COMPASS Synoptic CB Porewater: DOC

May 2024 Samples

2025-10-31

##Setup - Change things here & write any notes

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

Setup Information

```r
###### Run information - PLEASE CHANGE
  Date_Run = "6/03/24"  #Date that instrument was run
  Run_by = "Stephanie J. Wilson"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = "Second NPOC Curve did not look good. One duplicate out of range and some checks
  below expected concentration, but not by much - run okay."  #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_50mgC_2mgN"  #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_202405.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_202405_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_202405.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 202405_SWH_UP_LysA_10cm      14.5   0.373 5/31/2024 9:08:46 PM
## 2 202405_SWH_UP_LysA_20cm      17.5   0.525 5/31/2024 9:33:40 PM
## 3 202405_SWH_UP_LysA_45cm      13.6   0.395 5/31/2024 9:58:11 PM
## 4 202405_SWH_UP_LysB_10cm      29.9   0.626 5/31/2024 10:23:37 PM
## 5 202405_SWH_UP_LysB_20cm      52.7   1.33  5/31/2024 10:49:45 PM
## 6 202405_SWH_UP_LysC_10cm      27     0.616 5/31/2024 11:06:37 PM
```
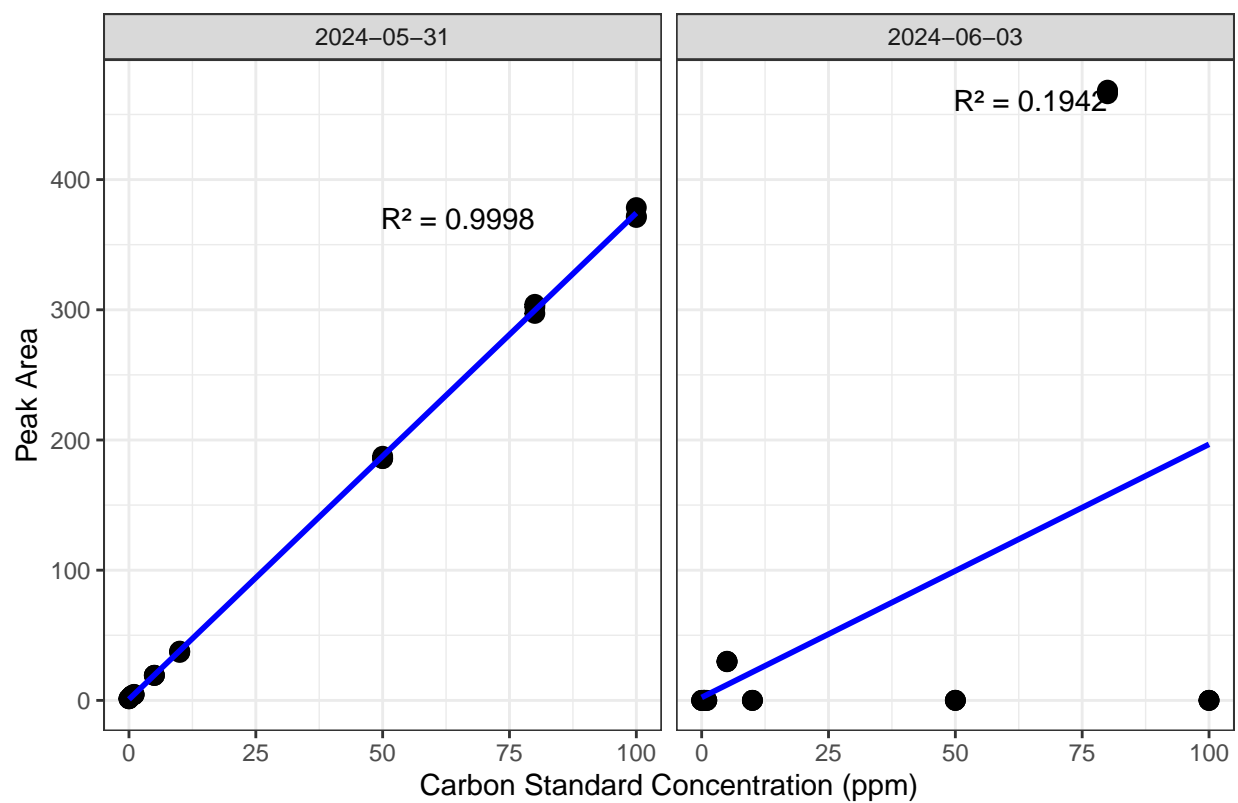
Assessing Standard Curves

```
## Assess the Standard Curves
```

```
## New names:
## * `` -> `...18`
```
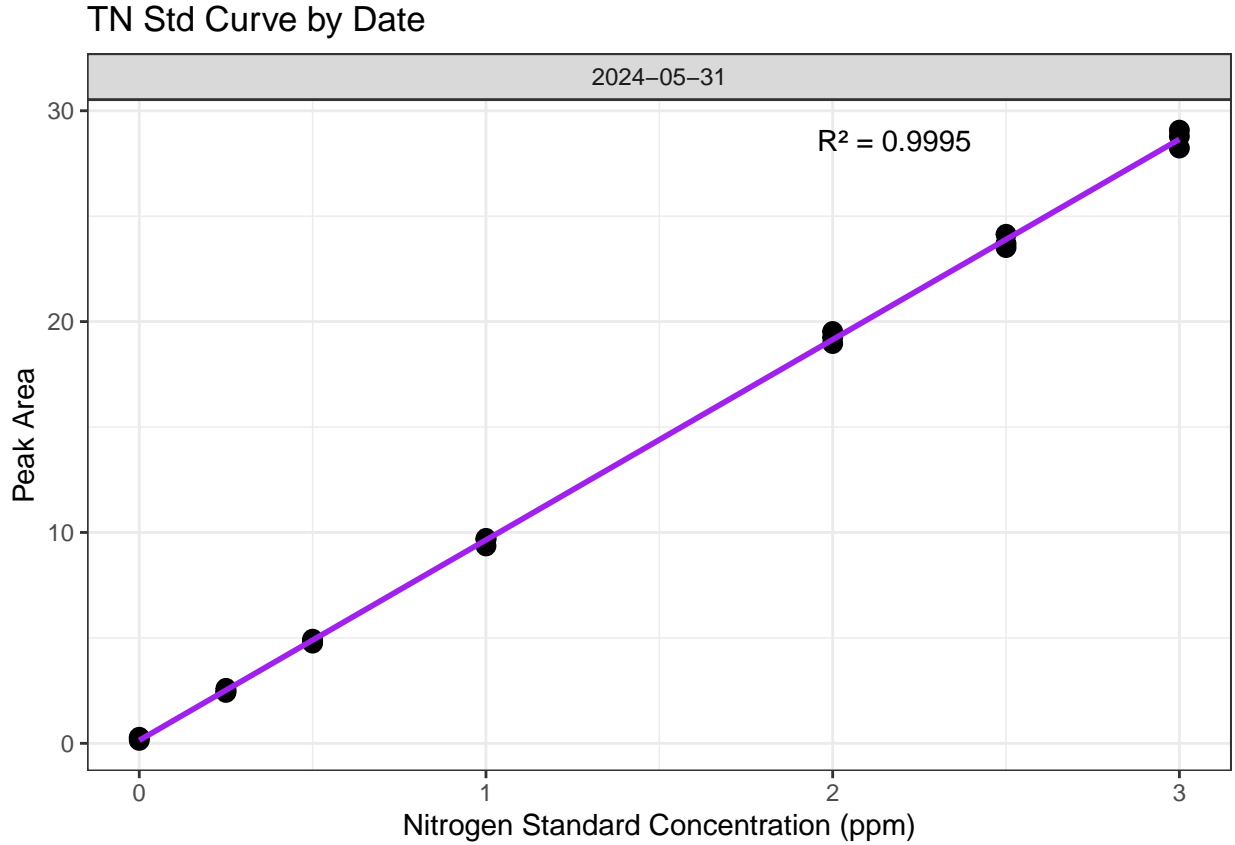
```
## Warning: One or more parsing issues, call `problems()` on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)
```
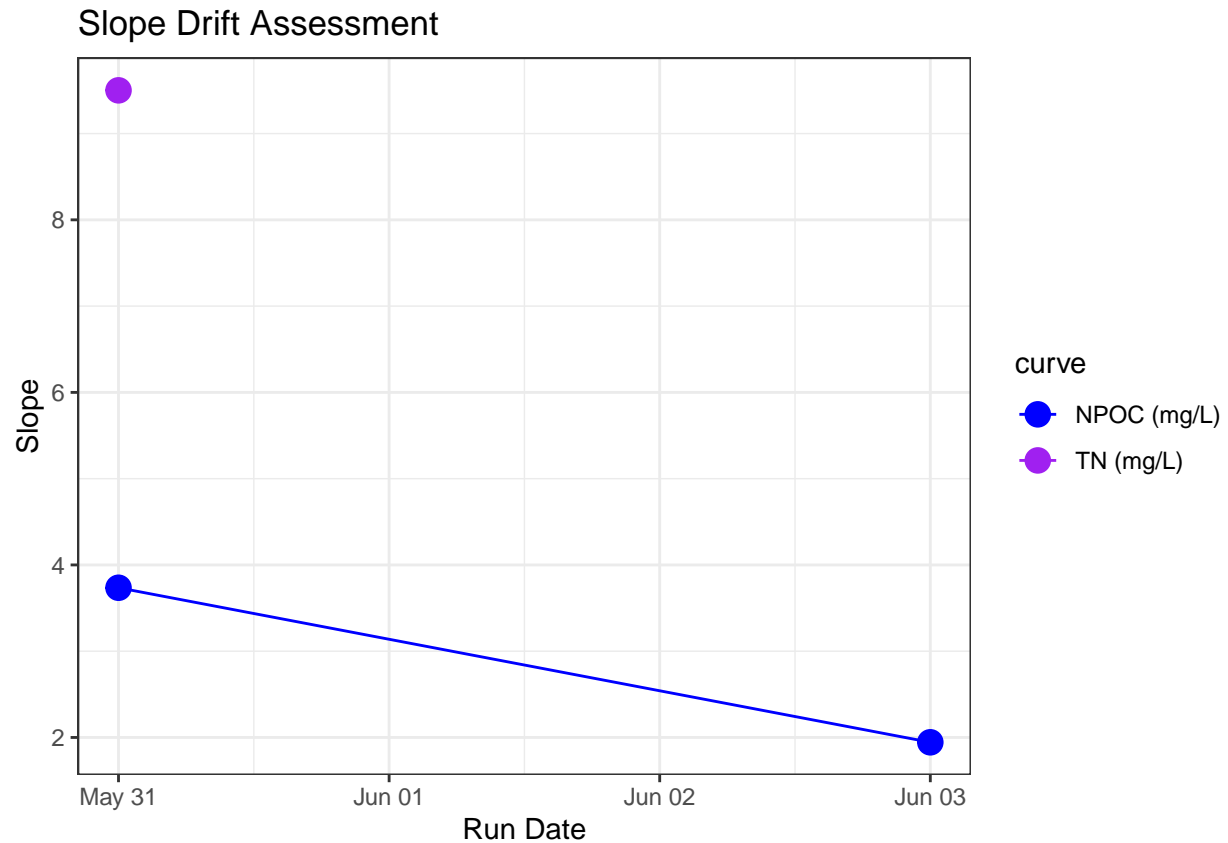
```
## `geom_smooth()` using formula = 'y ~ x'
```

