COMPASS: TEMPEST Discrete DIC Data QAQC

Freshwater Well Test: 2025-11-10

2025-11-25

Contents

##Setup - Change things here & write any notes

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

```
## Setup Information
```

```
###### Run information - PLEASE CHANGE
  Date_Run = "11/20/25"  #Date that instrument was run
  Run_by = "Stephanie J. Wilson"  #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = "Blanks / Background running high, may need to subtract blanks from
    sample concentrations as they were ~3 to 4mgL. The auto fill IC rxn setting was on
    at the beginning of the run, turned on by a tech during service."  #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_AquiferWellTest_202511_DIC.txt"

#file path and name for raw all peaks file
    raw_allpeaks_name = "Raw Data/TMP_AquiferWellTest_202511_DIC_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/TMP_20251110_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: 4 x 3
##   sample_name             ic_raw run_datetime
```

```
##   <chr>                     <dbl> <chr>
## 1 TMP_AquiferWell_1330       31.4 11/20/2025 9:06:51 PM
## 2 TMP_AquiferWell_1330_dup   30.8 11/20/2025 9:29:55 PM
## 3 TMP_AquiferWell_1500       34.1 11/20/2025 9:52:54 PM
## 4 TMP_AquiferWell_1500_dup   34.5 11/20/2025 10:16:09 PM
```

