

COMPASS_Synoptic_SEAL_Data_Analysis_Aug2022

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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)

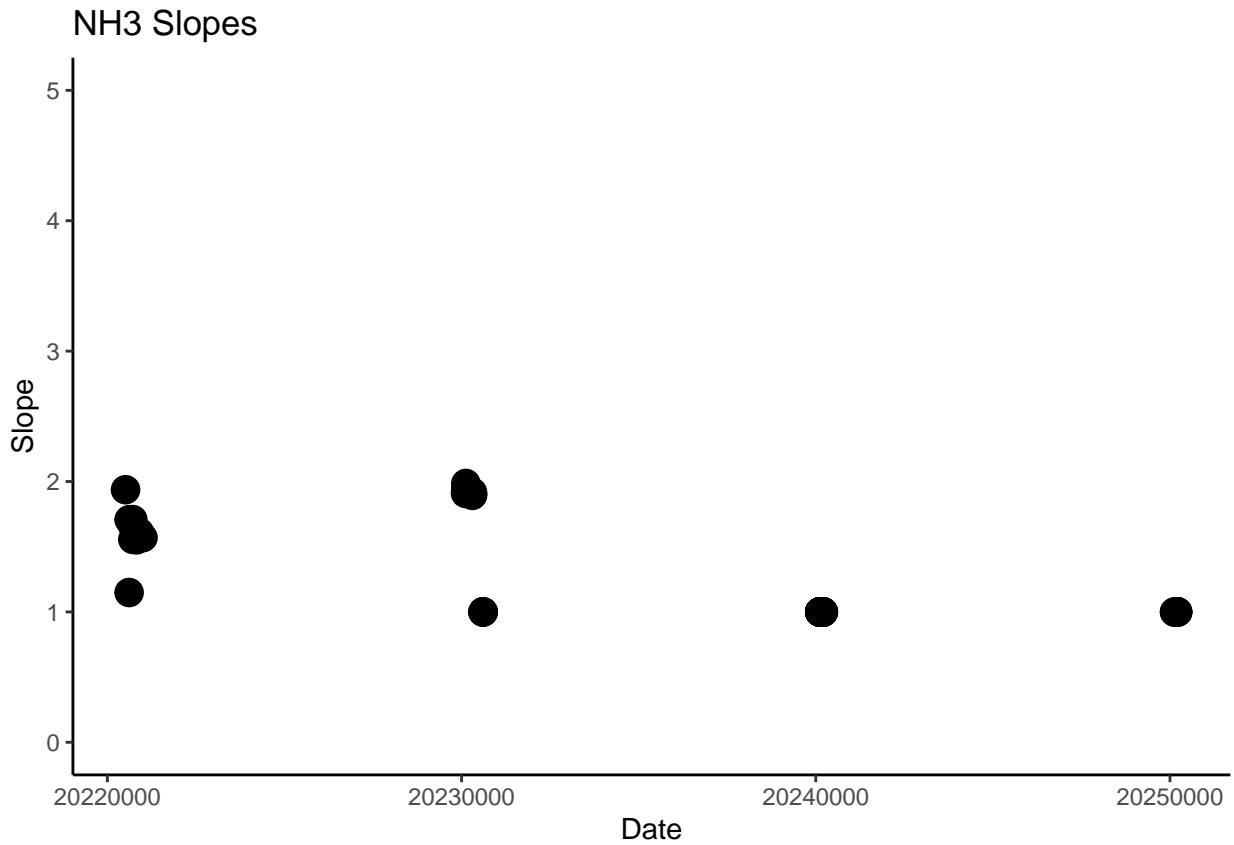
##           Date      User Machine Analysis Slope Intercept     R2
## 3 20220525 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9990
## 6 20220615 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9998
## 9 20220718 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9999
## 16 20220730 Stephanie Wilson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

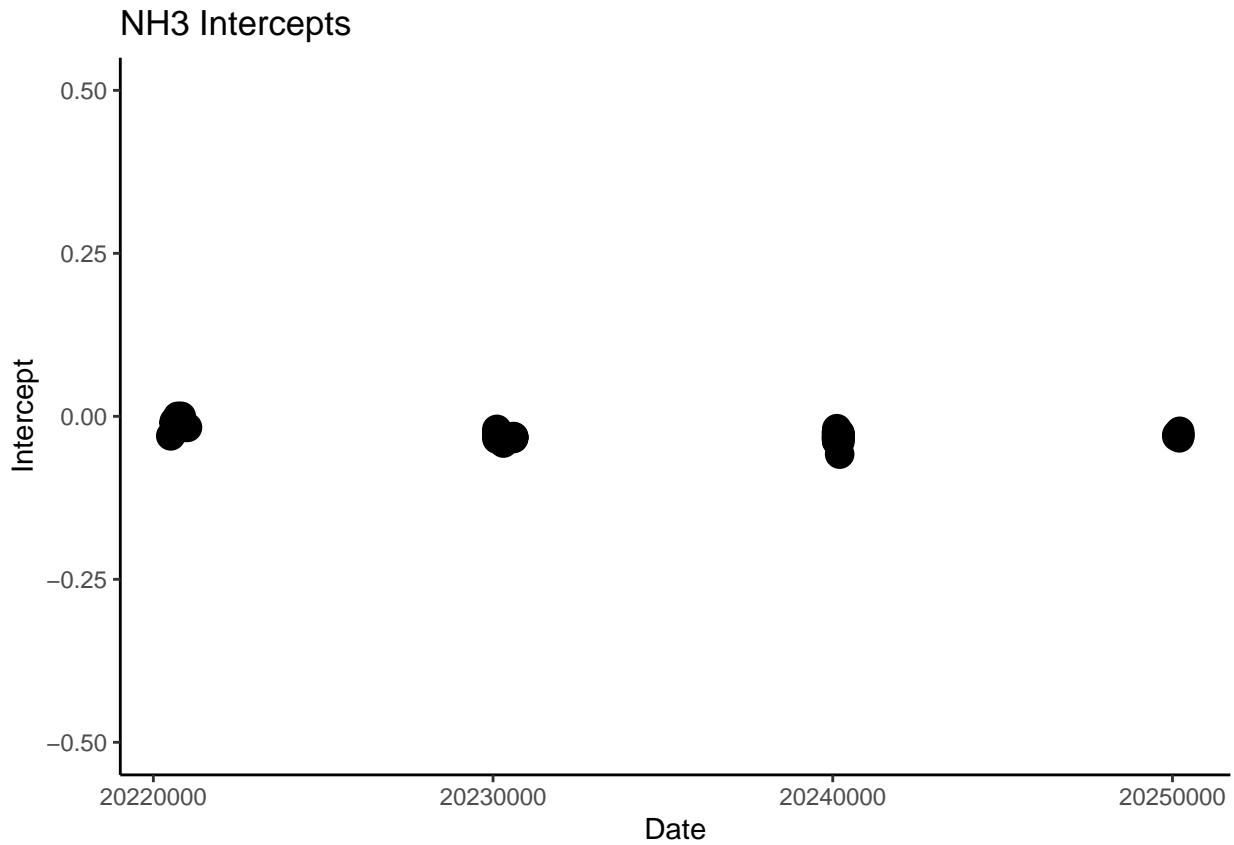
```



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

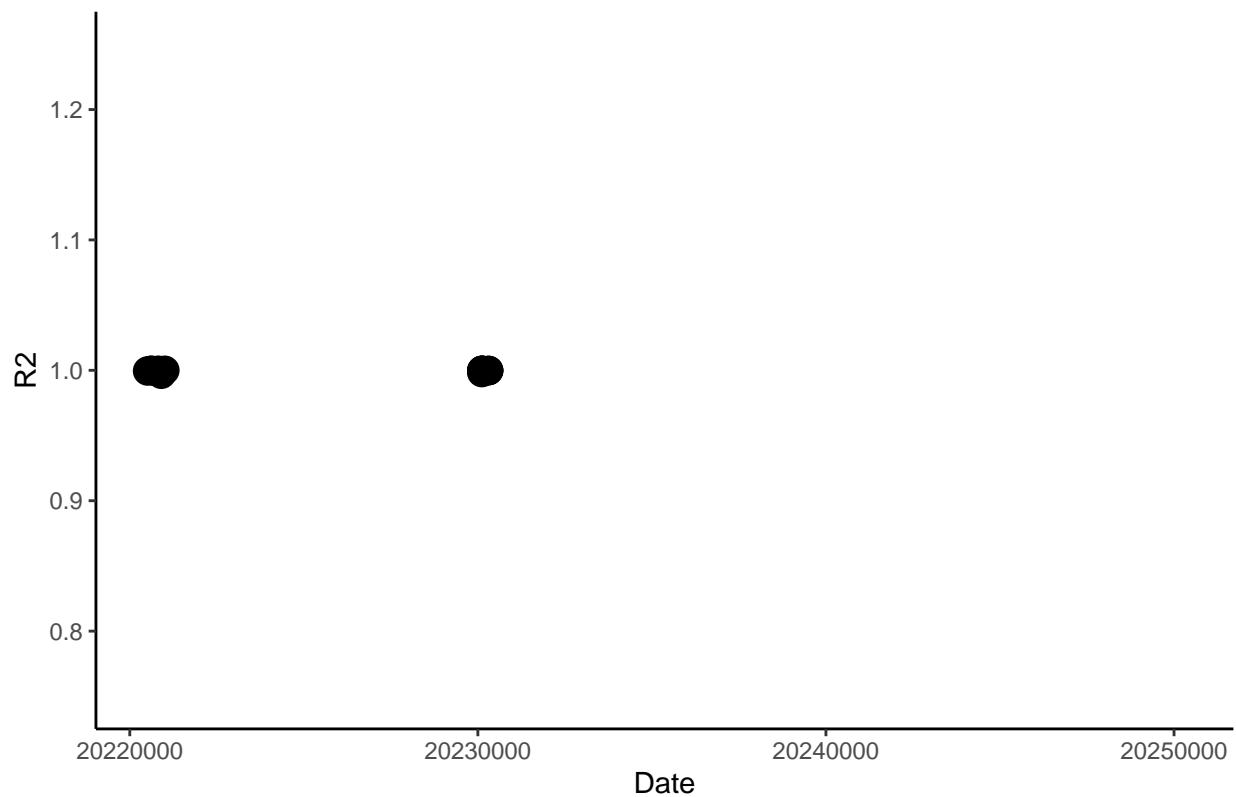


