

# COMPASS\_Synoptic\_SEAL\_Data\_Analysis\_May2022

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2023-03-03

## 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_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)

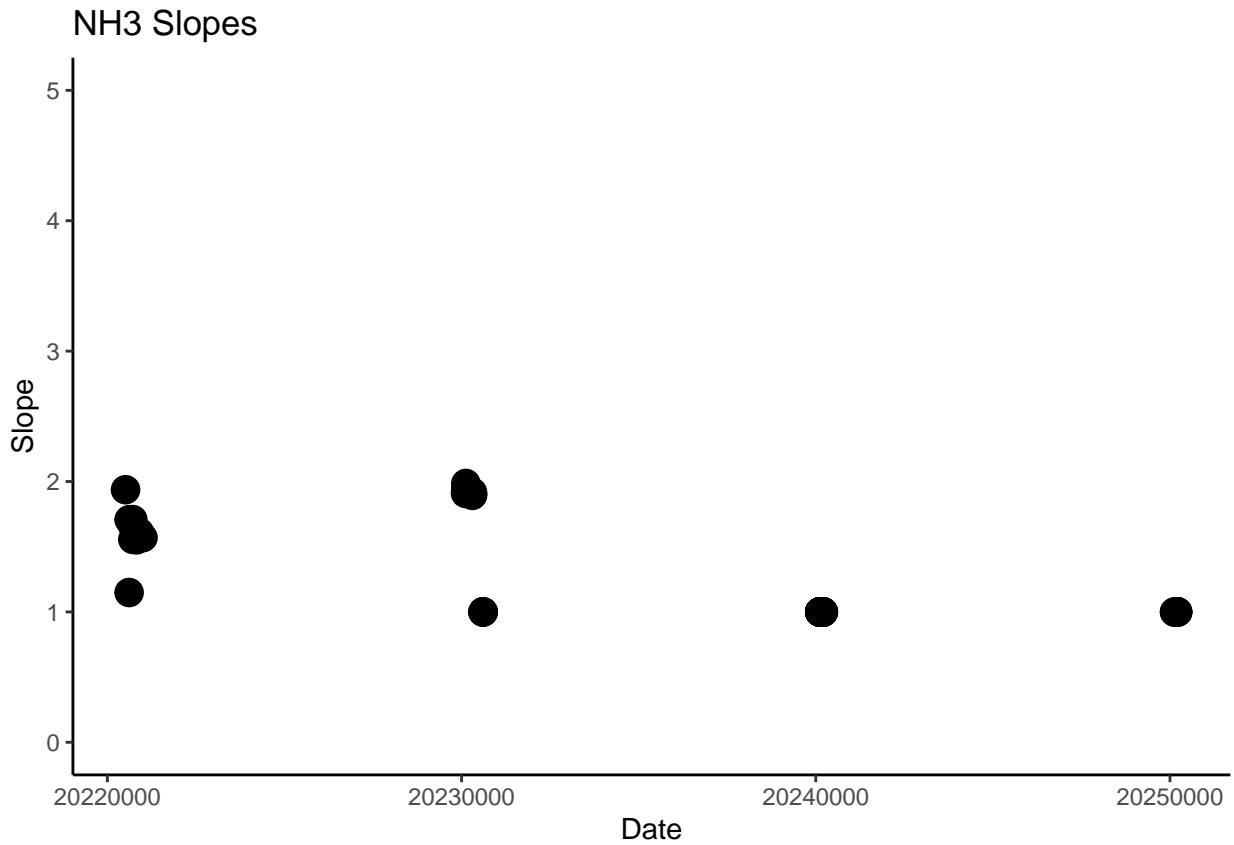
##           Date      User Machine Analysis Slope Intercept     R2
## 3 20220525 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9990
## 6 20220615 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9998
## 9 20220718 Stephanie Wilson SERC SEAL V-Nox     1        0 0.9999
## 16 20220730 Stephanie Wilson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

