

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 samples before/after and the NPOC in that sample is fine.  
One check at the end of the run came out odd - was prepped by TL, not SJW - can ignore."
```

```
#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

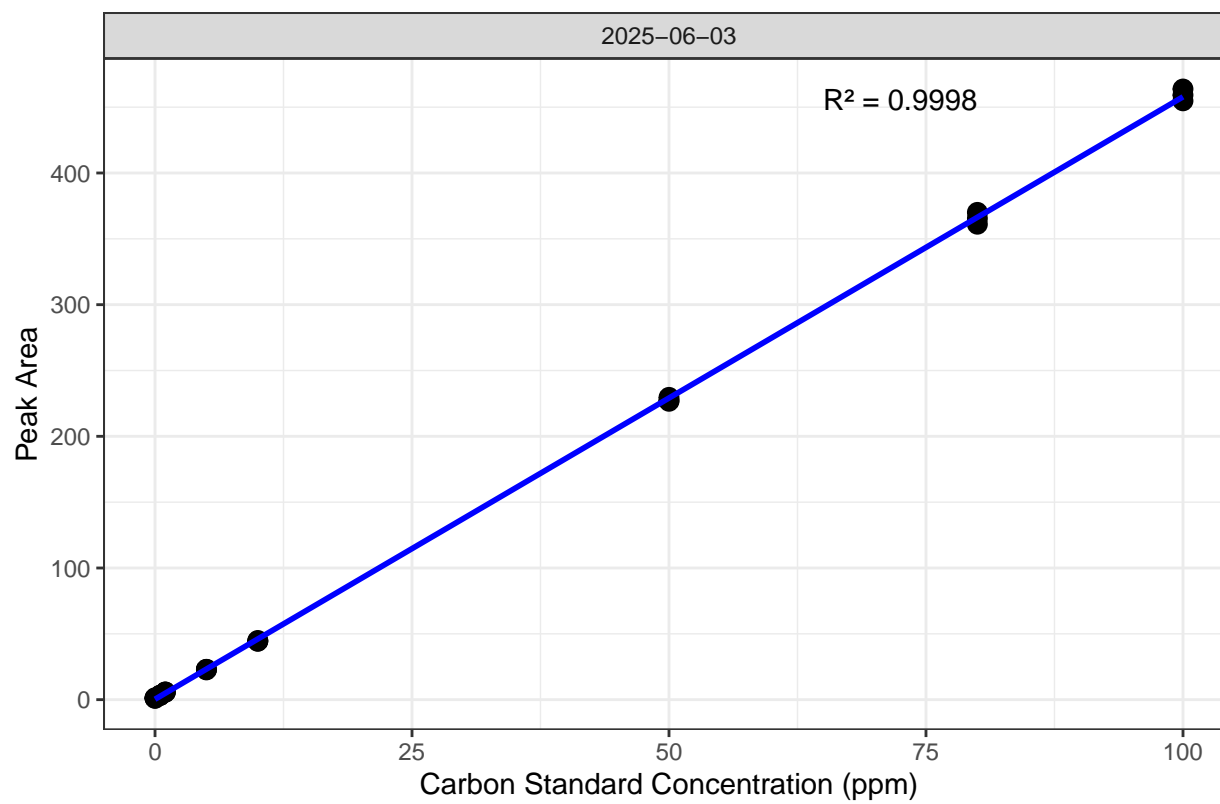
```
## Assess the Standard Curve
```

```
## New names:
```

