COMPASS TEMPEST Discrete DOC Data Workflow: 202505

May 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 = "05/22/25"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = "This run, the high check standard was remade halfway
  through run as a 60mg/L C, so checks are okay."

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2025/TMP_202505.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202505_allpeaks.txt"
  #file path and name for processed file
    processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202505.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
```

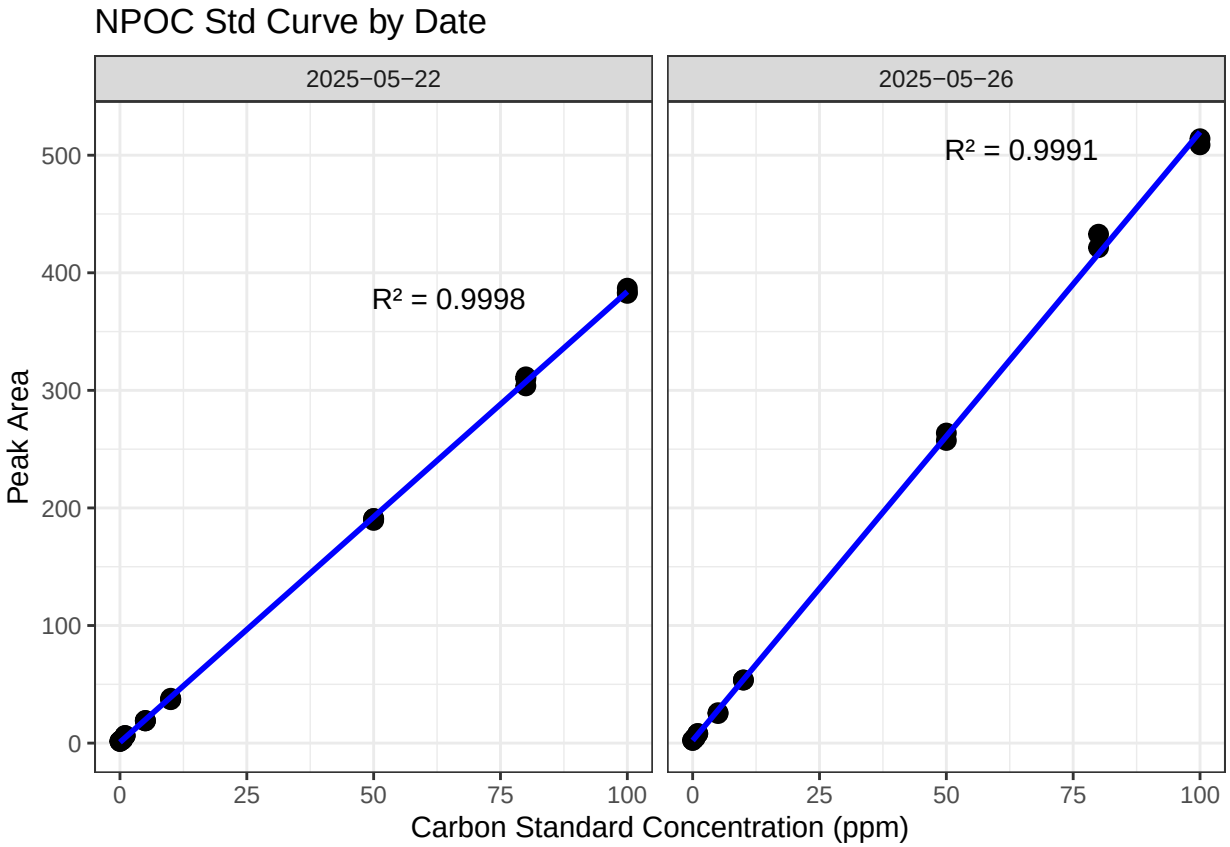
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 6 x 4
##   sample_name          npoc_raw tdn_raw run_datetime
##   <chr>                   <dbl>   <dbl> <chr>
## 1 TMP_CTRL_H3_20250509     25.5   0.977 5/23/2025 2:18:11 AM
## 2 TMP_CTRL_H6_20250509     29.9   0.975 5/23/2025 2:36:46 AM
## 3 TMP_CTRL_I5_20250509     21.5   0.568 5/23/2025 3:06:35 AM
## 4 TMP_FW_C6_20250509       10.3   0.365 5/23/2025 3:36:49 AM
## 5 TMP_FW_D5_20250509       18.4   0.657 5/23/2025 3:58:38 AM
## 6 TMP_FW_H3_20250509       13.9   0.748 5/23/2025 4:26:17 AM
```

