COMPASS: TEMPEST Discrete DOC Data QAQC

December 2024

2025-10-02

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 = "12/18/24"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = " SW_F4 is SW_F6 changed in this code. Rain water samples also
    collected, these are output to a separate file in processed data"

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2024/TMP_202412.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2024/TMP_202412_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2024/TMP_PW_DOC_Processed_202412.csv"
    processed_rain_data = "tmp_doc_processed_data_2024/TMP_RAIN_DOC_Processed_202412.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_2024/COMPASS_TMP_TOCTN_QAQClog_2024.csv"
```

Setup

Pull in active porewater tracking inventory sheet

```
## File already exists. No download needed.
```

Import Data Functions

Import Sample Data

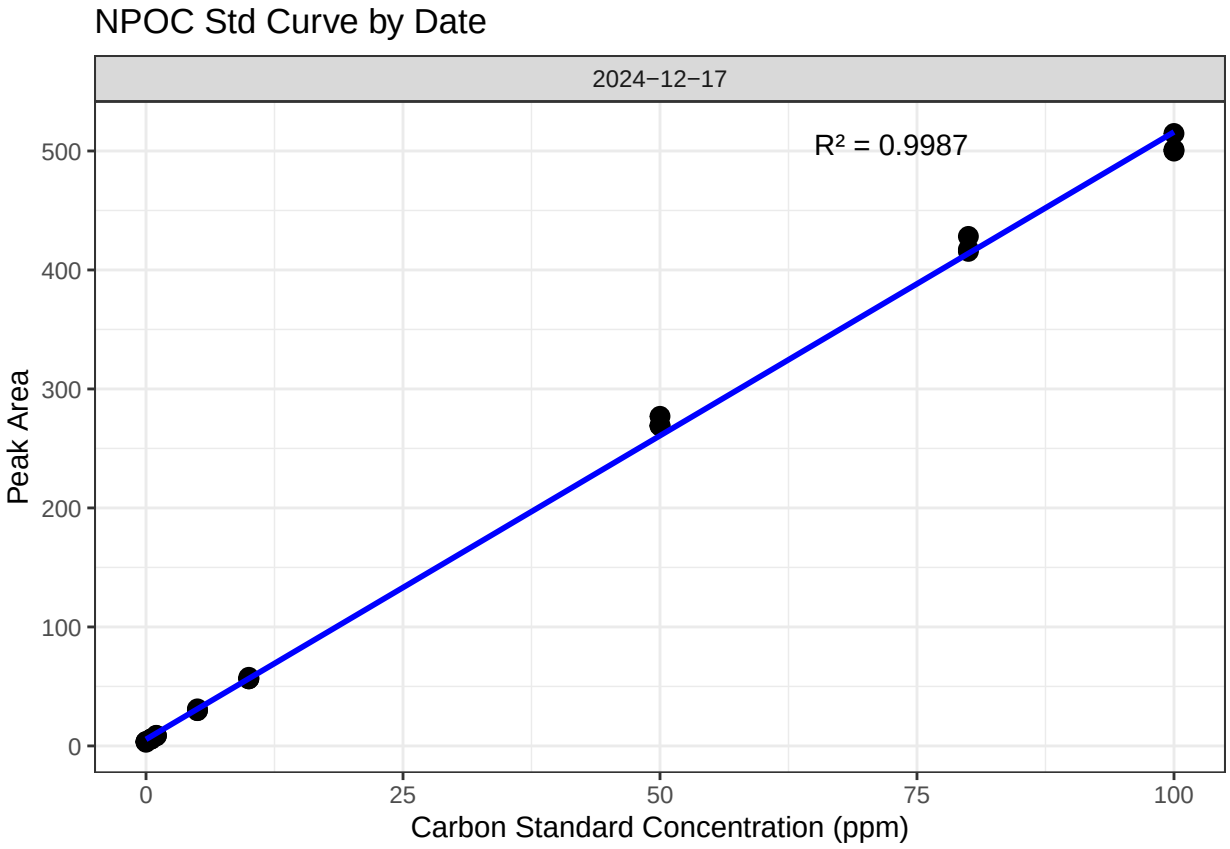
```
## Import Sample Data


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

```
## # A tibble: 6 x 4
##   sample_name          npoc_raw tdn_raw run_datetime
##   <chr>                   <dbl>   <dbl> <chr>
## 1 TMP_CTRL_C6_20241213     23.1   0.724 12/17/2024 11:28:40 PM
## 2 TMP_CTRL_D5_20241213     21.7   0.366 12/17/2024 11:51:36 PM
## 3 TMP_CTRL_E3_20241213     24.1   0.611 12/18/2024 12:22:13 AM
## 4 TMP_CTRL_F6_20241213     30.3   0.658 12/18/2024 12:47:24 AM
## 5 TMP_CTRL_H6_20241213     16.4   0.500 12/18/2024 1:16:17 AM
## 6 TMP_CTRL_I5_20241213     18.7   0.460 12/18/2024 1:46:03 AM
```

