COMPASS_Synoptic_SEAL_Data_Analysis_June2022

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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_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
  #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 ra
#these are run rouhgly 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 softare; if 80
#CCB's are DI blanks run every 10 samples, these are checked by the software; if 80% are within range w

  #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)

#set working directory
#setwd("S:/Biogeochemistry/People/Wilson (Steph)/Data/SEAL/Raw Data Files")

#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
```

```r
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
```

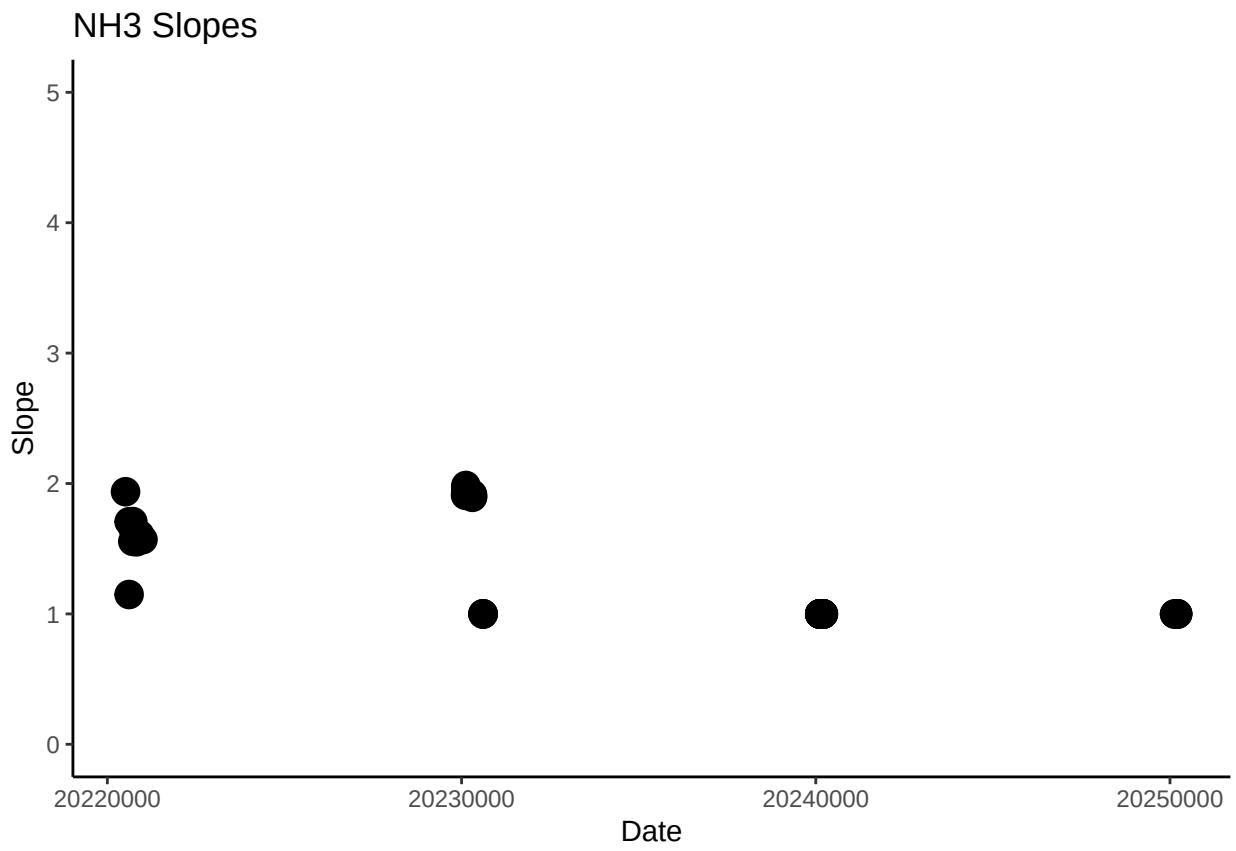
```r
qNOx <- qlog[qlog$Analysis %like% "V-Nox", ]
head(qNOx)
```

```
##        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
```

```r
########### 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
```

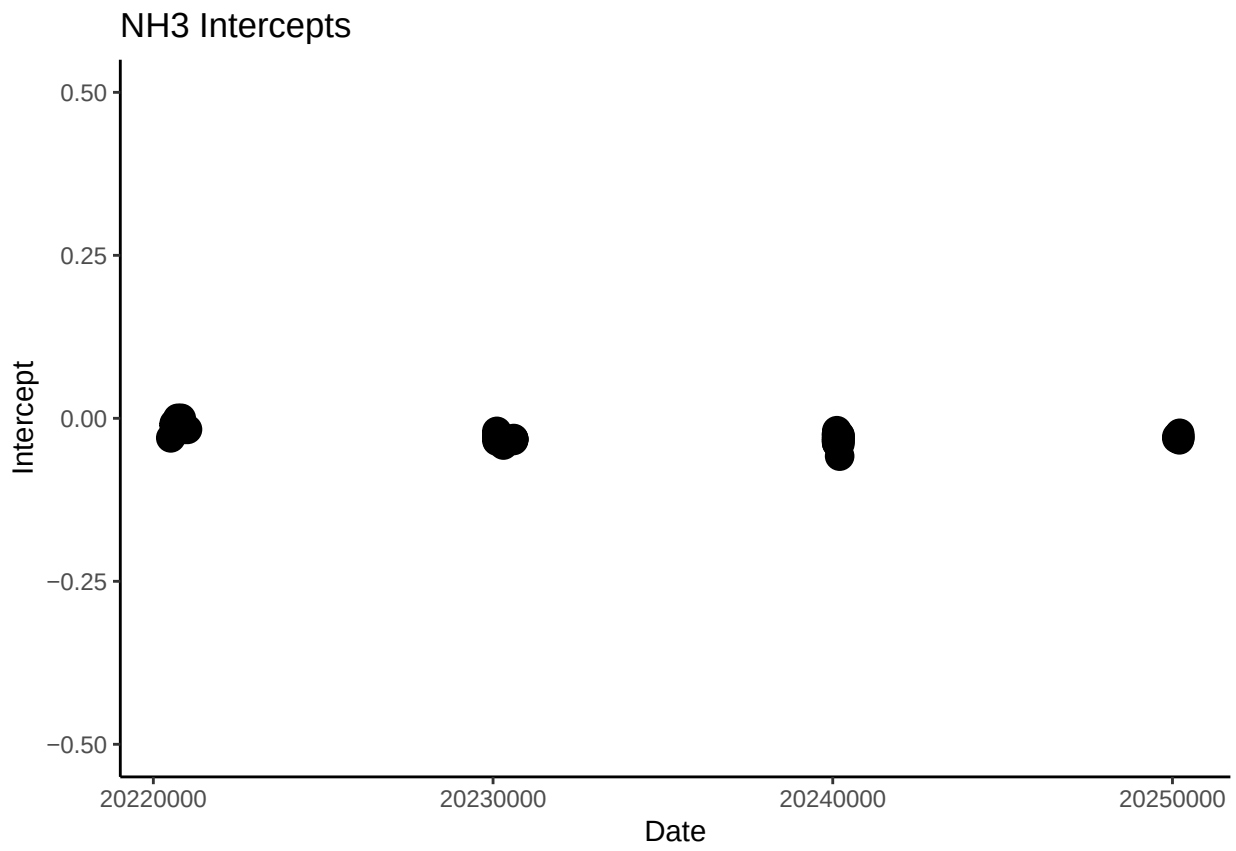
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#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
```

