

# 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
```

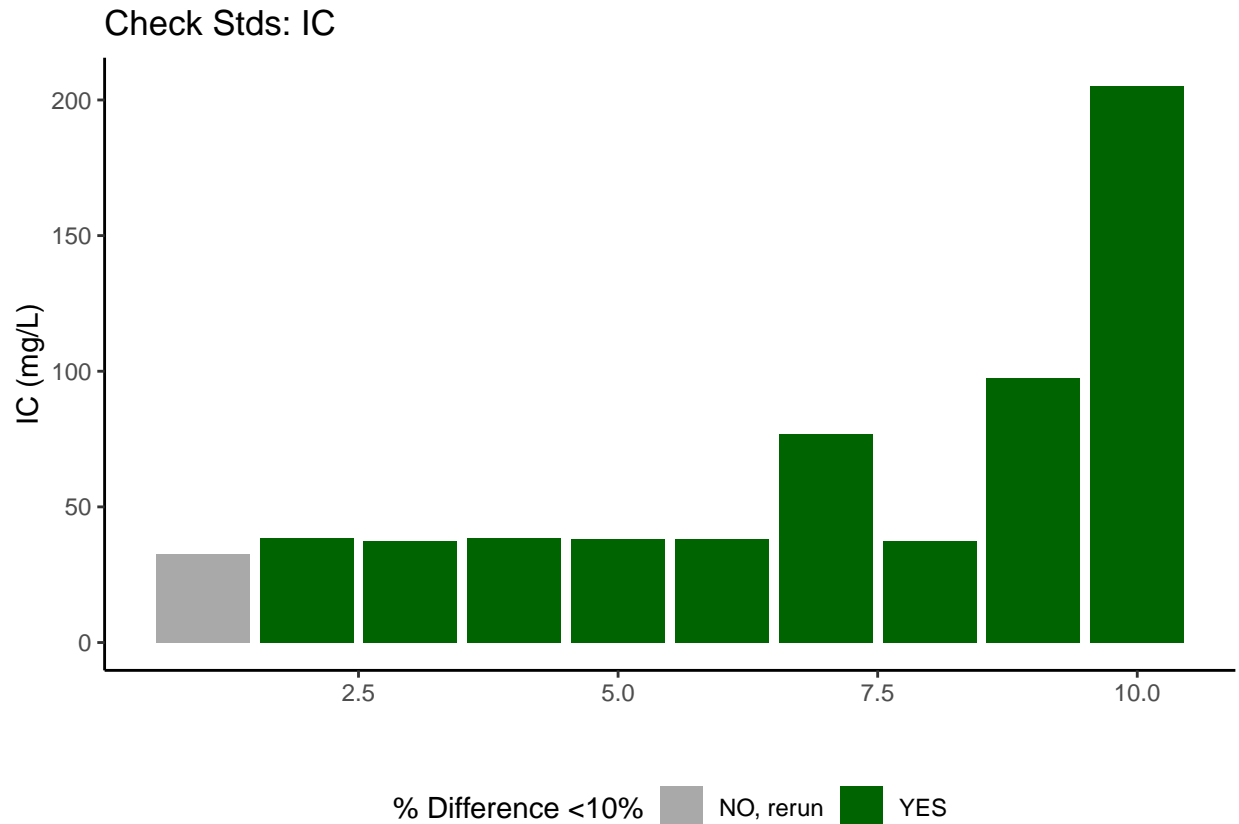
### 0.5 Assess Check Standards

