COMPASS: TEMPEST Discrete DOC Data QAQC

August 2024 run 1

2025-06-23

Run Information

```
#identify which section you are in
cat("Run Information")
```

```
## Run Information
```

```
#a link to the Gitbook or whatever protocol you are using for this analysis
  #steph will add this soon

#anything that needs to be changed do this in the first chunk
  Date_Run = "09/05/24"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = " "

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2024/TMP_202408_run1.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2024/TMP_202408_run1_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2024/TMP_PW_DOC_Processed_202408.csv"

#check standard concentrations - Update if running different checks:
   chk_std_c = 30
   chk_std_n = 2.5

#Log path
    Log_path = "tmp_doc_raw_data_2024/COMPASS_TMP_TOCTN_QAQClog_2024.csv"
```

Setup

Pull in active porewater tracking inventory sheet

```
## File already exists. No download needed.
```

Import Data Functions

Import Sample Data

```
## Import Sample Data
```

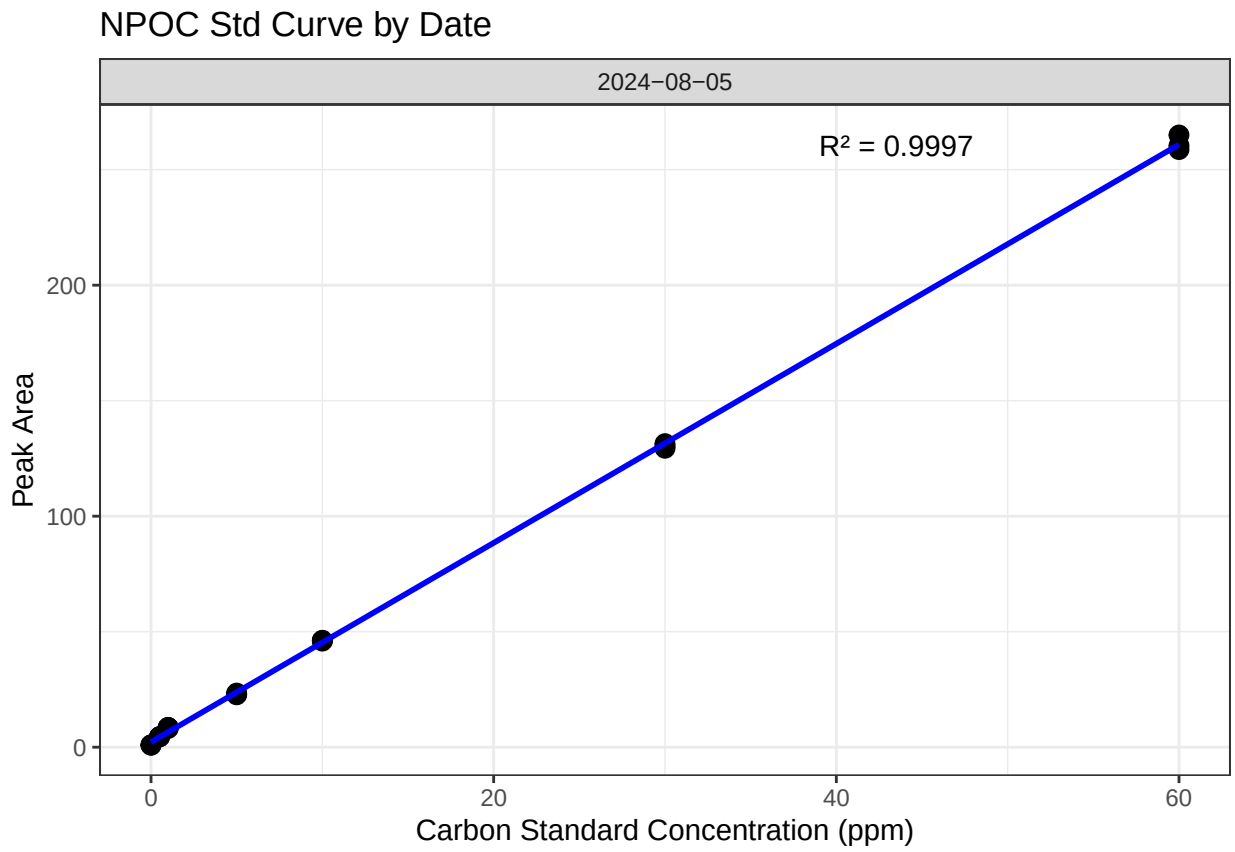
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 6 x 4
##   sample_name        npoc_raw tdn_raw run_datetime
##   <chr>                 <dbl>   <dbl> <chr>
## 1 TMP_FW_I5_20240808    28.8    4.37  8/9/2024 6:58:39 AM
## 2 TMP_SW_B4_20240805    10.8    0.623 8/9/2024 7:26:19 AM
## 3 TMP_SW_C3_20240802     8.80   1.03  8/9/2024 7:53:49 AM
## 4 TMP_SW_C3_20240805     9.92   0.639 8/9/2024 8:21:24 AM
## 5 TMP_SW_D5_20240802     4.01   0.466 8/9/2024 8:44:47 AM
## 6 TMP_SW_D5_20240805     6.32   0.471 8/9/2024 9:12:18 AM
```

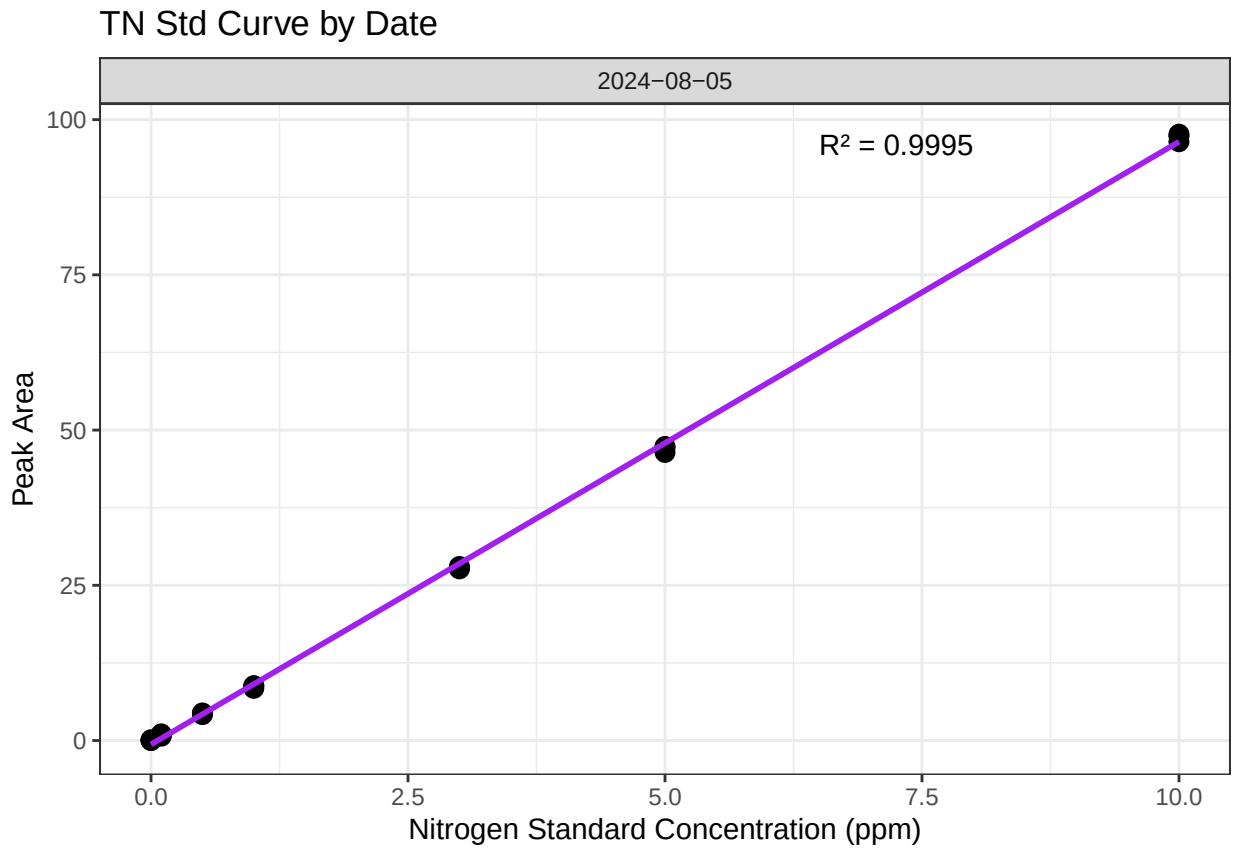
Assessing standard Curves

