PFHxS 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)  
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/PFHxS\_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("Decatur M Test", 9),  
 rep("Decatur F Test", 10),  
 'Paulsboro-Train','Horsham-Train',  
 'Warminster-Test','Warrington-Train'),   
 Sex = c(   
 rep("M", 9),  
 rep("F", 9),  
 rep("M", 9),  
 rep("F", 10),  
 'Mixed', 'Mixed', 'Mixed', 'Mixed'),  
 City = c(   
 rep("Decatur", 18),  
 rep("Decatur", 19),  
 'Paulsboro','Horsham','Warminster','Warrington'),   
 Train\_Test = c(   
 rep("Train", 9),  
 rep("Train", 9),  
 rep("Test", 9),  
 rep("Test", 10),  
 'Train', 'Train', 'Test', 'Test'),  
 datatype = c(  
 rep("Individual",9+9+9+10),  
 rep("Summary",4)),  
 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")) %>%  
 mutate( dataset = as.factor(dataset))  
  
nv <- data.frame(dataset =unique(indiv\_lut$dataset),   
 variable= rep("Pop GM", 4),  
 type= rep("Pop GM", 4), 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 match PFOA.

nrow(multicheck$df\_check)

## [1] 39000

nrow(id\_lut)

## [1] 41

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

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

## [1] 39000

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" ~ "G: PFHxS Train",  
 Train\_Test=="Test" ~ "H: PFHxS 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

#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` == "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("Male", "Female", "Mixed (all sexes)")))

## Joining, by = c("Level", "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 dataset  
## 1 1\_1\_1\_1\_1 1 Cserum 0.000 15.400 1\_1\_1\_1\_1 Decatur M Train  
## 2 1\_1\_1\_1\_1 1 Cserum 5.802 16.600 1\_1\_1\_1\_1 Decatur M Train  
## 3 1\_1\_1\_1\_2 2 Cserum 0.000 4.900 1\_1\_1\_1\_2 Decatur M Train  
## 4 1\_1\_1\_1\_2 2 Cserum 5.802 6.100 1\_1\_1\_1\_2 Decatur M Train  
## 5 1\_1\_1\_1\_3 3 Cserum 0.000 11.300 1\_1\_1\_1\_3 Decatur M Train  
## 6 1\_1\_1\_1\_3 3 Cserum 5.802 7.800 1\_1\_1\_1\_3 Decatur M Train  
## 7 1\_1\_1\_1\_4 4 Cserum 0.000 12.800 1\_1\_1\_1\_4 Decatur M Train  
## 8 1\_1\_1\_1\_4 4 Cserum 5.802 5.600 1\_1\_1\_1\_4 Decatur M Train  
## 9 1\_1\_1\_1\_5 5 Cserum 0.000 20.900 1\_1\_1\_1\_5 Decatur M Train  
## 10 1\_1\_1\_1\_5 5 Cserum 5.802 12.400 1\_1\_1\_1\_5 Decatur M Train  
## 11 1\_1\_1\_1\_6 6 Cserum 0.000 6.300 1\_1\_1\_1\_6 Decatur M Train  
## 12 1\_1\_1\_1\_6 6 Cserum 5.802 6.700 1\_1\_1\_1\_6 Decatur M Train  
## 13 1\_1\_1\_1\_7 7 Cserum 0.000 24.400 1\_1\_1\_1\_7 Decatur M Train  
## 14 1\_1\_1\_1\_7 7 Cserum 5.802 18.100 1\_1\_1\_1\_7 Decatur M Train  
## 15 1\_1\_1\_1\_8 8 Cserum 0.000 24.200 1\_1\_1\_1\_8 Decatur M Train  
## 16 1\_1\_1\_1\_8 8 Cserum 5.802 20.200 1\_1\_1\_1\_8 Decatur M Train  
## 17 1\_1\_1\_1\_9 9 Cserum 0.000 7.800 1\_1\_1\_1\_9 Decatur M Train  
## 18 1\_1\_1\_1\_9 9 Cserum 5.802 8.500 1\_1\_1\_1\_9 Decatur M Train  
## 19 1\_1\_1\_1\_10 10 Cserum 0.000 2.300 1\_1\_1\_1\_10 Decatur F Train  
## 20 1\_1\_1\_1\_10 10 Cserum 5.802 2.500 1\_1\_1\_1\_10 Decatur F Train  
## 21 1\_1\_1\_1\_11 11 Cserum 0.000 12.900 1\_1\_1\_1\_11 Decatur F Train  
## 22 1\_1\_1\_1\_11 11 Cserum 5.802 13.700 1\_1\_1\_1\_11 Decatur F Train  
## 23 1\_1\_1\_1\_12 12 Cserum 0.000 2.400 1\_1\_1\_1\_12 Decatur F Train  
## 24 1\_1\_1\_1\_12 12 Cserum 5.802 3.300 1\_1\_1\_1\_12 Decatur F Train  
## 25 1\_1\_1\_1\_13 13 Cserum 0.000 2.700 1\_1\_1\_1\_13 Decatur F Train  
## 26 1\_1\_1\_1\_13 13 Cserum 5.802 4.000 1\_1\_1\_1\_13 Decatur F Train  
## 27 1\_1\_1\_1\_14 14 Cserum 0.000 18.300 1\_1\_1\_1\_14 Decatur F Train  
## 28 1\_1\_1\_1\_14 14 Cserum 5.802 18.400 1\_1\_1\_1\_14 Decatur F Train  
## 29 1\_1\_1\_1\_15 15 Cserum 0.000 12.900 1\_1\_1\_1\_15 Decatur F Train  
## 30 1\_1\_1\_1\_15 15 Cserum 5.802 13.200 1\_1\_1\_1\_15 Decatur F Train  
## 31 1\_1\_1\_1\_16 16 Cserum 0.000 3.300 1\_1\_1\_1\_16 Decatur F Train  
## 32 1\_1\_1\_1\_16 16 Cserum 5.802 4.100 1\_1\_1\_1\_16 Decatur F Train  
## 33 1\_1\_1\_1\_17 17 Cserum 0.000 16.900 1\_1\_1\_1\_17 Decatur F Train  
## 34 1\_1\_1\_1\_17 17 Cserum 5.802 12.300 1\_1\_1\_1\_17 Decatur F Train  
## 35 1\_1\_1\_1\_18 18 Cserum 0.000 8.700 1\_1\_1\_1\_18 Decatur F Train  
## 36 1\_1\_1\_1\_18 18 Cserum 5.802 6.500 1\_1\_1\_1\_18 Decatur F Train  
## 37 1\_1\_1\_2\_1 19 Cserum 0.000 6.300 1\_1\_1\_2\_1 Decatur M Test  
## 38 1\_1\_1\_2\_1 19 Cserum 5.802 4.600 1\_1\_1\_2\_1 Decatur M Test  
## 39 1\_1\_1\_2\_2 20 Cserum 0.000 7.100 1\_1\_1\_2\_2 Decatur M Test  
## 40 1\_1\_1\_2\_2 20 Cserum 5.802 7.400 1\_1\_1\_2\_2 Decatur M Test  
## 41 1\_1\_1\_2\_3 21 Cserum 0.000 19.500 1\_1\_1\_2\_3 Decatur M Test  
## 42 1\_1\_1\_2\_3 21 Cserum 5.802 14.000 1\_1\_1\_2\_3 Decatur M Test  
## 43 1\_1\_1\_2\_4 22 Cserum 0.000 7.500 1\_1\_1\_2\_4 Decatur M Test  
## 44 1\_1\_1\_2\_4 22 Cserum 5.802 9.000 1\_1\_1\_2\_4 Decatur M Test  
## 45 1\_1\_1\_2\_5 23 Cserum 0.000 8.600 1\_1\_1\_2\_5 Decatur M Test  
## 46 1\_1\_1\_2\_5 23 Cserum 5.802 9.200 1\_1\_1\_2\_5 Decatur M Test  
## 47 1\_1\_1\_2\_6 24 Cserum 0.000 12.400 1\_1\_1\_2\_6 Decatur M Test  
## 48 1\_1\_1\_2\_6 24 Cserum 5.802 12.800 1\_1\_1\_2\_6 Decatur M Test  
## 49 1\_1\_1\_2\_7 25 Cserum 0.000 8.900 1\_1\_1\_2\_7 Decatur M Test  
## 50 1\_1\_1\_2\_7 25 Cserum 5.802 6.600 1\_1\_1\_2\_7 Decatur M Test  
## 51 1\_1\_1\_2\_8 26 Cserum 0.000 7.400 1\_1\_1\_2\_8 Decatur M Test  
## 52 1\_1\_1\_2\_8 26 Cserum 5.802 6.300 1\_1\_1\_2\_8 Decatur M Test  
## 53 1\_1\_1\_2\_9 27 Cserum 0.000 14.300 1\_1\_1\_2\_9 Decatur M Test  
## 54 1\_1\_1\_2\_9 27 Cserum 5.802 15.800 1\_1\_1\_2\_9 Decatur M Test  
## 55 1\_1\_1\_2\_10 28 Cserum 0.000 3.800 1\_1\_1\_2\_10 Decatur F Test  
## 56 1\_1\_1\_2\_10 28 Cserum 5.802 4.200 1\_1\_1\_2\_10 Decatur F Test  
## 57 1\_1\_1\_2\_11 29 Cserum 0.000 22.100 1\_1\_1\_2\_11 Decatur F Test  
## 58 1\_1\_1\_2\_11 29 Cserum 5.802 26.000 1\_1\_1\_2\_11 Decatur F Test  
## 59 1\_1\_1\_2\_12 30 Cserum 0.000 6.500 1\_1\_1\_2\_12 Decatur F Test  
## 60 1\_1\_1\_2\_12 30 Cserum 5.802 5.800 1\_1\_1\_2\_12 Decatur F Test  
## 61 1\_1\_1\_2\_13 31 Cserum 0.000 7.500 1\_1\_1\_2\_13 Decatur F Test  
## 62 1\_1\_1\_2\_13 31 Cserum 5.802 7.900 1\_1\_1\_2\_13 Decatur F Test  
## 63 1\_1\_1\_2\_14 32 Cserum 0.000 7.500 1\_1\_1\_2\_14 Decatur F Test  
## 64 1\_1\_1\_2\_14 32 Cserum 5.802 6.800 1\_1\_1\_2\_14 Decatur F Test  
## 65 1\_1\_1\_2\_15 33 Cserum 0.000 7.500 1\_1\_1\_2\_15 Decatur F Test  
## 66 1\_1\_1\_2\_15 33 Cserum 5.802 2.400 1\_1\_1\_2\_15 Decatur F Test  
## 67 1\_1\_1\_2\_16 34 Cserum 0.000 6.000 1\_1\_1\_2\_16 Decatur F Test  
## 68 1\_1\_1\_2\_16 34 Cserum 5.802 6.800 1\_1\_1\_2\_16 Decatur F Test  
## 69 1\_1\_1\_2\_17 35 Cserum 0.000 18.200 1\_1\_1\_2\_17 Decatur F Test  
## 70 1\_1\_1\_2\_17 35 Cserum 5.802 13.200 1\_1\_1\_2\_17 Decatur F Test  
## 71 1\_1\_1\_2\_18 36 Cserum 0.000 5.300 1\_1\_1\_2\_18 Decatur F Test  
## 72 1\_1\_1\_2\_18 36 Cserum 5.802 3.900 1\_1\_1\_2\_18 Decatur F Test  
## 73 1\_1\_1\_2\_19 37 Cserum 0.000 5.600 1\_1\_1\_2\_19 Decatur F Test  
## 74 1\_1\_1\_2\_19 37 Cserum 5.802 5.400 1\_1\_1\_2\_19 Decatur F Test  
## 75 1\_2\_1 38 M\_Cbgd\_Css 2.200 2.593 1\_2\_1 Paulsboro-Train  
## 76 1\_3\_1 39 M\_Cbgd\_Css 2.000 27.340 1\_3\_1 Horsham-Train  
## 77 1\_4\_1 40 M\_Cbgd\_Css 2.000 23.157 1\_4\_1 Warminster-Test  
## 78 1\_4\_2\_1 41 M\_Cbgd\_Css 2.000 14.851 1\_4\_2\_1 Warrington-Train  
## Sex City Train\_Test datatype variable  
## 1 Male Decatur Train Individual Decatur M Train 1  
## 2 Male Decatur Train Individual Decatur M Train 1  
## 3 Male Decatur Train Individual Decatur M Train 2  
## 4 Male Decatur Train Individual Decatur M Train 2  
## 5 Male Decatur Train Individual Decatur M Train 3  
## 6 Male Decatur Train Individual Decatur M Train 3  
## 7 Male Decatur Train Individual Decatur M Train 4  
## 8 Male Decatur Train Individual Decatur M Train 4  
## 9 Male Decatur Train Individual Decatur M Train 5  
## 10 Male Decatur Train Individual Decatur M Train 5  
## 11 Male Decatur Train Individual Decatur M Train 6  
## 12 Male Decatur Train Individual Decatur M Train 6  
## 13 Male Decatur Train Individual Decatur M Train 7  
## 14 Male Decatur Train Individual Decatur M Train 7  
## 15 Male Decatur Train Individual Decatur M Train 8  
## 16 Male Decatur Train Individual Decatur M Train 8  
## 17 Male Decatur Train Individual Decatur M Train 9  
## 18 Male Decatur Train Individual Decatur M Train 9  
## 19 Female Decatur Train Individual Decatur F Train 10  
## 20 Female Decatur Train Individual Decatur F Train 10  
## 21 Female Decatur Train Individual Decatur F Train 11  
## 22 Female Decatur Train Individual Decatur F Train 11  
## 23 Female Decatur Train Individual Decatur F Train 12  
## 24 Female Decatur Train Individual Decatur F Train 12  
## 25 Female Decatur Train Individual Decatur F Train 13  
## 26 Female Decatur Train Individual Decatur F Train 13  
## 27 Female Decatur Train Individual Decatur F Train 14  
## 28 Female Decatur Train Individual Decatur F Train 14  
## 29 Female Decatur Train Individual Decatur F Train 15  
## 30 Female Decatur Train Individual Decatur F Train 15  
## 31 Female Decatur Train Individual Decatur F Train 16  
## 32 Female Decatur Train Individual Decatur F Train 16  
## 33 Female Decatur Train Individual Decatur F Train 17  
## 34 Female Decatur Train Individual Decatur F Train 17  
## 35 Female Decatur Train Individual Decatur F Train 18  
## 36 Female Decatur Train Individual Decatur F Train 18  
## 37 Male Decatur Test Individual Decatur M Test 19  
## 38 Male Decatur Test Individual Decatur M Test 19  
## 39 Male Decatur Test Individual Decatur M Test 20  
## 40 Male Decatur Test Individual Decatur M Test 20  
## 41 Male Decatur Test Individual Decatur M Test 21  
## 42 Male Decatur Test Individual Decatur M Test 21  
## 43 Male Decatur Test Individual Decatur M Test 22  
## 44 Male Decatur Test Individual Decatur M Test 22  
## 45 Male Decatur Test Individual Decatur M Test 23  
## 46 Male Decatur Test Individual Decatur M Test 23  
## 47 Male Decatur Test Individual Decatur M Test 24  
## 48 Male Decatur Test Individual Decatur M Test 24  
## 49 Male Decatur Test Individual Decatur M Test 25  
## 50 Male Decatur Test Individual Decatur M Test 25  
## 51 Male Decatur Test Individual Decatur M Test 26  
## 52 Male Decatur Test Individual Decatur M Test 26  
## 53 Male Decatur Test Individual Decatur M Test 27  
## 54 Male Decatur Test Individual Decatur M Test 27  
## 55 Female Decatur Test Individual Decatur F Test 28  
## 56 Female Decatur Test Individual Decatur F Test 28  
## 57 Female Decatur Test Individual Decatur F Test 29  
## 58 Female Decatur Test Individual Decatur F Test 29  
## 59 Female Decatur Test Individual Decatur F Test 30  
## 60 Female Decatur Test Individual Decatur F Test 30  
## 61 Female Decatur Test Individual Decatur F Test 31  
## 62 Female Decatur Test Individual Decatur F Test 31  
## 63 Female Decatur Test Individual Decatur F Test 32  
## 64 Female Decatur Test Individual Decatur F Test 32  
## 65 Female Decatur Test Individual Decatur F Test 33  
## 66 Female Decatur Test Individual Decatur F Test 33  
## 67 Female Decatur Test Individual Decatur F Test 34  
## 68 Female Decatur Test Individual Decatur F Test 34  
## 69 Female Decatur Test Individual Decatur F Test 35  
## 70 Female Decatur Test Individual Decatur F Test 35  
## 71 Female Decatur Test Individual Decatur F Test 36  
## 72 Female Decatur Test Individual Decatur F Test 36  
## 73 Female Decatur Test Individual Decatur F Test 37  
## 74 Female Decatur Test Individual Decatur F Test 37  
## 75 Mixed (all sexes) Paulsboro Train Summary Paulsboro-Train 38  
## 76 Mixed (all sexes) Horsham Train Summary Horsham-Train 39  
## 77 Mixed (all sexes) Warminster Test Summary Warminster-Test 40  
## 78 Mixed (all sexes) Warrington Test Summary Warrington-Train 41  
## Dataset Time.desc Dataset.Time  
## 1 Decatur M Train 1 T=0 Decatur M Train 1.T=0  
## 2 Decatur M Train 1 T=5.802 Decatur M Train 1.T=5.802  
## 3 Decatur M Train 2 T=0 Decatur M Train 2.T=0  
## 4 Decatur M Train 2 T=5.802 Decatur M Train 2.T=5.802  
## 5 Decatur M Train 3 T=0 Decatur M Train 3.T=0  
## 6 Decatur M Train 3 T=5.802 Decatur M Train 3.T=5.802  
## 7 Decatur M Train 4 T=0 Decatur M Train 4.T=0  
## 8 Decatur M Train 4 T=5.802 Decatur M Train 4.T=5.802  
## 9 Decatur M Train 5 T=0 Decatur M Train 5.T=0  
## 10 Decatur M Train 5 T=5.802 Decatur M Train 5.T=5.802  
## 11 Decatur M Train 6 T=0 Decatur M Train 6.T=0  
## 12 Decatur M Train 6 T=5.802 Decatur M Train 6.T=5.802  
## 13 Decatur M Train 7 T=0 Decatur M Train 7.T=0  
## 14 Decatur M Train 7 T=5.802 Decatur M Train 7.T=5.802  
## 15 Decatur M Train 8 T=0 Decatur M Train 8.T=0  
## 16 Decatur M Train 8 T=5.802 Decatur M Train 8.T=5.802  
## 17 Decatur M Train 9 T=0 Decatur M Train 9.T=0  
## 18 Decatur M Train 9 T=5.802 Decatur M Train 9.T=5.802  
## 19 Decatur F Train 10 T=0 Decatur F Train 10.T=0  
## 20 Decatur F Train 10 T=5.802 Decatur F Train 10.T=5.802  
## 21 Decatur F Train 11 T=0 Decatur F Train 11.T=0  
## 22 Decatur F Train 11 T=5.802 Decatur F Train 11.T=5.802  
## 23 Decatur F Train 12 T=0 Decatur F Train 12.T=0  
## 24 Decatur F Train 12 T=5.802 Decatur F Train 12.T=5.802  
## 25 Decatur F Train 13 T=0 Decatur F Train 13.T=0  
## 26 Decatur F Train 13 T=5.802 Decatur F Train 13.T=5.802  
## 27 Decatur F Train 14 T=0 Decatur F Train 14.T=0  
## 28 Decatur F Train 14 T=5.802 Decatur F Train 14.T=5.802  
## 29 Decatur F Train 15 T=0 Decatur F Train 15.T=0  
## 30 Decatur F Train 15 T=5.802 Decatur F Train 15.T=5.802  
## 31 Decatur F Train 16 T=0 Decatur F Train 16.T=0  
## 32 Decatur F Train 16 T=5.802 Decatur F Train 16.T=5.802  
## 33 Decatur F Train 17 T=0 Decatur F Train 17.T=0  
## 34 Decatur F Train 17 T=5.802 Decatur F Train 17.T=5.802  
## 35 Decatur F Train 18 T=0 Decatur F Train 18.T=0  
## 36 Decatur F Train 18 T=5.802 Decatur F Train 18.T=5.802  
## 37 Decatur M Test 19 T=0 Decatur M Test 19.T=0  
## 38 Decatur M Test 19 T=5.802 Decatur M Test 19.T=5.802  
## 39 Decatur M Test 20 T=0 Decatur M Test 20.T=0  
## 40 Decatur M Test 20 T=5.802 Decatur M Test 20.T=5.802  
## 41 Decatur M Test 21 T=0 Decatur M Test 21.T=0  
## 42 Decatur M Test 21 T=5.802 Decatur M Test 21.T=5.802  
## 43 Decatur M Test 22 T=0 Decatur M Test 22.T=0  
## 44 Decatur M Test 22 T=5.802 Decatur M Test 22.T=5.802  
## 45 Decatur M Test 23 T=0 Decatur M Test 23.T=0  
## 46 Decatur M Test 23 T=5.802 Decatur M Test 23.T=5.802  
## 47 Decatur M Test 24 T=0 Decatur M Test 24.T=0  
## 48 Decatur M Test 24 T=5.802 Decatur M Test 24.T=5.802  
## 49 Decatur M Test 25 T=0 Decatur M Test 25.T=0  
## 50 Decatur M Test 25 T=5.802 Decatur M Test 25.T=5.802  
## 51 Decatur M Test 26 T=0 Decatur M Test 26.T=0  
## 52 Decatur M Test 26 T=5.802 Decatur M Test 26.T=5.802  
## 53 Decatur M Test 27 T=0 Decatur M Test 27.T=0  
## 54 Decatur M Test 27 T=5.802 Decatur M Test 27.T=5.802  
## 55 Decatur F Test 28 T=0 Decatur F Test 28.T=0  
## 56 Decatur F Test 28 T=5.802 Decatur F Test 28.T=5.802  
## 57 Decatur F Test 29 T=0 Decatur F Test 29.T=0  
## 58 Decatur F Test 29 T=5.802 Decatur F Test 29.T=5.802  
## 59 Decatur F Test 30 T=0 Decatur F Test 30.T=0  
## 60 Decatur F Test 30 T=5.802 Decatur F Test 30.T=5.802  
## 61 Decatur F Test 31 T=0 Decatur F Test 31.T=0  
## 62 Decatur F Test 31 T=5.802 Decatur F Test 31.T=5.802  
## 63 Decatur F Test 32 T=0 Decatur F Test 32.T=0  
## 64 Decatur F Test 32 T=5.802 Decatur F Test 32.T=5.802  
## 65 Decatur F Test 33 T=0 Decatur F Test 33.T=0  
## 66 Decatur F Test 33 T=5.802 Decatur F Test 33.T=5.802  
## 67 Decatur F Test 34 T=0 Decatur F Test 34.T=0  
## 68 Decatur F Test 34 T=5.802 Decatur F Test 34.T=5.802  
## 69 Decatur F Test 35 T=0 Decatur F Test 35.T=0  
## 70 Decatur F Test 35 T=5.802 Decatur F Test 35.T=5.802  
## 71 Decatur F Test 36 T=0 Decatur F Test 36.T=0  
## 72 Decatur F Test 36 T=5.802 Decatur F Test 36.T=5.802  
## 73 Decatur F Test 37 T=0 Decatur F Test 37.T=0  
## 74 Decatur F Test 37 T=5.802 Decatur F Test 37.T=5.802  
## 75 Paulsboro-Train 38 T=2.2 Paulsboro-Train 38.T=2.2  
## 76 Horsham-Train 39 T=2 Horsham-Train 39.T=2  
## 77 Warminster-Test 40 T=2 Warminster-Test 40.T=2  
## 78 Warrington-Train 41 T=2 Warrington-Train 41.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.

