

COMPASS_Synoptic_SEAL_Data_Analysis_July2022

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Information

```
#####
##### COMPASS Synoptic
##### Chesapeake Bay Sites
##### Data Analysis Code: Porewater Nutrients
##### MONTH: August 2022
#####

#####
##### Information #####
#Author: Stephanie J. Wilson
#Edited: 20220727

#Samples taken from Lysimeters & Sippers at CB Synoptic Sites
#Samples were filtered with 0.45 uM, kept on ice, frozen until analysis
#Field Protocol:
#Samples Analyzed on a SEAL discrete auto analyzer
#Lab Protocol: https://docs.google.com/document/d/1VaJT7Wb9AcdmM1tgsR_9ZtQ6kwcaoNmp/edit?usp=sharing&ou
#NOx method = https://drive.google.com/file/d/1sicqBFnzVxmDd5I2_pu8s8pj7iNUAuhF/view?usp=sharing
#NH4 method = https://drive.google.com/file/d/1ENGemUEvm_rfjZqv3lz9BjD0pAMX5nzu/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
#R2 and Slopes
#These are checked for drift or differences in this code

#Duplicates and Spikes
#This is checked by the SEAL software
#If 80% of the dups and spikes are within range we accept
#the only exceptions are NOx values that are below the detection limit - we do not count dups out of range
#these are run roughly every 10-12 samples per tray.

#CCV and CCBs
#CCV's are 50% of the top standard checks run every 10 samples, these are checked by the software; if 80%
#CCB's are DI blanks run every 10 samples, these are checked by the software; if 80% are within range we

#Third Party Standard
#This is checked within the code - must be within 20% of the peChk concentration
```

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")

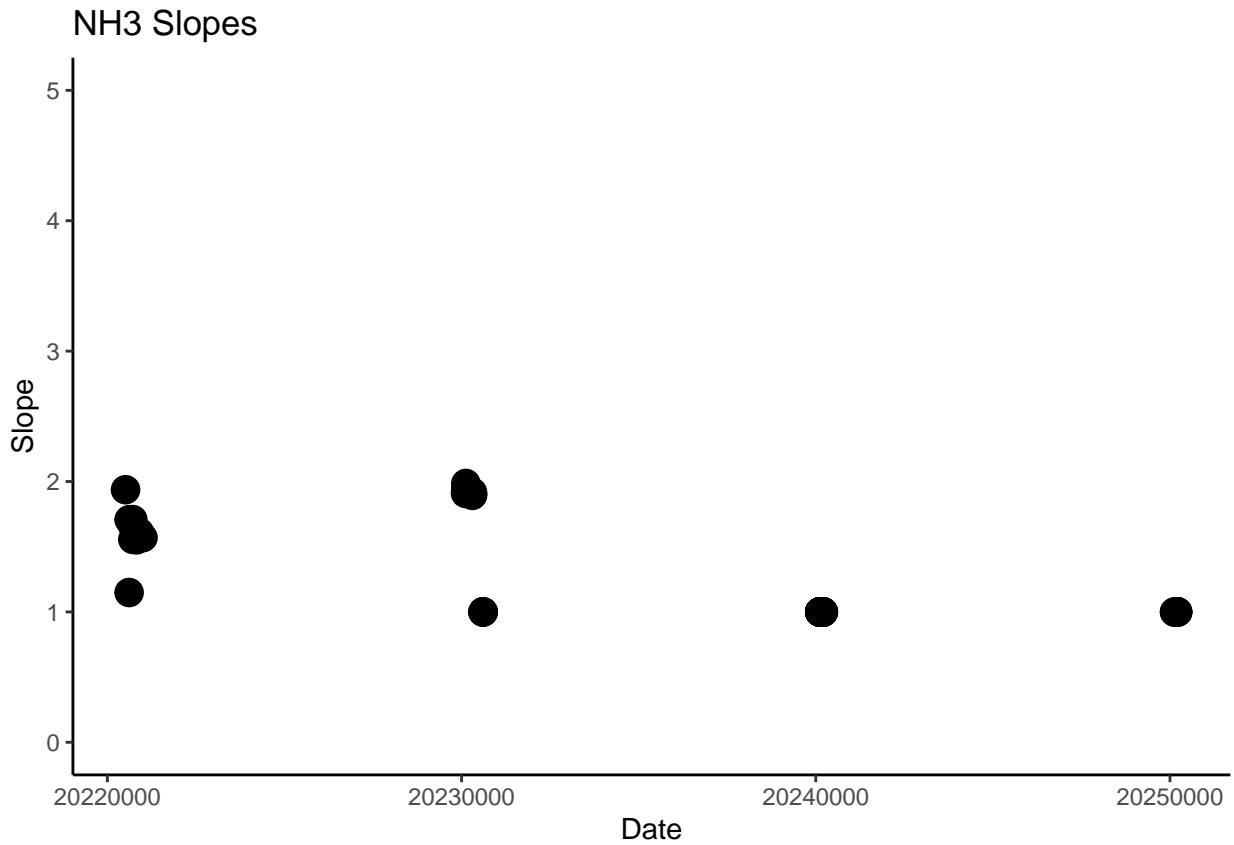
```

```
slope1
```

```

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

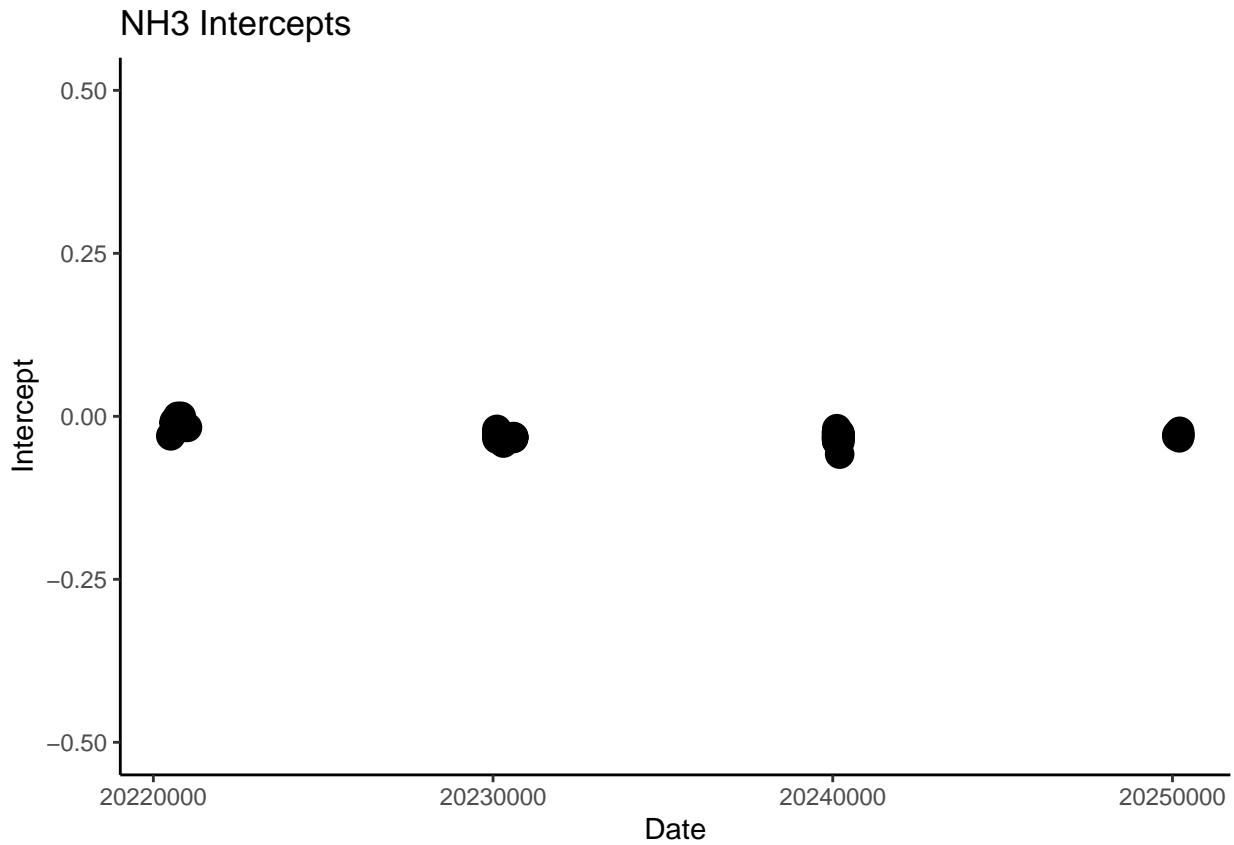
```



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

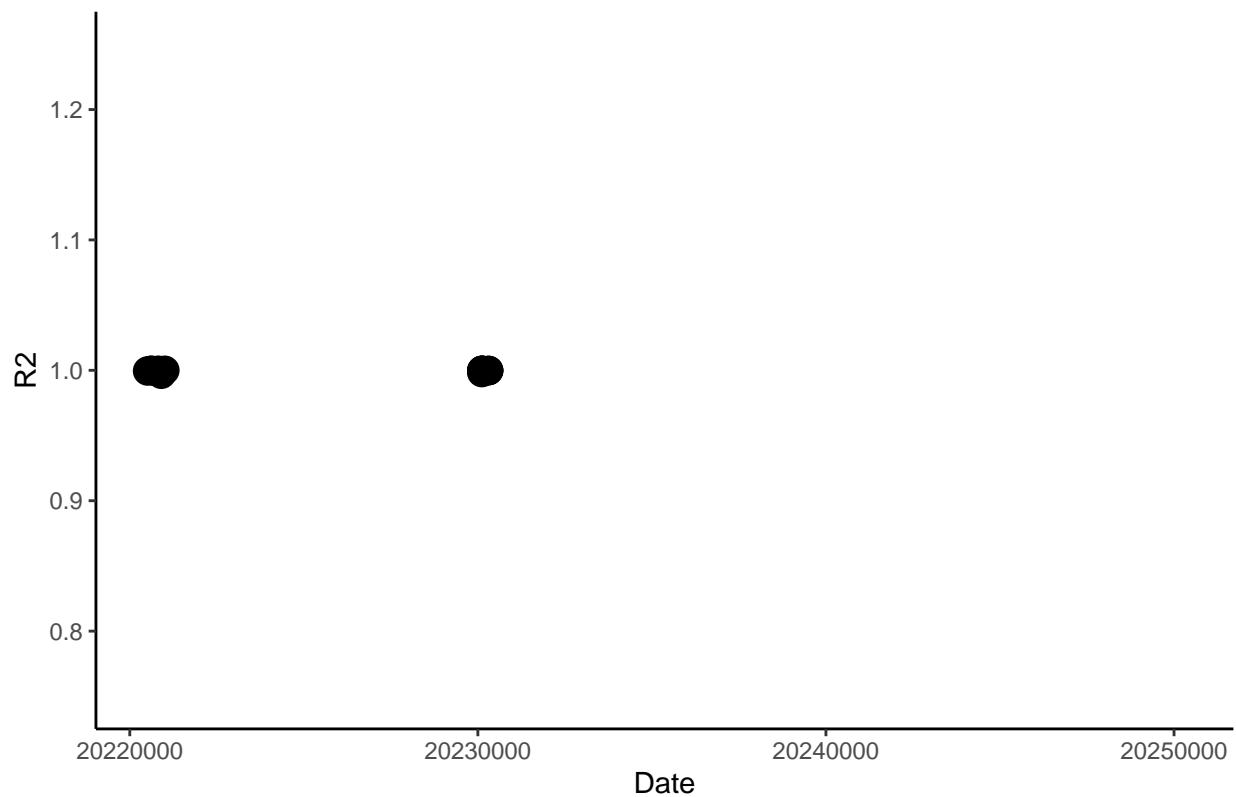


