

Synoptic CB: Porewater DIC

May 2023 Samples

2025-10-22

Contents

0.1	Import Data Functions	2
0.2	Import Sample Data	2
0.3	Assessing Standard Curves - this was done manually on the TOC, not included here	3
0.4	CRM Check - No CRMs 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 - in 2023 SWH Upland = UPCON and Swamp = UP	6
0.10	Convert data from mg/L to uMoles/L	7
0.11	Check to see if samples run match metadata & merge info - 2023 data needs entered	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 = "06/05/23" #Date that instrument was run
Run_by = "Instrument User" #Instrument user
Script_run_by = "Code User" #Code user
run_notes = " The standard curve for this run was checked manually on the instrument. " #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_202305.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_202305.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_202305_TR_LysB_10cm 39.5 6/5/2023 3:54:24 PM
## 2 GCW_202305_TR_LysB_20cm 35.5 6/5/2023 4:18:07 PM
## 3 GCW_202305_WC_LysA_10cm 69.5 6/5/2023 4:47:05 PM
## 4 GCW_202305_WC_LysA_20cm 82.3 6/5/2023 5:18:20 PM
## 5 GCW_202305_WC_LysA_45cm 151   6/5/2023 5:43:41 PM
## 6 GCW_202305_WC_LysB_10cm 72.5 6/5/2023 6:07:36 PM

```

0.3 Assessing Standard Curves - this was done manually on the TOC, not included here

0.4 CRM Check - No CRMs on this run

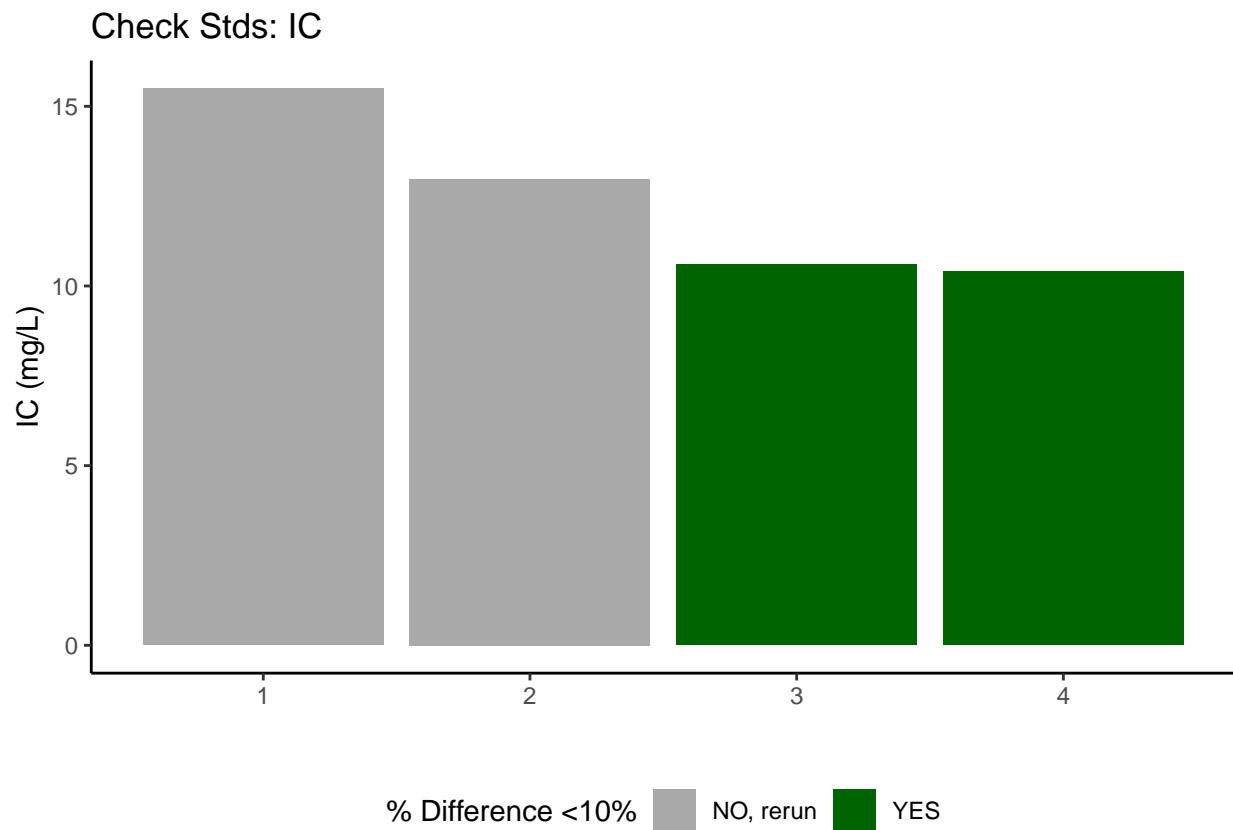
0.5 Assess Check Standards

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

