COMPASS: TEMPEST Discrete DOC Data QAQC

November 2025

2025-11-10

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 = "11/03/25"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = "NPOC check standards slightly out of range. Accepting run anyways.
      No diuplicates on this run."

  #file path and name for summary file
    raw_file_name = "tmp_doc_raw_data_2025/TMP_202511.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "tmp_doc_raw_data_2025/TMP_202511_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "tmp_doc_processed_data_2025/TMP_PW_DOC_Processed_202511.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_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
```

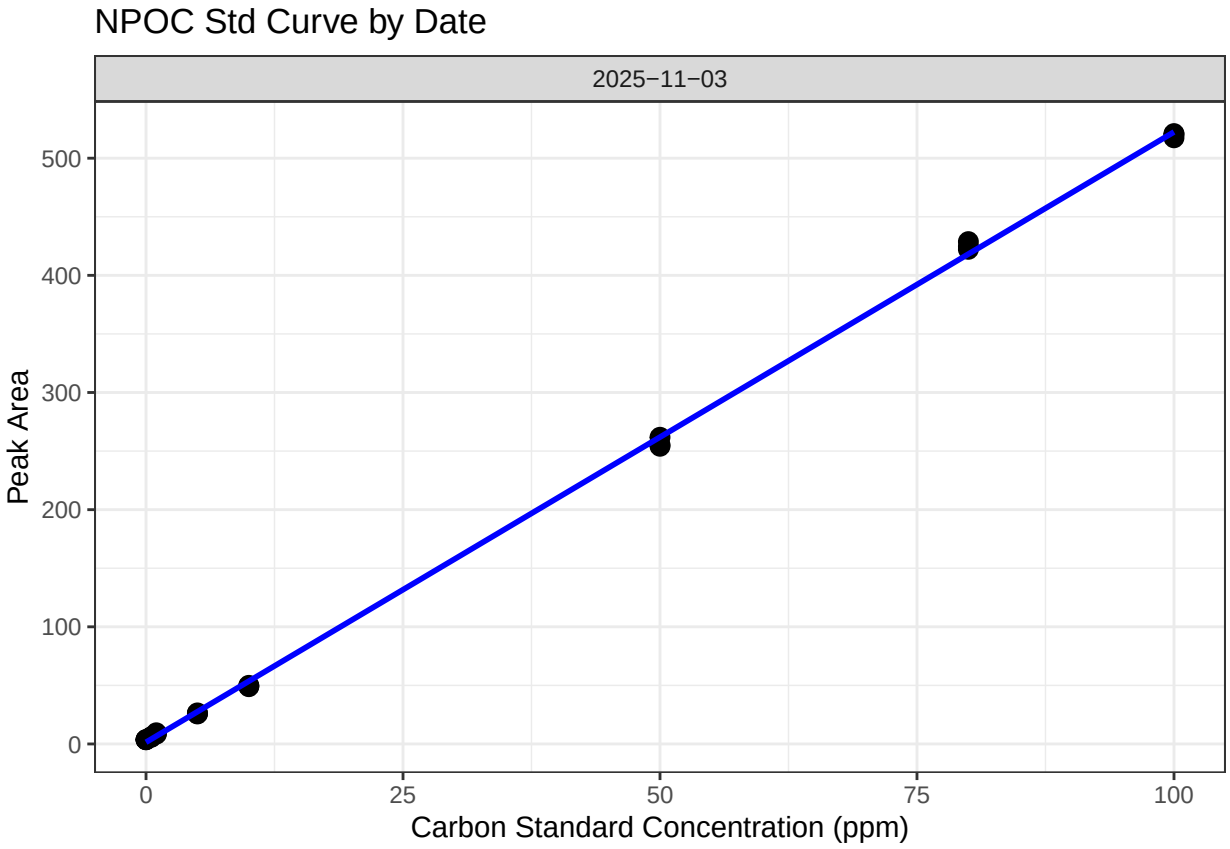
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 4 x 4
##   sample_name        npoc_raw tdn_raw run_datetime
##   <chr>                 <dbl>   <dbl> <chr>
## 1 TMP_C_I5_20251101      12.0   0.588 11/3/2025 7:41:06 PM
## 2 TMP_FW_I5_20251101     19.2   0.713 11/3/2025 8:12:39 PM
## 3 TMP_SW_F6_20251101     23.9   0.814 11/3/2025 8:38:56 PM
## 4 TMP_SW_H6_20251101     27.3   1.08  11/3/2025 9:10:49 PM
```

