COMPASS TEMPEST Discrete DOC Data Workflow: 202504

April 2025

2025-06-05

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 = "04/07/25"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = "NPOC Check Standard was a bit old and came out higher than expected."

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2025/TMP_202504.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202504_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202504.csv"

#check standard concentrations - Update if running different checks:
   chk_std_c = 1
   chk_std_n = 1

#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

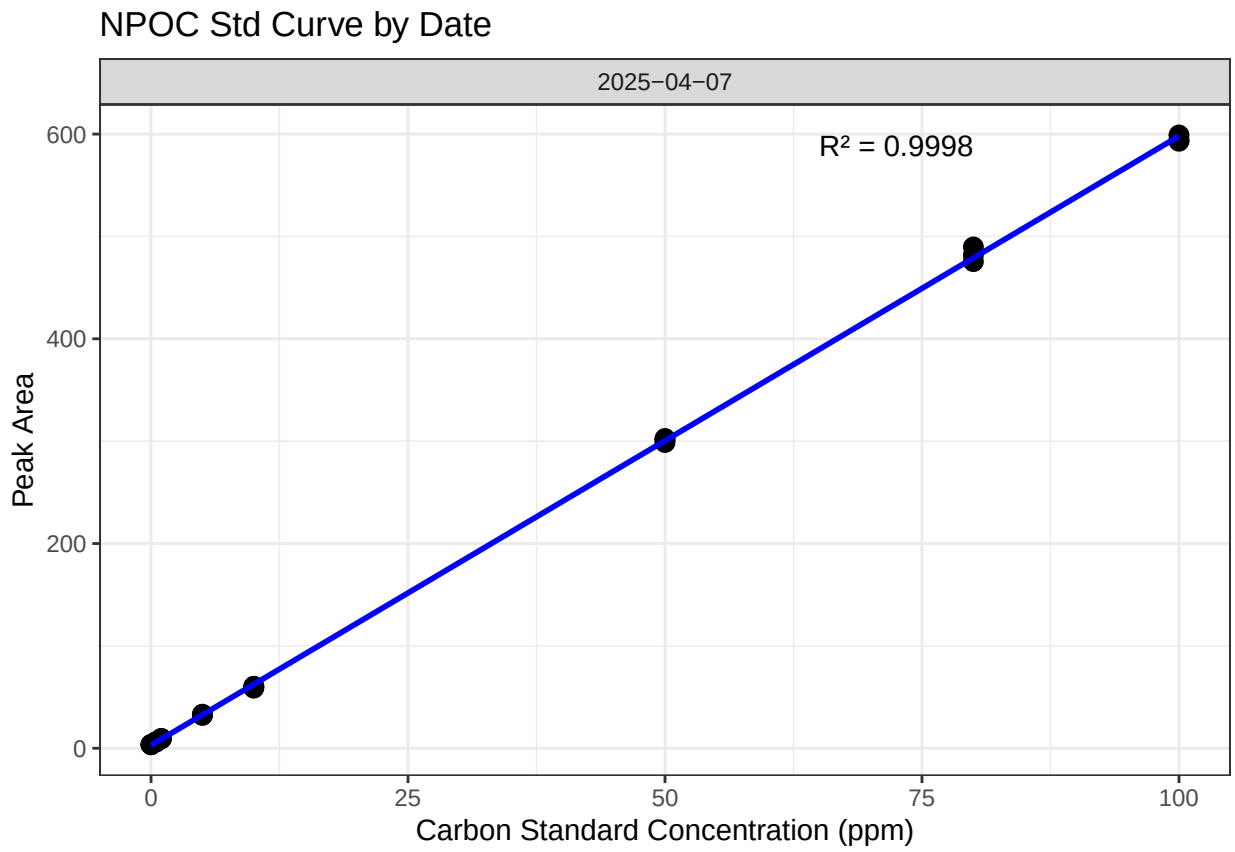
```
## Import Sample Data


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