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

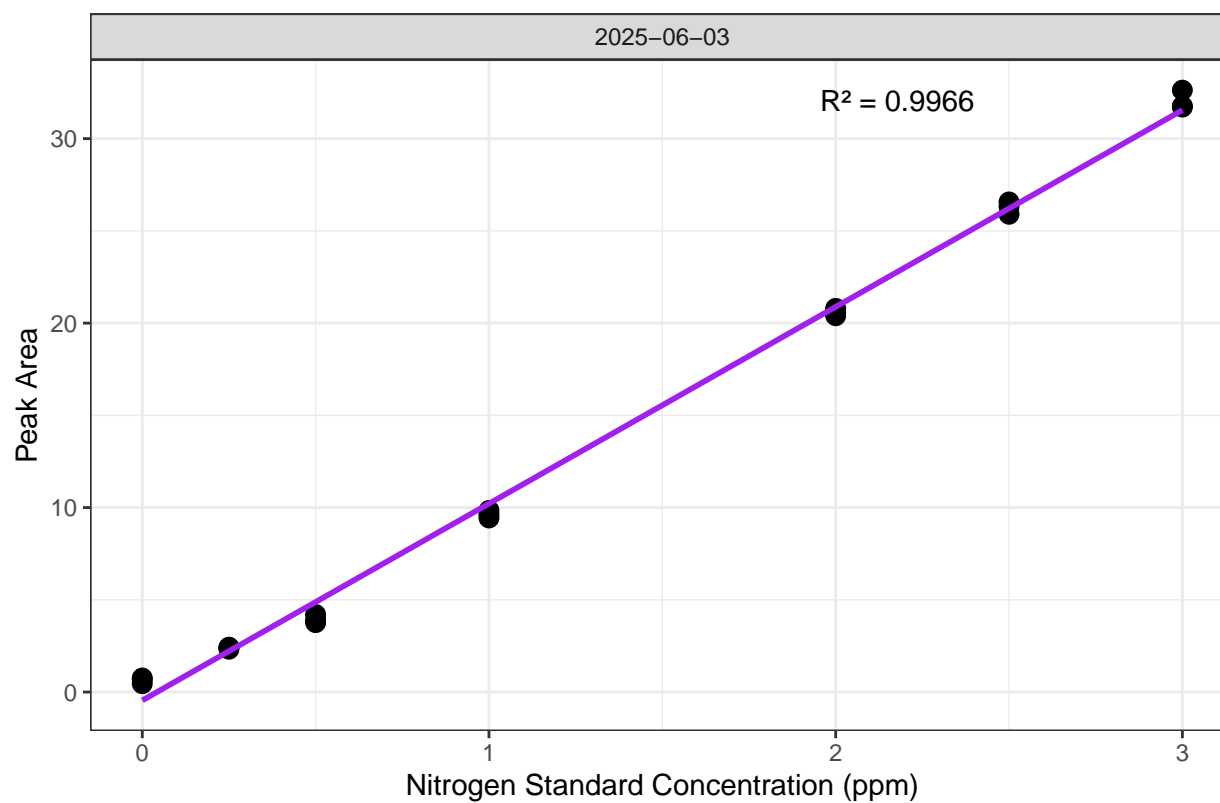
```
## * '' -> '...18'
```

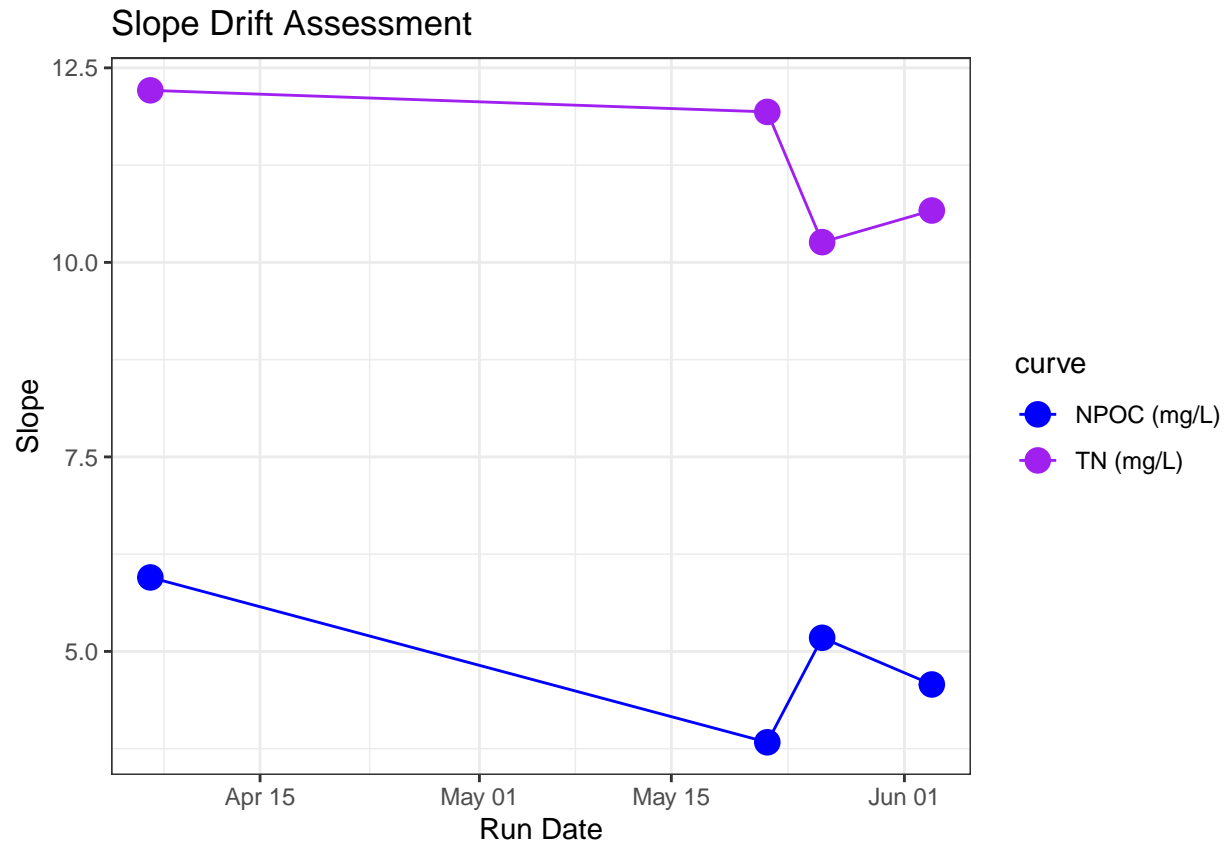
NPOC Std Curve by Date



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

TN Std Curve by Date





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

