

# Synoptic CB: Porewater DIC

May 2025 Samples

2025-10-21

## Contents

0.1	Import Data Functions . . . . .	2
0.2	Import Sample Data . . . . .	2
0.3	Assessing Standard Curves . . . . .	3
0.4	CRM Check - Don't run chunk if no CRMs run . . . . .	4
0.5	Assess Check Standards . . . . .	4
0.6	Assess Blanks . . . . .	5
0.7	Assess Duplicates . . . . .	6
0.8	Sample Flagging - Are samples Within the range of the curve? . . . . .	7
0.9	Visualize Data by Plot . . . . .	8
0.10	Convert data from mg/L to uMoles/L . . . . .	9
0.11	Check to see if samples run match metadata & merge info . . . . .	9
0.12	Export Processed Data . . . . .	9

```

##Setup - Change things here & write any notes

#identify section
cat("Setup Information")

## Setup Information

##### Run information - PLEASE CHANGE
Date_Run = "5/26/25" #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/COMPASS_SynopticCB_PW_DIC_202505.txt"

#file path and name for raw all peaks file
raw_allpeaks_name = "Raw Data/COMPASS_SynopticCB_PW_DIC_202505_allpeaks.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202505.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_2025.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'

## # A tibble: 6 x 3
##   sample_name          ic_raw run_datetime
##   <chr>                <dbl> <chr>

```

```

## 1 202505_GCW_TR_LysA_20cm 13.3 5/26/2025 10:43:57 PM
## 2 202505_GCW_TR_LysB_10cm 11.0 5/26/2025 10:56:35 PM
## 3 202505_GCW_TR_LysB_20cm 16.1 5/26/2025 11:09:42 PM
## 4 202505_GCW_TR_LysC_10cm 11.5 5/26/2025 11:22:34 PM
## 5 202505_GCW_TR_LysC_20cm 11.0 5/26/2025 11:35:16 PM
## 6 202505_GCW_WC_LysA_10cm 52.6 5/26/2025 11:50:20 PM

