

COMPASS Synoptic CB Porewater: DOC

June 2024 Samples

2025-10-31

##Setup - Change things here & write any notes

```
#identify section  
cat("Setup Information")
```

Setup Information

```
##### Run information - PLEASE CHANGE  
Date_Run = "06/29/24" #Date that instrument was run  
Run_by = "Stephanie J. Wilson" #Instrument user  
Script_run_by = "Stephanie J. Wilson" #Code user  
run_notes = "Couple of samples are above the top standard. Accidentally put in 2023 rather  
than 2024, so that is changed programmatically in this code." #any notes from the run  
samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names  
samples_pattern <- paste(samples, collapse = "|")  
  #samples_pattern <- "GCW" #use this instead of the line above if you have only one site code  
chks_name = "Chk_Std_50C_2N" #what did you name your check standards?  
  
##### File Names - PLEASE CHANGE  
#file path and name for raw summary data file  
  #raw_file_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202505.txt" #example  
  raw_file_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202406.txt"  
  
#file path and name for raw all peaks file  
  #raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202505_allpeaks.txt" #example  
  raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202406_allpeaks.txt"  
  
#file path and name of processed data file  
  #processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DOC_202505.csv" #example  
  processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DOC_202406.csv" #example  
  
##### Log Files - PLEASE CHECK  
#downloaded metadata csv - downloaded from Google drive as csv for this year  
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"  
  
#qaqc log file path for this year  
  Log_path = "Raw Data/COMPASS_Synoptic_TOCTN_QAQClog_2024.csv"
```

##Set Up Code

##Read in metadata and create similar sample IDs for matching to samples

Import Data Functions

Import Sample Data

```
## Import Sample Data

## New names:
## * `` -> '...14'

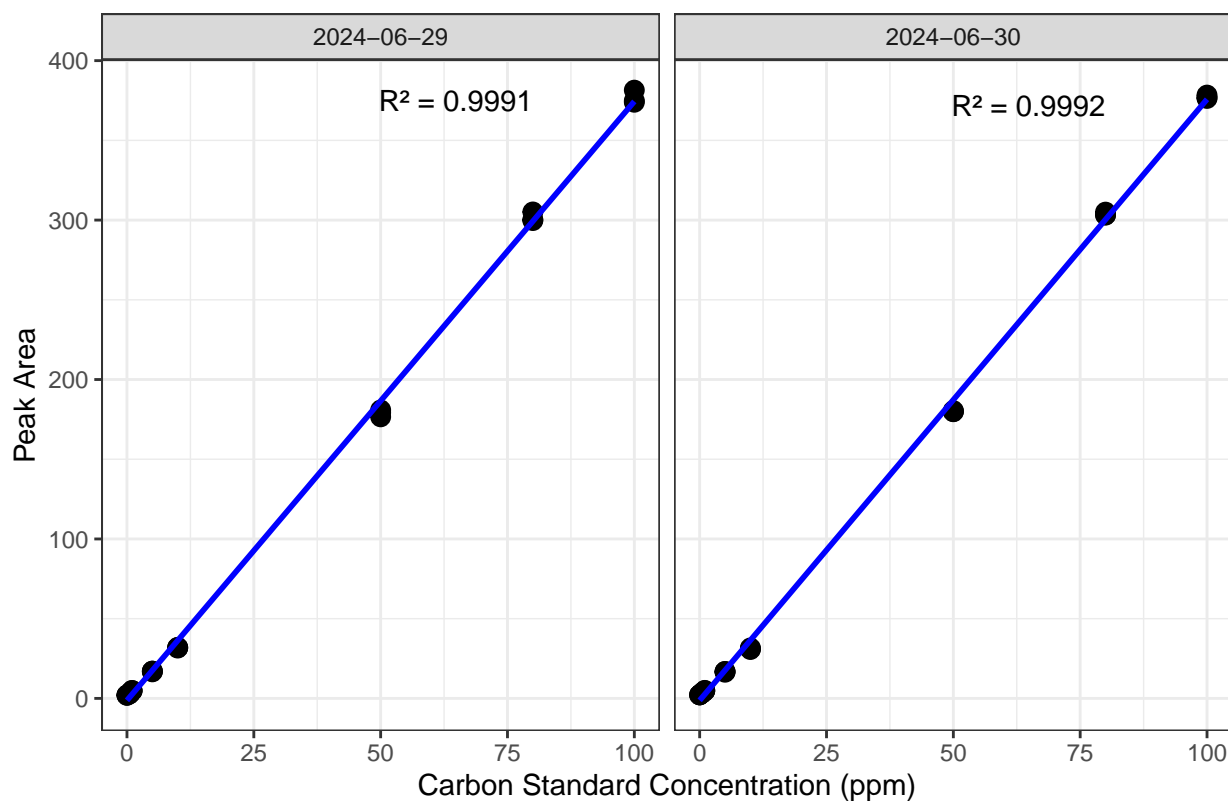
## # A tibble: 6 x 4
##   sample_name      npoc_raw tdn_raw run_datetime
##   <chr>          <dbl>   <dbl> <chr>
## 1 202406_SWH_UP_LysA_10cm  10.2    0.483 6/29/2024 6:44:46 PM
## 2 202406_SWH_UP_LysA_20cm   8.06    0.404 6/29/2024 7:09:08 PM
## 3 202406_SWH_UP_LysA_45cm  14.7    0.541 6/29/2024 7:34:09 PM
## 4 202406_SWH_UP_LysB_10cm  20.5    0.736 6/29/2024 7:56:34 PM
## 5 202406_SWH_UP_LysB_20cm  17.9    0.895 6/29/2024 8:18:55 PM
## 6 202406_SWH_UP_LysB_45cm  29.7    0.955 6/29/2024 8:44:15 PM
```