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

Assess Check Standards

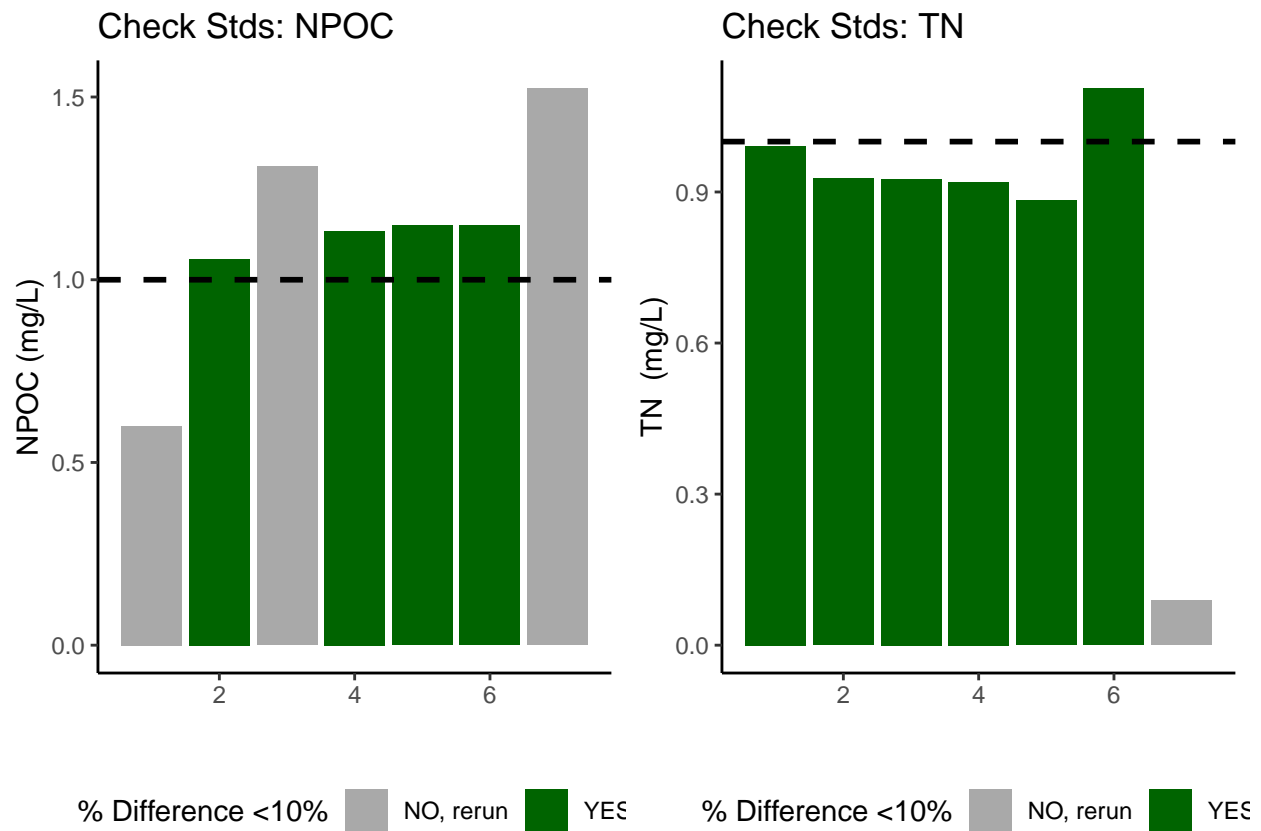
```
## Assess the Check Standards
```

```
## 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

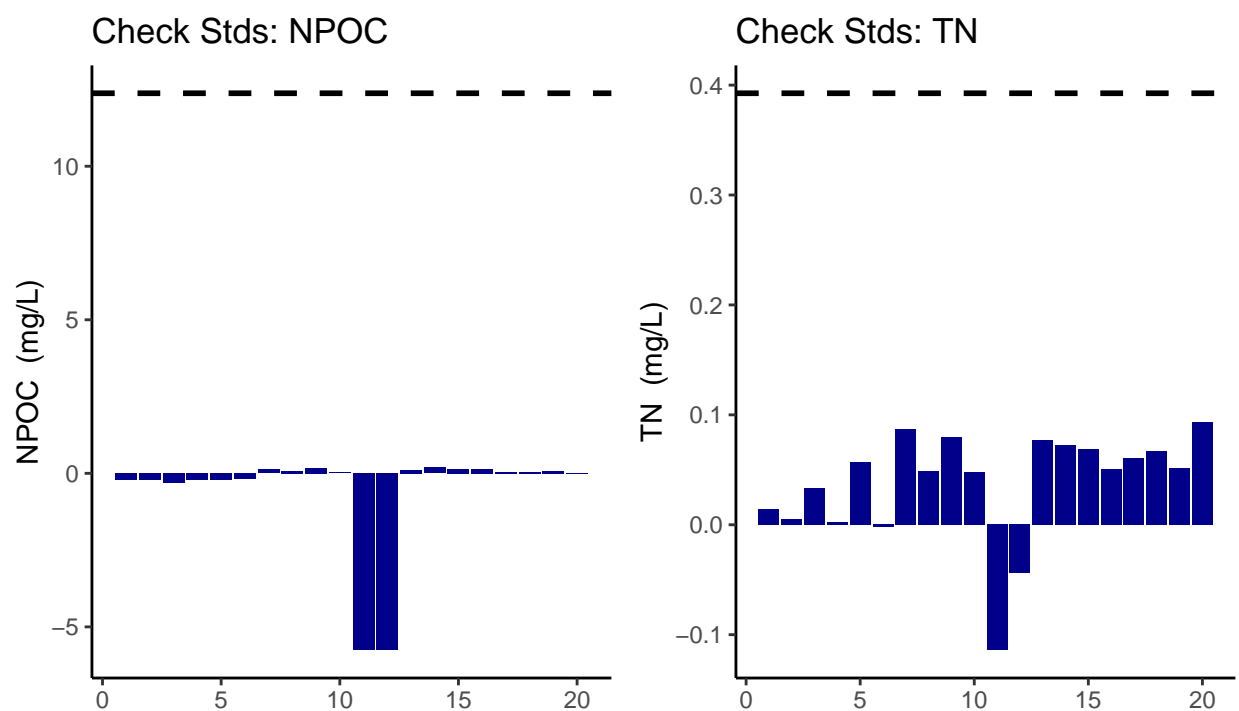
```
## Assess Blanks
```

```
## 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"
```



Blank Conc <25% Quartile Samples ■ YE

Blank Conc <25% Quartile Samples ■ Y

```
## carbon blanks:
```

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

```
## nitrogen blanks:
```

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

Assess Duplicates - if there are any