```
#plot the R2s to make sure there are no crazy outliers
Rsq1 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NH3 R2s")
```

```
Rsq1
```

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

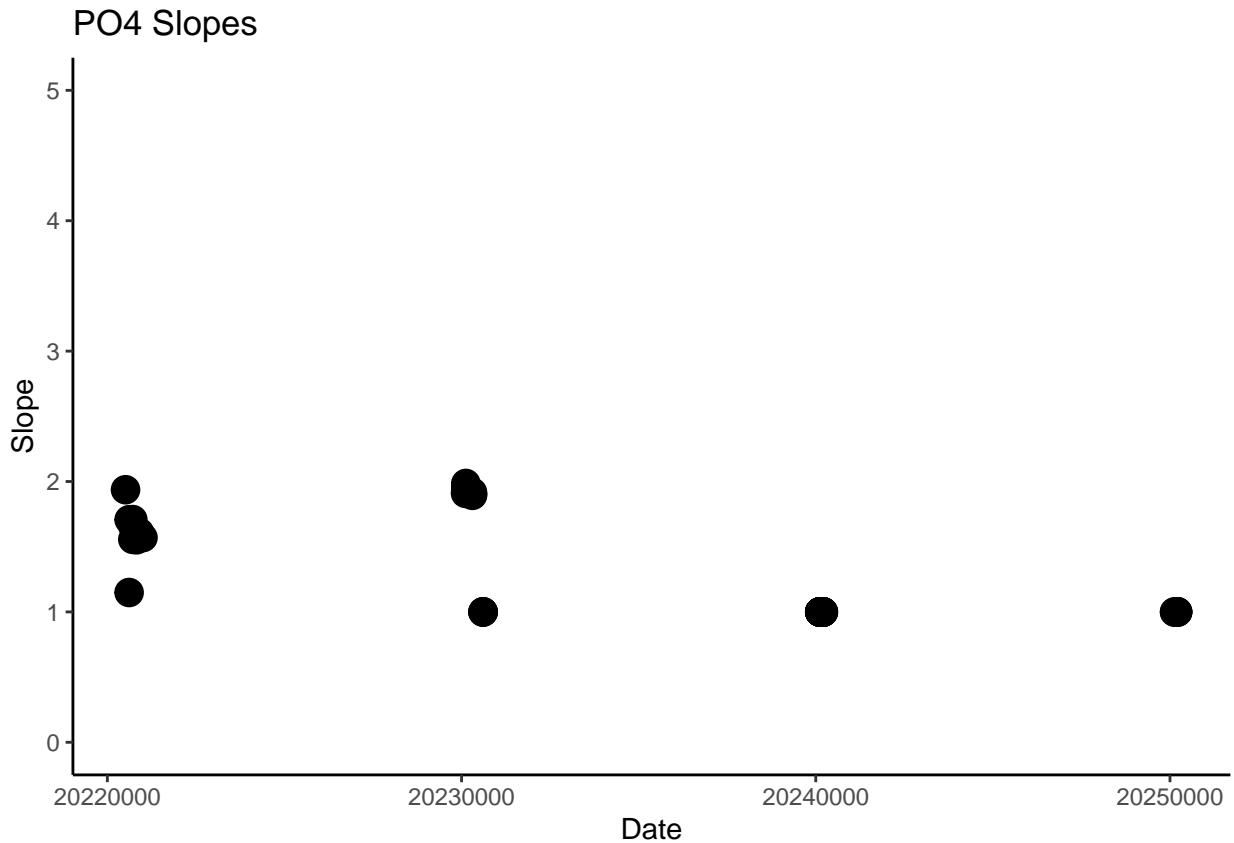
NH3 R2s



```
##### 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
```

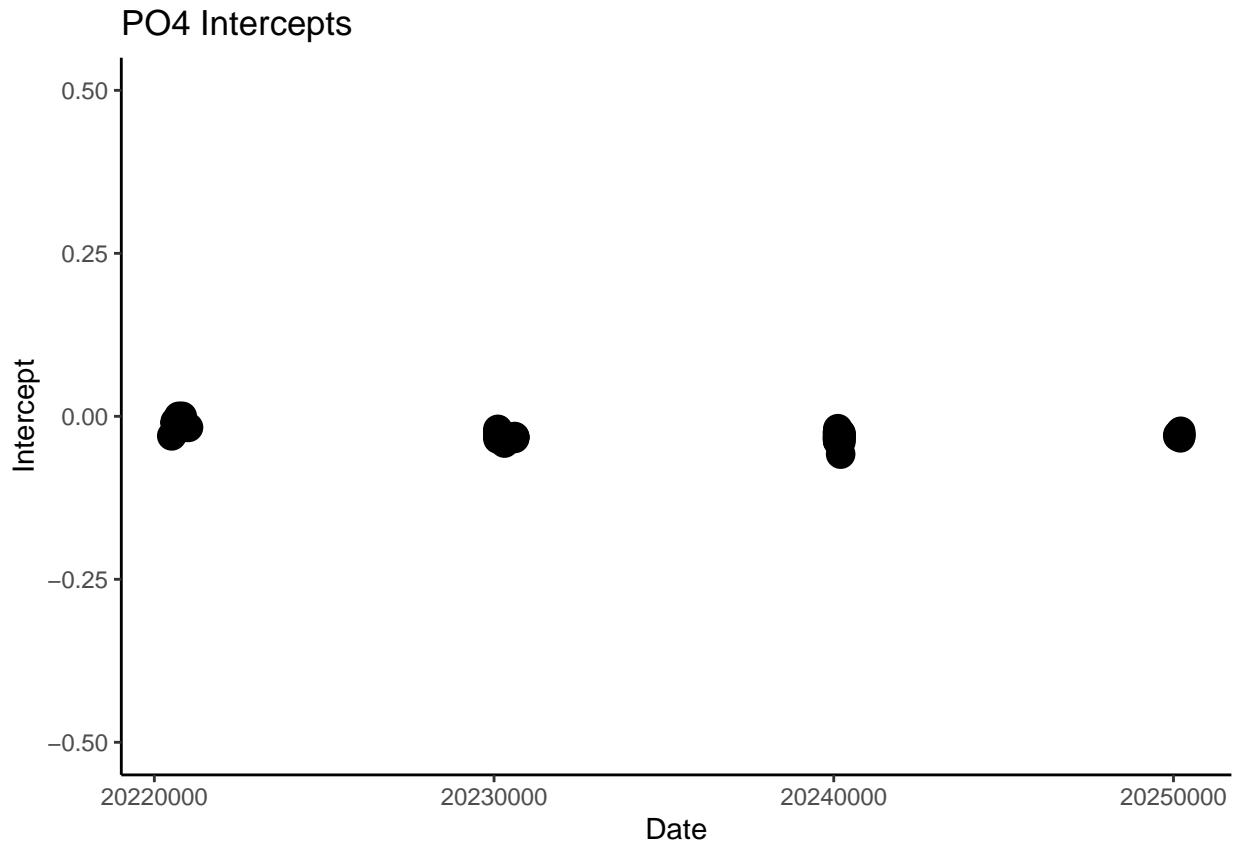
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

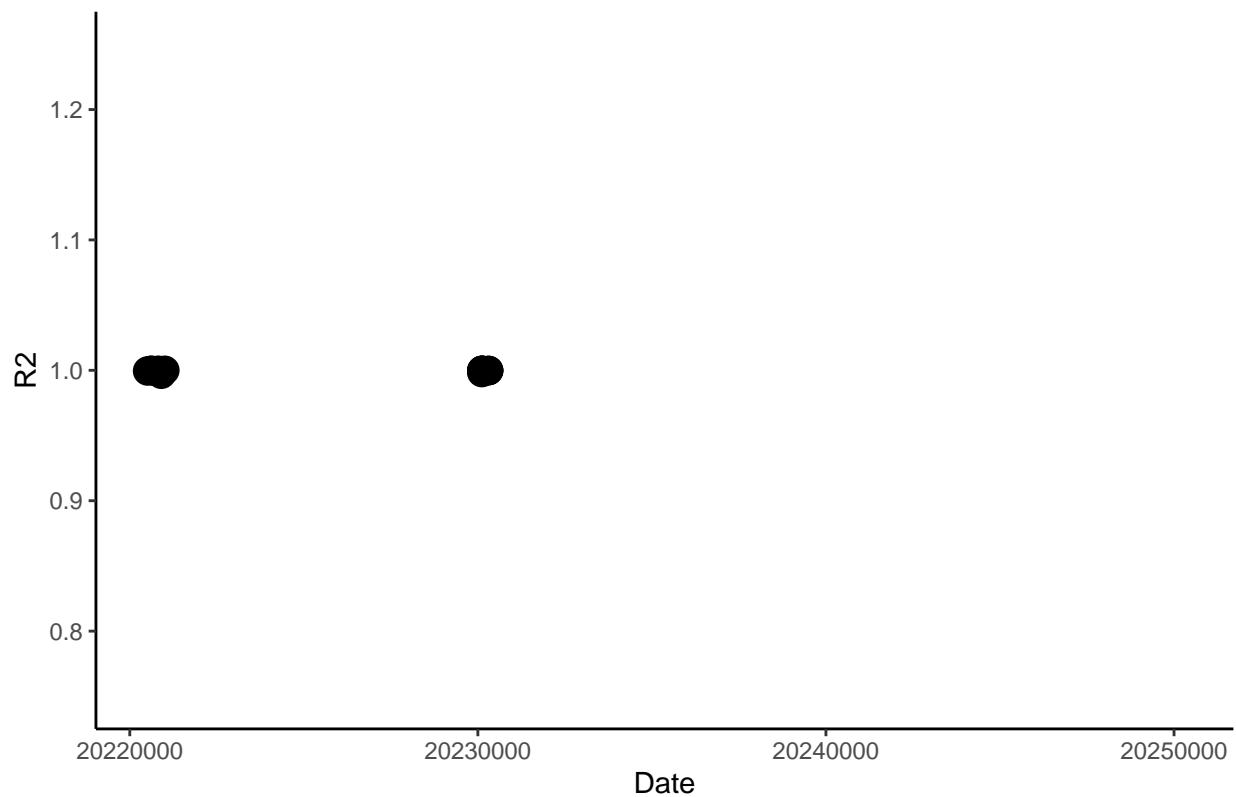


