

Synoptic CB: Porewater DIC

July 2024 Samples

2025-10-21

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```

##Setup - Change things here & write any notes

#identify section
cat("Setup Information")

## Setup Information

##### Run information - PLEASE CHANGE
Date_Run = "07/29/2024" #Date that instrument was run
Run_by = "Stephanie J. Wilson" #Instrument user
Script_run_by = "Stephanie J. Wilson" #Code user
run_notes = "One sample was entered into the instrument incorrectly and that is
fixed in this code: 202407_SWH_UP_LysB_45cm is 202407_SWH_UP_LysC_45cm" #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_202407.txt"

#file path and name for raw all peaks file
raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202407_allpeaks.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202407.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_QAAClog_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 202407_GCW_WC_LysA_10cm 111. 7/29/2024 3:29:12 PM
## 2 202407_GCW_WC_LysA_20cm 125. 7/29/2024 3:47:04 PM
## 3 202407_GCW_WC_LysA_45cm 185. 7/29/2024 4:04:53 PM
## 4 202407_GCW_WC_LysB_10cm 119. 7/29/2024 4:22:47 PM
## 5 202407_GCW_WC_LysB_20cm 126. 7/29/2024 4:40:38 PM
## 6 202407_GCW_WC_LysB_45cm 154. 7/29/2024 4:58:24 PM

```

0.3 Assessing Standard Curves

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

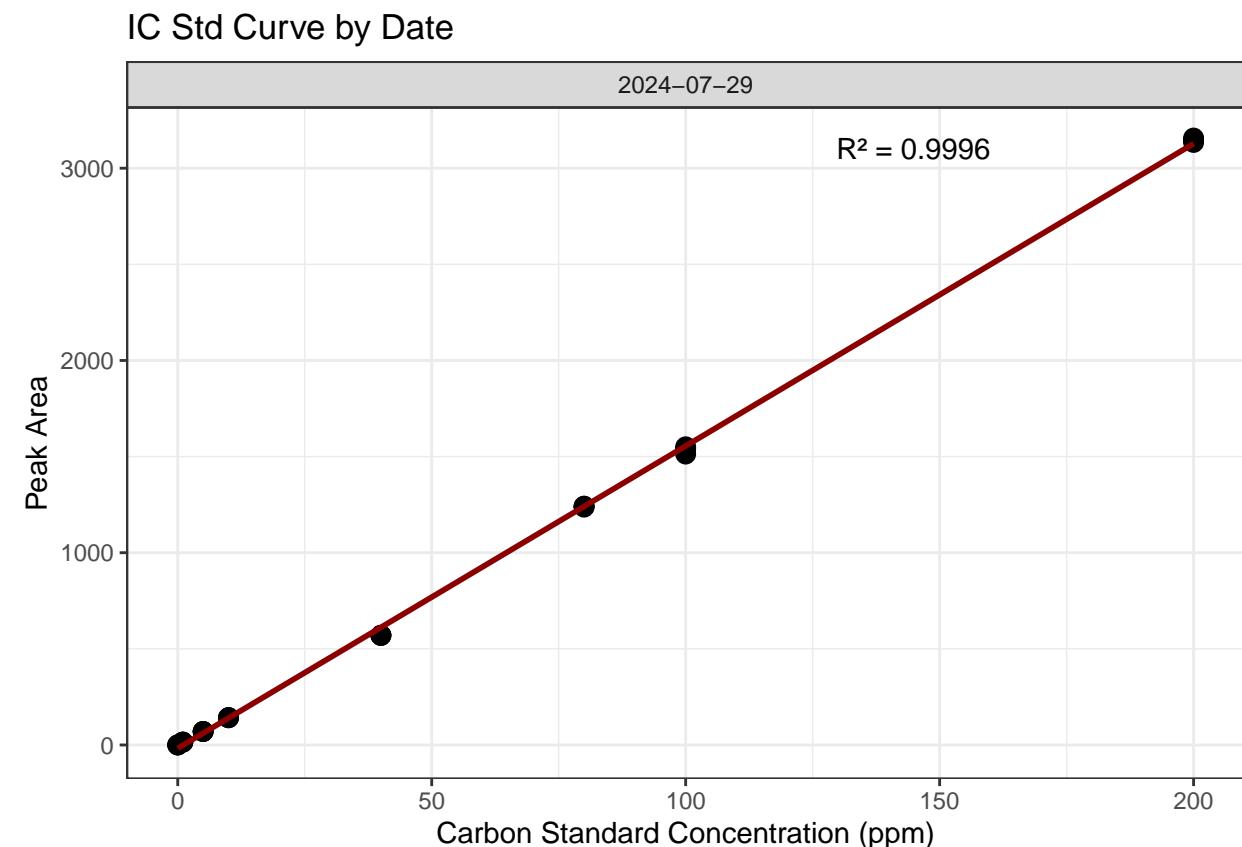
```

