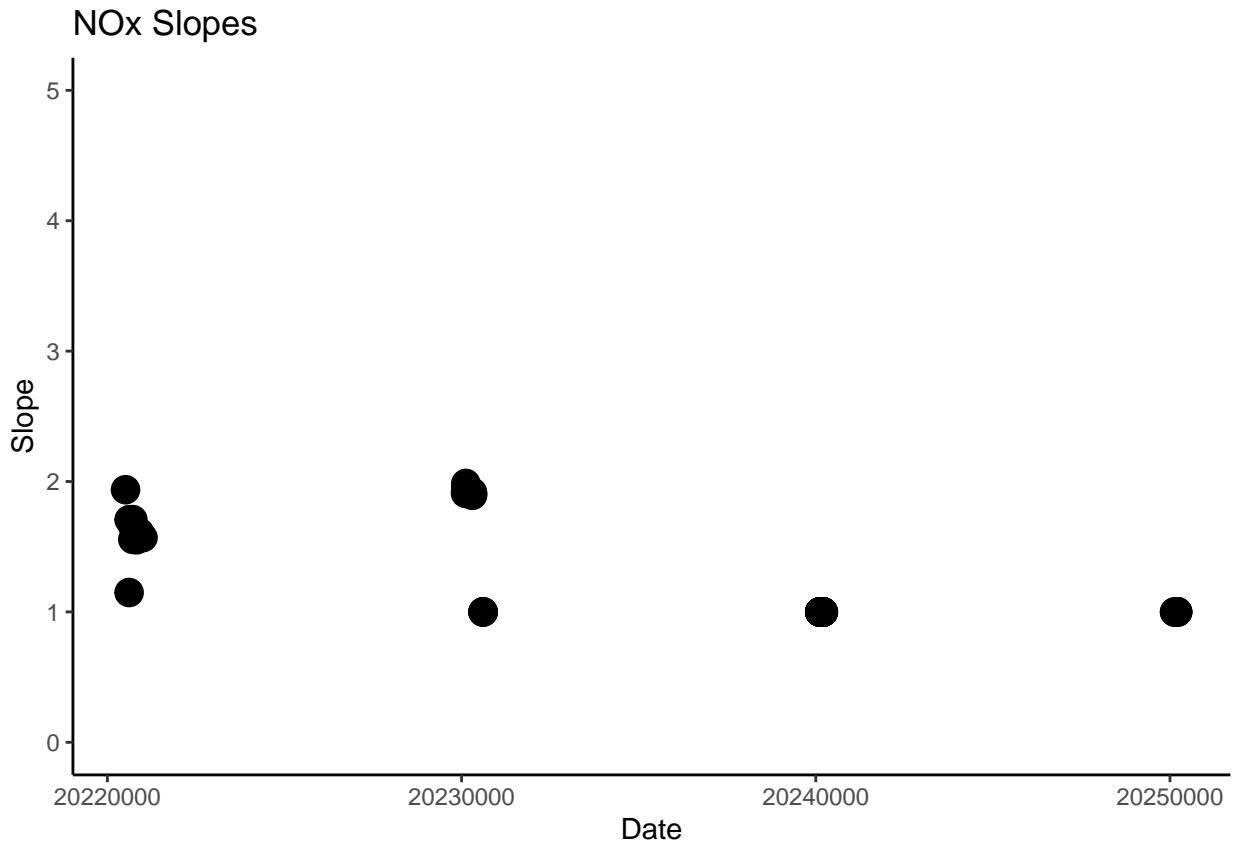
PO4 R2s



```
#####
# 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
```