#GH  
# 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("G: PFHxS Decatur Train", "H: PFHxS 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.

lets <- LETTERS;  
names(lets)[1:(length(unique(df\_check$dataset))-4)]<-as.character(unique(df\_check$dataset))[5: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)  
  
}

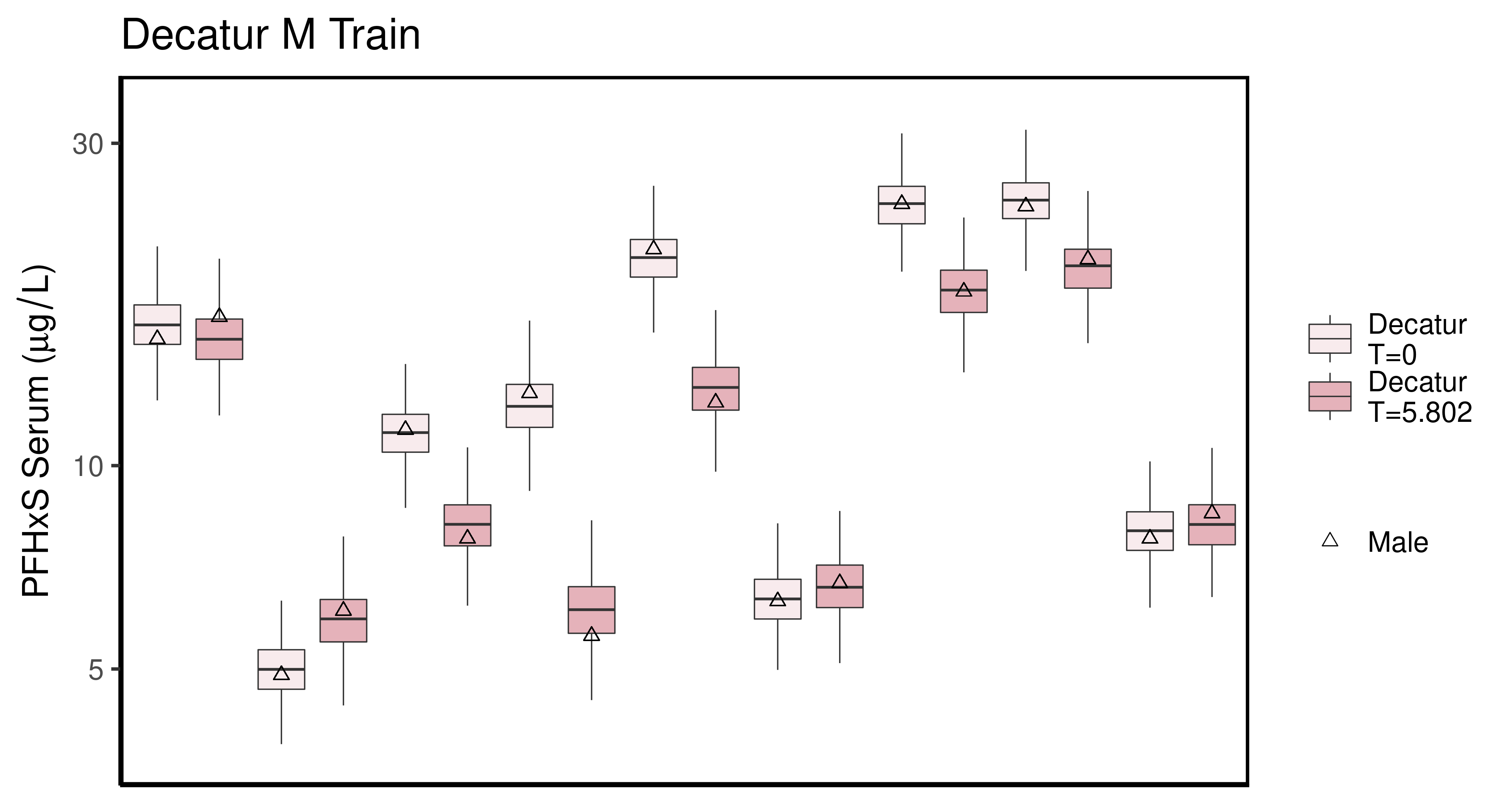
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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