```
#plot the R2s to make sure there are no crazy outliers
Rsq2 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("P04 R2s")
```

```
Rsq2
```

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

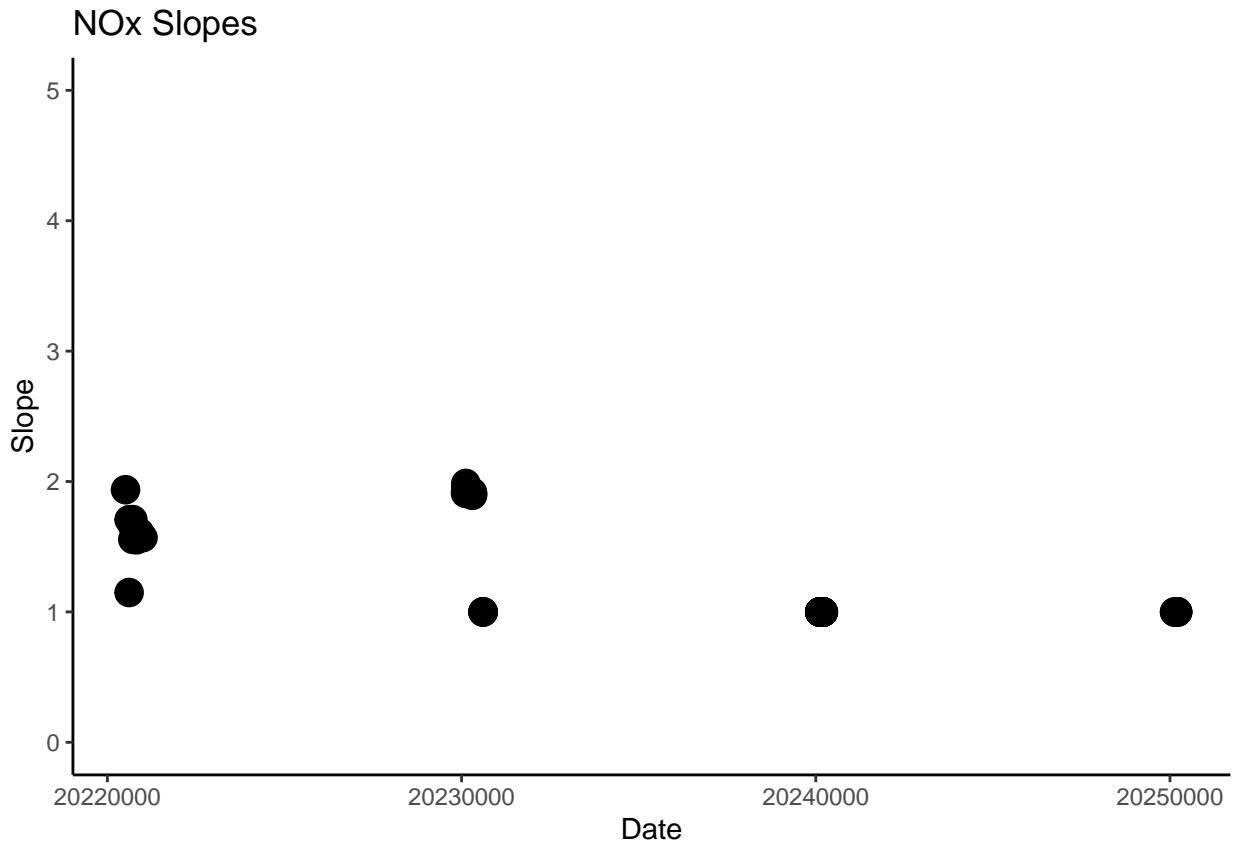
PO4 R2s



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

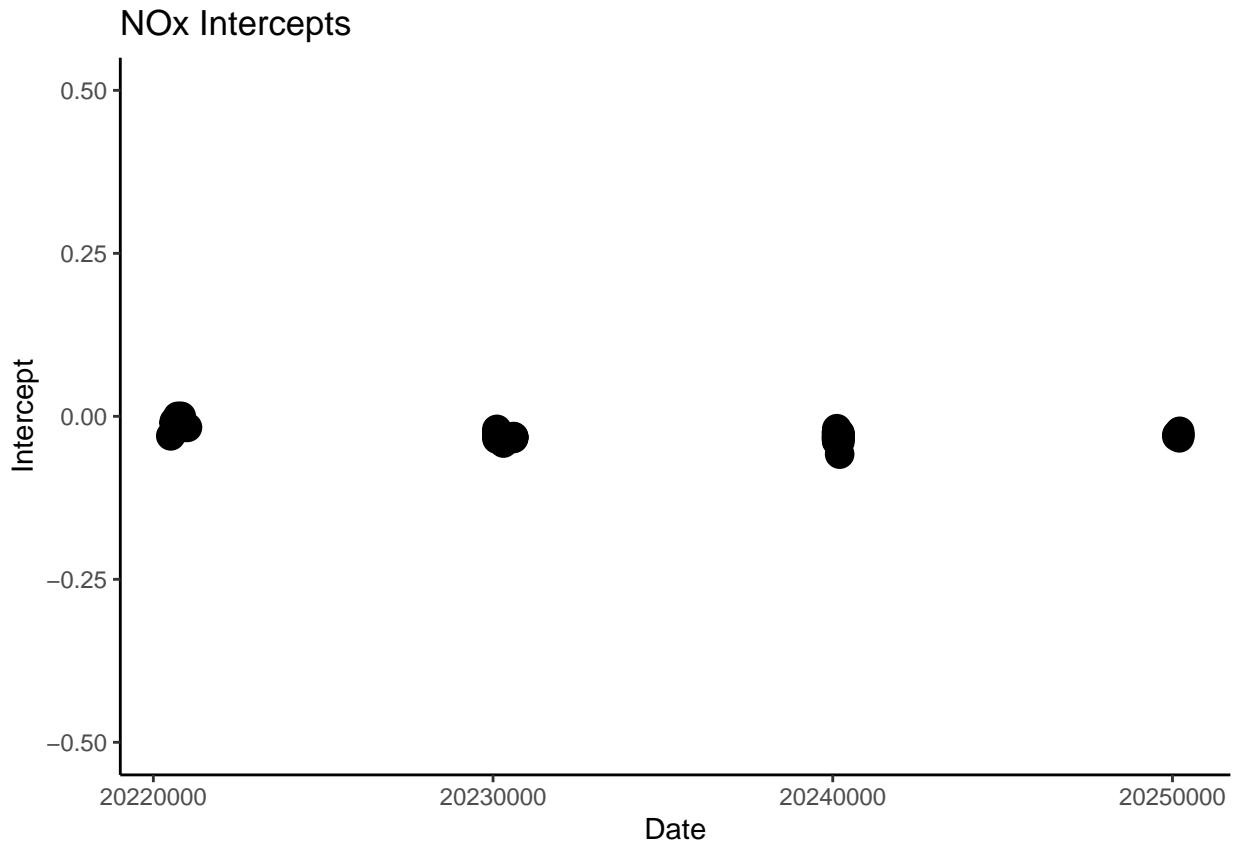
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_point()').
```



