COMPASS: TEMPEST Discrete DOC Data QAQC

Freshwater Well Test: 2025-11-10

2025-11-18

Contents

0.1 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 = "11/16/25"
  Run_by = "Stephanie J. Wilson"
  Script_run_by = "Stephanie J. Wilson"
  run_notes = " Instrument started, then there was a leak and once that was fixed a new standard curve
    was run for remaining samples."

  #file path and name for summary file
```

```
    raw_file_name = "Raw Data/TMP_AquiferWellTest_NPOC.txt"
  #file path and name for the all peaks file
    raw_allpeaks_name = "Raw Data/TMP_AquiferWellTest_NPOC_allpeaks.txt"
  #file path and name for processed data after QAQC
    processed_file_name = "Processed Data/TMP_20251110_FW_WellTest_DOC_Processed.csv"

#check standard concentrations - Update if running different checks:
   chk_std_c = 50
   chk_std_n = 2

#Log path
    Log_path = "Raw Data/COMPASS_TMP_TOCTN_QAQClog_2025.csv"
```

0.2 Setup

0.3 Import Data Functions

0.4 Import Sample Data

```
## Import Sample Data
```

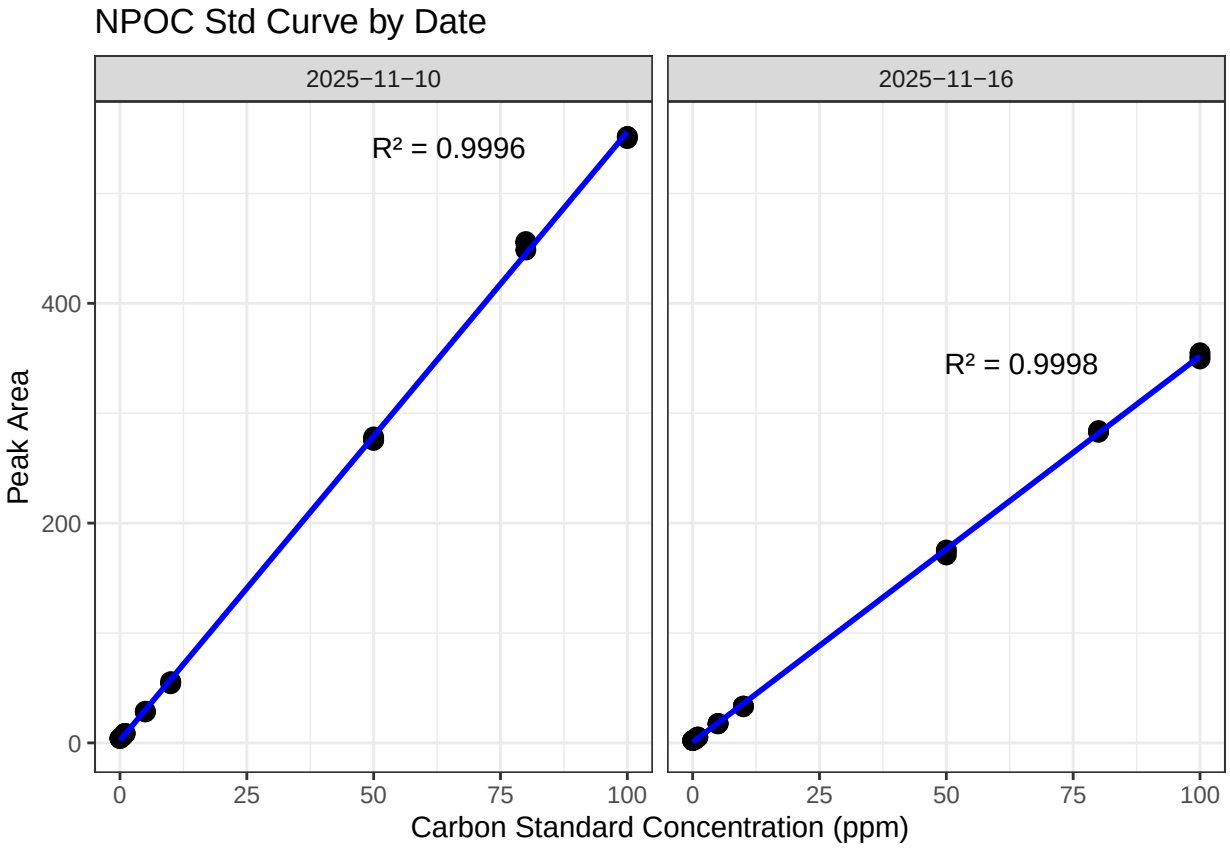
```
## New names:
## * `` -> `...14`
```