```
#plot the R2s to make sure there are no crazy outliers
Rsq1 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NH3 R2s")
```

```
Rsq1
```

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

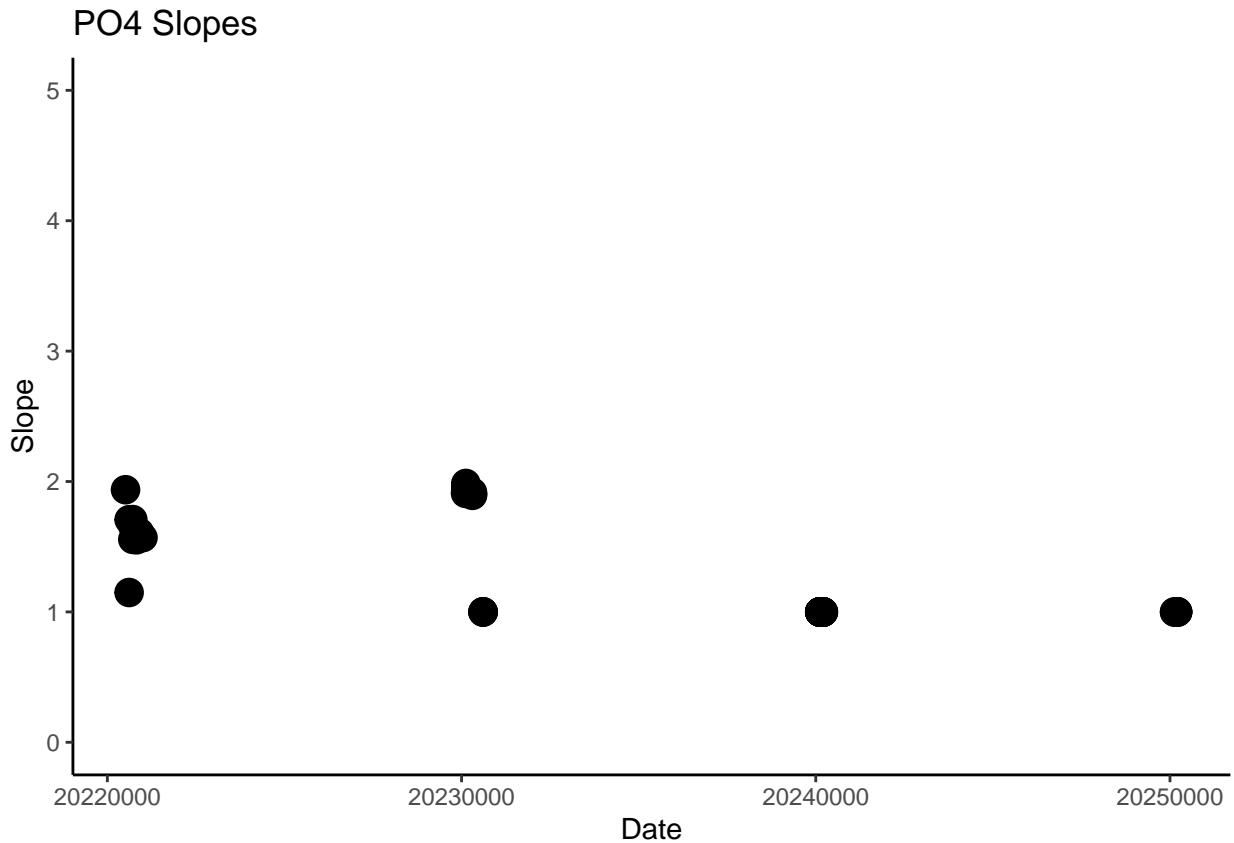
NH3 R2s



```
##### 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
```

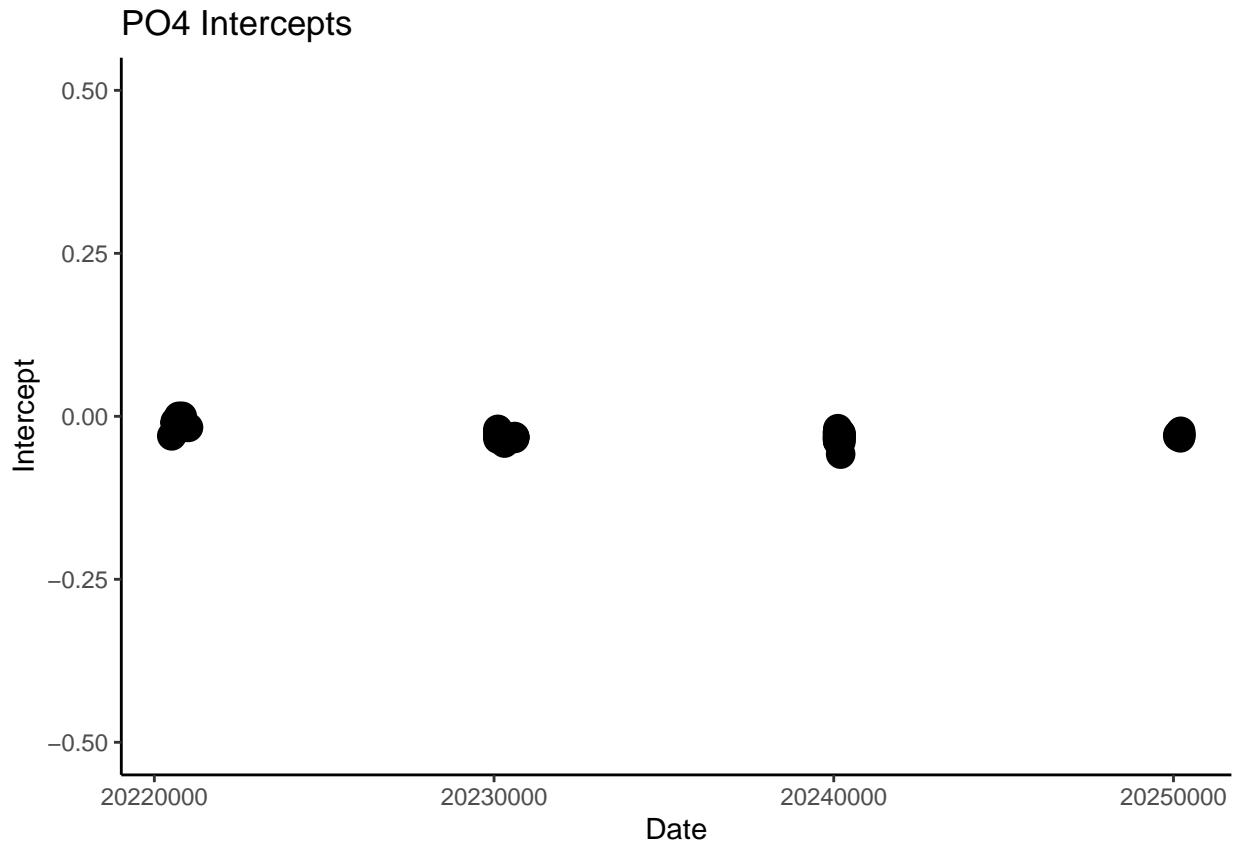
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

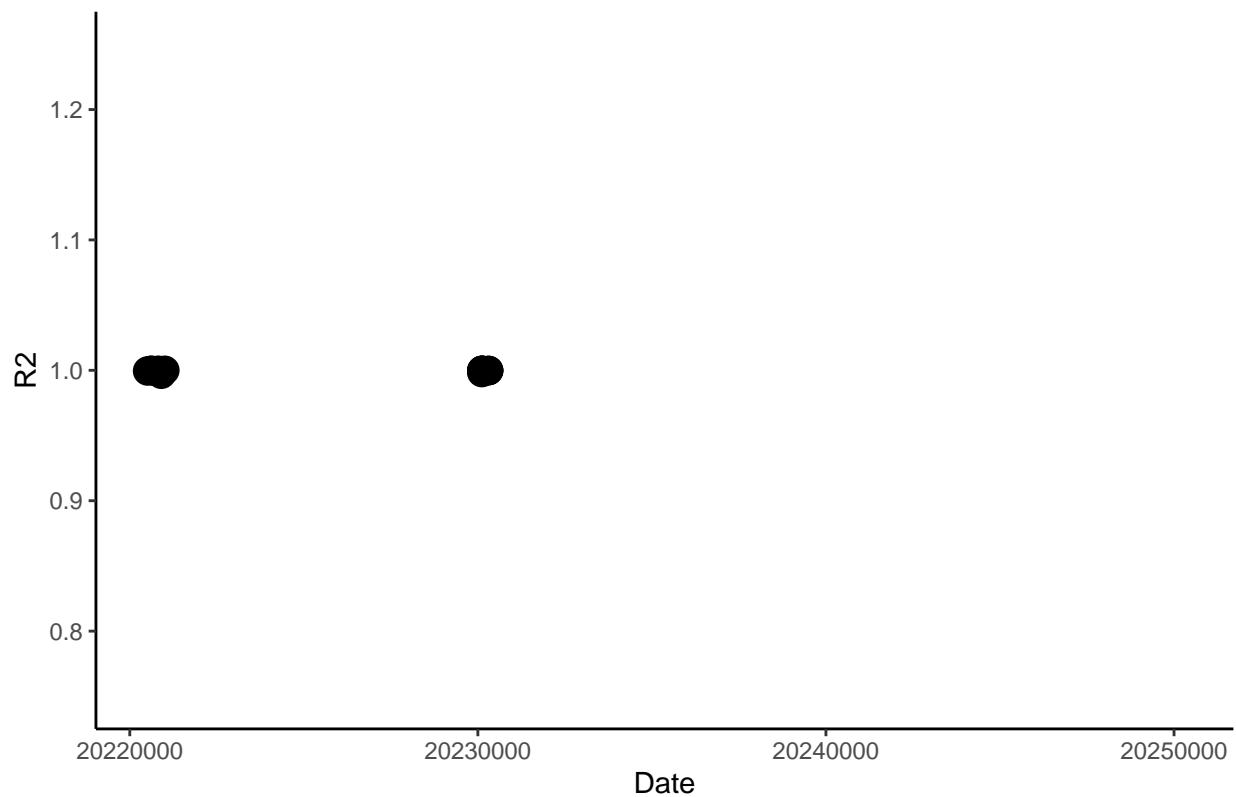