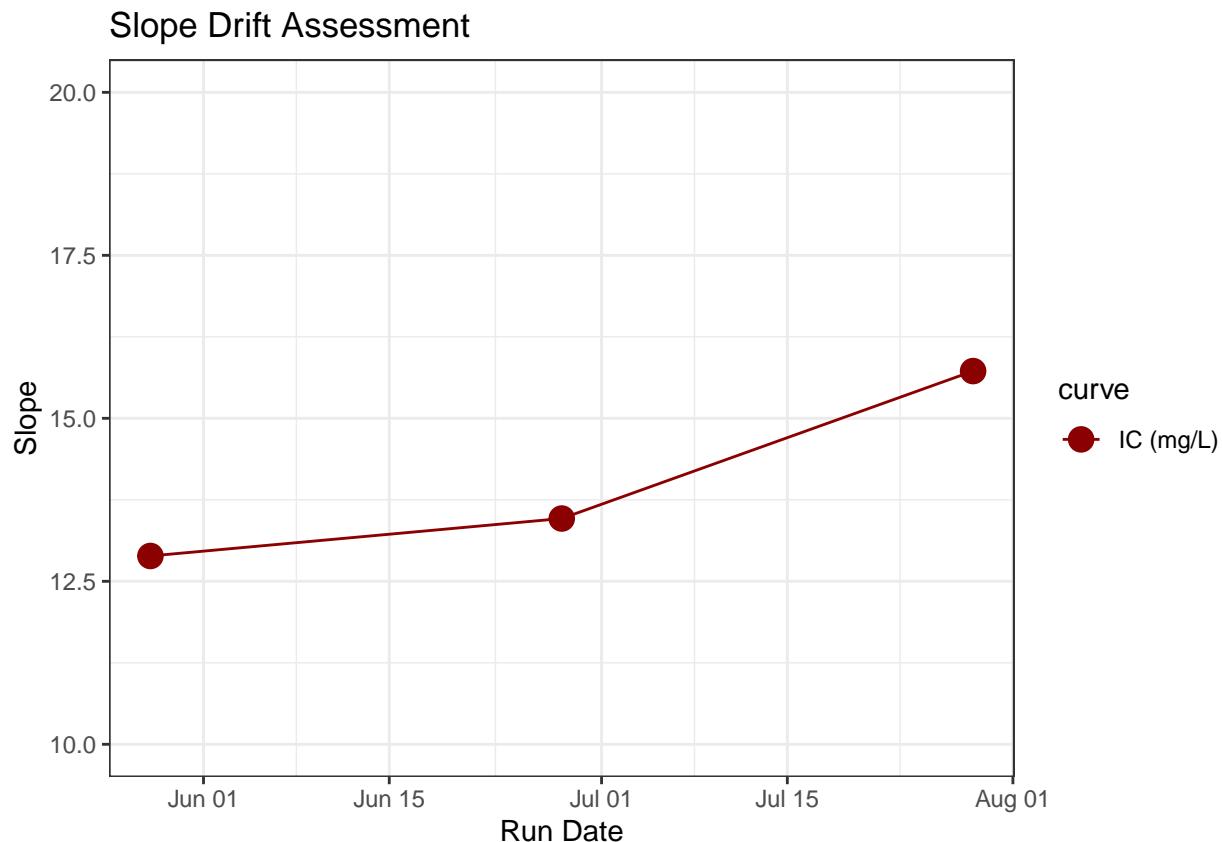
## New names:
## * ` ` -> '...18'

