COMPASS: TEMPEST Discrete DOC Data QAQC

September 2024

2025-06-23

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 = "09/10/24"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = "This run the samples names were not put in correctly, they are
      changed in the code to be the correct format"

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2024/TMP_202409.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2024/TMP_202409_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2024/TMP_PW_DOC_Processed_202409.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_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
```

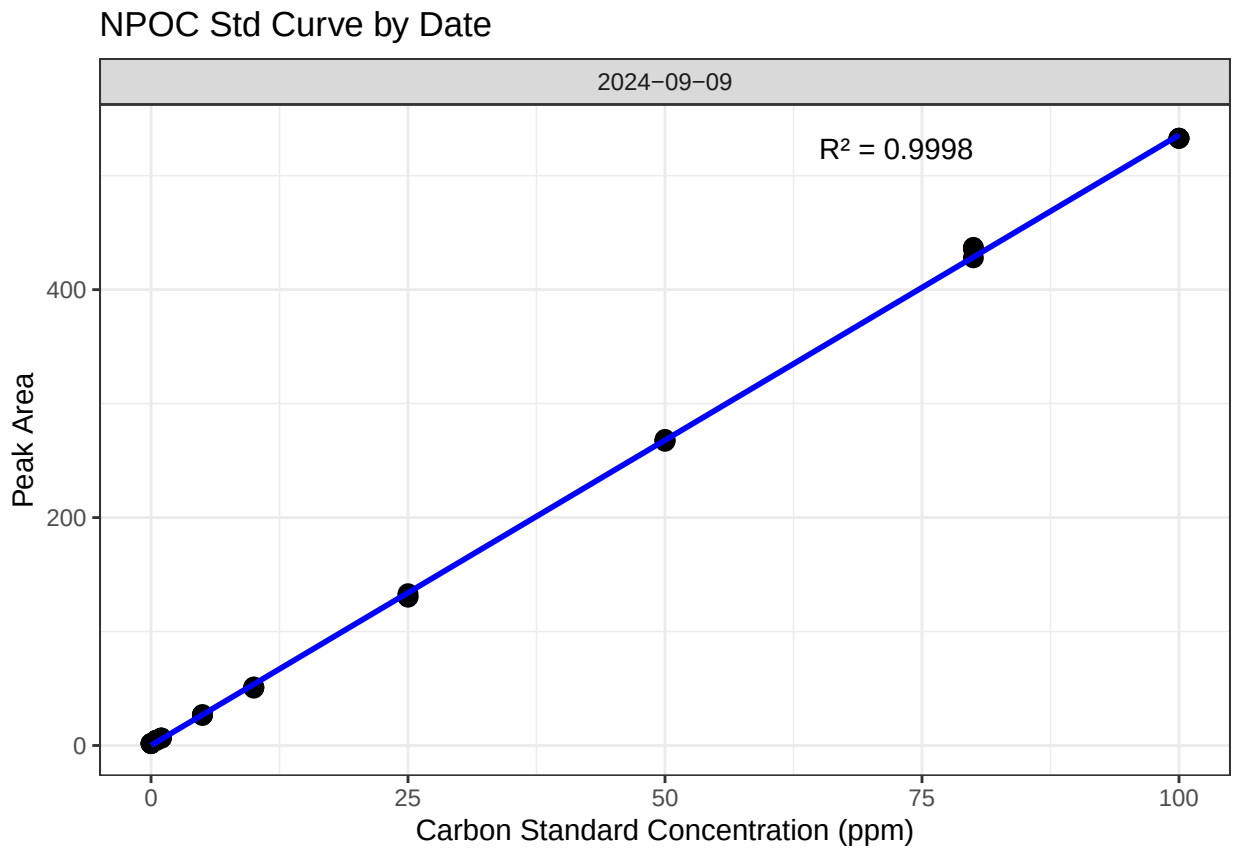
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 3 x 4
##   sample_name    npoc_raw tdn_raw run_datetime
##   <chr>              <dbl>   <dbl> <chr>
## 1 TMP_SW_C3_15cm     9.33   0.666 9/10/2024 3:03:33 PM
## 2 TMP_SW_D5_15cm     5.78   0.268 9/10/2024 3:32:19 PM
## 3 TMP_SW_F6_15cm     6.01   0.353 9/10/2024 4:01:16 PM
```

