Synoptic CB: Porewater DIC

May 2025 Samples

2025-09-23

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "9/20/25"  #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("TMP") #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/TMP_20250904_FW_WellTest_DIC.txt"

#file path and name for raw all peaks file
    raw_allpeaks_name = "Raw Data/TMP_20250904_FW_WellTest_DIC_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/TMP_20250904_FW_WellTest_DIC_Processed.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

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 TMP_FW_Well_20250904_1225_A   33.1 9/23/2025 12:04:12 AM
```

```
## 2 TMP_FW_Well_20250904_1225_B   30.2 9/23/2025 12:16:51 AM
## 3 TMP_FW_Well_20250904_1225_C   30.0 9/23/2025 12:29:32 AM
## 4 TMP_FW_Well_20250904_1300_A   25.7 9/23/2025 12:42:14 AM
## 5 TMP_FW_Well_20250904_1300_B   25.6 9/23/2025 12:54:59 AM
## 6 TMP_FW_Well_20250904_1300_C   26.3 9/23/2025 1:07:42 AM
```

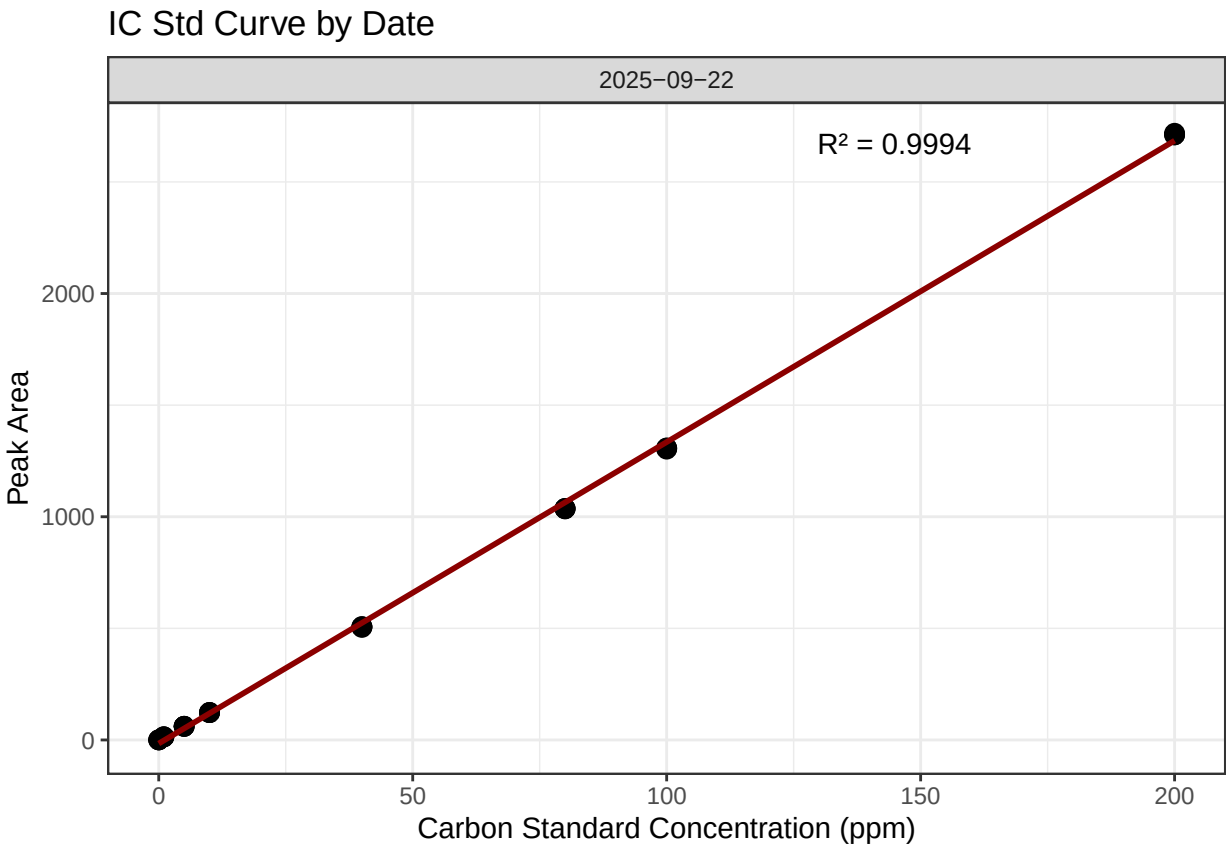
0.3 Assessing Standard Curves

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

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

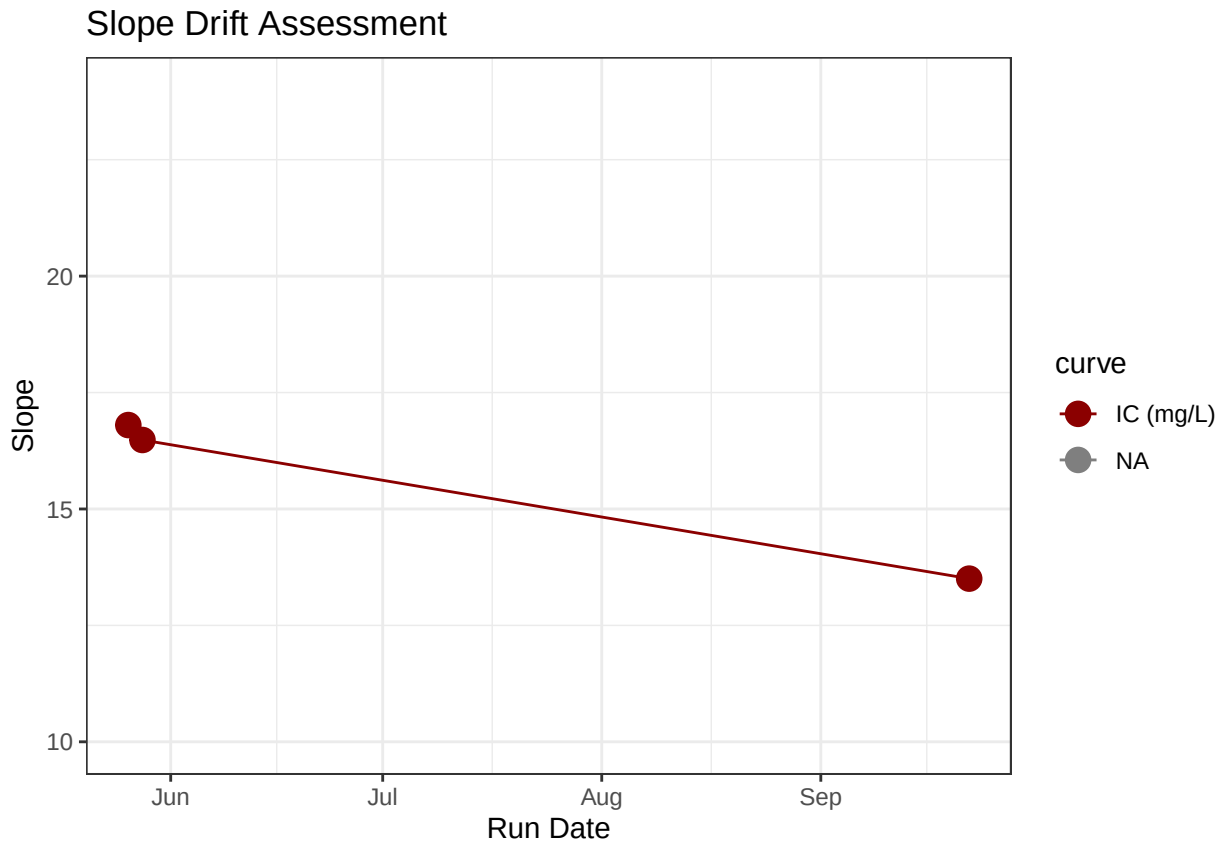
```
## Warning: One or more parsing issues, call `problems()` on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)
```

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




