PFOA 1 compartment Plots (v8)

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library(coda)  
library(bayesplot)

## This is bayesplot version 1.7.0

## - Online documentation and vignettes at mc-stan.org/bayesplot

## - bayesplot theme set to bayesplot::theme\_default()

## \* Does \_not\_ affect other ggplot2 plots

## \* See ?bayesplot\_theme\_set for details on theme setting

library(ggplot2)  
library(ggsci)  
library(khroma) # for colors  
library(tidyverse)

## ── Attaching packages ─────────────────────────────────────── tidyverse 1.3.0 ──

## ✔ tibble 2.1.3 ✔ dplyr 0.8.3  
## ✔ tidyr 1.0.0 ✔ stringr 1.4.0  
## ✔ readr 1.3.1 ✔ forcats 0.4.0  
## ✔ purrr 0.3.3

## ── Conflicts ────────────────────────────────────────── tidyverse\_conflicts() ──  
## ✖ dplyr::filter() masks stats::filter()  
## ✖ dplyr::lag() masks stats::lag()

library(reshape2)

##   
## Attaching package: 'reshape2'

## The following object is masked from 'package:tidyr':  
##   
## smiths

library(here)

## here() starts at /media/projects/Projects/PFAS\_PBPK/user/weihsueh\_2021/PFAS\_1cpt\_v8-main/PFOA\_1cpt\_v8

knitr::opts\_chunk$set(echo = TRUE, dpi = 300 )

Set up MCSim file

# this markdown file must be saved in top level directory for the following to work; the mcsim code depends on getwd results.  
mdir <- "MCSim"  
source(here::here(mdir,"setup\_MCSim.R"))  
# Make mod.exe (used to create mcsim executable from model file)  
makemod()

## The mod.exe had been created.

## Set filenames and load data

## Set up dataset

id\_lut <- multicheck$df\_check %>% select(Level) %>% unique () %>%  
 mutate(dataset = c(   
 rep("Decatur M Train", 9),  
 rep("Decatur F Train", 9),  
 rep("Arnsberg M Train", 41),  
 rep("Arnsberg F Train", 69),  
 rep("Decatur M Test", 9),  
 rep("Decatur F Test", 10),  
 rep("Arnsberg M Test", 41),  
 rep("Arnsberg F Test", 69),   
 rep("Minnesota Train", 48),  
 rep("Minnesota Test", 47),   
 'Lubeck-Bartell-Train', 'Lubeck-Bartell-Test',  
 'Little Hocking-Bartell-Train', 'Little Hocking-Bartell-Test',  
 'Little Hocking-Emmett-Test',  
 'Paulsboro-Train','Horsham-Train',  
 'Warminster-Test','Warrington-Train'  
 ),   
 Sex = c(   
 rep("M", 9),  
 rep("F", 9),  
 rep("M", 41),  
 rep("F", 69),  
 rep("M", 9),  
 rep("F", 10),  
 rep("M", 41),  
 rep("F", 69),   
 rep("Mixed",95),  
 rep('Mixed',9)),  
 City = c(   
 rep("Decatur", 18),  
 rep("Arnsberg", 110),  
 rep("Decatur", 19),  
 rep("Arnsberg", 110),  
 rep("Minnesota", 95),  
 rep('Lubeck-Bartell',2),  
 rep('Little Hocking-Bartell',2),  
 'Little Hocking-Emmett',   
 'Paulsboro','Horsham','Warminster','Warrington'),   
 Train\_Test = c(   
 rep("Train", 128),  
 rep("Test", 129),  
 rep("Train",48),  
 rep("Test",47),  
 'Train', 'Test',  
 'Train', 'Test',  
 'Test',  
 'Train','Train',  
 'Test','Test'),  
 datatype = c(  
 rep("Individual",9+9+41+69+9+10+41+69+95),  
 rep("Summary",9)),  
  
 Simulation = row\_number(),  
 variable = paste0(dataset, " ",Simulation))  
  
id\_lut$dataset <- factor(id\_lut$dataset,levels=  
 c("Decatur M Train","Decatur F Train","Arnsberg M Train",  
 "Arnsberg F Train","Decatur M Test","Decatur F Test","Arnsberg M Test",  
 "Arnsberg F Test","Minnesota Train","Minnesota Test",  
 'Lubeck-Bartell-Train', 'Lubeck-Bartell-Test',  
 'Little Hocking-Bartell-Train', 'Little Hocking-Bartell-Test',  
 'Little Hocking-Emmett-Test','Paulsboro-Train','Horsham-Train',  
 'Warminster-Test','Warrington-Train'))  
id\_lut$City <- factor(id\_lut$City,levels =   
 c("Decatur","Arnsberg","Minnesota",'Lubeck-Bartell',  
 'Little Hocking-Bartell','Little Hocking-Emmett',  
 'Paulsboro','Horsham','Warminster','Warrington'))  
  
indiv\_lut <- id\_lut %>%   
 filter(City %in% c("Decatur", "Arnsberg","Minnesota")) %>%  
 mutate( dataset = as.factor(dataset))  
  
nv <- data.frame(dataset =unique(indiv\_lut$dataset),   
 variable= rep("Pop GM", 10),  
 type= rep("Pop GM", 10), stringsAsFactors = FALSE)

## Scatter plot of predictions (median of multicheck samples) versus data.

This is a Figure 2 panel. Needed to use “scale=1.1” in ggsave to make sure “City” appeared.

nrow(multicheck$df\_check)

## [1] 312000

nrow(id\_lut)

## [1] 361

multicheck$df\_check %>% left\_join(id\_lut) %>% nrow()

## Joining, by = c("Level", "Simulation")

## [1] 312000

names(multicheck$df\_check)

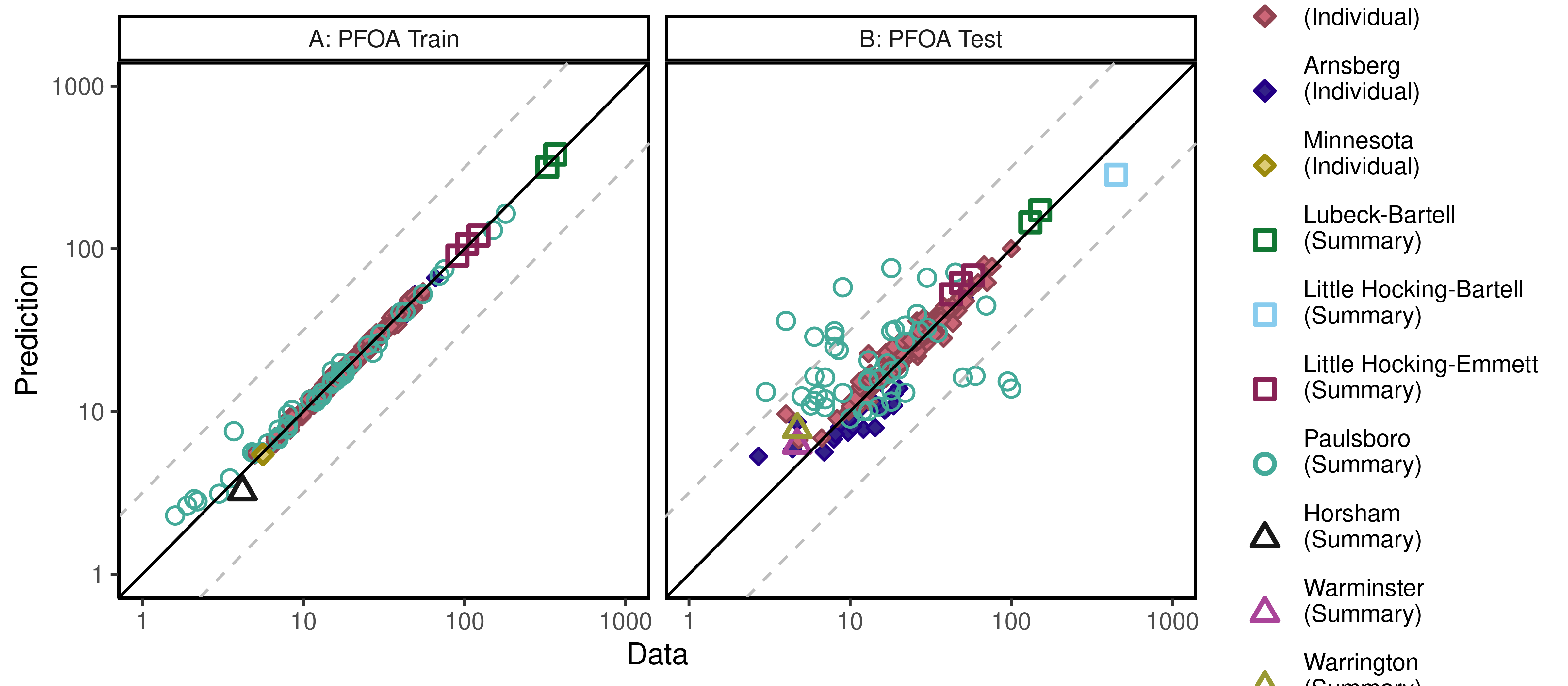
## [1] "Level" "Simulation" "Output\_Var" "Time" "Data"   
## [6] "Prediction"

multicheck2 <- multicheck$df\_check %>%   
 left\_join(id\_lut, by = c("Level", "Simulation"))%>%   
 group\_by\_at ( vars(-Prediction)) %>%   
 summarise(Prediction = median(Prediction)) %>%  
 ungroup() %>%  
 group\_by(City) %>%   
 mutate(Train\_Test = factor(Train\_Test, levels = c("Train", "Test")),  
 `City (datatype)` = factor (paste0(City, "\n(", datatype, ")\n") ),  
 label = case\_when(Train\_Test=="Train" ~ "A: PFOA Train",  
 Train\_Test=="Test" ~ "B: PFOA Test",  
 TRUE ~ ""))

## Warning in mutate\_impl(.data, dots, caller\_env()): Unequal factor levels:  
## coercing to character

## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector  
  
## Warning in mutate\_impl(.data, dots, caller\_env()): binding character and factor  
## vector, coercing into character vector

#define color for testing boxplots  
bp\_cols <- c (as.character (khroma::colour("muted")(9)) , "#191919")   
bp\_cols <-bp\_cols[c(1:7,10:8)]# plot\_scheme\_colourblind(bp\_cols)   
  
### Create aesthetics lookup  
aes\_lut <- multicheck2 %>% ungroup() %>%   
 group\_by(City, datatype, `City (datatype)` ) %>% summarise () %>% ungroup() %>%  
 mutate( cols = bp\_cols, city\_fills = bp\_cols ,   
 # for individual level on point plot (multicheck2), darken outlines for visibility, use standard colors otherwise  
 city\_outlines = if\_else(datatype == "Individual" , colorspace::darken(city\_fills, 0.3), city\_fills) ,   
 shapes = case\_when(datatype == "Individual" & `City` %in% c('Decatur', 'Arnsberg', 'Minnesota') ~ 23,  
 datatype == "Summary" &`City` %in% c("Horsham", "Warminster", "Warrington") ~ 2,  
 datatype == "Summary" & `City` %in%  
 c("Lubeck-Bartell", "Little Hocking-Bartell", "Little Hocking-Emmett") ~ 0,  
 datatype == "Summary" & `City` == "Paulsboro" ~ 1,  
 TRUE ~ 18 ),   
 size = if\_else(datatype =="Individual", 1.75, 2.5 ) )   
  
source( paste0(gsub(basename(here()), 'shared\_functions', here()), '/plot\_scatter\_mcheck.r'))  
  
p2 <- plot\_scatter\_mcheck(dframe = multicheck2, pfas\_nom = pfas\_name, aes\_lut\_fn = aes\_lut )  
print(p2)



ggsave(here ("output-plots", paste0( sa,"multicheckplot\_", pfas\_name,  
 ".pdf")),p2,dpi=600, scale=1.1)

## Saving 8.8 x 3.85 in image

## Parse multicheck

df\_check <- multicheck$df\_check  
df\_check <- subset(df\_check,Data > 0)   
  
n1 <- nrow(df\_check)  
id\_chks <- df\_check %>% select(Level) %>% unique() %>% bind\_cols(id\_lut) %>%  
 mutate(dataset = as.factor(dataset), Sex = as.factor(Sex), City = as.factor(City),   
 Train\_Test = as.factor(Train\_Test))  
  
df\_check <- df\_check %>% left\_join(id\_chks)%>%  
 mutate(Dataset = paste(as.character(dataset), Simulation),  
 Sex = ordered(Sex, levels = c("M", "F", "Mixed"),   
 labels = c("Female", "Male", "Mixed (all sexes)")))

## Joining, by = c("Level", "Simulation")

df\_check$Dataset = factor(df\_check$Dataset, levels =  
 unique(paste(as.character(df\_check$dataset), df\_check$Simulation)))  
n2 <- nrow(df\_check)  
if(n1 != n2)print("duplicates created in id-lut join")

df\_check$Time.desc <- as.character(paste0("T=",df\_check$Time))  
df\_check$Time.desc[df\_check$Time.desc == "T=1e-06"] <- "SteadyState"  
df\_check$Dataset.Time <- interaction(df\_check$Dataset,  
 df\_check$Time.desc,lex.order=TRUE)  
df\_check$Dataset.Time <- factor(df\_check$Dataset.Time,  
 levels=levels(df\_check$Dataset.Time))  
calibdata <- df\_check[,names(df\_check) != "Prediction"]  
calibdata <- calibdata[!duplicated(calibdata),]  
print(calibdata)

## Level Simulation Output\_Var Time Data Level1  
## 1 1\_1\_1 1 Cserum\_t 0.000000 41.000 1\_1\_1  
## 2 1\_1\_1 1 Cserum\_t 5.802000 29.300 1\_1\_1  
## 3 1\_1\_2 2 Cserum\_t 0.000000 13.100 1\_1\_2  
## 4 1\_1\_2 2 Cserum\_t 5.802000 10.300 1\_1\_2  
## 5 1\_1\_3 3 Cserum\_t 0.000000 25.700 1\_1\_3  
## 6 1\_1\_3 3 Cserum\_t 5.802000 10.100 1\_1\_3  
## 7 1\_1\_4 4 Cserum\_t 0.000000 47.700 1\_1\_4  
## 8 1\_1\_4 4 Cserum\_t 5.802000 11.300 1\_1\_4  
## 9 1\_1\_5 5 Cserum\_t 0.000000 51.200 1\_1\_5  
## 10 1\_1\_5 5 Cserum\_t 5.802000 19.300 1\_1\_5  
## 11 1\_1\_6 6 Cserum\_t 0.000000 12.600 1\_1\_6  
## 12 1\_1\_6 6 Cserum\_t 5.802000 9.800 1\_1\_6  
## 13 1\_1\_7 7 Cserum\_t 0.000000 44.300 1\_1\_7  
## 14 1\_1\_7 7 Cserum\_t 5.802000 12.700 1\_1\_7  
## 15 1\_1\_8 8 Cserum\_t 0.000000 47.400 1\_1\_8  
## 16 1\_1\_8 8 Cserum\_t 5.802000 15.600 1\_1\_8  
## 17 1\_1\_9 9 Cserum\_t 0.000000 19.600 1\_1\_9  
## 18 1\_1\_9 9 Cserum\_t 5.802000 12.700 1\_1\_9  
## 19 1\_1\_10 10 Cserum\_t 0.000000 7.600 1\_1\_10  
## 20 1\_1\_10 10 Cserum\_t 5.802000 5.500 1\_1\_10  
## 21 1\_1\_11 11 Cserum\_t 0.000000 46.100 1\_1\_11  
## 22 1\_1\_11 11 Cserum\_t 5.802000 30.900 1\_1\_11  
## 23 1\_1\_12 12 Cserum\_t 0.000000 10.900 1\_1\_12  
## 24 1\_1\_12 12 Cserum\_t 5.802000 9.800 1\_1\_12  
## 25 1\_1\_13 13 Cserum\_t 0.000000 6.700 1\_1\_13  
## 26 1\_1\_13 13 Cserum\_t 5.802000 7.300 1\_1\_13  
## 27 1\_1\_14 14 Cserum\_t 0.000000 65.900 1\_1\_14  
## 28 1\_1\_14 14 Cserum\_t 5.802000 31.500 1\_1\_14  
## 29 1\_1\_15 15 Cserum\_t 0.000000 49.100 1\_1\_15  
## 30 1\_1\_15 15 Cserum\_t 5.802000 42.400 1\_1\_15  
## 31 1\_1\_16 16 Cserum\_t 0.000000 13.000 1\_1\_16  
## 32 1\_1\_16 16 Cserum\_t 5.802000 8.500 1\_1\_16  
## 33 1\_1\_17 17 Cserum\_t 0.000000 45.500 1\_1\_17  
## 34 1\_1\_17 17 Cserum\_t 5.802000 17.700 1\_1\_17  
## 35 1\_1\_18 18 Cserum\_t 0.000000 34.300 1\_1\_18  
## 36 1\_1\_18 18 Cserum\_t 5.802000 15.000 1\_1\_18  
## 37 1\_2\_1 19 Cserum\_t 0.000000 15.700 1\_2\_1  
## 38 1\_2\_1 19 Cserum\_t 0.982900 16.000 1\_2\_1  
## 39 1\_2\_2 20 Cserum\_t 0.000000 14.300 1\_2\_2  
## 40 1\_2\_2 20 Cserum\_t 0.982900 15.000 1\_2\_2  
## 41 1\_2\_3 21 Cserum\_t 0.000000 40.500 1\_2\_3  
## 42 1\_2\_3 21 Cserum\_t 0.982900 32.000 1\_2\_3  
## 43 1\_2\_4 22 Cserum\_t 0.000000 45.000 1\_2\_4  
## 44 1\_2\_4 22 Cserum\_t 0.982900 48.000 1\_2\_4  
## 45 1\_2\_5 23 Cserum\_t 0.000000 38.330 1\_2\_5  
## 46 1\_2\_5 23 Cserum\_t 0.982900 32.000 1\_2\_5  
## 47 1\_2\_6 24 Cserum\_t 0.000000 16.500 1\_2\_6  
## 48 1\_2\_6 24 Cserum\_t 0.982900 13.600 1\_2\_6  
## 49 1\_2\_7 25 Cserum\_t 0.000000 40.200 1\_2\_7  
## 50 1\_2\_7 25 Cserum\_t 0.982900 35.700 1\_2\_7  
## 51 1\_2\_8 26 Cserum\_t 0.000000 21.400 1\_2\_8  
## 52 1\_2\_8 26 Cserum\_t 0.982900 16.300 1\_2\_8  
## 53 1\_2\_9 27 Cserum\_t 0.000000 45.000 1\_2\_9  
## 54 1\_2\_9 27 Cserum\_t 0.982900 46.500 1\_2\_9  
## 55 1\_2\_10 28 Cserum\_t 0.000000 11.670 1\_2\_10  
## 56 1\_2\_10 28 Cserum\_t 0.982900 8.200 1\_2\_10  
## 57 1\_2\_11 29 Cserum\_t 0.000000 21.300 1\_2\_11  
## 58 1\_2\_11 29 Cserum\_t 0.982900 20.000 1\_2\_11  
## 59 1\_2\_12 30 Cserum\_t 0.000000 21.500 1\_2\_12  
## 60 1\_2\_12 30 Cserum\_t 0.982900 16.000 1\_2\_12  
## 61 1\_2\_13 31 Cserum\_t 0.000000 26.900 1\_2\_13  
## 62 1\_2\_13 31 Cserum\_t 0.982900 20.300 1\_2\_13  
## 63 1\_2\_14 32 Cserum\_t 0.000000 13.300 1\_2\_14  
## 64 1\_2\_14 32 Cserum\_t 0.982900 11.670 1\_2\_14  
## 65 1\_2\_15 33 Cserum\_t 0.000000 23.330 1\_2\_15  
## 66 1\_2\_15 33 Cserum\_t 0.982900 18.330 1\_2\_15  
## 67 1\_2\_16 34 Cserum\_t 0.000000 50.000 1\_2\_16  
## 68 1\_2\_16 34 Cserum\_t 0.982900 46.800 1\_2\_16  
## 69 1\_2\_17 35 Cserum\_t 0.000000 31.500 1\_2\_17  
## 70 1\_2\_17 35 Cserum\_t 0.982900 30.000 1\_2\_17  
## 71 1\_2\_18 36 Cserum\_t 0.000000 7.500 1\_2\_18  
## 72 1\_2\_18 36 Cserum\_t 0.982900 7.500 1\_2\_18  
## 73 1\_2\_19 37 Cserum\_t 0.000000 9.500 1\_2\_19  
## 74 1\_2\_19 37 Cserum\_t 0.982900 8.000 1\_2\_19  
## 75 1\_2\_20 38 Cserum\_t 0.000000 26.670 1\_2\_20  
## 76 1\_2\_20 38 Cserum\_t 0.982900 23.330 1\_2\_20  
## 77 1\_2\_21 39 Cserum\_t 0.000000 11.670 1\_2\_21  
## 78 1\_2\_21 39 Cserum\_t 0.982900 10.000 1\_2\_21  
## 79 1\_2\_22 40 Cserum\_t 0.000000 15.000 1\_2\_22  
## 80 1\_2\_22 40 Cserum\_t 0.982900 13.330 1\_2\_22  
## 81 1\_2\_23 41 Cserum\_t 0.000000 9.400 1\_2\_23  
## 82 1\_2\_23 41 Cserum\_t 0.982900 9.800 1\_2\_23  
## 83 1\_2\_24 42 Cserum\_t 0.000000 41.670 1\_2\_24  
## 84 1\_2\_24 42 Cserum\_t 0.982900 38.000 1\_2\_24  
## 85 1\_2\_25 43 Cserum\_t 0.000000 45.000 1\_2\_25  
## 86 1\_2\_25 43 Cserum\_t 0.982900 46.500 1\_2\_25  
## 87 1\_2\_26 44 Cserum\_t 0.000000 13.500 1\_2\_26  
## 88 1\_2\_26 44 Cserum\_t 0.982900 11.670 1\_2\_26  
## 89 1\_2\_27 45 Cserum\_t 0.000000 30.000 1\_2\_27  
## 90 1\_2\_27 45 Cserum\_t 0.982900 26.500 1\_2\_27  
## 91 1\_2\_28 46 Cserum\_t 0.000000 31.300 1\_2\_28  
## 92 1\_2\_28 46 Cserum\_t 0.982900 28.300 1\_2\_28  
## 93 1\_2\_29 47 Cserum\_t 0.000000 21.300 1\_2\_29  
## 94 1\_2\_29 47 Cserum\_t 0.982900 20.500 1\_2\_29  
## 95 1\_2\_30 48 Cserum\_t 0.000000 45.000 1\_2\_30  
## 96 1\_2\_30 48 Cserum\_t 0.982900 40.500 1\_2\_30  
## 97 1\_2\_31 49 Cserum\_t 0.000000 38.330 1\_2\_31  
## 98 1\_2\_31 49 Cserum\_t 0.982900 36.500 1\_2\_31  
## 99 1\_2\_32 50 Cserum\_t 0.000000 18.000 1\_2\_32  
## 100 1\_2\_32 50 Cserum\_t 0.982900 16.670 1\_2\_32  
## 101 1\_2\_33 51 Cserum\_t 0.000000 36.700 1\_2\_33  
## 102 1\_2\_33 51 Cserum\_t 0.982900 33.500 1\_2\_33  
## 103 1\_2\_34 52 Cserum\_t 0.000000 34.800 1\_2\_34  
## 104 1\_2\_34 52 Cserum\_t 0.982900 36.670 1\_2\_34  
## 105 1\_2\_35 53 Cserum\_t 0.000000 38.600 1\_2\_35  
## 106 1\_2\_35 53 Cserum\_t 0.982900 36.300 1\_2\_35  
## 107 1\_2\_36 54 Cserum\_t 0.000000 6.670 1\_2\_36  
## 108 1\_2\_36 54 Cserum\_t 0.982900 6.670 1\_2\_36  
## 109 1\_2\_37 55 Cserum\_t 0.000000 45.200 1\_2\_37  
## 110 1\_2\_37 55 Cserum\_t 0.982900 46.700 1\_2\_37  
## 111 1\_2\_38 56 Cserum\_t 0.000000 15.000 1\_2\_38  
## 112 1\_2\_38 56 Cserum\_t 0.982900 14.700 1\_2\_38  
## 113 1\_2\_39 57 Cserum\_t 0.000000 22.000 1\_2\_39  
## 114 1\_2\_39 57 Cserum\_t 0.982900 18.000 1\_2\_39  
## 115 1\_2\_40 58 Cserum\_t 0.000000 41.000 1\_2\_40  
## 116 1\_2\_40 58 Cserum\_t 0.982900 38.300 1\_2\_40  
## 117 1\_2\_41 59 Cserum\_t 0.000000 20.500 1\_2\_41  
## 118 1\_2\_41 59 Cserum\_t 0.982900 20.500 1\_2\_41  
## 119 1\_2\_42 60 Cserum\_t 0.000000 13.000 1\_2\_42  
## 120 1\_2\_42 60 Cserum\_t 0.982900 13.000 1\_2\_42  
## 121 1\_2\_43 61 Cserum\_t 0.000000 16.800 1\_2\_43  
## 122 1\_2\_43 61 Cserum\_t 0.982900 13.600 1\_2\_43  
## 123 1\_2\_44 62 Cserum\_t 0.000000 18.000 1\_2\_44  
## 124 1\_2\_44 62 Cserum\_t 0.982900 17.700 1\_2\_44  
## 125 1\_2\_45 63 Cserum\_t 0.000000 10.300 1\_2\_45  
## 126 1\_2\_45 63 Cserum\_t 0.982900 8.300 1\_2\_45  
## 127 1\_2\_46 64 Cserum\_t 0.000000 23.330 1\_2\_46  
## 128 1\_2\_46 64 Cserum\_t 0.982900 18.330 1\_2\_46  
## 129 1\_2\_47 65 Cserum\_t 0.000000 10.300 1\_2\_47  
## 130 1\_2\_47 65 Cserum\_t 0.982900 8.500 1\_2\_47  
## 131 1\_2\_48 66 Cserum\_t 0.000000 55.200 1\_2\_48  
## 132 1\_2\_48 66 Cserum\_t 0.982900 43.500 1\_2\_48  
## 133 1\_2\_49 67 Cserum\_t 0.000000 48.330 1\_2\_49  
## 134 1\_2\_49 67 Cserum\_t 0.982900 38.330 1\_2\_49  
## 135 1\_2\_50 68 Cserum\_t 0.000000 36.700 1\_2\_50  
## 136 1\_2\_50 68 Cserum\_t 0.982900 33.330 1\_2\_50  
## 137 1\_2\_51 69 Cserum\_t 0.000000 26.000 1\_2\_51  
## 138 1\_2\_51 69 Cserum\_t 0.982900 25.000 1\_2\_51  
## 139 1\_2\_52 70 Cserum\_t 0.000000 28.330 1\_2\_52  
## 140 1\_2\_52 70 Cserum\_t 0.982900 24.600 1\_2\_52  
## 141 1\_2\_53 71 Cserum\_t 0.000000 18.330 1\_2\_53  
## 142 1\_2\_53 71 Cserum\_t 0.982900 12.900 1\_2\_53  
## 143 1\_2\_54 72 Cserum\_t 0.000000 20.000 1\_2\_54  
## 144 1\_2\_54 72 Cserum\_t 0.982900 20.200 1\_2\_54  
## 145 1\_2\_55 73 Cserum\_t 0.000000 18.330 1\_2\_55  
## 146 1\_2\_55 73 Cserum\_t 0.982900 13.330 1\_2\_55  
## 147 1\_2\_56 74 Cserum\_t 0.000000 21.700 1\_2\_56  
## 148 1\_2\_56 74 Cserum\_t 0.982900 16.700 1\_2\_56  
## 149 1\_2\_57 75 Cserum\_t 0.000000 12.500 1\_2\_57  
## 150 1\_2\_57 75 Cserum\_t 0.982900 5.000 1\_2\_57  
## 151 1\_2\_58 76 Cserum\_t 0.000000 15.200 1\_2\_58  
## 152 1\_2\_58 76 Cserum\_t 0.982900 14.900 1\_2\_58  
## 153 1\_2\_59 77 Cserum\_t 0.000000 26.500 1\_2\_59  
## 154 1\_2\_59 77 Cserum\_t 0.982900 15.400 1\_2\_59  
## 155 1\_2\_60 78 Cserum\_t 0.000000 11.670 1\_2\_60  
## 156 1\_2\_60 78 Cserum\_t 0.982900 8.330 1\_2\_60  
## 157 1\_2\_61 79 Cserum\_t 0.000000 35.000 1\_2\_61  
## 158 1\_2\_61 79 Cserum\_t 0.982900 26.400 1\_2\_61  
## 159 1\_2\_62 80 Cserum\_t 0.000000 29.700 1\_2\_62  
## 160 1\_2\_62 80 Cserum\_t 0.982900 25.000 1\_2\_62  
## 161 1\_2\_63 81 Cserum\_t 0.000000 26.700 1\_2\_63  
## 162 1\_2\_63 81 Cserum\_t 0.982900 23.330 1\_2\_63  
## 163 1\_2\_64 82 Cserum\_t 0.000000 10.300 1\_2\_64  
## 164 1\_2\_64 82 Cserum\_t 0.982900 8.600 1\_2\_64  
## 165 1\_2\_65 83 Cserum\_t 0.000000 25.000 1\_2\_65  
## 166 1\_2\_65 83 Cserum\_t 0.982900 19.600 1\_2\_65  
## 167 1\_2\_66 84 Cserum\_t 0.000000 35.400 1\_2\_66  
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## 610 Lubeck-Bartell-Train Mixed (all sexes) Lubeck-Bartell  
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## 612 Lubeck-Bartell-Train Mixed (all sexes) Lubeck-Bartell  
## 613 Lubeck-Bartell-Test Mixed (all sexes) Lubeck-Bartell  
## 614 Lubeck-Bartell-Test Mixed (all sexes) Lubeck-Bartell  
## 615 Lubeck-Bartell-Test Mixed (all sexes) Lubeck-Bartell  
## 616 Little Hocking-Bartell-Train Mixed (all sexes) Little Hocking-Bartell  
## 617 Little Hocking-Bartell-Train Mixed (all sexes) Little Hocking-Bartell  
## 618 Little Hocking-Bartell-Test Mixed (all sexes) Little Hocking-Bartell  
## 619 Little Hocking-Bartell-Test Mixed (all sexes) Little Hocking-Bartell  
## 620 Little Hocking-Emmett-Test Mixed (all sexes) Little Hocking-Emmett  
## 621 Paulsboro-Train Mixed (all sexes) Paulsboro  
## 622 Horsham-Train Mixed (all sexes) Horsham  
## 623 Warminster-Test Mixed (all sexes) Warminster  
## 624 Warrington-Train Mixed (all sexes) Warrington  
## Train\_Test datatype variable  
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## 609 Minnesota Test 352.SteadyState  
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## 612 Lubeck-Bartell-Train 353.T=1.25  
## 613 Lubeck-Bartell-Test 354.T=0  
## 614 Lubeck-Bartell-Test 354.T=0.5  
## 615 Lubeck-Bartell-Test 354.T=1.25  
## 616 Little Hocking-Bartell-Train 355.T=0  
## 617 Little Hocking-Bartell-Train 355.T=0.75  
## 618 Little Hocking-Bartell-Test 356.T=0  
## 619 Little Hocking-Bartell-Test 356.T=0.75  
## 620 Little Hocking-Emmett-Test 357.SteadyState  
## 621 Paulsboro-Train 358.T=2.2  
## 622 Horsham-Train 359.T=2  
## 623 Warminster-Test 360.T=2  
## 624 Warrington-Train 361.T=2