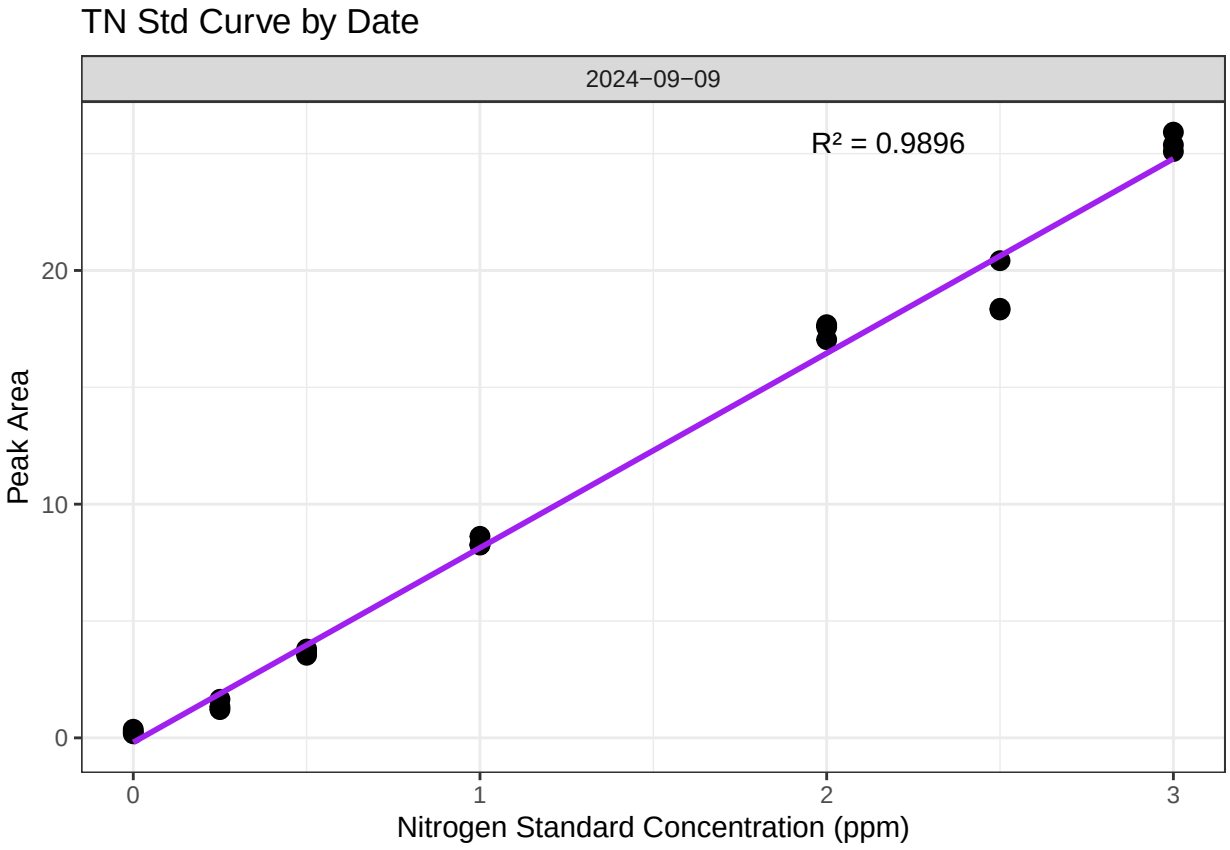
Assessing standard Curves

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

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