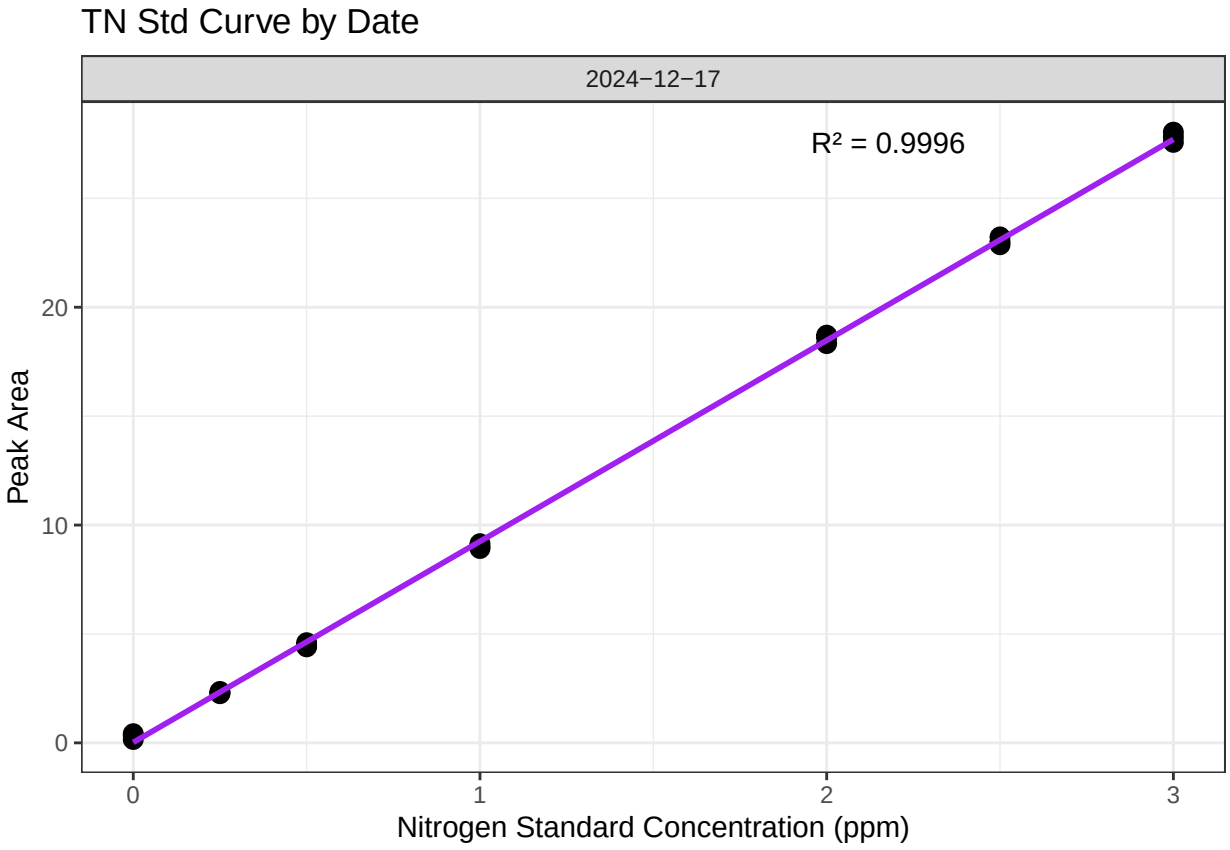
Assessing standard Curves

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

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

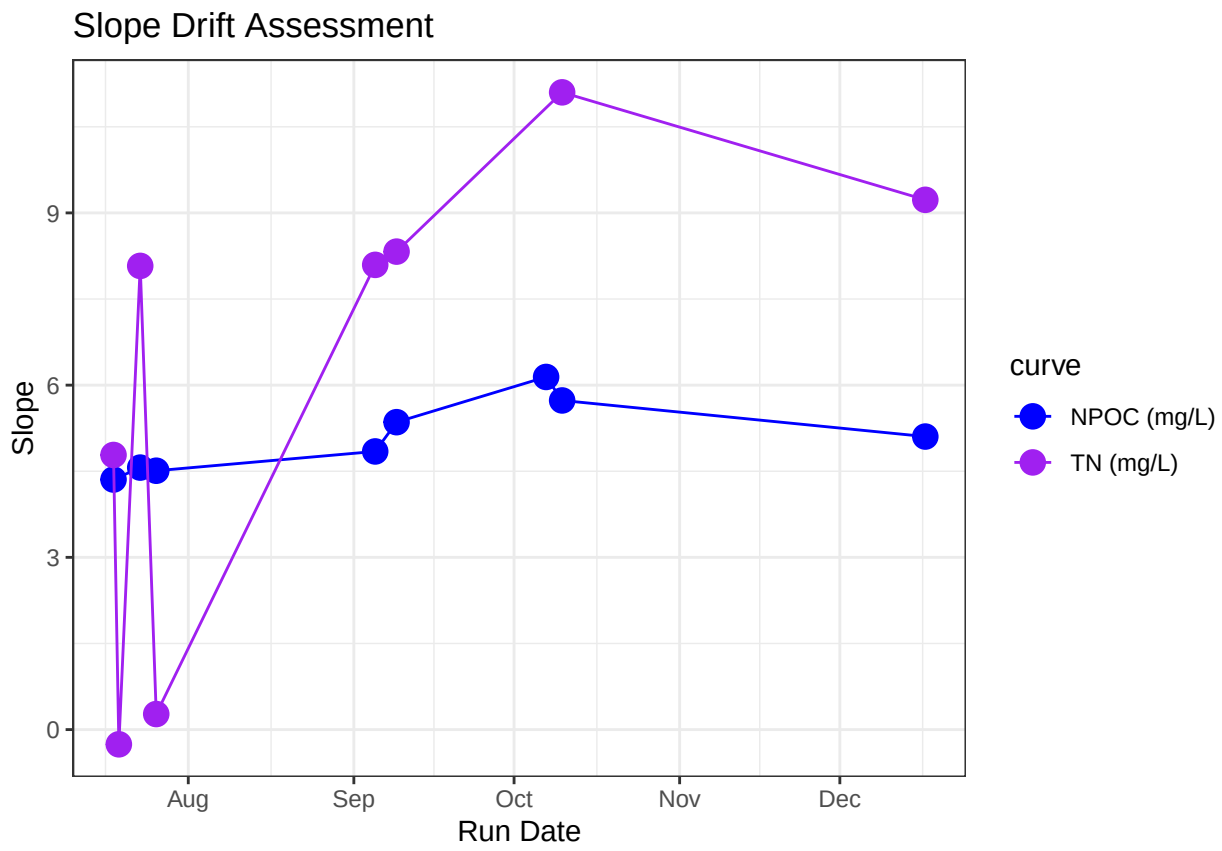



```
## ‘geom_smooth()‘ using formula = ’y ~ x’
```




```
## Warning: Removed 15 rows containing missing values or values outside the scale range
## (`geom_point()`).
```

```
## Warning: Removed 15 rows containing missing values or values outside the scale range
## (`geom_line()`).
```




