

# Synoptic CB: Porewater DIC

June 2023 Samples

2025-10-22

## Contents

0.1	Import Data Functions . . . . .	2
0.2	Import Sample Data . . . . .	2
0.3	Assessing Standard Curves - assessed on the instrument manually . . . . .	3
0.4	CRM Check - no CRMs included on this run . . . . .	3
0.5	Assess Check Standards . . . . .	3
0.6	Assess Blanks . . . . .	3
0.7	Assess Duplicates . . . . .	4
0.8	Sample Flagging - Are samples Within the range of the curve? . . . . .	5
0.9	Visualize Data by Plot . . . . .	6
0.10	Convert data from mg/L to uMoles/L . . . . .	7
0.11	Check to see if samples run match metadata & merge info . . . . .	7
0.12	Export Processed Data . . . . .	7

```

##Setup - Change things here & write any notes

#identify section
cat("Setup Information")

## Setup Information

##### Run information - PLEASE CHANGE
Date_Run = "MM/DD/YY" #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 was checked manually on the instrument for this run. " #any notes if
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_202306.txt"

#file path and name for raw all peaks file
#raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202305_allpeaks.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202306.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_2023.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_202306_TR_LysA_20cm 54.8 7/26/2023 9:29:24 PM
## 2 GCW_202306_TR_LysA_45cm 13.7 7/26/2023 9:41:29 PM
## 3 GCW_202306_TR_LysB_10cm 33.4 7/26/2023 10:01:20 PM
## 4 GCW_202306_TR_LysB_20cm 42.3 7/26/2023 10:15:17 PM
## 5 GCW_202306_TR_LysB_dup 26.3 7/26/2023 10:28:21 PM
## 6 GCW_202306_TR_LysC_10cm 21.2 7/26/2023 10:47:30 PM