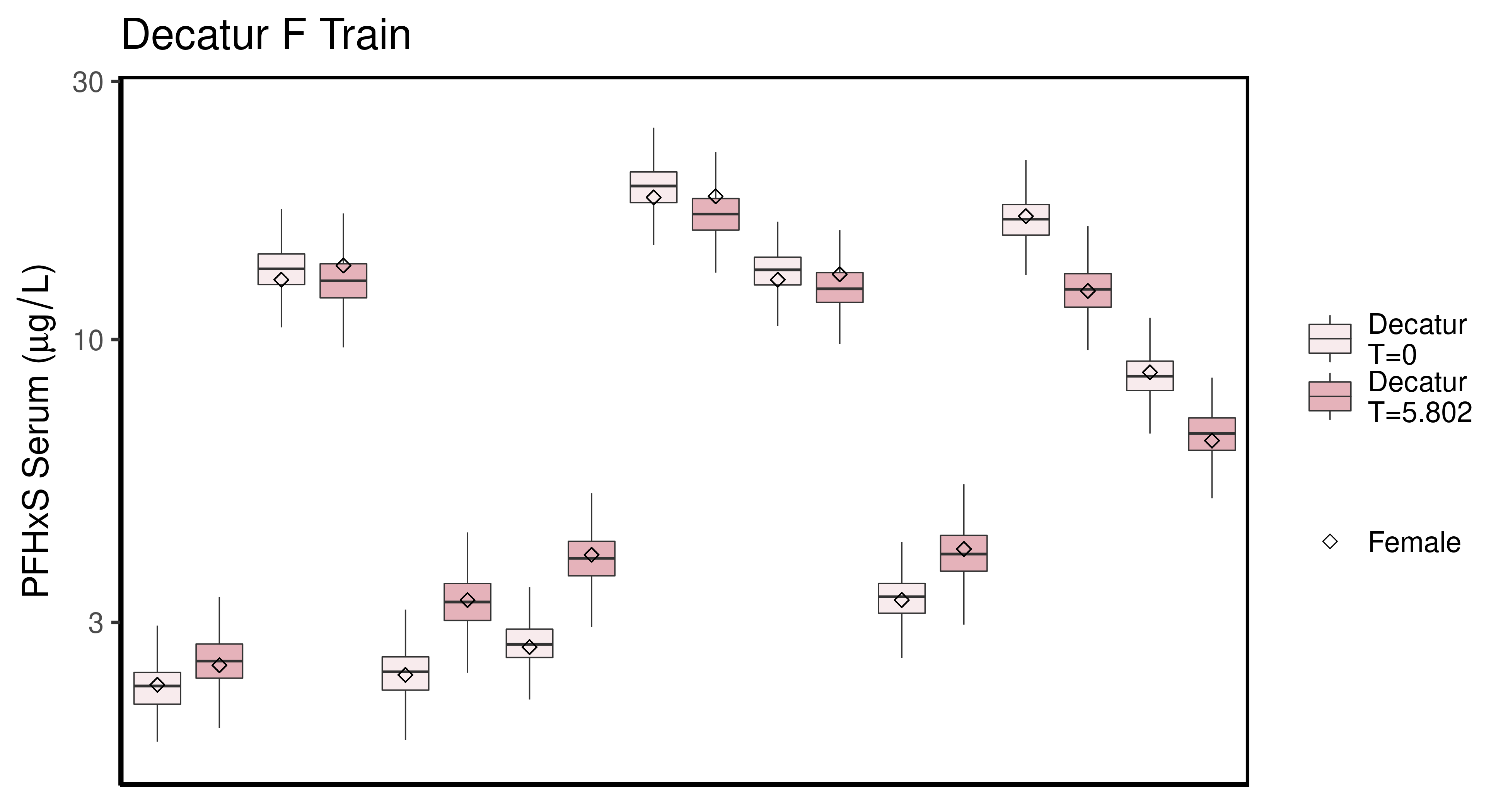
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



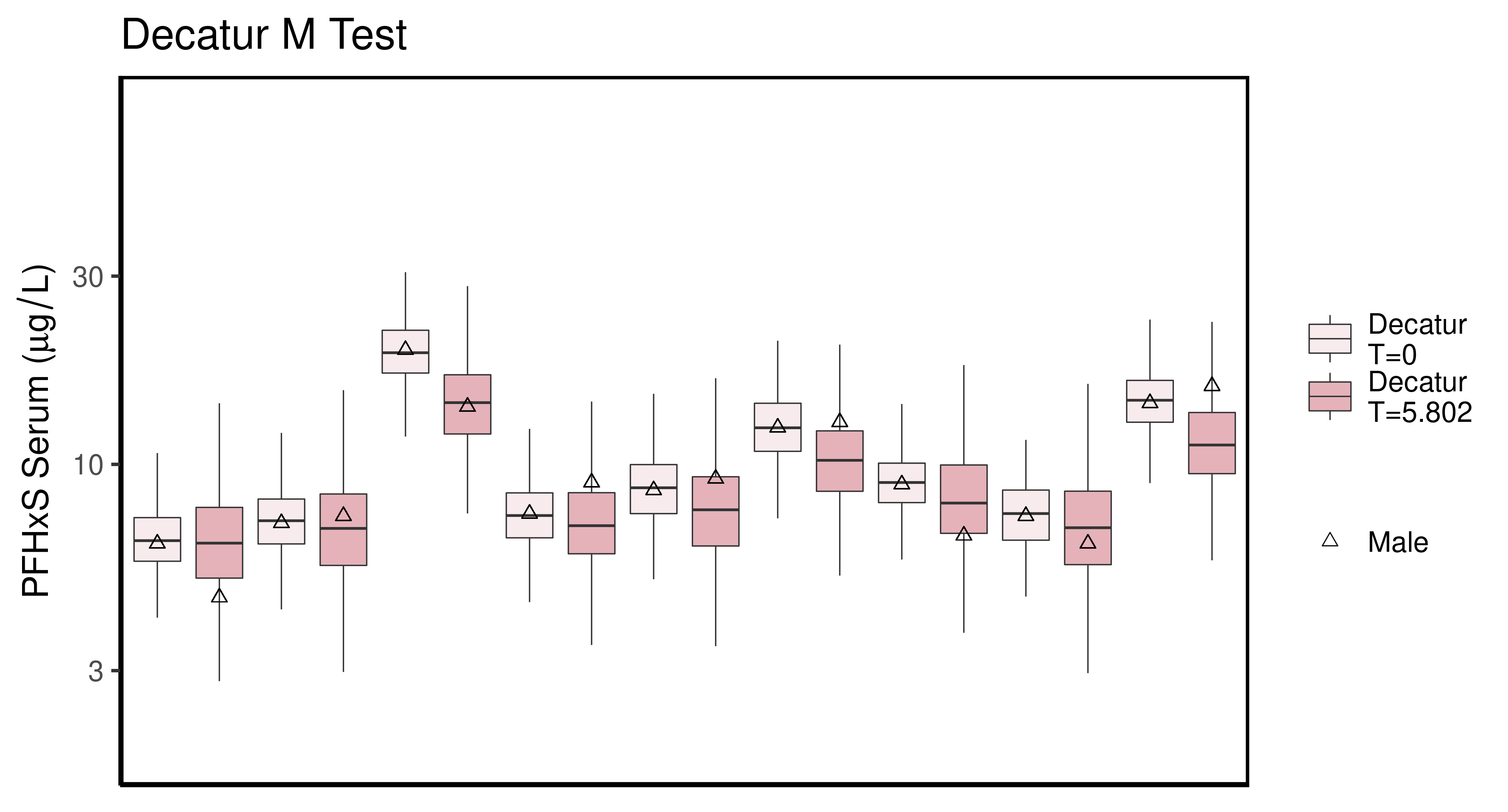
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



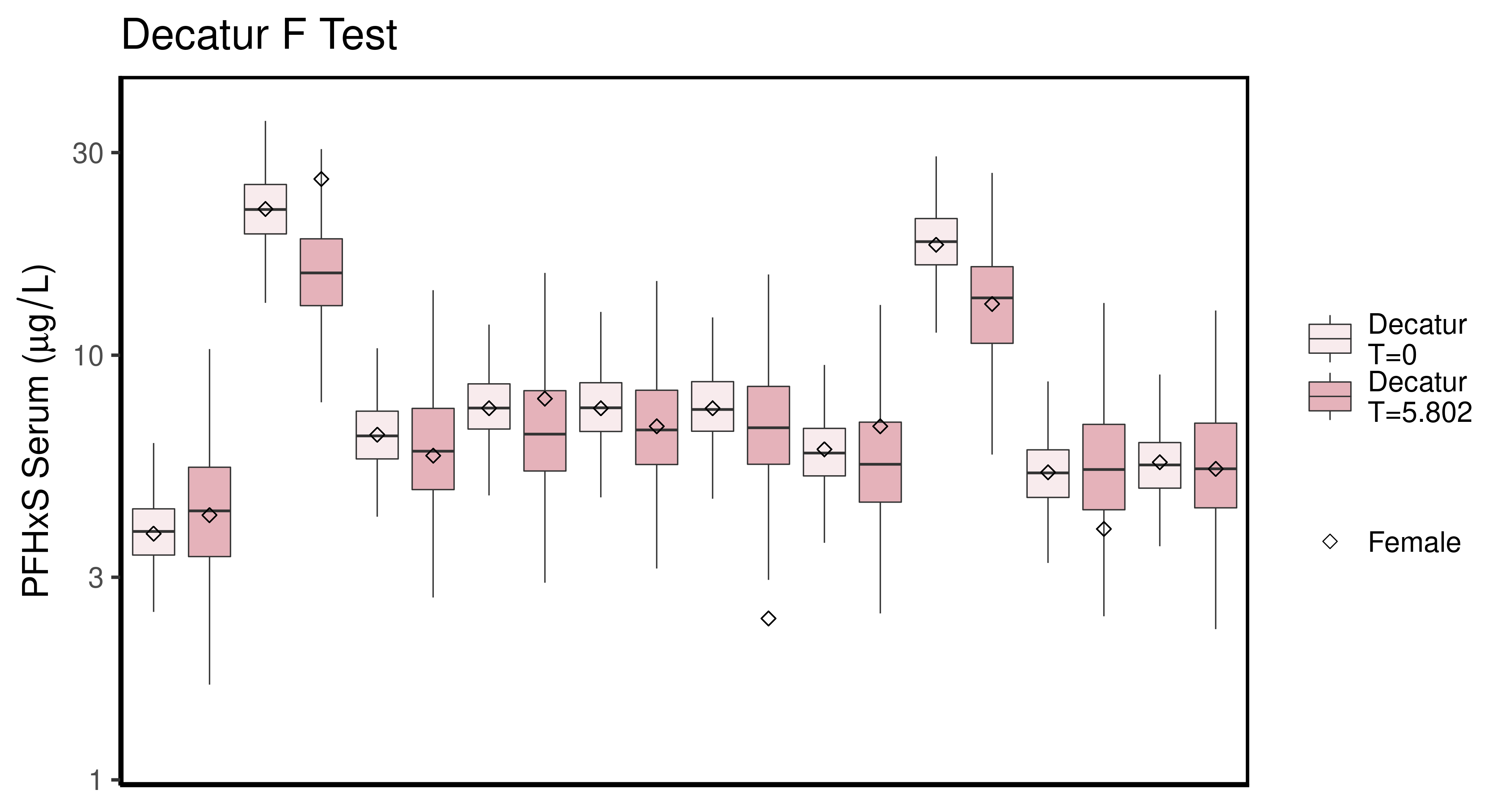
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



