COMPASS: TEMPEST Discrete DOC Data QAQC

August 2024 run 2

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 = "09/05/24"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = " "

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2024/TMP_202408.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2024/TMP_202408_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2024/TMP_PW_DOC_Processed_202408a.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

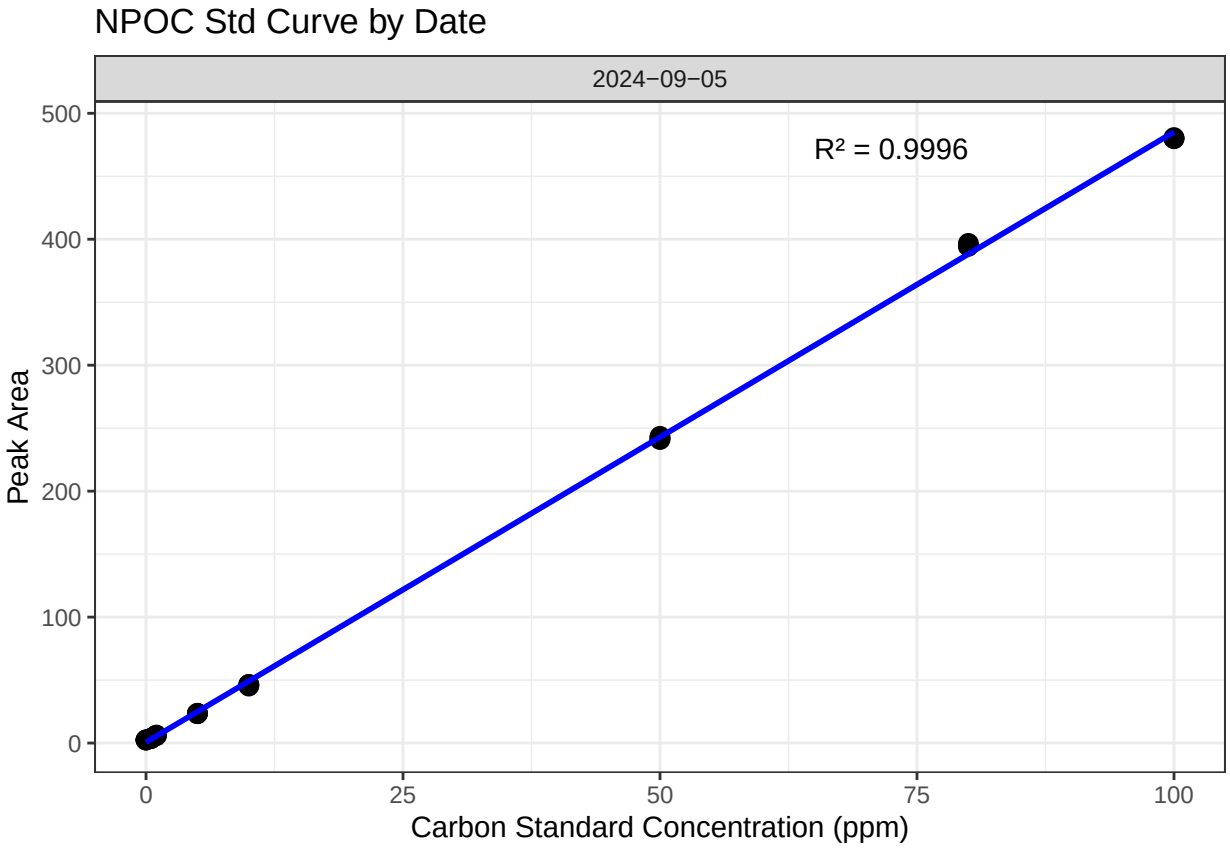
```
## Import Sample Data


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