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

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

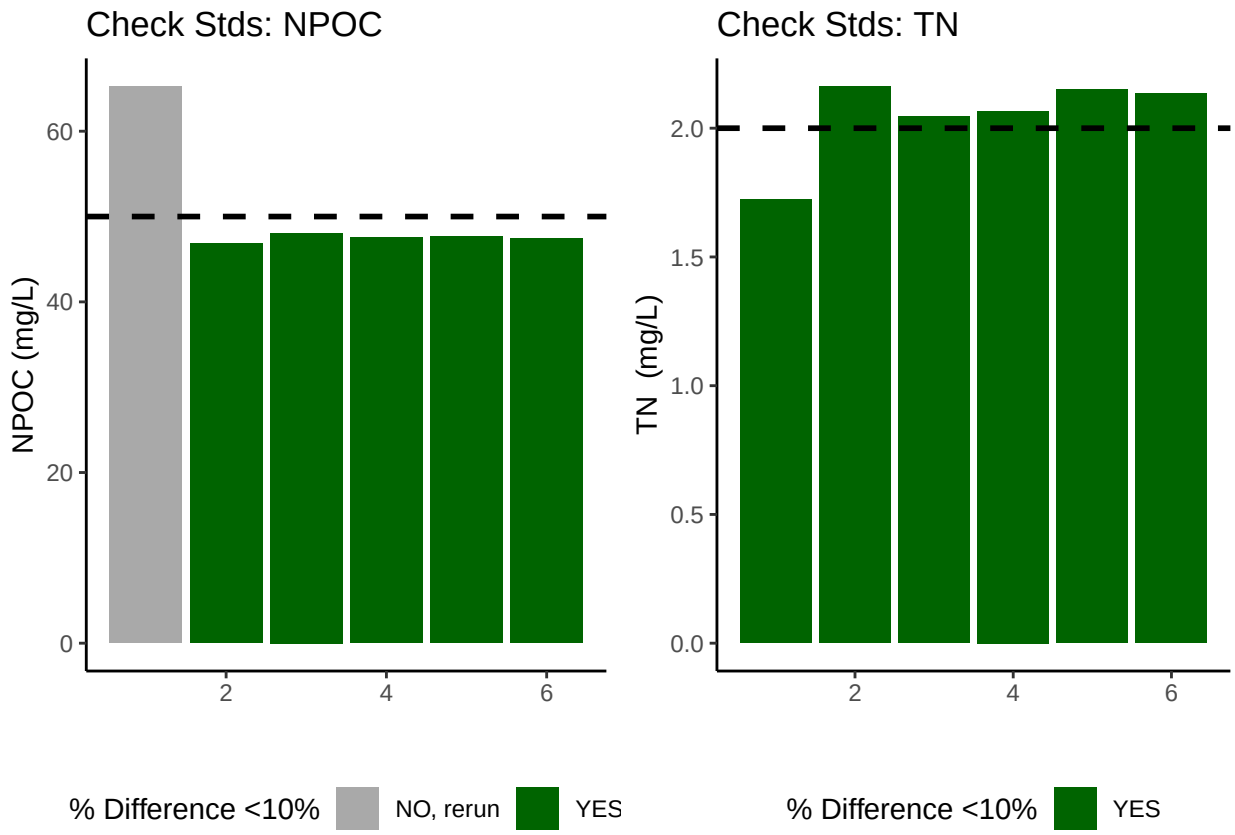
Assess Check Standards

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

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

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

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




```
## [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"
```