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

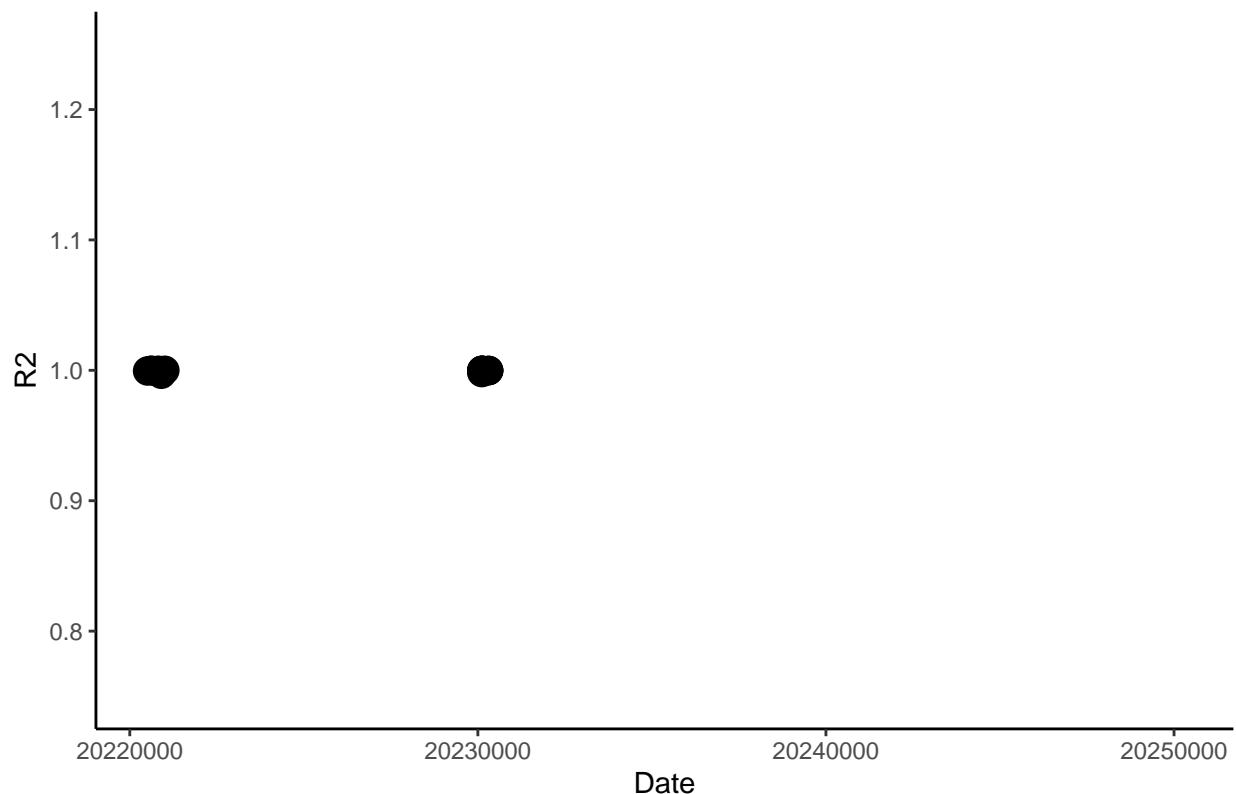


```
#plot the R2s to make sure there are no crazy outliers
Rsq3 <- ggplot(data=qNH3, aes(x=Date, y=R2)) +
  #geom_line()+
  geom_point(aes(size=3)) +
  theme_classic() + ylim(0.75, 1.25) +
  theme(legend.position="none")+
  ggtitle("NOx R2s")
```

```
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_202207_1.csv")
#Quick look at dataframe
head(file1)

##      RUNSTARTED X1658165226 X7.18.2022.13.27          X X.1      Conc      Abs
## 1  QCACTION    CONTINUE        1658165413          NA
## 2  RUNENDED    1658165413        COMPLETE          NA
## 3  RUNSTARTED   1658165922 7/18/2022 13:38          NA
## 4      RESULT      -1           S1 Standard 1 0 0.006887 0.006887
## 5      RESULT      -2           S90 Standard .0389 1 0.03206 0.03206
## 6      RESULT      -2           S91 Standard .1000 2 0.065922 0.065922
##      X.2 Dilution X.3 X.4      X.5      X.6      X.7          X.8
## 1     NA          NA  NA          NA          NA          NA
## 2     NA          NA  NA          NA          NA          NA
## 3     NA          NA  NA          NA          NA          NA
## 4     0            0  0 mg N/L Ammonia 2 1658167154 7/18/2022 13:59
## 5     0            0  0 mg N/L Ammonia 2 1658167314 7/18/2022 14:01
## 6     0            0  0 mg N/L Ammonia 2 1658167474 7/18/2022 14:04

#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  QCPROACTION
## 2    RUNENDED
## 3  RUNSTARTED
## 4      RESULT      Standard 1 0.006887 0.006887 mg N/L Ammonia 2
## 5      RESULT Standard .0389  0.03206 0.03206 mg N/L Ammonia 2
## 6      RESULT Standard .1000 0.065922 0.065922 mg N/L Ammonia 2

#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202207_2.csv")
#Quick look at dataframe
head(file2)

##      RUNSTARTED X1658190607      X7.18.2022.20.30      X X.1      X.2
## 1    RUNENDED   1658190628 STOP IMMEDIATE PRESSED          NA
## 2  RUNSTARTED   1658190693           7/18/2022 20:31          NA
## 3                               NA          NA Conc
## 4      RESULT      -1           S1 Standard 1 0 0.005962
## 5      RESULT      -2           S90 Standard .0389 1 0.030602
## 6      RESULT      -2           S91 Standard .1000 2 0.066232
##      X.3 X.4 X.5 X.6 X.7      X.8      X.9      X.10      X.11
## 1      NA      NA      NA          NA
## 2      NA      NA      NA          NA
## 3      Abs     NA Dil     NA      NA          NA
## 4 0.005962 0 0 0 512 mg N/L Ammonia 2 1658191931 7/18/2022 20:52
## 5 0.030602 0 0 0 512 mg N/L Ammonia 2 1658192091 7/18/2022 20:54
## 6 0.066232 0 0 0 512 mg N/L Ammonia 2 1658192251 7/18/2022 20:57

#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    RUNENDED
## 2  RUNSTARTED
## 3                               Conc      Abs
## 4      RESULT      Standard 1 0.005962 0.005962 mg N/L Ammonia 2
## 5      RESULT Standard .0389 0.030602 0.030602 mg N/L Ammonia 2
## 6      RESULT Standard .1000 0.066232 0.066232 mg N/L Ammonia 2

#read in data
file3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_202207_3.csv")
#Quick look at dataframe
head(file3)

##      RUNSTARTED X1658228831      X7.19.2022.7.07      X X.1      X.2
## 1  RUNSTARTED   1658230325           7/19/2022 7:32          NA      NA
## 2  RUNENDED    1658230365 STOP IMMEDIATE PRESSED          NA      NA
## 3  RUNSTARTED   1658230665           7/19/2022 7:37          NA      NA
## 4      RESULT      -1           S1 Standard 1 0 0.005266

```

```

## 5      RESULT          -2                      S90 Standard .0389   1 0.031630
## 6      RESULT          -2                      S91 Standard .1000   2 0.067535
##     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      NA  NA  NA  NA  NA                               NA
## 4 0.005266  0  0  0  0 mg N/L Ammonia 2 1658231899 7/19/2022 7:58
## 5 0.031630  0  0  0  0 mg N/L Ammonia 2 1658232059 7/19/2022 8:00
## 6 0.067535  0  0  0  0 mg N/L Ammonia 2 1658232219 7/19/2022 8:03

```

```

#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 RUNENDED             NA           NA
## 3 RUNSTARTED           NA           NA
## 4      RESULT      Standard 1 0.005266 0.005266 mg N/L Ammonia 2
## 5      RESULT Standard .0389 0.031630 0.031630 mg N/L Ammonia 2
## 6      RESULT Standard .1000 0.067535 0.067535 mg N/L Ammonia 2

```

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

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 4      RESULT      Standard 1 0.006887 0.006887 mg N/L Ammonia 2
## 5      RESULT Standard .0389 0.03206 0.03206 mg N/L Ammonia 2
## 6      RESULT Standard .1000 0.065922 0.065922 mg N/L Ammonia 2
## 7      RESULT Standard .2000 0.130039 0.130039 mg N/L Ammonia 2
## 8      RESULT Standard .5000 0.3005 0.3005 mg N/L Ammonia 2
## 9      RESULT Standard 1.0000 0.618677 0.618677 mg N/L Ammonia 2

```

```

#Pull out samples
alldat2 <- alldat[alldat$Sample_Name %like% "MSM_", ]
alldat2 <- rbind(alldat2, (alldat[alldat$Sample_Name %like% "GWI_", ]))
alldat2 <- rbind(alldat2, (alldat[alldat$Sample_Name %like% "GCrew_", ]))
head(alldat2)

```

```

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 398      RESULT MSM_UP_LysB_10cm 0.042758 0.035969 mg N/L Ammonia 2
## 405      RESULT MSM_UP_LysC_10cm 0.568162 0.352609 mg N/L Ammonia 2
## 406      RESULT MSM_UP_LysA_20cm 1.795753 1.092427 mg N/L Ammonia 2
## 414      RESULT MSM_UP_LysB_20cm 0.588825 0.365062 mg N/L Ammonia 2
## 415      RESULT MSM_UP_LysC_20cm 1.999664 1.215316 mg N/L Ammonia 2
## 418      RESULT MSM_UP_LysA_45cm 1.148694 0.702472 mg N/L Ammonia 2

```

NOx

```
#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202207_1.csv")
#Quick look at dataframe
head(Nfile1)

## RUNSTARTED X1658149249 X7.18.2022.9.00          X X.1      Conc      Abs X.2
## 1   RESULT      -1           S1 Standard 1  0 0.165420 0.165420 0
## 2   RESULT      -2           S90 Standard 90  1 0.182766 0.182766 0
## 3   RESULT      -2           S91 Standard 91  2 0.207313 0.207313 0
## 4   RESULT      -2           S92 Standard 92  3 0.248635 0.248635 0
## 5   RESULT      -2           S93 Standard 93  4 0.360514 0.360514 0
## 6   RESULT      -2           S94 Standard 94  5 0.563482 0.563482 0
## Dil X.3 X.4    X.5       X.6       X.7       X.8
## 1   0   0   0 mg N/L Vanadium NOx 1658151476 7/18/2022 9:37
## 2   0   0   0 mg N/L Vanadium NOx 1658151558 7/18/2022 9:39
## 3   0   0   0 mg N/L Vanadium NOx 1658151639 7/18/2022 9:40
## 4   0   0   0 mg N/L Vanadium NOx 1658151720 7/18/2022 9:42
## 5   0   0   0 mg N/L Vanadium NOx 1658151800 7/18/2022 9:43
## 6   0   0   0 mg N/L Vanadium NOx 1658151882 7/18/2022 9:44

#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 0.165420 0.165420 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.182766 0.182766 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.207313 0.207313 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.248635 0.248635 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.360514 0.360514 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.563482 0.563482 mg N/L Vanadium NOx

#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202207_2.csv")
#Quick look at dataframe
head(Nfile2)

