

COMPASS Synoptic CB Porewater: DOC

June 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 = "06/25/23" #Date that instrument was run  
Run_by = "Stephanie J. Wilson" #Instrument user  
Script_run_by = "Stephanie J. Wilson" #Code user  
run_notes = "NA" #any notes from the run  
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 = "Std_Chk_1ppmCN" #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 = c("Raw Data/TOCTN_COMPASS_Synoptic_TCTN_202306_1.txt",  
                 "Raw Data/TOCTN_COMPASS_Synoptic_TCTN_202306_2.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_202306.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:
## New names:
## * `` -> '...14'

## Warning: One or more parsing issues, call 'problems()' on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

## # A tibble: 6 x 4
##   sample_name      npoc_raw tdn_raw run_datetime
##   <chr>          <dbl>    <dbl> <chr>
## 1 202306_SWH_TR_LysA_10cm 39.6     2.17  6/25/2023 1:25:10 AM
## 2 202306_SWH_TR_LysA_20cm 14.9     3.90  6/25/2023 1:53:44 AM
## 3 202306_SWH_TR_LysA_20cm_dup 14.6     3.69  6/25/2023 2:16:08 AM
## 4 202306_SWH_TR_LysA_45cm 12.0     3.41  6/25/2023 2:34:44 AM
## 5 202306_SWH_TR_LysB_10cm  8.68    0.541 6/25/2023 3:00:23 AM
## 6 202306_SWH_TR_LysB_20cm 13.3     1.67  6/25/2023 3:28:44 AM
```

Assessing Standard Curves - assessed manually on the instrument

Assess Check Standards

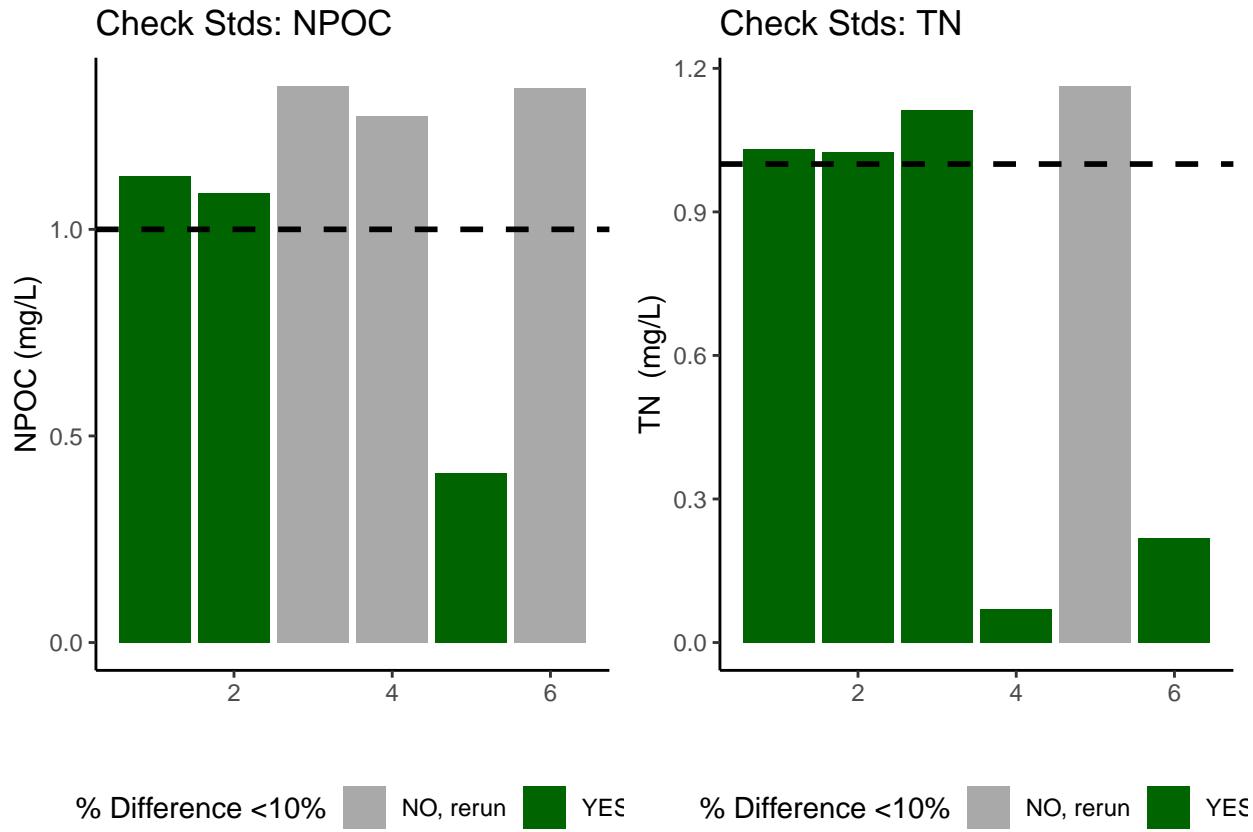
```
## Assess the Check Standards