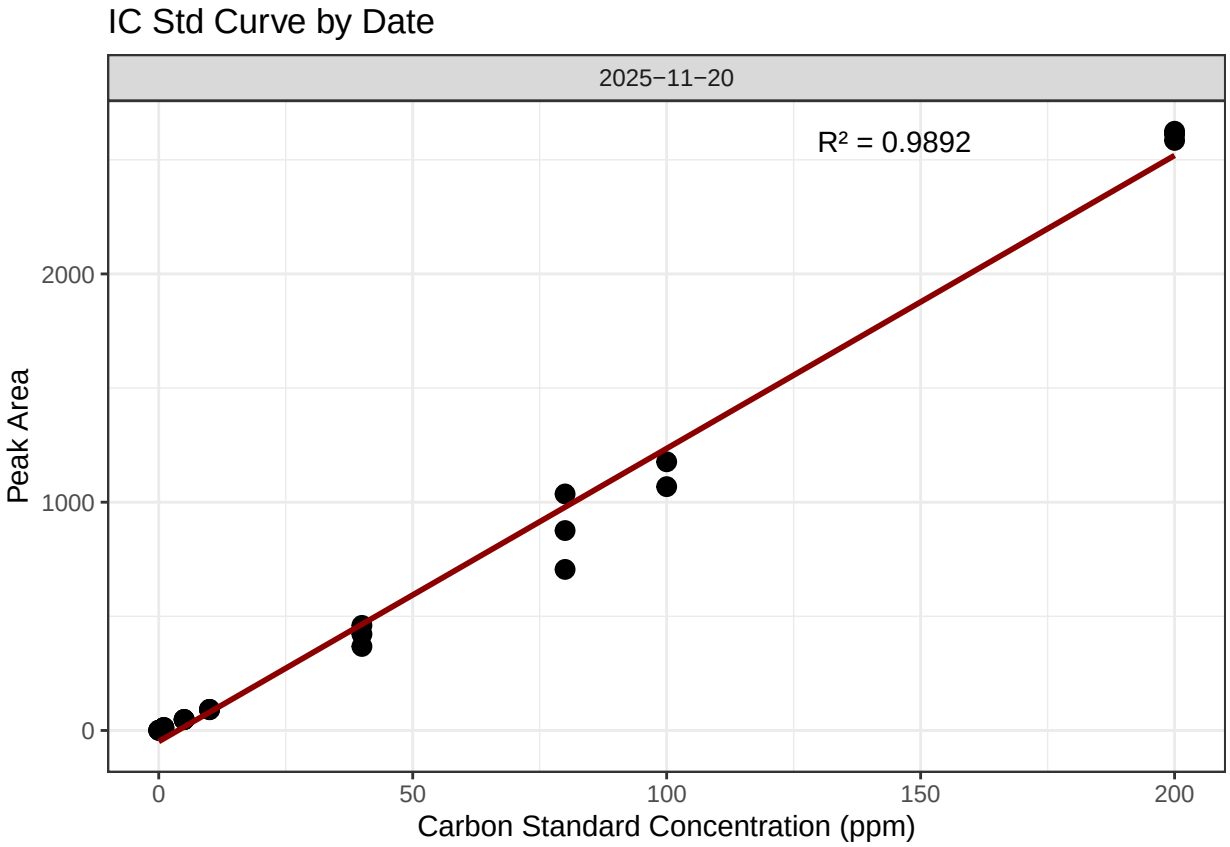
0.3 Assessing Standard Curves

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

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

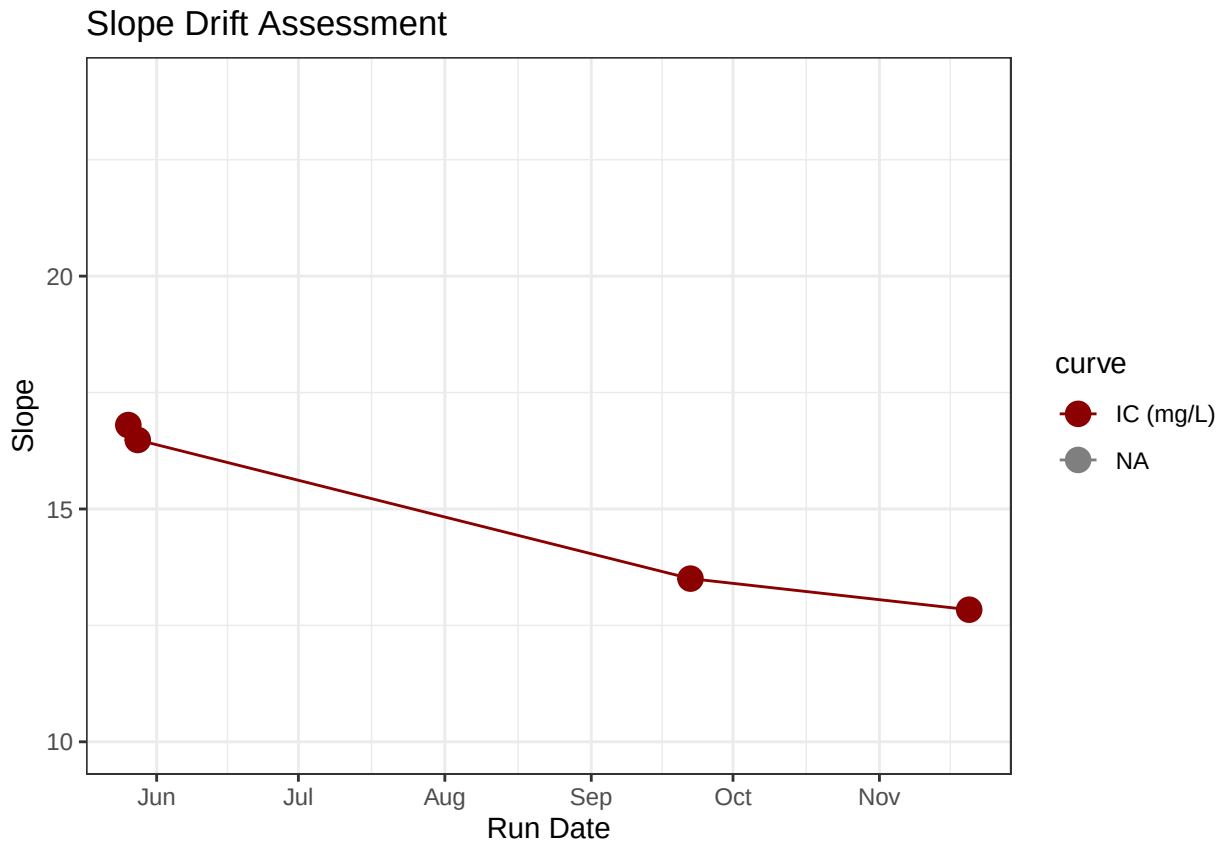
```
## Warning: One or more parsing issues, call `problems()` on your data frame for details,
## e.g.:
##   dat <- vroom(...)
##   problems(dat)
```

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




```
## 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 - REASSESS"
```

