

COMPASS Synoptic CB Porewater: DOC

August 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 = "09/02/23" #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 = "Chk_Std_50C_2N" #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_202308.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_202308.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"

#qac log file path for this year
#Log_path = "Raw Data/COMPASS_Synoptic_TOCTN_QAClog_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 202308_GCW_TR_LysA_20cm    52.4     2.41 9/2/2023 12:52:17 AM
## 2 202308_GCW_TR_LysB_10cm     4.75    0.357 9/2/2023 1:17:30 AM
## 3 202308_GCW_TR_LysB_20cm    15.2     1.74 9/2/2023 1:42:02 AM
## 4 202308_GCW_TR_LysC_10cm    21.4     0.596 9/2/2023 2:08:49 AM
## 5 202308_GCW_WC_LysA_10cm    17.4     1.32 9/2/2023 2:29:56 AM
## 6 202308_GCW_WC_LysA_20cm    15.3     1.40 9/2/2023 2:47:00 AM
```

Assessing Standard Curves - assessed manually on the instrument

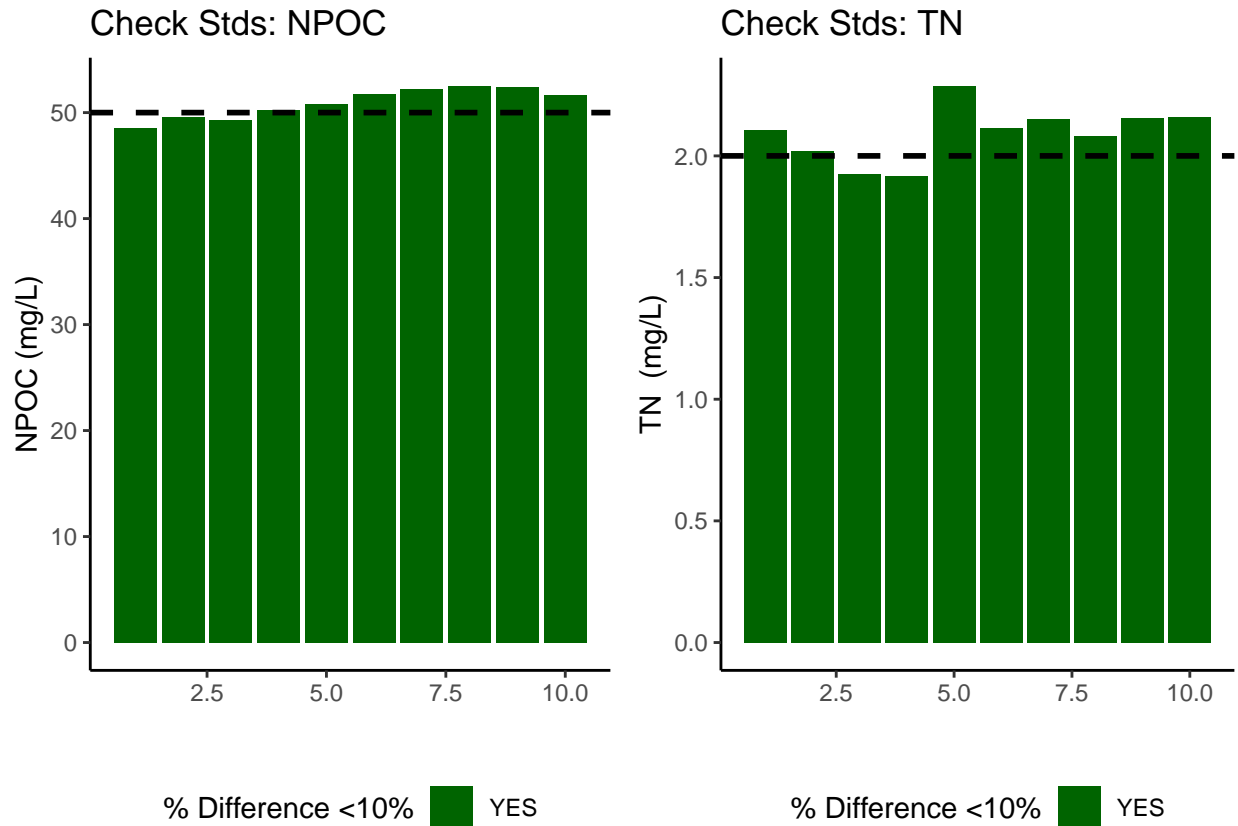
Assess Check Standards