```
## # A tibble: 4 x 4
##   sample_name                         npoc_raw tdn_raw run_datetime
##   <chr>                                  <dbl>   <dbl> <chr>
## 1 TMP_AquiferWell_13:30_halffull         0.865   0.165 11/17/2025 10:59:13 AM
## 2 TMP_AquiferWell_13:30_halffull_dup     0.870   0.161 11/17/2025 11:27:18 AM
## 3 TMP_AquiferWell_15:00_full             0.643   0.198 11/17/2025 11:54:54 AM
## 4 TMP_AquiferWell_15:00_full_dup         0.783   0.188 11/17/2025 12:20:54 PM
```

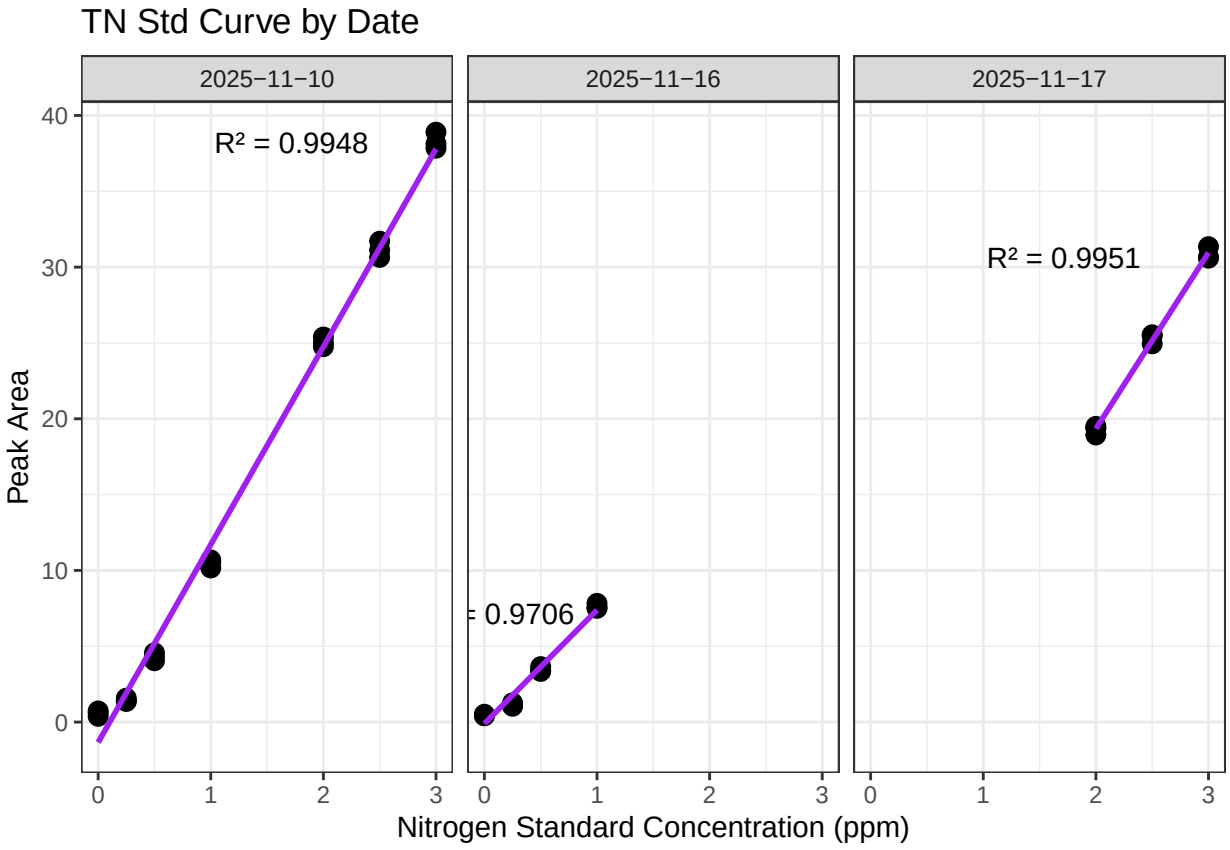
0.5 Assessing standard Curves

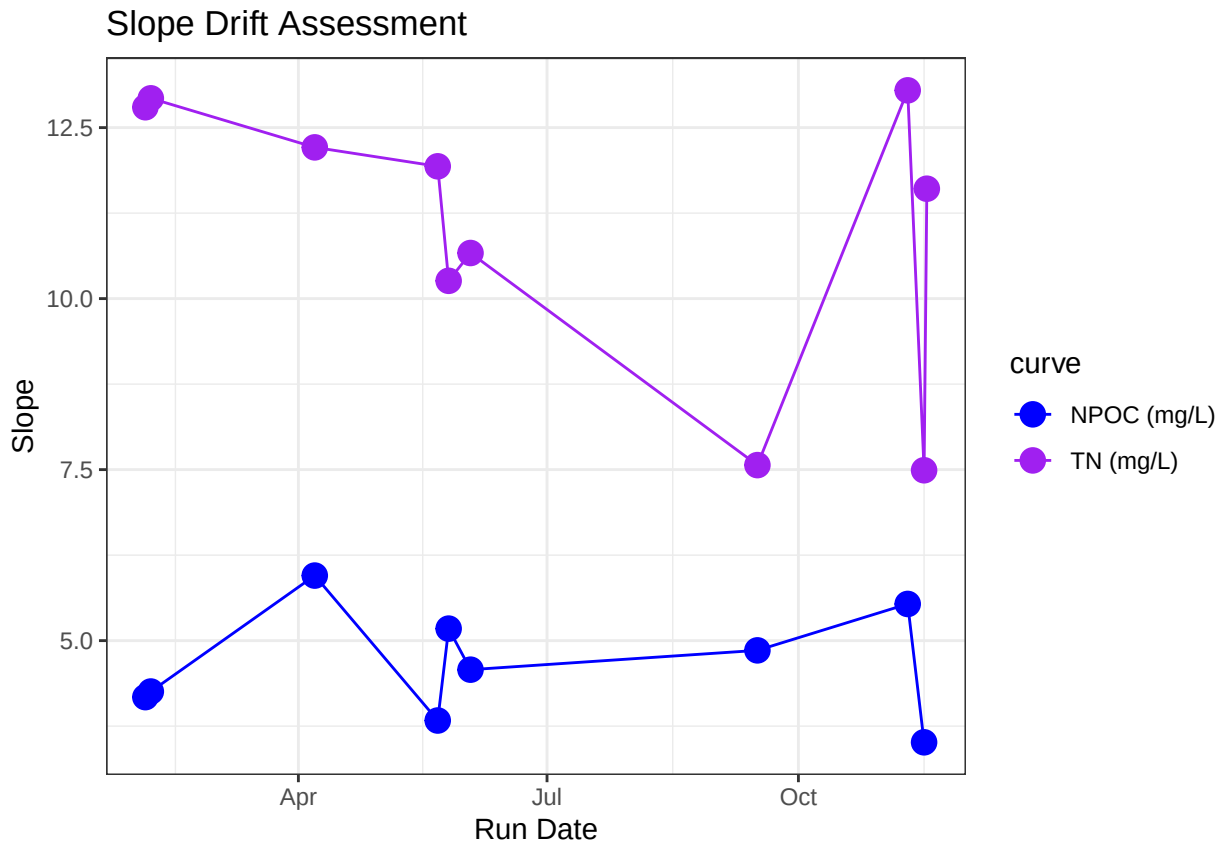
```
## Assess the Standard Curve
```

