Synoptic CB: Porewater DIC

November 2024 Samples

2025-10-21

Contents

##Setup - Change things here & write any notes

```
#identify section
cat("Setup Information")
```

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "11/25/2024"  #Date that instrument was run
  Run_by = "Stephanie J. Wilsonr"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = "There was only one duplicate included in this run and it is out of range,
    accepting the run. "  #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_202411.txt"

#file path and name for raw all peaks file
    raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202411_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202411.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_2024.csv"

#qaqc log file path for this year
  Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAQClog_2024.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 202411_SWH_UP_LysA_10cm   3.13 11/26/2024 12:18:08 PM
## 2 202411_SWH_UP_LysA_20cm   5.01 11/26/2024 12:28:48 PM
## 3 202411_SWH_UP_LysA_45cm  15.5  11/26/2024 12:44:57 PM
## 4 202411_SWH_UP_LysB_10cm   3.02 11/26/2024 12:55:18 PM
## 5 202411_SWH_UP_LysB_20cm  11.6  11/26/2024 1:06:21 PM
## 6 202411_SWH_UP_LysC_20cm   5.29 11/26/2024 1:17:01 PM
```

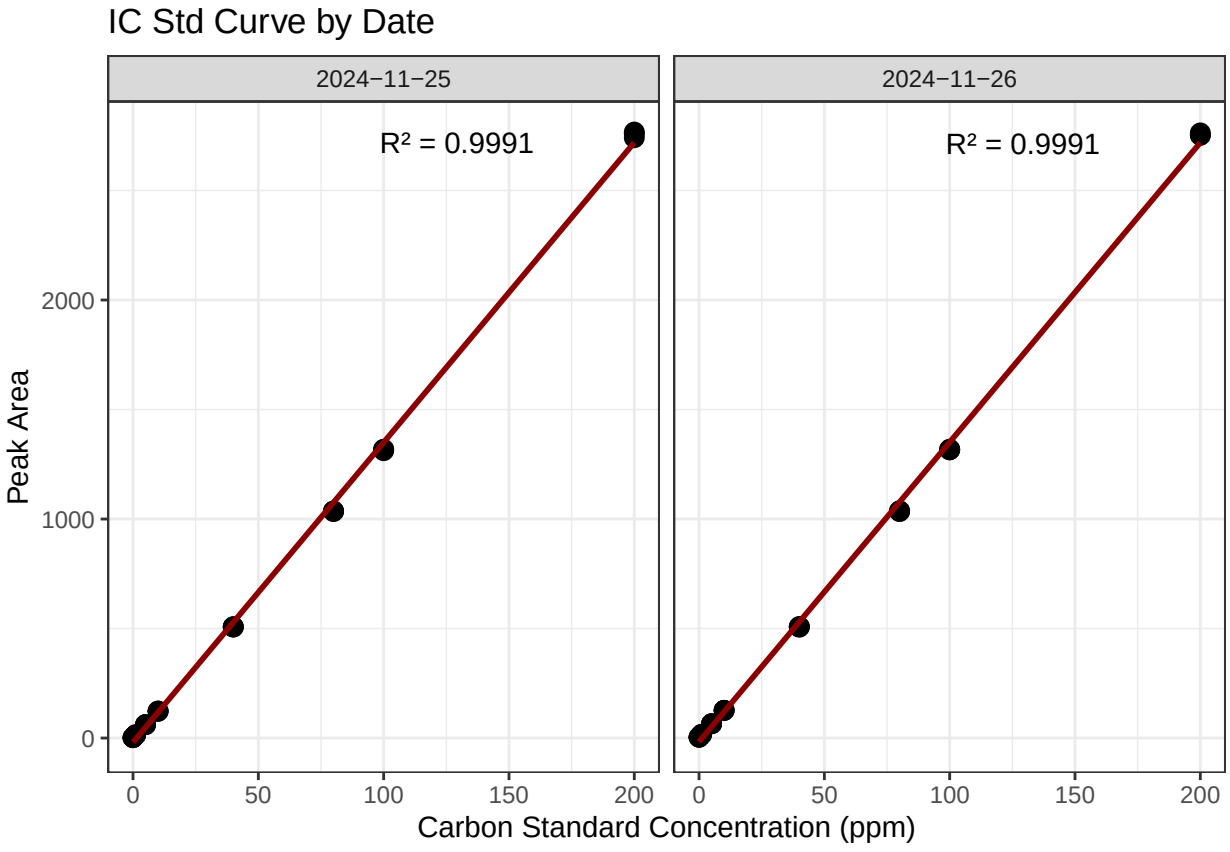
0.3 Assessing Standard Curves

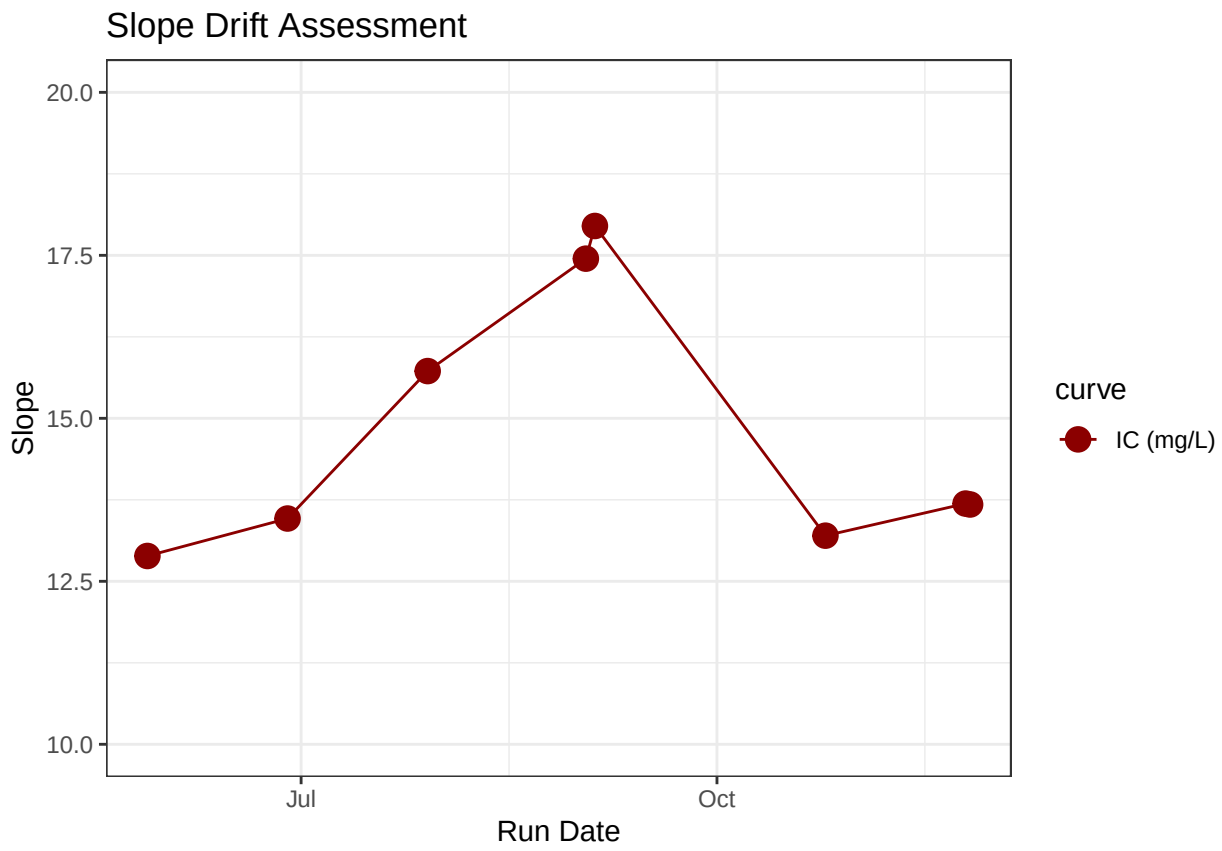
```
## Assess the Standard Curves
```

