

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

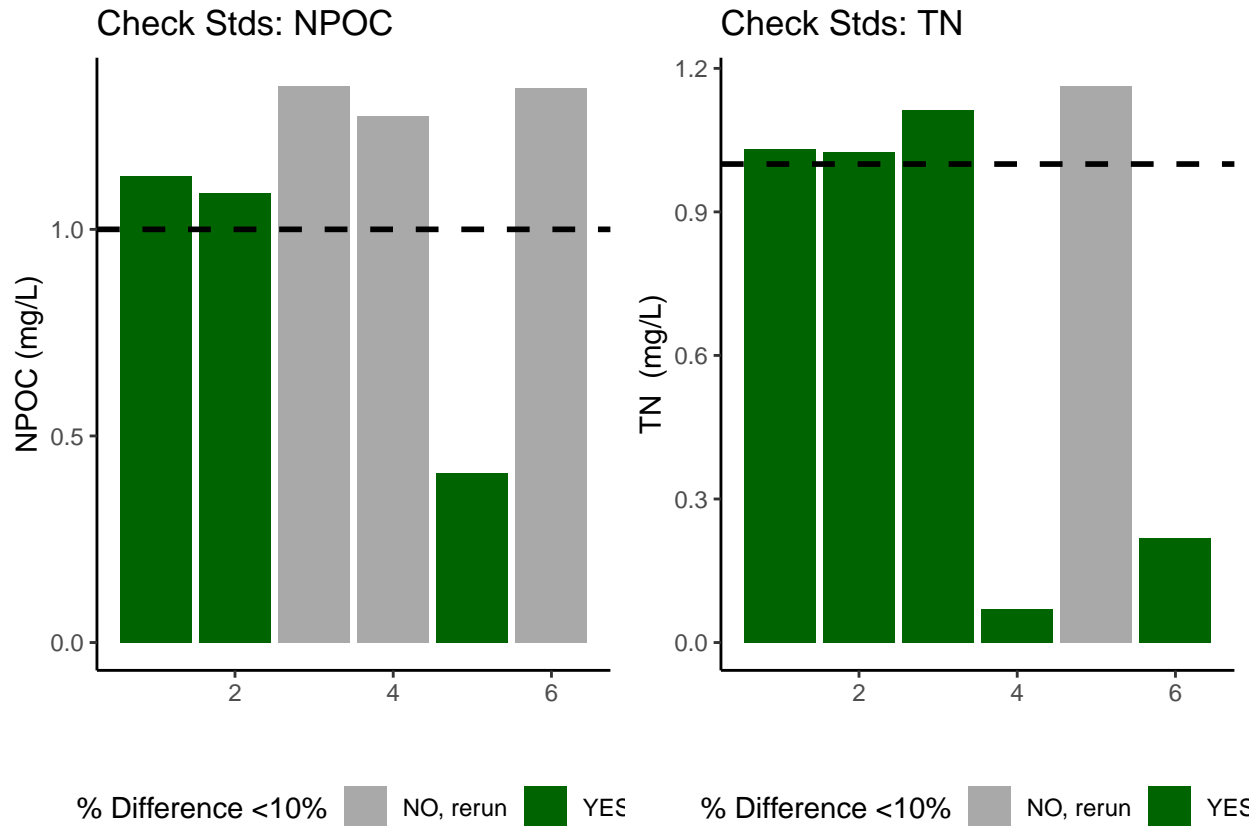
```
## Assess the Check Standards

## 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

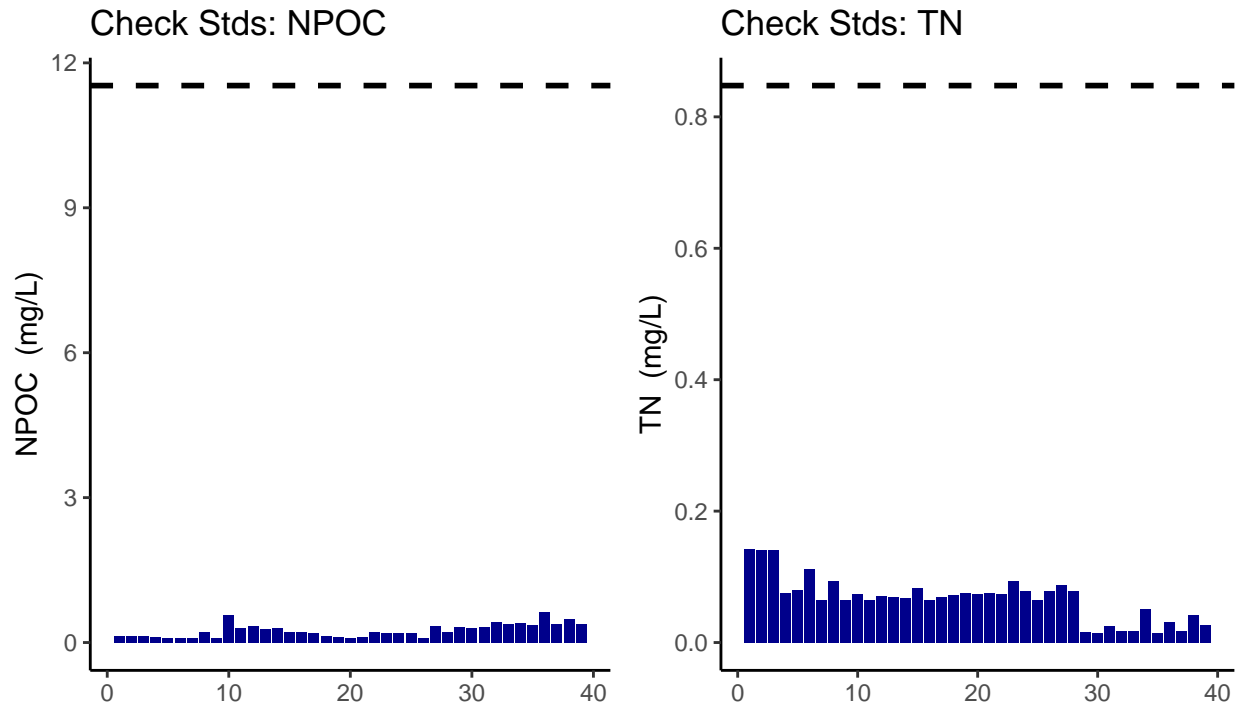
