

Synoptic CB: Porewater DIC

November 2023 Samples

2025-10-25

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```

##Setup - Change things here & write any notes

#identify section
cat("Setup Information")

## Setup Information

##### Run information - PLEASE CHANGE
Date_Run = "11/10/23" #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_202311.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_202311.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'

## Warning: One or more parsing issues, call 'problems()' on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

```

```

## # A tibble: 6 x 3
##   sample_name          ic_raw run_datetime
##   <chr>                <dbl> <chr>
## 1 202311_MSM_UP_LysB_10cm 13.1  11/10/2023 7:14:33 PM
## 2 202311_MSM_UP_LysC_10cm  9.71  11/10/2023 7:30:11 PM
## 3 202311_MSM_UP_LysC_20cm 17.0   11/10/2023 7:43:55 PM
## 4 202311_MSM_TR_LysA_10cm 12.5   11/10/2023 7:59:53 PM
## 5 202311_MSM_TR_LysA_20cm 41.4   11/10/2023 8:17:28 PM
## 6 202311_MSM_TR_LysB_10cm 27.2   11/10/2023 8:31:25 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‘

## Warning: One or more parsing issues, call ‘problems()’ on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

## [1] NA

## Run mean = NaN

## Expected = 22.19

```

0.5 Assess Check Standards

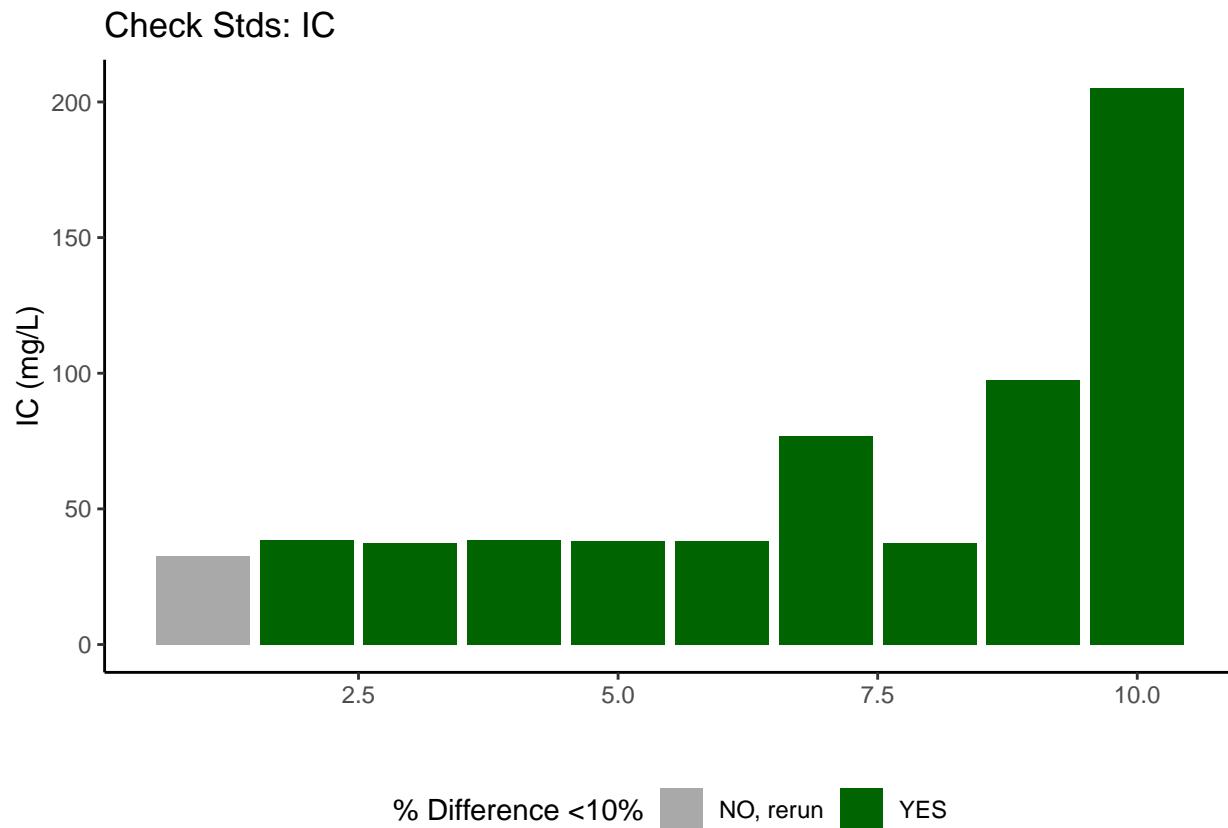
```

## Assess the Check Standards

## New names:
## * ‘‘ → ‘...14‘

## Warning: One or more parsing issues, call ‘problems()’ on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

```



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

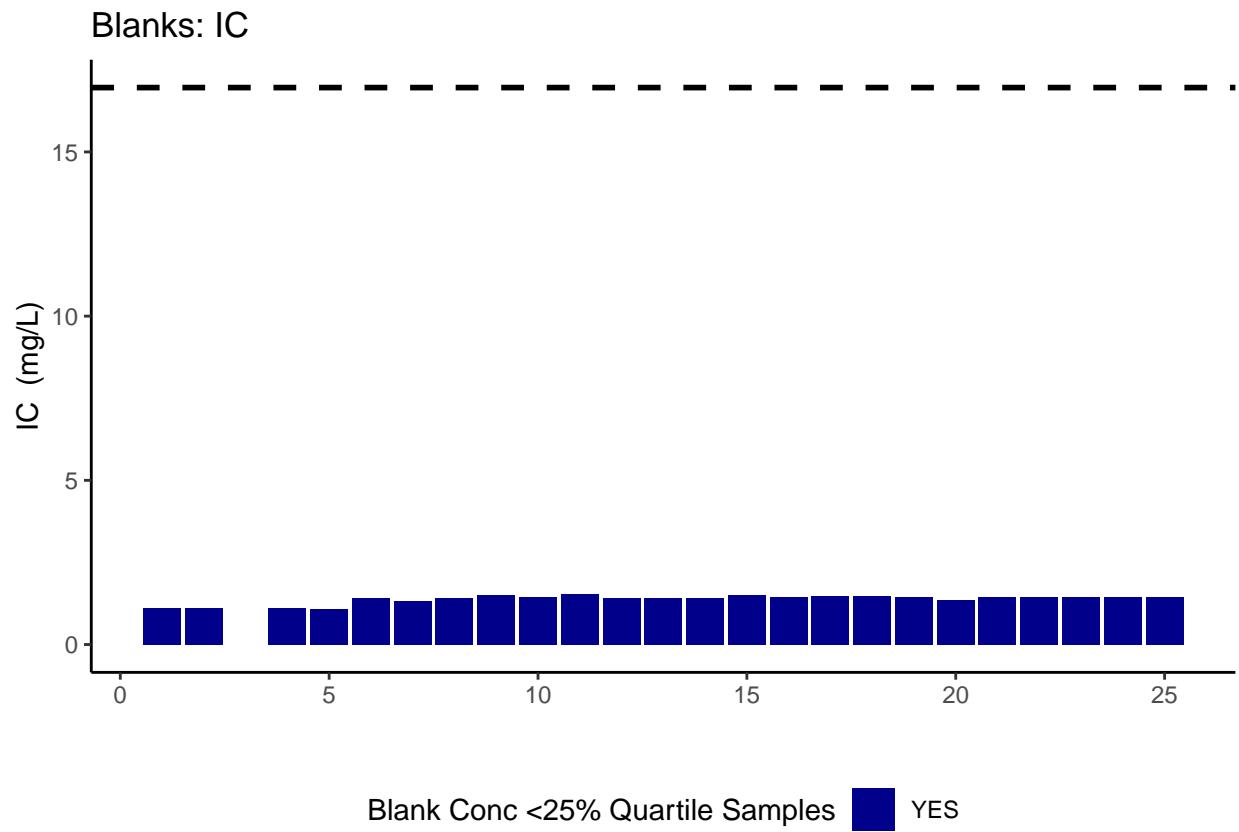
0.6 Assess Blanks

