COMPASS: TEMPEST Discrete DOC Data QAQC

June 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 = "06/03/25"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = "One CTRL (H6) sample has high TN, no issue with peaks or sample before/after.
  NPOC in that sample fine."

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2025/TMP_202506.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202506_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202506.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_20250602     47.0    1.18 6/3/2025 11:56:03 PM
## 2 TMP_SW_C3_20250602     65.2    1.80 6/4/2025 12:18:54 AM
## 3 TMP_SW_C6_20250602     54.2    1.87 6/4/2025 12:38:06 AM
## 4 TMP_SW_D5_20250602     33.0    1.04 6/4/2025 1:06:44 AM
## 5 TMP_SW_E3_20250602     33.6    1.08 6/4/2025 1:30:44 AM
## 6 TMP_SW_F4_20250602     41.3    1.45 6/4/2025 1:59:04 AM
```
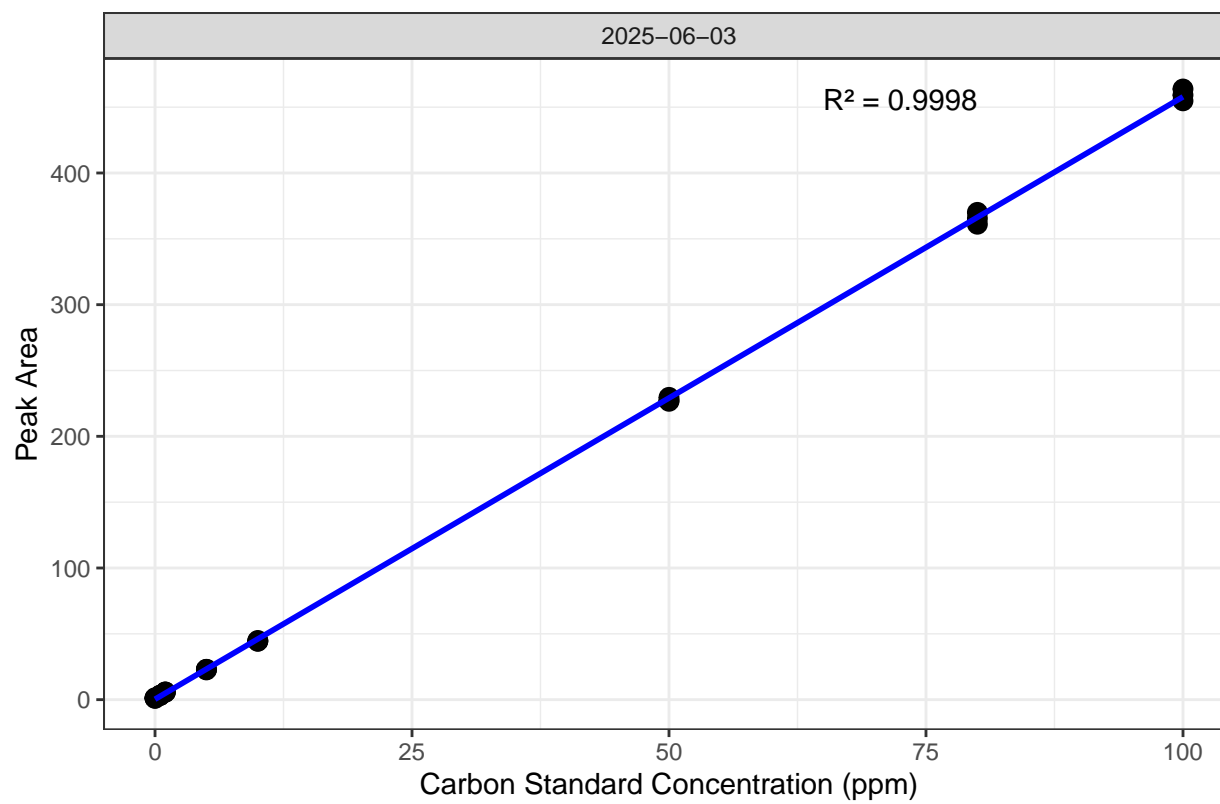
Assessing standard Curves

Assess the Standard Curve

New names:
`geom_smooth()` using formula = 'y ~ x'
* `` -> `...18`
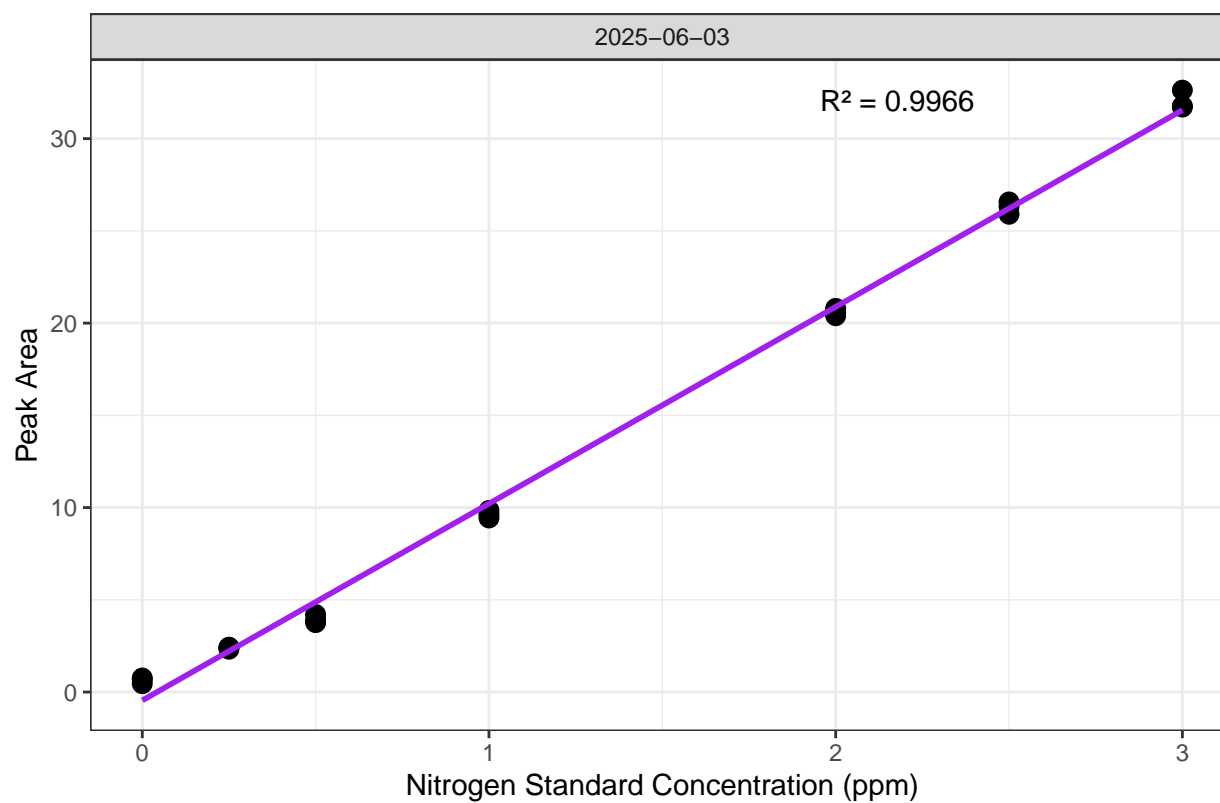
NPOC Std Curve by Date

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

TN Std Curve by Date

Slope Drift Assessment
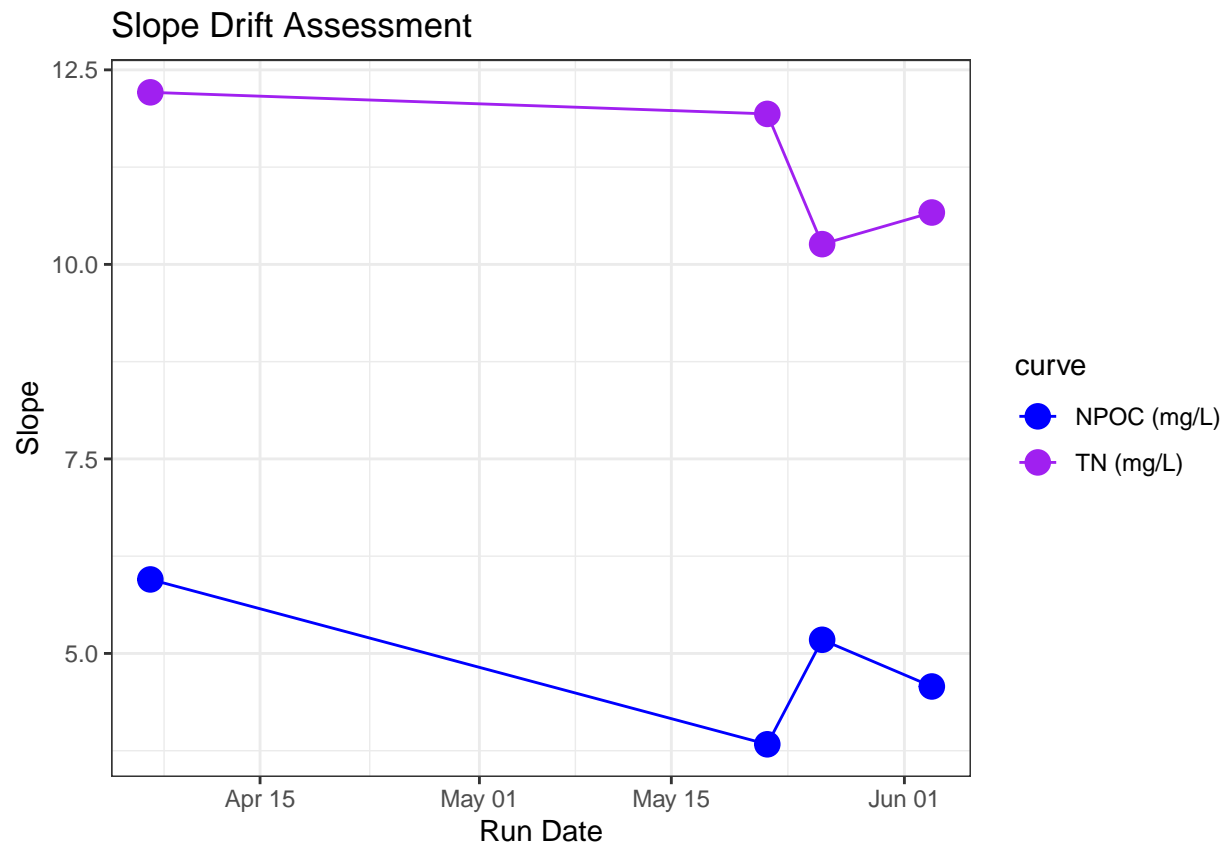
```
## [1] "NPOC Curve r2 GOOD"

## [1] "TN Curve r2 GOOD"
```