```

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

```



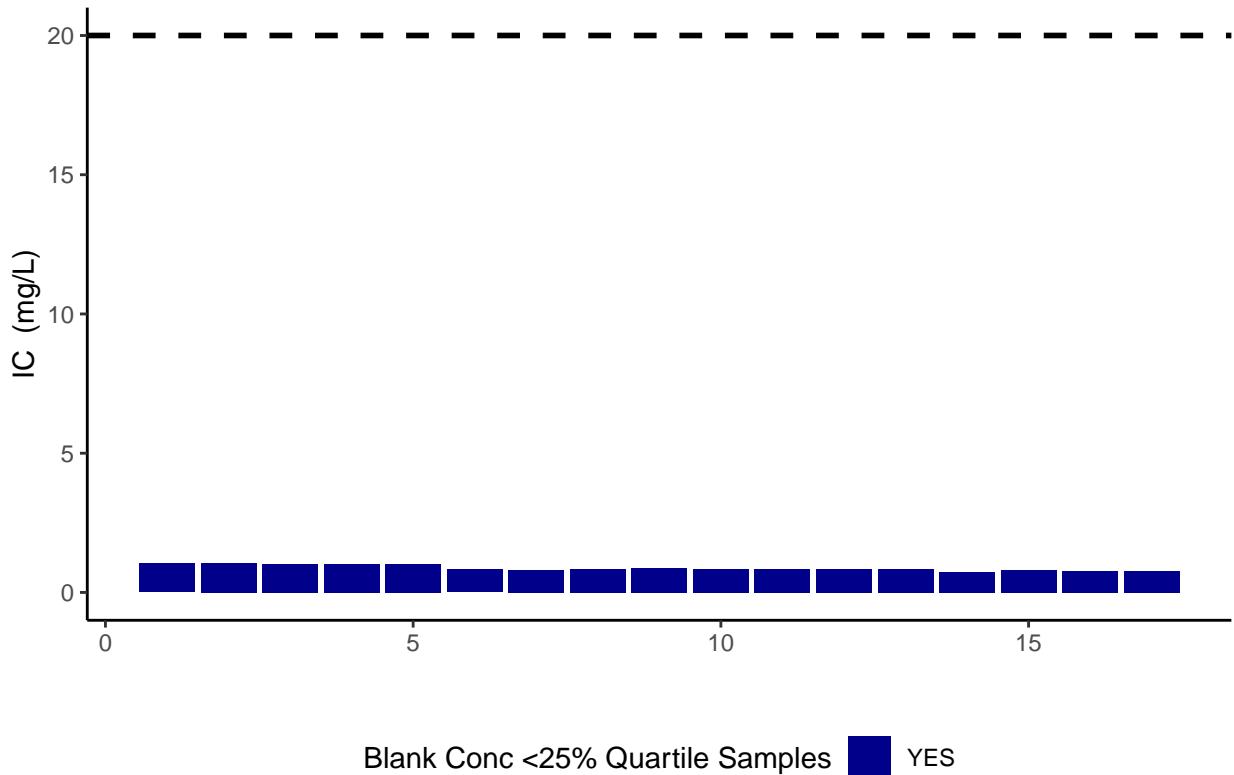
```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

