COMPASS_Synoptic_SEAL_Data_Analysis_Oct2022

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2023-03-03

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_pu8s8pj7iNOAuhF/view?usp=sharing
#NH4 method = https://drive.google.com/file/d/1ENGemUEvm_rffZqv3lz9BjDOpAMX5nzu/view?usp=sharing
#PO4 method = https://drive.google.com/file/d/1m3gXDZnJoIo_QmyhvZG4HRgGShCzm9Wq/view?usp=sharing
#Units from SEAL = mg/L and converted to uMoles/L
```

QAQC on Slopes

```
library(ggplot2)
```

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

```
library(data.table)

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

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

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

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

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

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

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

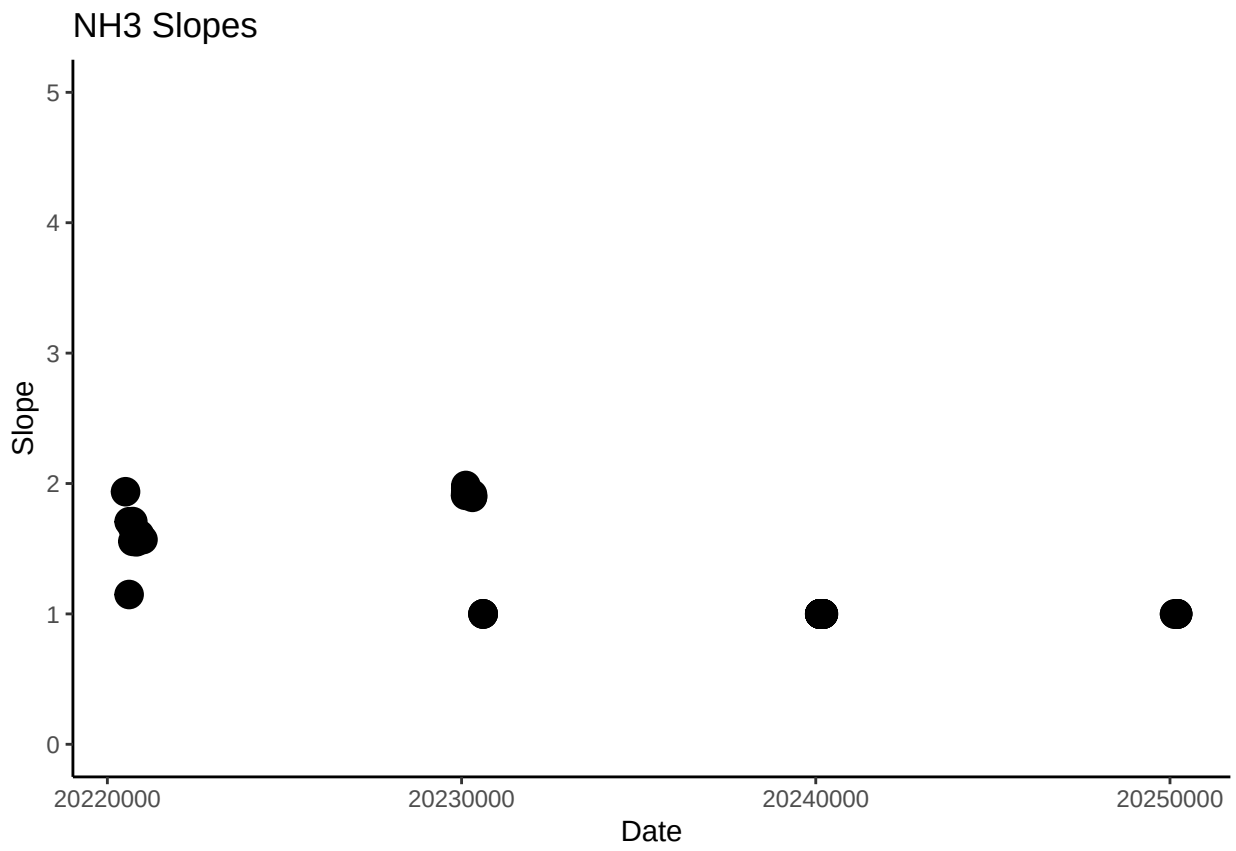
```
qNOx <- qlog[qlog$Analysis %like% "V-Nox", ]
head(qNOx)
```

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

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

slope1
```

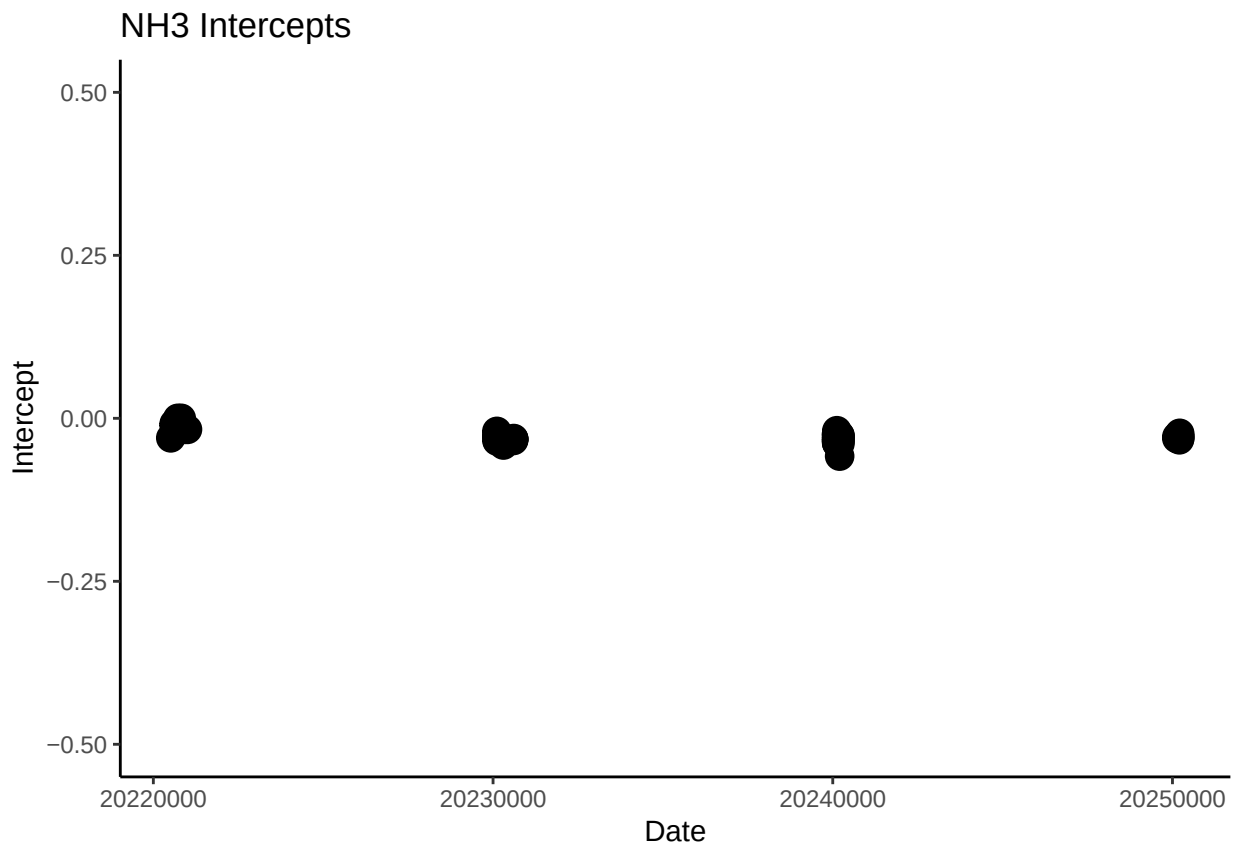
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




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

int1
```

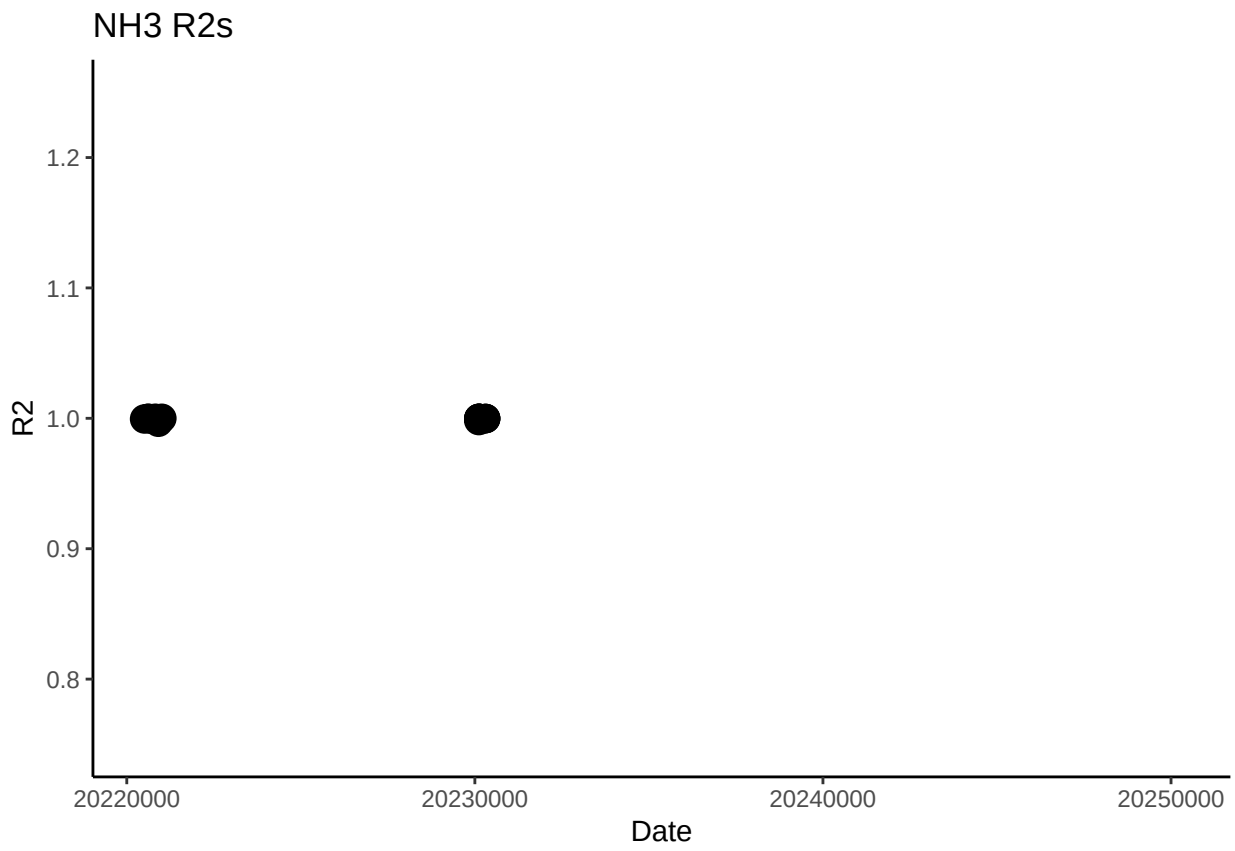
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




