COMPASS Synoptic CB Porewater: DOC

May 2023 Samples

2025-10-31

##Setup - Change things here & write any notes

```
#identify section
cat("Setup Information")
```

Setup Information

```
###### Run information - PLEASE CHANGE
  Date_Run = "06/02/23"   #Date that instrument was run
  Run_by = "Stephanie J. Wilson"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = "Standard Curve was assessed manually on the instrument.
    One duplicate out of range. A few samples above standard curve top standard."  #any notes from the
  samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names
  samples_pattern <- paste(samples, collapse = "|")
    #samples_pattern <- "GCW" #use this instead of the line above if you have only one site code
  chks_name = "ChkStd_1ppm_CN"   #what did you name your check standards?

###### File Names - PLEASE CHANGE
#file path and name for raw summary data file
    #raw_file_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202505.txt" #example
    raw_file_name = "Raw Data/TOCTN_COMPASS_Synoptic_TCTN_202305.txt"

#file path and name for raw all peaks file
    #raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202505_allpeaks.txt" #example
    # raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DOC_202411_allpeaks.txt"

#file path and name of processed data file
    #processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DOC_202505.csv" #example
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DOC_202305.csv" #example


###### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"

#qaqc log file path for this year
  #Log_path = "Raw Data/COMPASS_Synoptic_TOCTN_QAQClog_2024.csv"
```

##Set Up Code

##Read in metadata and create similar sample IDs for matching to samples

Import Data Functions

Import Sample Data

```
## Import Sample Data

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

## # A tibble: 6 x 4
##   sample_name                npoc_raw tdn_raw run_datetime
##   <chr>                         <dbl>   <dbl> <chr>
## 1 202305_GCW_TR_LysA_20cm        36.3   1.92  6/3/2023 12:12:25 AM
## 2 202305_GCW_TR_LysB_10cm        20.9   0.804 6/3/2023 12:37:36 AM
## 3 202305_GCW_TR_LysB_20cm        22.1   1.46  6/3/2023 1:04:36 AM
## 4 202305_GCW_TR_LysC_10cm        83.9   2.24  6/3/2023 1:23:43 AM
## 5 202305_GCW_WC_LysA_10cm         9.11  0.678 6/3/2023 1:50:02 AM
## 6 202305_GCW_WC_LysA_10cm_dup     8.85  0.670 6/3/2023 2:15:12 AM
```

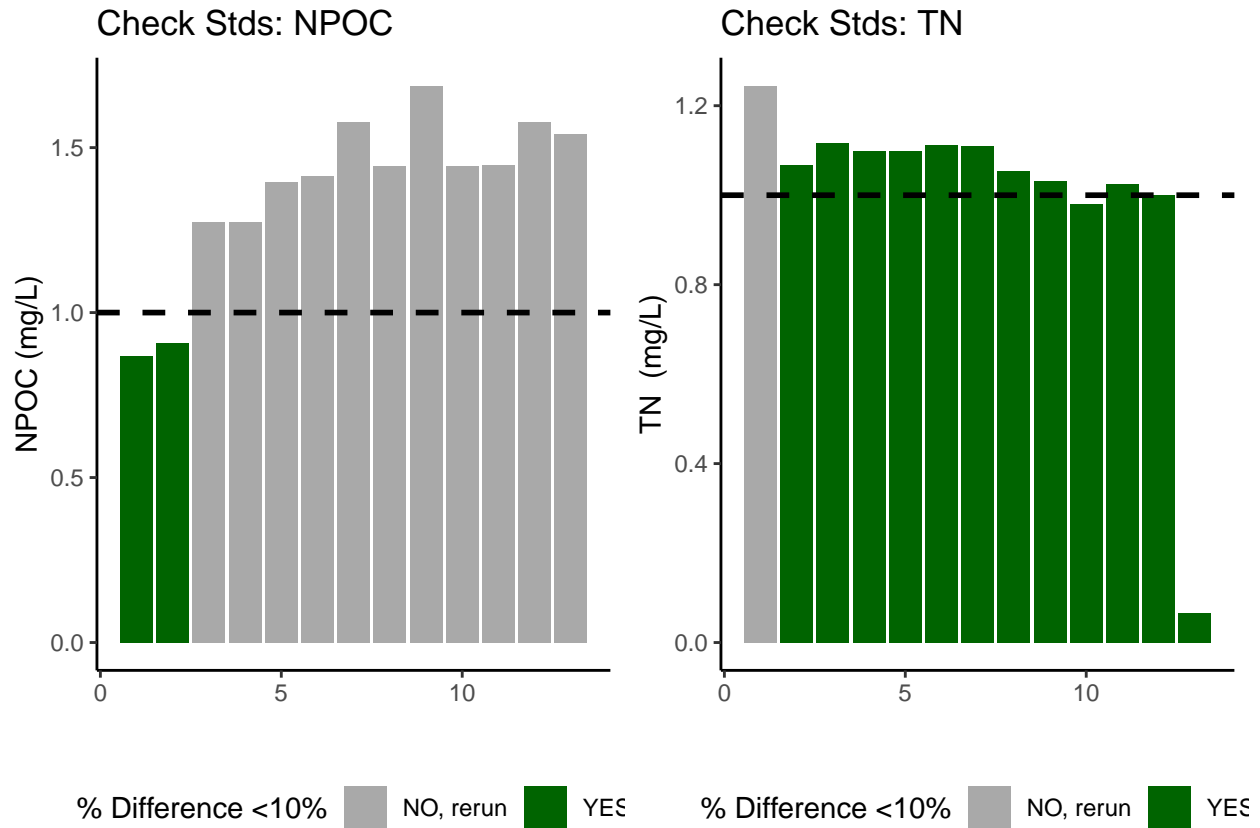## Assessing Standard Curves - assessed manually on the instrument