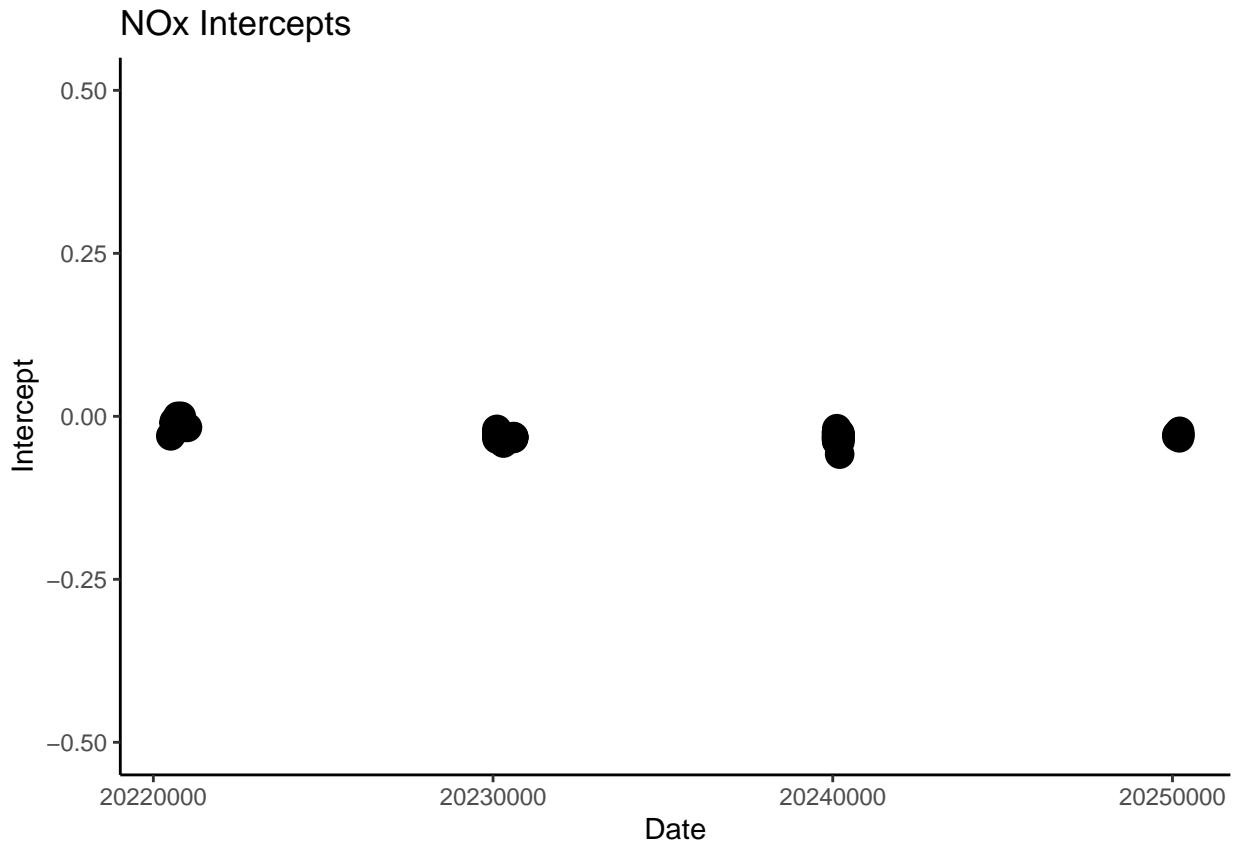
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#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()').
```

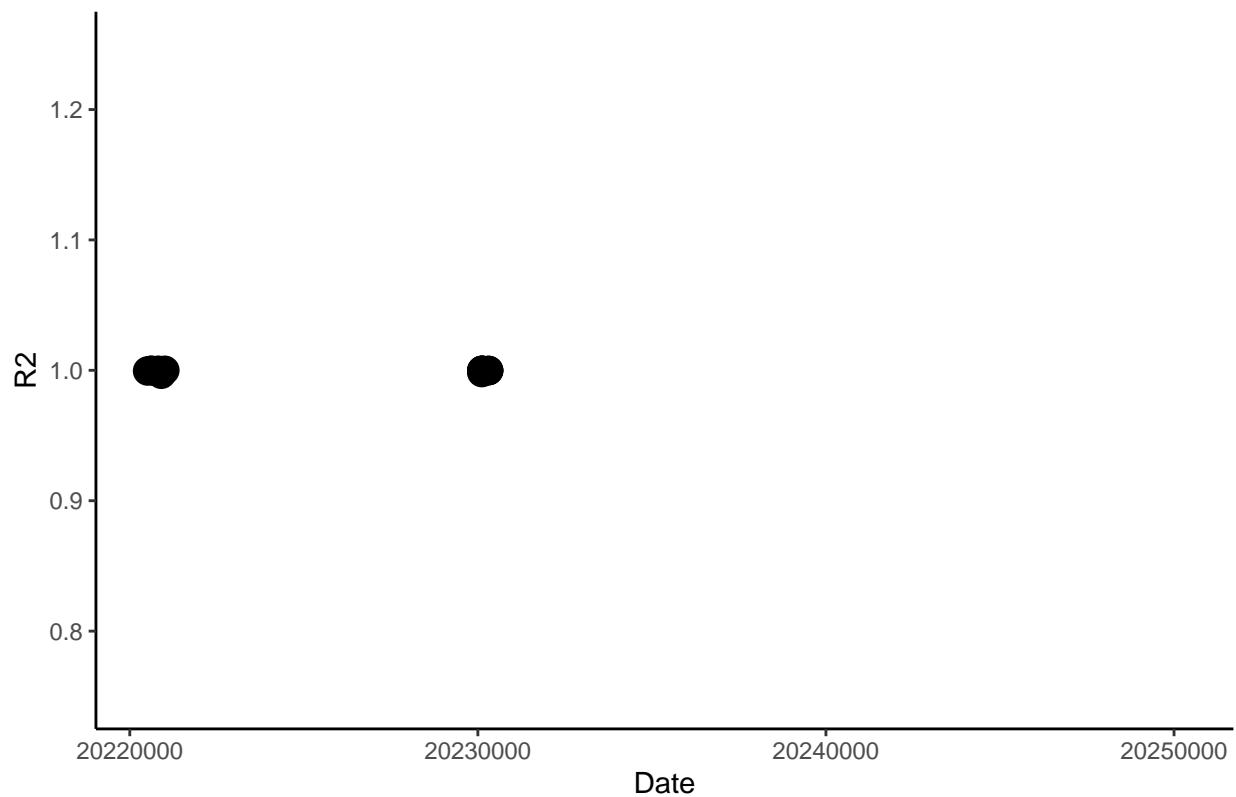


```
#plot the R2s to make sure there are no crazy outliers
Rsq3 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NOx R2s")
```

```
Rsq3
```

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

NOx R2s



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_P04_202209_1.csv")
#Quick look at dataframe
head(file1)

##   RUNSTARTED X1553789462 X3.28.2019.12.11      X X.1      X.2      X.3 X.4
## 1      RESULT      -1          S1 Standard 1  0 0.000019 0.000019  0
## 2      RESULT      -2          S90 Standard 90 1 0.008778 0.008778  0
## 3      RESULT      -2          S91 Standard 91 2 0.023144 0.023144  0
## 4      RESULT      -2          S92 Standard 92 3 0.045439 0.045439  0
## 5      RESULT      -2          S93 Standard 93 4 0.117195 0.117195  0
## 6      RESULT      -2          S94 Standard 94 5 0.237585 0.237585  0
##   X.5 X.6 X.7      X.8      X.9      X.10      X.11
## 1  0  0  0 mg N/L Nitrite 0.2 1553790057 3/28/2019 12:20
## 2  0  0  0 mg N/L Nitrite 0.2 1553790098 3/28/2019 12:21
## 3  0  0  0 mg N/L Nitrite 0.2 1553790139 3/28/2019 12:22
## 4  0  0  0 mg N/L Nitrite 0.2 1553790179 3/28/2019 12:22
## 5  0  0  0 mg N/L Nitrite 0.2 1553790220 3/28/2019 12:23
## 6  0  0  0 mg N/L Nitrite 0.2 1553790261 3/28/2019 12:24

#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 0.000019 0.000019 mg N/L Nitrite 0.2
## 2   RESULT Standard 90 0.008778 0.008778 mg N/L Nitrite 0.2
## 3   RESULT Standard 91 0.023144 0.023144 mg N/L Nitrite 0.2
## 4   RESULT Standard 92 0.045439 0.045439 mg N/L Nitrite 0.2
## 5   RESULT Standard 93 0.117195 0.117195 mg N/L Nitrite 0.2
## 6   RESULT Standard 94 0.237585 0.237585 mg N/L Nitrite 0.2

#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202209_2.csv")
#Quick look at dataframe
head(file2)

##   RUNSTARTED X1568815852 X9.18.2019.10.10          X X.1      X.2      X.3 X.4
## 1   RESULT      -1           S1 Standard 1 0 0.584576 0.584576 0
## 2   RESULT      -2           S90 Standard 90 1 0.518989 0.518989 0
## 3   RESULT      -2           S91 Standard 91 2 0.605939 0.605939 0
## 4   RESULT      -2           S92 Standard 92 3 0.684434 0.684434 0
## 5   RESULT      -2           S93 Standard 93 4 0.787007 0.787007 0
## 6   RESULT      -2           S94 Standard 94 5 0.938437 0.938437 0
##   X.5 X.6 X.7     X.8      X.9      X.10      X.11
## 1   0   0   0 mg N/L N03_N02 2 1568817080 9/18/2019 10:31
## 2   0   0   0 mg N/L N03_N02 2 1568817209 9/18/2019 10:33
## 3   0   0   0 mg N/L N03_N02 2 1568817338 9/18/2019 10:35
## 4   0   0   0 mg N/L N03_N02 2 1568817466 9/18/2019 10:37
## 5   0   0   0 mg N/L N03_N02 2 1568817594 9/18/2019 10:39
## 6   0   0   0 mg N/L N03_N02 2 1568817722 9/18/2019 10:42

#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 0.584576 0.584576 mg N/L N03_N02 2
## 2   RESULT Standard 90 0.518989 0.518989 mg N/L N03_N02 2
## 3   RESULT Standard 91 0.605939 0.605939 mg N/L N03_N02 2
## 4   RESULT Standard 92 0.684434 0.684434 mg N/L N03_N02 2
## 5   RESULT Standard 93 0.787007 0.787007 mg N/L N03_N02 2
## 6   RESULT Standard 94 0.938437 0.938437 mg N/L N03_N02 2

#read in data
file3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202209_3.csv")
#Quick look at dataframe
head(file3)

##   RUNSTARTED X1673644940 X1.13.2023.16.22          X X.1      X.2      X.3
## 1   RESULT      -1           S1 Standard 1 0 0.009933 0.009933
## 2   RESULT      -2           S90 Standard .0389 1 0.029260 0.029260
## 3   RESULT      -2           S91 Standard .1000 2 0.063726 0.063726
## 4   RESULT      -2           S92 Standard .2000 3 0.094039 0.094039