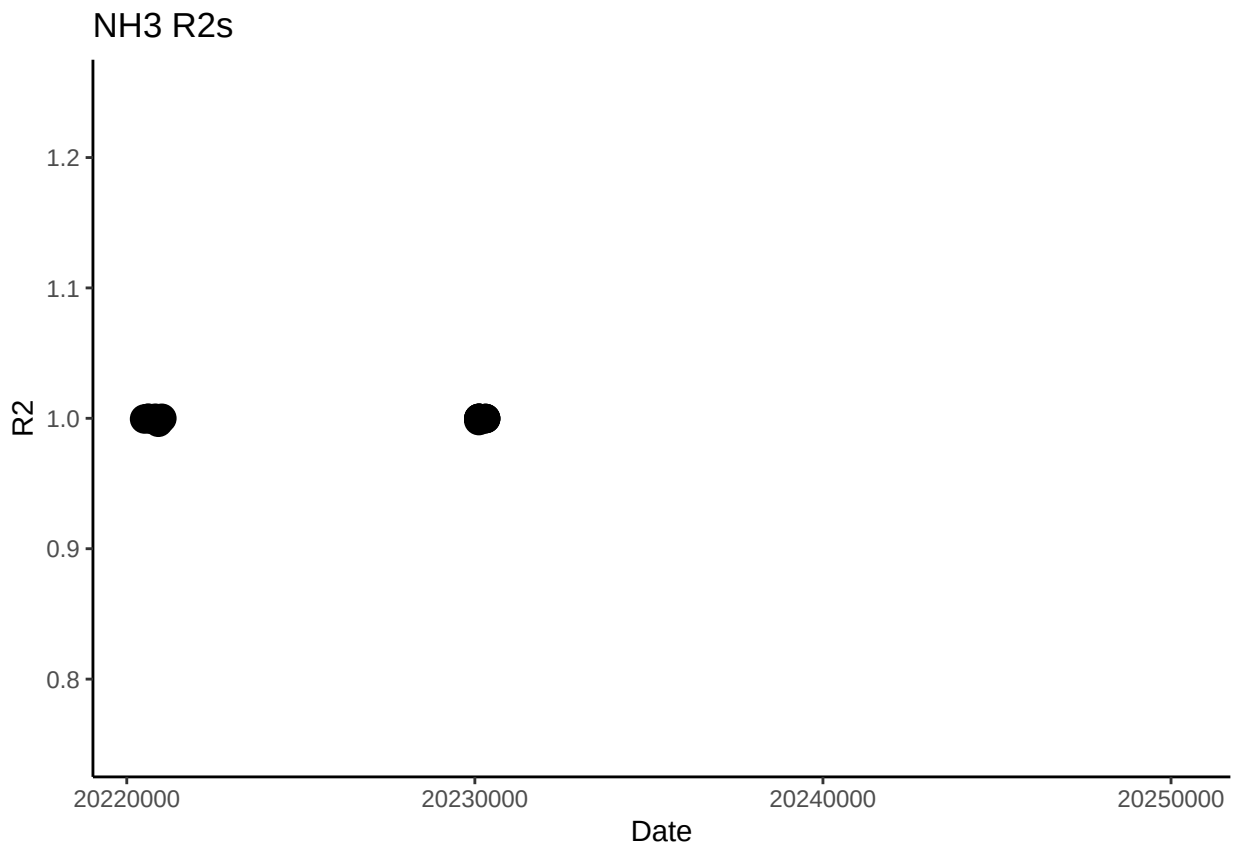
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#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
```

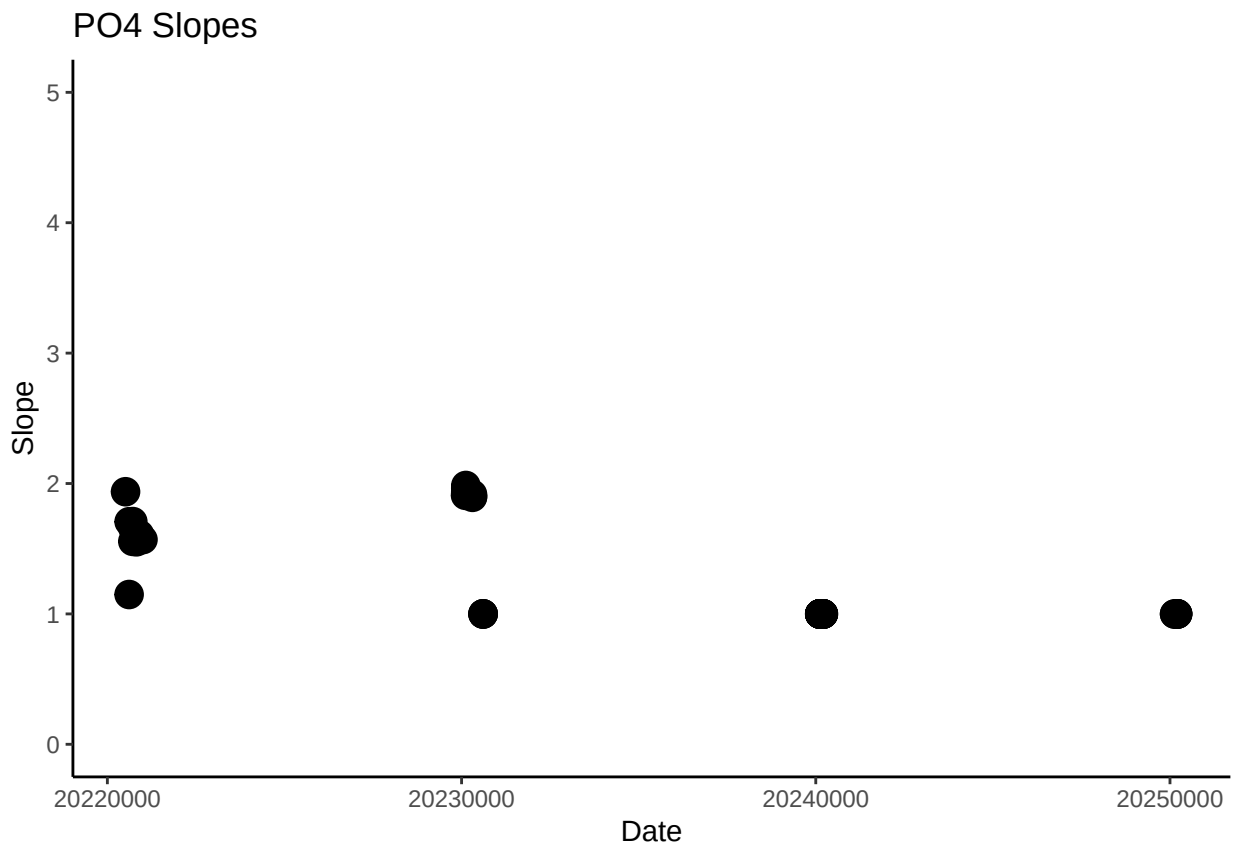
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




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

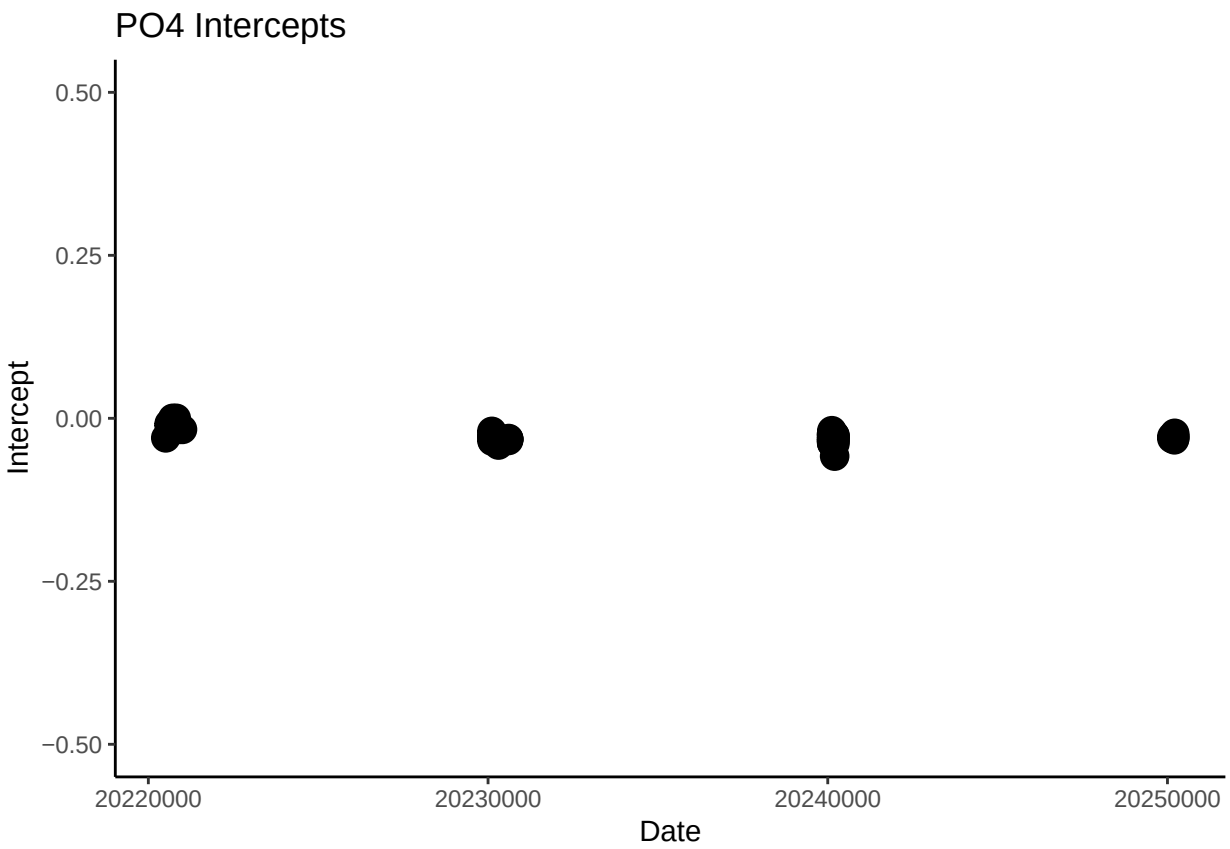
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#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
```

