COMPASS: TEMPEST Discrete DOC Data QAQC

July 2025

2025-10-02

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 = "07/03/25"
  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_2025/TMP_202507.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202507_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202507.csv"

#check standard concentrations - Update if running different checks:
   chk_std_c = 50
   chk_std_n = 2

#Log path
    Log_path = "tmp_doc_raw_data_2025/COMPASS_TMP_TOCTN_QAQClog_2025.csv"
```

Setup

Pull in active porewater tracking inventory sheet

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

Import Data Functions

Import Sample Data

```
## Import Sample Data
```

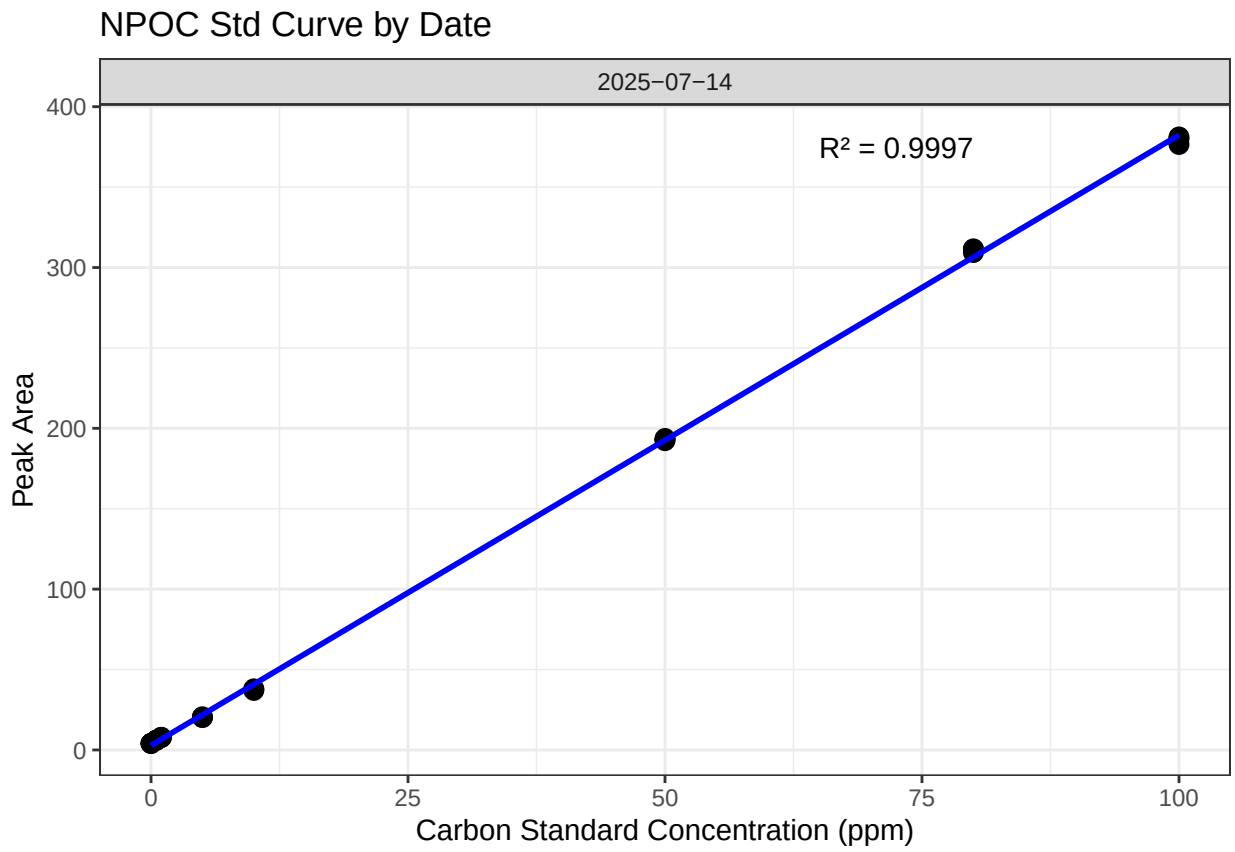
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 6 x 4
##   sample_name           npoc_raw tdn_raw run_datetime
##   <chr>                    <dbl>   <dbl> <chr>
## 1 TMP_C_F6_20250711         24.8   0.824 7/14/2025 9:35:40 PM
## 2 TMP_C_H3_20250711         25.4   0.926 7/14/2025 10:04:08 PM
## 3 TMP_C_H3_20250711_dup     25.7   1.01  7/14/2025 10:33:15 PM
## 4 TMP_C_H6_20250711         25.8   0.862 7/14/2025 11:45:04 PM
## 5 TMP_C_I5_20250711         18.0   0.584 7/15/2025 12:12:38 AM
## 6 TMP_SW_B4_20250711        75.8   2.60  7/15/2025 12:34:38 AM
```

