

COMPASS_Synoptic_SEAL_Data_Analysis_May2022

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Information

```
#####  
##### COMPASS Synoptic  
##### Chesapeake Bay Sites  
##### Data Analysis Code: Porewater Nutrients  
##### MONTH: May 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\_rffZqv3lz9BjD0pAMX5nzu/view?usp=sharing  
#PO4 method = https://drive.google.com/file/d/1m3gXDZnJoIo\_QmyhvuZG4HRgGShCzm9Wq/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
```

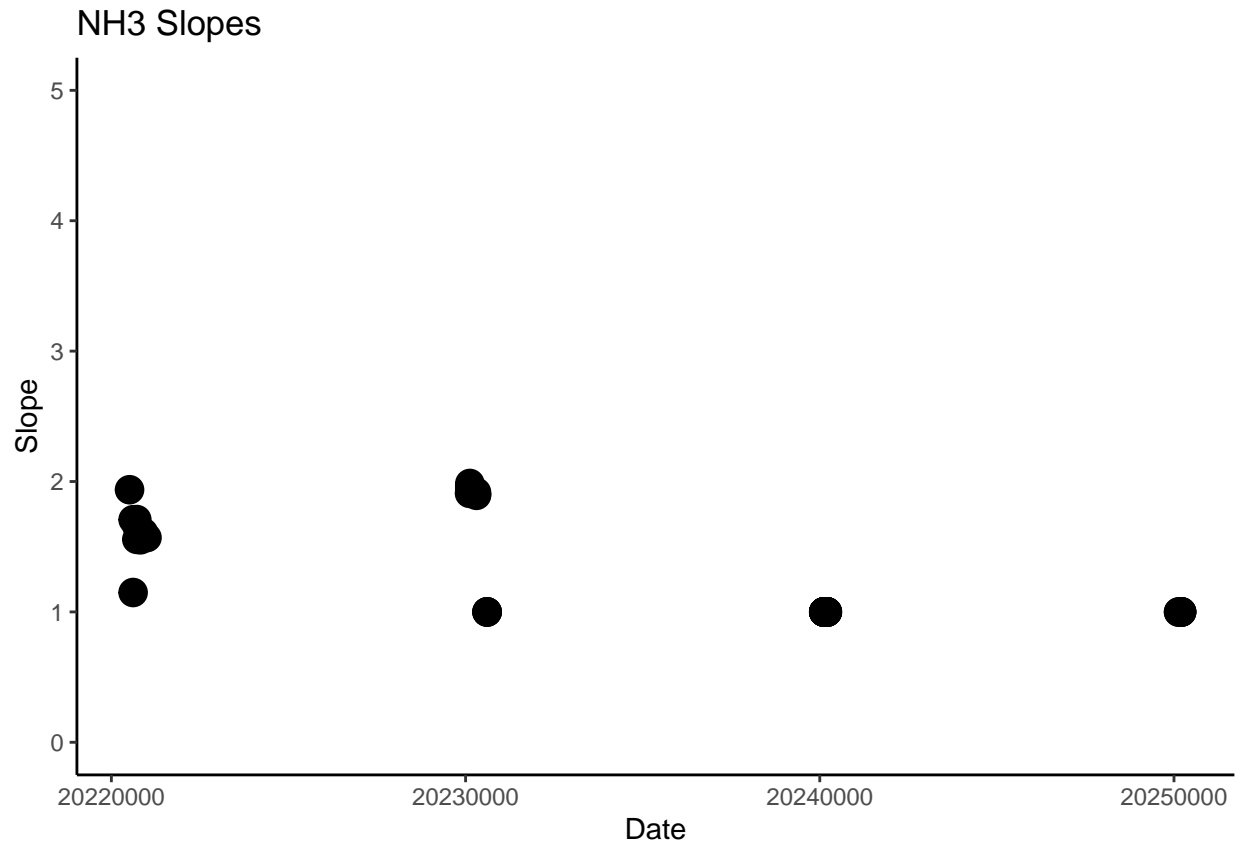
```
qNOx <- qlog[qlog$Analysis %like% "V-Nox", ]
head(qNOx)
```

```
##      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
```