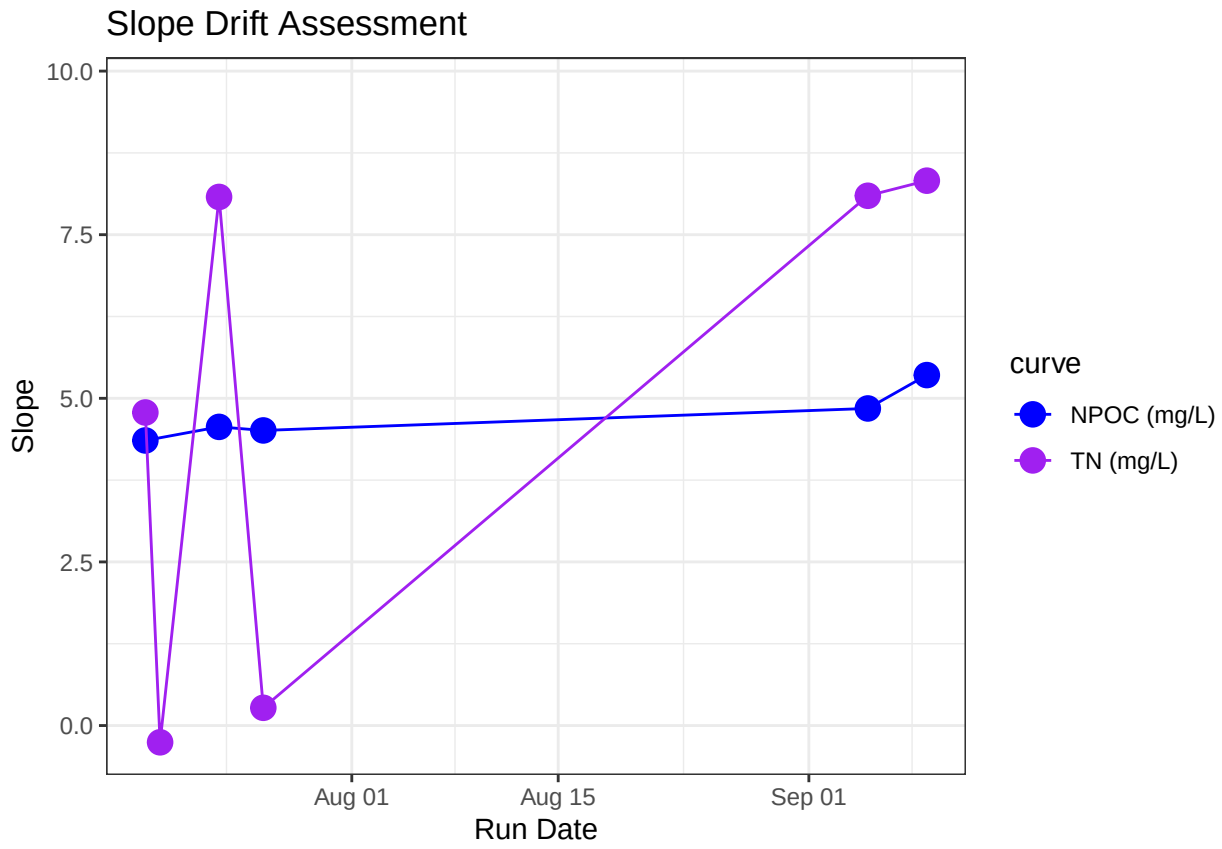



```
## ‘geom_smooth()‘ using formula = ’y ~ x’
```




```
## 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"
```