#Multicheck plot  
  
# Split Steady State Group into different populations for boxplot grouping  
#df\_check[df\_check$Time.desc == "SteadyState" & grepl("Lubeck",df\_check$Dataset),]$Time.desc <- "Lubeck"  
#df\_check[df\_check$Time.desc == "SteadyState" & grepl("Little Hocking",df\_check$Dataset),]$Time.desc <- "Little Hocking"

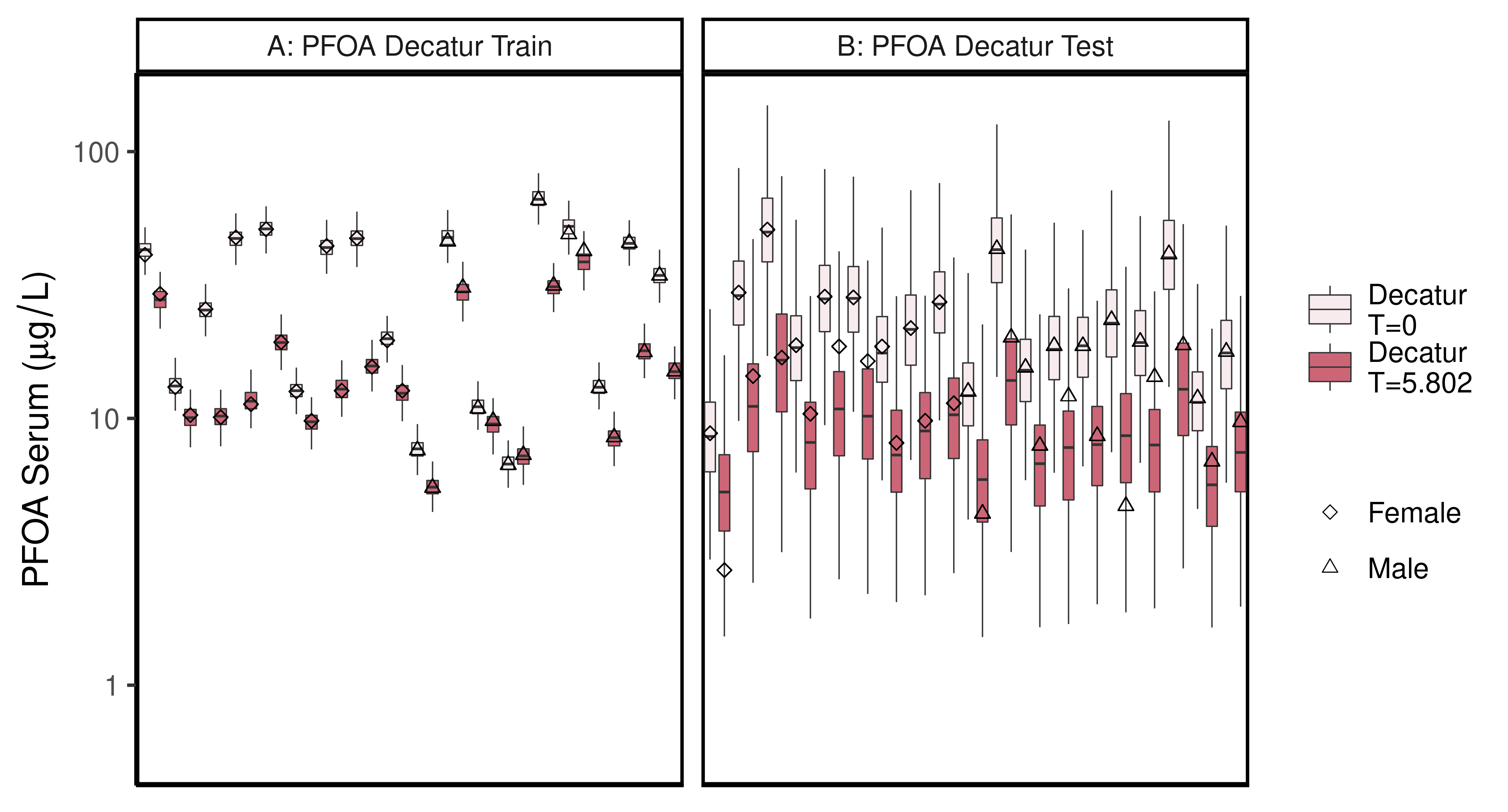
Modify aesthetics lookup table for boxplots

## additional source aesthetic lookup table for grey-scale time (years); merged legends save space on plotting output  
times <- df\_check%>% select(Time.desc, Time) %>% unique () %>%   
 mutate(rank = rank(Time) , grey = grey.colors(start=1,end=0.4, n = n()),  
 alpha = (rank)/8) %>%   
 select(-Time)  
   
df\_check <- df\_check %>% mutate (legend\_label = (paste0(City, "\n", Time.desc ) )) # add legend-labels  
aes\_lut <- df\_check %>%   
 select(City, Train\_Test, datatype,Time, Time.desc, legend\_label) %>% unique () %>%  
 left\_join(aes\_lut[, c("City", "cols")], by = "City") %>% ungroup () %>% unique ()%>%  
 left\_join (times, by = "Time.desc") %>%   
 arrange(datatype, City, Train\_Test, Time) %>%   
 mutate(alpha = if\_else(City == "Horsham", alpha/2, alpha)) %>% # otherwise too dark with this color  
 mutate\_if(is.factor, as.character)

## Decatur boxplots

Changed grey start to 1 instead of 0.8, end at 0.6 instead of 0.4. Changed shape of symbols so they are filled.

# Decatur   
  
df\_decat <- df\_check %>%   
 filter(City == "Decatur" & Train\_Test %in% c ("Train", "Test")) %>%   
 mutate(panel = ordered (Train\_Test, levels = c ("Train", "Test"),   
 labels = c("A: PFOA Decatur Train", "B: PFOA Decatur Test") ) )  
  
aes\_lut\_df\_df\_decat <- aes\_lut %>%   
 filter(City == "Decatur" & Train\_Test %in% c ("Train", "Test")) %>%   
 mutate\_if(is.factor, as.character)   
  
source( paste0(gsub(basename(here()), 'shared\_functions', here()), '/plot\_sum\_boxplot.r'))  
  
  
plt\_train <- plot\_sum\_boxplot (dframe = df\_decat, aes\_lut= aes\_lut\_df\_df\_decat, facets = TRUE , pfas\_nom = pfas\_name )   
print(plt\_train)



ggsave(here ("output-plots",paste0( sa,"DecaturTrainTestboxplot",pfas\_name,".pdf")),plt\_train,dpi=600)

## Saving 6.5 x 3.5 in image

## All boxplots

Changed grey start to 1 instead of 0.8, end at 0.6 instead of 0.4. Added shapes and fills to data points.

print(pfas\_name)

## [1] "PFOA"

lets <- LETTERS;  
names(lets)[1:(length(unique(df\_check$dataset))-4)]<-as.character(unique(df\_check$dataset))[c(3,4,7:length(unique(df\_check$dataset)))]  
  
for (d in unique(df\_check$dataset)) { # d = unique(df\_check$dataset)[11]  
  
 ddset <- df\_check %>%   
 filter(dataset == d)   
   
 aes\_lut\_ddset <- ddset %>% select(legend\_label, City,Train\_Test,datatype, Time.desc ) %>% unique () %>% inner\_join(aes\_lut)  
   
 gt <- ifelse(is.na(lets[d]),d,paste0(lets[d],": ", d))  
 plt <- plot\_sum\_boxplot(dframe = ddset, aes\_lut= aes\_lut\_ddset, gtitle= gt, facets = FALSE, pfas\_nom = pfas\_name)  
   
 print(plt)  
 ggsave(here ("output-plots",  
 paste0( sa, d,"-boxplot-",   
 pfas\_name,".pdf")) ,  
 plt,dpi=600)  
  
}

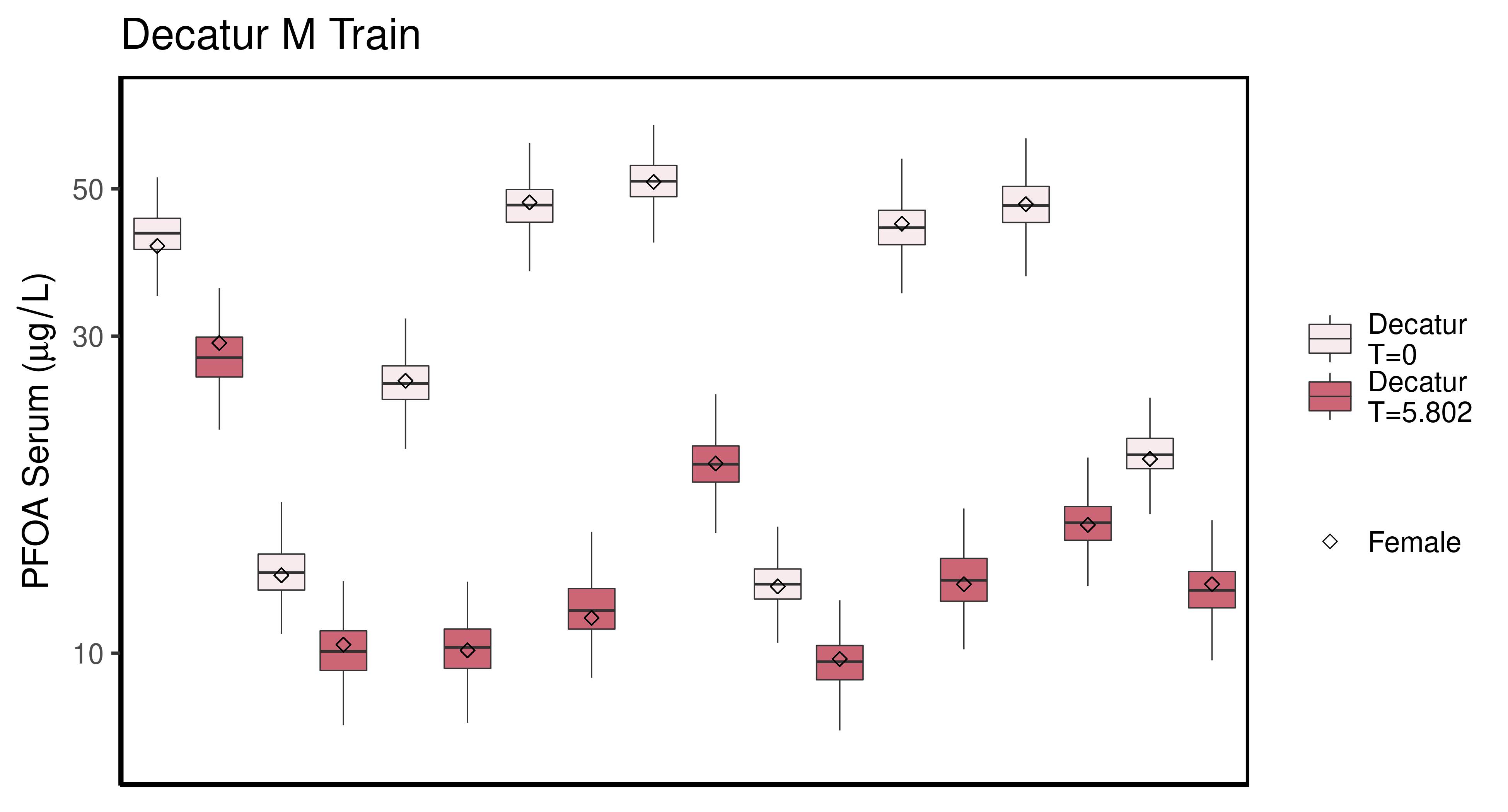
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector

## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector

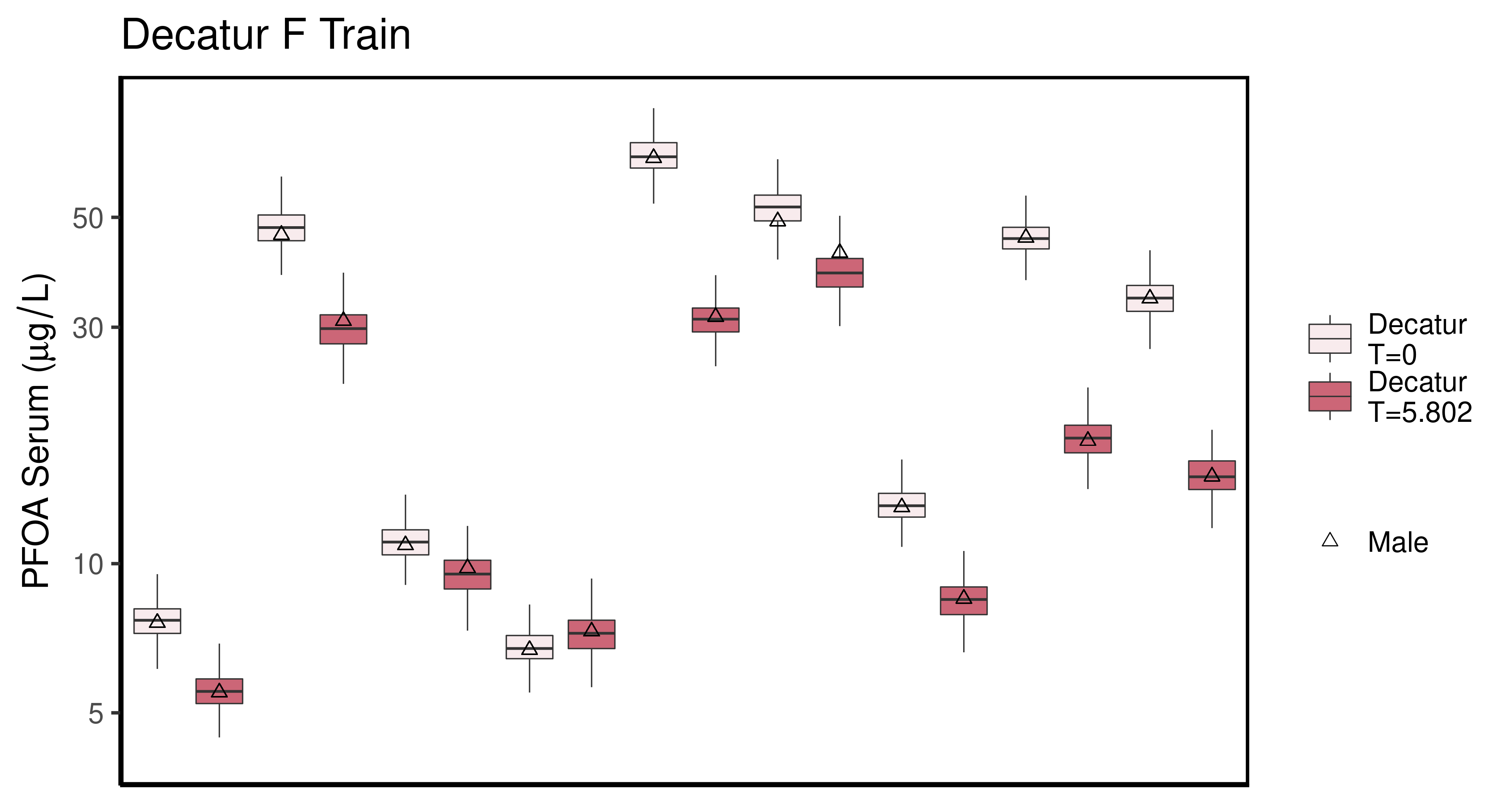
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



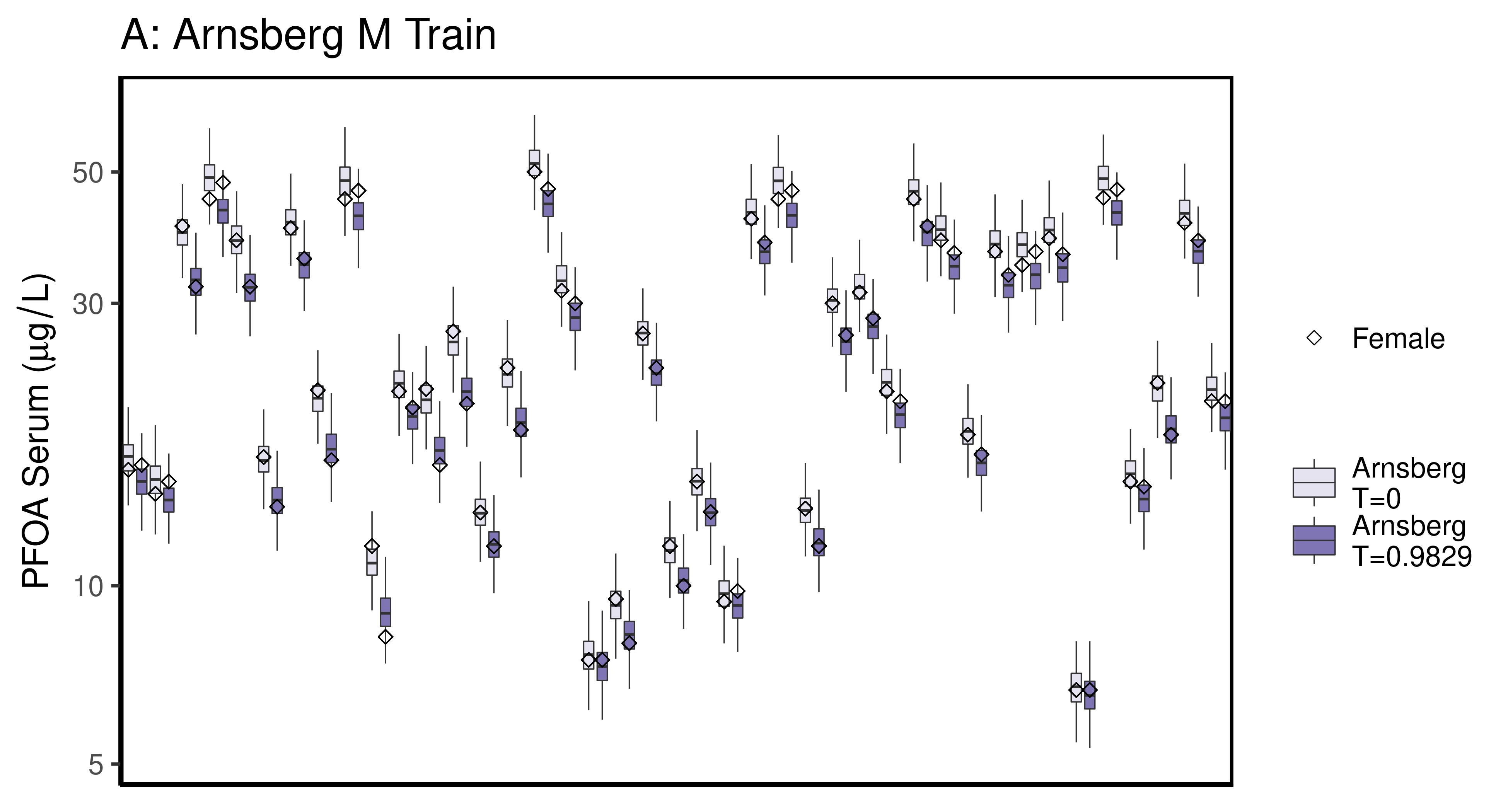
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