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

Rsq1
```

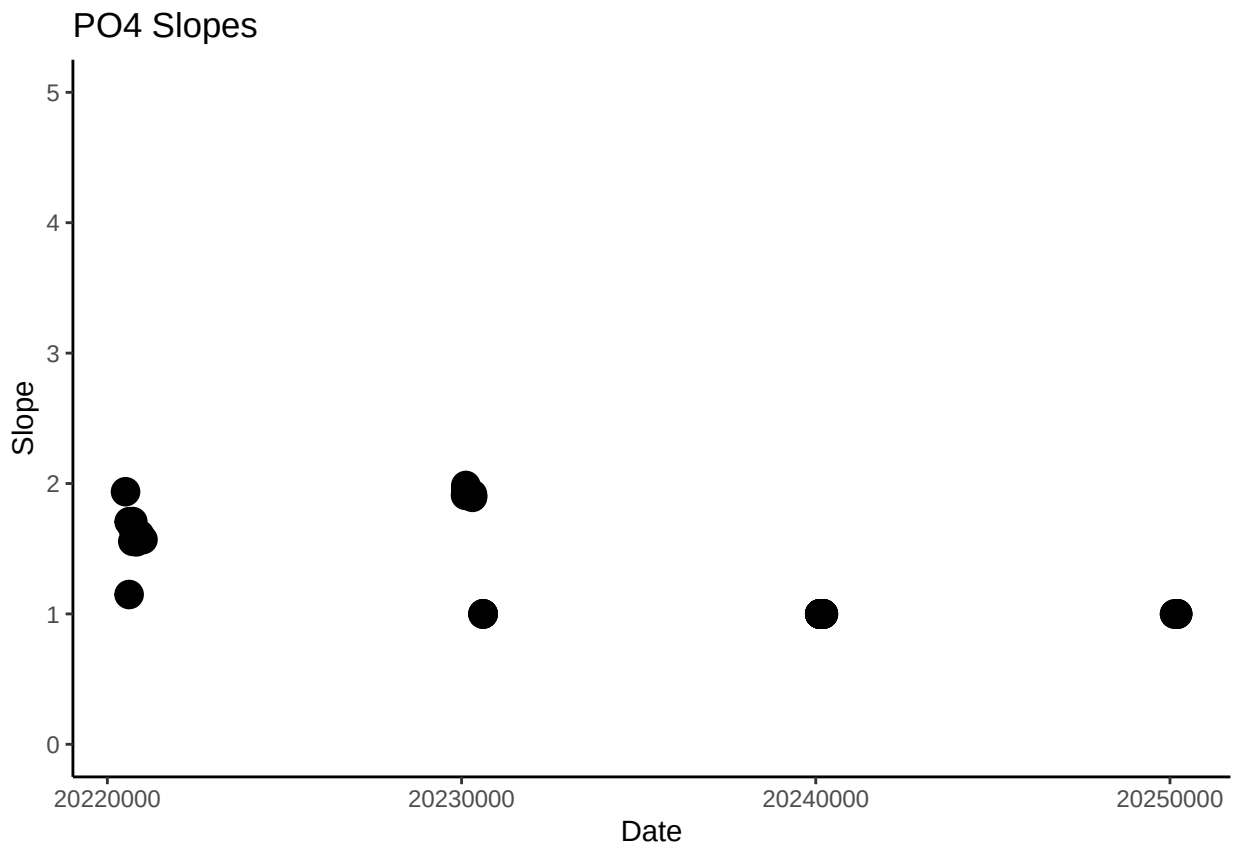
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




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

slope2
```

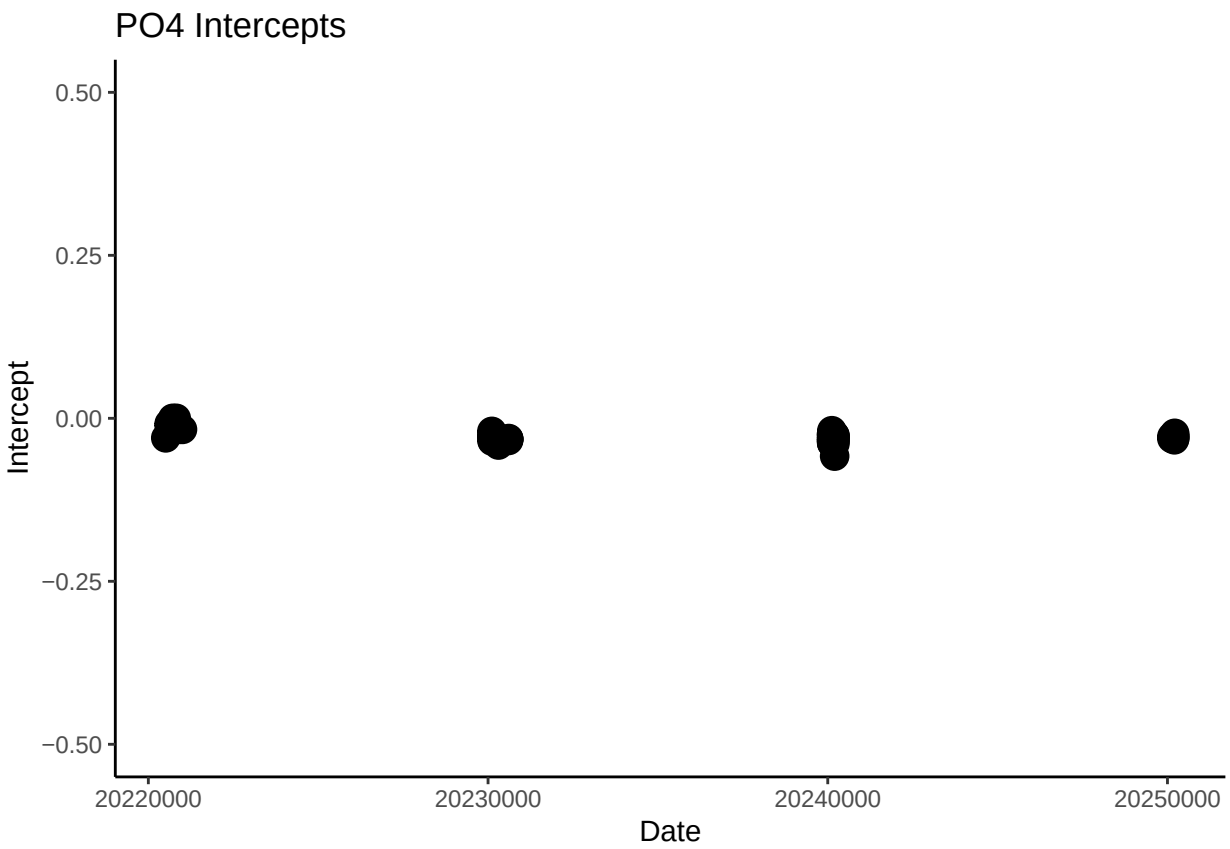
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