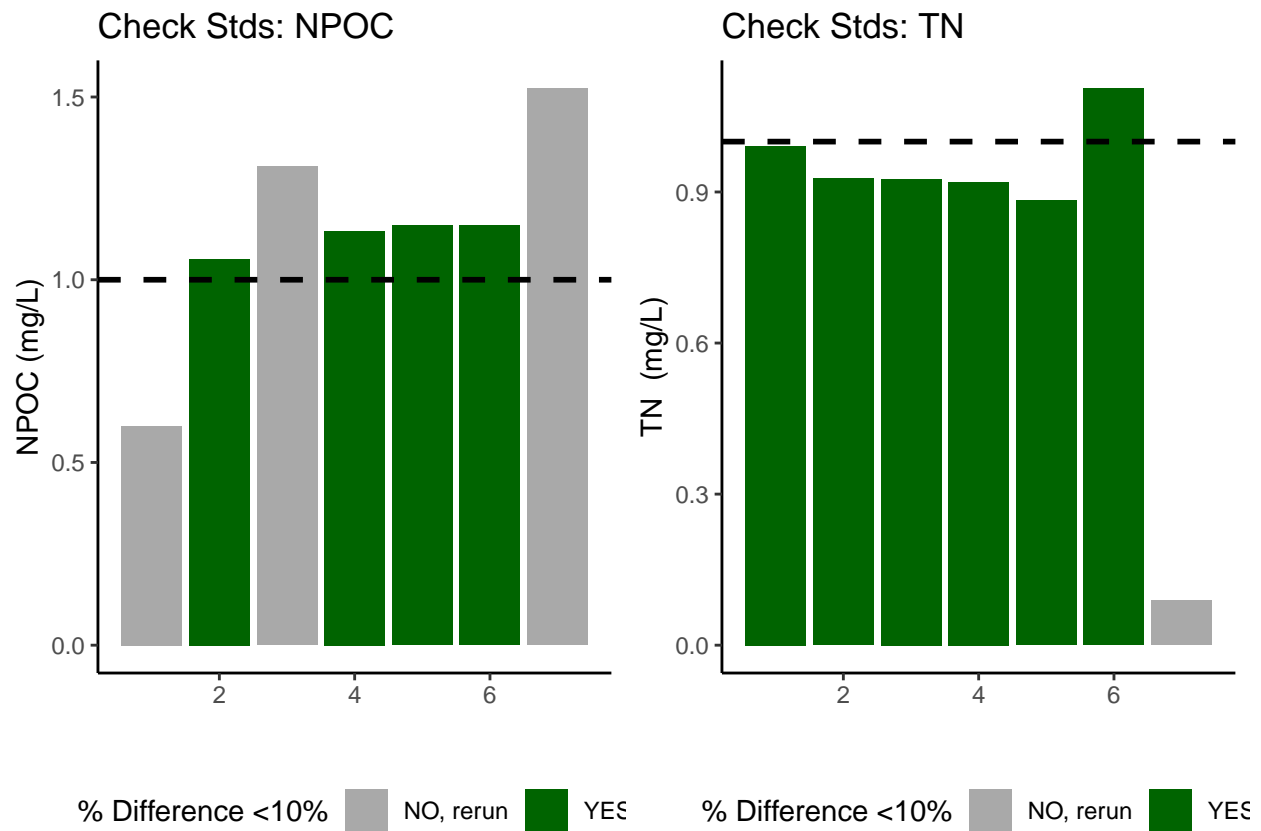
Assess Check Standards

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

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

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

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



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

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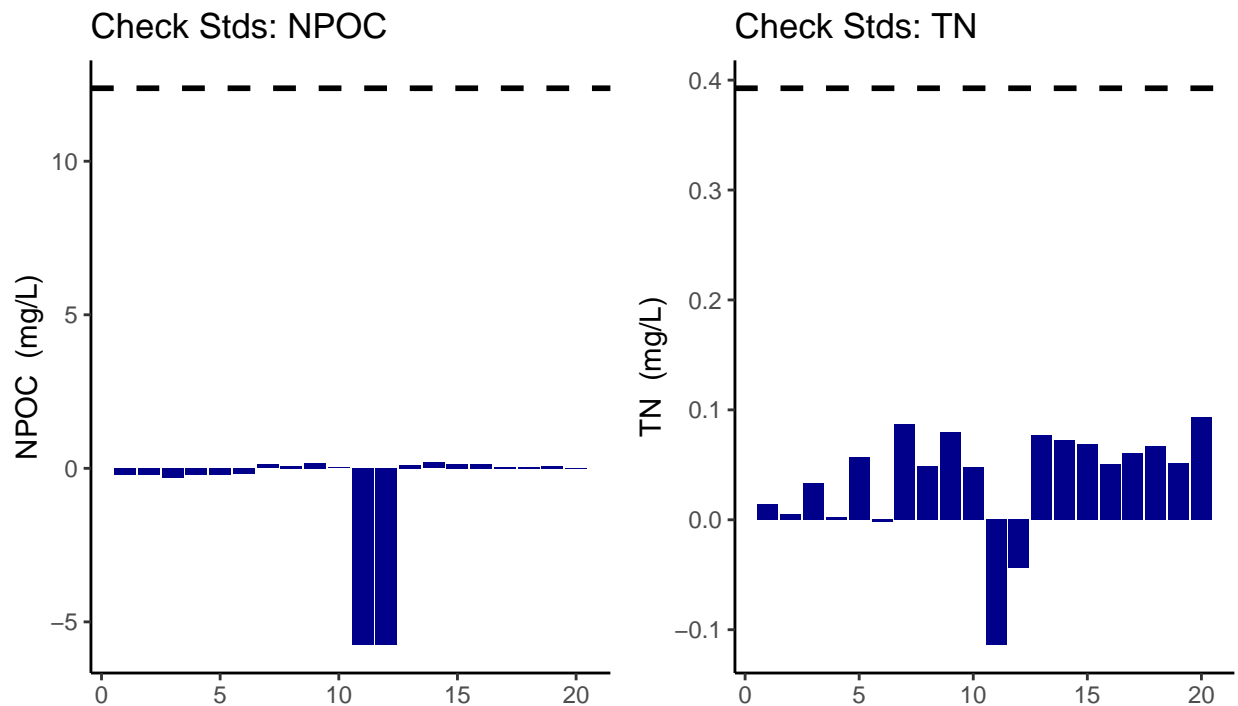
Assess Blanks

```
## 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"
```



```
## carbon blanks:
```

```
## [1] -0.5818205
```

```
## nitrogen blanks:
```

```
## [1] 0.0377145
```

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_SW_H6_20250602         34.0        1.01
## 2 TMP_FW_I5_20250602         12.2        0.422
## 3 TMP_CTRL_I5_20250602       15.3        0.389


##            sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_CTRL_I5_20250602    15.11  0.3941 6/4/2025 1:52:56 PM
## 2   TMP_FW_I5_20250602    12.27  0.3950 6/4/2025 9:05:23 AM
## 3   TMP_SW_H6_20250602    34.14  1.0460 6/4/2025 3:19:30 AM
##                npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup
## 1 NPOC checks out of range              15.28      0.3890
## 2 NPOC checks out of range              12.15      0.4225
## 3 NPOC checks out of range              33.99      1.0140


