Synoptic CB: Porewater DIC

August 2023 Samples

2025-10-25

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```r
###### Run information - PLEASE CHANGE
  Date_Run = "08/18/23"   #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 = c("Raw Data/TOCTN_COMPASS_Synoptic_DIC_202308_1.txt",
                      "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202308_2.txt")

#file path and name for raw all peaks file
   # raw_allpeaks_name = c("Raw Data/COMPASS_SynopticCB_PW_DIC_202308_1_allpeaks.txt",
    #                      "Raw Data/COMPASS_SynopticCB_PW_DIC_202308_2_allpeaks.txt")

#file path and name of processed data file
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202308.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_2023.csv"

#qaqc log file path for this year
  #Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAQClog_2023.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:
## New names:
## * `` -> `...14`
```

```
## # A tibble: 6 x 3
##   sample_name              ic_raw run_datetime
##   <chr>                     <dbl> <chr>
## 1 GCW_202308_TR_LysB_10cm    28.1 8/19/2023 9:50:53 AM
## 2 GCW_202308_WC_LysA_10cm   162.  8/19/2023 10:08:13 AM
## 3 GCW_202308_WC_LysA_20cm   148.  8/19/2023 10:26:42 AM
## 4 GCW_202308_WC_LysA_45cm   170.  8/19/2023 10:44:08 AM
## 5 GCW_202308_WC_LysB_10cm   198.  8/19/2023 11:00:44 AM
## 6 GCW_202308_WC_LysB_20cm   165.  8/19/2023 11:18:50 AM
```

0.3 Assessing Standard Curves - assessed on the instrument manually

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

```
## Assess the CRMs
```

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

```
## [1] "IC crm has a % Difference <25% of expected - PROCEED"
```
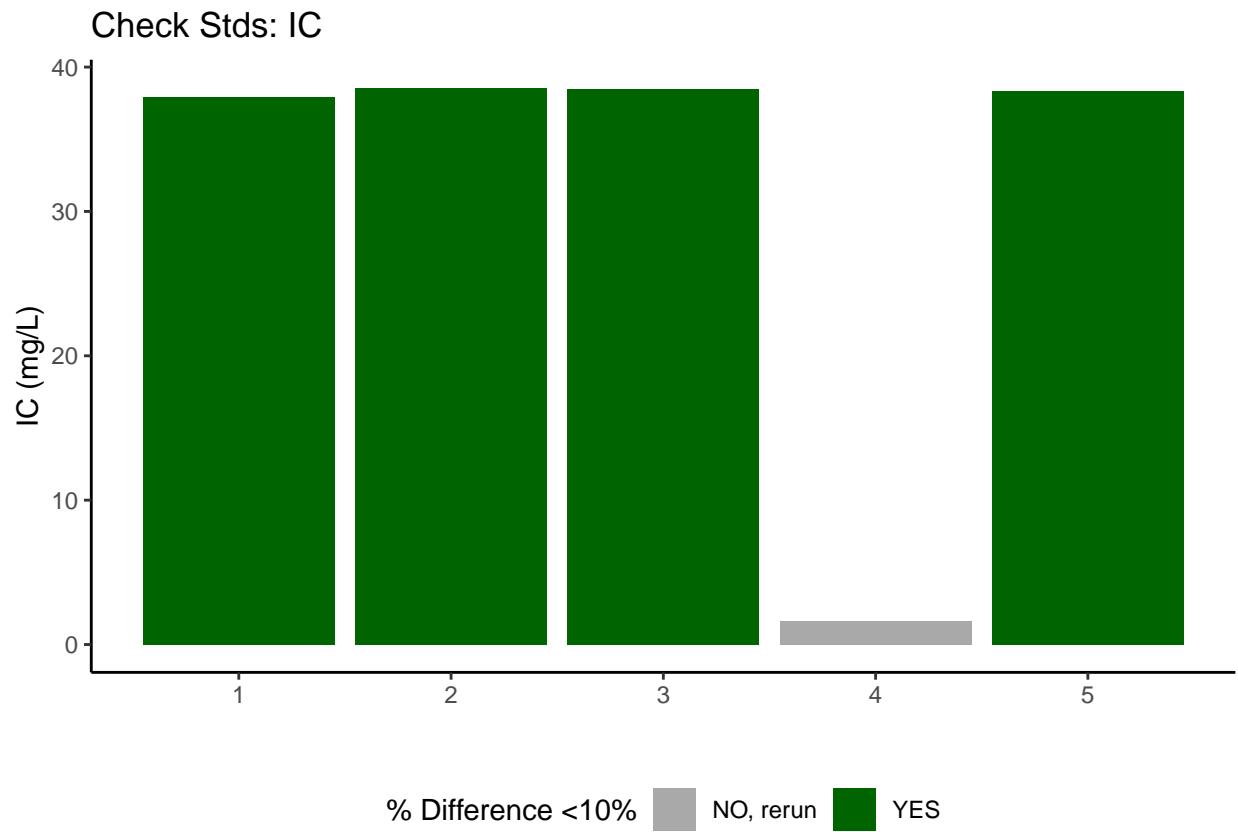
```
## Run mean = 23.1575
```