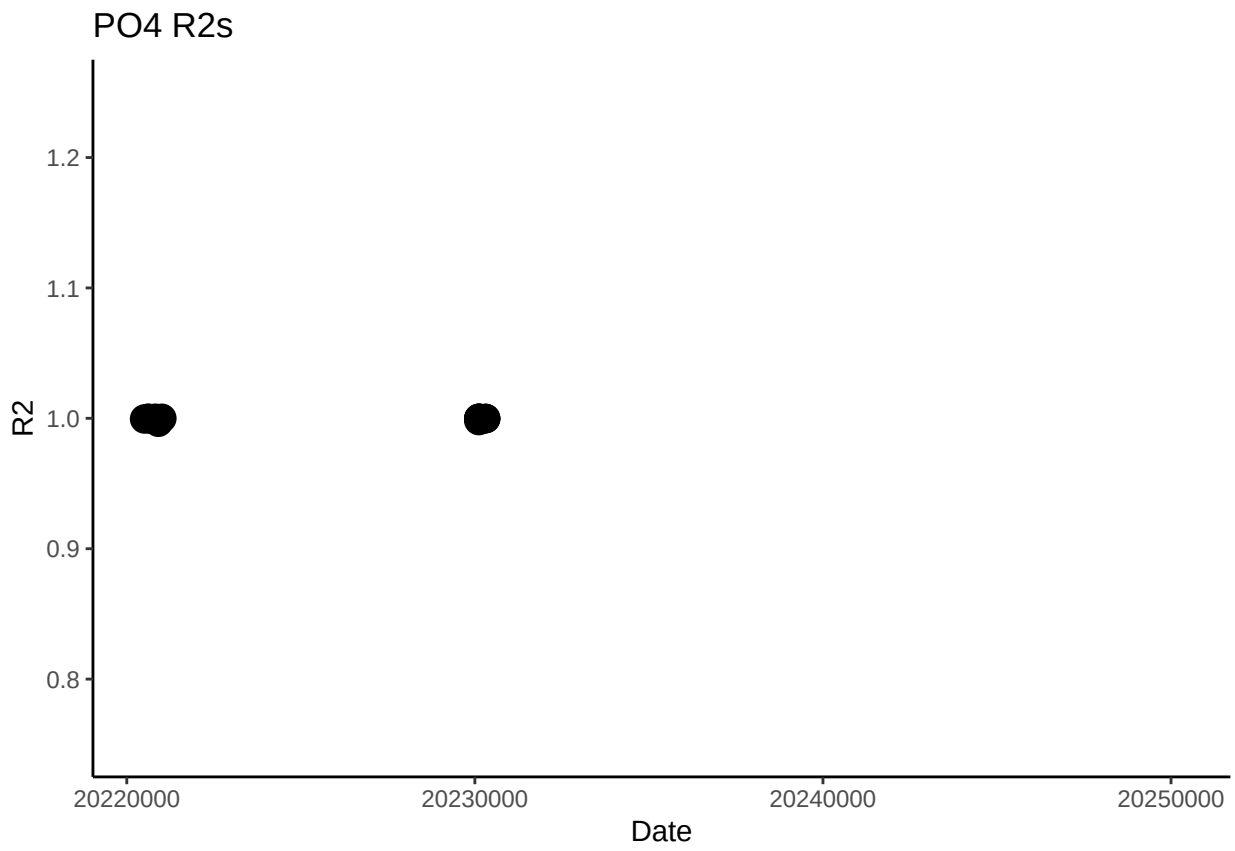
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




```
#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
```

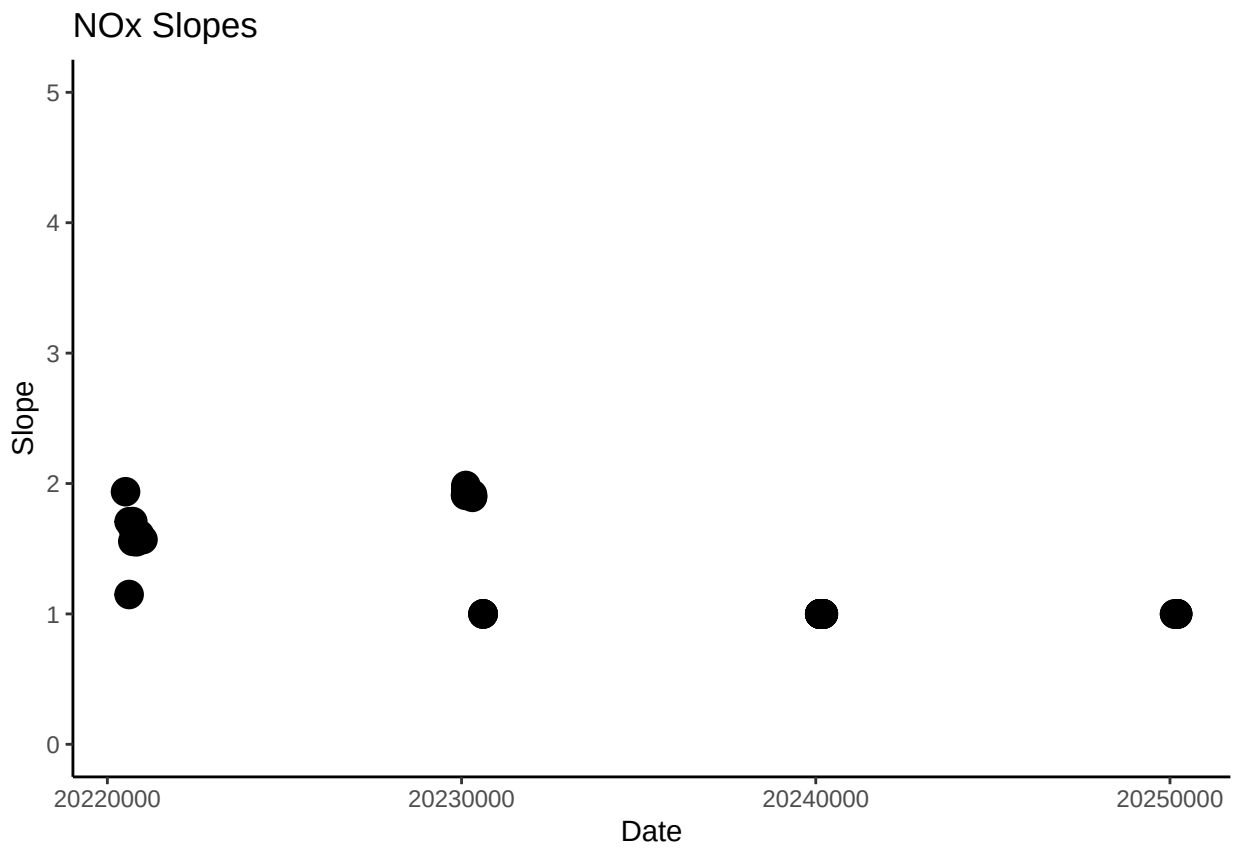
```
## Warning: Removed 39 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




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

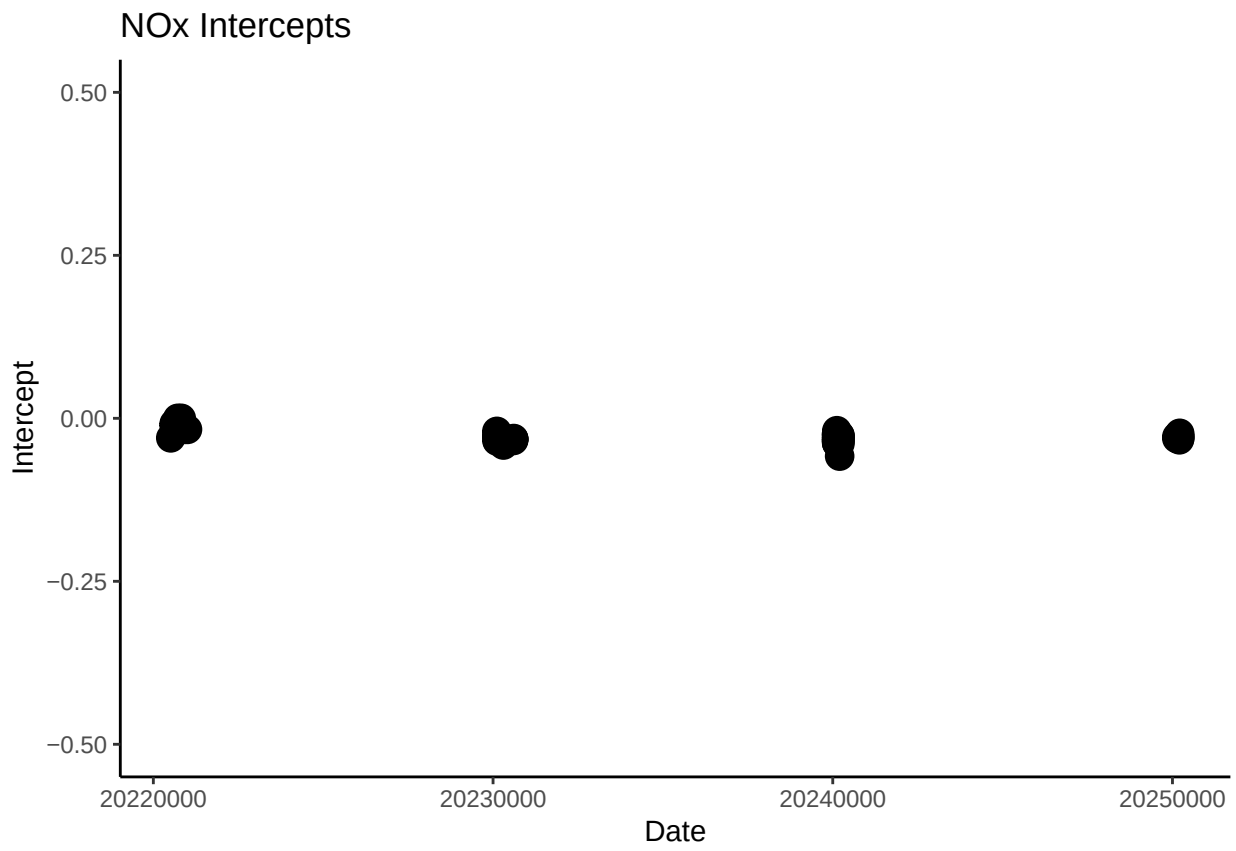
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_point()`).
```




```
#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
```