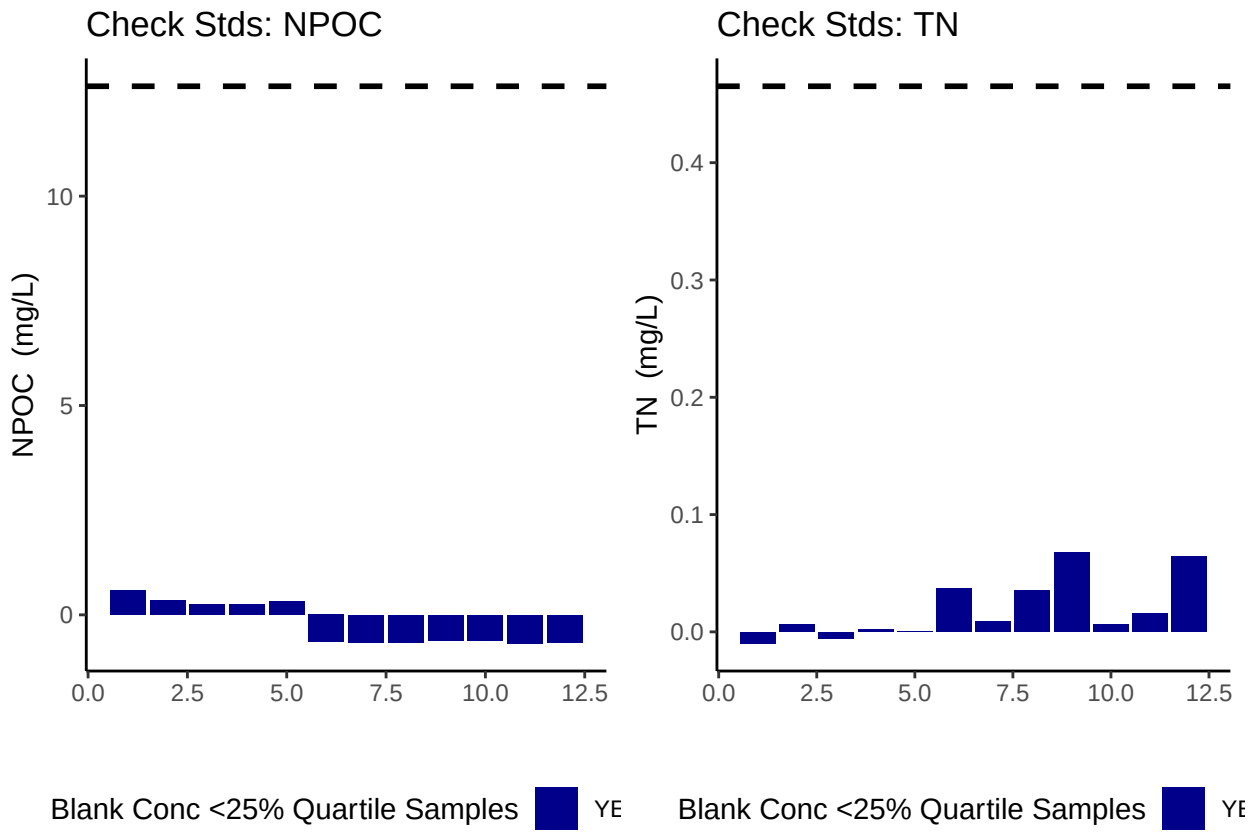
Assess Blanks

```
## 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"
```




```
## carbon blanks:
```

```
## [1] -0.2328583
```

```
## nitrogen blanks:
```

```
## [1] 0.01915167
```

Assess Duplicates - if there are any

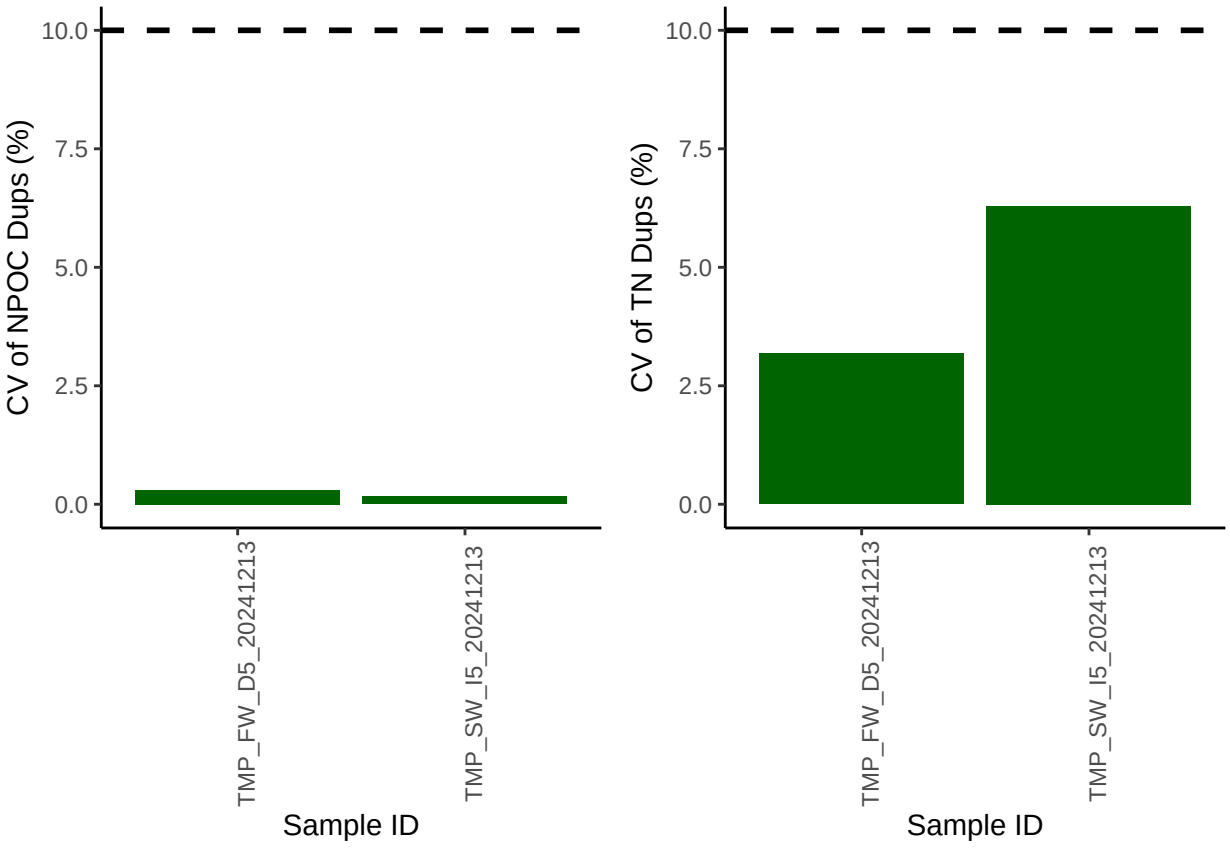
```
## Assess Duplicates
```

```
## # A tibble: 2 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_FW_D5_20241213         27.7       0.622
## 2 TMP_SW_I5_20241213         12.6       0.787
```

```
##          sample_name npoc_raw tdn_raw          run_datetime npoc_flag tdn_flag
## 1 TMP_FW_D5_20241213    27.75  0.6039 12/18/2024 3:42:26 AM
## 2 TMP_SW_I5_20241213    12.62  0.8358 12/18/2024 9:35:51 AM
##   npoc_raw_dup tdn_raw_dup
## 1        27.67      0.6225
## 2        12.64      0.7866
```

```
##          sample_name npoc_raw tdn_raw          run_datetime npoc_flag tdn_flag
## 1 TMP_FW_D5_20241213    27.75  0.6039 12/18/2024 3:42:26 AM
## 2 TMP_SW_I5_20241213    12.62  0.8358 12/18/2024 9:35:51 AM
##   npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv
## 1        27.67      0.6225    0.3059051               YES    3.183130
## 2        12.64      0.7866    0.1678649               YES    6.297949
##   tdn_dups_cv_flag
## 1              YES
## 2              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.
```