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




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


TN Std Curve by Date
2025−11−10
2025−11−16
2025−11−17
R² = 0.9948
= 0.9706
R² = 0.9951
Peak Area
Nitrogen Standard Concentration (ppm)
0
10
20
30
40
0
1
2
3




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

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

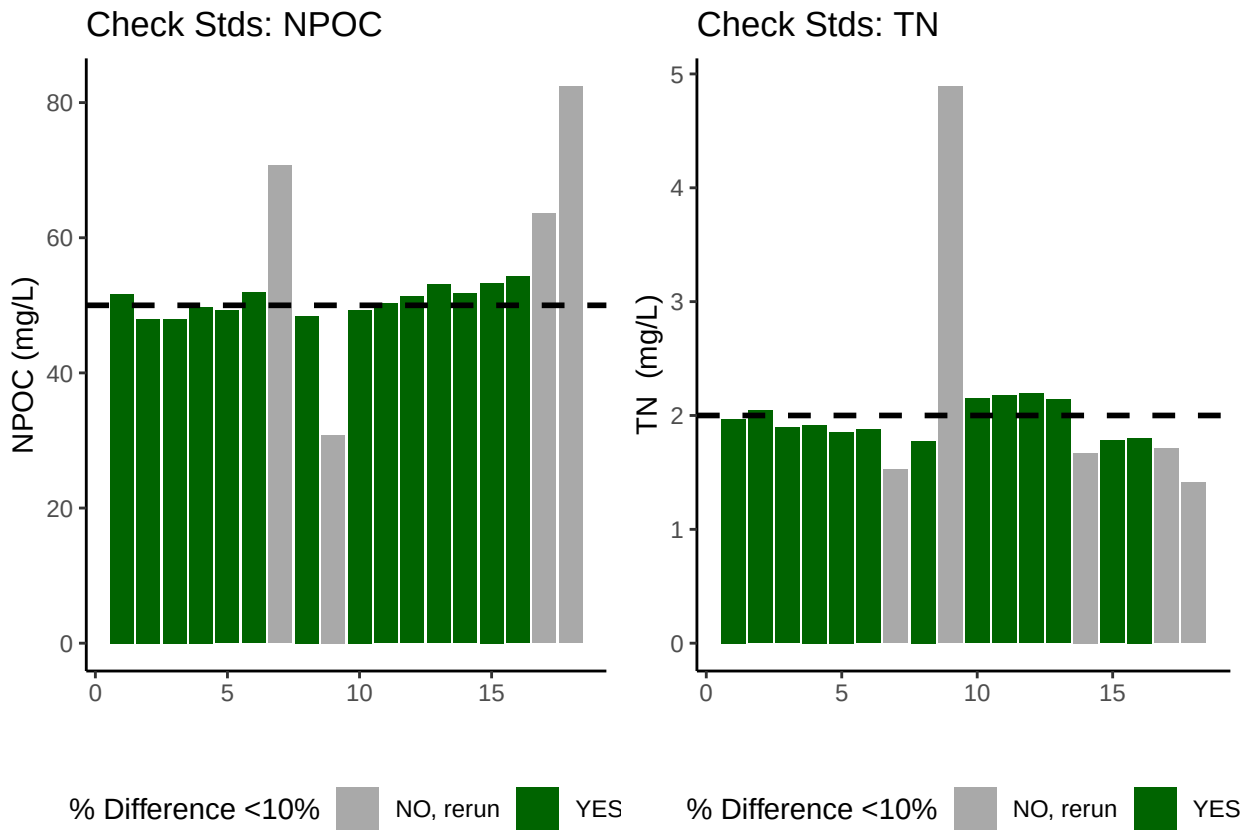
0.6 Assess Check Standards

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

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

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

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