```

### 0.3 Assessing Standard Curves - assessed on the instrument manually

### 0.4 CRM Check - no CRMs included on this run

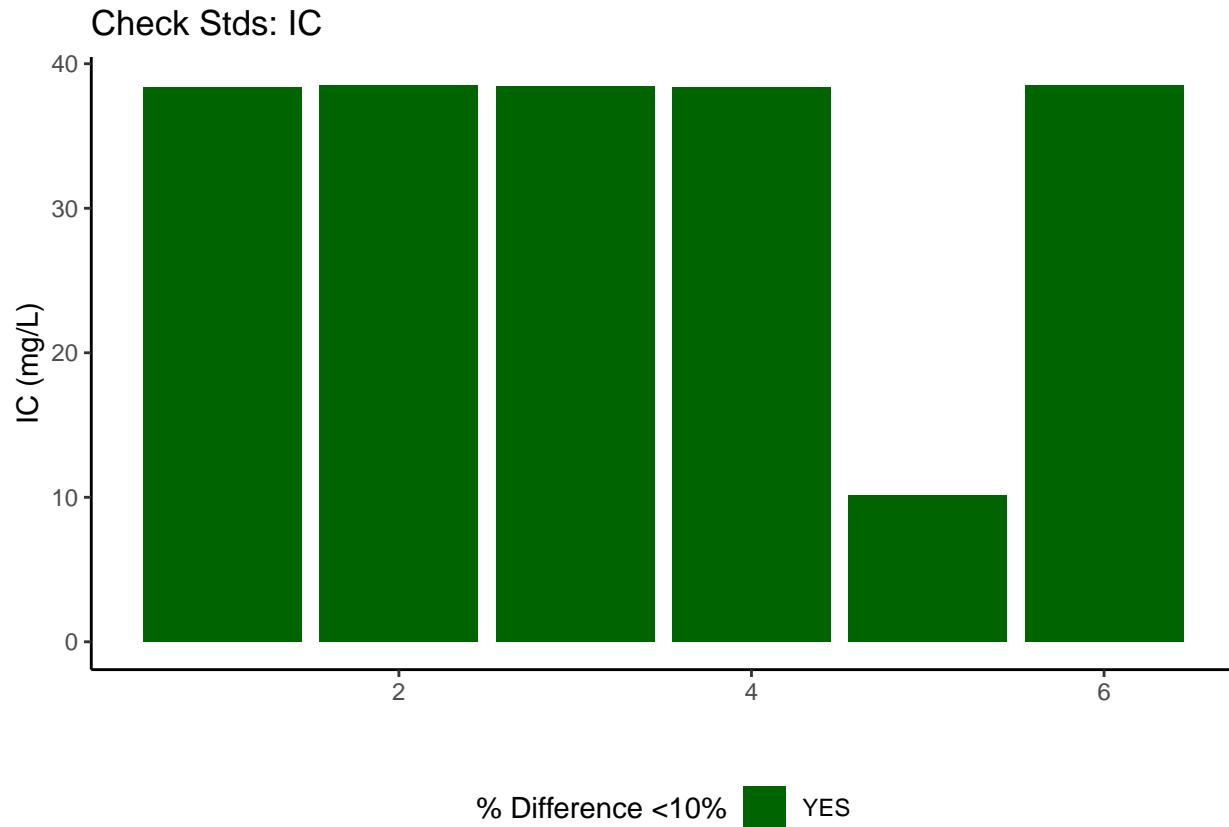
### 0.5 Assess Check Standards

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

```

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

```

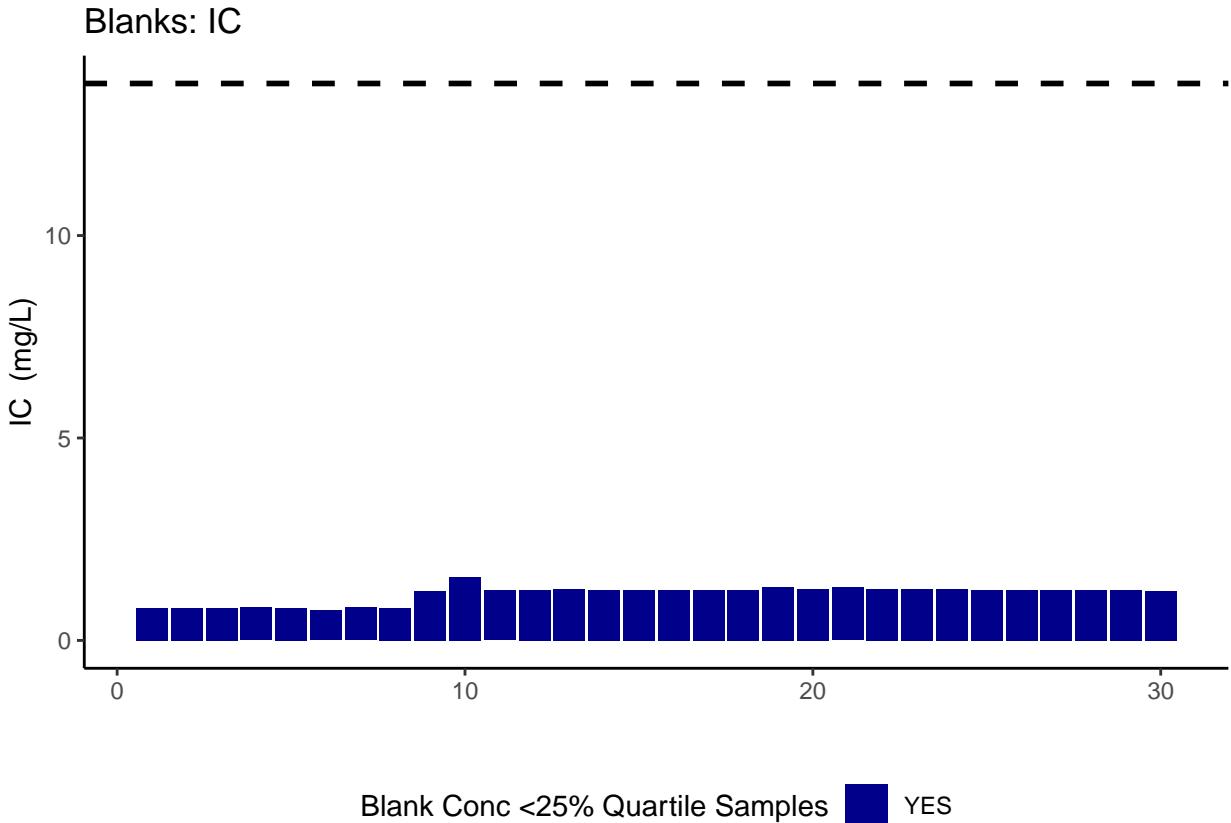


```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

### 0.6 Assess Blanks