NPOC Std Curve by Date


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

TN Std Curve by Date

2024−05−31

R² = 0.9995

Peak Area

Nitrogen Standard Concentration (ppm)

Slope Drift Assessment


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

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

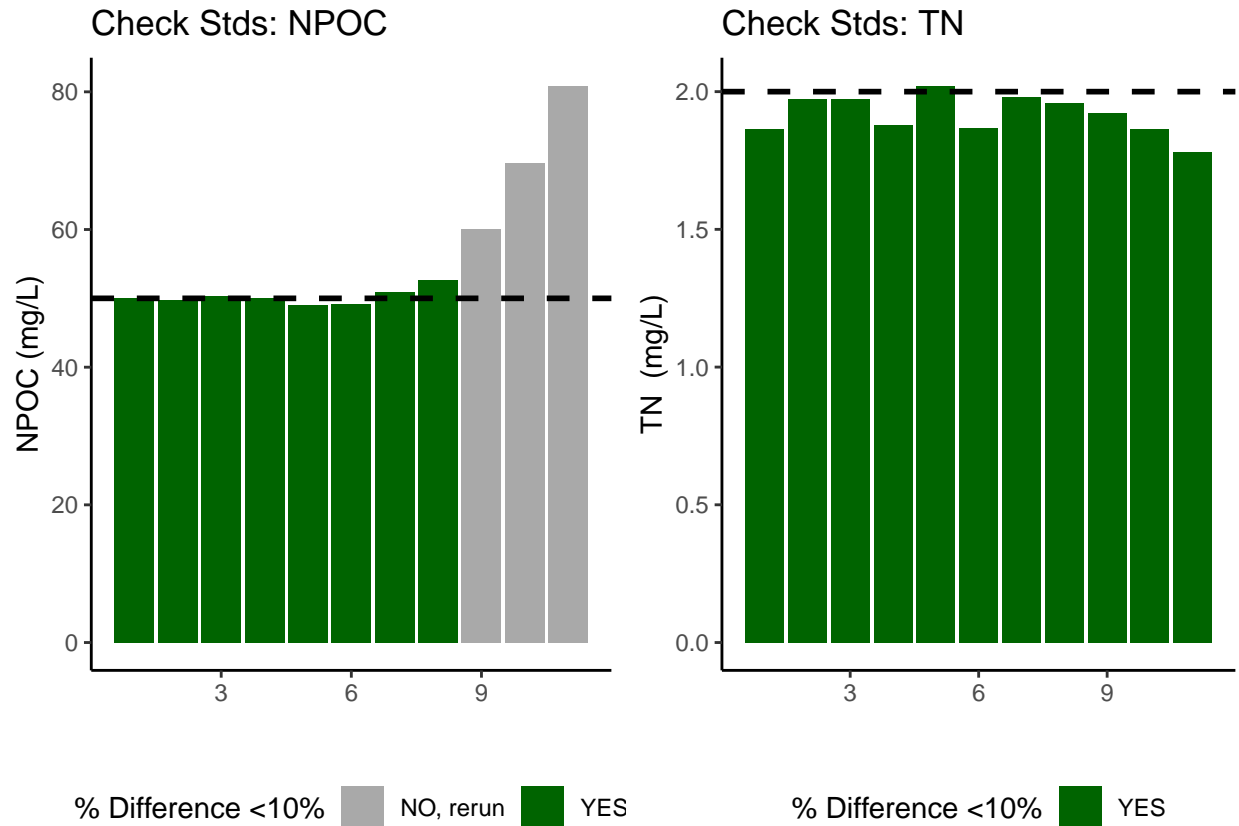## Assess Check Standards

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

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

```
## [1] "Carbon CHECK STANDARD RSD TOO HIGH - REASSESS"
```

