

Synoptic CB: Porewater DIC

June 2023 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 = "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 f  
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
```

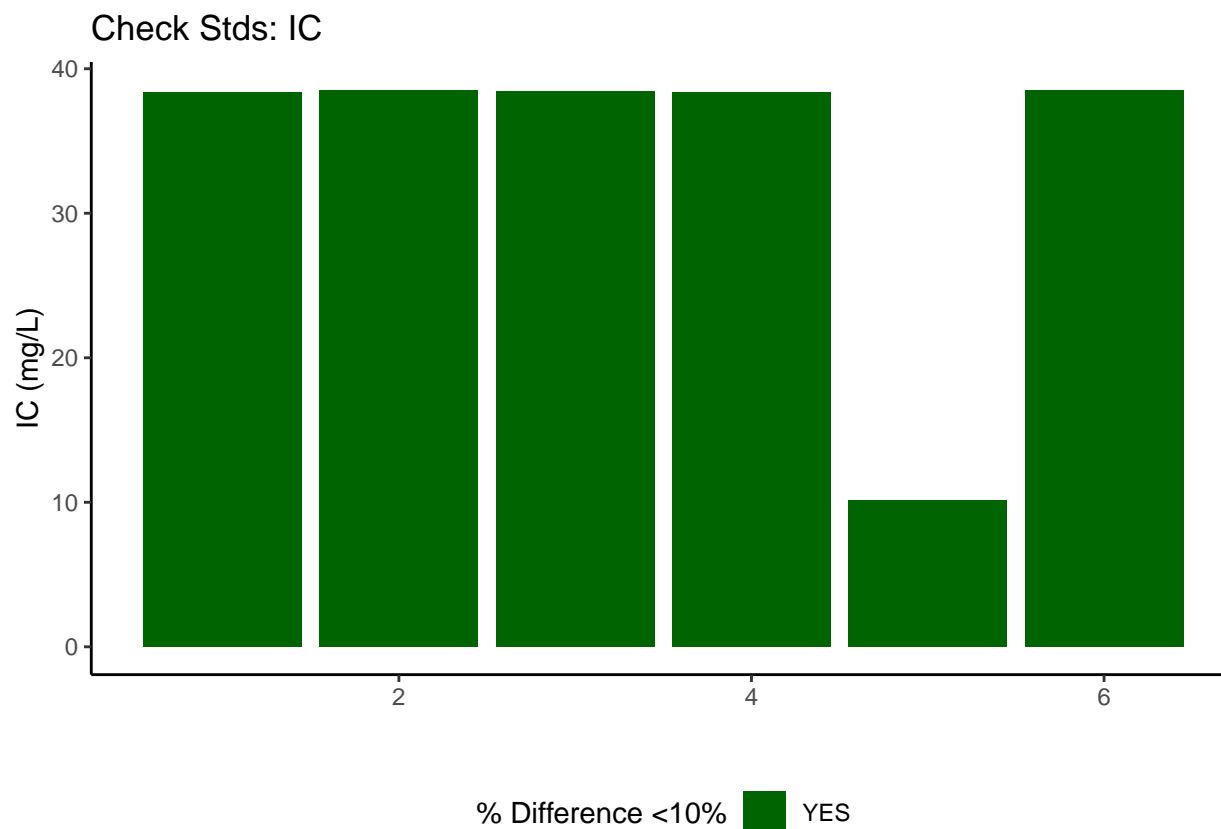
0.3 Assessing Standard Curves - assessed on the instrument manually

