Synoptic CB: Porewater DIC

October 2022 Samples

2025-10-22

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "11/14/22"  #Date that instrument was run
  Run_by = "Stephanie J. Wilson"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = " The standard curve for this run was checked manually on the instrument.
    This run contains data from multiple months."  #any notes from the run
  samples <- c("GCW", "GWI", "MSM", "SWH", "GCrew") #whatever identifies your samples within the same n
  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_"  #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_202210.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_202210.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_2022.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 GWI_202209_UP_LysA_20cm  12.3  11/14/2022 11:25:37 PM
## 2 GWI_202209_UP_LysB_10cm   5.34 11/14/2022 11:37:44 PM
## 3 GWI_202209_UP_LysB_20cm  13.9  11/14/2022 11:53:12 PM
## 4 GWI_202209_UP_LysB_45cm  16.5  11/15/2022 12:05:53 AM
## 5 GWI_202209_UP_LysC_10cm  15.0  11/15/2022 12:18:26 AM
## 6 GWI_202209_UP_LysC_20cm  15.4  11/15/2022 12:31:04 AM
```

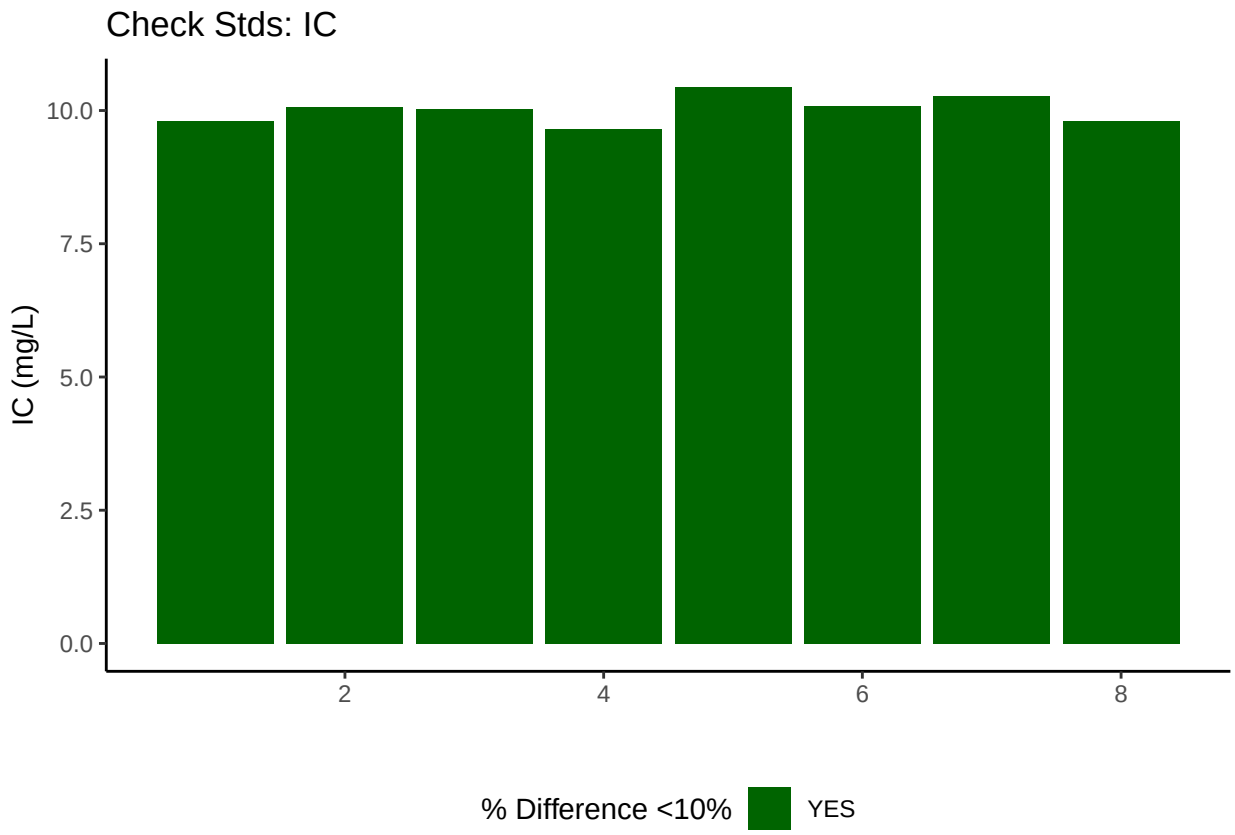
0.3 Assessing Standard Curves - done manually on the instrument

0.4 CRM Check - No CRMs included on this run

0.5 Assess Check Standards