```

```

## 5      RESULT          -2           S93 Standard .5000   4 0.271131 0.271131
## 6      RESULT          -2           S94 Standard 1.0000   5 0.558844 0.558844
## 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 1673646166 1/13/2023 16:42
## 2  0  0  0  0 mg N/L Ammonia 2 1673646326 1/13/2023 16:45
## 3  0  0  0  0 mg N/L Ammonia 2 1673646486 1/13/2023 16:48
## 4  0  0  0  0 mg N/L Ammonia 2 1673646646 1/13/2023 16:50
## 5  0  0  0  0 mg N/L Ammonia 2 1673646806 1/13/2023 16:53
## 6  0  0  0  0 mg N/L Ammonia 2 1673646966 1/13/2023 16:56

#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 0.009933 0.009933 mg N/L Ammonia 2
## 2  RESULT      Standard .0389 0.029260 0.029260 mg N/L Ammonia 2
## 3  RESULT      Standard .1000 0.063726 0.063726 mg N/L Ammonia 2
## 4  RESULT      Standard .2000 0.094039 0.094039 mg N/L Ammonia 2
## 5  RESULT      Standard .5000 0.271131 0.271131 mg N/L Ammonia 2
## 6  RESULT      Standard 1.0000 0.558844 0.558844 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 0.000019 0.000019 mg N/L Nitrite 0.2
## 2  RESULT Standard 90 0.008778 0.008778 mg N/L Nitrite 0.2
## 3  RESULT Standard 91 0.023144 0.023144 mg N/L Nitrite 0.2
## 4  RESULT Standard 92 0.045439 0.045439 mg N/L Nitrite 0.2
## 5  RESULT Standard 93 0.117195 0.117195 mg N/L Nitrite 0.2
## 6  RESULT Standard 94 0.237585 0.237585 mg N/L Nitrite 0.2

#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
## 122  RESULT MSM_202209_UP_LysA_20cm 1.390346 0.896168 mg N/L Ammonia 2
## 123  RESULT MSM_202209_UP_LysA_45cm 0.681030 0.444370 mg N/L Ammonia 2
## 124  RESULT MSM_202209_UP_LysB_10cm 0.029888 0.029626 mg N/L Ammonia 2
## 125  RESULT MSM_202209_UP_LysB_20cm 0.194465 0.134453 mg N/L Ammonia 2
## 126  RESULT MSM_202209_UP_LysB_45cm 0.395437 0.262462 mg N/L Ammonia 2
## 127  RESULT MSM_202209_UP_LysC_10cm 0.375479 0.249749 mg N/L Ammonia 2

```

NOx

```
#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202209_1.csv")
#Quick look at dataframe
head(Nfile1)

##    RUNSTARTED X1674261103      X1.20.2023.19.31          X X.1      X.2      X.3
## 1  RUNENDED   1674261139 INSUFFICIENT REAGENT           NA      NA      NA
## 2 RUNSTARTED   1674261195      1/20/2023 19:33           NA      NA      NA
## 3    RESULT     -1                  S1 Standard 1  0 0.184456 0.184456
## 4    RESULT     -2                  S90 Standard 90  1 0.203401 0.203401
## 5    RESULT     -2                  S91 Standard 91  2 0.227204 0.227204
## 6    RESULT     -2                  S92 Standard 92  3 0.266972 0.266972
##    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 1674263383 1/20/2023 20:09
## 4  0   0   0 512 mg N/L Vanadium NOx 1674263465 1/20/2023 20:11
## 5  0   0   0 512 mg N/L Vanadium NOx 1674263546 1/20/2023 20:12
## 6  0   0   0 512 mg N/L Vanadium NOx 1674263627 1/20/2023 20:13

#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    RESULT Standard 1 0.184456 0.184456 mg N/L Vanadium NOx
## 4    RESULT Standard 90 0.203401 0.203401 mg N/L Vanadium NOx
## 5    RESULT Standard 91 0.227204 0.227204 mg N/L Vanadium NOx
## 6    RESULT Standard 92 0.266972 0.266972 mg N/L Vanadium NOx

#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202209_2.csv")
#Quick look at dataframe
head(Nfile2)

##    RUNSTARTED X1673807323 X1.15.2023.13.28          X X.1      X.2      X.3 X.4
## 1    RESULT     -1                  S1 Standard 1  0 0.140496 0.140496  0
## 2    RESULT     -2                  S90 Standard 90  1 0.158302 0.158302  0
## 3    RESULT     -2                  S91 Standard 91  2 0.182799 0.182799  0
## 4    RESULT     -2                  S92 Standard 92  3 0.223878 0.223878  0
## 5    RESULT     -2                  S93 Standard 93  4 0.344134 0.344134  0
## 6    RESULT     -2                  S94 Standard 94  5 0.553945 0.553945  0
##    X.5 X.6 X.7      X.8      X.9      X.10      X.11
## 1  0   0   0 mg N/L Vanadium NOx 1673809505 1/15/2023 14:05
## 2  0   0   0 mg N/L Vanadium NOx 1673809585 1/15/2023 14:06
```

```

## 3 0 0 0 mg N/L Vanadium NOx 1673809665 1/15/2023 14:07
## 4 0 0 0 mg N/L Vanadium NOx 1673809745 1/15/2023 14:09
## 5 0 0 0 mg N/L Vanadium NOx 1673809825 1/15/2023 14:10
## 6 0 0 0 mg N/L Vanadium NOx 1673809905 1/15/2023 14:11

#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 0.140496 0.140496 mg N/L Vanadium NOx
## 2    RESULT Standard 90 0.158302 0.158302 mg N/L Vanadium NOx
## 3    RESULT Standard 91 0.182799 0.182799 mg N/L Vanadium NOx
## 4    RESULT Standard 92 0.223878 0.223878 mg N/L Vanadium NOx
## 5    RESULT Standard 93 0.344134 0.344134 mg N/L Vanadium NOx
## 6    RESULT Standard 94 0.553945 0.553945 mg N/L Vanadium NOx