```
#plot the R2s to make sure there are no crazy outliers
Rsq2 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("P04 R2s")
```

```
Rsq2
```

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

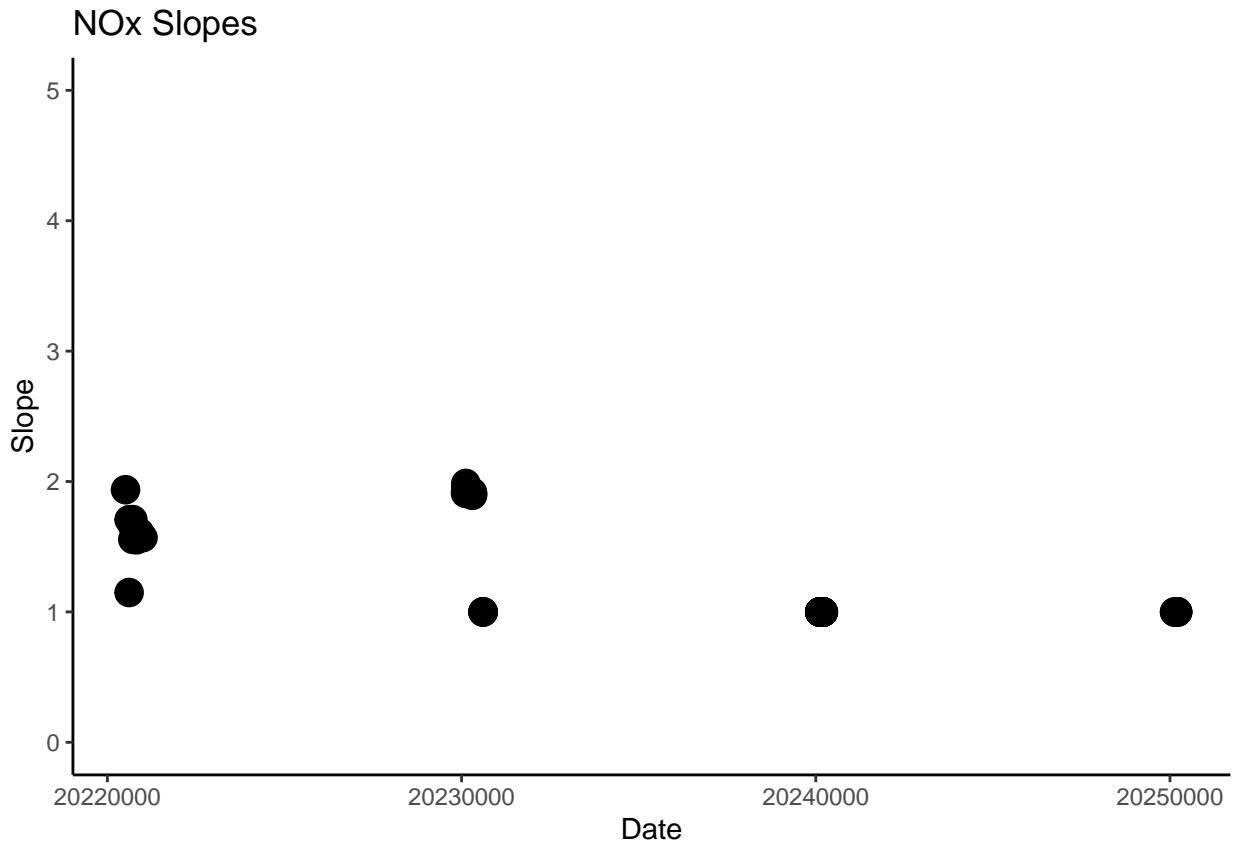
PO4 R2s



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

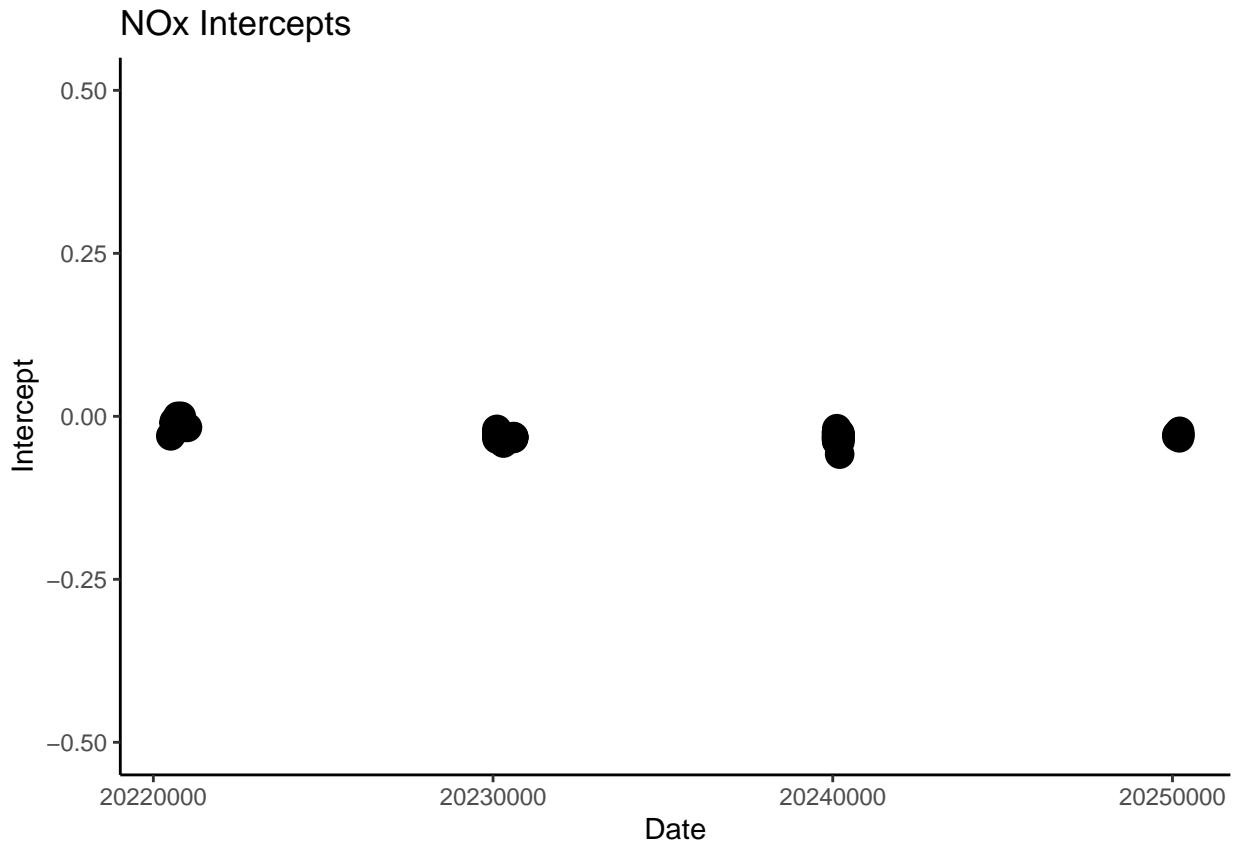
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

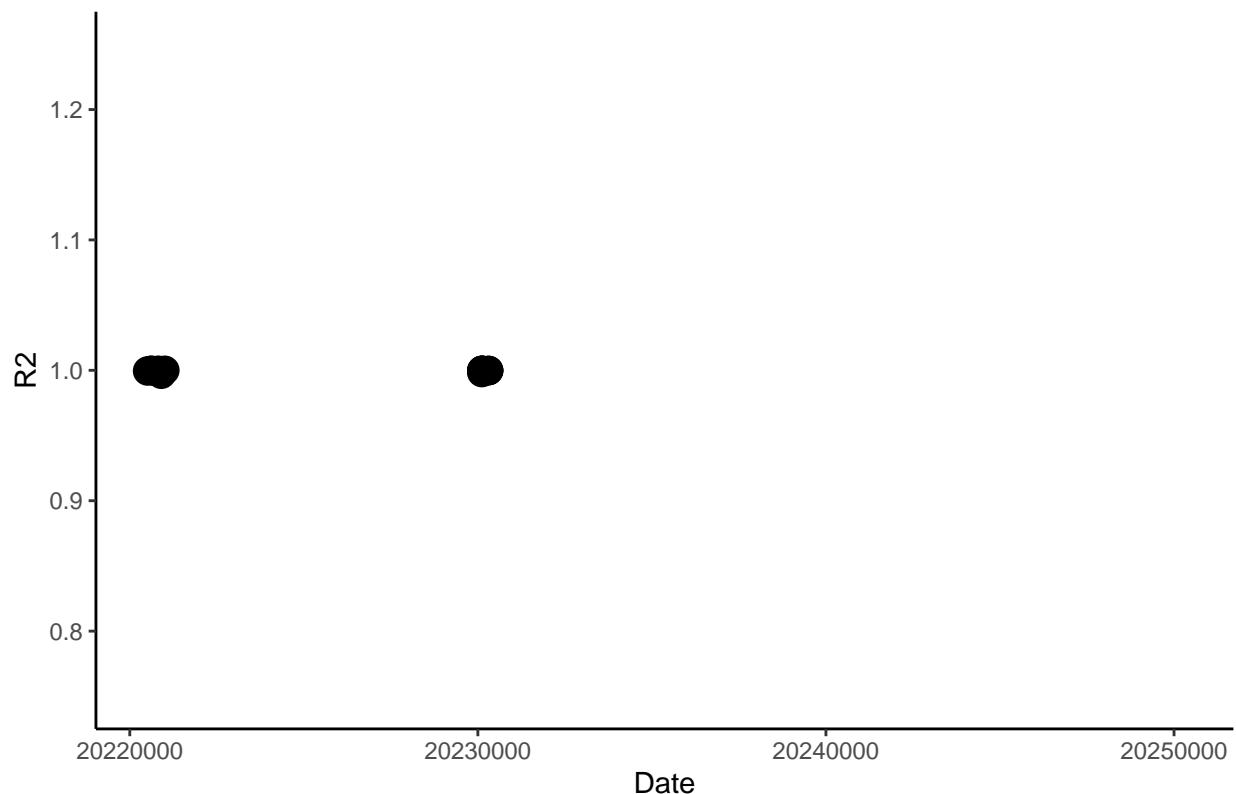