Assessing Standard Curves

```
## Assess the Standard Curves

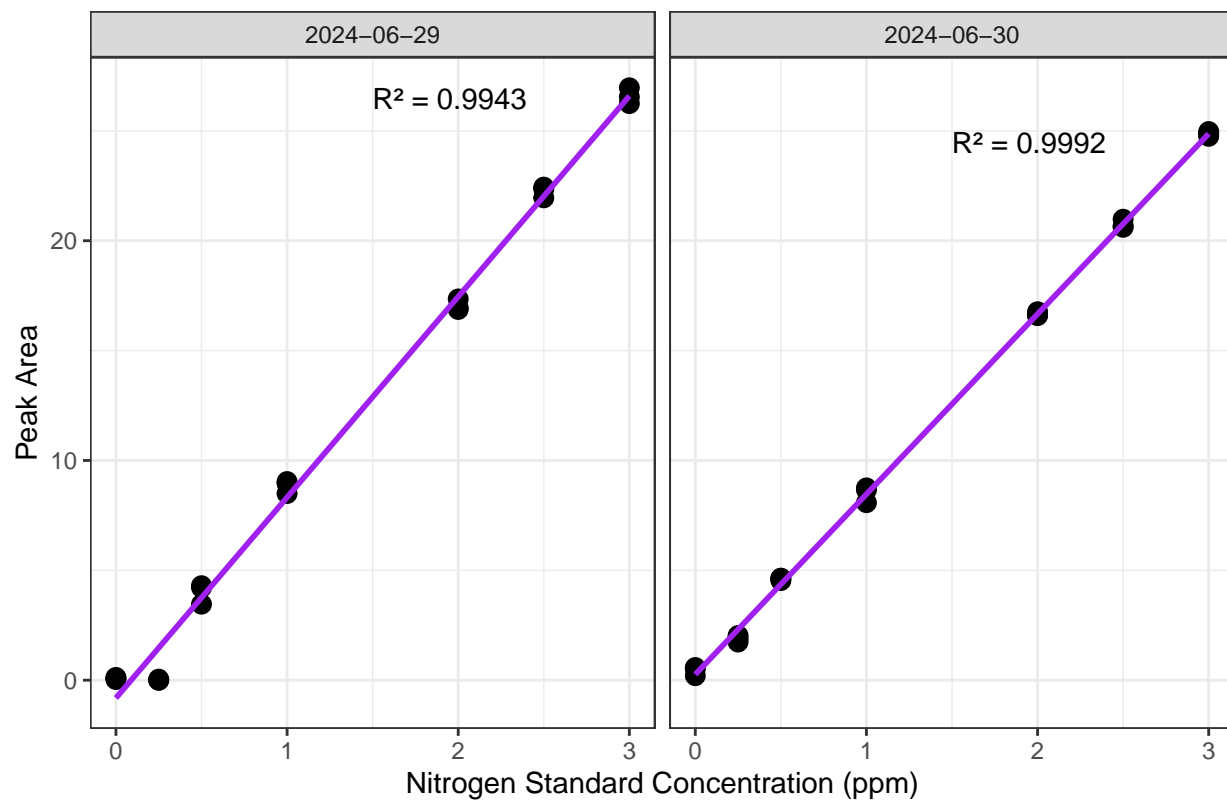
## New names:
## 'geom_smooth()' using formula = 'y ~ x'
## * `` -> '...18'
```