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"
```

Check Stds: NPOC

Check Stds: TN

% Difference <10% NO, rerun YES % Difference <10% NO, rerun YES

[1] ">60% of Carbon Check Standards are within range of expected concentration"

[1] ">60% of Nitrogen Check Standards are within range of expected concentration"
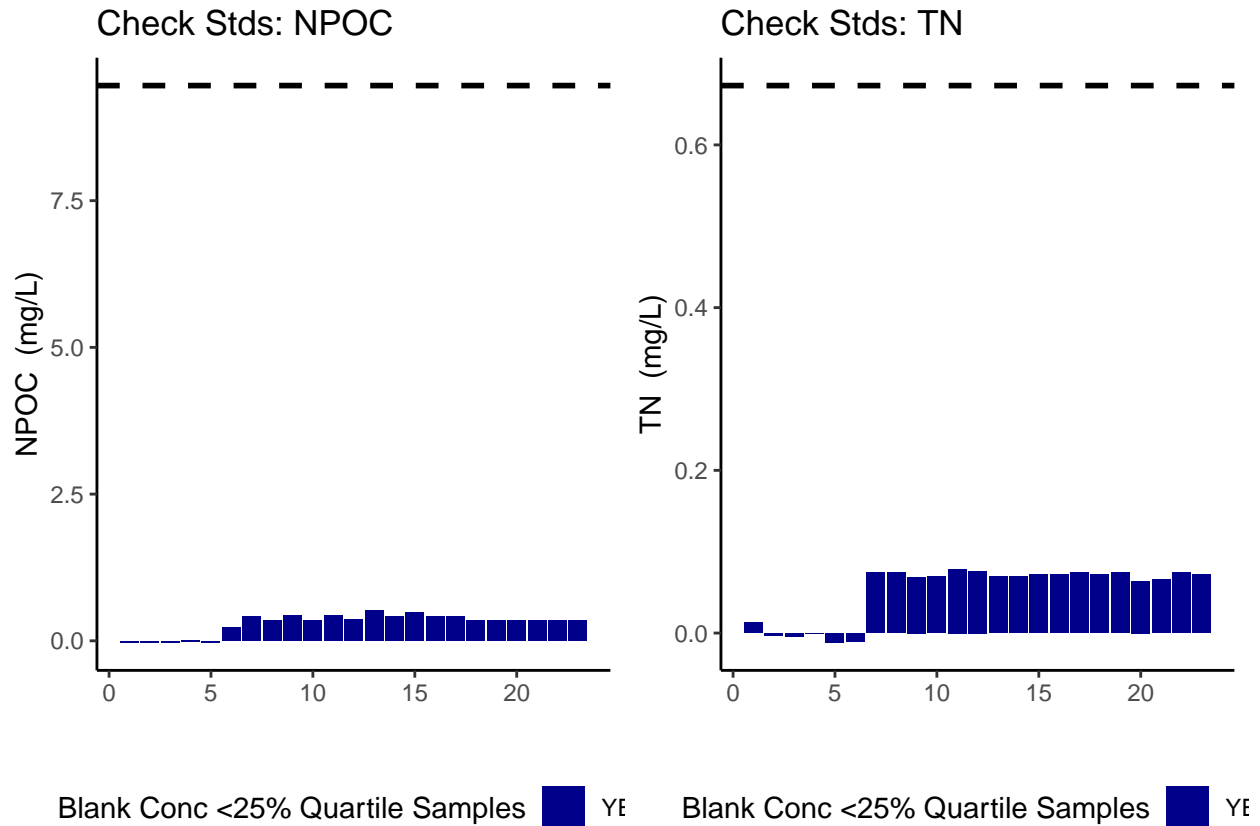
Assess Blanks

Assess Blanks

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