```
## # A tibble: 3 x 4
##   sample_name            npoc_raw tdn_raw run_datetime
##   <chr>                     <dbl>   <dbl> <chr>
## 1 TMP_20240812_SW_C6        11.6    2.10  9/5/2024 9:35:07 PM
## 2 TMP_20240812_SW_C6_dup    11.6    2.17  9/5/2024 10:07:22 PM
## 3 TMP_20240812_SW_E3         4.86   0.316 9/5/2024 10:38:39 PM
```

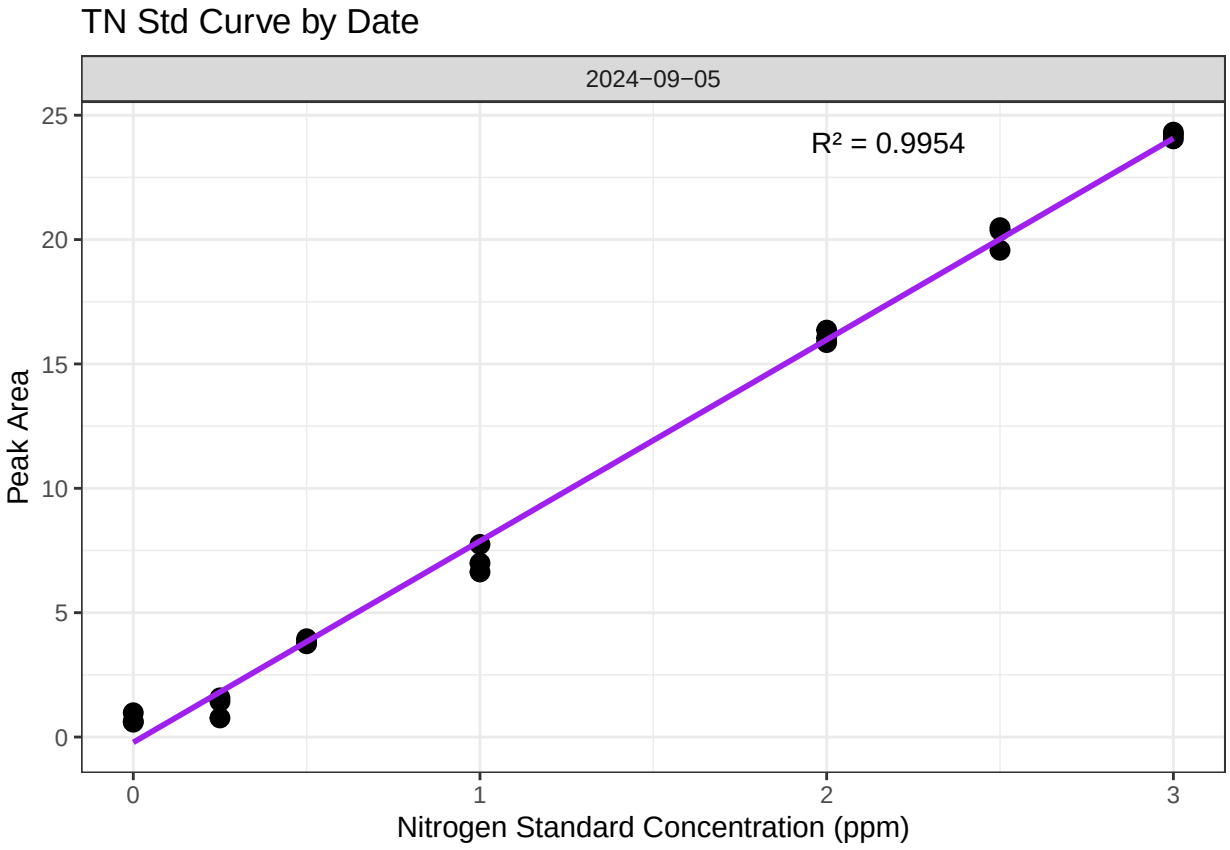
Assessing standard Curves

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

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

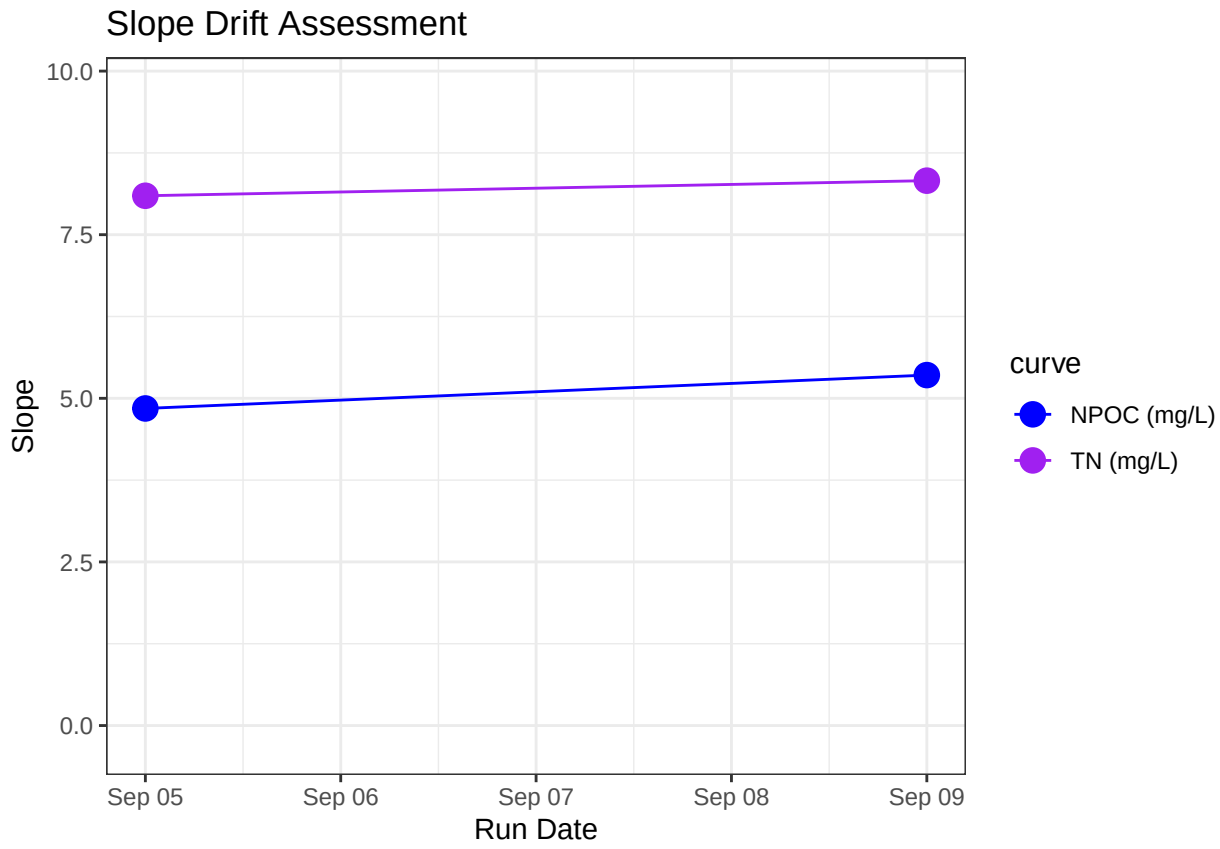