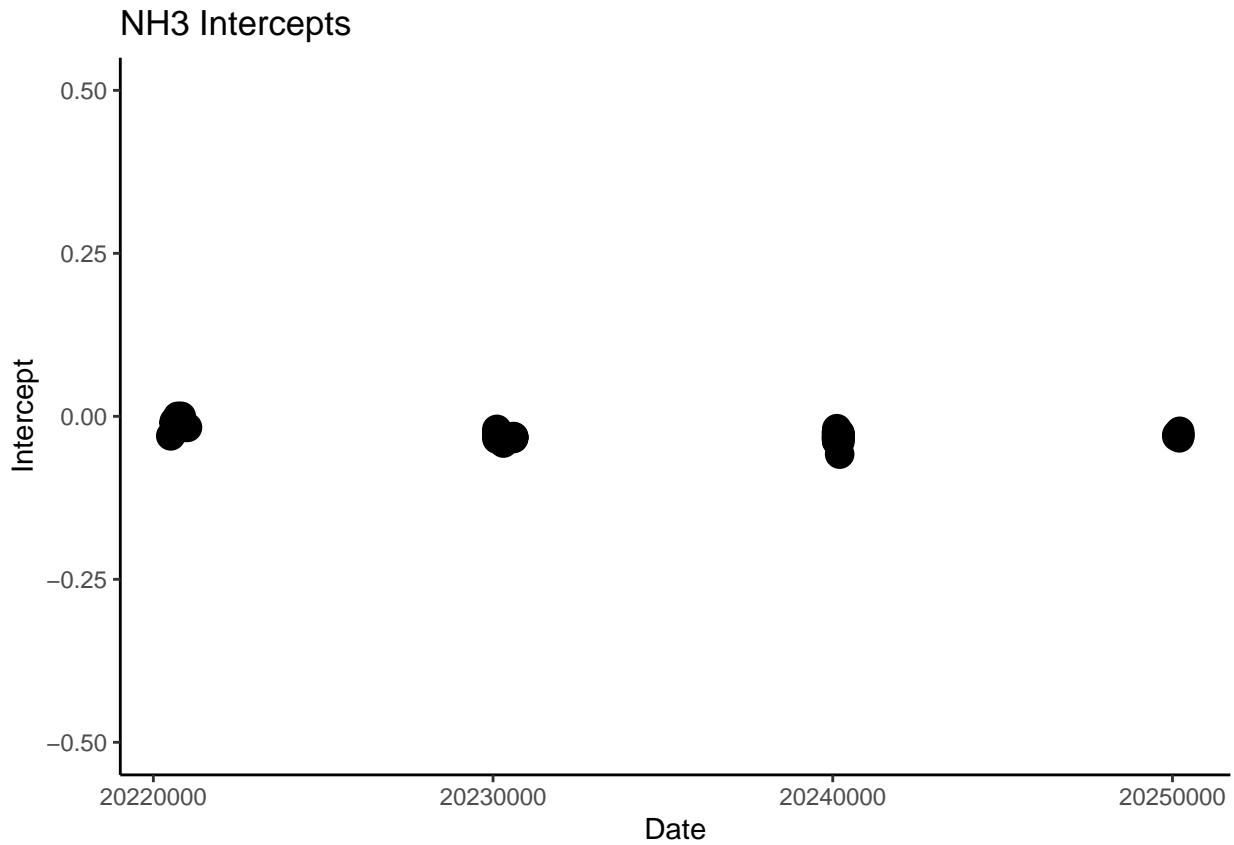
```



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

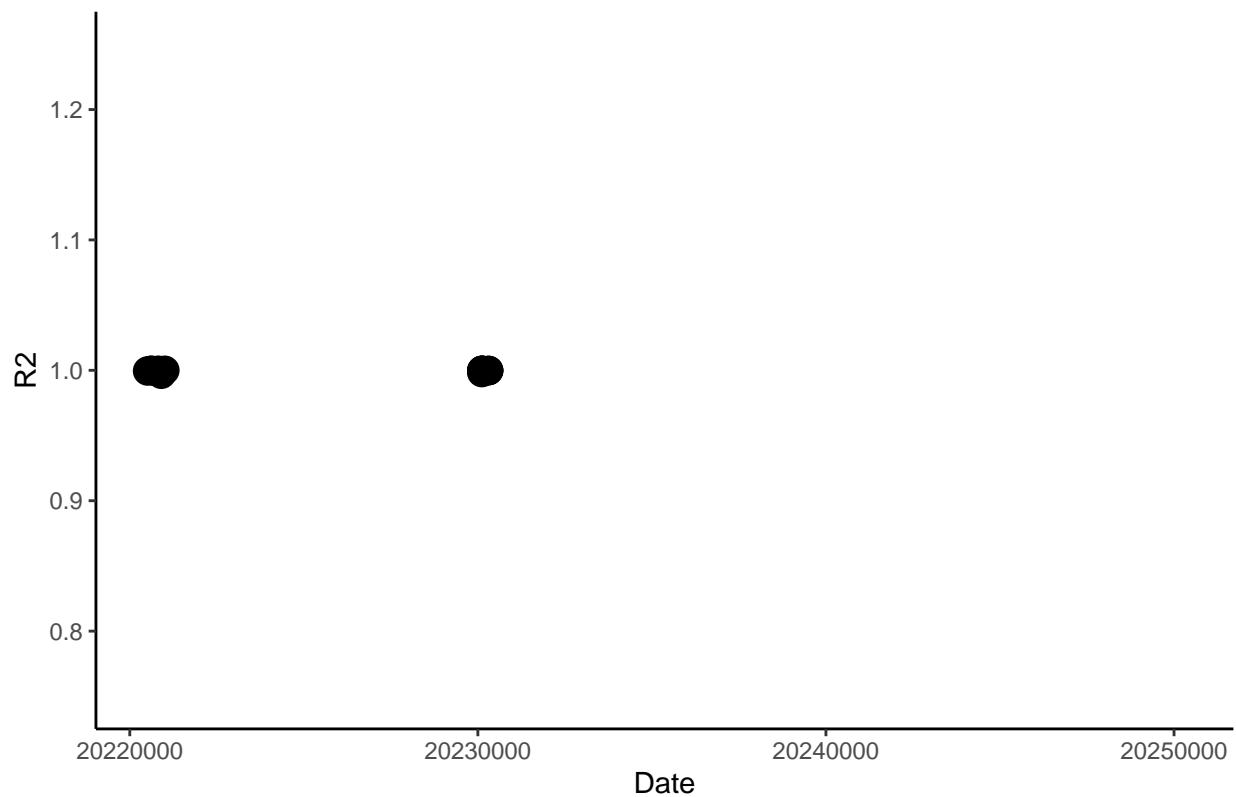