##            sample_name npoc_raw tdn_raw         run_datetime
## 1 TMP_CTRL_I5_20250602    15.11  0.3941 6/4/2025 1:52:56 PM
## 2   TMP_FW_I5_20250602    12.27  0.3950 6/4/2025 9:05:23 AM
## 3   TMP_SW_H6_20250602    34.14  1.0460 6/4/2025 3:19:30 AM
##                npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup npoc_dups_cv
## 1 NPOC checks out of range              15.28      0.3890    1.1819797
## 2 NPOC checks out of range              12.15      0.4225    1.0388083
## 3 NPOC checks out of range              33.99      1.0140    0.4663195
##   npoc_dups_cv_flag tdn_dups_cv tdn_dups_cv_flag
## 1               YES    1.375194              YES
## 2               YES    6.970145              YES
## 3               YES    3.259452              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.
```
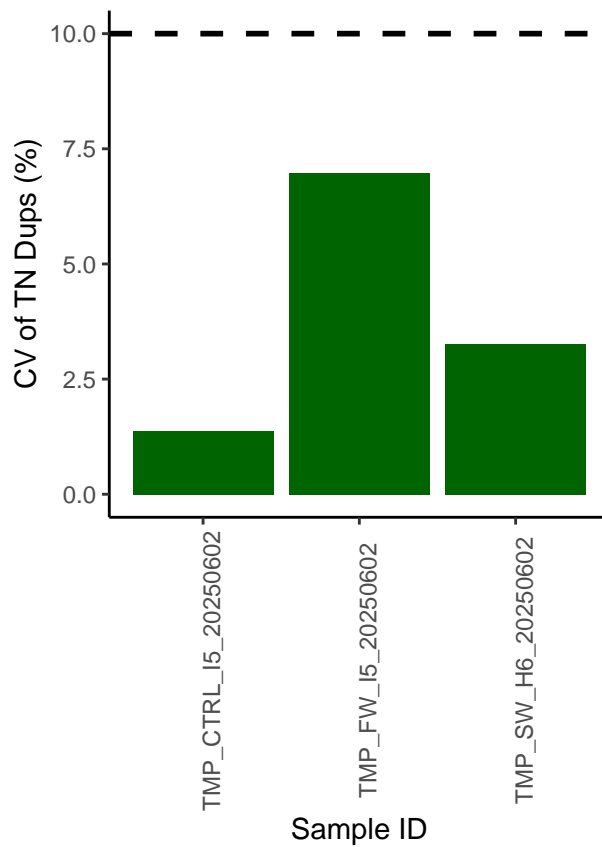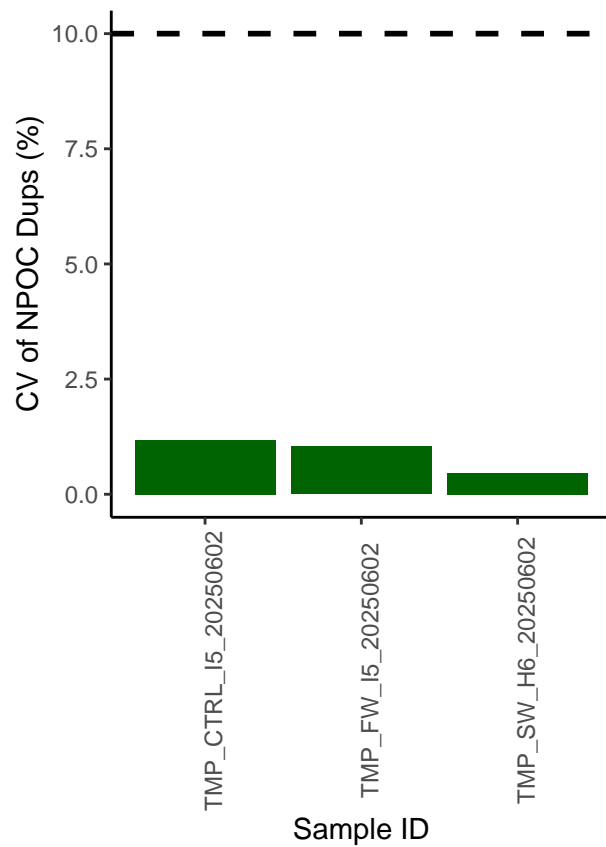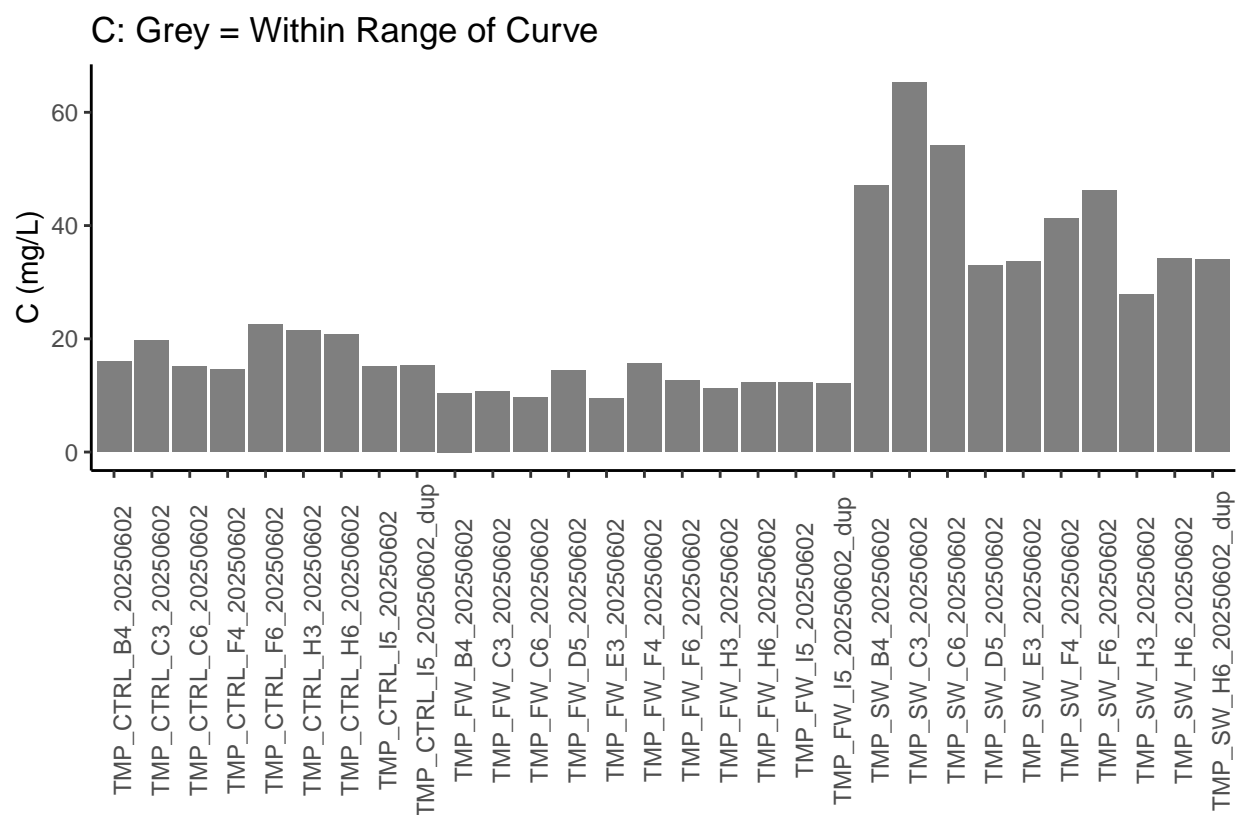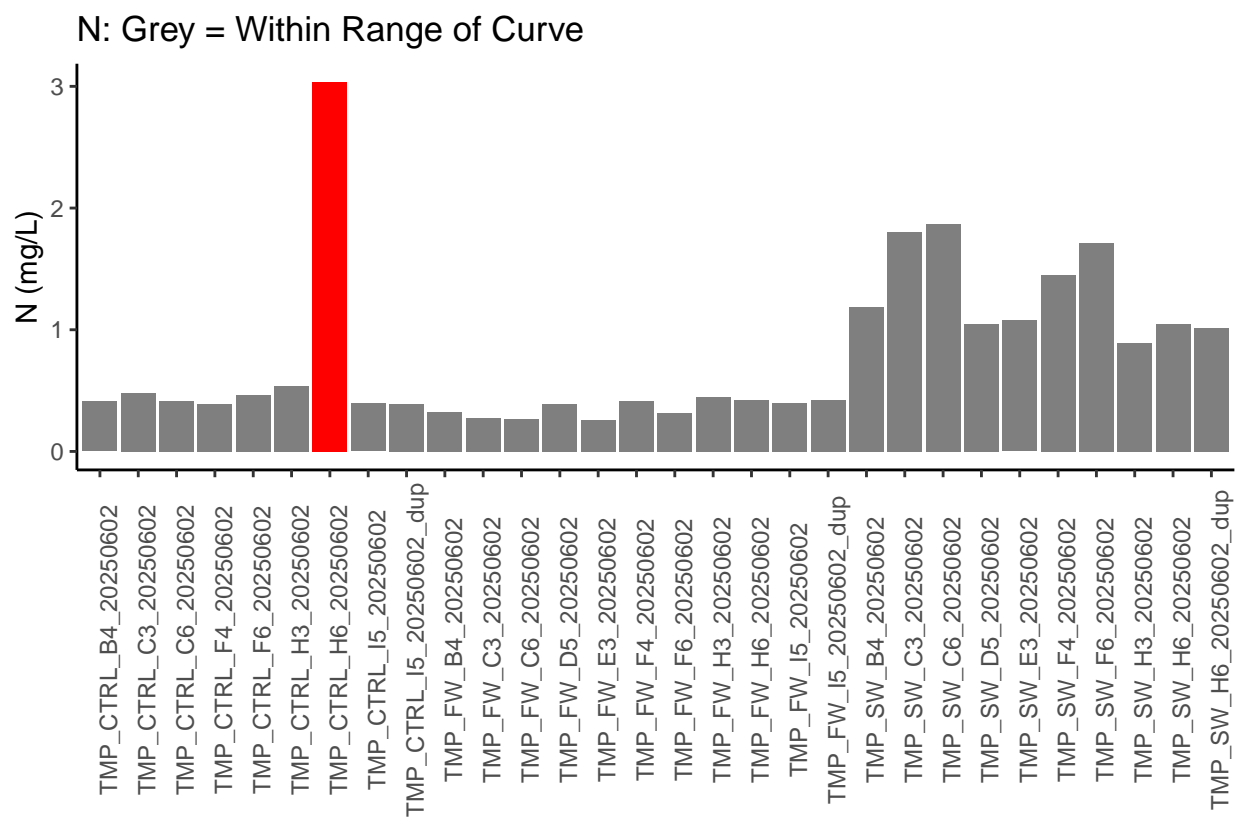
