Synoptic CB: Porewater DIC

May 2025 Samples

2025-07-11

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "5/26/25"   #Date that instrument was run
  Run_by = "Stephanie J. Wilson"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = " "   #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/COMPASS_SynopticCB_PW_DIC_202505.txt"

#file path and name for raw all peaks file
    raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DIC_202505_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202505.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_2025.csv"

#qaqc log file path for this year
  Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAQClog_2025.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 202505_GCW_TR_LysA_20cm    13.3 5/26/2025 10:43:57 PM
## 2 202505_GCW_TR_LysB_10cm    11.0 5/26/2025 10:56:35 PM
## 3 202505_GCW_TR_LysB_20cm    16.1 5/26/2025 11:09:42 PM
## 4 202505_GCW_TR_LysC_10cm    11.5 5/26/2025 11:22:34 PM
## 5 202505_GCW_TR_LysC_20cm    11.0 5/26/2025 11:35:16 PM
## 6 202505_GCW_WC_LysA_10cm    52.6 5/26/2025 11:50:20 PM
```

0.3 Assessing Standard Curves
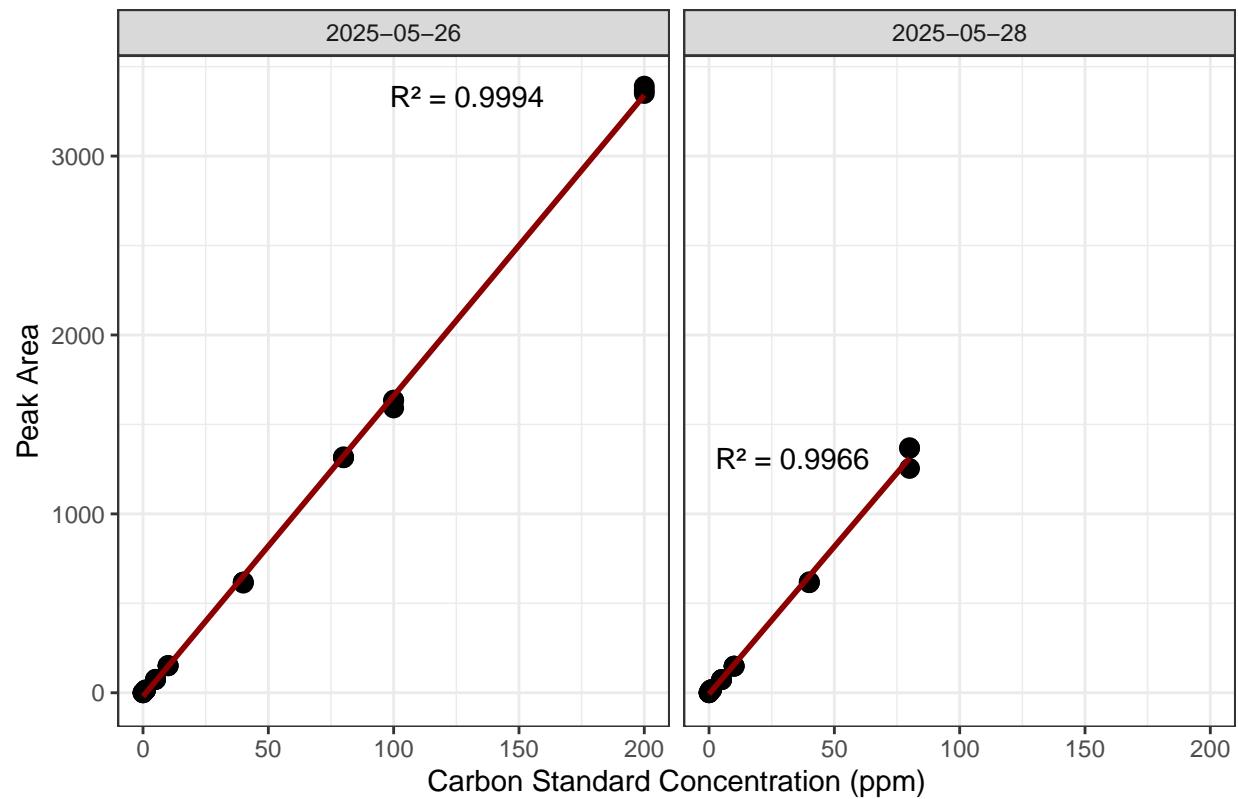
```
## Assess the Standard Curves