```
## Assess the Check Standards

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

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

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



```
## [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

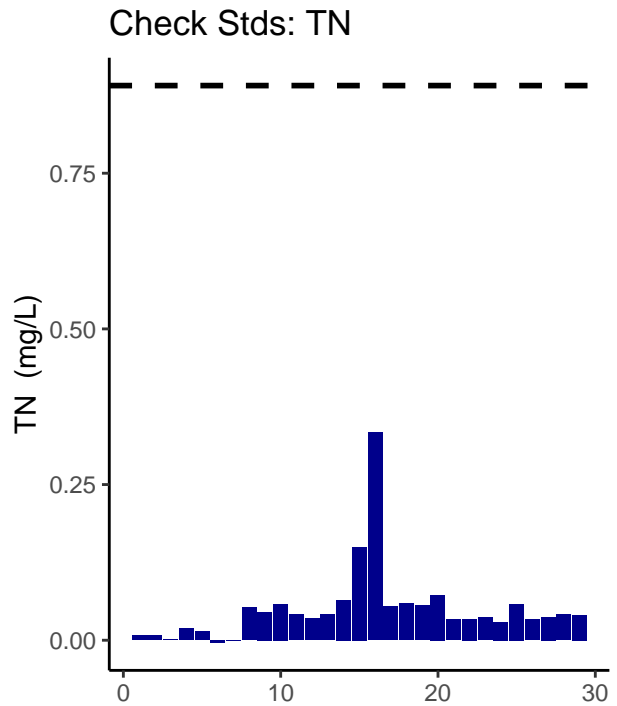
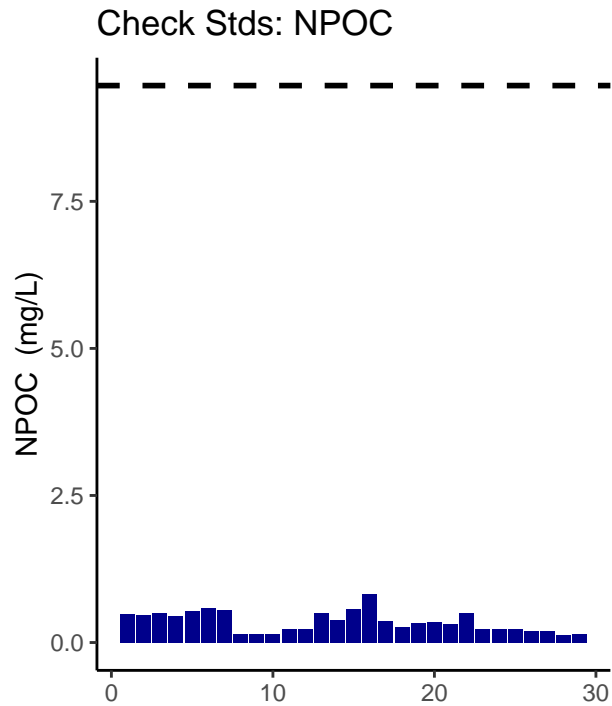
```
## Assess Blanks
```

```
## 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"
```



Blank Conc <25% Quartile Samples Y

Blank Conc <25% Quartile Samples Y

