COMPASS_Synoptic_TGW_2023: November Samples that got Skipped

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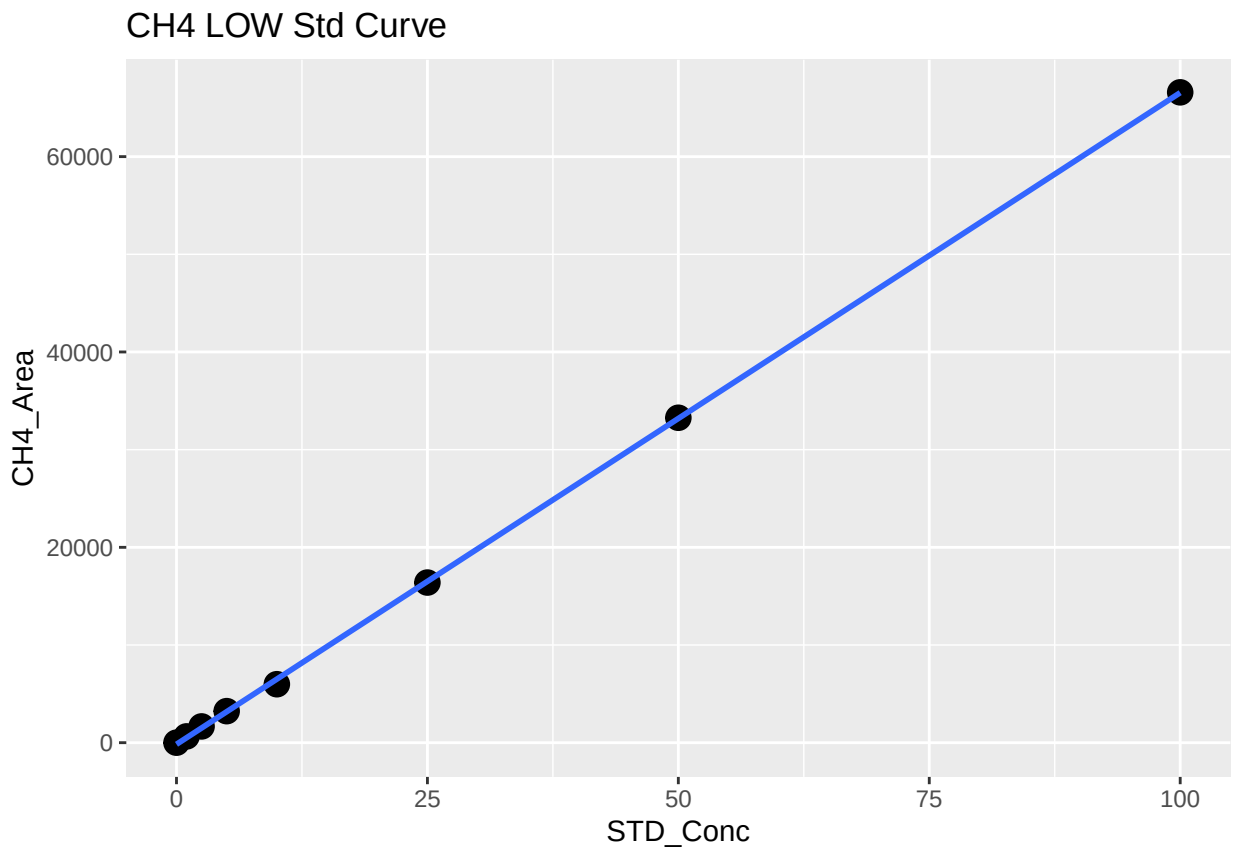
##Set Up