```
## Assess the Standard Curve
```

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

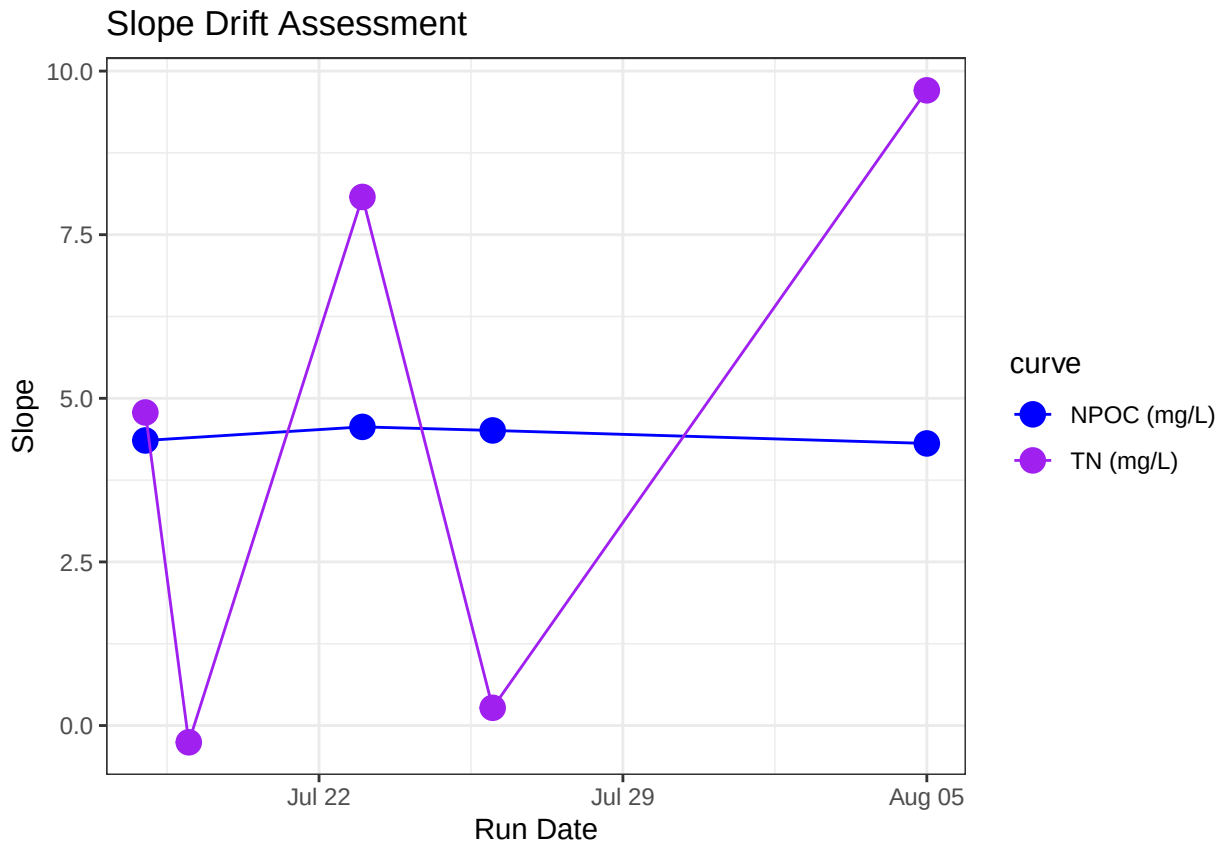