```
#plot the R2s to make sure there are no crazy outliers
Rsq3 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NOx R2s")
```

```
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_202208_1.csv")
#Quick look at dataframe
head(file1)

##    RUNSTARTED X1661176810 X8.22.2022.10.00          X X.1      X.2      X.3
## 1      RESULT      -1           S1 Standard 1  0 0.004353 0.004353
## 2      RESULT      -2           S90 Standard .0389  1 0.029444 0.029444
## 3      RESULT      -2           S91 Standard .1000  2 0.067392 0.067392
## 4      RESULT      -2           S92 Standard .2000  3 0.127815 0.127815
## 5      RESULT      -2           S93 Standard .5000  4 0.314373 0.314373
## 6      RESULT      -2           S94 Standard 1.0000  5 0.642907 0.642907
##    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 1661178089 8/22/2022 10:21
## 2  0  0  0  0 mg N/L Ammonia 2 1661178249 8/22/2022 10:24
## 3  0  0  0  0 mg N/L Ammonia 2 1661178409 8/22/2022 10:26
## 4  0  0  0  0 mg N/L Ammonia 2 1661178569 8/22/2022 10:29
## 5  0  0  0  0 mg N/L Ammonia 2 1661178729 8/22/2022 10:32
## 6  0  0  0  0 mg N/L Ammonia 2 1661178889 8/22/2022 10:34

#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 0.004353 0.004353 mg N/L Ammonia 2
## 2   RESULT      Standard .0389 0.029444 0.029444 mg N/L Ammonia 2
## 3   RESULT      Standard .1000 0.067392 0.067392 mg N/L Ammonia 2
## 4   RESULT      Standard .2000 0.127815 0.127815 mg N/L Ammonia 2
## 5   RESULT      Standard .5000 0.314373 0.314373 mg N/L Ammonia 2
## 6   RESULT      Standard 1.0000 0.642907 0.642907 mg N/L Ammonia 2

#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202208_2.csv")
#Quick look at dataframe
head(file2)

##   RUNSTARTED X1661199121 X8.22.2022.16.12          X X.1      X.2      X.3
## 1   RESULT      -1           S1      Standard 1 0 0.004933 0.004933
## 2   RESULT      -2           S90     Standard .0389 1 0.031041 0.031041
## 3   RESULT      -2           S91     Standard .1000 2 0.065687 0.065687
## 4   RESULT      -2           S92     Standard .2000 3 0.128546 0.128546
## 5   RESULT      -2           S93     Standard .5000 4 0.310806 0.310806
## 6   RESULT      -2           S94     Standard 1.0000 5 0.624441 0.624441
##   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 1661200356 8/22/2022 16:32
## 2   0   0   0   0   mg N/L Ammonia 2 1661200516 8/22/2022 16:35
## 3   0   0   0   0   mg N/L Ammonia 2 1661200676 8/22/2022 16:37
## 4   0   0   0   0   mg N/L Ammonia 2 1661200836 8/22/2022 16:40
## 5   0   0   0   0   mg N/L Ammonia 2 1661200996 8/22/2022 16:43
## 6   0   0   0   0   mg N/L Ammonia 2 1661201156 8/22/2022 16:45

#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 0.004933 0.004933 mg N/L Ammonia 2
## 2   RESULT      Standard .0389 0.031041 0.031041 mg N/L Ammonia 2
## 3   RESULT      Standard .1000 0.065687 0.065687 mg N/L Ammonia 2
## 4   RESULT      Standard .2000 0.128546 0.128546 mg N/L Ammonia 2
## 5   RESULT      Standard .5000 0.310806 0.310806 mg N/L Ammonia 2
## 6   RESULT      Standard 1.0000 0.624441 0.624441 mg N/L Ammonia 2

#read in data
file3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202208_3.csv")
#Quick look at dataframe
head(file3)

##   RUNSTARTED X1662562456 X9.7.2022.10.54          X X.1      X.2      X.3
## 1   RESULT      -1           S1      Standard 1 0 0.010229 0.010229
## 2   RESULT      -2           S90     Standard .0389 1 0.035526 0.035526
## 3   RESULT      -2           S91     Standard .1000 2 0.074637 0.074637
## 4   RESULT      -2           S92     Standard .2000 3 0.134298 0.134298

```