```
## 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()`).
```




```
## [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"
```

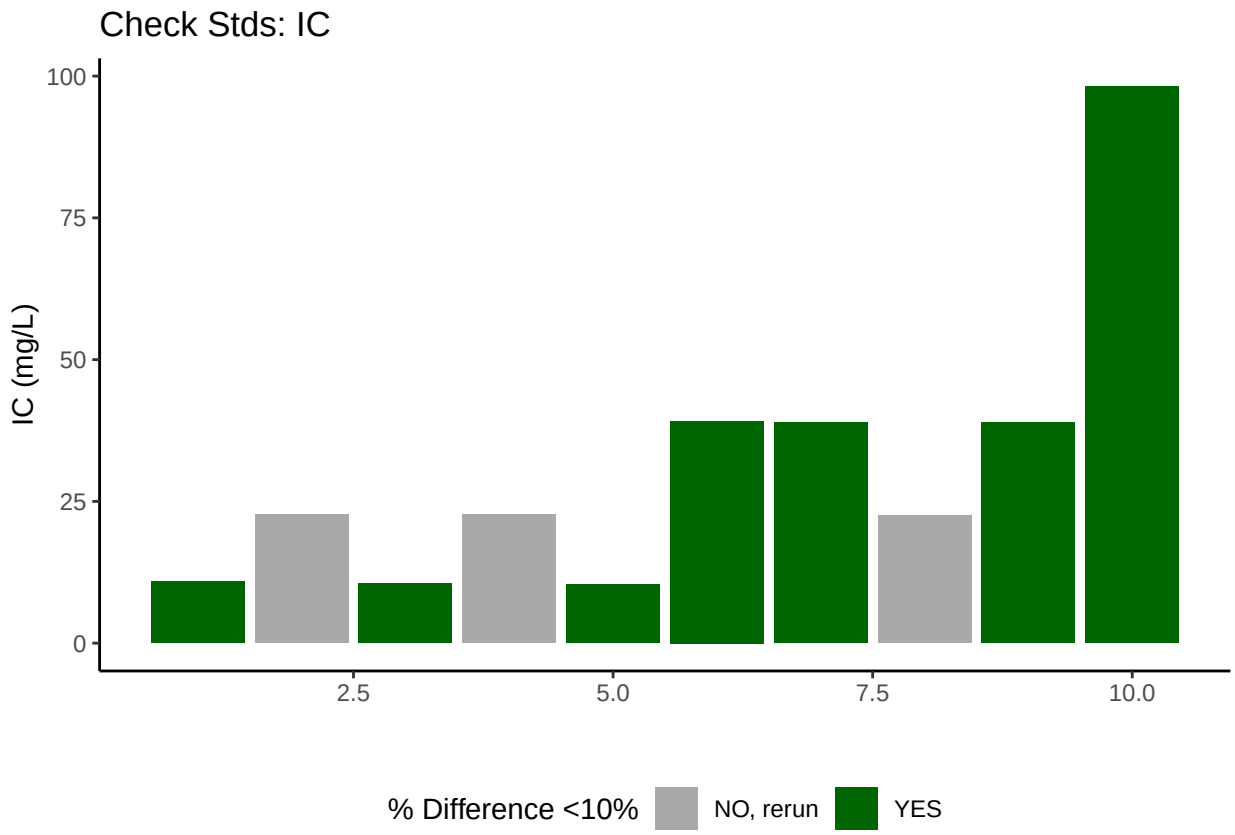
```
## Run mean = 22.63667
```