```
## [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"
```

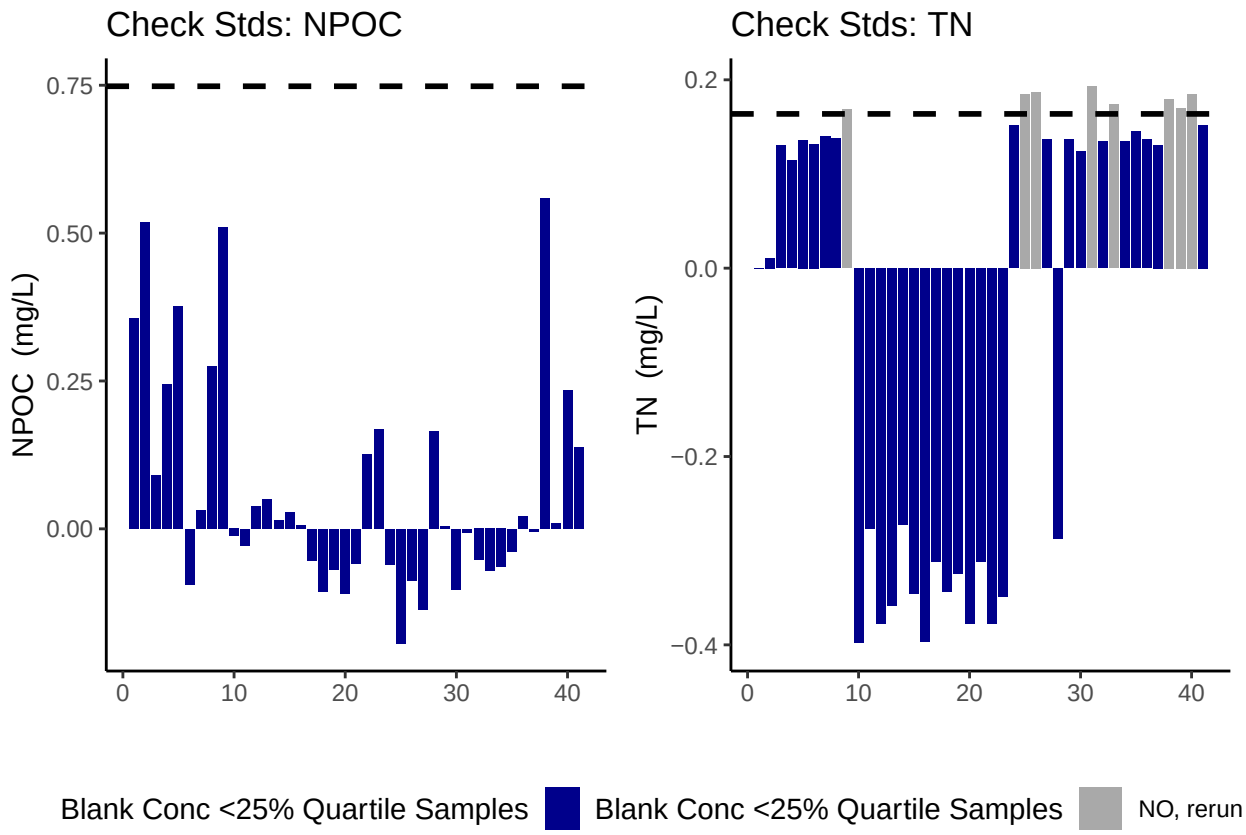
0.7 Assess Blanks

