

Synoptic CB: Porewater DIC

August 2022 Samples

2025-10-22

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```

##Setup - Change things here & write any notes

#identify section
cat("Setup Information")

## Setup Information

##### Run information - PLEASE CHANGE
Date_Run = "09/08/22" #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", "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_202208.txt"

#file path and name for raw all peaks file
# raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202208_allpeaks.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202208.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 GCW_202208_UP_LysB_20cm 4.96 9/8/2022 1:37:11 PM
## 2 GCW_202208_TR_LysA_20cm 42.1 9/8/2022 1:52:30 PM
## 3 GCW_202208_TR_LysC_20cm 92.4 9/8/2022 2:09:52 PM
## 4 GCW_202208_WC_SipA_10cm 113. 9/8/2022 2:31:47 PM
## 5 GCW_202208_WC_SipA_20cm 124. 9/8/2022 2:49:55 PM
## 6 GCW_202208_WC_SipA_45cm 201. 9/8/2022 3:08:07 PM

```

0.3 Assessing Standard Curves - done manually on the instrument

0.4 CRM Check - No CRMS included on this run

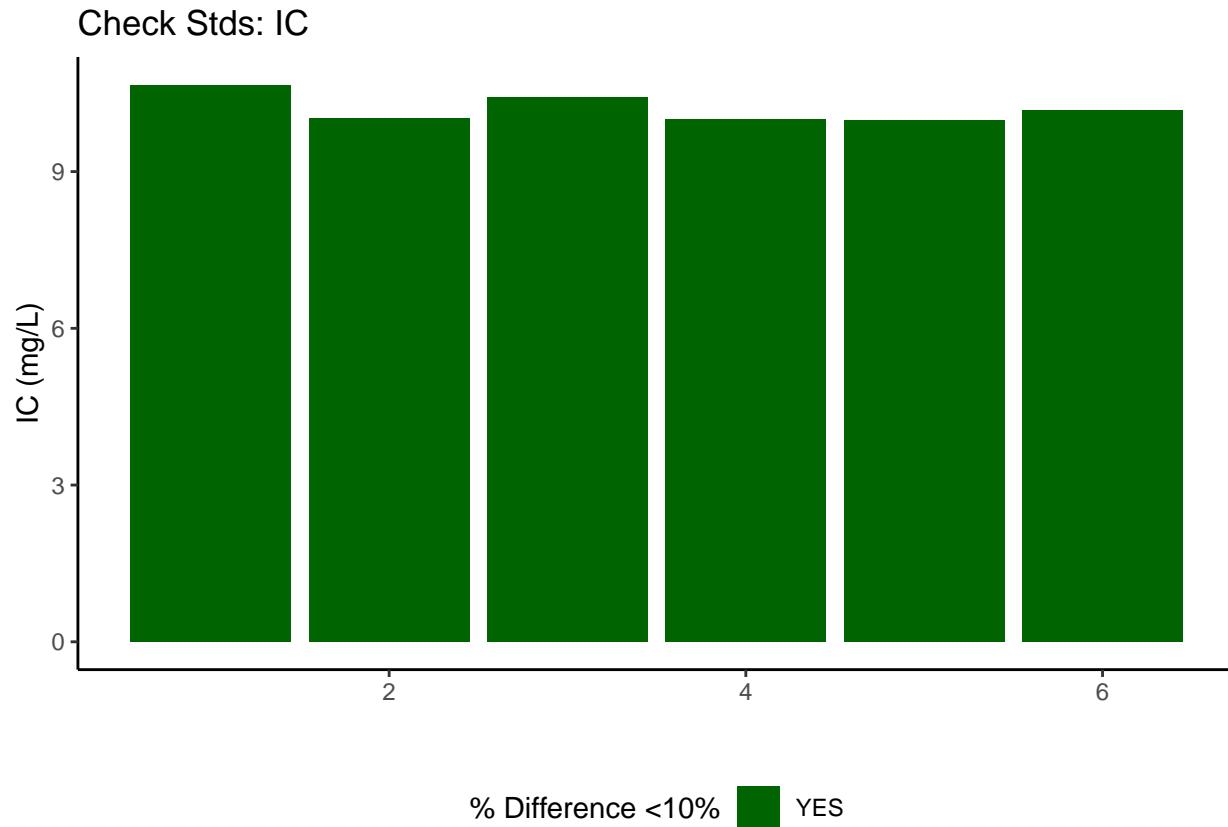
0.5 Assess Check Standards

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