## New names:
## `geom_smooth()` using formula = 'y ~ x'
## * `` -> `...18`
```
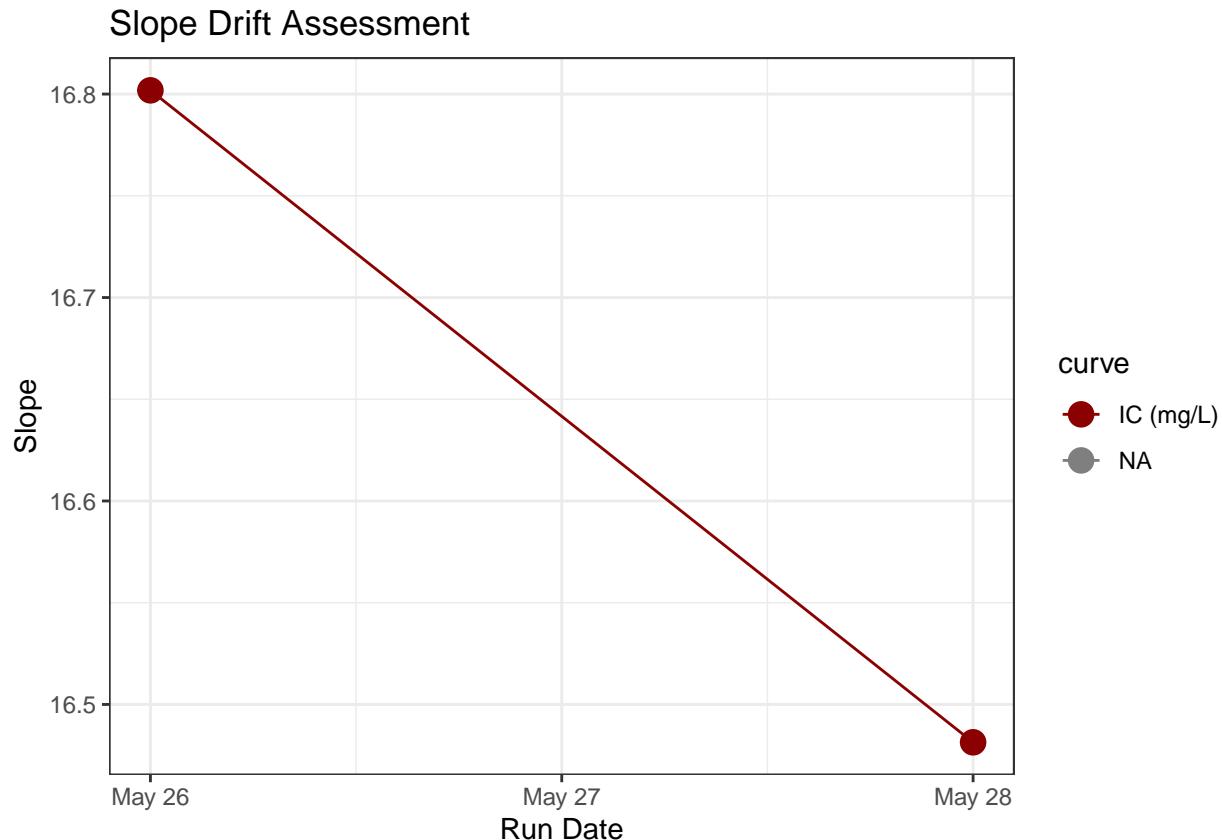
IC Std Curve by Date


```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_point()').
```

```
## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_line()').
```

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

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

```
## Assess the CRMs
```

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