```

## 5      RESULT          -2           S93 Standard .5000   4 0.322347 0.322347
## 6      RESULT          -2           S94 Standard 1.0000   5 0.636797 0.636797
## 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 1662563717 9/7/2022 11:15
## 2  0  0  0  0 mg N/L Ammonia 2 1662563877 9/7/2022 11:17
## 3  0  0  0  0 mg N/L Ammonia 2 1662564037 9/7/2022 11:20
## 4  0  0  0  0 mg N/L Ammonia 2 1662564197 9/7/2022 11:23
## 5  0  0  0  0 mg N/L Ammonia 2 1662564357 9/7/2022 11:25
## 6  0  0  0  0 mg N/L Ammonia 2 1662564517 9/7/2022 11:28

```

```

#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 0.010229 0.010229 mg N/L Ammonia 2
## 2  RESULT      Standard .0389 0.035526 0.035526 mg N/L Ammonia 2
## 3  RESULT      Standard .1000 0.074637 0.074637 mg N/L Ammonia 2
## 4  RESULT      Standard .2000 0.134298 0.134298 mg N/L Ammonia 2
## 5  RESULT      Standard .5000 0.322347 0.322347 mg N/L Ammonia 2
## 6  RESULT      Standard 1.0000 0.636797 0.636797 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 0.004353 0.004353 mg N/L Ammonia 2
## 2  RESULT      Standard .0389 0.029444 0.029444 mg N/L Ammonia 2
## 3  RESULT      Standard .1000 0.067392 0.067392 mg N/L Ammonia 2
## 4  RESULT      Standard .2000 0.127815 0.127815 mg N/L Ammonia 2
## 5  RESULT      Standard .5000 0.314373 0.314373 mg N/L Ammonia 2
## 6  RESULT      Standard 1.0000 0.642907 0.642907 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
## 653  RESULT MSM_202208_UP_LysA_20cm 1.751941 1.099048 mg N/L Ammonia 2
## 654  RESULT MSM_202208_UP_LysA_45cm 0.970558 0.613498 mg N/L Ammonia 2
## 655  RESULT MSM_202208_UP_LysB_10cm 0.067022 0.052042 mg N/L Ammonia 2
## 656  RESULT MSM_202208_UP_LysB_20cm 0.289288 0.190158 mg N/L Ammonia 2
## 657  RESULT MSM_202208_UP_LysB_45cm 0.495821 0.318497 mg N/L Ammonia 2
## 658  RESULT MSM_202208_UP_LysC_10cm 0.566208 0.362236 mg N/L Ammonia 2

```

NOx

```
#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202208_1.csv")
#Quick look at dataframe
head(Nfile1)
```

```
##    RUNSTARTED X1661365293      X8.24.2022.14.21          X X.1      X.2      X.3
## 1    RUNENDED  1661365463 INSUFFICIENT REAGENT          NA      NA      NA
## 2  RUNSTARTED  1661365472      8/24/2022 14:24          NA      NA      NA
## 3    RESULT      -1          S1 Standard 1  0 0.158878 0.158878
## 4    RESULT      -2          S90 Standard 90  1 0.173292 0.173292
## 5    RESULT      -2          S91 Standard 91  2 0.196489 0.196489
## 6    RESULT      -2          S92 Standard 92  3 0.236722 0.236722
##    X.4 X.5 X.6 X.7      X.8          X.9      X.10          X.11
## 1  NA  NA  NA  NA          NA          NA
## 2  NA  NA  NA  NA          NA          NA
## 3  0   0   0 512 mg N/L Vanadium NOx 1661367660 8/24/2022 15:01
## 4  0   0   0 512 mg N/L Vanadium NOx 1661367741 8/24/2022 15:02
## 5  0   0   0 512 mg N/L Vanadium NOx 1661367822 8/24/2022 15:03
## 6  0   0   0 512 mg N/L Vanadium NOx 1661367903 8/24/2022 15:05
```

```
#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 0.158878 0.158878 mg N/L Vanadium NOx
## 4    RESULT Standard 90 0.173292 0.173292 mg N/L Vanadium NOx
## 5    RESULT Standard 91 0.196489 0.196489 mg N/L Vanadium NOx
## 6    RESULT Standard 92 0.236722 0.236722 mg N/L Vanadium NOx
```

```
#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202208_2.csv")
#Quick look at dataframe
head(Nfile2)
```

```
##    RUNSTARTED X1661365293      X8.24.2022.14.21          X X.1      X.2      X.3
## 1    RUNENDED  1661365463 INSUFFICIENT REAGENT          NA      NA      NA
## 2  RUNSTARTED  1661365472      8/24/2022 14:24          NA      NA      NA
## 3    RESULT      -1          S1 Standard 1  0 0.158878 0.158878
## 4    RESULT      -2          S90 Standard 90  1 0.173292 0.173292
## 5    RESULT      -2          S91 Standard 91  2 0.196489 0.196489
## 6    RESULT      -2          S92 Standard 92  3 0.236722 0.236722
##    X.4 X.5 X.6 X.7      X.8          X.9      X.10          X.11
## 1  NA  NA  NA  NA          NA          NA
## 2  NA  NA  NA  NA          NA          NA
```

```

## 3 0 0 0 512 mg N/L Vanadium NOx 1661367660 8/24/2022 15:01
## 4 0 0 0 512 mg N/L Vanadium NOx 1661367741 8/24/2022 15:02
## 5 0 0 0 512 mg N/L Vanadium NOx 1661367822 8/24/2022 15:03
## 6 0 0 0 512 mg N/L Vanadium NOx 1661367903 8/24/2022 15:05

#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 RUNENDED NA NA
## 2 RUNSTARTED NA NA
## 3 RESULT Standard 1 0.158878 0.158878 mg N/L Vanadium NOx
## 4 RESULT Standard 90 0.173292 0.173292 mg N/L Vanadium NOx
## 5 RESULT Standard 91 0.196489 0.196489 mg N/L Vanadium NOx
## 6 RESULT Standard 92 0.236722 0.236722 mg N/L Vanadium NOx

```

```

#read in data
Nfile3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202208_3.csv")
#Quick look at dataframe
head(Nfile3)

```

```

## RUNSTARTED X1662589677 X9.7.2022.18.27 X X.1 X.2 X.3 X.4
## 1 RESULT -1 S1 Standard 1 0 0.132385 0.132385 0
## 2 RESULT -2 S90 Standard 90 1 0.150861 0.150861 0
## 3 RESULT -2 S91 Standard 91 2 0.176037 0.176037 0
## 4 RESULT -2 S92 Standard 92 3 0.214585 0.214585 0
## 5 RESULT -2 S93 Standard 93 4 0.336491 0.336491 0
## 6 RESULT -2 S94 Standard 94 5 0.533887 0.533887 0
## X.5 X.6 X.7 X.8 X.9 X.10 X.11
## 1 0 0 0 mg N/L Vanadium NOx 1662591874 9/7/2022 19:04
## 2 0 0 0 mg N/L Vanadium NOx 1662591956 9/7/2022 19:05
## 3 0 0 0 mg N/L Vanadium NOx 1662592037 9/7/2022 19:07
## 4 0 0 0 mg N/L Vanadium NOx 1662592118 9/7/2022 19:08
## 5 0 0 0 mg N/L Vanadium NOx 1662592199 9/7/2022 19:09
## 6 0 0 0 mg N/L Vanadium NOx 1662592280 9/7/2022 19:11

```

```

#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 RESULT Standard 1 0.132385 0.132385 mg N/L Vanadium NOx
## 2 RESULT Standard 90 0.150861 0.150861 mg N/L Vanadium NOx
## 3 RESULT Standard 91 0.176037 0.176037 mg N/L Vanadium NOx
## 4 RESULT Standard 92 0.214585 0.214585 mg N/L Vanadium NOx
## 5 RESULT Standard 93 0.336491 0.336491 mg N/L Vanadium NOx
## 6 RESULT Standard 94 0.533887 0.533887 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 0.158878 0.158878 mg N/L Vanadium NOx
## 4   RESULT Standard 90 0.173292 0.173292 mg N/L Vanadium NOx
## 5   RESULT Standard 91 0.196489 0.196489 mg N/L Vanadium NOx
## 6   RESULT Standard 92 0.236722 0.236722 mg N/L Vanadium NOx
## 7   RESULT Standard 93 0.362256 0.362256 mg N/L Vanadium NOx
## 8   RESULT Standard 94 0.575194 0.575194 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
## 303  RESULT MSM_202208_UP_LysA_20cm 0.004871 0.137970 mg N/L Vanadium NOx
## 304  RESULT MSM_202208_UP_LysA_45cm 0.004033 0.137299 mg N/L Vanadium NOx
## 305  RESULT MSM_202208_UP_LysB_10cm 0.004512 0.137682 mg N/L Vanadium NOx
## 306  RESULT MSM_202208_UP_LysB_20cm 0.004184 0.137420 mg N/L Vanadium NOx
## 307  RESULT MSM_202208_UP_LysB_45cm 0.003101 0.136551 mg N/L Vanadium NOx
## 308  RESULT MSM_202208_UP_LysC_10cm 0.004130 0.137376 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
## 653  RESULT MSM_202208_UP_LysA_20cm 1.751941 1.099048 mg N/L Ammonia 2
## 654  RESULT MSM_202208_UP_LysA_45cm 0.970558 0.613498 mg N/L Ammonia 2
## 655  RESULT MSM_202208_UP_LysB_10cm 0.067022 0.052042 mg N/L Ammonia 2
## 656  RESULT MSM_202208_UP_LysB_20cm 0.289288 0.190158 mg N/L Ammonia 2
## 657  RESULT MSM_202208_UP_LysB_45cm 0.495821 0.318497 mg N/L Ammonia 2
## 658  RESULT MSM_202208_UP_LysC_10cm 0.566208 0.362236 mg N/L Ammonia 2

```