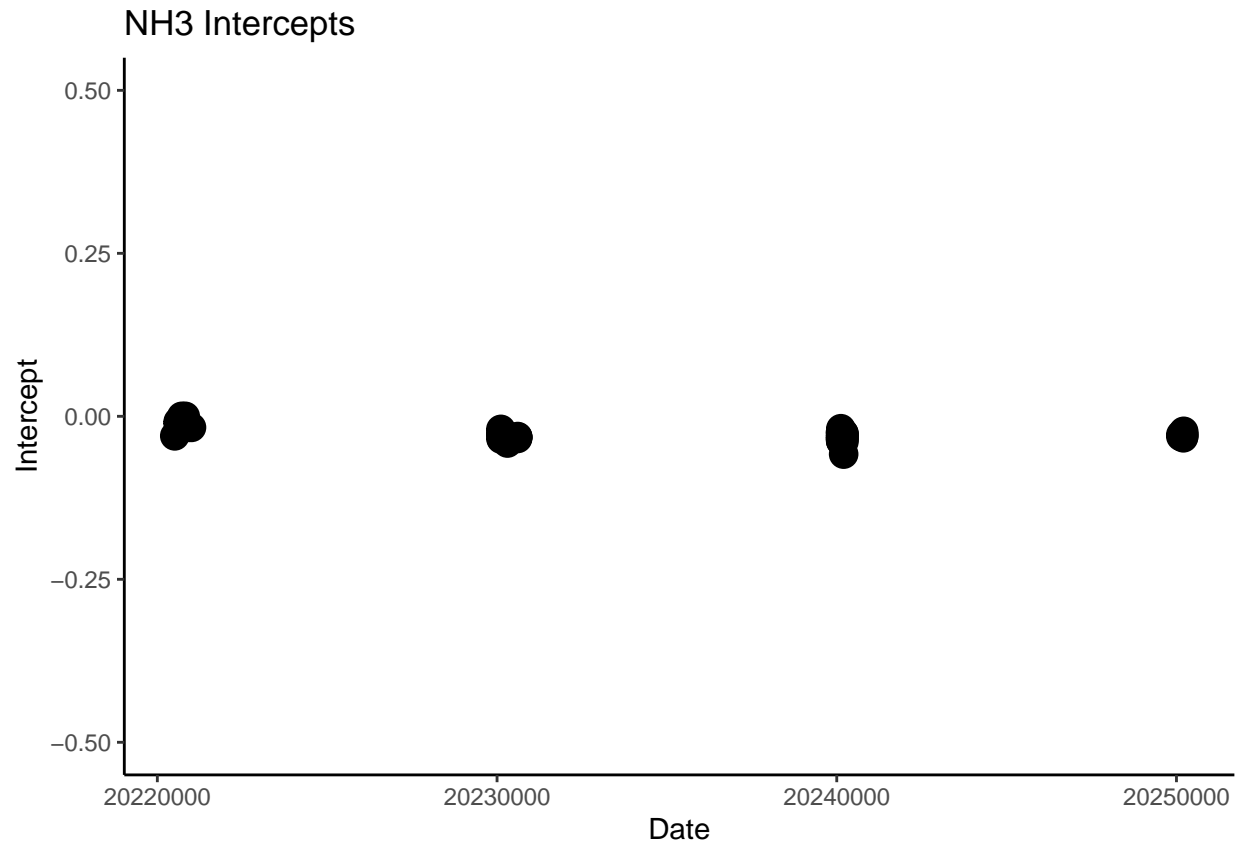
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#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
```

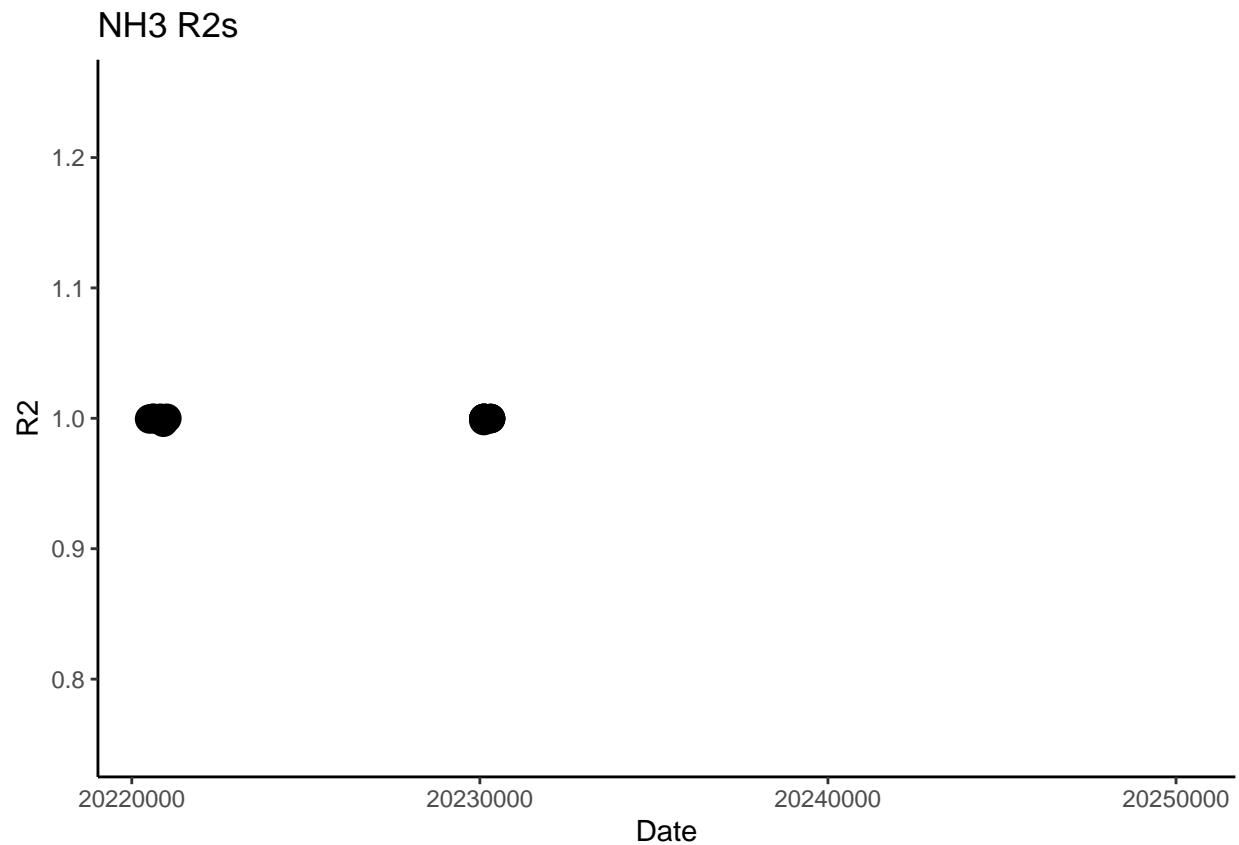
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#plot the R2s to make sure there are no crazy outliers
Rsqr1 <- 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")
```

Rsqr1

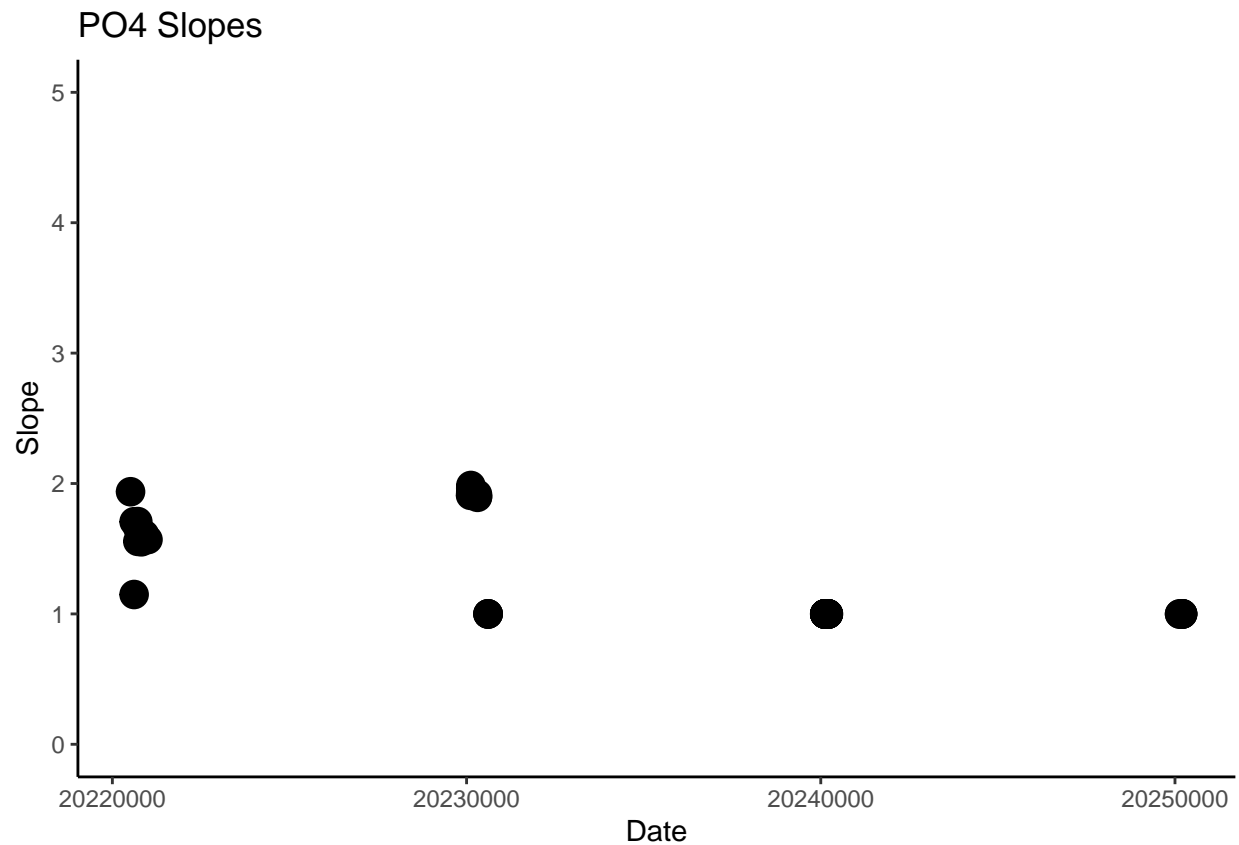
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## ('geom_point()').
```