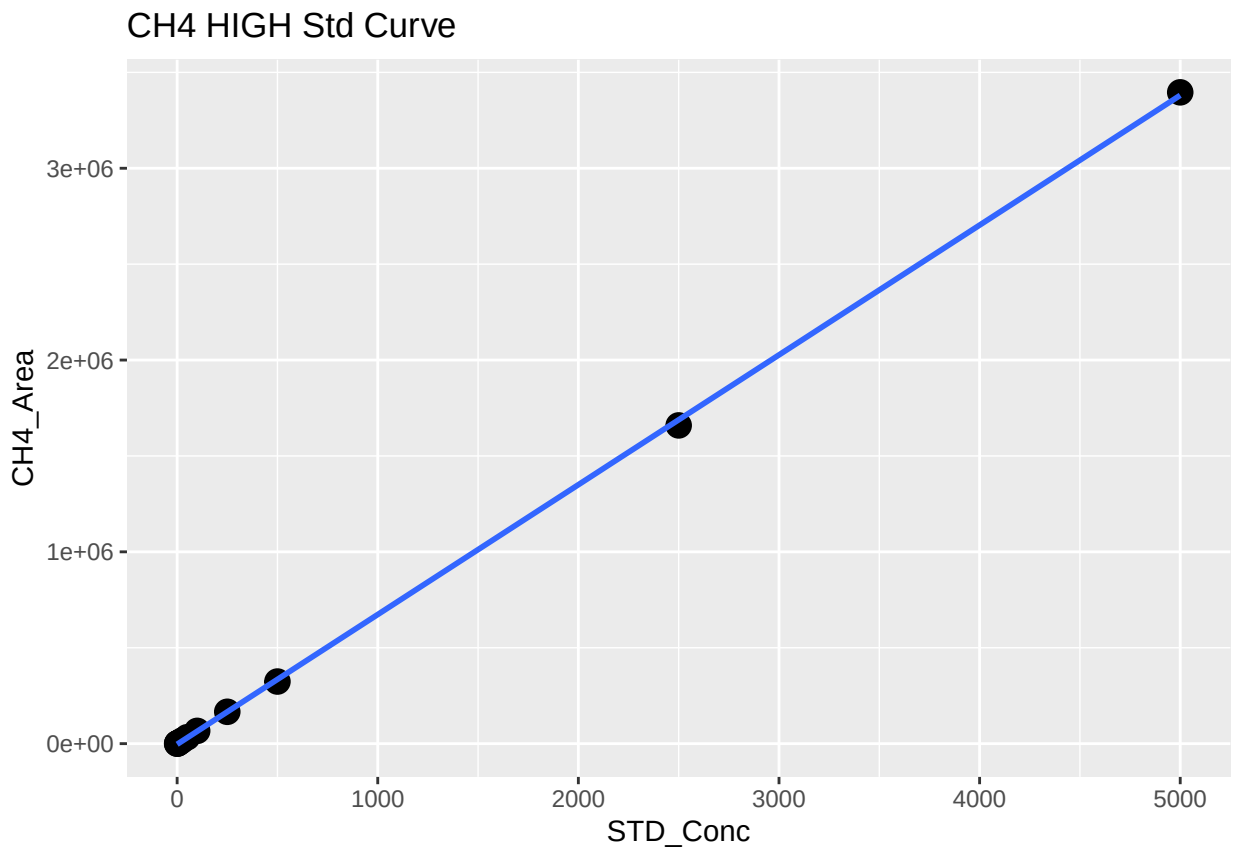
Read in first data file and assess standard curves

```
##     Machine   User Run_Date Sample_Type   Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240311       Blank   Blank        2024         <NA>
## 2 Varian GC Wegner 20240311     STD_CH4 STD_CH4        2024         <NA>
## 3 Varian GC Wegner 20240311     STD_CO2 STD_CO2        2024         <NA>
## 4 Varian GC Wegner 20240311     STD_CH4 STD_CH4        2024         <NA>
## 5 Varian GC Wegner 20240311     STD_CH4 STD_CH4        2024         <NA>
## 6 Varian GC Wegner 20240311     STD_CH4 STD_CH4        2024         <NA>
##              Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1              Blank_0               1      0.0     8170        0          NA
## 2 Blank_0_repeatforCH4               1      0.0     8170        0          NA
## 3 Blank_0_repeatforCO2               1      0.0     8170        0          NA
## 4         STD_1ppm_CH4               1      1.0    25120      642          NA
## 5       STD_2.5ppm_CH4               1      2.5    69200     1664          NA
## 6         STD_5ppm_CH4               1      5.0   141017     3228          NA
##   Lab.Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

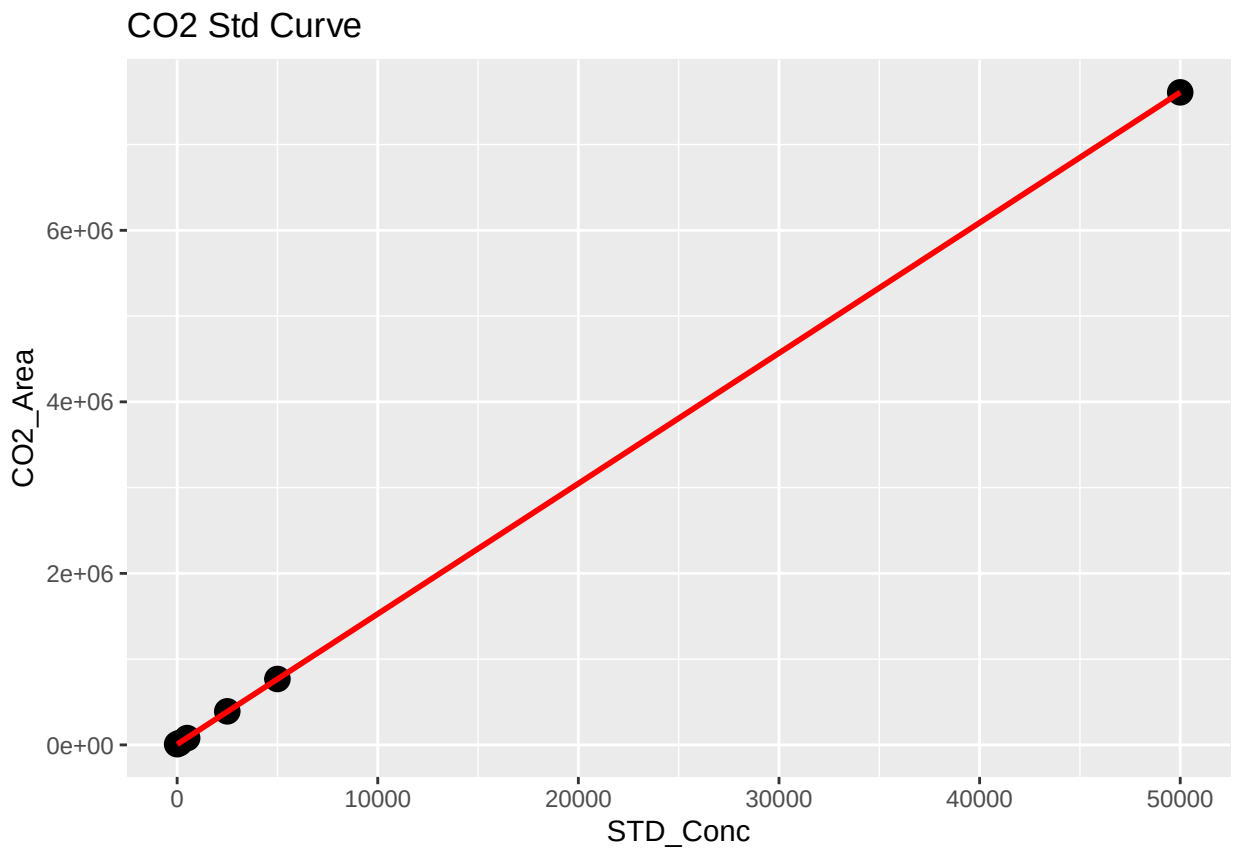
```
## `geom_smooth()` using formula = 'y ~ x'
```



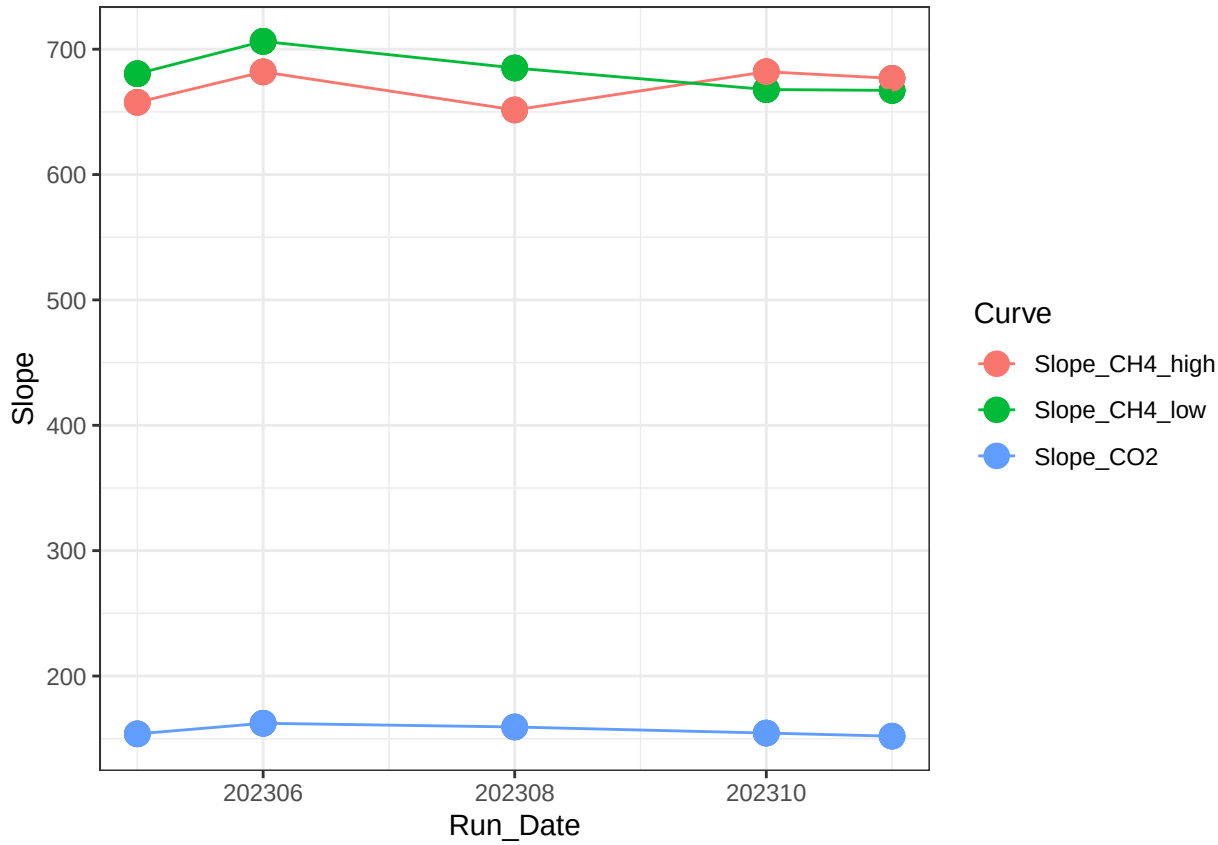

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -520.10   -2.44   66.29  146.31  166.10
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -166.101    108.922  -1.525    0.178
## stds_ch4_low$STD_Conc  667.120      2.676 249.328 2.81e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 247.8 on 6 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 6.216e+04 on 1 and 6 DF,  p-value: 2.809e-13

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -29185   1847   2900   3416  15587
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)       -3448.891   3644.622  -0.946    0.366
## stds_ch4$STD_Conc   676.747      2.247 301.204   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 11380 on 10 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 9.072e+04 on 1 and 10 DF,  p-value: < 2.2e-16

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




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##       1       2       3       4       5       6
##  1296.2 -3146.3 -3365.7  4181.7  1335.2  -301.1
##
## Coefficients:
##                     Estimate Std. Error  t value Pr(>|t|)
## (Intercept)       6.874e+03  1.505e+03    4.567   0.0103 *
## stds_co2$STD_Conc 1.520e+02  7.327e-02 2075.176 3.24e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3251 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 4.306e+06 on 1 and 4 DF,  p-value: 3.235e-13

##   X          Curve        R2    Slope Intercept Run_Date
## 1 1  Slope_CH4_low 0.9984062 680.4131 -473.3666   202305
## 2 2 Slope_CH4_high 0.9998709 657.6131 3119.1378   202305
## 3 3      Slope_CO2 0.9999897 153.8752 9651.4986   202305
## 4 4  Slope_CH4_low 0.9984062 680.4131 -473.3666   202305
## 5 5 Slope_CH4_high 0.9998709 657.6131 3119.1378   202305
## 6 6      Slope_CO2 0.9999897 153.8752 9651.4986   202305
```