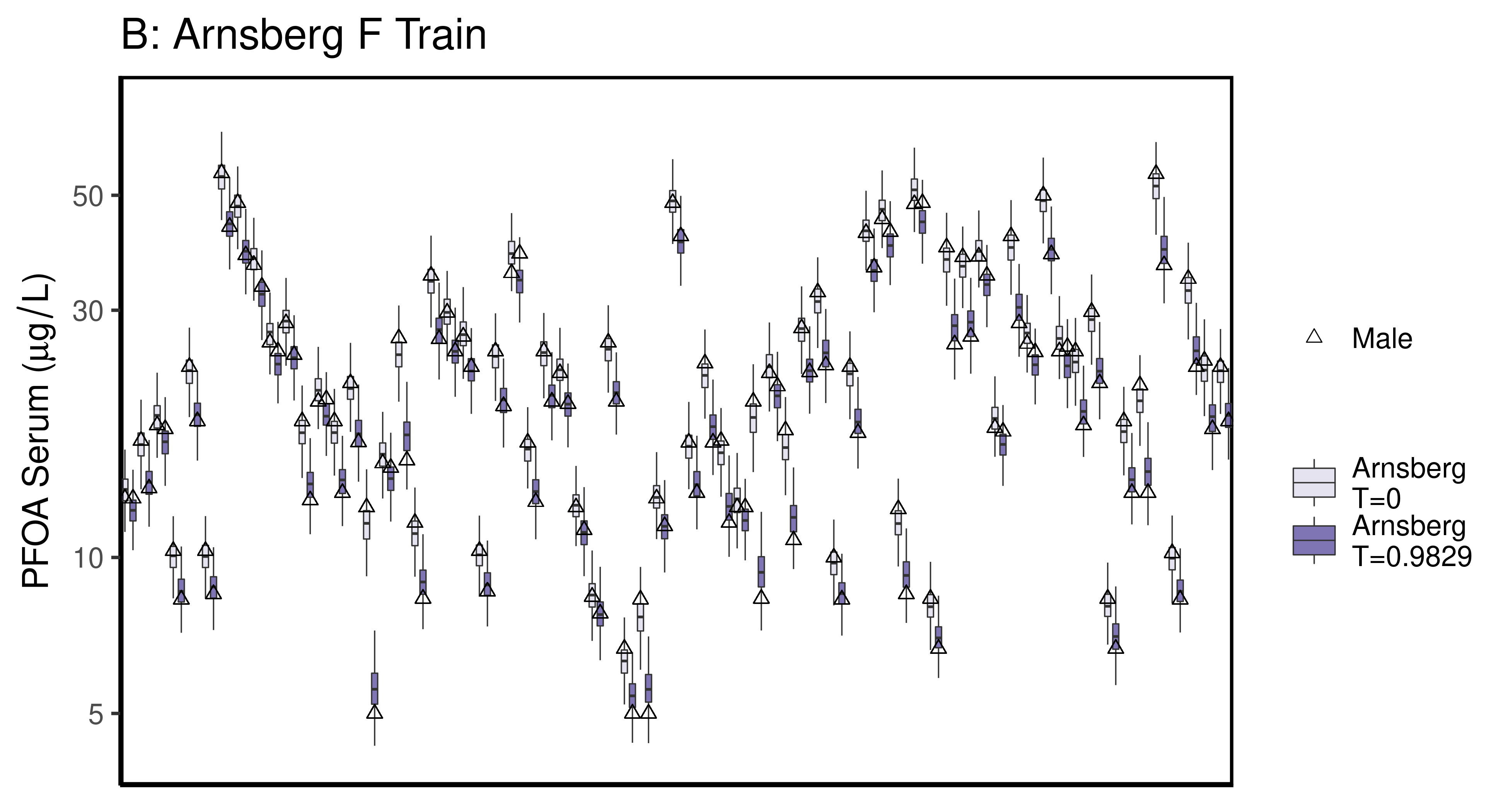
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



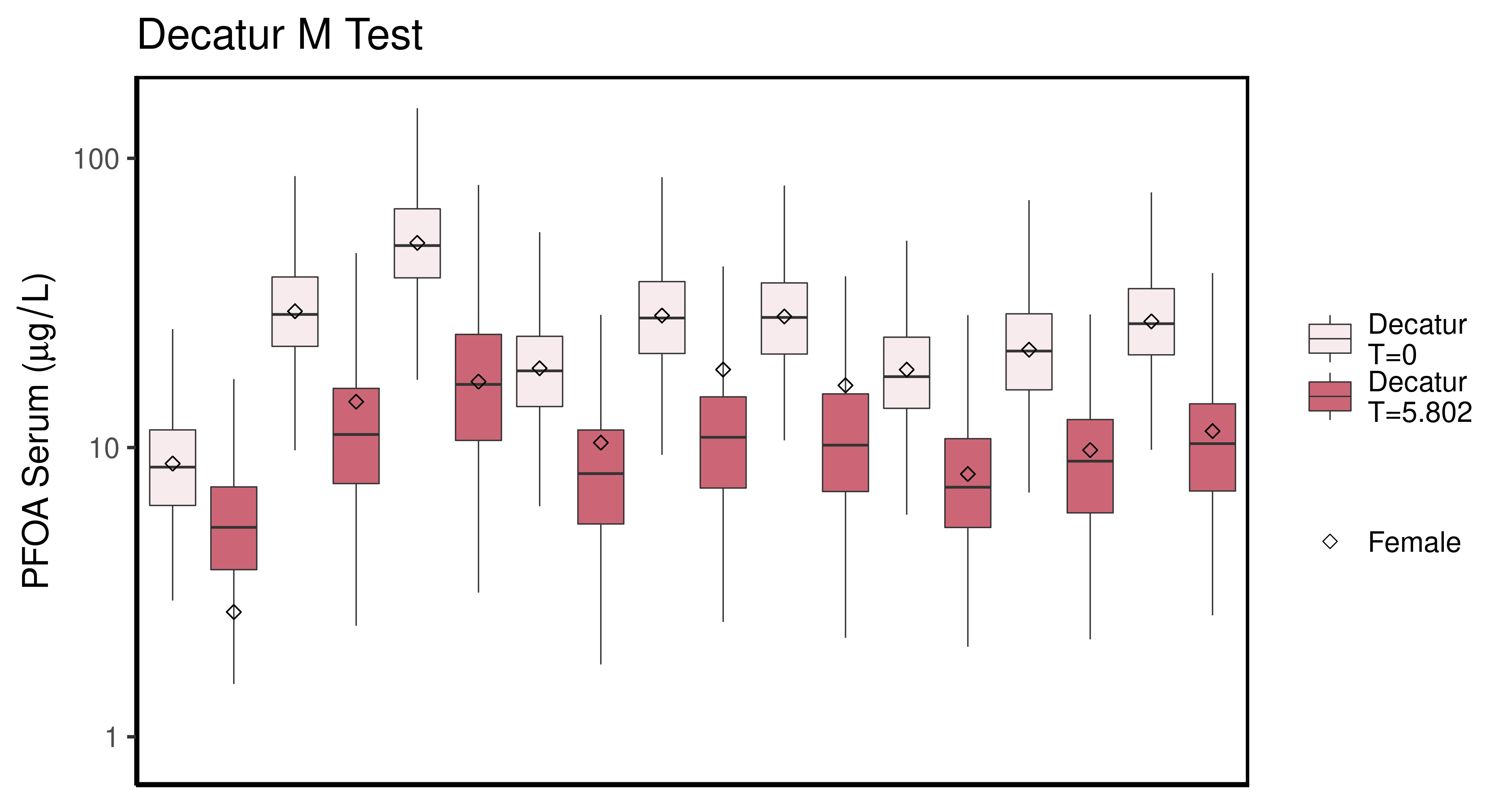
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



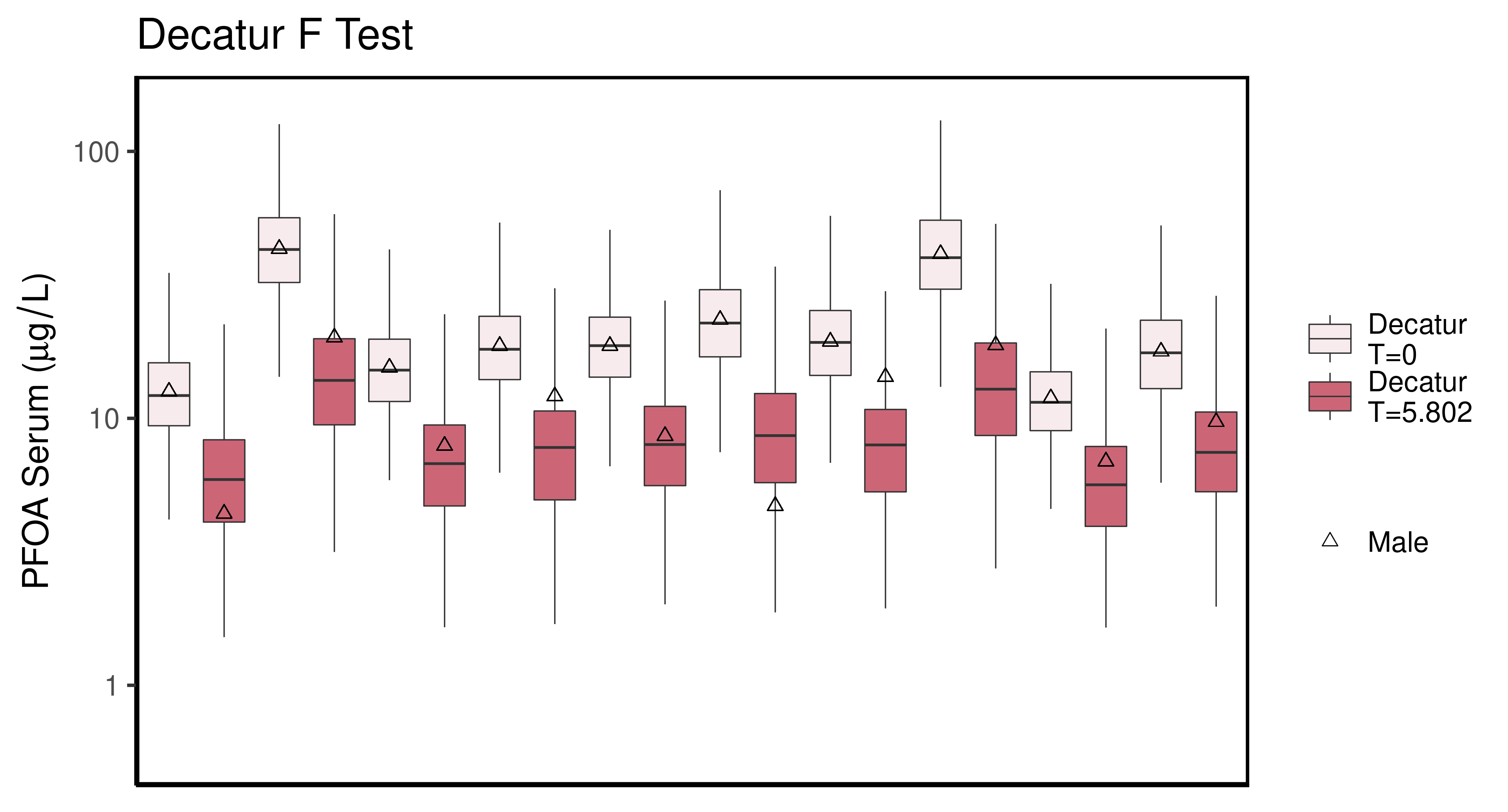
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



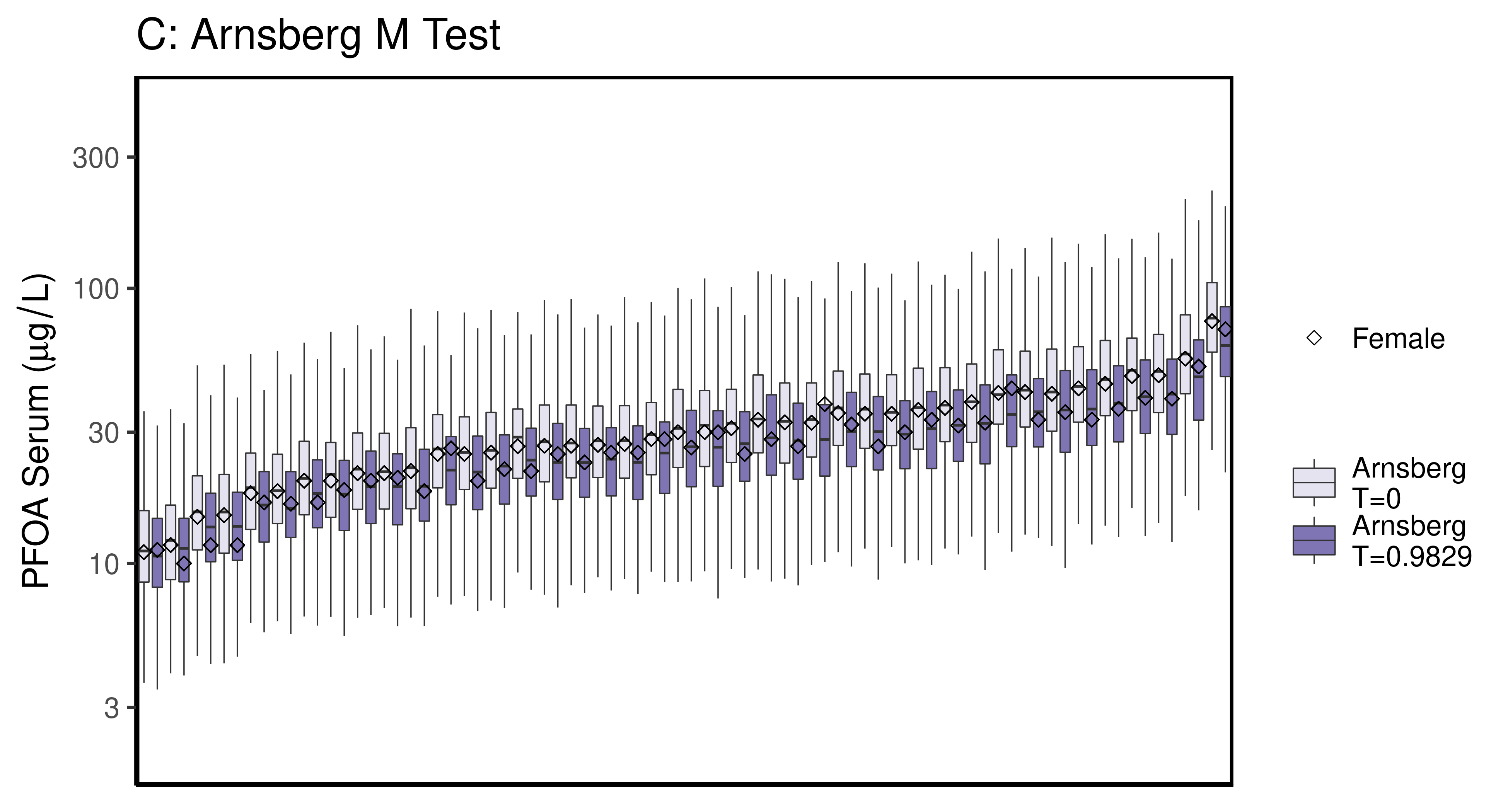
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



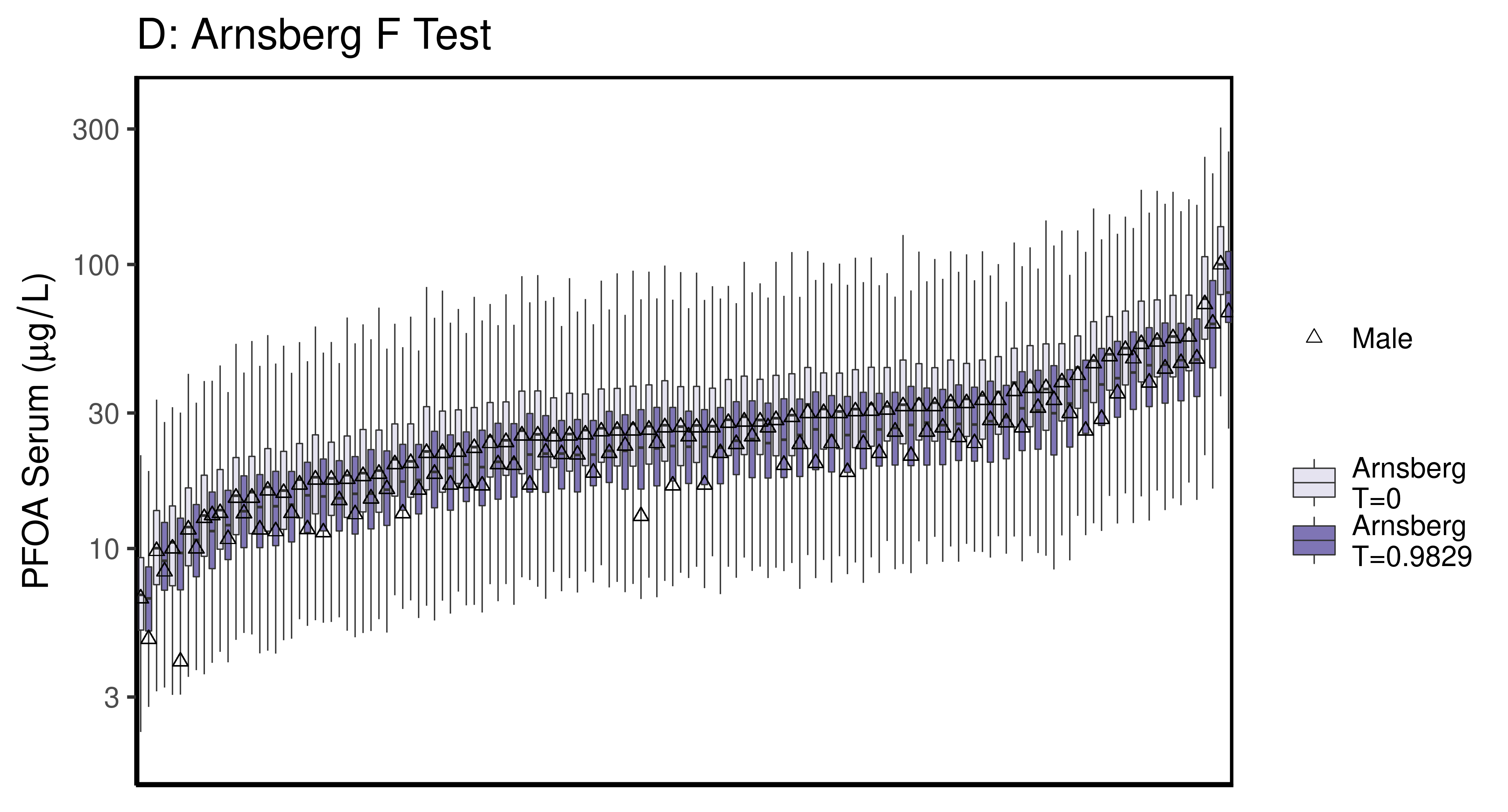
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



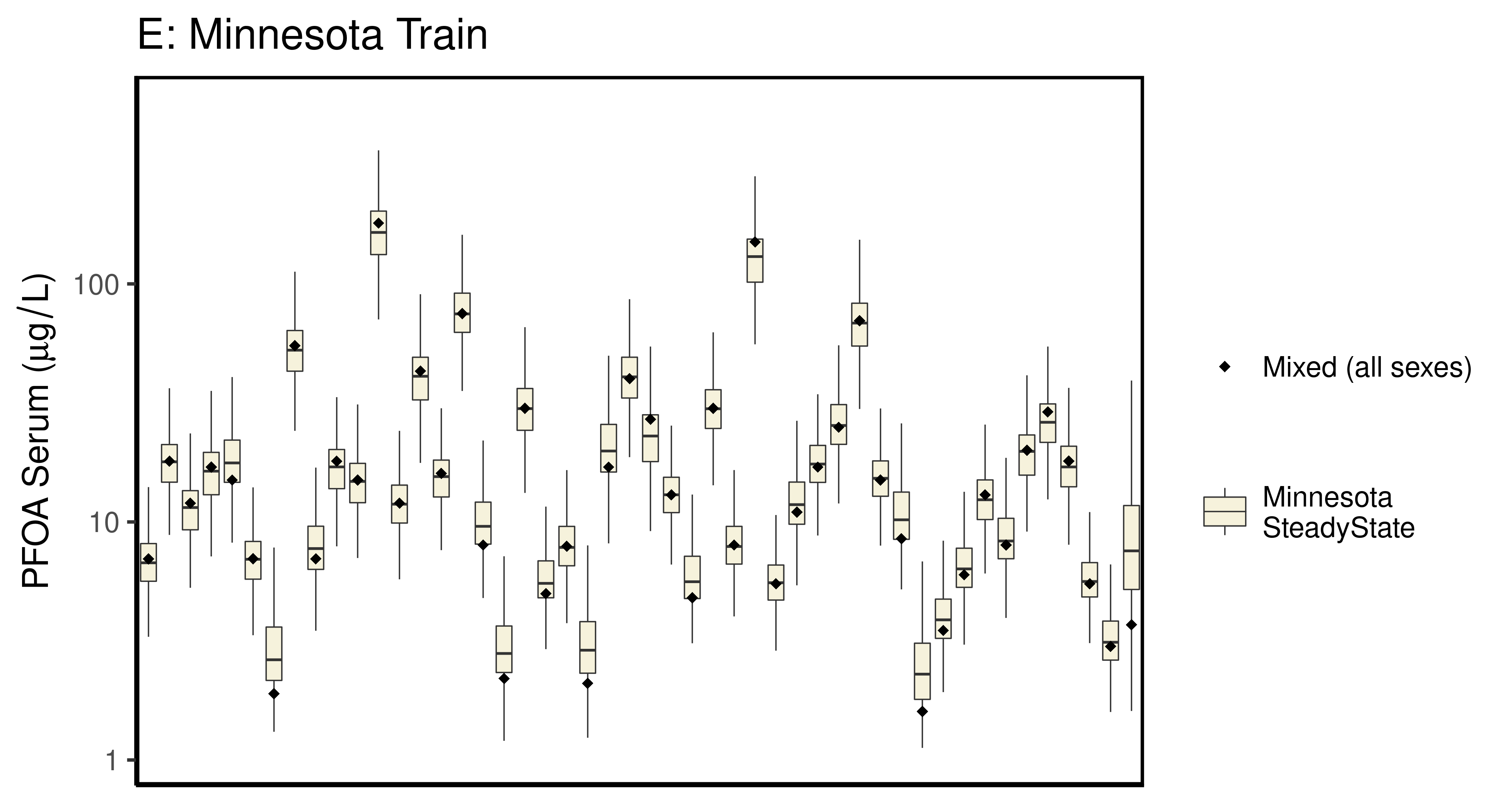
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



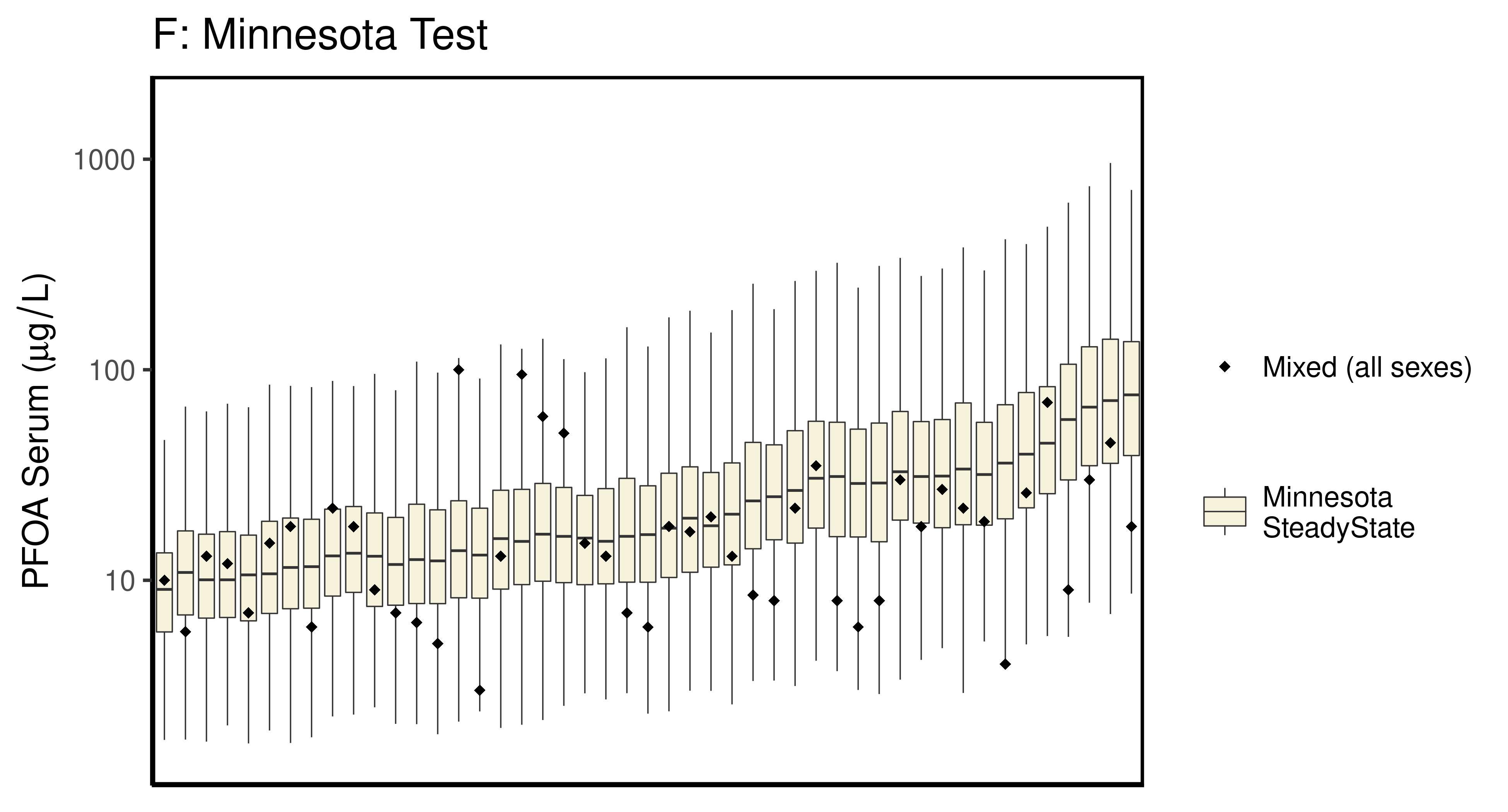
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