```
head(Nalldat2)
```

```
##     Run_Info             Sample_Name    Conc      Abs  Units      Test
## 303   RESULT MSM_202208_UP_LysA_20cm 0.004871 0.137970 mg N/L Vanadium NOx
## 304   RESULT MSM_202208_UP_LysA_45cm 0.004033 0.137299 mg N/L Vanadium NOx
## 305   RESULT MSM_202208_UP_LysB_10cm 0.004512 0.137682 mg N/L Vanadium NOx
## 306   RESULT MSM_202208_UP_LysB_20cm 0.004184 0.137420 mg N/L Vanadium NOx
## 307   RESULT MSM_202208_UP_LysB_45cm 0.003101 0.136551 mg N/L Vanadium NOx
## 308   RESULT MSM_202208_UP_LysC_10cm 0.004130 0.137376 mg N/L Vanadium NOx
```

```
#subset by test
```

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

```
##     Run_Info             Sample_Name    Conc      Abs  Units      Test
## 653   RESULT MSM_202208_UP_LysA_20cm 1.751941 1.099048 mg N/L Ammonia 2
## 654   RESULT MSM_202208_UP_LysA_45cm 0.970558 0.613498 mg N/L Ammonia 2
## 655   RESULT MSM_202208_UP_LysB_10cm 0.067022 0.052042 mg N/L Ammonia 2
## 656   RESULT MSM_202208_UP_LysB_20cm 0.289288 0.190158 mg N/L Ammonia 2
## 657   RESULT MSM_202208_UP_LysB_45cm 0.495821 0.318497 mg N/L Ammonia 2
## 658   RESULT MSM_202208_UP_LysC_10cm 0.566208 0.362236 mg N/L Ammonia 2
```

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

```
##     Run_Info             Sample_Name    Conc      Abs  Units      Test
## 813   RESULT MSM_202208_UP_LysA_20cm 0.040826 0.018384 mg P/L o-PHOS 0.3
## 814   RESULT MSM_202208_UP_LysA_45cm 0.044884 0.020104 mg P/L o-PHOS 0.3
## 815   RESULT MSM_202208_UP_LysB_10cm 0.023058 0.010857 mg P/L o-PHOS 0.3
## 816   RESULT MSM_202208_UP_LysB_20cm 0.016900 0.008248 mg P/L o-PHOS 0.3
## 817   RESULT MSM_202208_UP_LysB_45cm 0.060440 0.026694 mg P/L o-PHOS 0.3
## 818   RESULT MSM_202208_UP_LysC_10cm 0.025075 0.011711 mg P/L o-PHOS 0.3
```

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

```
##     Run_Info             Sample_Name    Conc      Abs  Units      Test
## 303   RESULT MSM_202208_UP_LysA_20cm 0.004871 0.137970 mg N/L Vanadium NOx
## 304   RESULT MSM_202208_UP_LysA_45cm 0.004033 0.137299 mg N/L Vanadium NOx
## 305   RESULT MSM_202208_UP_LysB_10cm 0.004512 0.137682 mg N/L Vanadium NOx
## 306   RESULT MSM_202208_UP_LysB_20cm 0.004184 0.137420 mg N/L Vanadium NOx
## 307   RESULT MSM_202208_UP_LysB_45cm 0.003101 0.136551 mg N/L Vanadium NOx
## 308   RESULT MSM_202208_UP_LysC_10cm 0.004130 0.137376 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
## 653   RESULT MSM_202208_UP_LysA_20cm 1.751941 1.099048 mg N/L Ammonia 2
## 654   RESULT MSM_202208_UP_LysA_45cm 0.970558 0.613498 mg N/L Ammonia 2
```

```

## 655 RESULT MSM_202208_UP_LysB_10cm 0.067022 0.052042 mg N/L Ammonia 2
## 656 RESULT MSM_202208_UP_LysB_20cm 0.289288 0.190158 mg N/L Ammonia 2
## 657 RESULT MSM_202208_UP_LysB_45cm 0.495821 0.318497 mg N/L Ammonia 2
## 658 RESULT MSM_202208_UP_LysC_10cm 0.566208 0.362236 mg N/L Ammonia 2
## Conc_uM
## 653 125.078784
## 654 69.292410
## 655 4.784996
## 656 20.653544
## 657 35.398845
## 658 40.424083

```

```

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

```

```

## Run_Info Sample_Name Conc Abs Units Test
## 813 RESULT MSM_202208_UP_LysA_20cm 0.040826 0.018384 mg P/L o-PHOS 0.3
## 814 RESULT MSM_202208_UP_LysA_45cm 0.044884 0.020104 mg P/L o-PHOS 0.3
## 815 RESULT MSM_202208_UP_LysB_10cm 0.023058 0.010857 mg P/L o-PHOS 0.3
## 816 RESULT MSM_202208_UP_LysB_20cm 0.016900 0.008248 mg P/L o-PHOS 0.3
## 817 RESULT MSM_202208_UP_LysB_45cm 0.060440 0.026694 mg P/L o-PHOS 0.3
## 818 RESULT MSM_202208_UP_LysC_10cm 0.025075 0.011711 mg P/L o-PHOS 0.3
## Conc_uM
## 813 2.914748
## 814 3.204466
## 815 1.646212
## 816 1.206565
## 817 4.315078
## 818 1.790215

```

```

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

```

```

## Run_Info Sample_Name Conc Abs Units Test
## 303 RESULT MSM_202208_UP_LysA_20cm 0.004871 0.137970 mg N/L Vanadium NOx
## 304 RESULT MSM_202208_UP_LysA_45cm 0.004033 0.137299 mg N/L Vanadium NOx
## 305 RESULT MSM_202208_UP_LysB_10cm 0.004512 0.137682 mg N/L Vanadium NOx
## 306 RESULT MSM_202208_UP_LysB_20cm 0.004184 0.137420 mg N/L Vanadium NOx
## 307 RESULT MSM_202208_UP_LysB_45cm 0.003101 0.136551 mg N/L Vanadium NOx
## 308 RESULT MSM_202208_UP_LysC_10cm 0.004130 0.137376 mg N/L Vanadium NOx
## Conc_uM_raw
## 303 0.3477621
## 304 0.2879336
## 305 0.3221316
## 306 0.2987142
## 307 0.2213940
## 308 0.2948589

```

```

#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
## 303   RESULT MSM_202208_UP_LysA_20cm 0.004871 0.137970 mg N/L Vanadium NOx
## 304   RESULT MSM_202208_UP_LysA_45cm 0.004033 0.137299 mg N/L Vanadium NOx
## 305   RESULT MSM_202208_UP_LysB_10cm 0.004512 0.137682 mg N/L Vanadium NOx
## 306   RESULT MSM_202208_UP_LysB_20cm 0.004184 0.137420 mg N/L Vanadium NOx
## 307   RESULT MSM_202208_UP_LysB_45cm 0.003101 0.136551 mg N/L Vanadium NOx
## 308   RESULT MSM_202208_UP_LysC_10cm 0.004130 0.137376 mg N/L Vanadium NOx
##      Conc_uM_raw    Conc_uM
## 303    0.3477621 0.3477621
## 304    0.2879336 0.2879336
## 305    0.3221316 0.3221316
## 306    0.2987142 0.2987142
## 307    0.2213940 0.2213940
## 308    0.2948589 0.2948589

```

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
## 653 MSM_202208_UP_LysA_20cm 1.751941 125.078784
## 654 MSM_202208_UP_LysA_45cm 0.970558 69.292410
## 655 MSM_202208_UP_LysB_10cm 0.067022 4.784996
## 656 MSM_202208_UP_LysB_20cm 0.289288 20.653544
## 657 MSM_202208_UP_LysB_45cm 0.495821 35.398845
## 658 MSM_202208_UP_LysC_10cm 0.566208 40.424083