## 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] NA
```

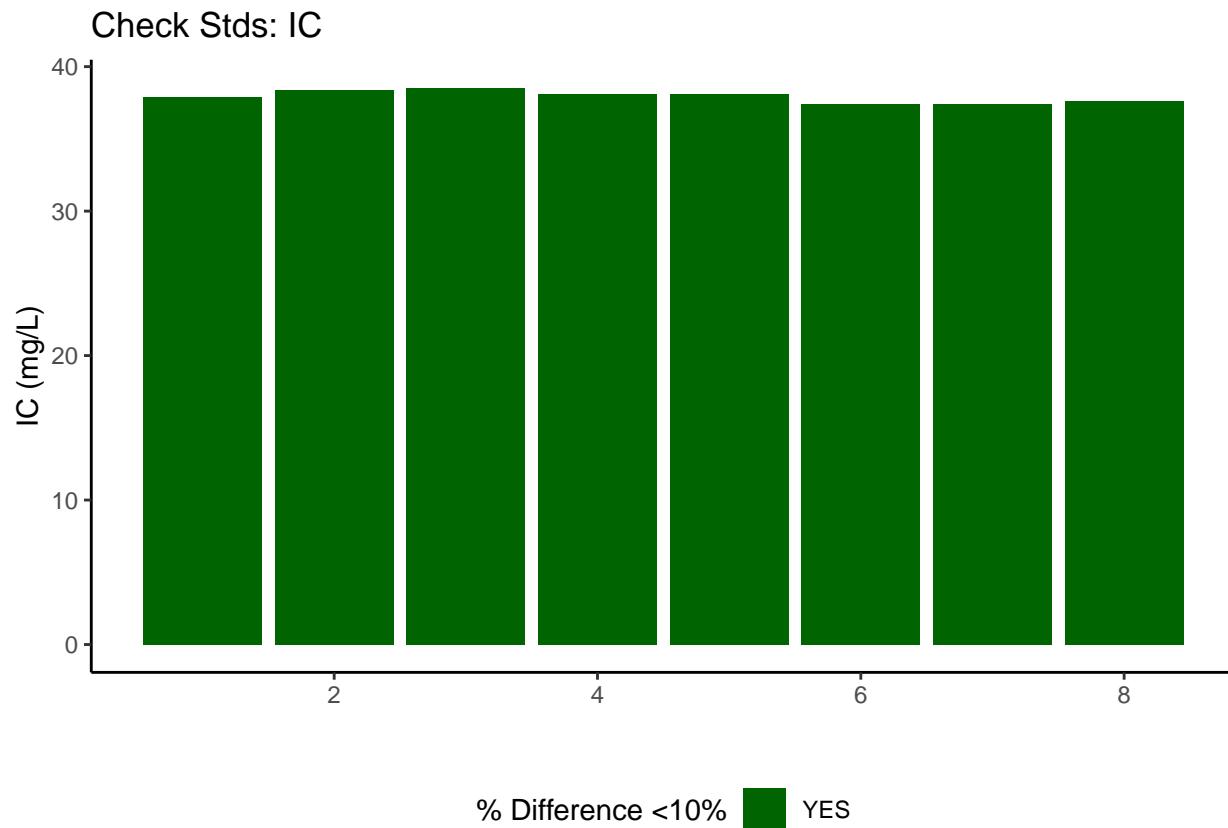
```
## Run mean = NaN
```

```
## Expected = 22.19
```

0.5 Assess Check Standards

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

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



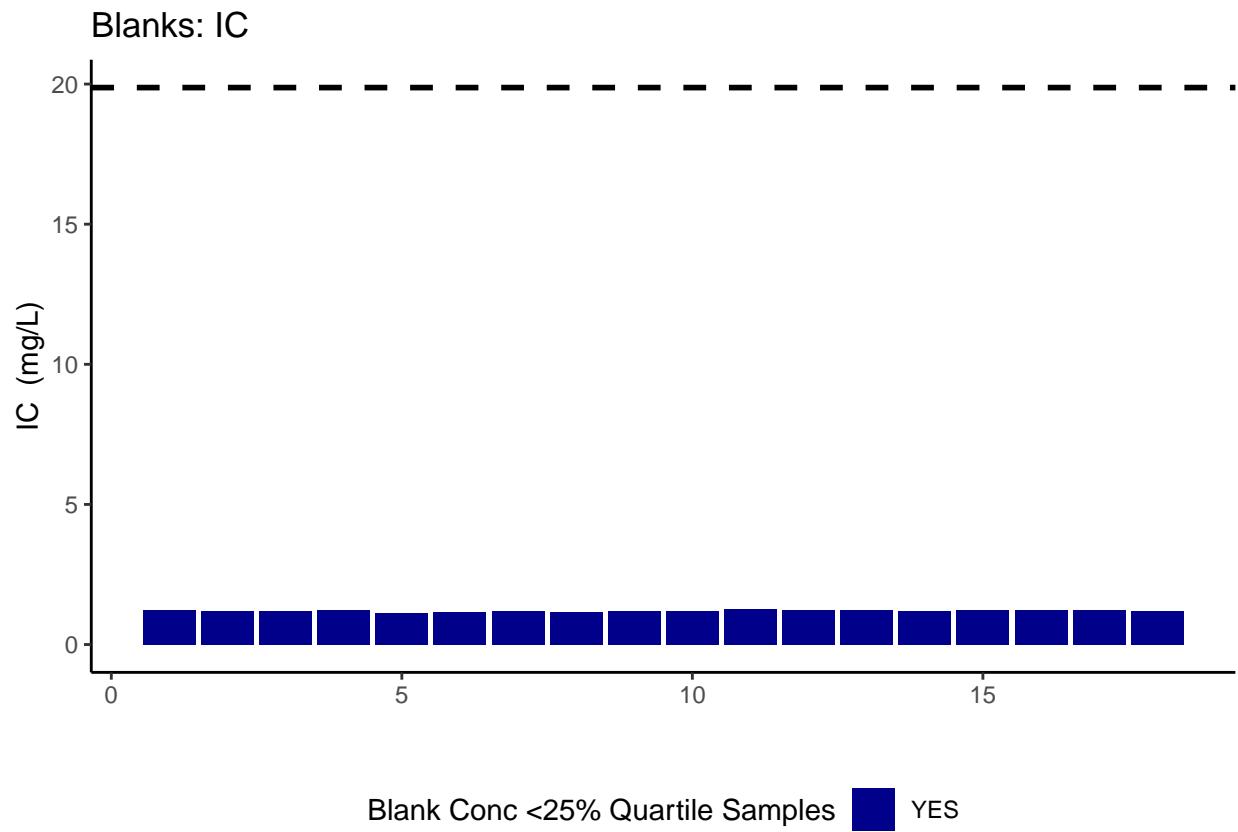
```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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



```
## carbon blanks:
```