```
## Expected  = 22.19
```

0.5 Assess Check Standards

```
## Assess the Check Standards
```
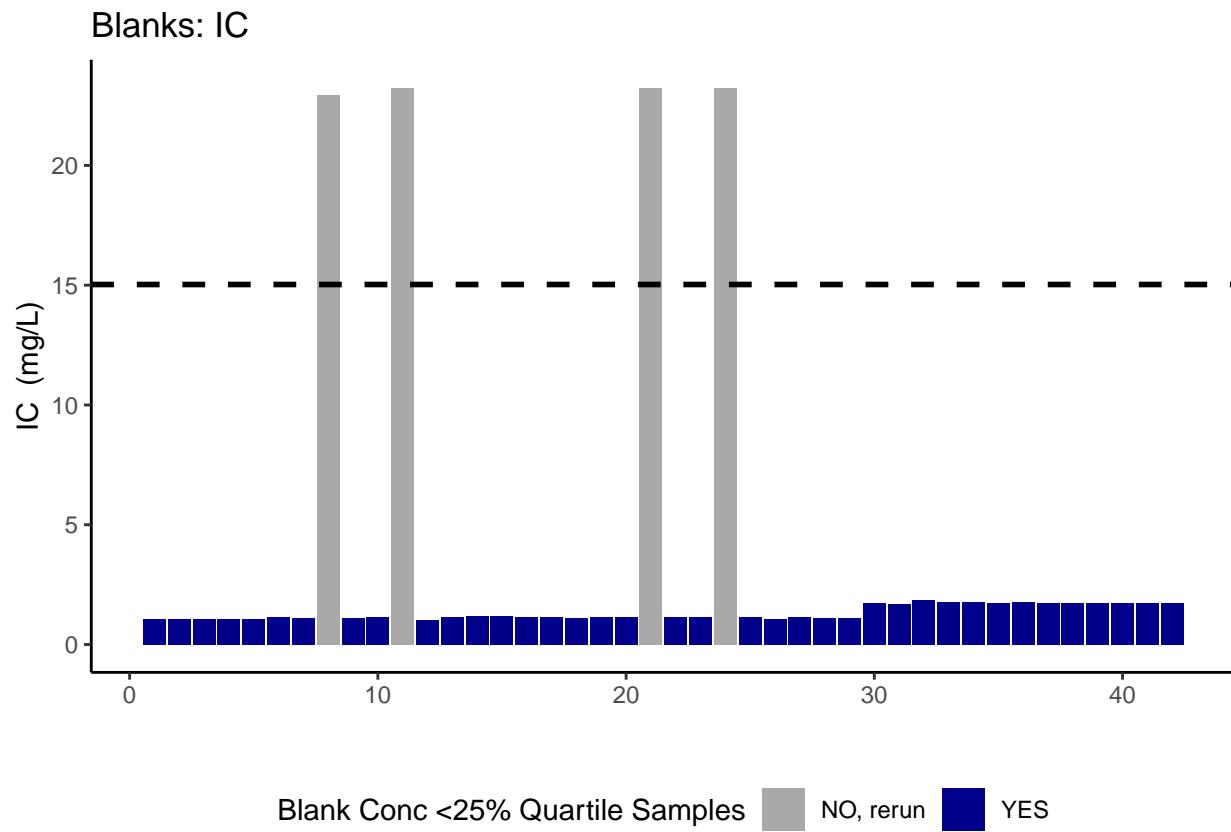
```
## New names:
## New names:
## * '' -> '...14'
```

Check Stds: IC

IC (mg/L)

Bar chart showing five bars along the x-axis (1–5), with the y-axis ranging from 0 to 40. Bars 1, 2, 3, and 5 are green (~38 mg/L). Bar 4 is gray (~1.5 mg/L).

% Difference <10%   ▨ NO, rerun   ▮ YES

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

0.6 Assess Blanks

