

# COMPASS TEMPEST Discrete DOC Data Workflow: 202502

January & February 2025

2025-07-09

## 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 = "Standard curve for TN is not good, reanalyzed with a
recently run standard curve to get values."

#file path and name for summary file
raw_file_name = "tmp_doc_raw_data_2025/TMP_202502.txt"
#file path and name for the all peaks file
raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202502_allpeaks.txt"
#file path and name for processed data after QAQC
processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202502.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_B4_20250131    31.4    0.985 2/4/2025 9:12:13 PM
## 2 TMP_CTRL_C3_20250131    30.5    0.660 2/4/2025 9:42:02 PM
## 3 TMP_CTRL_D5_20250131    21.1    0.560 2/4/2025 10:00:23 PM
## 4 TMP_CTRL_E3_20250131    25.9    0.772 2/4/2025 10:29:44 PM
## 5 TMP_CTRL_H6_20250131    36.8    1.23  2/4/2025 10:58:13 PM
## 6 TMP_CTRL_I5_20250131    16.8    0.526 2/4/2025 11:26:31 PM
```

## Assessing standard Curves

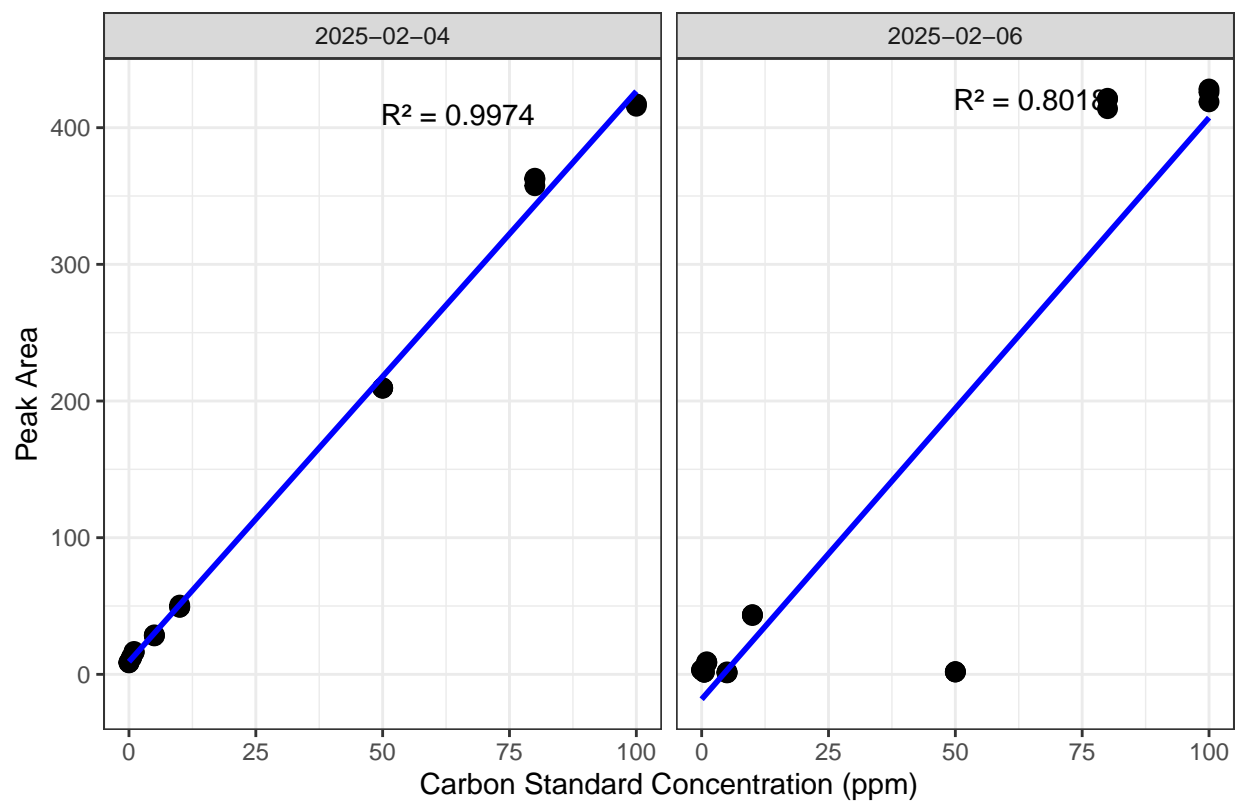
```
## Assess the Standard Curve
```