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

Check Stds: NPOC — Check Stds: TN

% Difference <10%   NO, rerun   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"
```
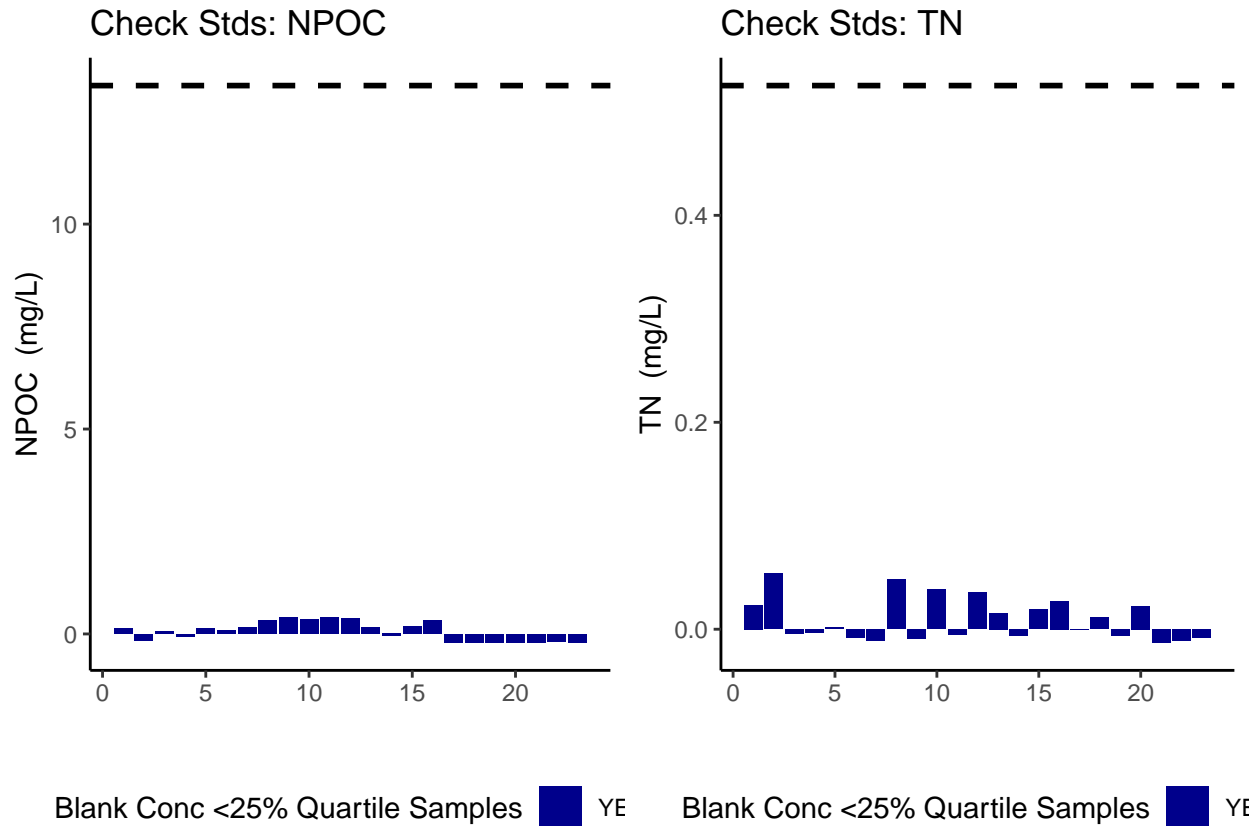
Assess Blanks

```
## 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"
```

Check Stds: NPOC

NPOC (mg/L)

Check Stds: TN

TN (mg/L)

Blank Conc <25% Quartile Samples ■ YE

Blank Conc <25% Quartile Samples ■ YE

```
## carbon blanks:

## [1] 0.06258217

## nitrogen blanks:

## [1] 0.009127391
```
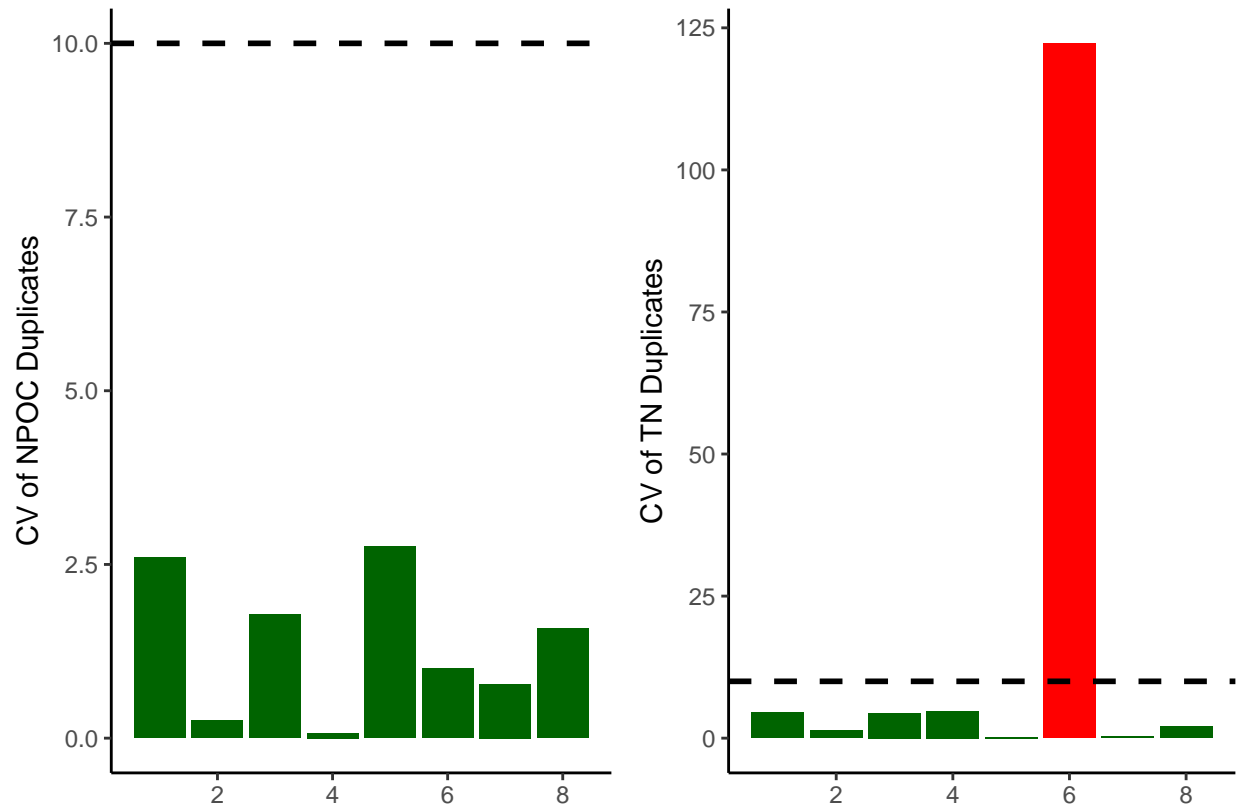
Assess Duplicates

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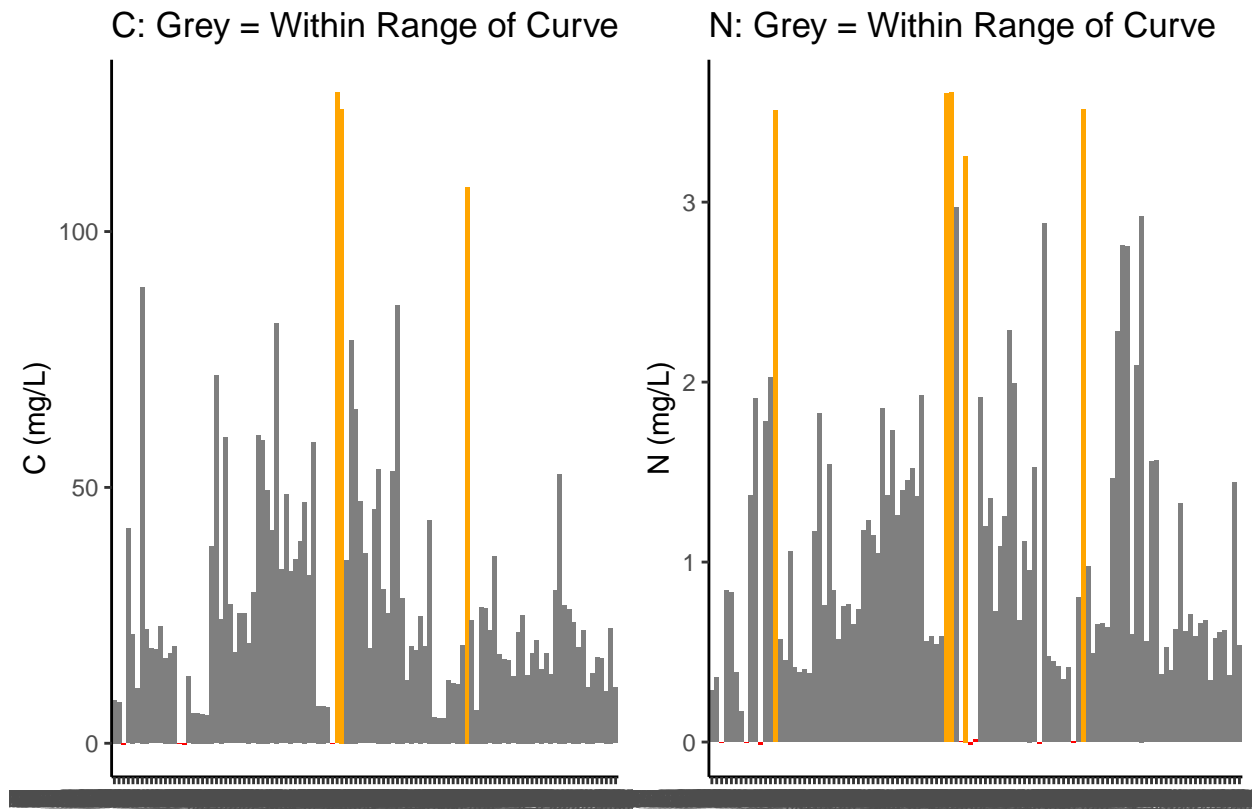
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

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