```
## Assess Duplicates
```

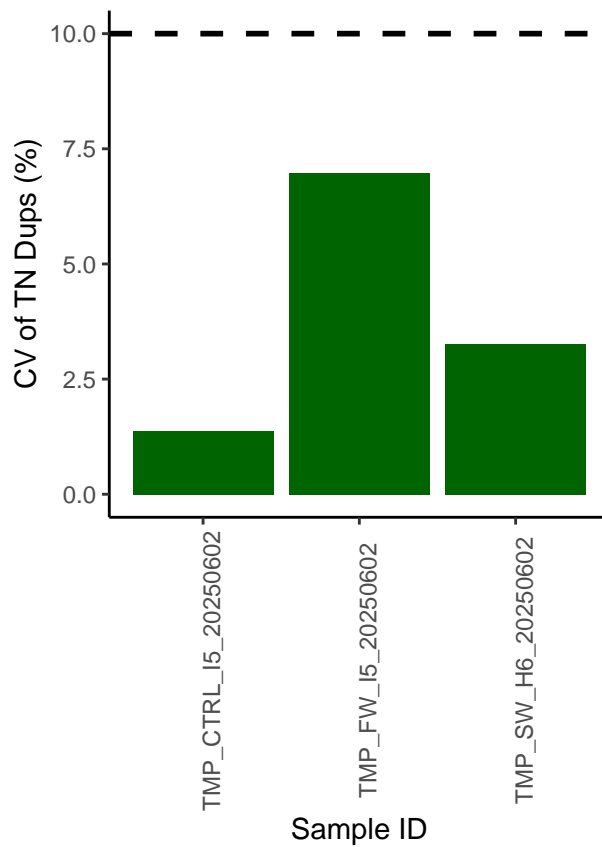
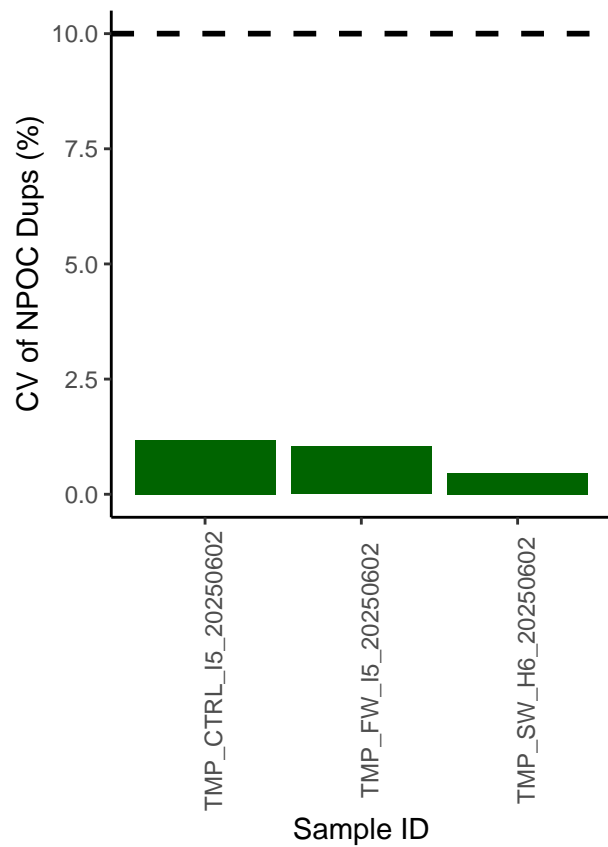
```
## # A tibble: 3 x 3
```