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

## Warning: One or more parsing issues, call 'problems()' on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

## [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 expected concentration"

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

Assess Blanks

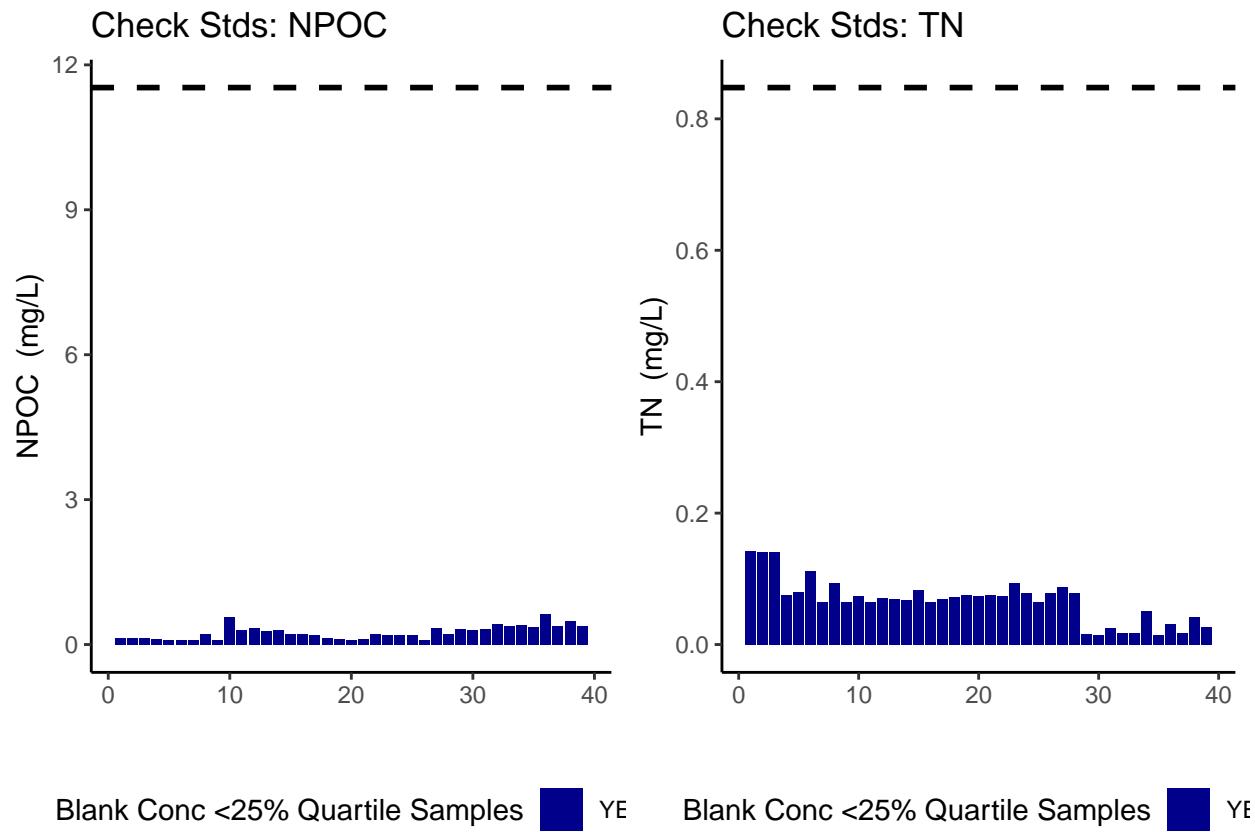
## Assess Blanks

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

## Warning: One or more parsing issues, call 'problems()' on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

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

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



```
## carbon blanks:
```

```
## [1] 0.252639
```