```

```

#read in data
Nfile3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202209_3.csv")
#Quick look at dataframe
head(Nfile3)

```

```

##    RUNSTARTED X1673913818 X1.16.2023.19.03          X X.1      X.2      X.3 X.4
## 1 RUNSTARTED 1673918924 1/16/2023 20:28          NA      NA      NA  NA
## 2    RESULT      -1          S1 Standard 1 0 0.139612 0.139612 0
## 3    RESULT      -2          S90 Standard 90 1 0.156868 0.156868 0
## 4    RESULT      -2          S91 Standard 91 2 0.177989 0.177989 0
## 5    RESULT      -2          S92 Standard 92 3 0.220473 0.220473 0
## 6    RESULT      -2          S93 Standard 93 4 0.339950 0.339950 0
##   X.5 X.6 X.7    X.8      X.9      X.10      X.11
## 1  NA  NA  NA          NA
## 2  0  0  0 mg N/L Vanadium NOx 1673921121 1/16/2023 21:05
## 3  0  0  0 mg N/L Vanadium NOx 1673921200 1/16/2023 21:06
## 4  0  0  0 mg N/L Vanadium NOx 1673921281 1/16/2023 21:08
## 5  0  0  0 mg N/L Vanadium NOx 1673921360 1/16/2023 21:09
## 6  0  0  0 mg N/L Vanadium NOx 1673921441 1/16/2023 21:10

```

```

#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 RUNSTARTED          NA      NA
## 2    RESULT Standard 1 0.139612 0.139612 mg N/L Vanadium NOx
## 3    RESULT Standard 90 0.156868 0.156868 mg N/L Vanadium NOx
## 4    RESULT Standard 91 0.177989 0.177989 mg N/L Vanadium NOx
## 5    RESULT Standard 92 0.220473 0.220473 mg N/L Vanadium NOx
## 6    RESULT Standard 93 0.339950 0.339950 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
## 3   RESULT Standard 1 0.184456 0.184456 mg N/L Vanadium NOx
## 4   RESULT Standard 90 0.203401 0.203401 mg N/L Vanadium NOx
## 5   RESULT Standard 91 0.227204 0.227204 mg N/L Vanadium NOx
## 6   RESULT Standard 92 0.266972 0.266972 mg N/L Vanadium NOx
## 7   RESULT Standard 93 0.382567 0.382567 mg N/L Vanadium NOx
## 8   RESULT Standard 94 0.583302 0.583302 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
## 23  RESULT MSM_202209_UP_LysA_20cm 0.005178 0.189194 mg N/L Vanadium NOx
## 24  RESULT MSM_202209_UP_LysA_45cm 0.004450 0.188606 mg N/L Vanadium NOx
## 25  RESULT MSM_202209_UP_LysB_10cm -0.000600 0.184527 mg N/L Vanadium NOx
## 26  RESULT MSM_202209_UP_LysB_20cm -0.000584 0.184540 mg N/L Vanadium NOx
## 27  RESULT MSM_202209_UP_LysB_45cm 0.020174 0.201302 mg N/L Vanadium NOx
## 28  RESULT MSM_202209_UP_LysC_10cm -0.002939 0.182637 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
## 122  RESULT MSM_202209_UP_LysA_20cm 1.390346 0.896168 mg N/L Ammonia 2
## 123  RESULT MSM_202209_UP_LysA_45cm 0.681030 0.444370 mg N/L Ammonia 2
## 124  RESULT MSM_202209_UP_LysB_10cm 0.029888 0.029626 mg N/L Ammonia 2
## 125  RESULT MSM_202209_UP_LysB_20cm 0.194465 0.134453 mg N/L Ammonia 2
## 126  RESULT MSM_202209_UP_LysB_45cm 0.395437 0.262462 mg N/L Ammonia 2
## 127  RESULT MSM_202209_UP_LysC_10cm 0.375479 0.249749 mg N/L Ammonia 2

```

```

head(Nalldat2)

##      Run_Info          Sample_Name    Conc     Abs Units      Test
## 23  RESULT MSM_202209_UP_LysA_20cm 0.005178 0.189194 mg N/L Vanadium NOx
## 24  RESULT MSM_202209_UP_LysA_45cm 0.004450 0.188606 mg N/L Vanadium NOx
## 25  RESULT MSM_202209_UP_LysB_10cm -0.000600 0.184527 mg N/L Vanadium NOx
## 26  RESULT MSM_202209_UP_LysB_20cm -0.000584 0.184540 mg N/L Vanadium NOx
## 27  RESULT MSM_202209_UP_LysB_45cm  0.020174 0.201302 mg N/L Vanadium NOx
## 28  RESULT MSM_202209_UP_LysC_10cm -0.002939 0.182637 mg N/L Vanadium NOx

```

```

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

```

```

##      Run_Info          Sample_Name    Conc     Abs Units      Test
## 122 RESULT MSM_202209_UP_LysA_20cm 1.390346 0.896168 mg N/L Ammonia 2
## 123 RESULT MSM_202209_UP_LysA_45cm 0.681030 0.444370 mg N/L Ammonia 2
## 124 RESULT MSM_202209_UP_LysB_10cm 0.029888 0.029626 mg N/L Ammonia 2
## 125 RESULT MSM_202209_UP_LysB_20cm 0.194465 0.134453 mg N/L Ammonia 2
## 126 RESULT MSM_202209_UP_LysB_45cm 0.395437 0.262462 mg N/L Ammonia 2
## 127 RESULT MSM_202209_UP_LysC_10cm 0.375479 0.249749 mg N/L Ammonia 2