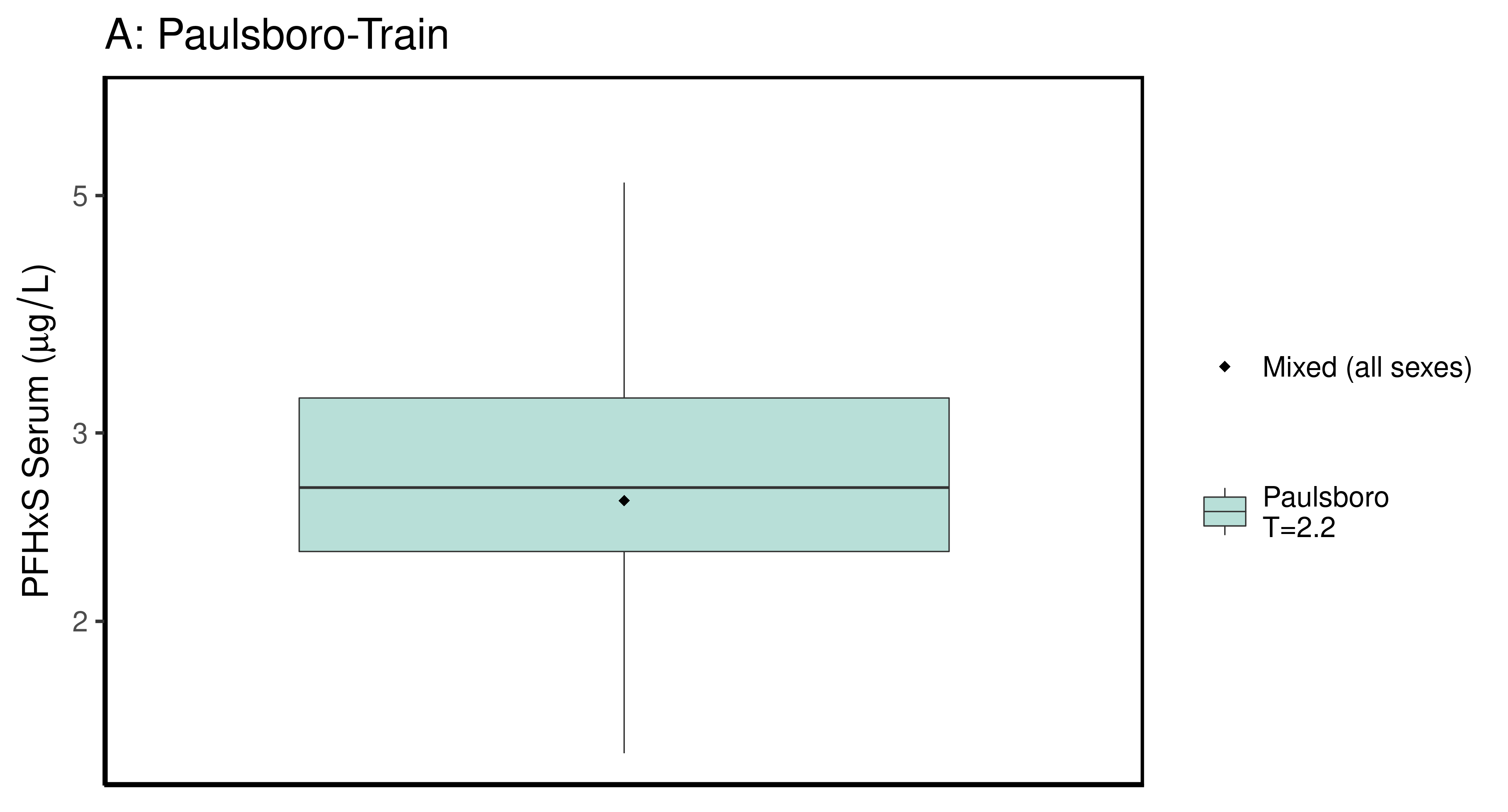
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



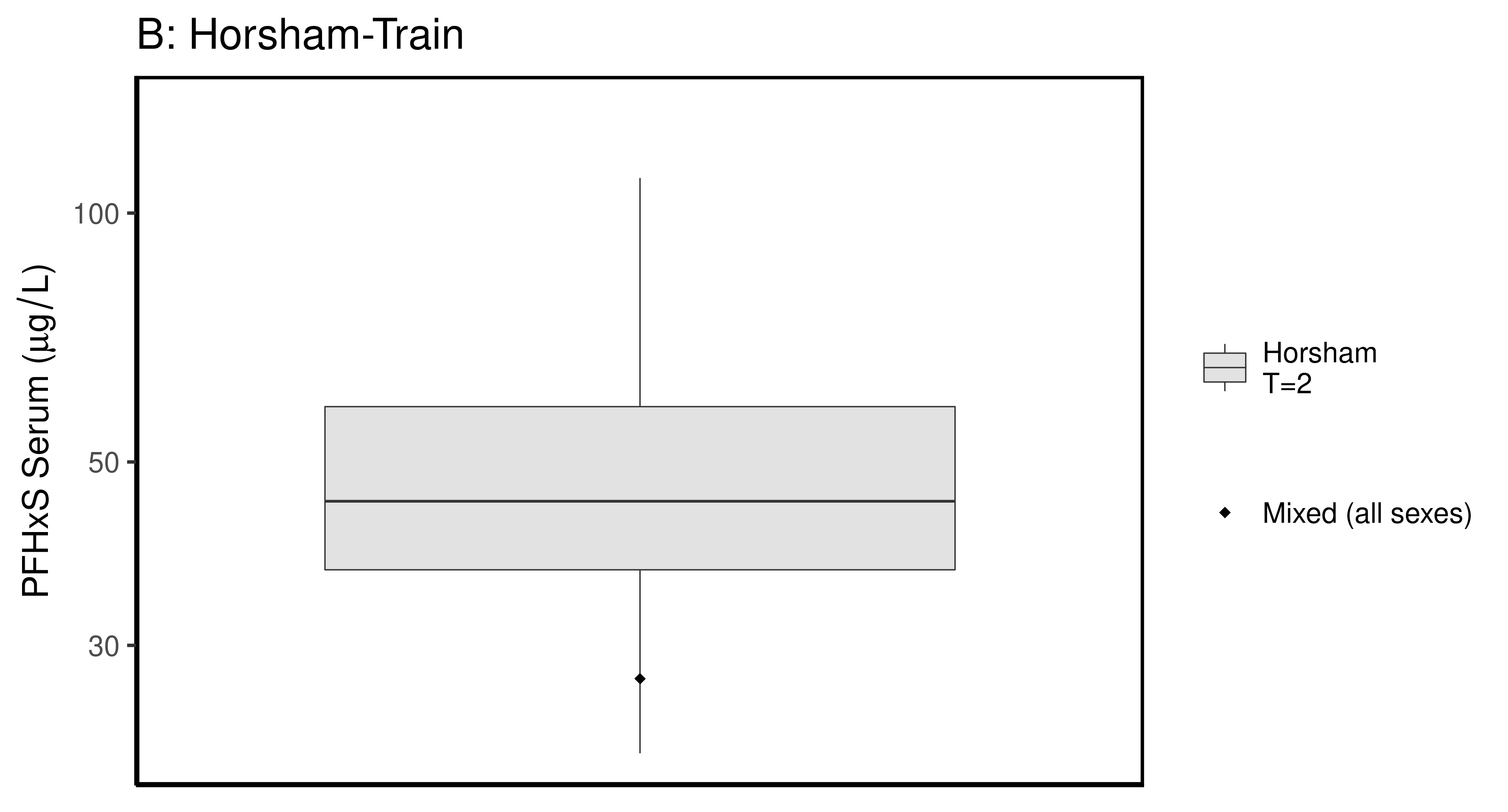
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



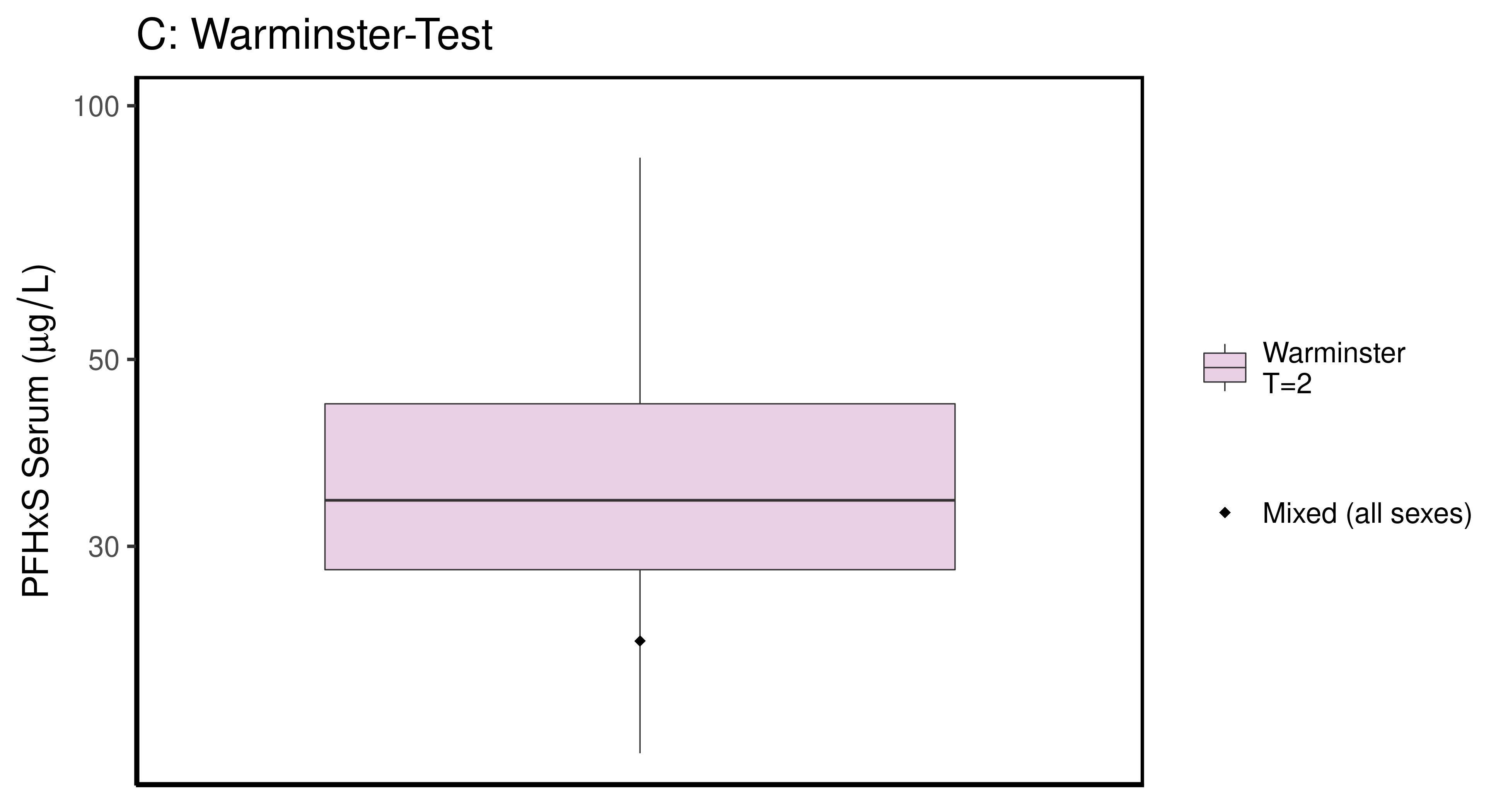
## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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