```
## ‘geom_smooth()‘ using formula = ’y ~ x’
```




```
## 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"
```

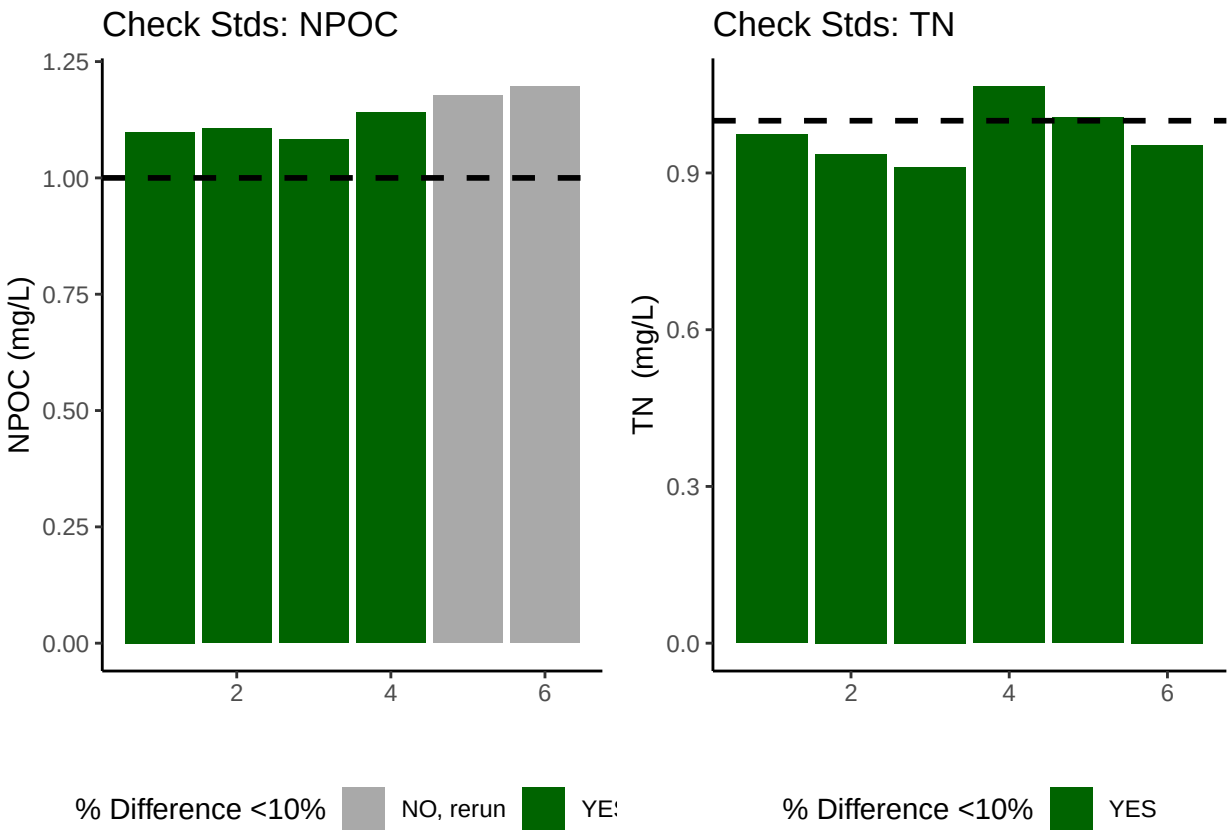
Assess Check Standards