[1] ">60% of Carbon Blank concentrations are lower 25% quartile of samples"

[1] ">60% of Nitrogen Blank concentrations are lower 25% quartile of samples"

Check Stds: NPOC

Check Stds: TN

NPOC (mg/L)

7.5

5.0

2.5

0.0

0   5   10   15   20

TN (mg/L)

0.6

0.4

0.2

0.0

0   5   10   15   20

Blank Conc <25% Quartile Samples   YE

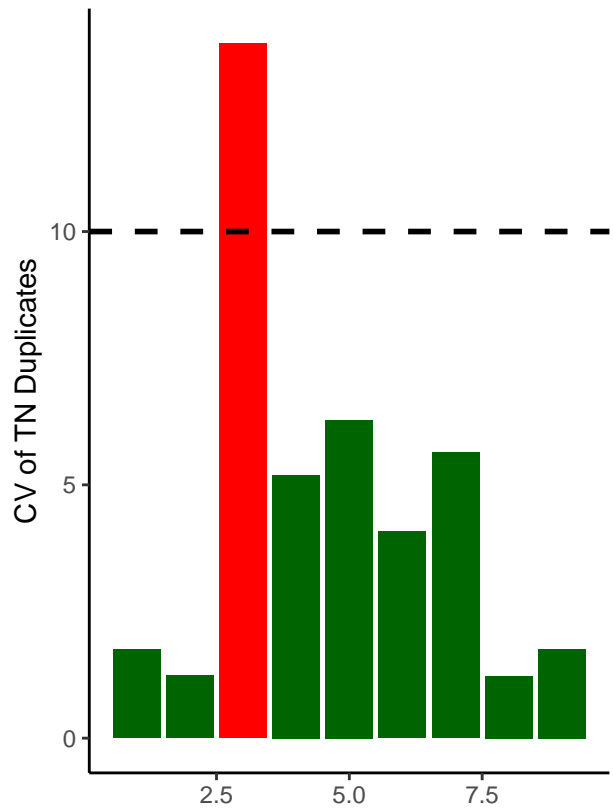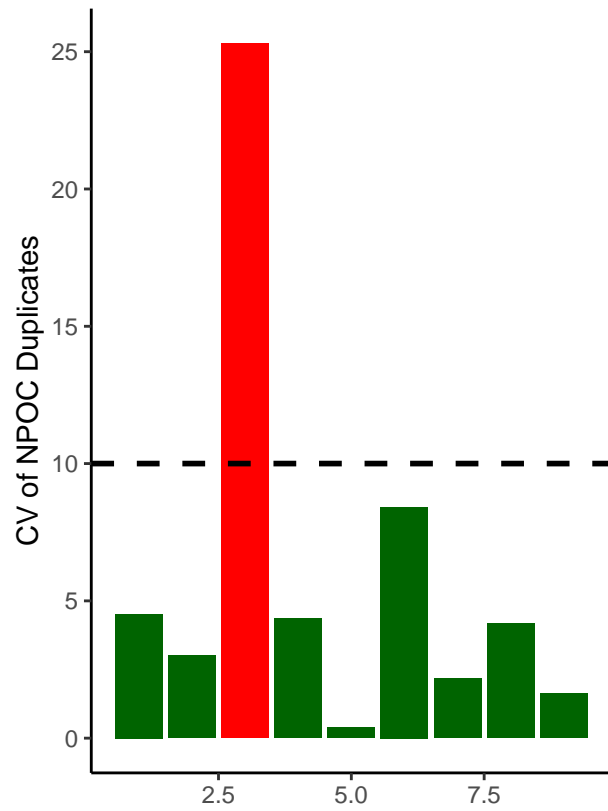Blank Conc <25% Quartile Samples   YE