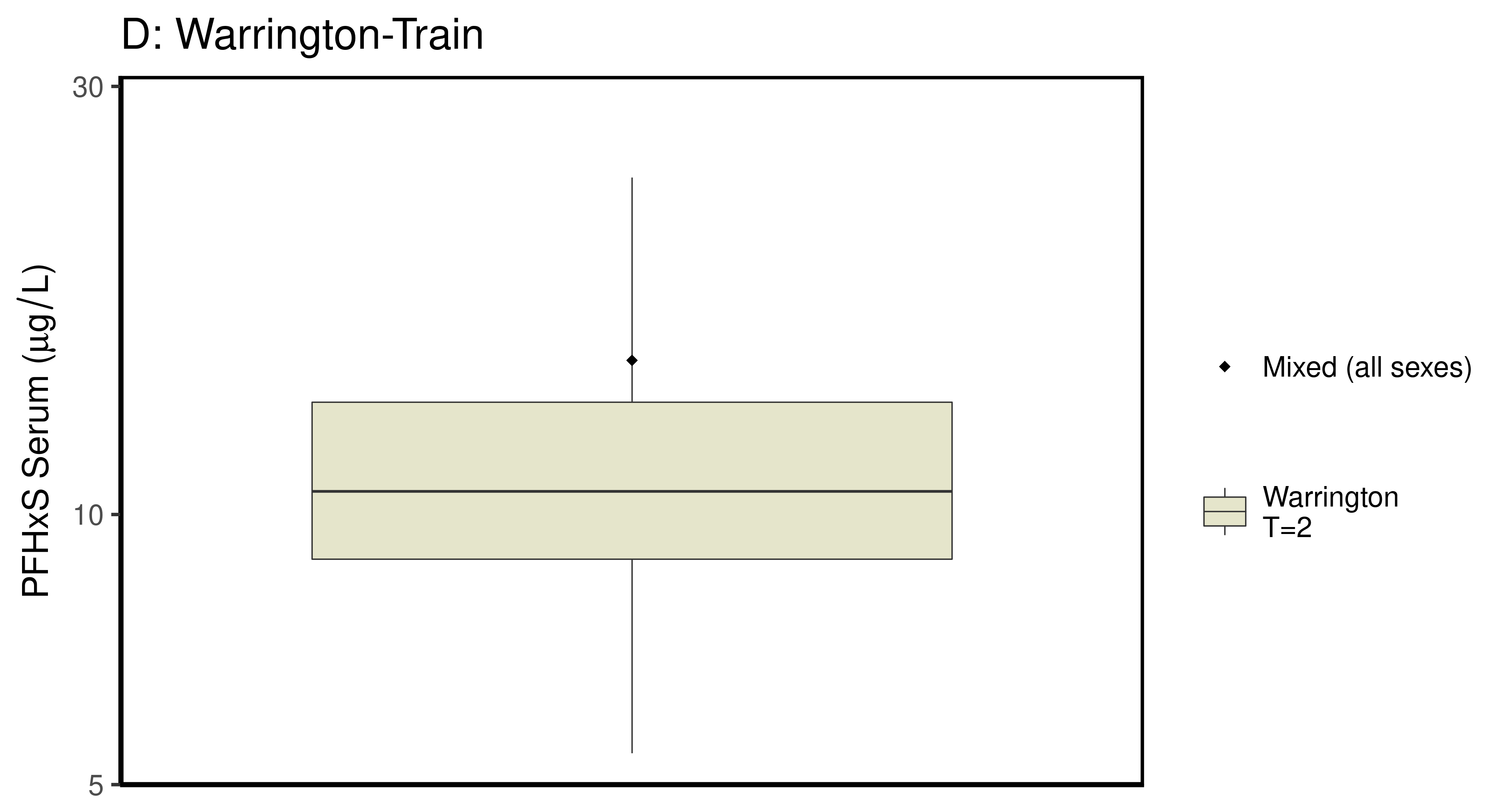


## Saving 6.5 x 3.5 in image  
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")

## 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



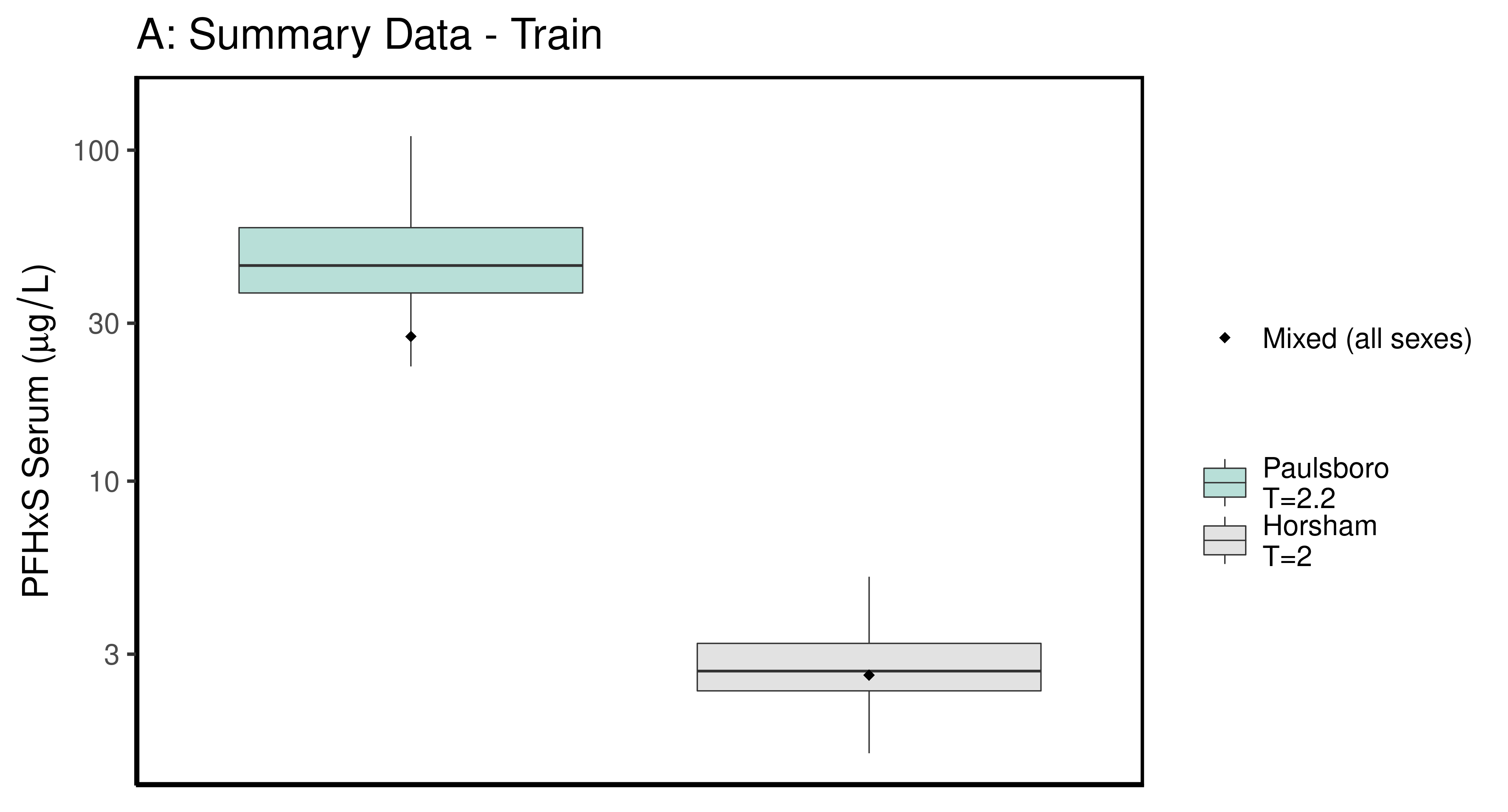
## Saving 6.5 x 3.5 in image



### 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="A: Summary Data - Train" , facets = FALSE,   
 pfas\_nom = pfas\_name )  
 print(plt\_train)



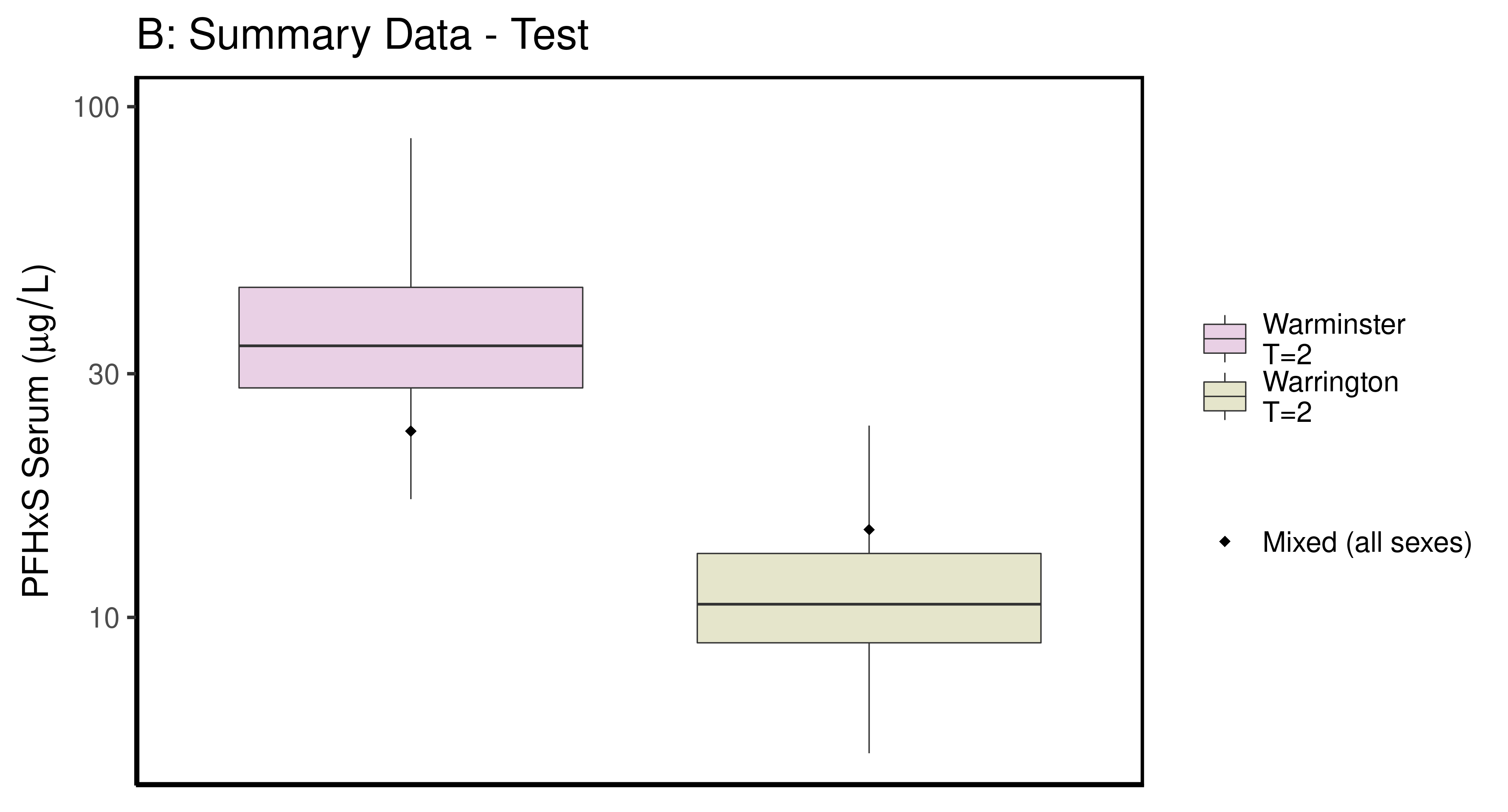
ggsave(here ("output-plots", paste0( sa, "SummaryTrainDataboxplot",pfas\_name,".pdf")), plt\_train,dpi=600)

## 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="B: 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)

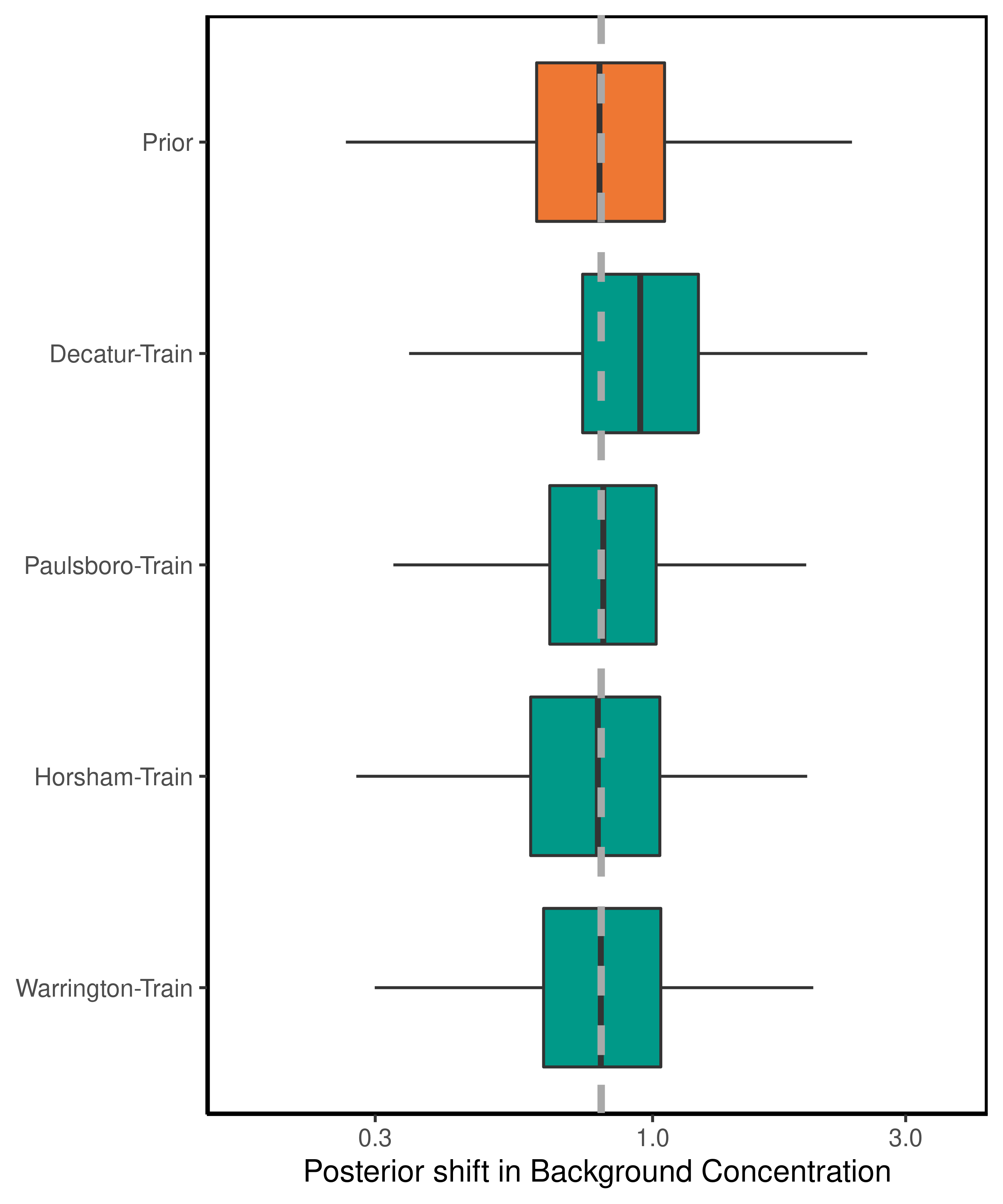
## Saving 6.5 x 3.5 in image

## PFHxS

### 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$dataset))  
datasetnames <- gsub(" Train","-Train",datasetnames)  
datasetnames <- gsub(" Test","-Train",datasetnames)  
datasetnames <- gsub(" M","",datasetnames)  
datasetnames <- gsub(" F","",datasetnames)  
datasetnames<-datasetnames[!duplicated(datasetnames)]  
datasetnames <- datasetnames[grep("Train",datasetnames)]  
names(dat) <- datasetnames  
dat <- dat[,grep("Train",names(dat))]  
dat.df <- pivot\_longer(dat,1:ncol(dat))  
dat.df <- rbind(dat.df,  
 data.frame(name="Prior",value=rnorm(5000,m=log(gmscale),sd=0.4055)))  
dat.df$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=NULL,   
 values=c("#009988", "#EE7733" )) +  
 theme\_classic() +   
 theme(axis.title.y.left = element\_blank())+  
 geom\_hline(yintercept = gmscale, color="darkgrey", linetype = 2, size = 1.25)+  
 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, "PFHxS\_GM\_Cbgd.pdf")) ,p,dpi=600)