```
## New names:
```

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

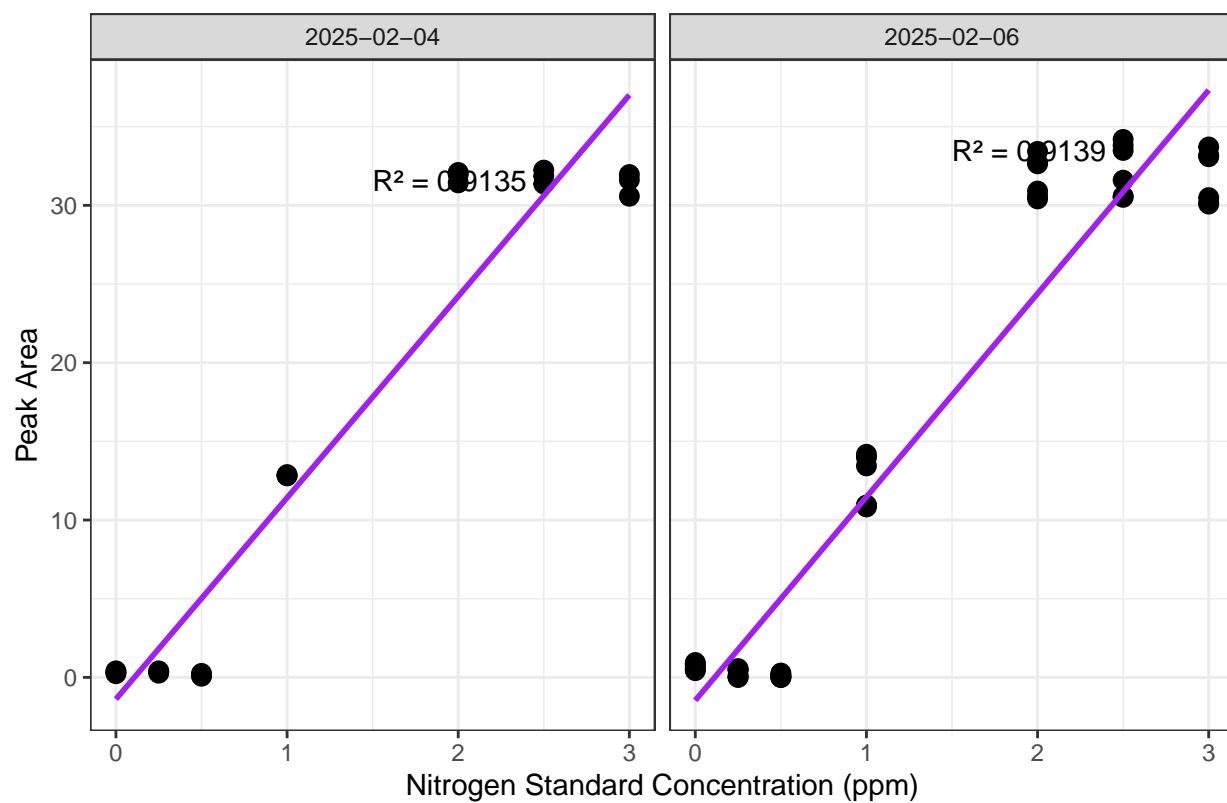
```
## * '' -> '...18'
```

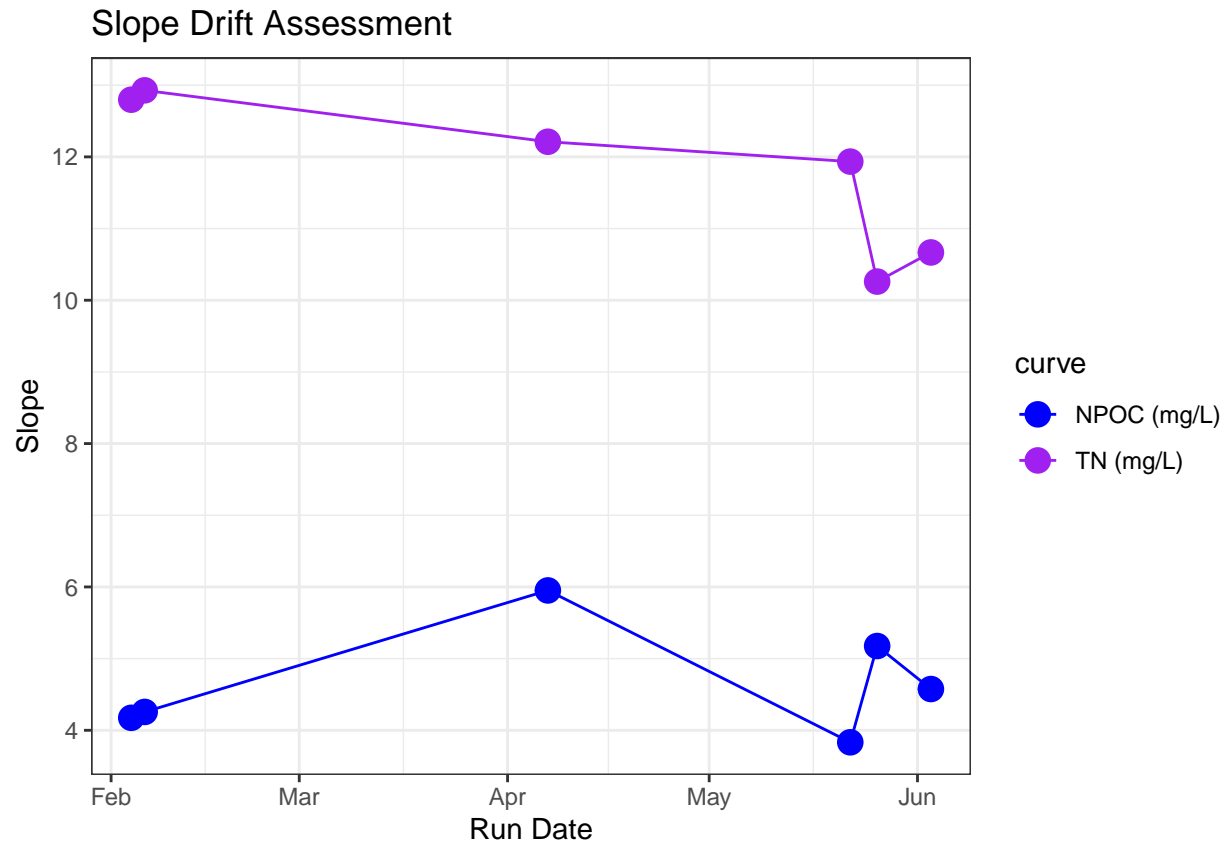
NPOC Std Curve by Date



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

TN Std Curve by Date





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