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

int2
```

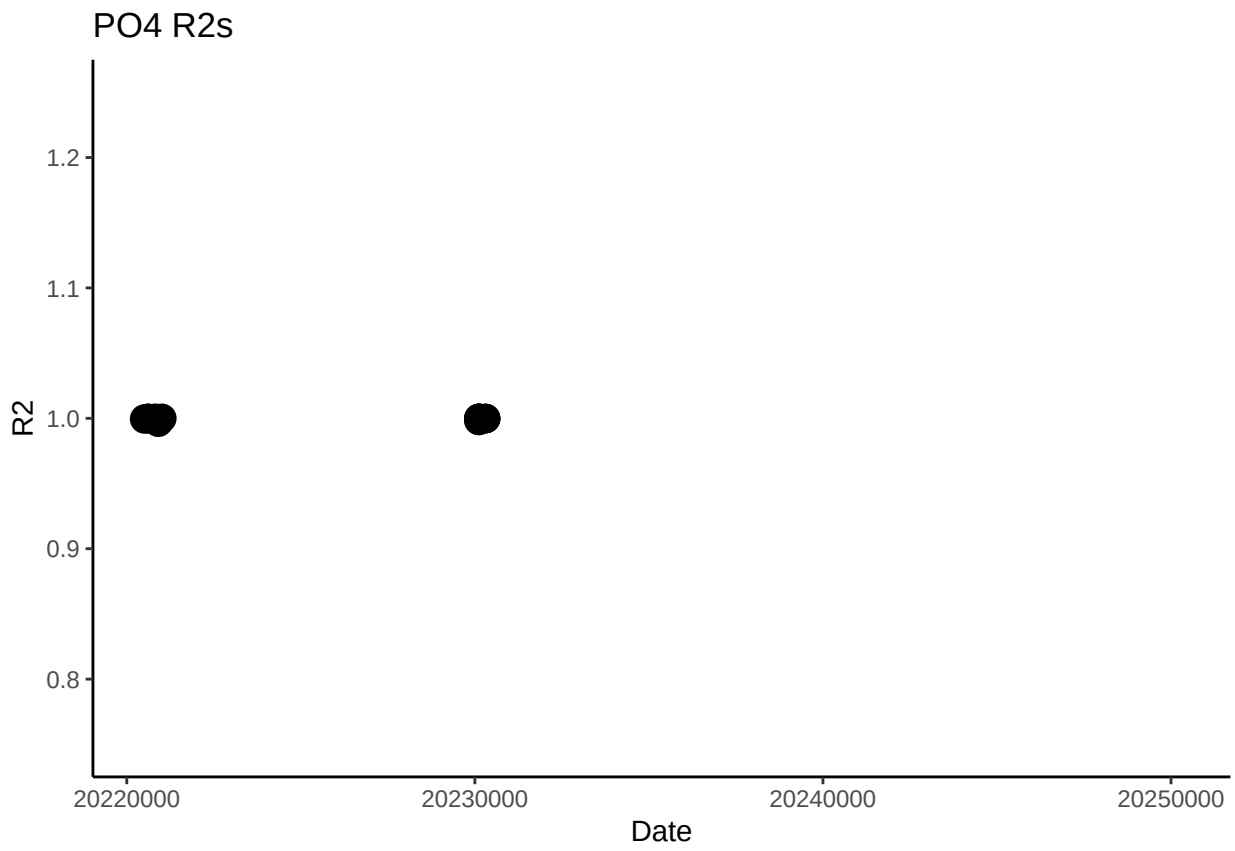
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




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

Rsq2
```

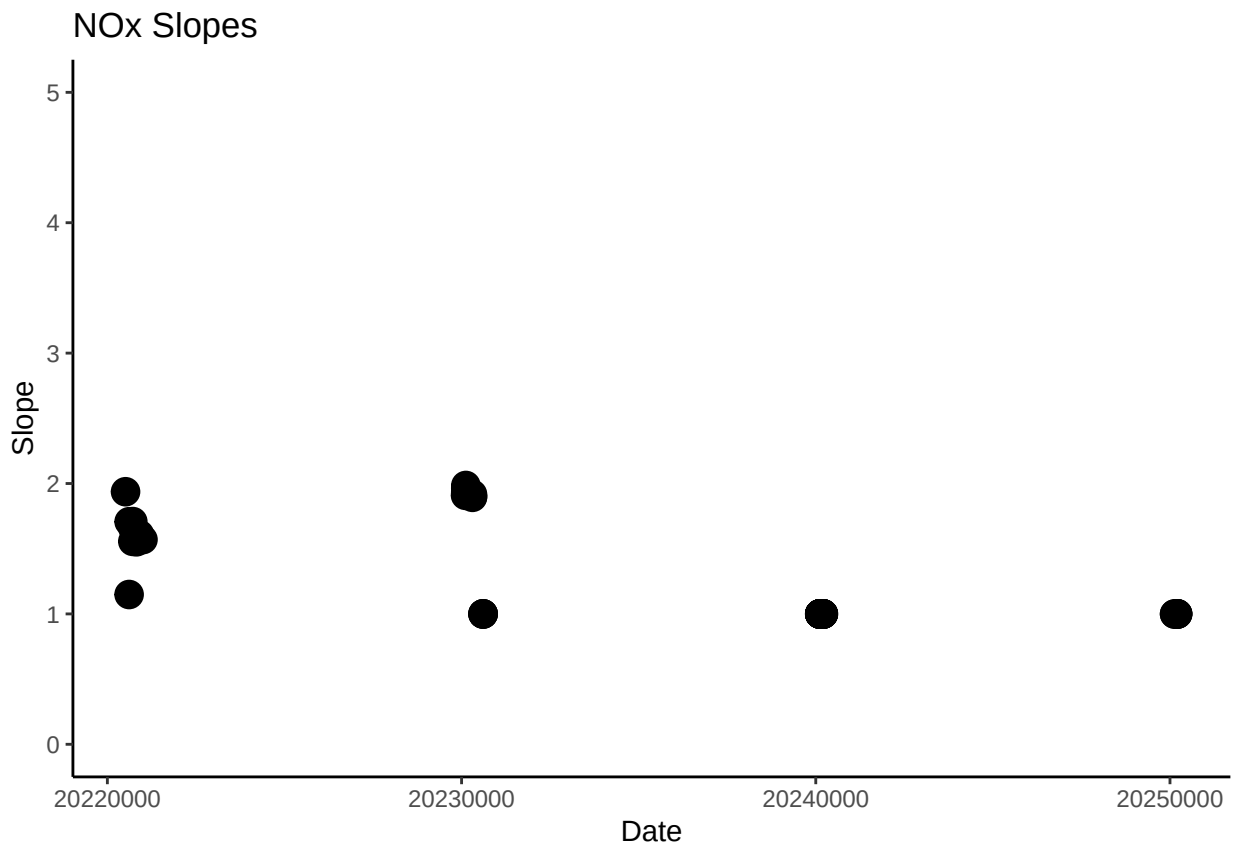
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




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

slope3
```

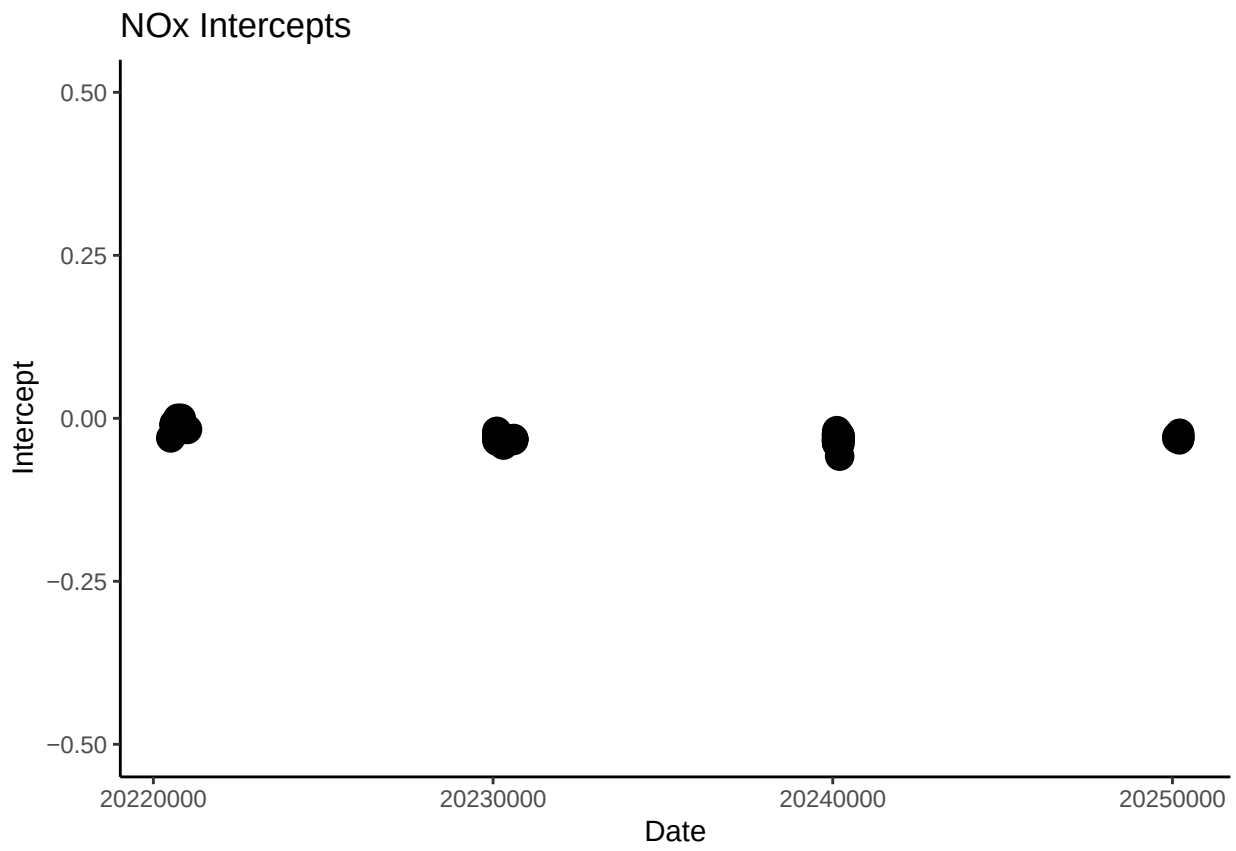
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




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

int3
```