```
## carbon blanks:
```

```
## [1] 0.352431
```

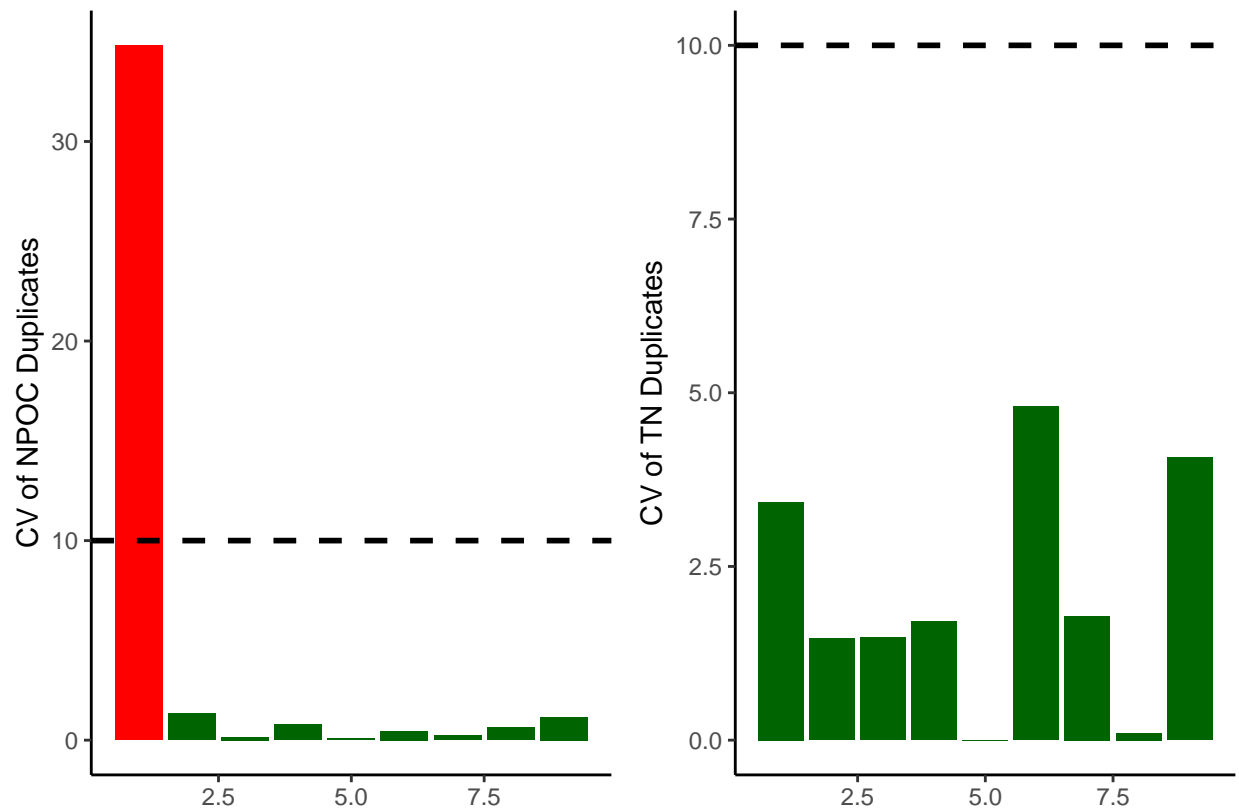
```
## nitrogen blanks:
```

```
## [1] 0.05007724
```

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.
```