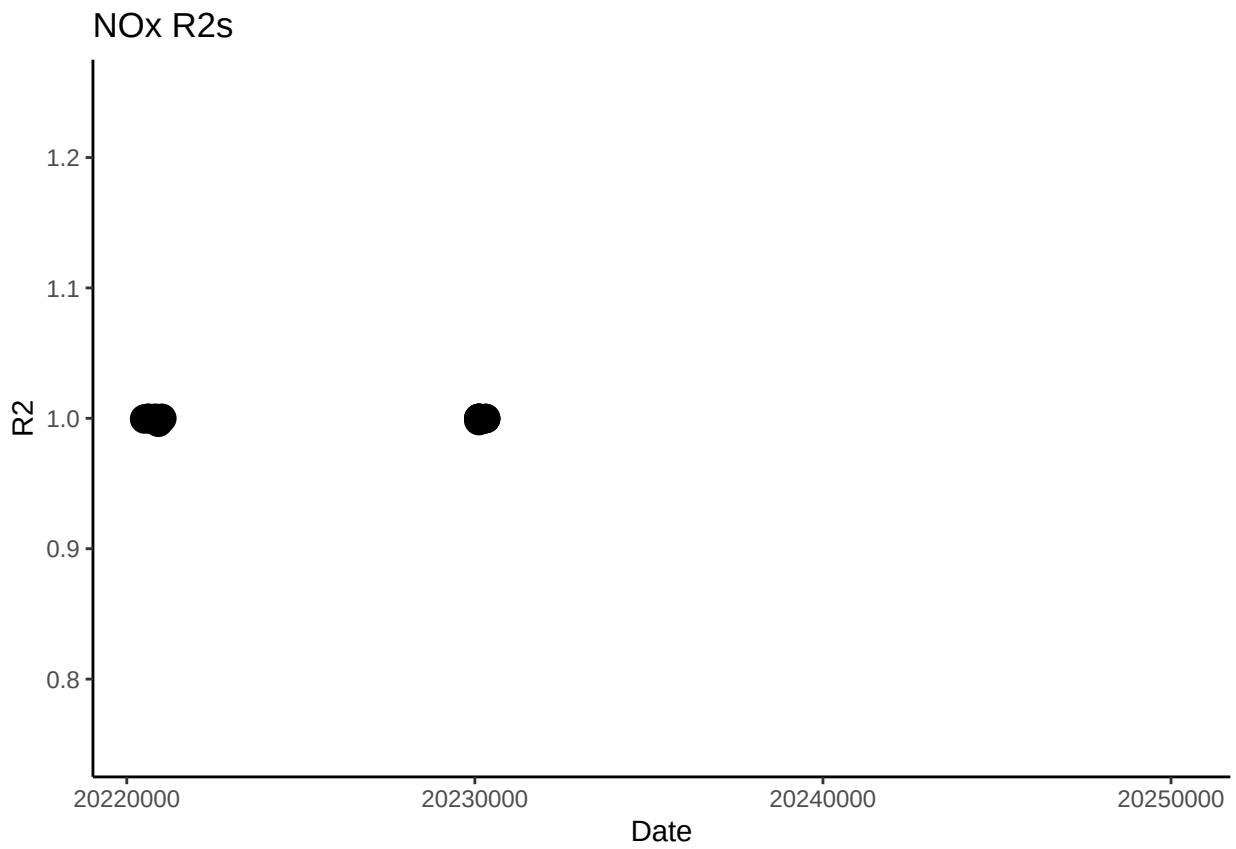
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (‘geom_point()‘).
```




```
#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

```
#set working directory
#setwd("S:/Biogeochemistry/People/Wilson (Steph)/Data/SEAL/Raw Data Files")

#read in data
file1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202206_1.csv")

#Quick look at dataframe
head(file1)
```

```
##   RUNSTARTED X1655221488 X6.14.2022.11.44               X X.1     Conc      Abs
## 1     RESULT          -1               S1      Standard 1   0 0.007059 0.007059
## 2     RESULT          -2              S90  Standard .0389   1 0.028945 0.028945
## 3     RESULT          -2              S91  Standard .1000   2 0.062415 0.062415
## 4     RESULT          -2              S92  Standard .2000   3 0.122412 0.122412
## 5     RESULT          -2              S93  Standard .5000   4 0.288107 0.288107
## 6     RESULT          -2              S94 Standard 1.0000   5 0.596654 0.596654
##   X.2 Dil X.3 X.4    X.5       X.6        X.7             X.8
## 1   0   0   0 512 mg N/L Ammonia 2 1655241586 6/14/2022 17:19
## 2   0   0   0 512 mg N/L Ammonia 2 1655241746 6/14/2022 17:22
## 3   0   0   0 512 mg N/L Ammonia 2 1655241906 6/14/2022 17:25
## 4   0   0   0 512 mg N/L Ammonia 2 1655242066 6/14/2022 17:27
## 5   0   0   0 512 mg N/L Ammonia 2 1655242226 6/14/2022 17:30
## 6   0   0   0 512 mg N/L Ammonia 2 1655242386 6/14/2022 17:33
```

```r
#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 0.007059 0.007059 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.028945 0.028945 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.062415 0.062415 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.122412 0.122412 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.288107 0.288107 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.596654 0.596654 mg N/L Ammonia 2
```

```r
#read in data
file2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_202206_2.csv")

#Quick look at dataframe
head(file2)
```

```
##   RUNSTARTED X1655221488 X6.14.2022.11.44               X X.1     Conc      Abs
## 1     RESULT          -1               S1      Standard 1   0 0.006822 0.006822
## 2     RESULT          -2              S90  Standard .0389   1 0.029314 0.029314
## 3     RESULT          -2              S91  Standard .1000   2 0.063427 0.063427
## 4     RESULT          -2              S92  Standard .2000   3 0.122820 0.122820
## 5     RESULT          -2              S93  Standard .5000   4 0.297338 0.297338
## 6     RESULT          -2              S94 Standard 1.0000   5 0.585606 0.585606
##   X.2 Dil X.3 X.4    X.5       X.6        X.7             X.8
## 1   0   0   0   0 mg N/L Ammonia 2 1655315545 6/15/2022 13:52
## 2   0   0   0   0 mg N/L Ammonia 2 1655315705 6/15/2022 13:55
## 3   0   0   0   0 mg N/L Ammonia 2 1655315865 6/15/2022 13:57
## 4   0   0   0   0 mg N/L Ammonia 2 1655316025 6/15/2022 14:00
## 5   0   0   0   0 mg N/L Ammonia 2 1655316185 6/15/2022 14:03
## 6   0   0   0   0 mg N/L Ammonia 2 1655316345 6/15/2022 14:05
```

```r
#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 0.006822 0.006822 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.029314 0.029314 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.063427 0.063427 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.122820 0.122820 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.297338 0.297338 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.585606 0.585606 mg N/L Ammonia 2
```

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

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

```
##   Run_Info     Sample_Name     Conc      Abs  Units      Test
## 1   RESULT      Standard 1 0.007059 0.007059 mg N/L Ammonia 2
## 2   RESULT  Standard .0389 0.028945 0.028945 mg N/L Ammonia 2
## 3   RESULT  Standard .1000 0.062415 0.062415 mg N/L Ammonia 2
## 4   RESULT  Standard .2000 0.122412 0.122412 mg N/L Ammonia 2
## 5   RESULT  Standard .5000 0.288107 0.288107 mg N/L Ammonia 2
## 6   RESULT Standard 1.0000 0.596654 0.596654 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
## 17   RESULT MSM_UP_LysB_10cm 0.115540 0.073369 mg N/L Ammonia 2
## 21   RESULT MSM_UP_LysC_10cm 0.862642 0.505136 mg N/L Ammonia 2
## 25   RESULT MSM_UP_LysA_20cm 1.880653 1.093465 mg N/L Ammonia 2
## 31   RESULT MSM_UP_LysB_20cm 0.478298 0.283015 mg N/L Ammonia 2
## 35   RESULT MSM_UP_LysC_20cm 2.220213 1.289704 mg N/L Ammonia 2
## 49   RESULT MSM_UP_LysA_45cm 1.003960 0.586806 mg N/L Ammonia 2
```