```
#plot the R2s to make sure there are no crazy outliers
Rsq1 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NH3 R2s")
```

```
Rsq1
```

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

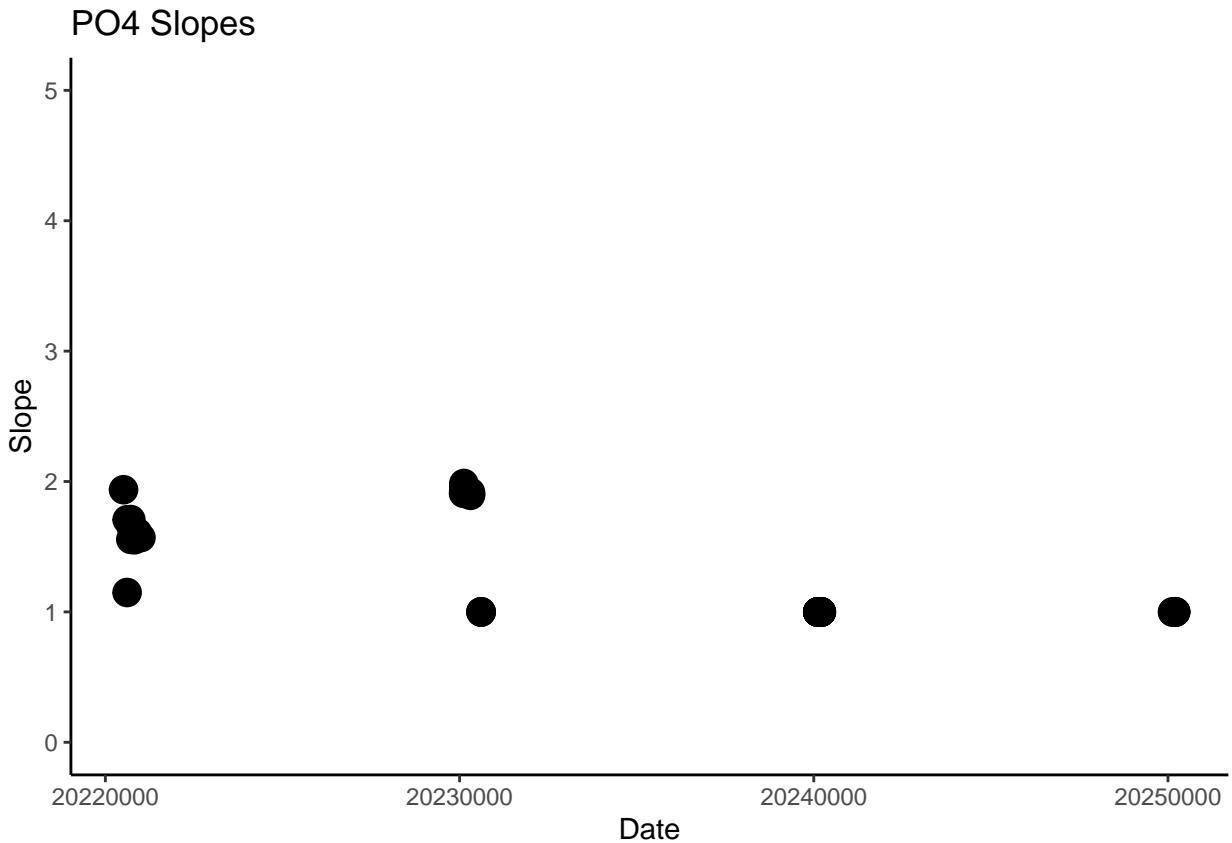
## NH3 R2s