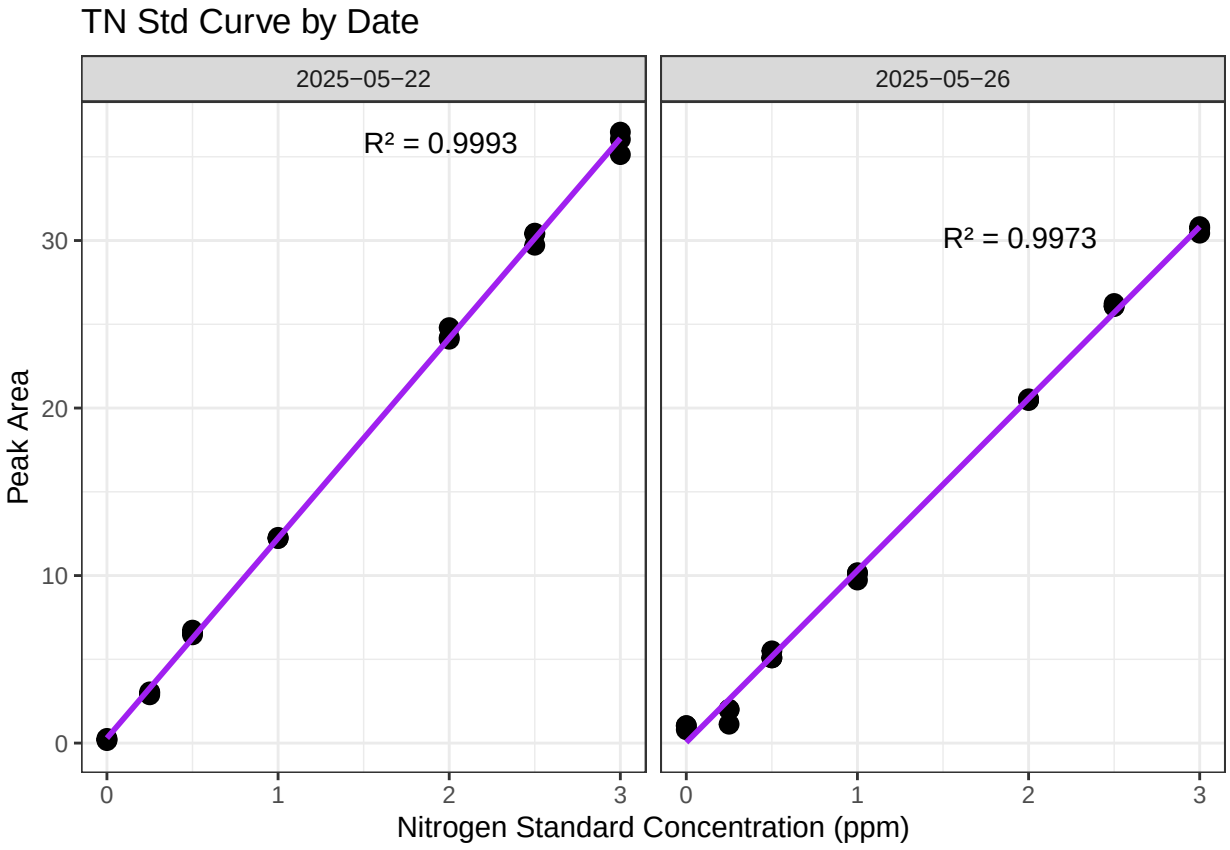
Assessing standard Curves

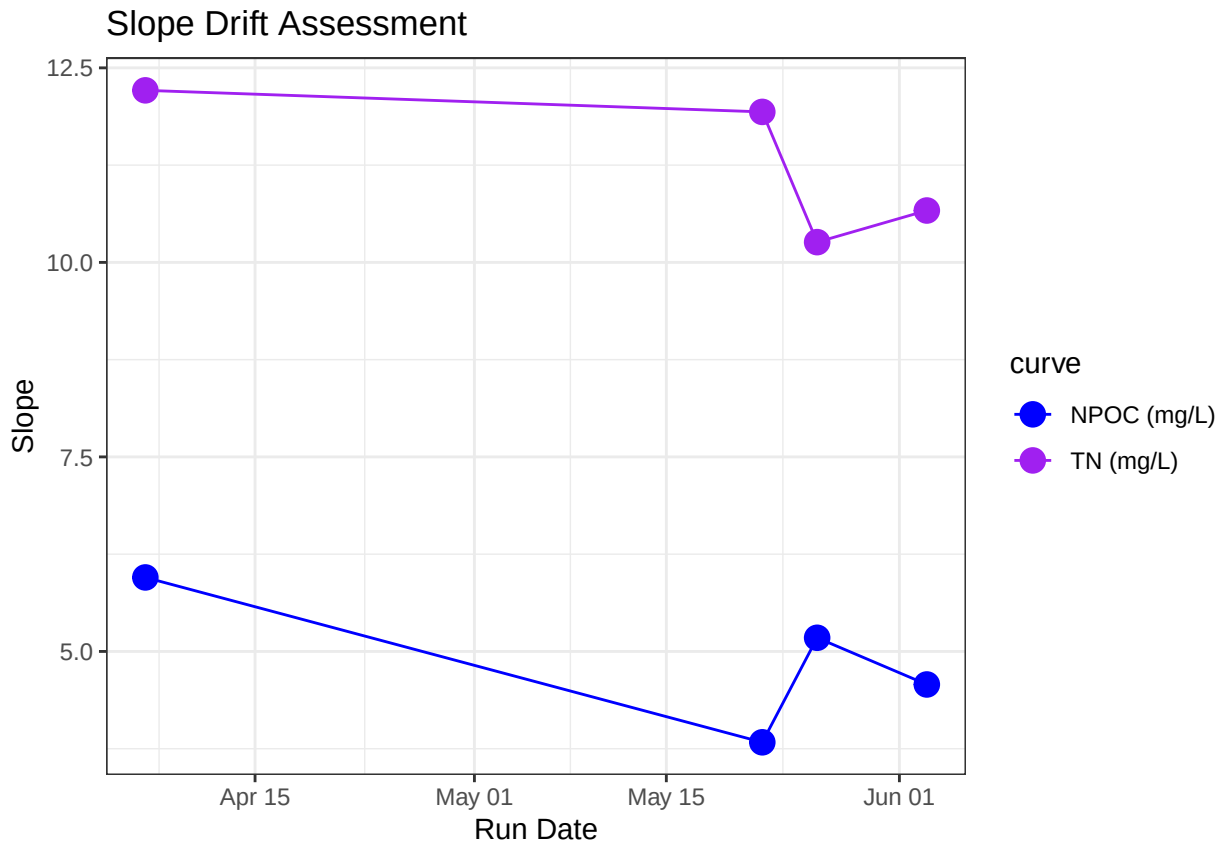
```
## Assess the Standard Curve
```

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




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


TN Std Curve by Date
2025−05−22
2025−05−26
R² = 0.9993
R² = 0.9973