```

```

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

```

```

##          Sample_Name    Conc    Conc_uM
## 813 MSM_202208_UP_LysA_20cm 0.040826 2.914748
## 814 MSM_202208_UP_LysA_45cm 0.044884 3.204466
## 815 MSM_202208_UP_LysB_10cm 0.023058 1.646212
## 816 MSM_202208_UP_LysB_20cm 0.016900 1.206565
## 817 MSM_202208_UP_LysB_45cm 0.060440 4.315078
## 818 MSM_202208_UP_LysC_10cm 0.025075 1.790215

```

```

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

```

```

##          Sample_Name    Conc    Conc_uM
## 303 MSM_202208_UP_LysA_20cm 0.004871 0.3477621
## 304 MSM_202208_UP_LysA_45cm 0.004033 0.2879336
## 305 MSM_202208_UP_LysB_10cm 0.004512 0.3221316
## 306 MSM_202208_UP_LysB_20cm 0.004184 0.2987142
## 307 MSM_202208_UP_LysB_45cm 0.003101 0.2213940
## 308 MSM_202208_UP_LysC_10cm 0.004130 0.2948589

```

```

#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 Conc_uM
## 1 GCrew_202208_SW_A 2.232714 159.40329 0.615367 43.93376 NA      NA
## 2 GCrew_202208_SW_A 2.232714 159.40329 0.696618 49.73463 NA      NA
## 3 GCrew_202208_SW_A 2.577261 184.00201 0.615367 43.93376 NA      NA
## 4 GCrew_202208_SW_A 2.577261 184.00201 0.696618 49.73463 NA      NA
## 5 GCrew_202208_SW_B 0.885919 63.24966 0.206491 14.74230 NA      NA
## 6 GCrew_202208_SW_C 0.593469 42.37037 0.199273 14.22698 NA      NA

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 NOx_uM
## 1 GCrew_202208_SW_A 2.232714 159.40329 0.615367 43.93376 NA      NA
## 2 GCrew_202208_SW_A 2.232714 159.40329 0.696618 49.73463 NA      NA
## 3 GCrew_202208_SW_A 2.577261 184.00201 0.615367 43.93376 NA      NA
## 4 GCrew_202208_SW_A 2.577261 184.00201 0.696618 49.73463 NA      NA
## 5 GCrew_202208_SW_B 0.885919 63.24966 0.206491 14.74230 NA      NA
## 6 GCrew_202208_SW_C 0.593469 42.37037 0.199273 14.22698 NA      NA

#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 NOx_uM
## 1 GCrew_202208_SW_A 2.232714 159.40329 0.615367 43.93376 NA      NA
## 2 GCrew_202208_SW_A 2.232714 159.40329 0.696618 49.73463 NA      NA
## 3 GCrew_202208_SW_A 2.577261 184.00201 0.615367 43.93376 NA      NA
## 4 GCrew_202208_SW_A 2.577261 184.00201 0.696618 49.73463 NA      NA
## 5 GCrew_202208_SW_B 0.885919 63.24966 0.206491 14.74230 NA      NA
## 6 GCrew_202208_SW_C 0.593469 42.37037 0.199273 14.22698 NA      NA

##           NH3_range   PO4_range NOx_range
## 1          adl Within_Range    <NA>
## 2          adl Within_Range    <NA>
## 3          adl Within_Range    <NA>
## 4          adl Within_Range    <NA>
## 5 Within_Range Within_Range    <NA>
## 6 Within_Range Within_Range    <NA>

```

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") +

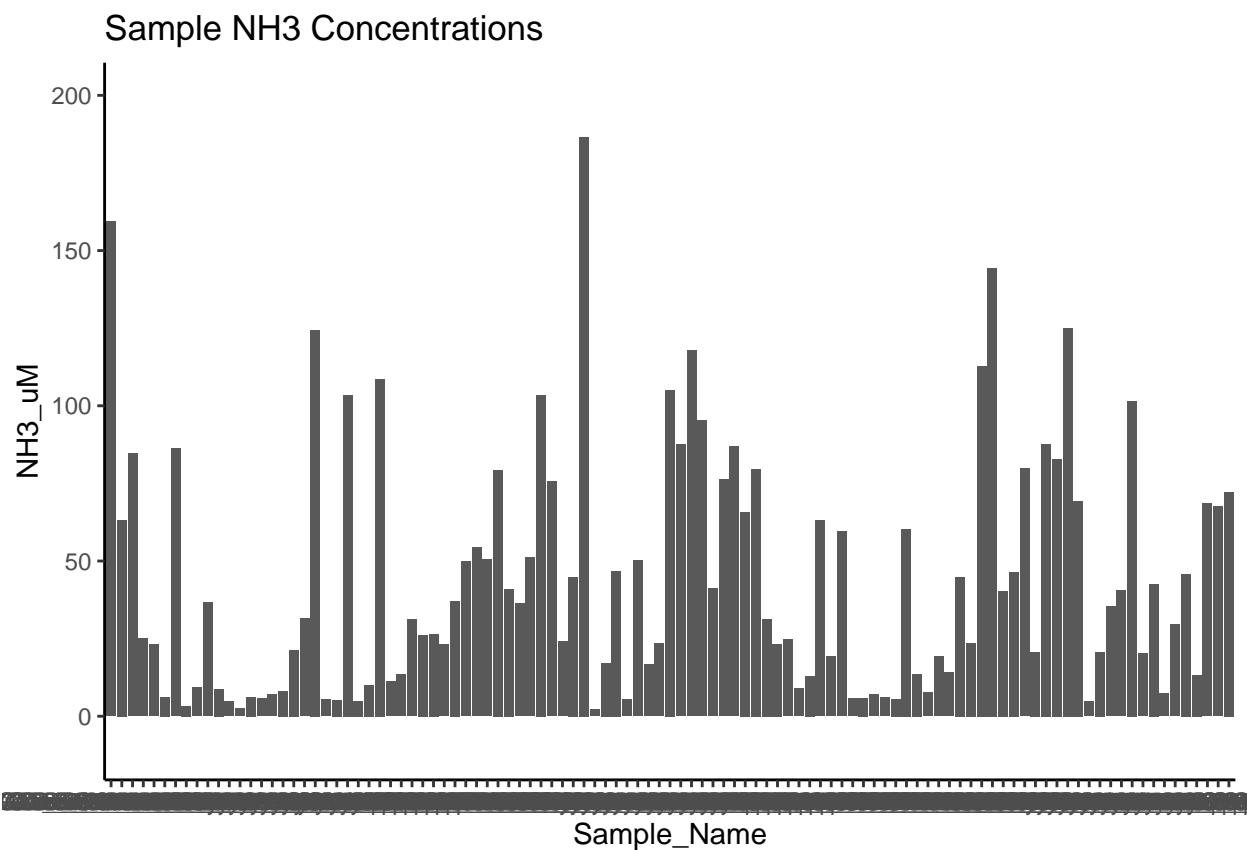
```

```

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()').

```



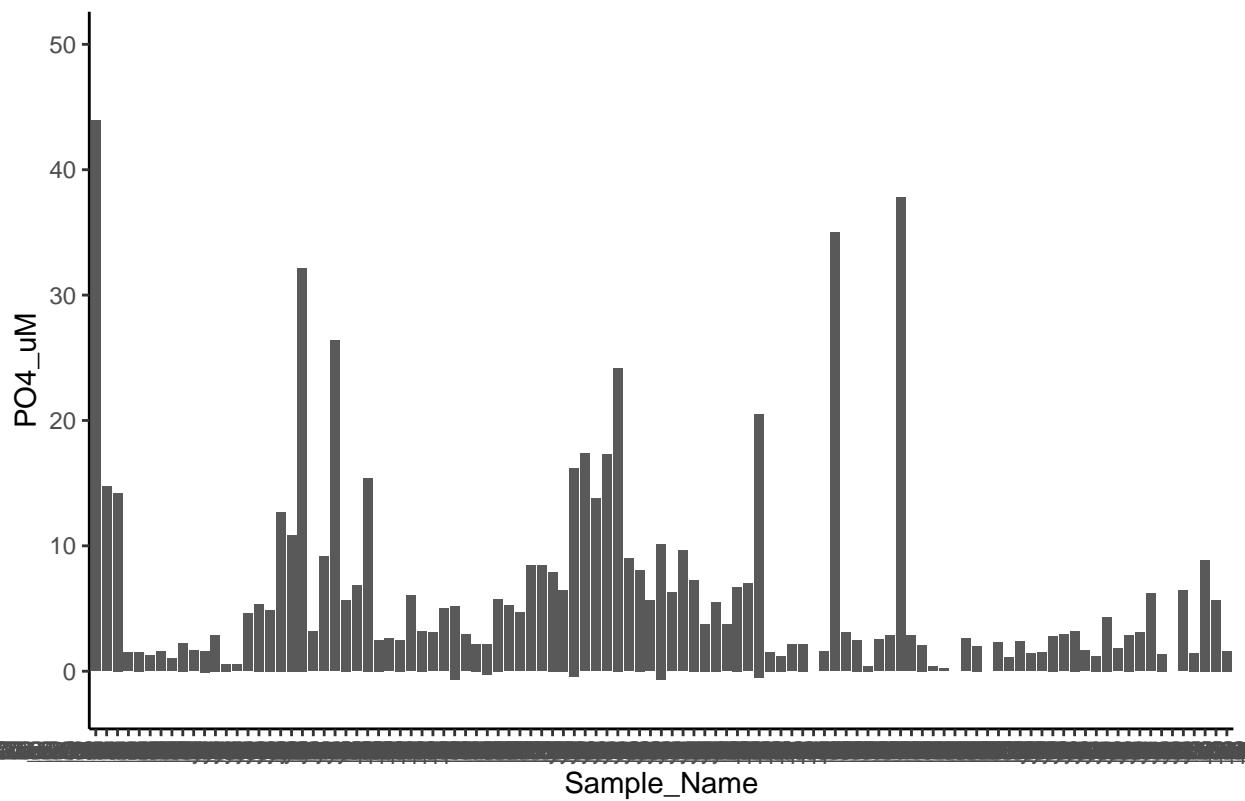
```