```

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

```

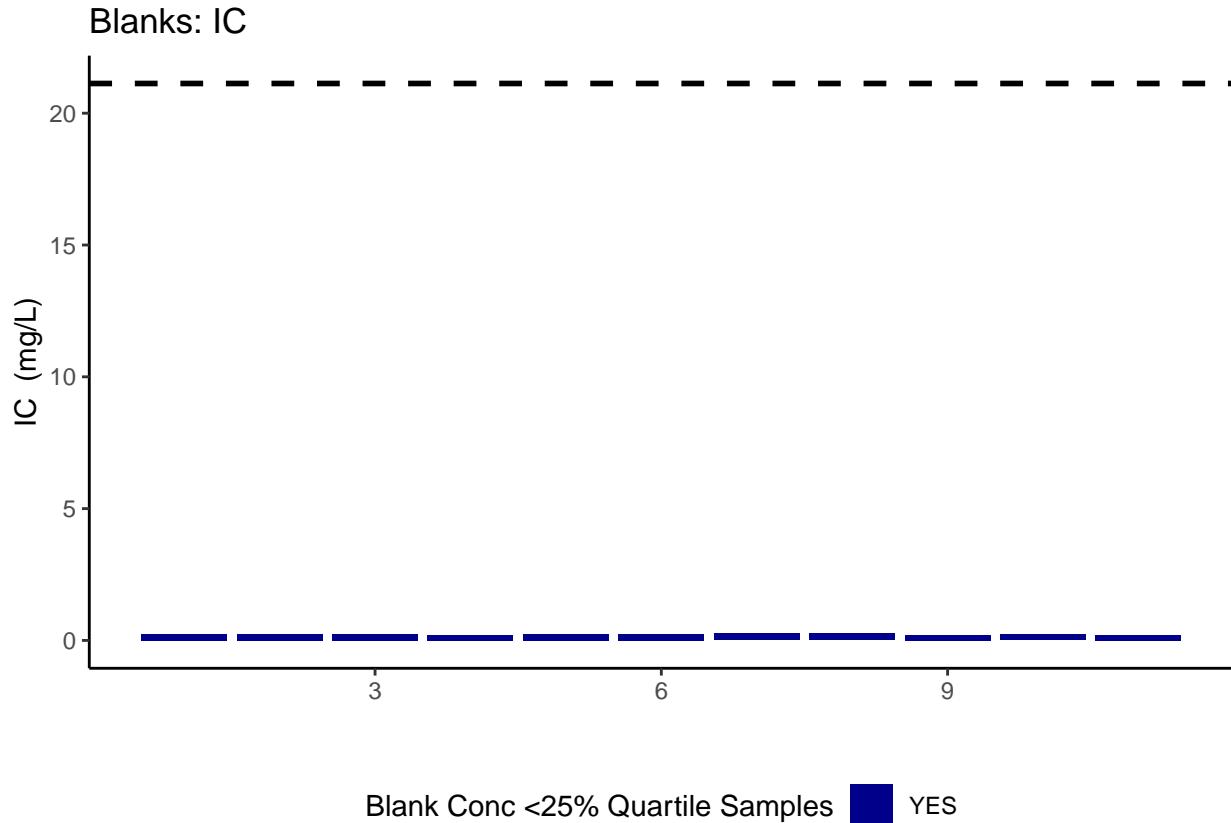


```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

```
## New names:  
## * ' ' -> '...14'  
  
## [1] ">60% of Carbon Blank concentrations are lower 25% quartile of samples"
```



```
## carbon blanks:
```