Peak Area
0
10
20
30
0
1
2
3
Nitrogen Standard Concentration (ppm)




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

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

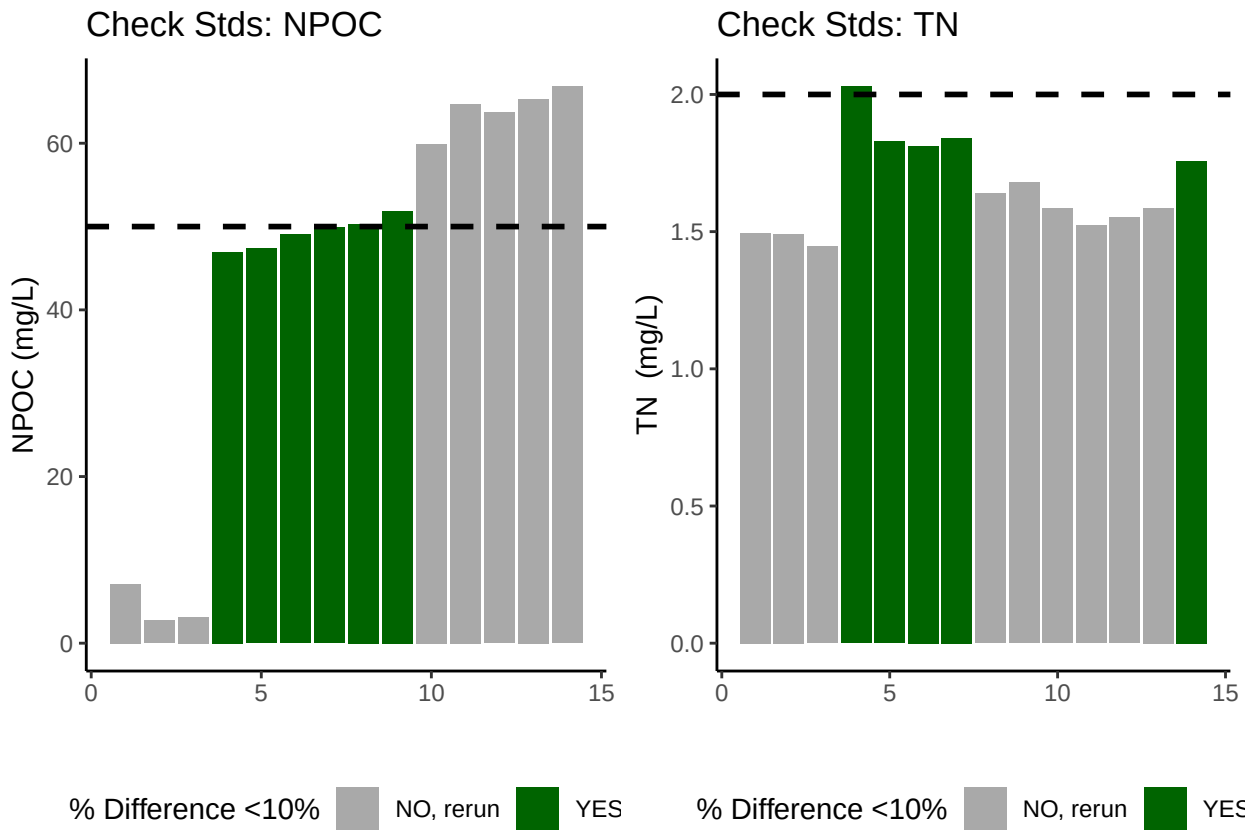
Assess Check Standards

```
## 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 - REASSESS"
```