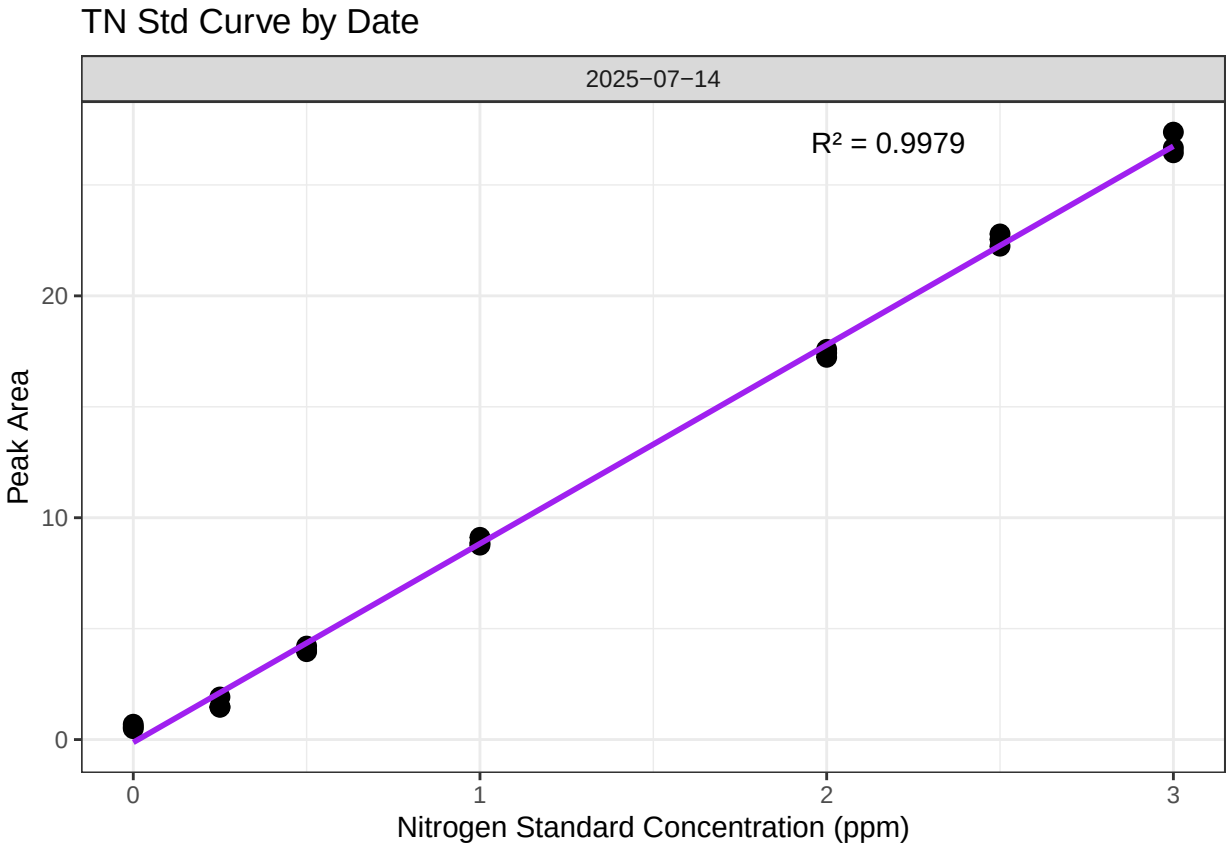
Assessing standard Curves

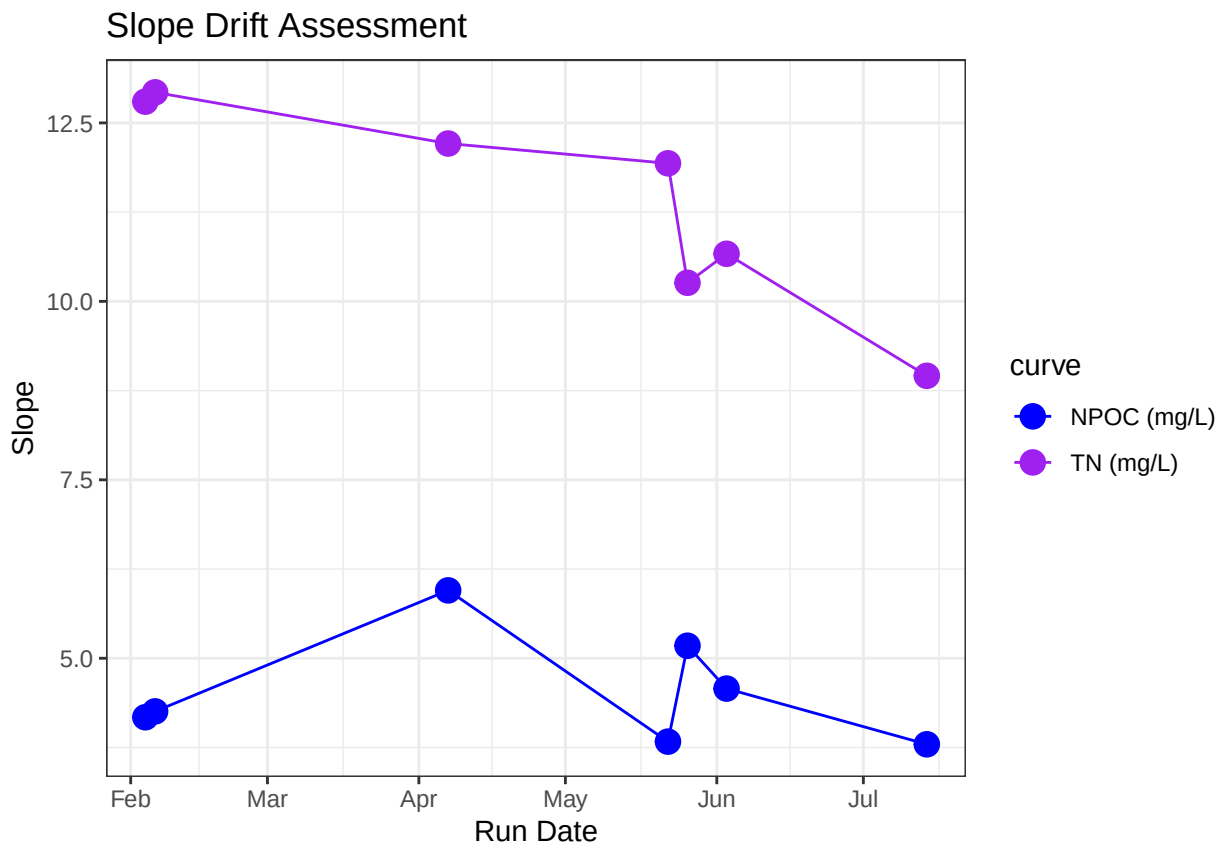
```
## Assess the Standard Curve
```

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




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


TN Std Curve by Date
2025−07−14
R² = 0.9979
Peak Area
20
10
0
0
1
2
3
Nitrogen Standard Concentration (ppm)




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

