

COMPASS_SynopticCB_PW_DIC_202505_Data

Stephanie J. Wilson

2025-05-30

##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"  
  
#qac log file path for this year  
Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAClog_2025.csv"
```

##Set Up Code

##Read in metadata and create similar sample IDs for matching to samples

Import Data Functions

Import Sample Data

```
## Import Sample Data

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

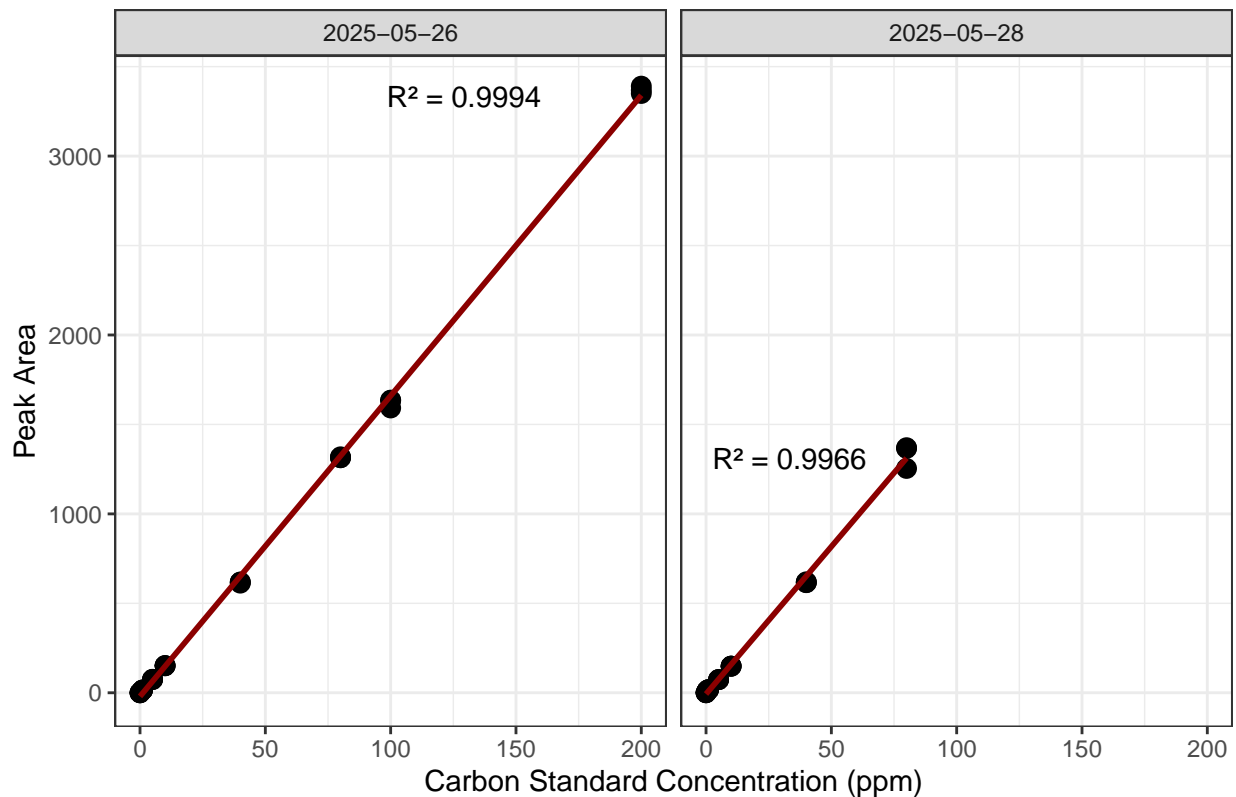
## # A tibble: 6 x 3
##   sample_name      ic_raw run_datetime
##   <chr>          <dbl> <chr>
## 1 202505_GCW_TR_LysA_20cm  13.3 5/26/2025 10:43:57 PM
## 2 202505_GCW_TR_LysB_10cm  11.0 5/26/2025 10:56:35 PM
## 3 202505_GCW_TR_LysB_20cm  16.1 5/26/2025 11:09:42 PM
## 4 202505_GCW_TR_LysC_10cm  11.5 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
```

Assessing Standard Curves

```
## Assess the Standard Curves

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

IC Std Curve by Date



```
## 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"
```