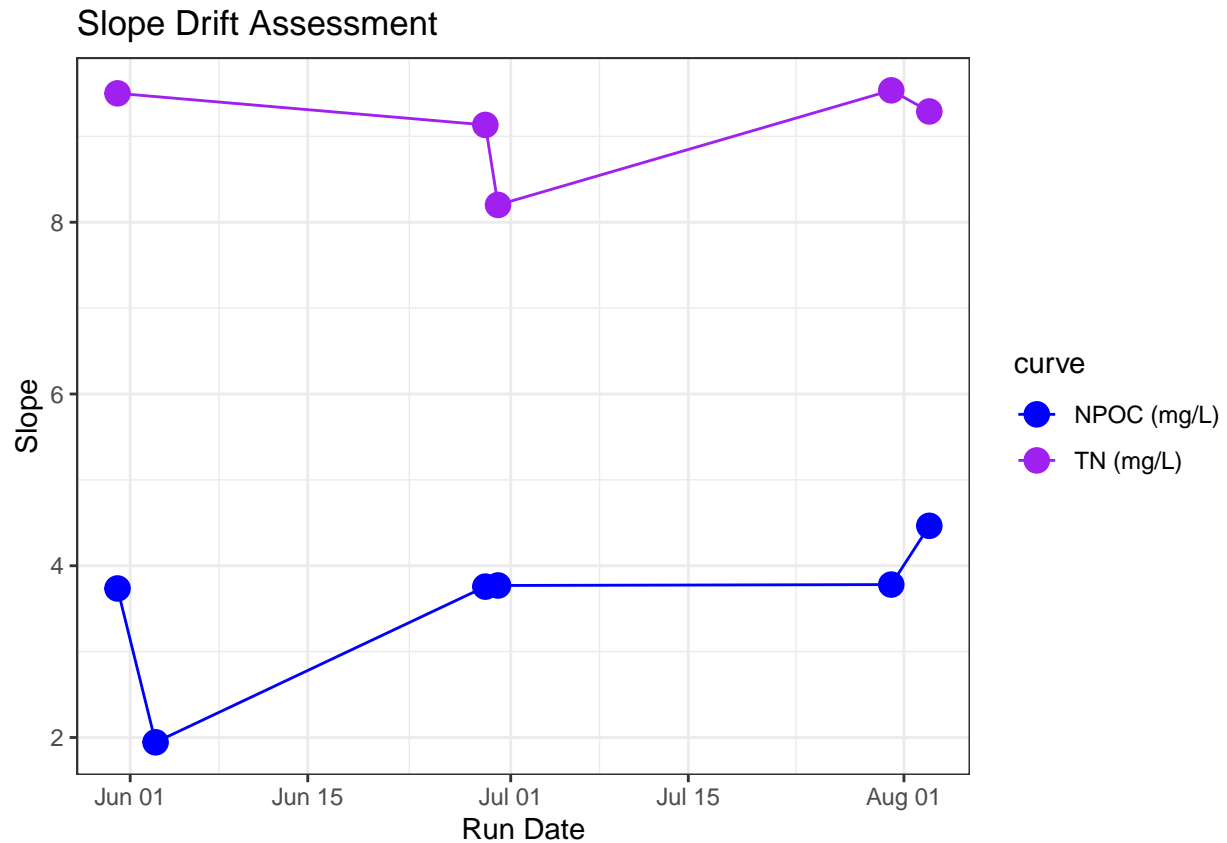
NPOC Std Curve by Date



```
## 'geom_smooth()' using formula = 'y ~ x'
```

TN Std Curve by Date





```
## [1] "NPOC Curve r2 GOOD"
```

```
## [1] "TN Curve r2 GOOD"
```