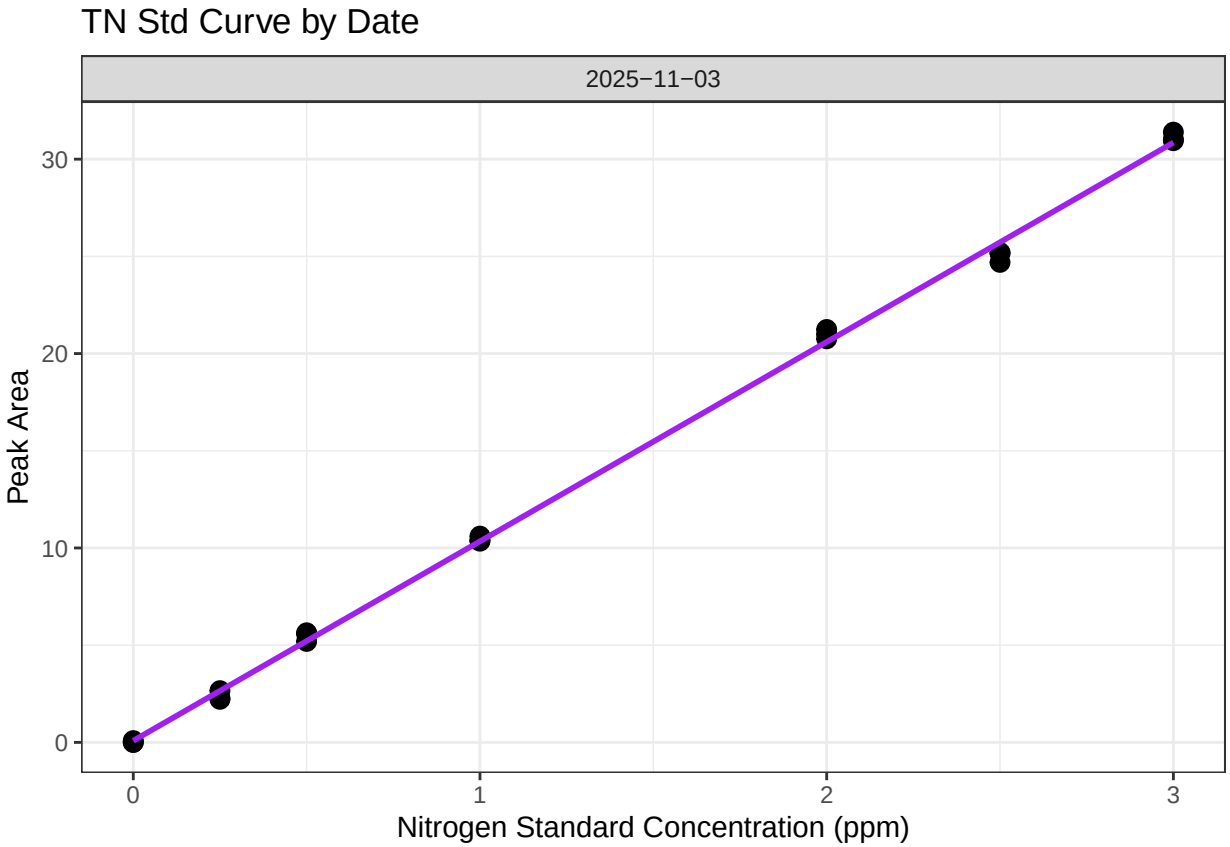
Assessing standard Curves

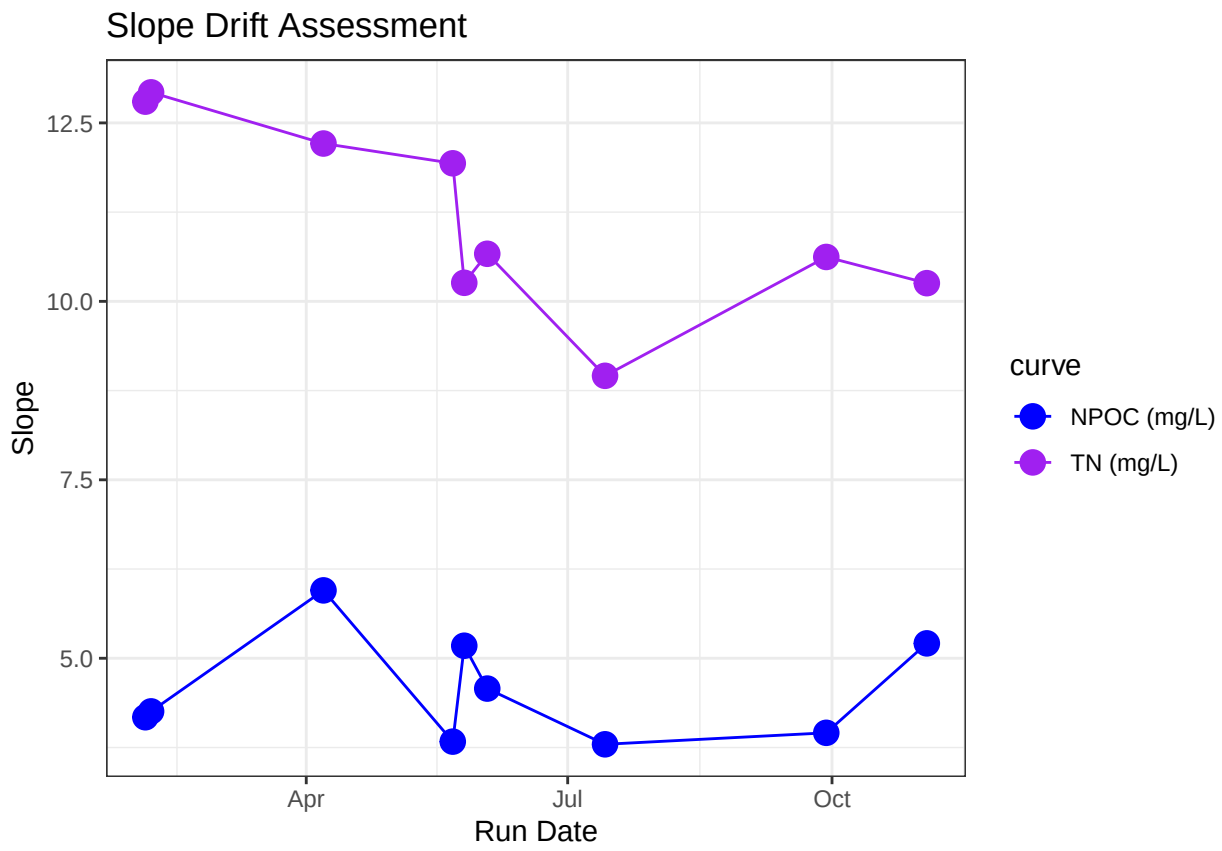
```
## Assess the Standard Curve
```

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




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


TN Std Curve by Date
2025−11−03
Peak Area
0
10
20
30
0
1
2
3
Nitrogen Standard Concentration (ppm)




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