```
## ‘geom_smooth()‘ using formula = ’y ~ x’
```




```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## (`geom_point()`).
```

```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## (`geom_line()`).
```




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

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

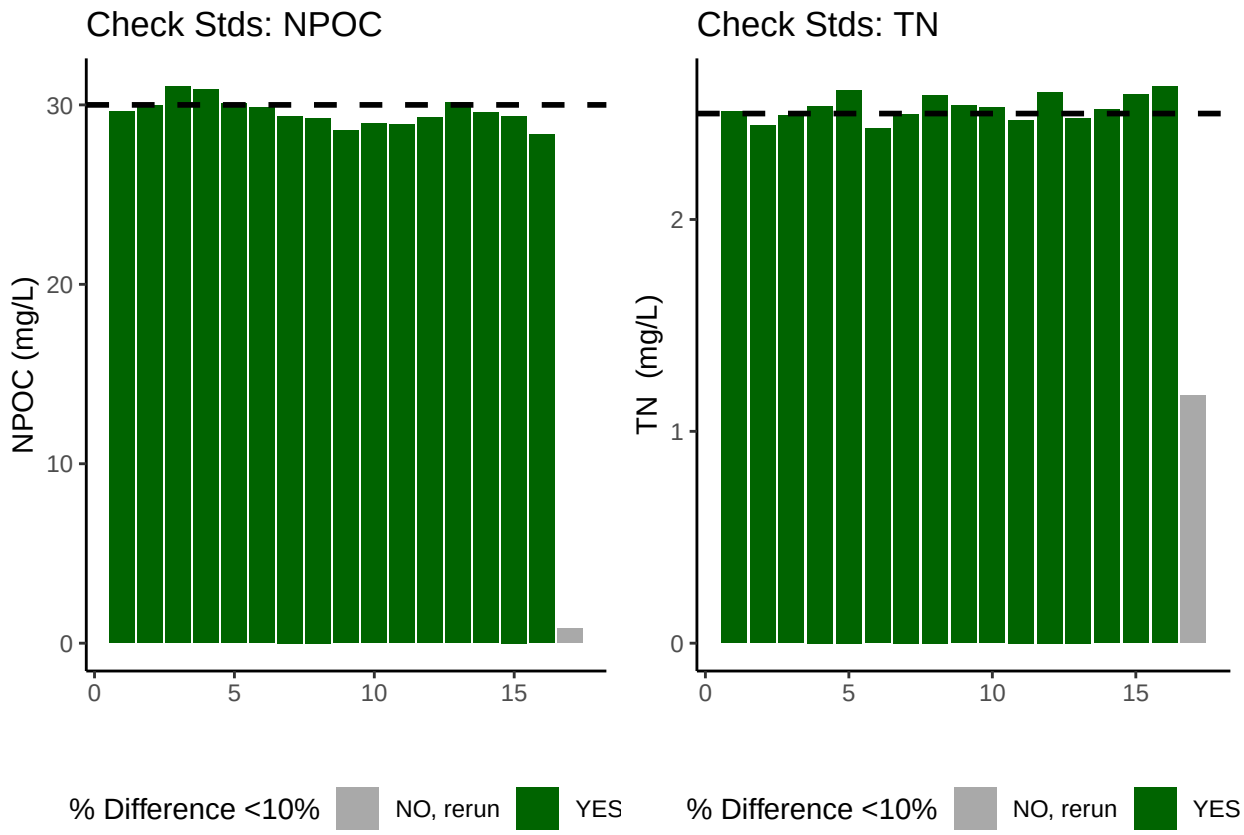
Assess Check Standards

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

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

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

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




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

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

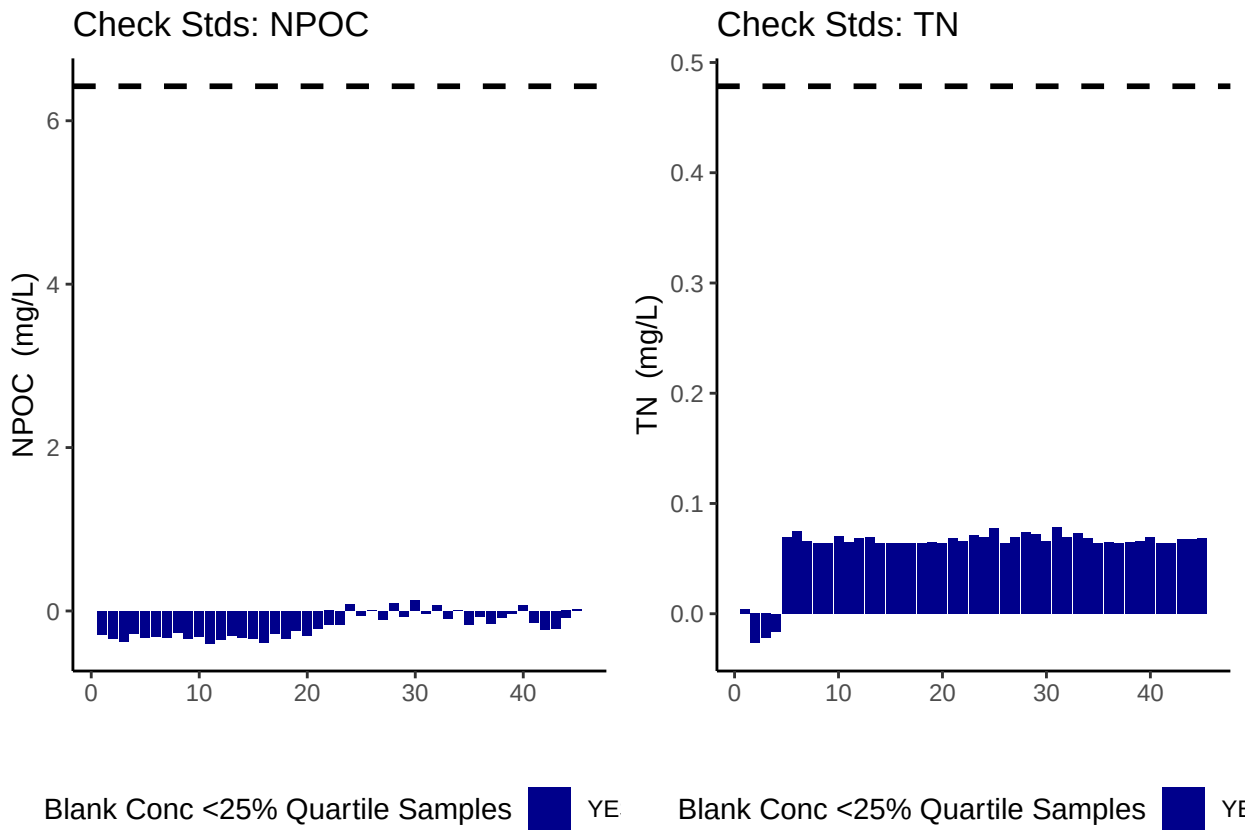
Assess Blanks

```
## Assess Blanks
```

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

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

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