```

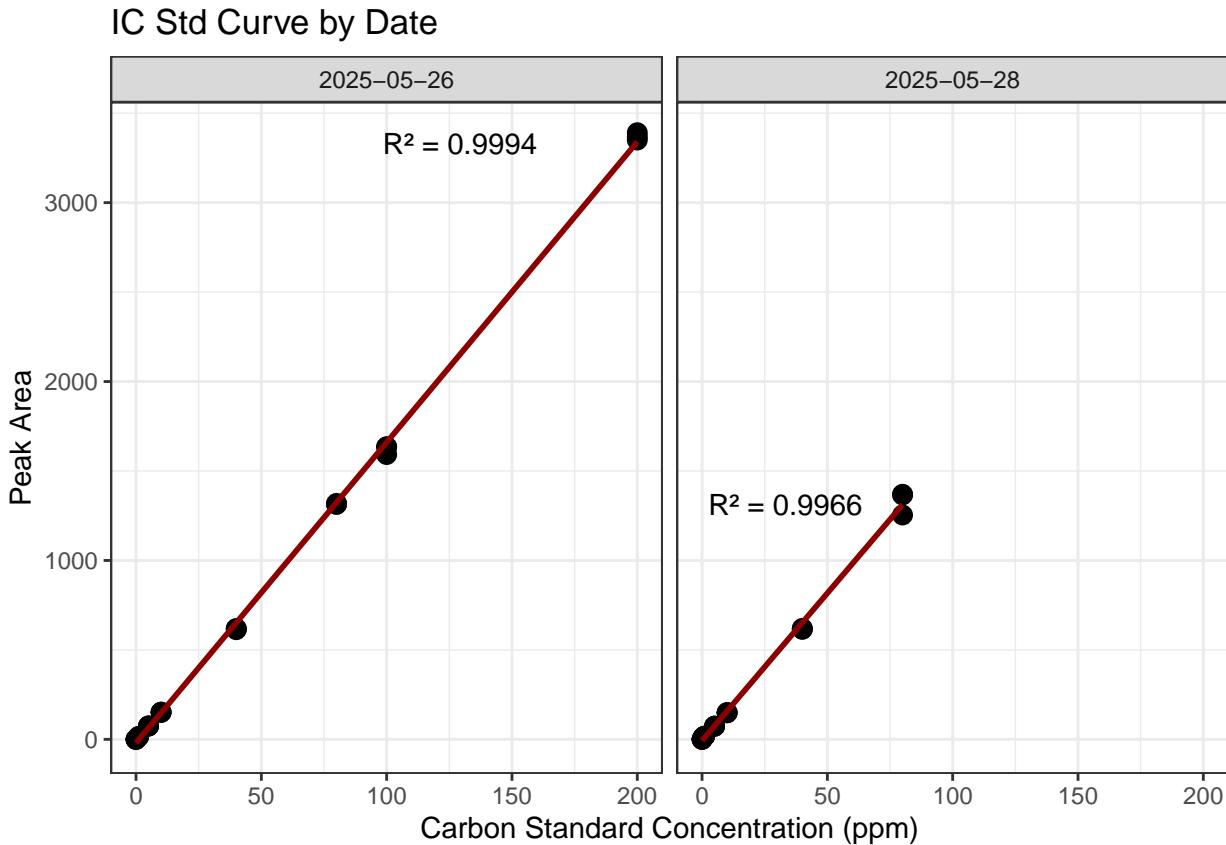
### 0.3 Assessing Standard Curves

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

```

## New names:
## `geom_smooth()` using formula = 'y ~ x'
## * `-->` '...18'

```



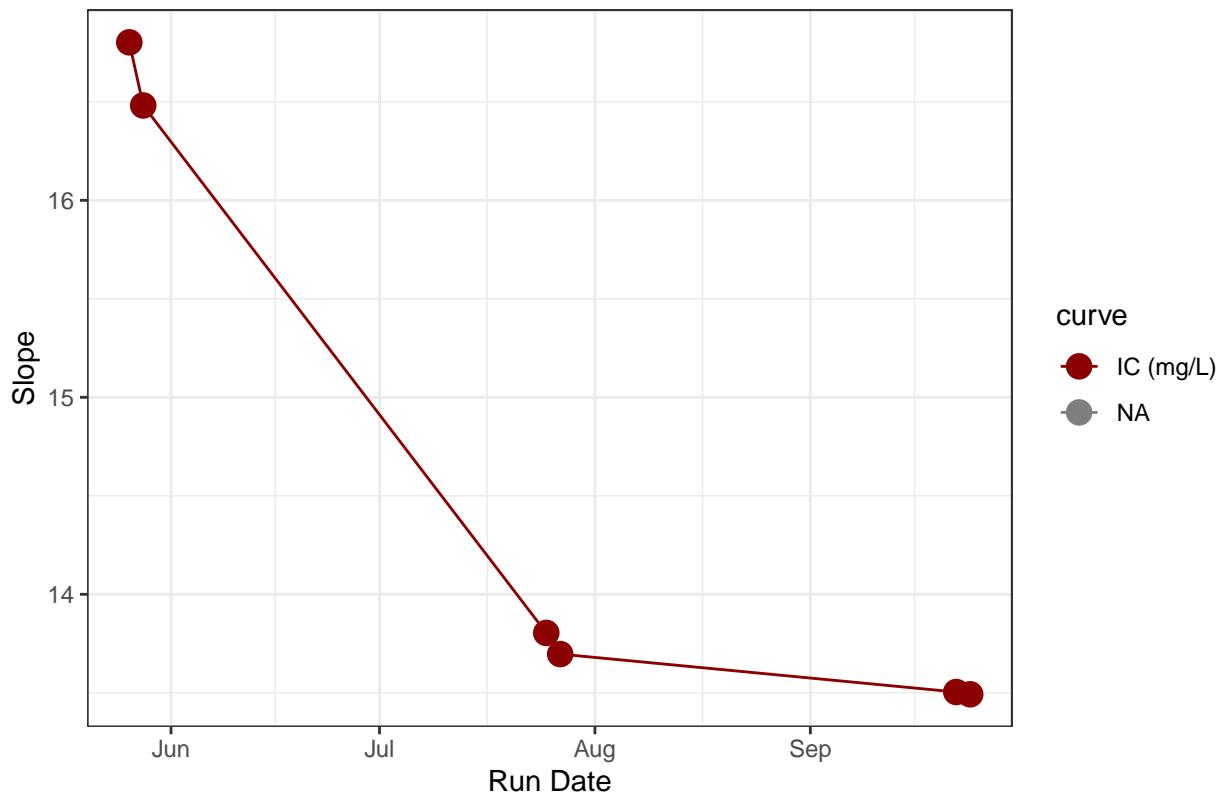
```

## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_point()').

## Warning: Removed 4 rows containing missing values or values outside the scale range
## ('geom_line()').