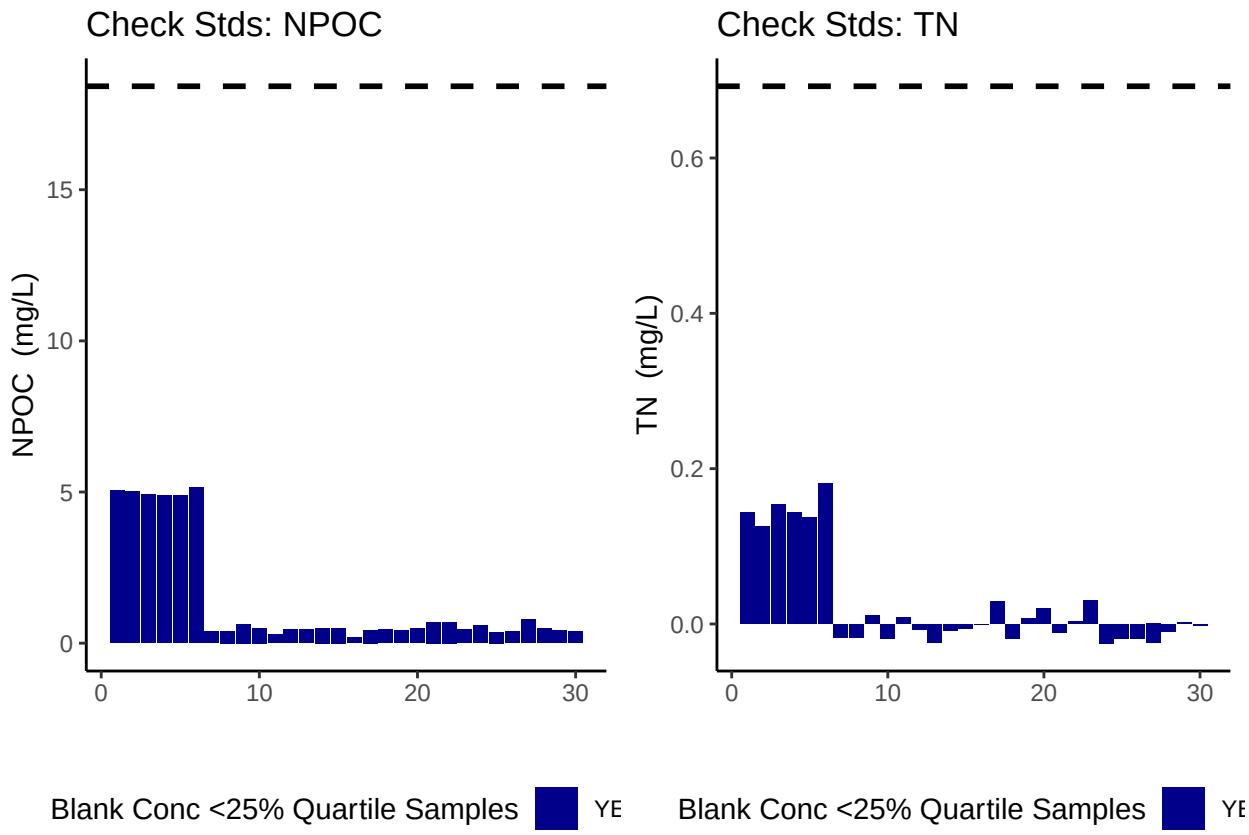
Assess Blanks

```
## 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] 1.37688
```

```
## nitrogen blanks:
```

```
## [1] 0.025593
```