```
## 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"
```

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

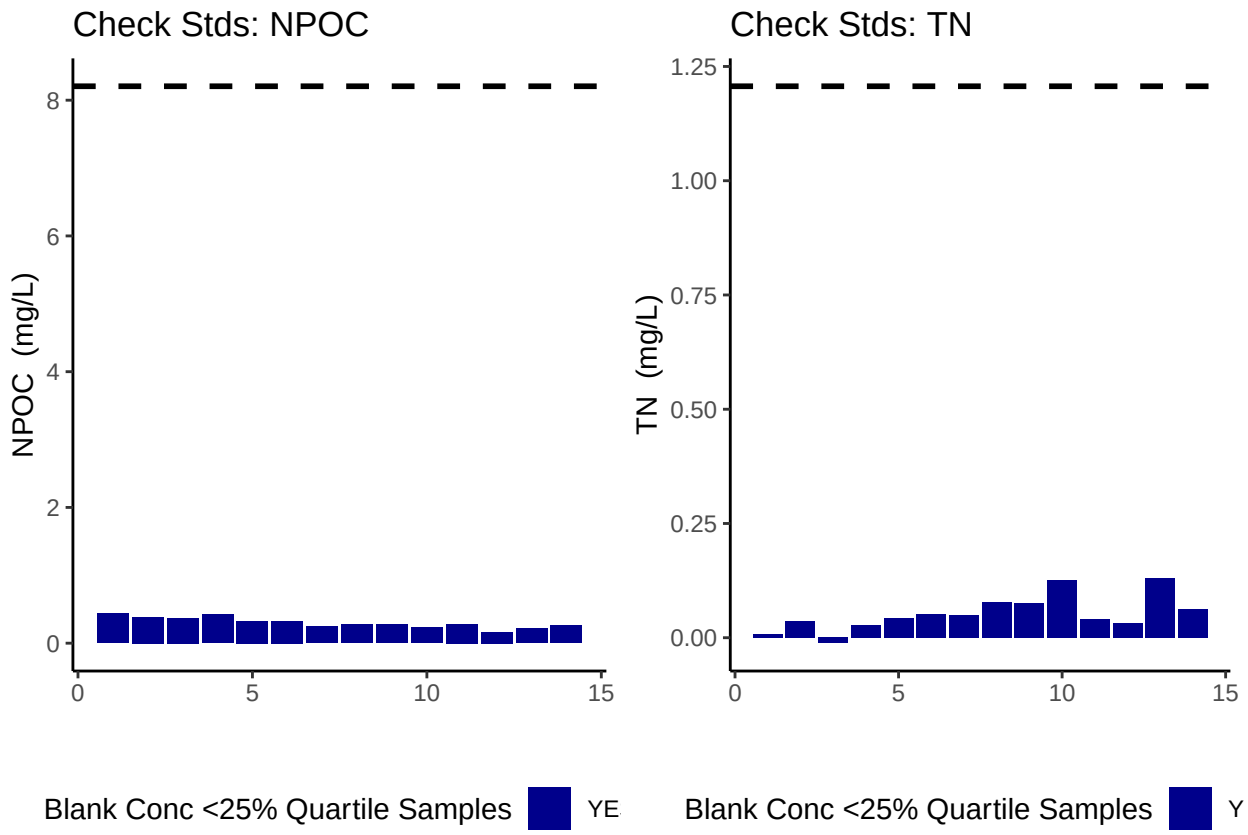
Assess Blanks

