

Synoptic CB: Porewater DIC

September 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 = "09/20/22" #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_202209.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_202209.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 MSM_202209_UP_LysA_20cm 21.8 9/20/2022 6:16:02 PM
## 2 MSM_202209_UP_LysB_10cm 19.2 9/20/2022 6:30:09 PM
## 3 MSM_202209_UP_LysC_10cm 21.6 9/20/2022 6:44:16 PM
## 4 MSM_202209_UP_LysC_20cm 34.4 9/20/2022 6:58:51 PM
## 5 MSM_202209_TR_LysA_10cm 62.6 9/20/2022 7:20:49 PM
## 6 MSM_202209_TR_LysA_20cm 39.6 9/20/2022 7:40:07 PM

```

0.3 Assessing Standard Curves - done manually on the instrument

0.4 CRM Check - No CRMs included on this run

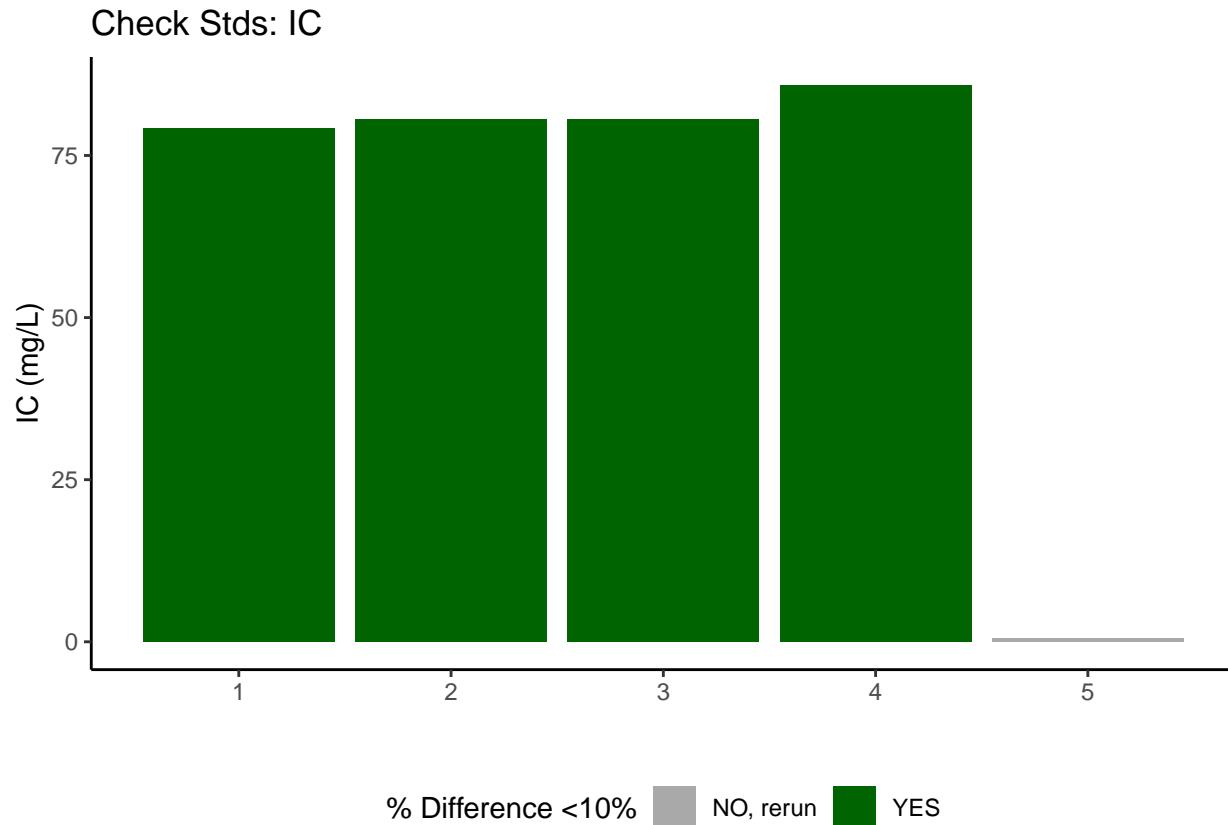
0.5 Assess Check Standards

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