```
## 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] 0.06378463
```

```
## nitrogen blanks:
```

```
## [1] -0.03622024
```

0.8 Assess Duplicates - if there are any

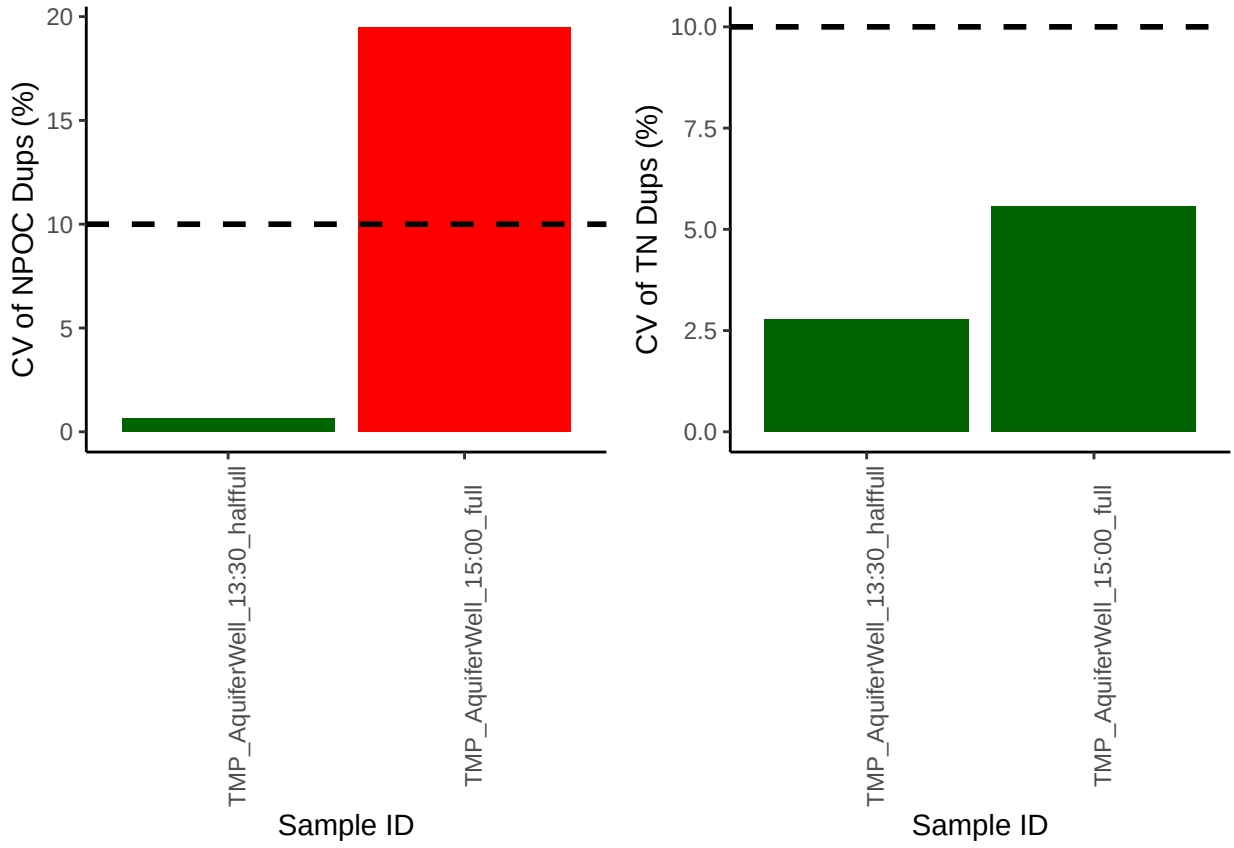
```
## Assess Duplicates
```

```
## # A tibble: 2 x 3
##   sample_name                    npoc_raw_dup tdn_raw_dup
##   <chr>                                 <dbl>       <dbl>
## 1 TMP_AquiferWell_13:30_halffull        0.870       0.161
## 2 TMP_AquiferWell_15:00_full            0.783       0.188
```

```
##                       sample_name npoc_raw tdn_raw           run_datetime
## 1 TMP_AquiferWell_13:30_halffull   0.8650  0.1649 11/17/2025 10:59:13 AM
## 2     TMP_AquiferWell_15:00_full   0.6431  0.1979 11/17/2025 11:54:54 AM
##   npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup
## 1                          0.8703      0.1606
## 2                          0.7834      0.1876
```