```
## [1] ">60% of Carbon Duplicates have a CV <10%"

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

Sample Flagging

C: Grey = Within Range of Curve

N: Grey = Within Range of Curve

Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "SW", "B4", "20250602"), 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 20250602 TMP
## 2       TMP   SW          C3 20250602 TMP
## 3       TMP   SW          C6 20250602 TMP
## 4       TMP   SW          D5 20250602 TMP
## 5       TMP   SW          E3 20250602 TMP
## 6       TMP   SW          F4 20250602 TMP
```

```
##   Site_Code Plot Grid_Square     Date  NA         sample_name npoc_raw tdn_raw
## 1       TMP   SW          B4 20250602 TMP TMP_SW_B4_20250602    47.02   1.185
## 2       TMP   SW          C3 20250602 TMP TMP_SW_C3_20250602    65.21   1.804
## 3       TMP   SW          C6 20250602 TMP TMP_SW_C6_20250602    54.19   1.871
## 4       TMP   SW          D5 20250602 TMP TMP_SW_D5_20250602    33.01   1.045
## 5       TMP   SW          E3 20250602 TMP TMP_SW_E3_20250602    33.58   1.076
## 6       TMP   SW          F4 20250602 TMP TMP_SW_F4_20250602    41.28   1.453
##            run_datetime               npoc_flag tdn_flag
## 1 6/3/2025 11:56:03 PM NPOC checks out of range
## 2 6/4/2025 12:18:54 AM NPOC checks out of range
## 3 6/4/2025 12:38:06 AM NPOC checks out of range
## 4  6/4/2025 1:06:44 AM NPOC checks out of range
## 5  6/4/2025 1:30:44 AM NPOC checks out of range
## 6  6/4/2025 1:59:04 AM NPOC checks out of range
```

Carbon by Plot

Nitrogen by Plot
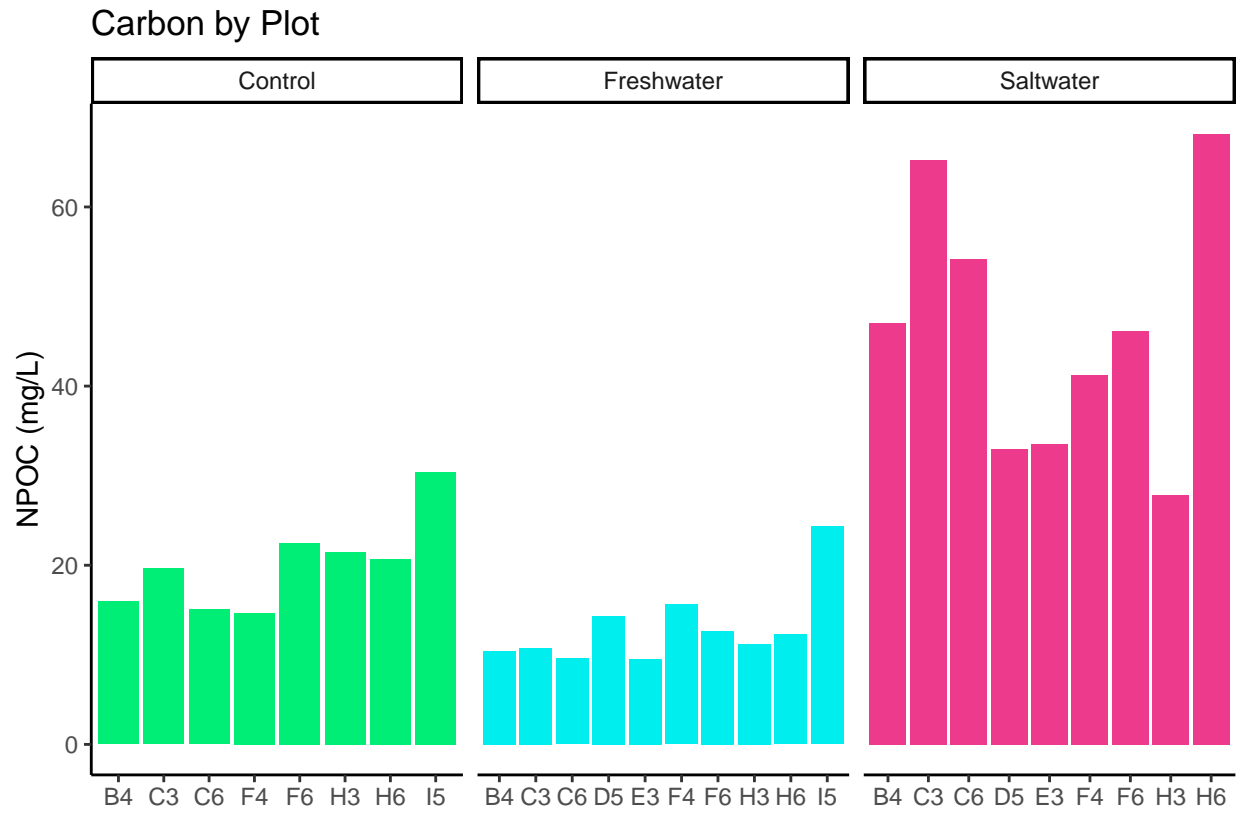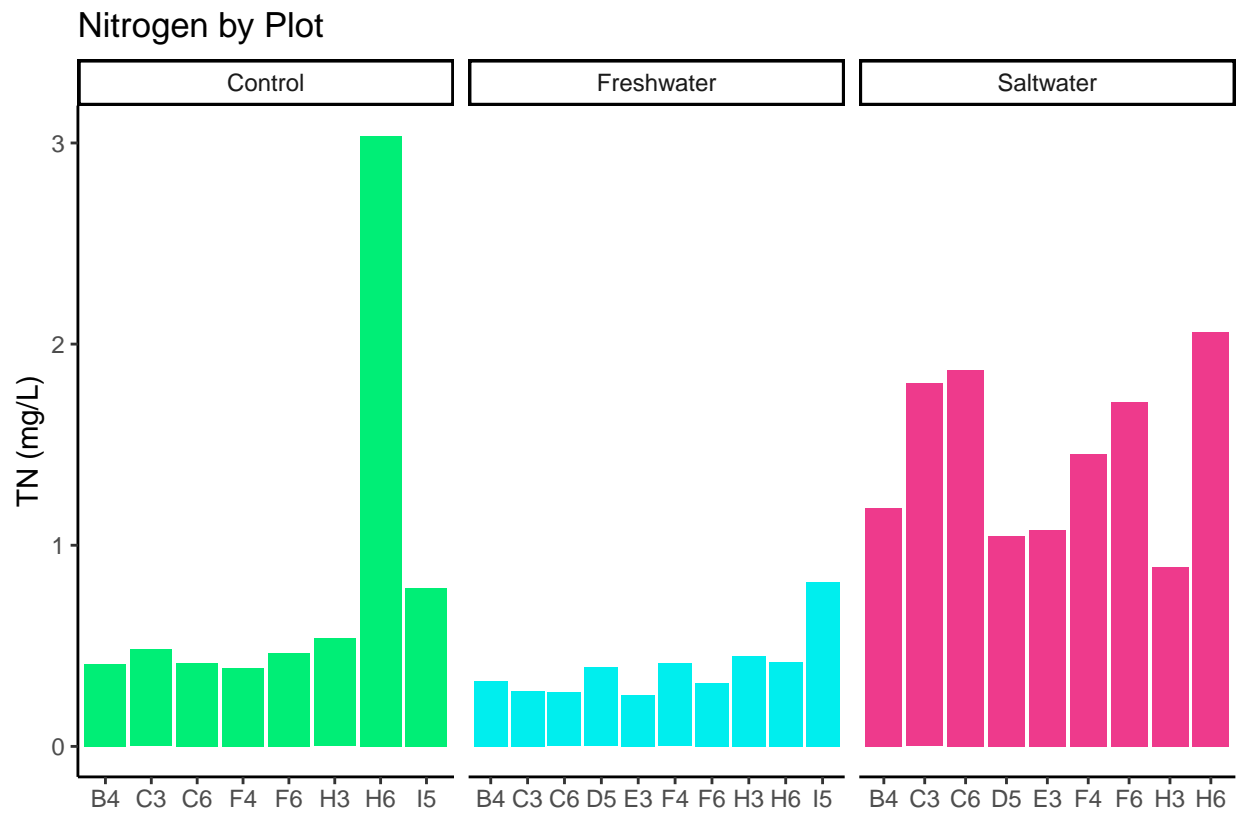
Convert data from mg/L to uMoles/L

Add in/check metadata

```