NOx

```
#set working directory
#setwd("S:/Biogeochemistry/People/Wilson (Steph)/Data/SEAL/Raw Data Files")

#read in data
Nfile1 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202206_1.csv")

#Quick look at dataframe
head(Nfile1)
```

```
##   RUNSTARTED X1655221488      X6.14.2022.11.44                X X.1     Conc
## 1   RUNENDED  1655221531 CANCELLED NOT STARTED                   NA       NA
## 2 RUNSTARTED  1655221552       6/14/2022 11:45                   NA       NA
## 3   RUNENDED  1655221634  INSUFFICIENT REAGENT                   NA       NA
## 4 RUNSTARTED  1655221640       6/14/2022 11:47                   NA       NA
## 5     RESULT           2                   C21 Nitrate Standard   0 0.497297
## 6     RESULT           3                   C22 Nitrite Standard   1 0.515290
##        Abs X.2 Dil 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       NA  NA  NA  NA  NA                                NA
## 5 0.498512   0   0   0 512 mg N/L Vanadium NOx 1655223776 6/14/2022 12:22
## 6 0.512669   0   0   0 512 mg N/L Vanadium NOx 1655223857 6/14/2022 12:24
```

```
#take out only the columns that we need
Ndat1 <- Nfile1[ ,c(1,4,6,7, 12, 13)]

# assigning new names to the columns of the data frame
colnames(Ndat1) <- c('Run_Info','Sample_Name','Conc', "Abs", "Units", "Test")
head(Ndat1)
```

```
##     Run_Info      Sample_Name     Conc      Abs  Units         Test
## 1   RUNENDED                        NA       NA
## 2 RUNSTARTED                        NA       NA
## 3   RUNENDED                        NA       NA
## 4 RUNSTARTED                        NA       NA
## 5     RESULT Nitrate Standard 0.497297 0.498512 mg N/L Vanadium NOx
## 6     RESULT Nitrite Standard 0.515290 0.512669 mg N/L Vanadium NOx
```

```
#read in data
Nfile2 <- read.csv("Raw Data/SEAL_COMPASS_Synoptic_NOx_202206_2.csv")

#Quick look at dataframe
head(Nfile2)
```

```
##   RUNSTARTED X1655297957 X6.15.2022.8.59           X X.1     Conc      Abs X.2
## 1     RESULT          -1              S1  Standard 1   0 0.104187 0.104187   0
## 2     RESULT          -2             S90 Standard 90   1 0.122856 0.122856   0
## 3     RESULT          -2             S91 Standard 91   2 0.156137 0.156137   0
## 4     RESULT          -2             S92 Standard 92   3 0.192336 0.192336   0
## 5     RESULT          -2             S93 Standard 93   4 0.318678 0.318678   0
## 6     RESULT          -2             S94 Standard 94   5 0.508615 0.508615   0
##   Dil X.3 X.4    X.5          X.6        X.7            X.8
## 1   0   0   0 mg N/L Vanadium NOx 1655300153 6/15/2022 9:35
## 2   0   0   0 mg N/L Vanadium NOx 1655300234 6/15/2022 9:37
## 3   0   0   0 mg N/L Vanadium NOx 1655300315 6/15/2022 9:38
## 4   0   0   0 mg N/L Vanadium NOx 1655300396 6/15/2022 9:39
## 5   0   0   0 mg N/L Vanadium NOx 1655300477 6/15/2022 9:41
## 6   0   0   0 mg N/L Vanadium NOx 1655300558 6/15/2022 9:42
```

```
#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 0.104187 0.104187 mg N/L Vanadium NOx
## 2   RESULT Standard 90 0.122856 0.122856 mg N/L Vanadium NOx
## 3   RESULT Standard 91 0.156137 0.156137 mg N/L Vanadium NOx
## 4   RESULT Standard 92 0.192336 0.192336 mg N/L Vanadium NOx
## 5   RESULT Standard 93 0.318678 0.318678 mg N/L Vanadium NOx
## 6   RESULT Standard 94 0.508615 0.508615 mg N/L Vanadium NOx
```

```
Nalldat <- rbind(Ndat1, Ndat2)

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

```
##     Run_Info      Sample_Name     Conc      Abs  Units         Test
## 5     RESULT Nitrate Standard 0.497297 0.498512 mg N/L Vanadium NOx
## 6     RESULT Nitrite Standard 0.515290 0.512669 mg N/L Vanadium NOx
## 225   RESULT       Standard 1 0.104187 0.104187 mg N/L Vanadium NOx
## 226   RESULT      Standard 90 0.122856 0.122856 mg N/L Vanadium NOx
## 227   RESULT      Standard 91 0.156137 0.156137 mg N/L Vanadium NOx
## 228   RESULT      Standard 92 0.192336 0.192336 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
## 15   RESULT MSM_UP_LysA_10cm -0.010845 0.105420 mg N/L Vanadium NOx
## 19   RESULT MSM_UP_LysB_10cm -0.008500 0.107205 mg N/L Vanadium NOx
## 23   RESULT MSM_UP_LysC_10cm -0.008269 0.107381 mg N/L Vanadium NOx
## 27   RESULT MSM_UP_LysA_20cm -0.007655 0.107848 mg N/L Vanadium NOx
## 31   RESULT MSM_UP_LysB_20cm -0.008364 0.107309 mg N/L Vanadium NOx
## 41   RESULT MSM_UP_LysC_20cm -0.009718 0.106278 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       Test
## 187    RESULT                     peCheck 1.140970 0.665987 mg N/L  Ammonia 2
## 411    RESULT                     peCheck 0.769670 0.321612 mg P/L o-PHOS 0.3
## 662    RESULT peCheck_948ppmNH4_818ppmPO4 1.201878 0.708806 mg N/L  Ammonia 2
## 1021   RESULT peCheck_948ppmNH4_818ppmPO4 0.799204 0.340360 mg P/L o-PHOS 0.3
```

```
Nchks <- Nalldat[Nalldat$Sample_Name %like% "peCheck", ]
NH4chk <- subset(chks, Test == "Ammonia 2")
NH4chk$ConcTrue <- 0.948
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      Test
## 187   RESULT                    peCheck 1.140970 0.665987 mg N/L Ammonia 2
```

```
## 662   RESULT peCheck_948ppmNH4_818ppmPO4 1.201878 0.708806 mg N/L Ammonia 2
##     ConcTrue Chk_diff Chk_dff_flag
## 187    0.948 18.47513          YES
## 662    0.948 23.61790          YES
```

```
PO4chk <- subset(chks, Test == "o-PHOS 0.3")
PO4chk$ConcTrue <- 0.818
PO4chk$Chk_diff <- (PO4chk$Conc - PO4chk$ConcTrue)/((PO4chk$Conc+PO4chk$ConcTrue)/2) * 100
PO4chk$Chk_dff_flag <-  ifelse(PO4chk$Chk_diff <25, 'YES', 'NO, rerun')
head(PO4chk)
```

```
##      Run_Info                Sample_Name     Conc      Abs  Units       Test
## 411    RESULT                    peCheck 0.769670 0.321612 mg P/L o-PHOS 0.3
## 1021   RESULT peCheck_948ppmNH4_818ppmPO4 0.799204 0.340360 mg P/L o-PHOS 0.3
##      ConcTrue  Chk_diff Chk_dff_flag
## 411     0.818 -6.088167          YES
## 1021    0.818 -2.324506          YES
```

```
NOXchk <- subset(Nchks, Test == "Vanadium NOx")
NOXchk$ConcTrue <- 0.706
NOXchk$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         Test
## 192   RESULT peCheck_706ppm_Nitrate 0.713231 0.669542 mg N/L Vanadium NOx
## 430   RESULT peCheck_706ppm_Nitrate 0.690136 0.674198 mg N/L Vanadium NOx
##     ConcTrue  Chk_diff Chk_dff_flag
## 192    0.706  1.019003          YES
## 430    0.706 -2.272558          YES
```

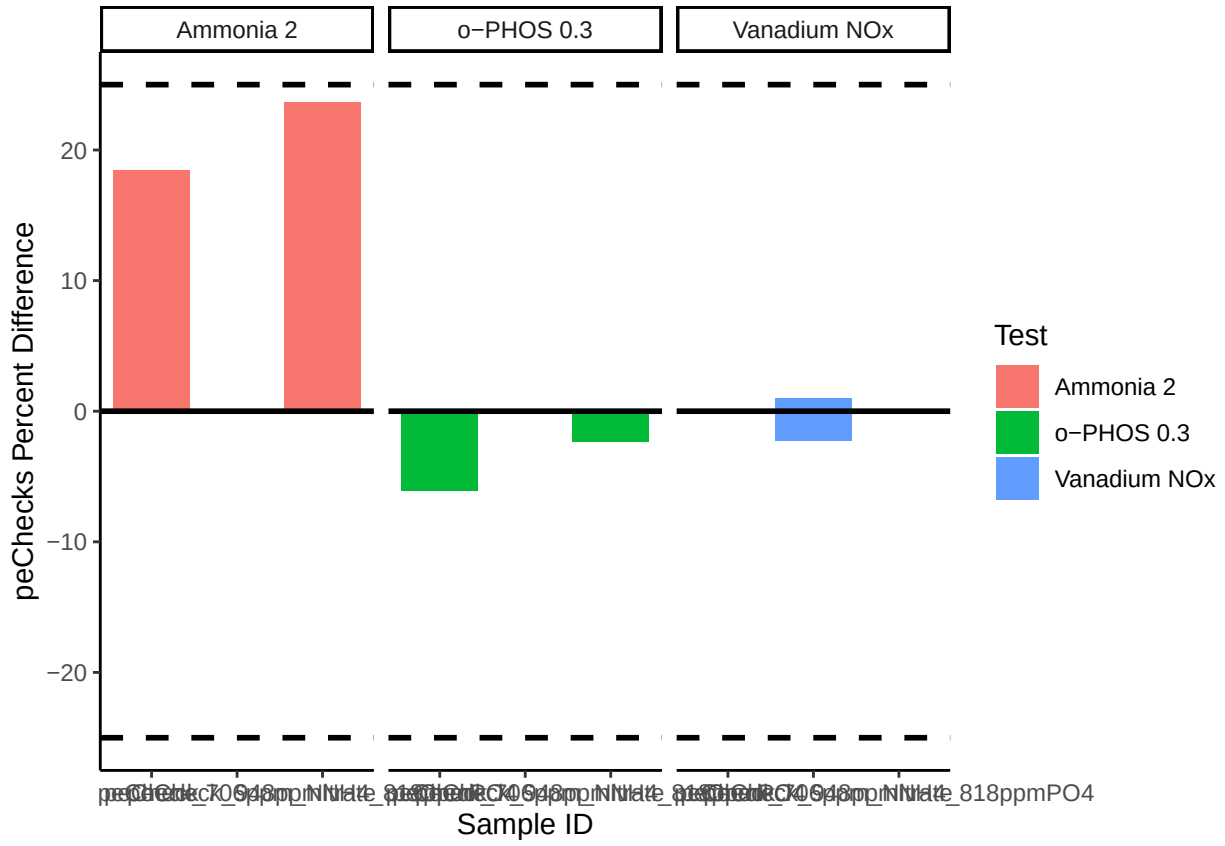
```
Allchks <- rbind(NH4chk, PO4chk)
Allchks <- rbind(Allchks, NOXchk)
head(Allchks)
```