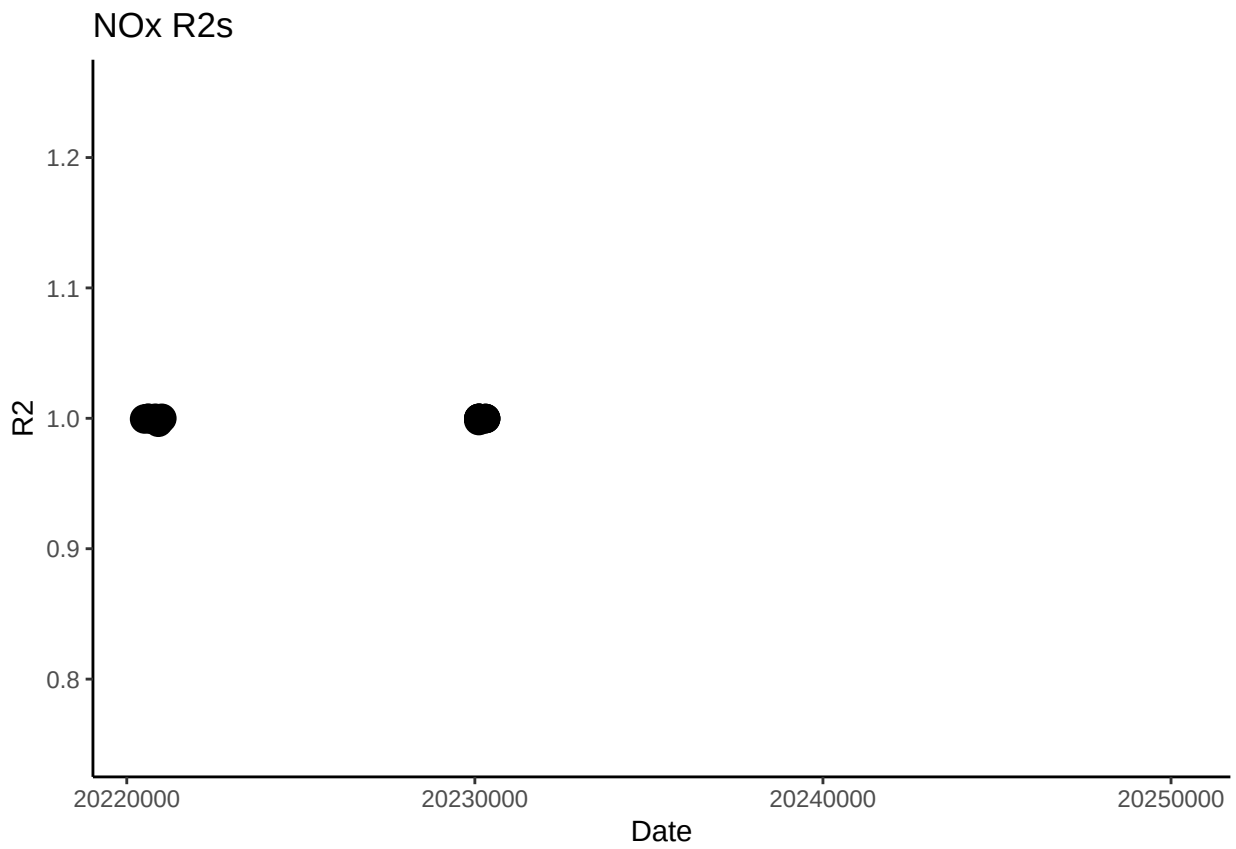
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




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

Rsq3
```

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



Code Set up

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

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

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

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

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

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

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

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

```
library(gridExtra)
```

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

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

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

Ammonia & Phosphate

```
#read in data
file1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202210_1.csv")
#Quick look at dataframe
head(file1)
```

```
##   RUNSTARTED X1674009384 X1.17.2023.21.36               X X.1      X.2      X.3
## 1     RESULT          -1               S1      Standard 1   0 0.013208 0.013208
## 2     RESULT          -2              S90  Standard .0389   1 0.033938 0.033938
## 3     RESULT          -2              S91  Standard .1000   2 0.064862 0.064862
## 4     RESULT          -2              S92  Standard .2000   3 0.118781 0.118781
## 5     RESULT          -2              S93  Standard .5000   4 0.274742 0.274742
## 6     RESULT          -2              S94 Standard 1.0000   5 0.536226 0.536226
##   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 1674010634 1/17/2023 21:57
## 2   0   0   0   0 mg N/L Ammonia 2 1674010794 1/17/2023 21:59
## 3   0   0   0   0 mg N/L Ammonia 2 1674010954 1/17/2023 22:02
## 4   0   0   0   0 mg N/L Ammonia 2 1674011114 1/17/2023 22:05
## 5   0   0   0   0 mg N/L Ammonia 2 1674011274 1/17/2023 22:07
## 6   0   0   0   0 mg N/L Ammonia 2 1674011434 1/17/2023 22:10
```

```
#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 0.013208 0.013208 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.033938 0.033938 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.064862 0.064862 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.118781 0.118781 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.274742 0.274742 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.536226 0.536226 mg N/L Ammonia 2
```

```
#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202210_2.csv")
#Quick look at dataframe
head(file2)
```

```
##   RUNSTARTED X1674070636 X1.18.2023.14.37              X X.1      X.2      X.3
## 1     RESULT          -1               S1      Standard 1   0 0.015211 0.015211
## 2     RESULT          -2              S90  Standard .0389   1 0.034194 0.034194
## 3     RESULT          -2              S91  Standard .1000   2 0.064507 0.064507
## 4     RESULT          -2              S92  Standard .2000   3 0.117400 0.117400
## 5     RESULT          -2              S93  Standard .5000   4 0.265003 0.265003
## 6     RESULT          -2              S94 Standard 1.0000   5 0.536287 0.536287
##   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 1674071922 1/18/2023 14:58
## 2   0   0   0   0 mg N/L Ammonia 2 1674072082 1/18/2023 15:01
## 3   0   0   0   0 mg N/L Ammonia 2 1674072242 1/18/2023 15:04
## 4   0   0   0   0 mg N/L Ammonia 2 1674072402 1/18/2023 15:06
## 5   0   0   0   0 mg N/L Ammonia 2 1674072562 1/18/2023 15:09
## 6   0   0   0   0 mg N/L Ammonia 2 1674072722 1/18/2023 15:12
```

```
#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 0.015211 0.015211 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.034194 0.034194 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.064507 0.064507 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.117400 0.117400 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.265003 0.265003 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.536287 0.536287 mg N/L Ammonia 2
```

```
#read in data
file3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202210_3.csv")
#Quick look at dataframe
head(file3)
```

```
##   RUNSTARTED X1674261032 X1.20.2023.19.30              X X.1      X.2      X.3
## 1 RUNSTARTED  1674261064  1/20/2023 19:31                 NA       NA       NA
## 2 RUNSTARTED  1674270611  1/20/2023 22:10                 NA       NA       NA
## 3     RESULT          -1               S1     Standard 1   0 0.015424 0.015424
## 4     RESULT          -2              S90 Standard .0389   1 0.037041 0.037041
```

```
## 5     RESULT          -2              S91 Standard .1000   2 0.065641 0.065641
## 6     RESULT          -2              S92 Standard .2000   3 0.120285 0.120285
##   X.4 X.5 X.6 X.7    X.8       X.9       X.10            X.11
## 1  NA  NA  NA  NA                           NA
## 2  NA  NA  NA  NA                           NA
## 3   0   0   0   0 mg N/L Ammonia 2 1674271855 1/20/2023 22:30
## 4   0   0   0   0 mg N/L Ammonia 2 1674272015 1/20/2023 22:33
## 5   0   0   0   0 mg N/L Ammonia 2 1674272175 1/20/2023 22:36
## 6   0   0   0   0 mg N/L Ammonia 2 1674272335 1/20/2023 22:38
```

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

```
##     Run_Info    Sample_Name     Conc      Abs  Units      Test
## 1 RUNSTARTED                     NA       NA
## 2 RUNSTARTED                     NA       NA
## 3     RESULT     Standard 1 0.015424 0.015424 mg N/L Ammonia 2
## 4     RESULT Standard .0389 0.037041 0.037041 mg N/L Ammonia 2
## 5     RESULT Standard .1000 0.065641 0.065641 mg N/L Ammonia 2
## 6     RESULT Standard .2000 0.120285 0.120285 mg N/L Ammonia 2
```

```
#read in data
file4 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202210_4.csv")
#Quick look at dataframe
head(file4)
```

```
##   RUNSTARTED X1674261032 X1.20.2023.19.30             X X.1      X.2      X.3
## 1 RUNSTARTED  1674261064  1/20/2023 19:31                NA       NA       NA
## 2 RUNSTARTED  1674270611  1/20/2023 22:10                NA       NA       NA
## 3     RESULT          -1               S1     Standard 1   0 0.015424 0.015424
## 4     RESULT          -2              S90 Standard .0389   1 0.037041 0.037041
## 5     RESULT          -2              S91 Standard .1000   2 0.065641 0.065641
## 6     RESULT          -2              S92 Standard .2000   3 0.120285 0.120285
##   X.4 X.5 X.6 X.7    X.8       X.9       X.10            X.11
## 1  NA  NA  NA  NA                           NA
## 2  NA  NA  NA  NA                           NA
## 3   0   0   0   0 mg N/L Ammonia 2 1674271855 1/20/2023 22:30
## 4   0   0   0   0 mg N/L Ammonia 2 1674272015 1/20/2023 22:33
## 5   0   0   0   0 mg N/L Ammonia 2 1674272175 1/20/2023 22:36
## 6   0   0   0   0 mg N/L Ammonia 2 1674272335 1/20/2023 22:38
```

```
#take out only the columns that we need
dat4 <- file4[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(dat4) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(dat4)
```

```
##     Run_Info    Sample_Name     Conc      Abs  Units      Test
## 1 RUNSTARTED                     NA       NA
```

```
## 2 RUNSTARTED                      NA       NA
## 3     RESULT     Standard 1 0.015424 0.015424 mg N/L Ammonia 2
## 4     RESULT Standard .0389 0.037041 0.037041 mg N/L Ammonia 2
## 5     RESULT Standard .1000 0.065641 0.065641 mg N/L Ammonia 2
## 6     RESULT Standard .2000 0.120285 0.120285 mg N/L Ammonia 2
```