```
## Expected  = 22.19
```

0.5 Assess Check Standards

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

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



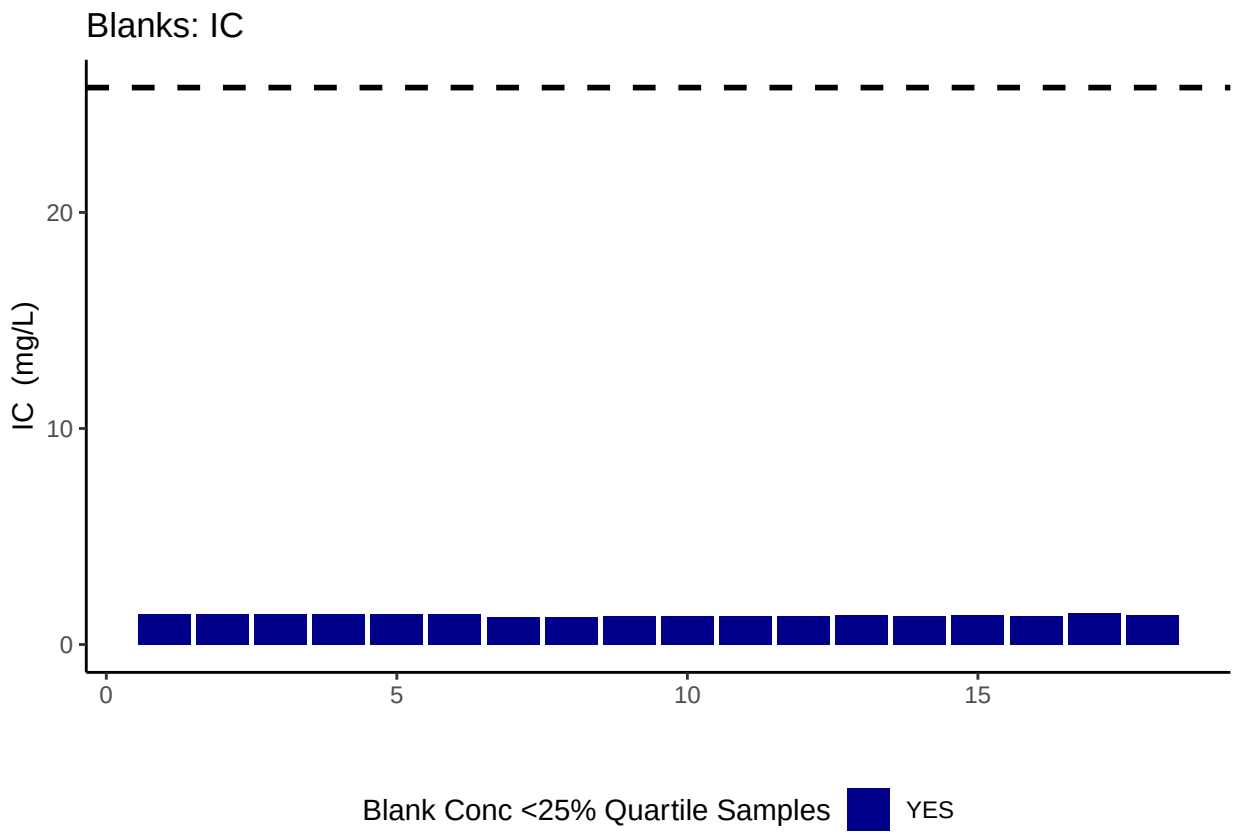

```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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

