

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
```

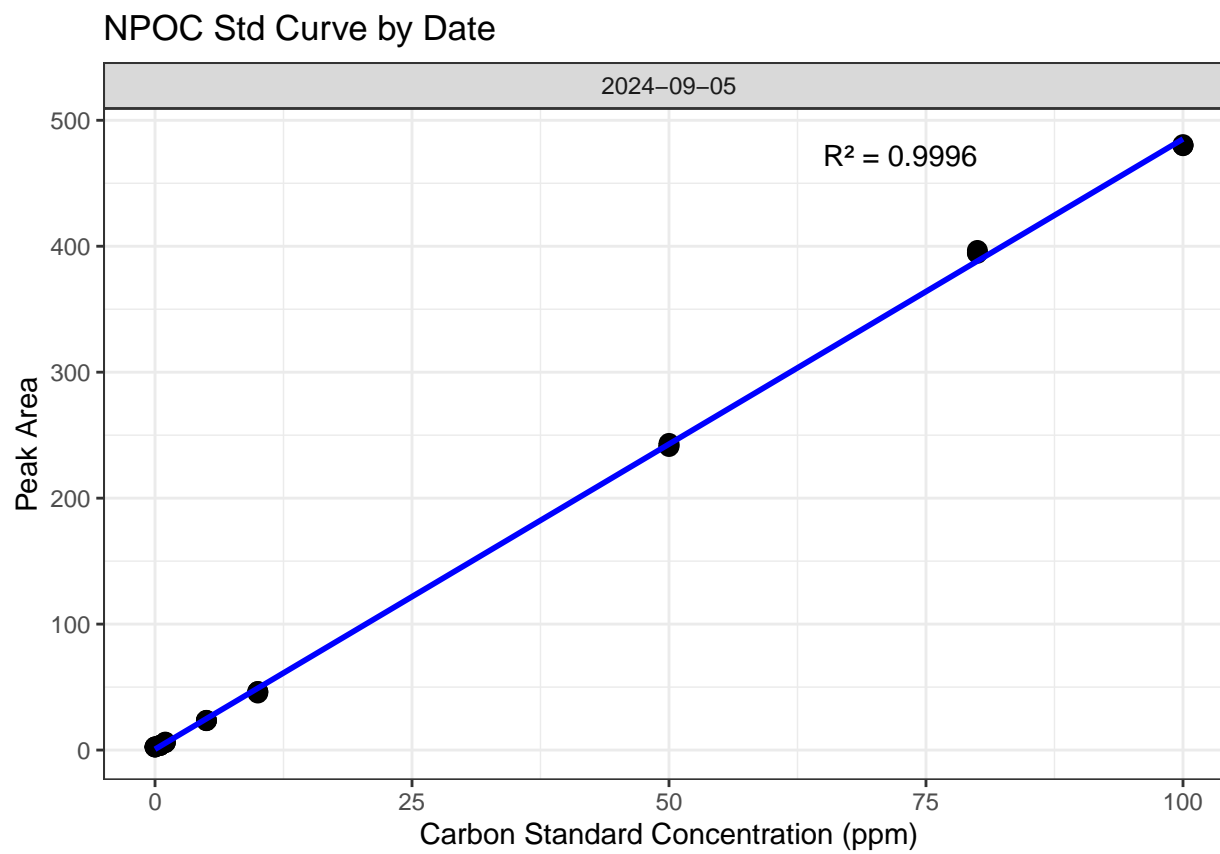
Assessing standard Curves

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

```
## New names:
```

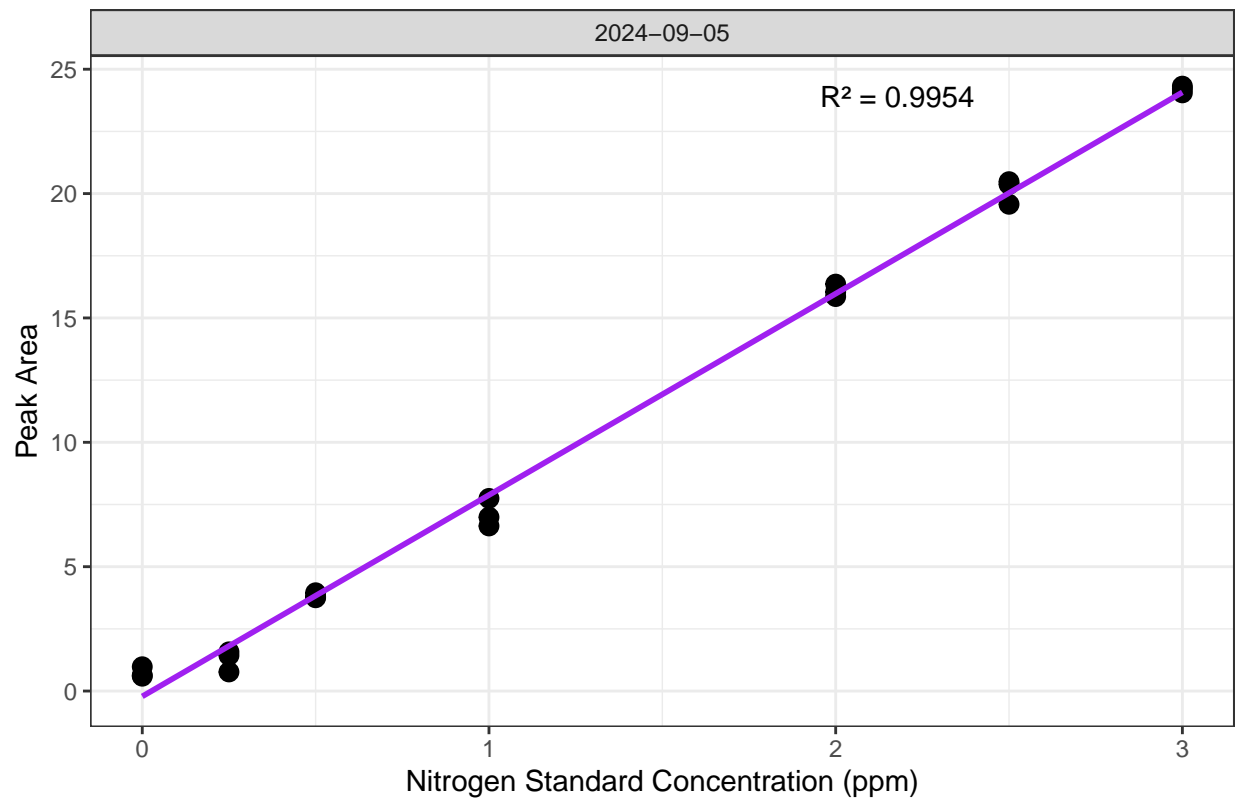
```