```

## Slope Drift Assessment



```
## [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"

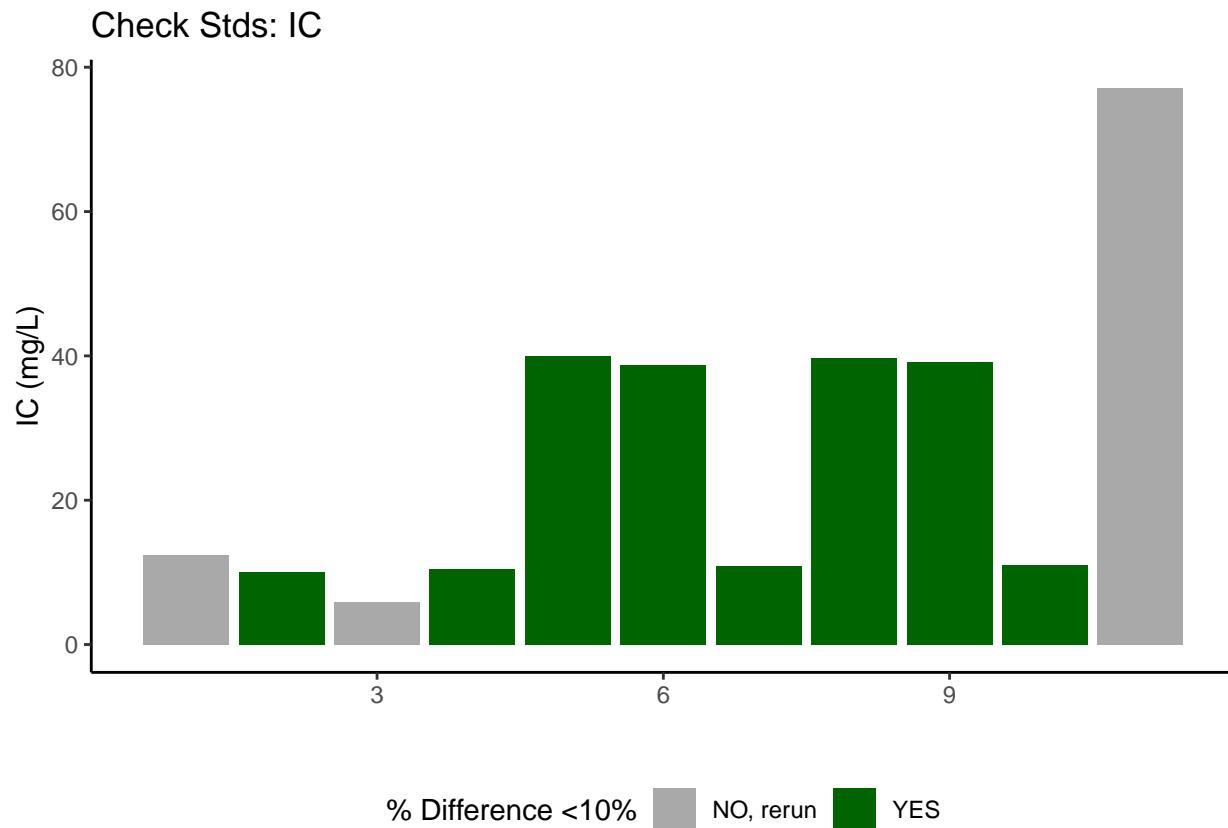
## Run mean = 22.17

## 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"
```