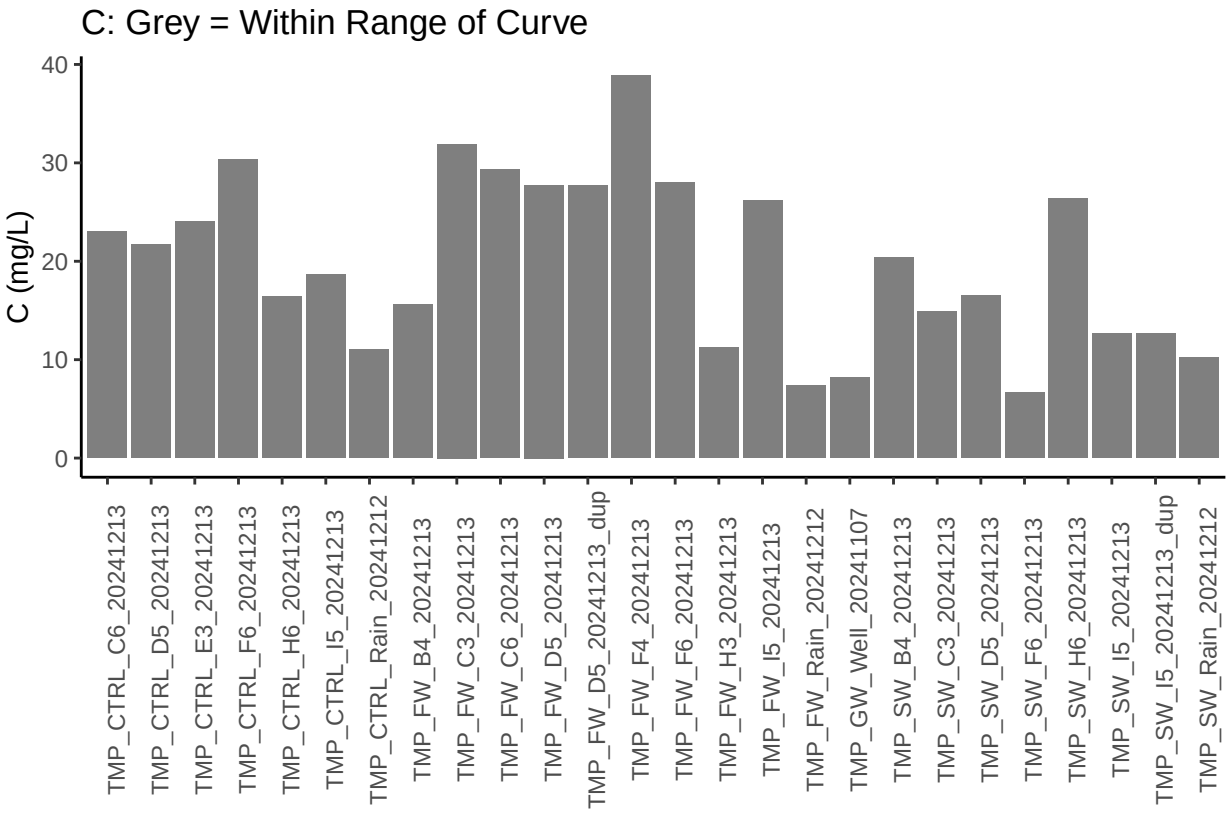


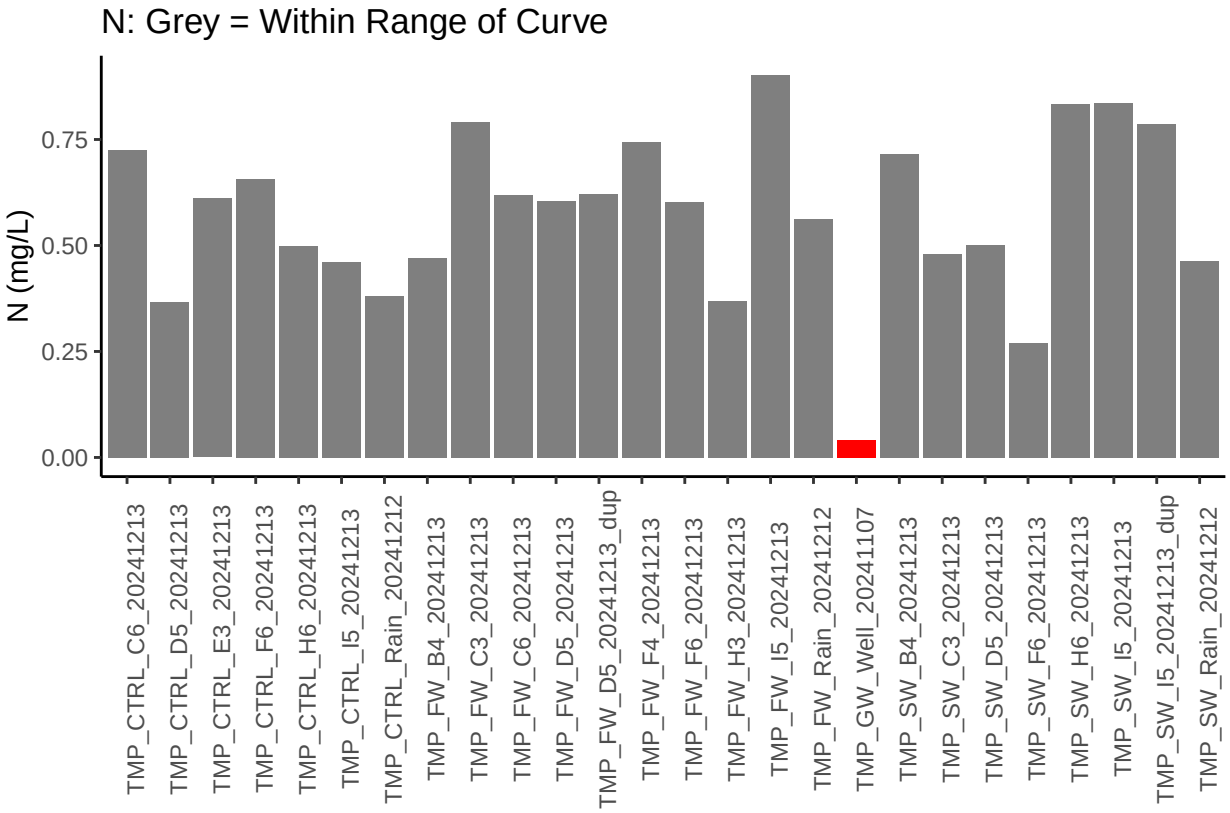

```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