## 'geom_smooth()' using formula = 'y ~ x'
```

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



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

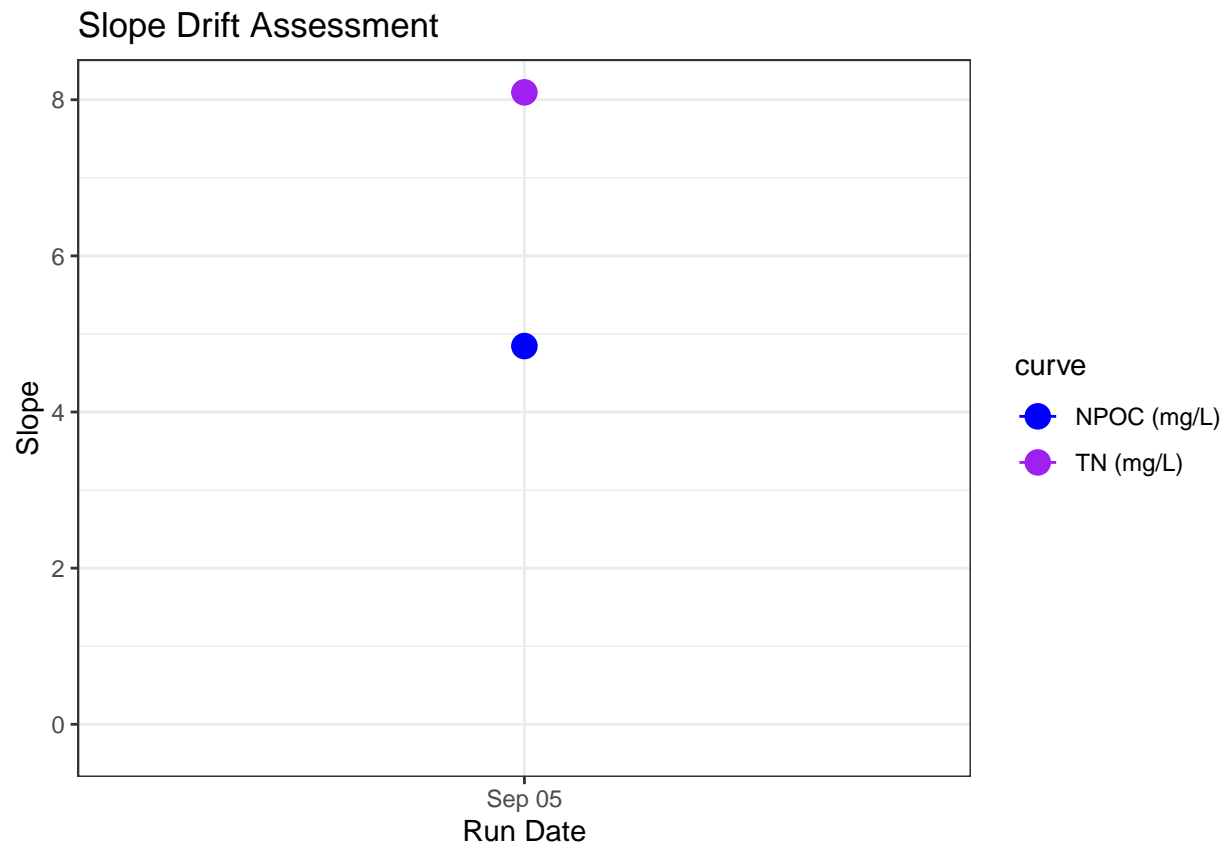
TN Std Curve by Date



```
## Warning: Removed 19 rows containing missing values or values