```
## [1] "TN Curve r2 is below cutoff! - REASSESS"
```

## Assess Check Standards

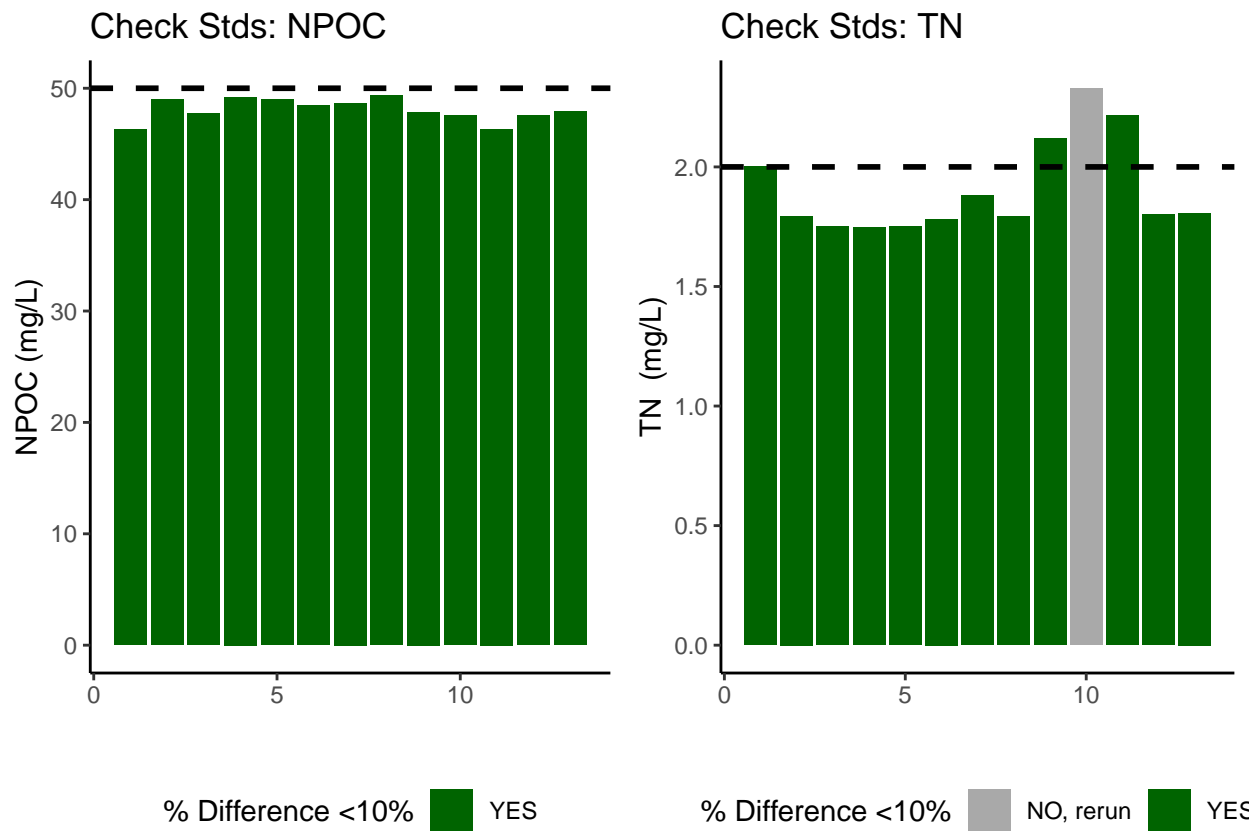
```
## Assess the Check Standards
```

```
## New names:
```

```
## * ' ' -> '...14'
```

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

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