## RUNSTARTED X1659202700 X7.30.2022.13.38          X X.1      X.2      X.3 X.4
## 1 RUNSTARTED 1659202912 7/30/2022 13:41          NA       NA       NA  NA
## 2   RESULT      -1           S1 Standard 1  0 0.165839 0.165839 0
## 3   RESULT      -2           S90 Standard 90  1 0.178468 0.178468 0
## 4   RESULT      -2           S91 Standard 91  2 0.202958 0.202958 0
## 5   RESULT      -2           S92 Standard 92  3 0.240962 0.240962 0
## 6   RESULT      -2           S93 Standard 93  4 0.359596 0.359596 0
## X.5 X.6 X.7    X.8       X.9       X.10      X.11
## 1   NA  NA  NA          NA
## 2   0   0   0 mg N/L Vanadium NOx 1659205111 7/30/2022 14:18
```

```

## 3 0 0 0 mg N/L Vanadium NOx 1659205193 7/30/2022 14:19
## 4 0 0 0 mg N/L Vanadium NOx 1659205274 7/30/2022 14:21
## 5 0 0 0 mg N/L Vanadium NOx 1659205354 7/30/2022 14:22
## 6 0 0 0 mg N/L Vanadium NOx 1659205435 7/30/2022 14:23

#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 RUNSTARTED          NA        NA
## 2      RESULT Standard 1 0.165839 0.165839 mg N/L Vanadium NOx
## 3      RESULT Standard 90 0.178468 0.178468 mg N/L Vanadium NOx
## 4      RESULT Standard 91 0.202958 0.202958 mg N/L Vanadium NOx
## 5      RESULT Standard 92 0.240962 0.240962 mg N/L Vanadium NOx
## 6      RESULT Standard 93 0.359596 0.359596 mg N/L Vanadium NOx

```

```

#read in data
Nfile3 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202207_3.csv")
#Quick look at dataframe
head(Nfile3)

```

```

##   RUNSTARTED X1659298379 X7.31.2022.16.12           X X.1      X.2      X.3 X.4
## 1      RESULT      -1           S1 Standard 1 0 0.172549 0.172549 0
## 2      RESULT      -2           S90 Standard 90 1 0.194234 0.194234 0
## 3      RESULT      -2           S91 Standard 91 2 0.214575 0.214575 0
## 4      RESULT      -2           S92 Standard 92 3 0.253198 0.253198 0
## 5      RESULT      -2           S93 Standard 93 4 0.377676 0.377676 0
## 6      RESULT      -2           S94 Standard 94 5 0.585169 0.585169 0
##   X.5 X.6 X.7     X.8      X.9      X.10      X.11
## 1 0 0 0 mg N/L Vanadium NOx 1659300574 7/31/2022 16:49
## 2 0 0 0 mg N/L Vanadium NOx 1659300655 7/31/2022 16:50
## 3 0 0 0 mg N/L Vanadium NOx 1659300737 7/31/2022 16:52
## 4 0 0 0 mg N/L Vanadium NOx 1659300817 7/31/2022 16:53
## 5 0 0 0 mg N/L Vanadium NOx 1659300899 7/31/2022 16:54
## 6 0 0 0 mg N/L Vanadium NOx 1659300980 7/31/2022 16:56

```

```

#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 0.172549 0.172549 mg N/L Vanadium NOx
## 2      RESULT Standard 90 0.194234 0.194234 mg N/L Vanadium NOx
## 3      RESULT Standard 91 0.214575 0.214575 mg N/L Vanadium NOx
## 4      RESULT Standard 92 0.253198 0.253198 mg N/L Vanadium NOx
## 5      RESULT Standard 93 0.377676 0.377676 mg N/L Vanadium NOx
## 6      RESULT Standard 94 0.585169 0.585169 mg N/L Vanadium NOx

```

```

Nalldat <- rbind(Ndat1, Ndat2, Ndat3)

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

##   Run_Info Sample_Name      Conc      Abs Units       Test
## 1    RESULT Standard 1 0.165420 0.165420 mg N/L Vanadium NOx
## 2    RESULT Standard 90 0.182766 0.182766 mg N/L Vanadium NOx
## 3    RESULT Standard 91 0.207313 0.207313 mg N/L Vanadium NOx
## 4    RESULT Standard 92 0.248635 0.248635 mg N/L Vanadium NOx
## 5    RESULT Standard 93 0.360514 0.360514 mg N/L Vanadium NOx
## 6    RESULT Standard 94 0.563482 0.563482 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
## 282    RESULT MSM_UP_LysB_10cm 0.001102 0.162520 mg N/L Vanadium NOx
## 290    RESULT MSM_UP_LysC_10cm 0.002487 0.163655 mg N/L Vanadium NOx
## 291    RESULT MSM_UP_LysA_20cm 0.001262 0.162651 mg N/L Vanadium NOx
## 299    RESULT MSM_UP_LysB_20cm 0.003195 0.164234 mg N/L Vanadium NOx
## 300    RESULT MSM_UP_LysC_20cm -0.001923 0.160043 mg N/L Vanadium NOx
## 301    RESULT MSM_UP_LysA_45cm 0.000066 0.161672 mg N/L Vanadium NOx

```

peCheck Checks

```

#pull out peChecks from alldat and Nalldat
chks <- alldat[alldat$Sample_Name %like% "peCheck", ]
head(chks)

##   Run_Info                               Sample_Name      Conc      Abs Units
## 142    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 1.285274 0.762447 mg N/L
## 149    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 1.270126 0.753577 mg N/L
## 327    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 0.79617 0.326971 mg P/L
## 336    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 0.7993 0.328251 mg P/L
## 376    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 0.929474 0.077364 mg P/L
## 377    RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 0.89814 0.074801 mg P/L
##           Test
## 142 Ammonia 2
## 149 Ammonia 2
## 327 o-PHOS 0.3
## 336 o-PHOS 0.3
## 376 o-PHOS 0.3
## 377 o-PHOS 0.3

```

```

Nchks <- Nalldat[Nalldat$Sample_Name %like% "peCheck", ]

NH4chk <- subset(chks, Test == "Ammonia 2")
NH4chk$ConcTrue <- 0.948
NH4chk$Conc <- as.numeric(NH4chk$Conc)
NH4chk$Chk_diff <- (NH4chk$Conc - NH4chk$ConcTrue) / ((NH4chk$Conc + NH4chk$ConcTrue) / 2) * 100
NH4chk$Chk_dff_flag <- ifelse(NH4chk$Chk_diff < 25, 'YES', 'NO, rerun')
head(NH4chk)

```

	Run_Info	Sample_Name	Conc	Abs	Units
## 142	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	1.285274	0.762447	mg	N/L
## 149	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	1.270126	0.753577	mg	N/L
## 571	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04	1.229047	0.750897	mg	N/L
## 1060	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04_A	1.061506	0.682024	mg	N/L
## 1061	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04_B	1.079544	0.693616	mg	N/L
##	Test ConcTrue Chk_diff Chk_dff_flag				
## 142	Ammonia 2 0.948 30.20444	NO, rerun			
## 149	Ammonia 2 0.948 29.04488	NO, rerun			
## 571	Ammonia 2 0.948 25.81910	NO, rerun			
## 1060	Ammonia 2 0.948 11.29691	YES			
## 1061	Ammonia 2 0.948 12.97570	YES			

```

P04chk <- subset(chks, Test == "o-PHOS 0.3")
P04chk$ConcTrue <- 0.818
P04chk$Conc <- as.numeric(P04chk$Conc)
P04chk$Chk_diff <- (P04chk$Conc - P04chk$ConcTrue) / ((P04chk$Conc + P04chk$ConcTrue) / 2) * 100
P04chk$Chk_dff_flag <- ifelse(P04chk$Chk_diff < 25, 'YES', 'NO, rerun')
head(P04chk)

```

	Run_Info	Sample_Name	Conc	Abs	Units
## 327	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	0.796170	0.326971	mg	P/L
## 336	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	0.799300	0.328251	mg	P/L
## 376	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	0.929474	0.077364	mg	P/L
## 377	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe	0.898140	0.074801	mg	P/L
## 800	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04	0.745772	0.319165	mg	P/L
## 895	RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04	0.803470	0.070133	mg	P/L
##	Test ConcTrue Chk_diff Chk_dff_flag				
## 327	o-PHOS 0.3 0.818 -2.704796	YES			
## 336	o-PHOS 0.3 0.818 -2.312496	YES			
## 376	o-PHOS 0.3 0.818 12.758301	YES			
## 377	o-PHOS 0.3 0.818 9.339564	YES			
## 800	o-PHOS 0.3 0.818 -9.237664	YES			
## 895	o-PHOS 0.3 0.818 -1.792201	YES			

```

NOXchk <- subset(Nchks, Test == "Vanadium NOx")
NOXchk$ConcTrue <- 0.706
NOXchk$Conc <- as.numeric(NOXchk$Conc)
NOXchk$Chk_diff <- (NOXchk$Conc - NOXchk$ConcTrue) / ((NOXchk$Conc + NOXchk$ConcTrue) / 2) * 100
NOXchk$Chk_dff_flag <- ifelse(NOXchk$Chk_diff < 25, 'YES', 'NO, rerun')
head(NOXchk)

```

	Run_Info	Sample_Name	Conc	Abs	Units
--	----------	-------------	------	-----	-------

```

## 246  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04 0.717276 0.742243 mg N/L
## 253  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04 0.722862 0.746443 mg N/L
## 451  RESULT                               peCheck_N03_706 0.711677 0.726175 mg N/L
## 452  RESULT                               peCheck_N03_706 0.684810 0.705487 mg N/L
## 629  RESULT                               peCheck_N03_706ppm_A 0.671314 0.714344 mg N/L
## 630  RESULT                               peCheck_N03_706ppm_B 0.673346 0.715908 mg N/L
##          Test ConcTrue   Chk_diff Chk_dff_flag
## 246 Vanadium NOx    0.706  1.5845135      YES
## 253 Vanadium NOx    0.706  2.3601999      YES
## 451 Vanadium NOx    0.706  0.8008876      YES
## 452 Vanadium NOx    0.706 -3.0471452      YES
## 629 Vanadium NOx    0.706 -5.0367600      YES
## 630 Vanadium NOx    0.706 -4.7347076      YES

```

```

Allchks <- rbind(NH4chk, P04chk)
Allchks <- rbind(Allchks, NOXchk)
head(Allchks)

```