```
##                       sample_name npoc_raw tdn_raw           run_datetime
## 1 TMP_AquiferWell_13:30_halffull   0.8650  0.1649 11/17/2025 10:59:13 AM
## 2     TMP_AquiferWell_15:00_full   0.6431  0.1979 11/17/2025 11:54:54 AM
##   npoc_flag tdn_flag npoc_raw_dup tdn_raw_dup npoc_dups_cv npoc_dups_cv_flag
## 1                          0.8703      0.1606    0.6465031               YES
## 2                          0.7834      0.1876   19.5071025         NO, rerun
##   tdn_dups_cv tdn_dups_cv_flag
## 1    2.776424              YES
## 2    5.562763              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.
```

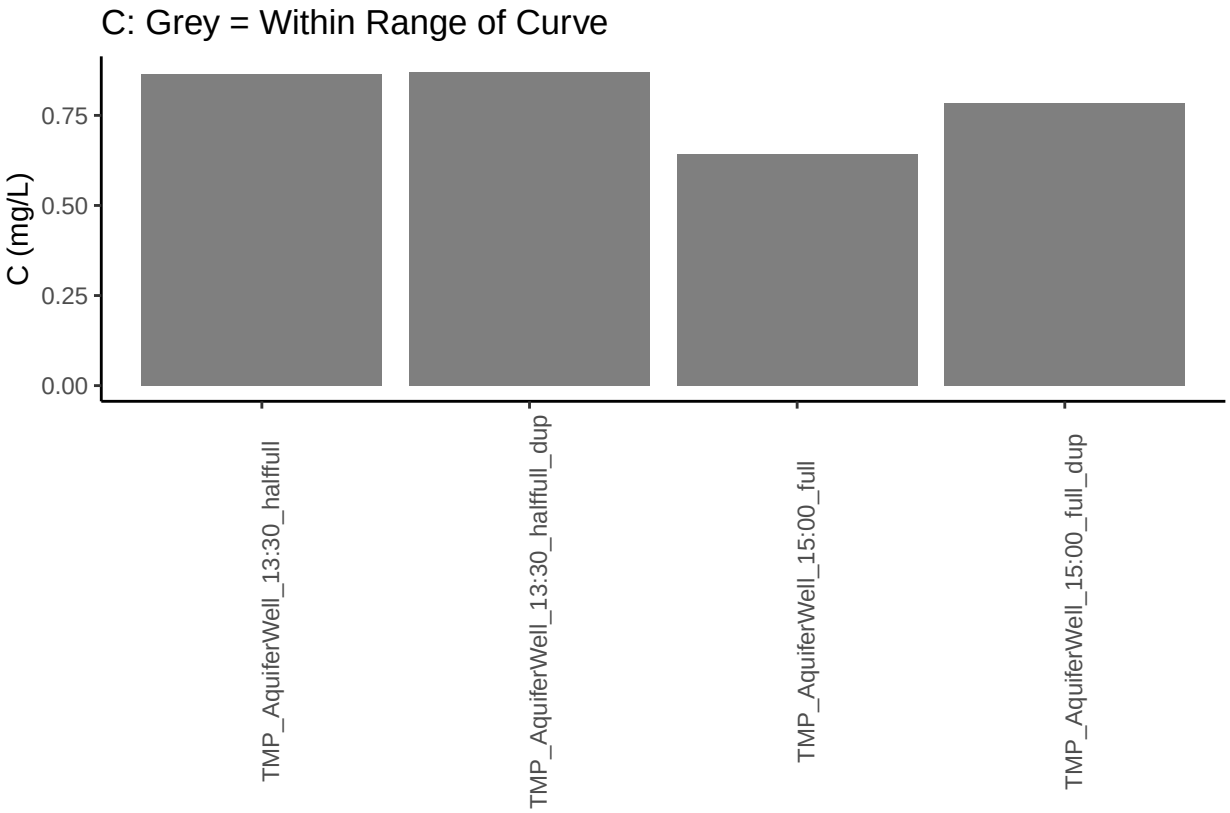


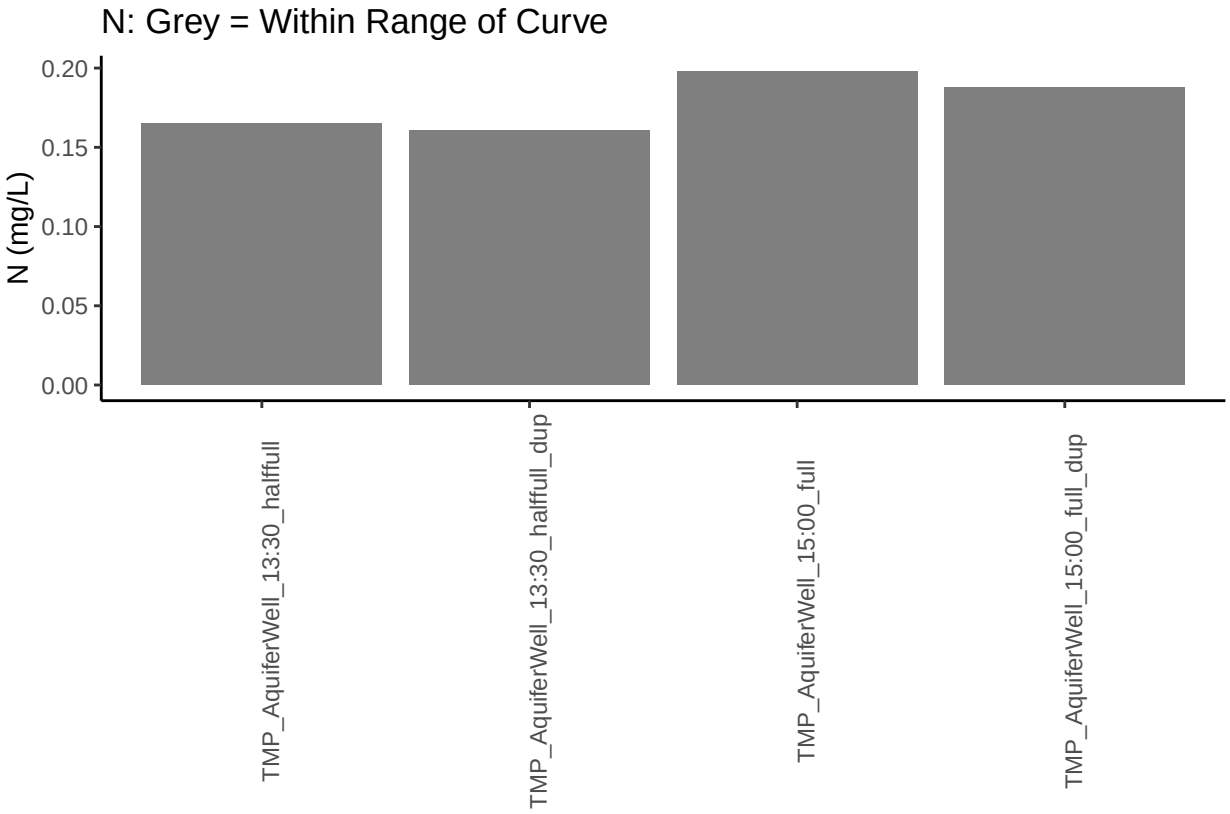