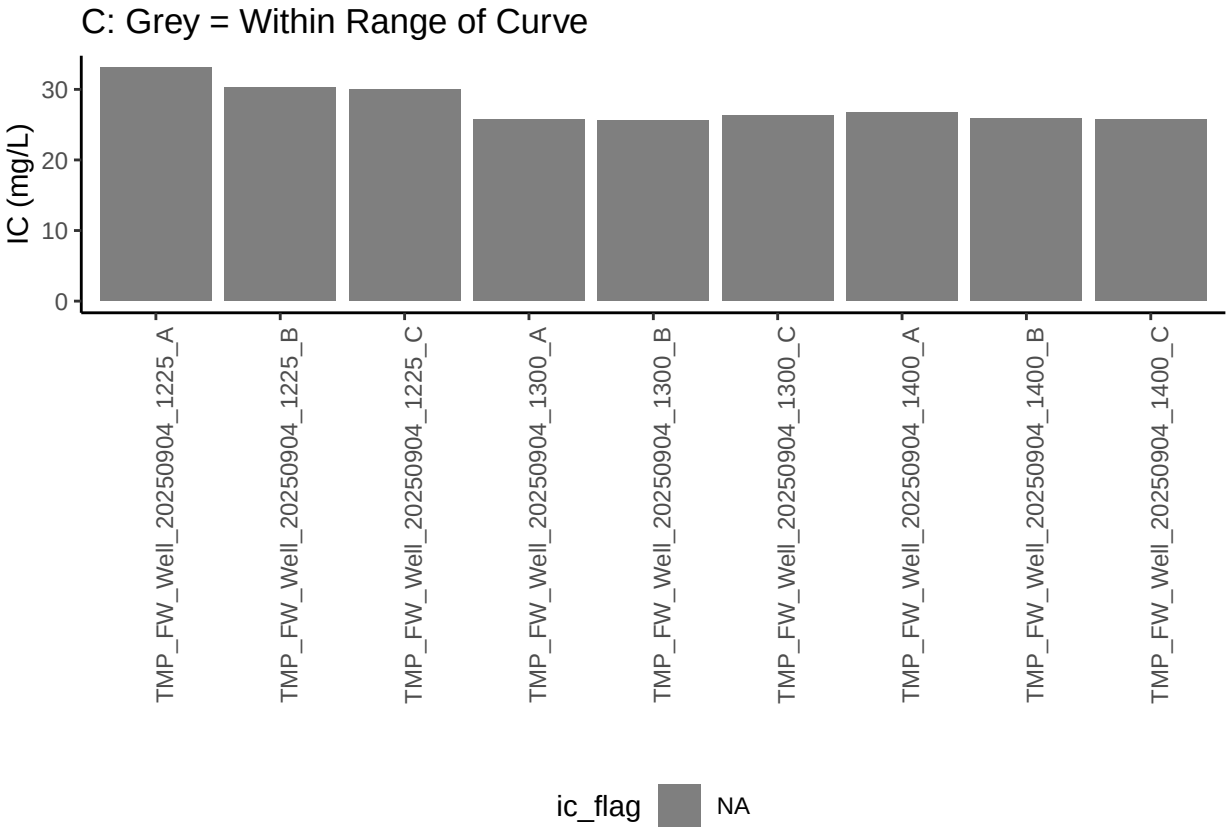



```
## carbon blanks:
```

```
## [1] 1.362
```