Assess Duplicates - if there are any

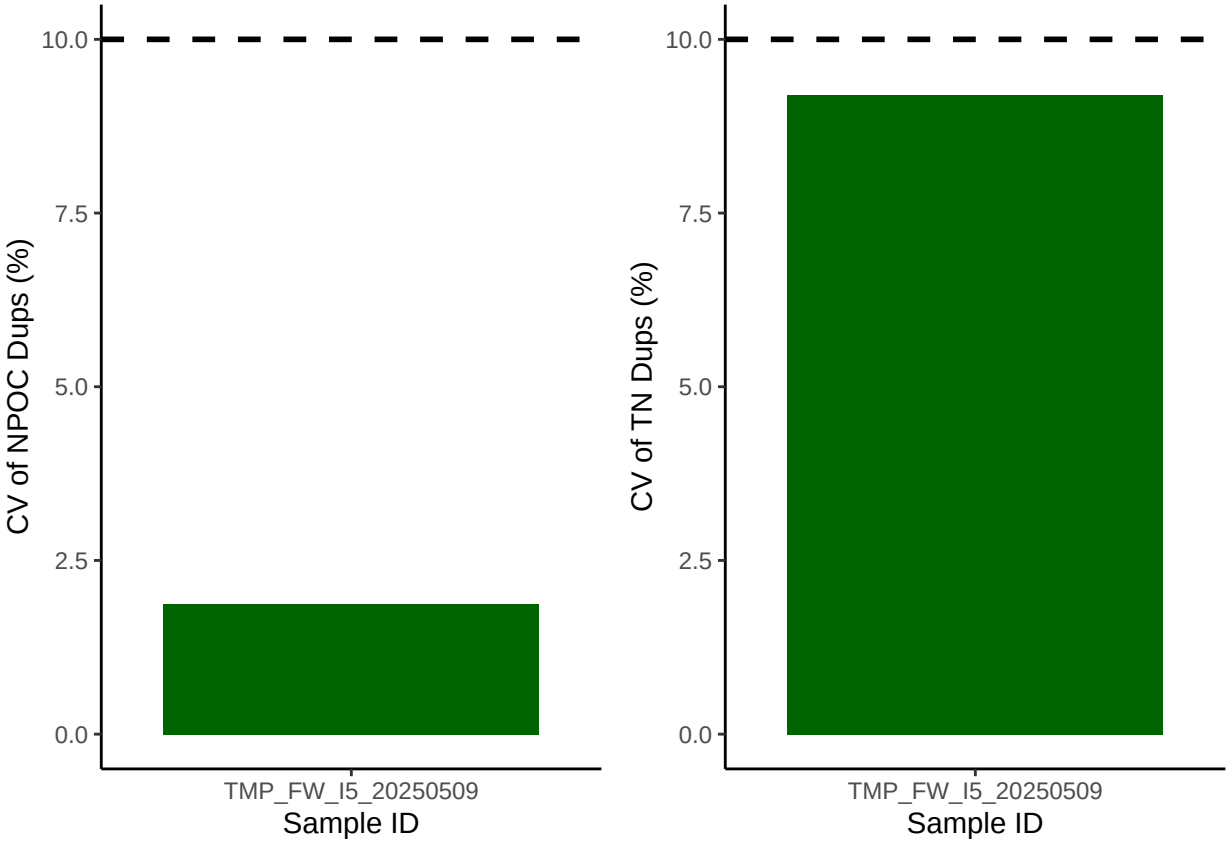
```
## Assess Duplicates

## # A tibble: 1 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_FW_I5_20250509         19.0       0.710

##          sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_FW_I5_20250509     19.3  0.7764 5/23/2025 5:29:16 AM
##                  npoc_flag               tdn_flag npoc_raw_dup tdn_raw_dup
## 1 NPOC checks out of range TN checks out of range        18.96      0.7099

##          sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_FW_I5_20250509     19.3  0.7764 5/23/2025 5:29:16 AM
##                  npoc_flag               tdn_flag npoc_raw_dup tdn_raw_dup
## 1 NPOC checks out of range TN checks out of range        18.96      0.7099
##   npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv tdn_dups_cv_flag
## 1     1.873354               YES    9.200138               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.
```