## Check Sample IDs with Metadata


## # A tibble: 27 x 2
##    sample_name       metadata_recorded
##    <chr>             <lgl>
##  1 TMP_SW_B4_20250602 TRUE
##  2 TMP_SW_C3_20250602 TRUE
##  3 TMP_SW_C6_20250602 TRUE
##  4 TMP_SW_D5_20250602 TRUE
##  5 TMP_SW_E3_20250602 TRUE
##  6 TMP_SW_F4_20250602 TRUE
##  7 TMP_SW_F6_20250602 TRUE
##  8 TMP_SW_H3_20250602 TRUE
##  9 TMP_SW_H6_20250602 TRUE
## 10 TMP_FW_B4_20250602 TRUE
## # i 17 more rows
```

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~     47.0   3918.
## 2 COMPASS: TEMP~ SW   C3          15 DOC         SW_C3_~ 2025~     65.2   5434.
## 3 COMPASS: TEMP~ SW   C6          15 DOC         SW_C6_~ 2025~     54.2   4516.
## 4 COMPASS: TEMP~ SW   D5          15 DOC         SW_D5_~ 2025~     33.0   2751.
## 5 COMPASS: TEMP~ SW   E3          15 DOC         SW_E3_~ 2025~     33.6   2798.
## 6 COMPASS: TEMP~ SW   F4          15 DOC         SW_F4_~ 2025~     41.3   3440
## # 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