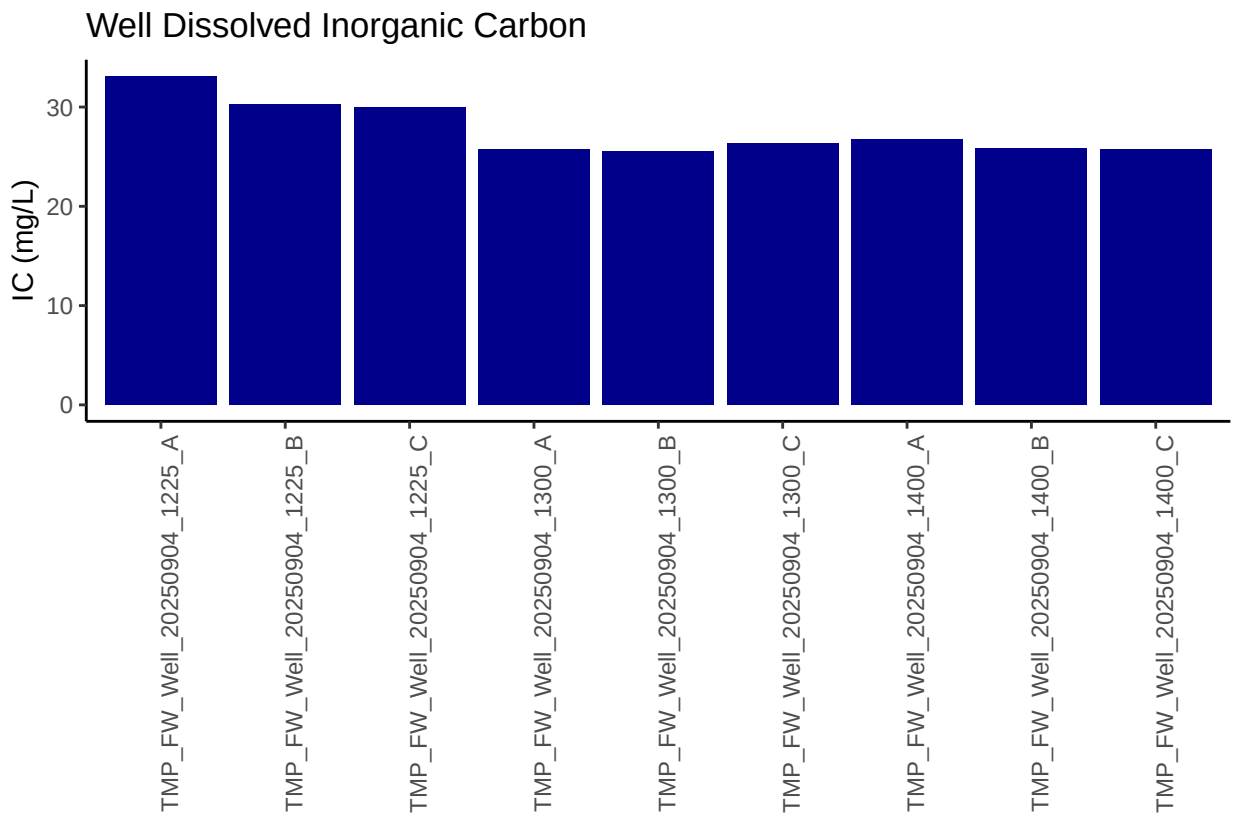
0.7 Sample Flagging - Are samples Within the range of the curve?

```
## Sample Flagging
```



0.8 Visualize Data by Plot

```
## Visualize Data
```



0.9 Convert data from mg/L to uMoles/L

0.10 Export Processed Data

```
## # A tibble: 6 x 11
##   Project Experiment  Sample_Date Sample_Time Replicate sample_name ic_mgL ic_uM
##   <chr>   <chr>       <chr>       <chr>       <chr>     <chr>        <dbl> <dbl>
## 1 COMPASS TEMPEST: W~ 2025-09-04  12:25       A         TMP_FW_Wel~   33.1 2757.
## 2 COMPASS TEMPEST: W~ 2025-09-04  12:25       B         TMP_FW_Wel~   30.2 2516.
## 3 COMPASS TEMPEST: W~ 2025-09-04  12:25       C         TMP_FW_Wel~   30.0 2497.
## 4 COMPASS TEMPEST: W~ 2025-09-04  13:00       A         TMP_FW_Wel~   25.7 2139.
## 5 COMPASS TEMPEST: W~ 2025-09-04  13:00       B         TMP_FW_Wel~   25.6 2129.
## 6 COMPASS TEMPEST: W~ 2025-09-04  13:00       C         TMP_FW_Wel~   26.3 2193.
## # i 3 more variables: ic_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>
```

#end