```
##### 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
```

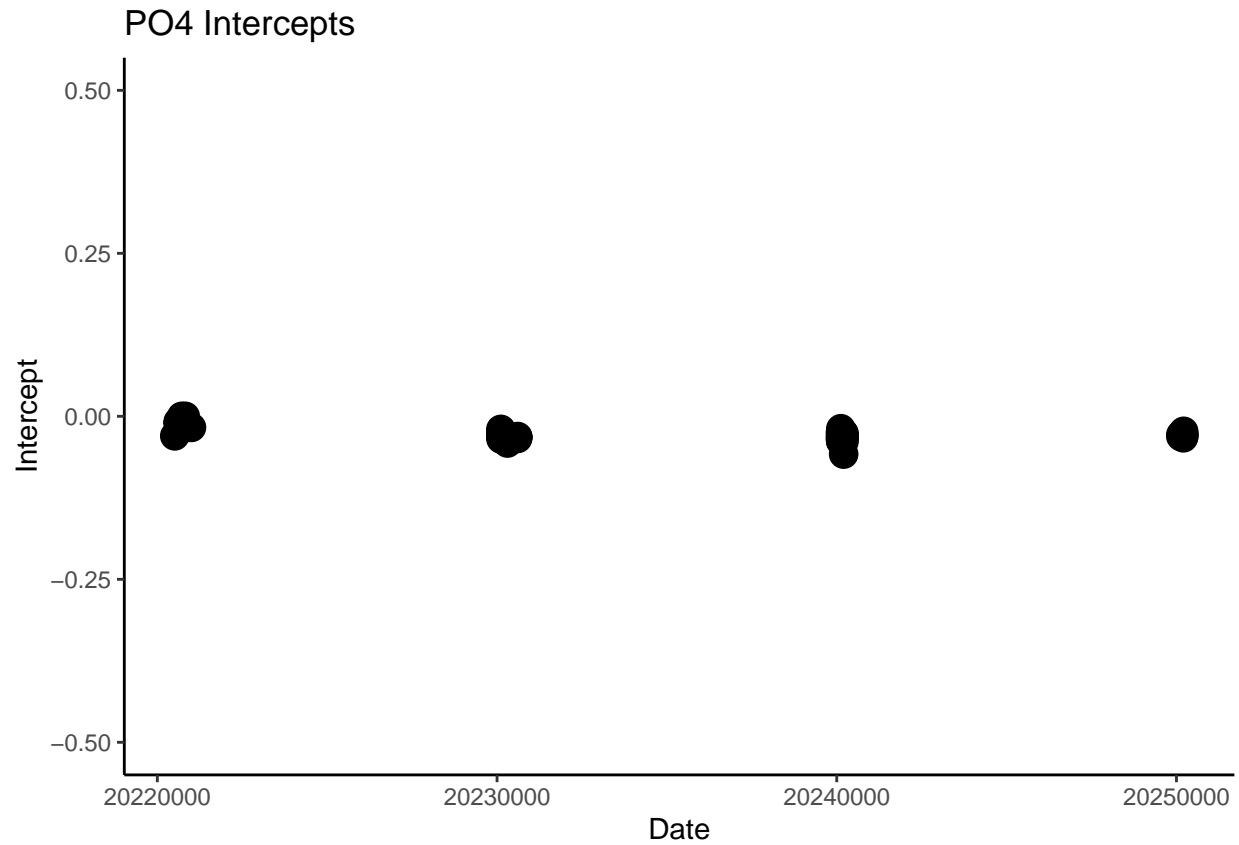
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#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
```