```
## [1] "IC crm has a % Difference <25% of expected - PROCEED"
```
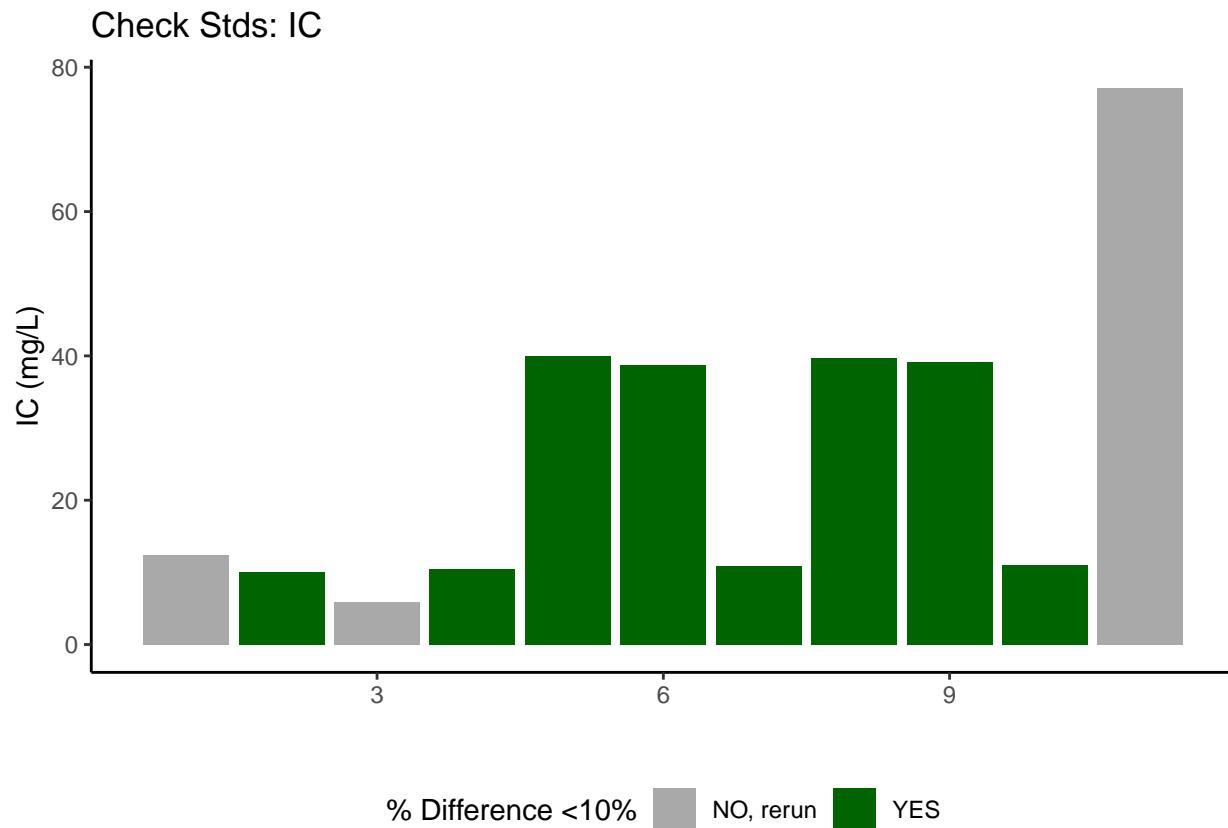
```
## Run mean = 22.17
```