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
```

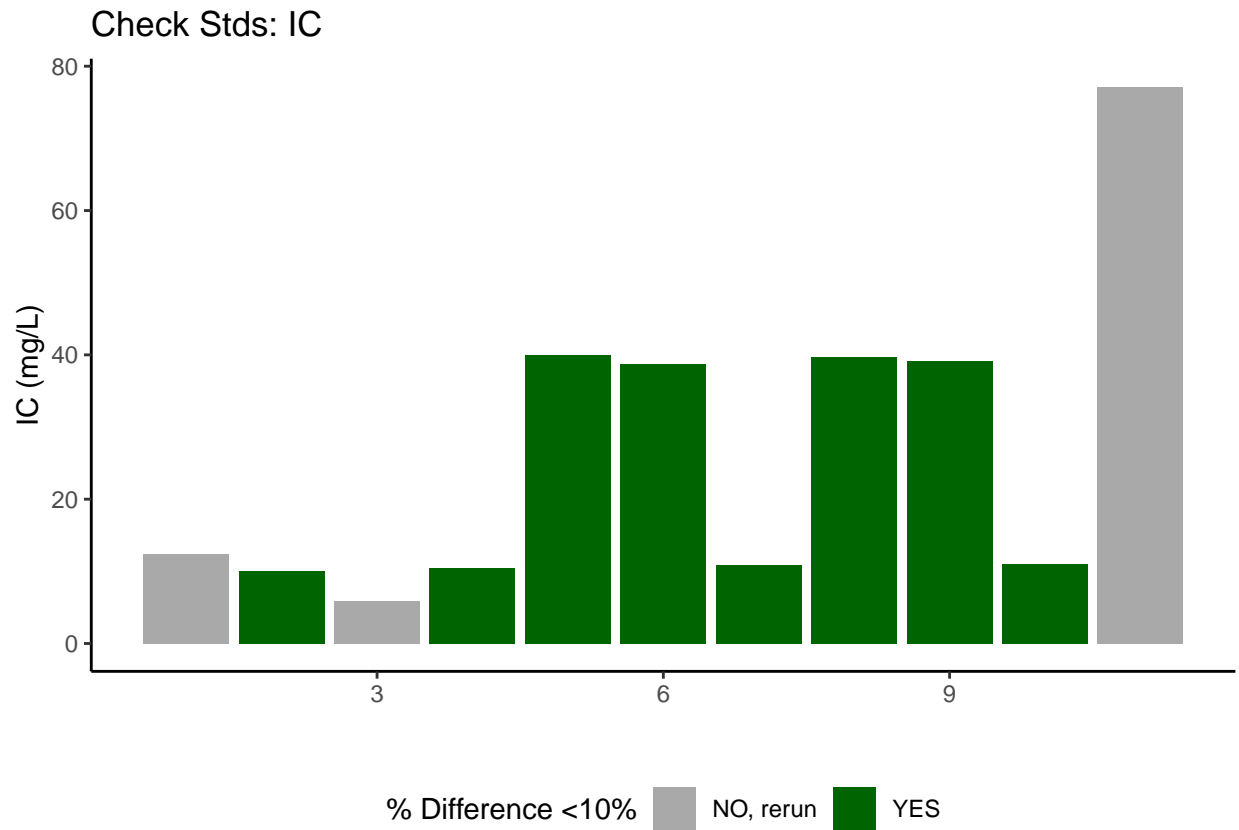
```
## Expected = 22.19
```

Assess Check Standards

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