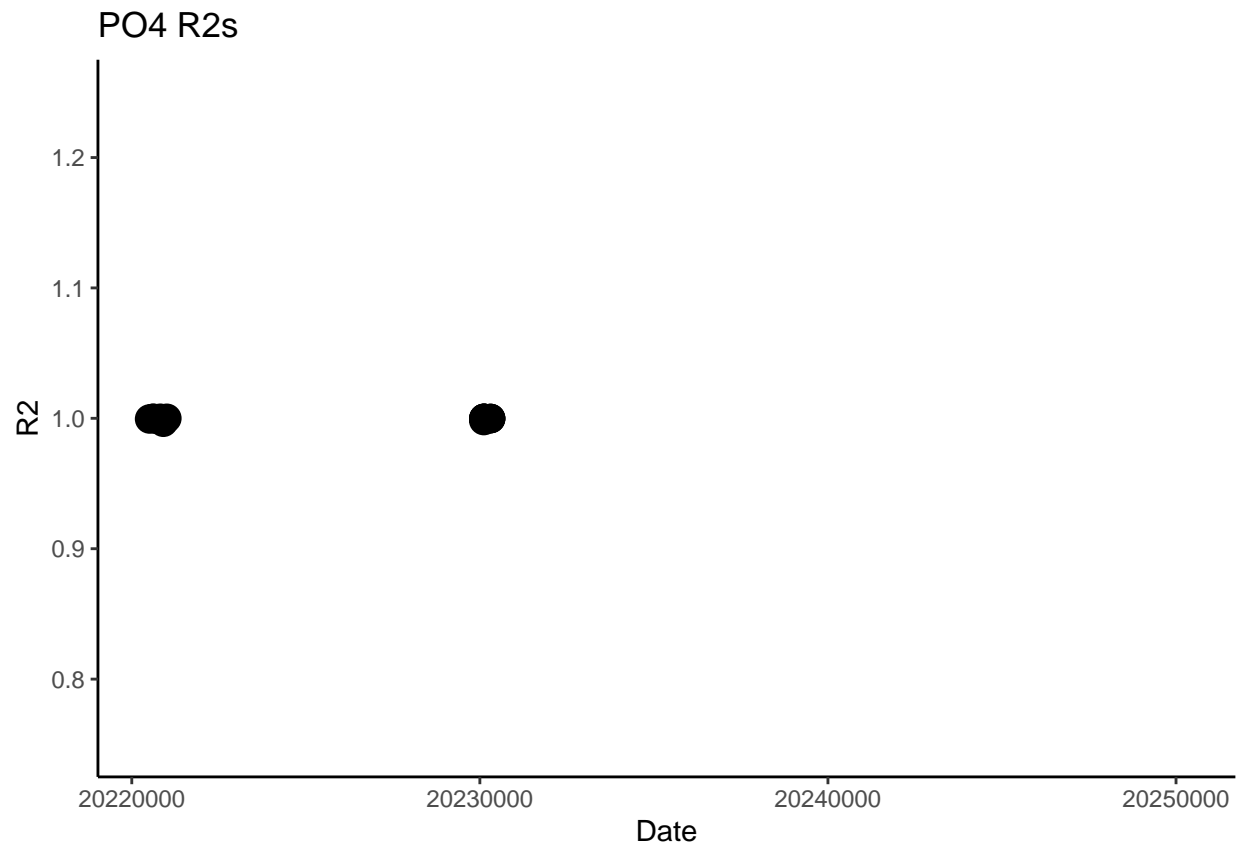
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#plot the R2s to make sure there are no crazy outliers
Rsqr2 <- 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")
```

Rsqr2

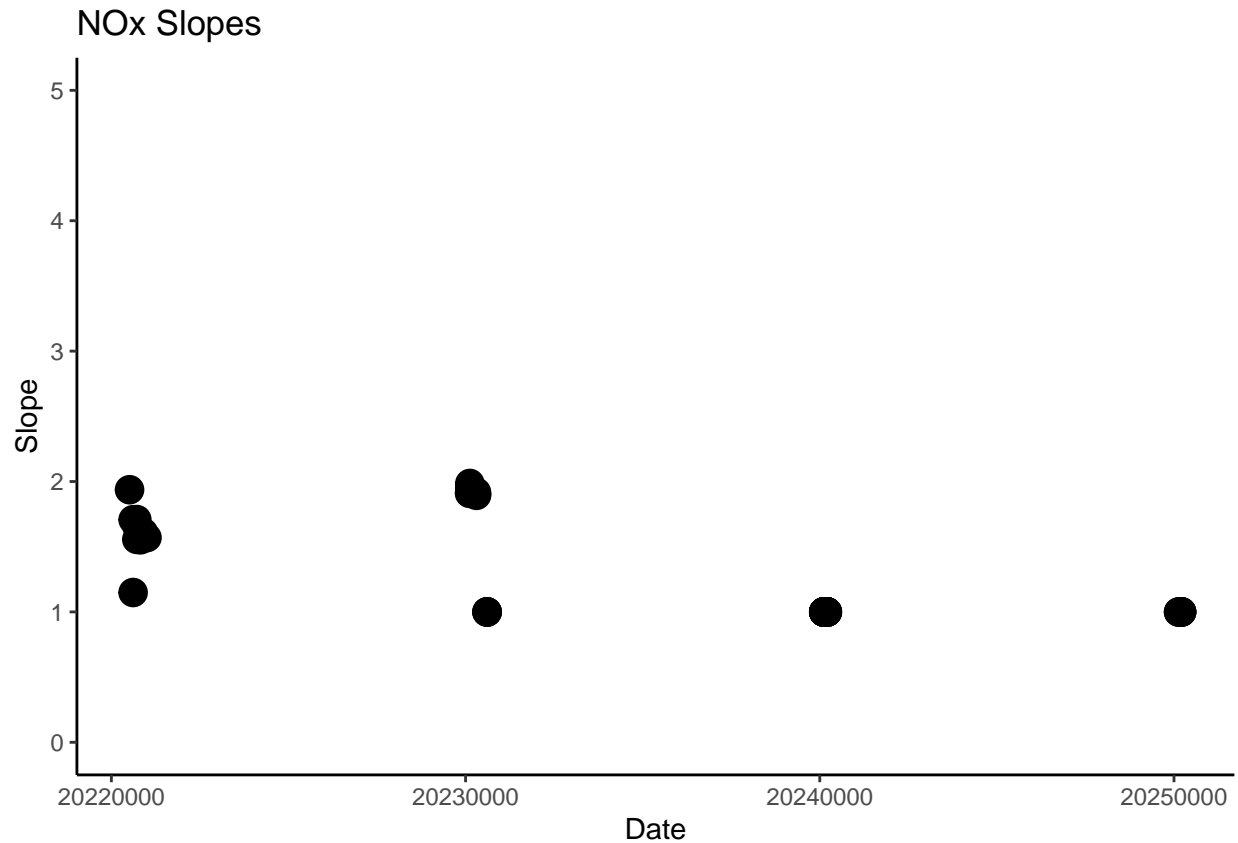
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## ('geom_point()').
```

```
##### 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
```