0.4 CRM Check - no CRMs included on this run

0.5 Assess Check Standards

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

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



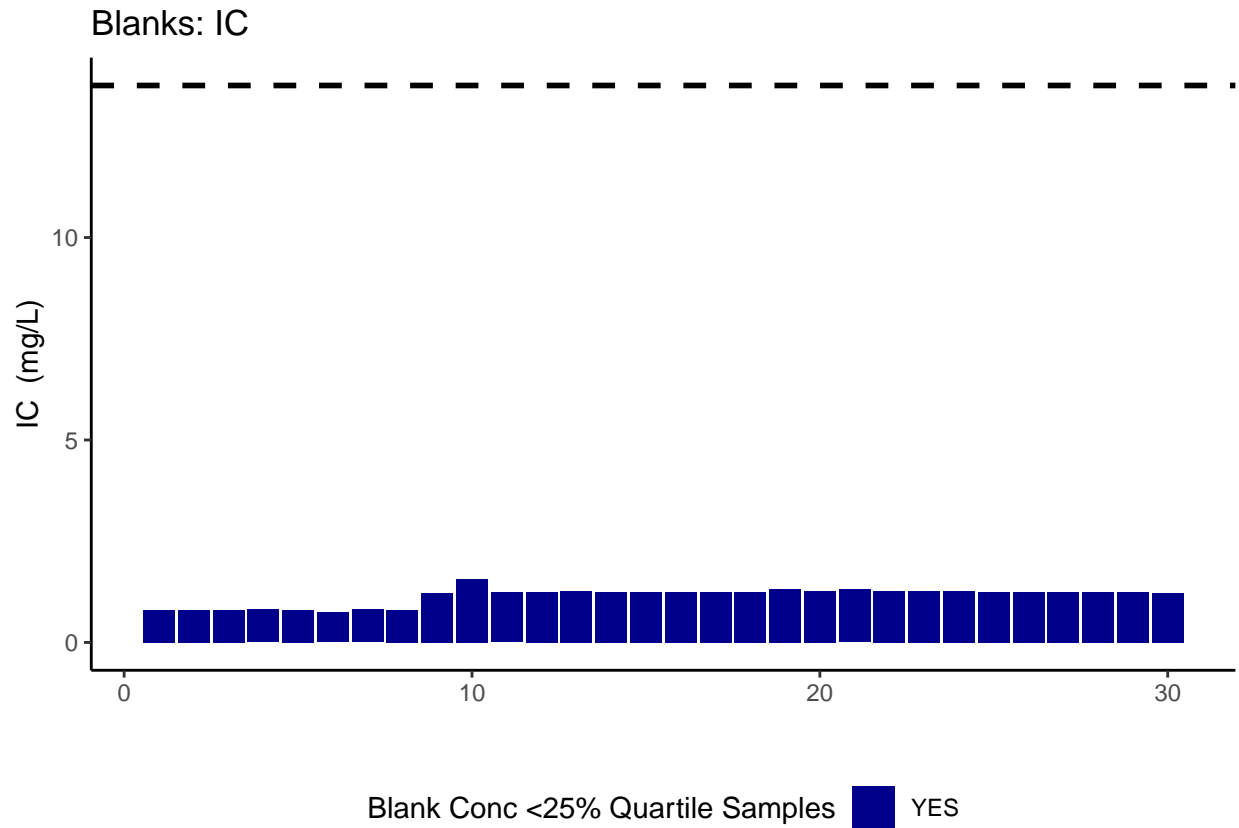
```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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