Assess Blanks

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

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

Blanks: IC

Blank Conc <25% Quartile Samples   NO, rerun   YES
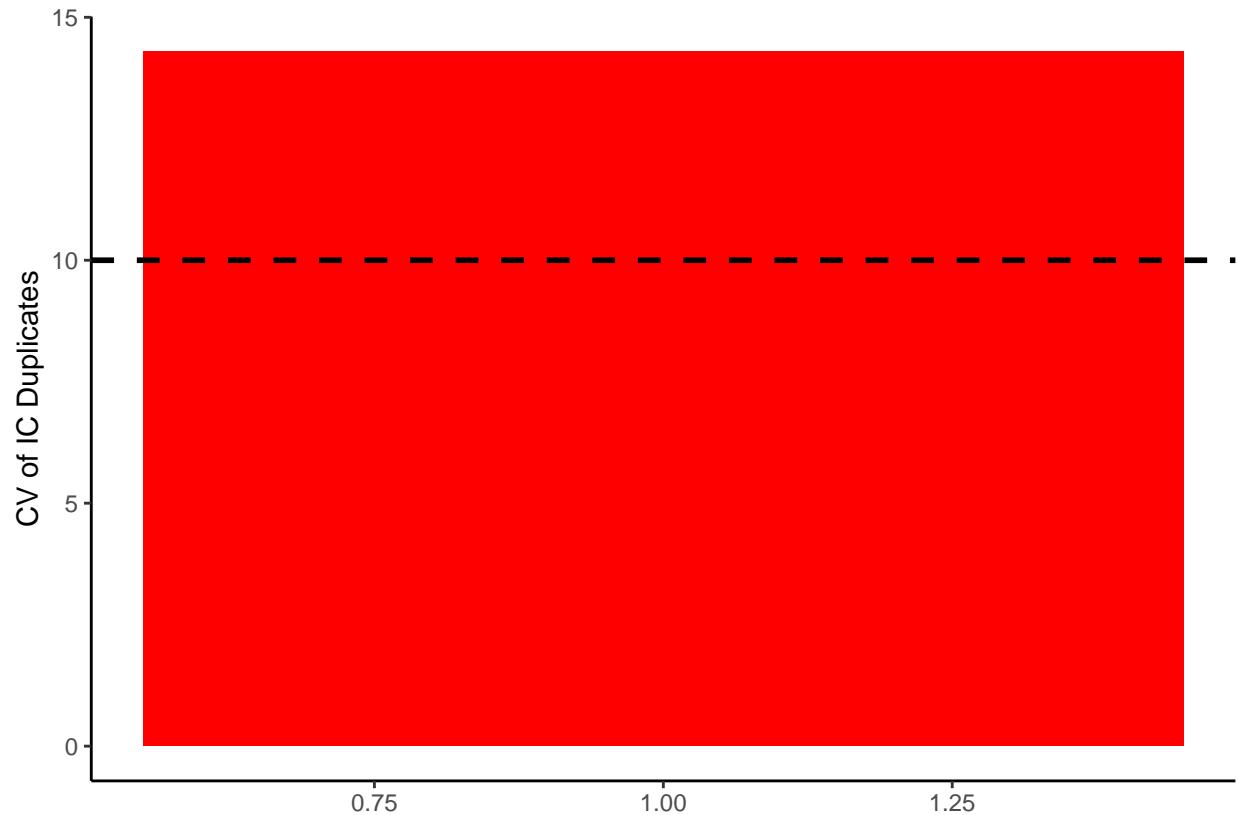
carbon blanks:

[1] 3.413595

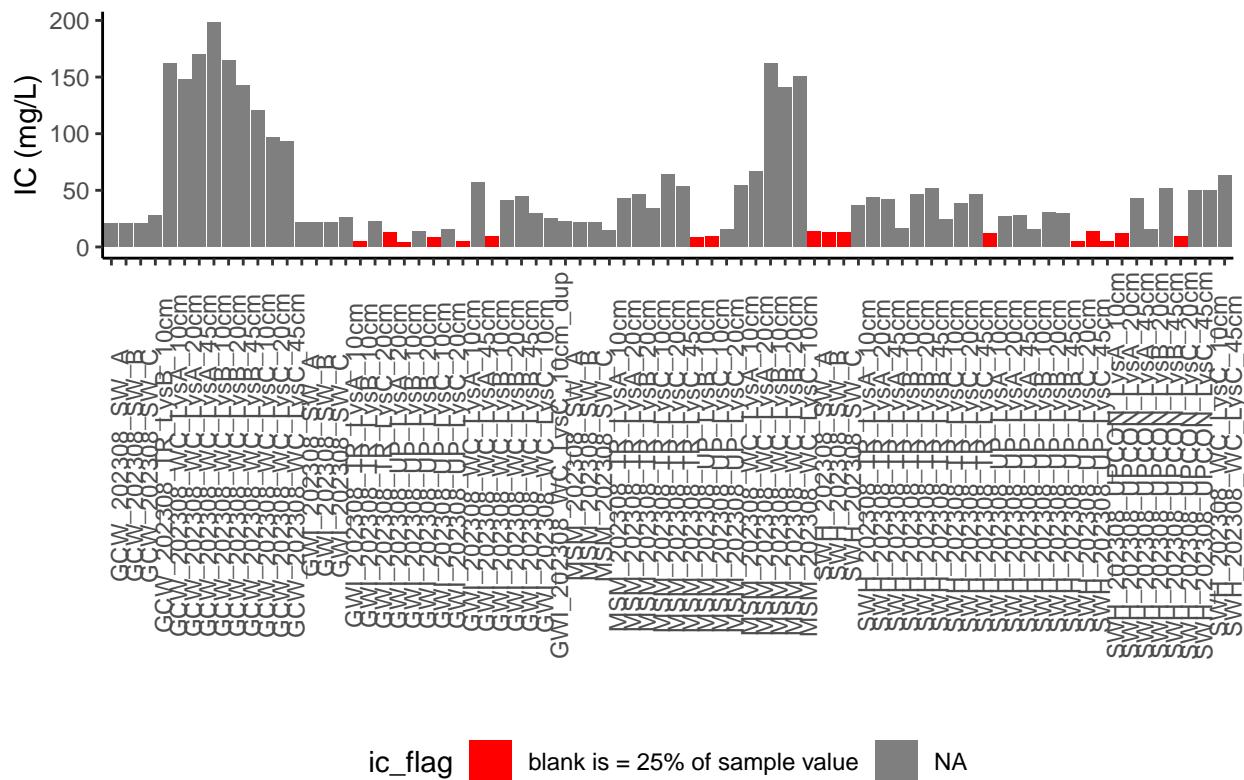## 0.7 Assess Duplicates

Assess Duplicates

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

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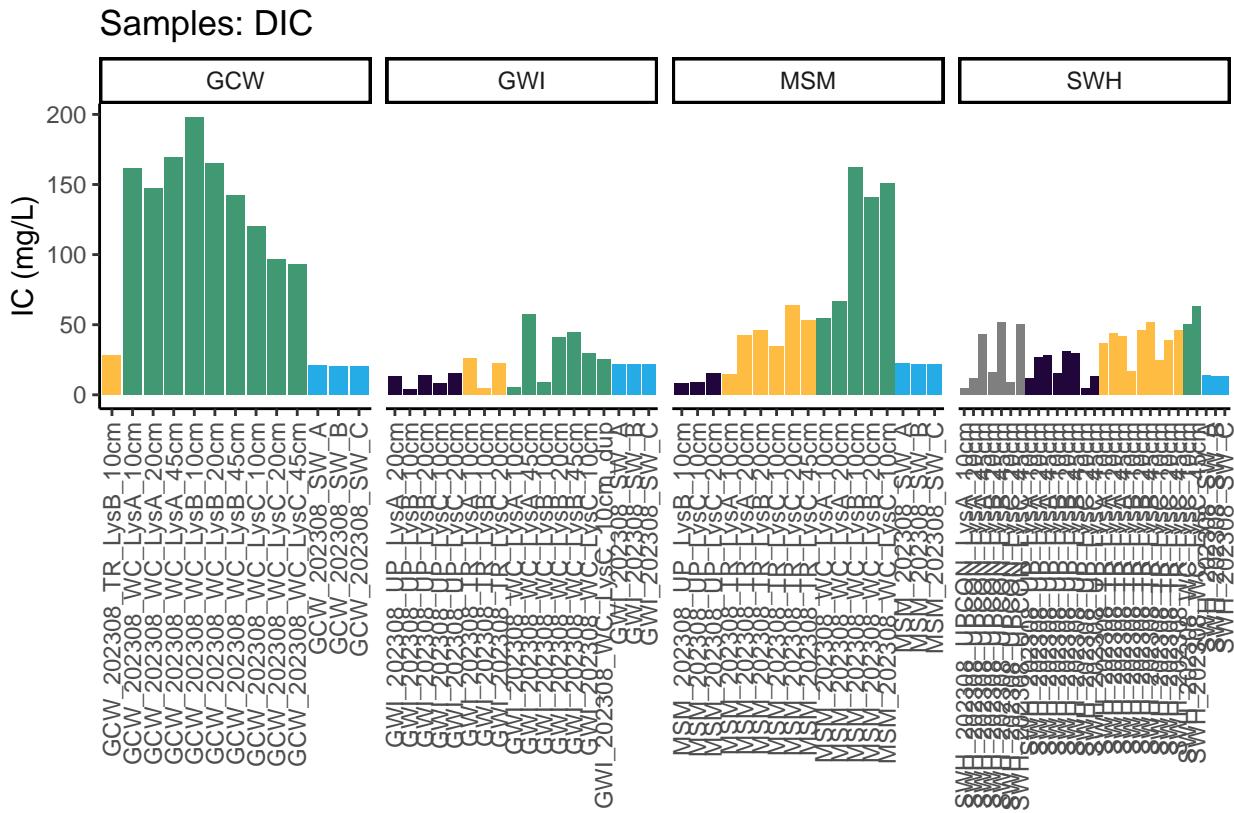
```
## Sample Flagging
```

C: Grey = Within Range of Curve

ic_flag | [red box] blank is = 25% of sample value | [grey box] NA

0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("GCW", "202308", "TR", "LysB", "10cm"), c("GCW", "202308", :
## 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> <fct> <chr>        <int> <chr>     <int> <int> <int>
## 1 COMPASS: Sy~  CB     SWH   UPCON A               10 SWH_2023~  2023     8    23
## 2 COMPASS: Sy~  CB     SWH   UPCON A               20 SWH_2023~  2023     8    23
## 3 COMPASS: Sy~  CB     SWH   UPCON A               45 SWH_2023~  2023     8    23
## 4 COMPASS: Sy~  CB     SWH   UPCON B               20 SWH_2023~  2023     8    23
## 5 COMPASS: Sy~  CB     SWH   UPCON B               45 SWH_2023~  2023     8    23
## 6 COMPASS: Sy~  CB     SWH   UPCON C               20 SWH_2023~  2023     8    23
## # i 8 more variables: Time <lgl>, Time_Zone <lgl>, ic_mgL <dbl>, ic_uM <dbl>,
## #   ic_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>
```

#end