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

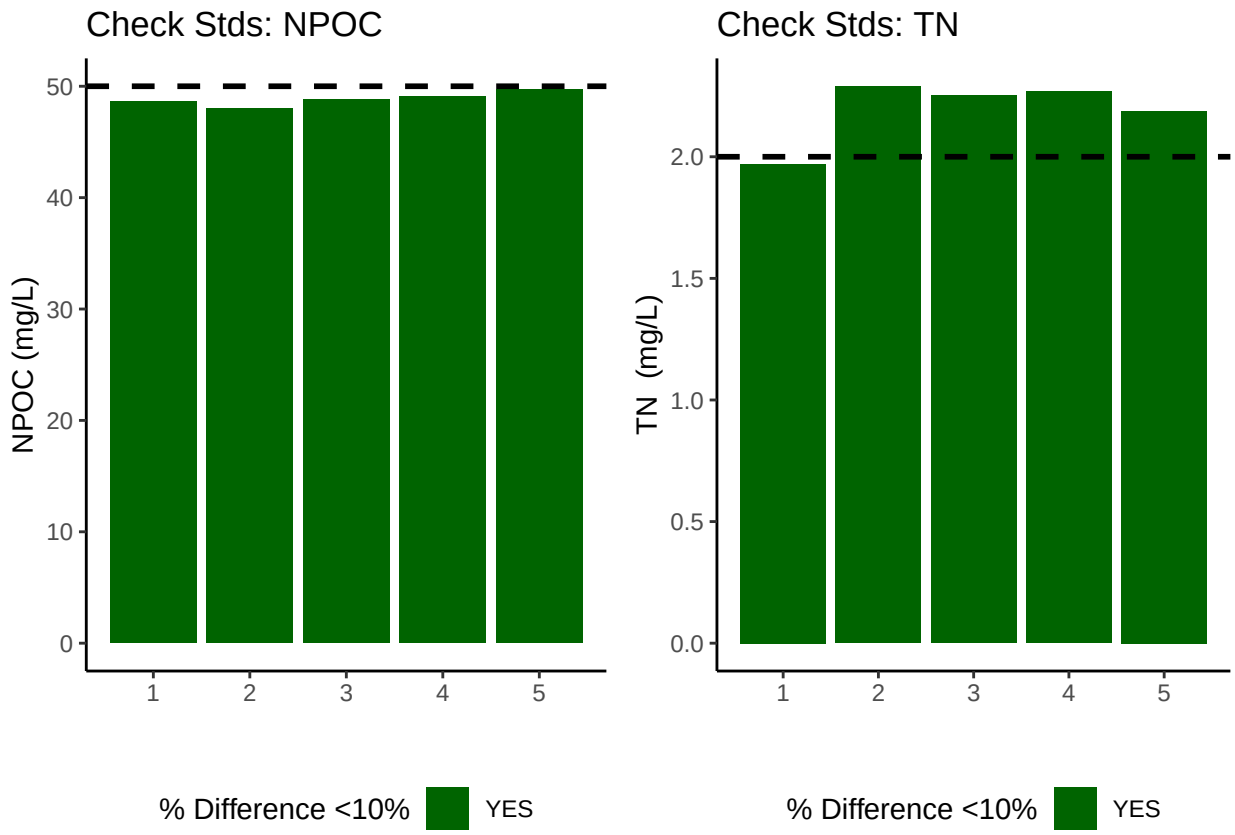
Assess Check Standards

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

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

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

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




```
## [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"
```

