Synoptic CB: Porewater DIC

October 2023 Samples

2025-10-25

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "10/27/23"  #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 = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202310.txt"

#file path and name for raw all peaks file
   # raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DIC_2025MM_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202310.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_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 202310_MSM_UP_LysB_10cm   28.0 10/27/2023 8:18:39 PM
## 2 202310_MSM_UP_LysC_10cm   16.2 10/27/2023 8:33:39 PM
## 3 202310_MSM_UP_LysC_20cm   23.4 10/27/2023 8:48:54 PM
## 4 202310_MSM_TR_LysA_10cm   31.6 10/27/2023 9:04:28 PM
## 5 202310_MSM_TR_LysA_20cm   35.9 10/27/2023 9:26:26 PM
## 6 202310_MSM_TR_LysB_10cm   32.3 10/27/2023 9:54:27 PM
```

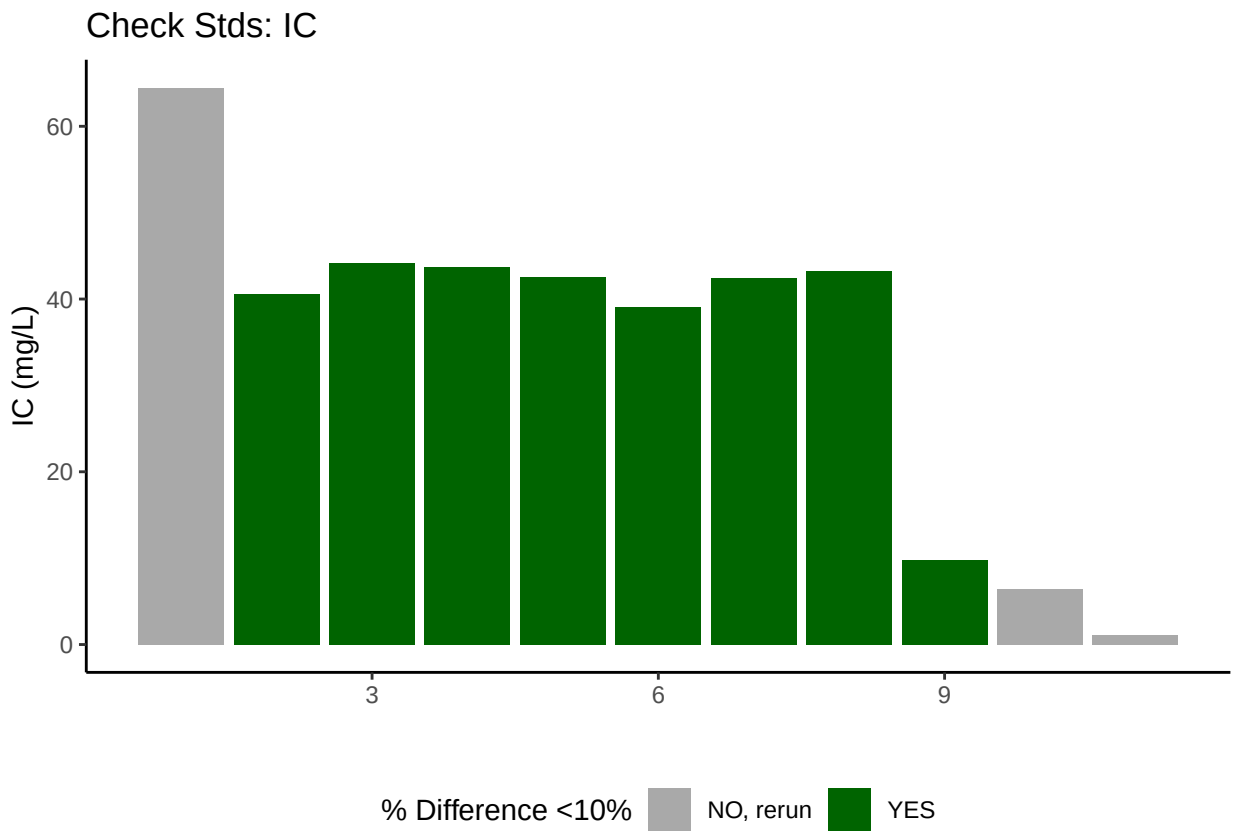
0.3 Assessing Standard Curves - the curve was assessed manually on the instrument

0.4 CRM Check - No CRMs on this run