```

##      Run_Info                         Sample_Name     Conc     Abs Units
## 142  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 1.285274 0.762447 mg N/L
## 149  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 1.270126 0.753577 mg N/L
## 571  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04 1.229047 0.750897 mg N/L
## 1060 RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04_A 1.061506 0.682024 mg N/L
## 1061 RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04_B 1.079544 0.693616 mg N/L
## 327  RESULT peCheck_706ppmN03_948ppmNH4_818ppmP04pe 0.796170 0.326971 mg P/L
##          Test ConcTrue   Chk_diff Chk_dff_flag
## 142 Ammonia 2    0.948 30.204444    NO, rerun
## 149 Ammonia 2    0.948 29.044878    NO, rerun
## 571 Ammonia 2    0.948 25.819103    NO, rerun
## 1060 Ammonia 2   0.948 11.296906      YES
## 1061 Ammonia 2   0.948 12.975699      YES
## 327 o-PHOS 0.3   0.818 -2.704796      YES

```

```

#plot dups output as a bar graph to easily check - want any over 10% to be red need to work on this
Chksbar <- ggplot(data = Allchks, aes(x = Sample_Name, y = Chk_diff, fill=Test)) +
  geom_bar(stat = 'identity') +
  facet_wrap(~Test) +
  theme_classic() + labs(x= "Sample ID", y="peChecks Percent Difference") +
  theme(legend.position="right") +
  geom_hline(yintercept=25, linetype="dashed", color = "black", size=1) +
  geom_hline(yintercept=0, color = "black", size=1) +
  geom_hline(yintercept=-25, linetype="dashed", color = "black", size=1)

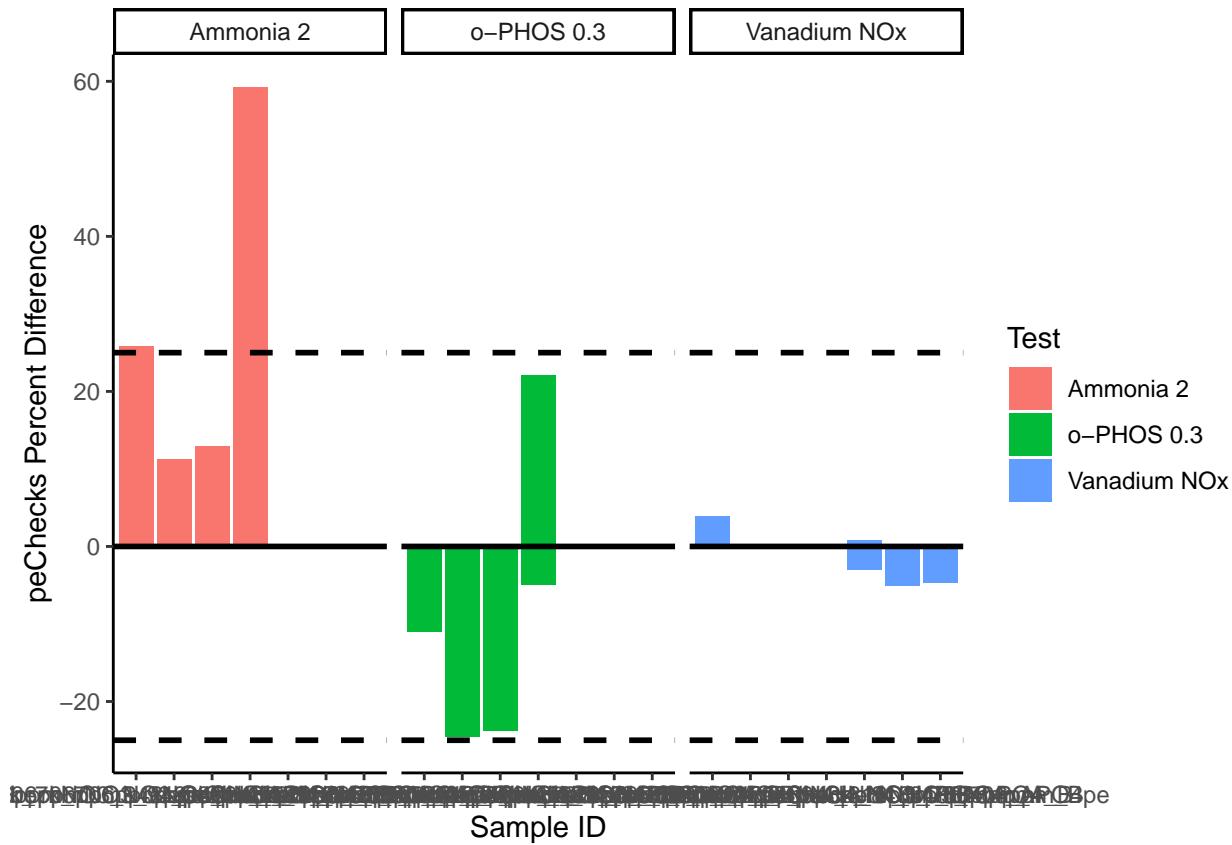
```

```

## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.

```

```
Chksbar
```



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
## 398   RESULT MSM_UP_LysB_10cm 0.042758 0.035969 mg N/L Ammonia 2
## 405   RESULT MSM_UP_LysC_10cm 0.568162 0.352609 mg N/L Ammonia 2
## 406   RESULT MSM_UP_LysA_20cm 1.795753 1.092427 mg N/L Ammonia 2
## 414   RESULT MSM_UP_LysB_20cm 0.588825 0.365062 mg N/L Ammonia 2
## 415   RESULT MSM_UP_LysC_20cm 1.999664 1.215316 mg N/L Ammonia 2
## 418   RESULT MSM_UP_LysA_45cm 1.148694 0.702472 mg N/L Ammonia 2
```

```

head(Nalldat2)

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 282   RESULT MSM_UP_LysB_10cm  0.001102 0.162520 mg N/L Vanadium NOx
## 290   RESULT MSM_UP_LysC_10cm  0.002487 0.163655 mg N/L Vanadium NOx
## 291   RESULT MSM_UP_LysA_20cm  0.001262 0.162651 mg N/L Vanadium NOx
## 299   RESULT MSM_UP_LysB_20cm  0.003195 0.164234 mg N/L Vanadium NOx
## 300   RESULT MSM_UP_LysC_20cm -0.001923 0.160043 mg N/L Vanadium NOx
## 301   RESULT MSM_UP_LysA_45cm  0.000066 0.161672 mg N/L Vanadium NOx

```

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 398   RESULT MSM_UP_LysB_10cm  0.042758 0.035969 mg N/L Ammonia 2
## 405   RESULT MSM_UP_LysC_10cm  0.568162 0.352609 mg N/L Ammonia 2
## 406   RESULT MSM_UP_LysA_20cm  1.795753 1.092427 mg N/L Ammonia 2
## 414   RESULT MSM_UP_LysB_20cm  0.588825 0.365062 mg N/L Ammonia 2
## 415   RESULT MSM_UP_LysC_20cm  1.999664 1.215316 mg N/L Ammonia 2
## 418   RESULT MSM_UP_LysA_45cm  1.148694 0.702472 mg N/L Ammonia 2

```

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 595   RESULT MSM_UP_LysB_10cm  0.168261 0.073354 mg P/L o-PHOS 0.3
## 606   RESULT MSM_UP_LysC_10cm  0.122153 0.053728 mg P/L o-PHOS 0.3
## 607   RESULT MSM_UP_LysA_20cm  0.161279 0.070382 mg P/L o-PHOS 0.3
## 618   RESULT MSM_UP_LysB_20cm  0.099871 0.044244 mg P/L o-PHOS 0.3
## 619   RESULT MSM_UP_LysC_20cm  0.155479 0.067913 mg P/L o-PHOS 0.3
## 620   RESULT MSM_UP_LysA_45cm  0.171565 0.07476 mg P/L o-PHOS 0.3

```

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs      Units      Test
## 282   RESULT MSM_UP_LysB_10cm  0.001102 0.162520 mg N/L Vanadium NOx
## 290   RESULT MSM_UP_LysC_10cm  0.002487 0.163655 mg N/L Vanadium NOx
## 291   RESULT MSM_UP_LysA_20cm  0.001262 0.162651 mg N/L Vanadium NOx
## 299   RESULT MSM_UP_LysB_20cm  0.003195 0.164234 mg N/L Vanadium NOx
## 300   RESULT MSM_UP_LysC_20cm -0.001923 0.160043 mg N/L Vanadium NOx
## 301   RESULT MSM_UP_LysA_45cm  0.000066 0.161672 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
## 398   RESULT MSM_UP_LysB_10cm  0.042758 0.035969 mg N/L Ammonia 2    3.052682
## 405   RESULT MSM_UP_LysC_10cm  0.568162 0.352609 mg N/L Ammonia 2   40.563587

```

```

## 406  RESULT MSM_UP_LysA_20cm 1.795753 1.092427 mg N/L Ammonia 2 128.206715
## 414  RESULT MSM_UP_LysB_20cm 0.588825 0.365062 mg N/L Ammonia 2 42.038810
## 415  RESULT MSM_UP_LysC_20cm 1.999664 1.215316 mg N/L Ammonia 2 142.764820
## 418  RESULT MSM_UP_LysA_45cm 1.148694 0.702472 mg N/L Ammonia 2 82.010324

```

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs  Units      Test    Conc_uM
## 595  RESULT MSM_UP_LysB_10cm 0.168261 0.073354 mg P/L o-PHOS 0.3 12.012894
## 606  RESULT MSM_UP_LysC_10cm 0.122153 0.053728 mg P/L o-PHOS 0.3 8.721041
## 607  RESULT MSM_UP_LysA_20cm 0.161279 0.070382 mg P/L o-PHOS 0.3 11.514418
## 618  RESULT MSM_UP_LysB_20cm 0.099871 0.044244 mg P/L o-PHOS 0.3 7.130231
## 619  RESULT MSM_UP_LysC_20cm 0.155479 0.067913 mg P/L o-PHOS 0.3 11.100331
## 620  RESULT MSM_UP_LysA_45cm 0.171565 0.07476 mg P/L o-PHOS 0.3 12.248781