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

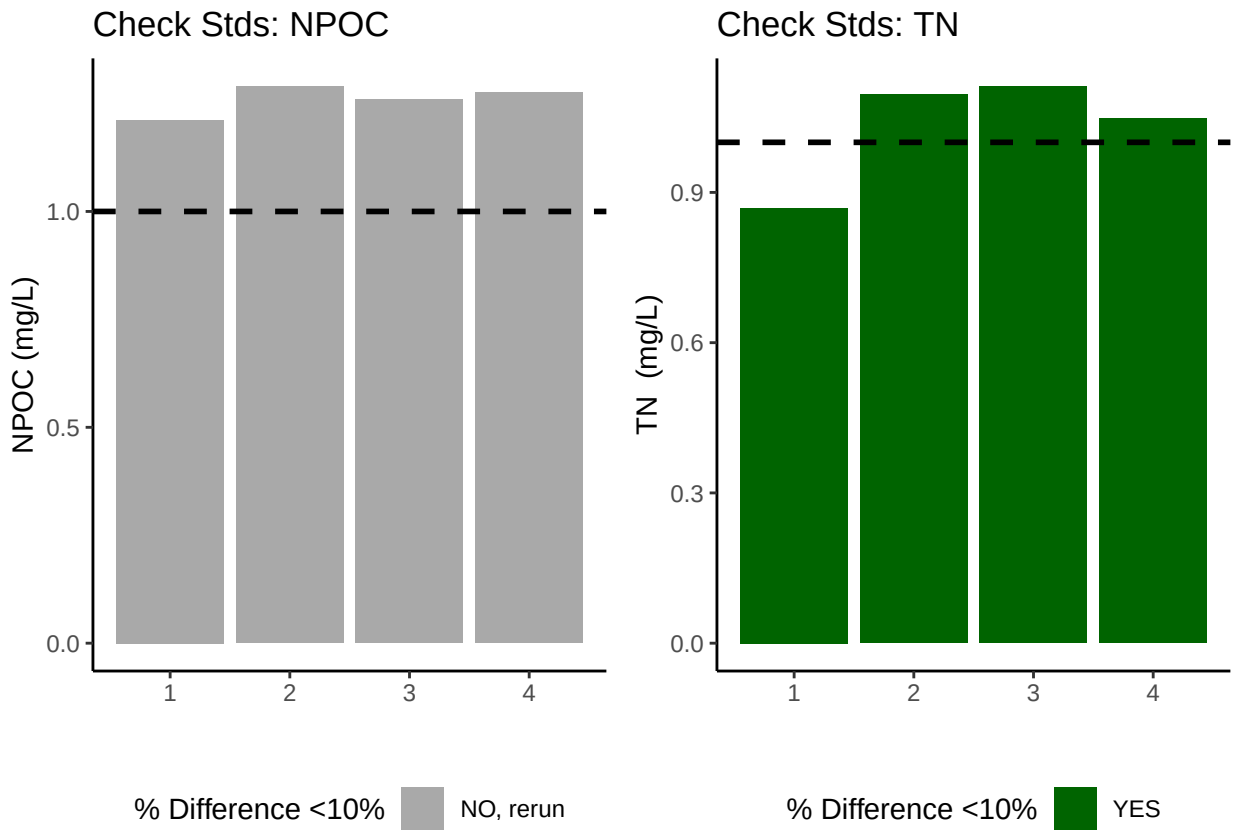
Assess Check Standards

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

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

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

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




```
## [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"
```