```
#read in data
file5 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202210-11_4.csv")
#Quick look at dataframe
head(file5)
```

```
##   RUNSTARTED X1674434960       X1.22.2023.19.49              X X.1      X.2
## 1   RUNENDED  1674434979 STOP IMMEDIATE PRESSED                 NA       NA
## 2 RUNSTARTED  1674435072        1/22/2023 19:51                 NA       NA
## 3     RESULT          -1                    S1     Standard 1   0 0.015639
## 4     RESULT          -2                   S90 Standard .0389   1 0.035279
## 5     RESULT          -2                   S91 Standard .1000   2 0.064059
## 6     RESULT          -2                   S92 Standard .2000   3 0.117862
##        X.3 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 0.015639   0   0   0 512 mg N/L Ammonia 2 1674436305 1/22/2023 20:11
## 4 0.035279   0   0   0 512 mg N/L Ammonia 2 1674436465 1/22/2023 20:14
## 5 0.064059   0   0   0 512 mg N/L Ammonia 2 1674436625 1/22/2023 20:17
## 6 0.117862   0   0   0 512 mg N/L Ammonia 2 1674436785 1/22/2023 20:19
```

```
#take out only the columns that we need
dat5 <- file5[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(dat5) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(dat5)
```

```
##     Run_Info    Sample_Name     Conc      Abs  Units      Test
## 1   RUNENDED                      NA       NA
## 2 RUNSTARTED                      NA       NA
## 3     RESULT     Standard 1 0.015639 0.015639 mg N/L Ammonia 2
## 4     RESULT Standard .0389 0.035279 0.035279 mg N/L Ammonia 2
## 5     RESULT Standard .1000 0.064059 0.064059 mg N/L Ammonia 2
## 6     RESULT Standard .2000 0.117862 0.117862 mg N/L Ammonia 2
```

```
alldat <- rbind(dat1, dat2, dat3, dat4, dat5)

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

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.013208 0.013208 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.033938 0.033938 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.064862 0.064862 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.118781 0.118781 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.274742 0.274742 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.536226 0.536226 mg N/L Ammonia 2
```

```r
#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
## 489   RESULT MSM_202210_UP_PPR_1 0.313359 0.178272 mg N/L Ammonia 2
## 490   RESULT MSM_202210_UP_PPR_2 0.343022 0.193470 mg N/L Ammonia 2
## 491   RESULT MSM_202210_UP_PPR_3 0.467758 0.257378 mg N/L Ammonia 2
## 492   RESULT MSM_202210_UP_PPR_4 0.645589 0.348490 mg N/L Ammonia 2
## 493   RESULT MSM_202210_UP_PPR_5 0.794490 0.424779 mg N/L Ammonia 2
## 494   RESULT MSM_202210_UP_PPR_6 0.450865 0.248723 mg N/L Ammonia 2
```

NOx

```r
#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202210_1.csv")
#Quick look at dataframe
head(Nfile1)
```

```
##   RUNSTARTED X1674058557 X1.18.2023.11.15           X X.1      X.2      X.3 X.4
## 1     RESULT          -1               S1  Standard 1   0 0.138425 0.138425   0
## 2     RESULT          -2              S90 Standard 90   1 0.156085 0.156085   0
## 3     RESULT          -2              S91 Standard 91   2 0.181254 0.181254   0
## 4     RESULT          -2              S92 Standard 92   3 0.224592 0.224592   0
## 5     RESULT          -2              S93 Standard 93   4 0.338805 0.338805   0
## 6     RESULT          -2              S94 Standard 94   5 0.546026 0.546026   0
##   X.5 X.6 X.7    X.8          X.9       X.10            X.11
## 1   0   0   0 mg N/L Vanadium NOx 1674060737 1/18/2023 11:52
## 2   0   0   0 mg N/L Vanadium NOx 1674060816 1/18/2023 11:53
## 3   0   0   0 mg N/L Vanadium NOx 1674060896 1/18/2023 11:54
## 4   0   0   0 mg N/L Vanadium NOx 1674060977 1/18/2023 11:56
## 5   0   0   0 mg N/L Vanadium NOx 1674061057 1/18/2023 11:57
## 6   0   0   0 mg N/L Vanadium NOx 1674061137 1/18/2023 11:58
```

```r
#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   RESULT  Standard 1 0.138425 0.138425 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.156085 0.156085 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.181254 0.181254 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.224592 0.224592 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.338805 0.338805 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.546026 0.546026 mg N/L Vanadium NOx
```

```r
#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202210_2.csv")
#Quick look at dataframe
head(Nfile2)
```

```
##   RUNSTARTED X1674088994 X1.18.2023.19.43           X X.1      X.2      X.3 X.4
## 1     RESULT          -1               S1  Standard 1   0 0.142252 0.142252   0
## 2     RESULT          -2              S90 Standard 90   1 0.161788 0.161788   0
## 3     RESULT          -2              S91 Standard 91   2 0.187268 0.187268   0
## 4     RESULT          -2              S92 Standard 92   3 0.229701 0.229701   0
## 5     RESULT          -2              S93 Standard 93   4 0.350446 0.350446   0
## 6     RESULT          -2              S94 Standard 94   5 0.552649 0.552649   0
##   X.5 X.6 X.7    X.8          X.9       X.10            X.11
## 1   0   0   0 mg N/L Vanadium NOx 1674091173 1/18/2023 20:19
## 2   0   0   0 mg N/L Vanadium NOx 1674091253 1/18/2023 20:20
## 3   0   0   0 mg N/L Vanadium NOx 1674091334 1/18/2023 20:22
## 4   0   0   0 mg N/L Vanadium NOx 1674091413 1/18/2023 20:23
## 5   0   0   0 mg N/L Vanadium NOx 1674091493 1/18/2023 20:24
## 6   0   0   0 mg N/L Vanadium NOx 1674091573 1/18/2023 20:26
```

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

```
##   Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RESULT  Standard 1 0.142252 0.142252 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.161788 0.161788 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.187268 0.187268 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.229701 0.229701 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.350446 0.350446 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.552649 0.552649 mg N/L Vanadium NOx
```

```r
#read in data
Nfile3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202210_3.csv")
#Quick look at dataframe
head(Nfile3)
```

```
##   RUNSTARTED X1674251527 X1.20.2023.16.52           X X.1      X.2      X.3 X.4
## 1     RESULT          -1               S1  Standard 1   0 0.181183 0.181183   0
## 2     RESULT          -2              S90 Standard 90   1 0.198214 0.198214   0
## 3     RESULT          -2              S91 Standard 91   2 0.223312 0.223312   0
## 4     RESULT          -2              S92 Standard 92   3 0.265110 0.265110   0
## 5     RESULT          -2              S93 Standard 93   4 0.383191 0.383191   0
## 6     RESULT          -2              S94 Standard 94   5 0.579907 0.579907   0
##   X.5 X.6 X.7    X.8          X.9       X.10            X.11
## 1   0   0   0 mg N/L Vanadium NOx 1674253722 1/20/2023 17:28
## 2   0   0   0 mg N/L Vanadium NOx 1674253804 1/20/2023 17:30
## 3   0   0   0 mg N/L Vanadium NOx 1674253884 1/20/2023 17:31
## 4   0   0   0 mg N/L Vanadium NOx 1674253966 1/20/2023 17:32
## 5   0   0   0 mg N/L Vanadium NOx 1674254046 1/20/2023 17:34
## 6   0   0   0 mg N/L Vanadium NOx 1674254127 1/20/2023 17:35
```

```r
#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 0.181183 0.181183 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.198214 0.198214 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.223312 0.223312 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.265110 0.265110 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.383191 0.383191 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.579907 0.579907 mg N/L Vanadium NOx
```

```r
#read in data
Nfile4 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202210_4.csv")
#Quick look at dataframe
head(Nfile4)
```

```
##   RUNSTARTED X1674330201 X1.21.2023.14.43           X X.1      X.2      X.3 X.4
## 1     RESULT          -1               S1  Standard 1   0 0.182628 0.182628   0
## 2     RESULT          -2              S90 Standard 90   1 0.201200 0.201200   0
## 3     RESULT          -2              S91 Standard 91   2 0.224336 0.224336   0
## 4     RESULT          -2              S92 Standard 92   3 0.264526 0.264526   0
## 5     RESULT          -2              S93 Standard 93   4 0.384563 0.384563   0
## 6     RESULT          -2              S94 Standard 94   5 0.587757 0.587757   0
##   X.5 X.6 X.7    X.8          X.9       X.10            X.11
## 1   0   0   0 mg N/L Vanadium NOx 1674332394 1/21/2023 15:19
## 2   0   0   0 mg N/L Vanadium NOx 1674332475 1/21/2023 15:21
## 3   0   0   0 mg N/L Vanadium NOx 1674332556 1/21/2023 15:22
## 4   0   0   0 mg N/L Vanadium NOx 1674332637 1/21/2023 15:23
## 5   0   0   0 mg N/L Vanadium NOx 1674332718 1/21/2023 15:25
## 6   0   0   0 mg N/L Vanadium NOx 1674332799 1/21/2023 15:26
```

```r
#take out only the columns that we need
Ndat4 <- Nfile4[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(Ndat4) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat4)
```

```
##   Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RESULT  Standard 1 0.182628 0.182628 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.201200 0.201200 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.224336 0.224336 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.264526 0.264526 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.384563 0.384563 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.587757 0.587757 mg N/L Vanadium NOx
```

```r
#read in data
Nfile5 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202210-11_4.csv")
#Quick look at dataframe
head(Nfile5)
```