```
## 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:
```

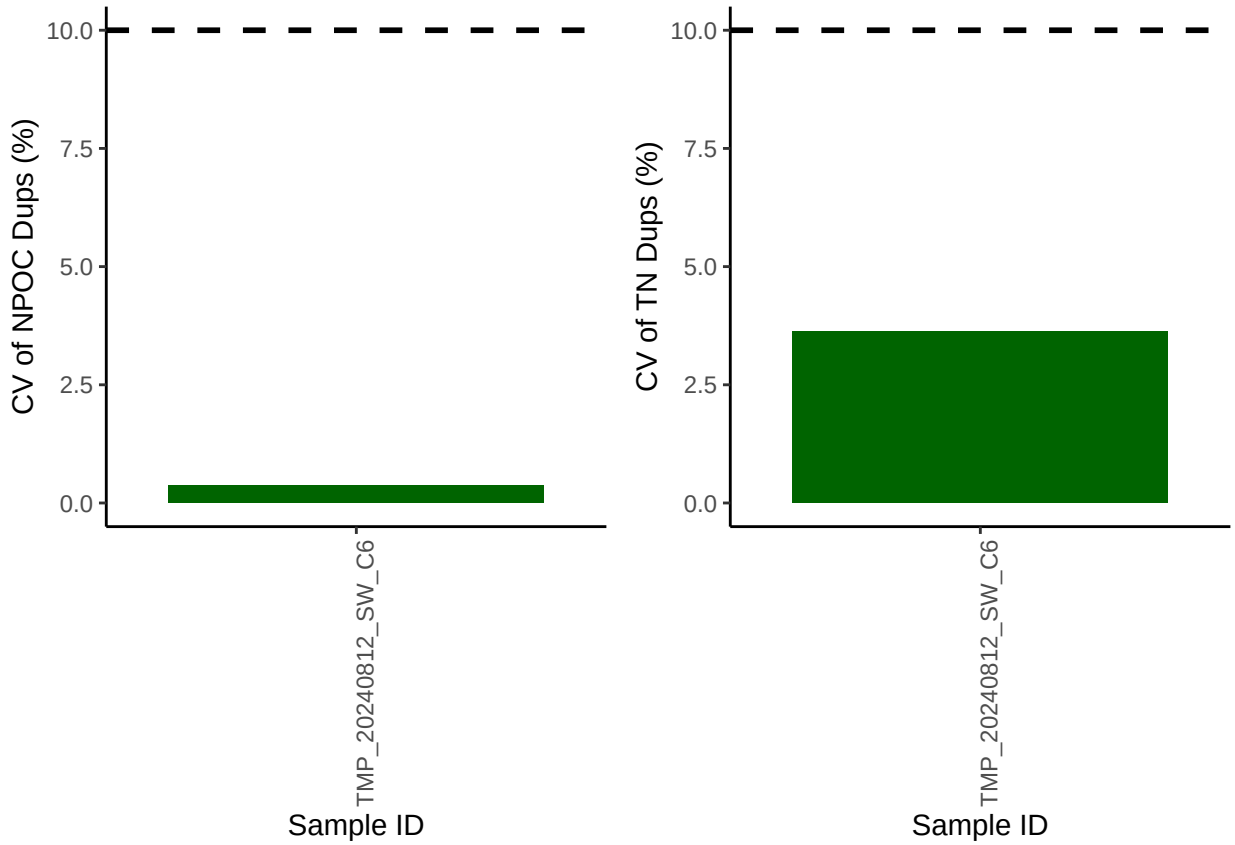
```
## [1] 0.3019643
```

```
## nitrogen blanks:
```

```
## [1] 0.05335857
```

Assess Duplicates - if there are any

```
## Assess Duplicates

## # A tibble: 1 x 3
##   sample_name        npoc_raw_dup tdn_raw_dup
##   <chr>                     <dbl>       <dbl>
## 1 TMP_20240812_SW_C6         11.6        2.17

##          sample_name npoc_raw tdn_raw        run_datetime npoc_flag tdn_flag
## 1 TMP_20240812_SW_C6    11.55   2.097 9/5/2024 9:35:07 PM
##   npoc_raw_dup tdn_raw_dup
## 1        11.59       2.171