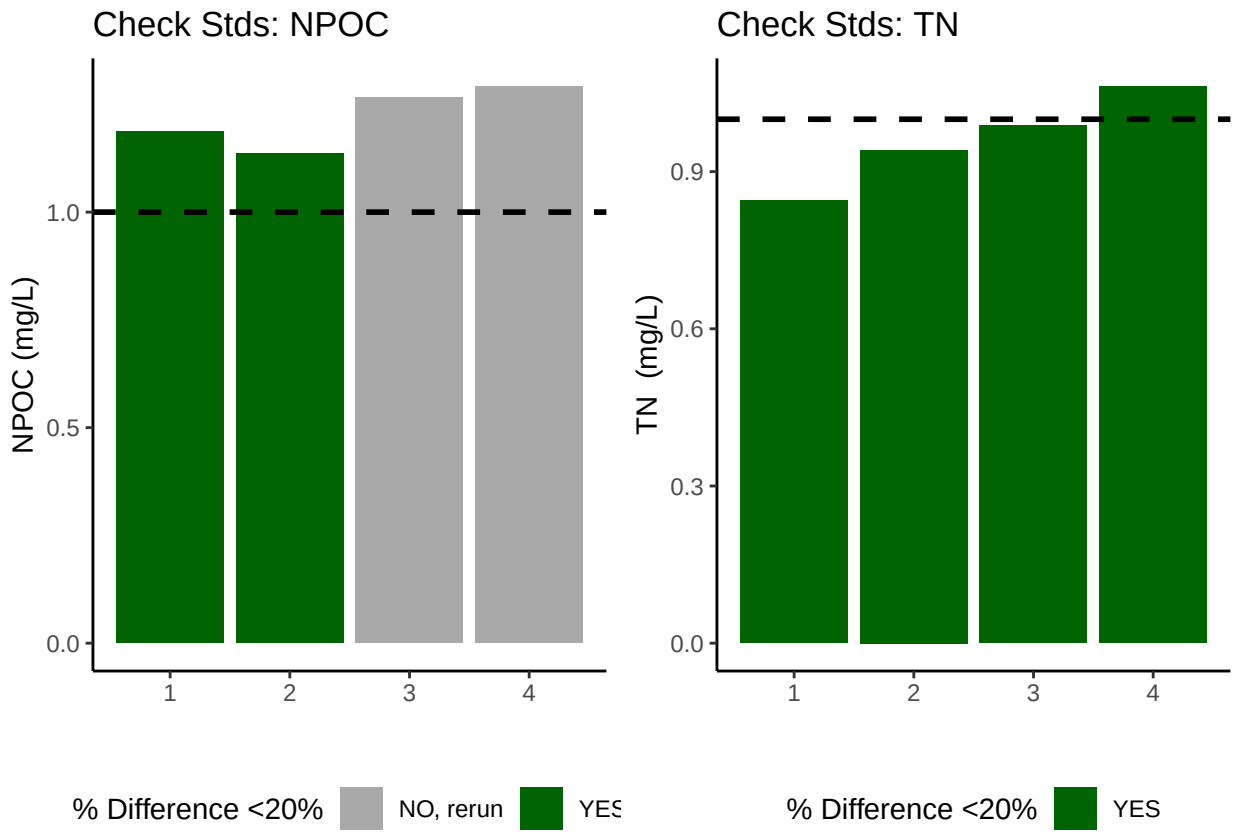
Assess Check Standards

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

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

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

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




