

Synoptic CB: Porewater DIC

July 2024 Samples

2025-10-21

Contents

0.1	Import Data Functions	2
0.2	Import Sample Data	2
0.3	Assessing Standard Curves	3
0.4	CRM Check - Don't run chunk if no CRMs run	4
0.5	Assess Check Standards	4
0.6	Assess Blanks	5
0.7	Assess Duplicates - no duplicates on this run	6
0.8	Sample Flagging - Are samples Within the range of the curve?	6
0.9	Visualize Data by Plot	7
0.10	Convert data from mg/L to uMoles/L	8
0.11	Check to see if samples run match metadata & merge info	8
0.12	Export Processed Data	8

```
##Setup - Change things here & write any notes
```

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

```
## Setup Information
```

```
##### Run information - PLEASE CHANGE  
Date_Run = "07/29/2024" #Date that instrument was run  
Run_by = "Stephanie J. Wilson" #Instrument user  
Script_run_by = "Stephanie J. Wilson" #Code user  
run_notes = "One sample was entered into the instrument incorrectly and that is  
fixed in this code: 202407_SWH_UP_LysB_45cm is 202407_SWH_UP_LysC_45cm" #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_" #what did you name your check standards?  
crm_name = "CRM|crm" #what did you name your CRMS?  
  
##### File Names - PLEASE CHANGE  
#file path and name for raw summary data file  
raw_file_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202407.txt"  
  
#file path and name for raw all peaks file  
raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202407_allpeaks.txt"  
  
#file path and name of processed data file  
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202407.csv"  
  
##### Log Files - PLEASE CHECK  
#downloaded metadata csv - downloaded from Google drive as csv for this year  
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"  
  
#qaqc log file path for this year  
Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAQClog_2024.csv"
```

```
##Set Up Code
```

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

0.1 Import Data Functions

0.2 Import Sample Data

```
## Import Sample Data
```

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

```
## # A tibble: 6 x 3  
##   sample_name          ic_raw run_datetime
```

```
##   <chr>                                <dbl> <chr>
## 1 202407_GCW_WC_LysA_10cm             111. 7/29/2024 3:29:12 PM
## 2 202407_GCW_WC_LysA_20cm             125. 7/29/2024 3:47:04 PM
## 3 202407_GCW_WC_LysA_45cm             185. 7/29/2024 4:04:53 PM
## 4 202407_GCW_WC_LysB_10cm             119. 7/29/2024 4:22:47 PM
## 5 202407_GCW_WC_LysB_20cm             126. 7/29/2024 4:40:38 PM
## 6 202407_GCW_WC_LysB_45cm             154. 7/29/2024 4:58:24 PM
```