```
## Assess the CRMs

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

## [1] NA

## Run mean = NaN

## Expected  = 22.19
```

0.5 Assess Check Standards

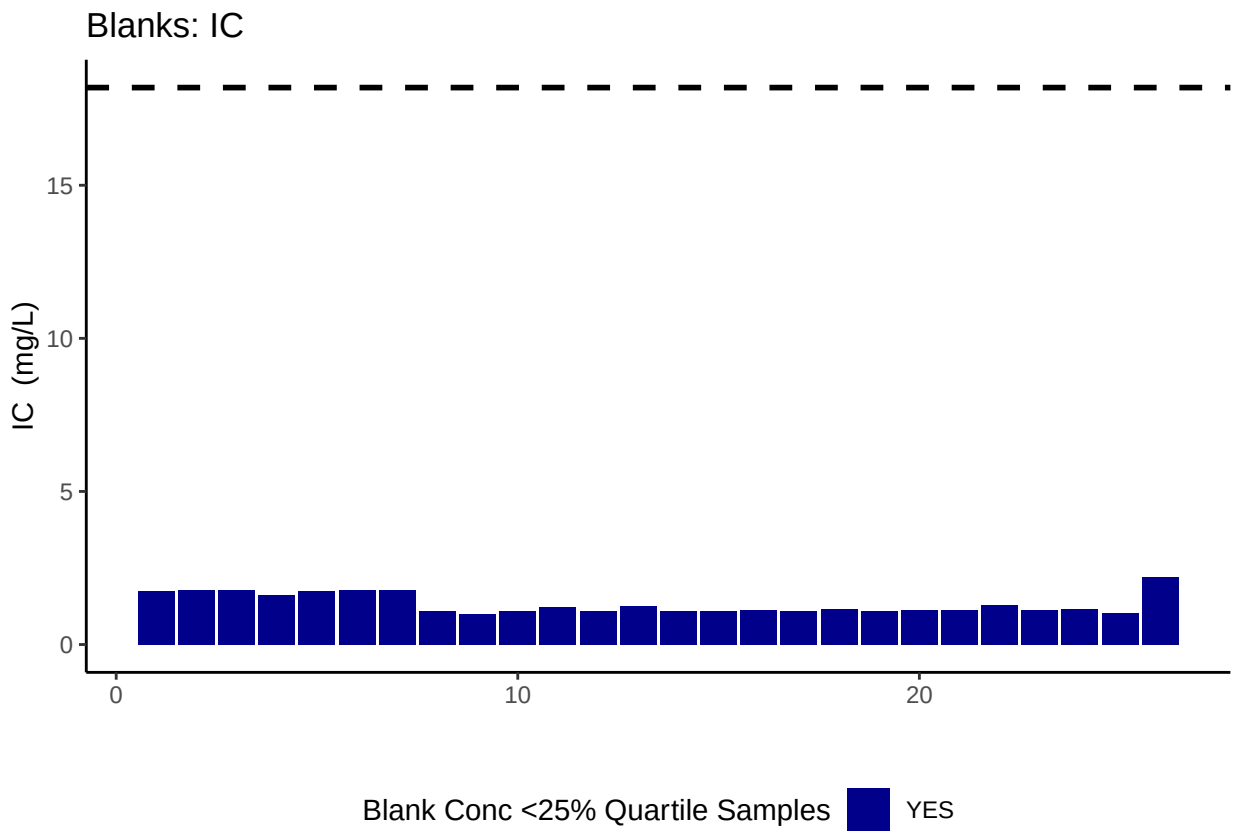
```
## Assess the Check Standards