## Saving 5 x 6 in image

### Half-life

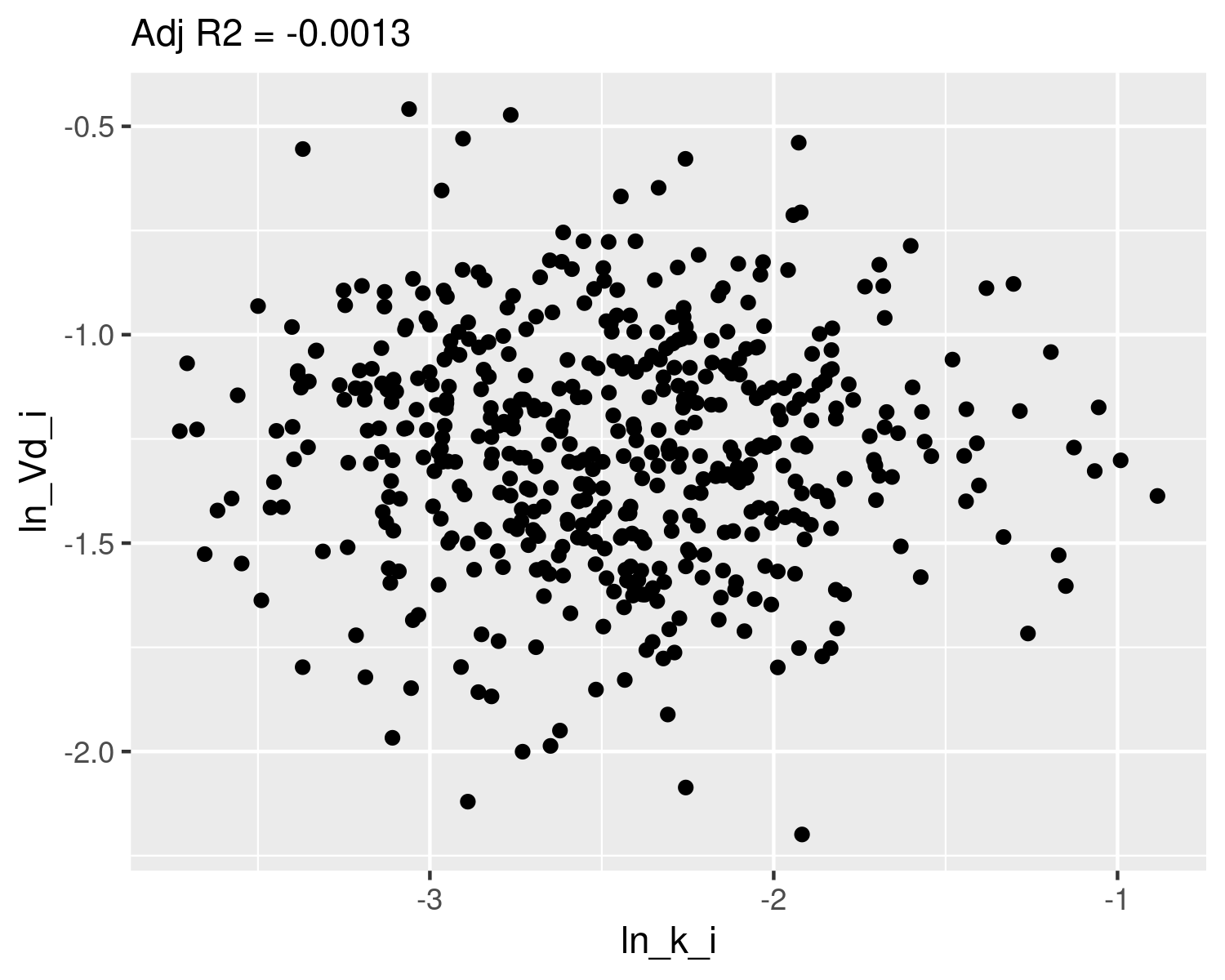
For PFHxS, the population GM of the half-life has a posterior distribution that is narrower than the prior, with a posterior median (95% CI) estimate of 3.06 (2.16-4.37) years. The population GSD posterior is larger than the prior at 1.47(1.44-1.75).

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.

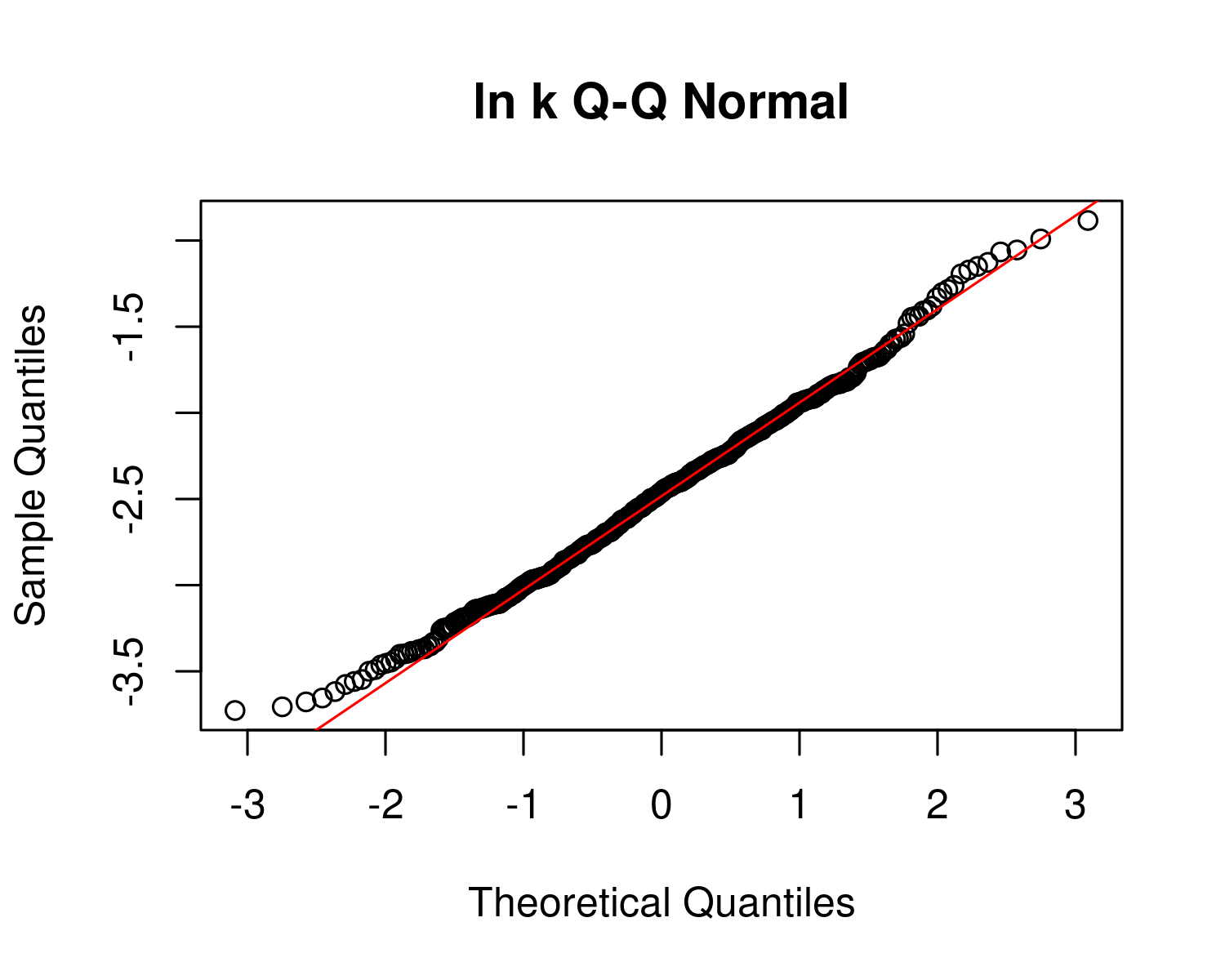
## M\_ln\_k(1) V\_ln\_k(1) M\_ln\_Vd(1) SD\_ln\_Vd(1) z\_ln\_k z\_ln\_Vd  
## 12503 -2.75291 0.2041830 -1.412470 0.191222000 -0.961933416 -2.139841913  
## 15901 -2.72905 0.3388370 -1.262040 0.095982100 -0.292525723 -1.263479244  
## 17543 -2.67035 0.2659090 -1.390400 0.286419000 0.258788216 0.083307969  
## 18721 -2.31531 0.1939420 -1.200790 0.132528000 -1.152131886 0.188325130  
## 11662 -2.51794 0.1579330 -1.097060 0.082538200 0.195782826 0.189814193  
## 13403 -2.83577 0.1720120 -1.244460 0.207939000 0.030123945 0.217615352  
## 13192 -2.36731 0.2929010 -1.090200 0.063831600 0.085417732 -0.648814142  
## 15663 -2.35551 0.1869580 -1.423570 0.188954000 1.116610213 0.254774383  
## 1246 -2.48740 0.2047250 -1.167350 0.026815800 -1.218857416 -0.468830015  
## 16132 -2.28657 0.2310820 -1.212640 0.007859580 1.267368722 -1.192510054  
## 10602 -2.76543 0.2356490 -1.451400 0.008926270 -0.744781596 0.121228235  
## 10563 -2.46342 0.1863690 -1.042400 0.109301000 -1.131218571 -1.035932658  
## 15932 -2.70822 0.2264000 -0.840291 0.133664000 -0.716358490 -0.191888295  
## 1114 -2.74916 0.1426340 -1.200700 0.064772000 0.252652370 -0.970546336  
## 1699 -2.69943 0.2717080 -1.233420 0.034752200 0.152045707 0.057771938  
## 1141 -2.74801 0.2122340 -1.339750 0.076209900 -0.307656430 -2.110692675  
## 13383 -2.96621 0.1474260 -1.060710 0.021755100 -0.953017331 0.978176274  
## 12832 -2.69611 0.2346190 -1.002450 0.113141000 -0.648242811 0.371021737  
## 19552 -2.51489 0.3228540 -1.223570 0.030571700 1.224313624 0.720910931  
## 14423 -2.40016 0.1580630 -1.223940 0.064784600 0.199811608 1.879594880  
## 12372 -2.65261 0.1251740 -1.018450 0.030116200 -0.578483722 -0.396316112  
## 12042 -2.29333 0.1725240 -1.497460 0.131016000 -0.942300733 0.110322947  
## 10473 -2.32319 0.1890660 -1.383060 0.158345000 -0.203728180 -0.593140881  
## 1509 -2.87891 0.2592500 -1.324400 0.221668000 -1.666474840 0.419621770  
## 1552 -2.34423 0.2684330 -1.264770 0.072917700 -0.484455109 -0.545738743  
## 19513 -2.04339 0.1517460 -1.563720 0.002395420 -0.741072661 1.160921499  
## 17471 -2.44949 0.1714430 -1.134580 0.009712250 1.160615779 0.639817834  
## 18092 -2.92293 0.2649380 -0.749883 0.212432000 1.012067125 -0.122020443  
## 1613 -2.62062 0.1960020 -1.583610 0.051115900 -0.072078474 0.184645026  
## 14383 -2.07859 0.1494270 -1.473980 0.147827000 -1.136782298 -0.517806023  
## 14263 -2.35721 0.1679390 -1.817640 0.286360000 0.900624729 0.067988352  
## 18291 -2.16099 0.1645120 -1.694750 0.054638300 0.851770447 -0.184797156  
## 1945 -2.41898 0.2266590 -1.056890 0.050055700 0.727715174 -1.403691615  
## 19613 -2.12554 0.2178070 -1.204940 0.374359000 0.736502146 0.229740706  
## 1842 -2.26703 0.2282840 -1.489630 0.185089000 -0.352129617 -0.889081301  
## 1873 -2.30463 0.1012290 -1.017190 0.105298000 0.705515513 -0.160401177  
## 19423 -2.29065 0.1188390 -1.376410 0.095319000 1.300357989 -0.242136794  
## 19352 -2.83644 0.1681330 -1.866550 0.041875600 0.038252014 -0.028837196  
## 11812 -2.36280 0.1702990 -1.223170 0.385055000 -0.979283770 -0.316215474  
## 14982 -2.19641 0.1326170 -1.220060 0.117067000 0.793761231 -0.416160087  
## 11263 -2.66246 0.1561150 -1.449460 0.154783000 0.786506872 -1.023895957  
## 1028 -3.11690 0.4711690 -1.141750 0.094573500 -0.310463131 1.099495275  
## 1051 -2.36686 0.2249400 -1.372110 0.141351000 1.698884846 0.817712470  
## 17222 -2.58380 0.2625230 -1.444480 0.194389000 -0.794593709 0.168875510  
## 1747 -2.39220 0.2981630 -1.534210 0.165598000 0.348437716 0.038665440  
## 1284 -2.63369 0.2122760 -1.286310 0.054794600 -2.265401074 1.078174892  
## 1564 -2.38815 0.2185380 -1.107500 0.116141000 -0.162205279 0.379427297  
## 18632 -2.39139 0.1617920 -1.278670 0.067979300 1.130864991 -1.078174559  
## 19142 -2.35800 0.1688640 -1.359770 0.006053020 -0.455545976 0.188763468  
## 15793 -2.33111 0.1659800 -1.205790 0.022403200 -0.899166316 1.583133508  
## 1126 -2.30517 0.1680520 -1.373240 0.174320000 0.726838902 -0.250112295  
## 16502 -2.46539 0.1421920 -1.093550 0.137344000 -0.809440902 0.342994219  
## 15103 -2.22348 0.1332940 -1.259620 0.085270400 0.267085116 -0.124701883  
## 11251 -2.29728 0.1875460 -1.587920 0.097563800 -1.737263711 -0.993314763  
## 11732 -2.68818 0.1392170 -1.631840 0.087352100 -1.411425136 -1.021439085  
## 18382 -2.90847 0.1900410 -1.513860 0.051897200 -0.453551227 0.840642928  
## 13433 -2.94800 0.1661000 -1.828890 0.036808300 -1.035491275 0.849573118  
## 16403 -2.48109 0.1899540 -1.169690 0.049453500 1.362142893 0.469618942  
## 11871 -2.81063 0.2940520 -1.020030 0.010292700 0.917456737 -1.269655261  
## 1988 -2.30920 0.2368420 -1.316840 0.144035000 -0.785142161 -1.105120219  
## 1589 -2.55007 0.1595040 -1.389440 0.204108000 0.573518173 -1.897945965  
## 1449 -2.69991 0.2258280 -1.252910 0.158285000 0.918196208 0.491787265  
## 1232 -2.52956 0.1945000 -1.265820 0.207718000 0.256287273 -0.704722317  
## 10171 -2.43987 0.2402250 -1.119880 0.061807300 0.351966556 1.777576130  
## 1259 -2.04854 0.2679840 -1.376630 0.094045200 1.174337357 -0.245389029  
## 18503 -2.58795 0.1304050 -1.068760 0.065600100 -0.480846375 -2.111252318  
## 10801 -2.81228 0.2198140 -1.138300 0.154019000 -0.418829722 -0.585314536  
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## 18351 -2.07196 0.2859340 -1.773640 0.067483100 -0.405077513 0.164593185  
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## 19111 -2.42786 0.1817920 -1.124380 0.067765000 -1.632153479 -0.109166877  
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## 1504 -2.41772 0.1536940 -1.039570 0.223998000 1.443928256 -0.318596856  
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## 19693 -2.42895 0.1916690 -1.137700 0.089808500 -1.306438327 0.532403631  
## 13331 -2.46457 0.2337390 -0.922659 0.241005000 -0.877198993 -0.197683940  
## 18422 -2.37022 0.1760710 -1.118770 0.161377000 -1.164380459 1.664379027  
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## 1170 -2.33214 0.1450430 -2.173590 0.146048000 1.088442705 -0.174111691  
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## 1468 -2.63761 0.2137270 -1.200060 0.012087000 0.052200047 0.278350539  
## 17953 -2.69536 0.2201650 -0.944860 0.117315000 -1.083698485 -1.202692142  
## 1557 -2.28829 0.2691060 -1.096310 0.117185000 -0.008856207 0.642761817  
## 19642 -2.45008 0.1746040 -0.757825 0.047770600 2.030643112 -0.605973945  
## 16191 -2.07468 0.1367260 -1.307650 0.200690000 -1.113328933 -1.377257613  
## 17011 -2.54155 0.1779580 -1.088670 0.200049000 1.138271925 -0.925992687  
## 1820 -2.67781 0.2744160 -1.130930 0.272739000 -0.614892642 0.567243857  
## 10851 -2.61594 0.1918340 -1.604430 0.081496100 -2.193536615 2.595481260  
## 13483 -2.97149 0.2244890 -1.520540 0.118417000 -1.215686372 -0.239984547  
## 13183 -2.69848 0.2226620 -1.059710 0.105705000 -0.045326362 0.687536401  
## 18462 -2.44366 0.1458040 -1.460300 0.028477800 1.598812624 -0.151788986  
## 15542 -2.37954 0.2782630 -1.224820 0.084755500 0.927542200 0.227544260  
## 18752 -2.64053 0.1648670 -1.638830 0.101685000 0.829284552 -0.668648038  
## 12081 -2.39692 0.2183460 -1.381470 0.028250100 1.024603876 0.030829067  
## 1014 -2.75811 0.1743640 -1.221350 0.103274000 -0.476238068 0.028429558  
## 15612 -2.76002 0.1996990 -1.089480 0.134250000 1.638868393 -0.365455074  
## 14833 -1.95189 0.1598310 -1.265820 0.036476900 -0.632050958 -2.208012195  
## 1639 -2.73364 0.2009320 -1.162480 0.169149000 -1.379618576 0.297039427  
## 10353 -2.15850 0.1615210 -1.368610 0.192932000 -0.257455748 2.129700659  
## 15011 -2.55299 0.2621500 -0.913079 0.061140100 1.679972711 1.325041143  
## 12253 -2.36845 0.1232820 -1.094110 0.230603000 -2.545858038 -0.116171447  
## 10793 -1.94338 0.2035550 -1.535410 0.026017300 0.012078784 -1.470146221  
## 10103 -2.87468 0.1556830 -1.345700 0.022665200 1.960925111 -0.379271835  
## 1903 -2.71520 0.2042490 -1.459870 0.450800000 -0.385905481 -1.465005931  
## 1679 -2.30976 0.2779830 -1.179630 0.181344000 0.910757548 1.075148263  
## 1795 -2.62165 0.1818670 -1.292130 0.177647000 -1.448130794 -1.226124877  
## 1489 -2.65237 0.1656490 -1.472160 0.161936000 -1.121614596 -3.056328234  
## 1881 -2.69172 0.2042330 -1.243580 0.238797000 -0.973617906 1.450657775  
## 15061 -2.69719 0.1883980 -1.343580 0.262119000 -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)))