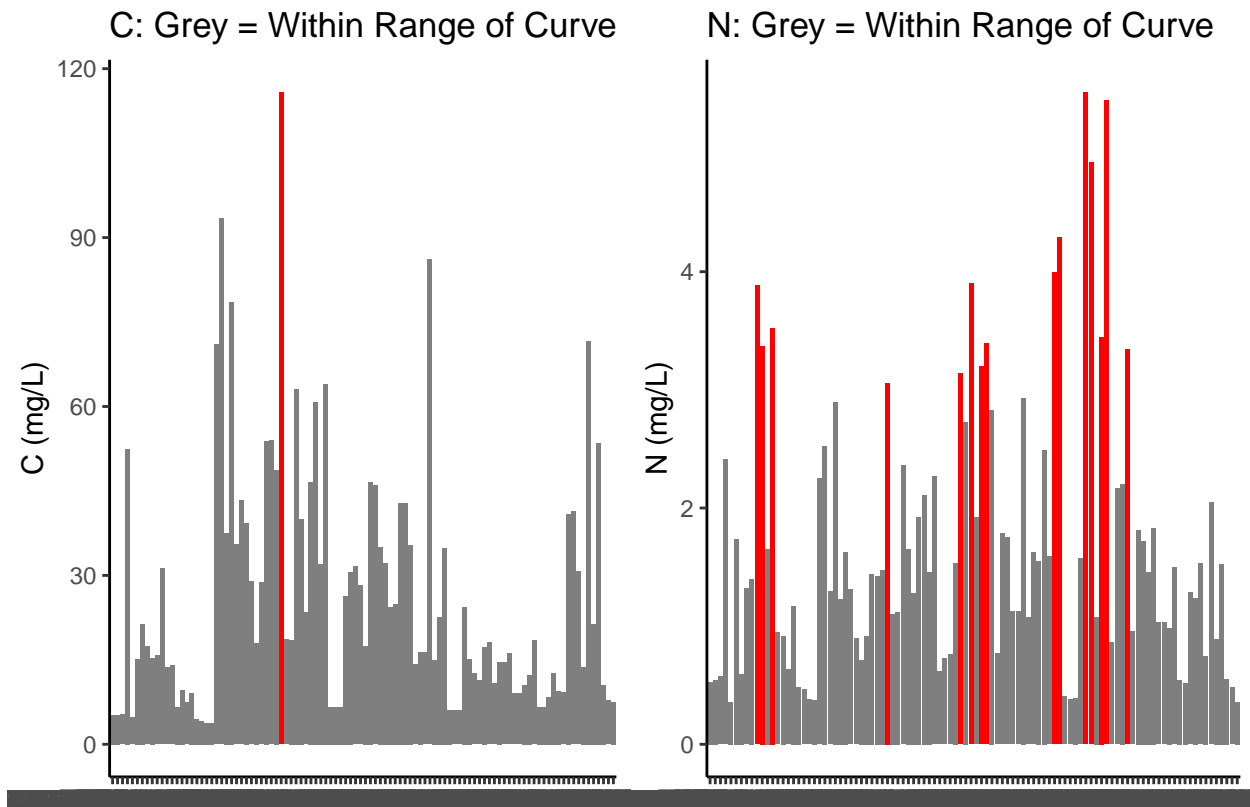


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

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

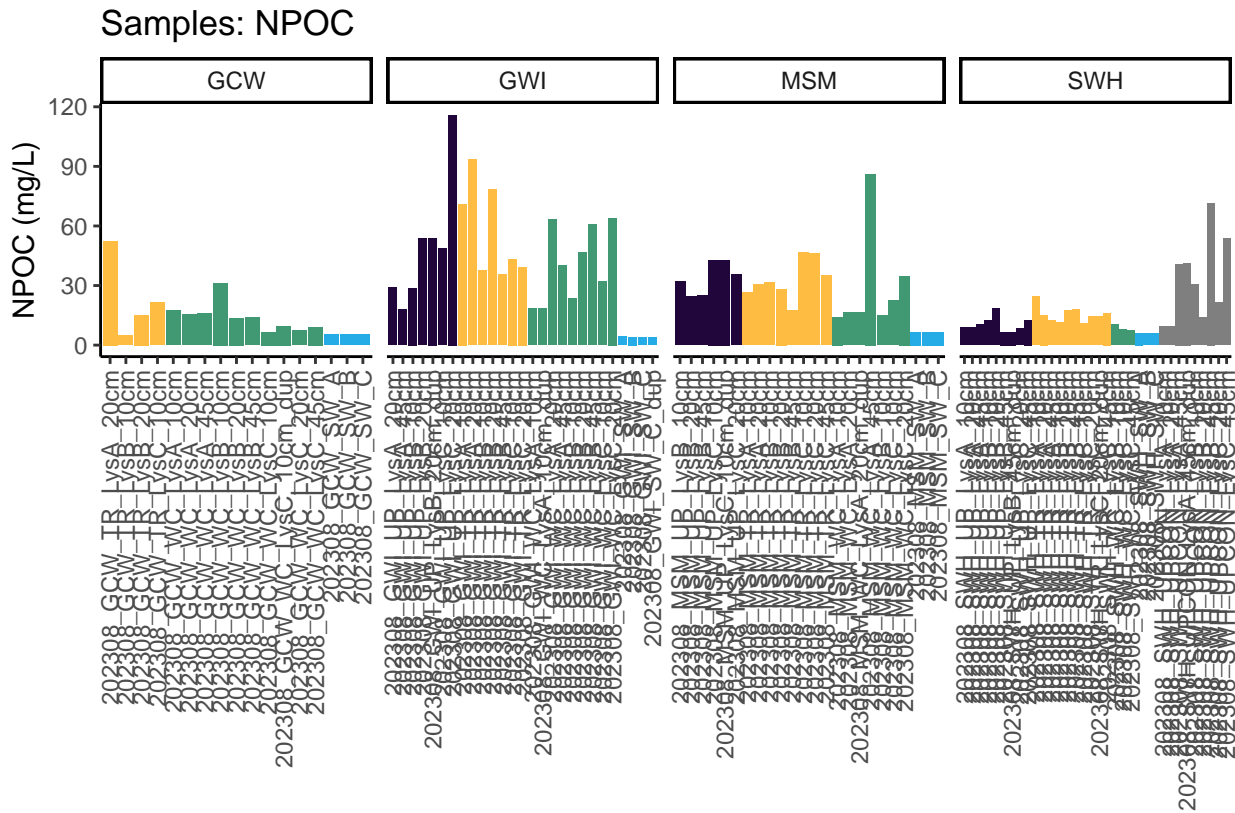
```
## Sample Flagging
```

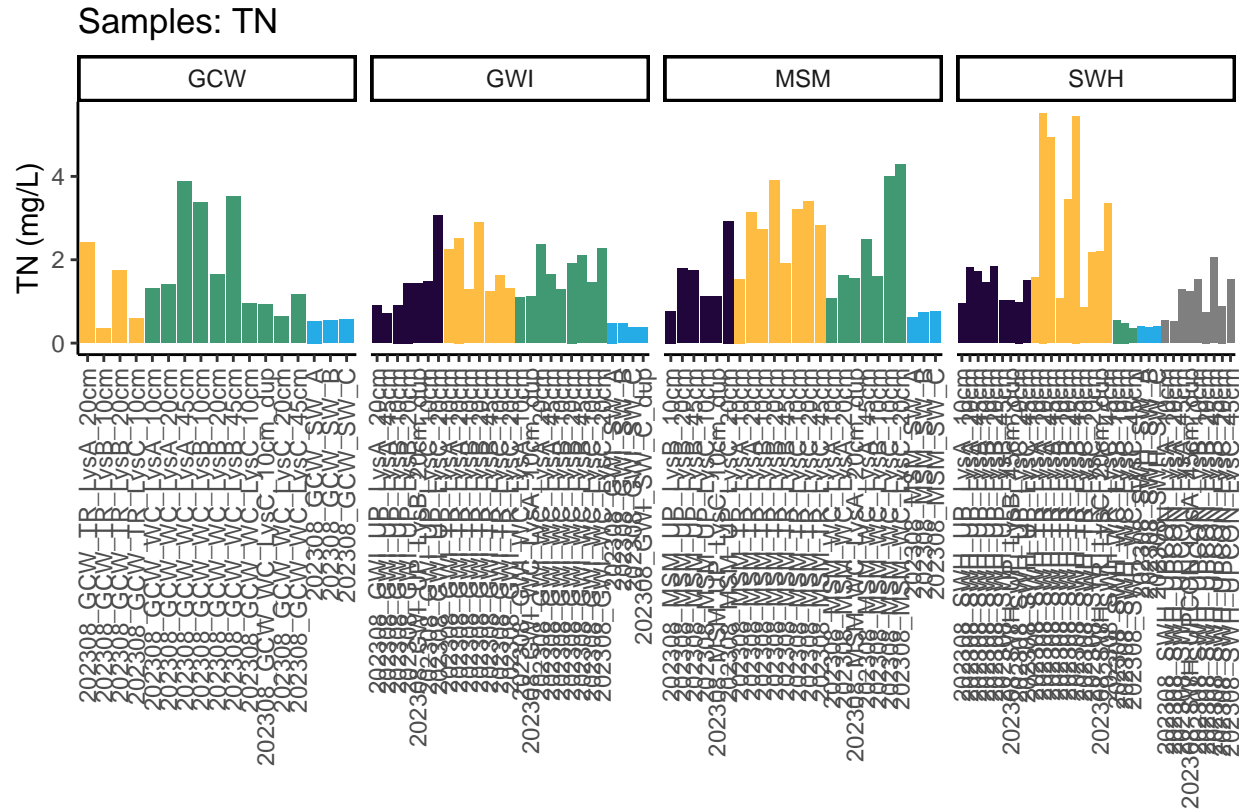


Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202308", "GCW", "TR", "LysA", "20cm"), c("202308", "GCW", :
## number of columns of result is not a multiple of vector length (arg 1)
```





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    B          10 202308_M~ 2023    8    17
## 2 COMPASS: Sy~ CB    MSM  UP    B          20 202308_M~ 2023    8    17
## 3 COMPASS: Sy~ CB    MSM  UP    B          45 202308_M~ 2023    8    17
## 4 COMPASS: Sy~ CB    MSM  UP    C          10 202308_M~ 2023    8    17
## 5 COMPASS: Sy~ CB    MSM  UP    C          20 202308_M~ 2023    8    17
## 6 COMPASS: Sy~ CB    SWH  UP    A          10 202308_S~ 2023    8    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