```
## # A tibble: 6 x 4
##   sample_name            npoc_raw tdn_raw run_datetime
##   <chr>                     <dbl>   <dbl> <chr>
## 1 TMP_SW_B4_20250403         85      2.17 4/8/2025 12:21:11 AM
## 2 TMP_SW_C3_20250403         67.3    1.82 4/8/2025 12:48:14 AM
## 3 TMP_SW_C3_20250403_dup     66.2    1.79 4/8/2025 1:20:48 AM
## 4 TMP_SW_C6_20250403         60.4    2.04 4/8/2025 1:52:33 AM
## 5 TMP_SW_D5_20250403         39.1    1.31 4/8/2025 2:22:45 AM
## 6 TMP_SW_E3_20250403         46.0    1.56 4/8/2025 2:54:49 AM
```

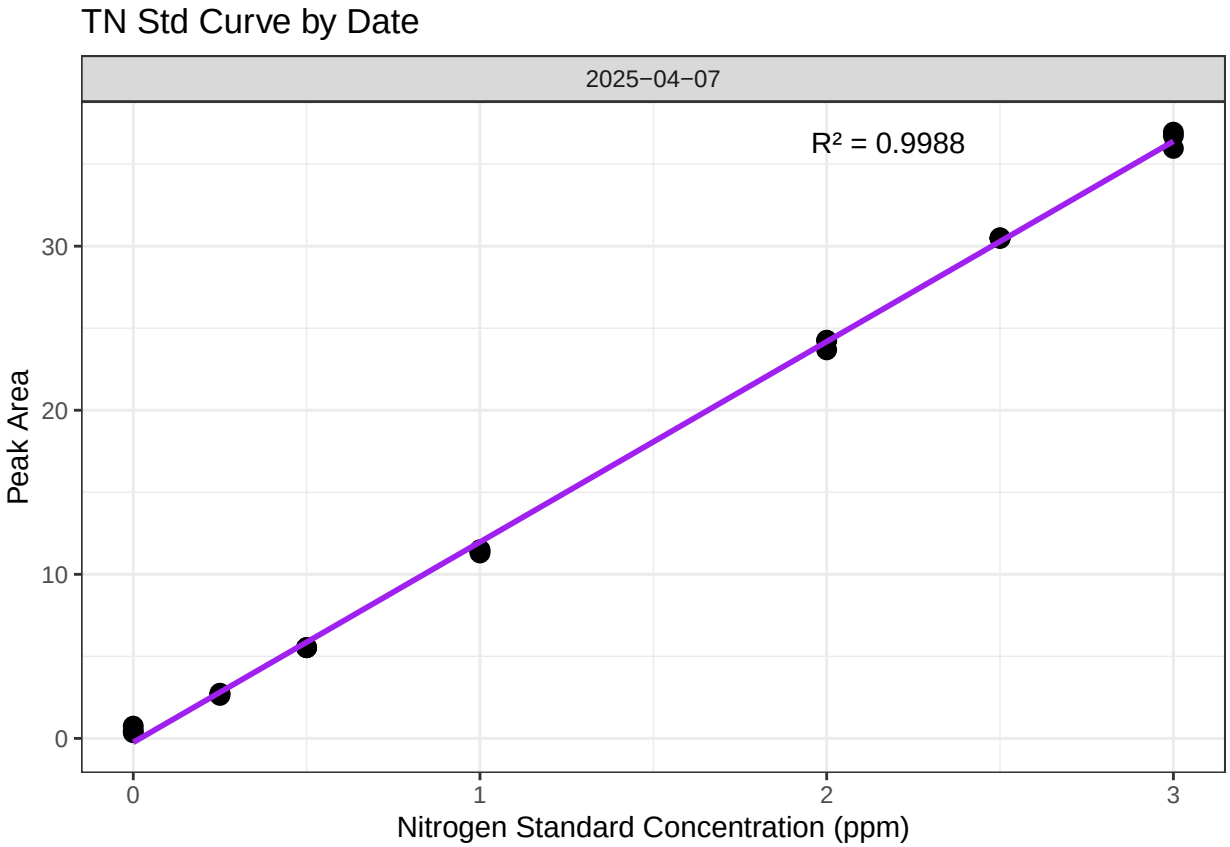
Assessing standard Curves

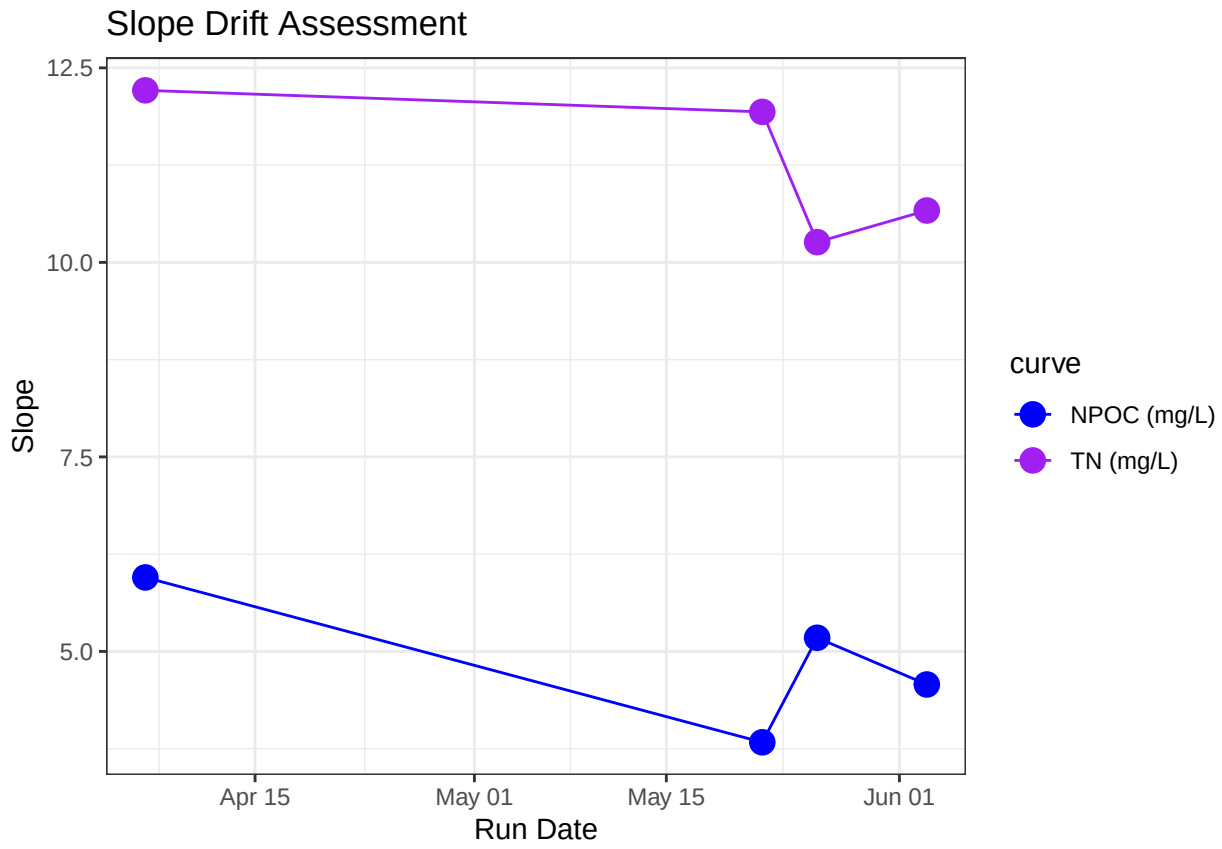
```
## Assess the Standard Curve
```

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




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


TN Std Curve by Date
2025−04−07
R² = 0.9988
Peak Area
0
10
20
30
0
1
2
3
Nitrogen Standard Concentration (ppm)

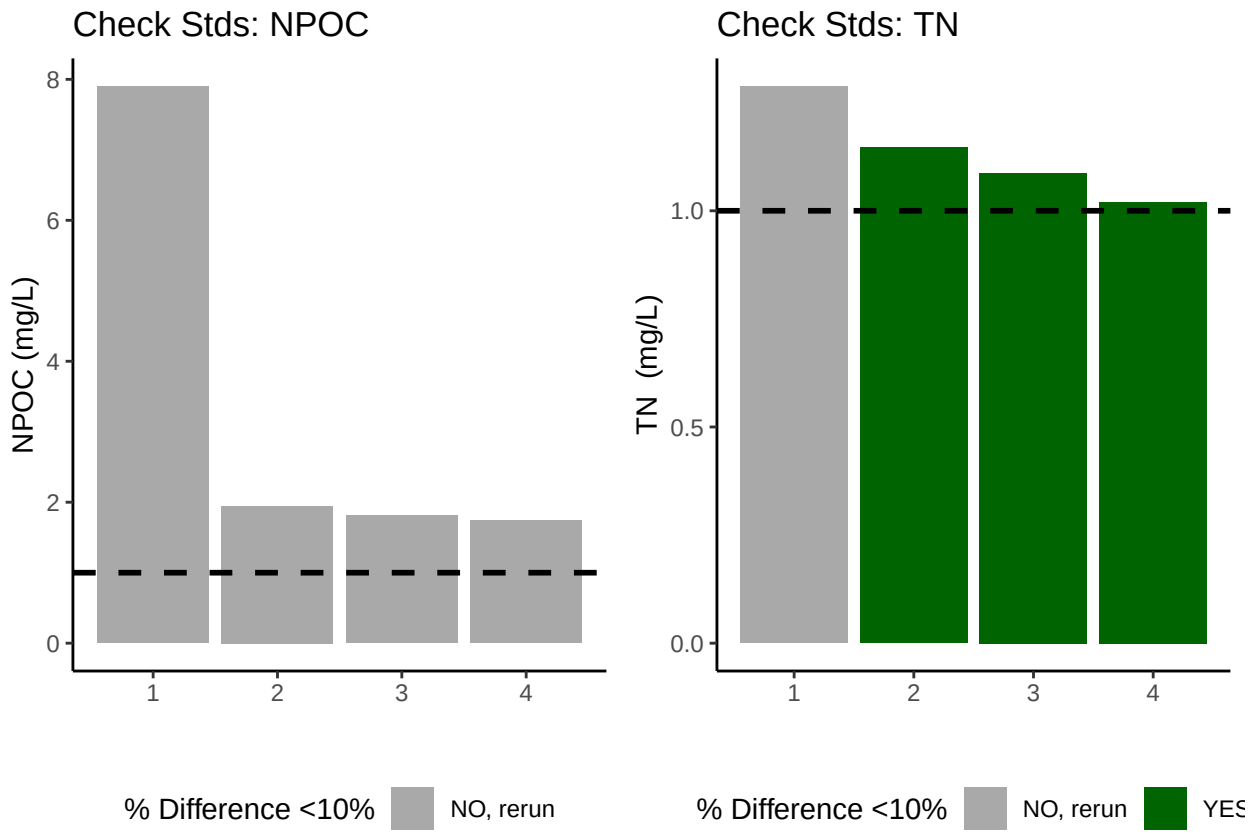