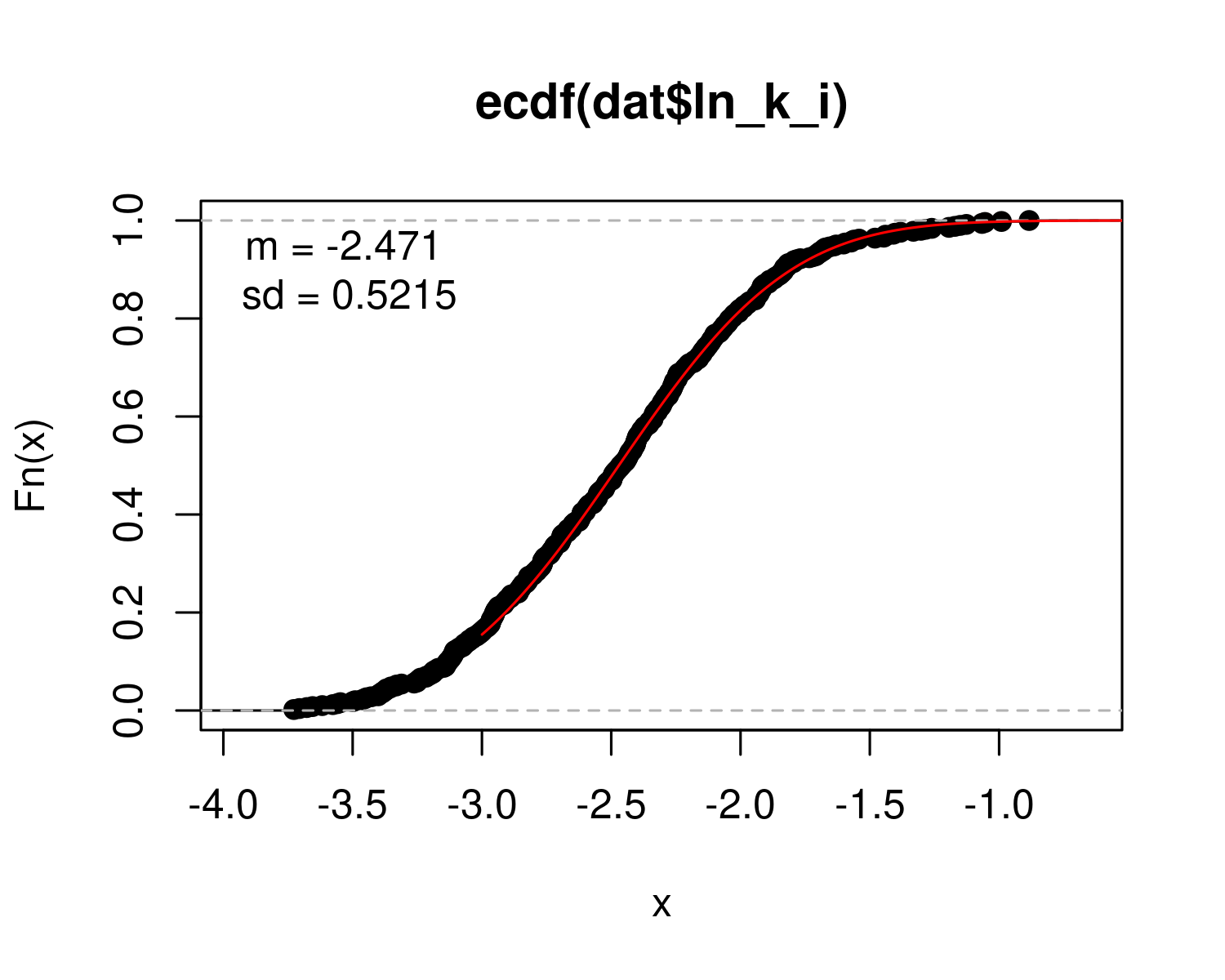


## Check normality

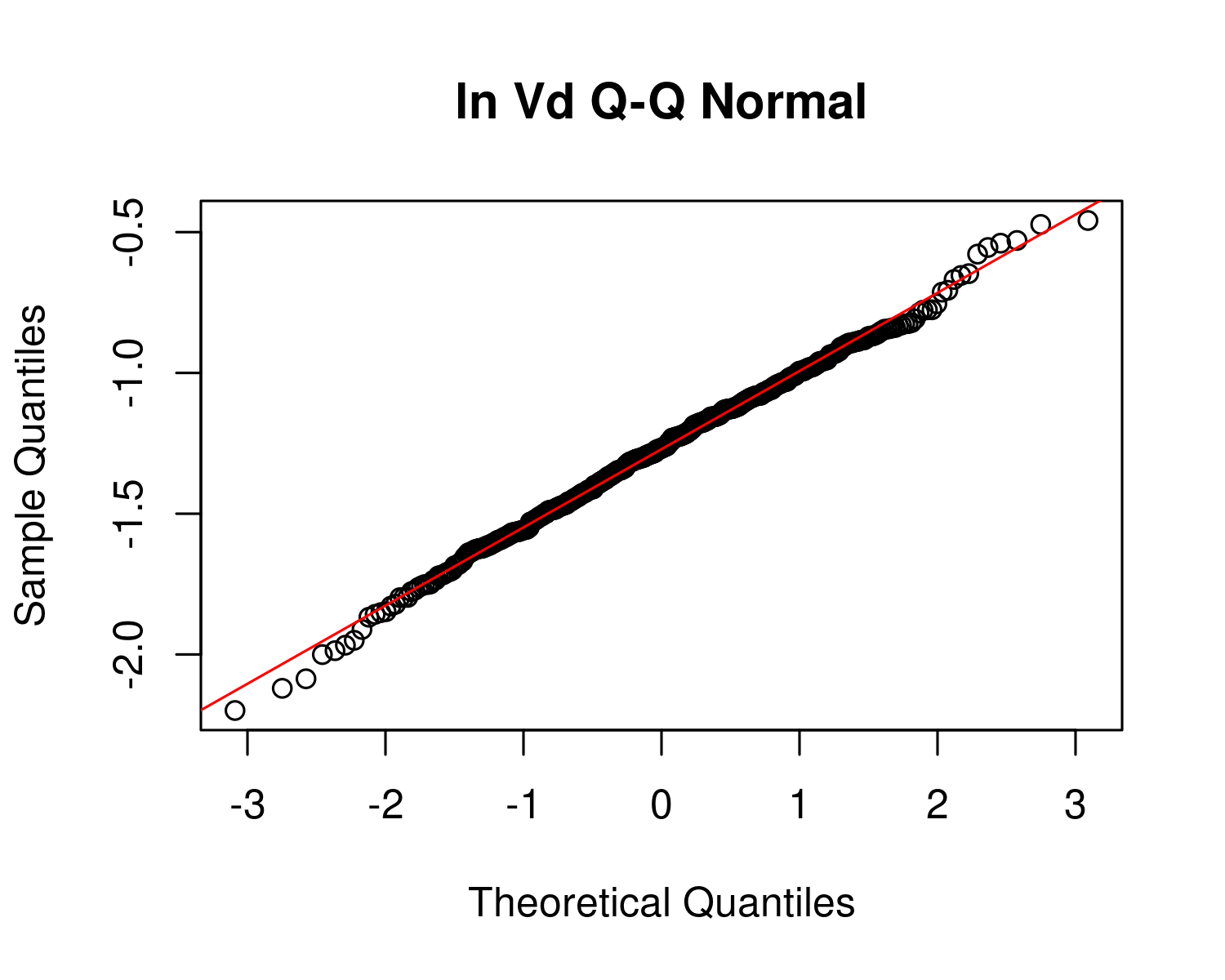
qqnorm(dat$ln\_k\_i,main="ln k Q-Q Normal")  
qqline(dat$ln\_k\_i,col="red")