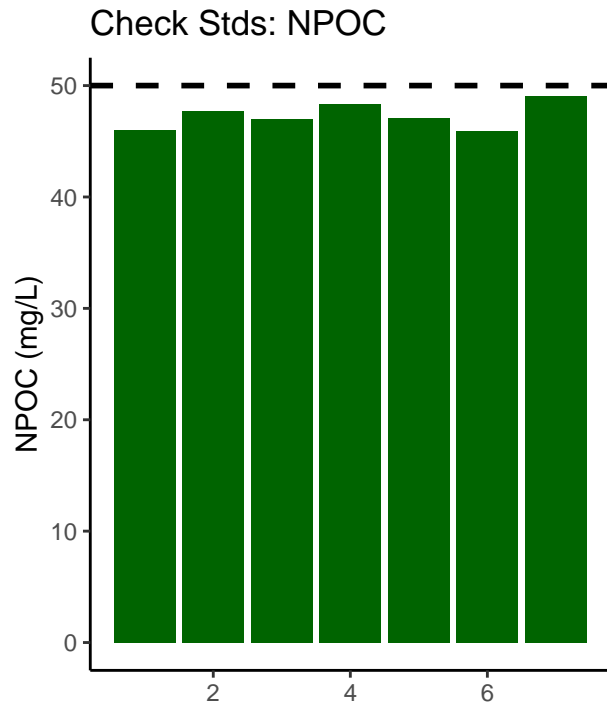
Assess Check Standards

```
## Assess the Check Standards
```

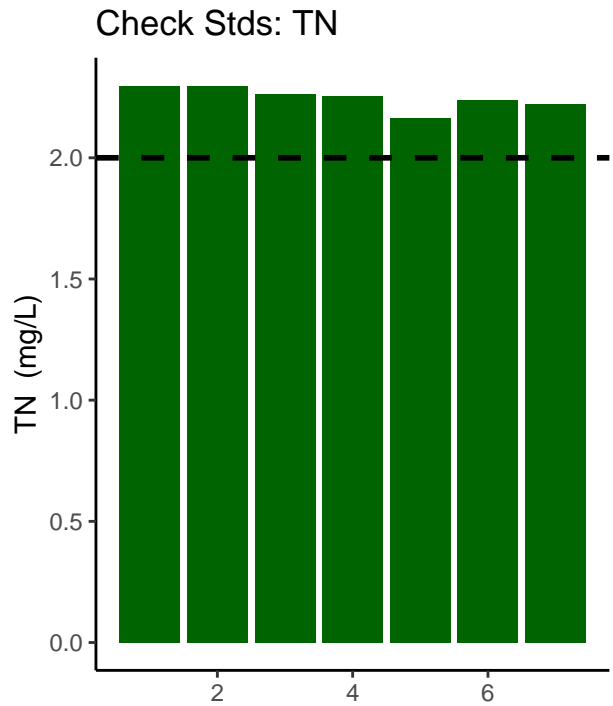
```
## New names:
## * ' ' -> '...14'
```

```
## [1] "Carbon Check Standard RSD within Range"
```

```
## [1] "Nitrogen Check Standard RSD within Range"
```



% Difference <10% ■ YES



% Difference <10% ■ YES

```
## [1] ">60% of Carbon Check Standards are within range of expected concentration"
```

```
## [1] ">60% of Nitrogen Check Standards are within range of expected concentration"
```