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 P04 Concentrations")
P04look

## Warning: Removed 9 rows containing missing values or values outside the scale range
## ('geom_bar()').

```

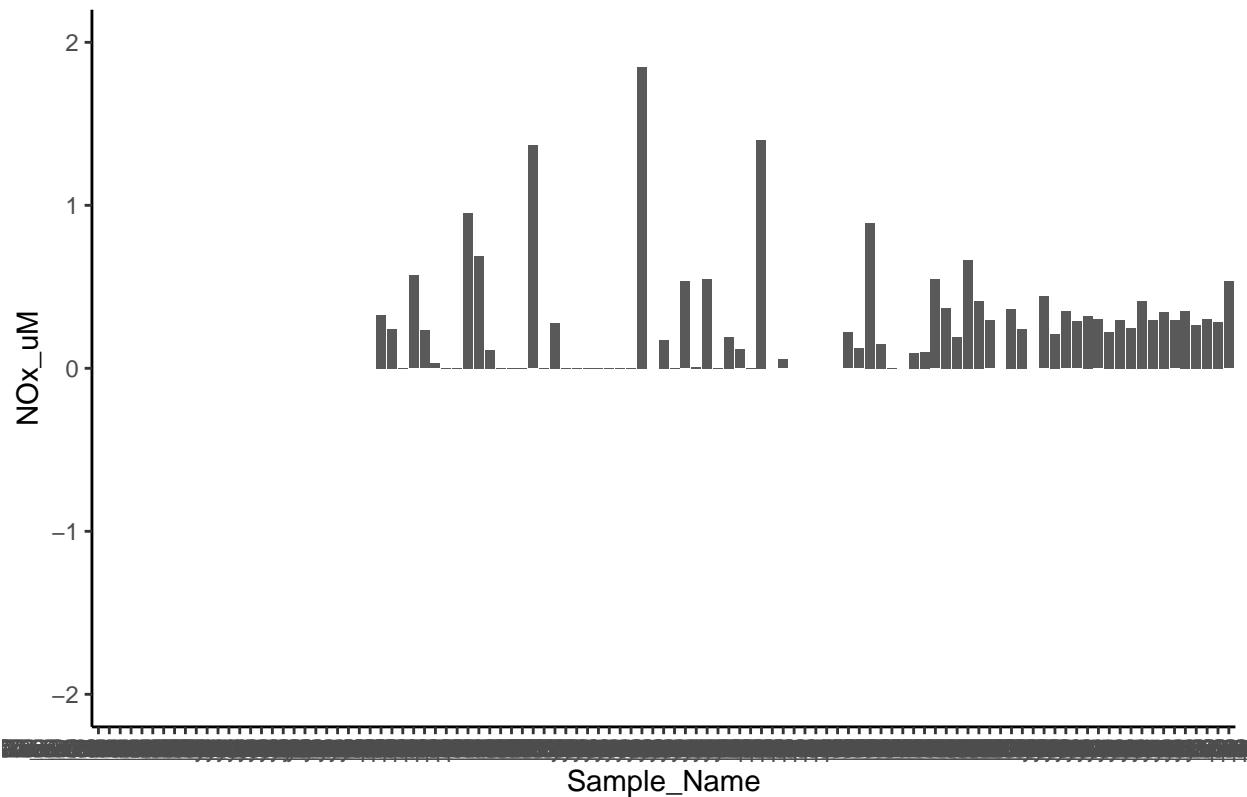
Sample PO4 Concentrations



```
NOXlook <- ggplot(data=all_data, aes(x=Sample_Name, y=N0x_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 2) +
  theme(legend.position="none") +
  ggtitle("Sample N0x Concentrations")
NOXlook
```

```
## Warning: Removed 49 rows containing missing values or values outside the scale range
## ('geom_bar()').
```

Sample NOx Concentrations



Pull out data you need, make IDs

```
head(all_data)

##           Sample_Name  NH3_mgL    NH3_uM  P04_mgL   P04_uM NOx_mgL NOx_uM
## 1 GCrew_202208_SW_A 2.232714 159.40329 0.615367 43.93376     NA     NA
## 2 GCrew_202208_SW_A 2.232714 159.40329 0.696618 49.73463     NA     NA
## 3 GCrew_202208_SW_A 2.577261 184.00201 0.615367 43.93376     NA     NA
## 4 GCrew_202208_SW_A 2.577261 184.00201 0.696618 49.73463     NA     NA
## 5 GCrew_202208_SW_B 0.885919  63.24966 0.206491 14.74230     NA     NA
## 6 GCrew_202208_SW_C 0.593469  42.37037 0.199273 14.22698     NA     NA
##           NH3_range  P04_range NOx_range
## 1      adl Within_Range     <NA>
## 2      adl Within_Range     <NA>
## 3      adl Within_Range     <NA>
## 4      adl Within_Range     <NA>
## 5 Within_Range Within_Range     <NA>
## 6 Within_Range Within_Range     <NA>

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

```
##           Sample_Name    NH3_uM    P04_uM NOx_uM    NH3_range    P04_range
```

```

## 1 GCrew_202208_SW_A 159.40329 43.93376      NA      adl Within_Range
## 2 GCrew_202208_SW_A 159.40329 49.73463      NA      adl Within_Range
## 3 GCrew_202208_SW_A 184.00201 43.93376      NA      adl Within_Range
## 4 GCrew_202208_SW_A 184.00201 49.73463      NA      adl Within_Range
## 5 GCrew_202208_SW_B 63.24966 14.74230      NA Within_Range Within_Range
## 6 GCrew_202208_SW_C 42.37037 14.22698      NA Within_Range Within_Range
##   NOx_range
## 1 <NA>
## 2 <NA>
## 3 <NA>
## 4 <NA>
## 5 <NA>
## 6 <NA>

#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", "202208", "SW", "A"), c("GCrew", "202208", "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 <- "August"
head(IDs)

##     Site Date Zone Replicate Depth Tree Month
## 1 GCrew 202208 SW      A GCrew 202208 August
## 2 GCrew 202208 SW      A GCrew 202208 August
## 3 GCrew 202208 SW      A GCrew 202208 August
## 4 GCrew 202208 SW      A GCrew 202208 August
## 5 GCrew 202208 SW      B GCrew 202208 August
## 6 GCrew 202208 SW      C GCrew 202208 August

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

##     Site Date Zone Replicate Depth Tree Month     Sample_Name NH3_uM
## 1 GCrew 202208 SW      A GCrew 202208 August GCrew_202208_SW_A 159.40329
## 2 GCrew 202208 SW      A GCrew 202208 August GCrew_202208_SW_A 159.40329
## 3 GCrew 202208 SW      A GCrew 202208 August GCrew_202208_SW_A 184.00201
## 4 GCrew 202208 SW      A GCrew 202208 August GCrew_202208_SW_A 184.00201
## 5 GCrew 202208 SW      B GCrew 202208 August GCrew_202208_SW_B 63.24966
## 6 GCrew 202208 SW      C GCrew 202208 August GCrew_202208_SW_C 42.37037
##   P04_uM NOx_uM NH3_range P04_range NOx_range
## 1 43.93376    NA      adl Within_Range    <NA>
## 2 49.73463    NA      adl Within_Range    <NA>
## 3 43.93376    NA      adl Within_Range    <NA>
## 4 49.73463    NA      adl Within_Range    <NA>
## 5 14.74230    NA Within_Range Within_Range    <NA>
## 6 14.22698    NA Within_Range Within_Range    <NA>

```

Export final data with flags

```
#Export Data  
write.csv(alldat, file="Processed Data/COMPASS_SynopticCB_Nutrients_202208.csv")
```