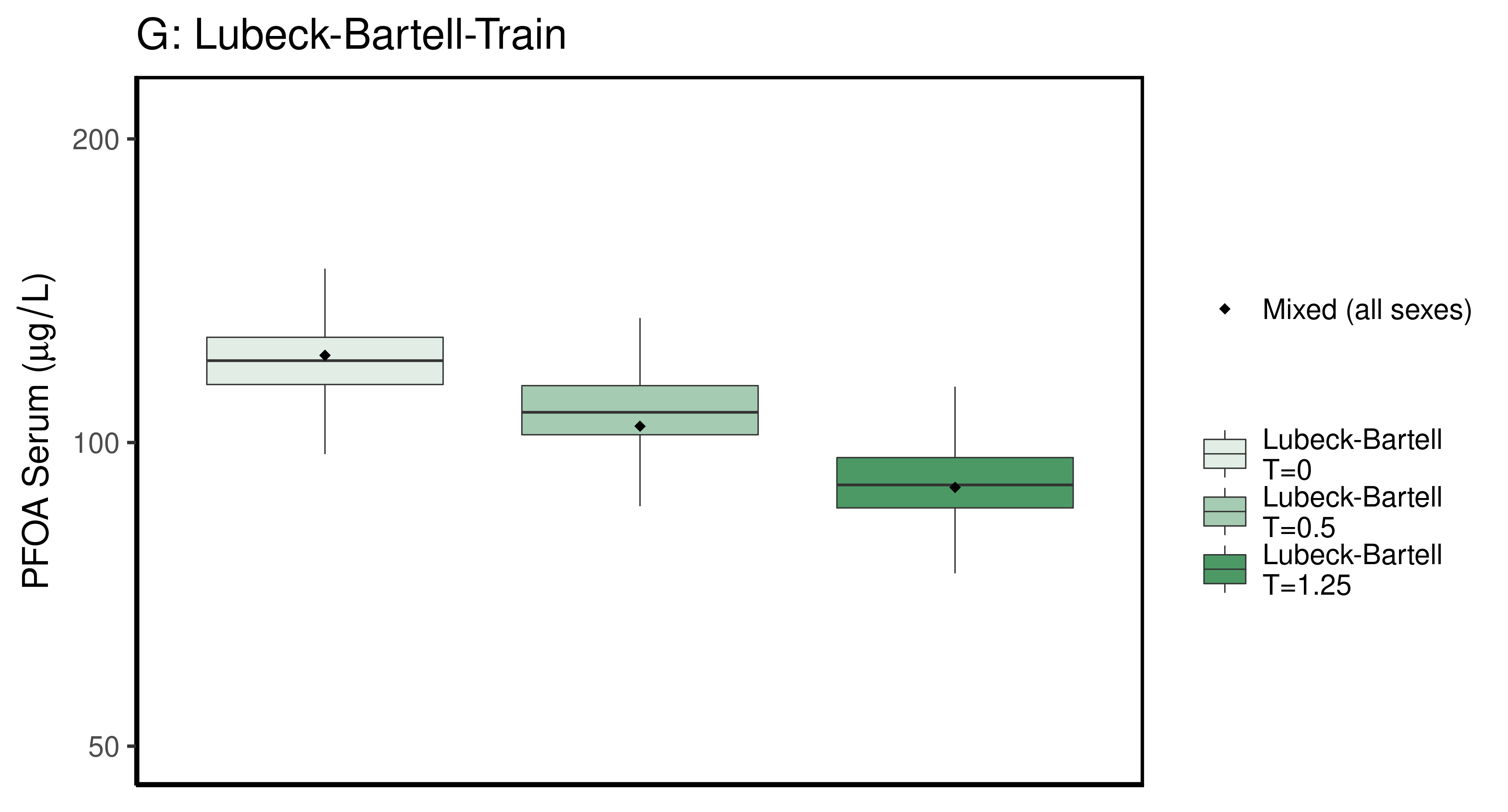
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



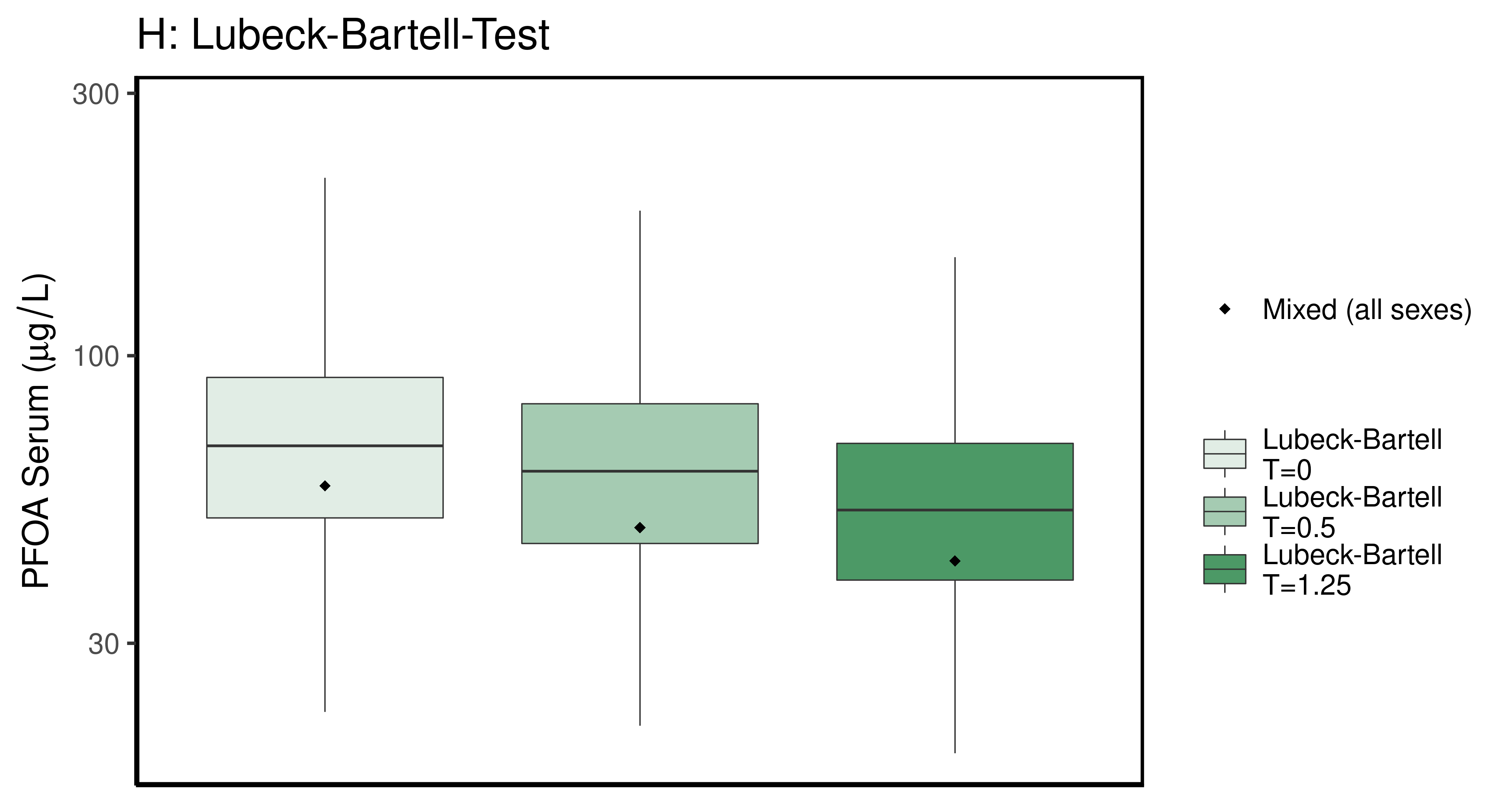
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



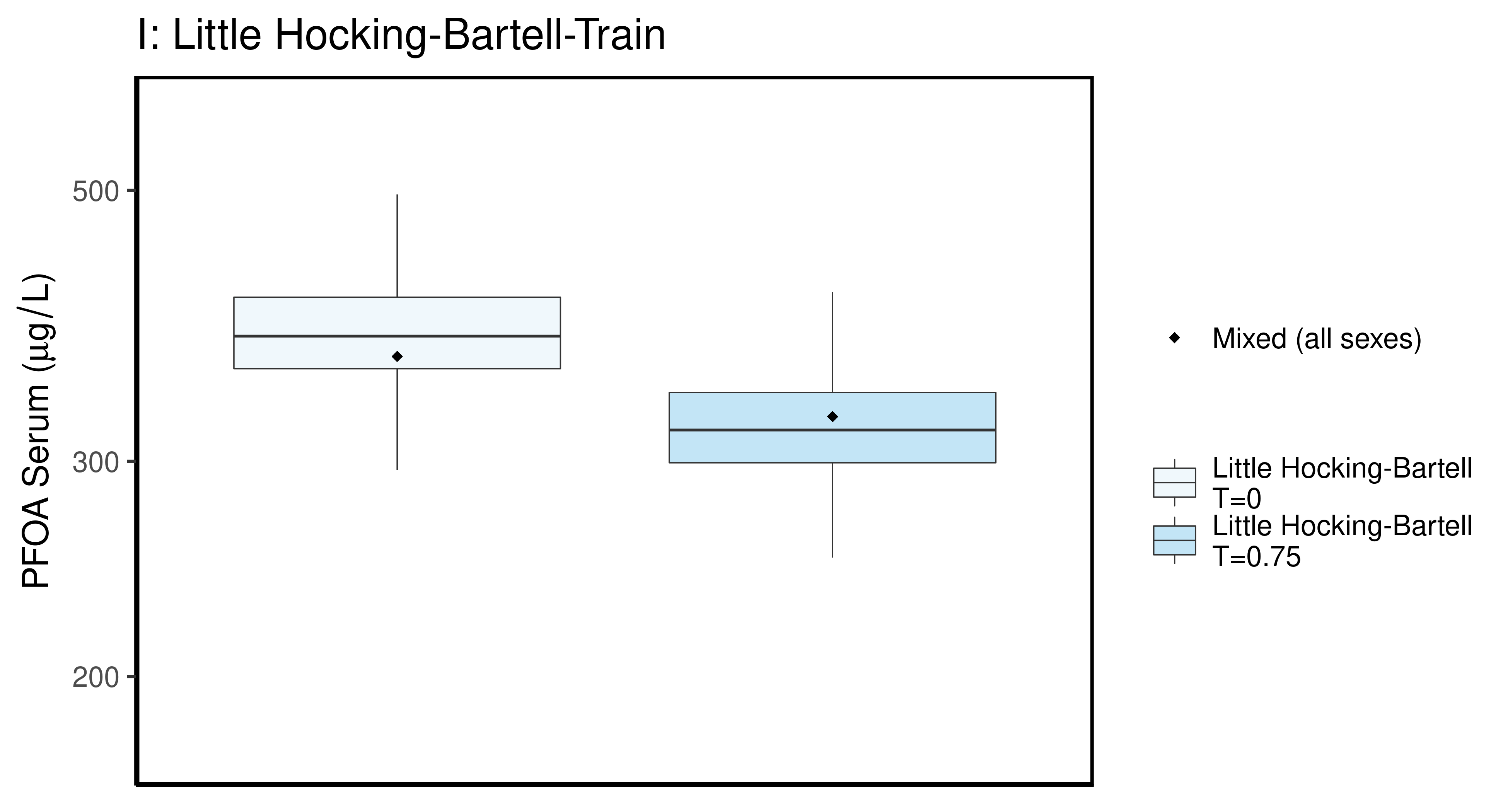
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



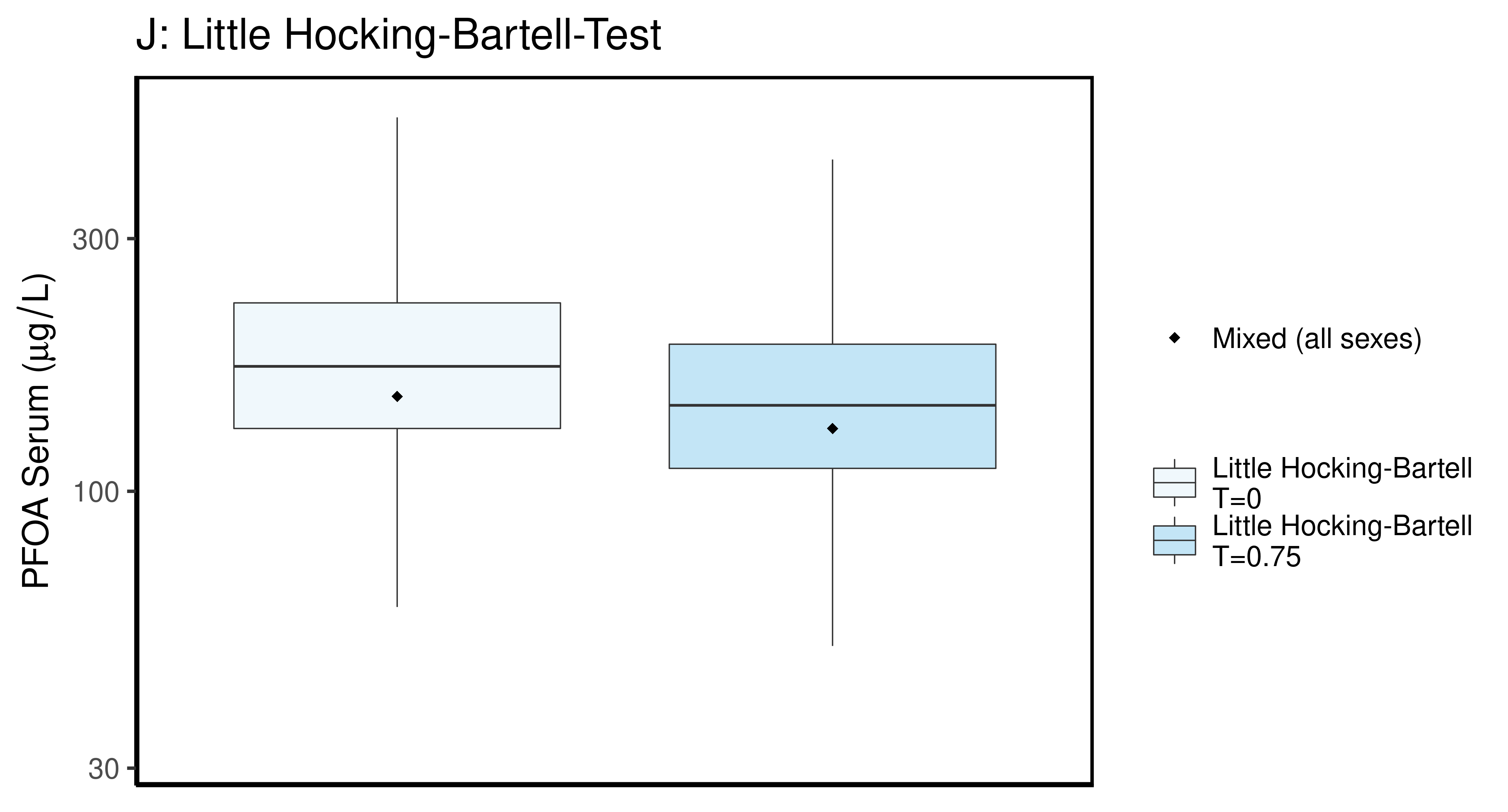
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



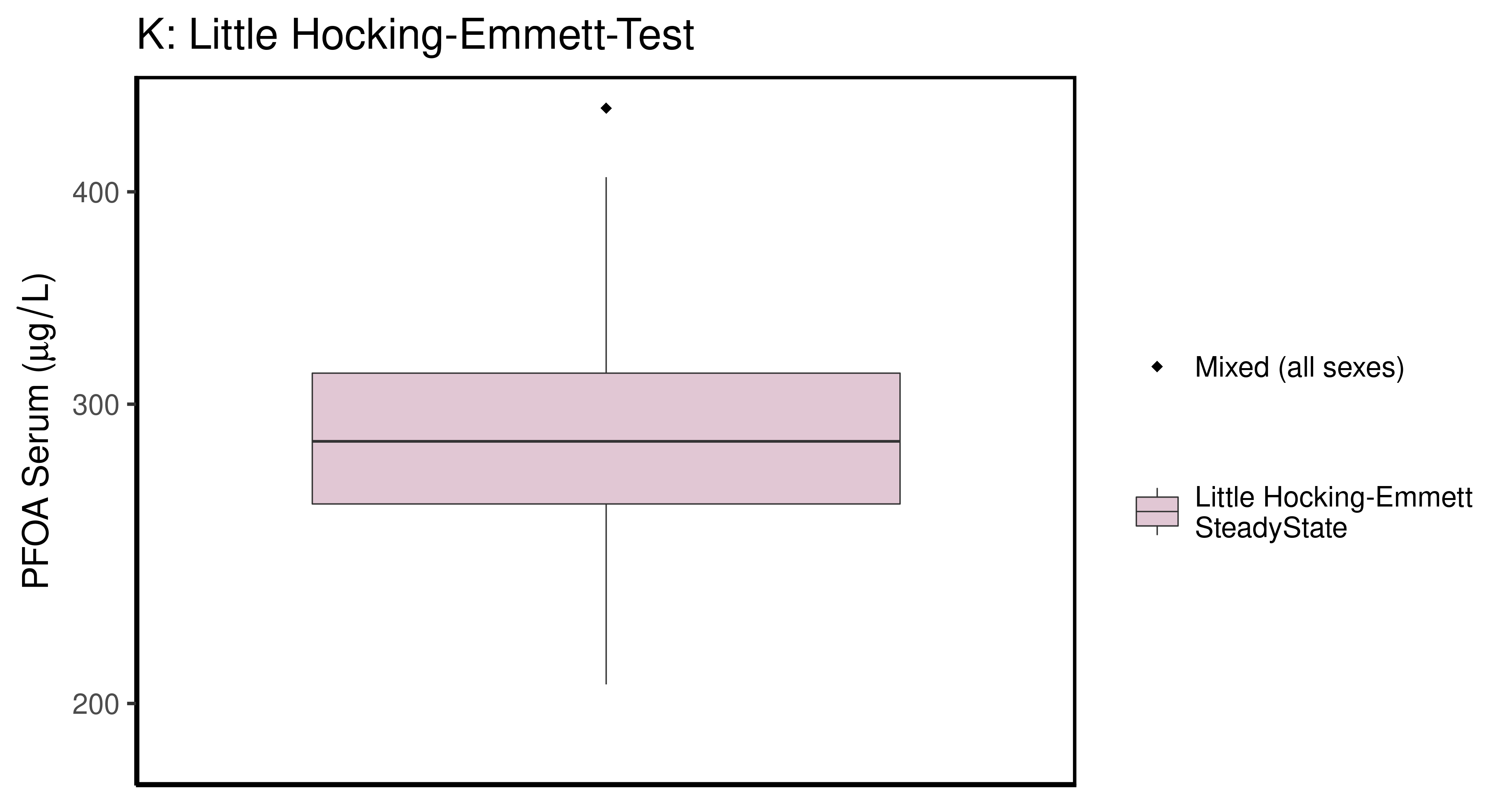
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



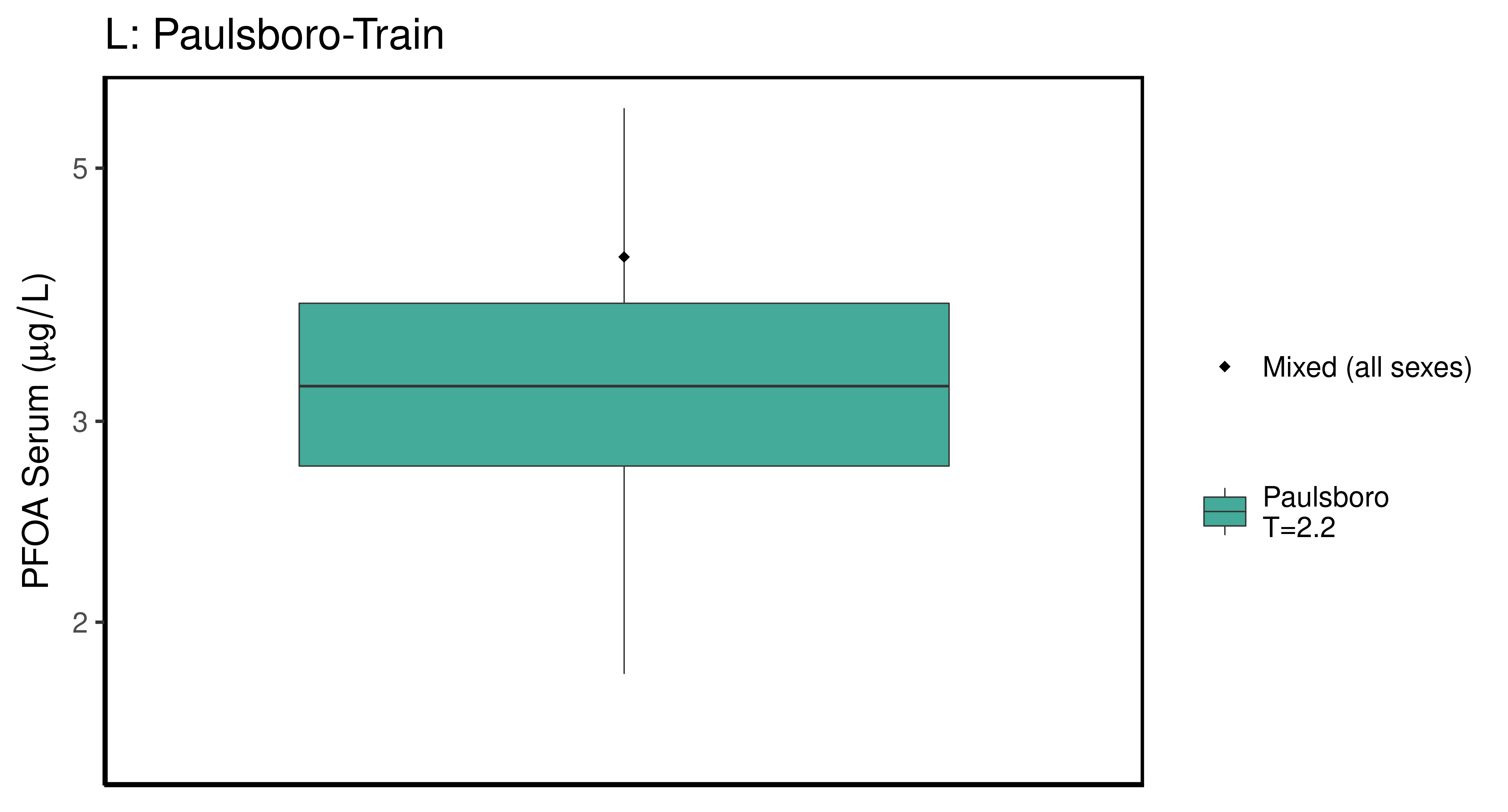
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



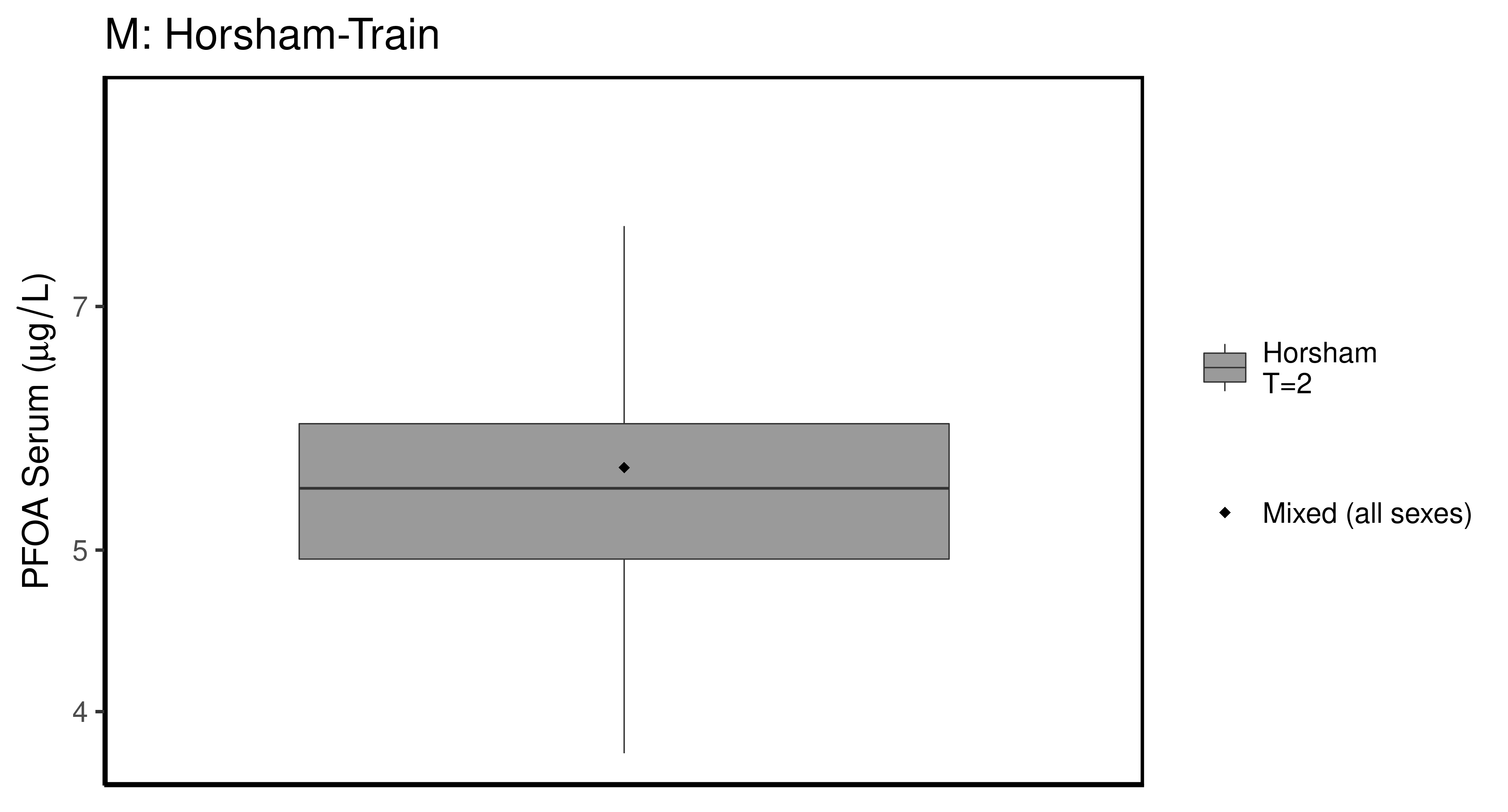
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