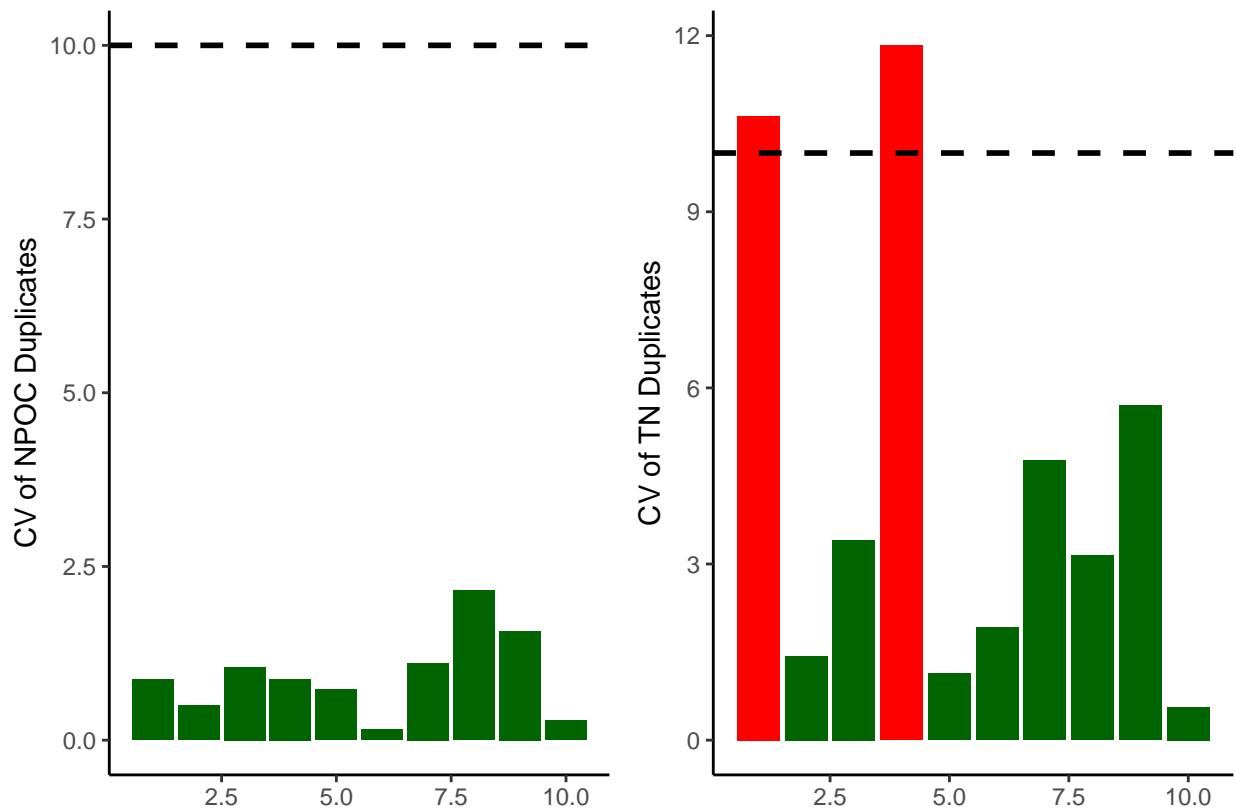
```
## nitrogen blanks:
```

```
## [1] 0.06674872
```