```

```

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

```

```

##      Run_Info      Sample_Name      Conc      Abs  Units      Test
## 282  RESULT MSM_UP_LysB_10cm 0.001102 0.162520 mg N/L Vanadium NOx
## 290  RESULT MSM_UP_LysC_10cm 0.002487 0.163655 mg N/L Vanadium NOx
## 291  RESULT MSM_UP_LysA_20cm 0.001262 0.162651 mg N/L Vanadium NOx
## 299  RESULT MSM_UP_LysB_20cm 0.003195 0.164234 mg N/L Vanadium NOx
## 300  RESULT MSM_UP_LysC_20cm -0.001923 0.160043 mg N/L Vanadium NOx
## 301  RESULT MSM_UP_LysA_45cm 0.000066 0.161672 mg N/L Vanadium NOx
##      Conc_uM_raw
## 282  0.078676633
## 290  0.177557883
## 291  0.090099738
## 299  0.228105121
## 300  -0.137291439
## 301  0.004712031

```

#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
## 282  RESULT MSM_UP_LysB_10cm 0.001102 0.162520 mg N/L Vanadium NOx
## 290  RESULT MSM_UP_LysC_10cm 0.002487 0.163655 mg N/L Vanadium NOx
## 291  RESULT MSM_UP_LysA_20cm 0.001262 0.162651 mg N/L Vanadium NOx
## 299  RESULT MSM_UP_LysB_20cm 0.003195 0.164234 mg N/L Vanadium NOx
## 300  RESULT MSM_UP_LysC_20cm -0.001923 0.160043 mg N/L Vanadium NOx
## 301  RESULT MSM_UP_LysA_45cm 0.000066 0.161672 mg N/L Vanadium NOx
##      Conc_uM_raw      Conc_uM
## 282  0.078676633  0.078676633
## 290  0.177557883  0.177557883
## 291  0.090099738  0.090099738
## 299  0.228105121  0.228105121
## 300  -0.137291439  0.000000000
## 301  0.004712031  0.004712031

```

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
## 398 MSM_UP_LysB_10cm 0.042758  3.052682
## 405 MSM_UP_LysC_10cm 0.568162 40.563587
## 406 MSM_UP_LysA_20cm 1.795753 128.206715
## 414 MSM_UP_LysB_20cm 0.588825 42.038810
## 415 MSM_UP_LysC_20cm 1.999664 142.764820
## 418 MSM_UP_LysA_45cm 1.148694 82.010324
```

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

```
##           Sample_Name      Conc      Conc_uM
## 595 MSM_UP_LysB_10cm 0.168261 12.012894
## 606 MSM_UP_LysC_10cm 0.122153 8.721041
## 607 MSM_UP_LysA_20cm 0.161279 11.514418
## 618 MSM_UP_LysB_20cm 0.099871 7.130231
## 619 MSM_UP_LysC_20cm 0.155479 11.100331
## 620 MSM_UP_LysA_45cm 0.171565 12.248781
```

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

```
##           Sample_Name      Conc      Conc_uM
## 282 MSM_UP_LysB_10cm 0.001102 0.078676633
## 290 MSM_UP_LysC_10cm 0.002487 0.177557883
## 291 MSM_UP_LysA_20cm 0.001262 0.090099738
## 299 MSM_UP_LysB_20cm 0.003195 0.228105121
## 300 MSM_UP_LysC_20cm -0.001923 0.000000000
## 301 MSM_UP_LysA_45cm 0.000066 0.004712031
```

```
#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      Conc
## 1 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 0.000036
## 2 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 1.457371
## 3 GCrew_TR_LysA_45cm 0.073945 5.279259 0.025919 1.850472 -0.004228
## 4 GCrew_TR_LysA_45cm 0.073945 5.279259 0.025919 1.850472 0.243058
## 5 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.001133
## 6 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.457136
##           Conc_uM
## 1 2.570199e-03
```

```

## 2 1.040481e+02
## 3 0.000000e+00
## 4 1.735298e+01
## 5 8.088986e-02
## 6 3.263695e+01

colnames(all_data) <- c("Sample_Name", "NH3_mgL", "NH3_uM", "PO4_mgL", "PO4_uM", "NOx_mgL", "NOx_uM")
head(all_data)

##           Sample_Name  NH3_mgL   NH3_uM  PO4_mgL  PO4_uM  NOx_mgL
## 1 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 0.000036
## 2 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 1.457371
## 3 GCrew_TR_LysA_45cm 0.073945  5.279259 0.025919 1.850472 -0.004228
## 4 GCrew_TR_LysA_45cm 0.073945  5.279259 0.025919 1.850472  0.243058
## 5 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.001133
## 6 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.457136
##           NOx_uM
## 1 2.570199e-03
## 2 1.040481e+02
## 3 0.000000e+00
## 4 1.735298e+01
## 5 8.088986e-02
## 6 3.263695e+01

#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  NOx_mgL
## 1 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 0.000036
## 2 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 1.457371
## 3 GCrew_TR_LysA_45cm 0.073945  5.279259 0.025919 1.850472 -0.004228
## 4 GCrew_TR_LysA_45cm 0.073945  5.279259 0.025919 1.850472  0.243058
## 5 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.001133
## 6 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.457136
##           NOx_uM  NH3_range  PO4_range  NOx_range
## 1 2.570199e-03 Within_Range Within_Range      bdl
## 2 1.040481e+02 Within_Range Within_Range      adl
## 3 0.000000e+00 Within_Range Within_Range      bdl
## 4 1.735298e+01 Within_Range Within_Range Within_Range
## 5 8.088986e-02 Within_Range Within_Range      bdl
## 6 3.263695e+01 Within_Range Within_Range Within_Range

```

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) +

```

```

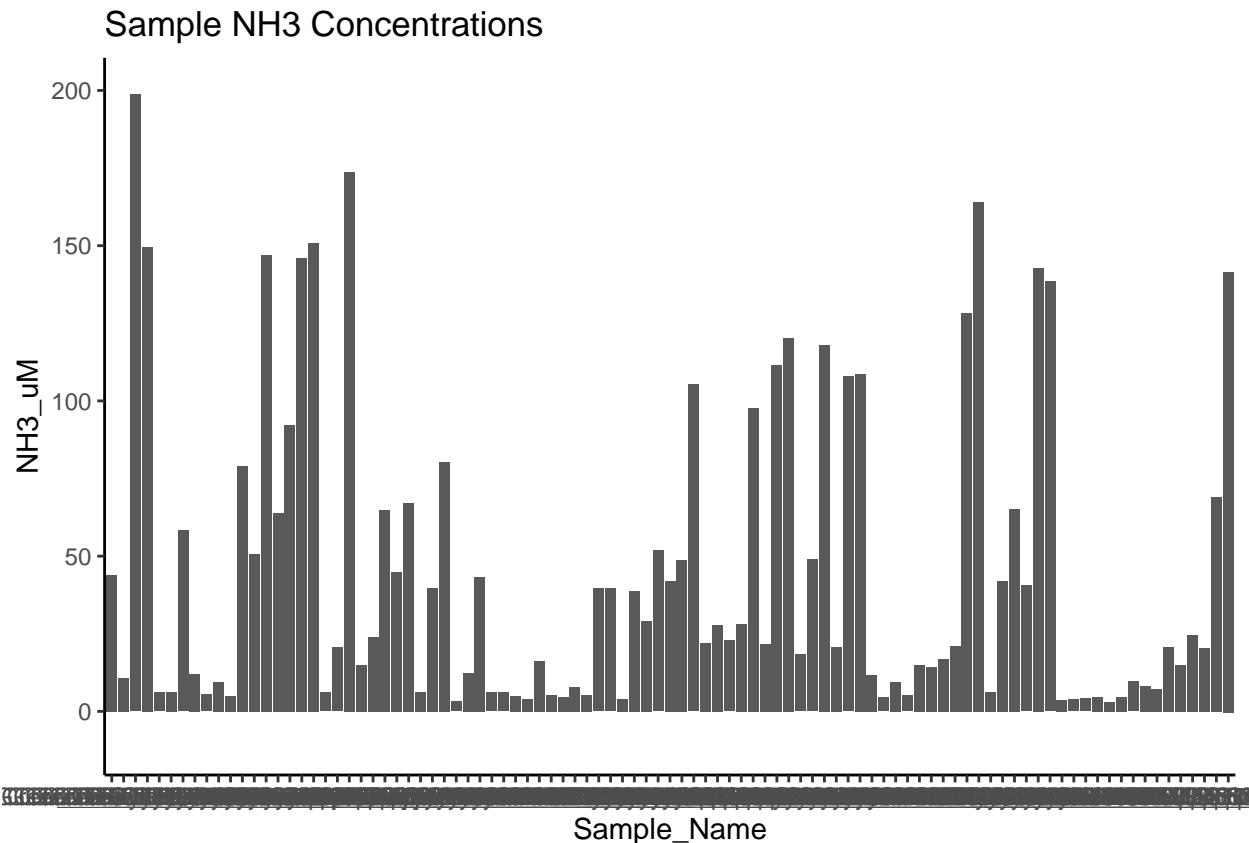
theme(legend.position="none") +
ggtitle("Sample NH3 Concentrations")
NH3look

```

```

## Warning: Removed 6 rows containing missing values or values outside the scale range
## ('geom_bar()').

```



```

P04look <- ggplot(data=all_data, aes(x=Sample_Name, y=P04_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 50) +
  theme(legend.position="none") +
  ggtitle("Sample P04 Concentrations")
P04look