```
##   RUNSTARTED X1674567913      X1.24.2023.8.45           X X.1      X.2      X.3
## 1   RUNENDED  1674567954 INSUFFICIENT REAGENT              NA       NA       NA
## 2 RUNSTARTED  1674569191       1/24/2023 9:06              NA       NA       NA
## 3     RESULT          -1                  S1  Standard 1   0 0.178421 0.178421
## 4     RESULT          -2                 S90 Standard 90   1 0.198991 0.198991
## 5     RESULT          -2                 S91 Standard 91   2 0.218318 0.218318
## 6     RESULT          -2                 S92 Standard 92   3 0.260783 0.260783
##   X.4 X.5 X.6 X.7    X.8          X.9       X.10           X.11
## 1  NA  NA  NA  NA                            NA
## 2  NA  NA  NA  NA                            NA
## 3   0   0   0 512 mg N/L Vanadium NOx 1674571379 1/24/2023 9:42
## 4   0   0   0 512 mg N/L Vanadium NOx 1674571460 1/24/2023 9:44
## 5   0   0   0 512 mg N/L Vanadium NOx 1674571540 1/24/2023 9:45
## 6   0   0   0 512 mg N/L Vanadium NOx 1674571621 1/24/2023 9:47
```

```
#take out only the columns that we need
Ndat5 <- Nfile5[ ,c(1,4,6,7, 12, 13)]
# assigning new names to the columns of the data frame
colnames(Ndat5) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat5)
```

```
##     Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RUNENDED                   NA       NA
## 2 RUNSTARTED                   NA       NA
## 3     RESULT  Standard 1 0.178421 0.178421 mg N/L Vanadium NOx
## 4     RESULT Standard 90 0.198991 0.198991 mg N/L Vanadium NOx
## 5     RESULT Standard 91 0.218318 0.218318 mg N/L Vanadium NOx
## 6     RESULT Standard 92 0.260783 0.260783 mg N/L Vanadium NOx
```

```
Nalldat <- rbind(Ndat1, Ndat2, Ndat3, Ndat4, Ndat5)

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

```
##   Run_Info Sample_Name     Conc      Abs  Units         Test
## 1   RESULT  Standard 1 0.138425 0.138425 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.156085 0.156085 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.181254 0.181254 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.224592 0.224592 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.338805 0.338805 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.546026 0.546026 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
## 231   RESULT MSM_202210_UP_LysA_20cm  0.000456 0.182796 mg N/L Vanadium NOx
## 232   RESULT MSM_202210_UP_LysA_45cm  0.000638 0.182941 mg N/L Vanadium NOx
```

```
## 233   RESULT MSM_202210_UP_LysB_10cm -0.002491 0.180455 mg N/L Vanadium NOx
## 234   RESULT MSM_202210_UP_LysB_20cm  0.001671 0.183762 mg N/L Vanadium NOx
## 235   RESULT MSM_202210_UP_LysB_45cm -0.001690 0.181091 mg N/L Vanadium NOx
## 236   RESULT MSM_202210_UP_LysC_10cm -0.005525 0.178046 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
## 489   RESULT MSM_202210_UP_PPR_1 0.313359 0.178272 mg N/L Ammonia 2
## 490   RESULT MSM_202210_UP_PPR_2 0.343022 0.193470 mg N/L Ammonia 2
## 491   RESULT MSM_202210_UP_PPR_3 0.467758 0.257378 mg N/L Ammonia 2
## 492   RESULT MSM_202210_UP_PPR_4 0.645589 0.348490 mg N/L Ammonia 2
## 493   RESULT MSM_202210_UP_PPR_5 0.794490 0.424779 mg N/L Ammonia 2
## 494   RESULT MSM_202210_UP_PPR_6 0.450865 0.248723 mg N/L Ammonia 2
```

```
head(Nalldat2)
```

```
##     Run_Info             Sample_Name      Conc      Abs  Units         Test
## 231   RESULT MSM_202210_UP_LysA_20cm  0.000456 0.182796 mg N/L Vanadium NOx
## 232   RESULT MSM_202210_UP_LysA_45cm  0.000638 0.182941 mg N/L Vanadium NOx
## 233   RESULT MSM_202210_UP_LysB_10cm -0.002491 0.180455 mg N/L Vanadium NOx
## 234   RESULT MSM_202210_UP_LysB_20cm  0.001671 0.183762 mg N/L Vanadium NOx
## 235   RESULT MSM_202210_UP_LysB_45cm -0.001690 0.181091 mg N/L Vanadium NOx
## 236   RESULT MSM_202210_UP_LysC_10cm -0.005525 0.178046 mg N/L Vanadium NOx
```

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

```
##     Run_Info         Sample_Name     Conc      Abs  Units      Test
## 489   RESULT MSM_202210_UP_PPR_1 0.313359 0.178272 mg N/L Ammonia 2
## 490   RESULT MSM_202210_UP_PPR_2 0.343022 0.193470 mg N/L Ammonia 2
## 491   RESULT MSM_202210_UP_PPR_3 0.467758 0.257378 mg N/L Ammonia 2
## 492   RESULT MSM_202210_UP_PPR_4 0.645589 0.348490 mg N/L Ammonia 2
## 493   RESULT MSM_202210_UP_PPR_5 0.794490 0.424779 mg N/L Ammonia 2
## 494   RESULT MSM_202210_UP_PPR_6 0.450865 0.248723 mg N/L Ammonia 2
```

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

```
##     Run_Info         Sample_Name     Conc      Abs  Units       Test
## 631   RESULT MSM_202210_UP_PPR_1 0.003792 0.003058 mg P/L o-PHOS 0.3
## 632   RESULT MSM_202210_UP_PPR_2 0.003947 0.003122 mg P/L o-PHOS 0.3
## 633   RESULT MSM_202210_UP_PPR_3 0.007060 0.004405 mg P/L o-PHOS 0.3
## 634   RESULT MSM_202210_UP_PPR_4 0.009802 0.005535 mg P/L o-PHOS 0.3
## 635   RESULT MSM_202210_UP_PPR_5 0.009451 0.005390 mg P/L o-PHOS 0.3
## 636   RESULT MSM_202210_UP_PPR_6 0.005077 0.003588 mg P/L o-PHOS 0.3
```

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

```
##     Run_Info             Sample_Name      Conc      Abs  Units         Test
## 231   RESULT MSM_202210_UP_LysA_20cm  0.000456 0.182796 mg N/L Vanadium NOx
## 232   RESULT MSM_202210_UP_LysA_45cm  0.000638 0.182941 mg N/L Vanadium NOx
## 233   RESULT MSM_202210_UP_LysB_10cm -0.002491 0.180455 mg N/L Vanadium NOx
## 234   RESULT MSM_202210_UP_LysB_20cm  0.001671 0.183762 mg N/L Vanadium NOx
## 235   RESULT MSM_202210_UP_LysB_45cm -0.001690 0.181091 mg N/L Vanadium NOx
## 236   RESULT MSM_202210_UP_LysC_10cm -0.005525 0.178046 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  Conc_uM
## 489   RESULT MSM_202210_UP_PPR_1 0.313359 0.178272 mg N/L Ammonia 2 22.37208
## 490   RESULT MSM_202210_UP_PPR_2 0.343022 0.193470 mg N/L Ammonia 2 24.48985
## 491   RESULT MSM_202210_UP_PPR_3 0.467758 0.257378 mg N/L Ammonia 2 33.39530
## 492   RESULT MSM_202210_UP_PPR_4 0.645589 0.348490 mg N/L Ammonia 2 46.09144
## 493   RESULT MSM_202210_UP_PPR_5 0.794490 0.424779 mg N/L Ammonia 2 56.72214
## 494   RESULT MSM_202210_UP_PPR_6 0.450865 0.248723 mg N/L Ammonia 2 32.18924
```

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

```
##     Run_Info         Sample_Name     Conc      Abs  Units       Test   Conc_uM
## 631   RESULT MSM_202210_UP_PPR_1 0.003792 0.003058 mg P/L o-PHOS 0.3 0.2707276
## 632   RESULT MSM_202210_UP_PPR_2 0.003947 0.003122 mg P/L o-PHOS 0.3 0.2817937
## 633   RESULT MSM_202210_UP_PPR_3 0.007060 0.004405 mg P/L o-PHOS 0.3 0.5040445
## 634   RESULT MSM_202210_UP_PPR_4 0.009802 0.005535 mg P/L o-PHOS 0.3 0.6998079
## 635   RESULT MSM_202210_UP_PPR_5 0.009451 0.005390 mg P/L o-PHOS 0.3 0.6747485
## 636   RESULT MSM_202210_UP_PPR_6 0.005077 0.003588 mg P/L o-PHOS 0.3 0.3624694
```

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

```
##     Run_Info             Sample_Name      Conc      Abs  Units         Test
## 231   RESULT MSM_202210_UP_LysA_20cm  0.000456 0.182796 mg N/L Vanadium NOx
## 232   RESULT MSM_202210_UP_LysA_45cm  0.000638 0.182941 mg N/L Vanadium NOx
```

```
## 233   RESULT MSM_202210_UP_LysB_10cm -0.002491 0.180455 mg N/L Vanadium NOx
## 234   RESULT MSM_202210_UP_LysB_20cm  0.001671 0.183762 mg N/L Vanadium NOx
## 235   RESULT MSM_202210_UP_LysB_45cm -0.001690 0.181091 mg N/L Vanadium NOx
## 236   RESULT MSM_202210_UP_LysC_10cm -0.005525 0.178046 mg N/L Vanadium NOx
##     Conc_uM_raw
## 231  0.03255585
## 232  0.04554963
## 233 -0.17784346
## 234  0.11930005
## 235 -0.12065654
## 236 -0.39445408
```

```
#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
## 231   RESULT MSM_202210_UP_LysA_20cm  0.000456 0.182796 mg N/L Vanadium NOx
## 232   RESULT MSM_202210_UP_LysA_45cm  0.000638 0.182941 mg N/L Vanadium NOx
## 233   RESULT MSM_202210_UP_LysB_10cm -0.002491 0.180455 mg N/L Vanadium NOx
## 234   RESULT MSM_202210_UP_LysB_20cm  0.001671 0.183762 mg N/L Vanadium NOx
## 235   RESULT MSM_202210_UP_LysB_45cm -0.001690 0.181091 mg N/L Vanadium NOx
## 236   RESULT MSM_202210_UP_LysC_10cm -0.005525 0.178046 mg N/L Vanadium NOx
##     Conc_uM_raw    Conc_uM
## 231  0.03255585 0.03255585
## 232  0.04554963 0.04554963
## 233 -0.17784346 0.00000000
## 234  0.11930005 0.11930005
## 235 -0.12065654 0.00000000
## 236 -0.39445408 0.00000000
```