```
## Sample Flagging
```




N: Grey = Within Range of Curve
N (mg/L)
0.00
0.25
0.50
0.75
TMP_CTRL_C6_20241213
TMP_CTRL_D5_20241213
TMP_CTRL_E3_20241213
TMP_CTRL_F6_20241213
TMP_CTRL_H6_20241213
TMP_CTRL_I5_20241213
TMP_CTRL_Rain_20241212
TMP_FW_B4_20241213
TMP_FW_C3_20241213
TMP_FW_C6_20241213
TMP_FW_D5_20241213
TMP_FW_D5_20241213_dup
TMP_FW_F4_20241213
TMP_FW_F6_20241213
TMP_FW_H3_20241213
TMP_FW_I5_20241213
TMP_FW_Rain_20241212
TMP_GW_Well_20241107
TMP_SW_B4_20241213
TMP_SW_C3_20241213
TMP_SW_D5_20241213
TMP_SW_F6_20241213
TMP_SW_H6_20241213
TMP_SW_I5_20241213
TMP_SW_I5_20241213_dup
TMP_SW_Rain_20241212

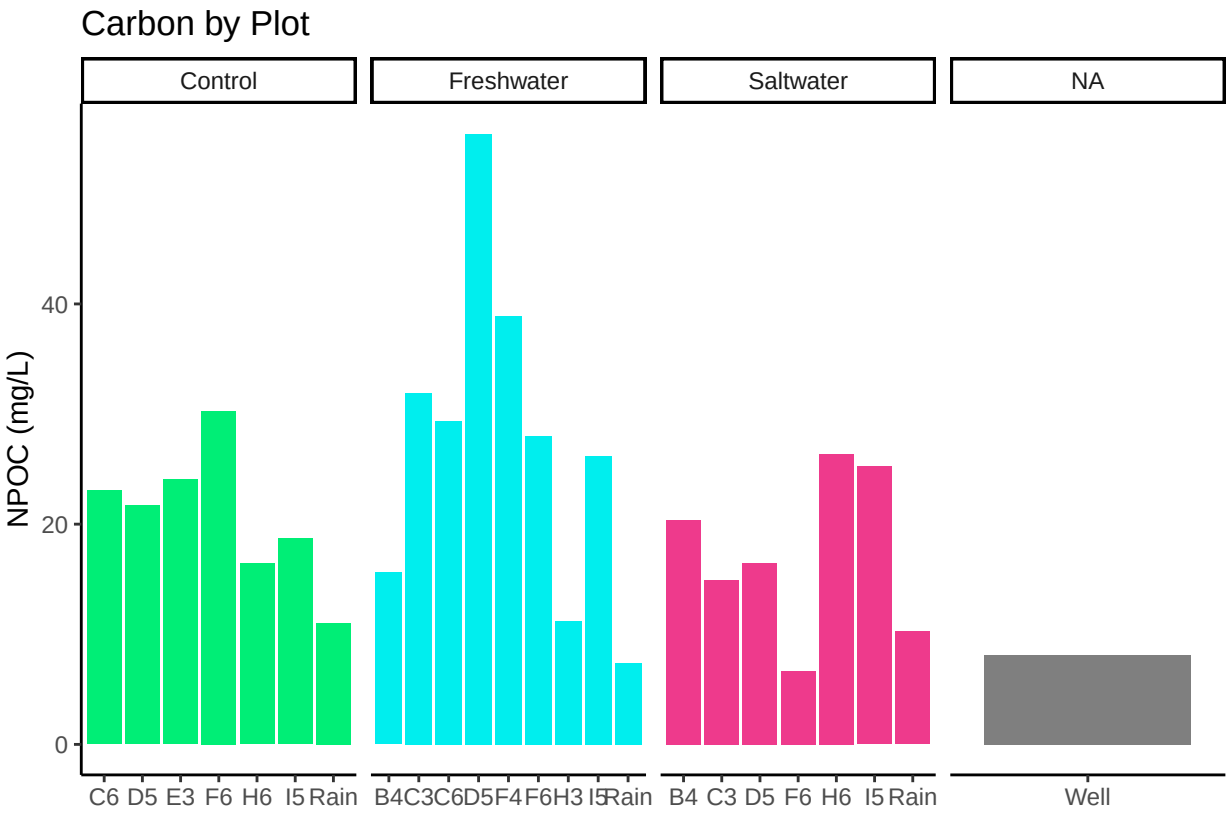
Visualize Data by Plot

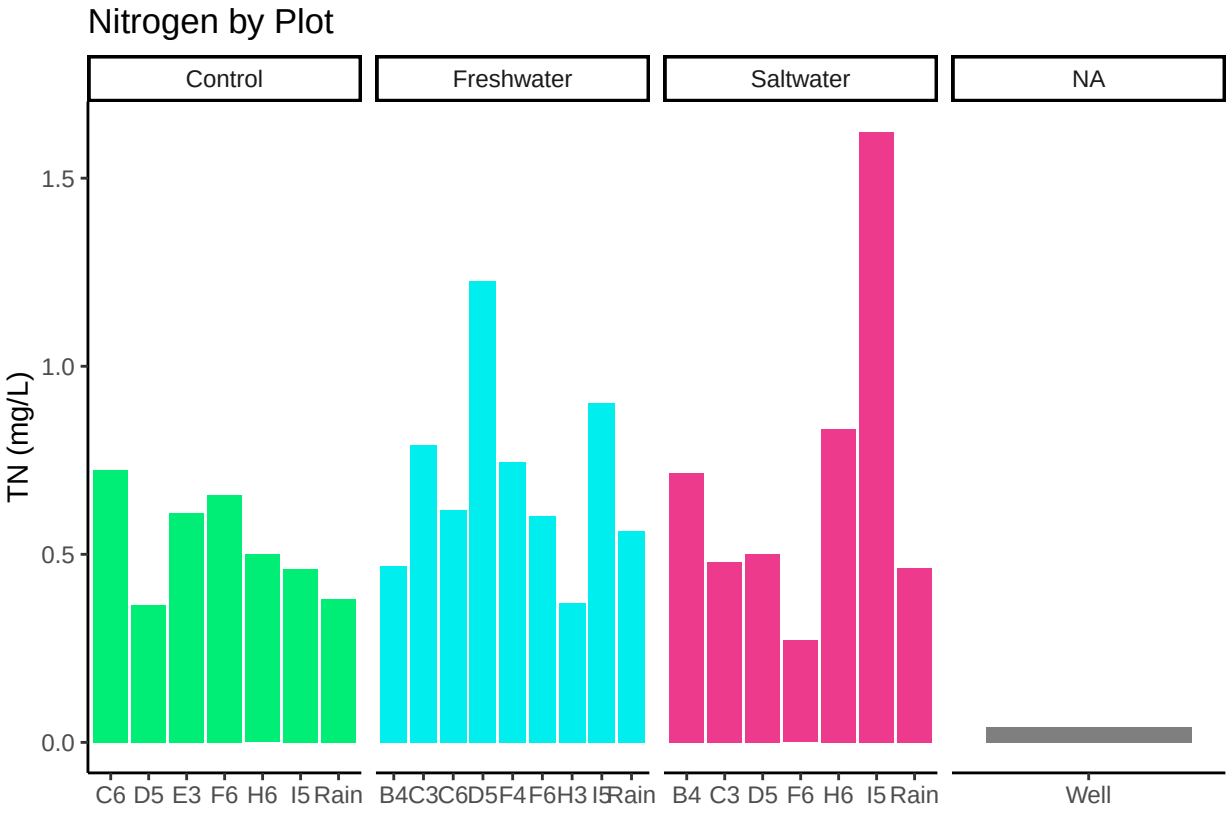
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "CTRL", "C6", "20241213"), c("TMP", "CTRL", "D5", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code Plot Grid_Square     Date Extra