```
## [1] "<60% of Carbon Duplicates have a CB <10% - REASSESS"
```

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

0.9 Sample Flagging

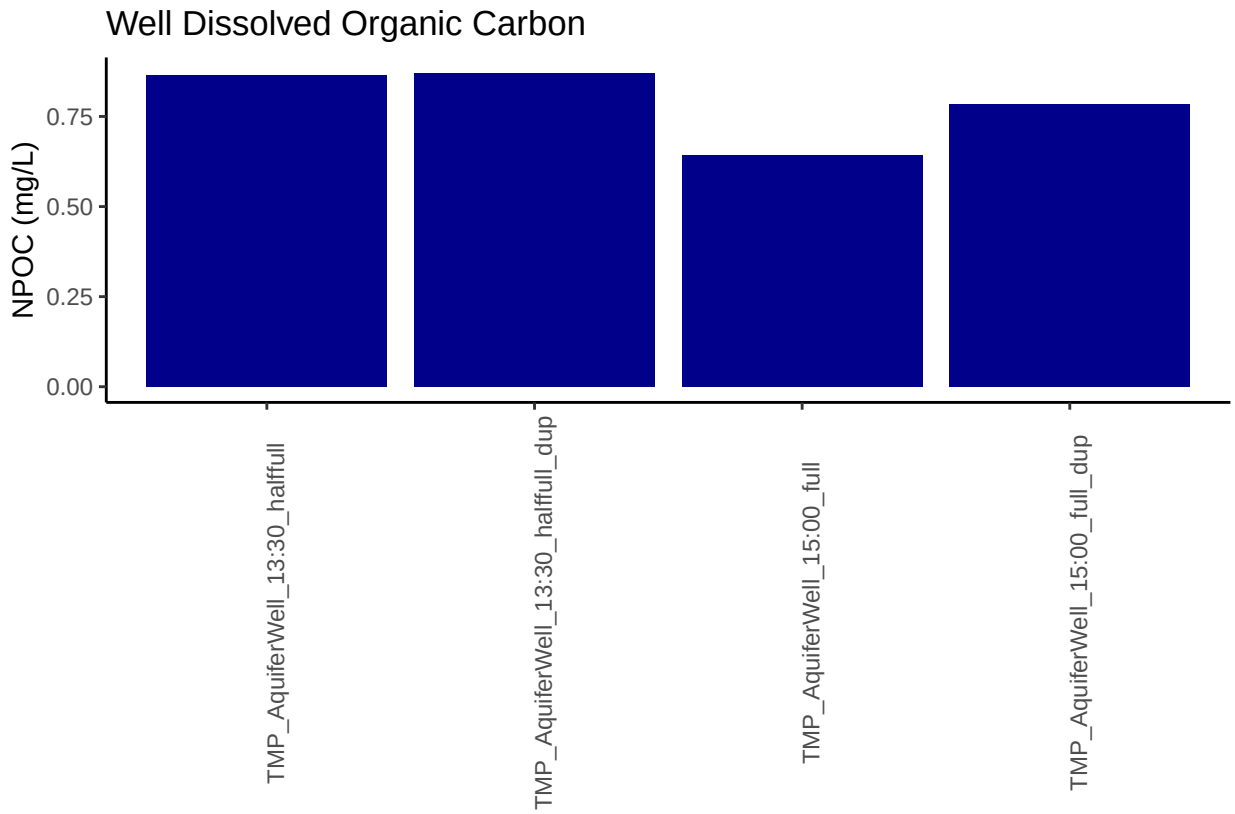
```
## Sample Flagging
```

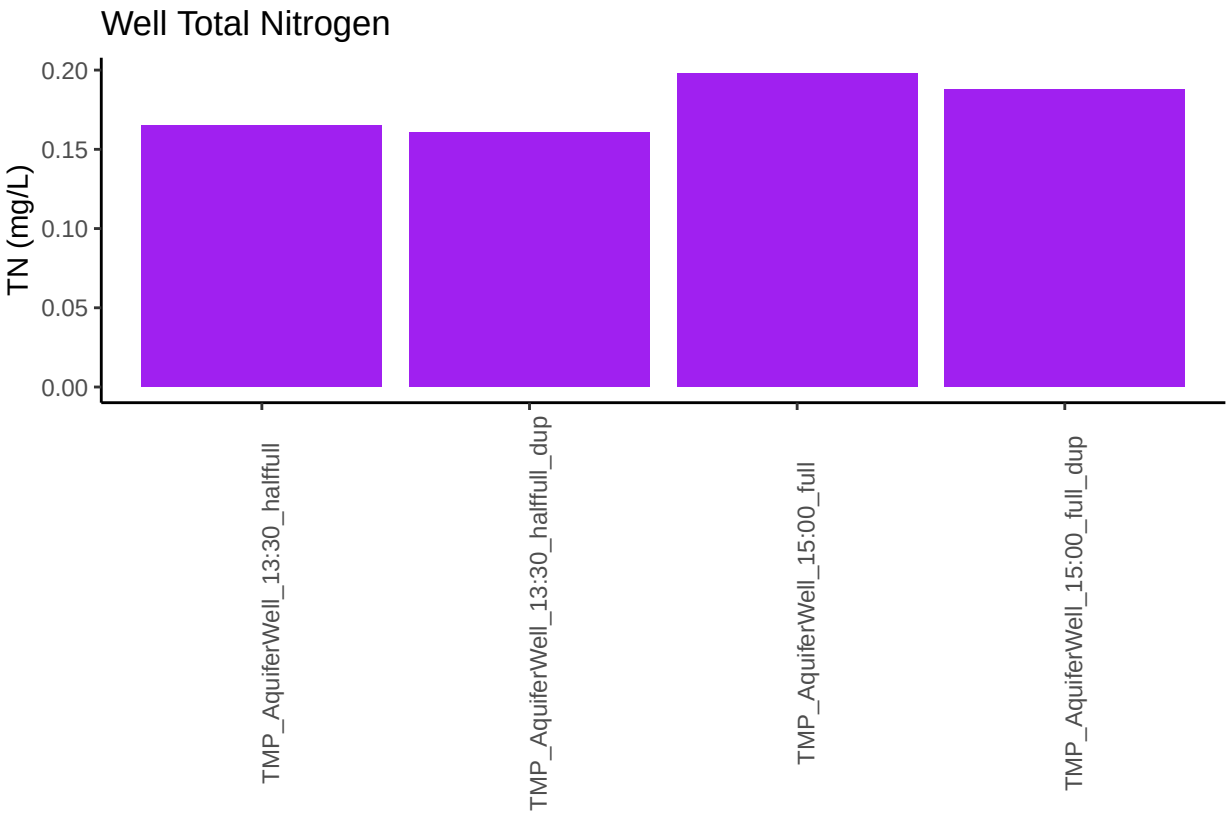



N: Grey = Within Range of Curve
N (mg/L)
0.20
0.15
0.10
0.05
0.00
TMP_AquiferWell_13:30_halffull
TMP_AquiferWell_13:30_halffull_dup
TMP_AquiferWell_15:00_full
TMP_AquiferWell_15:00_full_dup

0.10 Visualize Data by Plot