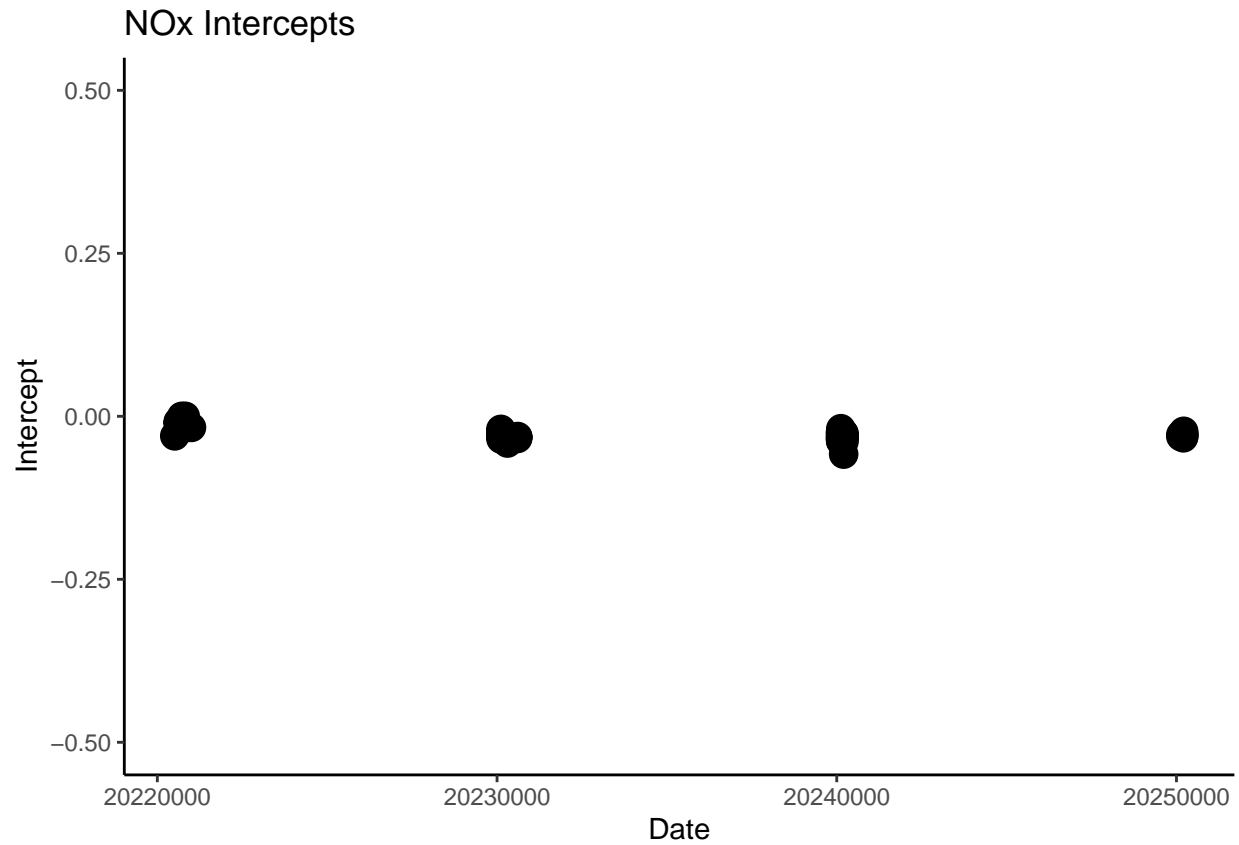
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#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
```

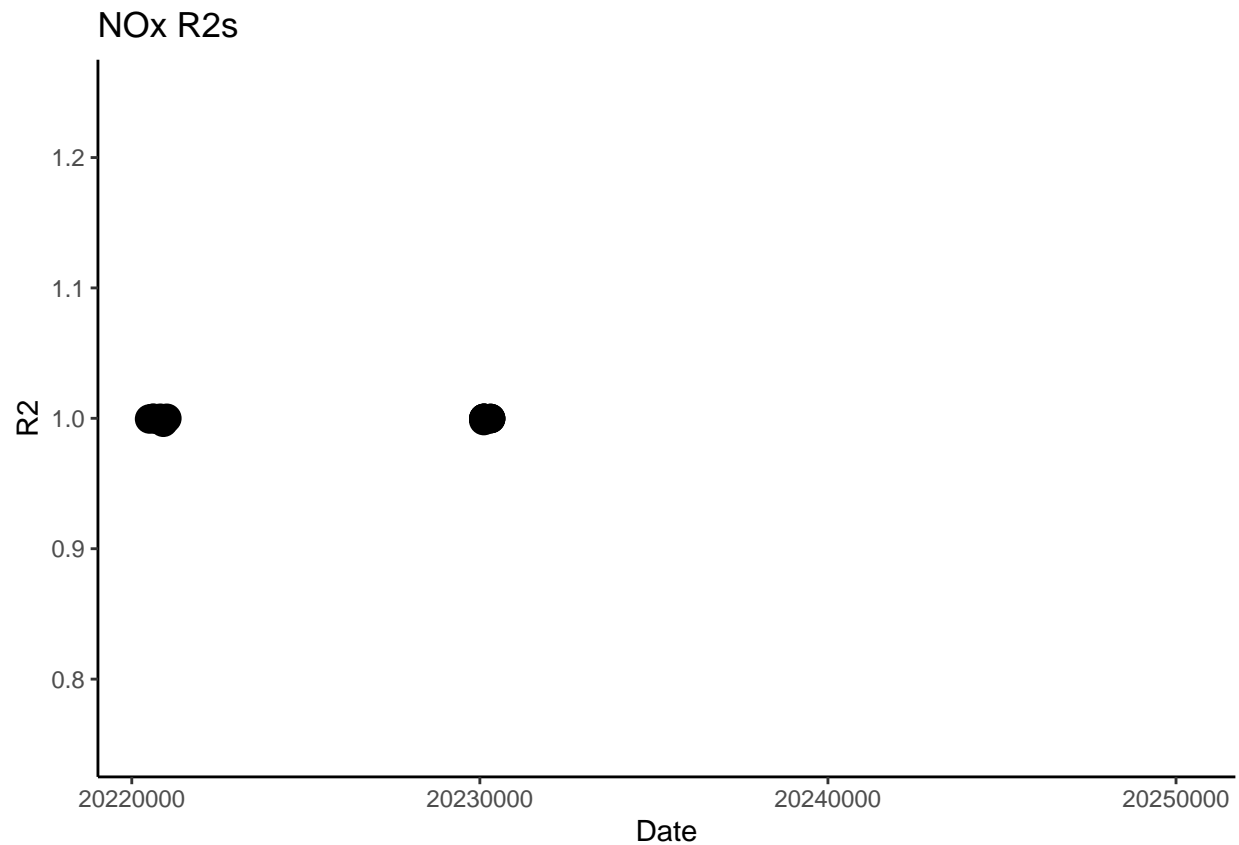
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



```
#plot the R2s to make sure there are no crazy outliers
Rsqr3 <- 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")
```

Rsqr3

```
## 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_202205.csv")
#Quick look at dataframe
head(file1)
```

```
##      RUNSTARTED X1652457973 X5.13.2022.12.06          X X.1      Conc      abs.
## 1      RESULT          -1          S1      Standard 1    0 0.010914 0.010914
## 2      RESULT          -2          S90 Standard .0389    1 0.033695 0.033695
## 3      RESULT          -2          S91 Standard .1000    2 0.065531 0.065531
## 4      RESULT          -2          S92 Standard .2000    3 0.123799 0.123799
## 5      RESULT          -2          S93 Standard .5000    4 0.273219 0.273219
## 6      RESULT          -2          S94 Standard 1.0000    5 0.537588 0.537588
##      X.2 dilution X.3 X.4      X.5      X.6      X.7      X.8
## 1    0          0    0    0 mg N/L Ammonia 2 1652459189 5/13/2022 12:26
## 2    0          0    0    0 mg N/L Ammonia 2 1652459349 5/13/2022 12:29
## 3    0          0    0    0 mg N/L Ammonia 2 1652459509 5/13/2022 12:31
## 4    0          0    0    0 mg N/L Ammonia 2 1652459669 5/13/2022 12:34
## 5    0          0    0    0 mg N/L Ammonia 2 1652459829 5/13/2022 12:37
## 6    0          0    0    0 mg N/L Ammonia 2 1652459989 5/13/2022 12:39
```