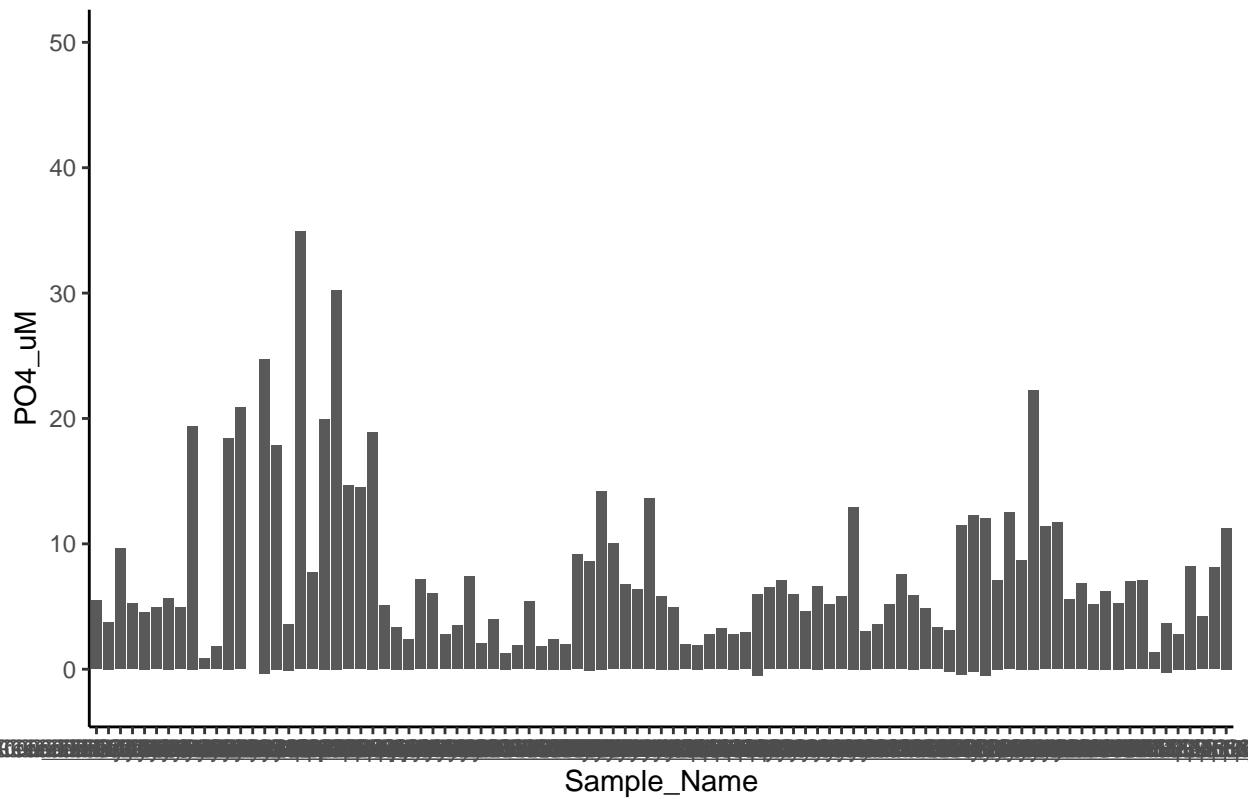
```

```

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

```

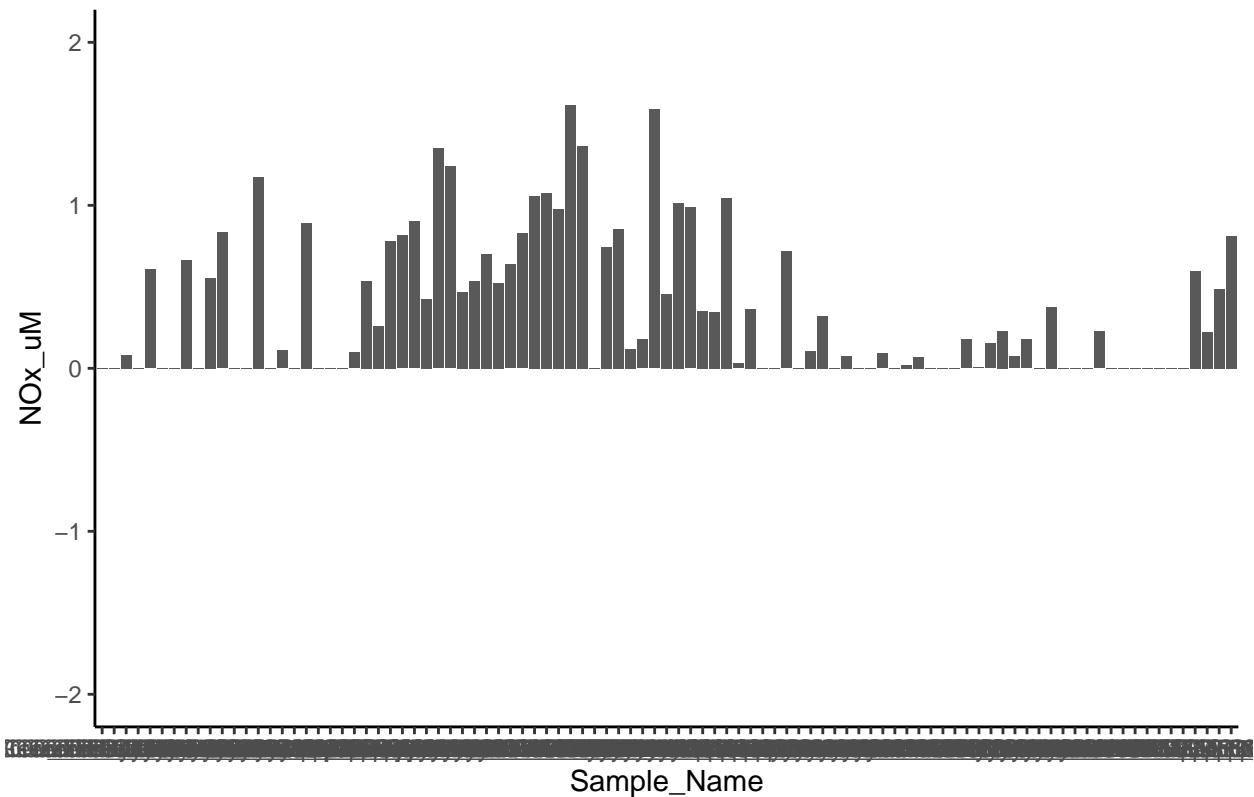
Sample PO4 Concentrations



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

```
## Warning: Removed 13 rows containing missing values or values outside the scale range
## ('geom_bar()').
```

Sample NOx Concentrations



Pull out data you need, make IDs

```
head(all_data)

##           Sample_Name  NH3_mgL    NH3_uM  PO4_mgL  PO4_uM  NOx_mgL
## 1 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 0.000036
## 2 GCrew_TR_LysA_20cm 0.306868 21.908658 0.038776 2.768389 1.457371
## 3 GCrew_TR_LysA_45cm 0.073945 5.279259 0.025919 1.850472 -0.004228
## 4 GCrew_TR_LysA_45cm 0.073945 5.279259 0.025919 1.850472 0.243058
## 5 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.001133
## 6 GCrew_TR_LysB_10cm 1.393605 99.495599 0.067836 4.843111 0.457136
##           NOx_uM    NH3_range    PO4_range    NOx_range
## 1 2.570199e-03 Within_Range Within_Range      bdl
## 2 1.040481e+02 Within_Range Within_Range      adl
## 3 0.000000e+00 Within_Range Within_Range      bdl
## 4 1.735298e+01 Within_Range Within_Range Within_Range
## 5 8.088986e-02 Within_Range Within_Range      bdl
## 6 3.263695e+01 Within_Range Within_Range Within_Range
```

```
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_TR_LysA_20cm 21.908658 2.768389 2.570199e-03 Within_Range Within_Range
## 2 GCrew_TR_LysA_20cm 21.908658 2.768389 1.040481e+02 Within_Range Within_Range
## 3 GCrew_TR_LysA_45cm 5.279259 1.850472 0.000000e+00 Within_Range Within_Range
## 4 GCrew_TR_LysA_45cm 5.279259 1.850472 1.735298e+01 Within_Range Within_Range
## 5 GCrew_TR_LysB_10cm 99.495599 4.843111 8.088986e-02 Within_Range Within_Range
## 6 GCrew_TR_LysB_10cm 99.495599 4.843111 3.263695e+01 Within_Range Within_Range
##           NOx_range
## 1             bdl
## 2             adl
## 3             bdl
## 4 Within_Range
## 5             bdl
## 6 Within_Range

#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", "TR", "LysA", "20cm"), c("GCrew", "TR", "LysA", :
## number of columns of result is not a multiple of vector length (arg 1)

colnames(IDs) <- c("Site" , "Zone", "Replicate", "Depth", "Tree")
IDs$date <- 202207
IDs$Month <- "July"
head(IDs)

##      Site Zone Replicate Depth Tree Date Month
## 1 GCrew   TR     LysA    20cm GCrew 202207 July
## 2 GCrew   TR     LysA    20cm GCrew 202207 July
## 3 GCrew   TR     LysA    45cm GCrew 202207 July
## 4 GCrew   TR     LysA    45cm GCrew 202207 July
## 5 GCrew   TR     LysB    10cm GCrew 202207 July
## 6 GCrew   TR     LysB    10cm GCrew 202207 July

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

##      Site Zone Replicate Depth Tree Date Month      Sample_Name   NH3_uM
## 1 GCrew   TR     LysA    20cm GCrew 202207 July GCrew_TR_LysA_20cm 21.908658
## 2 GCrew   TR     LysA    20cm GCrew 202207 July GCrew_TR_LysA_20cm 21.908658
## 3 GCrew   TR     LysA    45cm GCrew 202207 July GCrew_TR_LysA_45cm  5.279259
## 4 GCrew   TR     LysA    45cm GCrew 202207 July GCrew_TR_LysA_45cm  5.279259
## 5 GCrew   TR     LysB    10cm GCrew 202207 July GCrew_TR_LysB_10cm 99.495599
## 6 GCrew   TR     LysB    10cm GCrew 202207 July GCrew_TR_LysB_10cm 99.495599
##           P04_uM   NOx_uM  NH3_range   P04_range   NOx_range
## 1 2.768389 2.570199e-03 Within_Range Within_Range          bdl
## 2 2.768389 1.040481e+02 Within_Range Within_Range          adl
## 3 1.850472 0.000000e+00 Within_Range Within_Range          bdl
## 4 1.850472 1.735298e+01 Within_Range Within_Range Within_Range
## 5 4.843111 8.088986e-02 Within_Range Within_Range          bdl
## 6 4.843111 3.263695e+01 Within_Range Within_Range Within_Range

```

Export final data with flags

```
#Export Data  
#setwd("S:/Biogeochemistry/People/Wilson (Steph)/Data/SEAL/Final Data Files")  
write.csv(alldat, file="Processed Data/COMPASS_SynopticCB_Nutrients_202207.csv")
```