```
## Visualize Data
```




Well Total Nitrogen
TN (mg/L)
0.20
0.15
0.10
0.05
0.00
TMP_AquiferWell_13:30_halffull
TMP_AquiferWell_13:30_halffull_dup
TMP_AquiferWell_15:00_full
TMP_AquiferWell_15:00_full_dup

0.11 Convert data from mg/L to uMoles/L

0.12 Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 4 x 15
##   Project Experiment   Sample_Date Sample_Time Tank_Status Replicate sample_name
##   <chr>   <chr>        <chr>       <chr>       <chr>       <chr>     <chr>
## 1 COMPASS TEMPEST: We~ 2025-11-10  13:30       half full   A         TMP_Aquife~
## 2 COMPASS TEMPEST: We~ 2025-11-10  13:30       half full   B         TMP_Aquife~
## 3 COMPASS TEMPEST: We~ 2025-11-10  15:00       full        A         TMP_Aquife~
## 4 COMPASS TEMPEST: We~ 2025-11-10  15:00       full        B         TMP_Aquife~
## # i 8 more variables: npoc_mgL <dbl>, npoc_uM <dbl>, npoc_flag <chr>,
## #   tdn_mgL <dbl>, tdn_uM <dbl>, tdn_flag <chr>, Analysis_runtime <chr>,
## #   Run_notes <chr>
```

#end