```
## carbon blanks:

## [1] 0.2947074

## nitrogen blanks:

## [1] 0.05238348
```

Assess Duplicates

```
## Assess Duplicates

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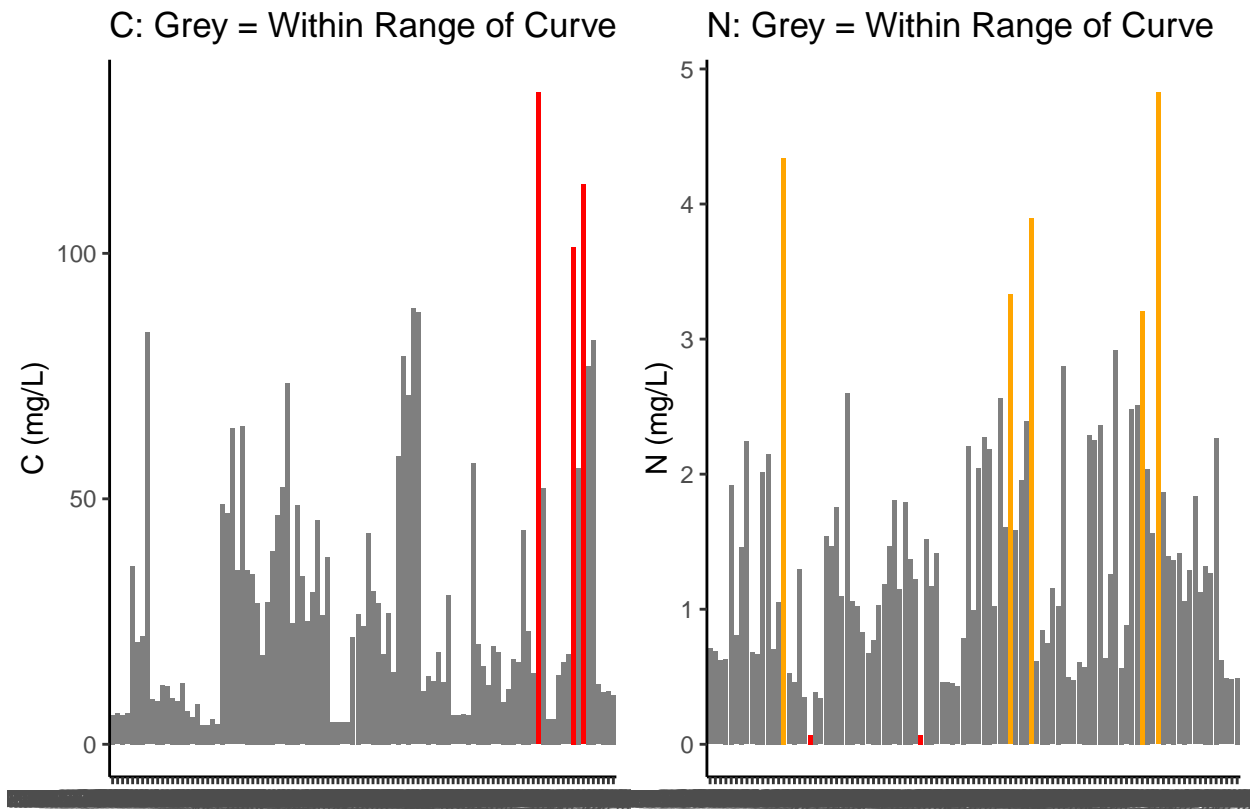
[1] ">60% of Carbon Duplicates have a CV <10%"

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

Sample Flagging - Are samples Within the range of the curve?