```
##### 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
```

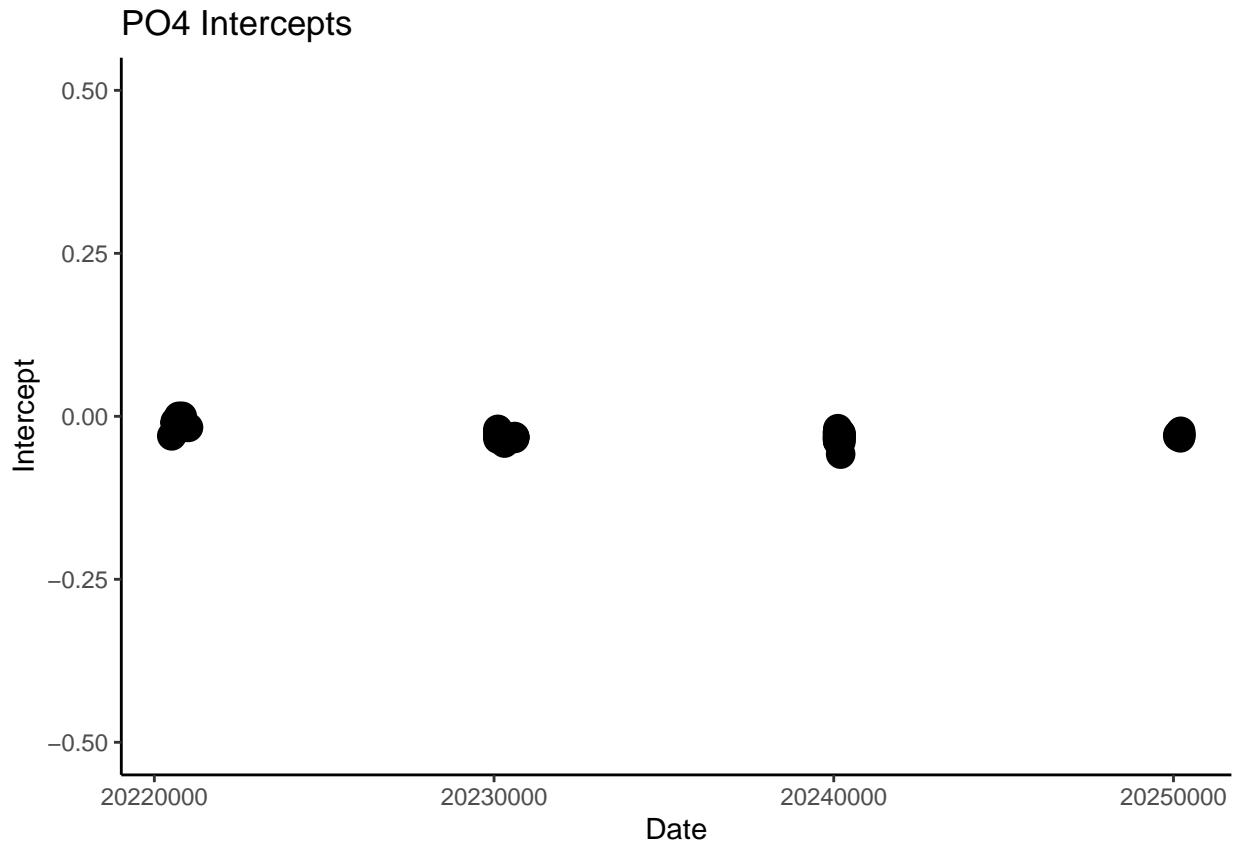
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

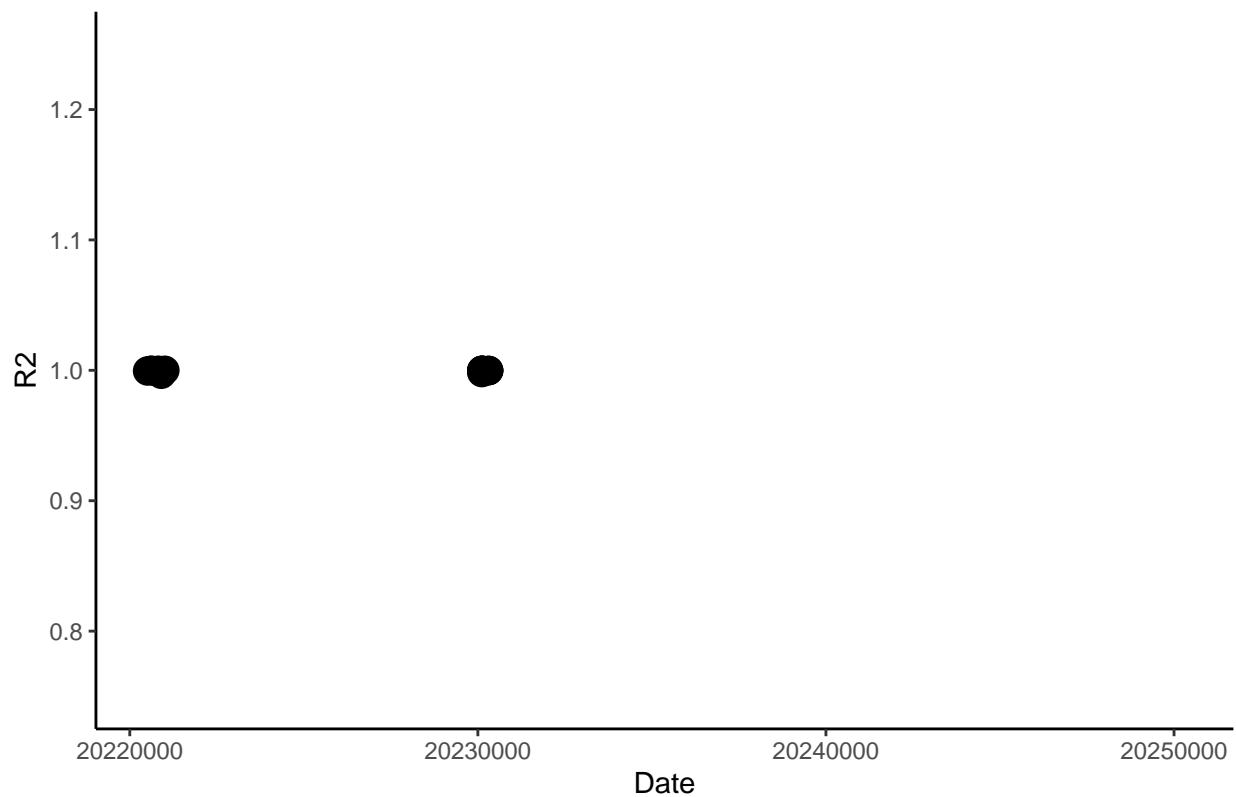