```
#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 0.010914 0.010914 mg N/L Ammonia 2
## 2  RESULT Standard .0389 0.033695 0.033695 mg N/L Ammonia 2
## 3  RESULT Standard .1000 0.065531 0.065531 mg N/L Ammonia 2
## 4  RESULT Standard .2000 0.123799 0.123799 mg N/L Ammonia 2
## 5  RESULT Standard .5000 0.273219 0.273219 mg N/L Ammonia 2
## 6  RESULT Standard 1.0000 0.537588 0.537588 mg N/L Ammonia 2
```

```
alldat <- dat1
```

```
#Pull out standards
```

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

```
## Run_Info      Sample_Name      Conc      Abs Units      Test
## 1  RESULT      Standard 1 0.010914 0.010914 mg N/L Ammonia 2
## 2  RESULT Standard .0389 0.033695 0.033695 mg N/L Ammonia 2
## 3  RESULT Standard .1000 0.065531 0.065531 mg N/L Ammonia 2
## 4  RESULT Standard .2000 0.123799 0.123799 mg N/L Ammonia 2
## 5  RESULT Standard .5000 0.273219 0.273219 mg N/L Ammonia 2
## 6  RESULT Standard 1.0000 0.537588 0.537588 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
## 17 RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 0.085440 mg N/L
## 21 RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.124875 0.079907 mg N/L
## 25 RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.060283 0.046558 mg N/L
## 29 RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 0.152037 mg N/L
## 33 RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.222125 0.130119 mg N/L
## 43 RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.077934 0.055671 mg N/L
## Test
## 17 Ammonia 2
## 21 Ammonia 2
## 25 Ammonia 2
## 29 Ammonia 2
## 33 Ammonia 2
## 43 Ammonia 2
```

NOx - Not run for the first month

```
#read in data
```

```
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202211_1.csv")
```

```
#Quick look at dataframe
```

```
head(Nfile1)
```

```
#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)

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

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

Nalldat <- rbind(Ndat1, Ndat2, Ndat3)

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

#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)

```

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
## 17  RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 0.085440 mg N/L
## 21  RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.124875 0.079907 mg N/L
## 25  RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.060283 0.046558 mg N/L
## 29  RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 0.152037 mg N/L
## 33  RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.222125 0.130119 mg N/L
## 43  RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.077934 0.055671 mg N/L
##      Test
## 17 Ammonia 2
## 21 Ammonia 2
## 25 Ammonia 2
## 29 Ammonia 2
## 33 Ammonia 2
## 43 Ammonia 2
```

```
#head(Nalldat2)
```

```
#subset by test
```

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

```
head(NH4samples)
```

```
##      Run_Info                Sample_Name      Conc      Abs  Units
## 17  RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 0.085440 mg N/L
## 21  RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.124875 0.079907 mg N/L
## 25  RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.060283 0.046558 mg N/L
## 29  RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 0.152037 mg N/L
## 33  RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.222125 0.130119 mg N/L
## 43  RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.077934 0.055671 mg N/L
##      Test
## 17 Ammonia 2
## 21 Ammonia 2
## 25 Ammonia 2
## 29 Ammonia 2
## 33 Ammonia 2
## 43 Ammonia 2
```

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

```
head(P04samples)
```

```
##      Run_Info                Sample_Name      Conc      Abs  Units
## 98  RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.031756 0.010427 mg P/L
## 102 RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.027584 0.008972 mg P/L
## 106 RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.022317 0.007136 mg P/L
## 110 RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.066781 0.022635 mg P/L
## 114 RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.070832 0.024048 mg P/L
## 124 RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.058239 0.019658 mg P/L
##      Test
```



```
## 98 o-PHOS 0.3
## 102 o-PHOS 0.3
## 106 o-PHOS 0.3
## 110 o-PHOS 0.3
## 114 o-PHOS 0.3
## 124 o-PHOS 0.3
```

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

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

```
##      Run_Info      Sample_Name      Conc      Abs Units
## 17  RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 0.085440 mg N/L
## 21  RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.124875 0.079907 mg N/L
## 25  RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.060283 0.046558 mg N/L
## 29  RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 0.152037 mg N/L
## 33  RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.222125 0.130119 mg N/L
## 43  RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.077934 0.055671 mg N/L
##      Test      Conc_uM
## 17 Ammonia 2  9.680439
## 21 Ammonia 2  8.915376
## 25 Ammonia 2  4.303869
## 29 Ammonia 2 18.889246
## 33 Ammonia 2 15.858482
## 43 Ammonia 2  5.564051
```

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

```
##      Run_Info      Sample_Name      Conc      Abs Units
## 98  RESULT MSM_WC_PW_MonMon_20220502_SipA_10cm 0.031756 0.010427 mg P/L
## 102 RESULT MSM_WC_PW_MonMon_20220502_SipB_10cm 0.027584 0.008972 mg P/L
## 106 RESULT MSM_WC_PW_MonMon_20220502_SipC_10cm 0.022317 0.007136 mg P/L
## 110 RESULT MSM_WC_PW_MonMon_20220502_SipA_20cm 0.066781 0.022635 mg P/L
## 114 RESULT MSM_WC_PW_MonMon_20220502_SipB_20cm 0.070832 0.024048 mg P/L
## 124 RESULT MSM_WC_PW_MonMon_20220502_SipC_20cm 0.058239 0.019658 mg P/L
##      Test      Conc_uM
## 98  o-PHOS 0.3 2.267201
## 102 o-PHOS 0.3 1.969343
## 106 o-PHOS 0.3 1.593309
## 110 o-PHOS 0.3 4.767790
## 114 o-PHOS 0.3 5.057008
## 124 o-PHOS 0.3 4.157939
```

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

```
#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)
```

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  
## 17 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 9.680439  
## 21 MSM_WC_PW_MonMon_20220502_SipB_10cm 0.124875 8.915376  
## 25 MSM_WC_PW_MonMon_20220502_SipC_10cm 0.060283 4.303869  
## 29 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 18.889246  
## 33 MSM_WC_PW_MonMon_20220502_SipB_20cm 0.222125 15.858482  
## 43 MSM_WC_PW_MonMon_20220502_SipC_20cm 0.077934 5.564051
```

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

```
##              Sample_Name      Conc  Conc_uM  
## 98 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.031756 2.267201  
## 102 MSM_WC_PW_MonMon_20220502_SipB_10cm 0.027584 1.969343  
## 106 MSM_WC_PW_MonMon_20220502_SipC_10cm 0.022317 1.593309  
## 110 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.066781 4.767790  
## 114 MSM_WC_PW_MonMon_20220502_SipB_20cm 0.070832 5.057008  
## 124 MSM_WC_PW_MonMon_20220502_SipC_20cm 0.058239 4.157939
```

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