```
## [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"
```

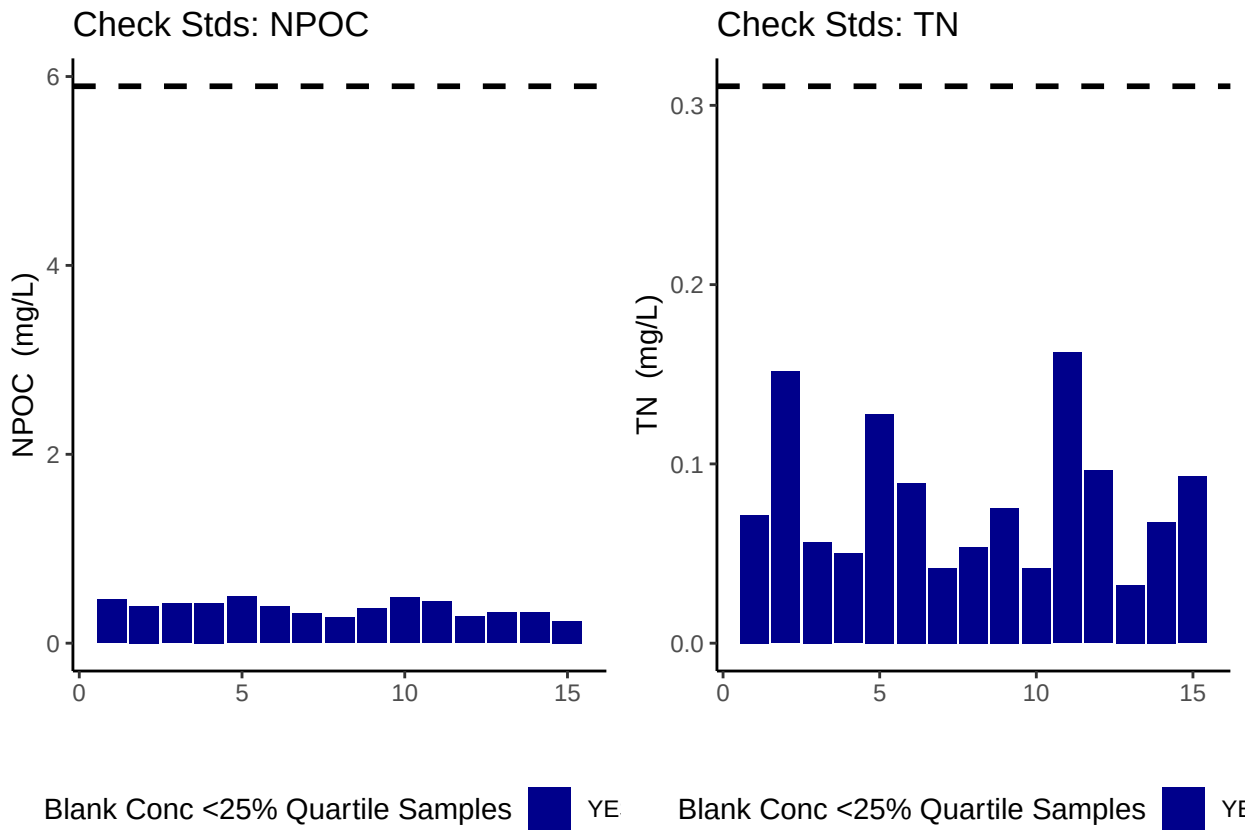
Assess Blanks

```
## 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"
```




```
## carbon blanks:
```

```
## [1] 0.3744933
```