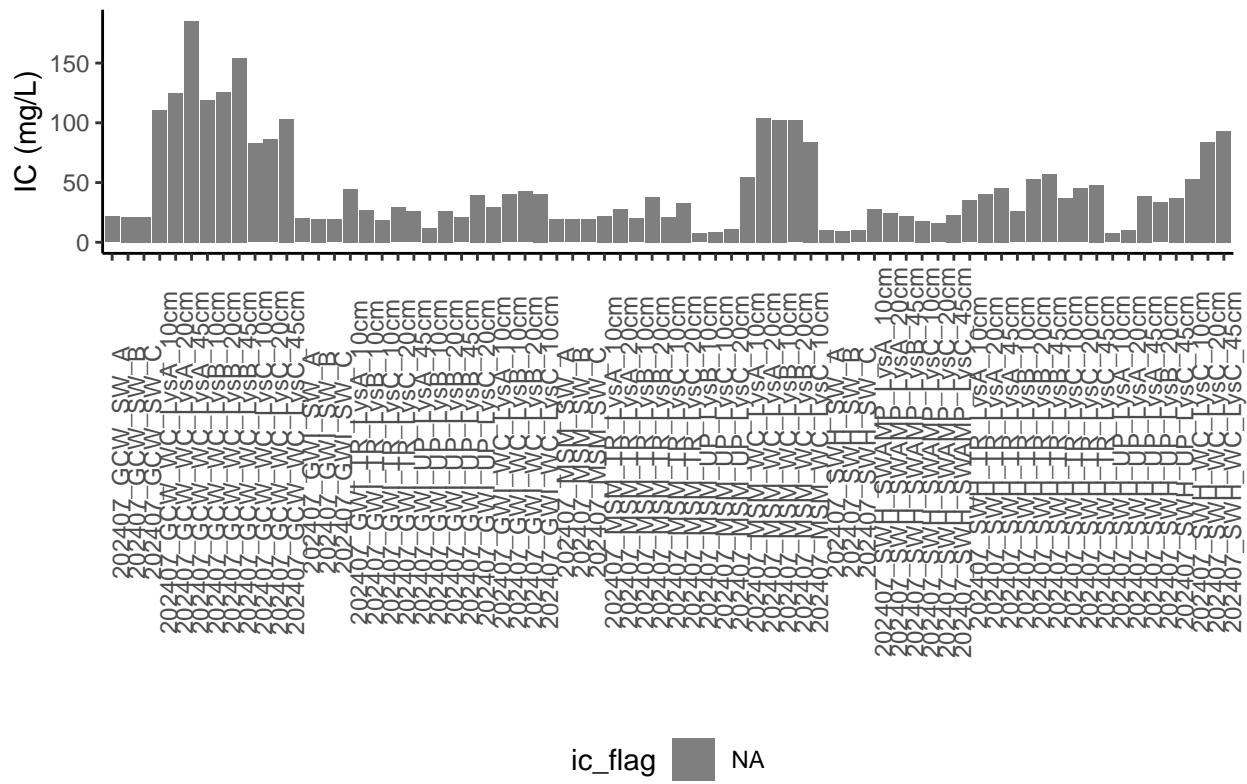
```
## [1] 1.2045
```

0.7 Assess Duplicates - no duplicates on this run

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

```
## Sample Flagging
```