```
## carbon blanks:
```

```
## [1] -0.1773447
```

```
## nitrogen blanks:
```

```
## [1] 0.060252
```

Assess Duplicates - if there are any

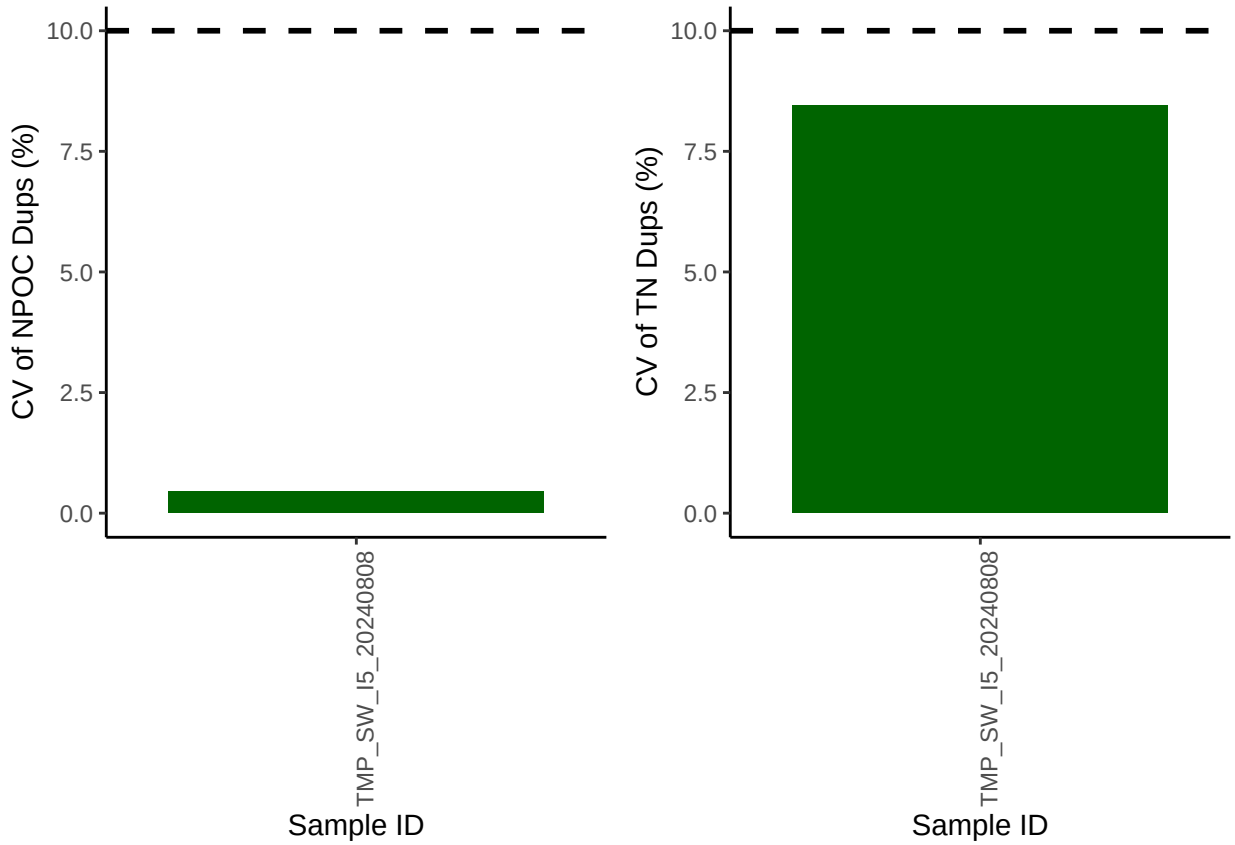
```
## Assess Duplicates

## # A tibble: 1 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_SW_I5_20240808         11.7       0.974

##          sample_name npoc_raw tdn_raw         run_datetime npoc_flag tdn_flag
## 1 TMP_SW_I5_20240808    11.67  0.8969 8/9/2024 10:58:21 AM
##   npoc_raw_dup tdn_raw_dup
## 1        11.72      0.9736

##          sample_name npoc_raw tdn_raw         run_datetime npoc_flag tdn_flag
## 1 TMP_SW_I5_20240808    11.67  0.8969 8/9/2024 10:58:21 AM
##   npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv
## 1        11.72      0.9736     0.452783               YES    8.453385
##   tdn_dups_cv_flag
## 1              YES