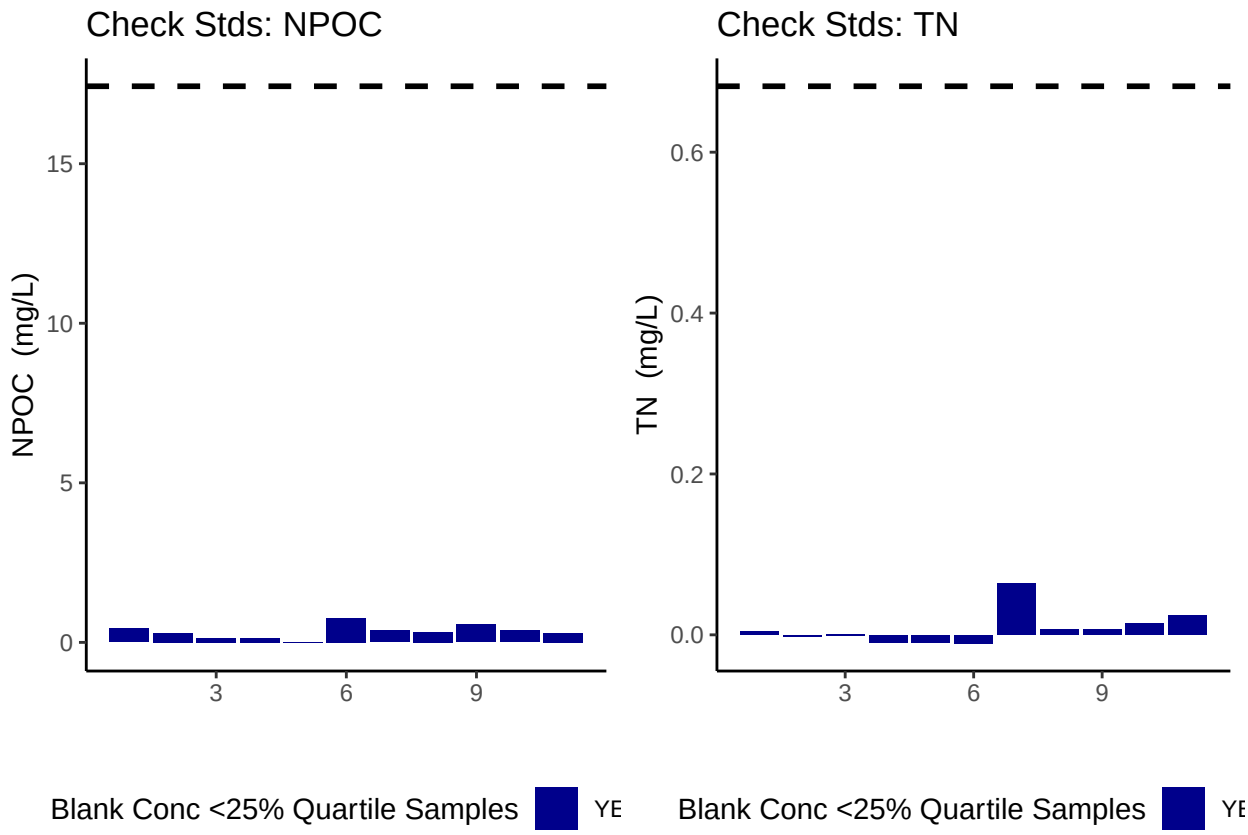
Assess Blanks

```
## 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:
```