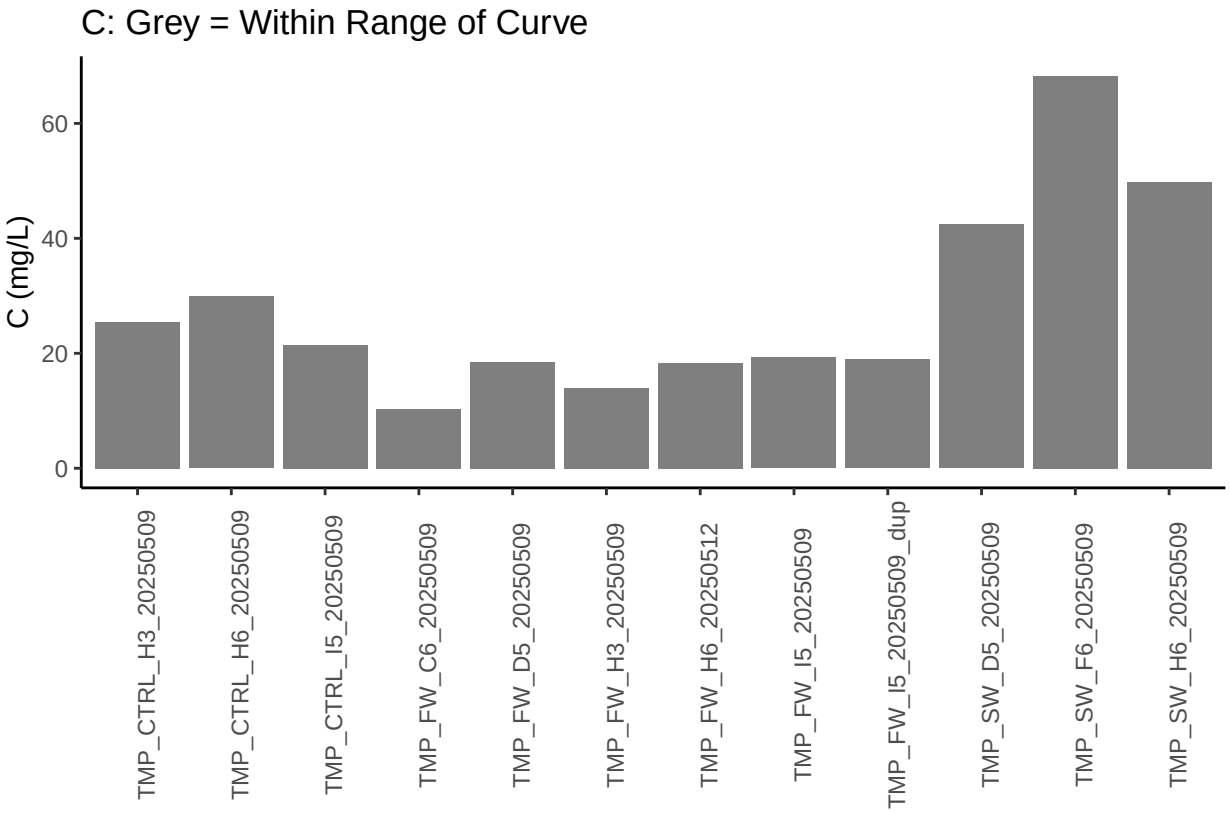


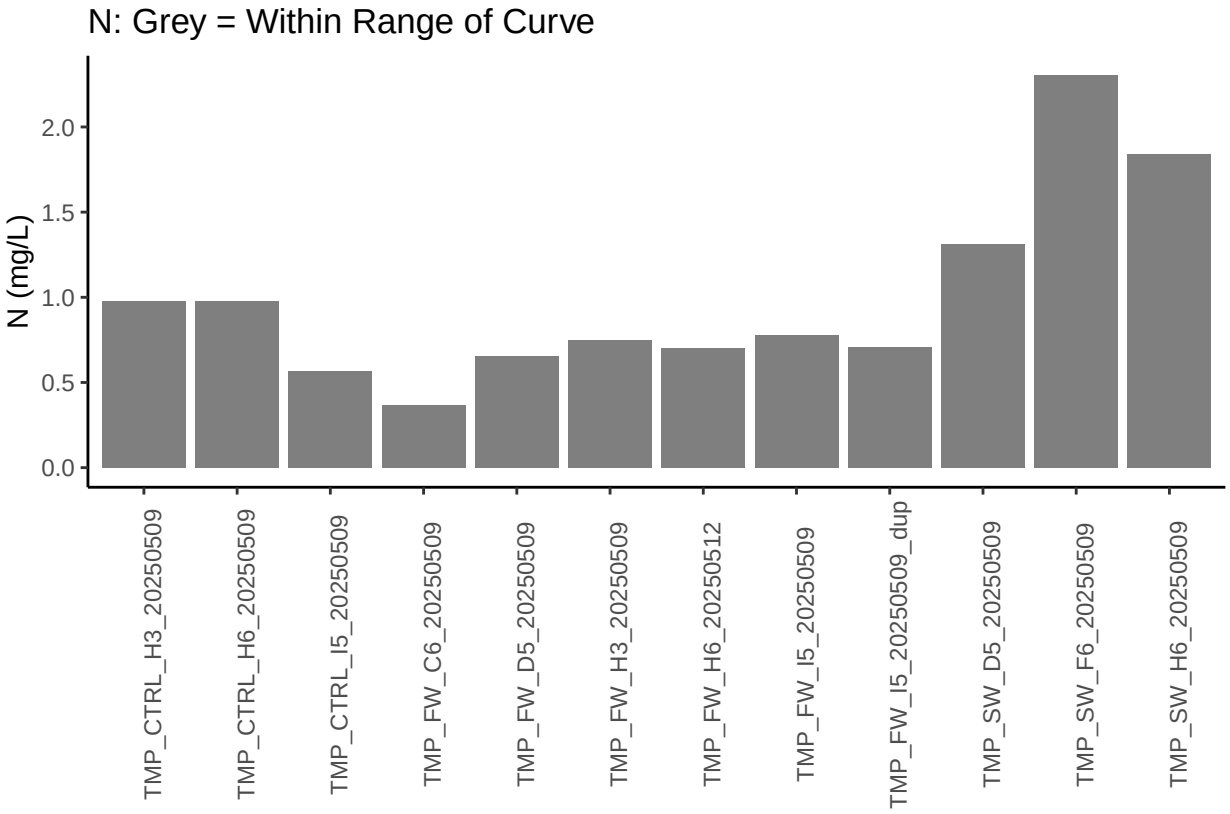
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

```
## [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_H3_20250509
TMP_CTRL_H6_20250509
TMP_CTRL_I5_20250509
TMP_FW_C6_20250509
TMP_FW_D5_20250509
TMP_FW_H3_20250509
TMP_FW_H6_20250512
TMP_FW_I5_20250509
TMP_FW_I5_20250509_dup
TMP_SW_D5_20250509
TMP_SW_F6_20250509
TMP_SW_H6_20250509

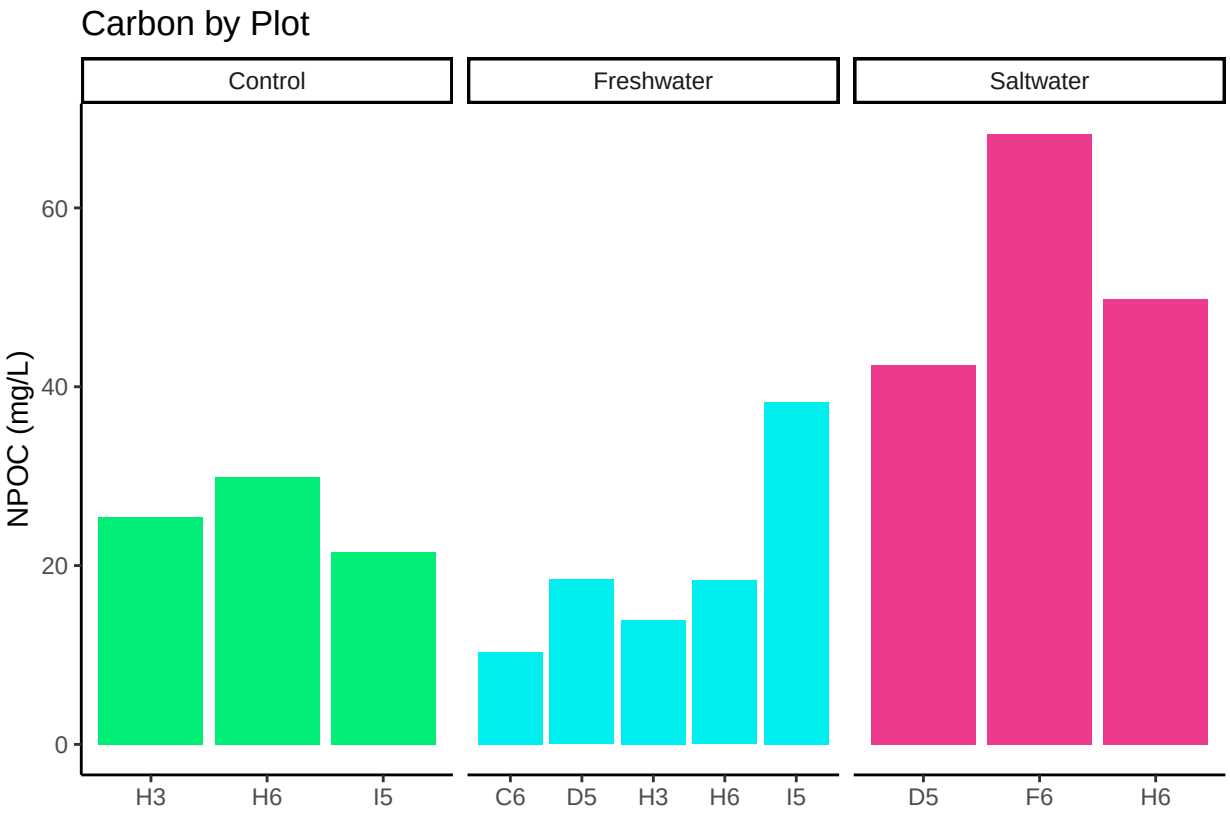
Visualize Data by Plot

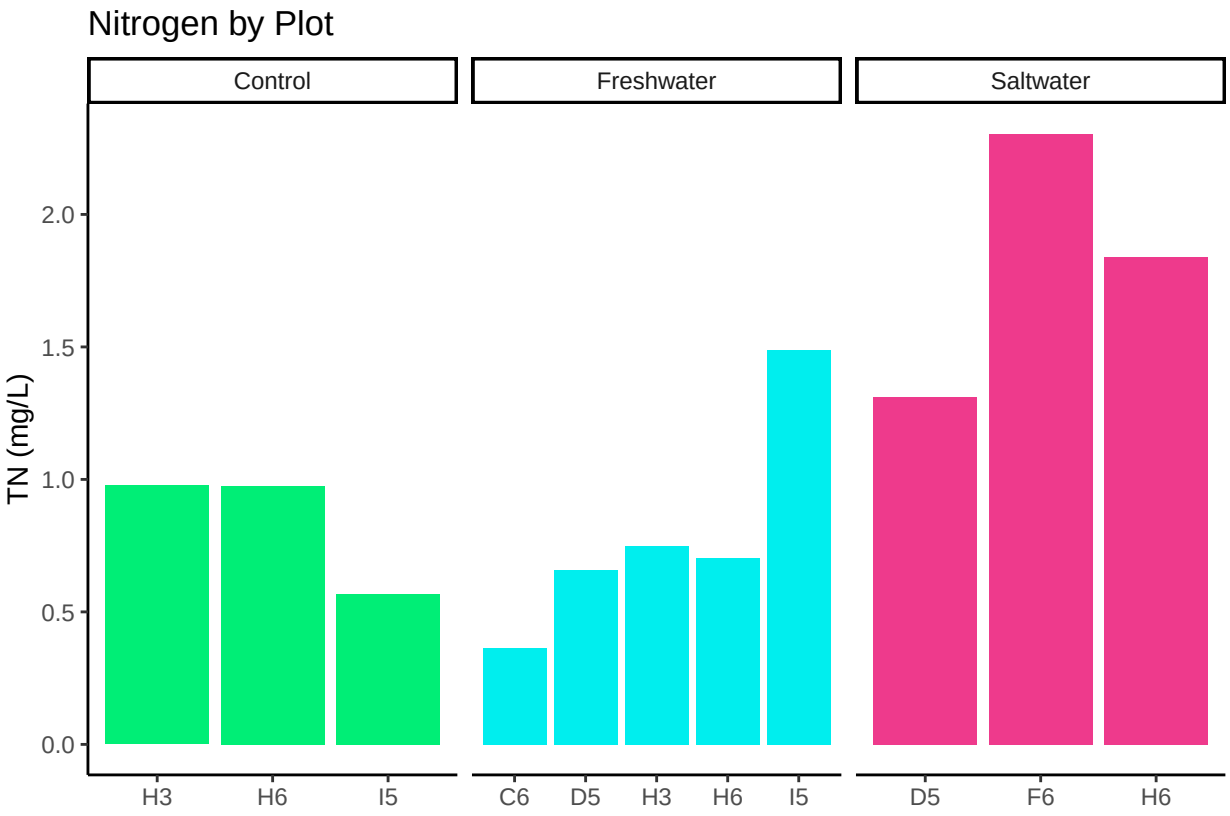
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "CTRL", "H3", "20250509"), c("TMP", "CTRL", "H6", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code Plot Grid_Square     Date  NA
## 1       TMP CTRL          H3 20250509 TMP
## 2       TMP CTRL          H6 20250509 TMP
## 3       TMP CTRL          I5 20250509 TMP
## 4       TMP   FW          C6 20250509 TMP
## 5       TMP   FW          D5 20250509 TMP
## 6       TMP   FW          H3 20250509 TMP
```

```