## 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.
```

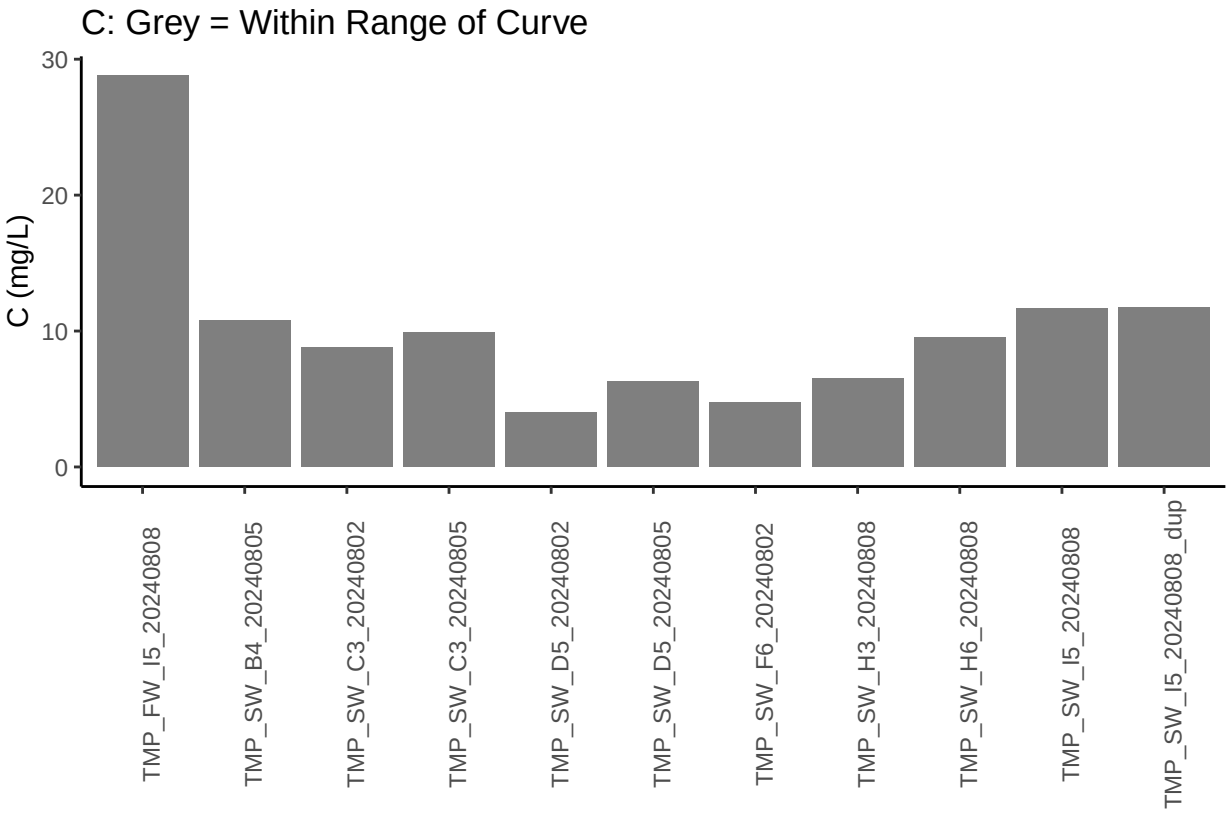


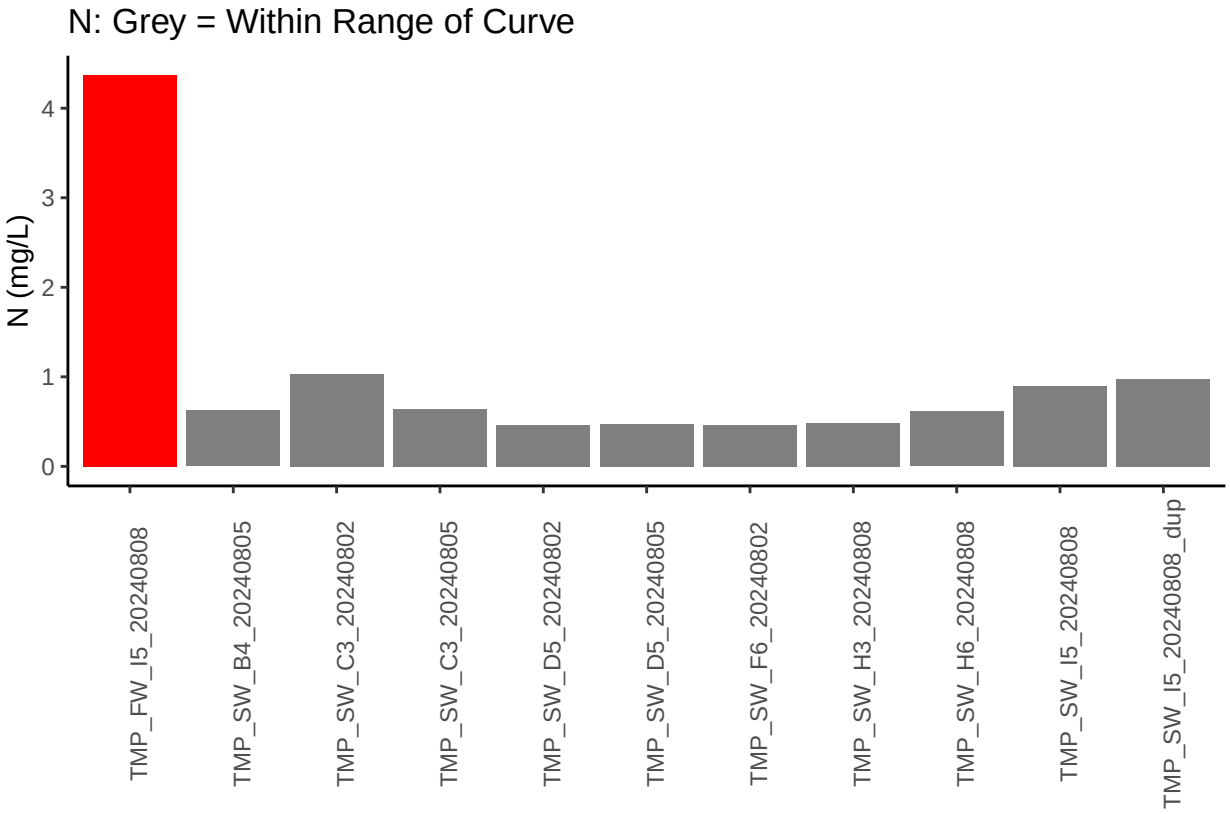
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