outside the scale range
## ('geom_point()').
```

```
## Warning: Removed 19 rows containing missing values or values outside the scale range
## ('geom_line()').
```

```
## 'geom_line()': Each group consists of only one observation.
## i Do you need to adjust the group aesthetic?
```



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

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

Assess Check Standards

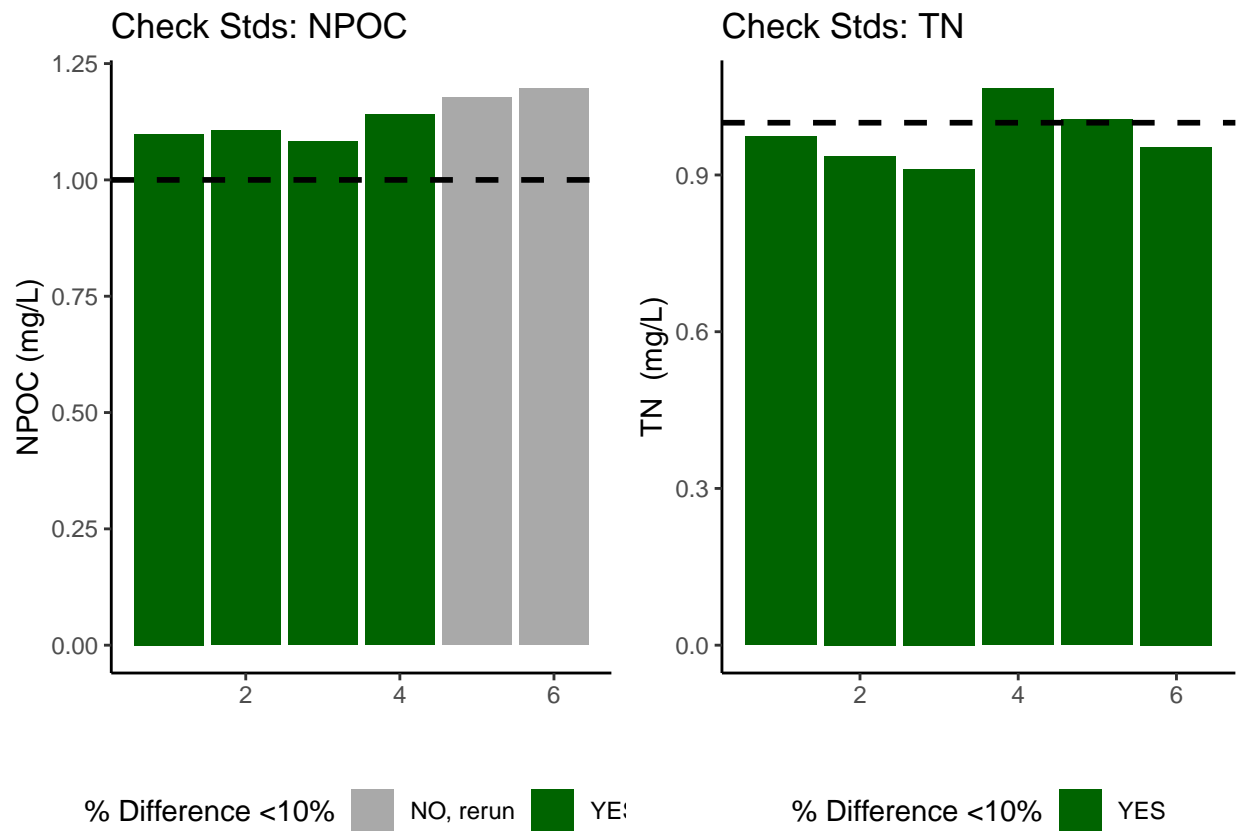
```
## Assess the Check Standards
```

```