```

```

P04samples <- subset(alldat2, Test == "o-PHOS 0.3")
head(P04samples)

```

```

##      Run_Info          Sample_Name    Conc     Abs Units      Test
## 274 RESULT MSM_202209_UP_LysA_20cm 0.015957 0.007203 mg P/L o-PHOS 0.3
## 275 RESULT MSM_202209_UP_LysA_45cm 0.042254 0.018219 mg P/L o-PHOS 0.3
## 276 RESULT MSM_202209_UP_LysB_10cm 0.011573 0.005367 mg P/L o-PHOS 0.3
## 277 RESULT MSM_202209_UP_LysB_20cm 0.009140 0.004347 mg P/L o-PHOS 0.3
## 278 RESULT MSM_202209_UP_LysB_45cm 0.039296 0.016980 mg P/L o-PHOS 0.3
## 279 RESULT MSM_202209_UP_LysC_10cm 0.013091 0.006002 mg P/L o-PHOS 0.3

```

```

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

```

```

##      Run_Info          Sample_Name    Conc     Abs Units      Test
## 23  RESULT MSM_202209_UP_LysA_20cm 0.005178 0.189194 mg N/L Vanadium NOx
## 24  RESULT MSM_202209_UP_LysA_45cm 0.004450 0.188606 mg N/L Vanadium NOx
## 25  RESULT MSM_202209_UP_LysB_10cm -0.000600 0.184527 mg N/L Vanadium NOx
## 26  RESULT MSM_202209_UP_LysB_20cm -0.000584 0.184540 mg N/L Vanadium NOx
## 27  RESULT MSM_202209_UP_LysB_45cm  0.020174 0.201302 mg N/L Vanadium NOx
## 28  RESULT MSM_202209_UP_LysC_10cm -0.002939 0.182637 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
## 122 RESULT MSM_202209_UP_LysA_20cm 1.390346 0.896168 mg N/L Ammonia 2
## 123 RESULT MSM_202209_UP_LysA_45cm 0.681030 0.444370 mg N/L Ammonia 2

```

```

## 124  RESULT MSM_202209_UP_LysB_10cm 0.029888 0.029626 mg N/L Ammonia 2
## 125  RESULT MSM_202209_UP_LysB_20cm 0.194465 0.134453 mg N/L Ammonia 2
## 126  RESULT MSM_202209_UP_LysB_45cm 0.395437 0.262462 mg N/L Ammonia 2
## 127  RESULT MSM_202209_UP_LysC_10cm 0.375479 0.249749 mg N/L Ammonia 2
##      Conc_uM
## 122  99.262924
## 123  48.621731
## 124  2.133836
## 125  13.883713
## 126  28.231989
## 127  26.807099

```

```

P04samples$Conc_uM <- (((as.numeric(P04samples$Conc))/Con1)/N_mw)*Con2
head(P04samples)

```

	Run_Info	Sample_Name	Conc	Abs	Units	Test
## 274	RESULT MSM_202209_UP_LysA_20cm	0.015957	0.007203	mg P/L	o-PHOS	0.3
## 275	RESULT MSM_202209_UP_LysA_45cm	0.042254	0.018219	mg P/L	o-PHOS	0.3
## 276	RESULT MSM_202209_UP_LysB_10cm	0.011573	0.005367	mg P/L	o-PHOS	0.3
## 277	RESULT MSM_202209_UP_LysB_20cm	0.009140	0.004347	mg P/L	o-PHOS	0.3
## 278	RESULT MSM_202209_UP_LysB_45cm	0.039296	0.016980	mg P/L	o-PHOS	0.3
## 279	RESULT MSM_202209_UP_LysC_10cm	0.013091	0.006002	mg P/L	o-PHOS	0.3
	Conc_uM					
## 274	1.1392405					
## 275	3.0166992					
## 276	0.8262474					
## 277	0.6525449					
## 278	2.8055145					
## 279	0.9346241					

```

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

```

	Run_Info	Sample_Name	Conc	Abs	Units	Test
## 23	RESULT MSM_202209_UP_LysA_20cm	0.005178	0.189194	mg N/L	Vanadium	NOx
## 24	RESULT MSM_202209_UP_LysA_45cm	0.004450	0.188606	mg N/L	Vanadium	NOx
## 25	RESULT MSM_202209_UP_LysB_10cm	-0.000600	0.184527	mg N/L	Vanadium	NOx
## 26	RESULT MSM_202209_UP_LysB_20cm	-0.000584	0.184540	mg N/L	Vanadium	NOx
## 27	RESULT MSM_202209_UP_LysB_45cm	0.020174	0.201302	mg N/L	Vanadium	NOx
## 28	RESULT MSM_202209_UP_LysC_10cm	-0.002939	0.182637	mg N/L	Vanadium	NOx
	Conc_uM_raw					
## 23	0.36968022					
## 24	0.31770510					
## 25	-0.04283664					
## 26	-0.04169433					
## 27	1.44031071					
## 28	-0.20982815					

```

#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
## 23  RESULT MSM_202209_UP_LysA_20cm  0.005178 0.189194 mg N/L Vanadium NOx
## 24  RESULT MSM_202209_UP_LysA_45cm  0.004450 0.188606 mg N/L Vanadium NOx
## 25  RESULT MSM_202209_UP_LysB_10cm -0.000600 0.184527 mg N/L Vanadium NOx
## 26  RESULT MSM_202209_UP_LysB_20cm -0.000584 0.184540 mg N/L Vanadium NOx
## 27  RESULT MSM_202209_UP_LysB_45cm  0.020174 0.201302 mg N/L Vanadium NOx
## 28  RESULT MSM_202209_UP_LysC_10cm -0.002939 0.182637 mg N/L Vanadium NOx
##      Conc_uM_raw   Conc_uM
## 23  0.36968022 0.3696802
## 24  0.31770510 0.3177051
## 25 -0.04283664 0.0000000
## 26 -0.04169433 0.0000000
## 27  1.44031071 1.4403107
## 28 -0.20982815 0.0000000

```

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
## 122 MSM_202209_UP_LysA_20cm 1.390346 99.262924
## 123 MSM_202209_UP_LysA_45cm 0.681030 48.621731
## 124 MSM_202209_UP_LysB_10cm 0.029888 2.133836
## 125 MSM_202209_UP_LysB_20cm 0.194465 13.883713
## 126 MSM_202209_UP_LysB_45cm 0.395437 28.231989
## 127 MSM_202209_UP_LysC_10cm 0.375479 26.807099

```