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
## 489 MSM_202210_UP_PPR_1 0.313359 22.37208
## 490 MSM_202210_UP_PPR_2 0.343022 24.48985
## 491 MSM_202210_UP_PPR_3 0.467758 33.39530
## 492 MSM_202210_UP_PPR_4 0.645589 46.09144
## 493 MSM_202210_UP_PPR_5 0.794490 56.72214
## 494 MSM_202210_UP_PPR_6 0.450865 32.18924
```

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

```
##             Sample_Name     Conc   Conc_uM
## 631 MSM_202210_UP_PPR_1 0.003792 0.2707276
```

```
## 632 MSM_202210_UP_PPR_2 0.003947 0.2817937
## 633 MSM_202210_UP_PPR_3 0.007060 0.5040445
## 634 MSM_202210_UP_PPR_4 0.009802 0.6998079
## 635 MSM_202210_UP_PPR_5 0.009451 0.6747485
## 636 MSM_202210_UP_PPR_6 0.005077 0.3624694
```

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

```
##                 Sample_Name      Conc    Conc_uM
## 231 MSM_202210_UP_LysA_20cm  0.000456 0.03255585
## 232 MSM_202210_UP_LysA_45cm  0.000638 0.04554963
## 233 MSM_202210_UP_LysB_10cm -0.002491 0.00000000
## 234 MSM_202210_UP_LysB_20cm  0.001671 0.11930005
## 235 MSM_202210_UP_LysB_45cm -0.001690 0.00000000
## 236 MSM_202210_UP_LysC_10cm -0.005525 0.00000000
```

```
#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_202210_SW_A 0.249386 17.804765 0.125976 8.9939815  0.007561 0.5398131
## 2 GCrew_202210_SW_B 0.305534 21.813418 0.137691 9.8303669  0.008117 0.5795084
## 3 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421 -0.069967 0.0000000
## 4 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421  0.004603 0.3286284
## 5 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489 -0.069967 0.0000000
## 6 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489  0.004603 0.3286284
```

```
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_202210_SW_A 0.249386 17.804765 0.125976 8.9939815  0.007561 0.5398131
## 2 GCrew_202210_SW_B 0.305534 21.813418 0.137691 9.8303669  0.008117 0.5795084
## 3 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421 -0.069967 0.0000000
## 4 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421  0.004603 0.3286284
## 5 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489 -0.069967 0.0000000
## 6 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489  0.004603 0.3286284
```

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

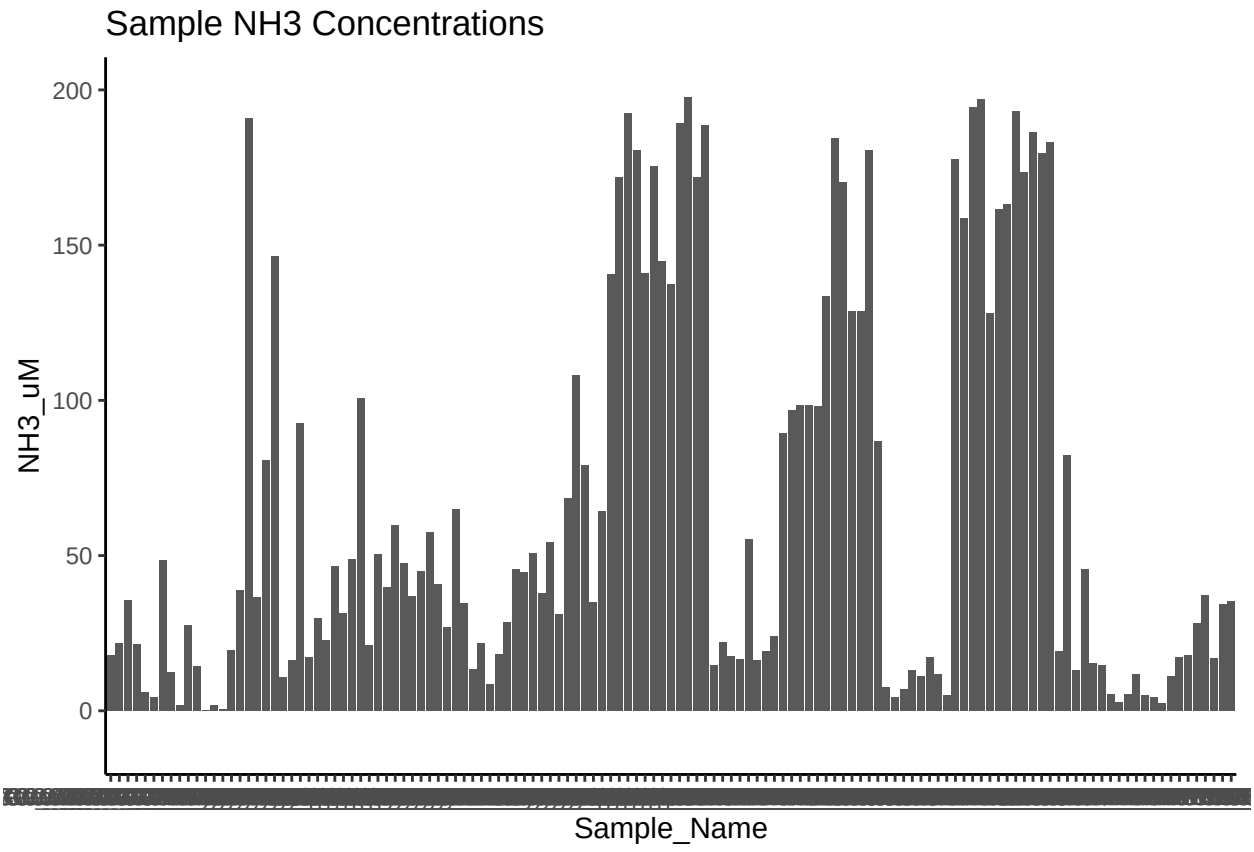
```
##         Sample_Name  NH3_mgL    NH3_uM  PO4_mgL    PO4_uM   NOx_mgL    NOx_uM
## 1 GCrew_202210_SW_A 0.249386 17.804765 0.125976 8.9939815  0.007561 0.5398131
## 2 GCrew_202210_SW_B 0.305534 21.813418 0.137691 9.8303669  0.008117 0.5795084
## 3 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421 -0.069967 0.0000000
```

```
## 4 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421  0.004603 0.3286284
## 5 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489 -0.069967 0.0000000
## 6 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489  0.004603 0.3286284
##      NH3_range    PO4_range NOx_range
## 1 Within_Range Within_Range       bdl
## 2 Within_Range Within_Range       bdl
## 3 Within_Range          bdl       bdl
## 4 Within_Range          bdl       bdl
## 5 Within_Range Within_Range       bdl
## 6 Within_Range Within_Range       bdl
```

Take an initial look at concentrations

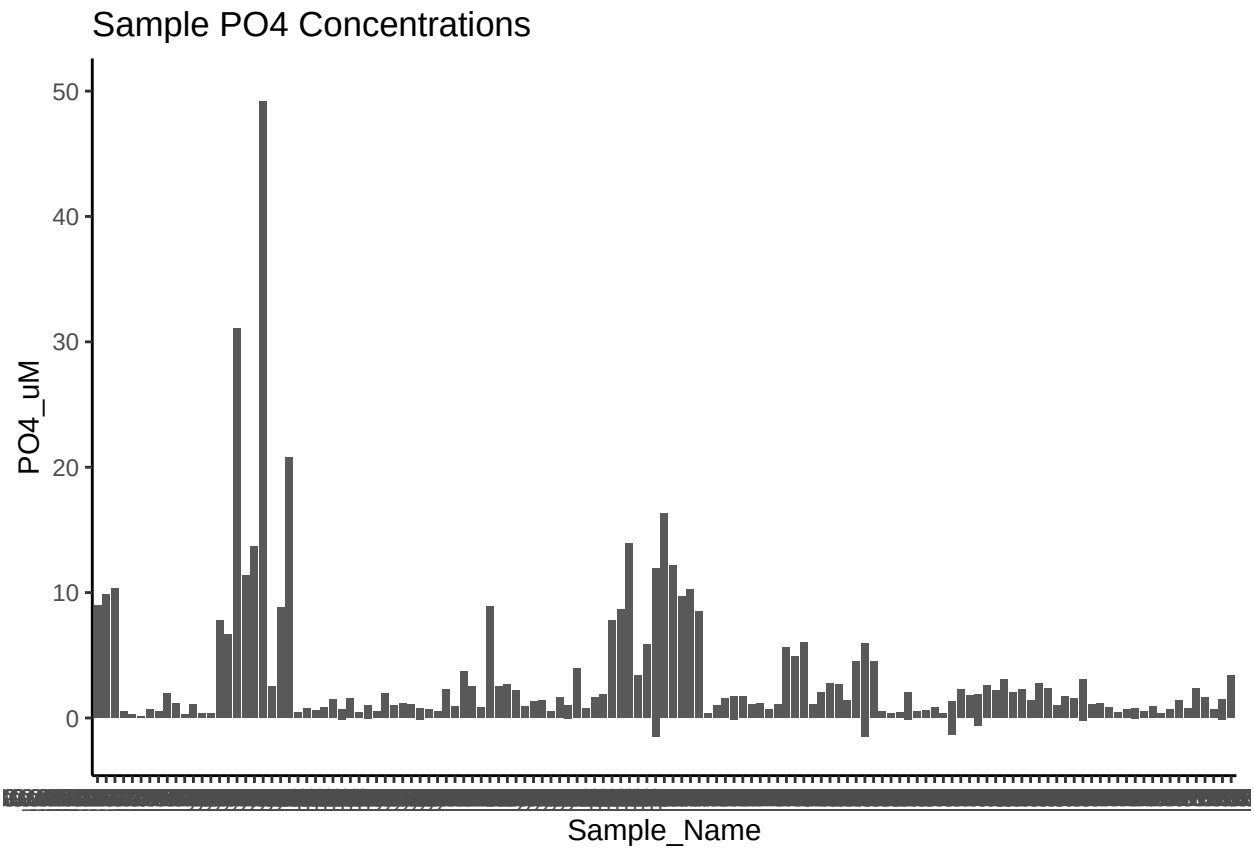
```
#plot data to get a sense of any outliers
NH3look <- ggplot(data=all_data, aes(x=Sample_Name, y=NH3_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-10, 200) +
  theme(legend.position="none") +
  ggtitle("Sample NH3 Concentrations")
NH3look
```