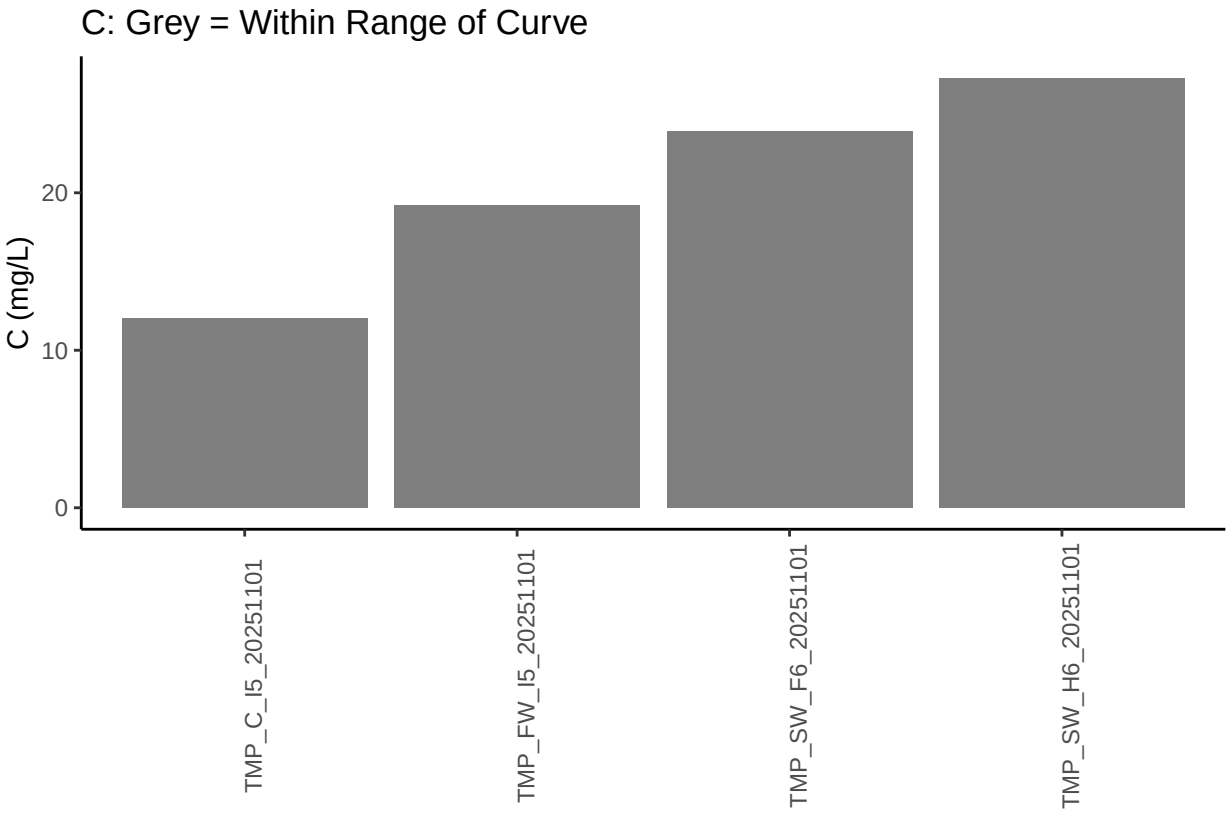
```
## [1] 0.3324136
```

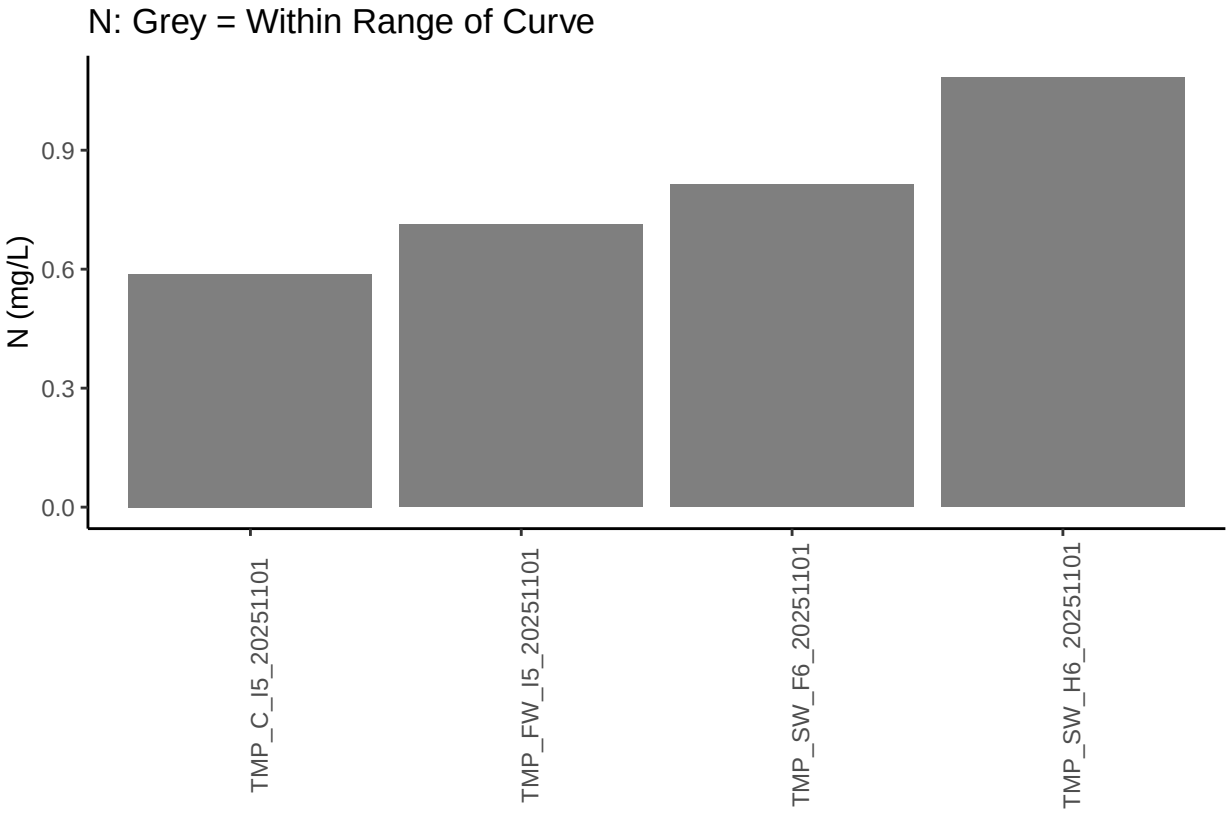
```
## nitrogen blanks:
```

```
## [1] 0.007966364
```