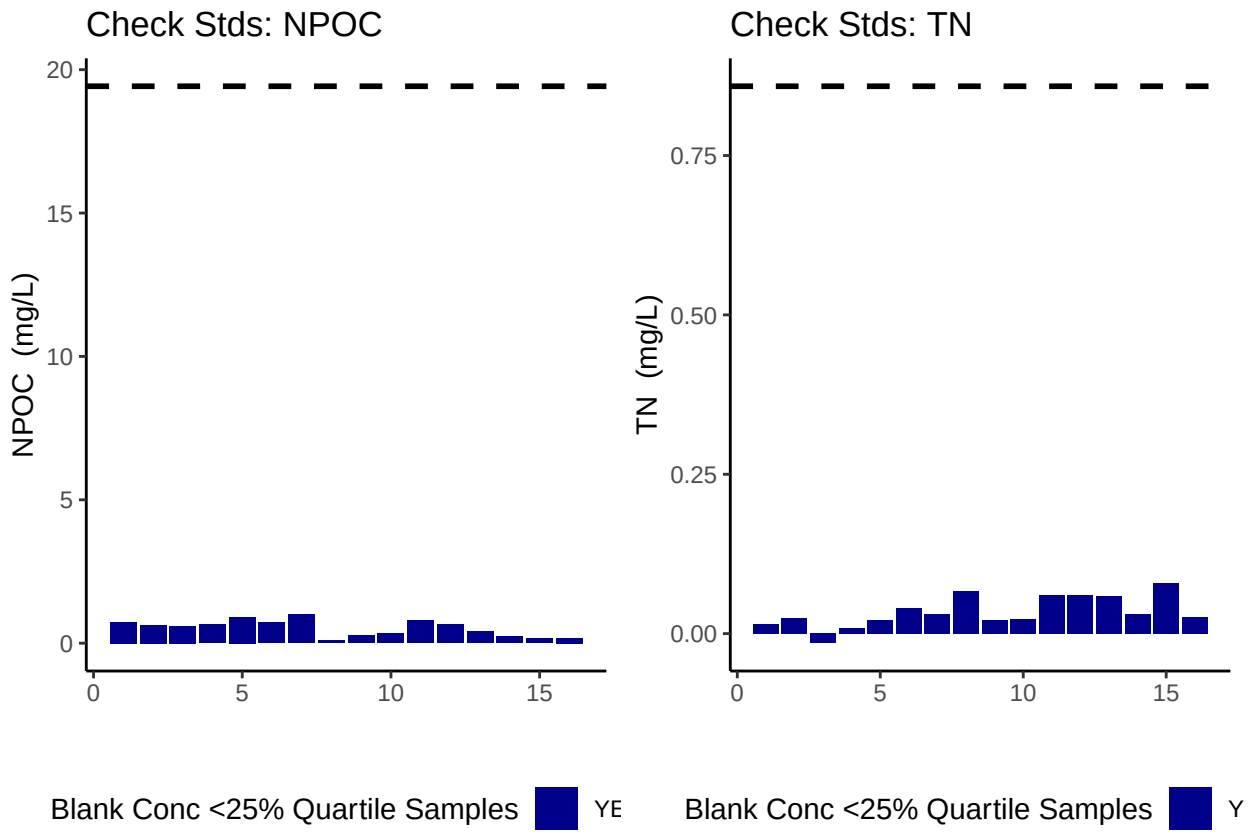
Assess Blanks

```
## 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] 0.5250037
```

```
## nitrogen blanks:
```

```
## [1] 0.03449812
```