## 1       TMP CTRL          C6 20241213   TMP
## 2       TMP CTRL          D5 20241213   TMP
## 3       TMP CTRL          E3 20241213   TMP
## 4       TMP CTRL          F6 20241213   TMP
## 5       TMP CTRL          H6 20241213   TMP
## 6       TMP CTRL          I5 20241213   TMP
```

```
##   Site_Code Plot Grid_Square     Date Extra          sample_name npoc_raw
## 1       TMP CTRL          C6 20241213   TMP TMP_CTRL_C6_20241213    23.06
## 2       TMP CTRL          D5 20241213   TMP TMP_CTRL_D5_20241213    21.69
## 3       TMP CTRL          E3 20241213   TMP TMP_CTRL_E3_20241213    24.06
## 4       TMP CTRL          F6 20241213   TMP TMP_CTRL_F6_20241213    30.31
## 5       TMP CTRL          H6 20241213   TMP TMP_CTRL_H6_20241213    16.43
## 6       TMP CTRL          I5 20241213   TMP TMP_CTRL_I5_20241213    18.69
##   tdn_raw           run_datetime npoc_flag tdn_flag
## 1  0.7241 12/17/2024 11:28:40 PM
## 2  0.3660 12/17/2024 11:51:36 PM
## 3  0.6108 12/18/2024 12:22:13 AM
## 4  0.6577 12/18/2024 12:47:24 AM
## 5  0.4995  12/18/2024 1:16:17 AM
## 6  0.4601  12/18/2024 1:46:03 AM
```