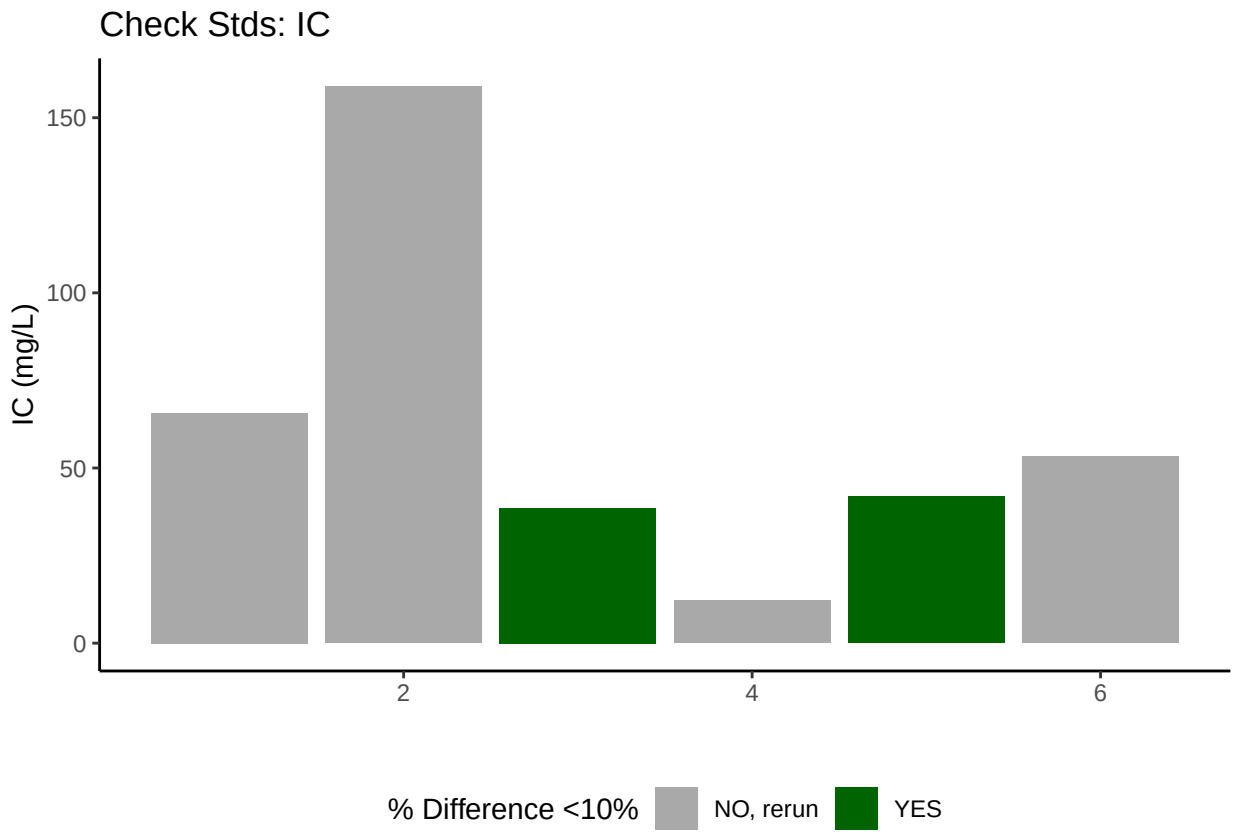
```
## Run mean = 29.16
```

```
## Expected  = 22.19
```