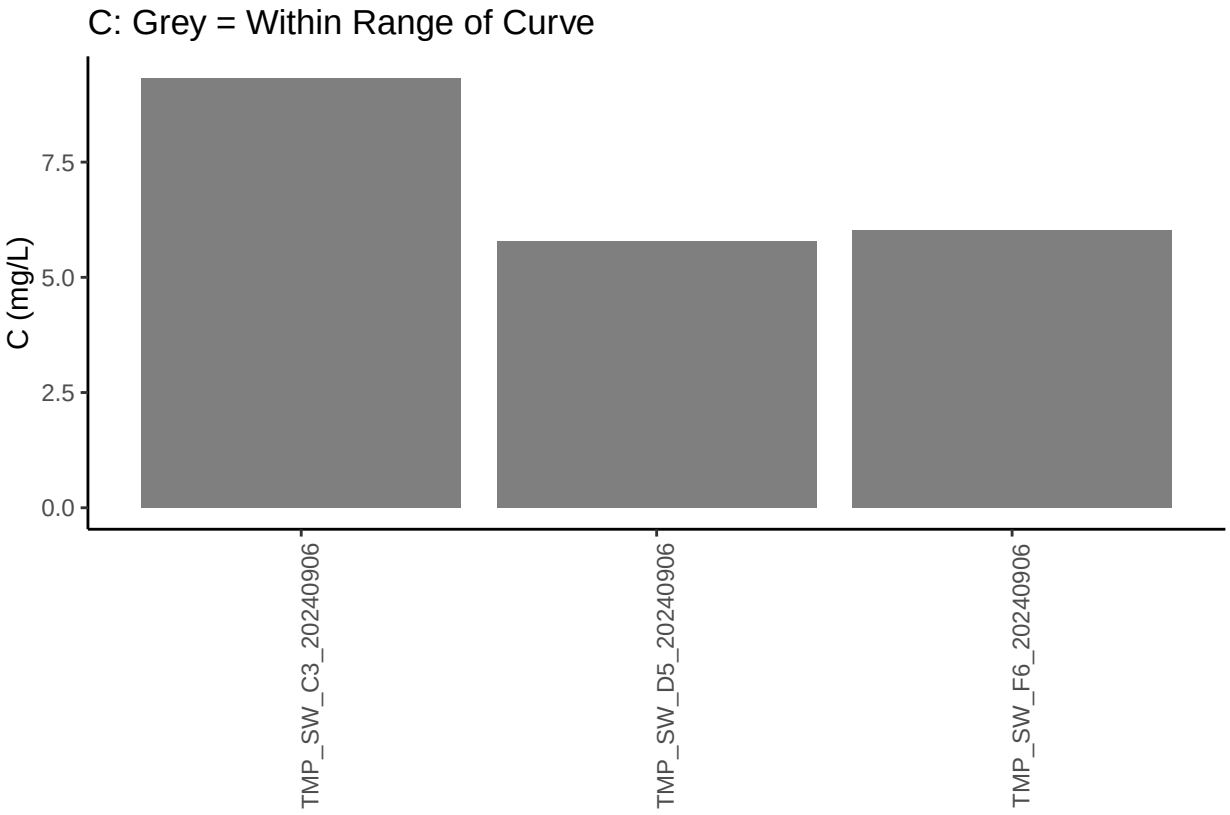
```
## nitrogen blanks:
```

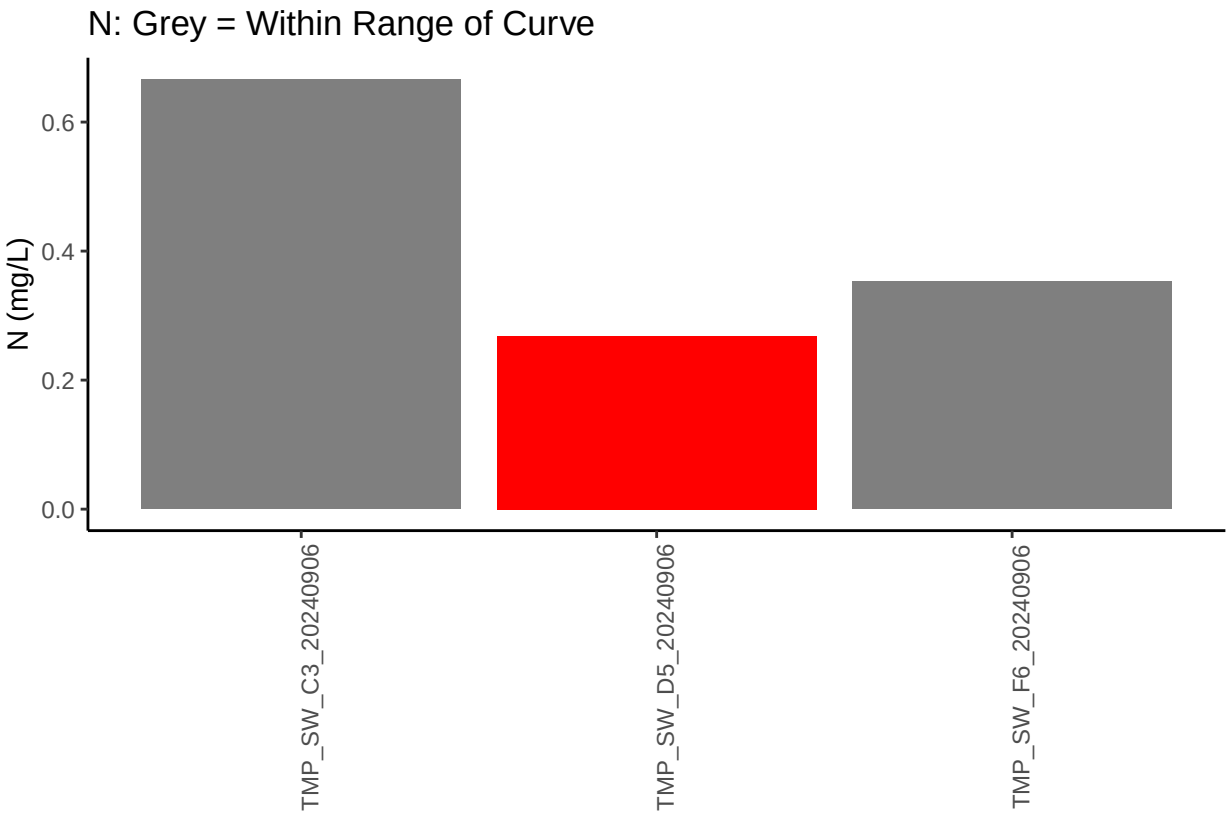
```
## [1] 0.08074067
```

Assess Duplicates - NO Duplicates in this run

Sample Flagging