```
## [1] "NPOC Curve r2 GOOD"
```

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

Assess Check Standards

```
## Assess the Check Standards

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

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

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




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

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

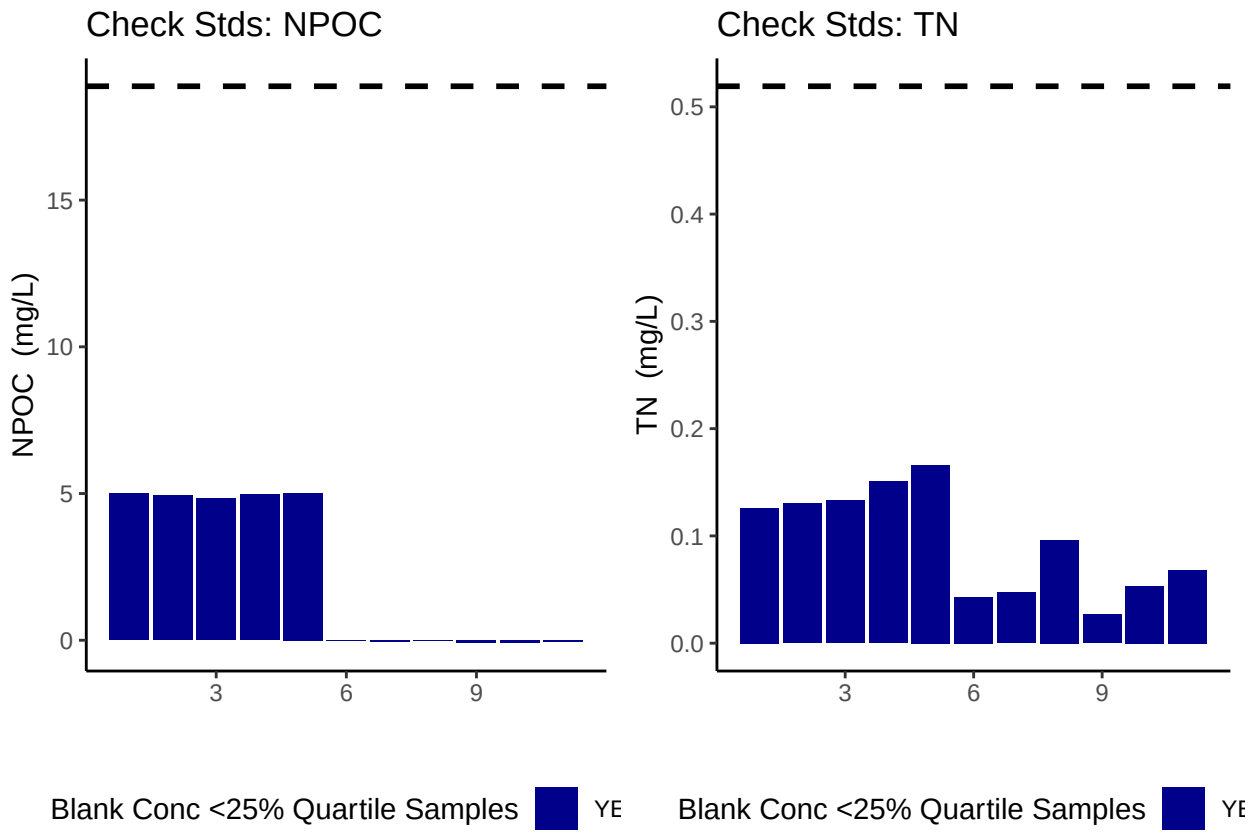
Assess Blanks

```
## 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] 2.220664
```

```
## nitrogen blanks:
```

```
## [1] 0.09457545
```