```
##      Run_Info                Sample_Name     Conc      Abs  Units         Test
## 187    RESULT                    peCheck 1.140970 0.665987 mg N/L    Ammonia 2
## 662    RESULT peCheck_948ppmNH4_818ppmPO4 1.201878 0.708806 mg N/L    Ammonia 2
## 411    RESULT                    peCheck 0.769670 0.321612 mg P/L   o-PHOS 0.3
## 1021   RESULT peCheck_948ppmNH4_818ppmPO4 0.799204 0.340360 mg P/L   o-PHOS 0.3
## 192    RESULT      peCheck_706ppm_Nitrate 0.713231 0.669542 mg N/L Vanadium NOx
## 430    RESULT      peCheck_706ppm_Nitrate 0.690136 0.674198 mg N/L Vanadium NOx
##      ConcTrue  Chk_diff Chk_dff_flag
## 187     0.948 18.475134          YES
## 662     0.948 23.617898          YES
## 411     0.818 -6.088167          YES
## 1021    0.818 -2.324506          YES
## 192     0.706  1.019003          YES
## 430     0.706 -2.272558          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) +
        #facet_grid(cols = Allchks$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
```

```r
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

```r
head(alldat2)
```

```
##    Run_Info      Sample_Name     Conc      Abs  Units      Test
## 17   RESULT MSM_UP_LysB_10cm 0.115540 0.073369 mg N/L Ammonia 2
## 21   RESULT MSM_UP_LysC_10cm 0.862642 0.505136 mg N/L Ammonia 2
## 25   RESULT MSM_UP_LysA_20cm 1.880653 1.093465 mg N/L Ammonia 2
## 31   RESULT MSM_UP_LysB_20cm 0.478298 0.283015 mg N/L Ammonia 2
## 35   RESULT MSM_UP_LysC_20cm 2.220213 1.289704 mg N/L Ammonia 2
## 49   RESULT MSM_UP_LysA_45cm 1.003960 0.586806 mg N/L Ammonia 2
```

```r
head(Nalldat2)
```

```
##    Run_Info      Sample_Name      Conc      Abs  Units         Test
## 15   RESULT MSM_UP_LysA_10cm -0.010845 0.105420 mg N/L Vanadium NOx
## 19   RESULT MSM_UP_LysB_10cm -0.008500 0.107205 mg N/L Vanadium NOx
## 23   RESULT MSM_UP_LysC_10cm -0.008269 0.107381 mg N/L Vanadium NOx
## 27   RESULT MSM_UP_LysA_20cm -0.007655 0.107848 mg N/L Vanadium NOx
## 31   RESULT MSM_UP_LysB_20cm -0.008364 0.107309 mg N/L Vanadium NOx
## 41   RESULT MSM_UP_LysC_20cm -0.009718 0.106278 mg N/L Vanadium NOx
```

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

```
##    Run_Info      Sample_Name     Conc      Abs  Units      Test
## 17   RESULT MSM_UP_LysB_10cm 0.115540 0.073369 mg N/L Ammonia 2
## 21   RESULT MSM_UP_LysC_10cm 0.862642 0.505136 mg N/L Ammonia 2
## 25   RESULT MSM_UP_LysA_20cm 1.880653 1.093465 mg N/L Ammonia 2
## 31   RESULT MSM_UP_LysB_20cm 0.478298 0.283015 mg N/L Ammonia 2
## 35   RESULT MSM_UP_LysC_20cm 2.220213 1.289704 mg N/L Ammonia 2
## 49   RESULT MSM_UP_LysA_45cm 1.003960 0.586806 mg N/L Ammonia 2
```

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

```
##     Run_Info      Sample_Name     Conc      Abs  Units       Test
## 237   RESULT MSM_UP_LysB_10cm 0.009014 0.004034 mg P/L o-PHOS 0.3
## 241   RESULT MSM_UP_LysC_10cm 0.011445 0.005049 mg P/L o-PHOS 0.3
## 245   RESULT MSM_UP_LysA_20cm 0.013253 0.005804 mg P/L o-PHOS 0.3
## 249   RESULT MSM_UP_LysB_20cm 0.009683 0.004314 mg P/L o-PHOS 0.3
## 253   RESULT MSM_UP_LysC_20cm 0.017500 0.007577 mg P/L o-PHOS 0.3
## 264   RESULT MSM_UP_LysA_45cm 0.013808 0.006036 mg P/L o-PHOS 0.3
```

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

```
##    Run_Info      Sample_Name      Conc      Abs  Units         Test
## 15   RESULT MSM_UP_LysA_10cm -0.010845 0.105420 mg N/L Vanadium NOx
## 19   RESULT MSM_UP_LysB_10cm -0.008500 0.107205 mg N/L Vanadium NOx
## 23   RESULT MSM_UP_LysC_10cm -0.008269 0.107381 mg N/L Vanadium NOx
## 27   RESULT MSM_UP_LysA_20cm -0.007655 0.107848 mg N/L Vanadium NOx
## 31   RESULT MSM_UP_LysB_20cm -0.008364 0.107309 mg N/L Vanadium NOx
## 41   RESULT MSM_UP_LysC_20cm -0.009718 0.106278 mg N/L Vanadium NOx
```

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

```
##    Run_Info      Sample_Name     Conc      Abs  Units      Test    Conc_uM
## 17   RESULT MSM_UP_LysB_10cm 0.115540 0.073369 mg N/L Ammonia 2   8.248909
## 21   RESULT MSM_UP_LysC_10cm 0.862642 0.505136 mg N/L Ammonia 2  61.587812
## 25   RESULT MSM_UP_LysA_20cm 1.880653 1.093465 mg N/L Ammonia 2 134.268100
## 31   RESULT MSM_UP_LysB_20cm 0.478298 0.283015 mg N/L Ammonia 2  34.147801
## 35   RESULT MSM_UP_LysC_20cm 2.220213 1.289704 mg N/L Ammonia 2 158.510784
## 49   RESULT MSM_UP_LysA_45cm 1.003960 0.586806 mg N/L Ammonia 2  71.677126
```

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

```
##     Run_Info      Sample_Name     Conc      Abs  Units       Test   Conc_uM
## 237   RESULT MSM_UP_LysB_10cm 0.009014 0.004034 mg P/L o-PHOS 0.3 0.6435492
## 241   RESULT MSM_UP_LysC_10cm 0.011445 0.005049 mg P/L o-PHOS 0.3 0.8171090
## 245   RESULT MSM_UP_LysA_20cm 0.013253 0.005804 mg P/L o-PHOS 0.3 0.9461900
## 249   RESULT MSM_UP_LysB_20cm 0.009683 0.004314 mg P/L o-PHOS 0.3 0.6913120
## 253   RESULT MSM_UP_LysC_20cm 0.017500 0.007577 mg P/L o-PHOS 0.3 1.2494021
## 264   RESULT MSM_UP_LysA_45cm 0.013808 0.006036 mg P/L o-PHOS 0.3 0.9858139
```

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

```
##    Run_Info      Sample_Name      Conc      Abs  Units         Test Conc_uM_raw
## 15   RESULT MSM_UP_LysA_10cm -0.010845 0.105420 mg N/L Vanadium NOx  -0.7742723
## 19   RESULT MSM_UP_LysB_10cm -0.008500 0.107205 mg N/L Vanadium NOx  -0.6068524
## 23   RESULT MSM_UP_LysC_10cm -0.008269 0.107381 mg N/L Vanadium NOx  -0.5903603
## 27   RESULT MSM_UP_LysA_20cm -0.007655 0.107848 mg N/L Vanadium NOx  -0.5465242
## 31   RESULT MSM_UP_LysB_20cm -0.008364 0.107309 mg N/L Vanadium NOx  -0.5971428
## 41   RESULT MSM_UP_LysC_20cm -0.009718 0.106278 mg N/L Vanadium NOx  -0.6938108
```

```r
#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 Conc_uM_raw
## 15   RESULT MSM_UP_LysA_10cm -0.010845 0.105420 mg N/L Vanadium NOx  -0.7742723
```

```
## 19   RESULT MSM_UP_LysB_10cm -0.008500 0.107205 mg N/L Vanadium NOx  -0.6068524
## 23   RESULT MSM_UP_LysC_10cm -0.008269 0.107381 mg N/L Vanadium NOx  -0.5903603
## 27   RESULT MSM_UP_LysA_20cm -0.007655 0.107848 mg N/L Vanadium NOx  -0.5465242
## 31   RESULT MSM_UP_LysB_20cm -0.008364 0.107309 mg N/L Vanadium NOx  -0.5971428
## 41   RESULT MSM_UP_LysC_20cm -0.009718 0.106278 mg N/L Vanadium NOx  -0.6938108
##    Conc_uM
## 15       0
## 19       0
## 23       0
## 27       0
## 31       0
## 41       0
```

Pull all data back together and add flags

```
#pull out the columns we want from each dataframe
NH4_pull <- NH4samples[ ,c(2,3,7) ]
head(NH4_pull)
```

```
##         Sample_Name     Conc    Conc_uM
## 17 MSM_UP_LysB_10cm 0.115540   8.248909
## 21 MSM_UP_LysC_10cm 0.862642  61.587812
## 25 MSM_UP_LysA_20cm 1.880653 134.268100
## 31 MSM_UP_LysB_20cm 0.478298  34.147801
## 35 MSM_UP_LysC_20cm 2.220213 158.510784
## 49 MSM_UP_LysA_45cm 1.003960  71.677126
```