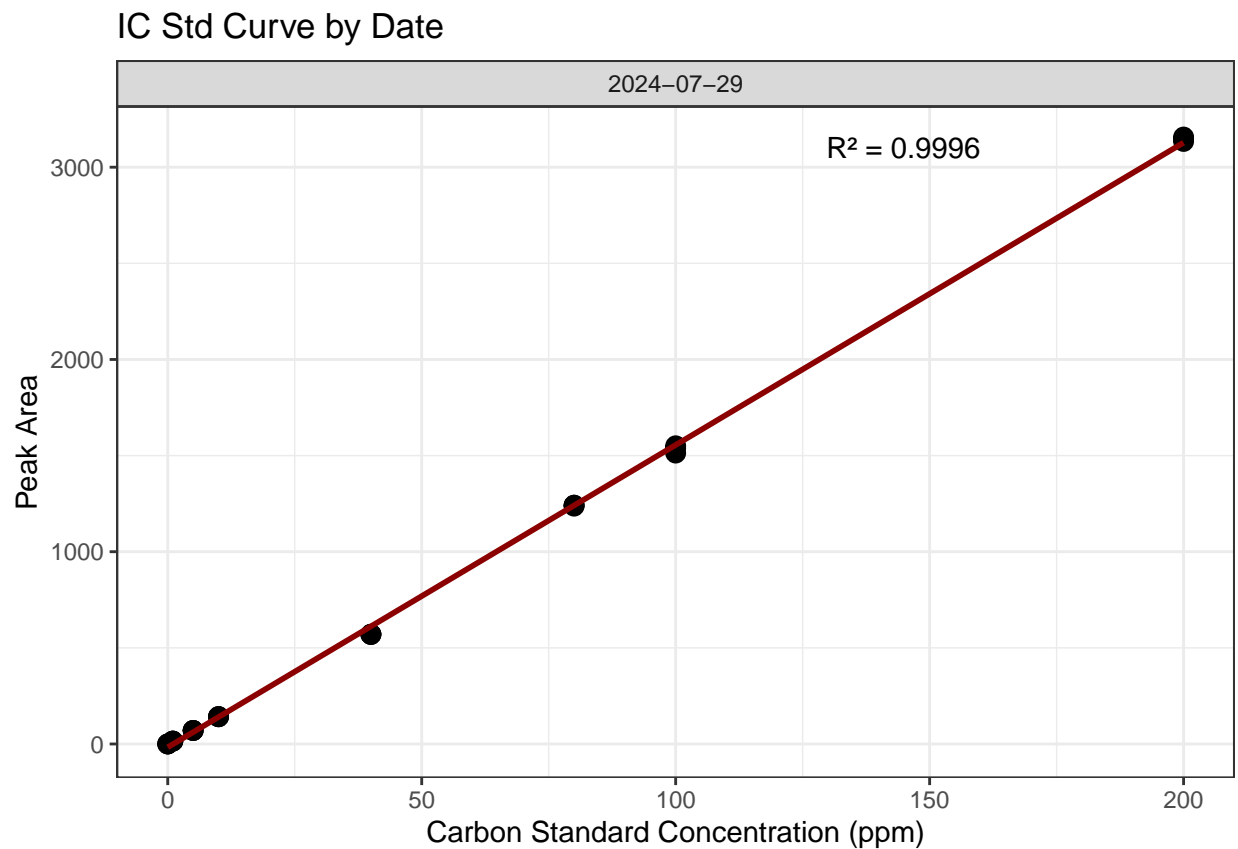
0.3 Assessing Standard Curves

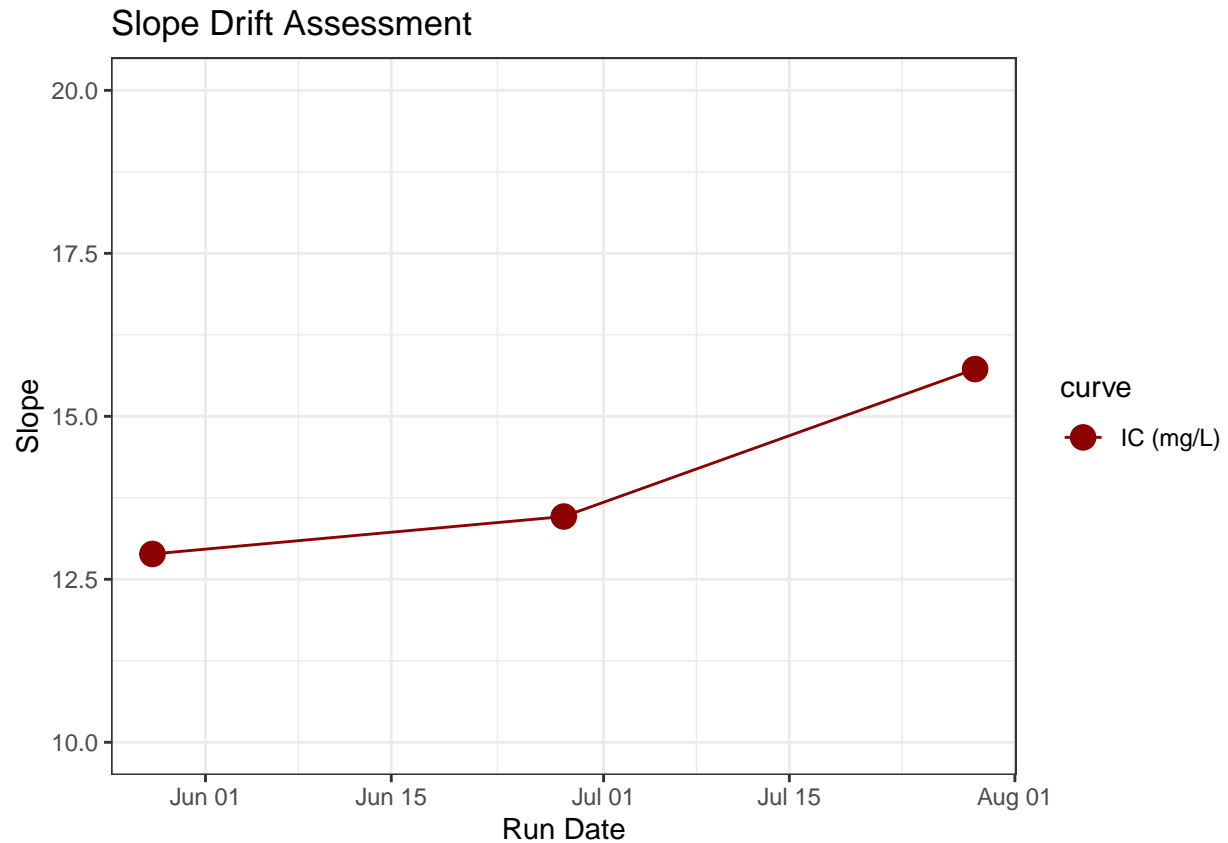
```
## Assess the Standard Curves
```

```
## New names:
## * ' ' -> '...18'
```