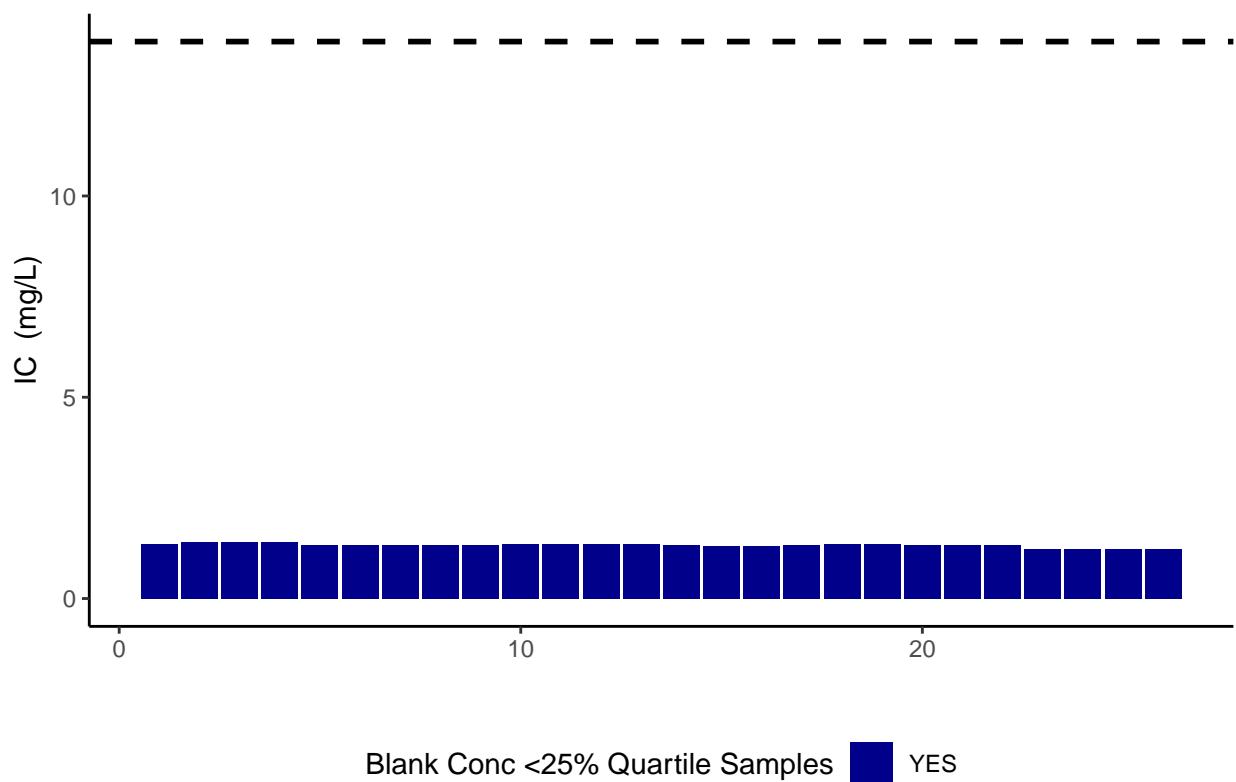
## 0.6 Assess Blanks

```
## Assess Blanks
```

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

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

Blanks: IC

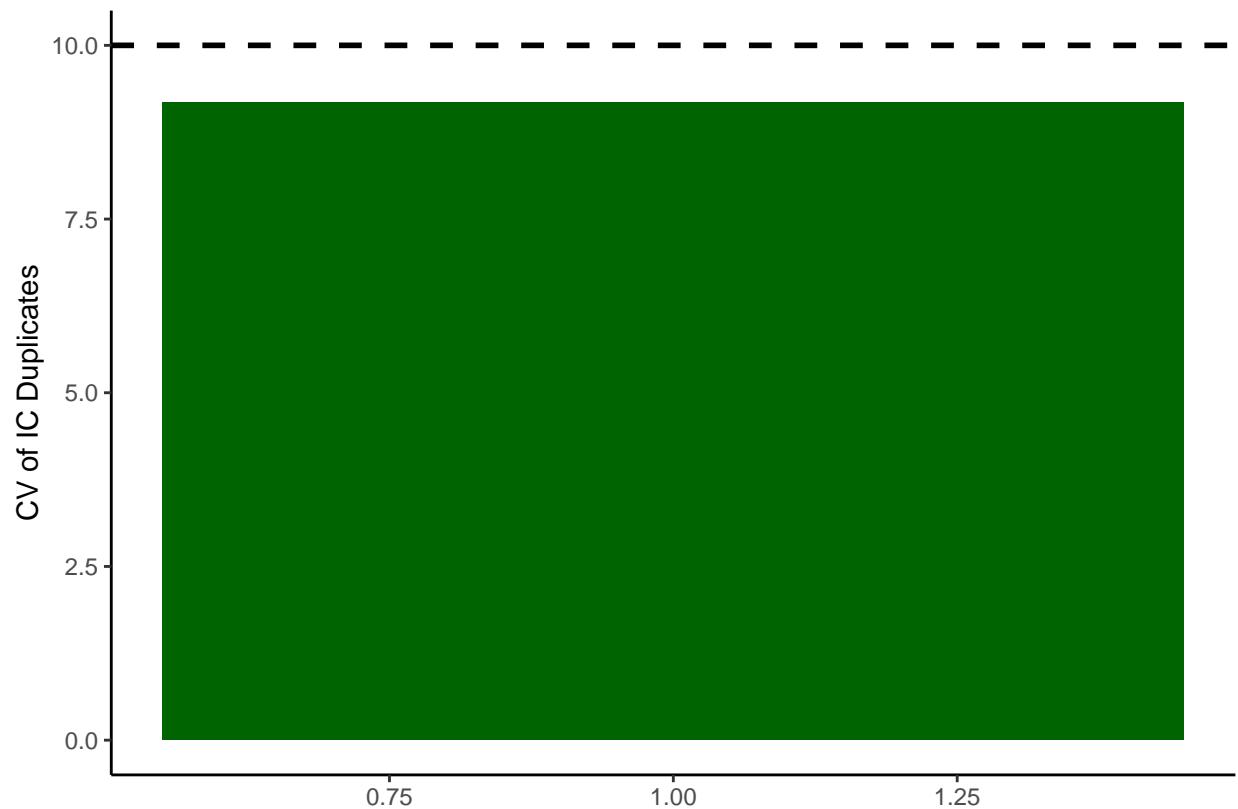


```
## carbon blanks:
```

```
## [1] 1.329
```