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

```
##          Sample_Name     Conc   Conc_uM
## 237 MSM_UP_LysB_10cm 0.009014 0.6435492
## 241 MSM_UP_LysC_10cm 0.011445 0.8171090
## 245 MSM_UP_LysA_20cm 0.013253 0.9461900
## 249 MSM_UP_LysB_20cm 0.009683 0.6913120
## 253 MSM_UP_LysC_20cm 0.017500 1.2494021
## 264 MSM_UP_LysA_45cm 0.013808 0.9858139
```

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

```
##         Sample_Name      Conc Conc_uM
## 15 MSM_UP_LysA_10cm -0.010845       0
## 19 MSM_UP_LysB_10cm -0.008500       0
## 23 MSM_UP_LysC_10cm -0.008269       0
## 27 MSM_UP_LysA_20cm -0.007655       0
## 31 MSM_UP_LysB_20cm -0.008364       0
## 41 MSM_UP_LysC_20cm -0.009718       0
```

```r
#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_TR_LysA_10cm 0.368399 26.301627 0.004501 0.3213462 -0.000079 0.00000000
## 2 GCrew_TR_LysA_20cm 0.252957 18.059714 0.003840 0.2741545  0.001369 0.09773894
## 3 GCrew_TR_LysA_45cm 0.081743  5.835993 0.003779 0.2697995  0.001238 0.08838627
## 4 GCrew_TR_LysB_10cm 1.170921 83.597207 0.008058 0.5752961 -0.002973 0.00000000
## 5 GCrew_TR_LysB_20cm 0.752796 53.745422 0.006376 0.4552107 -0.003554 0.00000000
## 6 GCrew_TR_LysB_45cm 0.172726 12.331670 0.003679 0.2626600 -0.005670 0.00000000
```

```r
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_TR_LysA_10cm 0.368399 26.301627 0.004501 0.3213462 -0.000079 0.00000000
## 2 GCrew_TR_LysA_20cm 0.252957 18.059714 0.003840 0.2741545  0.001369 0.09773894
## 3 GCrew_TR_LysA_45cm 0.081743  5.835993 0.003779 0.2697995  0.001238 0.08838627
## 4 GCrew_TR_LysB_10cm 1.170921 83.597207 0.008058 0.5752961 -0.002973 0.00000000
## 5 GCrew_TR_LysB_20cm 0.752796 53.745422 0.006376 0.4552107 -0.003554 0.00000000
## 6 GCrew_TR_LysB_45cm 0.172726 12.331670 0.003679 0.2626600 -0.005670 0.00000000
```

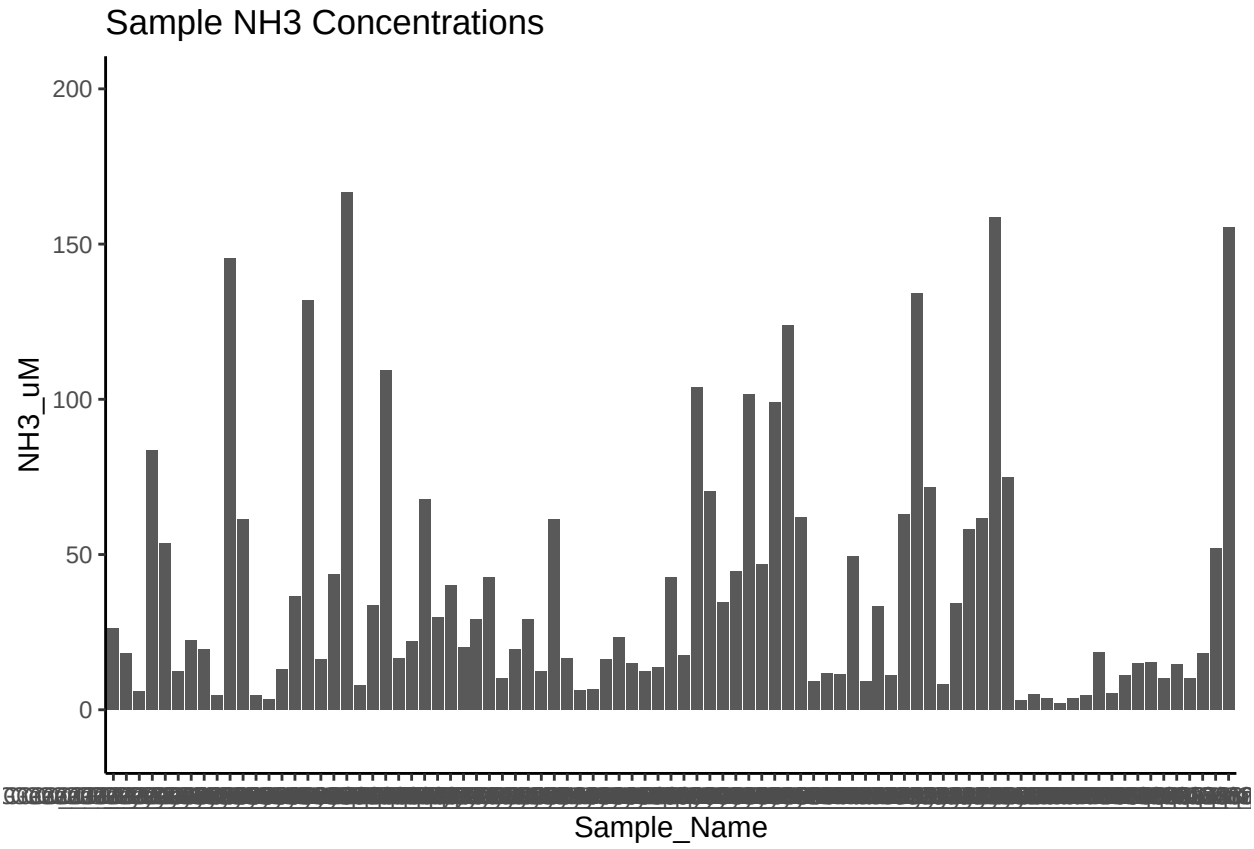
```r
#add in an if then statement that tells us if they are within the range of the test - check this after
all_data$NH3_range <- ifelse(all_data$NH3_mgL<0.02, "bdl",  ifelse(all_data$NH3_mgL>2, "adl", "Within_Ra
all_data$PO4_range <- ifelse(all_data$PO4_mgL<0.003, "bdl",  ifelse(all_data$PO4_mgL>3, "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_TR_LysA_10cm 0.368399 26.301627 0.004501 0.3213462 -0.000079 0.00000000
## 2 GCrew_TR_LysA_20cm 0.252957 18.059714 0.003840 0.2741545  0.001369 0.09773894
## 3 GCrew_TR_LysA_45cm 0.081743  5.835993 0.003779 0.2697995  0.001238 0.08838627
## 4 GCrew_TR_LysB_10cm 1.170921 83.597207 0.008058 0.5752961 -0.002973 0.00000000
## 5 GCrew_TR_LysB_20cm 0.752796 53.745422 0.006376 0.4552107 -0.003554 0.00000000
## 6 GCrew_TR_LysB_45cm 0.172726 12.331670 0.003679 0.2626600 -0.005670 0.00000000
##      NH3_range    PO4_range NOx_range
## 1 Within_Range Within_Range       bdl
## 2 Within_Range Within_Range       bdl
## 3 Within_Range Within_Range       bdl
## 4 Within_Range Within_Range       bdl
## 5 Within_Range Within_Range       bdl
## 6 Within_Range Within_Range       bdl
```

Take an initial look at concentrations

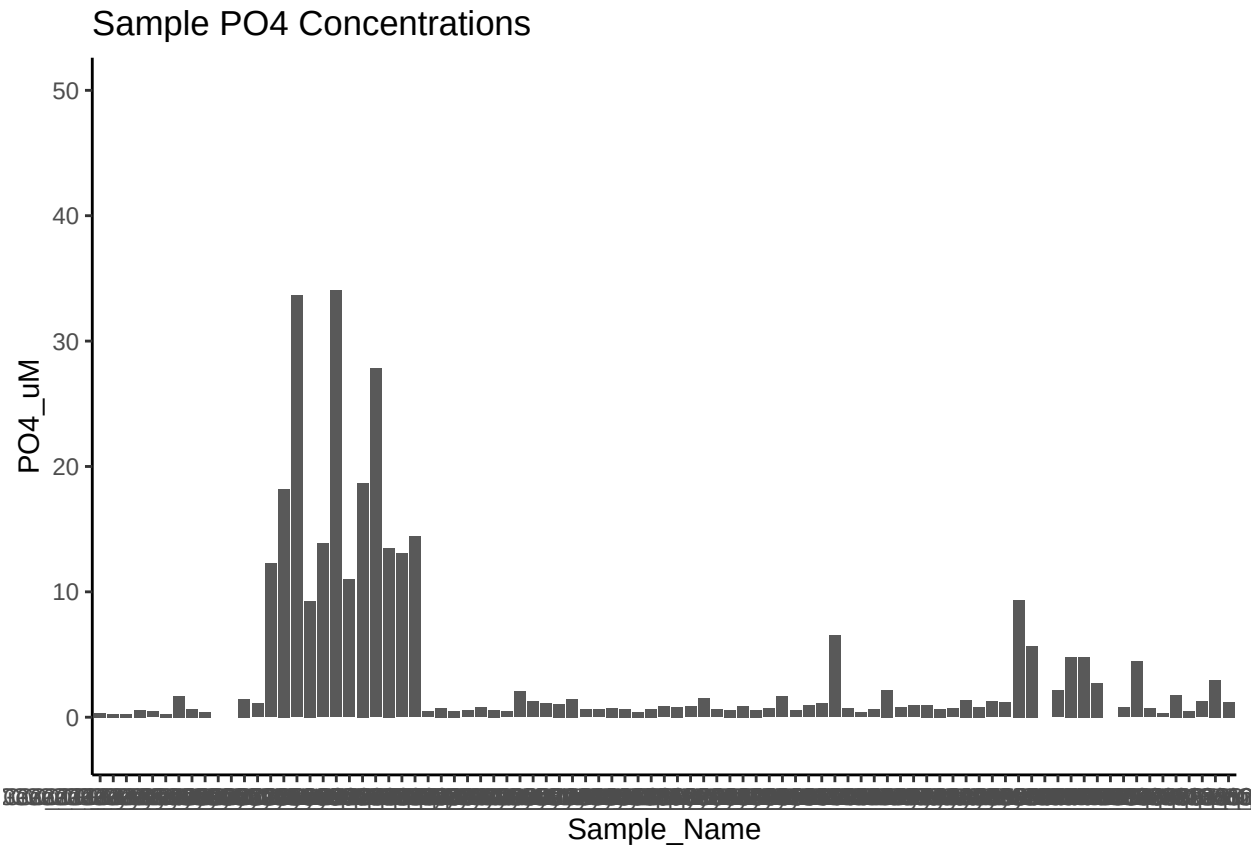
```r
#plot data to get a sense of any outliers
NH3look <- ggplot(data=all_data, aes(x=Sample_Name, y=NH3_uM)) +
  geom_bar(stat="identity") +
```

```
  theme_classic() + ylim(-10, 200) +
  theme(legend.position="none") +
  ggtitle("Sample NH3 Concentrations")
NH3look
```