## 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

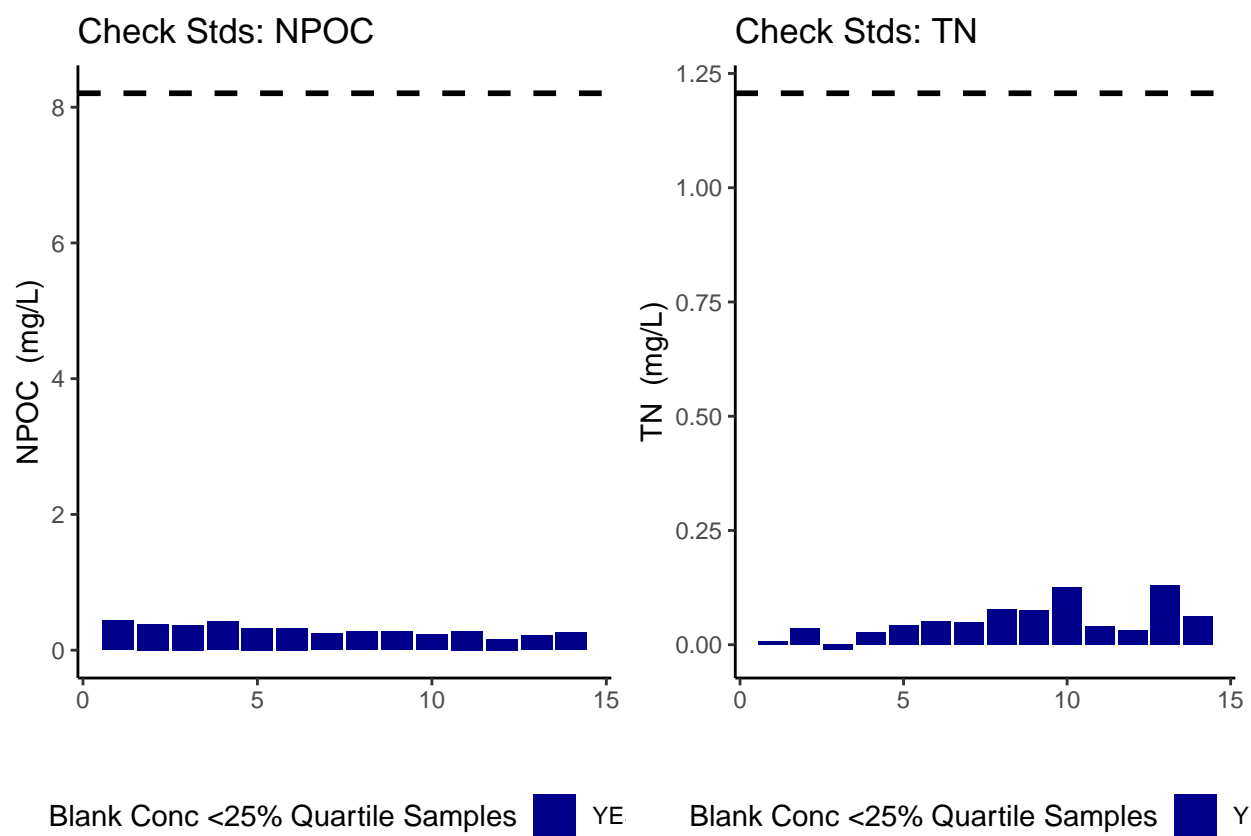
```
## Assess Blanks
```

```
## 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
```

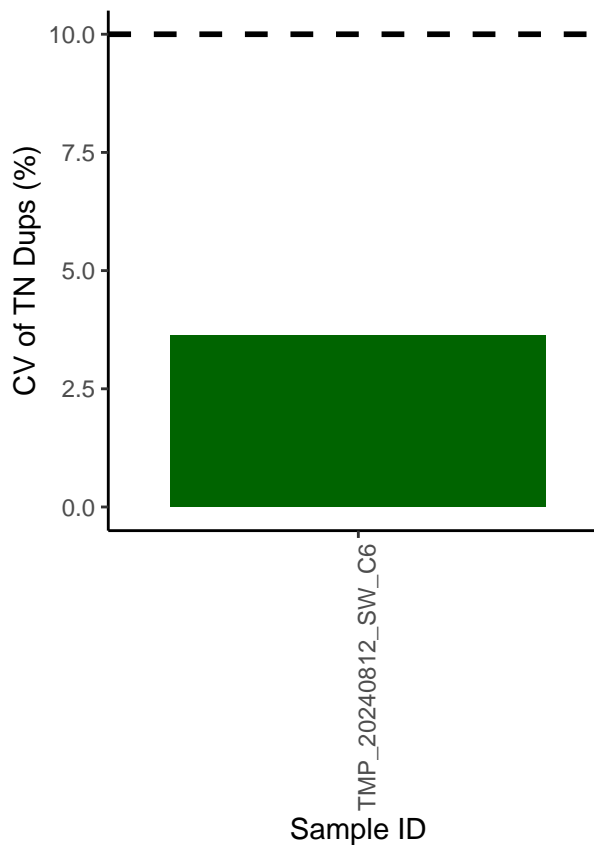
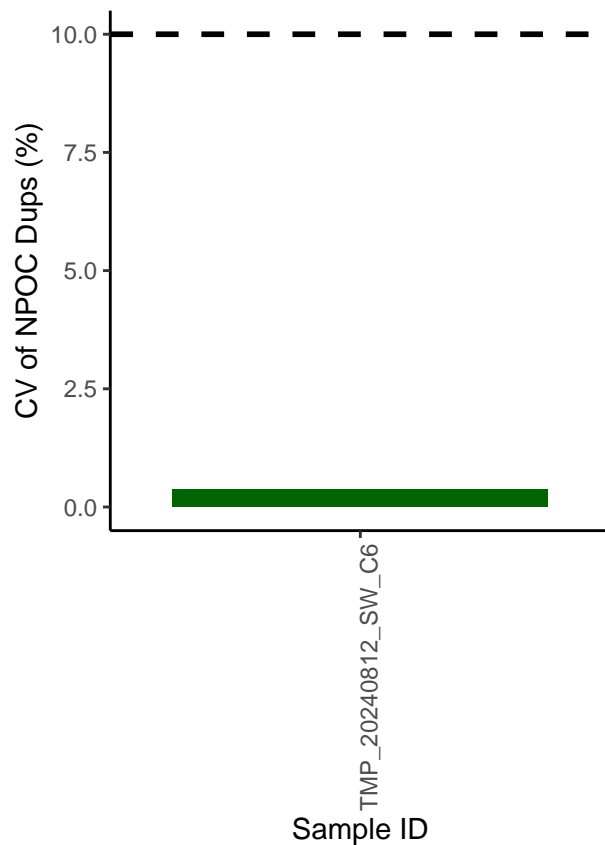
```
## # A tibble: 1 x 3
```