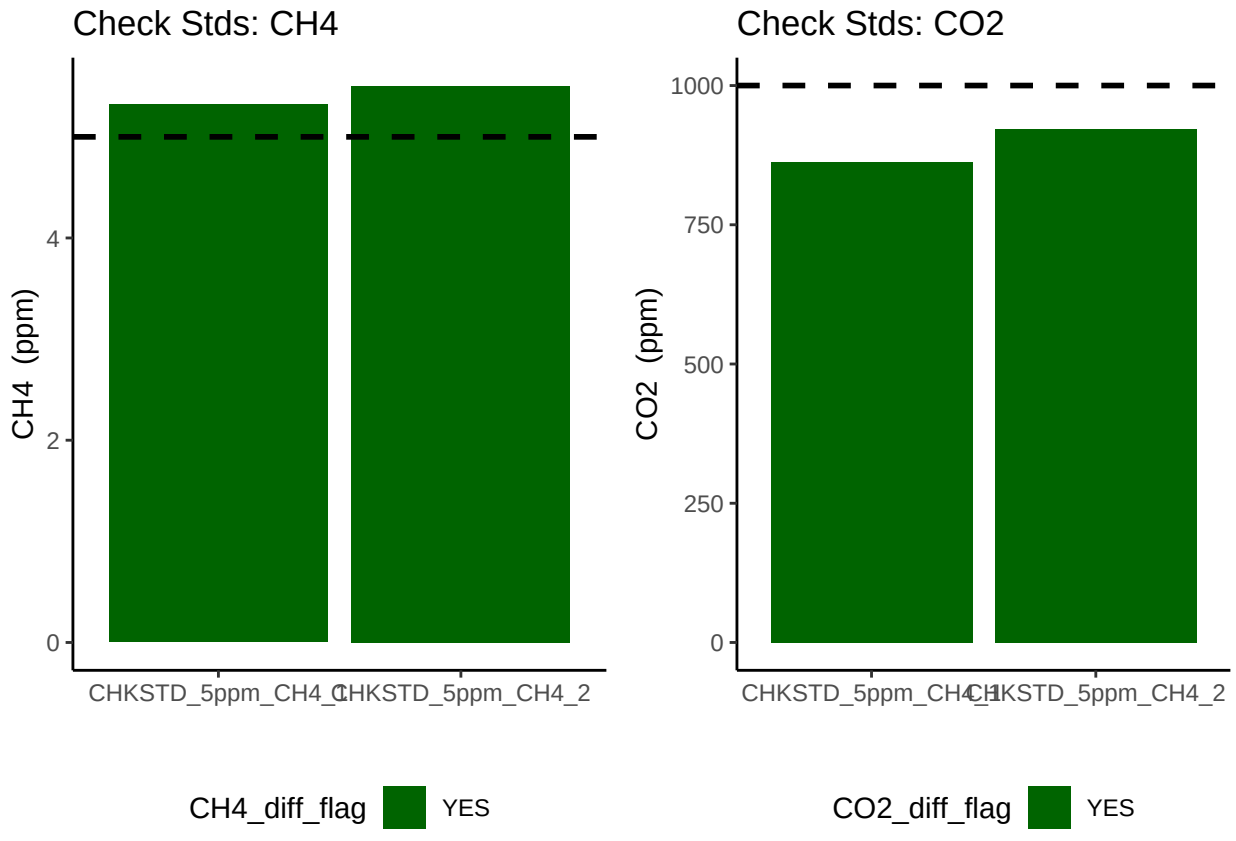
Now calculate the CH4 & CO2 concentrations in ppm

```
#head(raw)

#pull out methane standards
Samples <-  raw %>%
  filter(!str_detect(Sample_Type, "STD_CH4")) %>%
  filter(!str_detect(Sample_Type, "STD_CO2")) %>%
  filter(!str_detect(Sample_Type, "Blank")) %>%
  filter(!str_detect(Sample_Type, "Chk_STD")) %>%
   filter(!str_detect(Sample_Type, "CHKSTD")) %>%
  filter(!str_detect(Sample_Type, "CHK_STD")) %>%
    filter(!str_detect(Sample_ID, "Blank")) %>%
  filter(!str_detect(Sample_ID, "CHKSTD")) %>%
  filter(!str_detect(Sample_Type, "NA"))
#head(Samples)

#Now flag any areas that are above the 100ppm area for CH4
Samples$CH4_Curve <- ifelse(Samples$CH4_Area >71000, "High", "Low")
#head(Samples)

#Calculate CH4 concentrations in ppm
Samples$CH4_Conc_ppm <- ifelse(Samples$CH4_Area >71000, (Samples$CH4_Area-Slope_CH4_high$Intercept)/Slo
```

```r
#Calculate CO2 concentrations in ppm
Samples$CO2_Conc_ppm <- ((Samples$CO2_Area-Slope_CO2$Intercept)/Slope_CO2$Slope)

#head(Samples)

##########make flags for any dilutions needed
#highest CH4 standard = 10000
#highest CO2 standard = 50000

Samples$CH4_Flag <- ifelse(Samples$CH4_Conc_ppm >10000, "Needs Dilution", "Within Range")
Samples$CO2_Flag <- ifelse(Samples$CO2_Conc_ppm >50000, "Needs Dilution", "Within Range")
#head(Samples)
```