Assess Blanks

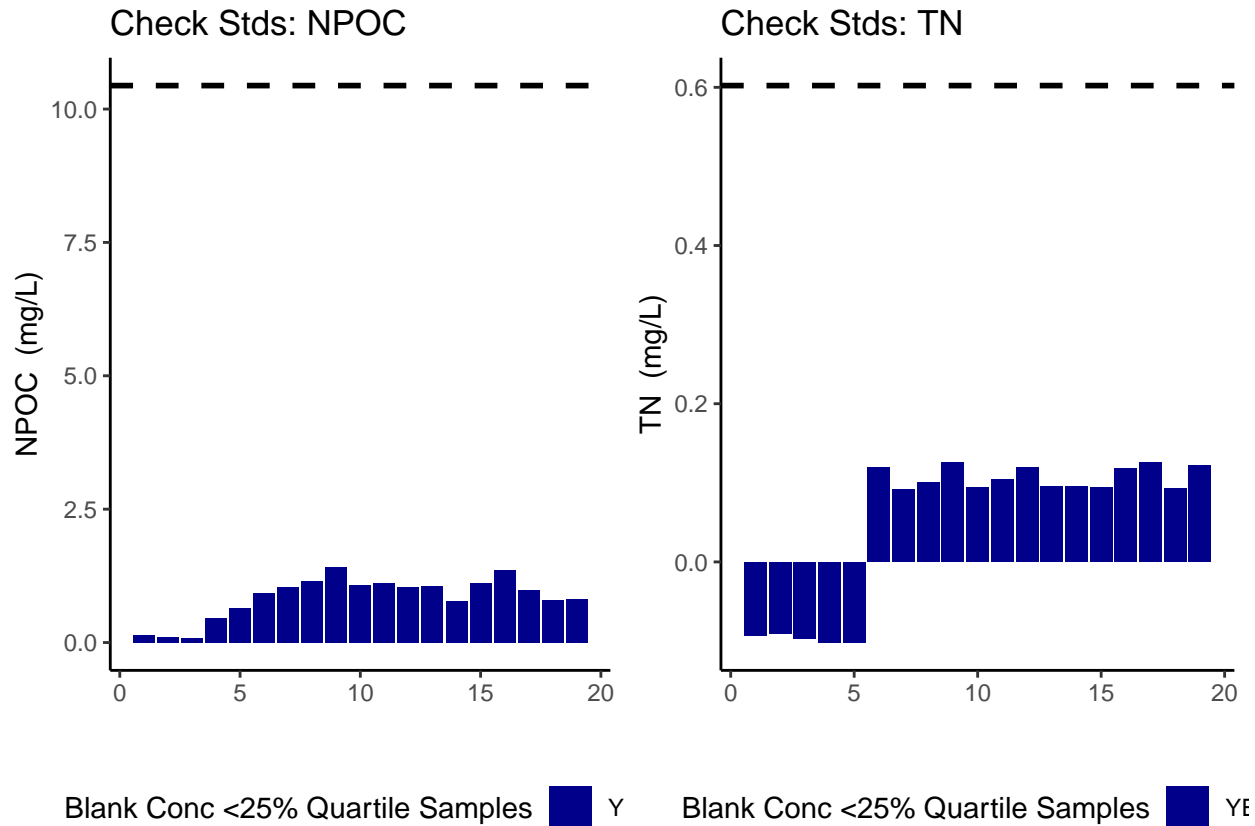
```
## Assess Blanks
```

```
## New names:
```

```
## * ' ' -> '...14'
```

```
## [1] ">60% of Carbon Blank concentrations are lower 25% quartile of samples"
```

```
## [1] ">60% of Nitrogen Blank concentrations are lower 25% quartile of samples"
```



```
## carbon blanks:
```

```
## [1] 0.8467211
```

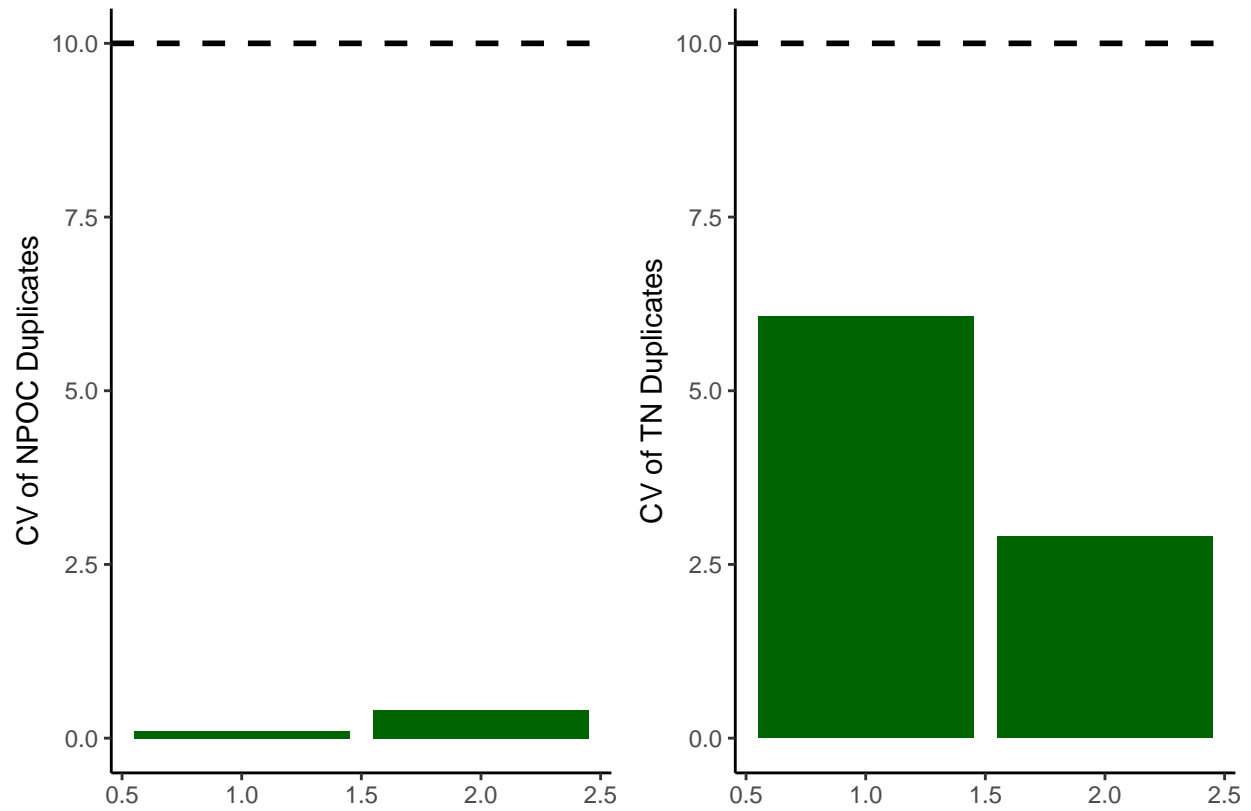
```
## nitrogen blanks:
```

```
## [1] 0.05334105
```