```
## Expected  = 22.19
```

0.5 Assess Check Standards

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

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

Check Stds: IC

% Difference <10% [gray] NO, rerun [green] YES

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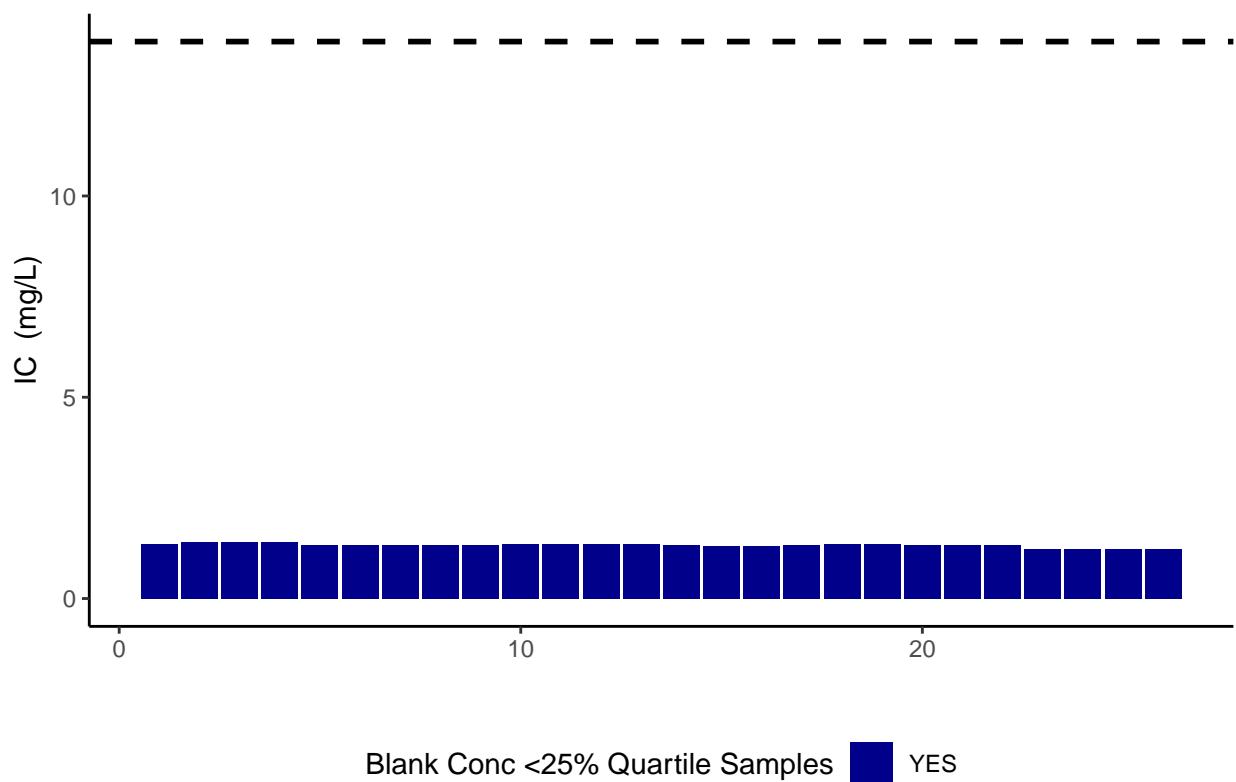
0.6 Assess Blanks

Assess Blanks

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

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

Blanks: IC

IC (mg/L)

Blank Conc <25% Quartile Samples ▮ YES
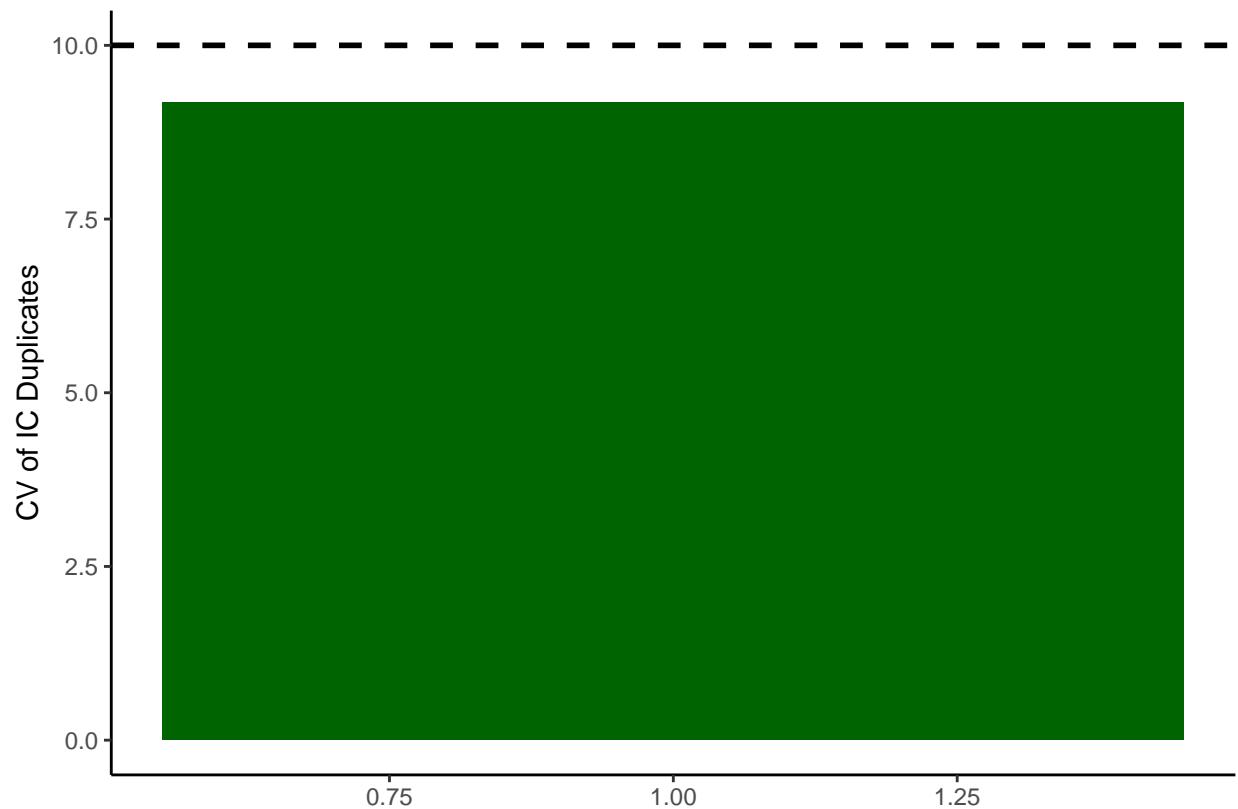
```
## carbon blanks:

## [1] 1.329
```

0.7 Assess Duplicates

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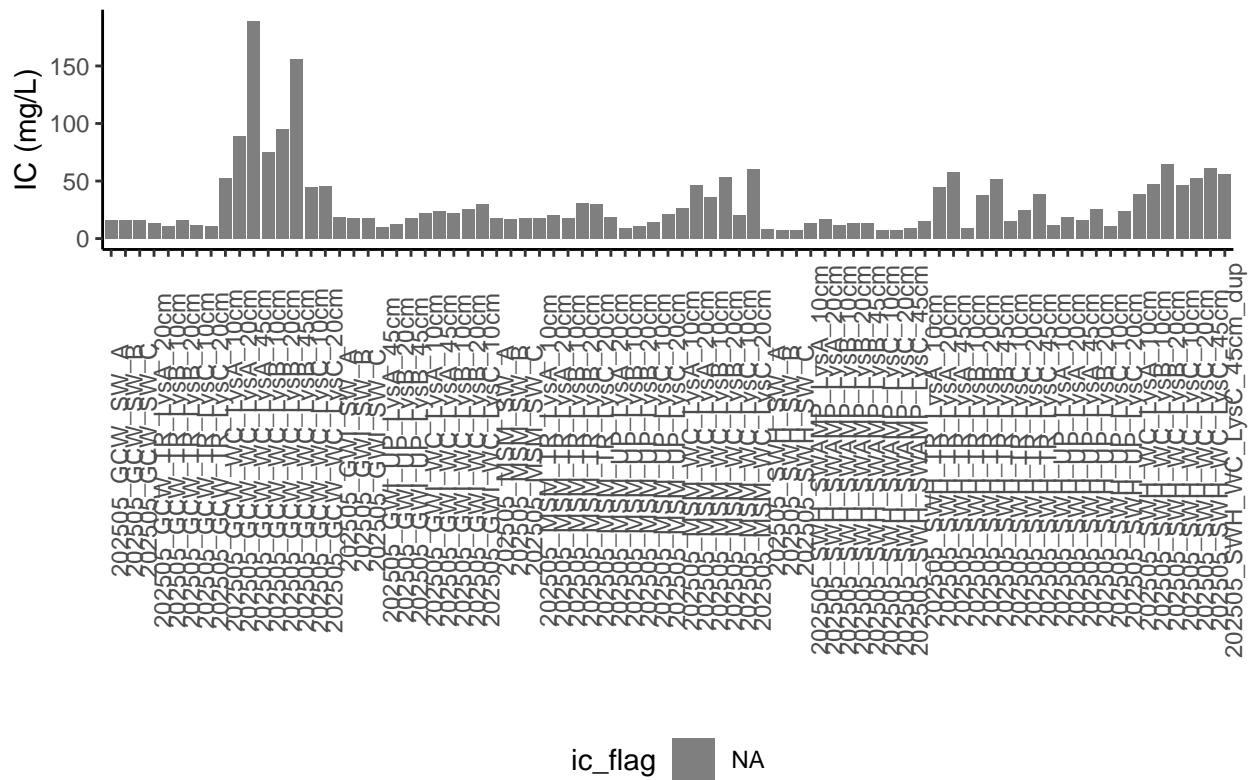
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