0.5 Assess Check Standards

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

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



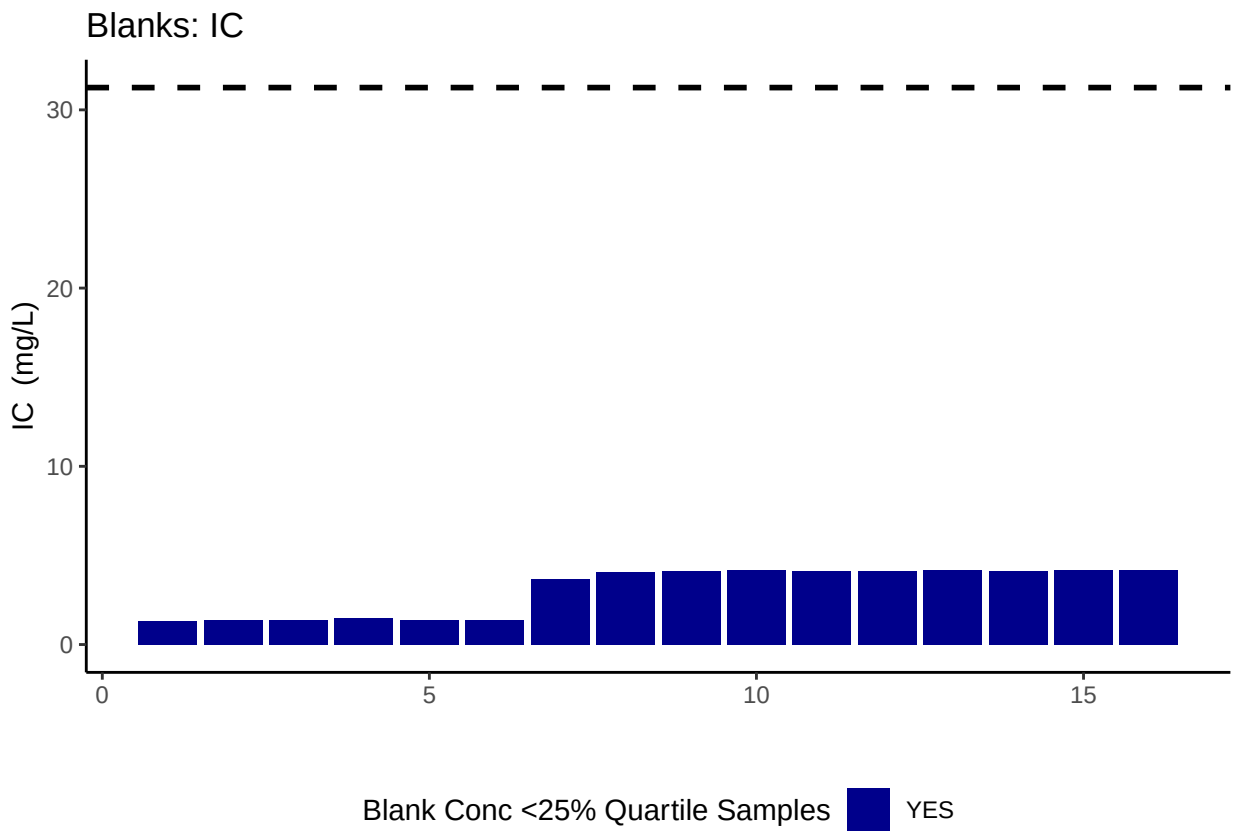

```
## [1] ">60% of IC Check Standards are within range of expected concentration"
```

0.6 Assess Blanks

```
## Assess Blanks
```

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

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

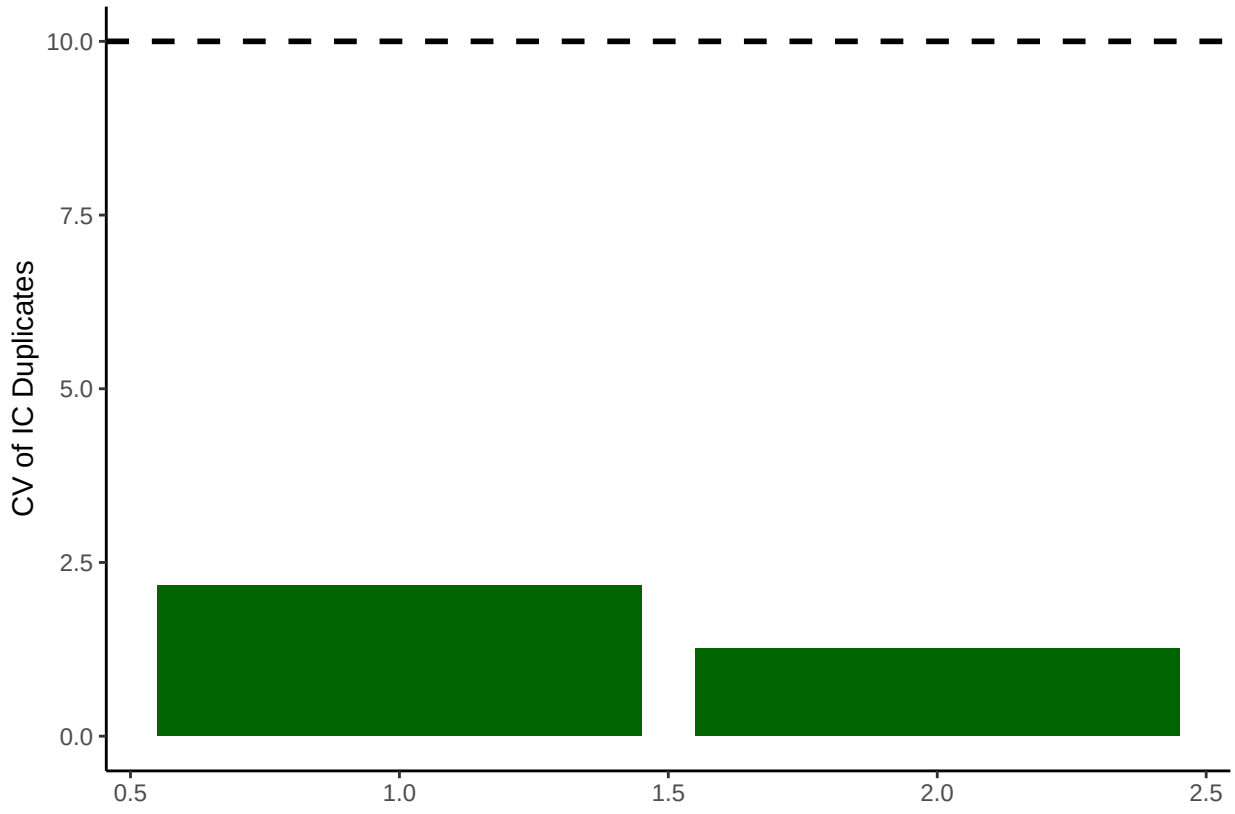



```
## carbon blanks:
```

```
## [1] 3.078562
```