```

P04_pull <- P04samples[ ,c(2,3,7) ]
head(P04_pull)

```

```

##          Sample_Name    Conc  Conc_uM
## 274 MSM_202209_UP_LysA_20cm 0.015957 1.1392405
## 275 MSM_202209_UP_LysA_45cm 0.042254 3.0166992
## 276 MSM_202209_UP_LysB_10cm 0.011573 0.8262474
## 277 MSM_202209_UP_LysB_20cm 0.009140 0.6525449
## 278 MSM_202209_UP_LysB_45cm 0.039296 2.8055145
## 279 MSM_202209_UP_LysC_10cm 0.013091 0.9346241

```

```

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

```

```

##          Sample_Name    Conc  Conc_uM
## 23  MSM_202209_UP_LysA_20cm  0.005178 0.3696802
## 24  MSM_202209_UP_LysA_45cm  0.004450 0.3177051
## 25  MSM_202209_UP_LysB_10cm -0.000600 0.0000000
## 26  MSM_202209_UP_LysB_20cm -0.000584 0.0000000
## 27  MSM_202209_UP_LysB_45cm  0.020174 1.4403107
## 28  MSM_202209_UP_LysC_10cm -0.002939 0.0000000

```

```

#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_202209_SW_A 0.267645 19.108355 0.065339 4.6648390 0.018448
## 2      GCrew_202209_SW_B 0.174531 12.460537 0.060568 4.3242163 0.004947
## 3      GCrew_202209_SW_C 0.095026  6.784325 0.038633 2.7581800 0.009035
## 4 GCrew_202209_TR_LysA_20cm 0.288862 20.623130 0.007691 0.5490944        NA
## 5 GCrew_202209_TR_LysA_45cm 0.110145  7.863737 0.008317 0.5937873        NA
## 6 GCrew_202209_TR_LysB_10cm 0.454608 32.456467 0.007700 0.5497369 0.006141
##           Conc_uM
## 1 1.3170840
## 2 0.3531881
## 3 0.6450484
## 4       NA
## 5       NA
## 6 0.4384330

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_202209_SW_A 0.267645 19.108355 0.065339 4.6648390 0.018448
## 2      GCrew_202209_SW_B 0.174531 12.460537 0.060568 4.3242163 0.004947
## 3      GCrew_202209_SW_C 0.095026  6.784325 0.038633 2.7581800 0.009035
## 4 GCrew_202209_TR_LysA_20cm 0.288862 20.623130 0.007691 0.5490944        NA
## 5 GCrew_202209_TR_LysA_45cm 0.110145  7.863737 0.008317 0.5937873        NA
## 6 GCrew_202209_TR_LysB_10cm 0.454608 32.456467 0.007700 0.5497369 0.006141
##           NOx_uM
## 1 1.3170840
## 2 0.3531881
## 3 0.6450484
## 4       NA
## 5       NA
## 6 0.4384330

#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$NH3_mgL>2, "adl", "Within_R"))
all_data$PO4_range <- ifelse(all_data$PO4_mgL<0.003, "bdl", ifelse(all_data$PO4_mgL>3, "adl", "Within_R"))
all_data$NOx_range <- ifelse(all_data$NOx_mgL<0.025, "bdl", ifelse(all_data$NOx_mgL>1, "adl", "Within_R"))
head(all_data)

##           Sample_Name NH3_mgL   NH3_uM  PO4_mgL   PO4_uM  NOx_mgL
## 1      GCrew_202209_SW_A 0.267645 19.108355 0.065339 4.6648390 0.018448
## 2      GCrew_202209_SW_B 0.174531 12.460537 0.060568 4.3242163 0.004947
## 3      GCrew_202209_SW_C 0.095026  6.784325 0.038633 2.7581800 0.009035
## 4 GCrew_202209_TR_LysA_20cm 0.288862 20.623130 0.007691 0.5490944        NA
## 5 GCrew_202209_TR_LysA_45cm 0.110145  7.863737 0.008317 0.5937873        NA
## 6 GCrew_202209_TR_LysB_10cm 0.454608 32.456467 0.007700 0.5497369 0.006141
##           NOx_uM   NH3_range   PO4_range NOx_range
```

```

## 1 1.3170840 Within_Range Within_Range      bdl
## 2 0.3531881 Within_Range Within_Range      bdl
## 3 0.6450484 Within_Range Within_Range      bdl
## 4       NA Within_Range Within_Range <NA>
## 5       NA Within_Range Within_Range <NA>
## 6 0.4384330 Within_Range Within_Range      bdl

```

Take an initial look at concentrations

```

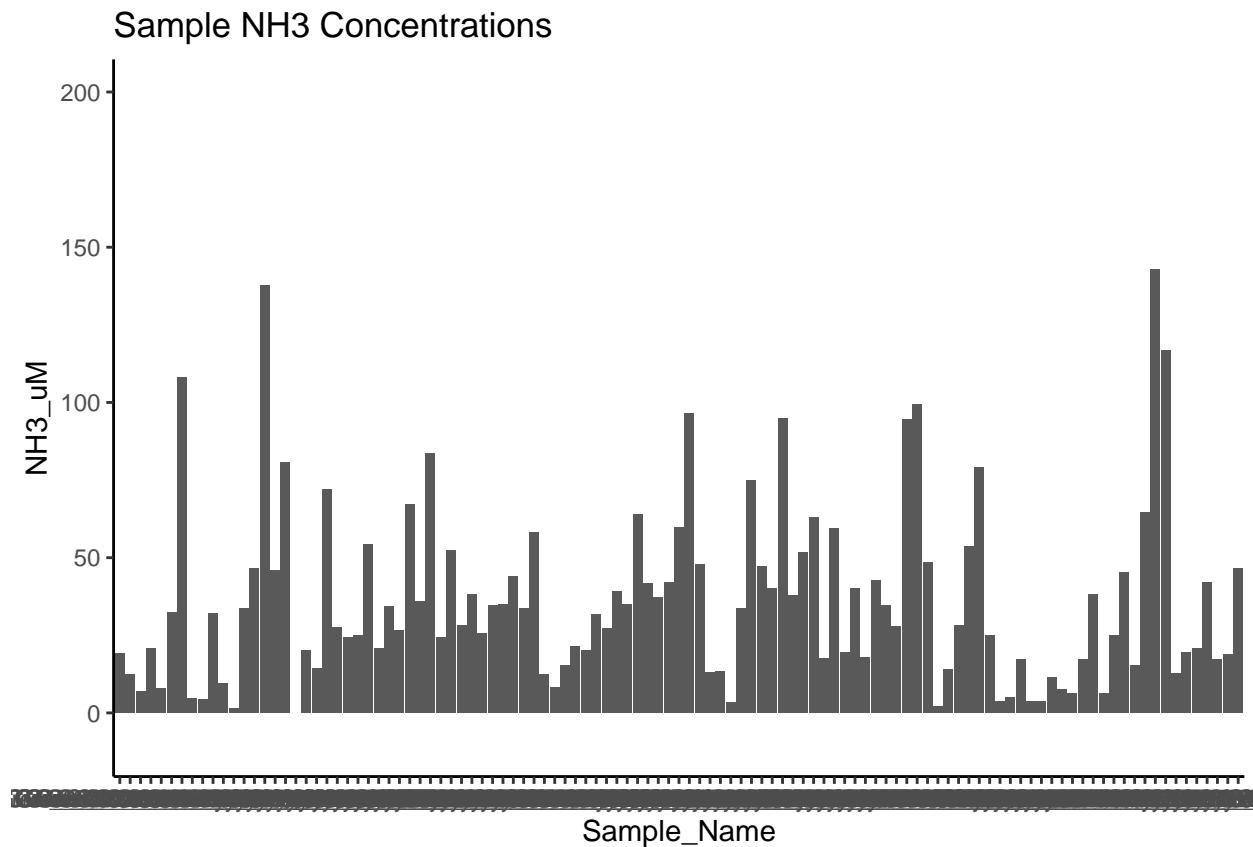
#plot data to get a sense of any outliers
NH3look <- ggplot(data=all_data, aes(x=Sample_Name, y=NH3_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-10, 200) +
  theme(legend.position="none") +
  ggtitle("Sample NH3 Concentrations")
NH3look

```