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.
```



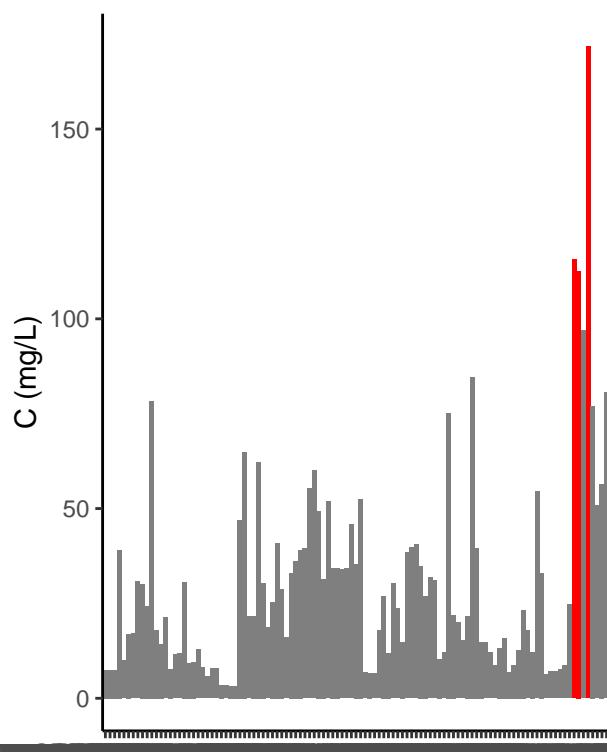
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

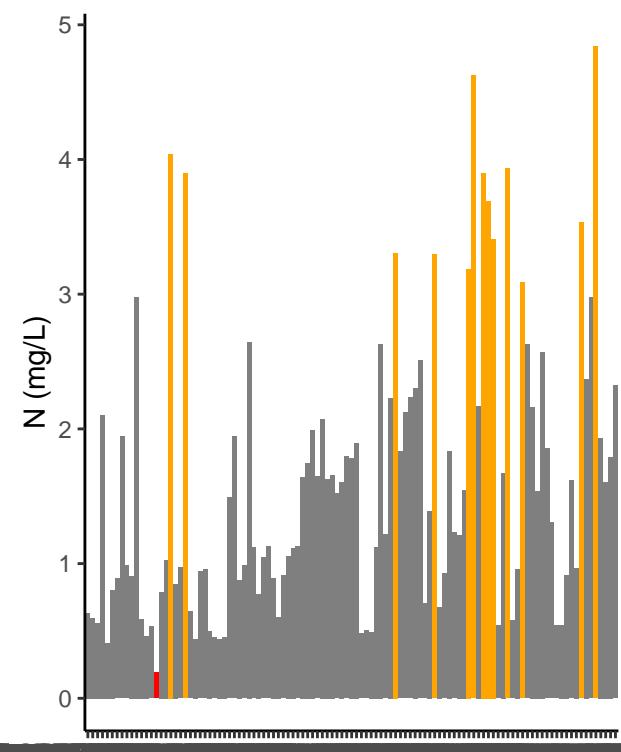
Sample Flagging - Are samples Within the range of the curve?