Blanks: IC

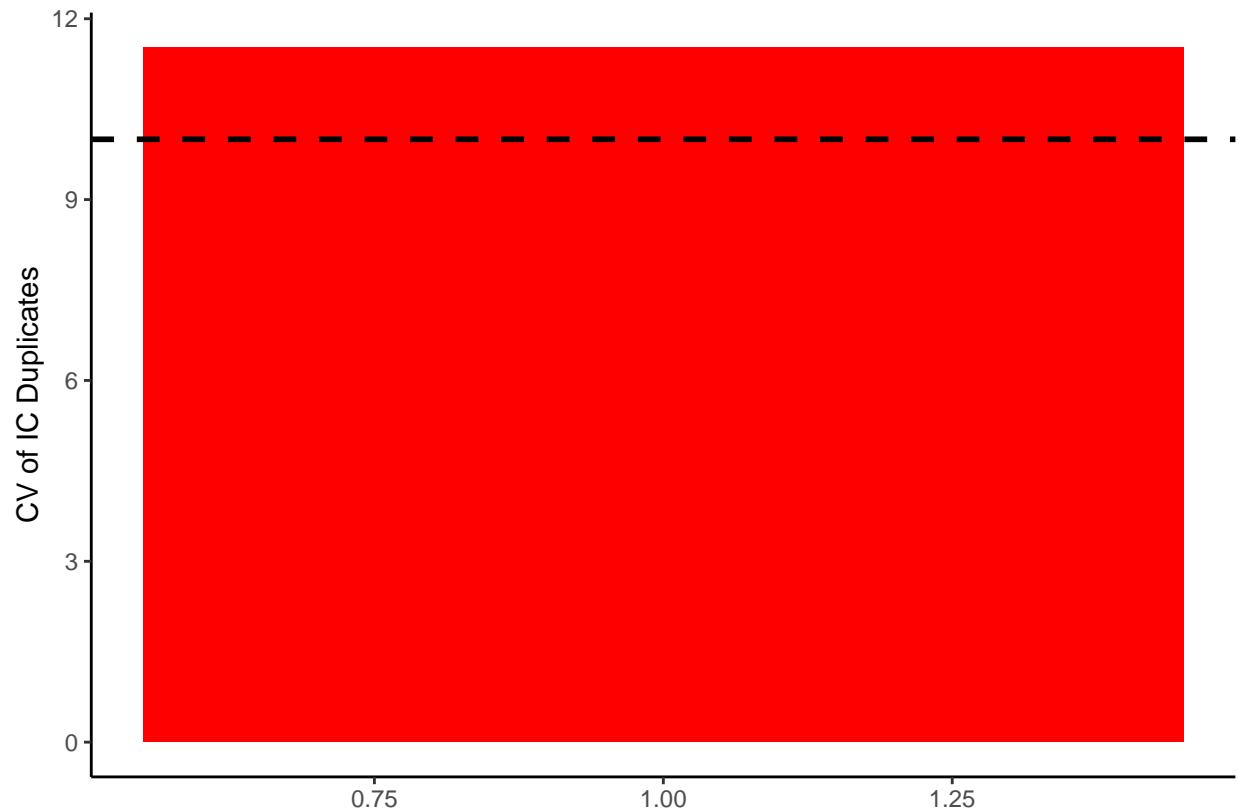


```
## carbon blanks:
```

```
## [1] 0.8814941
```

0.7 Assess Duplicates

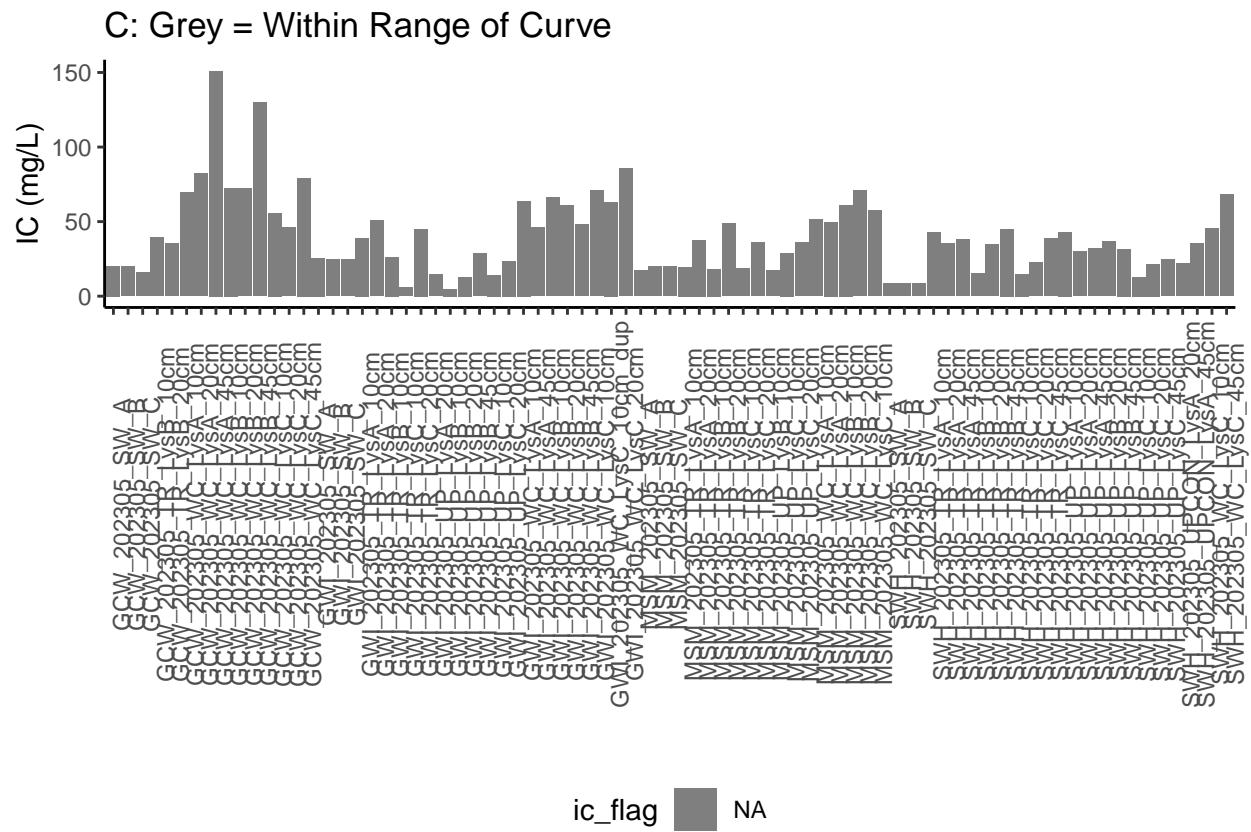
```
## Assess Duplicates
```



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

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

```
## Sample Flagging
```