Carbon by Plot
Control
Freshwater
Saltwater
NA
NPOC (mg/L)
40
20
0
C6 D5 E3 F6 H6 I5 Rain
B4 C3 C6 D5 F4 F6 H3 I5 Rain
B4 C3 D5 F6 H6 I5 Rain
Well


Nitrogen by Plot
Control
Freshwater
Saltwater
NA
TN (mg/L)
1.5
1.0
0.5
0.0
C6 D5 E3 F6 H6 I5 Rain
B4 C3 C6 D5 F4 F6 H3 I5 Rain
B4 C3 D5 F6 H6 I5 Rain
Well

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 24 x 2
##    sample_name        metadata_recorded
##    <chr>              <lgl>
##  1 TMP_C_C6_20241213  TRUE
##  2 TMP_C_D5_20241213  TRUE
##  3 TMP_C_E3_20241213  TRUE
##  4 TMP_C_F6_20241213  TRUE
##  5 TMP_C_H6_20241213  TRUE
##  6 TMP_C_I5_20241213  TRUE
##  7 TMP_FW_B4_20241213 TRUE
##  8 TMP_FW_C3_20241213 TRUE
##  9 TMP_FW_C6_20241213 TRUE
## 10 TMP_FW_D5_20241213 TRUE
## # i 14 more rows
```

Export PW 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     C6          15 DOC         C_C6_D~ 2024~     23.1   1922.
## 2 COMPASS: TEMP~ C     D5          15 DOC         C_D5_D~ 2024~     21.7   1808.
## 3 COMPASS: TEMP~ C     E3          15 DOC         C_E3_D~ 2024~     24.1   2005
## 4 COMPASS: TEMP~ C     F6          15 DOC         C_F6_D~ 2024~     30.3   2526.
## 5 COMPASS: TEMP~ C     H6          15 DOC         C_H6_D~ 2024~     16.4   1369.
## 6 COMPASS: TEMP~ C     I5          15 DOC         C_I5_D~ 2024~     18.7   1558.
## # 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>
```

Export Processed Rain Data

```
## Export Processed Rain Data
```

```
##            Project plot Type sample_type                Vial_ID     date
## 1 COMPASS: TEMPEST CTRL Rain         DOC TMP_CTRL_Rain_20241212 20241212
## 2 COMPASS: TEMPEST   FW Rain         DOC   TMP_FW_Rain_20241212 20241212
## 3 COMPASS: TEMPEST   SW Rain         DOC   TMP_SW_Rain_20241212 20241212
##   npoc_mgL  npoc_uM npoc_flag tdn_mgL   tdn_uM tdn_flag       Analysis_runtime
## 1   11.050 920.8333           0.3805 27.17857          12/18/2024 11:18:36 AM
## 2    7.418 618.1667           0.5626 40.18571          12/18/2024 11:45:14 AM
```

```
## 3   10.260 855.0000            0.4637 33.12143          12/18/2024 12:14:38 PM
##
## 1  SW_F4 is SW_F6 changed in this code. Rain water samples also\n    collected, these are output to a
## 2  SW_F4 is SW_F6 changed in this code. Rain water samples also\n    collected, these are output to a
## 3  SW_F4 is SW_F6 changed in this code. Rain water samples also\n    collected, these are output to a
```

#end