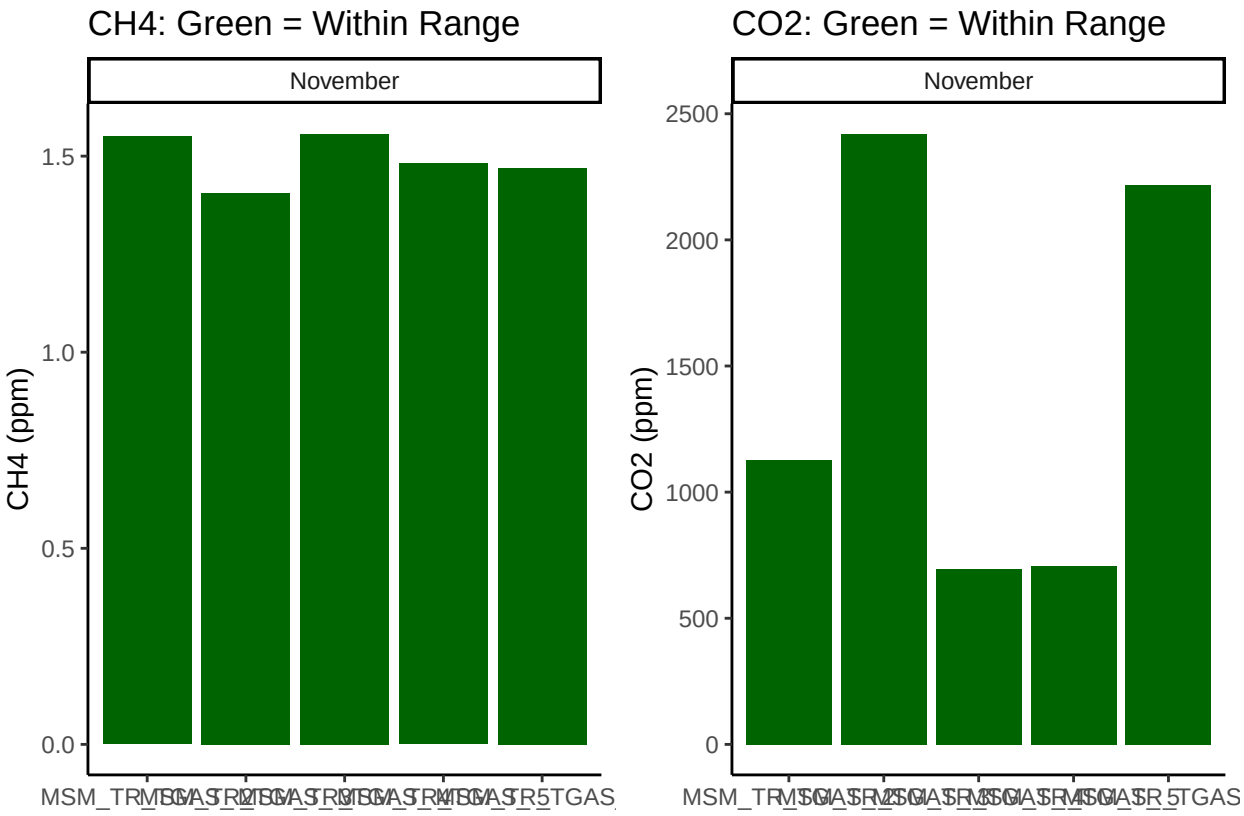
Check the Check Standards

```
## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```



Dilution correct samples