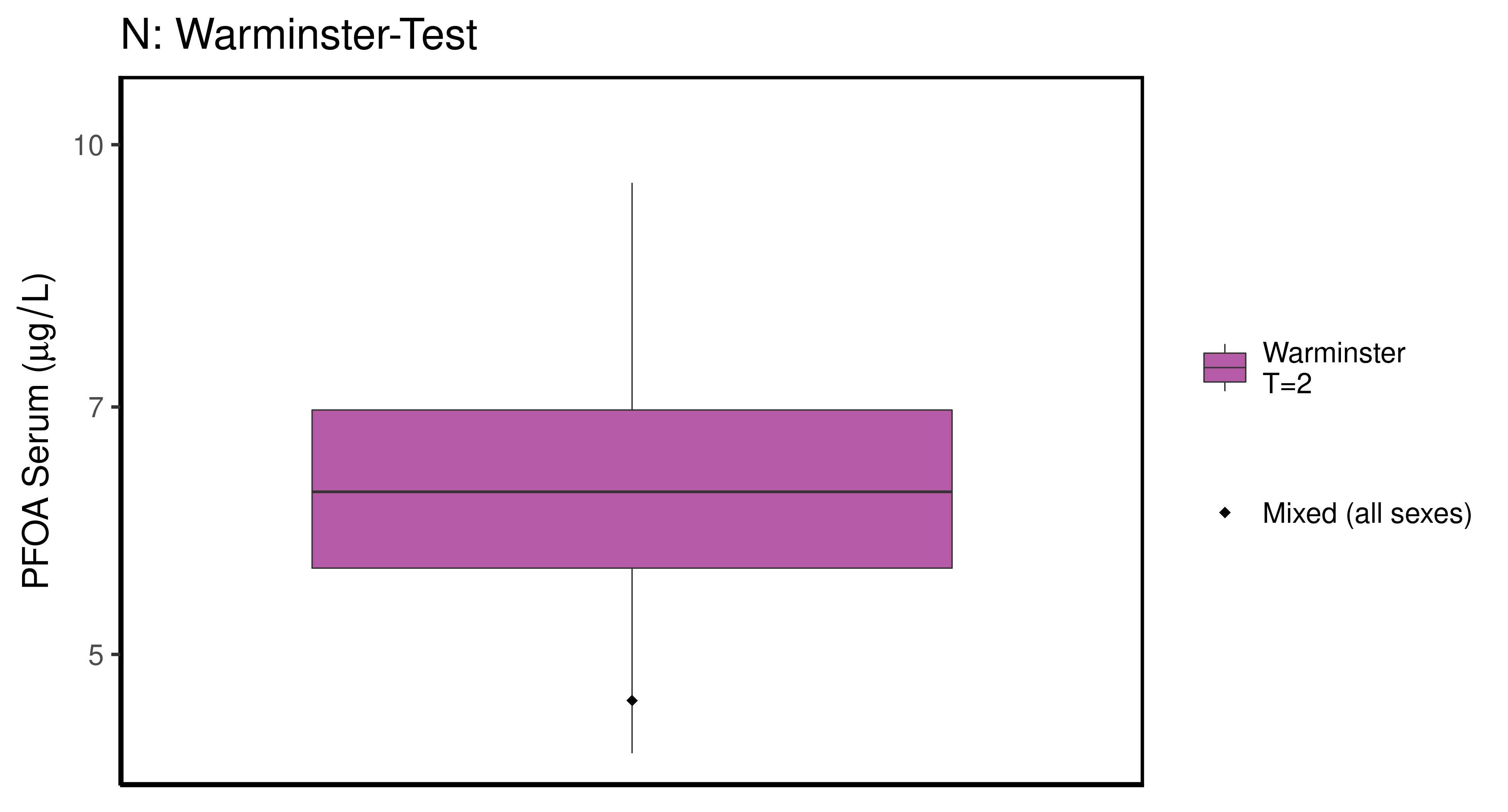
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector

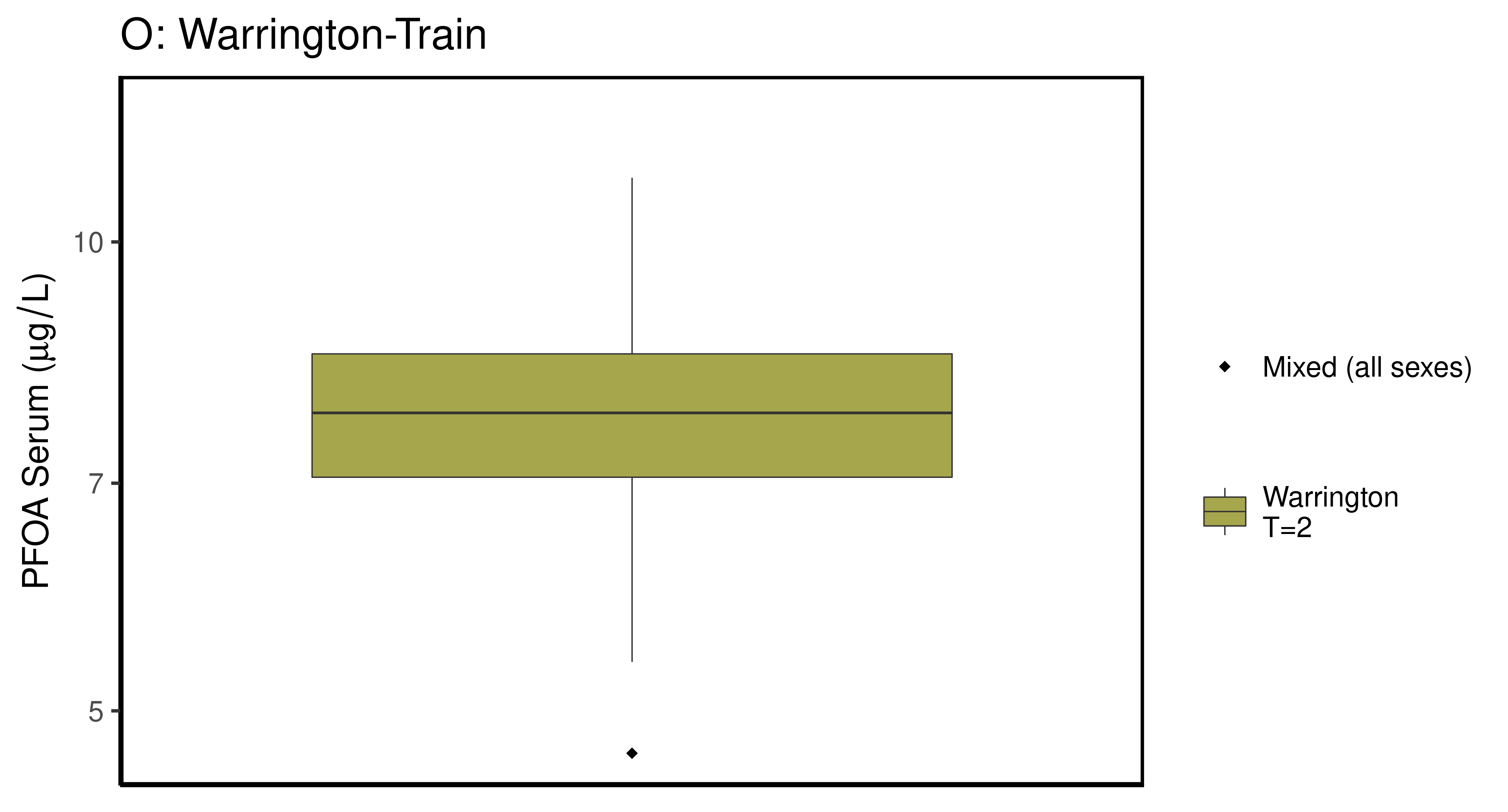


## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## Warning: Column `City` joining factor and character vector, coercing into  
## character vector  
  
## Warning: Column `Train\_Test` joining factor and character vector, coercing into  
## character vector



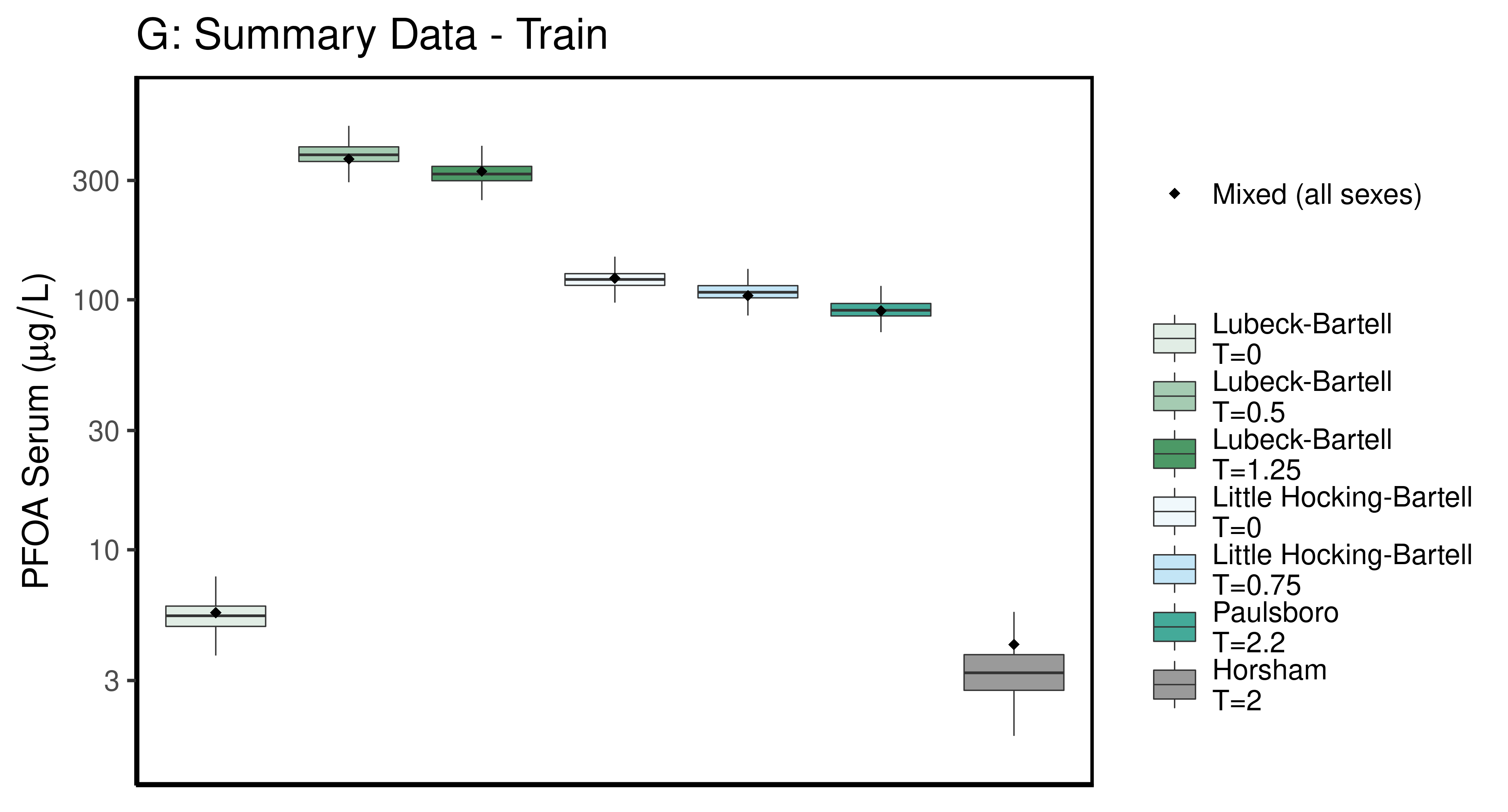
## Saving 6.5 x 3.5 in image



### make Training plot   
  
df\_d\_trt <- df\_check %>%   
 filter( (Train\_Test == "Train") & ((Output\_Var == "M\_Cbgd\_Css") | (Output\_Var == "M\_Cserum"))) %>%  
 mutate\_if(is.factor, as.character) %>% # drop factor levels unused  
 mutate(Dataset.Time = factor(Dataset.Time))   
   
  
 aes\_lut\_df\_d\_trt <- df\_d\_trt %>% select(City, datatype,Time, Time.desc, legend\_label) %>%   
 inner\_join(aes\_lut ) %>%   
 select(-Train\_Test) %>% ungroup () %>% unique ()

## Joining, by = c("City", "datatype", "Time", "Time.desc", "legend\_label")

plt\_train <- plot\_sum\_boxplot(dframe = df\_d\_trt, aes\_lut= aes\_lut\_df\_d\_trt,   
 gtitle="G: Summary Data - Train" , facets = FALSE,   
 pfas\_nom = pfas\_name )  
 print(plt\_train)



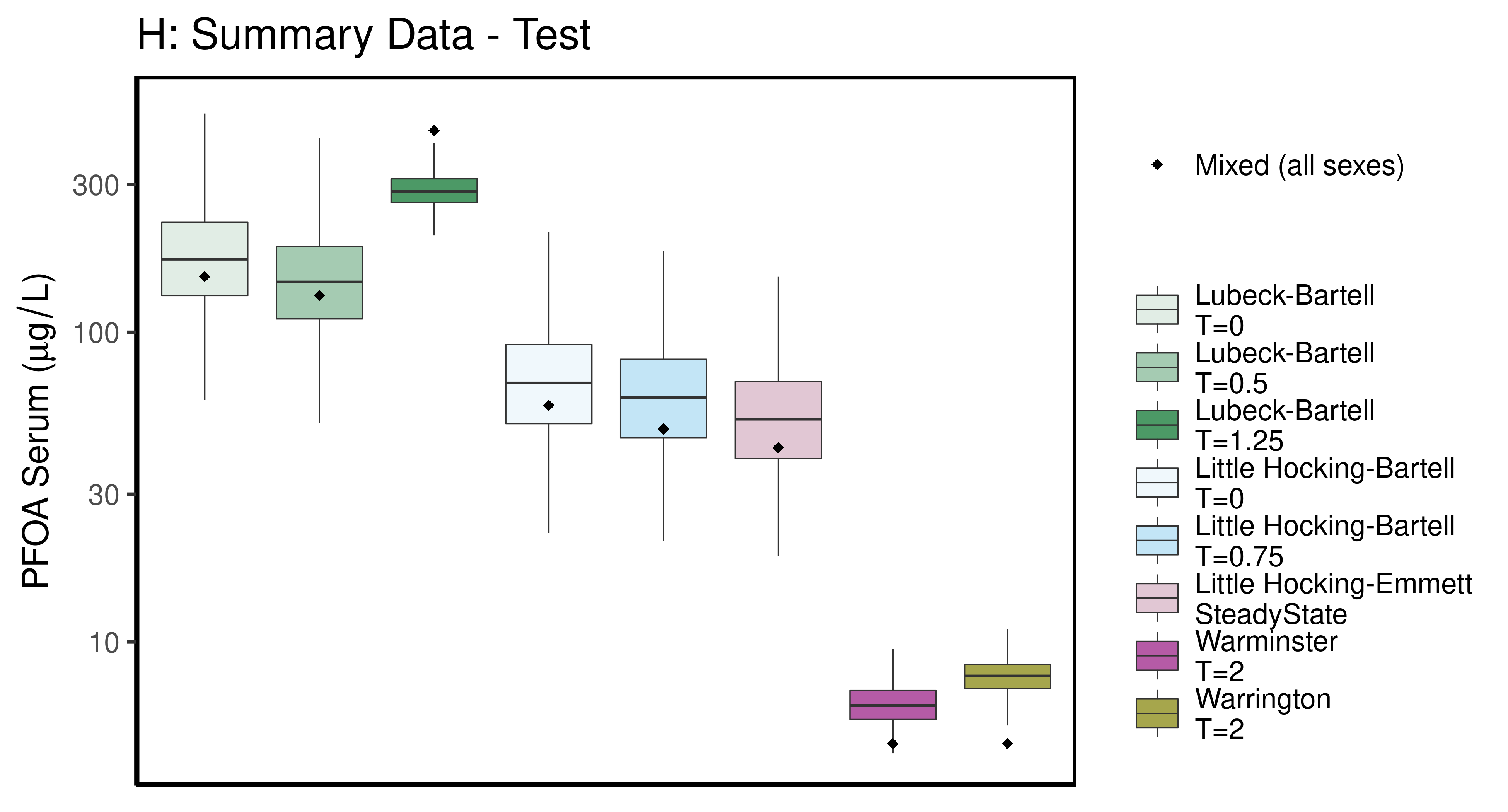
ggsave(here ("output-plots", paste0( sa, "SummaryTrainDataboxplot",pfas\_name,".pdf")), plt\_train,dpi=600)

## Saving 6.5 x 3.5 in image

### make Test plot  
df\_d\_test <- df\_check %>%   
 filter((Train\_Test == "Test") &   
 ((Output\_Var == "M\_Cbgd\_Css") | (Output\_Var == "M\_Cserum"))) %>%  
 mutate\_if(is.factor, as.character) %>% # drop factor levels unused  
 mutate(Dataset.Time = factor(Dataset.Time))   
  
aes\_lut\_df\_d\_test <- df\_d\_test %>% select(City, datatype,Time, Time.desc, legend\_label) %>%   
 inner\_join(aes\_lut ) %>%   
 select(-Train\_Test) %>% ungroup () %>% unique ()

## Joining, by = c("City", "datatype", "Time", "Time.desc", "legend\_label")

plt\_test <- plot\_sum\_boxplot(dframe = df\_d\_test, aes\_lut= aes\_lut\_df\_d\_test,   
 gtitle="H: Summary Data - Test", facets = FALSE,   
 pfas\_nom = pfas\_name)  
 print(plt\_test)



ggsave(here ("output-plots",paste0( sa, "SummaryTestDataboxplot",pfas\_name,".pdf")), plt\_test,dpi=600)

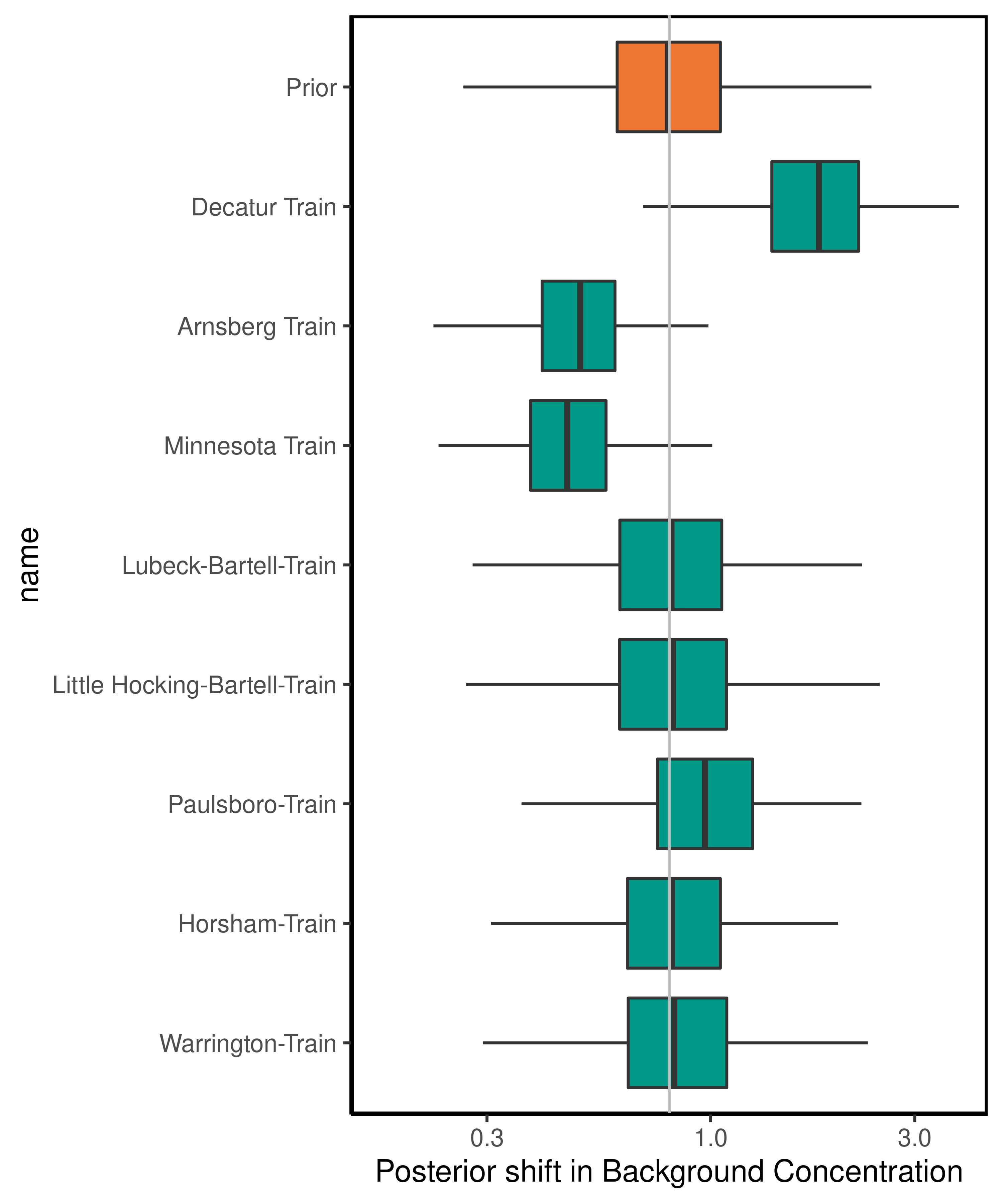
## Saving 6.5 x 3.5 in image

## PFOA

### Background posteriors

Shows shift in background estimate.

gmscale<-0.8  
  
dat <- multicheck$parms.samp[,grep("M\_ln\_Cbgd",names(multicheck$parms.samp))]  
datasetnames <- as.character(unique(calibdata$dataset))  
datasetnames <- gsub(" M","",datasetnames)  
datasetnames <- gsub(" F","",datasetnames)  
datasetnames<-datasetnames[!duplicated(datasetnames)]  
names(dat) <- datasetnames  
dat <- dat[,grep("Train",names(dat))]  
dat.df <- pivot\_longer(dat,1:ncol(dat))  
dat.df <- rbind(dat.df,  
 data.frame(name="Prior",value=rnorm(5000,m=log(gmscale),sd=0.4055)))  
dat.df$name <- factor(dat.df$name,levels=rev(  
 c("Prior",datasetnames[grep("Train",datasetnames)])))  
dat.df$value <- exp(dat.df$value)  
  
p<-ggplot(dat.df)+  
 #geom\_violin(aes(x=name,y=value,fill=name=="Prior"))+  
 geom\_boxplot(aes(x=name,y=value,fill=name=="Prior"),outlier.shape=NA)+  
 scale\_y\_log10()+coord\_flip()+  
 scale\_fill\_manual(name="Prior",   
 values=c("#009988", "#EE7733" )) +  
 theme\_classic() +   
 geom\_hline(yintercept = gmscale,color="grey")+  
 theme(legend.position="none",  
 panel.background = element\_rect(color="black",size=1))+  
 ylab("Posterior shift in Background Concentration")  
  
print(p)



ggsave(here ("output-plots",paste0( sa, "PFOA\_GM\_Cbgd.pdf")), p,dpi=600)

## Saving 5 x 6 in image

### Half-life

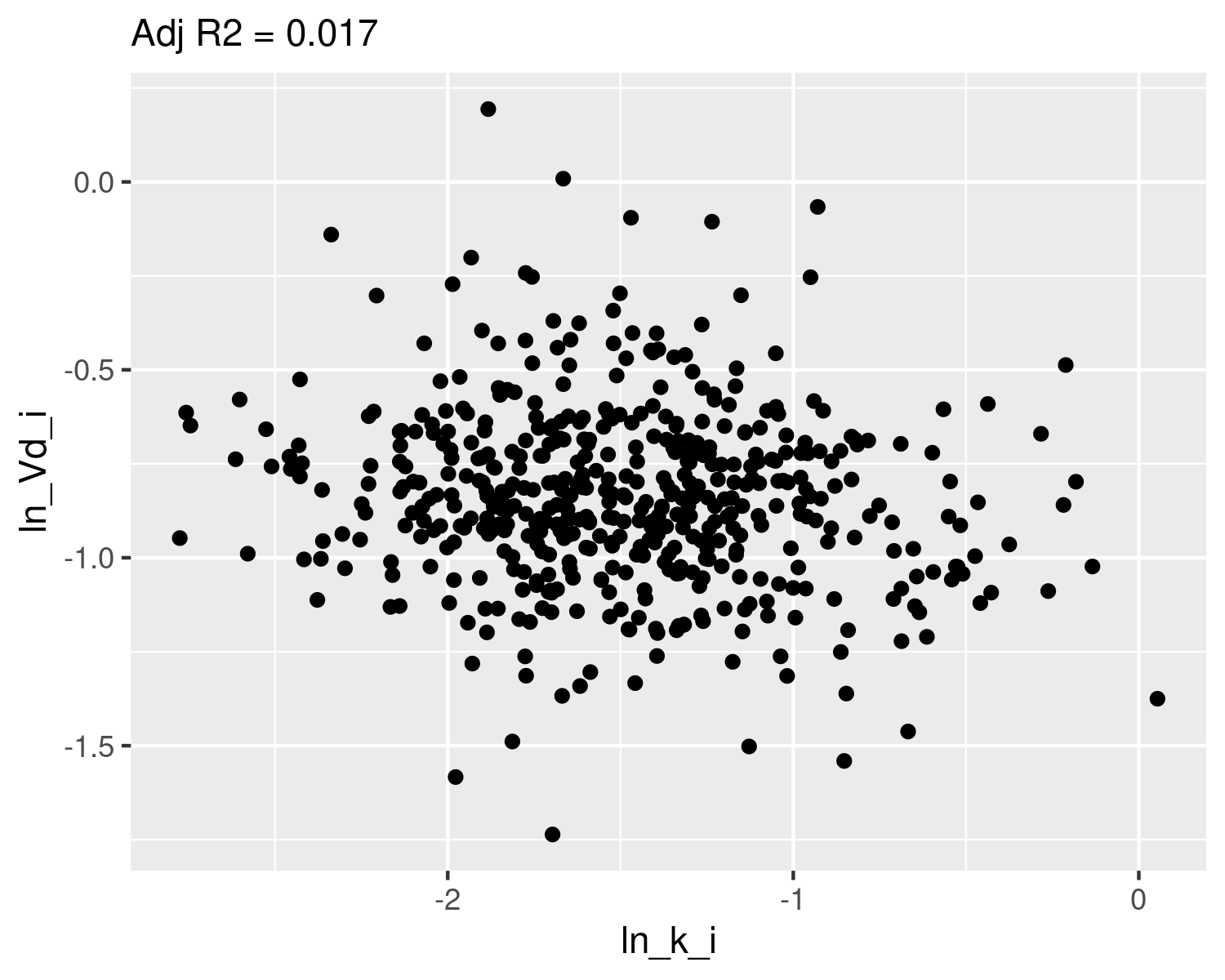
For PFOA, the population GM of the half-life has a posterior distribution that is narrower than the prior, with a posterior median (95% CI) estimate of 3.06 (2.16-4.37) years. The population GSD posterior is larger than the prior at 1.47(1.44-1.75).

dat <- multicheck$parms.samp[,c("M\_ln\_k.1.","V\_ln\_k.1.", "M\_ln\_Vd.1.", "SD\_ln\_Vd.1.")]  
names(dat) <- c("M\_ln\_k(1)","V\_ln\_k(1)", "M\_ln\_Vd(1)", "SD\_ln\_Vd(1)")  
  
set.seed(3.14159)  
dat$z\_ln\_k <- rnorm(nrow(dat))  
dat$z\_ln\_Vd <- rnorm(nrow(dat))  
dat %>% rename\_()

## Warning: rename\_() is deprecated.   
## Please use rename() instead  
##   
## The 'programming' vignette or the tidyeval book can help you  
## to program with rename() : https://tidyeval.tidyverse.org  
## This warning is displayed once per session.