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

```
## 'geom_smooth()' using formula = 'y ~ x'
```





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

0.4 CRM Check - Don't run chunk if no CRMs run

```
## Assess the CRMs
```

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

```
## [1] NA
```

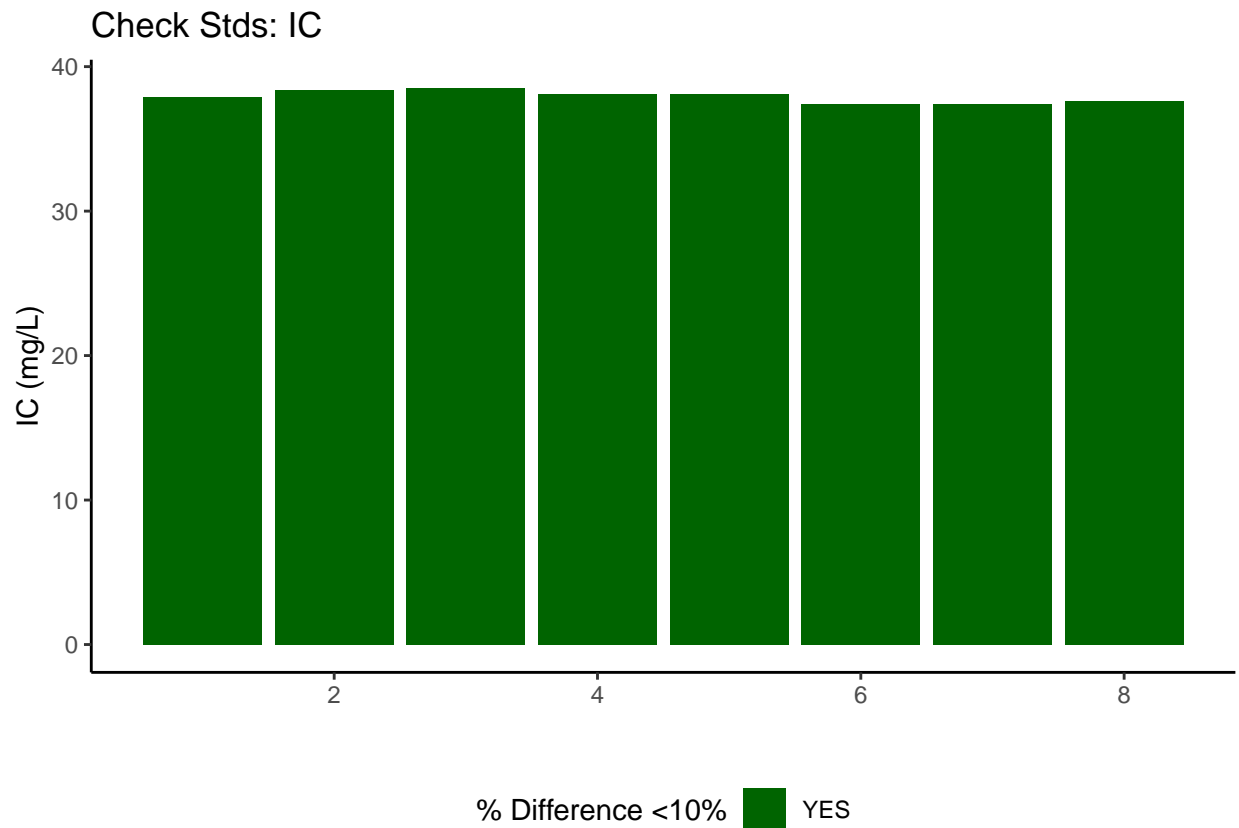
```
## Run mean = NaN
```

```
## Expected = 22.19
```