```
## Assess the Check Standards

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



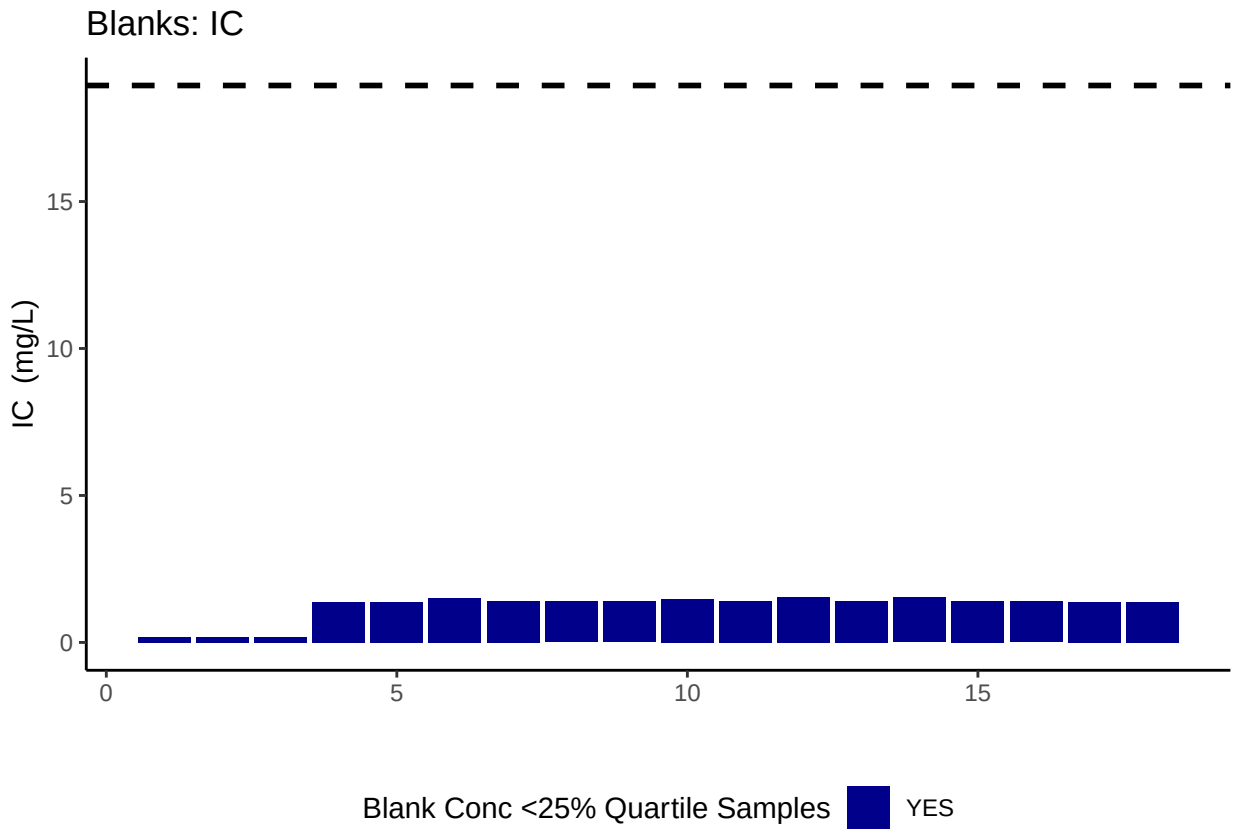

```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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



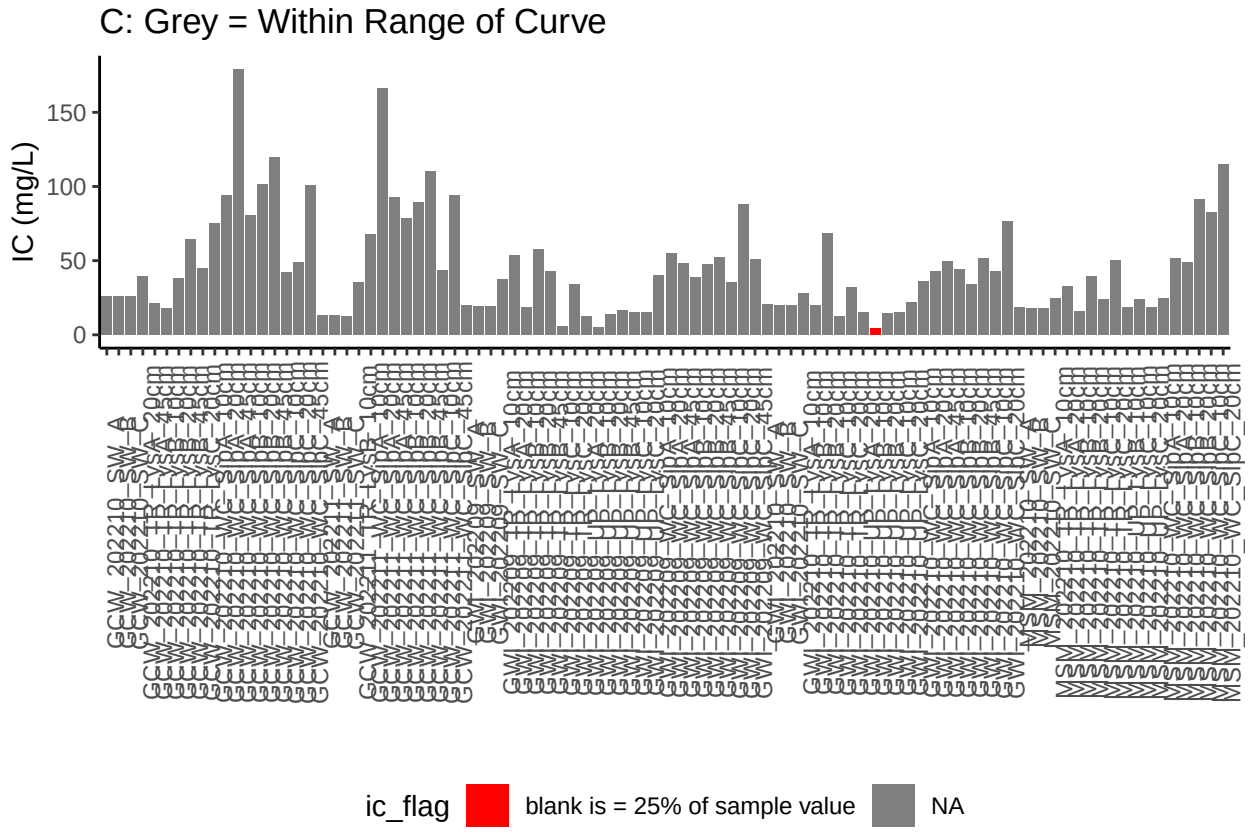