##          sample_name npoc_raw tdn_raw        run_datetime npoc_flag tdn_flag
## 1 TMP_20240812_SW_C6    11.55   2.097 9/5/2024 9:35:07 PM
##   npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag tdn_dups_cv
## 1        11.59       2.171    0.3662456               YES    3.633469
##   tdn_dups_cv_flag
## 1              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.
```

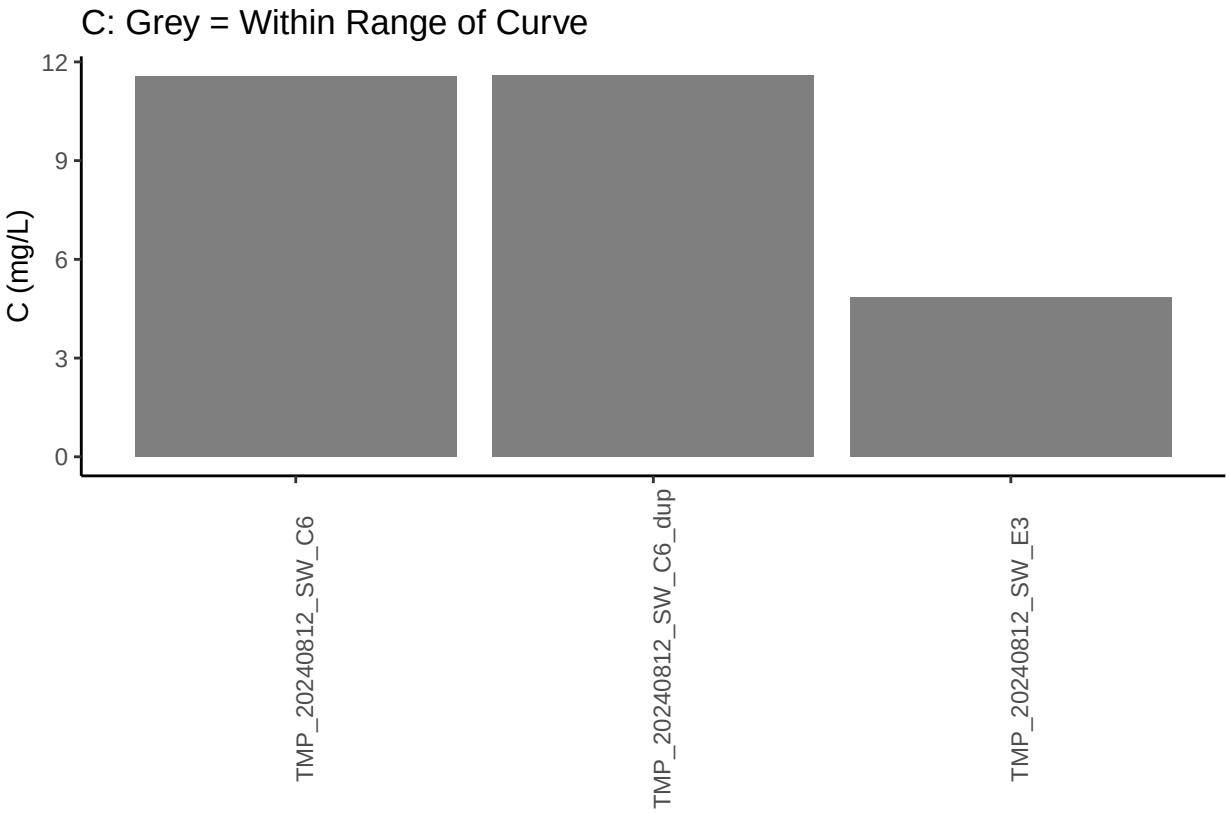


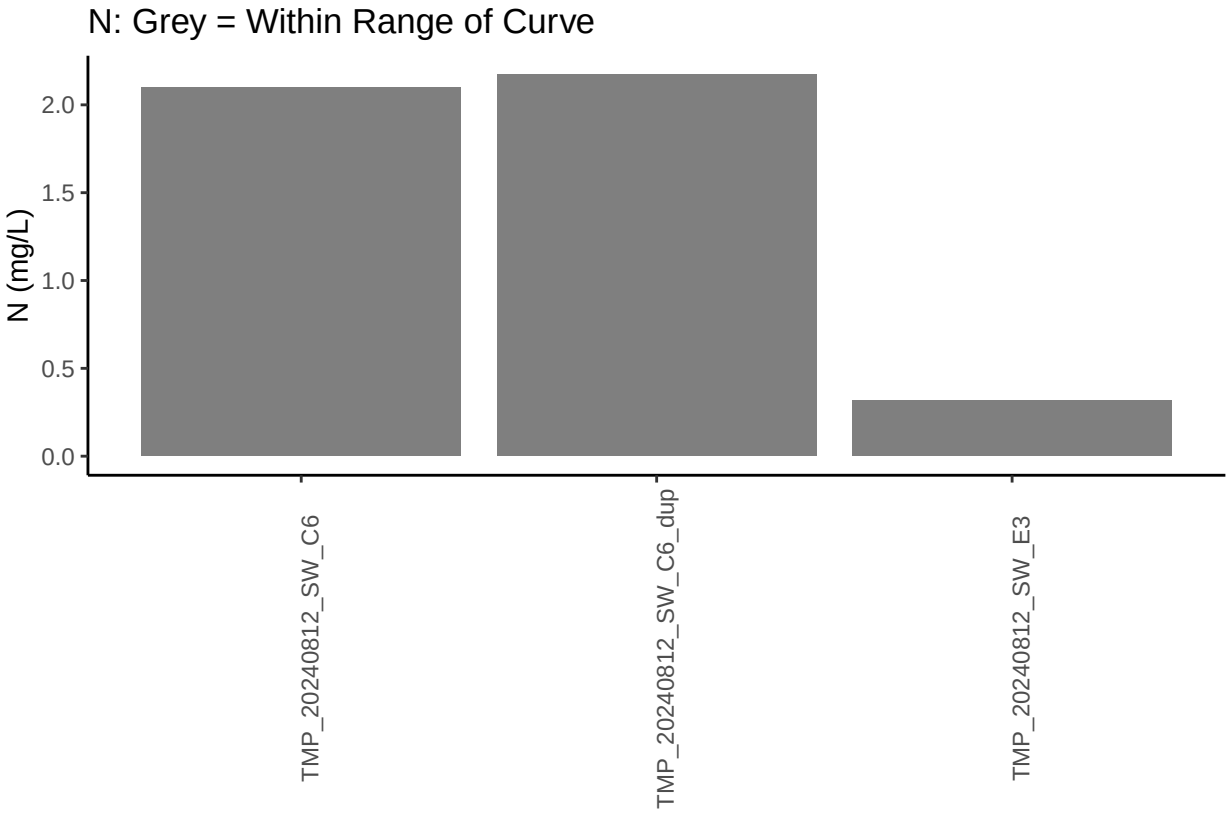
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