```
## Assess Blanks

## New names:
## * ‘‘ -> ‘...14‘

## Warning: One or more parsing issues, call ‘problems()’ on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)

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

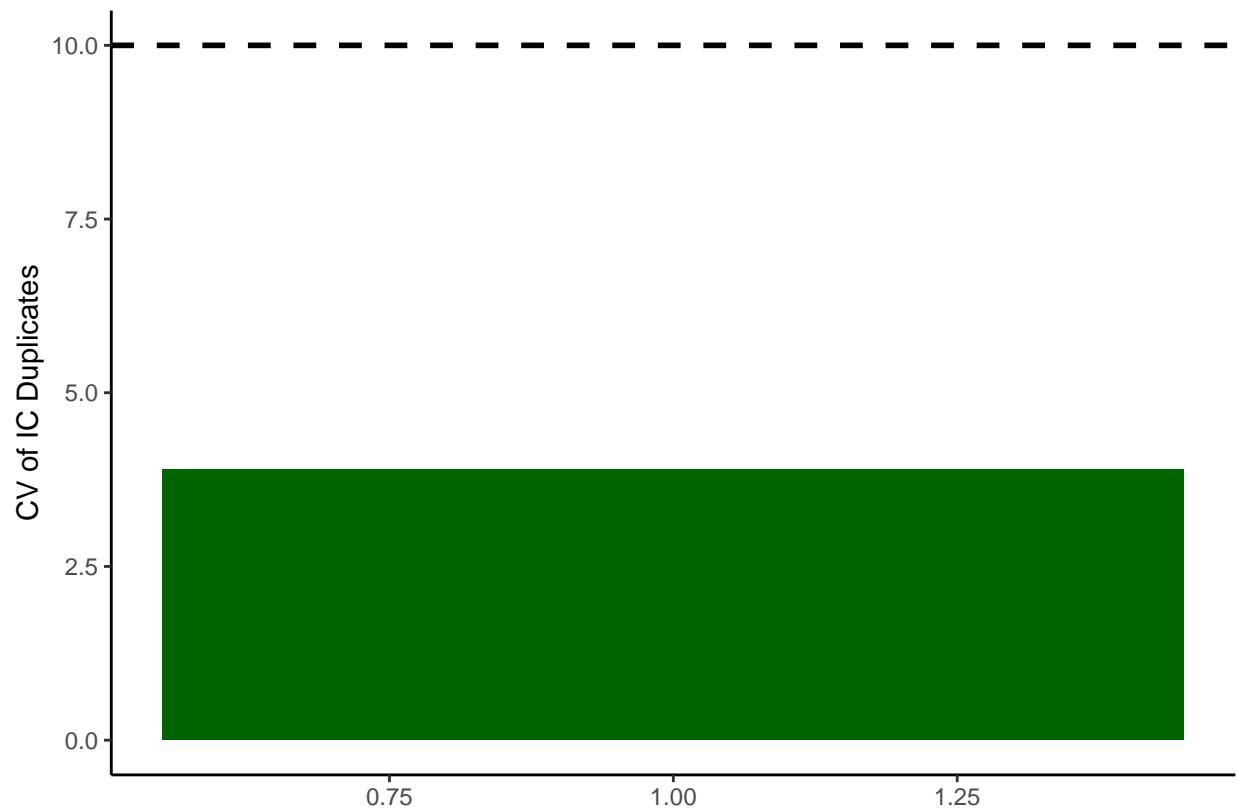


```
## carbon blanks:
```

```
## [1] 1.384792
```