```
## carbon blanks:
```

```
## [1] 1.218711
```

0.7 Assess Duplicates - no duplicates included on this run

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

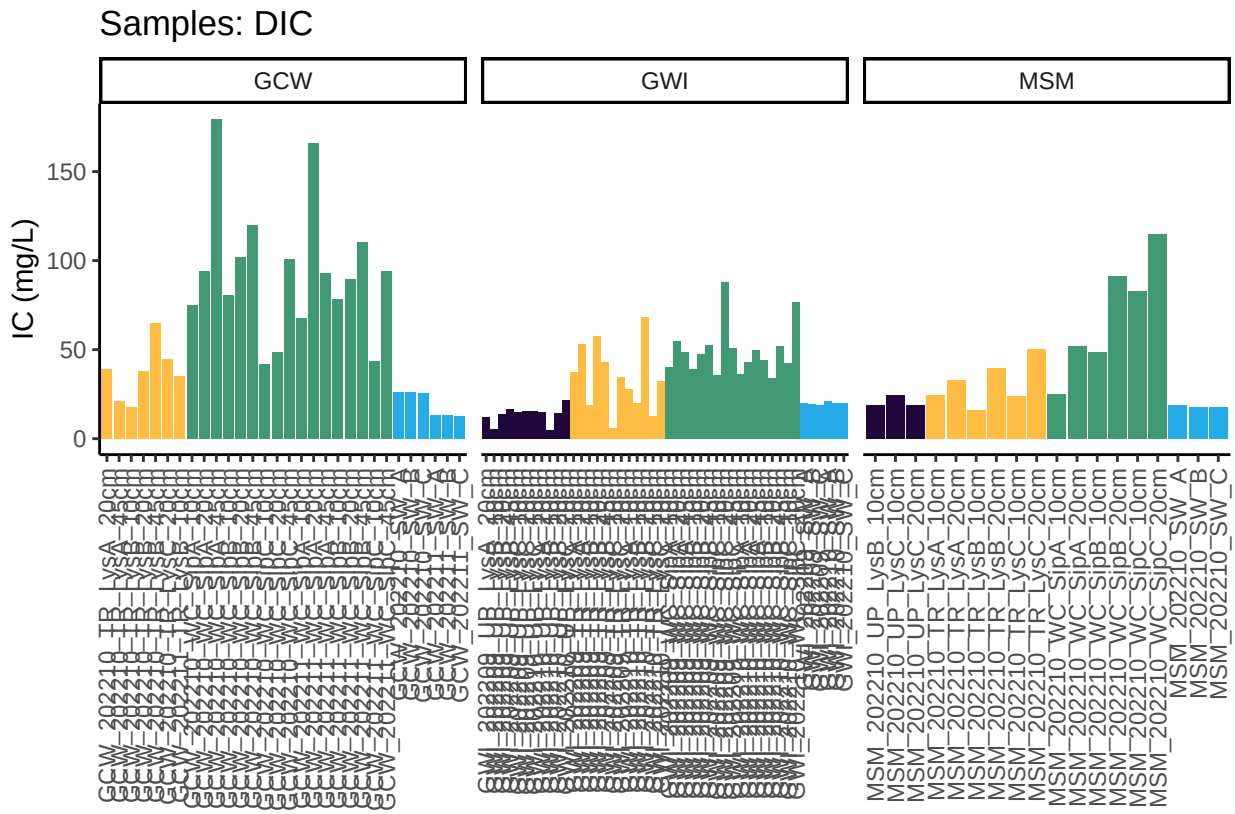
```
## Sample Flagging
```



0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("GWI", "202209", "UP", "LysA", "20cm"), c("GWI", "202209", :
## number of columns of result is not a multiple of vector length (arg 23)
```