```
##   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.
```

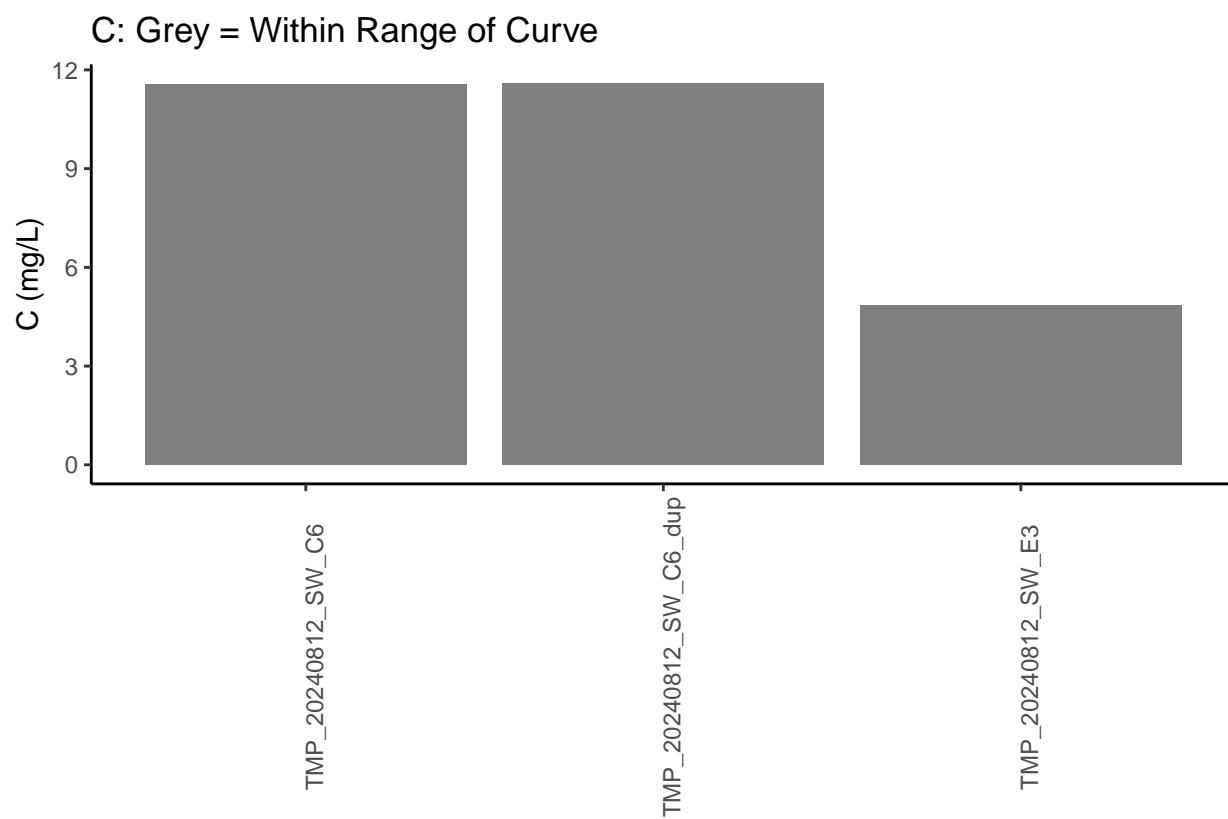


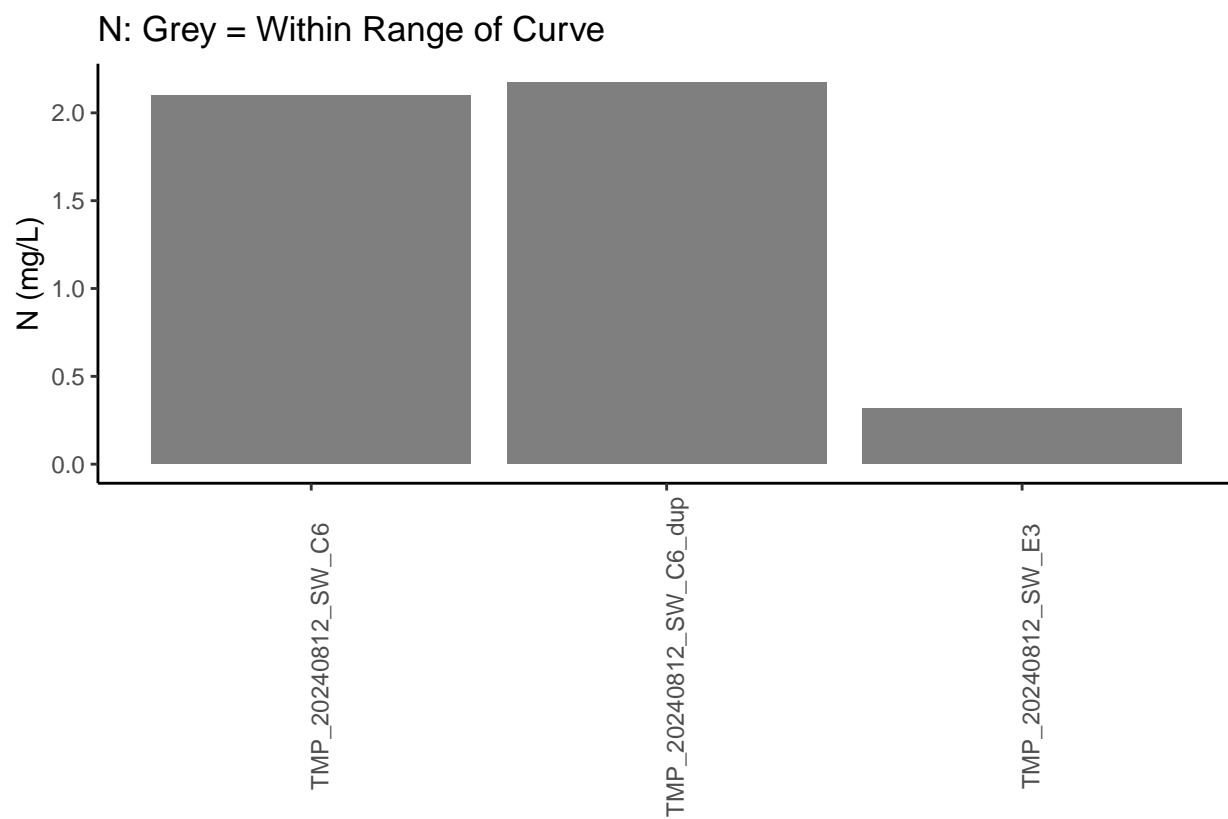