```
#plot the R2s to make sure there are no crazy outliers
Rsq2 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("P04 R2s")
```

```
Rsq2
```

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

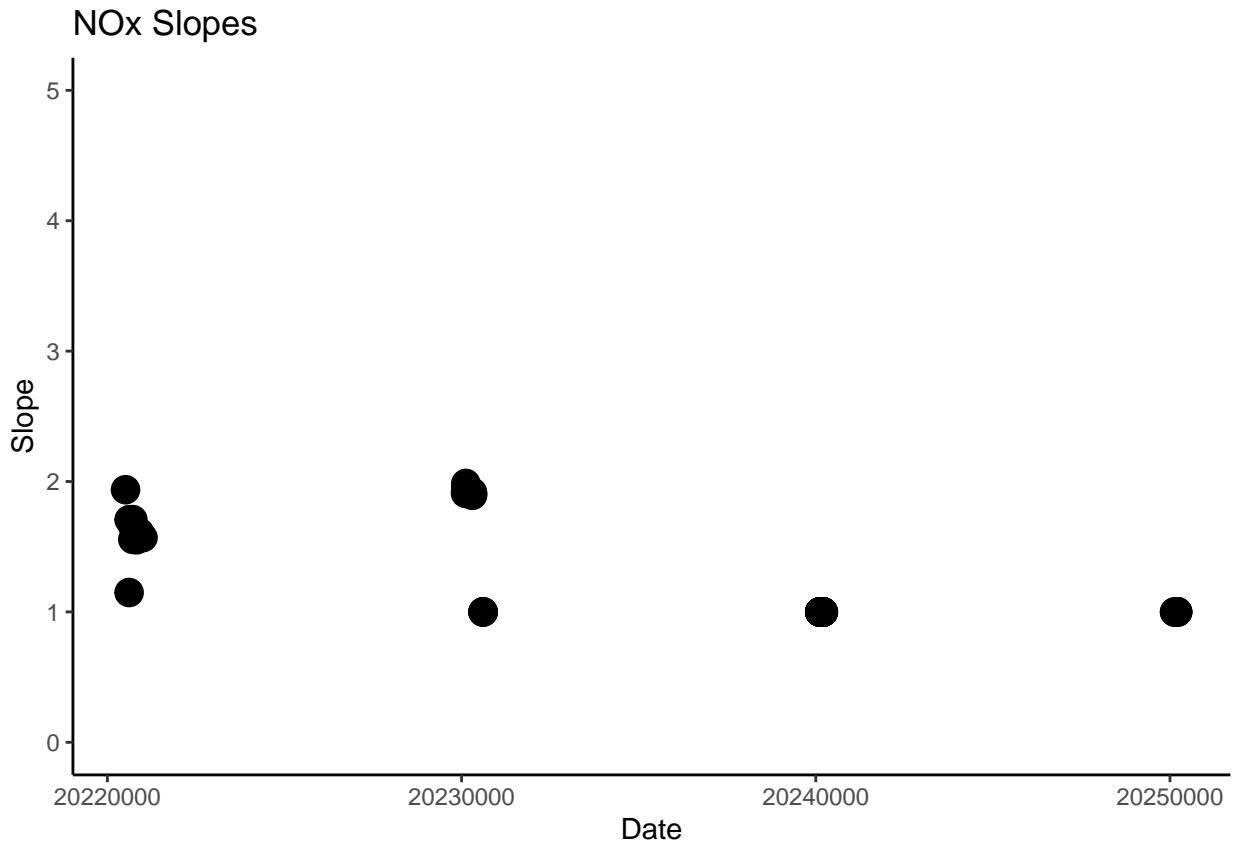