```
## Assess Blanks
```

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

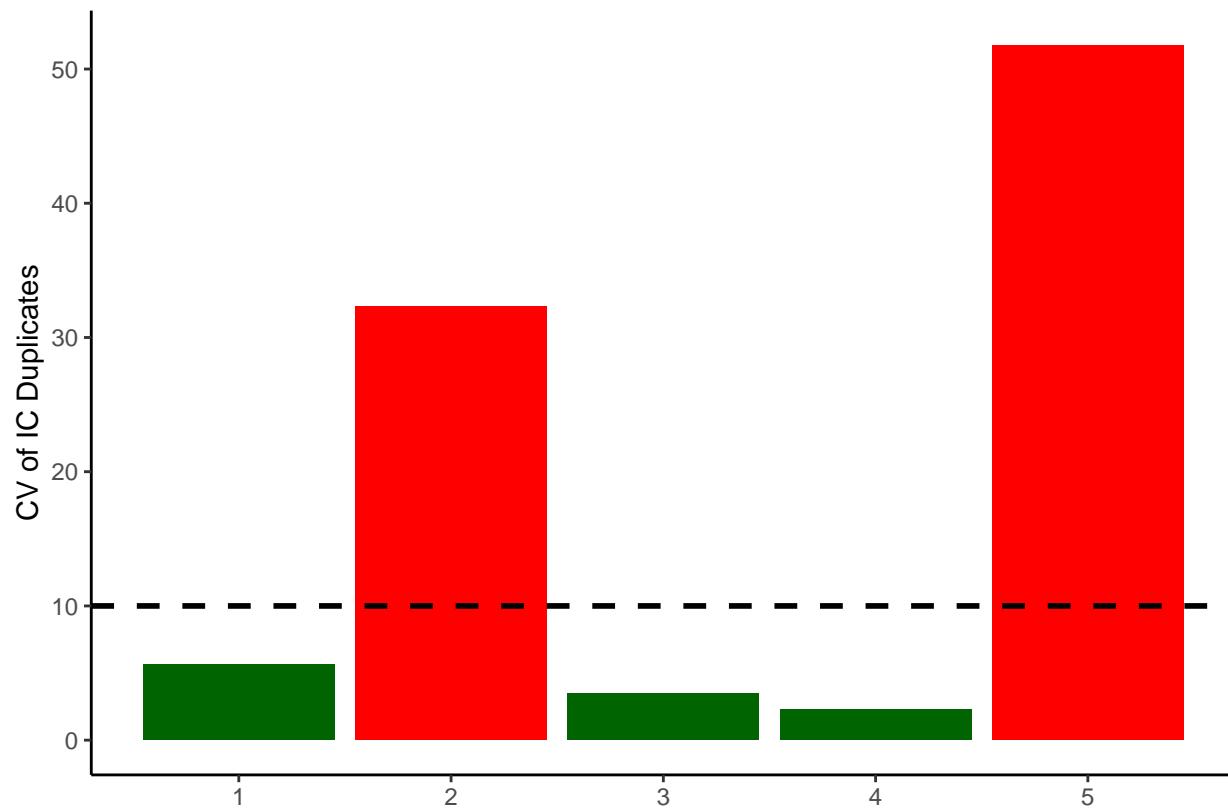