Assess Duplicates - if there are any

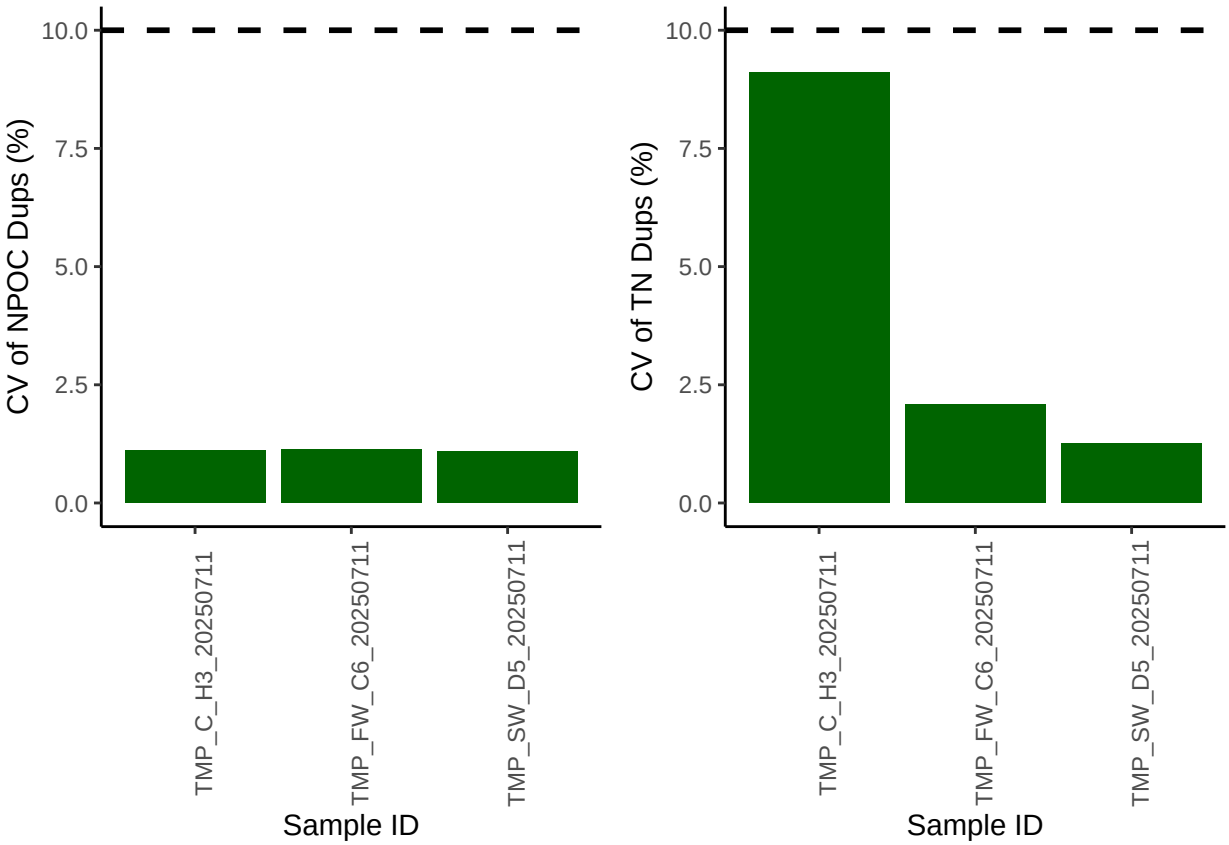
```
## Assess Duplicates
```

```
## # A tibble: 3 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_C_H3_20250711          25.7       1.01
## 2 TMP_SW_D5_20250711         31.9       1.27
## 3 TMP_FW_C6_20250711         10.2       0.437
```

```
##          sample_name npoc_raw tdn_raw          run_datetime npoc_flag tdn_flag
## 1  TMP_C_H3_20250711    25.42  0.9261 7/14/2025 10:04:08 PM
## 2 TMP_FW_C6_20250711    10.30  0.4455  7/15/2025 5:55:18 AM
## 3 TMP_SW_D5_20250711    32.21  1.2600  7/15/2025 1:22:53 AM
##   npoc_raw_dup tdn_raw_dup
## 1        25.69      1.0120
## 2        10.19      0.4368
## 3        31.88      1.2750
```

```
##          sample_name npoc_raw tdn_raw          run_datetime npoc_flag tdn_flag
## 1  TMP_C_H3_20250711    25.42  0.9261 7/14/2025 10:04:08 PM
## 2 TMP_FW_C6_20250711    10.30  0.4455  7/15/2025 5:55:18 AM
## 3 TMP_SW_D5_20250711    32.21  1.2600  7/15/2025 1:22:53 AM
##   npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv
## 1        25.69      1.0120     1.116464               YES    9.116356
## 2        10.19      0.4368     1.134518               YES    2.077264
## 3        31.88      1.2750     1.088307               YES    1.249989
##   tdn_dups_cv_flag
## 1              YES
## 2              YES
## 3              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.
```