```
#Bring all this data back together:
```

```
all_data <- merge(NH4_pull, P04_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  
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 0.156415 11.167156 0.014272 1.0189409  
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 0.233058 16.639037 0.006308 0.4503559  
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 0.170483 12.171532 0.008936 0.6379804  
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 0.213778 15.262553 0.011143 0.7955478  
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 9.680439 0.031756 2.2672007  
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 18.889246 0.066781 4.7677897
```

```
all_data$NOx_mgL <- NA  
all_data$NOx_uM <- NA
```

```
colnames(all_data) <- c("Sample_Name", "NH3_mgL", "NH3_uM", "P04_mgL", "P04_uM", "NOx_mgL", "NOx_uM")  
head(all_data)
```

```
##              Sample_Name      NH3_mgL      NH3_uM      P04_mgL      P04_uM  
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 0.156415 11.167156 0.014272 1.0189409
```

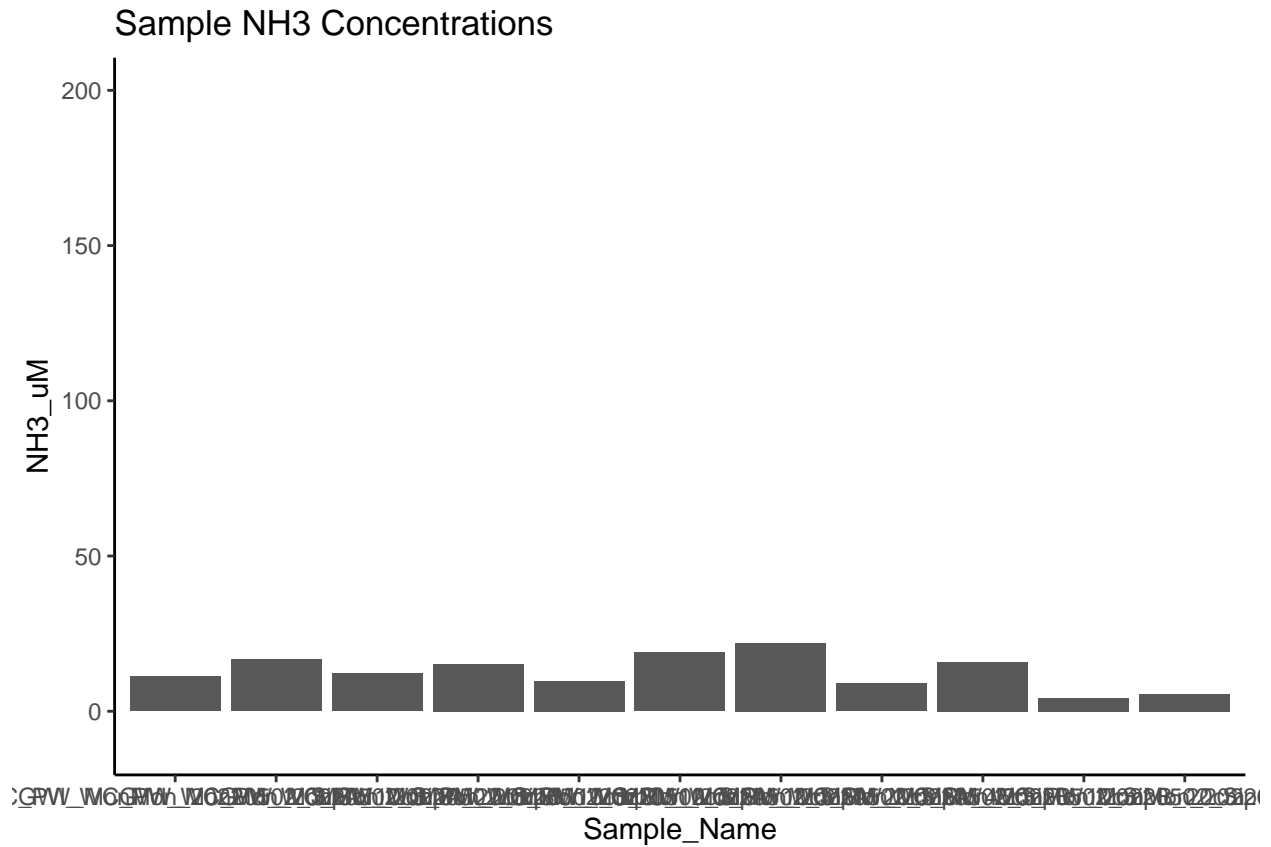
```
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 0.233058 16.639037 0.006308 0.4503559
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 0.170483 12.171532 0.008936 0.6379804
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 0.213778 15.262553 0.011143 0.7955478
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 9.680439 0.031756 2.2672007
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 18.889246 0.066781 4.7677897
## NOx_mgL NOx_uM
## 1 NA NA
## 2 NA NA
## 3 NA NA
## 4 NA NA
## 5 NA NA
## 6 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$NH3_mgL>2, "adl", "Within_Range"))
all_data$PO4_range <- ifelse(all_data$PO4_mgL<0.003, "bdl", ifelse(all_data$PO4_mgL>3, "adl", "Within_Range"))
all_data$NOx_range <- ifelse(all_data$NOx_mgL<0.025, "bdl", ifelse(all_data$NOx_mgL>1, "adl", "Within_Range"))
head(all_data)
```

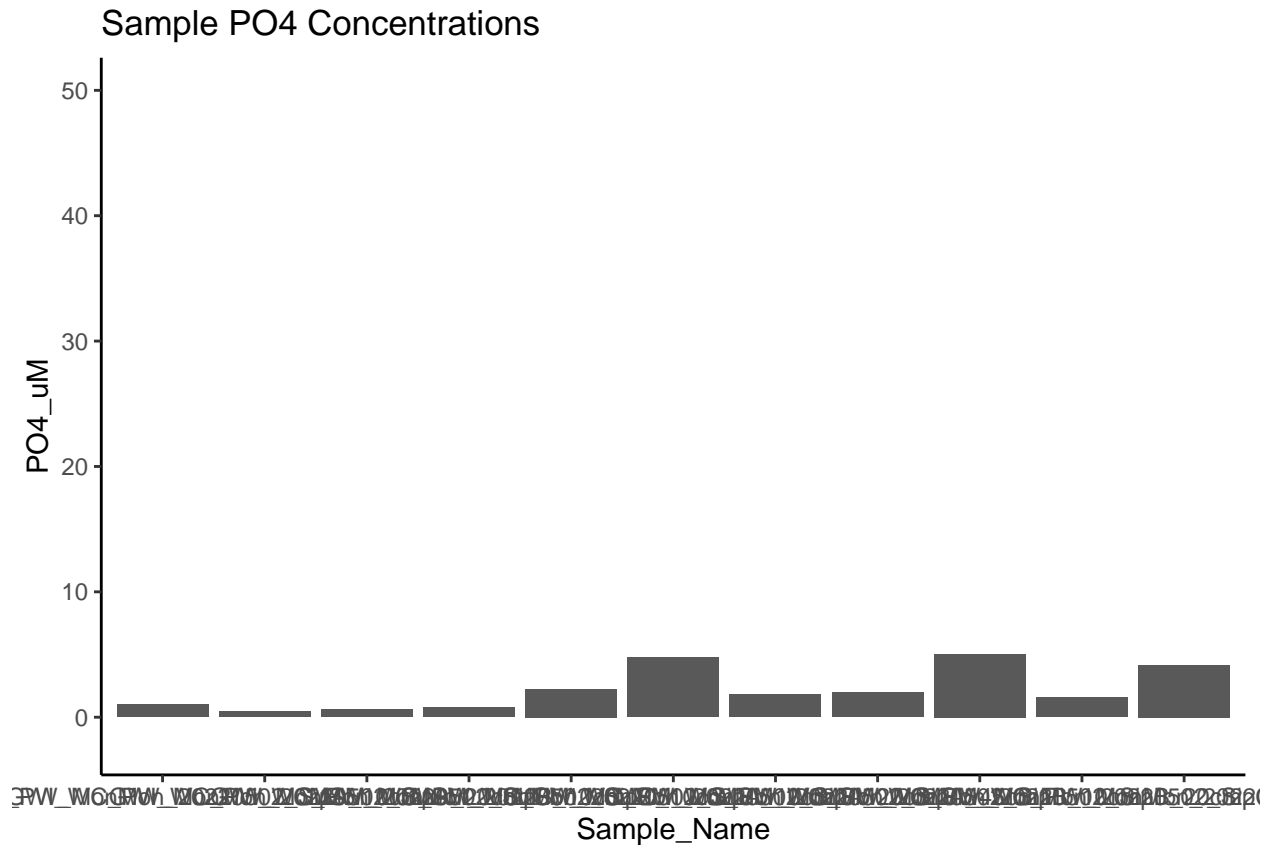
```
## Sample_Name NH3_mgL NH3_uM PO4_mgL PO4_uM
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 0.156415 11.167156 0.014272 1.0189409
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 0.233058 16.639037 0.006308 0.4503559
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 0.170483 12.171532 0.008936 0.6379804
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 0.213778 15.262553 0.011143 0.7955478
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591 9.680439 0.031756 2.2672007
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 18.889246 0.066781 4.7677897
## NOx_mgL NOx_uM NH3_range PO4_range NOx_range
## 1 NA NA Within_Range Within_Range NA
## 2 NA NA Within_Range Within_Range NA
## 3 NA NA Within_Range Within_Range NA
## 4 NA NA Within_Range Within_Range NA
## 5 NA NA Within_Range Within_Range NA
## 6 NA NA 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
```