```
##   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.
```

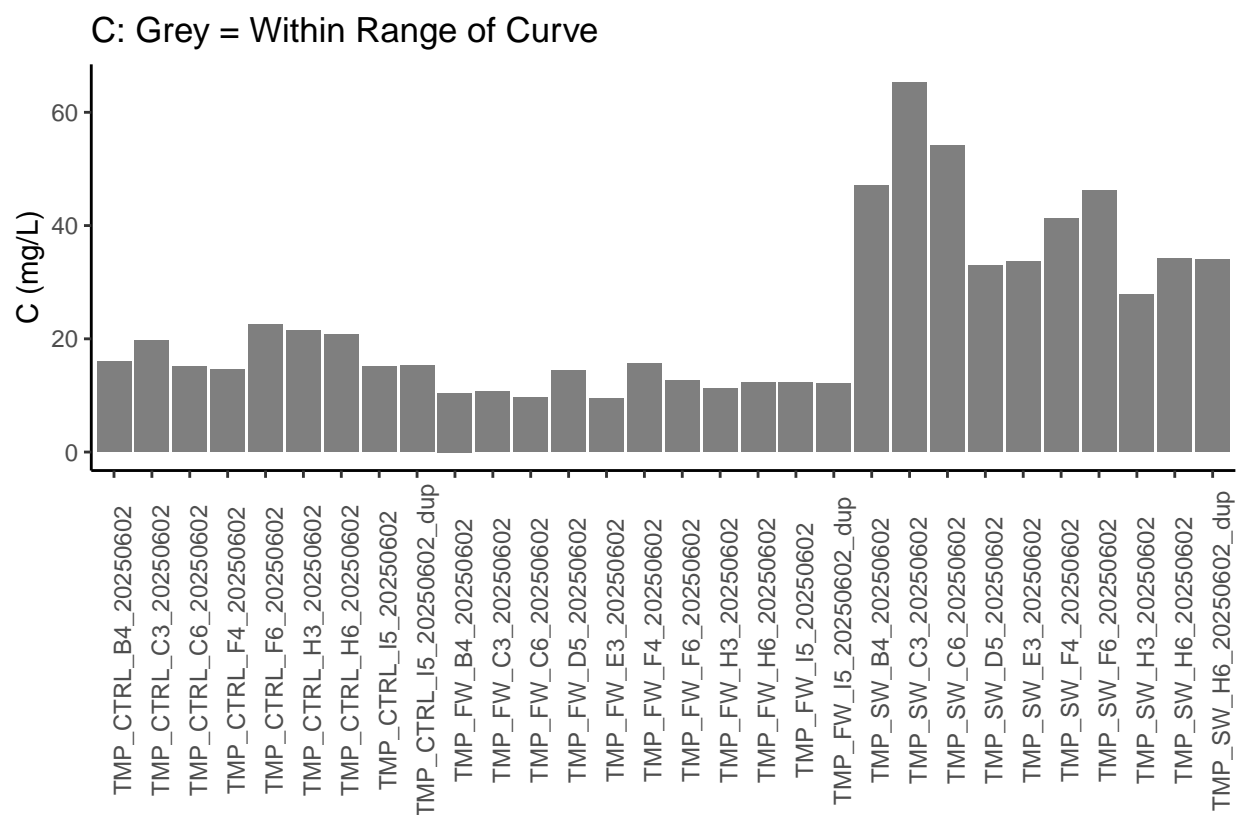



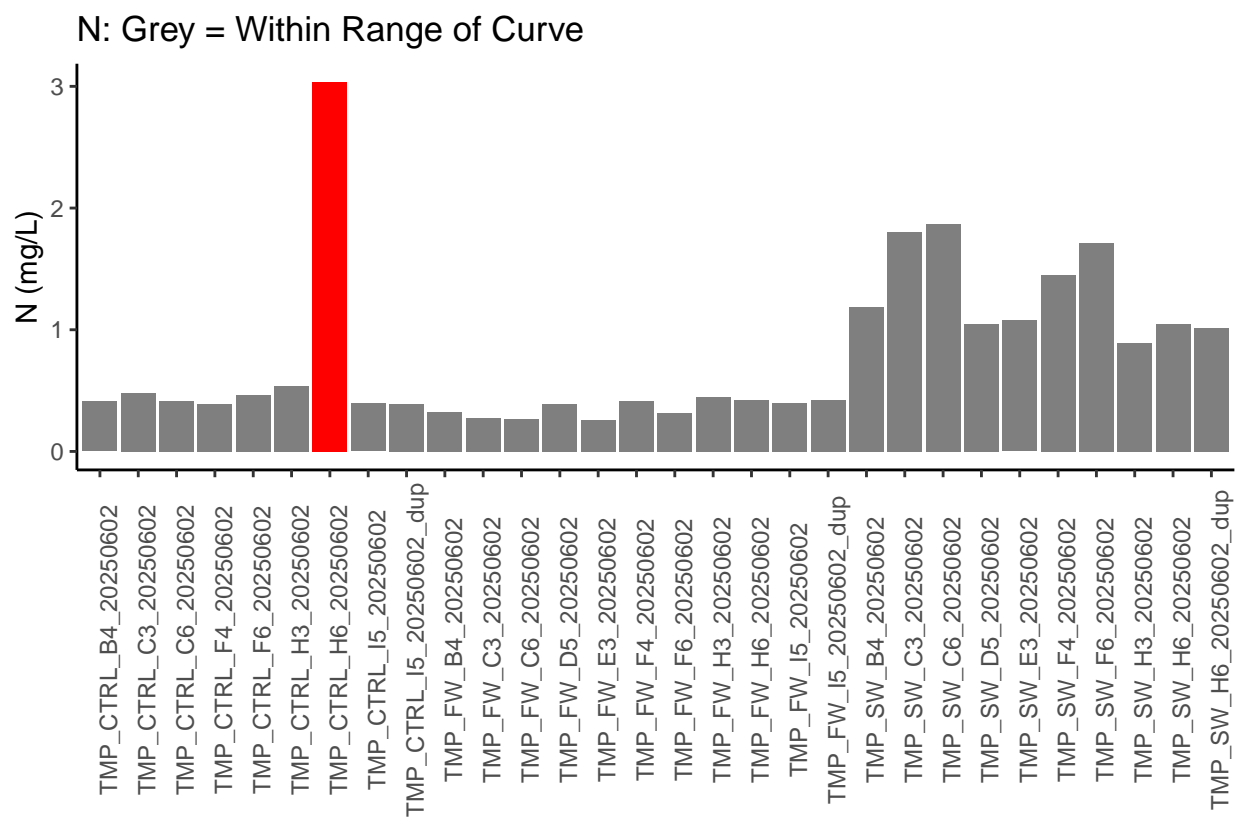
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

Sample Flagging