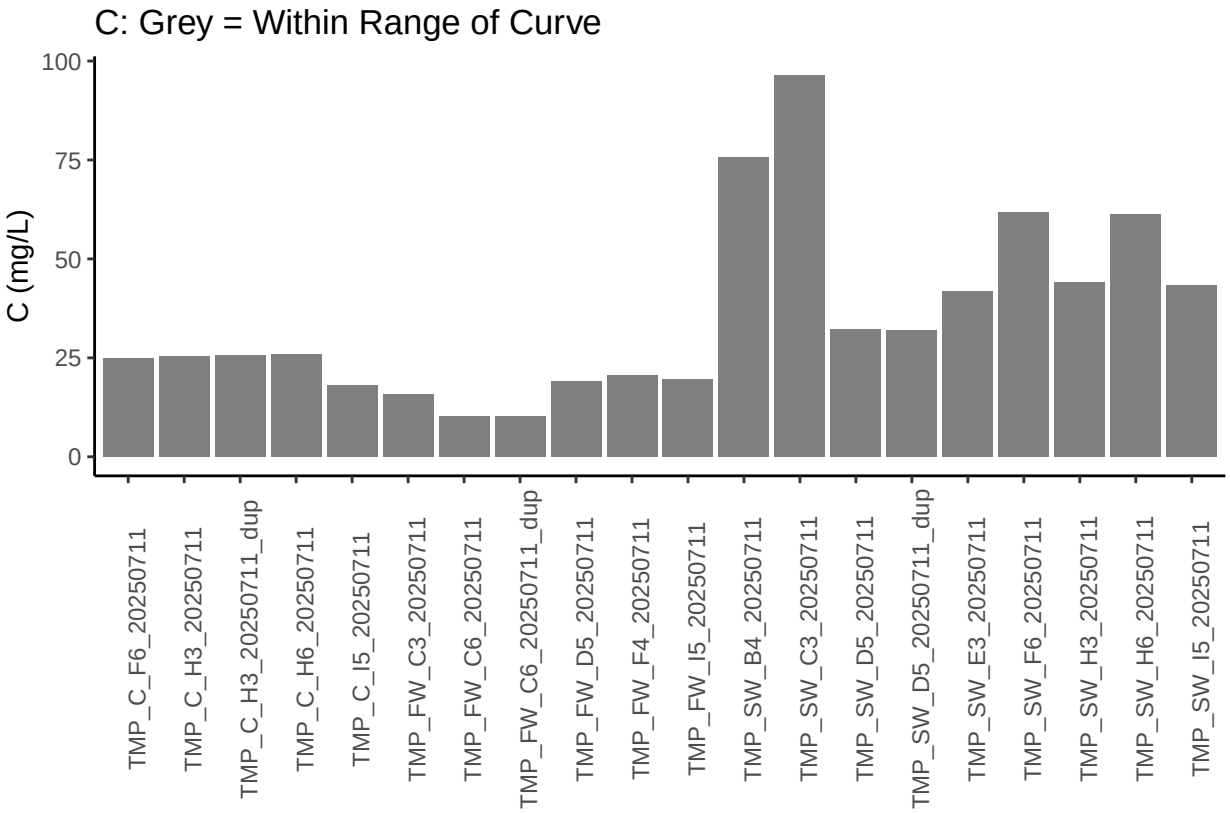


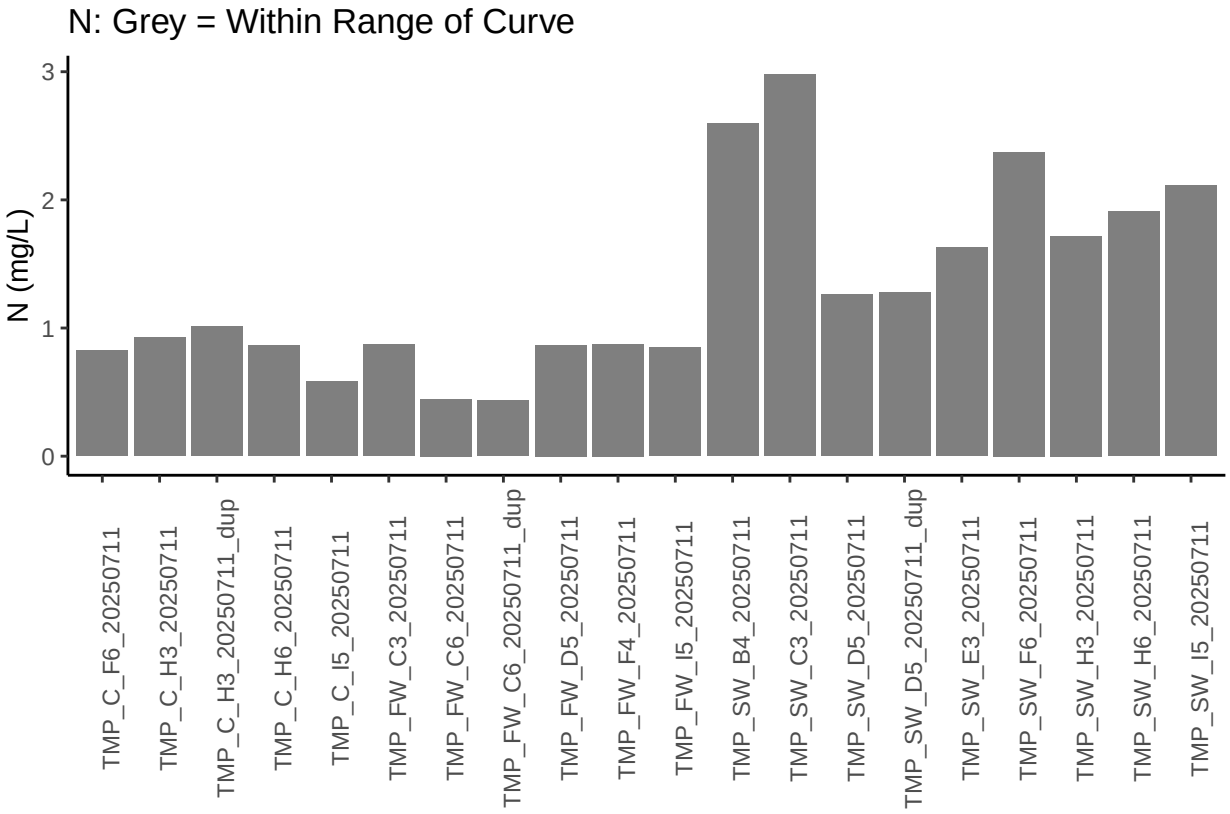

```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

```
## [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
TMP_C_F6_20250711
TMP_C_H3_20250711
TMP_C_H3_20250711_dup
TMP_C_H6_20250711
TMP_C_I5_20250711
TMP_FW_C3_20250711
TMP_FW_C6_20250711
TMP_FW_C6_20250711_dup
TMP_FW_D5_20250711
TMP_FW_F4_20250711
TMP_FW_I5_20250711
TMP_SW_B4_20250711
TMP_SW_C3_20250711
TMP_SW_D5_20250711
TMP_SW_D5_20250711_dup
TMP_SW_E3_20250711
TMP_SW_F6_20250711
TMP_SW_H3_20250711
TMP_SW_H6_20250711
TMP_SW_I5_20250711