```
## Sample Flagging
```




N: Grey = Within Range of Curve
N (mg/L)
0
1
2
3
4
TMP_FW_I5_20240808
TMP_SW_B4_20240805
TMP_SW_C3_20240802
TMP_SW_C3_20240805
TMP_SW_D5_20240802
TMP_SW_D5_20240805
TMP_SW_F6_20240802
TMP_SW_H3_20240808
TMP_SW_H6_20240808
TMP_SW_I5_20240808
TMP_SW_I5_20240808_dup

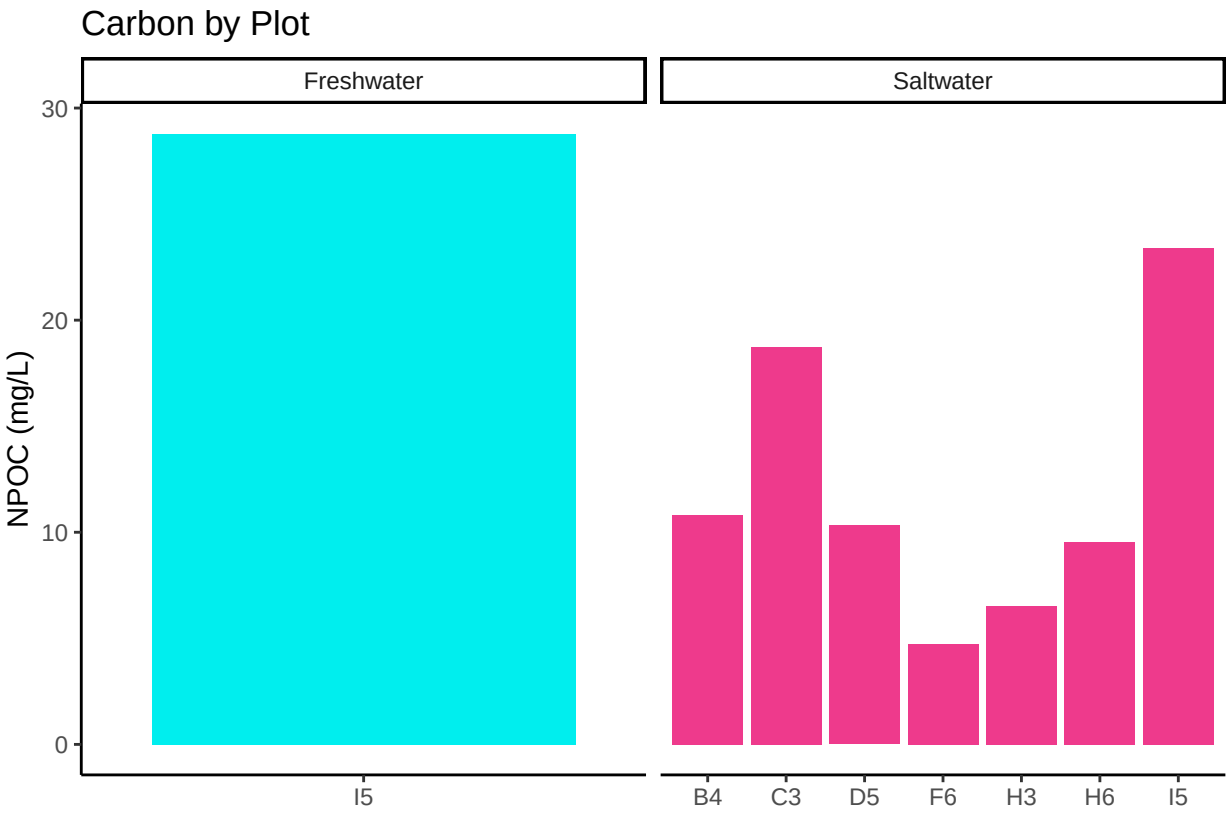
Visualize Data by Plot

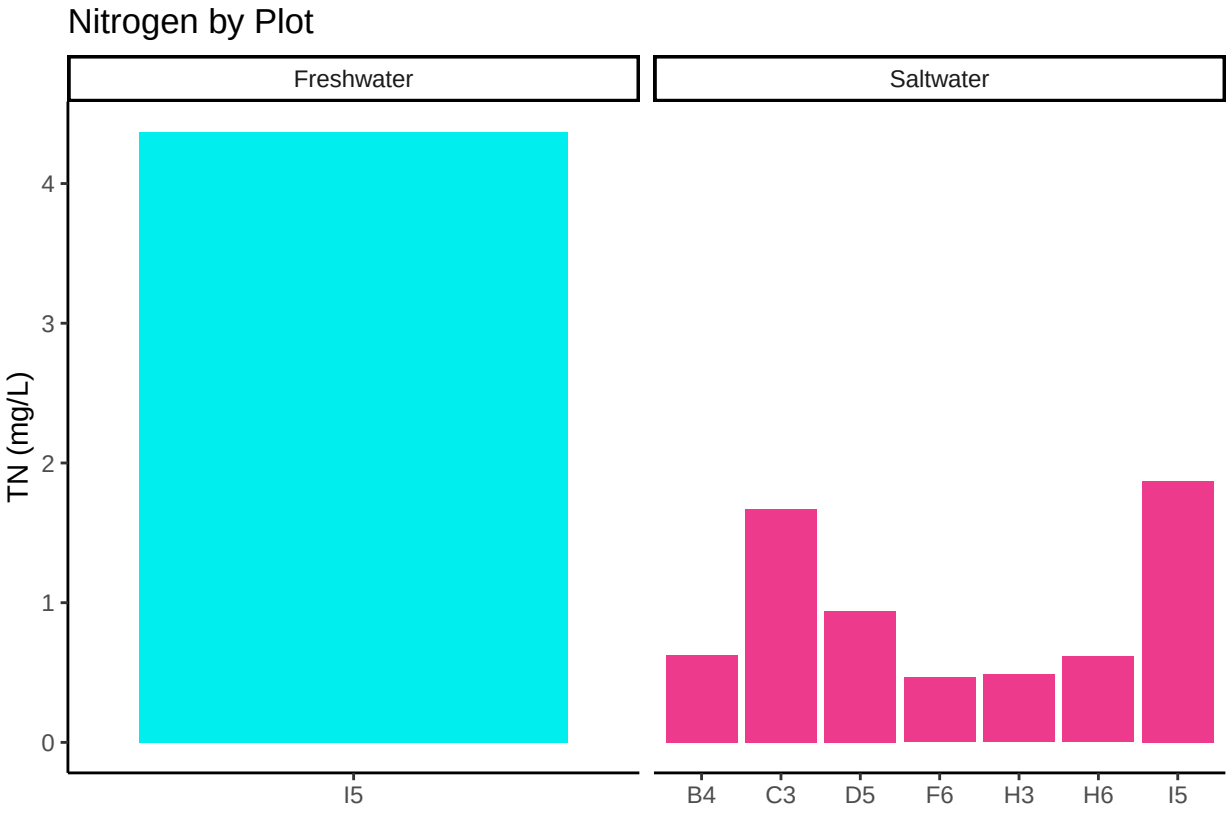
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "FW", "I5", "20240808"), c("TMP", "SW", "B4", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code Plot Grid_Square     Date Extra
## 1       TMP   FW          I5 20240808   TMP
## 2       TMP   SW          B4 20240805   TMP
## 3       TMP   SW          C3 20240802   TMP
## 4       TMP   SW          C3 20240805   TMP
## 5       TMP   SW          D5 20240802   TMP
## 6       TMP   SW          D5 20240805   TMP
```

```
##   Site_Code Plot Grid_Square     Date Extra        sample_name npoc_raw tdn_raw
## 1       TMP   FW          I5 20240808   TMP TMP_FW_I5_20240808   28.770  4.3680
## 2       TMP   SW          B4 20240805   TMP TMP_SW_B4_20240805   10.800  0.6228
## 3       TMP   SW          C3 20240802   TMP TMP_SW_C3_20240802    8.801  1.0310
## 4       TMP   SW          C3 20240805   TMP TMP_SW_C3_20240805    9.924  0.6386
## 5       TMP   SW          D5 20240802   TMP TMP_SW_D5_20240802    4.006  0.4656
## 6       TMP   SW          D5 20240805   TMP TMP_SW_D5_20240805    6.315  0.4707
##          run_datetime npoc_flag              tdn_flag
## 1 8/9/2024 6:58:39 AM           value above cal curve
## 2 8/9/2024 7:26:19 AM
## 3 8/9/2024 7:53:49 AM
## 4 8/9/2024 8:21:24 AM
## 5 8/9/2024 8:44:47 AM
## 6 8/9/2024 9:12:18 AM
```