Assess Duplicates - if there are any

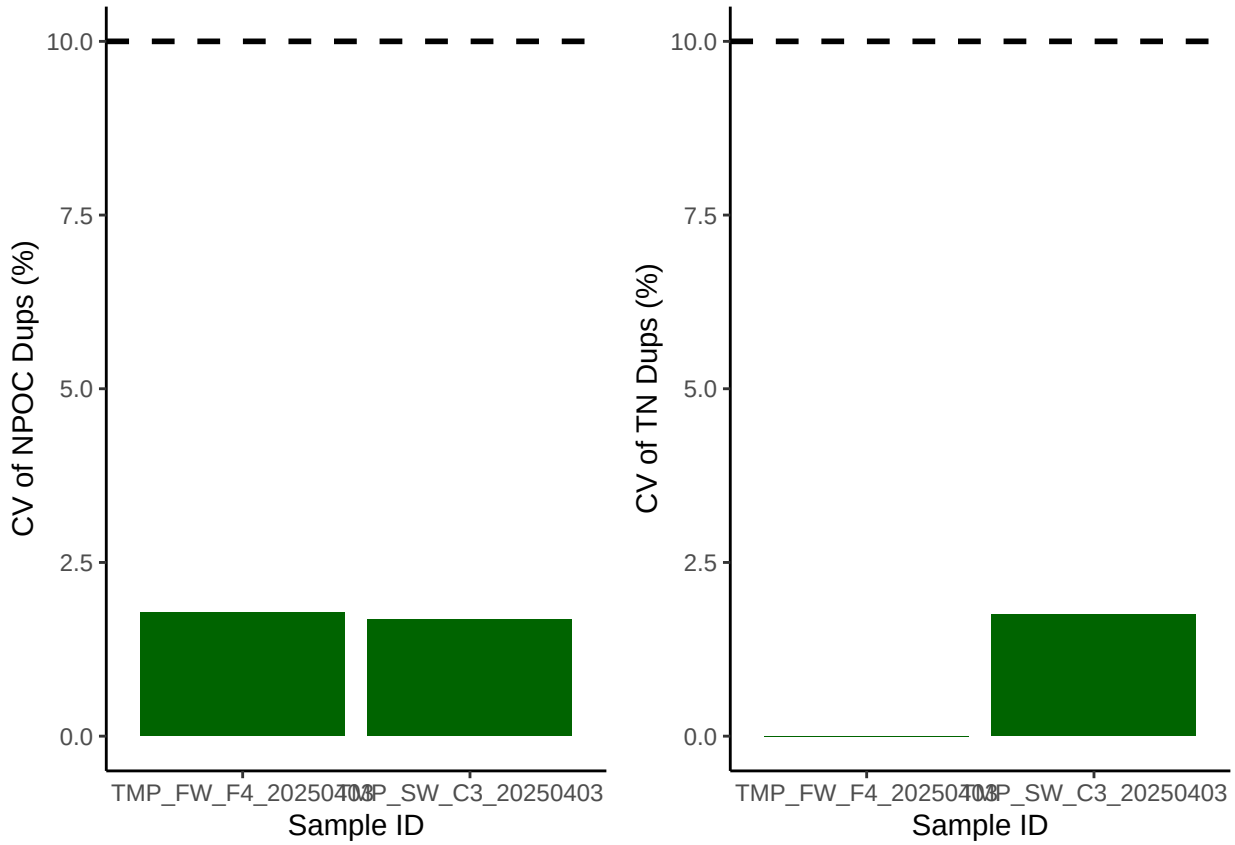
```
## Assess Duplicates
```

```
## # A tibble: 2 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_SW_C3_20250403         66.2       1.79
## 2 TMP_FW_F4_20250403         20.4       0.542
```

```
##          sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_FW_F4_20250403    20.02  0.5415  4/8/2025 5:25:48 AM
## 2 TMP_SW_C3_20250403    67.30  1.8190 4/8/2025 12:48:14 AM
##                  npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup
## 1 NPOC checks out of range                 20.36      0.5415
## 2 NPOC checks out of range                 66.24      1.7890
```

```
##          sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_FW_F4_20250403    20.02  0.5415  4/8/2025 5:25:48 AM
## 2 TMP_SW_C3_20250403    67.30  1.8190 4/8/2025 12:48:14 AM
##                  npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup npoc_dups_cv
## 1 NPOC checks out of range                 20.36      0.5415     1.775582
## 2 NPOC checks out of range                 66.24      1.7890     1.674441
##   npoc_dups_cv_flag tdn_dups_cv tdn_dups_cv_flag
## 1               YES    0.000000              YES
## 2               YES    1.753537              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.
```