Sample Flagging

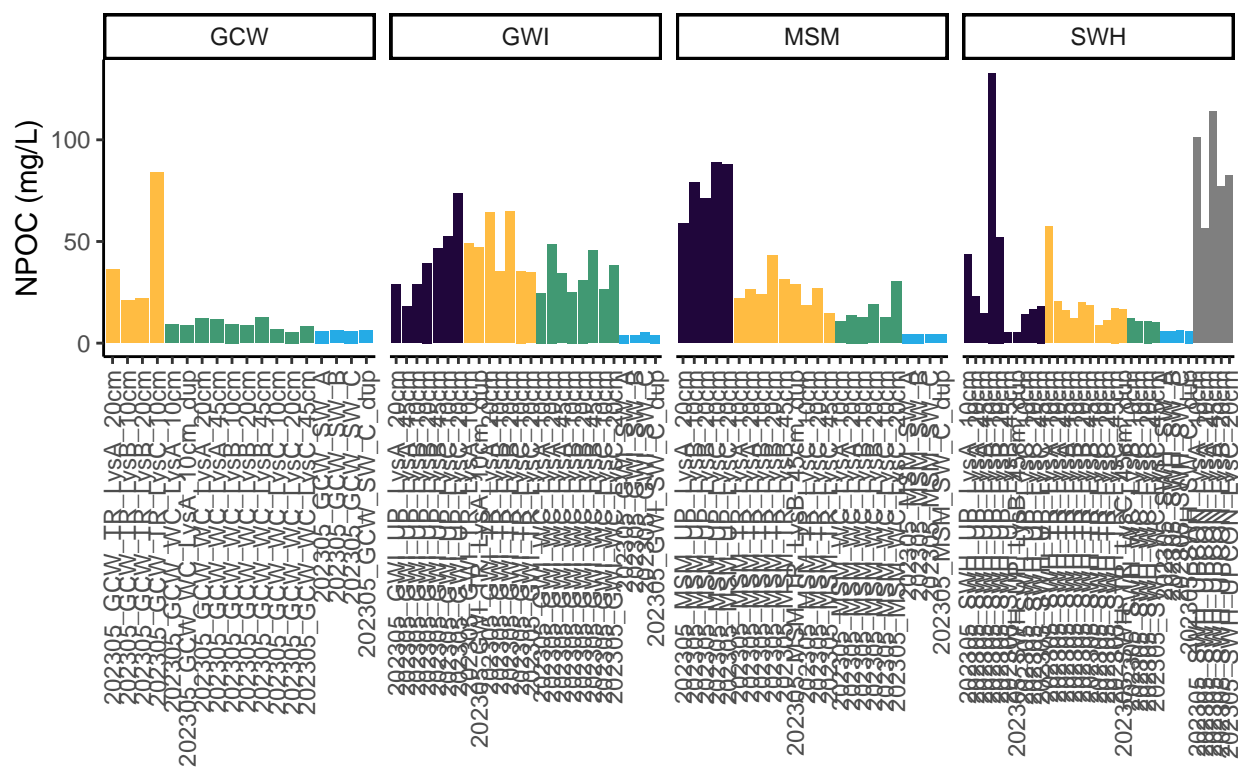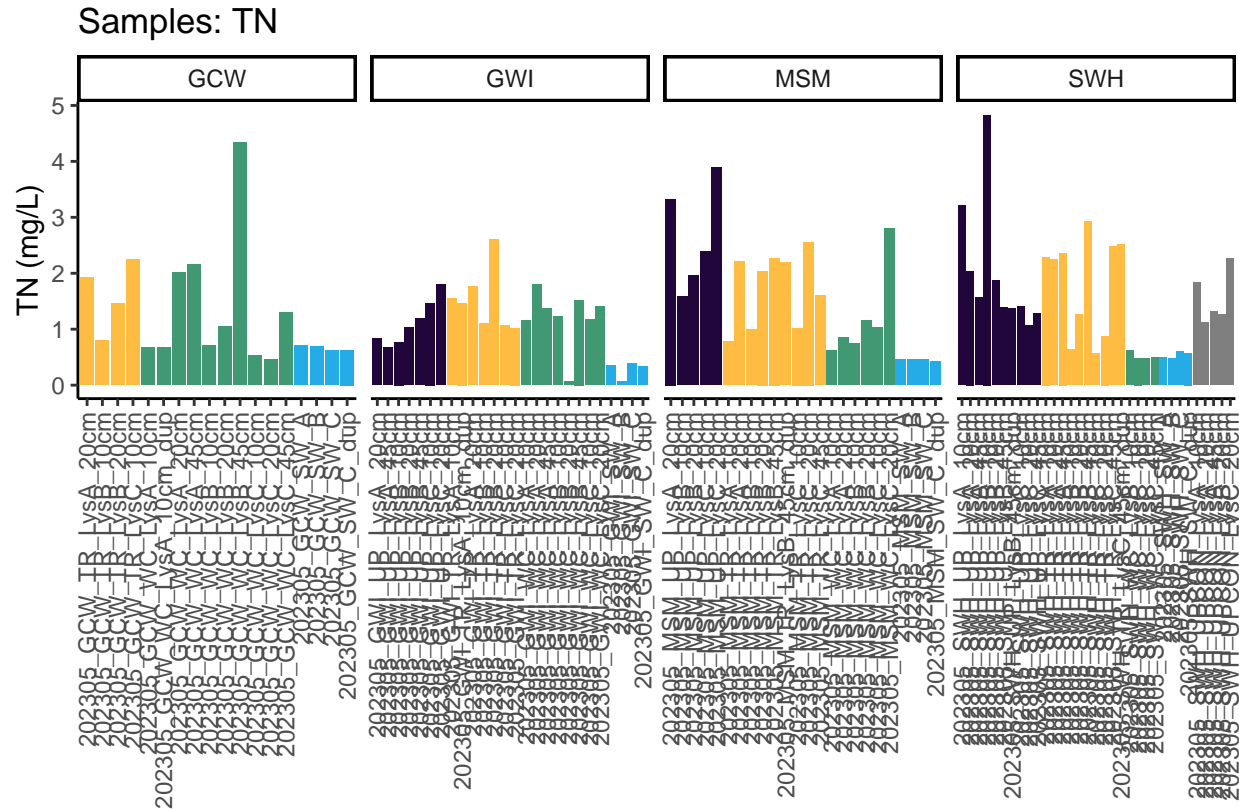C: Grey = Within Range of Curve   N: Grey = Within Range of Curve

Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202305", "GCW", "TR", "LysA", "20cm"), c("202305", "GCW", :
## number of columns of result is not a multiple of vector length (arg 1)
```

Samples: NPOC

Samples: TN

Convert data from mg/L to uMoles/L

Check to see if samples run match metadata & merge info

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

```
## All sample IDs are present in metadata.
```

Export Processed Data

```
## Export Processed Data
```

```
## # A tibble: 6 x 21
##   Project      Region Site  Zone  Replicate Depth_cm Sample_ID Year Month   Day
##   <chr>        <chr>  <chr> <fct> <chr>        <int> <chr>    <int> <int> <int>
## 1 COMPASS: Sy~ CB     MSM   UP    A               20 202305_M~ 2023     5    19
## 2 COMPASS: Sy~ CB     MSM   UP    B               10 202305_M~ 2023     5    19
## 3 COMPASS: Sy~ CB     MSM   UP    B               20 202305_M~ 2023     5    19
## 4 COMPASS: Sy~ CB     MSM   UP    C               10 202305_M~ 2023     5    19
## 5 COMPASS: Sy~ CB     MSM   UP    C               20 202305_M~ 2023     5    19
## 6 COMPASS: Sy~ CB     GWI   UP    A               20 202305_G~ 2023     5    23
## # i 11 more variables: Time <lgl>, Time_Zone <lgl>, npoc_mgL <dbl>,
## #   npoc_uM <dbl>, npoc_flag <chr>, tdn_mgL <dbl>, tdn_uM <dbl>,
## #   tdn_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>
```

#end