0.7 Assess Duplicates

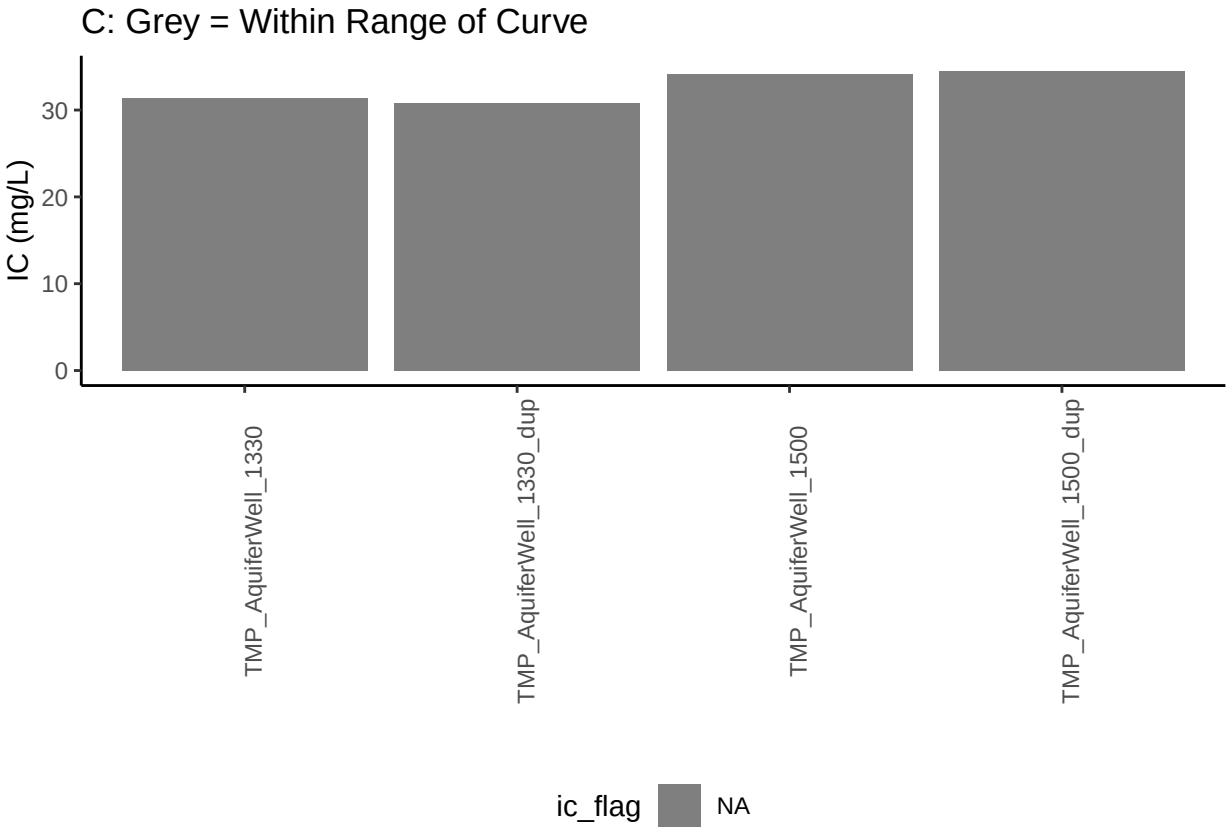
```
## Assess Duplicates
```




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

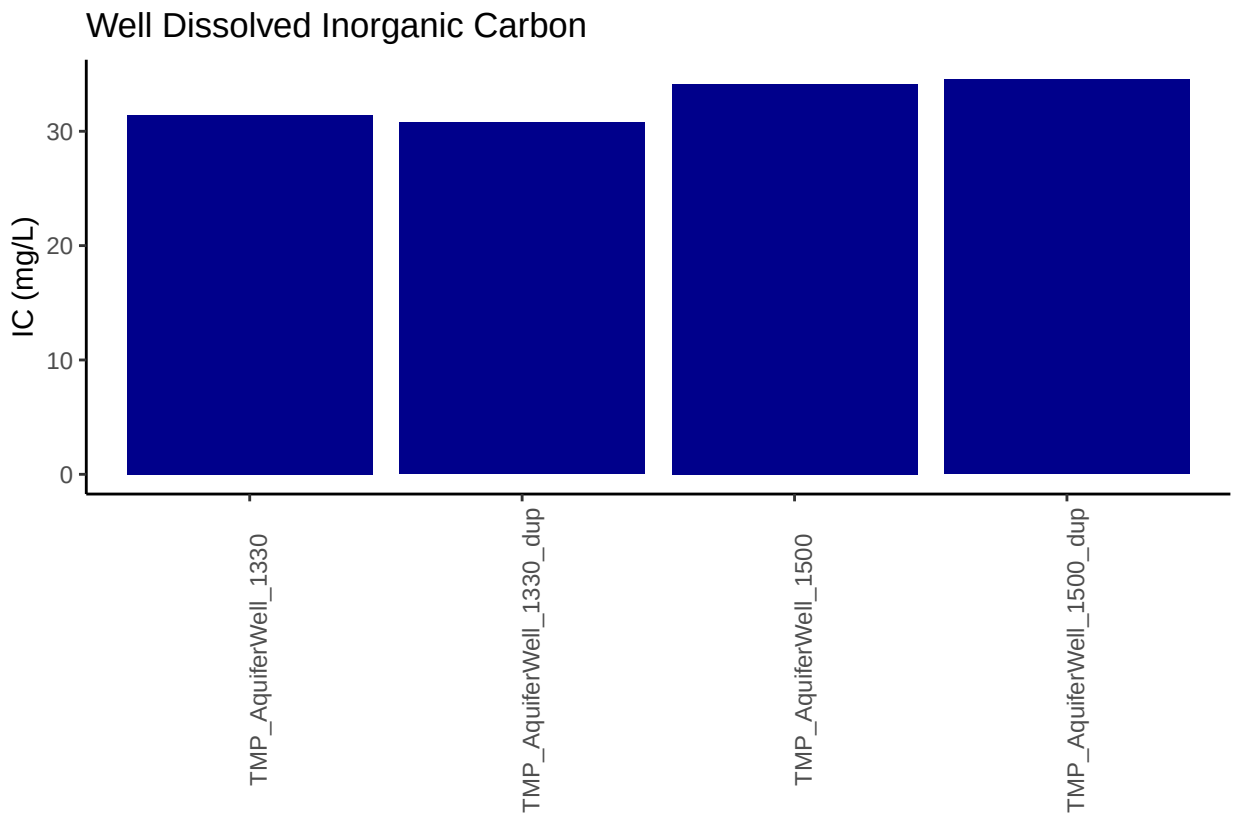
0.8 Sample Flagging - Are samples Within the range of the curve?

```
## Sample Flagging
```



0.9 Visualize Data by Plot

```
## Visualize Data
```



0.10 Convert data from mg/L to uMoles/L

0.11 Export Processed Data

```
## # A tibble: 4 x 12
##   Project Experiment   Sample_Date Sample_Time Tank_Status Replicate sample_name
##   <chr>   <chr>        <chr>       <chr>       <chr>       <chr>     <chr>
## 1 COMPASS TEMPEST: We~ 2025-11-10  13:30       half full   A         TMP_Aquife~
## 2 COMPASS TEMPEST: We~ 2025-11-10  13:30       half full   B         TMP_Aquife~
## 3 COMPASS TEMPEST: We~ 2025-11-10  15:00       full        A         TMP_Aquife~
## 4 COMPASS TEMPEST: We~ 2025-11-10  15:00       full        B         TMP_Aquife~
## # i 5 more variables: ic_mgL <dbl>, ic_uM <dbl>, ic_flag <chr>,
## #   Analysis_runtime <chr>, Run_notes <chr>
```

#end