```
## New names:
```

```
## * ' ' -> '...14'
```



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

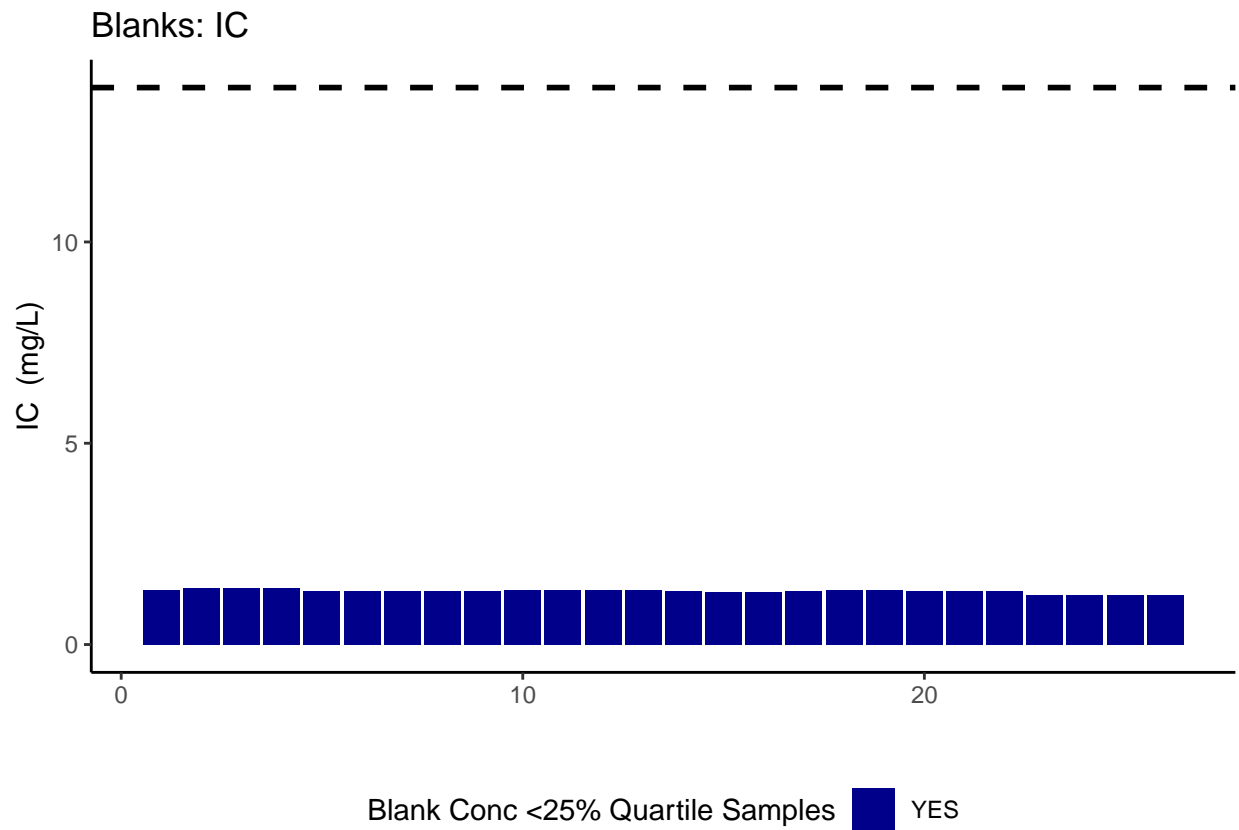
Assess Blanks

```
## Assess Blanks
```

```
## New names:
```

```
## * ' ' -> '...14'
```

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

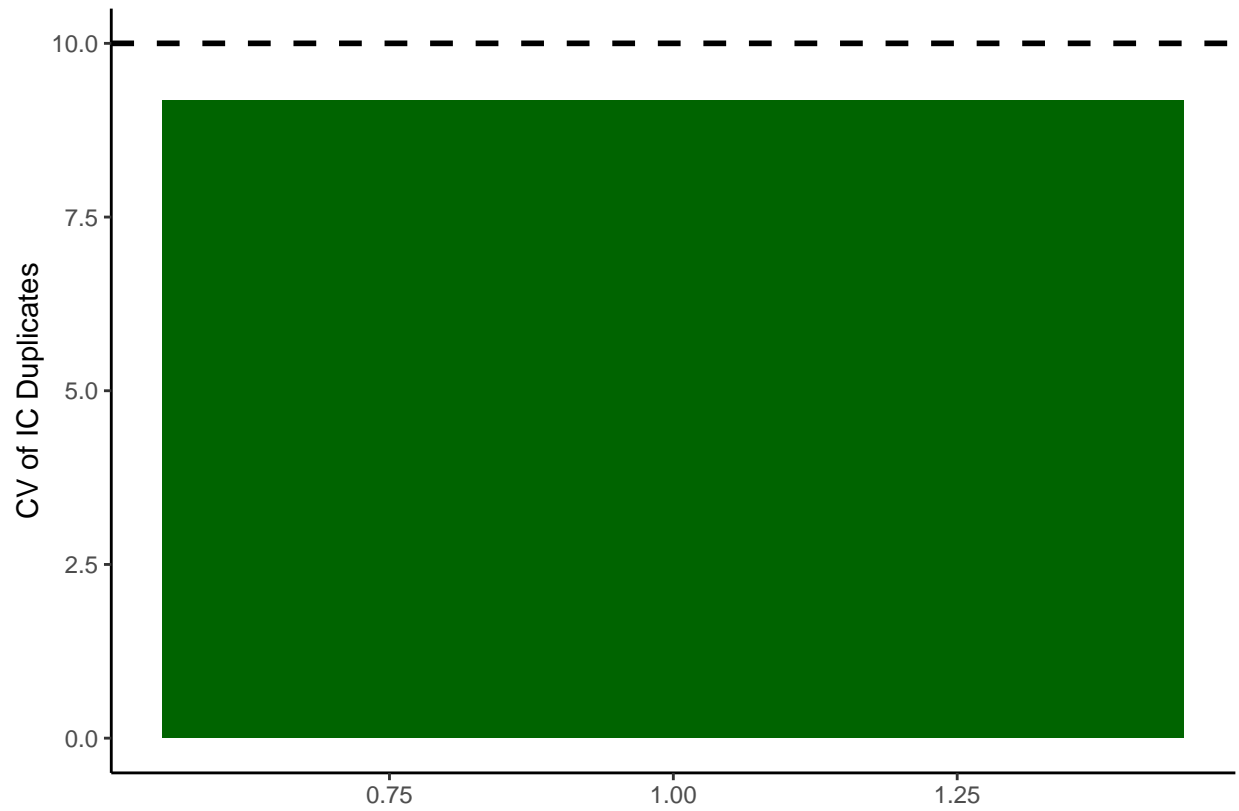