```
## New names:
## * `` -> `...18`
```

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

```
## `geom_smooth()` using formula = 'y ~ x'
```





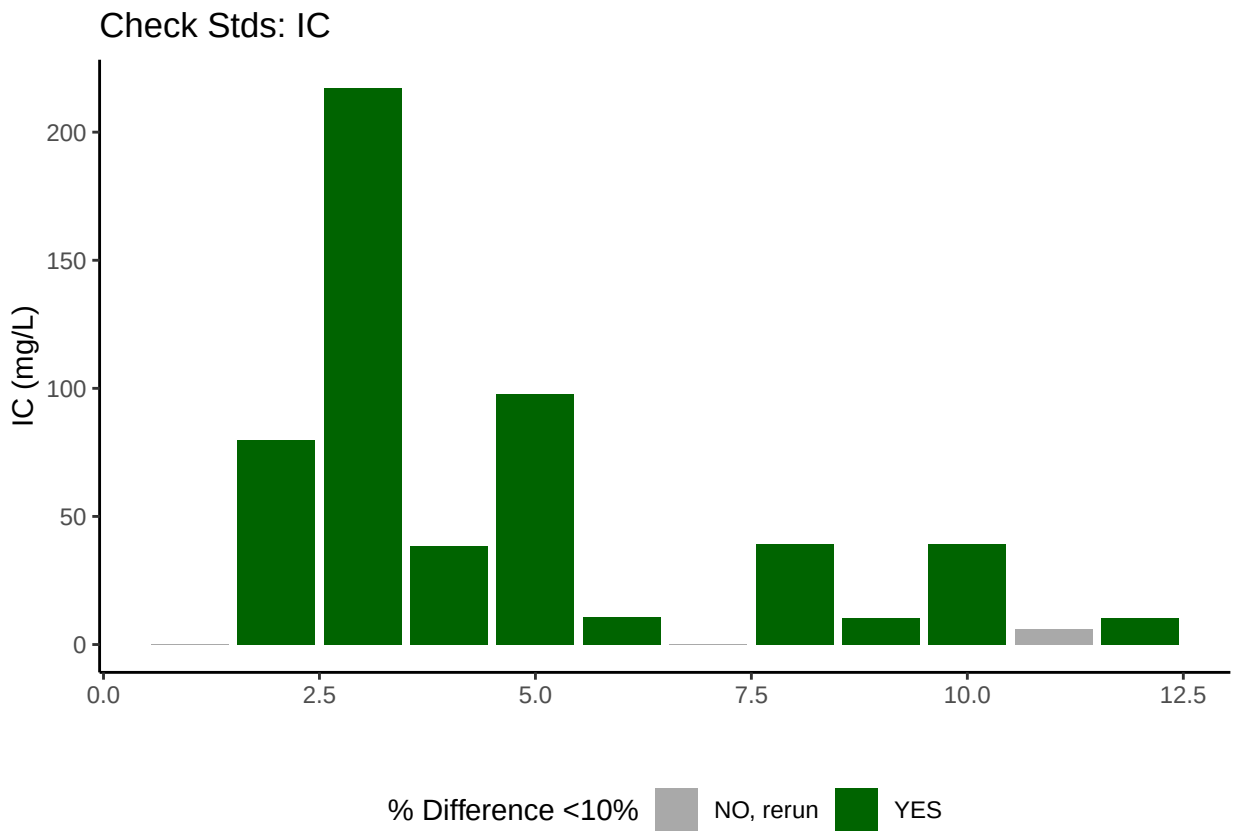

```
## [1] "IC Curve r2 GOOD"
```

0.4 CRM Check - Don't run chunk if no CRMs run