```

## Warning: Removed 7 rows containing missing values or values outside the scale range
## ('geom_bar()').

```



```

P04look <- ggplot(data=all_data, aes(x=Sample_Name, y=P04_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 50) +

```

```

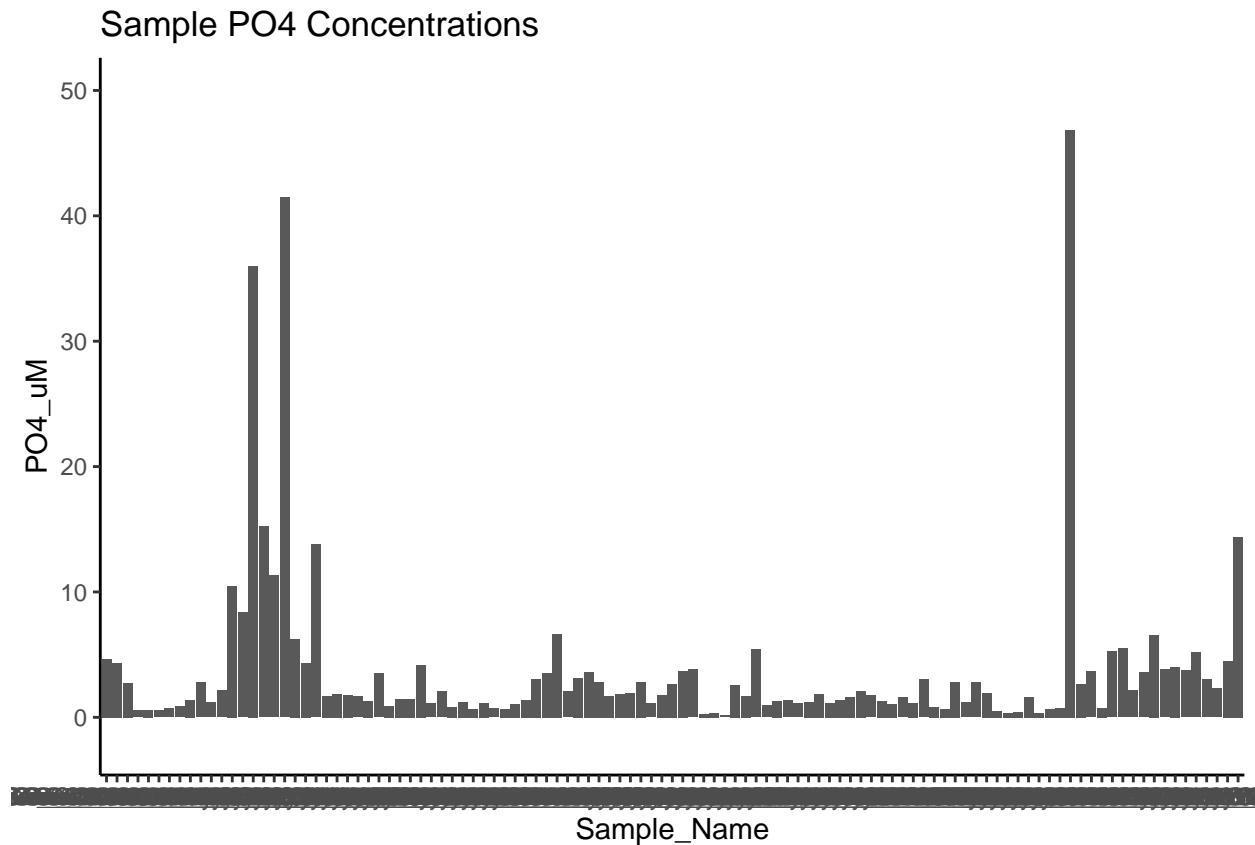
theme(legend.position="none") +
ggtitle("Sample PO4 Concentrations")
P04look