Assess Duplicates

```
## Assess Duplicates
```

```
## 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.
```

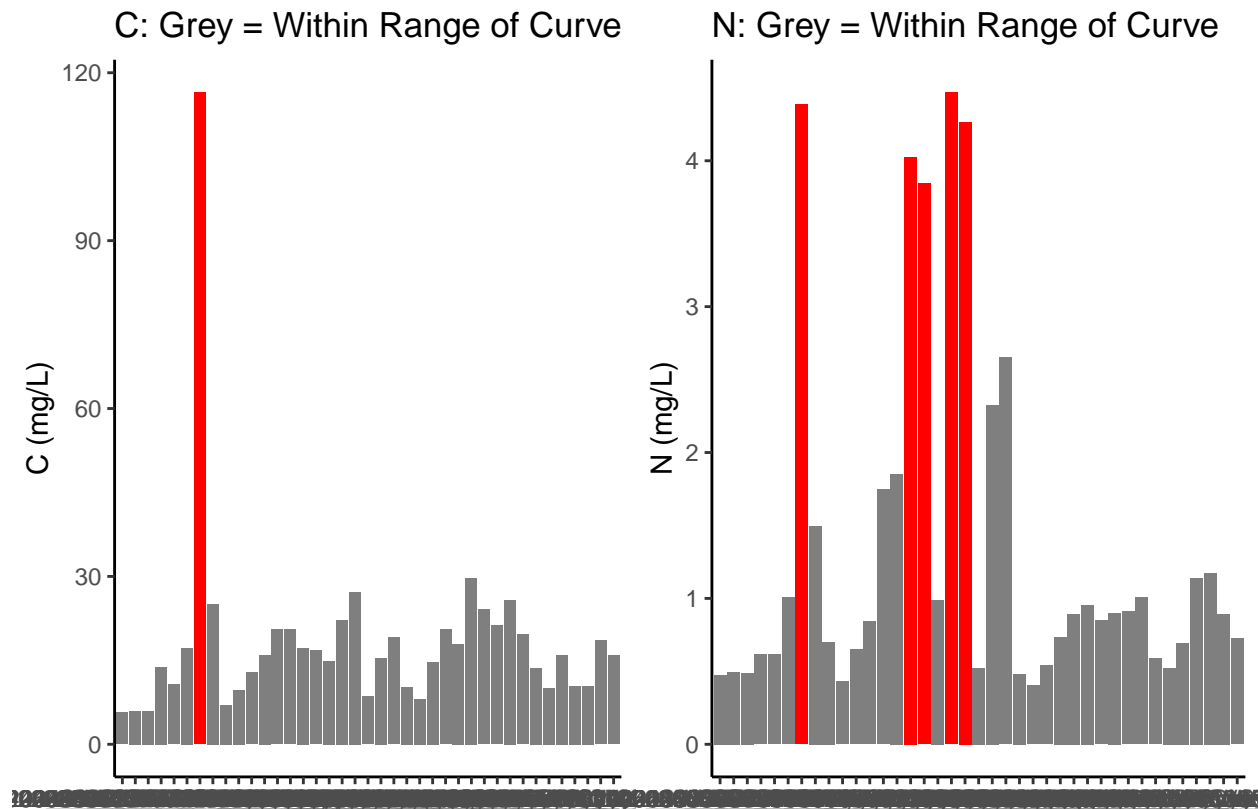


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

```
## [1] ">60% of Nitrogen Duplicates have a CV <10%"
```

Sample Flagging - Are samples Within the range of the curve?