```
## Sample Flagging
```



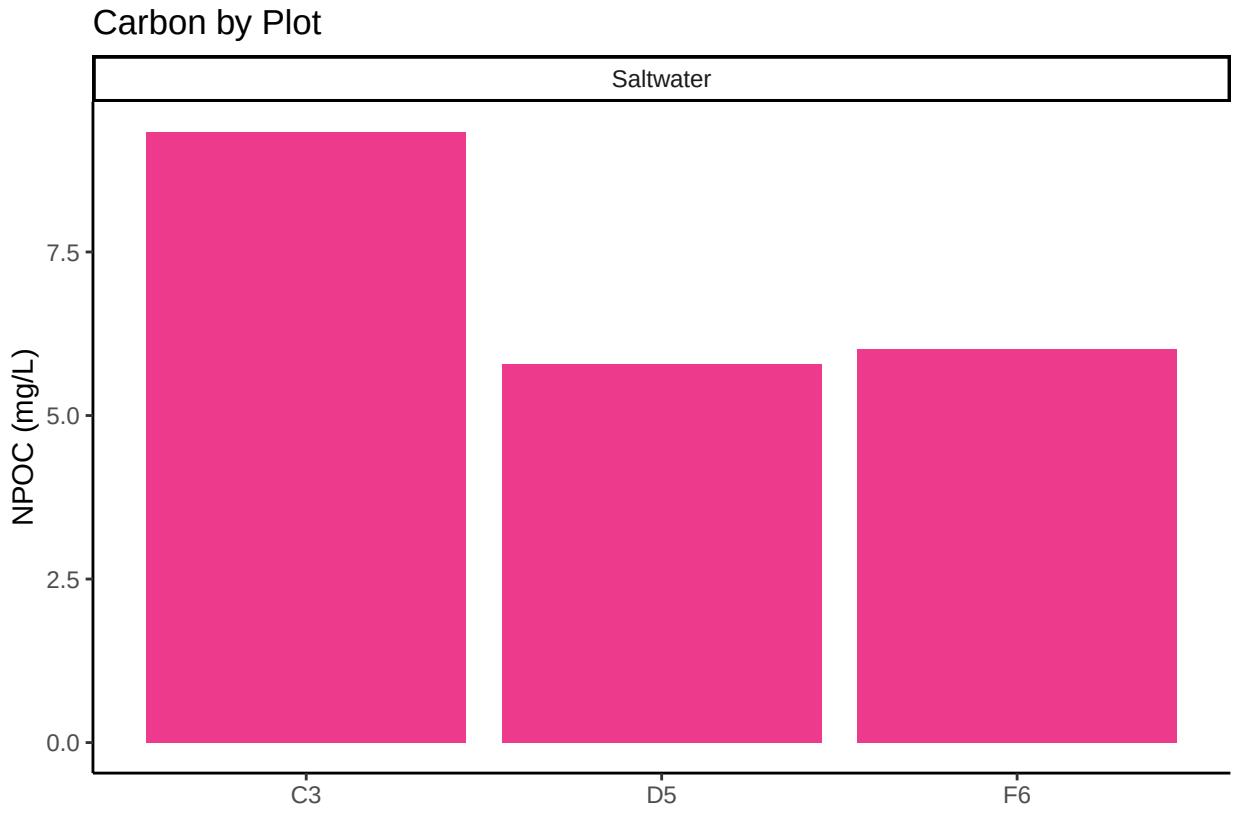

N: Grey = Within Range of Curve
N (mg/L)
0.0
0.2
0.4
0.6
TMP_SW_C3_20240906
TMP_SW_D5_20240906
TMP_SW_F6_20240906