Sample Flagging

```
## Sample Flagging
```



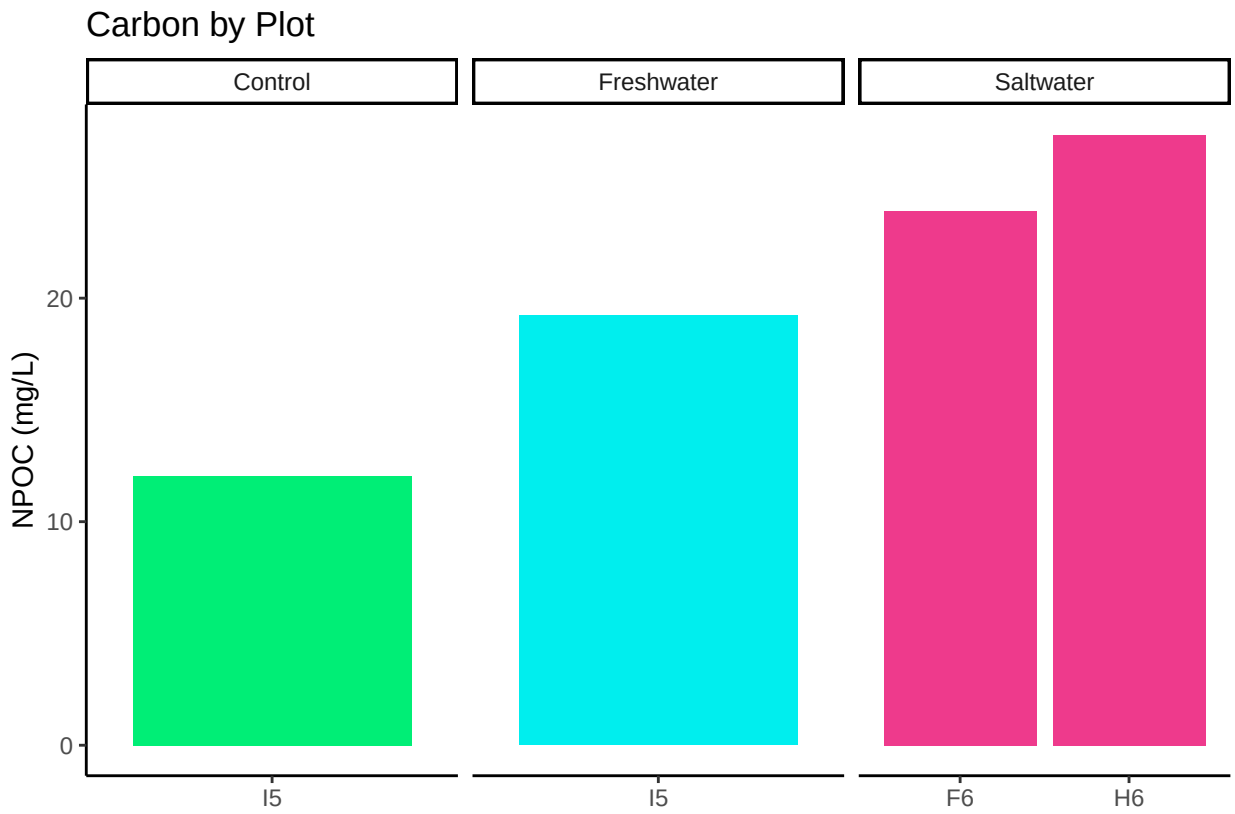

N: Grey = Within Range of Curve
N (mg/L)
0.0
0.3
0.6
0.9
TMP_C_I5_20251101
TMP_FW_I5_20251101
TMP_SW_F6_20251101
TMP_SW_H6_20251101