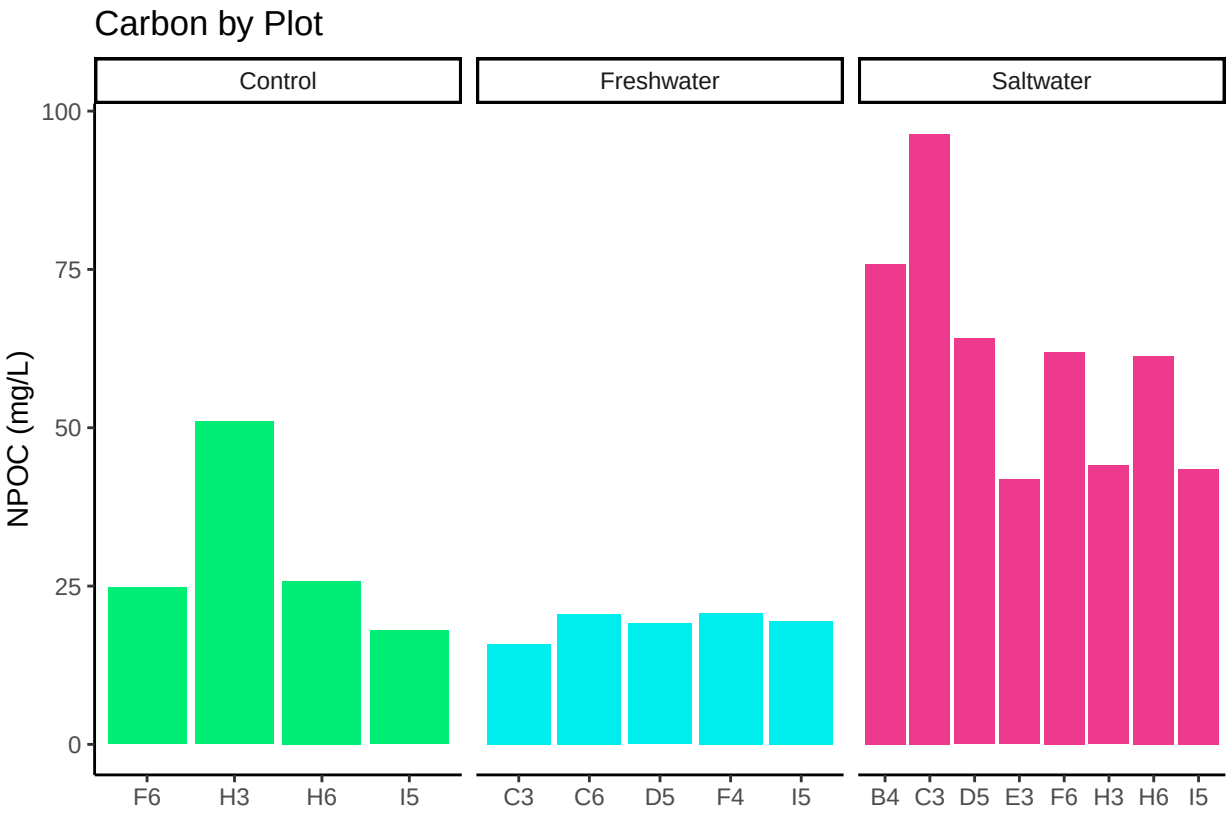
Visualize Data by Plot

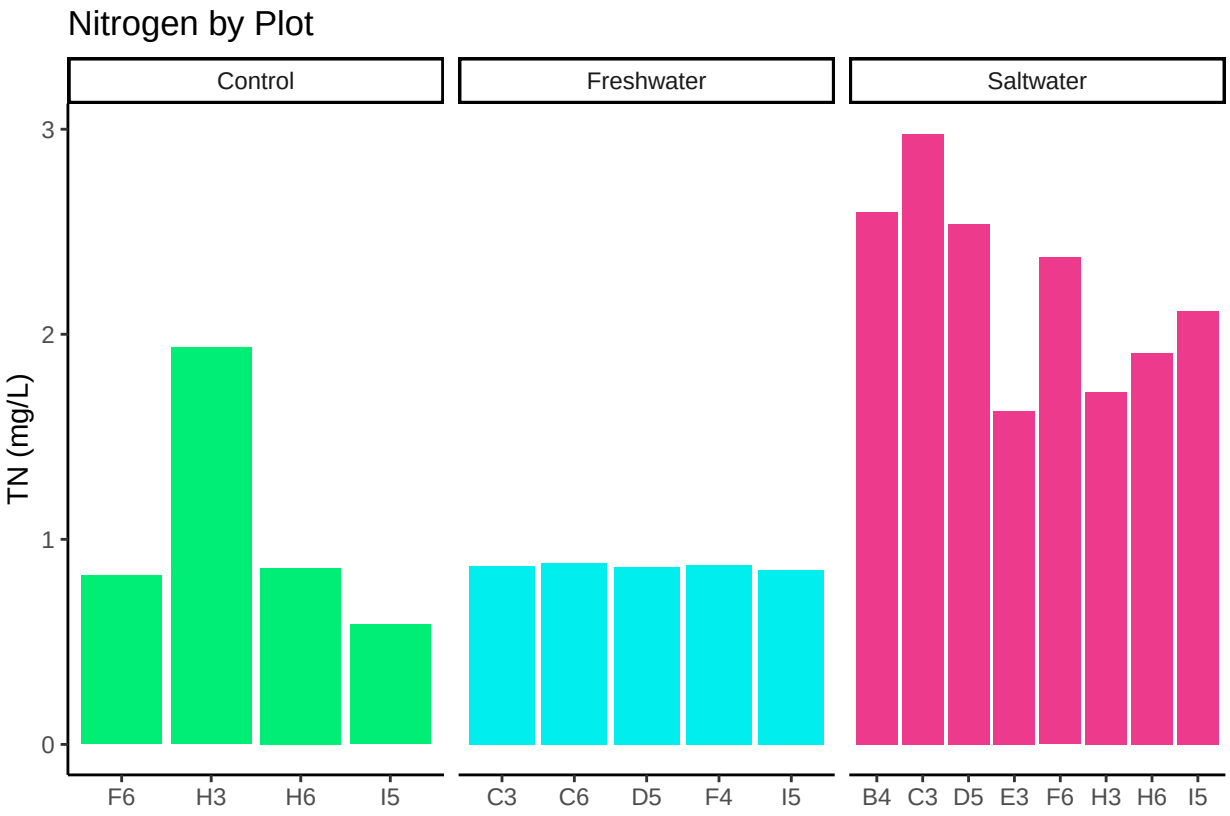
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "C", "F6", "20250711"), c("TMP", "C", "H3",
## "20250711": number of columns of result is not a multiple of vector length (arg
## 1)
```