```
## Assess Blanks
```

```
## 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"
```



Blank Conc <25% Quartile Samples ■ YE

Blank Conc <25% Quartile Samples ■ YE

```
## carbon blanks:
```

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

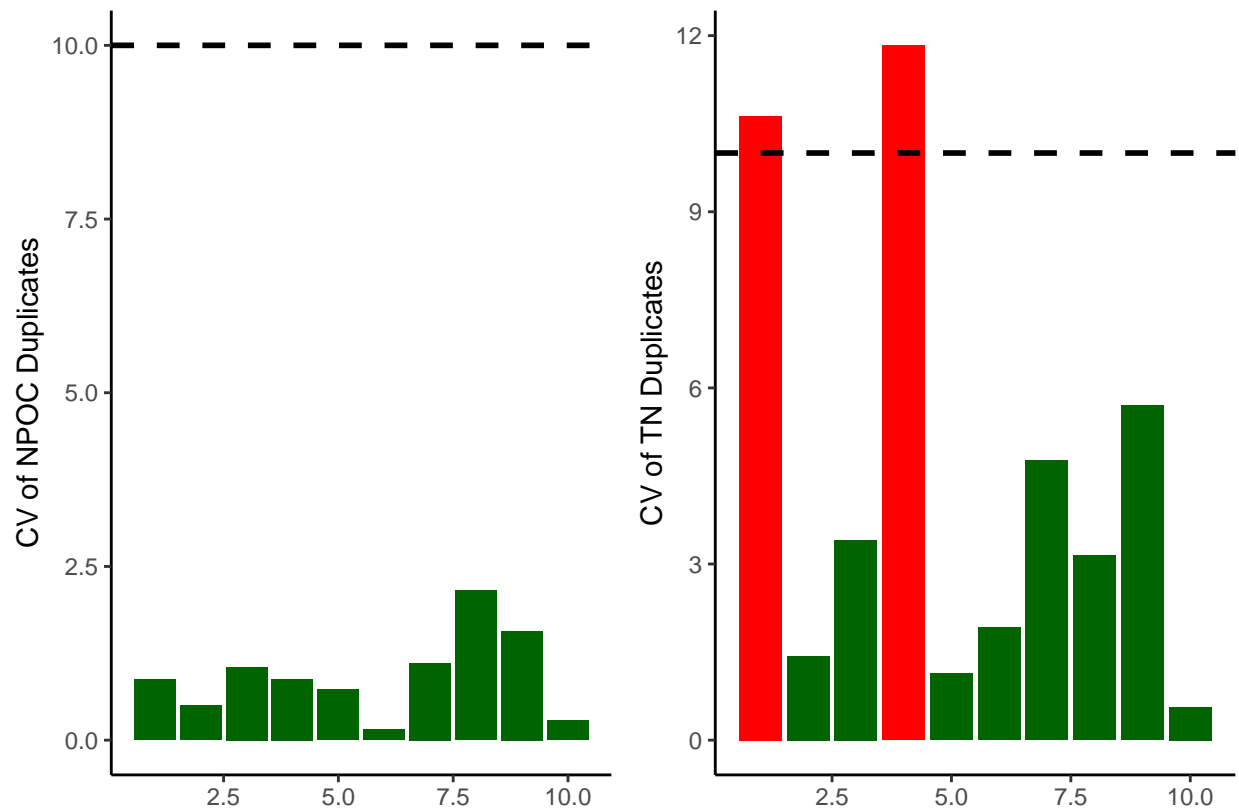
```
## nitrogen blanks:
```

```
## [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.
```