```
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
```



```
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
```

Pull out data you need, make IDs

```
head(all_data)
```

```
##           Sample_Name NH3_mgL  NH3_uM  P04_mgL  P04_uM
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 0.156415 11.167156 0.014272 1.0189409
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 0.233058 16.639037 0.006308 0.4503559
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 0.170483 12.171532 0.008936 0.6379804
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 0.213778 15.262553 0.011143 0.7955478
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm 0.135591  9.680439 0.031756 2.2672007
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 0.264576 18.889246 0.066781 4.7677897
##   NOx_mgL NOx_uM   NH3_range   P04_range NOx_range
## 1      NA      NA Within_Range Within_Range      NA
## 2      NA      NA Within_Range Within_Range      NA
## 3      NA      NA Within_Range Within_Range      NA
## 4      NA      NA Within_Range Within_Range      NA
```

```
## 5      NA      NA Within_Range Within_Range      NA
## 6      NA      NA Within_Range Within_Range      NA
```

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

```
##              Sample_Name    NH3_uM    PO4_uM NOx_uM    NH3_range
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 11.167156 1.0189409      NA Within_Range
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 16.639037 0.4503559      NA Within_Range
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 12.171532 0.6379804      NA Within_Range
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 15.262553 0.7955478      NA Within_Range
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm  9.680439 2.2672007      NA Within_Range
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 18.889246 4.7677897      NA Within_Range
##      PO4_range NOx_range
## 1 Within_Range      NA
## 2 Within_Range      NA
## 3 Within_Range      NA
## 4 Within_Range      NA
## 5 Within_Range      NA
## 6 Within_Range      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$Sample_Name), '_', fixed=TRUE)))
colnames(IDs) <- c("Site", "Date", "Zone", "Replicate", "Depth")
IDs$Month <- "May"
head(IDs)
```

```
##   Site Date Zone Replicate    Depth    NA    NA Month
## 1  GWI   WC   PW   MonMon 20220502 SipA 10cm   May
## 2  GWI   WC   PW   MonMon 20220502 SipA 20cm   May
## 3  GWI   WC   PW   MonMon 20220502 SipB 10cm   May
## 4  GWI   WC   PW   MonMon 20220502 SipC 10cm   May
## 5  MSM   WC   PW   MonMon 20220502 SipA 10cm   May
## 6  MSM   WC   PW   MonMon 20220502 SipA 20cm   May
```

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

```
##   Site Date Zone Replicate    Depth    NA    NA Month
## 1  GWI   WC   PW   MonMon 20220502 SipA 10cm   May
## 2  GWI   WC   PW   MonMon 20220502 SipA 20cm   May
## 3  GWI   WC   PW   MonMon 20220502 SipB 10cm   May
## 4  GWI   WC   PW   MonMon 20220502 SipC 10cm   May
## 5  MSM   WC   PW   MonMon 20220502 SipA 10cm   May
## 6  MSM   WC   PW   MonMon 20220502 SipA 20cm   May
##              Sample_Name    NH3_uM    PO4_uM NOx_uM    NH3_range
## 1 GWI_WC_PW_MonMon_20220502_SipA_10cm 11.167156 1.0189409      NA Within_Range
## 2 GWI_WC_PW_MonMon_20220502_SipA_20cm 16.639037 0.4503559      NA Within_Range
## 3 GWI_WC_PW_MonMon_20220502_SipB_10cm 12.171532 0.6379804      NA Within_Range
## 4 GWI_WC_PW_MonMon_20220502_SipC_10cm 15.262553 0.7955478      NA Within_Range
```

```
## 5 MSM_WC_PW_MonMon_20220502_SipA_10cm 9.680439 2.2672007 NA Within_Range
## 6 MSM_WC_PW_MonMon_20220502_SipA_20cm 18.889246 4.7677897 NA Within_Range
##      PO4_range NOx_range
## 1 Within_Range      NA
## 2 Within_Range      NA
## 3 Within_Range      NA
## 4 Within_Range      NA
## 5 Within_Range      NA
## 6 Within_Range      NA
```

Export final data with flags

#Export Data

```
write.csv(alldat, file="Processed Data/COMPASS_Synoptic_CB_SEAL_NUTR_202205.csv")
```