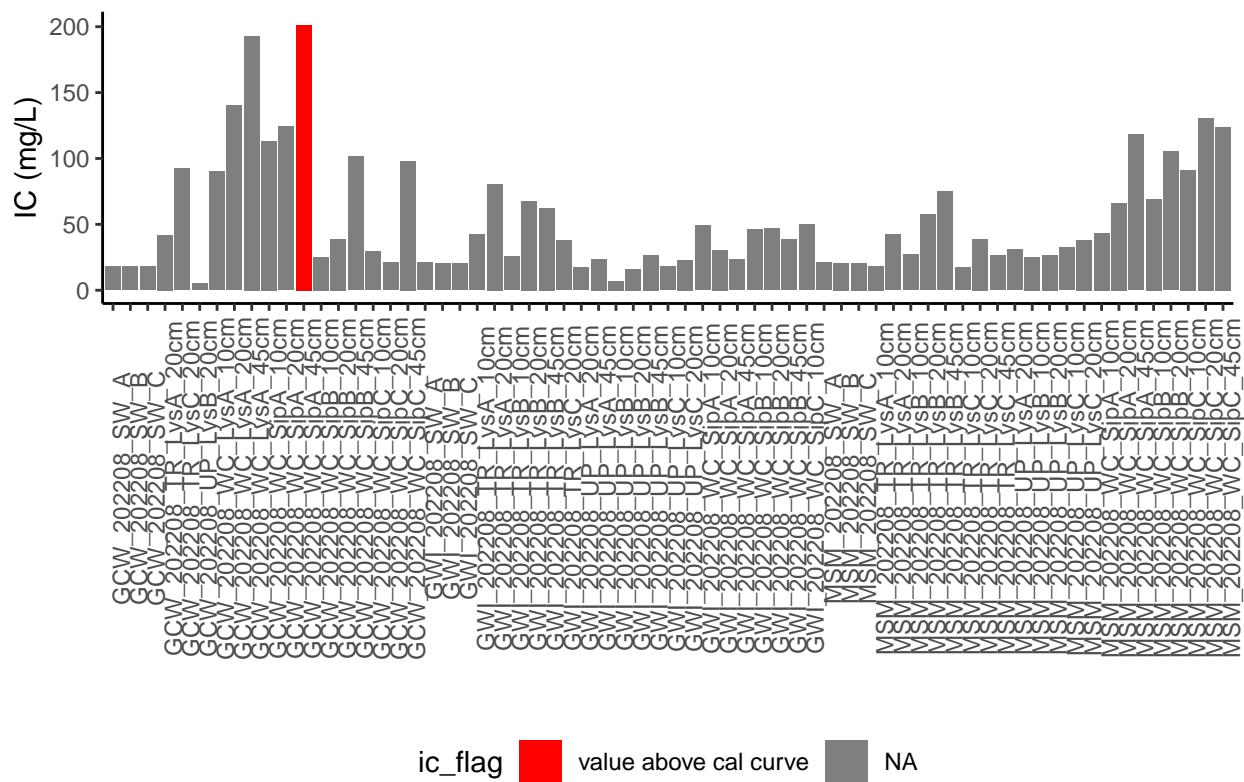
```
## [1] 0.2358818
```

0.7 Assess Duplicates - no duplicates included on this run

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

```
## Sample Flagging
```