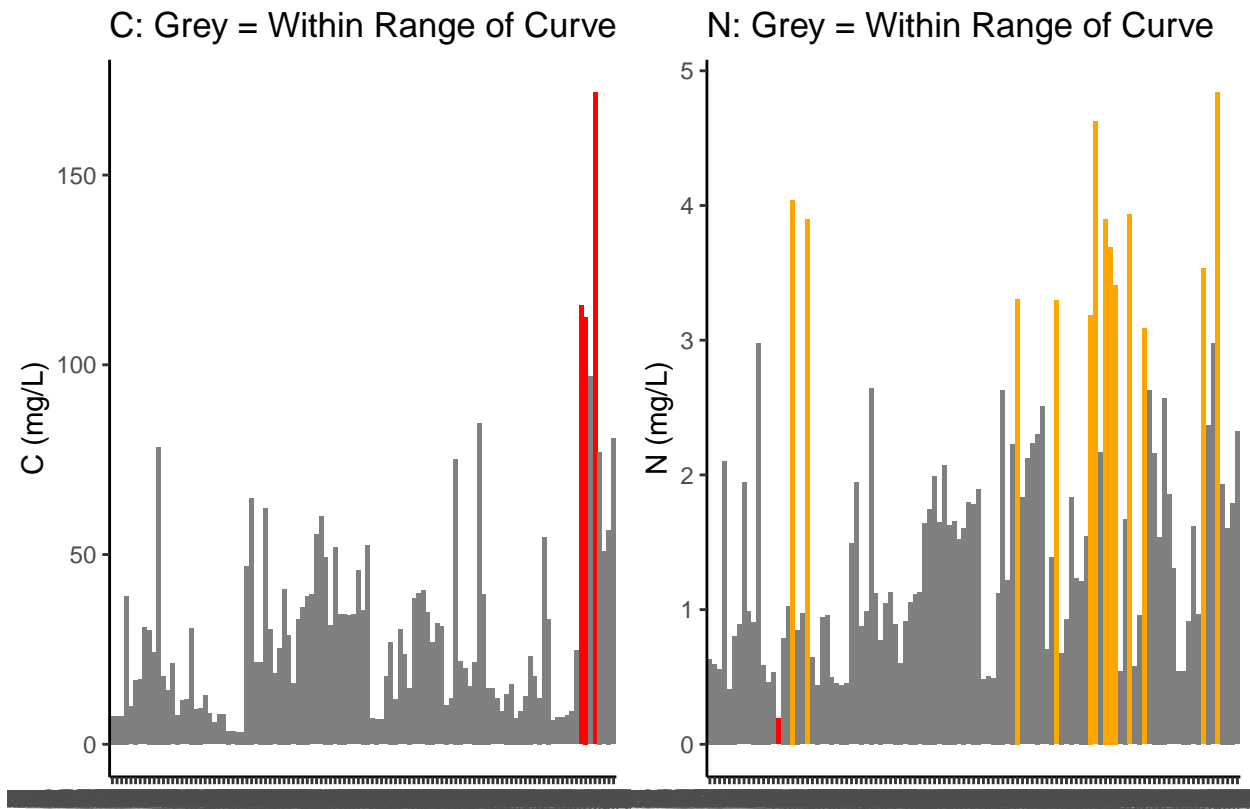


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

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

```
## Sample Flagging
```