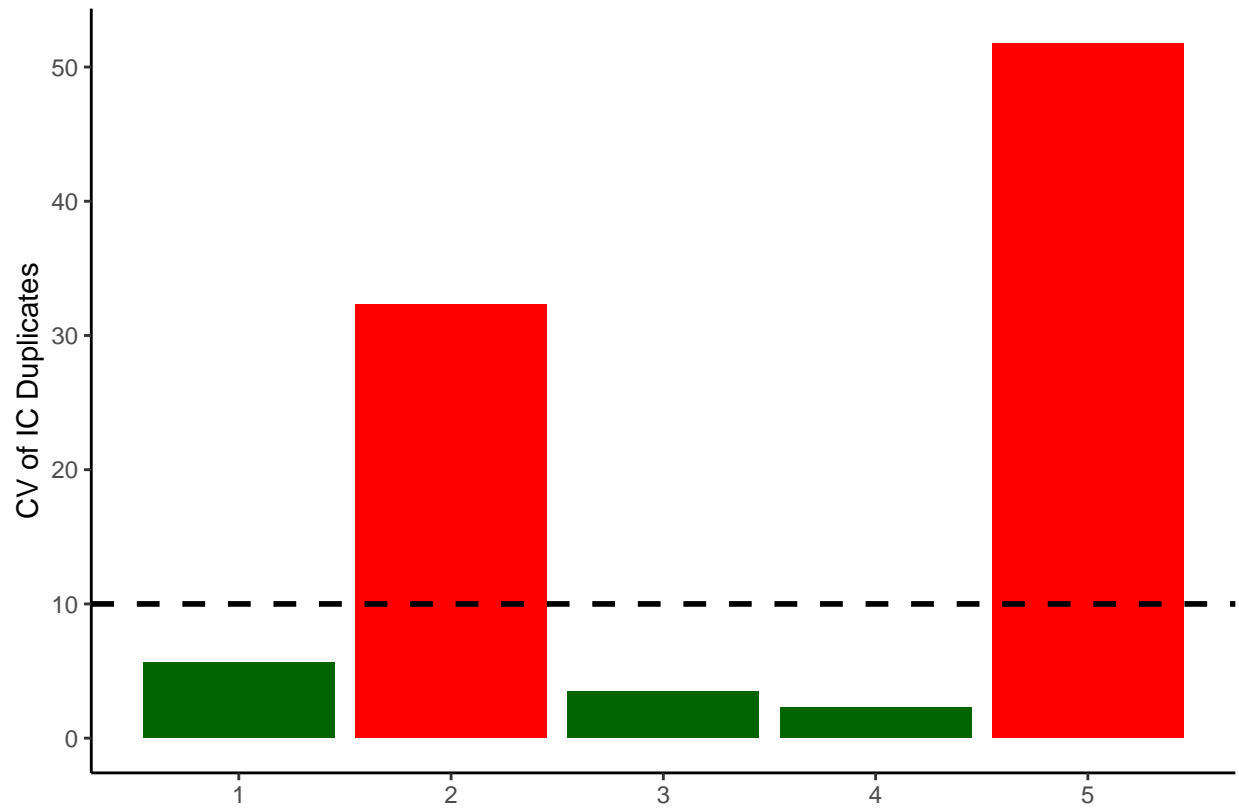


```
## carbon blanks:
```

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

0.7 Assess Duplicates

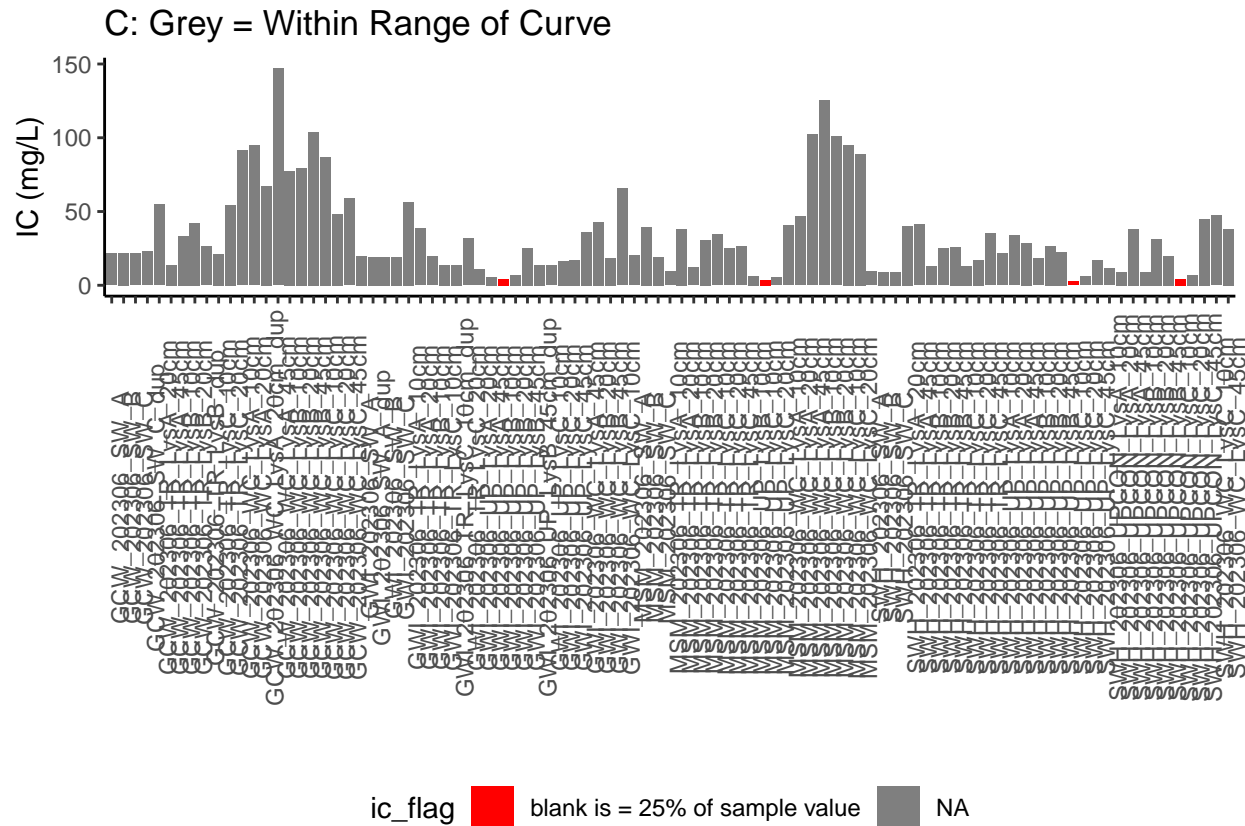
```
## Assess Duplicates
```