```
##   Site_Code Plot Grid_Square     Date  NA
## 1       TMP    C          F6 20250711 TMP
## 2       TMP    C          H3 20250711 TMP
## 3       TMP    C          H3 20250711 dup
## 4       TMP    C          H6 20250711 TMP
## 5       TMP    C          I5 20250711 TMP
## 6       TMP   SW          B4 20250711 TMP
```

```
##   Site_Code Plot Grid_Square     Date  NA           sample_name npoc_raw
## 1       TMP    C          F6 20250711 TMP     TMP_C_F6_20250711    24.78
## 2       TMP    C          H3 20250711 TMP     TMP_C_H3_20250711    25.42
## 3       TMP    C          H3 20250711 dup TMP_C_H3_20250711_dup    25.69
## 4       TMP    C          H6 20250711 TMP     TMP_C_H6_20250711    25.83
## 5       TMP    C          I5 20250711 TMP     TMP_C_I5_20250711    17.98
## 6       TMP   SW          B4 20250711 TMP    TMP_SW_B4_20250711    75.80
##   tdn_raw          run_datetime npoc_flag tdn_flag
## 1  0.8238  7/14/2025 9:35:40 PM
## 2  0.9261 7/14/2025 10:04:08 PM
## 3  1.0120 7/14/2025 10:33:15 PM
## 4  0.8619 7/14/2025 11:45:04 PM
## 5  0.5845 7/15/2025 12:12:38 AM
## 6  2.5970 7/15/2025 12:34:38 AM
```


Carbon by Plot
Control
Freshwater
Saltwater
NPOC (mg/L)
100
75
50
25
0
F6
H3
H6
I5
C3
C6
D5
F4
I5
B4
C3
D5
E3
F6
H3
H6
I5


Nitrogen by Plot
Control
Freshwater
Saltwater
TN (mg/L)
3
2
1
0
F6
H3
H6
I5
C3
C6
D5
F4
I5
B4
C3
D5
E3
F6
H3
H6
I5

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 17 x 2
##    sample_name        metadata_recorded
##    <chr>              <lgl>
##  1 TMP_C_F6_20250711  TRUE
##  2 TMP_C_H3_20250711  TRUE
##  3 TMP_C_H6_20250711  TRUE
##  4 TMP_C_I5_20250711  TRUE
##  5 TMP_SW_B4_20250711 TRUE
##  6 TMP_SW_C3_20250711 TRUE
##  7 TMP_SW_D5_20250711 TRUE
##  8 TMP_SW_E3_20250711 TRUE
##  9 TMP_SW_F6_20250711 TRUE
## 10 TMP_SW_H3_20250711 TRUE
## 11 TMP_SW_H6_20250711 TRUE
## 12 TMP_SW_I5_20250711 TRUE
## 13 TMP_FW_C3_20250711 TRUE
## 14 TMP_FW_C6_20250711 TRUE
## 15 TMP_FW_D5_20250711 TRUE
## 16 TMP_FW_F4_20250711 TRUE
## 17 TMP_FW_I5_20250711 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~ C     F6          15 DOC         C_F6_D~ 2025~     24.8   2065
## 2 COMPASS: TEMP~ C     H3          15 DOC         C_H3_D~ 2025~     25.4   2118.
## 3 COMPASS: TEMP~ C     H6          15 DOC         C_H6_D~ 2025~     25.8   2152.
## 4 COMPASS: TEMP~ C     I5          15 DOC         C_I5_D~ 2025~     18.0   1498.
## 5 COMPASS: TEMP~ SW    B4          15 DOC         SW_B4_~ 2025~     75.8   6317.
## 6 COMPASS: TEMP~ SW    C3          15 DOC         SW_C3_~ 2025~     96.4   8030
## # i 12 more variables: npoc_flag <chr>, tdn_mgL <dbl>, tdn_uM <dbl>,
## #   tdn_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>,
## #   Evacuation_date_YYYYMMDD <dbl>, Collection_Date_YYYYMMDD <dbl>,
## #   Collection_Start_Time_24hrs <dbl>, Collection_End_Time_24hrs <dbl>,
## #   EST_EDT <chr>, Volume_mL <dbl>
```

#end