C: Grey = Within Range of Curve

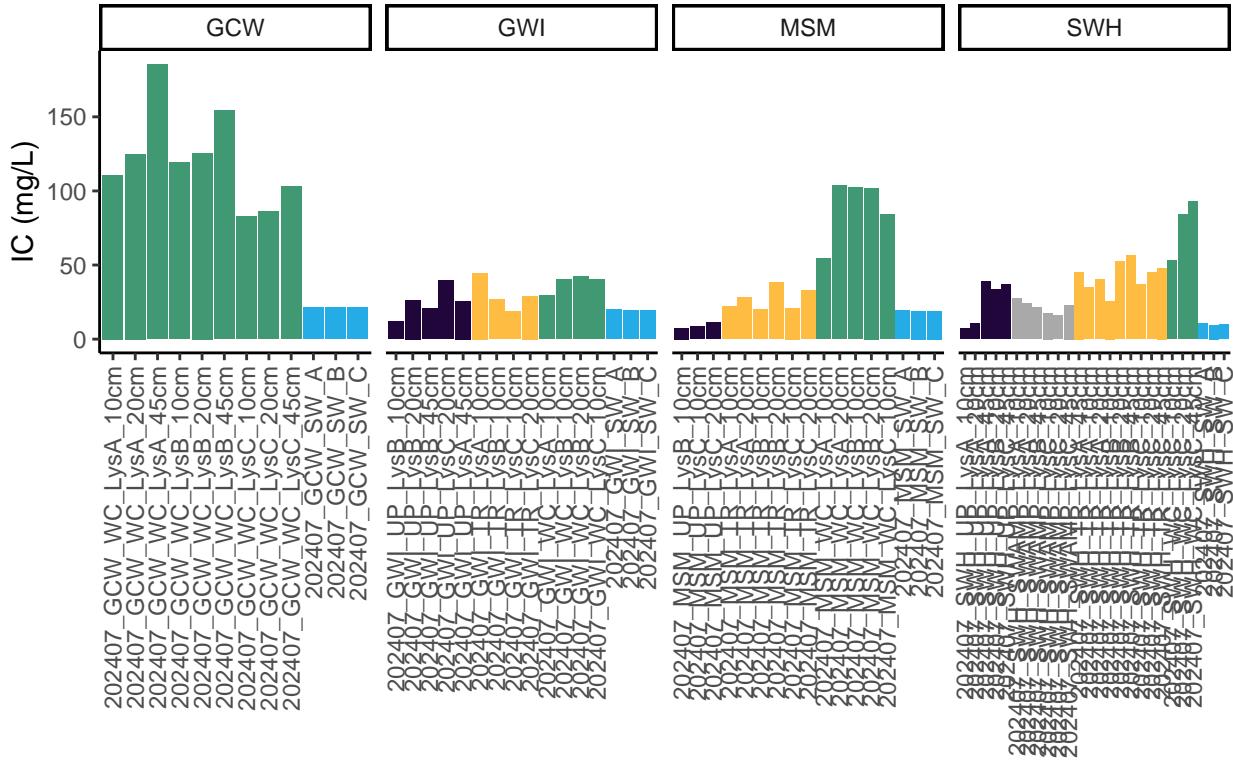


0.9 Visualize Data by Plot

Visualize Data

```
## Warning in rbind(c("202407", "GCW", "WC", "LysA", "10cm"), c("202407", "GCW", :  
## number of columns of result is not a multiple of vector length (arg 10)
```

Samples: DIC



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     B          10 202407_M~ 2024    7    18
## 2 COMPASS: Sy~ CB    MSM    UP     C          10 202407_M~ 2024    7    18
## 3 COMPASS: Sy~ CB    MSM    UP     C          20 202407_M~ 2024    7    18
## 4 COMPASS: Sy~ CB    SWH   UP     A          10 202407_S~ 2024    7    23
## 5 COMPASS: Sy~ CB    SWH   UP     A          20 202407_S~ 2024    7    23
## 6 COMPASS: Sy~ CB    SWH   UP     A          45 202407_S~ 2024    7    23
## # 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
```