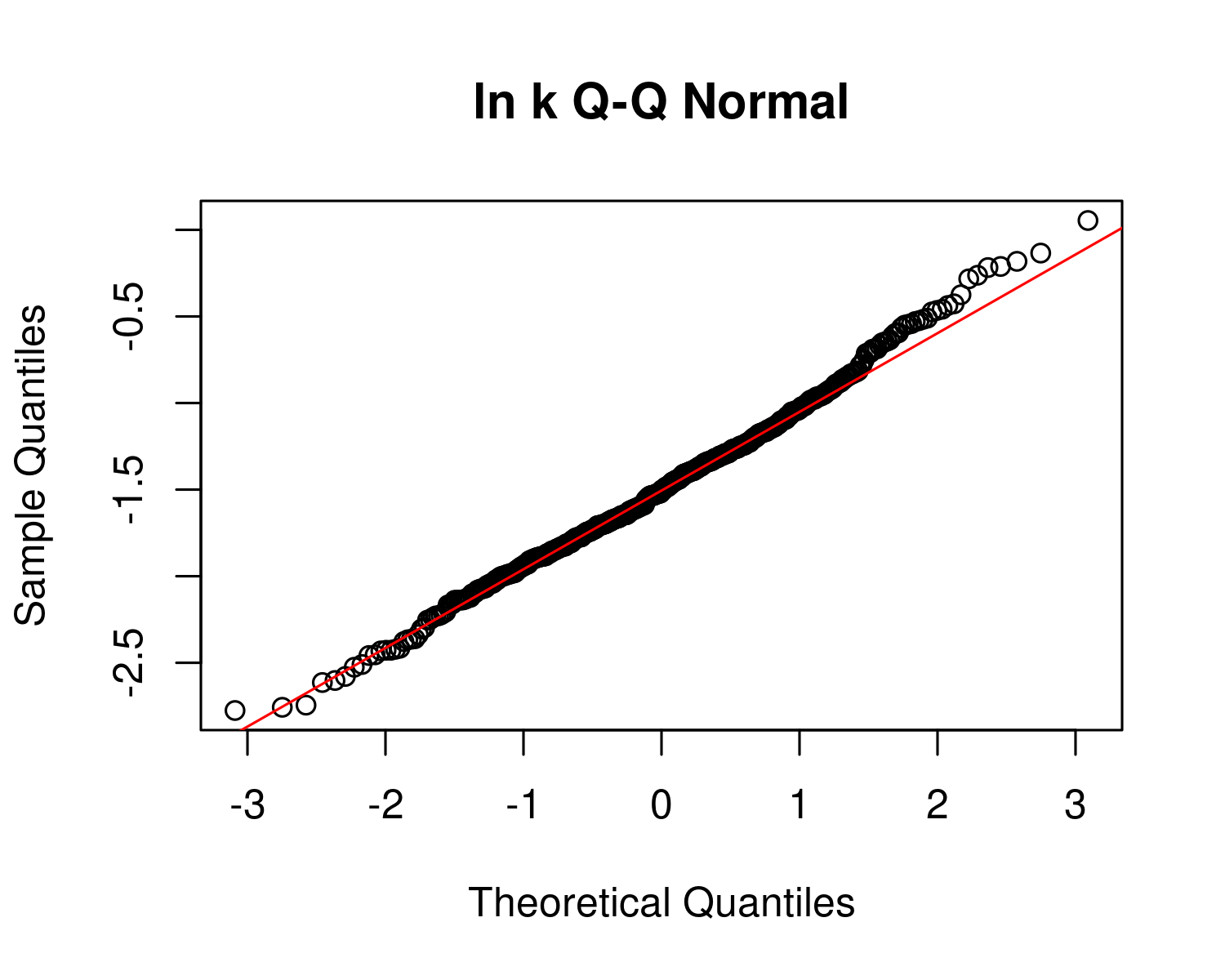
## M\_ln\_k(1) V\_ln\_k(1) M\_ln\_Vd(1) SD\_ln\_Vd(1) z\_ln\_k z\_ln\_Vd  
## 12503 -1.47166 0.2259770 -1.027430 0.11872900 -0.961933416 -2.139841913  
## 15901 -1.57172 0.1917550 -0.981910 0.12890300 -0.292525723 -1.263479244  
## 17543 -1.44315 0.2218600 -0.846605 0.05661850 0.258788216 0.083307969  
## 18721 -1.63377 0.2671930 -0.803807 0.00251033 -1.152131886 0.188325130  
## 11662 -1.63952 0.2442100 -0.641437 0.19616300 0.195782826 0.189814193  
## 13403 -1.50146 0.1316760 -0.912848 0.04207130 0.030123945 0.217615352  
## 13192 -1.52804 0.2576120 -0.836255 0.00522934 0.085417732 -0.648814142  
## 15663 -1.62322 0.2206230 -0.833671 0.12510900 1.116610213 0.254774383  
## 1246 -1.46340 0.1607610 -0.864602 0.11869500 -1.218857416 -0.468830015  
## 16132 -1.35944 0.1421860 -1.046470 0.05301980 1.267368722 -1.192510054  
## 10602 -1.31808 0.1962300 -1.020060 0.07258270 -0.744781596 0.121228235  
## 10563 -1.57564 0.2097090 -0.575507 0.08585640 -1.131218571 -1.035932658  
## 15932 -1.63592 0.2893040 -0.441297 0.46389700 -0.716358490 -0.191888295  
## 1114 -1.50220 0.1654030 -0.812117 0.12570300 0.252652370 -0.970546336  
## 1699 -1.61622 0.1952380 -0.655576 0.06439360 0.152045707 0.057771938  
## 1141 -1.44708 0.0791159 -0.824623 0.03169700 -0.307656430 -2.110692675  
## 13383 -1.53241 0.1373040 -0.898336 0.06439640 -0.953017331 0.978176274  
## 12832 -1.58927 0.2061870 -0.757849 0.09033650 -0.648242811 0.371021737  
## 19552 -1.65200 0.1755320 -0.922508 0.35681400 1.224313624 0.720910931  
## 14423 -1.56912 0.2473010 -0.613524 0.27567500 0.199811608 1.879594880  
## 12372 -1.58129 0.2054630 -0.863814 0.01532240 -0.578483722 -0.396316112  
## 12042 -1.44236 0.2313180 -0.930943 0.08416760 -0.942300733 0.110322947  
## 10473 -1.56596 0.2387790 -0.504892 0.05603230 -0.203728180 -0.593140881  
## 1509 -1.63181 0.2301430 -0.703216 0.00560974 -1.666474840 0.419621770  
## 1552 -1.60037 0.2947500 -0.756522 0.00787158 -0.484455109 -0.545738743  
## 19513 -1.60375 0.2381920 -0.640758 0.10491500 -0.741072661 1.160921499  
## 17471 -1.43266 0.1720730 -0.896787 0.09401620 1.160615779 0.639817834  
## 18092 -1.51021 0.2343130 -0.663190 0.09107450 1.012067125 -0.122020443  
## 1613 -1.42880 0.1599680 -1.366620 0.17959100 -0.072078474 0.184645026  
## 14383 -1.50389 0.3123290 -0.591951 0.14044200 -1.136782298 -0.517806023  
## 14263 -1.48924 0.2104700 -0.621222 0.18017100 0.900624729 0.067988352  
## 18291 -1.63622 0.2309160 -0.890736 0.07126660 0.851770447 -0.184797156  
## 1945 -1.52990 0.3078630 -1.009580 0.08054770 0.727715174 -1.403691615  
## 19613 -1.43231 0.2006660 -0.824693 0.34993200 0.736502146 0.229740706  
## 1842 -1.57472 0.2309900 -0.884116 0.02773450 -0.352129617 -0.889081301  
## 1873 -1.52882 0.1832970 -0.846448 0.09996610 0.705515513 -0.160401177  
## 19423 -1.50740 0.1751370 -0.797601 0.07921920 1.300357989 -0.242136794  
## 19352 -1.51582 0.1875540 -1.128120 0.31836300 0.038252014 -0.028837196  
## 11812 -1.45436 0.1943910 -0.839713 0.17480700 -0.979283770 -0.316215474  
## 14982 -1.54901 0.1428640 -0.848721 0.30714300 0.793761231 -0.416160087  
## 11263 -1.56783 0.2199070 -0.710211 0.41491600 0.786506872 -1.023895957  
## 1028 -1.54302 0.2678610 -0.871150 0.19559700 -0.310463131 1.099495275  
## 1051 -1.46362 0.1975220 -0.995615 0.01698190 1.698884846 0.817712470  
## 17222 -1.62549 0.1728590 -0.610798 0.04805740 -0.794593709 0.168875510  
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## 17573 -1.58928 0.1933030 -0.762938 0.00918553 -0.463031038 0.175989014  
## 19872 -1.58679 0.2888820 -0.631627 0.05272770 -0.279741696 -0.437523579  
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## 18271 -1.66192 0.2490240 -0.735196 0.26331900 0.143156356 -0.636048007  
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## 1920 -1.58874 0.1819160 -0.719057 0.23716200 -2.403663727 -0.079333090  
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## 16771 -1.53435 0.1623060 -0.837161 0.13471800 -0.878893050 0.118181119  
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## 1048 -1.48919 0.1993050 -0.821110 0.23316200 0.013969708 0.164813527  
## 12143 -1.54976 0.2504290 -0.779318 0.17970800 -1.633423995 -1.243838156  
## 1075 -1.55142 0.2850860 -0.728439 0.01539880 0.488932473 0.116308174  
## 18021 -1.43885 0.1650170 -0.676836 0.10744900 -1.019179409 1.197547370  
## 17623 -1.56458 0.2481620 -0.675031 0.06439390 1.090553483 -0.698130988  
## 1499 -1.47933 0.2354970 -0.842719 0.03511180 -1.139469805 0.293604948  
## 18673 -1.60311 0.1643570 -0.821628 0.09756690 -0.015725635 0.437297744  
## 1093 -1.49444 0.1846610 -0.717872 0.05115940 0.297491282 0.627762573  
## 13553 -1.42957 0.1519730 -0.786311 0.00982651 3.200590040 -1.160543514  
## 12592 -1.47815 0.1860290 -0.869114 0.01620470 0.089244244 -0.020788418  
## 12912 -1.54680 0.1815310 -0.892300 0.02948780 0.570972338 1.044724089  
## 1785 -1.42669 0.2171790 -0.991846 0.08288900 0.528685630 1.311594585  
## 14041 -1.56975 0.2135000 -0.883118 0.00203215 -0.440904798 -0.082439028  
## 1624 -1.46589 0.1993470 -0.957345 0.01713570 -0.672793368 0.919224762  
## 1841 -1.58289 0.2296940 -0.873117 0.07100870 2.154313365 -0.243269921  
## 19553 -1.54739 0.2263010 -0.391179 0.03320420 0.593852716 0.351094377  
## 12722 -1.43217 0.1634400 -0.994116 0.23131900 -0.384063768 -1.340384172  
## 15122 -1.41179 0.1467770 -0.927081 0.28481400 0.719783276 0.425846094  
## 1348 -1.42482 0.1731270 -0.832138 0.09016220 1.708173402 -0.814353733  
## 15183 -1.52820 0.2273670 -0.873265 0.10598700 1.075215667 0.693374081  
## 14432 -1.54149 0.1837410 -0.986642 0.33243600 0.777420367 0.705544556  
## 1468 -1.52714 0.2273480 -0.652243 0.11856900 0.052200047 0.278350539  
## 17953 -1.51122 0.1888740 -0.909895 0.12429800 -1.083698485 -1.202692142  
## 1557 -1.43841 0.1971180 -0.971405 0.00120255 -0.008856207 0.642761817  
## 19642 -1.43905 0.2482490 -0.986455 0.17539200 2.030643112 -0.605973945  
## 16191 -1.52013 0.2185760 -0.769066 0.11450600 -1.113328933 -1.377257613  
## 17011 -1.44545 0.1573750 -1.033650 0.13570000 1.138271925 -0.925992687  
## 1820 -1.52520 0.2170930 -0.880422 0.13424200 -0.614892642 0.567243857  
## 10851 -1.55563 0.2999810 -0.626022 0.00471981 -2.193536615 2.595481260  
## 13483 -1.38049 0.2561920 -1.084550 0.14871900 -1.215686372 -0.239984547  
## 13183 -1.59476 0.2636340 -0.807156 0.24493800 -0.045326362 0.687536401  
## 18462 -1.60507 0.2672580 -0.884388 0.02973600 1.598812624 -0.151788986  
## 15542 -1.61982 0.1783290 -0.602758 0.10187000 0.927542200 0.227544260  
## 18752 -1.41439 0.2021660 -1.021410 0.07233720 0.829284552 -0.668648038  
## 12081 -1.54116 0.1885010 -0.655092 0.03394090 1.024603876 0.030829067  
## 1014 -1.26405 0.1476700 -1.160320 0.03269000 -0.476238068 0.028429558  
## 15612 -1.76674 0.3375280 -0.667801 0.08488970 1.638868393 -0.365455074  
## 14833 -1.47812 0.2484540 -0.867909 0.13378900 -0.632050958 -2.208012195  
## 1639 -1.55076 0.1809390 -0.832294 0.02823040 -1.379618576 0.297039427  
## 10353 -1.46452 0.2528490 -0.771122 0.03499700 -0.257455748 2.129700659  
## 15011 -1.51556 0.1389780 -0.776806 0.02513700 1.679972711 1.325041143  
## 12253 -1.52683 0.1784320 -0.536272 0.36808800 -2.545858038 -0.116171447  
## 10793 -1.40285 0.1793950 -0.935126 0.17230300 0.012078784 -1.470146221  
## 10103 -1.45496 0.1923700 -1.018330 0.05143680 1.960925111 -0.379271835  
## 1903 -1.53717 0.1939060 -0.793830 0.00493727 -0.385905481 -1.465005931  
## 1679 -1.42264 0.1686210 -0.978543 0.10852200 0.910757548 1.075148263  
## 1795 -1.62570 0.1734150 -0.570858 0.04275820 -1.448130794 -1.226124877  
## 1489 -1.43750 0.2315680 -0.742989 0.27496200 -1.121614596 -3.056328234  
## 1881 -1.61298 0.2184480 -0.630581 0.13860100 -0.973617906 1.450657775  
## 15061 -1.32537 0.1226480 -0.867043 0.05831050 -0.067186922 0.717976859

dat$ln\_k\_i <- dat$`M\_ln\_k(1)` + sqrt(dat$`V\_ln\_k(1)`)\*dat$z\_ln\_k  
dat$ln\_Vd\_i <- dat$`M\_ln\_Vd(1)`+ dat$`SD\_ln\_Vd(1)`\*dat$z\_ln\_Vd  
linmod <- lm(ln\_Vd\_i ~ ln\_k\_i,data=dat)  
ggplot(dat) + geom\_point(aes(ln\_k\_i,ln\_Vd\_i)) +   
 labs(subtitle=paste("Adj R2 =",signif(summary(linmod)$adj.r.squared,2)))

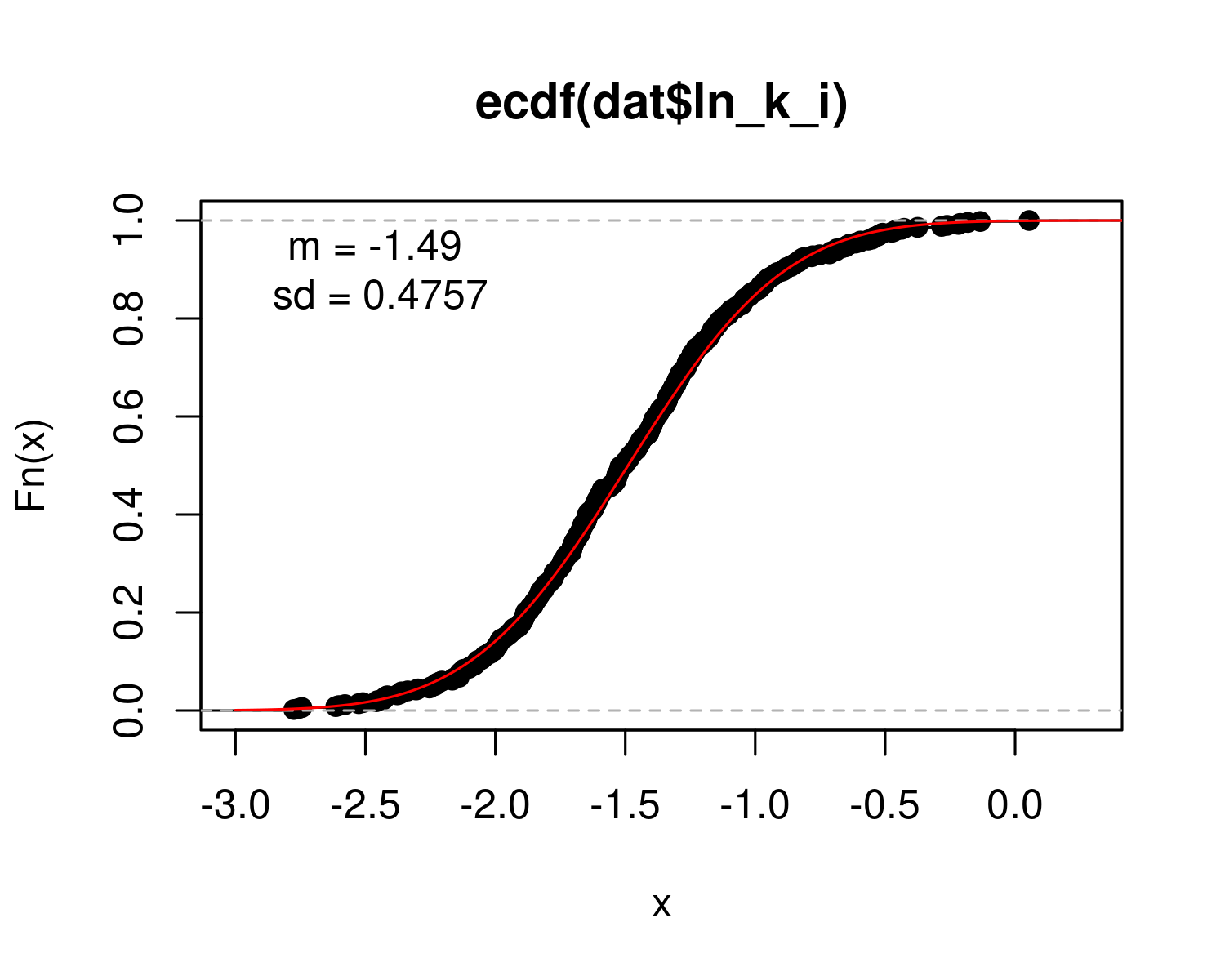


## Check normality

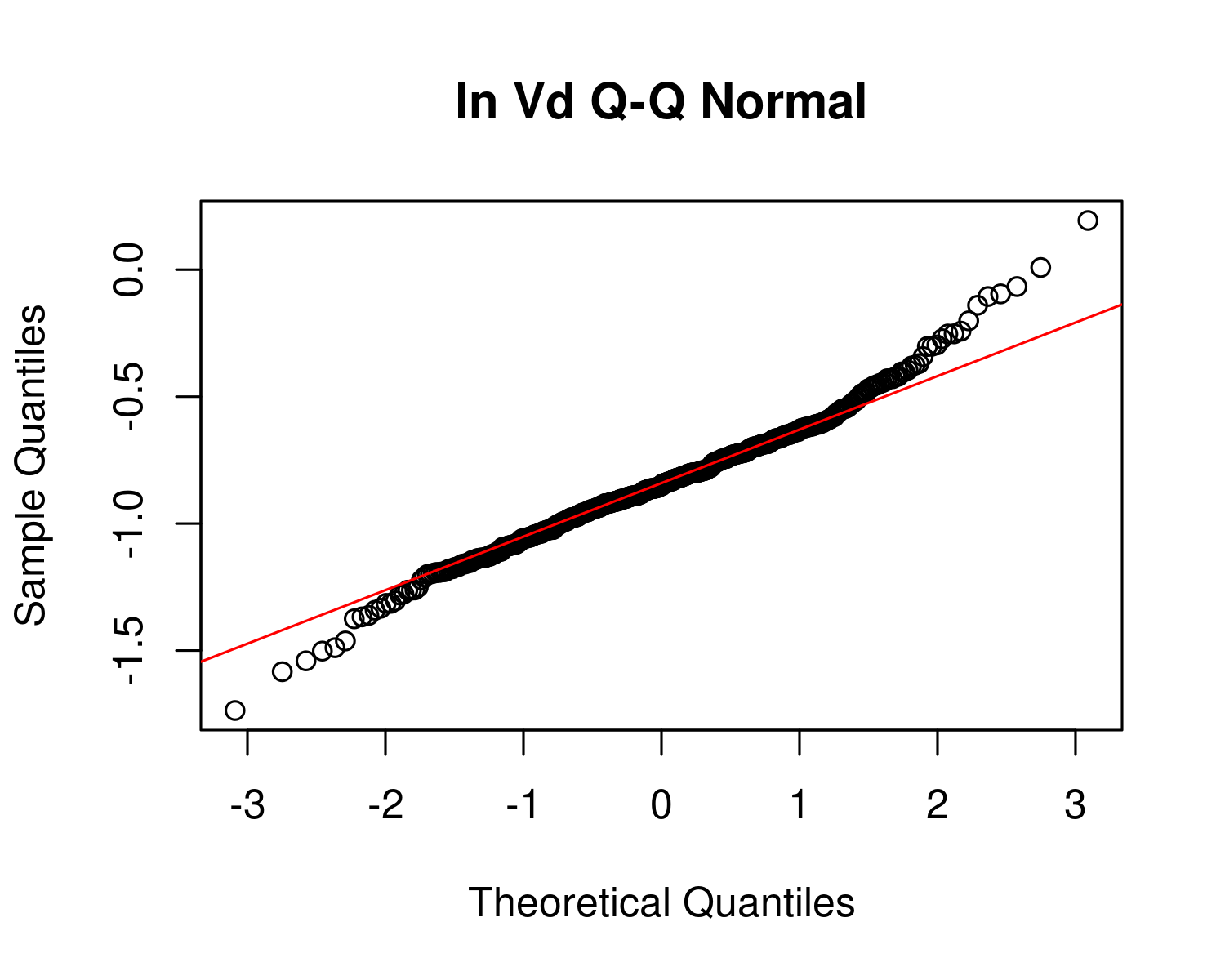
qqnorm(dat$ln\_k\_i,main="ln k Q-Q Normal")  
qqline(dat$ln\_k\_i,col="red")