```
## [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

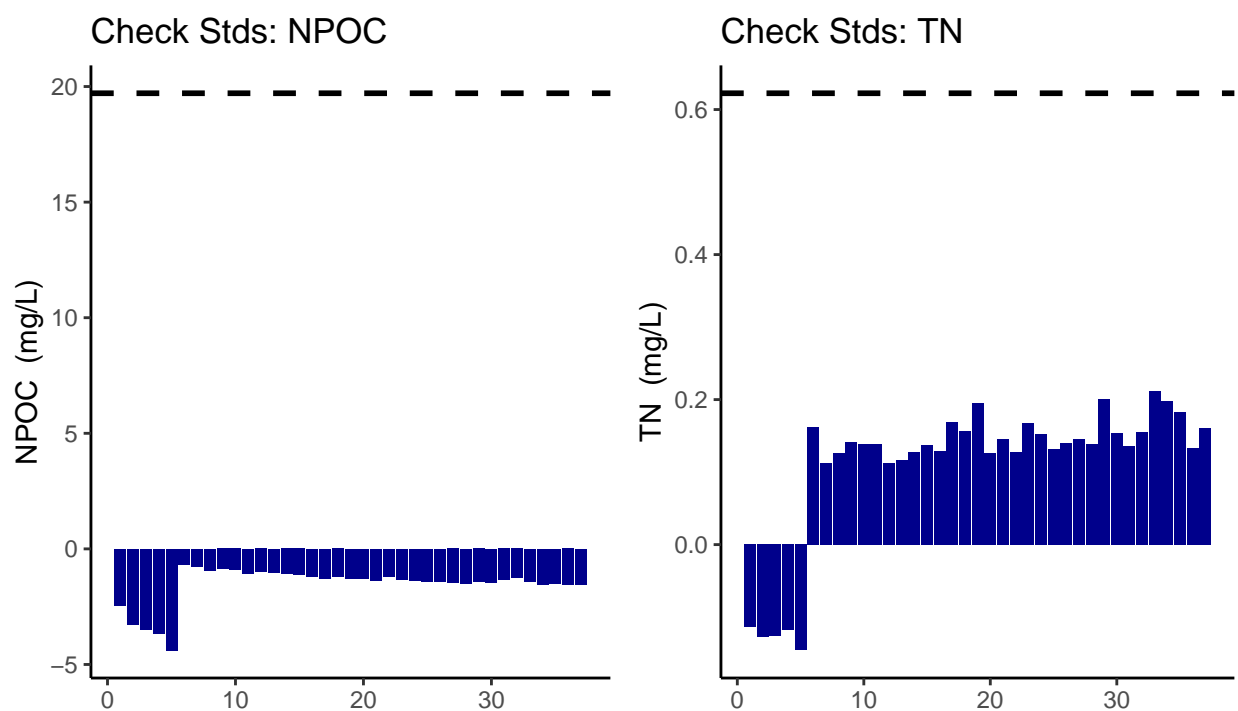
```
## Assess Blanks
```

```
## 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"
```



Blank Conc <25% Quartile Samples ☒ YE

Blank Conc <25% Quartile Samples ☒ YE

```
## carbon blanks:
```

```
## [1] -1.542005
```

```
## nitrogen blanks:
```

```
## [1] 0.111773
```