## PO4 R2s



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

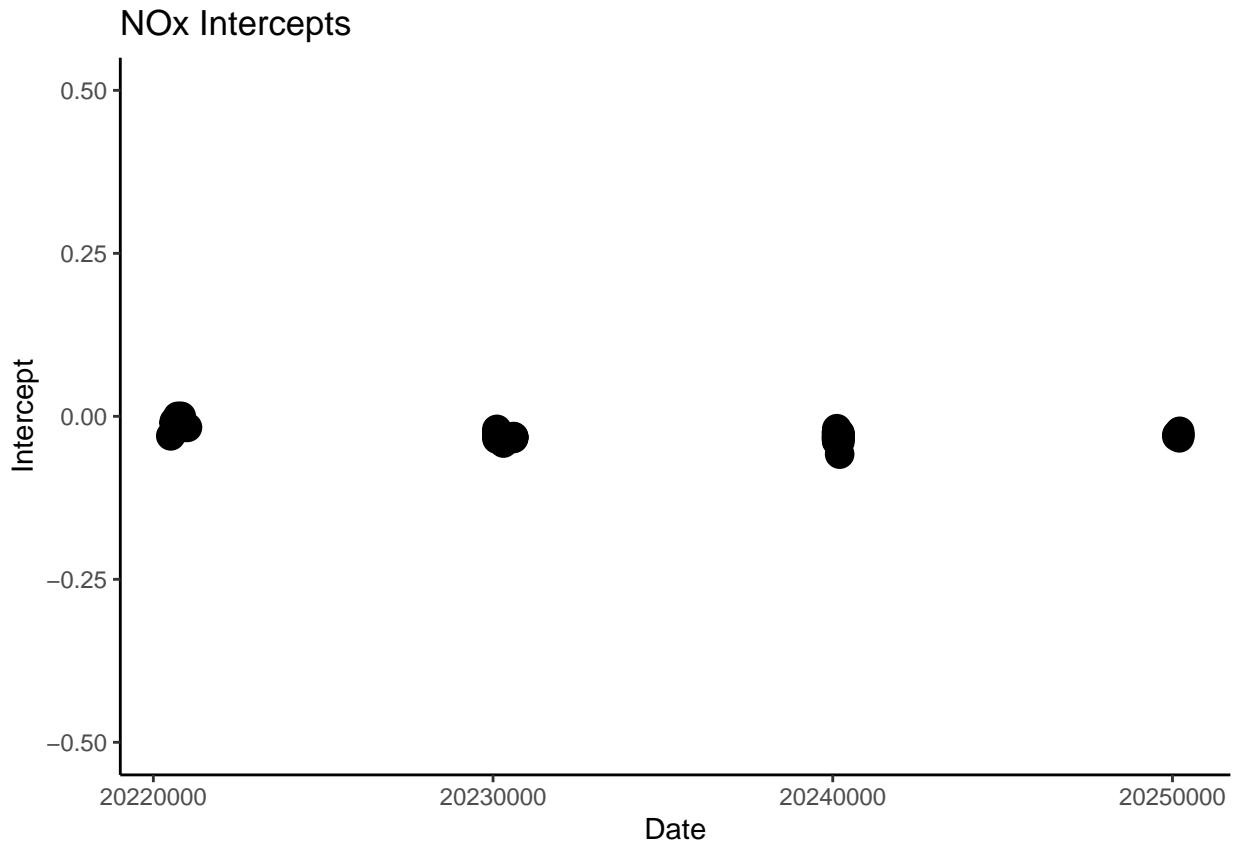
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

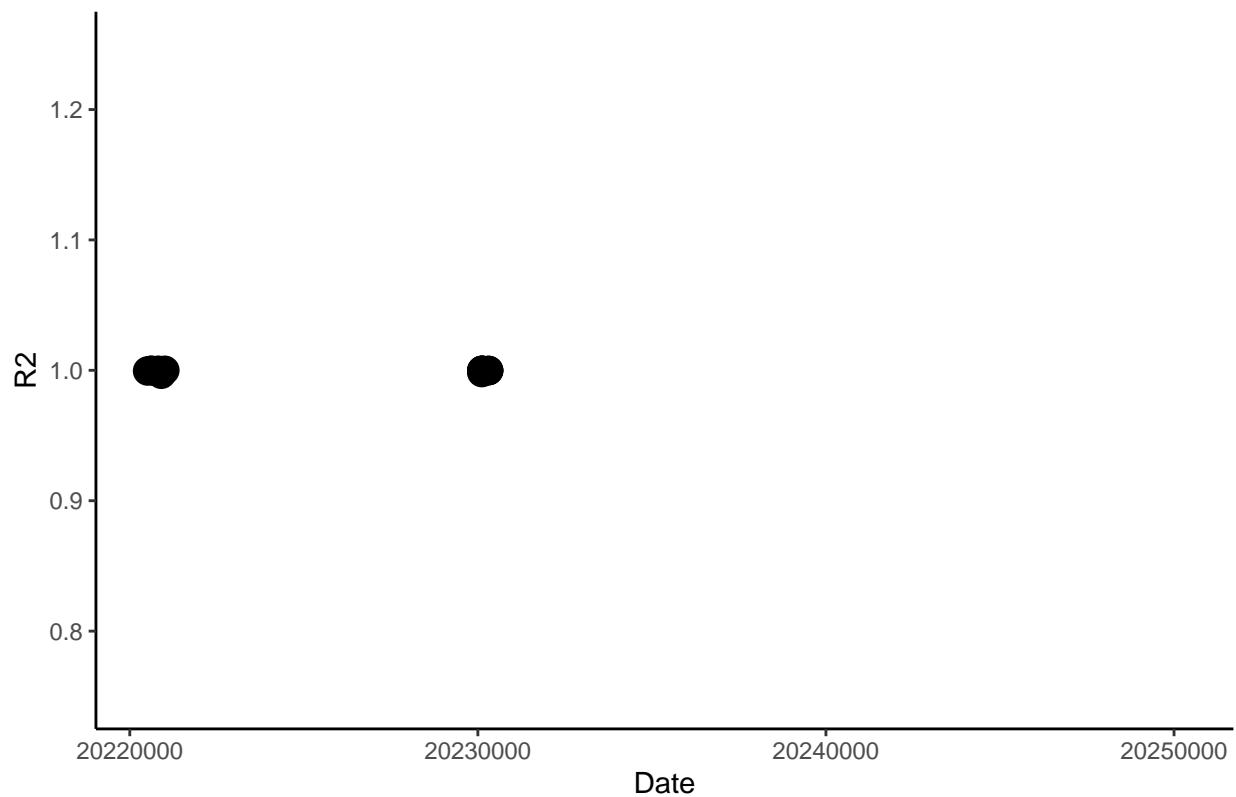