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

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

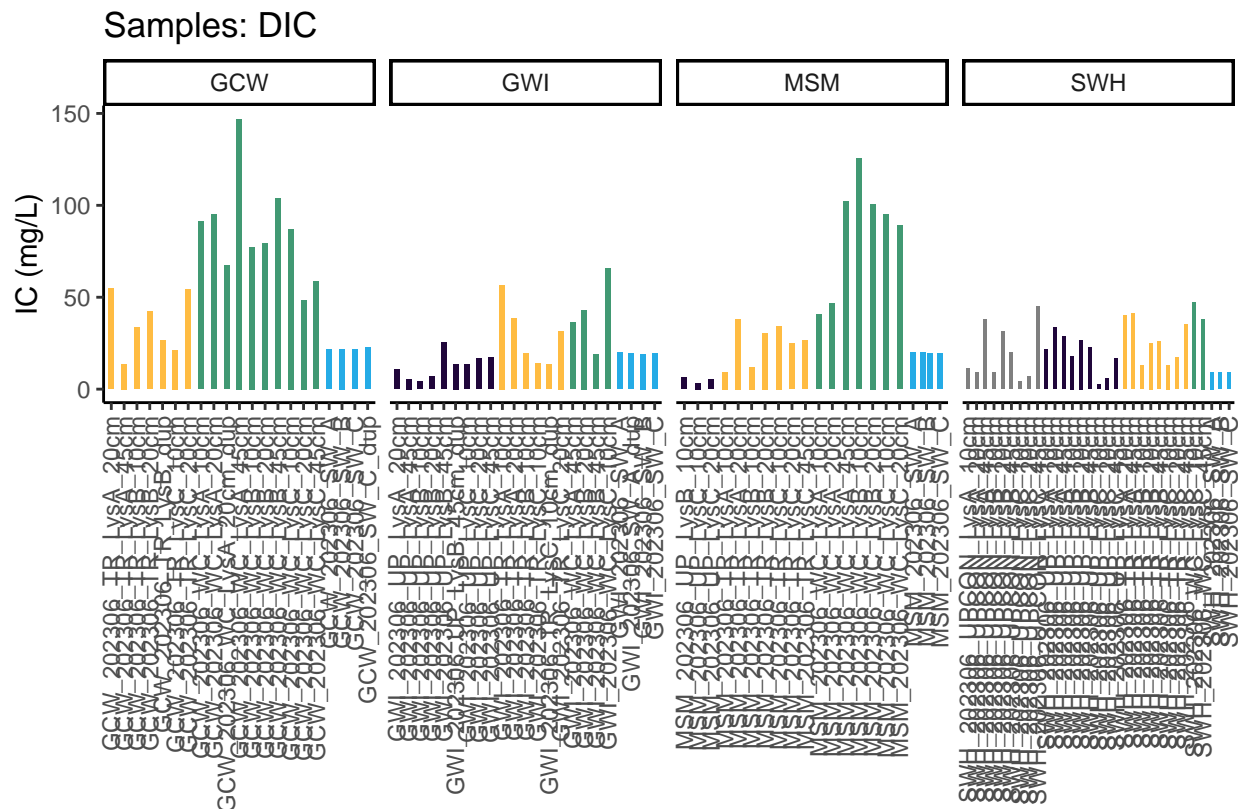
```
## Sample Flagging
```



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
```