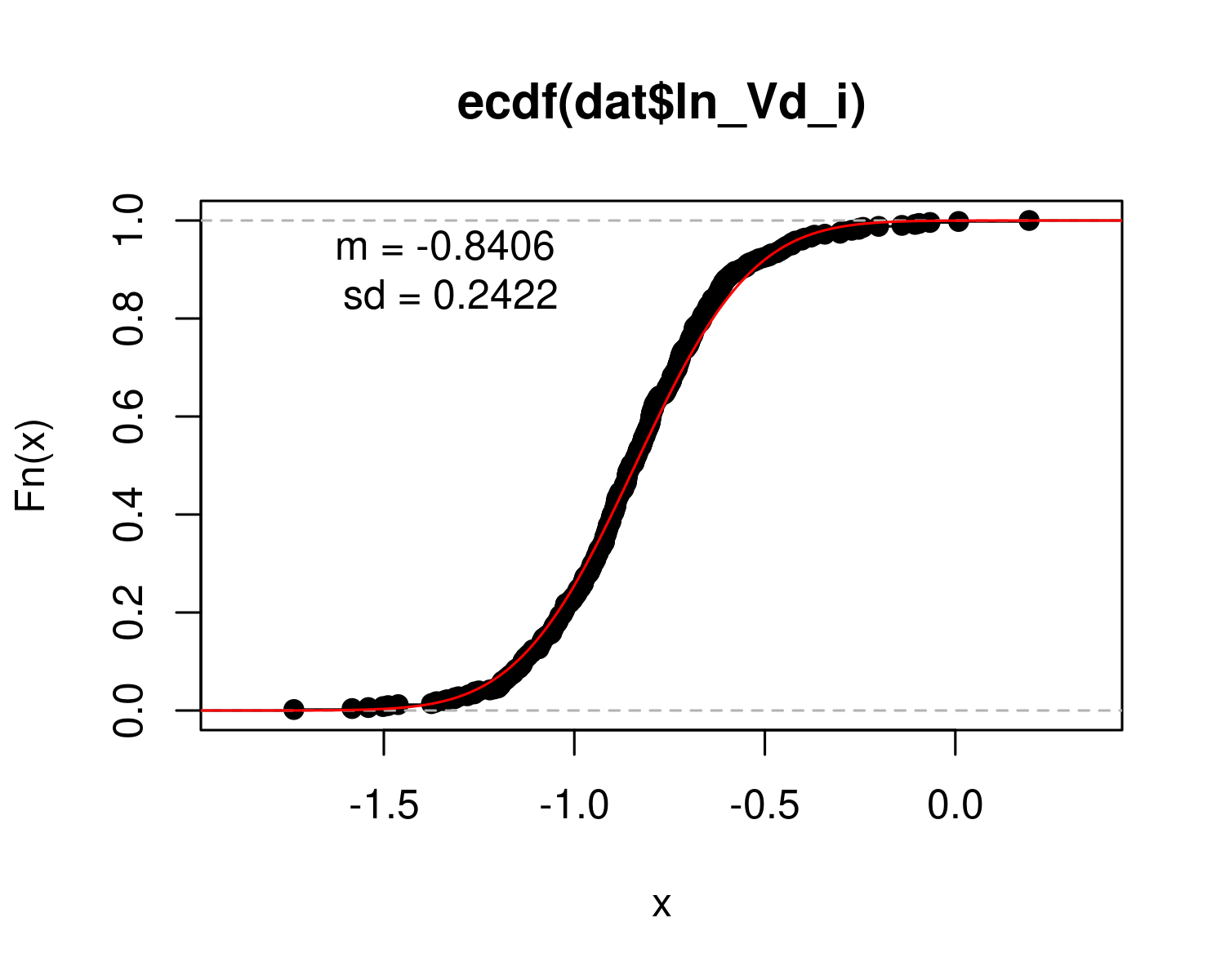
plot(ecdf(dat$ln\_k\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_k\_i <- mean(dat$ln\_k\_i)  
sd\_ln\_k\_i <- sd(dat$ln\_k\_i)  
lines(x,pnorm(x,mean=m\_ln\_k\_i,sd=sd\_ln\_k\_i),col="red")  
text(m\_ln\_k\_i-2\*sd\_ln\_k\_i,0.9,paste("m =",signif(m\_ln\_k\_i,4),"\nsd =",signif(sd\_ln\_k\_i,4)))



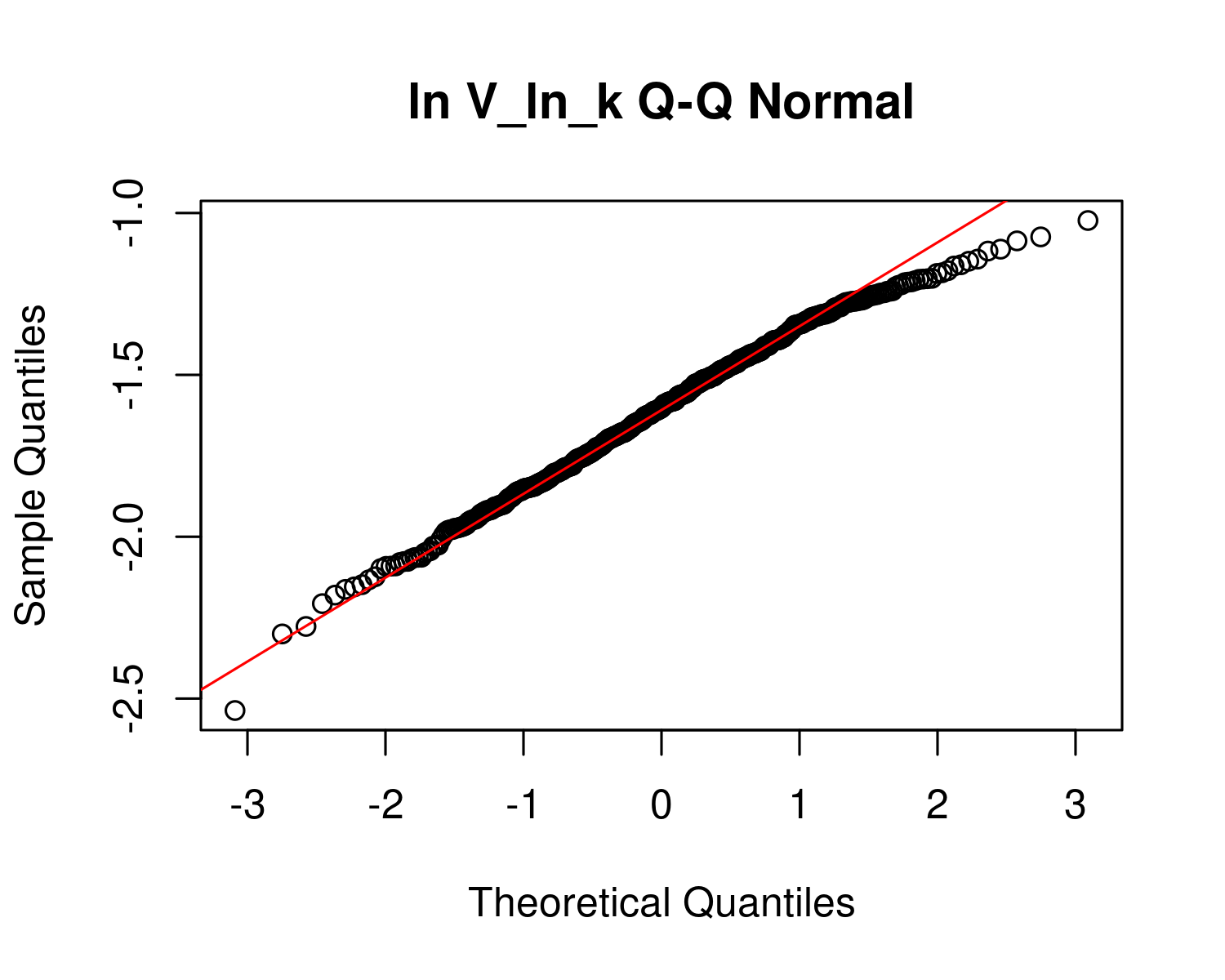
qqnorm(dat$ln\_Vd\_i,main="ln Vd Q-Q Normal")  
qqline(dat$ln\_Vd\_i,col="red")



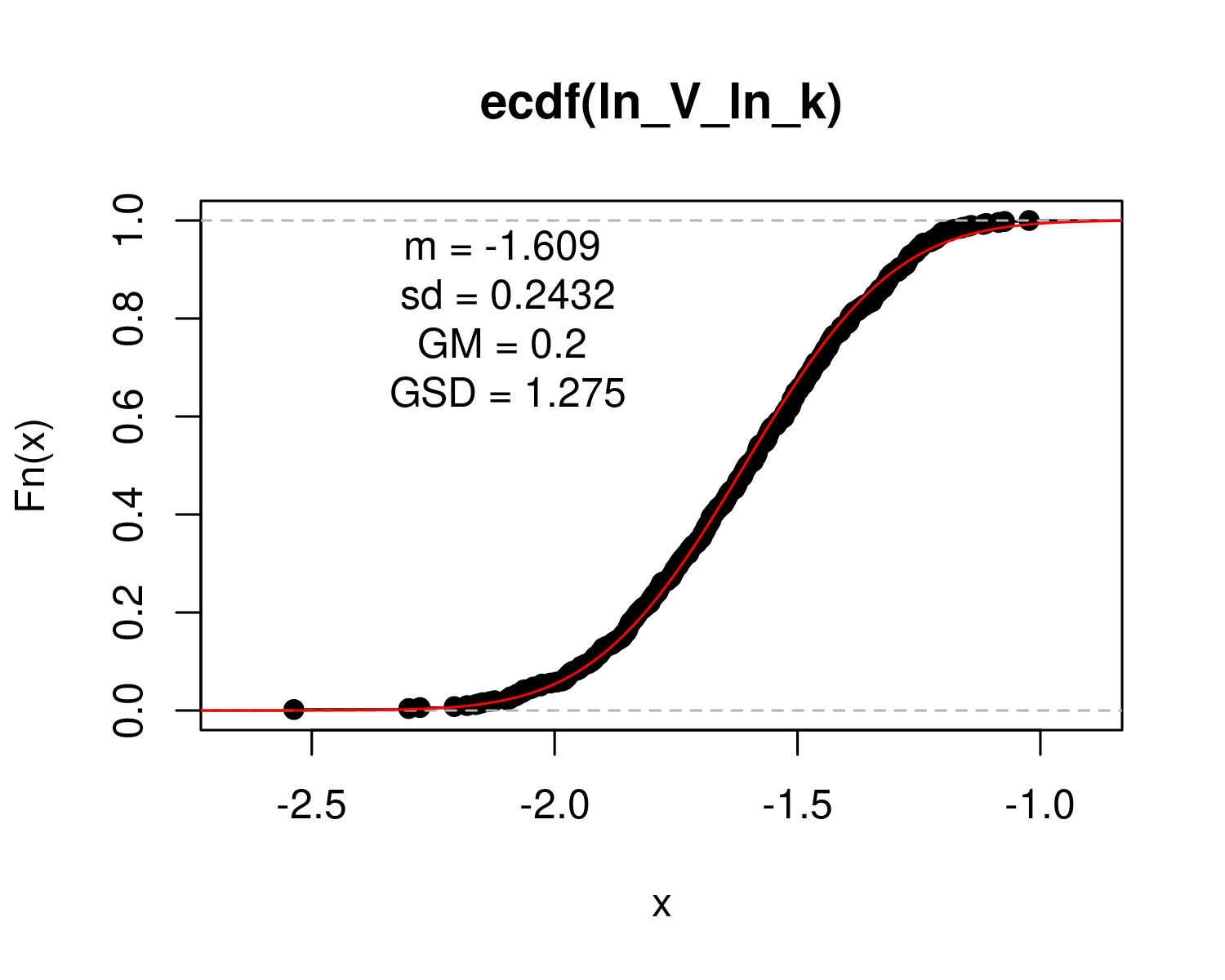
plot(ecdf(dat$ln\_Vd\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_Vd\_i <- mean(dat$ln\_Vd\_i)  
sd\_ln\_Vd\_i <- sd(dat$ln\_Vd\_i)  
  
lines(x,pnorm(x,mean=m\_ln\_Vd\_i,sd=sd\_ln\_Vd\_i),col="red")  
text(m\_ln\_Vd\_i-2\*sd\_ln\_Vd\_i,0.9,paste("m =",signif(m\_ln\_Vd\_i,4),"\nsd =",signif(sd\_ln\_Vd\_i,4)))

 ## Fit to posterior for half-life population variability

ln\_V\_ln\_k <- log(dat$`V\_ln\_k(1)`)  
qqnorm(ln\_V\_ln\_k,main="ln V\_ln\_k Q-Q Normal")  
qqline(ln\_V\_ln\_k,col="red")



plot(ecdf(ln\_V\_ln\_k))  
m\_ln\_V\_ln\_k <- mean(ln\_V\_ln\_k)  
sd\_ln\_V\_ln\_k <- sd(ln\_V\_ln\_k)  
x <- seq(-3,0,0.01)  
  
lines(x,pnorm(x,mean=m\_ln\_V\_ln\_k,sd=sd\_ln\_V\_ln\_k),col="red")  
text(m\_ln\_V\_ln\_k-2\*sd\_ln\_V\_ln\_k,0.9,paste("m =",signif(m\_ln\_V\_ln\_k,4),"\nsd =",signif(sd\_ln\_V\_ln\_k,4)))  
text(m\_ln\_V\_ln\_k-2\*sd\_ln\_V\_ln\_k,0.7,paste("GM =",signif(exp(m\_ln\_V\_ln\_k),4),"\nGSD =",signif(exp(sd\_ln\_V\_ln\_k),4)))

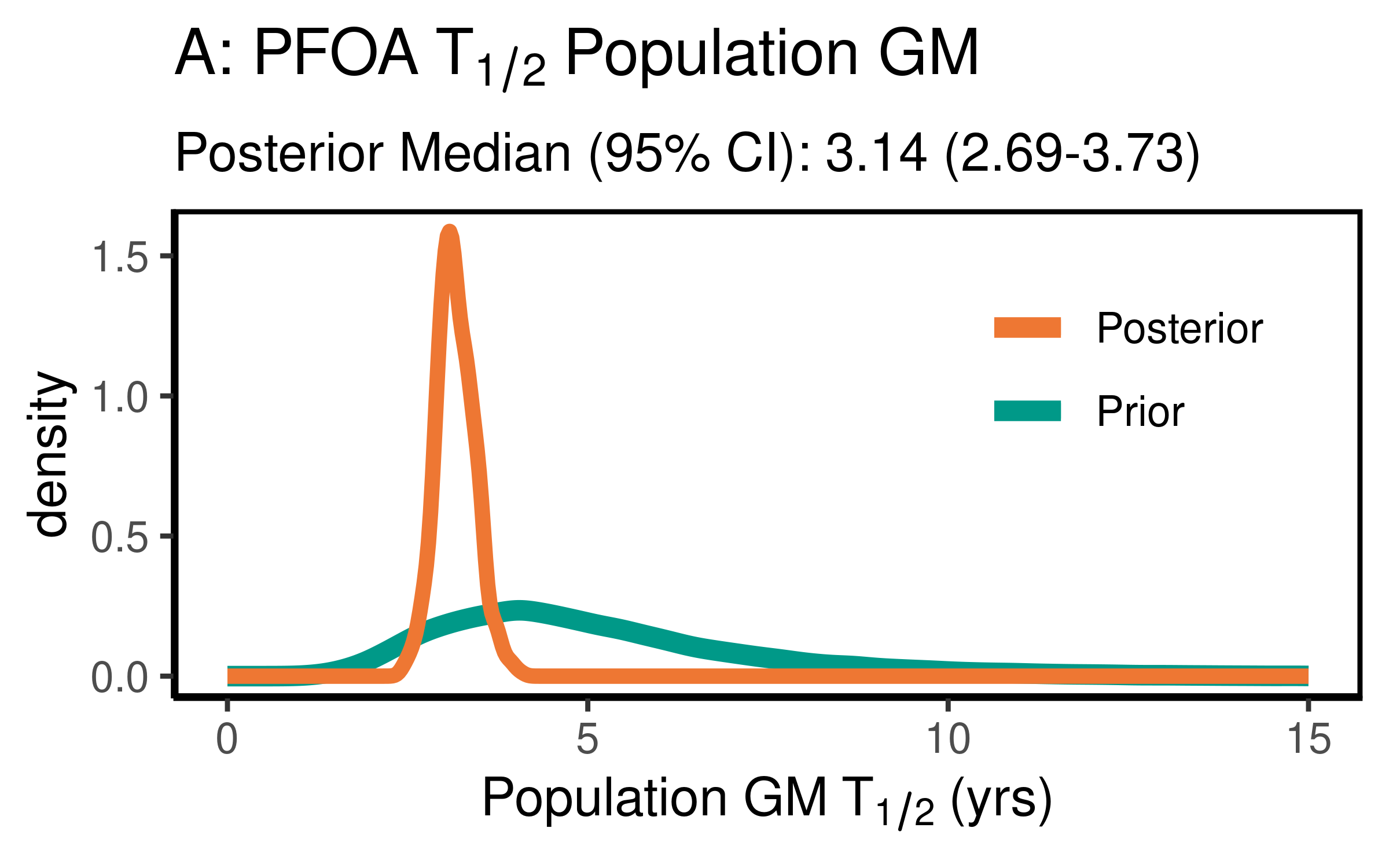


## Calculate table values for individual-level

hl\_i <- log(2)/ exp(dat$ln\_k\_i) # individual half-life   
med\_hl\_i <- paste(signif (median (hl\_i), 3)) # median of individual half-life  
ci\_med\_hl\_i <- paste(signif (quantile(hl\_i, prob=c(0.025,0.975)), 3),collapse="-") # 95ci med individual halflife  
gm\_hl\_i <- paste(signif (exp(mean(log(hl\_i))), 3)) # gm (which should be really close)  
gsd\_hl\_i <- paste(signif (exp(sd(log(hl\_i))), 3)) # gsd individual  
  
med\_Vd\_i <- paste(signif (median(exp(dat$ln\_Vd\_i)), 3)) # median individual Vd  
ci\_med\_Vd\_i <-paste(signif (quantile(exp(dat$ln\_Vd\_i), prob=c(0.025,0.975)), 3),collapse="-") # 95ci med individual Vd  
gm\_vd\_i <- paste(signif (exp(mean(dat$ln\_Vd\_i)), 3)) # gm (which should be really close)  
gsd\_vd\_i<- paste(signif (exp(sd(dat$ln\_Vd\_i)), 3)) # gsd indiv

PFOA\_priors <- data.frame(  
 halflife\_GM= log(2)/rlnorm(50000,  
 meanlog=-1.8971,sdlog=0.4055))  
  
M\_k <- exp(as.numeric(dat$`M\_ln\_k(1)`))  
PFOA\_halflife\_GM <- log(2)/M\_k  
  
pfoa\_hlgm\_pr\_med <- signif(median(PFOA\_priors$halflife\_GM,3))  
pfoa\_hlgm\_pr\_med\_95ci <-paste(signif(quantile(PFOA\_priors$halflife\_GM,  
 prob=c(0.025,0.975)),  
 3),  
 collapse="-")  
  
pfoa\_hl\_median\_gm <- signif(median(PFOA\_halflife\_GM),3)  
pfoa\_hl\_median\_gm\_95ci <- paste(signif(quantile(PFOA\_halflife\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(halflife\_GM, color = "Prior"),data=PFOA\_priors,geom="line",size=2 )+  
 stat\_density(aes(PFOA\_halflife\_GM,stat(density),color="Posterior"),geom="line",size=1.5 )+  
 xlim(0,15)+  
 labs(title = bquote("A: PFOA"~T[1/2]~"Population GM"),   
 subtitle=paste("Posterior Median (95% CI): ",  
 pfoa\_hl\_median\_gm," (",  
 pfoa\_hl\_median\_gm\_95ci,  
 ")",sep=""))+  
 xlab(bquote("Population GM"~T[1/2]~"(yrs)")) +  
 scale\_color\_manual(name=NULL,#  
 values=c(Prior="#009988", Posterior="#EE7733" )) +   
 theme\_classic() +   
 theme(legend.title = element\_blank(),legend.position=c(0.8,0.7),  
 panel.background = element\_rect(color="black",size=1),  
 legend.background = element\_rect(fill="transparent", color=NA))  
print(p)

## Warning: Removed 80 rows containing non-finite values (stat\_density).

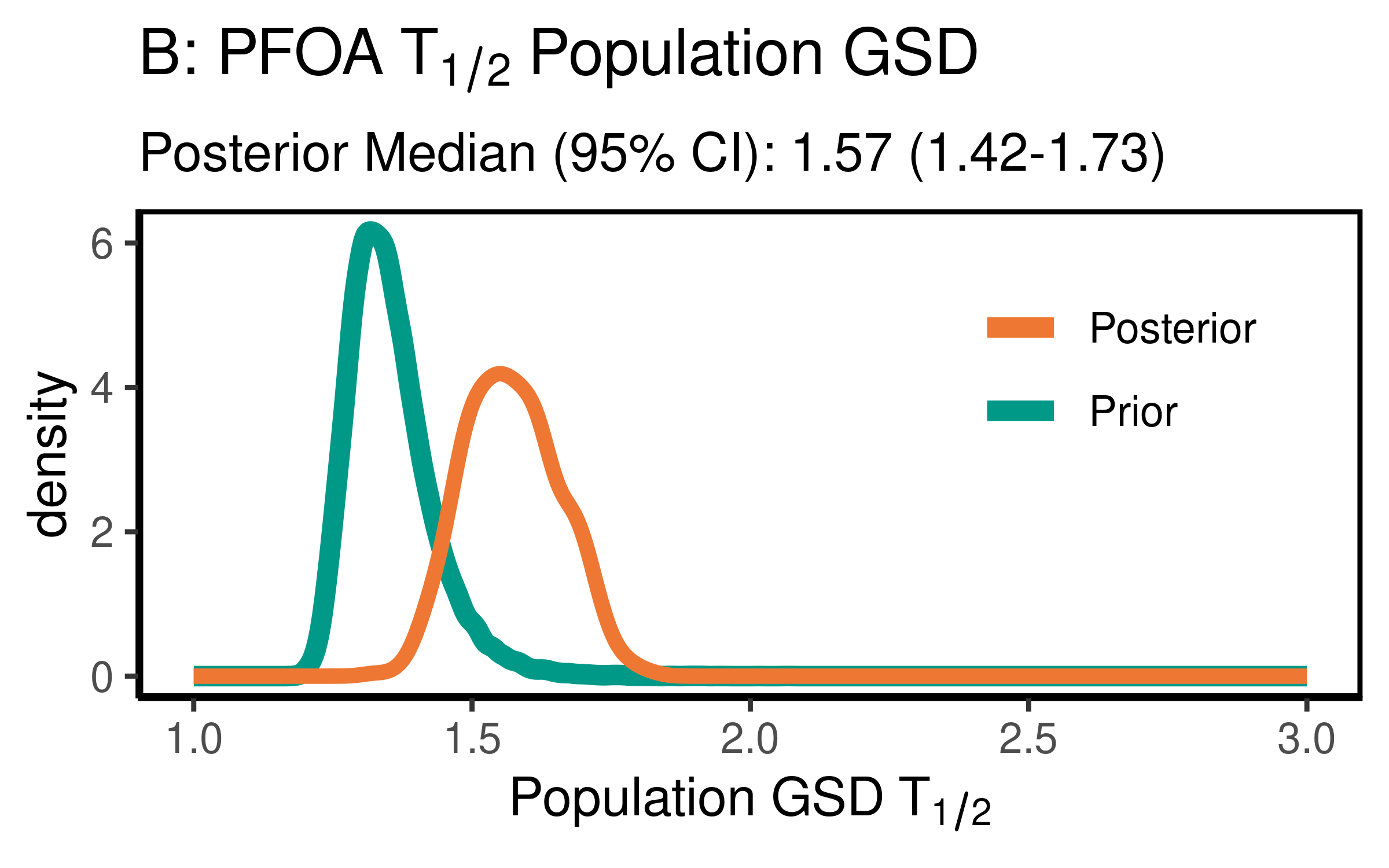


ggsave(here ("output-plots",paste0( sa, "PFOA\_hl\_gm.pdf")), p,dpi=600)

## Saving 4 x 2.5 in image

## Warning: Removed 80 rows containing non-finite values (stat\_density).

PFOA\_priors$halflife\_GSD = exp(sqrt(1/rgamma(50000,shape=9,rate=0.75))) #inverse gamma for the first trial  
PFOA\_halflife\_GSD <- exp(sqrt(dat$`V\_ln\_k(1)`))  
  
pfoa\_hlgsd\_pr\_med <- signif(median(PFOA\_priors$halflife\_GSD,3))  
pfoa\_hlgsd\_pr\_med\_95ci <-paste(signif(quantile(PFOA\_priors$halflife\_GSD,  
 prob=c(0.025,0.975)),  
 3),  
 collapse="-")  
pfoa\_hl\_gsd\_med <- signif(median(PFOA\_halflife\_GSD),3)  
pfoa\_hl\_gsd\_med\_95ci <- paste(signif(quantile(PFOA\_halflife\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
p<-ggplot()+  
 stat\_density(aes(halflife\_GSD, color = "Prior"),data=PFOA\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOA\_halflife\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote( "B: PFOA"~T[1/2]~"Population GSD"),   
 subtitle=paste("Posterior Median (95% CI): ",  
 pfoa\_hl\_gsd\_med," (",  
 pfoa\_hl\_gsd\_med\_95ci,  
 ")",sep=""))+  
 xlab(bquote("Population GSD"~T[1/2]))+  
 scale\_color\_manual(name=NULL,#  
 values=c(Prior="#009988", Posterior="#EE7733" ))+   
 theme\_classic() +   
 theme(legend.title = element\_blank(),legend.position=c(0.8,0.7),  
 panel.background = element\_rect(color="black",size=1),  
 legend.background = element\_rect(fill="transparent", color=NA))  
print(p)