```
## Assess the CRMs

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

## [1] "IC crm has a % Difference <25% of expected - PROCEED"

## Run mean = 21.95333

## Expected  = 22.19
```

0.5 Assess Check Standards

```
## Assess the Check Standards

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



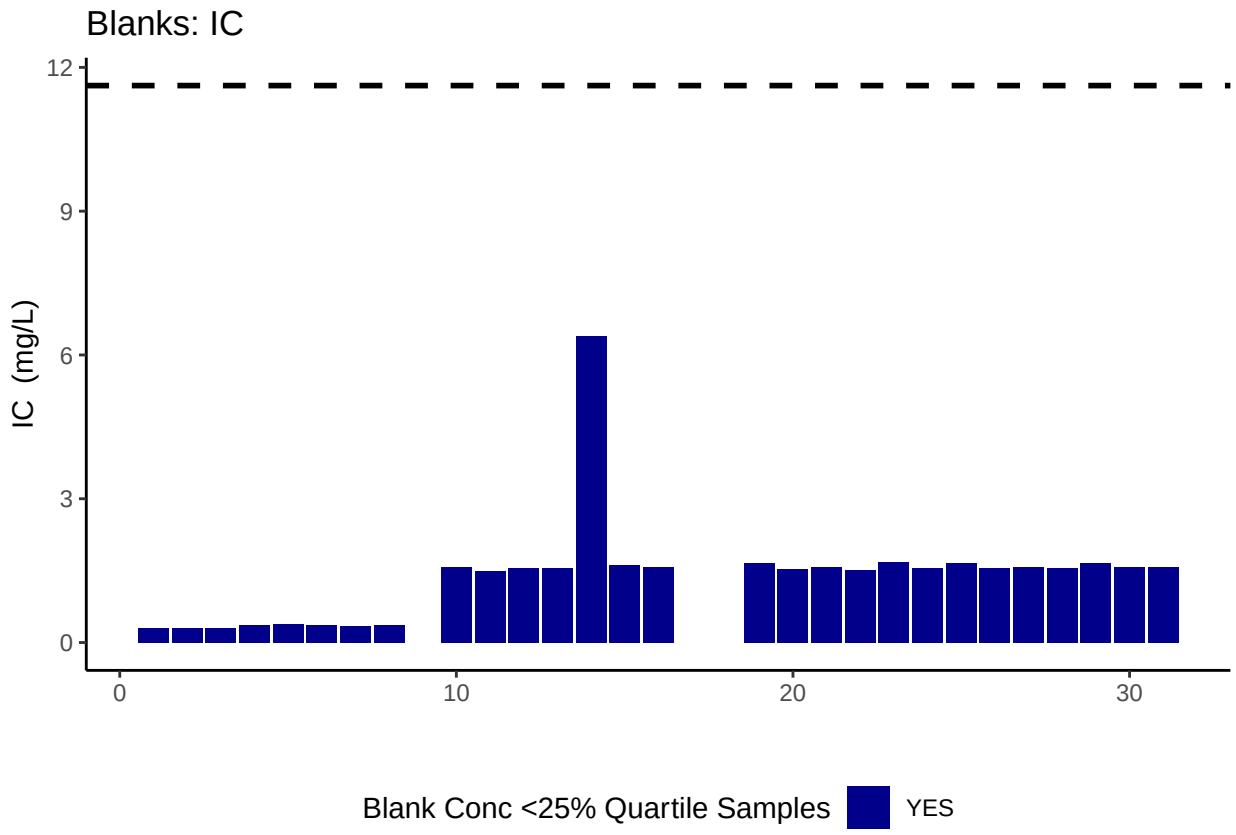

```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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

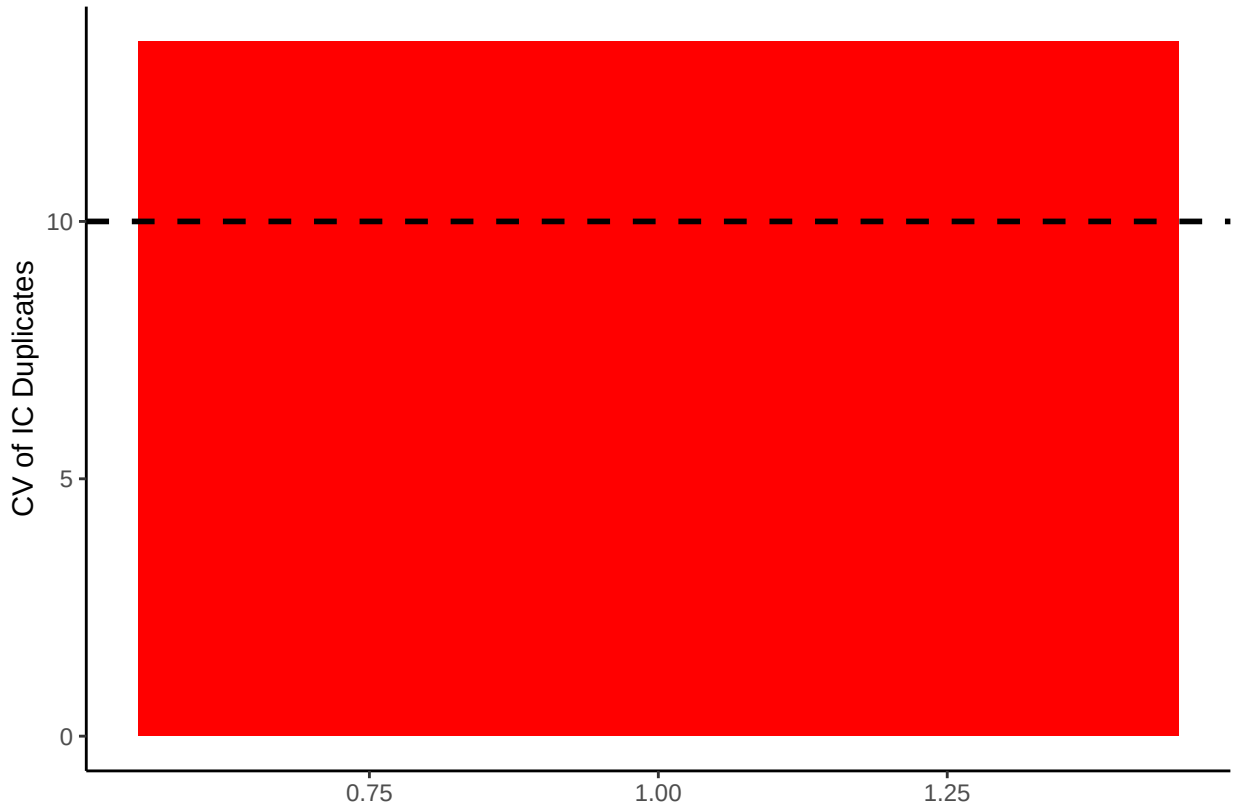