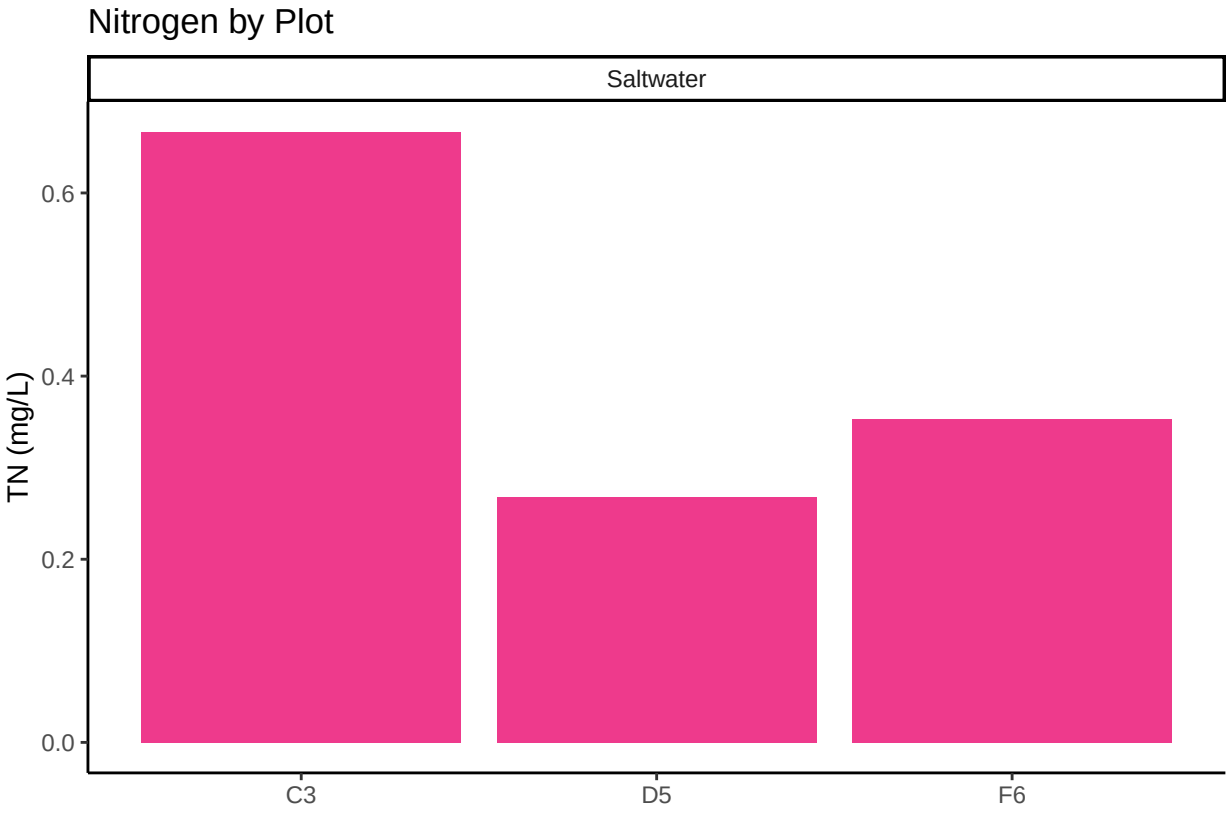
Visualize Data by Plot

```
## Visualize Data
```

```
##   Site_Code Plot Grid_Square     Date
## 1       TMP   SW          C3 20240906
## 2       TMP   SW          D5 20240906
## 3       TMP   SW          F6 20240906
```

```
##   Site_Code Plot Grid_Square     Date        sample_name npoc_raw tdn_raw
## 1       TMP   SW          C3 20240906 TMP_SW_C3_20240906    9.329  0.6664
## 2       TMP   SW          D5 20240906 TMP_SW_D5_20240906    5.781  0.2683
## 3       TMP   SW          F6 20240906 TMP_SW_F6_20240906    6.013  0.3530
##           run_datetime               npoc_flag                      tdn_flag
## 1 9/10/2024 3:03:33 PM NPOC checks out of range
## 2 9/10/2024 3:32:19 PM NPOC checks out of range blank is < 25% of sample value
## 3 9/10/2024 4:01:16 PM NPOC checks out of range
```




Nitrogen by Plot
Saltwater
TN (mg/L)
0.6
0.4
0.2
0.0
C3
D5
F6

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 3 x 2
##   sample_name        metadata_recorded
##   <chr>              <lgl>
## 1 TMP_SW_C3_20240906 TRUE
## 2 TMP_SW_D5_20240906 TRUE
## 3 TMP_SW_F6_20240906 TRUE
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 3 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    C3          15 DOC         SW_C3_~ 2024~     9.33    777.
## 2 COMPASS: TEMP~ SW    D5          15 DOC         SW_D5_~ 2024~     5.78    482.
## 3 COMPASS: TEMP~ SW    F6          15 DOC         SW_F6_~ 2024~     6.01    501.
## # 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