## 0.7 Assess Duplicates

```
## Assess Duplicates
```

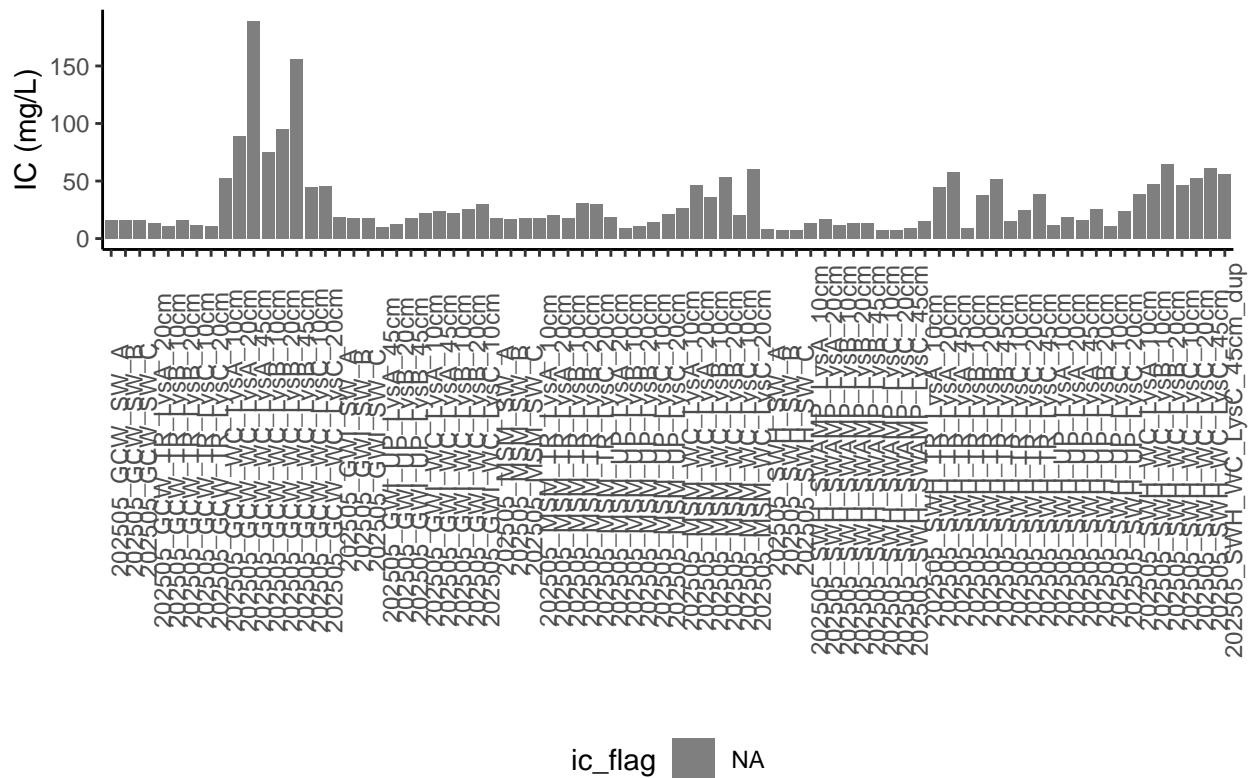


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

```
## Sample Flagging
```