```
## carbon blanks:
```

```
## [1] 1.144543
```

## 0.7 Assess Duplicates

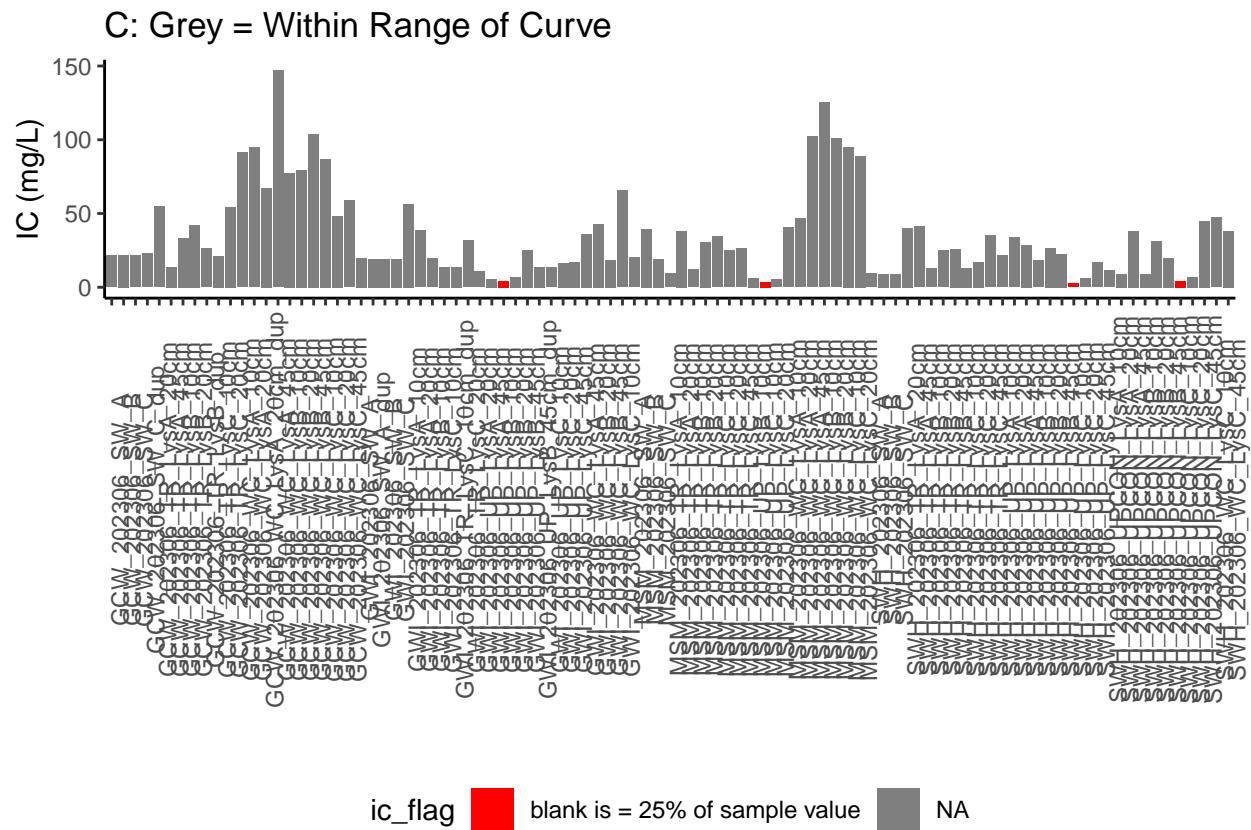
```
## Assess Duplicates
```



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

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

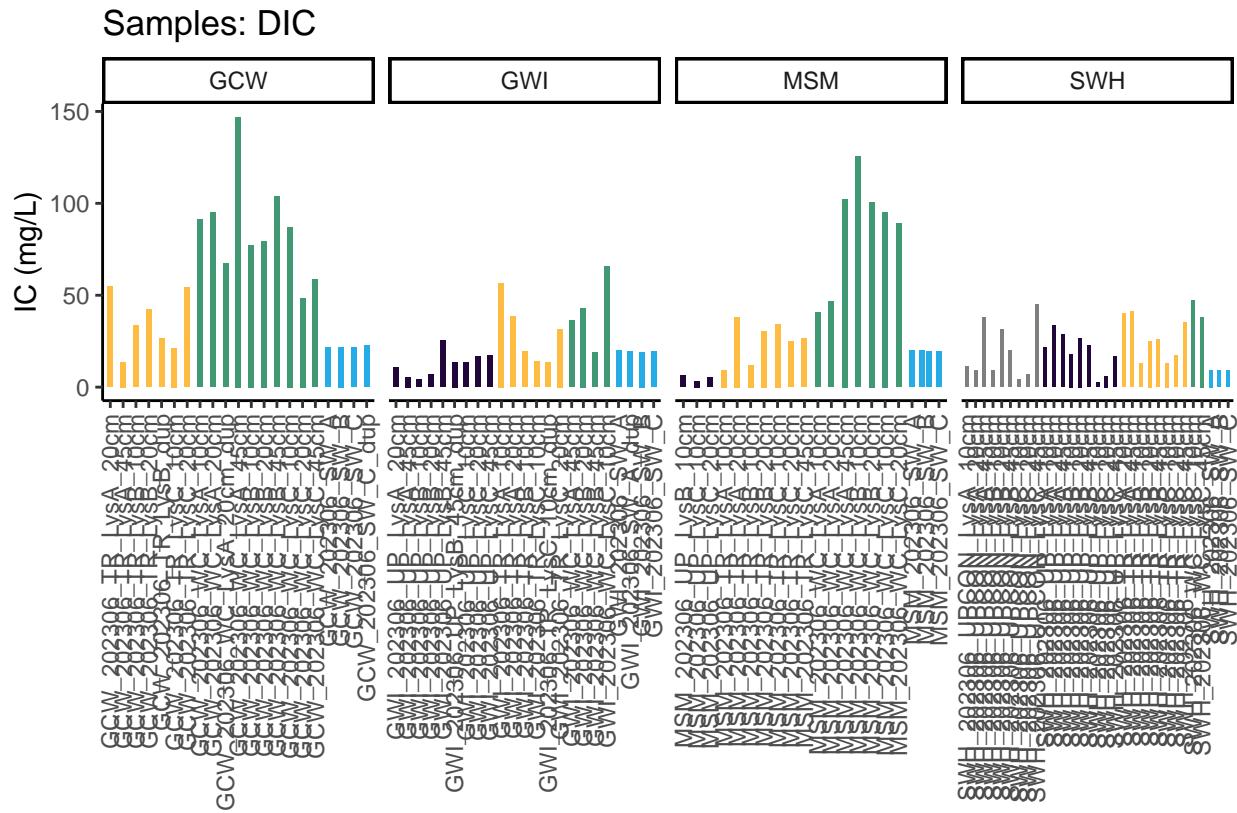
```
## Sample Flagging
```



## 0.9 Visualize Data by Plot

## ## Visualize Data

```
## Warning in rbind(c("GCW", "202306", "TR", "LysA", "20cm"), c("GCW", "202306", :  
## 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 SWH_2023~ 2023    6   21
## 2 COMPASS: Sy~ CB     SWH  UPCON A           20 SWH_2023~ 2023    6   21
## 3 COMPASS: Sy~ CB     SWH  UPCON A           45 SWH_2023~ 2023    6   21
## 4 COMPASS: Sy~ CB     SWH  UPCON B           10 SWH_2023~ 2023    6   21
## 5 COMPASS: Sy~ CB     SWH  UPCON B           20 SWH_2023~ 2023    6   21
## 6 COMPASS: Sy~ CB     SWH  UPCON B           45 SWH_2023~ 2023    6   21
## # 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
```