## Assess Duplicates - if there are any

```
## Assess Duplicates
```

```
## # A tibble: 4 x 3
```

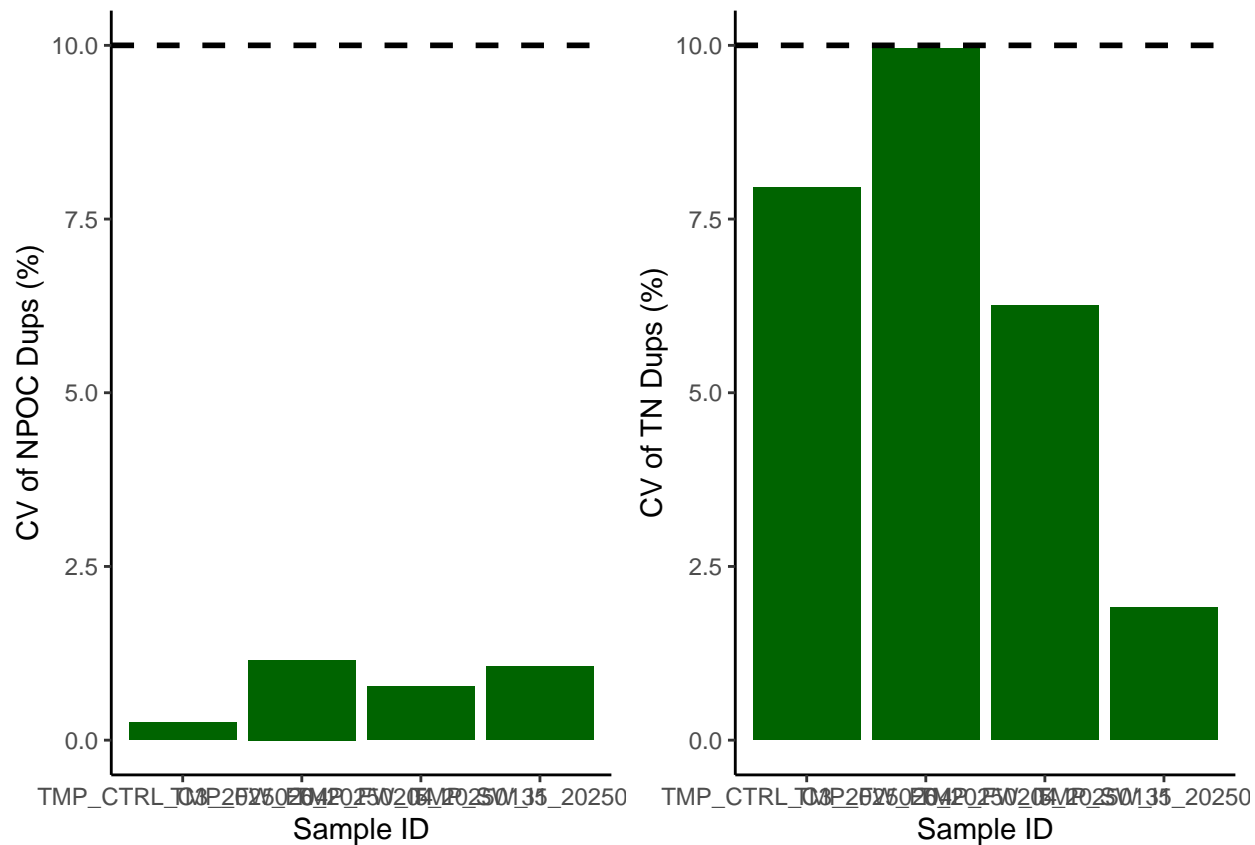
```
##   sample_name      npoc_raw_dup tdn_raw_dup
##   <chr>          <dbl>         <dbl>
## 1 TMP_FW_I5_20250131      32.7         1.03
## 2 TMP_CTRL_C3_20250204     29.6         0.619
## 3 TMP_FW_F6_20250204     18.4         0.576
## 4 TMP_SW_I5_20250204     60.8         1.73
```

```
##           sample_name npoc_raw tdn_raw      run_datetime npoc_flag
## 1 TMP_CTRL_C3_20250204   29.65  0.6686 2/5/2025 9:26:06 AM
## 2   TMP_FW_F6_20250204   18.19  0.5225 2/5/2025 6:00:06 PM
## 3   TMP_FW_I5_20250131   32.94  1.0940 2/5/2025 3:04:02 AM
## 4   TMP_SW_I5_20250204   61.38  1.6960 2/6/2025 12:58:02 AM
##   tdn_flag npoc_raw_dup tdn_raw_dup
## 1 TN r2 low    29.58      0.6190
## 2 TN r2 low    18.39      0.5758
## 3 TN r2 low    32.70      1.0300
## 4 TN r2 low    60.77      1.7270
```

```
##           sample_name npoc_raw tdn_raw      run_datetime npoc_flag
## 1 TMP_CTRL_C3_20250204   29.65  0.6686 2/5/2025 9:26:06 AM
## 2   TMP_FW_F6_20250204   18.19  0.5225 2/5/2025 6:00:06 PM
## 3   TMP_FW_I5_20250131   32.94  1.0940 2/5/2025 3:04:02 AM
## 4   TMP_SW_I5_20250204   61.38  1.6960 2/6/2025 12:58:02 AM
##   tdn_flag npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv
## 1 TN r2 low    29.58      0.6190    0.2504954      YES      7.954916
## 2 TN r2 low    18.39      0.5758    1.1553585      YES      9.953124
## 3 TN r2 low    32.70      1.0300    0.7736198      YES      6.258578
## 4 TN r2 low    60.77      1.7270    1.0556301      YES      1.908925
##   tdn_dups_cv_flag
## 1      YES
## 2      YES
## 3      YES
## 4      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.
```