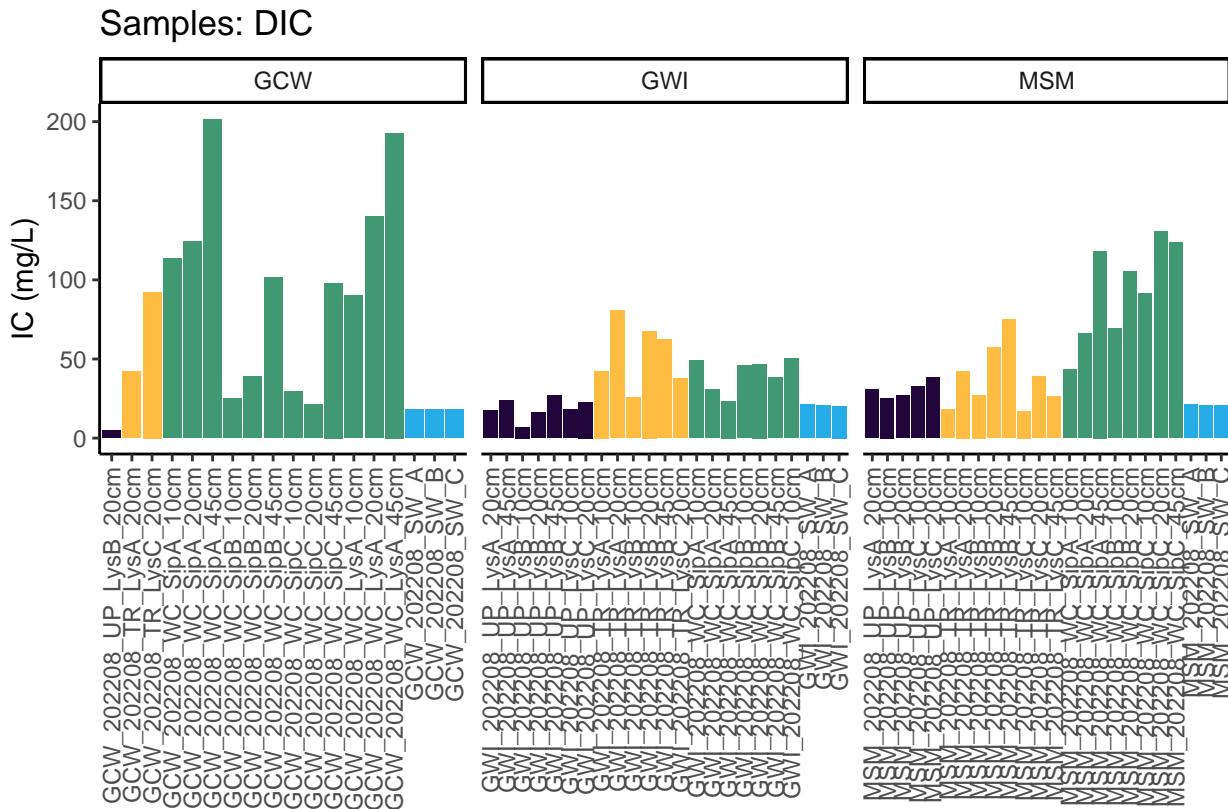
C: Grey = Within Range of Curve



0.9 Visualize Data by Plot

```
## Visualize Data

## Warning in rbind(c("GCW", "202208", "UP", "LysB", "20cm"), c("GCW", "202208", :
## number of columns of result is not a multiple of vector length (arg 16)
```



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] "GCW_202208_WC_SipA_10cm" "GCW_202208_WC_SipA_20cm"
## [3] "GCW_202208_WC_SipA_45cm" "GCW_202208_WC_SipB_10cm"
## [5] "GCW_202208_WC_SipB_20cm" "GCW_202208_WC_SipB_45cm"
## [7] "GCW_202208_WC_SipC_10cm" "GCW_202208_WC_SipC_20cm"
## [9] "GCW_202208_WC_SipC_45cm" "GWI_202208_WC_SipA_10cm"
## [11] "GWI_202208_WC_SipA_20cm" "GWI_202208_WC_SipA_45cm"
## [13] "GWI_202208_WC_SipB_10cm" "GWI_202208_WC_SipB_20cm"
## [15] "GWI_202208_WC_SipB_45cm" "GWI_202208_WC_SipC_10cm"
## [17] "MSM_202208_WC_SipA_10cm" "MSM_202208_WC_SipA_20cm"
## [19] "MSM_202208_WC_SipA_45cm" "MSM_202208_WC_SipB_10cm"
## [21] "MSM_202208_WC_SipB_20cm" "MSM_202208_WC_SipC_10cm"
## [23] "MSM_202208_WC_SipC_20cm" "MSM_202208_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     GCW    UP     B          20  GCW_2022~ 2022     8    15
## 2 COMPASS: Sy~ CB     GWI    UP     A          20  GWI_2022~ 2022     8    18
## 3 COMPASS: Sy~ CB     GWI    UP     A          45  GWI_2022~ 2022     8    18
## 4 COMPASS: Sy~ CB     GWI    UP     B          10  GWI_2022~ 2022     8    18
## 5 COMPASS: Sy~ CB     GWI    UP     B          20  GWI_2022~ 2022     8    18
## 6 COMPASS: Sy~ CB     GWI    UP     B          45  GWI_2022~ 2022     8    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
```