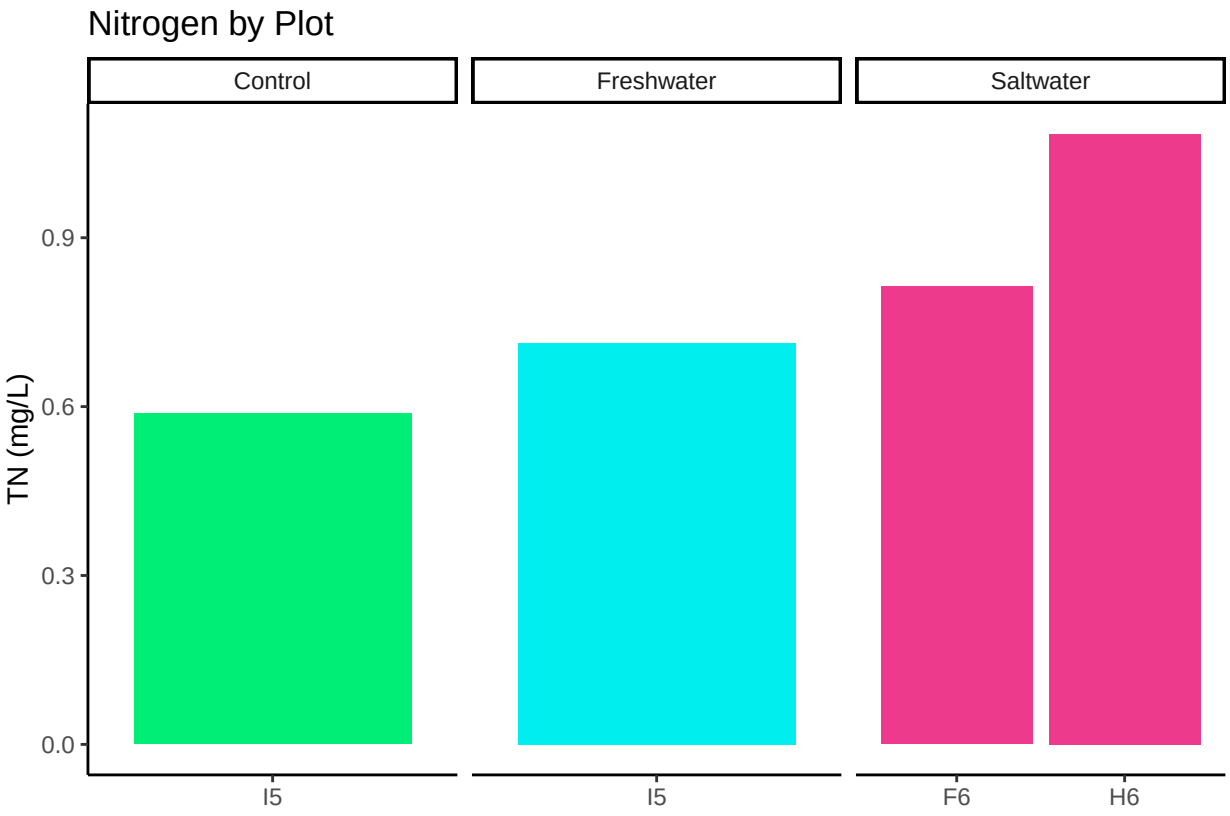
Visualize Data by Plot

```
## Visualize Data
```

```
##   Site_Code Plot Grid_Square     Date
## 1       TMP    C          I5 20251101
## 2       TMP   FW          I5 20251101
## 3       TMP   SW          F6 20251101
## 4       TMP   SW          H6 20251101
```

```
##   Site_Code Plot Grid_Square     Date        sample_name npoc_raw tdn_raw
## 1       TMP    C          I5 20251101  TMP_C_I5_20251101    12.05  0.5878
## 2       TMP   FW          I5 20251101 TMP_FW_I5_20251101    19.22  0.7134
## 3       TMP   SW          F6 20251101 TMP_SW_F6_20251101    23.89  0.8135
## 4       TMP   SW          H6 20251101 TMP_SW_H6_20251101    27.30  1.0840
##           run_datetime                npoc_flag tdn_flag
## 1 11/3/2025 7:41:06 PM NPOC checks out of range
## 2 11/3/2025 8:12:39 PM NPOC checks out of range
## 3 11/3/2025 8:38:56 PM NPOC checks out of range
## 4 11/3/2025 9:10:49 PM NPOC checks out of range
```




Nitrogen by Plot
Control
Freshwater
Saltwater
TN (mg/L)
0.9
0.6
0.3
0.0
I5
I5
F6
H6