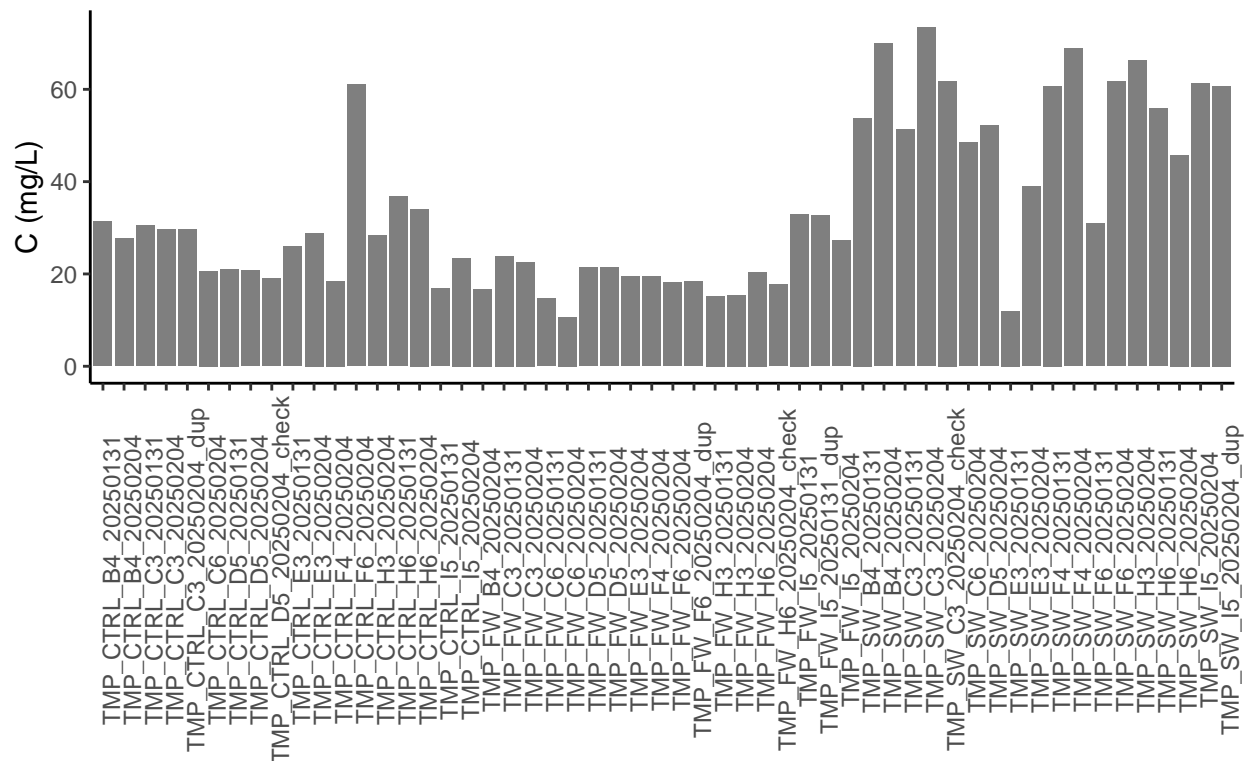
## [1] ">60% of Carbon Duplicates have a CV <10%"