```
## Sample Flagging
```




N: Grey = Within Range of Curve
N (mg/L)
2.0
1.5
1.0
0.5
0.0
TMP_20240812_SW_C6
TMP_20240812_SW_C6_dup
TMP_20240812_SW_E3

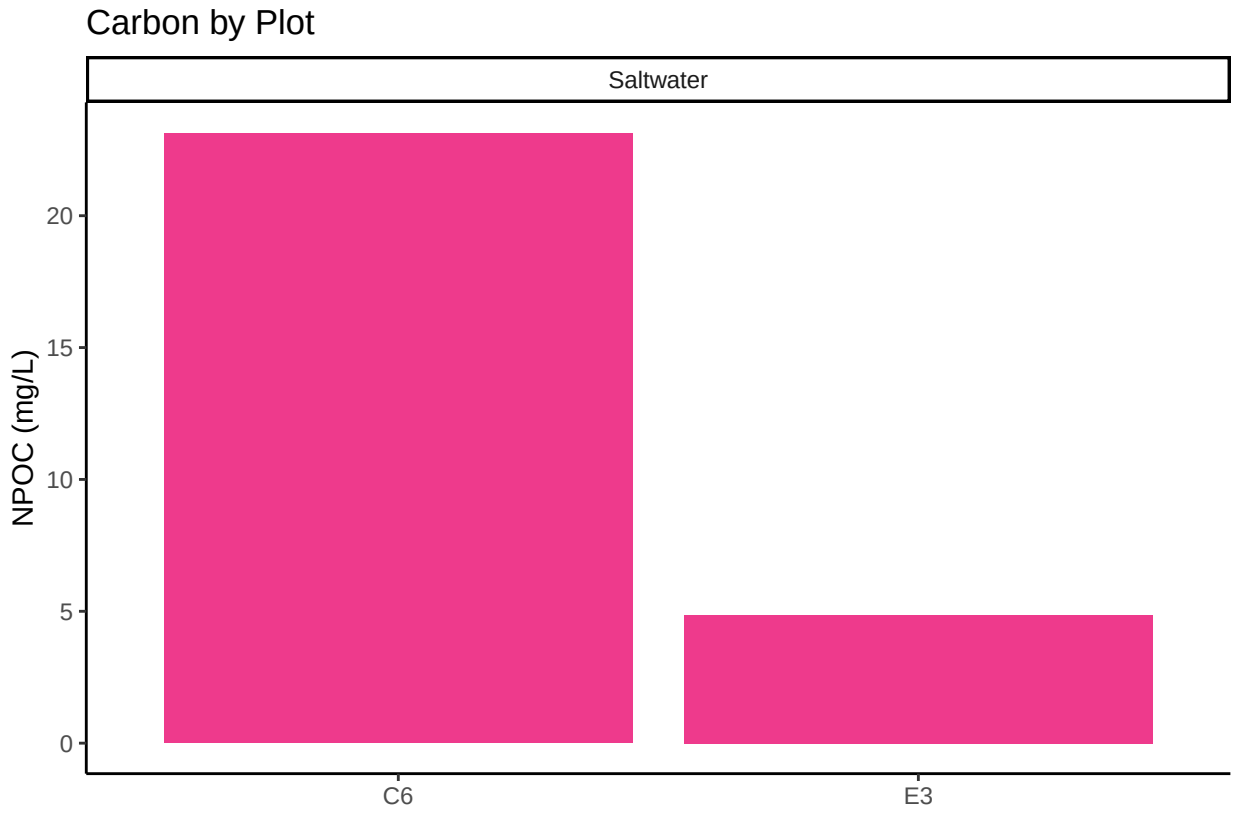
Visualize Data by Plot

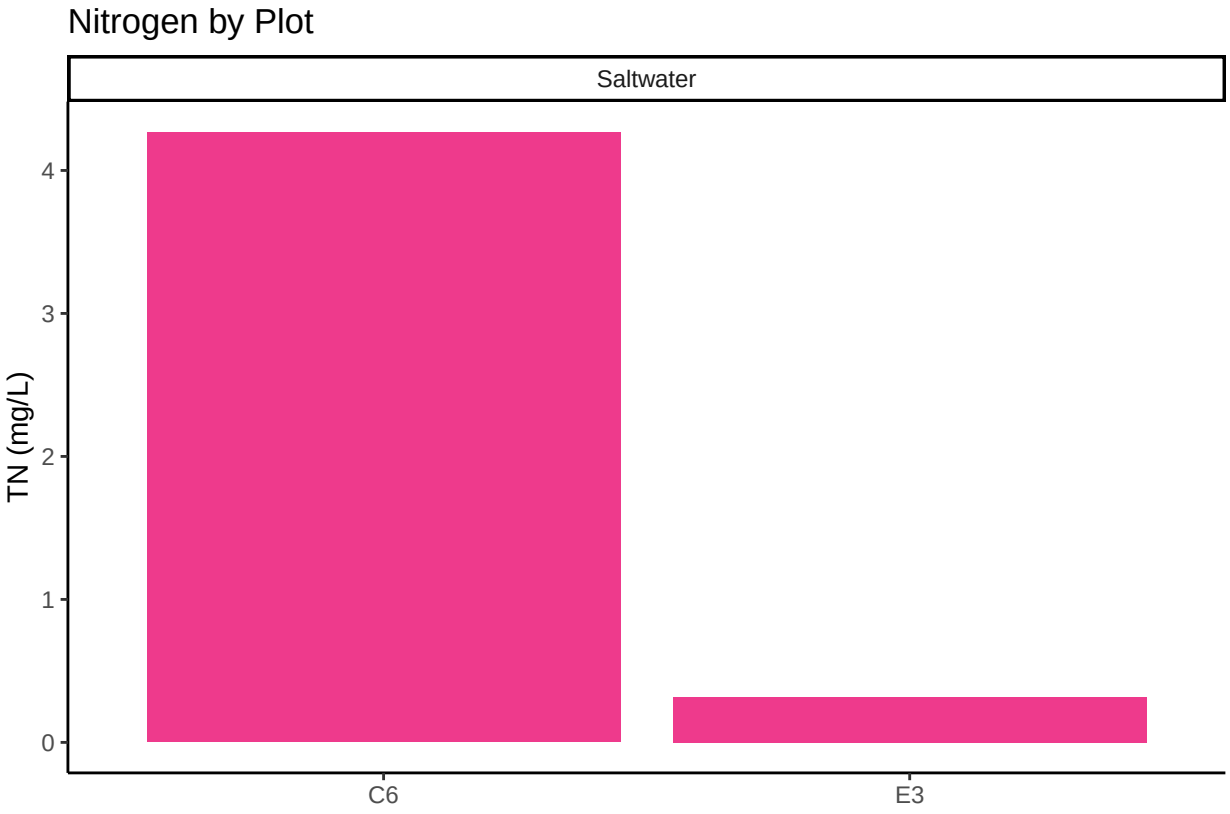
```
## Visualize Data
```