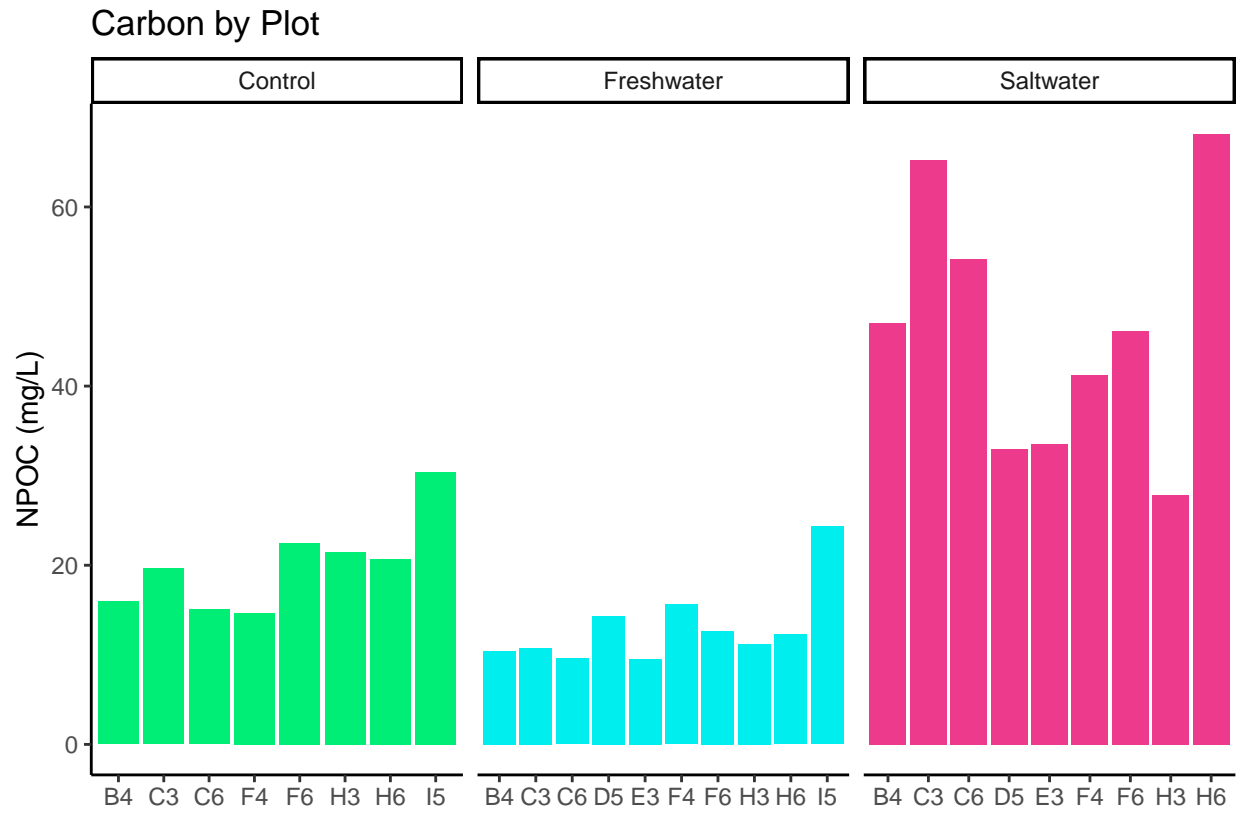
Visualize Data by Plot

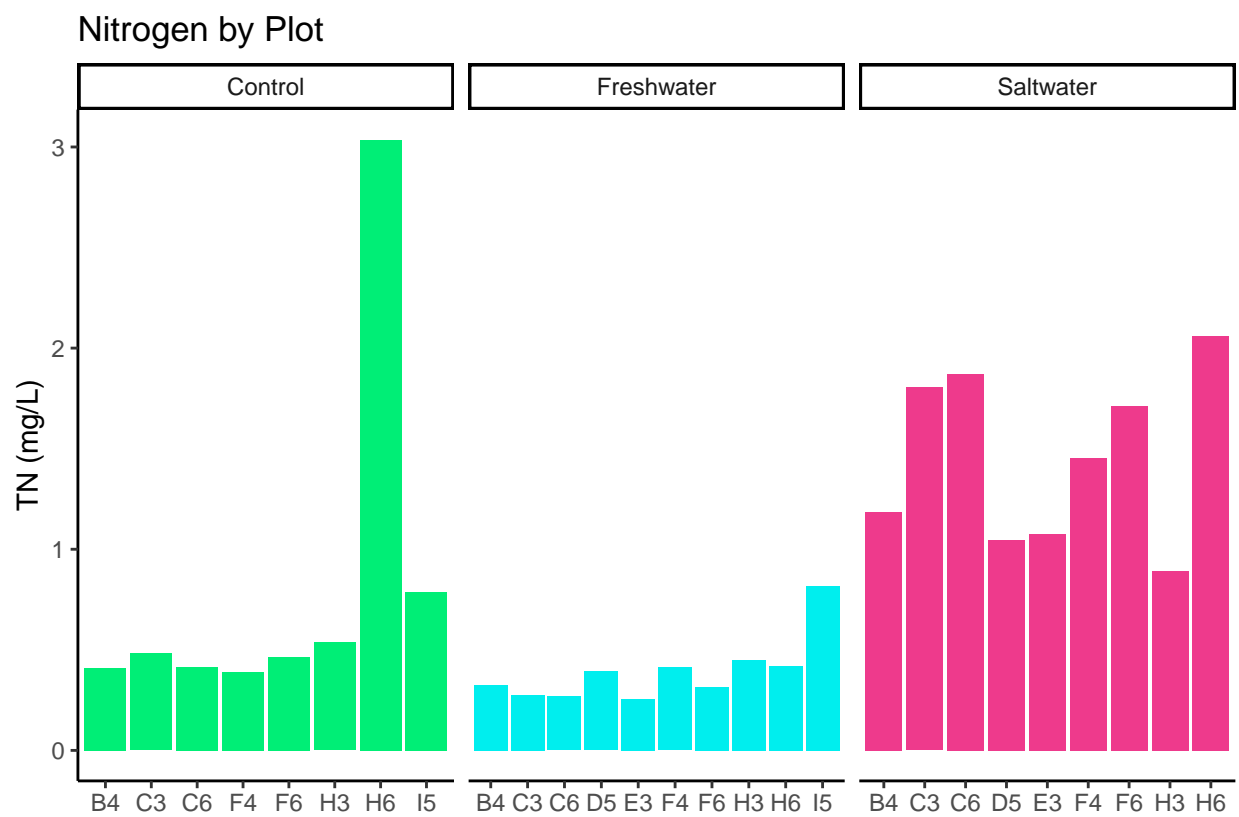
```
## Visualize Data
```

```
## 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
```





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_YYYYMMDD <dbl>, Collection_Date_YYYYMMDD <dbl>,
## #   Collection_Start_Time_24hrs <dbl>, Collection_End_Time_24hrs <dbl>,
## #   EST_EDT <chr>, Volume_mL <dbl>
```

```
#end
```