```
## 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,
```

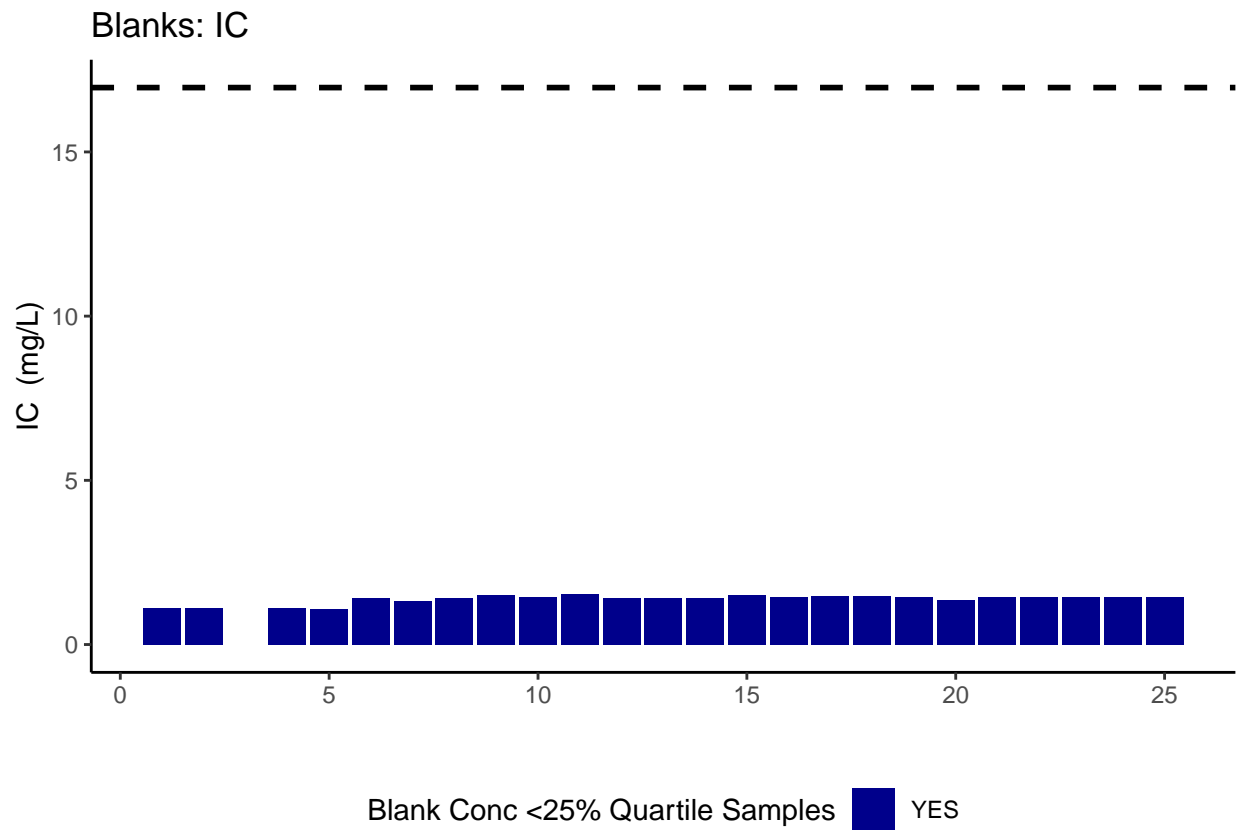
```
## e.g.:
```

```
##   dat <- vroom(...)
```

```
##   problems(dat)
```

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





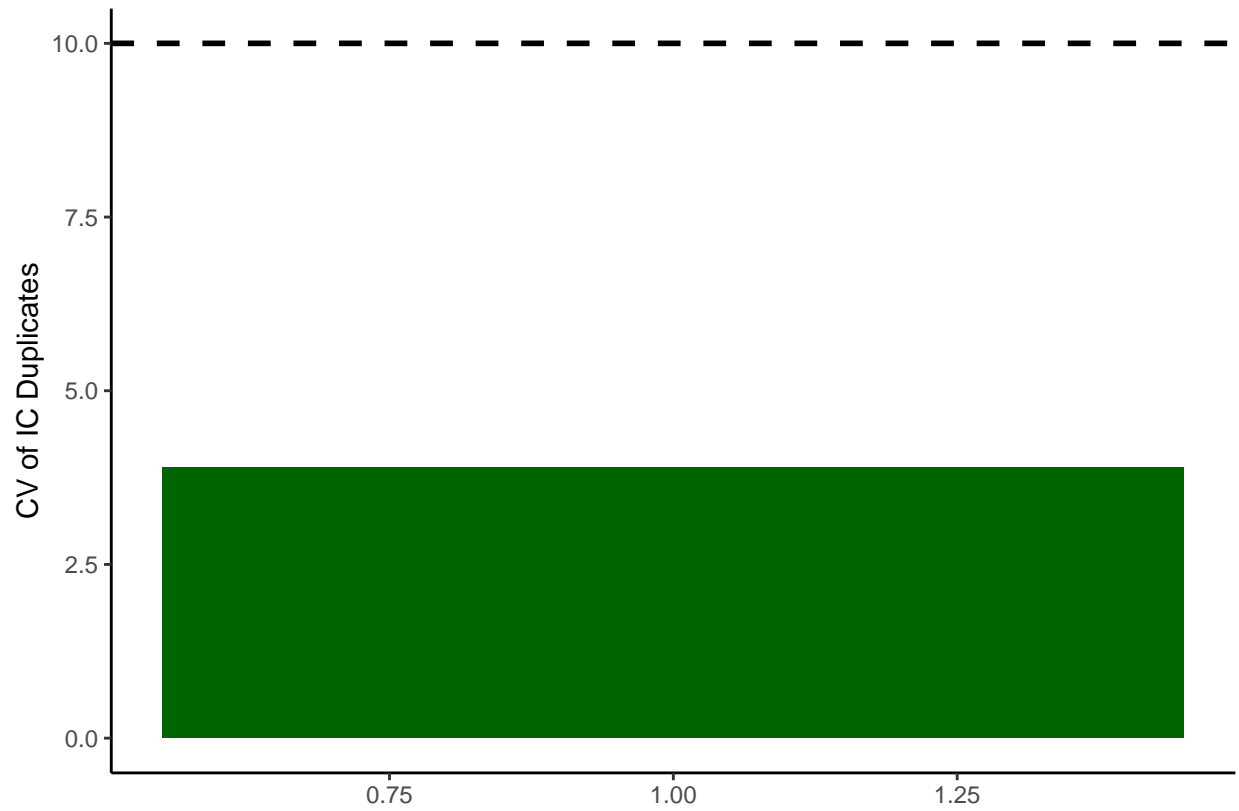
```
## carbon blanks:
```

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

## 0.7 Assess Duplicates