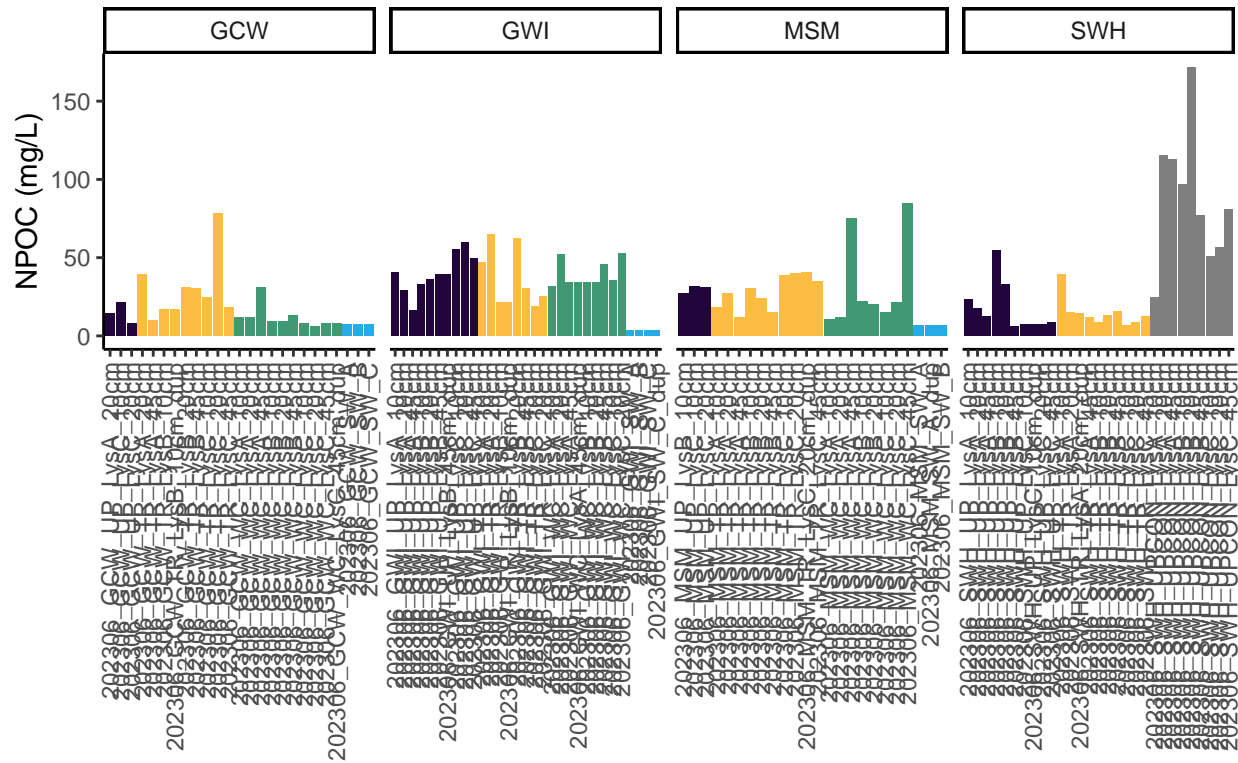


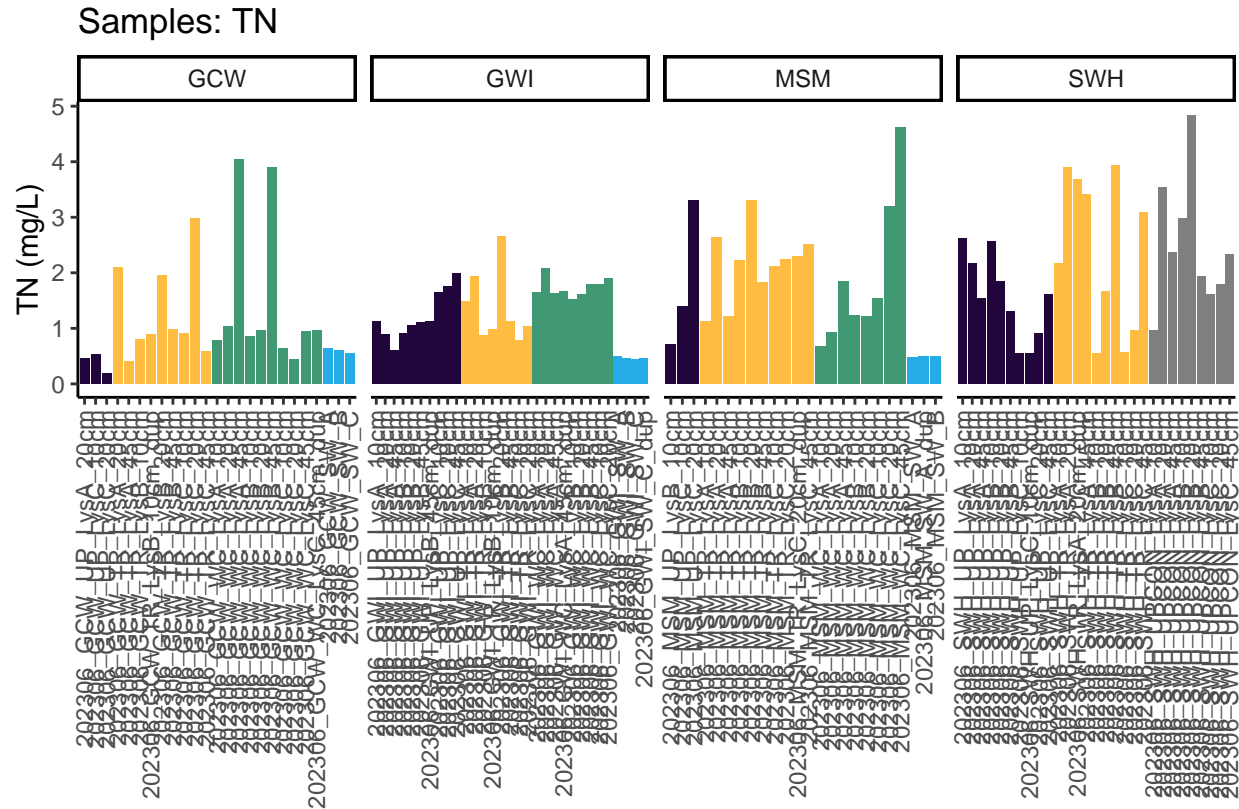
Visualize Data by Plot

```
## 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





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