```
## Sample Flagging
```

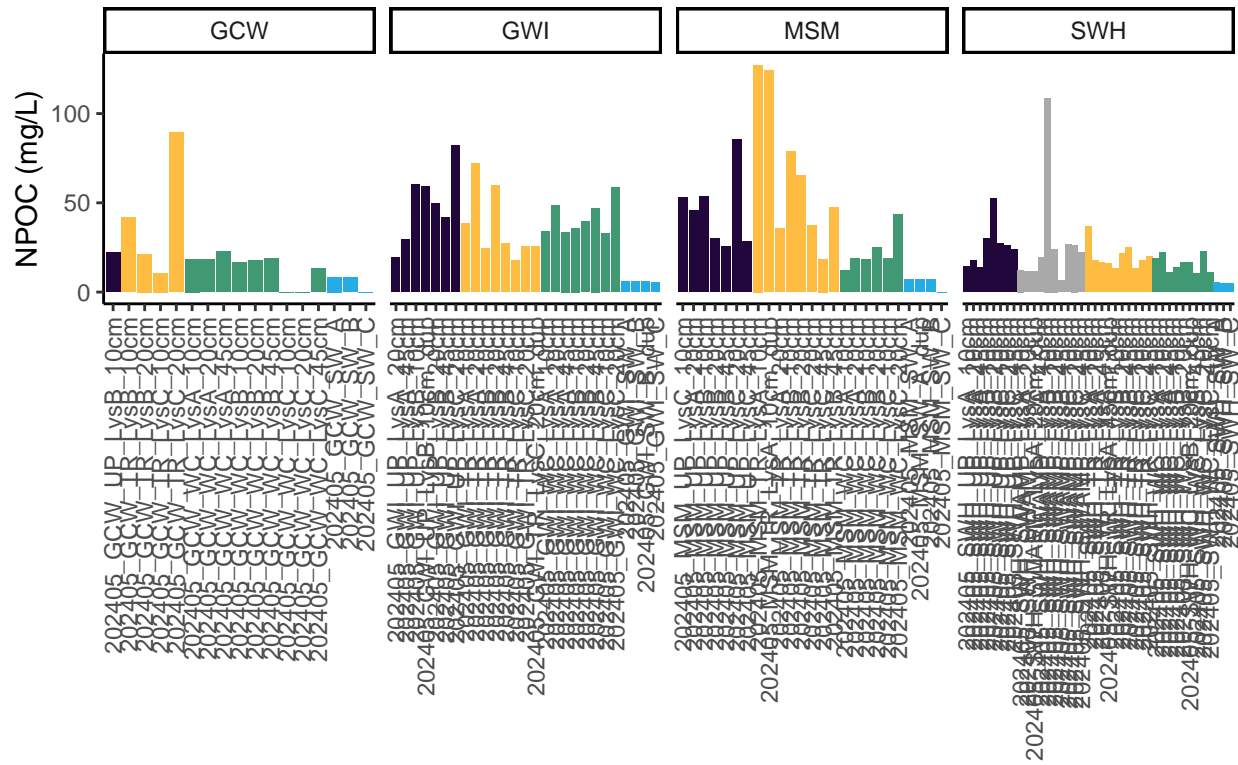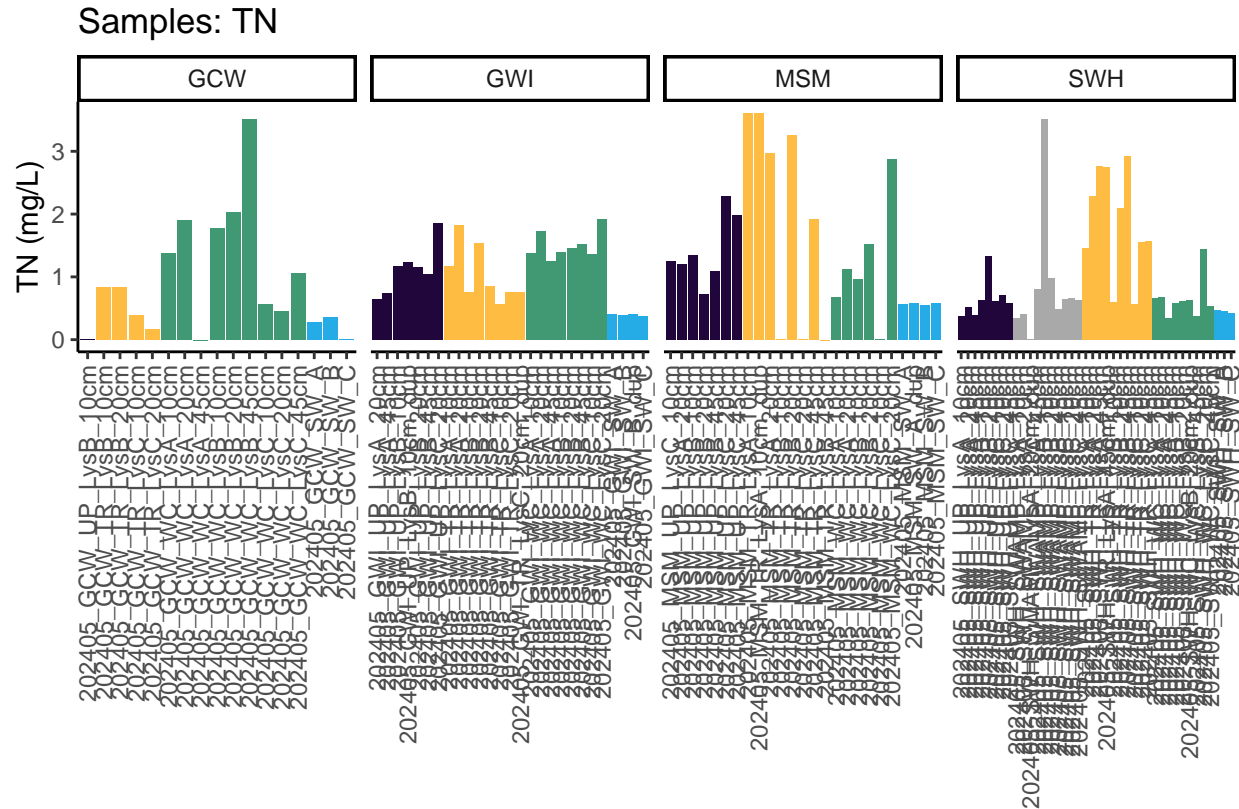C: Grey = Within Range of Curve   N: Grey = Within Range of Curve

Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202405", "SWH", "UP", "LysA", "10cm"), c("202405", "SWH", :
## number of columns of result is not a multiple of vector length (arg 1)
```

Samples: NPOC

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 202405_S~  2024     5    15
## 2 COMPASS: Sy~ CB     SWH   UP    A               20 202405_S~  2024     5    15
## 3 COMPASS: Sy~ CB     SWH   UP    A               45 202405_S~  2024     5    15
## 4 COMPASS: Sy~ CB     SWH   UP    B               10 202405_S~  2024     5    15
## 5 COMPASS: Sy~ CB     SWH   UP    B               20 202405_S~  2024     5    15
## 6 COMPASS: Sy~ CB     SWH   UP    C               10 202405_S~  2024     5    15
## # 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