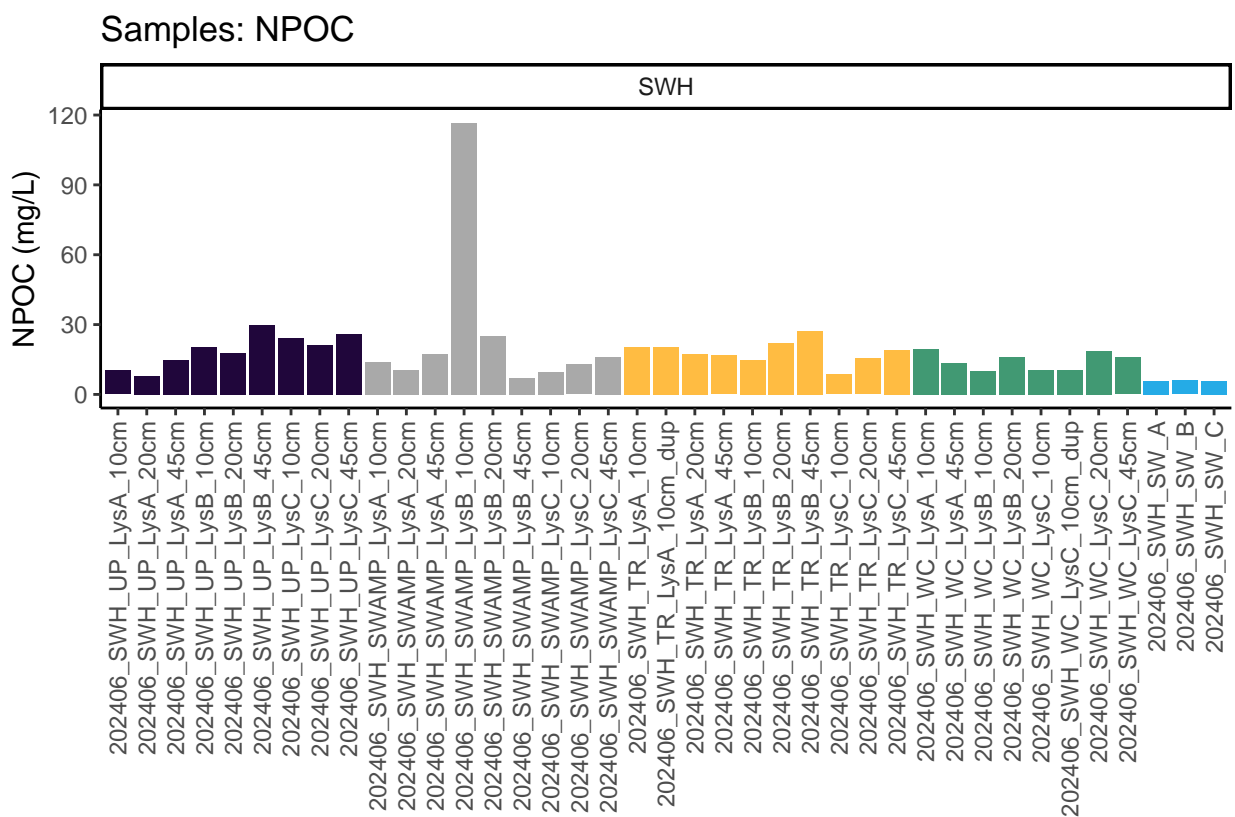
```
## Sample Flagging
```



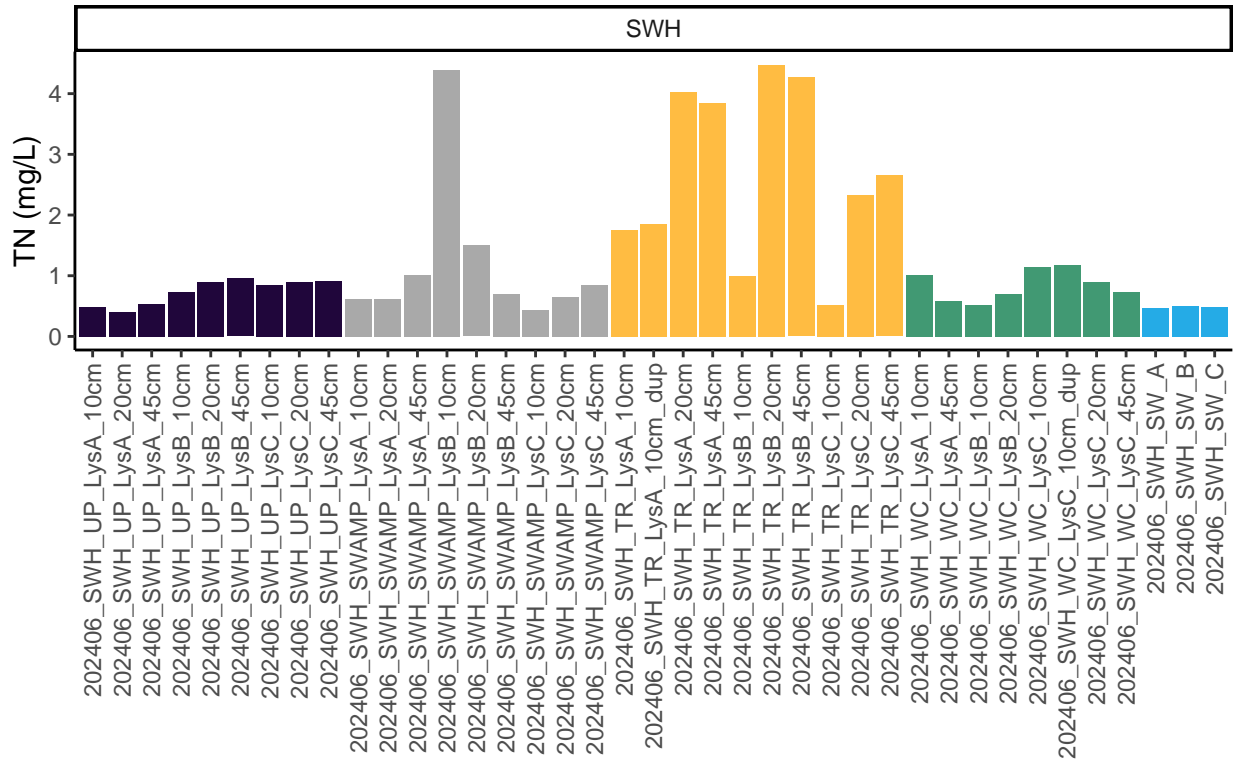
Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202406", "SWH", "UP", "LysA", "10cm"), c("202406", "SWH", :
## number of columns of result is not a multiple of vector length (arg 1)
```

Samples: TN



Convert data from mg/L to uMoles/L

Check to see if samples run match metadata & merge info

```
## Check Sample IDs with Metadata
```

```
## All sample IDs are present in metadata.
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 6 x 21
```

```
##   Project      Region Site  Zone Replicate Depth_cm Sample_ID   Year Month   Day
##   <chr>        <chr> <chr> <fct> <chr>      <int> <chr>      <int> <int> <int>
## 1 COMPASS: Sy~ CB    SWH  UP    A          10 202406_S~  2024    6    26
## 2 COMPASS: Sy~ CB    SWH  UP    A          20 202406_S~  2024    6    26
## 3 COMPASS: Sy~ CB    SWH  UP    A          45 202406_S~  2024    6    26
## 4 COMPASS: Sy~ CB    SWH  UP    B          10 202406_S~  2024    6    26
## 5 COMPASS: Sy~ CB    SWH  UP    B          20 202406_S~  2024    6    26
## 6 COMPASS: Sy~ CB    SWH  UP    B          45 202406_S~  2024    6    26
## # i 11 more variables: Time <chr>, Time_Zone <chr>, npoc_mgL <dbl>,
## #   npoc_uM <dbl>, npoc_flag <chr>, tdn_mgL <dbl>, tdn_uM <dbl>,
## #   tdn_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>
```

#end