```
#plot the R2s to make sure there are no crazy outliers
Rsq3 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NOx R2s")
```

```
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_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  mg N/L Ammonia 2 1652459189 5/13/2022 12:26
## 2  0        0  0  mg N/L Ammonia 2 1652459349 5/13/2022 12:29
## 3  0        0  0  mg N/L Ammonia 2 1652459509 5/13/2022 12:31
## 4  0        0  0  mg N/L Ammonia 2 1652459669 5/13/2022 12:34
## 5  0        0  0  mg N/L Ammonia 2 1652459829 5/13/2022 12:37
## 6  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_N0x_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_N0x_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

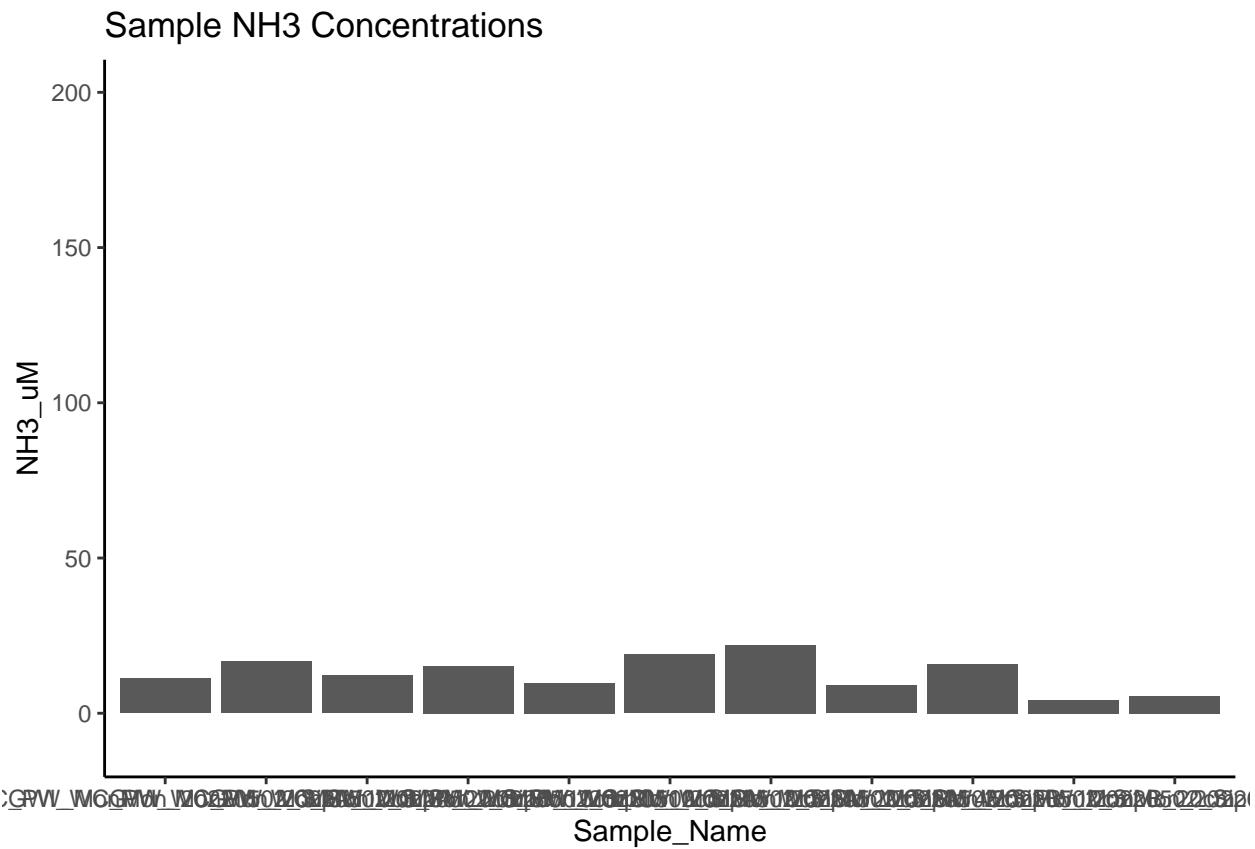
```

## Take an initial look at concentrations