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

## Some sample IDs are missing from metadata.

##  [1] "GWI_202209_WC_SipA_10cm" "GWI_202209_WC_SipA_20cm"
##  [3] "GWI_202209_WC_SipA_45cm" "GWI_202209_WC_SipB_10cm"
##  [5] "GWI_202209_WC_SipB_20cm" "GWI_202209_WC_SipB_45cm"
##  [7] "GWI_202209_WC_SipC_10cm" "GWI_202209_WC_SipC_20cm"
##  [9] "GWI_202209_WC_SipC_45cm" "GCW_202210_WC_SipA_10cm"
## [11] "GCW_202210_WC_SipA_20cm" "GCW_202210_WC_SipA_45cm"
## [13] "GCW_202210_WC_SipB_10cm" "GCW_202210_WC_SipB_20cm"
## [15] "GCW_202210_WC_SipB_45cm" "GCW_202210_WC_SipC_10cm"
## [17] "GCW_202210_WC_SipC_20cm" "GCW_202210_WC_SipC_45cm"
## [19] "GWI_202210_WC_SipA_10cm" "GWI_202210_WC_SipA_20cm"
## [21] "GWI_202210_WC_SipA_45cm" "GWI_202210_WC_SipB_10cm"
## [23] "GWI_202210_WC_SipB_20cm" "GWI_202210_WC_SipB_45cm"
## [25] "GWI_202210_WC_SipC_10cm" "GWI_202210_WC_SipC_20cm"
## [27] "MSM_202210_WC_SipA_10cm" "MSM_202210_WC_SipA_20cm"
## [29] "MSM_202210_WC_SipB_10cm" "MSM_202210_WC_SipB_20cm"
## [31] "MSM_202210_WC_SipC_10cm" "MSM_202210_WC_SipC_20cm"
```

```
## [33] "GCW_202211_WC_SipA_10cm" "GCW_202211_WC_SipA_20cm"
## [35] "GCW_202211_WC_SipA_45cm" "GCW_202211_WC_SipB_10cm"
## [37] "GCW_202211_WC_SipB_20cm" "GCW_202211_WC_SipB_45cm"
## [39] "GCW_202211_WC_SipC_10cm" "GCW_202211_WC_SipC_45cm"
```

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     GWI   UP    A               20 GWI_2022~  2022     9    22
## 2 COMPASS: Sy~ CB     GWI   UP    B               10 GWI_2022~  2022     9    22
## 3 COMPASS: Sy~ CB     GWI   UP    B               20 GWI_2022~  2022     9    22
## 4 COMPASS: Sy~ CB     GWI   UP    B               45 GWI_2022~  2022     9    22
## 5 COMPASS: Sy~ CB     GWI   UP    C               10 GWI_2022~  2022     9    22
## 6 COMPASS: Sy~ CB     GWI   UP    C               20 GWI_2022~  2022     9    22
## # 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