0.5 Assess Check Standards

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

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



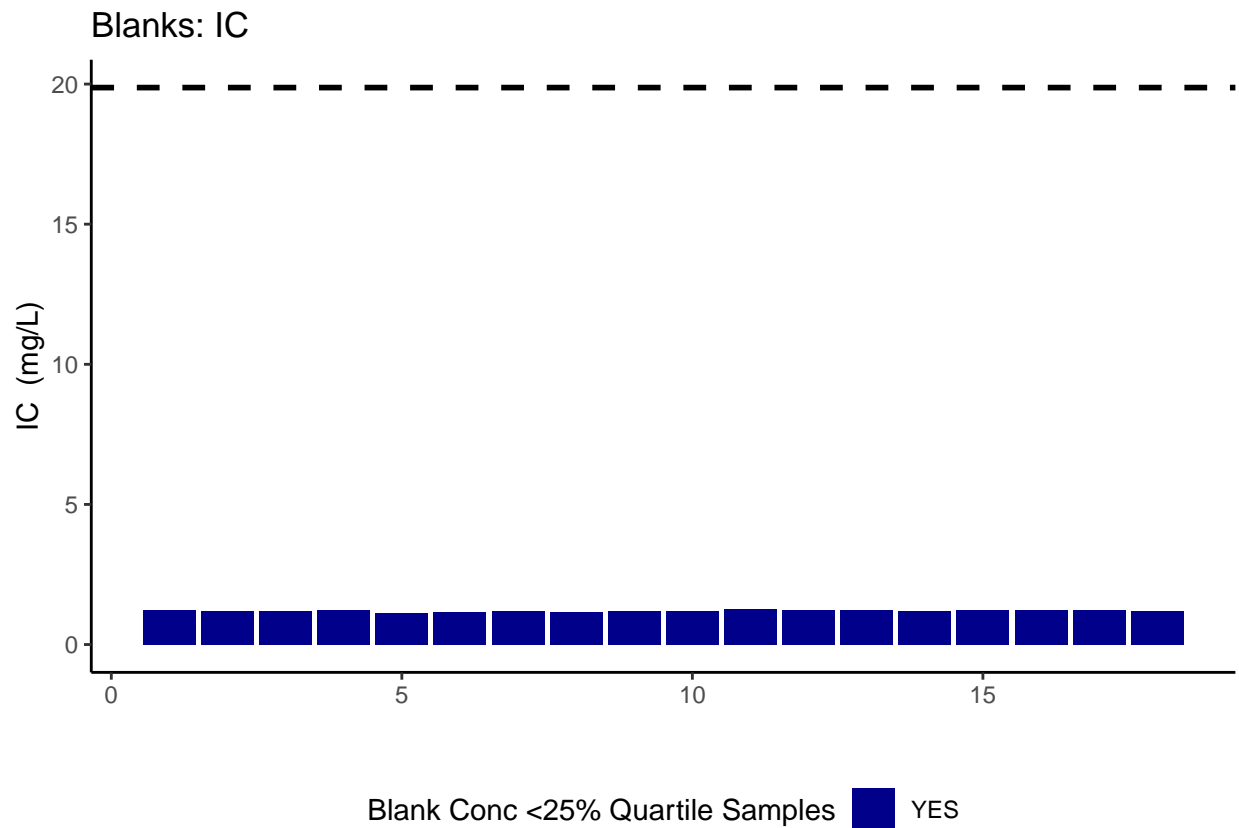
```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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



carbon blanks:

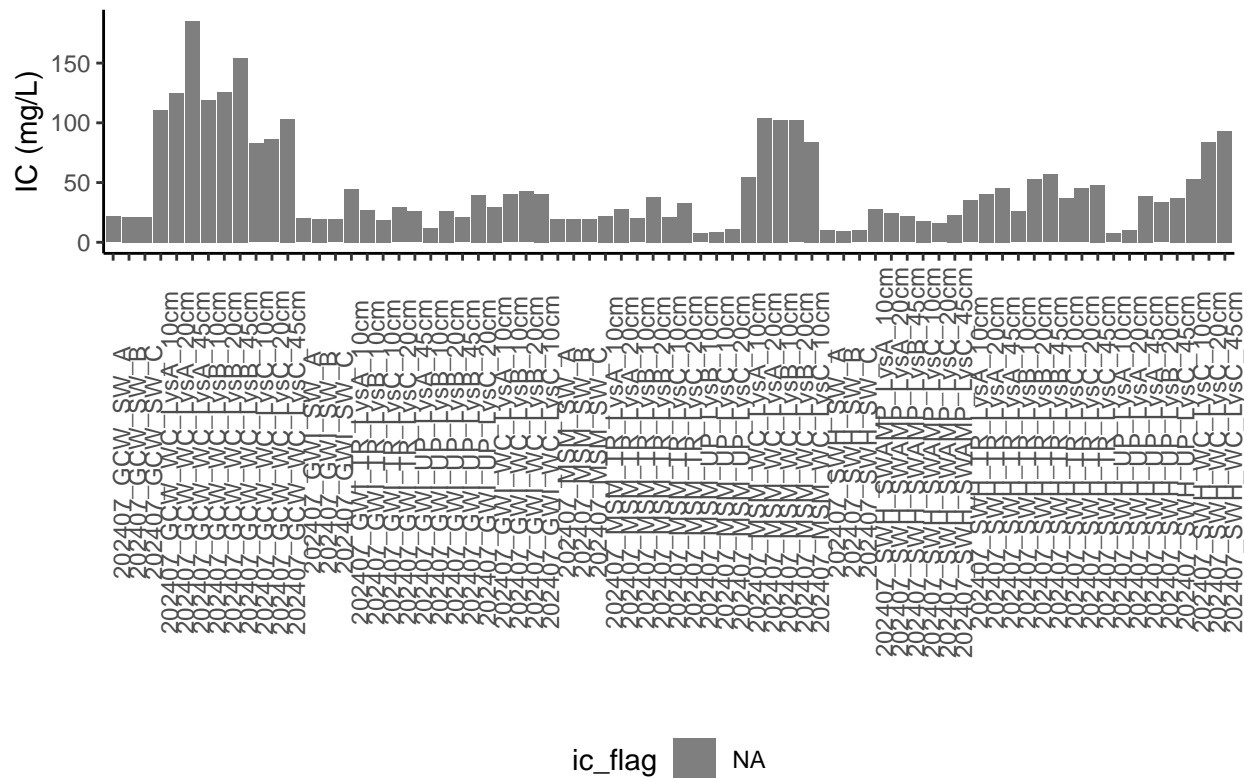
[1] 1.2045

0.7 Assess Duplicates - no duplicates on this run

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

Sample Flagging

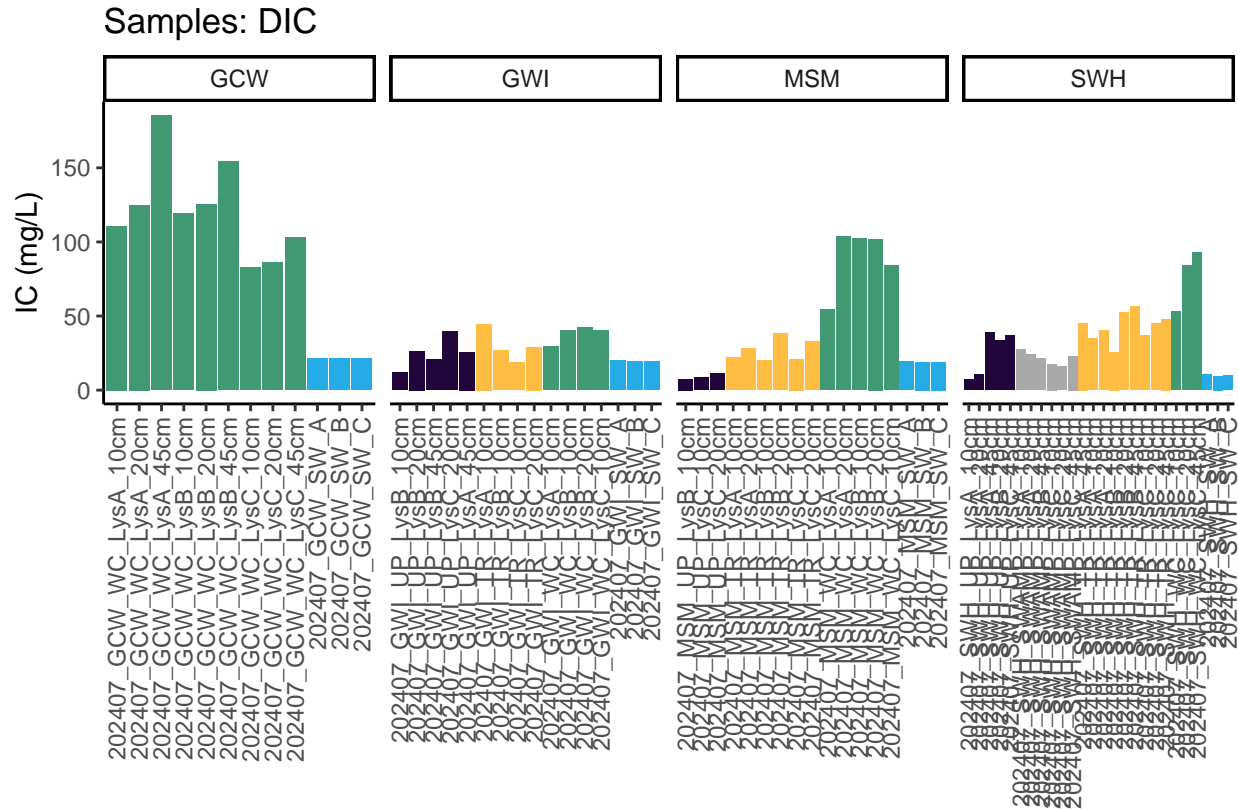
C: Grey = Within Range of Curve



0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202407", "GCW", "WC", "LysA", "10cm"), c("202407", "GCW", :
## number of columns of result is not a multiple of vector length (arg 10)
```



0.10 Convert data from mg/L to uMoles/L

0.11 Check to see if samples run match metadata & merge info

```
## Check Sample IDs with Metadata
## All sample IDs are present in metadata.
```

0.12 Export Processed Data

```
## Export Processed Data

## # A tibble: 6 x 18
##   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 202407_M~  2024    7   18
## 2 COMPASS: Sy~ CB    MSM  UP    C          10 202407_M~  2024    7   18
## 3 COMPASS: Sy~ CB    MSM  UP    C          20 202407_M~  2024    7   18
## 4 COMPASS: Sy~ CB    SWH  UP    A          10 202407_S~  2024    7   23
## 5 COMPASS: Sy~ CB    SWH  UP    A          20 202407_S~  2024    7   23
## 6 COMPASS: Sy~ CB    SWH  UP    A          45 202407_S~  2024    7   23
## # i 8 more variables: Time <chr>, Time_Zone <chr>, ic_mgL <dbl>, ic_uM <dbl>,
## #   ic_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>

#end
```