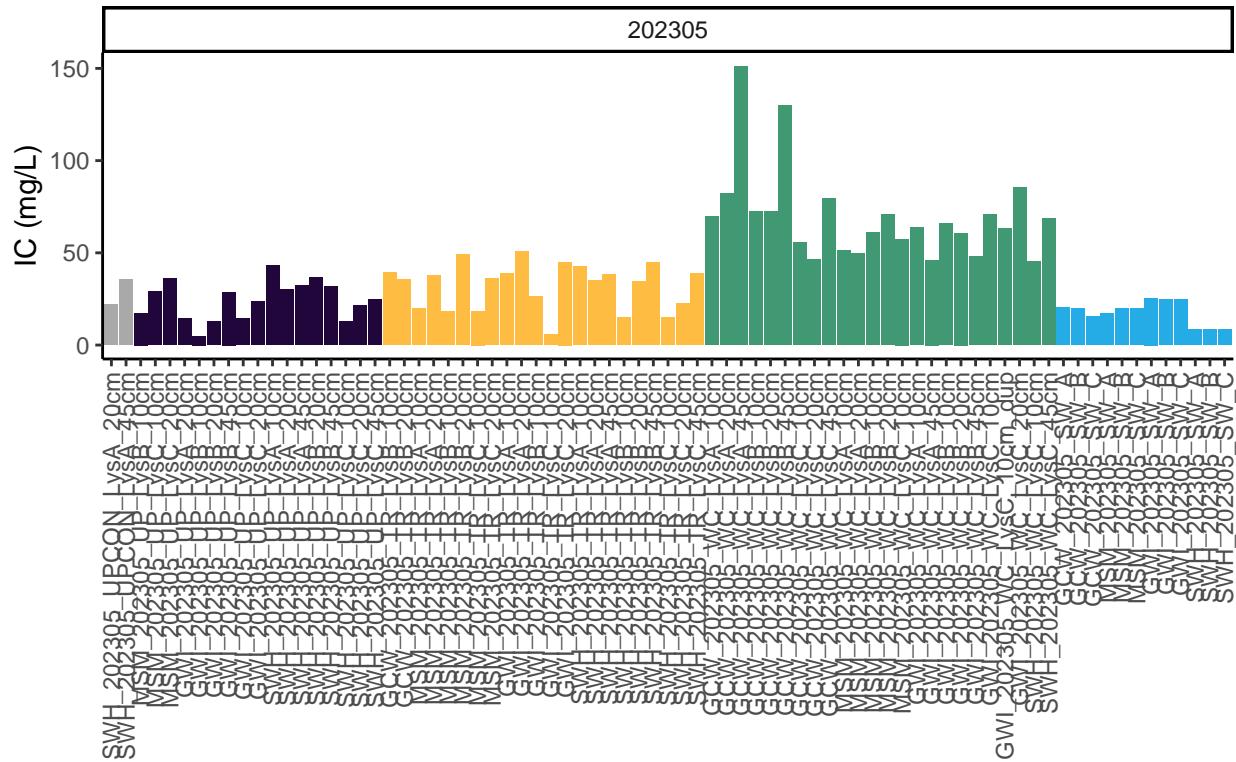


0.9 Visualize Data by Plot - in 2023 SWH Upland = UPCON and Swamp = UP

Visualize Data

```
## Warning in rbind(c("GCW", "202305", "TR", "LysB", "10cm"), c("GCW", "202305", :  
## 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 - 2023 data needs entered

```
## 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    2023~ UPCON A            20 SWH_2023~ 2023    5    24
## 2 COMPASS: Sy~ CB    2023~ UPCON A            45 SWH_2023~ 2023    5    24
## 3 COMPASS: Sy~ CB    2023~ UP    B            10 MSM_2023~ 2023    5    19
## 4 COMPASS: Sy~ CB    2023~ UP    C            10 MSM_2023~ 2023    5    19
## 5 COMPASS: Sy~ CB    2023~ UP    C            20 MSM_2023~ 2023    5    19
## 6 COMPASS: Sy~ CB    2023~ UP    A            20 GWI_2023~ 2023    5    23
## # 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