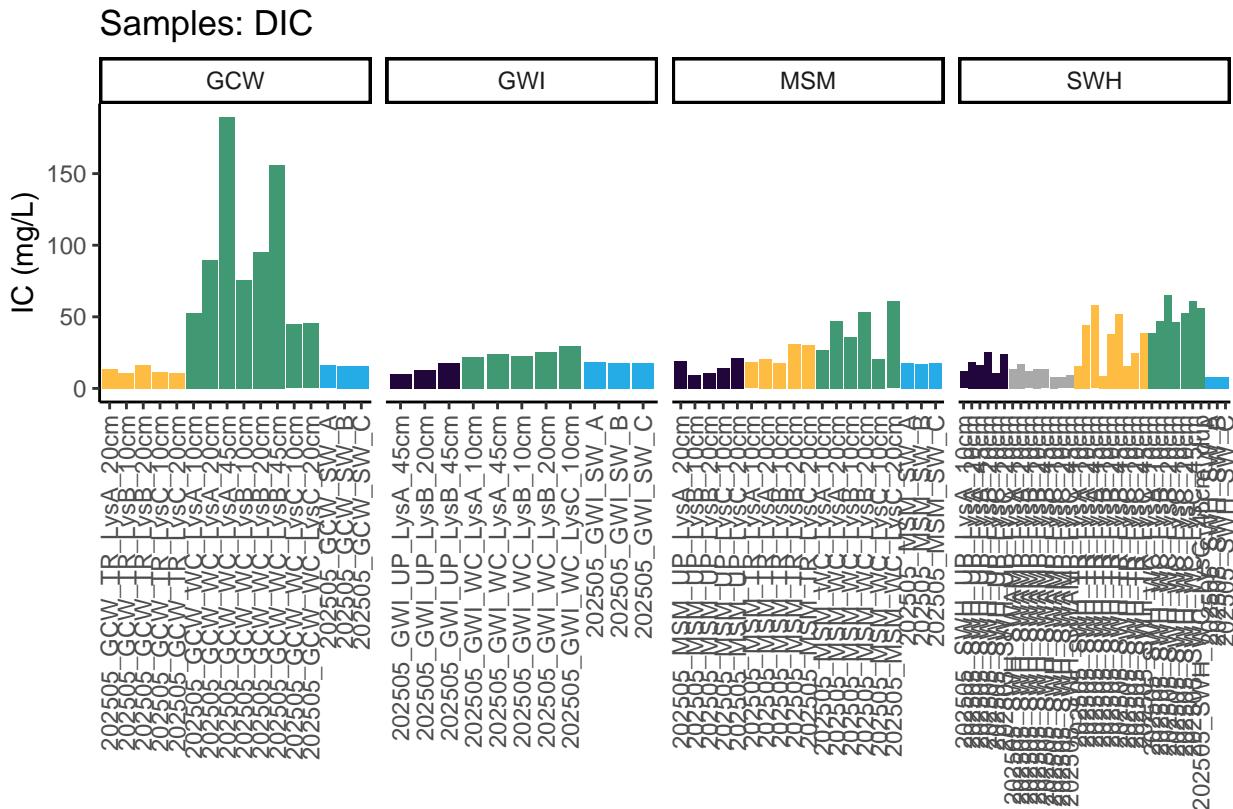
C: Grey = Within Range of Curve



## 0.9 Visualize Data by Plot

```
## Visualize Data

## Warning in rbind(c("202505", "GCW", "TR", "LysA", "20cm"), c("202505", "GCW", :
## 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     MSM   UP    A           20 202505_M~ 2025     5    15
## 2 COMPASS: Sy~ CB     MSM   UP    B           10 202505_M~ 2025     5    15
## 3 COMPASS: Sy~ CB     MSM   UP    B           20 202505_M~ 2025     5    15
## 4 COMPASS: Sy~ CB     MSM   UP    C           10 202505_M~ 2025     5    15
## 5 COMPASS: Sy~ CB     MSM   UP    C           20 202505_M~ 2025     5    15
## 6 COMPASS: Sy~ CB     GWI   UP    A           45 202505_G~ 2025     5    20
## # 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

```