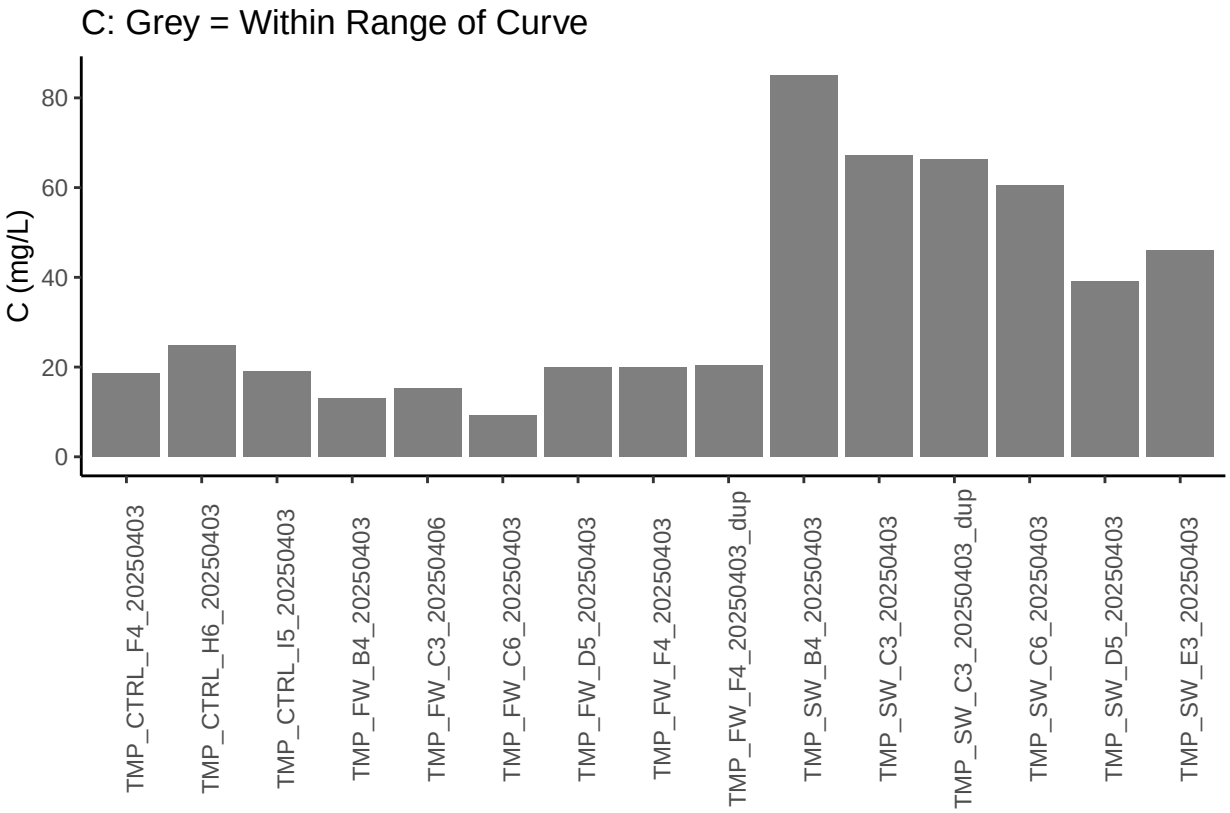


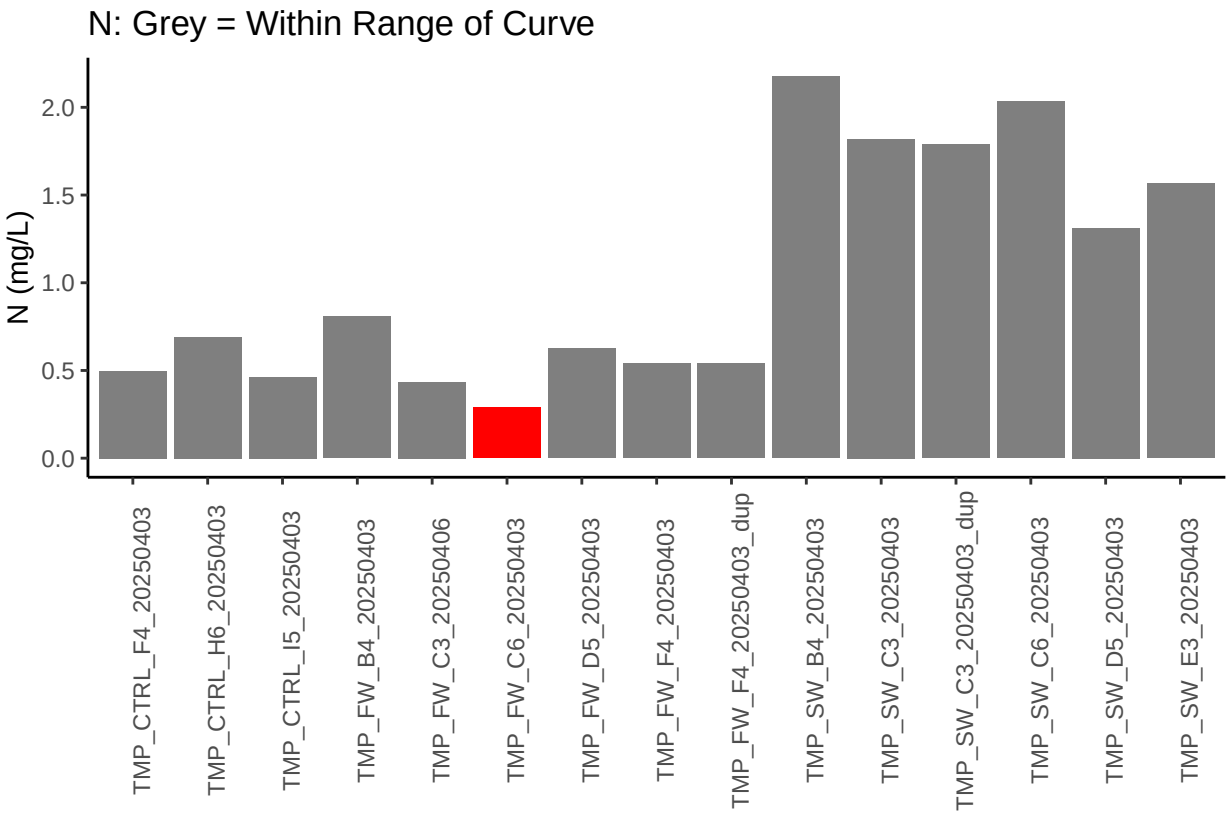

```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