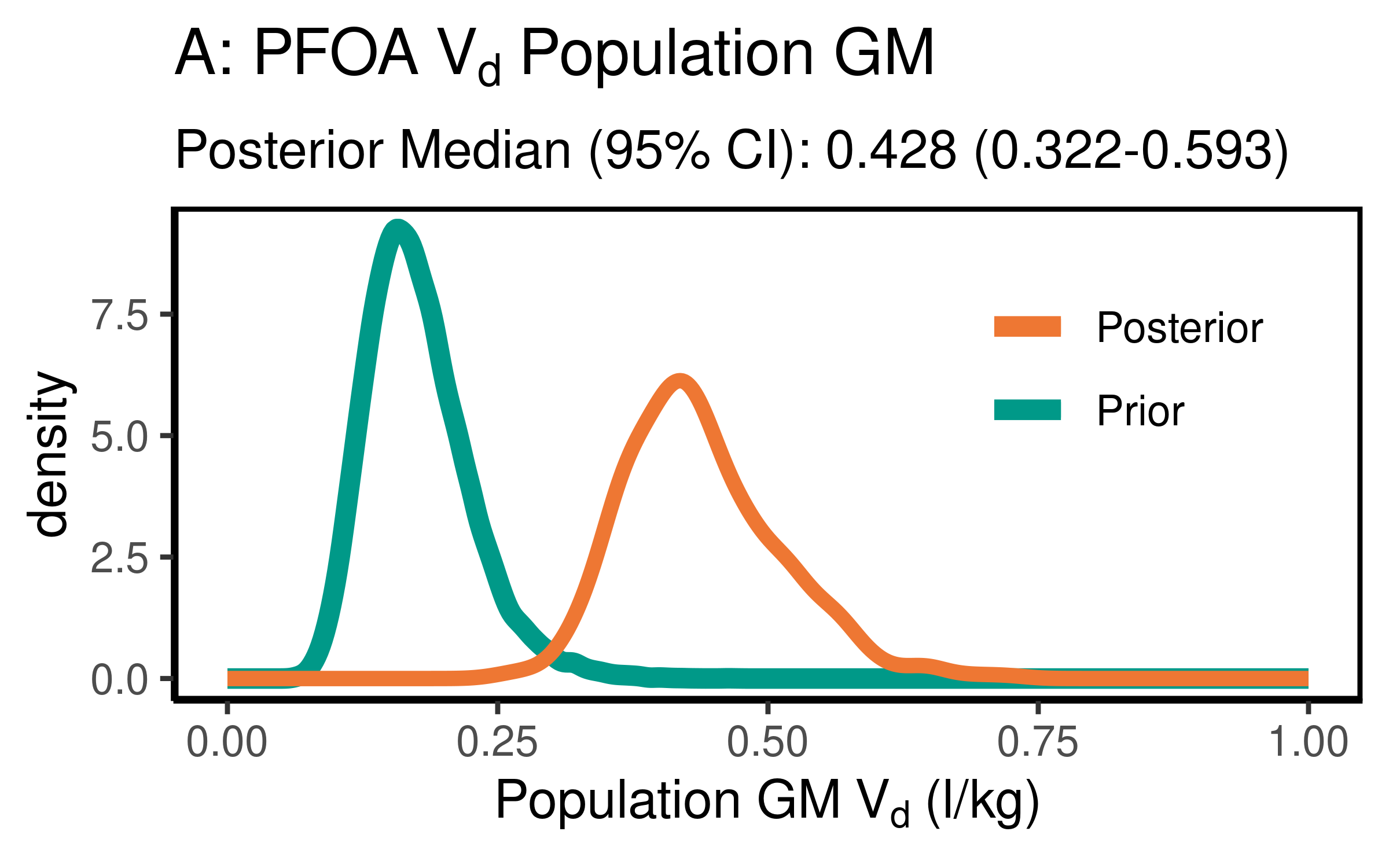


ggsave(here ("output-plots",paste0( sa, "PFOA\_hl\_gsd.pdf")) ,p,dpi=600)

### Distribution Volume

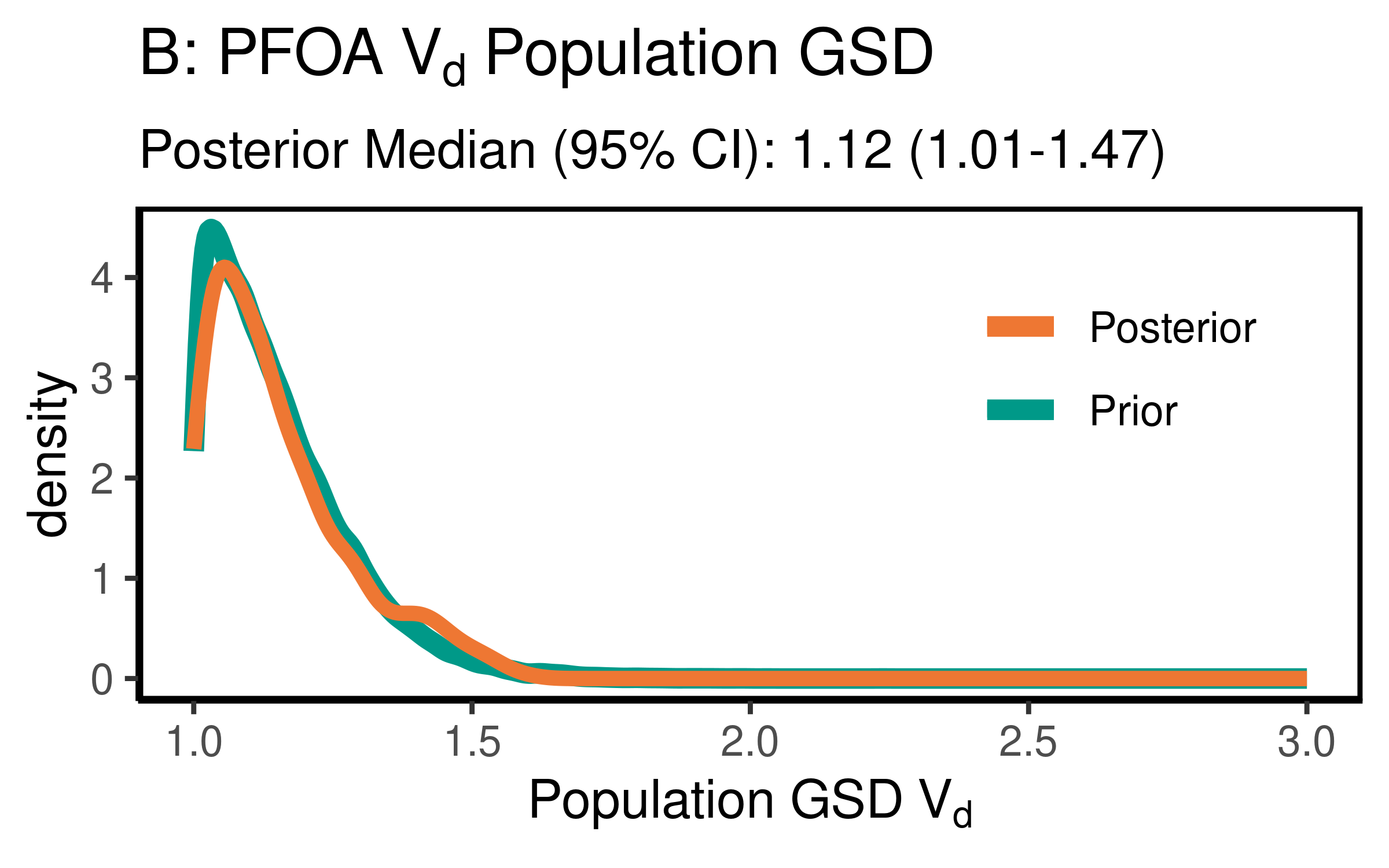
For PFOA, the data were not particularly informative, but slightly increased the estimate of the median to 0.308(0.223-0.548) slightly. They were not informative as to the population GSD, with the posterior distributions essentially unchanged from the priors.

PFOA\_priors$Vd\_GM <- rlnorm(50000,  
 meanlog=-1.7720,  
 sdlog=0.2624)  
PFOA\_Vd\_GM <- exp(dat$`M\_ln\_Vd(1)`)  
  
   
  
pfoa\_vd\_gm\_pr\_med <- signif(median(PFOA\_priors$Vd\_GM,3))  
pfoa\_vd\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFOA\_priors$Vd\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
pfoa\_vd\_gm\_med <- signif(median(PFOA\_Vd\_GM),3)  
pfoa\_vd\_gm\_med\_95ci <- paste(signif(quantile(PFOA\_Vd\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(Vd\_GM, color = "Prior"),data=PFOA\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOA\_Vd\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,1)+  
 labs(title = bquote( "A: PFOA"~V[d]~"Population GM"),  
 subtitle = paste0("Posterior Median (95% CI): ", pfoa\_vd\_gm\_med," (", pfoa\_vd\_gm\_med\_95ci, ")" )  
 )+  
 xlab(bquote("Population GM"~V[d]~"(l/kg)"))+  
 scale\_color\_manual(name=NULL,#  
 values=c(Prior="#009988", Posterior="#EE7733" )) +   
 theme\_classic() +   
 theme(legend.title = element\_blank(),legend.position=c(0.8,0.7),  
 panel.background = element\_rect(color="black",size=1),  
 legend.background = element\_rect(fill="transparent", color=NA))  
print(p)



ggsave(here ("output-plots",paste0( sa, "PFOA\_vd\_gm.pdf")) ,p,dpi=600)

PFOA\_priors$Vd\_GSD = exp(abs(rnorm(50000,sd=0.17)))  
PFOA\_Vd\_GSD <- exp(dat$`SD\_ln\_Vd(1)`)  
  
pfoa\_vd\_gsd\_pr\_med <- signif(median(PFOA\_priors$Vd\_GSD,3))  
pfoa\_vd\_gsd\_pr\_med\_95ci <- paste(signif(quantile(PFOA\_priors$Vd\_GSD,  
 prob=c(0.025,0.975)), 3), collapse="-")  
  
pfoa\_vd\_gsd\_med <- signif(median(PFOA\_Vd\_GSD),3)  
pfoa\_vd\_gsd\_med\_95ci <- paste(signif(quantile(PFOA\_Vd\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(Vd\_GSD, color = "Prior"),data=PFOA\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOA\_Vd\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("B: PFOA"~V[d]~"Population GSD "),  
 subtitle=paste("Posterior Median (95% CI): ",  
 pfoa\_vd\_gsd\_med," (",  
 pfoa\_vd\_gsd\_med\_95ci,  
 ")",sep=""))+  
 xlab(bquote("Population GSD"~V[d]))+  
 scale\_color\_manual(name=NULL,   
 values=c(Prior="#009988", Posterior="#EE7733" )) +   
 theme\_classic() +   
 theme(legend.title = element\_blank(),legend.position=c(0.8,0.7),  
 panel.background = element\_rect(color="black",size=1),  
 legend.background = element\_rect(fill="transparent", color=NA))  
print(p)

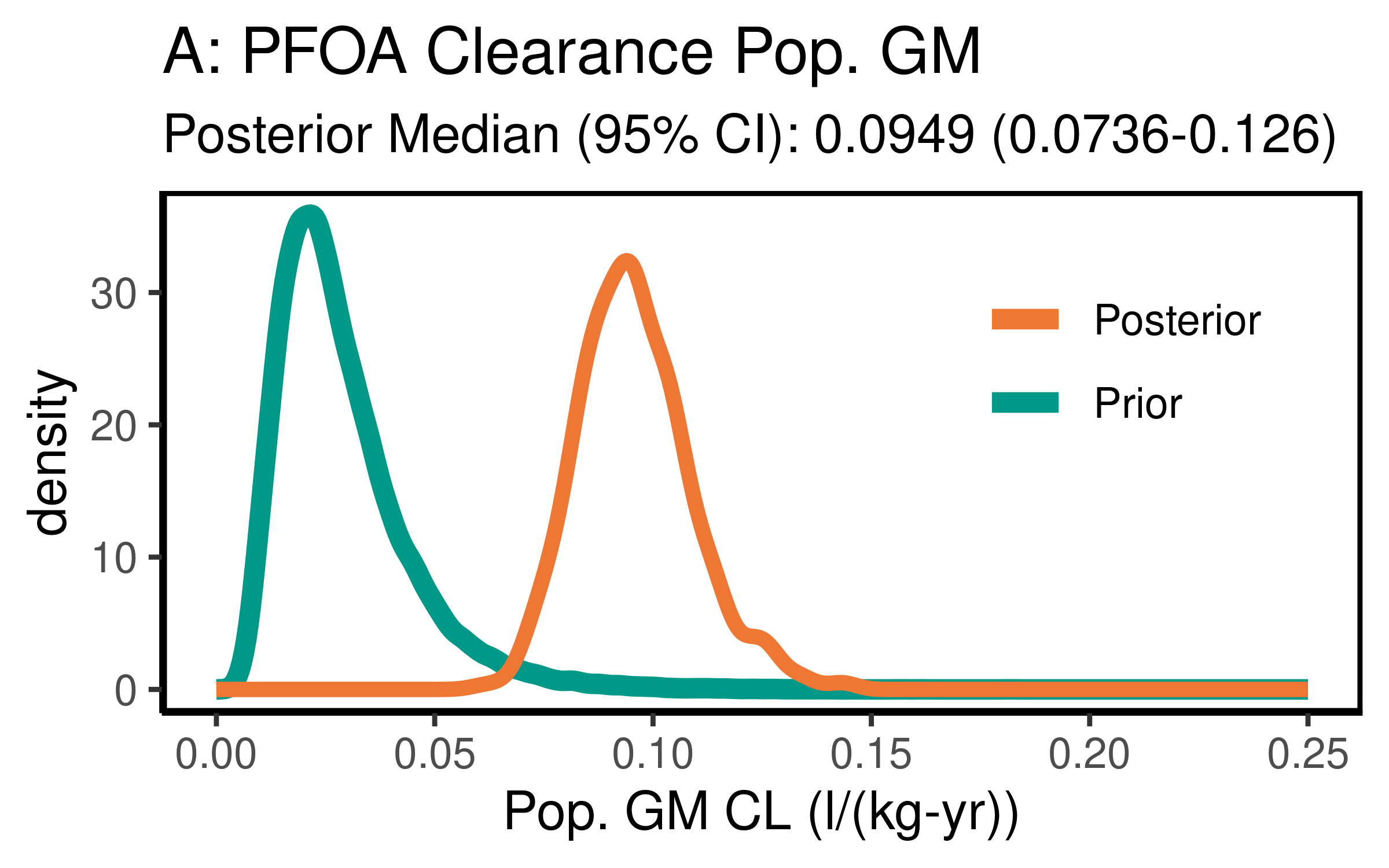


ggsave(here ("output-plots",paste0( sa, "PFOA\_vd\_gsd.pdf")) ,p,dpi=600)

### Clearance (just pop GM)

Cl is k \* Vd

PFOA\_priors$CL\_GM <- PFOA\_priors$Vd\_GM \* (log(2)/PFOA\_priors$halflife\_GM)  
PFOA\_CL\_GM <- exp(dat$`M\_ln\_Vd(1)` + dat$`M\_ln\_k(1)`)  
  
pfoa\_cl\_gm\_pr\_med <- signif(median(PFOA\_priors$CL\_GM,3))  
pfoa\_cl\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFOA\_priors$CL\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
pfoa\_cl\_gm\_med <- signif(median(PFOA\_CL\_GM),3)  
pfoa\_cl\_gm\_med\_95ci <- paste(signif(quantile(PFOA\_CL\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(CL\_GM, color = "Prior"),data=PFOA\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOA\_CL\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,0.25)+labs(title = "A: PFOA Clearance Pop. GM ",subtitle=paste("Posterior Median (95% CI): ",  
 pfoa\_cl\_gm\_med," (",  
 pfoa\_cl\_gm\_med\_95ci,  
 ")",sep=""))+  
 xlab("Pop. GM CL (l/(kg-yr))")+  
 scale\_color\_manual(name=NULL,#  
 values=c(Prior="#009988", Posterior="#EE7733" )) +   
 theme\_classic() +   
 theme(legend.title = element\_blank(),legend.position=c(0.8,0.7),  
 panel.background = element\_rect(color="black",size=1),  
 legend.background = element\_rect(fill="transparent", color=NA))  
print(p)



ggsave(here ("output-plots",paste0( sa, "PFOA\_CL\_gm.pdf")), p,dpi=600)

## Table significant digit values

pfoa\_hlgm\_pr\_med <- paste(signif(pfoa\_hlgm\_pr\_med, 3))  
pfoa\_hl\_median\_gm<- paste(signif(pfoa\_hl\_median\_gm, 3))  
pfoa\_hlgsd\_pr\_med<- paste(signif(pfoa\_hlgsd\_pr\_med, 3))  
pfoa\_hl\_gsd\_med<- paste(signif(pfoa\_hl\_gsd\_med, 3))  
pfoa\_vd\_gm\_pr\_med<- paste(signif(pfoa\_vd\_gm\_pr\_med, 3))  
pfoa\_vd\_gm\_med<- paste(signif(pfoa\_vd\_gm\_med, 3))  
pfoa\_vd\_gsd\_pr\_med<- paste(signif(pfoa\_vd\_gsd\_pr\_med, 3))  
pfoa\_vd\_gsd\_med<- paste(signif(pfoa\_vd\_gsd\_med, 3))  
pfoa\_cl\_gm\_pr\_med<- paste(signif(pfoa\_cl\_gm\_pr\_med, 3))  
pfoa\_cl\_gm\_med<- paste(signif(pfoa\_cl\_gm\_med, 3))

### Population median estimates [95% CI]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Prior GM | Posterior GM | Prior GSD | Posterior GSD |
| Half-life (years) | 4.62 | 3.14 | 1.34 | 1.57 |
| HL [95% CI] | [2.08-10.3] | [2.69-3.73] | [1.24-1.53] | [1.42-1.73] |
| Volume of distribution | 0.17 | 0.428 | 1.12 | 1.12 |
| [95% CI] | [0.102-0.286] | [0.322-0.593] | [1.01-1.46] | [1.01-1.47] |
| Clearance | 0.0255 | 0.0949 |  |  |
| [95% CI] | [0.00974-0.0664] | [0.0736-0.126] | [] | [] |

### Individual Posterior estimates

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | median GM [95% CI] | GM calculator input | GSD individual |
| Half-life (years) | 3.13 [ 1.13-7.83 ] | 3.07 | 1.61 |
| Volume of distribution | 0.427 [ 0.27-0.739 ] | 0.431 | 1.27 |

## ─ Session info ───────────────────────────────────────────────────────────────  
## setting value   
## version R version 3.6.1 (2019-07-05)   
## os Red Hat Enterprise Linux Server 7.9 (Maipo)  
## system x86\_64, linux-gnu   
## ui X11   
## language (EN)   
## collate en\_US.UTF-8   
## ctype en\_US.UTF-8   
## tz America/New\_York   
## date 2021-02-27   
##   
## ─ Packages ───────────────────────────────────────────────────────────────────  
## package \* version date lib source   
## assertthat 0.2.1 2019-03-21 [2] CRAN (R 3.6.1)  
## backports 1.1.5 2019-10-02 [2] CRAN (R 3.6.1)  
## bayesplot \* 1.7.0 2019-05-23 [2] CRAN (R 3.6.1)  
## broom 0.5.2 2019-04-07 [2] CRAN (R 3.6.1)  
## callr 3.3.2 2019-09-22 [2] CRAN (R 3.6.1)  
## cellranger 1.1.0 2016-07-27 [2] CRAN (R 3.6.1)  
## cli 1.1.0 2019-03-19 [2] CRAN (R 3.6.1)  
## coda \* 0.19-3 2019-07-05 [2] CRAN (R 3.6.1)  
## codetools 0.2-16 2018-12-24 [2] CRAN (R 3.6.1)  
## colorspace 1.4-1 2019-03-18 [2] CRAN (R 3.6.1)  
## crayon 1.3.4 2017-09-16 [2] CRAN (R 3.6.1)  
## DBI 1.0.0 2018-05-02 [2] CRAN (R 3.6.1)  
## dbplyr 1.4.2 2019-06-17 [2] CRAN (R 3.6.1)  
## desc 1.2.0 2018-05-01 [2] CRAN (R 3.6.1)  
## devtools 2.2.1 2019-09-24 [2] CRAN (R 3.6.1)  
## digest 0.6.23 2019-11-23 [2] CRAN (R 3.6.1)  
## dplyr \* 0.8.3 2019-07-04 [2] CRAN (R 3.6.1)  
## ellipsis 0.3.0 2019-09-20 [2] CRAN (R 3.6.1)  
## evaluate 0.14 2019-05-28 [2] CRAN (R 3.6.1)  
## farver 2.0.1 2019-11-13 [2] CRAN (R 3.6.1)  
## forcats \* 0.4.0 2019-02-17 [2] CRAN (R 3.6.1)  
## fs 1.3.1 2019-05-06 [2] CRAN (R 3.6.1)  
## generics 0.0.2 2018-11-29 [2] CRAN (R 3.6.1)  
## ggplot2 \* 3.2.1 2019-08-10 [2] CRAN (R 3.6.1)  
## ggridges 0.5.1 2018-09-27 [2] CRAN (R 3.6.1)  
## ggsci \* 2.9 2018-05-14 [2] CRAN (R 3.6.1)  
## glue 1.3.1 2019-03-12 [2] CRAN (R 3.6.1)  
## gridExtra 2.3 2017-09-09 [2] CRAN (R 3.6.1)  
## gtable 0.3.0 2019-03-25 [2] CRAN (R 3.6.1)  
## haven 2.2.0 2019-11-08 [2] CRAN (R 3.6.1)  
## here \* 0.1 2017-05-28 [2] CRAN (R 3.6.1)  
## hms 0.5.2 2019-10-30 [2] CRAN (R 3.6.1)  
## htmltools 0.4.0 2019-10-04 [2] CRAN (R 3.6.1)  
## httr 1.4.1 2019-08-05 [2] CRAN (R 3.6.1)  
## jsonlite 1.6 2018-12-07 [2] CRAN (R 3.6.1)  
## khroma \* 1.4.0 2020-10-05 [1] CRAN (R 3.6.1)  
## knitr 1.26 2019-11-12 [2] CRAN (R 3.6.1)  
## labeling 0.3 2014-08-23 [2] CRAN (R 3.6.1)  
## lattice 0.20-38 2018-11-04 [2] CRAN (R 3.6.1)  
## lazyeval 0.2.2 2019-03-15 [2] CRAN (R 3.6.1)  
## lifecycle 0.1.0 2019-08-01 [2] CRAN (R 3.6.1)  
## lubridate 1.7.4 2018-04-11 [2] CRAN (R 3.6.1)  
## magrittr 1.5 2014-11-22 [2] CRAN (R 3.6.1)  
## memoise 1.1.0 2017-04-21 [2] CRAN (R 3.6.1)  
## modelr 0.1.5 2019-08-08 [2] CRAN (R 3.6.1)  
## munsell 0.5.0 2018-06-12 [2] CRAN (R 3.6.1)  
## nlme 3.1-142 2019-11-07 [2] CRAN (R 3.6.1)  
## pillar 1.4.2 2019-06-29 [2] CRAN (R 3.6.1)  
## pkgbuild 1.0.6 2019-10-09 [2] CRAN (R 3.6.1)  
## pkgconfig 2.0.3 2019-09-22 [2] CRAN (R 3.6.1)  
## pkgload 1.0.2 2018-10-29 [2] CRAN (R 3.6.1)  
## plyr 1.8.4 2016-06-08 [2] CRAN (R 3.6.1)  
## prettyunits 1.0.2 2015-07-13 [2] CRAN (R 3.6.1)  
## processx 3.4.1 2019-07-18 [2] CRAN (R 3.6.1)  
## ps 1.3.0 2018-12-21 [2] CRAN (R 3.6.1)  
## purrr \* 0.3.3 2019-10-18 [2] CRAN (R 3.6.1)  
## R6 2.4.1 2019-11-12 [2] CRAN (R 3.6.1)  
## Rcpp 1.0.3 2019-11-08 [2] CRAN (R 3.6.1)  
## readr \* 1.3.1 2018-12-21 [2] CRAN (R 3.6.1)  
## readxl 1.3.1 2019-03-13 [2] CRAN (R 3.6.1)  
## remotes 2.1.0 2019-06-24 [2] CRAN (R 3.6.1)  
## reprex 0.3.0 2019-05-16 [2] CRAN (R 3.6.1)  
## reshape2 \* 1.4.3 2017-12-11 [2] CRAN (R 3.6.1)  
## rlang 0.4.2 2019-11-23 [2] CRAN (R 3.6.1)  
## rmarkdown 1.18 2019-11-27 [2] CRAN (R 3.6.1)  
## rprojroot 1.3-2 2018-01-03 [2] CRAN (R 3.6.1)  
## rstudioapi 0.10 2019-03-19 [2] CRAN (R 3.6.1)  
## rvest 0.3.5 2019-11-08 [2] CRAN (R 3.6.1)  
## scales 1.1.0 2019-11-18 [2] CRAN (R 3.6.1)  
## sessioninfo 1.1.1 2018-11-05 [2] CRAN (R 3.6.1)  
## stringi 1.4.3 2019-03-12 [2] CRAN (R 3.6.1)  
## stringr \* 1.4.0 2019-02-10 [2] CRAN (R 3.6.1)  
## testthat 2.3.0 2019-11-05 [2] CRAN (R 3.6.1)  
## tibble \* 2.1.3 2019-06-06 [2] CRAN (R 3.6.1)  
## tidyr \* 1.0.0 2019-09-11 [2] CRAN (R 3.6.1)  
## tidyselect 0.2.5 2018-10-11 [2] CRAN (R 3.6.1)  
## tidyverse \* 1.3.0 2019-11-21 [2] CRAN (R 3.6.1)  
## usethis 1.5.1 2019-07-04 [2] CRAN (R 3.6.1)  
## vctrs 0.2.0 2019-07-05 [2] CRAN (R 3.6.1)  
## viridis \* 0.5.1 2018-03-29 [2] CRAN (R 3.6.1)  
## viridisLite \* 0.3.0 2018-02-01 [2] CRAN (R 3.6.1)  
## withr 2.1.2 2018-03-15 [2] CRAN (R 3.6.1)  
## xfun 0.11 2019-11-12 [2] CRAN (R 3.6.1)  
## xml2 1.2.2 2019-08-09 [2] CRAN (R 3.6.1)  
## yaml 2.2.0 2018-07-25 [2] CRAN (R 3.6.1)  
## zeallot 0.1.0 2018-01-28 [2] CRAN (R 3.6.1)  
##   
## [1] /home/ad.abt.local/wchiu/R/library  
## [2] /opt/R/3.6.1/lib64/R/library