```

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

```

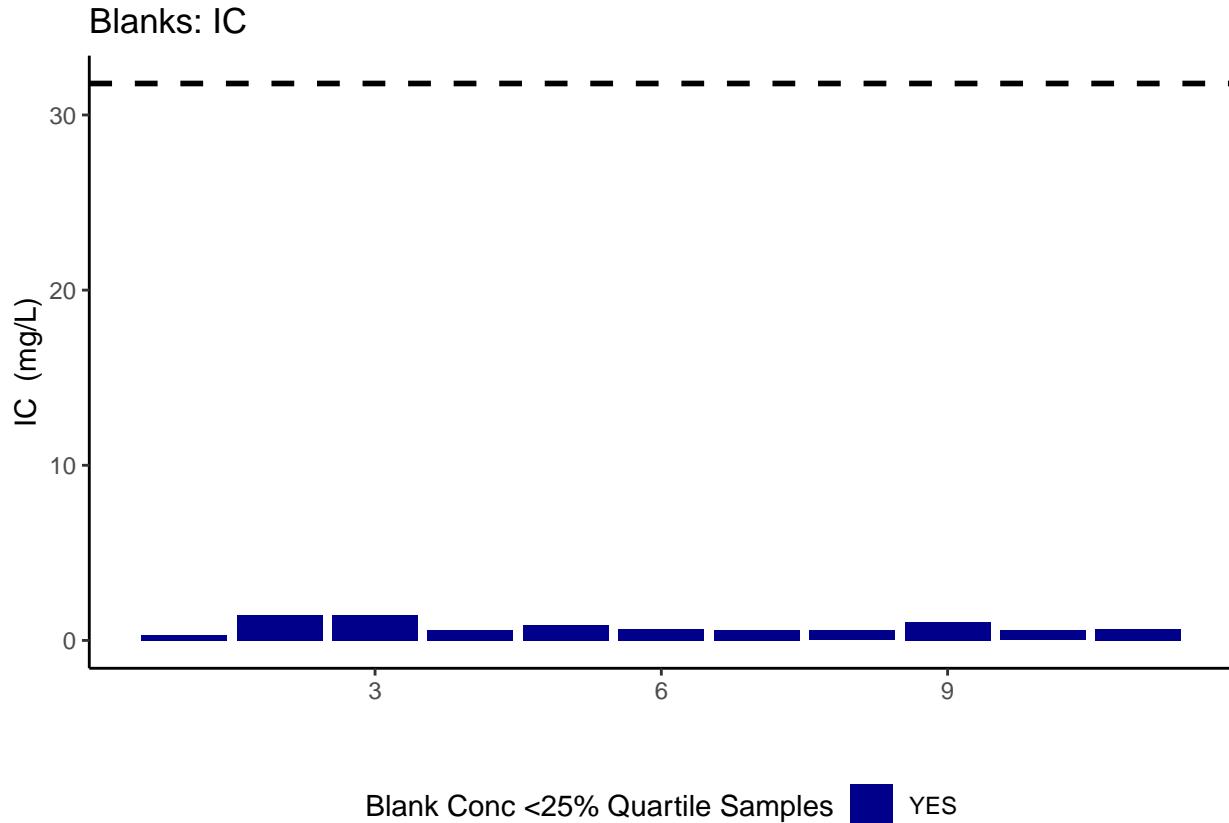


```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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



```
## carbon blanks:
```