```
## Sample Flagging
```

C: Grey = Within Range of Curve



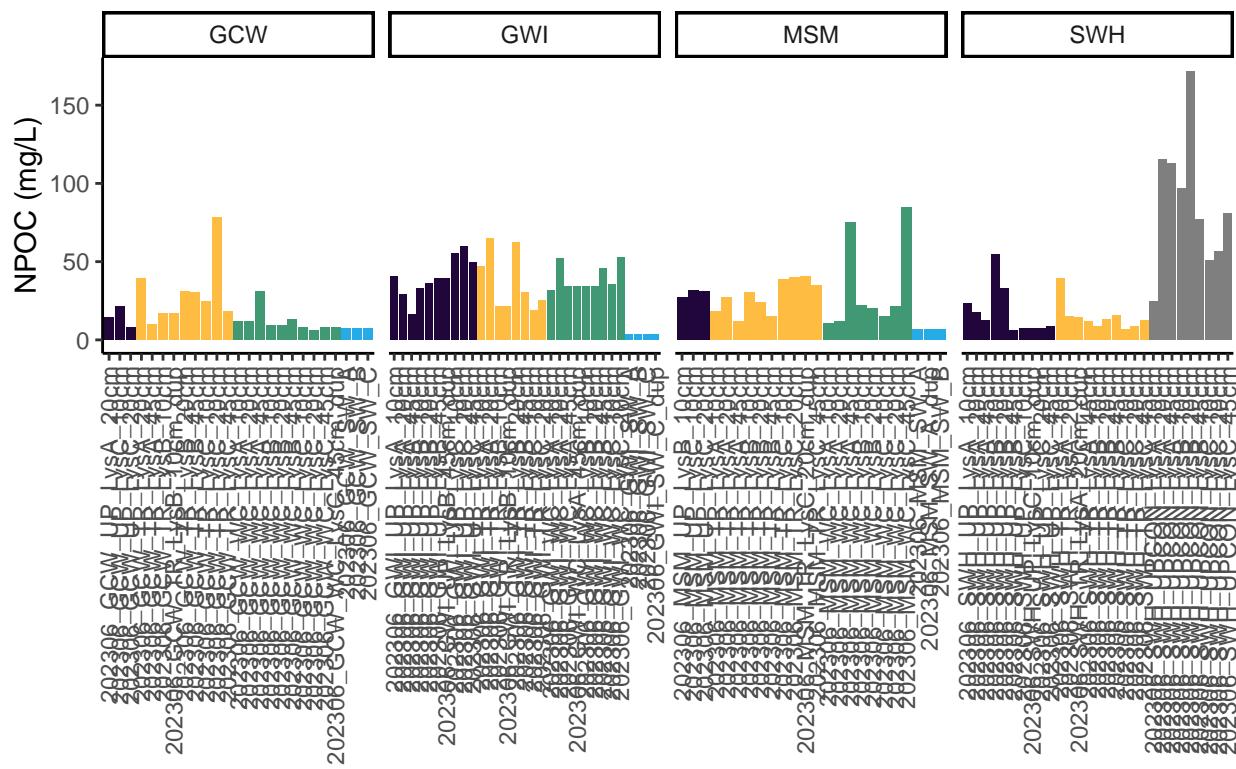
N: Grey = Within Range of Curve



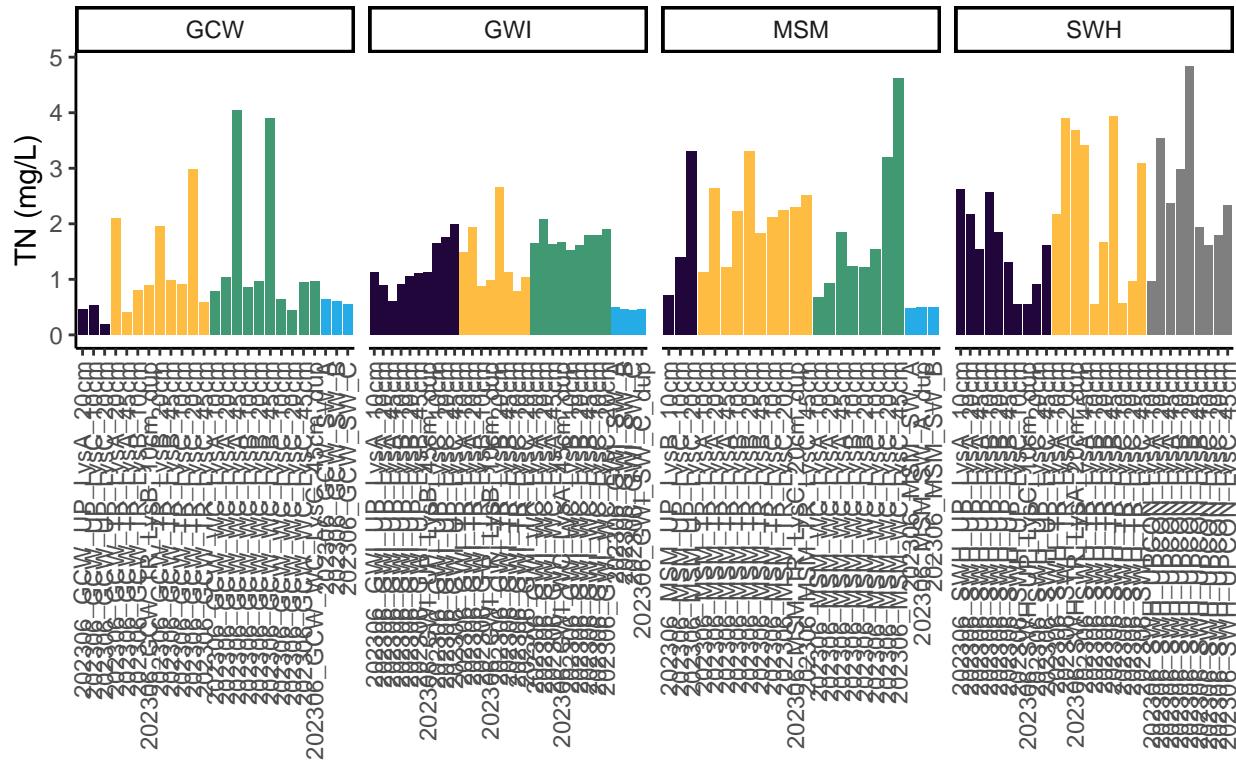
Visualize Data by Plot

```
## Visualize Data  
  
## Warning in rbind(c("202306", "SWH", "TR", "LysA", "10cm"), c("202306", "SWH", :  
## 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    SWH   UP    A          10 202306_S~ 2023   6    21
## 2 COMPASS: Sy~ CB    SWH   UP    A          20 202306_S~ 2023   6    21
## 3 COMPASS: Sy~ CB    SWH   UP    A          45 202306_S~ 2023   6    21
## 4 COMPASS: Sy~ CB    SWH   UP    B          10 202306_S~ 2023   6    21
## 5 COMPASS: Sy~ CB    SWH   UP    B          20 202306_S~ 2023   6    21
## 6 COMPASS: Sy~ CB    SWH   UP    B          45 202306_S~ 2023   6    21
## # 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