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

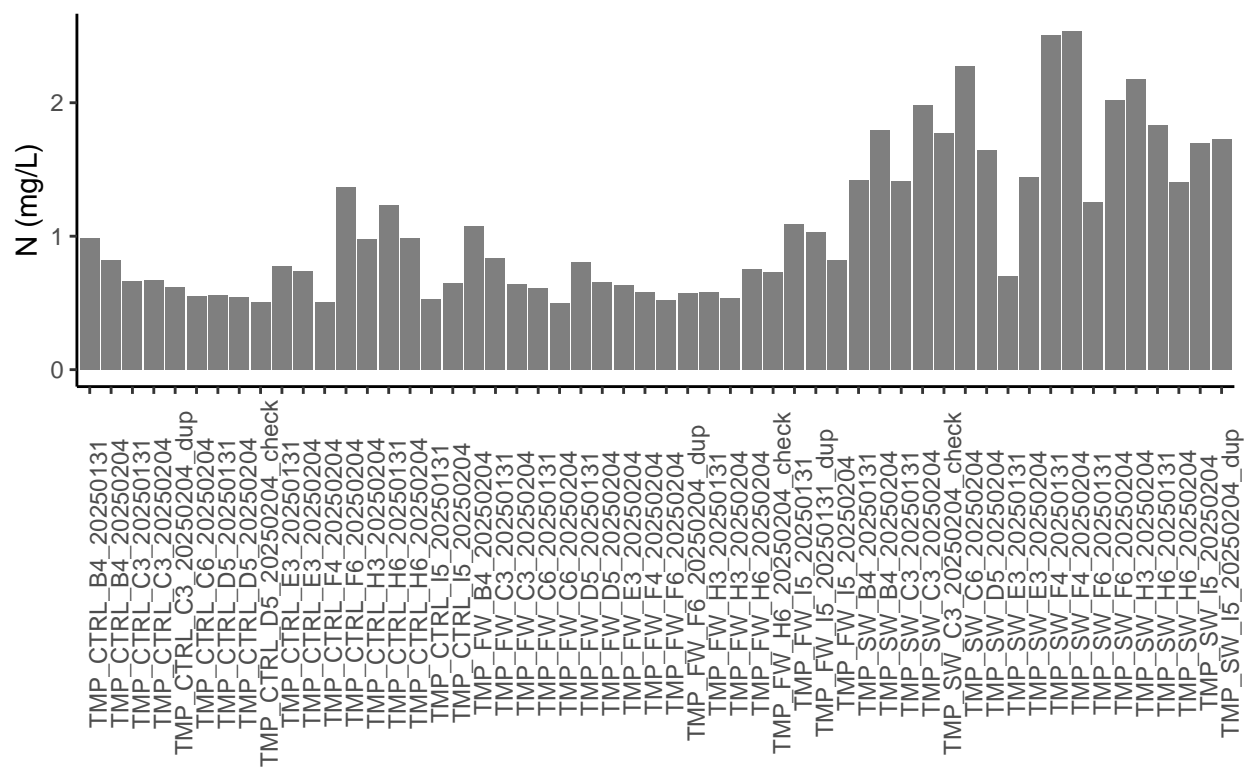
## Sample Flagging

## Sample Flagging

C: Grey = Within Range of Curve



N: Grey = Within Range of Curve



## Visualize Data by Plot

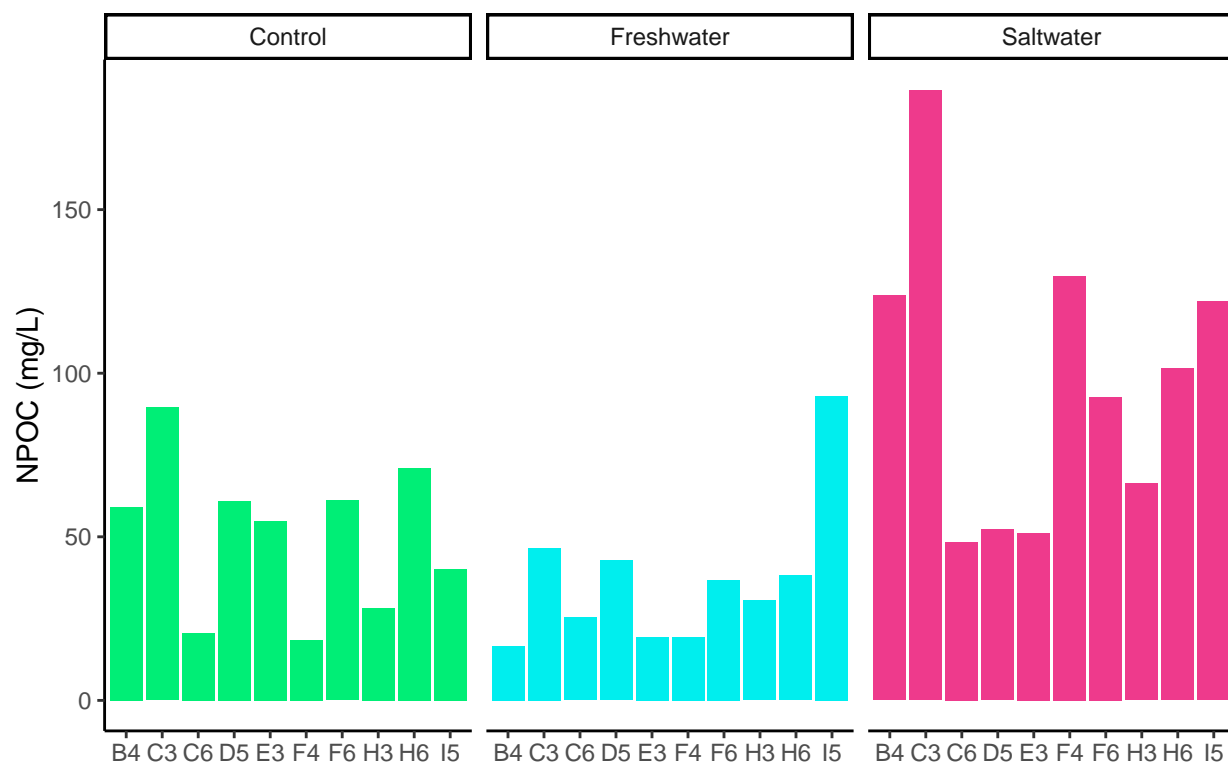
```
## Visualize Data
```

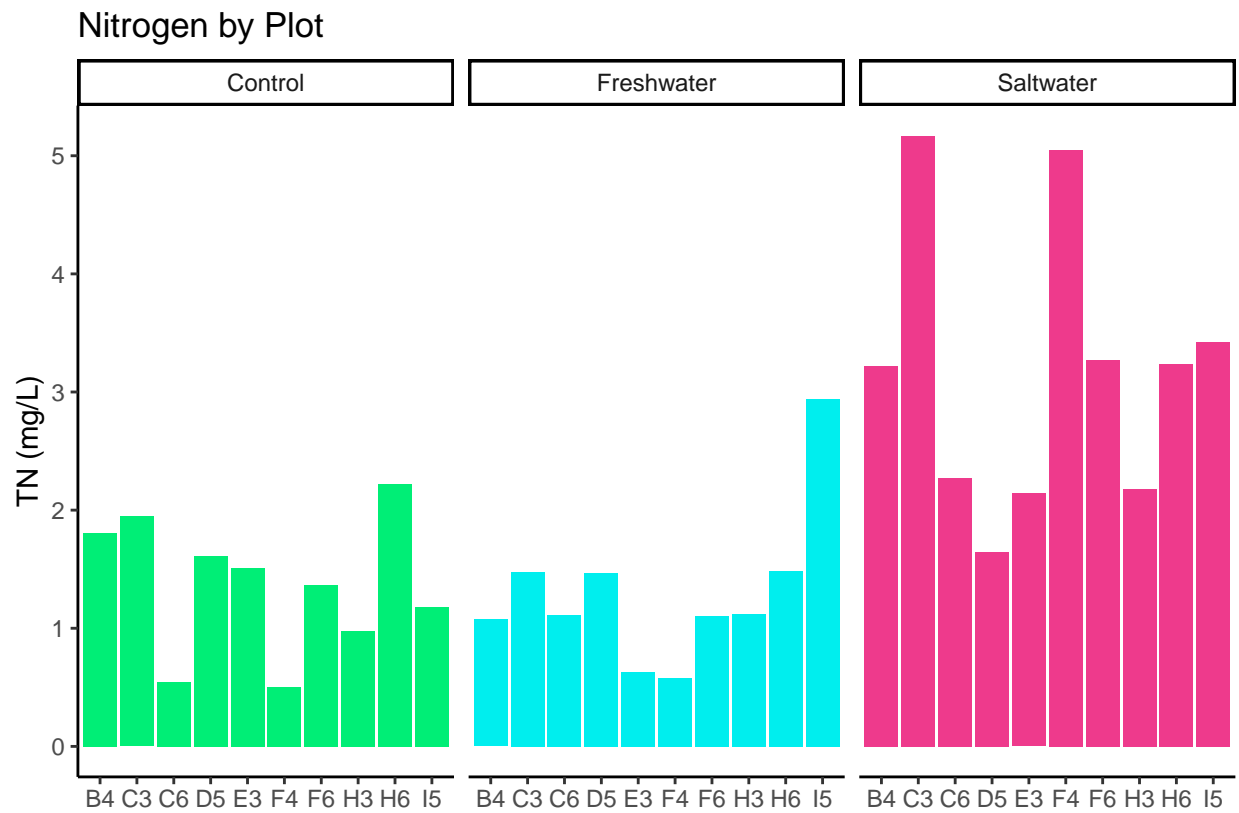
```
## Warning in rbind(c("TMP", "CTRL", "B4", "20250131"), c("TMP", "CTRL", "C3", :  
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code Plot Grid_Square    Date  NA  
## 1      TMP CTRL          B4 20250131 TMP  
## 2      TMP CTRL          C3 20250131 TMP  
## 3      TMP CTRL          D5 20250131 TMP  
## 4      TMP CTRL          E3 20250131 TMP  
## 5      TMP CTRL          H6 20250131 TMP  
## 6      TMP CTRL          I5 20250131 TMP
```

```
##   Site_Code Plot Grid_Square    Date  NA      sample_name npoc_raw tdn_raw  
## 1      TMP CTRL          B4 20250131 TMP TMP_CTRL_B4_20250131    31.35  0.9852  
## 2      TMP CTRL          C3 20250131 TMP TMP_CTRL_C3_20250131    30.54  0.6599  
## 3      TMP CTRL          D5 20250131 TMP TMP_CTRL_D5_20250131    21.09  0.5605  
## 4      TMP CTRL          E3 20250131 TMP TMP_CTRL_E3_20250131    25.90  0.7722  
## 5      TMP CTRL          H6 20250131 TMP TMP_CTRL_H6_20250131    36.77  1.2330  
## 6      TMP CTRL          I5 20250131 TMP TMP_CTRL_I5_20250131    16.82  0.5264  
##           