```
## Warning: Removed 28 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```



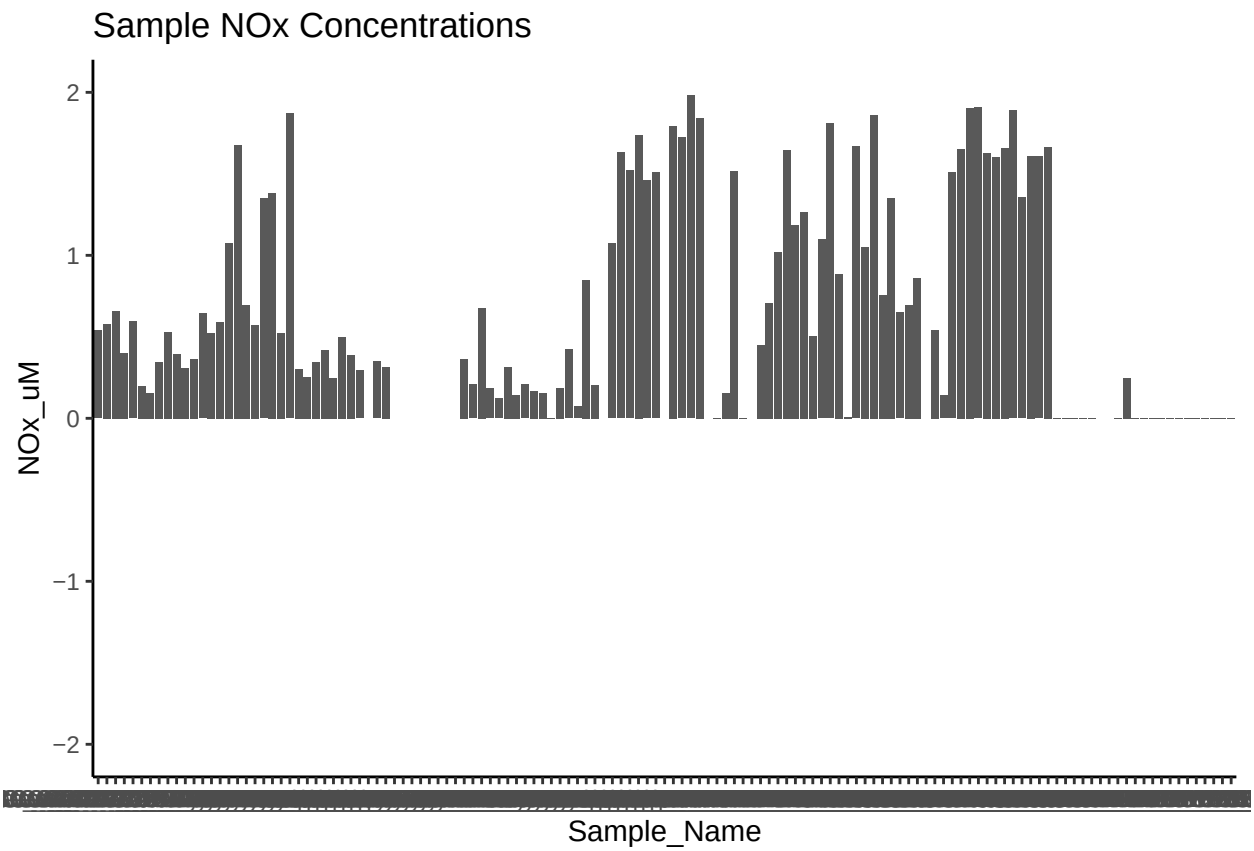
```
PO4look <- ggplot(data=all_data, aes(x=Sample_Name, y=PO4_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 50) +
  theme(legend.position="none") +
  ggtitle("Sample PO4 Concentrations")
PO4look
```

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




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

```
## Warning: Removed 80 rows containing missing values or values outside the scale range
## (`geom_bar()`).
```



Pull out data you need, make IDs

```
head(all_data)
```

```
##         Sample_Name  NH3_mgL    NH3_uM  PO4_mgL    PO4_uM   NOx_mgL    NOx_uM
## 1 GCrew_202210_SW_A 0.249386 17.804765 0.125976 8.9939815  0.007561 0.5398131
## 2 GCrew_202210_SW_B 0.305534 21.813418 0.137691 9.8303669  0.008117 0.5795084
## 3 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421 -0.069967 0.0000000
## 4 GCrew_202210_SW_C 0.124176  8.865472 0.002949 0.2105421  0.004603 0.3286284
## 5 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489 -0.069967 0.0000000
## 6 GCrew_202210_SW_C 0.124176  8.865472 0.069649 4.9725489  0.004603 0.3286284
##      NH3_range    PO4_range NOx_range
## 1 Within_Range Within_Range       bdl
## 2 Within_Range Within_Range       bdl
## 3 Within_Range          bdl       bdl
## 4 Within_Range          bdl       bdl
## 5 Within_Range Within_Range       bdl
## 6 Within_Range Within_Range       bdl
```

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

```
##         Sample_Name    NH3_uM    PO4_uM    NOx_uM    NH3_range    PO4_range
```

```
## 1 GCrew_202210_SW_A 17.804765 8.9939815 0.5398131 Within_Range Within_Range
## 2 GCrew_202210_SW_B 21.813418 9.8303669 0.5795084 Within_Range Within_Range
## 3 GCrew_202210_SW_C  8.865472 0.2105421 0.0000000 Within_Range          bdl
## 4 GCrew_202210_SW_C  8.865472 0.2105421 0.3286284 Within_Range          bdl
## 5 GCrew_202210_SW_C  8.865472 4.9725489 0.0000000 Within_Range Within_Range
## 6 GCrew_202210_SW_C  8.865472 4.9725489 0.3286284 Within_Range Within_Range
##   NOx_range
## 1       bdl
## 2       bdl
## 3       bdl
## 4       bdl
## 5       bdl
## 6       bdl
```

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

```
## Warning in rbind(c("GCrew", "202210", "SW", "A"), c("GCrew", "202210", "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$Month <- ifelse(IDs$Date == 202210,"October","November")
#IDs$Month <- "September"
head(IDs)
```

```
##    Site   Date Zone Replicate Depth   Tree   Month
## 1 GCrew 202210   SW         A GCrew 202210 October
## 2 GCrew 202210   SW         B GCrew 202210 October
## 3 GCrew 202210   SW         C GCrew 202210 October
## 4 GCrew 202210   SW         C GCrew 202210 October
## 5 GCrew 202210   SW         C GCrew 202210 October
## 6 GCrew 202210   SW         C GCrew 202210 October
```

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

```
##    Site   Date Zone Replicate Depth   Tree   Month       Sample_Name    NH3_uM
## 1 GCrew 202210   SW         A GCrew 202210 October GCrew_202210_SW_A 17.804765
## 2 GCrew 202210   SW         B GCrew 202210 October GCrew_202210_SW_B 21.813418
## 3 GCrew 202210   SW         C GCrew 202210 October GCrew_202210_SW_C  8.865472
## 4 GCrew 202210   SW         C GCrew 202210 October GCrew_202210_SW_C  8.865472
## 5 GCrew 202210   SW         C GCrew 202210 October GCrew_202210_SW_C  8.865472
## 6 GCrew 202210   SW         C GCrew 202210 October GCrew_202210_SW_C  8.865472
##      PO4_uM    NOx_uM    NH3_range    PO4_range NOx_range
## 1 8.9939815 0.5398131 Within_Range Within_Range       bdl
## 2 9.8303669 0.5795084 Within_Range Within_Range       bdl
## 3 0.2105421 0.0000000 Within_Range          bdl       bdl
## 4 0.2105421 0.3286284 Within_Range          bdl       bdl
## 5 4.9725489 0.0000000 Within_Range Within_Range       bdl
## 6 4.9725489 0.3286284 Within_Range Within_Range       bdl
```

Export final data with flags

```
#Export Data

write.csv(alldat, file="Processed Data/COMPASS_Synoptic_CB_SEAL_NUTR_202210-11.csv")
```