Carbon by Plot
Freshwater
Saltwater
NPOC (mg/L)
30
20
10
0
I5
B4
C3
D5
F6
H3
H6
I5


Nitrogen by Plot
Freshwater
Saltwater
TN (mg/L)
0
1
2
3
4
I5
B4
C3
D5
F6
H3
H6
I5

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 10 x 2
##    sample_name        metadata_recorded
##    <chr>              <lgl>
##  1 TMP_FW_I5_20240808 TRUE
##  2 TMP_SW_B4_20240805 TRUE
##  3 TMP_SW_C3_20240802 TRUE
##  4 TMP_SW_C3_20240805 TRUE
##  5 TMP_SW_D5_20240802 TRUE
##  6 TMP_SW_D5_20240805 TRUE
##  7 TMP_SW_F6_20240802 TRUE
##  8 TMP_SW_H3_20240808 TRUE
##  9 TMP_SW_H6_20240808 TRUE
## 10 TMP_SW_I5_20240808 TRUE
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 6 x 21
##   Project        plot  grid  Depth_cm sample_type Vial_ID date  npoc_mgL npoc_uM
##   <chr>          <chr> <chr>    <dbl> <chr>       <chr>   <chr>    <dbl>   <dbl>
## 1 COMPASS: TEMP~ FW    I5          15 DOC         FW_I5_~ 2024~    28.8    2398.
## 2 COMPASS: TEMP~ SW    B4          15 DOC         SW_B4_~ 2024~    10.8     900
## 3 COMPASS: TEMP~ SW    C3          15 DOC         SW_C3_~ 2024~     8.80    733.
## 4 COMPASS: TEMP~ SW    C3          15 DOC         SW_C3_~ 2024~     9.92    827
## 5 COMPASS: TEMP~ SW    D5          15 DOC         SW_D5_~ 2024~     4.01    334.
## 6 COMPASS: TEMP~ SW    D5          15 DOC         SW_D5_~ 2024~     6.32    526.
## # i 12 more variables: npoc_flag <chr>, tdn_mgL <dbl>, tdn_uM <dbl>,
## #   tdn_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>,
## #   Evacuation_date_YYYMMDD <dbl>, Collection_Date_YYYYMMDD <dbl>,
## #   Collection_Start_Time_24hrs <dbl>, Collection_End_Time_24hrs <dbl>,
## #   EST_EDT <chr>, Volume_mL <dbl>
```

#end