```
## Warning in rbind(c("TMP", "20240812", "SW", "C6"), c("TMP", "20240812", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
##   Site_Code     Date Plot Grid_Square Extra
## 1       TMP 20240812   SW          C6   TMP
## 2       TMP 20240812   SW          C6   dup
## 3       TMP 20240812   SW          E3   TMP
```

```
##   Site_Code     Date Plot Grid_Square Extra            sample_name npoc_raw
## 1       TMP 20240812   SW          C6   TMP     TMP_20240812_SW_C6   11.550
## 2       TMP 20240812   SW          C6   dup TMP_20240812_SW_C6_dup   11.590
## 3       TMP 20240812   SW          E3   TMP     TMP_20240812_SW_E3    4.861
##   tdn_raw         run_datetime npoc_flag tdn_flag
## 1  2.0970  9/5/2024 9:35:07 PM
## 2  2.1710 9/5/2024 10:07:22 PM
## 3  0.3165 9/5/2024 10:38:39 PM
```




Nitrogen by Plot
Saltwater
TN (mg/L)
0
1
2
3
4
C6
E3

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 2 x 2
##   sample_name        metadata_recorded
##   <chr>              <lgl>
## 1 TMP_20240812_SW_C6 FALSE
## 2 TMP_20240812_SW_E3 FALSE
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 2 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 <NA>    <NA>  <NA>        15 <NA>        <NA>    <NA>     11.6     963.
## 2 <NA>    <NA>  <NA>        15 <NA>        <NA>    <NA>      4.86    405.
## # 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