0.7 Assess Duplicates

```
## Assess Duplicates
```

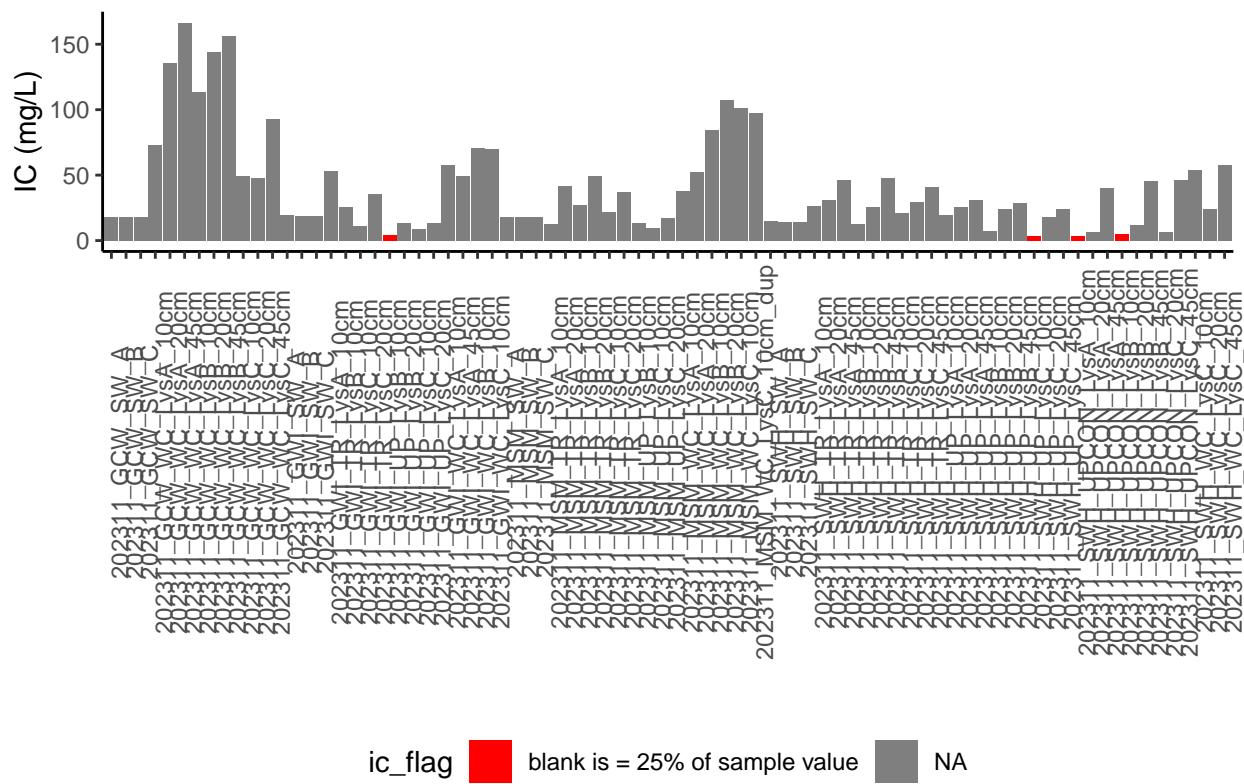


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

```
## Sample Flagging
```

C: Grey = Within Range of Curve

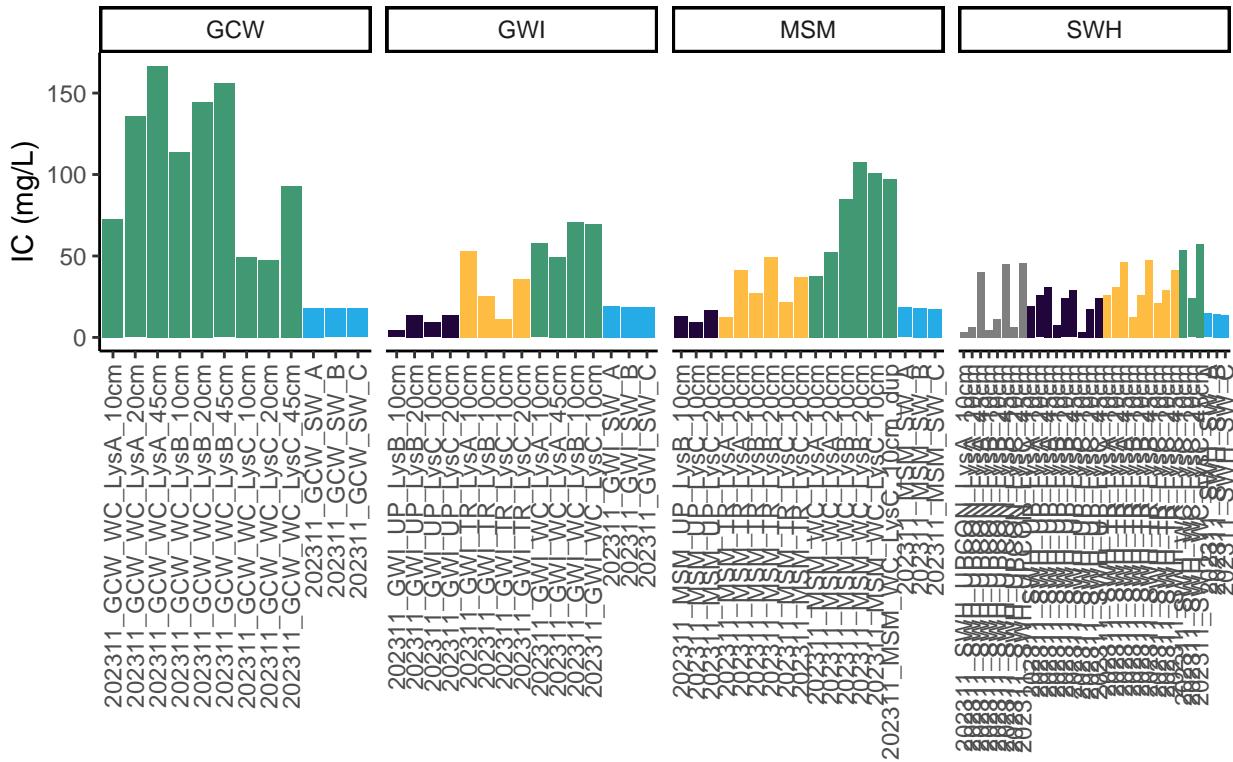


0.9 Visualize Data by Plot

```
## Visualize Data

## Warning in rbind(c("202311", "MSM", "UP", "LysB", "10cm"), c("202311", "MSM", :
## 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 202311_S~ 2023   11    8
## 2 COMPASS: Sy~ CB    SWH    UPCON A          20 202311_S~ 2023   11    8
## 3 COMPASS: Sy~ CB    SWH    UPCON A          45 202311_S~ 2023   11    8
## 4 COMPASS: Sy~ CB    SWH    UPCON B          10 202311_S~ 2023   11    8
## 5 COMPASS: Sy~ CB    SWH    UPCON B          20 202311_S~ 2023   11    8
## 6 COMPASS: Sy~ CB    SWH    UPCON B          45 202311_S~ 2023   11    8
## # 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
```