```
## Sample Flagging
```




N: Grey = Within Range of Curve
N (mg/L)
2.0
1.5
1.0
0.5
0.0
TMP_CTRL_F4_20250403
TMP_CTRL_H6_20250403
TMP_CTRL_I5_20250403
TMP_FW_B4_20250403
TMP_FW_C3_20250406
TMP_FW_C6_20250403
TMP_FW_D5_20250403
TMP_FW_F4_20250403
TMP_FW_F4_20250403_dup
TMP_SW_B4_20250403
TMP_SW_C3_20250403
TMP_SW_C3_20250403_dup
TMP_SW_C6_20250403
TMP_SW_D5_20250403
TMP_SW_E3_20250403

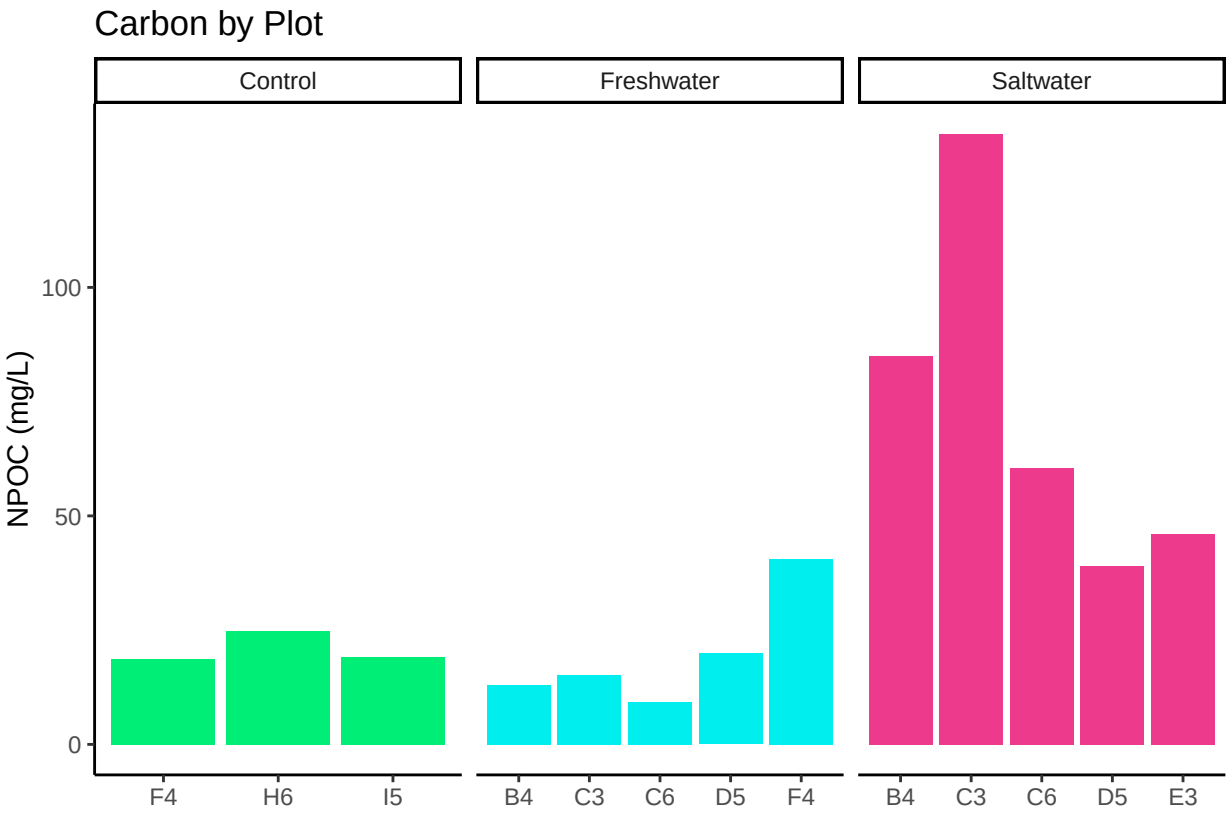
Visualize Data by Plot

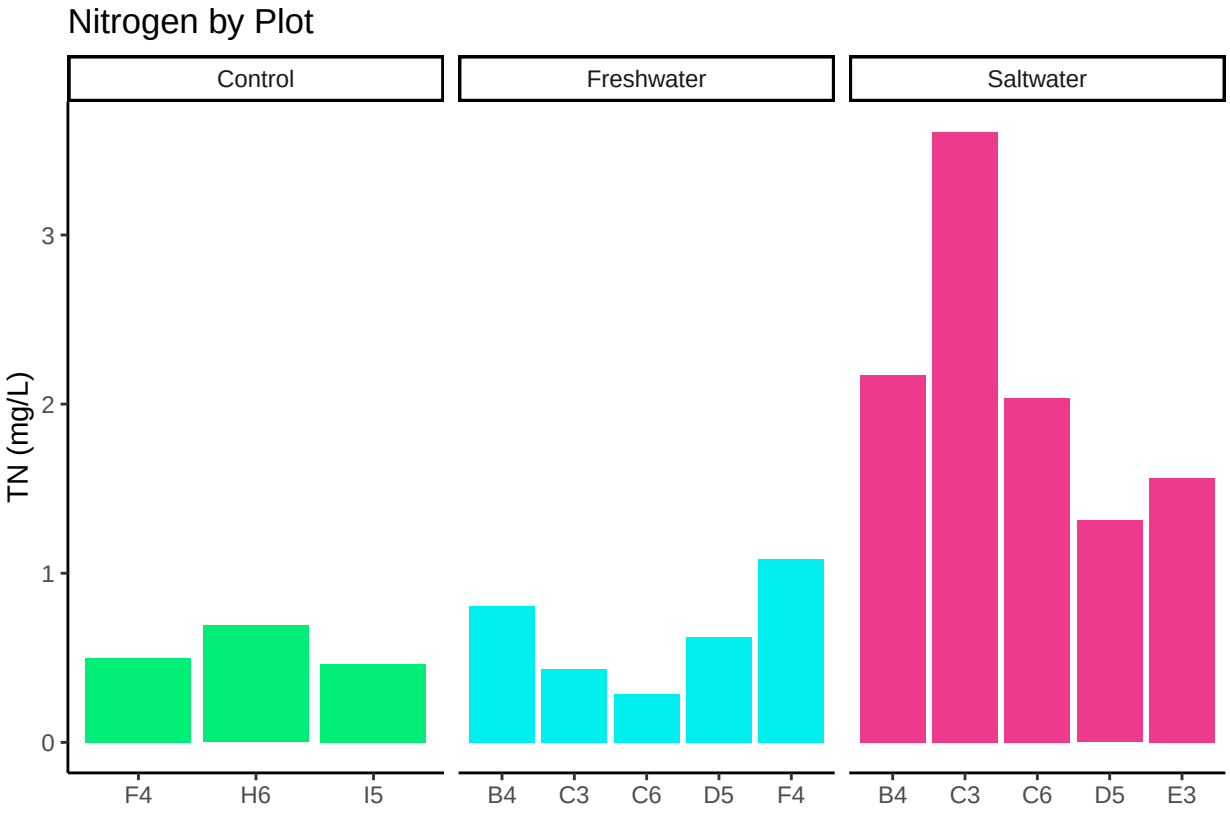
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "SW", "B4", "20250403"), c("TMP", "SW", "C3", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code Plot Grid_Square     Date  NA
## 1       TMP   SW          B4 20250403 TMP
## 2       TMP   SW          C3 20250403 TMP
## 3       TMP   SW          C3 20250403 dup
## 4       TMP   SW          C6 20250403 TMP
## 5       TMP   SW          D5 20250403 TMP
## 6       TMP   SW          E3 20250403 TMP
```

```
##   Site_Code Plot Grid_Square     Date  NA            sample_name npoc_raw
## 1       TMP   SW          B4 20250403 TMP     TMP_SW_B4_20250403    85.00
## 2       TMP   SW          C3 20250403 TMP     TMP_SW_C3_20250403    67.30
## 3       TMP   SW          C3 20250403 dup TMP_SW_C3_20250403_dup    66.24
## 4       TMP   SW          C6 20250403 TMP     TMP_SW_C6_20250403    60.40
## 5       TMP   SW          D5 20250403 TMP     TMP_SW_D5_20250403    39.07
## 6       TMP   SW          E3 20250403 TMP     TMP_SW_E3_20250403    46.02
##   tdn_raw         run_datetime                npoc_flag tdn_flag
## 1   2.174 4/8/2025 12:21:11 AM NPOC checks out of range
## 2   1.819 4/8/2025 12:48:14 AM NPOC checks out of range
## 3   1.789  4/8/2025 1:20:48 AM NPOC checks out of range
## 4   2.035  4/8/2025 1:52:33 AM NPOC checks out of range
## 5   1.312  4/8/2025 2:22:45 AM NPOC checks out of range
## 6   1.565  4/8/2025 2:54:49 AM NPOC checks out of range
```