Convert data from mg/L to uMoles/L

Add in/check metadata

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

```
## # A tibble: 4 x 2
##   sample_name        metadata_recorded
##   <chr>              <lgl>
## 1 TMP_C_I5_20251101  TRUE
## 2 TMP_FW_I5_20251101 TRUE
## 3 TMP_SW_F6_20251101 TRUE
## 4 TMP_SW_H6_20251101 TRUE
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 4 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     I5          15 DOC         C_I5_D~ 2025~     12.0   1004.
## 2 COMPASS: TEMP~ FW    I5          15 DOC         FW_I5_~ 2025~     19.2   1602.
## 3 COMPASS: TEMP~ SW    F6          15 DOC         SW_F6_~ 2025~     23.9   1991.
## 4 COMPASS: TEMP~ SW    H6          15 DOC         SW_H6_~ 2025~     27.3   2275
## # 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

Assess Duplicates - NO DUPLICATES ON THIS RUN

“‘{#r Check Duplicates, echo=FALSE}

cat(“Assess Duplicates”)

#Take a look at the raw data #head(dat_raw)

#pull out any rows that have “dup” in the sample_name column dups <- dat_raw %>% select(!c(npoc_flag, tdn_flag)) %>% filter(str_detect(sample_name, “dup”)) #have to change this to match data

#create a new dataframe and remove dups from sample dataframe dat_raw2 <- dat_raw %>% filter(!str_detect(sample_name, “dup”))

#remove the dup from these IDs so we will have duplicate sample names dups$sample_name <- gsub(”_dup”, ””, as.character(dups$sample_name)) dups <- dups[,-c(4)] #remove the run date time for colnames(dups) <- c(‘sample_name’, ‘npoc_raw_dup’, “tdn_raw_dup”) head(dups)

QAdups <- merge(dat_raw2, dups) head(QAdups)

df2 <- as.data.frame(QAdups$npoc_raw)df2dups <- QAdups$npoc_raw_dup

df2$sds <- apply(df2, 1, sd)df2$mean <- apply(df2, 1, mean)

QAdups$npoc_dups_cv <- (df2$sds/df2$mean)*100QAdups$npoc_dups_cv_flag <- ifelse(QAdups$npoc_dups_cv <10, 'YES', 'NO, rerun')

df3 <- as.data.frame(QAdups$tdn_raw)df3$dups <- QAdups$tdn_raw_dup

df3$sds <- apply(df3, 1, sd)df3$mean <- apply(df3, 1, mean)

QAdups$tdn_dups_cv <- (df3$sds/df3$mean) * 100QAdups$tdn_dups_cv_flag <- ifelse(QAdups$tdn_dups_cv <10, 'YES', 'NO, rerun')

head(QAdups)

#plot dups output as a bar graph to easily check - want any over 10% to be red need to work on this C_dups <- ggplot(data =QAdups, aes(x =sample_name, y =npoc_dups_cv, fill=npoc_dups_cv_flag)) + geom_bar(stat = 'identity') + theme_classic() + labs(x= "Sample ID", y="CV of NPOC Dups (%)") + scale_fill_manual(values = c("YES" = "darkgreen", "NO, rerun" = "red")) + theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed", color = "black", size=1) + guides(fill=guide_legend(title="CV Between Dups <10%")) + theme(axis.text.x = element_text(angle = 90, hjust = 0.5))

N_dups <- ggplot(data =QAdups, aes(x =sample_name, y =tdn_dups_cv, fill=tdn_dups_cv_flag)) + geom_bar(stat = 'identity') + theme_classic() + labs(x= "Sample ID", y="CV of TN Dups (%)") + scale_fill_manual(values = c("YES" = "darkgreen", "NO, rerun" = "red")) + theme(legend.position="none") + geom_hline(yintercept=10, linetype="dashed", color = "black", size=1) + guides(fill=guide_legend(title="CV Between Dups <10%"))+ theme(axis.text.x = element_text(angle = 90, hjust = 0.5))

ggarrange(C_dups, N_dups,ncol=2, nrow=1)

#calculate the percent of check standards that are within the range based on the flag c_dups_percent <- (sum(QAdups$npoc_dups_cv_flag == "YES")/nrow(QAdups))*100n_dups_percent <- (sum(QAdups$tdn_dups_cv_flag == "YES")/nrow(QAdups))*100

#report out if flags indicate need for rerun ifelse(c_dups_percent >= chks_flag, ">60% of Carbon Duplicates have a CV <10%", "<60% of Carbon Duplicates have a CB <10% - REASSESS") ifelse(n_dups_percent >= chks_flag, ">60% of Nitrogen Duplicates have a CV <10%", "<60% of Nitrogen Duplicates have a CB <10% - REASSESS")

#write out a flag to the sample dataframe if more than 60% of the dups have CVs out of range if (c_dups_percent <= chks_flag) { dat_raw$npoc_flag <- ifelse(dat_raw$npoc_flag != "", paste0(dat_raw$npoc_flag,"; NPOC dups out of range"), "NPOC dups out of range") }

if (n_dups_percent <= chks_flag) { # assuming you have tn_chks_percent similarly dat_raw$tdn_flag <- ifelse(dat_raw$tdn_flag != "", paste0(dat_raw$tdn_flag,"; TN dups out of range"), "TN dups out of range") }

```
```