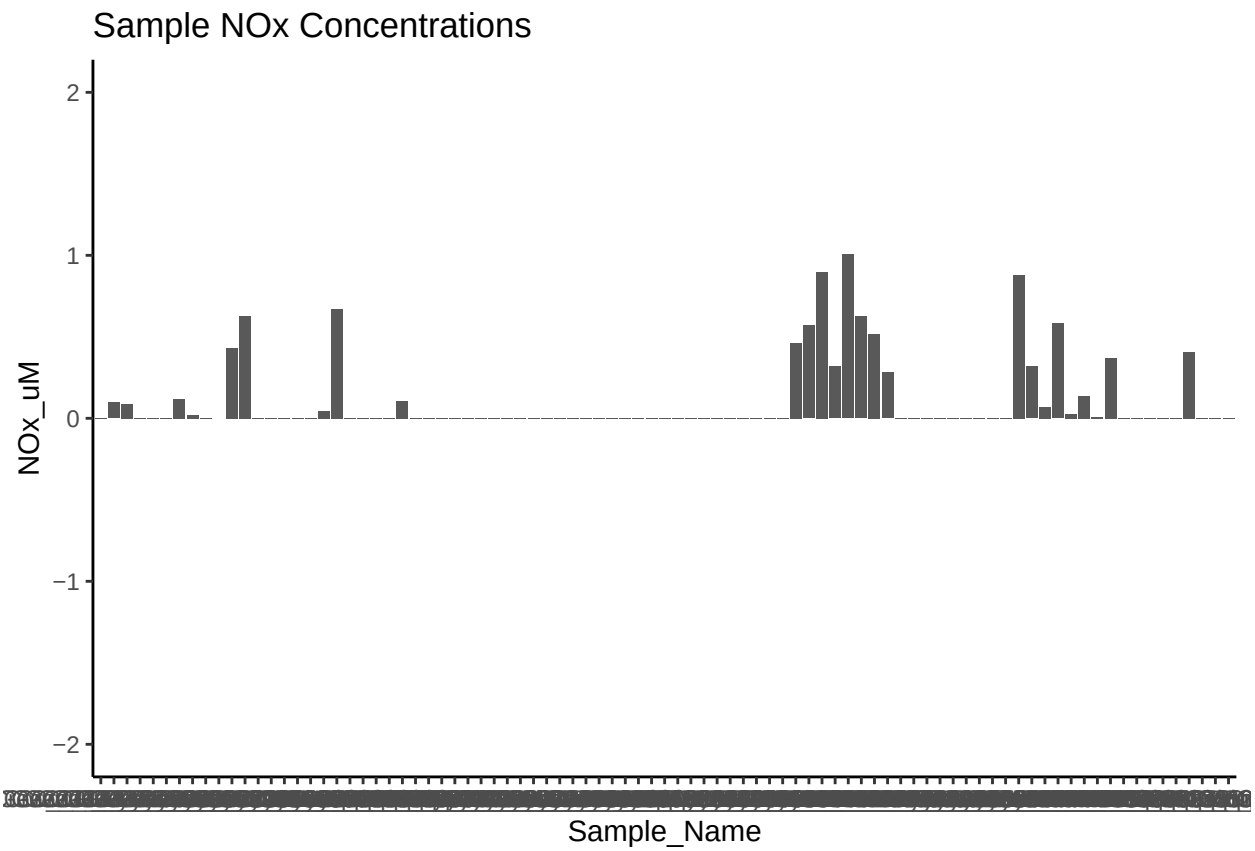

```
PO4look <- ggplot(data=all_data, aes(x=Sample_Name, y=PO4_uM)) +
  geom_bar(stat="identity") +
  theme_classic() + ylim(-2, 50) +
  theme(legend.position="none") +
  ggtitle("Sample PO4 Concentrations")
PO4look
```

```
## Warning: Removed 4 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 1 row 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_TR_LysA_10cm 0.368399 26.301627 0.004501 0.3213462 -0.000079 0.00000000
## 2 GCrew_TR_LysA_20cm 0.252957 18.059714 0.003840 0.2741545  0.001369 0.09773894
## 3 GCrew_TR_LysA_45cm 0.081743  5.835993 0.003779 0.2697995  0.001238 0.08838627
## 4 GCrew_TR_LysB_10cm 1.170921 83.597207 0.008058 0.5752961 -0.002973 0.00000000
## 5 GCrew_TR_LysB_20cm 0.752796 53.745422 0.006376 0.4552107 -0.003554 0.00000000
## 6 GCrew_TR_LysB_45cm 0.172726 12.331670 0.003679 0.2626600 -0.005670 0.00000000
##      NH3_range    PO4_range NOx_range
## 1 Within_Range Within_Range       bdl
## 2 Within_Range Within_Range       bdl
## 3 Within_Range Within_Range       bdl
## 4 Within_Range Within_Range       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_TR_LysA_10cm 26.301627 0.3213462 0.00000000 Within_Range Within_Range
## 2 GCrew_TR_LysA_20cm 18.059714 0.2741545 0.09773894 Within_Range Within_Range
## 3 GCrew_TR_LysA_45cm  5.835993 0.2697995 0.08838627 Within_Range Within_Range
## 4 GCrew_TR_LysB_10cm 83.597207 0.5752961 0.00000000 Within_Range Within_Range
## 5 GCrew_TR_LysB_20cm 53.745422 0.4552107 0.00000000 Within_Range Within_Range
## 6 GCrew_TR_LysB_45cm 12.331670 0.2626600 0.00000000 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$Sample_Name),'_',fixed=TRUE)))
colnames(IDs) <- c("Site" ,"Zone", "Replicate", "Depth")
IDs$Date <- 202206
IDs$Month <- "June"
head(IDs)
```

```
##    Site Zone Replicate Depth   Date Month
## 1 GCrew   TR      LysA  10cm 202206  June
## 2 GCrew   TR      LysA  20cm 202206  June
## 3 GCrew   TR      LysA  45cm 202206  June
## 4 GCrew   TR      LysB  10cm 202206  June
## 5 GCrew   TR      LysB  20cm 202206  June
## 6 GCrew   TR      LysB  45cm 202206  June
```

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

```
##    Site Zone Replicate Depth   Date Month        Sample_Name    NH3_uM
## 1 GCrew   TR      LysA  10cm 202206  June GCrew_TR_LysA_10cm 26.301627
## 2 GCrew   TR      LysA  20cm 202206  June GCrew_TR_LysA_20cm 18.059714
## 3 GCrew   TR      LysA  45cm 202206  June GCrew_TR_LysA_45cm  5.835993
## 4 GCrew   TR      LysB  10cm 202206  June GCrew_TR_LysB_10cm 83.597207
## 5 GCrew   TR      LysB  20cm 202206  June GCrew_TR_LysB_20cm 53.745422
## 6 GCrew   TR      LysB  45cm 202206  June GCrew_TR_LysB_45cm 12.331670
##      PO4_uM     NOx_uM    NH3_range    PO4_range NOx_range
## 1 0.3213462 0.00000000 Within_Range Within_Range       bdl
## 2 0.2741545 0.09773894 Within_Range Within_Range       bdl
## 3 0.2697995 0.08838627 Within_Range Within_Range       bdl
## 4 0.5752961 0.00000000 Within_Range Within_Range       bdl
## 5 0.4552107 0.00000000 Within_Range Within_Range       bdl
## 6 0.2626600 0.00000000 Within_Range Within_Range       bdl
```

Export final data with flags

```r
#Export Data
#setwd("S:/Biogeochemistry/People/Wilson (Steph)/Data/SEAL/Final Data Files")
write.csv(alldat, file="Processed Data/COMPASS_SynopticCB_Nutrients_202206.csv")
```