```
## Assess Duplicates
```





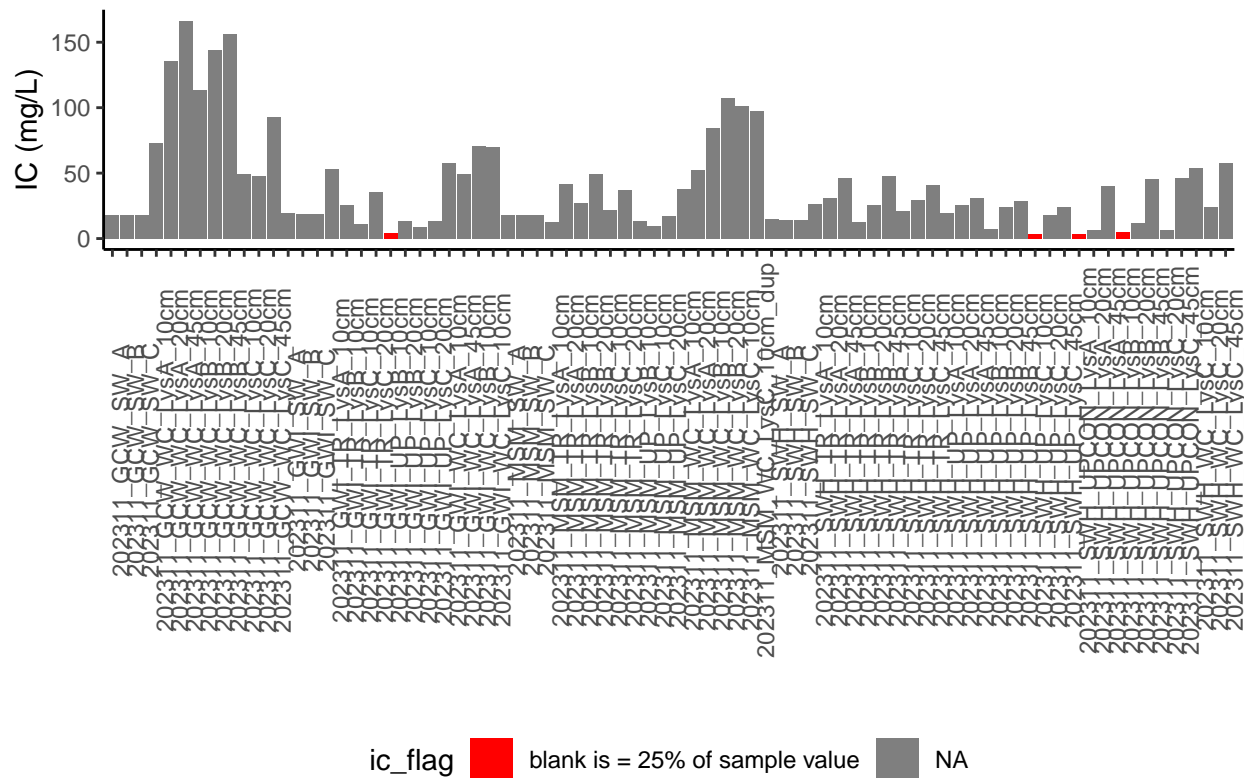
```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

## 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)
```



### 0.11 Check to see if samples run match metadata & merge info

```
## All sample IDs are present in metadata.
```

## ## Export Processed Data

#end