##   Site_Code Plot Grid_Square     Date  NA          sample_name npoc_raw tdn_raw
## 1       TMP CTRL          H3 20250509 TMP TMP_CTRL_H3_20250509    25.46  0.9769
## 2       TMP CTRL          H6 20250509 TMP TMP_CTRL_H6_20250509    29.91  0.9752
## 3       TMP CTRL          I5 20250509 TMP TMP_CTRL_I5_20250509    21.48  0.5675
## 4       TMP   FW          C6 20250509 TMP   TMP_FW_C6_20250509    10.30  0.3652
## 5       TMP   FW          D5 20250509 TMP   TMP_FW_D5_20250509    18.45  0.6574
## 6       TMP   FW          H3 20250509 TMP   TMP_FW_H3_20250509    13.93  0.7482
##            run_datetime                npoc_flag               tdn_flag
## 1 5/23/2025 2:18:11 AM NPOC checks out of range TN checks out of range
## 2 5/23/2025 2:36:46 AM NPOC checks out of range TN checks out of range
## 3 5/23/2025 3:06:35 AM NPOC checks out of range TN checks out of range
## 4 5/23/2025 3:36:49 AM NPOC checks out of range TN checks out of range
## 5 5/23/2025 3:58:38 AM NPOC checks out of range TN checks out of range
## 6 5/23/2025 4:26:17 AM NPOC checks out of range TN checks out of range
```