## 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"
```

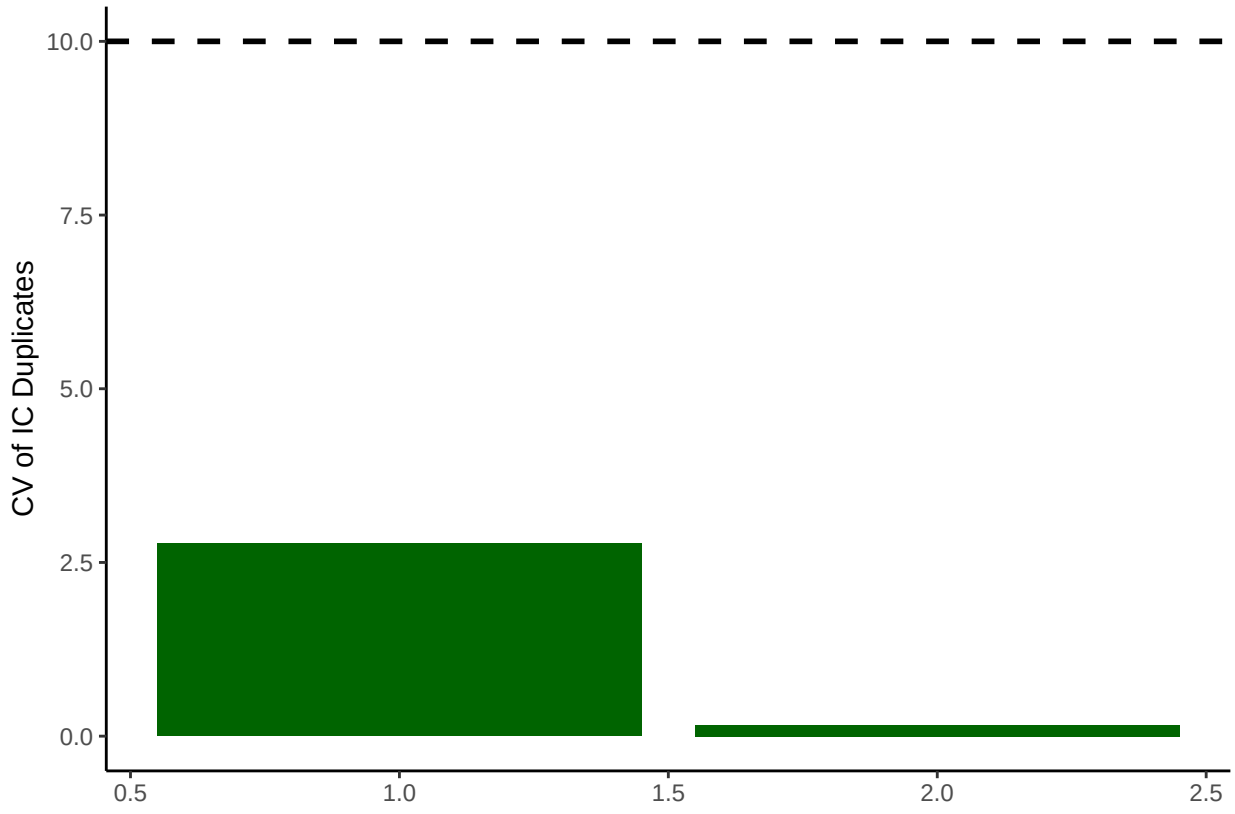



```
## carbon blanks:
```

```
## [1] 1.338454
```

0.7 Assess Duplicates

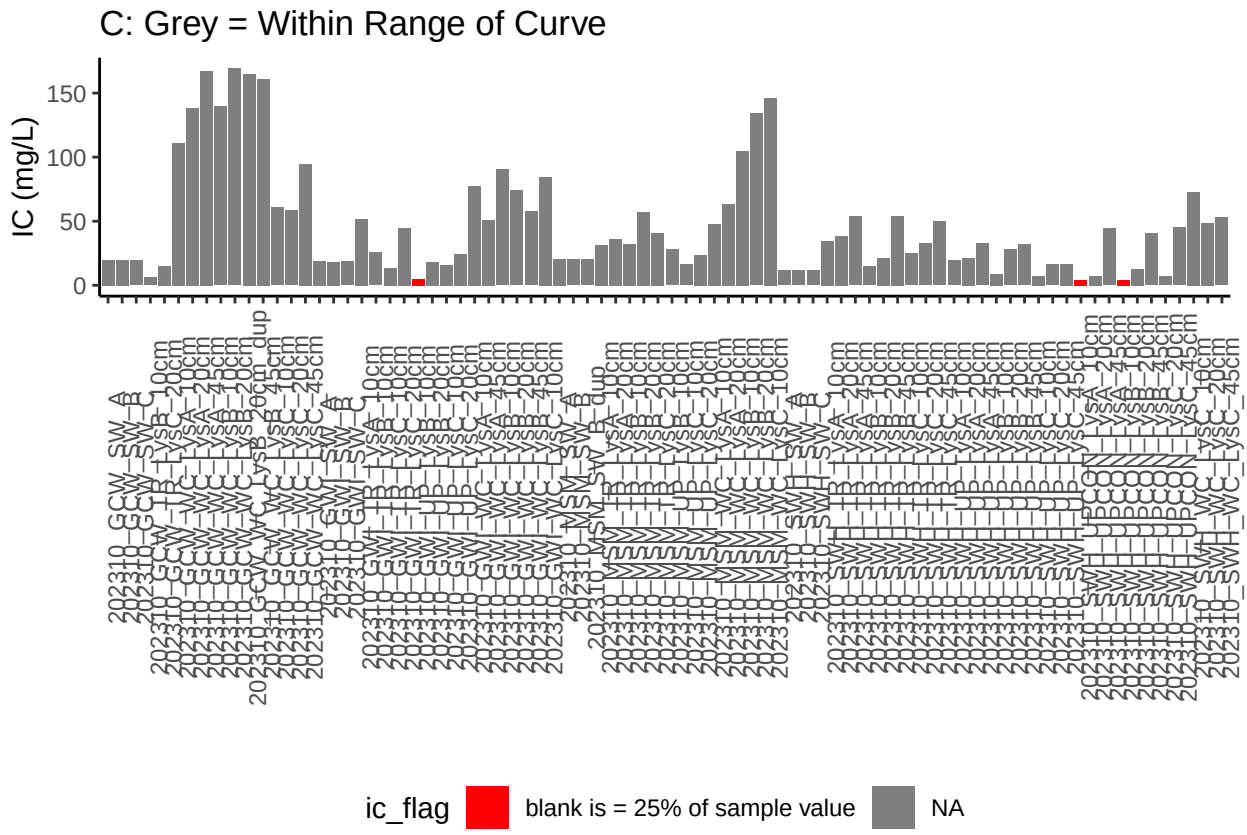
```
## Assess Duplicates
```




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

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

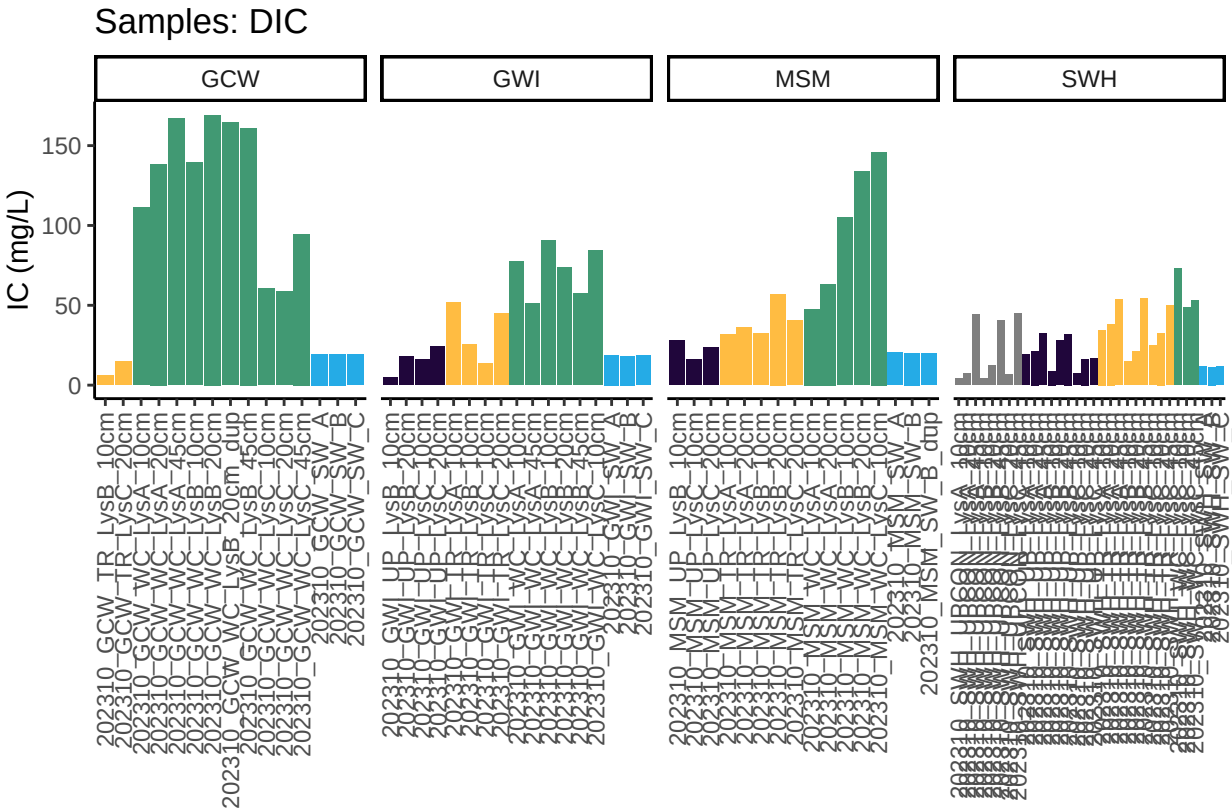
```
## Sample Flagging
```



0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202310", "MSM", "UP", "LysB", "10cm"), c("202310", "MSM", :
## number of columns of result is not a multiple of vector length (arg 1)
```



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 202310_S~  2023    10    18
## 2 COMPASS: Sy~ CB     SWH   UPCON A               20 202310_S~  2023    10    18
## 3 COMPASS: Sy~ CB     SWH   UPCON A               45 202310_S~  2023    10    18
## 4 COMPASS: Sy~ CB     SWH   UPCON B               10 202310_S~  2023    10    18
## 5 COMPASS: Sy~ CB     SWH   UPCON B               20 202310_S~  2023    10    18
## 6 COMPASS: Sy~ CB     SWH   UPCON B               45 202310_S~  2023    10    18
## # 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