```
## carbon blanks:
```

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

Assess Duplicates

```
## Assess Duplicates
```

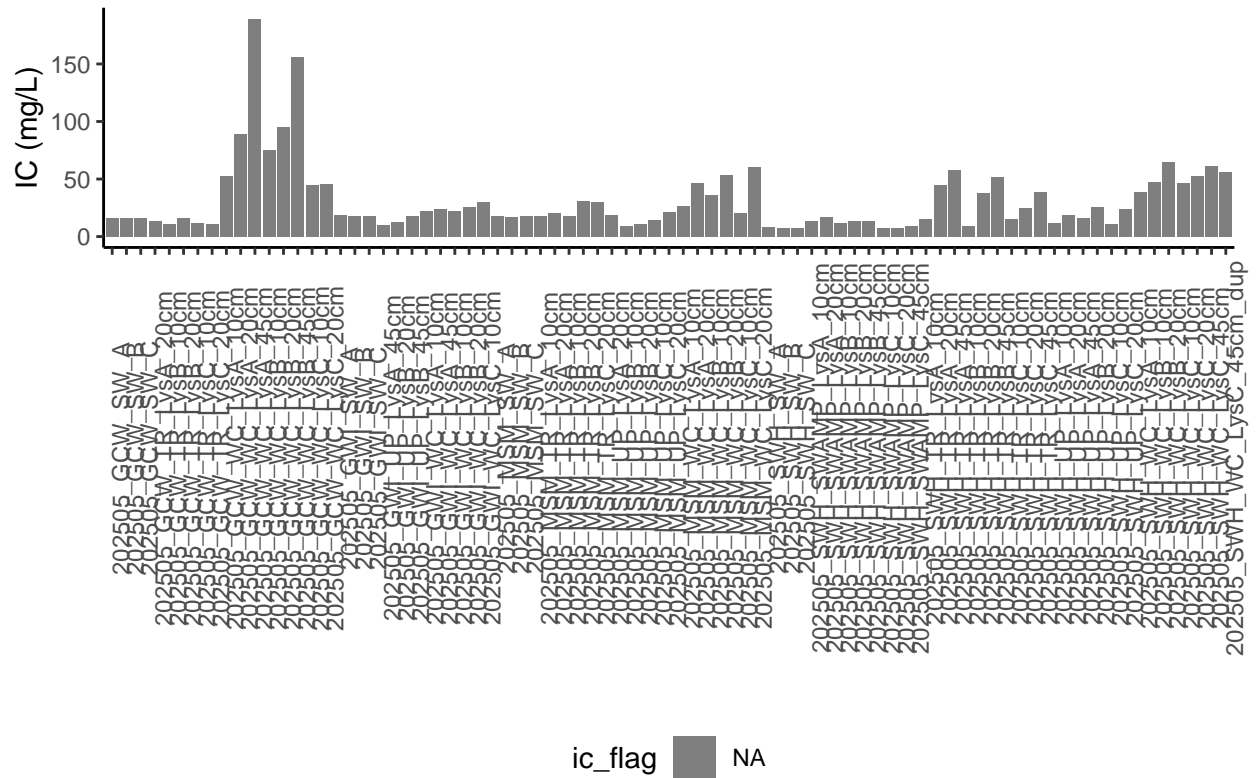


```
## [1] ">60% of Carbon Duplicates have a CV <10%"
```

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

```
## Sample Flagging
```

C: Grey = Within Range of Curve



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)
```