```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

Sample Flagging

Sample Flagging





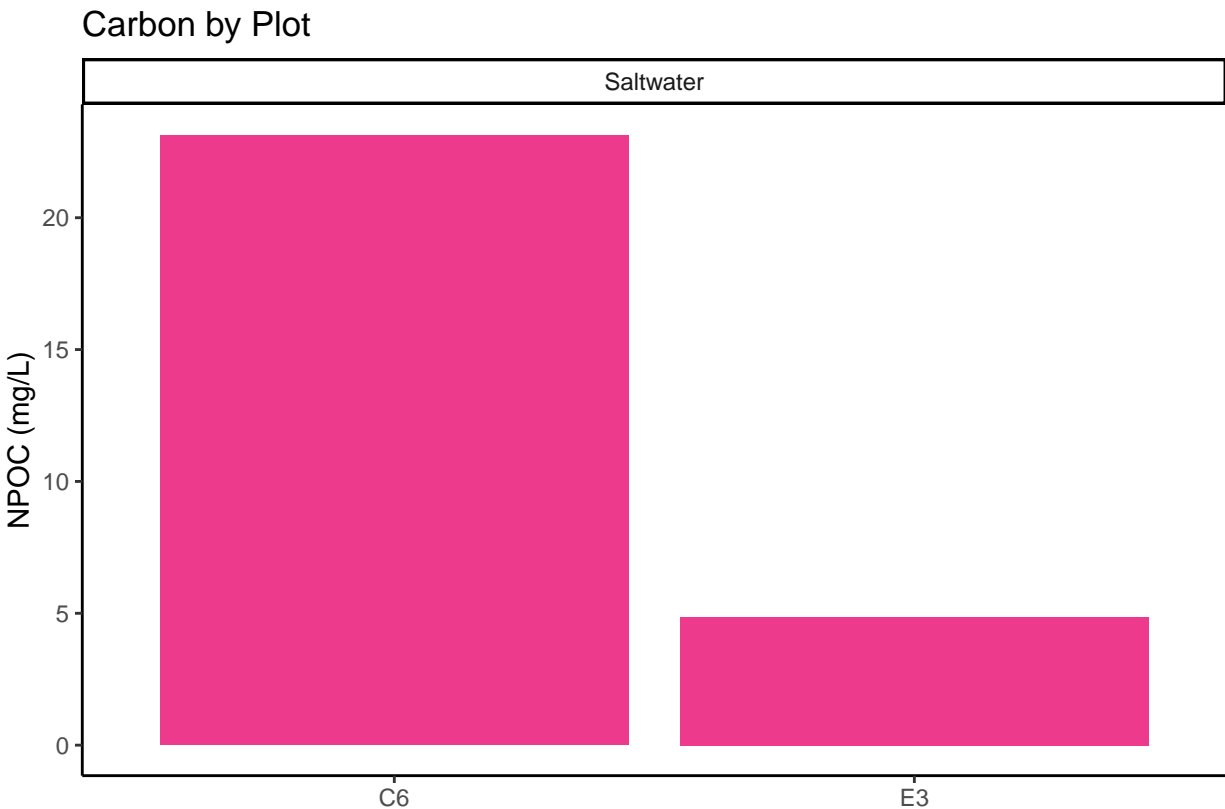
Visualize Data by Plot

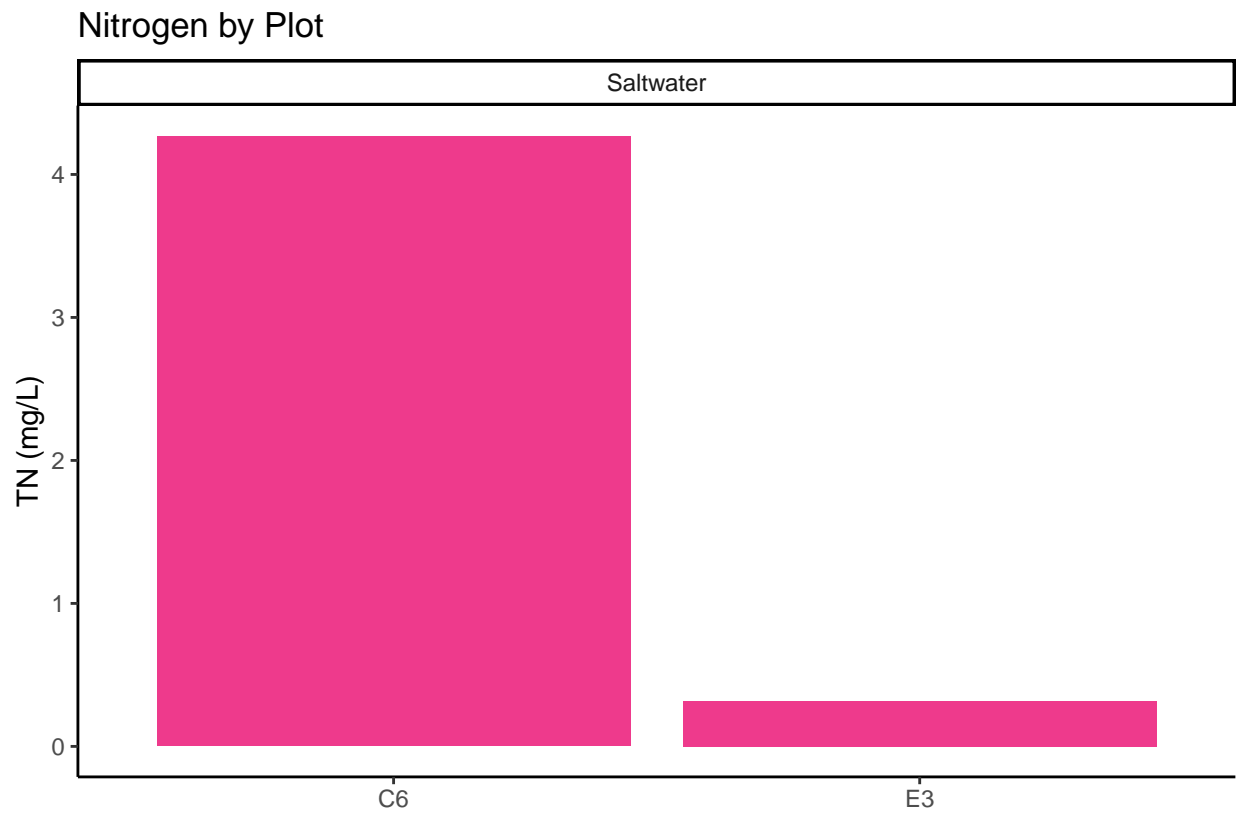
```
## Visualize Data

## 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
```





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

```
#end
```