```

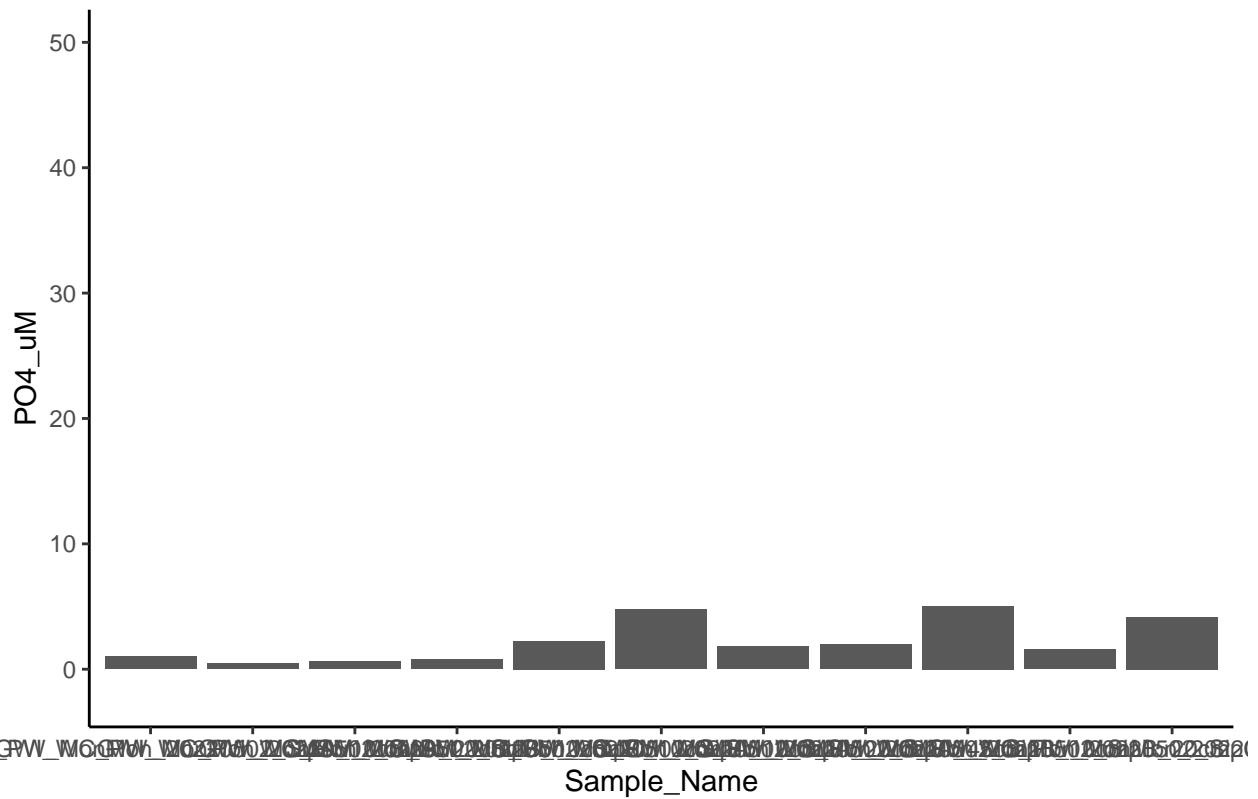
#plot data to get a sense of any outliers
NH3look <- ggplot(data=all_data, aes(x=Sample_Name, y=NH3_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-10, 200) +
  theme(legend.position="none") +
  ggtitle("Sample NH3 Concentrations")
NH3look

```



```
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
```

## Sample PO4 Concentrations



```
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
## P04_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")
```