Carbon by Plot
Control
Freshwater
Saltwater
NPOC (mg/L)
0
20
40
60
H3
H6
I5
C6
D5
H3
H6
I5
D5
F6
H6


Nitrogen by Plot
Control
Freshwater
Saltwater
TN (mg/L)
2.0
1.5
1.0
0.5
0.0
H3
H6
I5
C6
D5
H3
H6
I5
D5
F6
H6

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 11 x 2
##    sample_name        metadata_recorded
##    <chr>              <lgl>
##  1 TMP_C_H3_20250509  TRUE
##  2 TMP_C_H6_20250509  TRUE
##  3 TMP_C_I5_20250509  TRUE
##  4 TMP_FW_C6_20250509 TRUE
##  5 TMP_FW_D5_20250509 TRUE
##  6 TMP_FW_H3_20250509 TRUE
##  7 TMP_FW_H6_20250512 TRUE
##  8 TMP_FW_I5_20250509 TRUE
##  9 TMP_SW_D5_20250509 TRUE
## 10 TMP_SW_F6_20250509 TRUE
## 11 TMP_SW_H6_20250509 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     H3          15 DOC         C_H3_D~ 2025~     25.5   2122.
## 2 COMPASS: TEMP~ C     H6          15 DOC         C_H6_D~ 2025~     29.9   2492.
## 3 COMPASS: TEMP~ C     I5          15 DOC         C_I5_D~ 2025~     21.5   1790
## 4 COMPASS: TEMP~ FW    C6          15 DOC         FW_C6_~ 2025~     10.3    858.
## 5 COMPASS: TEMP~ FW    D5          15 DOC         FW_D5_~ 2025~     18.4   1537.
## 6 COMPASS: TEMP~ FW    H3          15 DOC         FW_H3_~ 2025~     13.9   1161.
## # 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