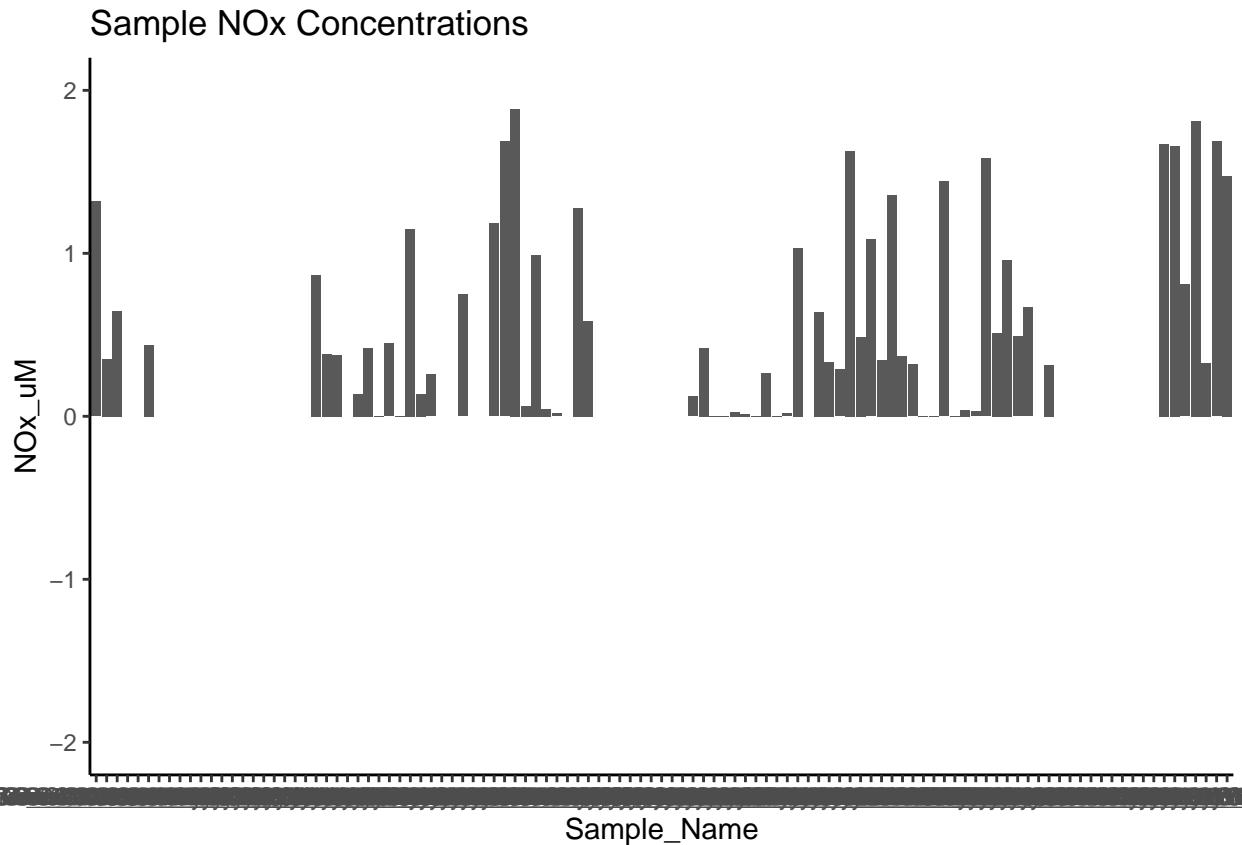
```

```

## Warning: Removed 5 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  P04_mgL    P04_uM  NOx_mgL
## 1      GCrew_202209_SW_A 0.267645 19.108355 0.065339 4.6648390 0.018448
## 2      GCrew_202209_SW_B 0.174531 12.460537 0.060568 4.3242163 0.004947
## 3      GCrew_202209_SW_C 0.095026  6.784325 0.038633 2.7581800 0.009035
## 4 GCrew_202209_TR_LysA_20cm 0.288862 20.623130 0.007691 0.5490944      NA
## 5 GCrew_202209_TR_LysA_45cm 0.110145  7.863737 0.008317 0.5937873      NA
## 6 GCrew_202209_TR_LysB_10cm 0.454608 32.456467 0.007700 0.5497369 0.006141
##       NOx_uM    NH3_range    P04_range NOx_range
## 1 1.3170840 Within_Range Within_Range      bdl
## 2 0.3531881 Within_Range Within_Range      bdl
## 3 0.6450484 Within_Range Within_Range      bdl
## 4      NA Within_Range Within_Range     <NA>
## 5      NA Within_Range Within_Range     <NA>
## 6 0.4384330 Within_Range Within_Range      bdl
```

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

##	Sample_Name	NH3_uM	P04_uM	NOx_uM	NH3_range
----	-------------	--------	--------	--------	-----------

```

## 1      GCrew_202209_SW_A 19.108355 4.6648390 1.3170840 Within_Range
## 2      GCrew_202209_SW_B 12.460537 4.3242163 0.3531881 Within_Range
## 3      GCrew_202209_SW_C  6.784325 2.7581800 0.6450484 Within_Range
## 4 GCrew_202209_TR_LysA_20cm 20.623130 0.5490944          NA Within_Range
## 5 GCrew_202209_TR_LysA_45cm  7.863737 0.5937873          NA Within_Range
## 6 GCrew_202209_TR_LysB_10cm 32.456467 0.5497369 0.4384330 Within_Range
##      P04_range NOx_range
## 1 Within_Range      bdl
## 2 Within_Range      bdl
## 3 Within_Range      bdl
## 4 Within_Range      <NA>
## 5 Within_Range      <NA>
## 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", "202209", "SW", "A"), c("GCrew", "202209", "SW", :
## number of columns of result is not a multiple of vector length (arg 1)

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

##   Site Date Zone Replicate Depth Tree Month
## 1 GCrew 202209 SW      A GCrew 202209 September
## 2 GCrew 202209 SW      B GCrew 202209 September
## 3 GCrew 202209 SW      C GCrew 202209 September
## 4 GCrew 202209 TR      LysA  20cm GCrew September
## 5 GCrew 202209 TR      LysA  45cm GCrew September
## 6 GCrew 202209 TR      LysB  10cm GCrew September

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

##   Site Date Zone Replicate Depth Tree Month Sample_Name
## 1 GCrew 202209 SW      A GCrew 202209 September GCrew_202209_SW_A
## 2 GCrew 202209 SW      B GCrew 202209 September GCrew_202209_SW_B
## 3 GCrew 202209 SW      C GCrew 202209 September GCrew_202209_SW_C
## 4 GCrew 202209 TR      LysA  20cm GCrew September GCrew_202209_TR_LysA_20cm
## 5 GCrew 202209 TR      LysA  45cm GCrew September GCrew_202209_TR_LysA_45cm
## 6 GCrew 202209 TR      LysB  10cm GCrew September GCrew_202209_TR_LysB_10cm
##      NH3_uM P04_uM NOx_uM NH3_range P04_range NOx_range
## 1 19.108355 4.6648390 1.3170840 Within_Range Within_Range      bdl
## 2 12.460537 4.3242163 0.3531881 Within_Range Within_Range      bdl
## 3 6.784325 2.7581800 0.6450484 Within_Range Within_Range      bdl
## 4 20.623130 0.5490944          NA Within_Range Within_Range      <NA>
## 5 7.863737 0.5937873          NA Within_Range Within_Range      <NA>
## 6 32.456467 0.5497369 0.4384330 Within_Range Within_Range      bdl

```

Export final data with flags

```
#Export Data  
  
write.csv(alldat, file="Processed Data/COMPASS_SynopticCB_Nutrients_202209.csv")
```