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


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

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 13 x 2
##    sample_name        metadata_recorded
##    <chr>              <lgl>
##  1 TMP_SW_B4_20250403 TRUE
##  2 TMP_SW_C3_20250403 TRUE
##  3 TMP_SW_C6_20250403 TRUE
##  4 TMP_SW_D5_20250403 TRUE
##  5 TMP_SW_E3_20250403 TRUE
##  6 TMP_FW_B4_20250403 TRUE
##  7 TMP_FW_C3_20250406 TRUE
##  8 TMP_FW_C6_20250403 TRUE
##  9 TMP_FW_D5_20250403 TRUE
## 10 TMP_FW_F4_20250403 TRUE
## 11 TMP_C_F4_20250403  TRUE
## 12 TMP_C_H6_20250403  TRUE
## 13 TMP_C_I5_20250403  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~ SW    B4          15 DOC         SW_B4_~ 2025~     85     7083.
## 2 COMPASS: TEMP~ SW    C3          15 DOC         SW_C3_~ 2025~     67.3   5608.
## 3 COMPASS: TEMP~ SW    C6          15 DOC         SW_C6_~ 2025~     60.4   5033.
## 4 COMPASS: TEMP~ SW    D5          15 DOC         SW_D5_~ 2025~     39.1   3256.
## 5 COMPASS: TEMP~ SW    E3          15 DOC         SW_E3_~ 2025~     46.0   3835
## 6 COMPASS: TEMP~ FW    B4          15 DOC         FW_B4_~ 2025~     13.1   1090
## # 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