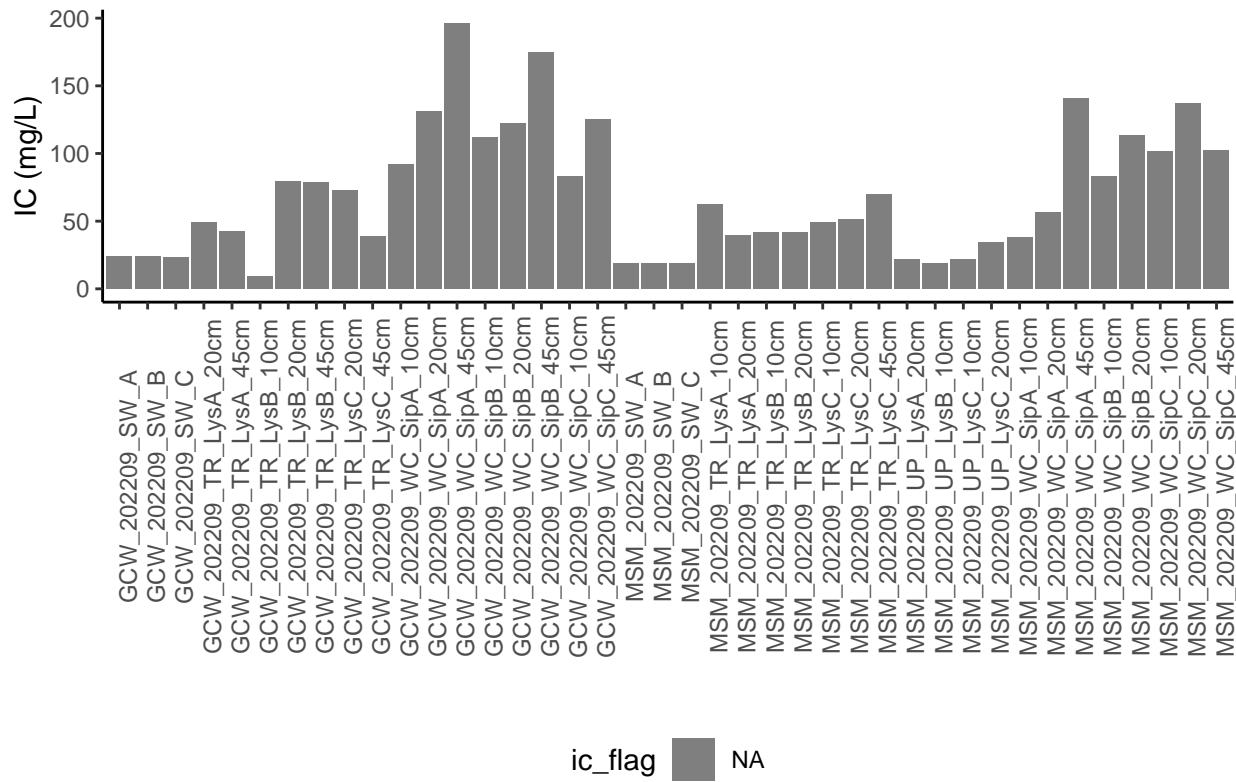
```
## [1] 0.7952091
```

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

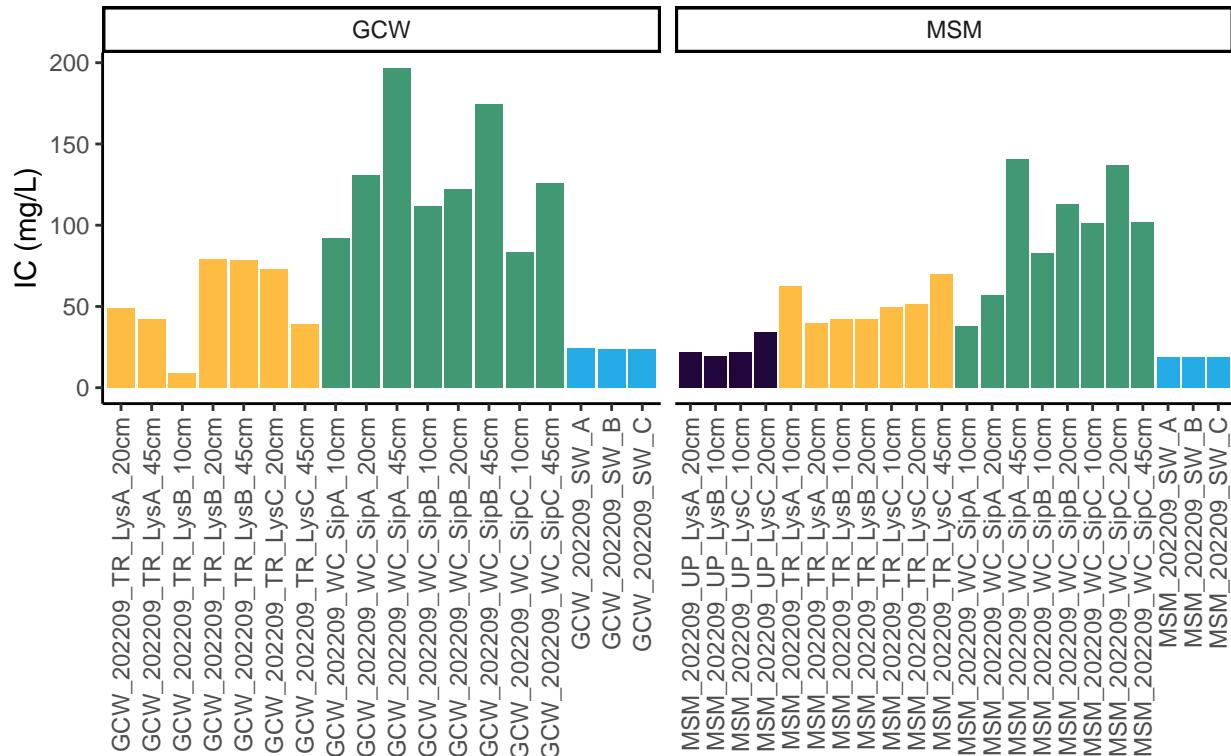


0.9 Visualize Data by Plot

```
## Visualize Data
```

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

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
```

```
## Some sample IDs are missing from metadata.
```

```
## [1] "MSM_202209_WC_SipA_10cm" "MSM_202209_WC_SipA_20cm"
## [3] "MSM_202209_WC_SipA_45cm" "MSM_202209_WC_SipB_10cm"
## [5] "MSM_202209_WC_SipB_20cm" "MSM_202209_WC_SipC_10cm"
## [7] "MSM_202209_WC_SipC_20cm" "MSM_202209_WC_SipC_45cm"
## [9] "GCW_202209_WC_SipA_10cm" "GCW_202209_WC_SipA_20cm"
## [11] "GCW_202209_WC_SipA_45cm" "GCW_202209_WC_SipB_10cm"
## [13] "GCW_202209_WC_SipB_20cm" "GCW_202209_WC_SipB_45cm"
## [15] "GCW_202209_WC_SipC_10cm" "GCW_202209_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    MSM    UP     A          20 MSM_2022~ 2022     9     18
## 2 COMPASS: Sy~ CB    MSM    UP     B          10 MSM_2022~ 2022     9     18
## 3 COMPASS: Sy~ CB    MSM    UP     C          10 MSM_2022~ 2022     9     18
## 4 COMPASS: Sy~ CB    MSM    UP     C          20 MSM_2022~ 2022     9     18
## 5 COMPASS: Sy~ CB    MSM    TR     A          10 MSM_2022~ 2022     9     18
## 6 COMPASS: Sy~ CB    MSM    TR     A          20 MSM_2022~ 2022     9     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
```