```
## carbon blanks:
```

```
## [1] 1.397504
```

0.7 Assess Duplicates - only one dup and it is out of range...

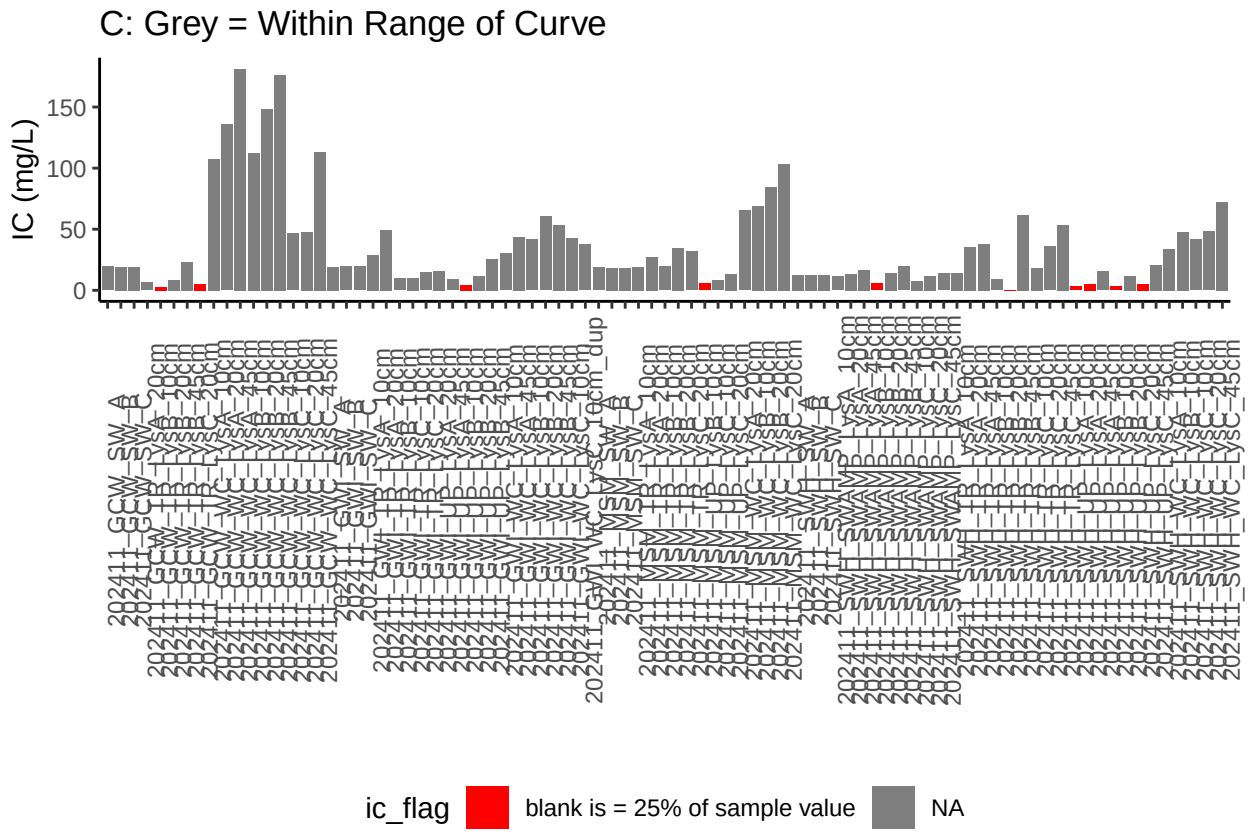
```
## Assess Duplicates
```




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

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

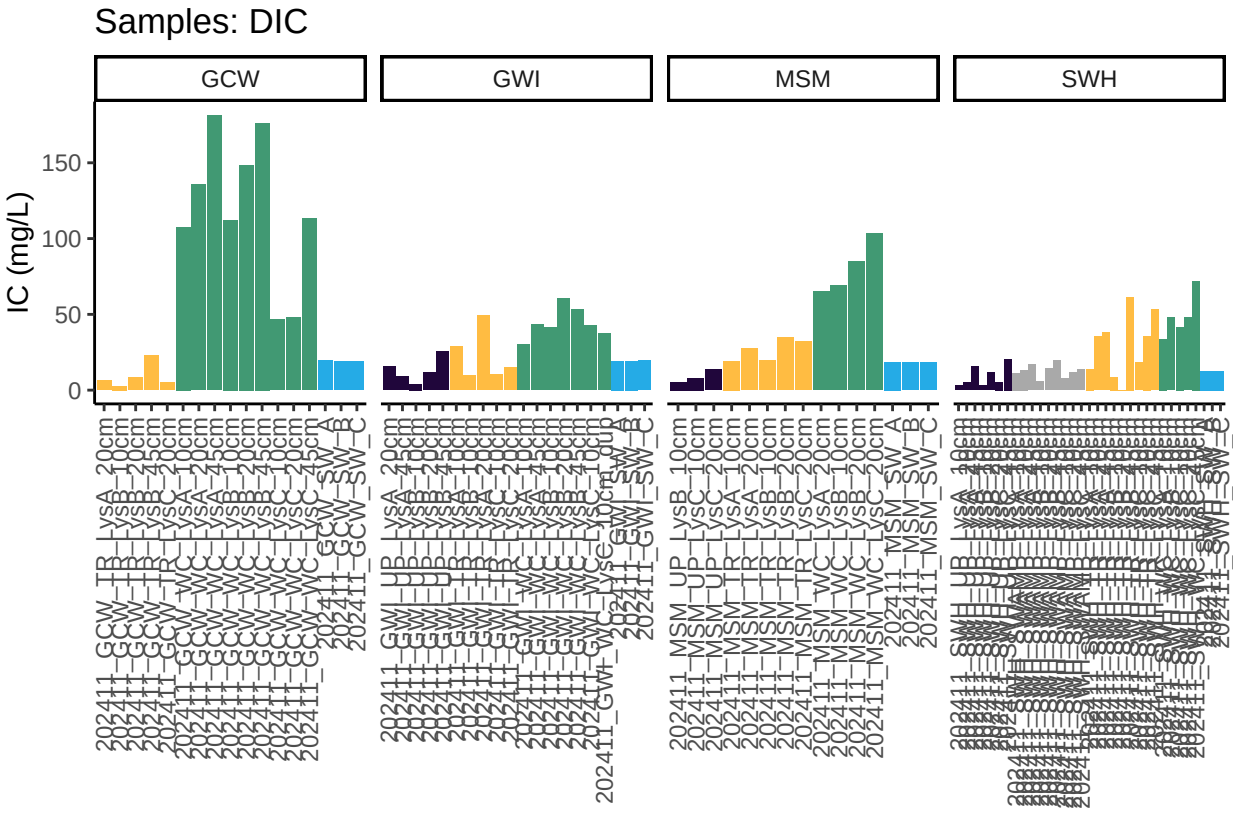
```
## Sample Flagging
```



0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202411", "SWH", "UP", "LysA", "10cm"), c("202411", "SWH", :
## 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   UP    A               10 202411_S~  2024    11    12
## 2 COMPASS: Sy~ CB     SWH   UP    A               20 202411_S~  2024    11    12
## 3 COMPASS: Sy~ CB     SWH   UP    A               45 202411_S~  2024    11    12
## 4 COMPASS: Sy~ CB     SWH   UP    B               10 202411_S~  2024    11    12
## 5 COMPASS: Sy~ CB     SWH   UP    B               20 202411_S~  2024    11    12
## 6 COMPASS: Sy~ CB     SWH   UP    C               20 202411_S~  2024    11    12
## # i 8 more variables: Time <chr>, Time_Zone <chr>, ic_mgL <dbl>, ic_uM <dbl>,
## #   ic_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>
```

#end