```
#multiply the concentration by the dilution factor
Samples$CH4_Conc_ppm_dilcorr <- (Samples$CH4_Conc_ppm * Samples$Dilution_Factor)

Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#check results
#head(Samples)

#quick first look at the samples
ch4_samples <-  ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
       geom_bar(stat = 'identity') +
        scale_fill_manual(values=c( "darkgreen", "red"))+
        #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
        theme_classic() + labs(x= " ", y="CH4 (ppm)", title="CH4: Green = Within Range") +
        theme(legend.position="none") +
        facet_grid(~Sample_Month)


co2_samples <-  ggplot(data = Samples, aes(x = Sample_ID, y = CO2_Conc_ppm, fill=CO2_Flag)) +
       geom_bar(stat = 'identity') +
        scale_fill_manual(values=c("darkgreen", "red"))+
        #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
        theme_classic() + labs(x= " ", y="CO2 (ppm)", title="CO2: Green = Within Range") +
        theme(legend.position="none") +
        facet_grid(~Sample_Month)

ggarrange(ch4_samples, co2_samples, nrow=1, ncol=2)
```



Write out processed data & slopes

```
#check results
head(Samples)
```

```
##     Machine   User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240311     Unknown   TGW        2023     November
## 2 Varian GC Wegner 20240311     Unknown   TGW        2023     November
## 3 Varian GC Wegner 20240311     Unknown   TGW        2023     November
## 4 Varian GC Wegner 20240311     Unknown   TGW        2023     November
## 5 Varian GC Wegner 20240311     Unknown   TGW        2023     November
##        Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1 MSM_TR_TGAS_ 2            2.83       NA   178484      868          NA
## 2 MSM_TR_TGAS_ 3            2.83       NA   374692      772          NA
## 3 MSM_TR_TGAS_ 4            2.83       NA   112466      872          NA
## 4 MSM_TR_TGAS_ 5            2.83       NA   114307      822          NA
## 5 MSM_TR_TGAS_ 6            2.83       NA   344017      815          NA
##                                                  Lab.Notes CH4_Curve
## 1 these got skipped on the first run; 10mL N2 added in the lab       Low
## 2                                  10mL N2 added in the lab       Low
## 3                                  10mL N2 added in the lab       Low
## 4                                  10mL N2 added in the lab       Low
## 5                                  10mL N2 added in the lab       Low
##   CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
```

```