```
## Sample Flagging
```

C: Grey = Within Range of Curve

IC (mg/L)

150
100
50
0

ic_flag █ NA
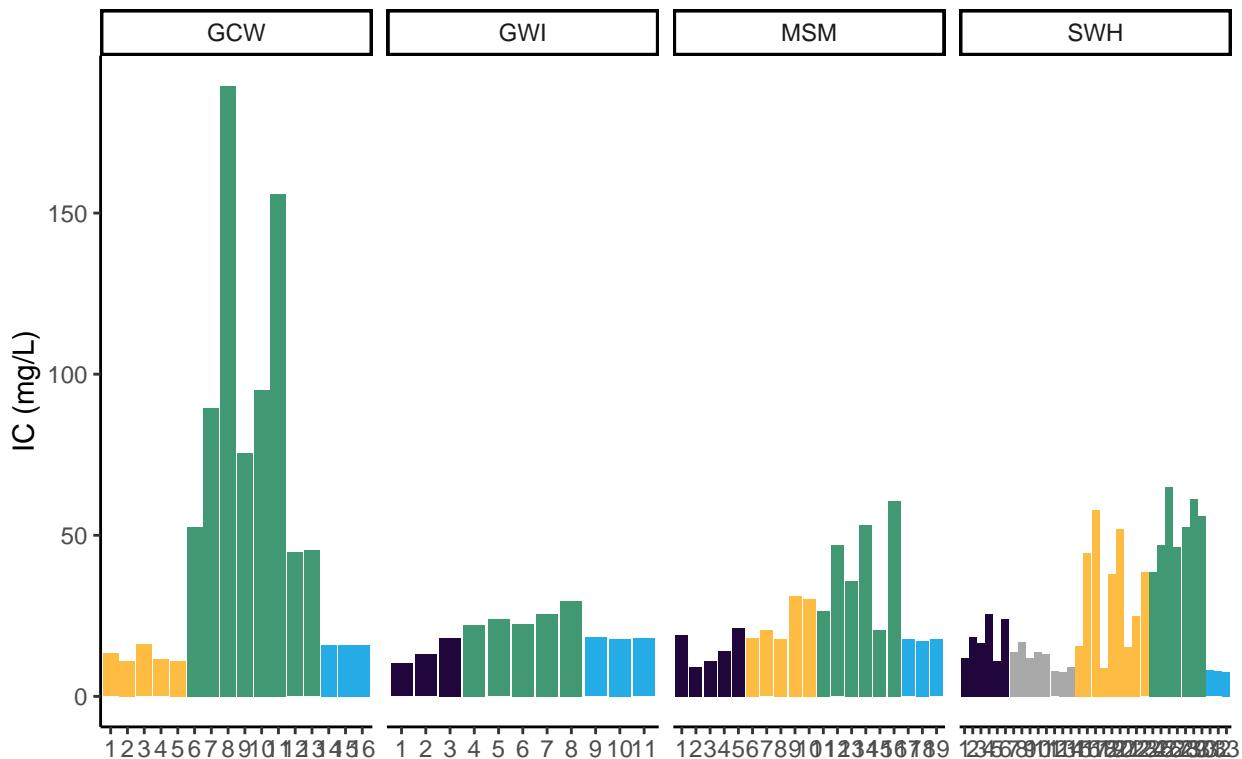
0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202505", "GCW", "TR", "LysA", "20cm"), c("202505", "GCW", :
## number of columns of result is not a multiple of vector length (arg 1)
```

Samples: DIC

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> <chr> <chr>        <int> <chr>     <int> <int> <int>
## 1 COMPASS: Sy~ CB     GCW   TR    A               20 202505_G~  2025     5    14
## 2 COMPASS: Sy~ CB     GCW   TR    B               10 202505_G~  2025     5    14
## 3 COMPASS: Sy~ CB     GCW   TR    B               20 202505_G~  2025     5    14
## 4 COMPASS: Sy~ CB     GCW   TR    C               10 202505_G~  2025     5    14
## 5 COMPASS: Sy~ CB     GCW   TR    C               20 202505_G~  2025     5    14
## 6 COMPASS: Sy~ CB     GCW   WC    A               10 202505_G~  2025     5    14
## # 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