run_datetime npoc_flag  tdn_flag  
## 1  2/4/2025 9:12:13 PM          TN r2 low  
## 2  2/4/2025 9:42:02 PM          TN r2 low  
## 3  2/4/2025 10:00:23 PM          TN r2 low  
## 4  2/4/2025 10:29:44 PM          TN r2 low  
## 5  2/4/2025 10:58:13 PM          TN r2 low  
## 6  2/4/2025 11:26:31 PM          TN r2 low
```

Carbon by Plot





## Convert data from mg/L to uMoles/L

### Add in/check metadata

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

```
## # A tibble: 50 x 2
##   sample_name      metadata_recorded
##   <chr>           <lgl>
## 1 TMP_C_B4_20250131 TRUE
## 2 TMP_C_C3_20250131 TRUE
## 3 TMP_C_D5_20250131 TRUE
## 4 TMP_C_E3_20250131 TRUE
## 5 TMP_C_H6_20250131 TRUE
## 6 TMP_C_I5_20250131 TRUE
## 7 TMP_FW_C3_20250131 TRUE
## 8 TMP_FW_C6_20250131 TRUE
## 9 TMP_FW_D5_20250131 TRUE
## 10 TMP_FW_H3_20250131 TRUE
## # i 40 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~ C    B4      15 DOC      C_B4_D~ 2025~    31.4    2613.
## 2 COMPASS: TEMP~ C    C3      15 DOC      C_C3_D~ 2025~    30.5    2545
## 3 COMPASS: TEMP~ C    D5      15 DOC      C_D5_D~ 2025~    21.1    1758.
## 4 COMPASS: TEMP~ C    E3      15 DOC      C_E3_D~ 2025~    25.9    2158.
## 5 COMPASS: TEMP~ C    H6      15 DOC      C_H6_D~ 2025~    36.8    3064.
## 6 COMPASS: TEMP~ C    I5      15 DOC      C_I5_D~ 2025~    16.8    1402.
## # 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
```