## 1     1.550096    1128.6891 Within Range Within Range             4.386772
## 2     1.406194    2419.1595 Within Range Within Range             3.979529
## 3     1.556092     694.4853 Within Range Within Range             4.403740
## 4     1.481143     706.5936 Within Range Within Range             4.191634
## 5     1.470650    2217.4084 Within Range Within Range             4.161940
##   CO2_Conc_ppm_dilcorr
## 1              3194.190
## 2              6846.221
## 3              1965.393
## 4              1999.660
## 5              6275.266
```

```
#pull out what we need
Samples1 <- Samples[ ,c(1:3,5:9,13, 18:21)]
head(Samples1)
```

```
##     Machine   User Run_Date Type1 Sample_Year Sample_Month      Sample_ID
## 1 Varian GC Wegner 20240311   TGW        2023     November MSM_TR_TGAS_ 2
## 2 Varian GC Wegner 20240311   TGW        2023     November MSM_TR_TGAS_ 3
## 3 Varian GC Wegner 20240311   TGW        2023     November MSM_TR_TGAS_ 4
## 4 Varian GC Wegner 20240311   TGW        2023     November MSM_TR_TGAS_ 5
## 5 Varian GC Wegner 20240311   TGW        2023     November MSM_TR_TGAS_ 6
##   Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
## 1            2.83          NA Within Range Within Range             4.386772
## 2            2.83          NA Within Range Within Range             3.979529
## 3            2.83          NA Within Range Within Range             4.403740
## 4            2.83          NA Within Range Within Range             4.191634
## 5            2.83          NA Within Range Within Range             4.161940
##   CO2_Conc_ppm_dilcorr
## 1              3194.190
## 2              6846.221
## 3              1965.393
## 4              1999.660
## 5              6275.266
```

```
Samples1 <- Samples1 %>%
  separate(Sample_ID, into = c("Site", "Gas_Sample", "Zone", "Replicate"), sep = "_", remove = FALSE) %>%
  mutate(Tree_Code = "SF") %>%
  mutate(Tree_Info = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Sapflow Monitoring",
    TRUE ~ "Other"  # Optional: handles any values that aren't DS or SF
  )) %>%
  mutate(Status = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Living",
    TRUE ~ "Other"
  )) %>%
  mutate(Project = "COMPASS: Synoptic",
         Region = "CB") %>%
  rename( Year = Sample_Year,
          Month = Sample_Month,
          CH4_ppm = CH4_Conc_ppm_dilcorr ,
```

```
          CO2_ppm = CO2_Conc_ppm_dilcorr )  %>%
  mutate(CH4_Flag = case_when(
    CH4_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  )) %>%
  mutate(CO2_Flag = case_when(
    CO2_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  ))

final <- Samples1 %>%
  select( "Project", "Region" , "Year","Month" ,"Site", "Zone", "Gas_Sample",
          "Sample_ID", "Tree_Code", "Replicate", "Status", "Tree_Info",
          "CH4_ppm", "CH4_Flag", "CO2_ppm", "CO2_Flag")

write.csv(final, "Processed Data/COMPASS_Synoptic_TGW_202311_Processed.csv")
```

#end