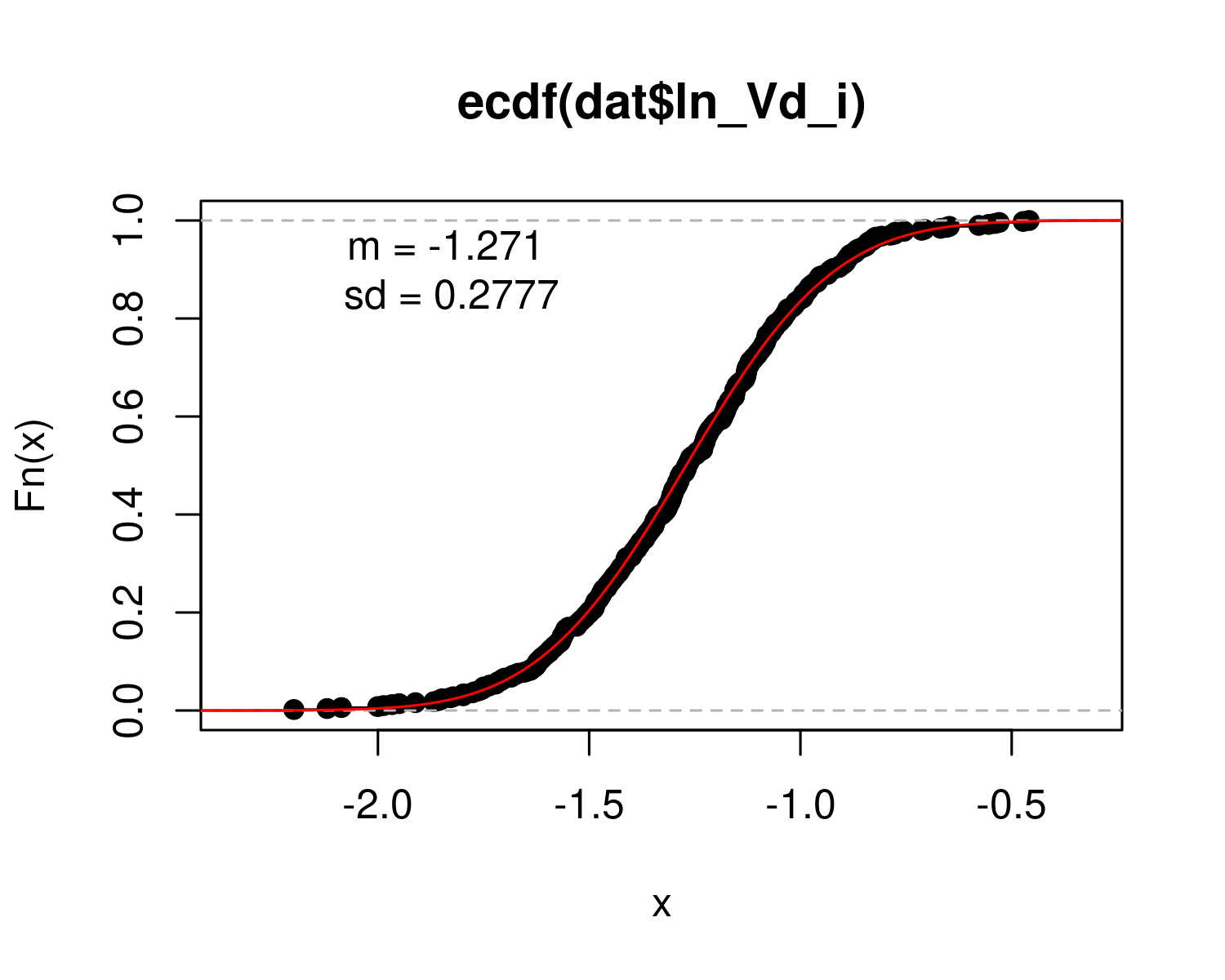
plot(ecdf(dat$ln\_k\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_k\_i <- mean(dat$ln\_k\_i)  
sd\_ln\_k\_i <- sd(dat$ln\_k\_i)  
lines(x,pnorm(x,mean=m\_ln\_k\_i,sd=sd\_ln\_k\_i),col="red")  
text(m\_ln\_k\_i-2\*sd\_ln\_k\_i,0.9,paste("m =",signif(m\_ln\_k\_i,4),"\nsd =",signif(sd\_ln\_k\_i,4)))



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)))



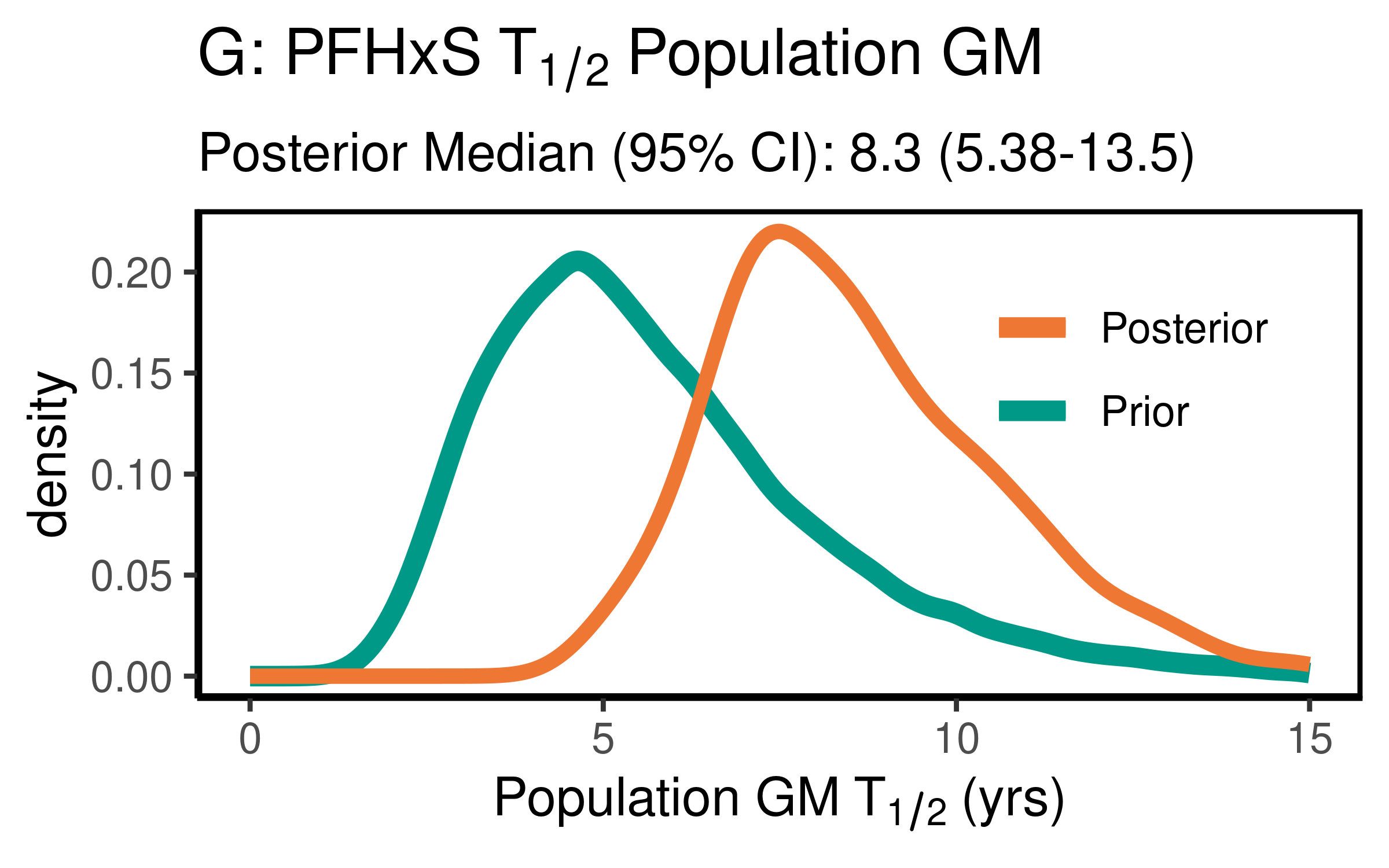
## Calculate table values for individual-level

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

PFHxS\_priors <- data.frame(  
 halflife\_GM= log(2)/rlnorm(50000,  
 meanlog=-2.03422,sdlog=0.4055))  
M\_k <- exp(as.numeric(dat$`M\_ln\_k(1)`))  
PFHxS\_halflife\_GM <- log(2)/M\_k  
  
PFHxS\_hlgm\_pr\_med <- signif(median(PFHxS\_priors$halflife\_GM,3))  
PFHxS\_hlgm\_pr\_med\_95ci <-paste(signif(quantile(PFHxS\_priors$halflife\_GM,  
 prob=c(0.025,0.975)),  
 3),  
 collapse="-")  
  
PFHxS\_hl\_median\_gm <- signif(median(PFHxS\_halflife\_GM),3)  
PFHxS\_hl\_median\_gm\_95ci <- paste(signif(quantile(PFHxS\_halflife\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(halflife\_GM, color = "Prior"),data=PFHxS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFHxS\_halflife\_GM, stat(density),color="Posterior"),geom="line",size=1.5 )+  
 xlim(0,15)+  
 labs(title = bquote("G: PFHxS"~T[1/2]~"Population GM") ,  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_hl\_median\_gm," (",  
 PFHxS\_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 250 rows containing non-finite values (stat\_density).

## Warning: Removed 6 rows containing non-finite values (stat\_density).

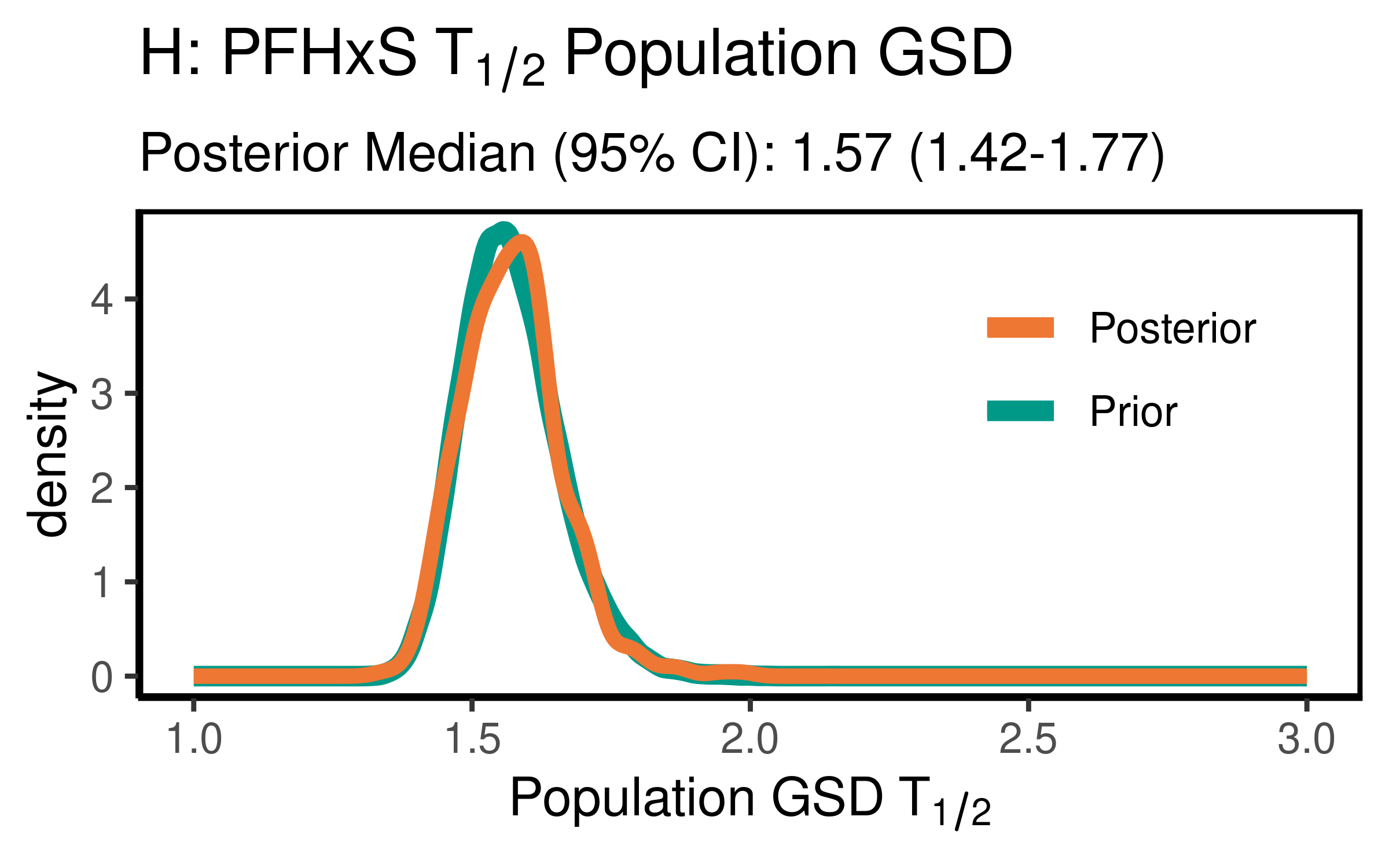


ggsave(here ("output-plots",paste0( sa, "PFHxS\_hl\_gm.pdf")),p,dpi=600)

## Saving 4 x 2.5 in image

## Warning: Removed 250 rows containing non-finite values (stat\_density).  
  
## Warning: Removed 6 rows containing non-finite values (stat\_density).

PFHxS\_priors$halflife\_GSD = exp(sqrt(exp(rnorm(50000,m=log(0.2),sd=log(1.275)))))   
PFHxS\_halflife\_GSD <- exp(sqrt(dat$`V\_ln\_k(1)`))  
  
PFHxS\_hlgsd\_pr\_med <- signif(median(PFHxS\_priors$halflife\_GSD,3))  
PFHxS\_hlgsd\_pr\_med\_95ci <-paste(signif(quantile(PFHxS\_priors$halflife\_GSD,  
 prob=c(0.025,0.975)),  
 3),  
 collapse="-")  
PFHxS\_hl\_gsd\_med <- signif(median(PFHxS\_halflife\_GSD),3)  
PFHxS\_hl\_gsd\_med\_95ci <- paste(signif(quantile(PFHxS\_halflife\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
p<-ggplot()+  
 stat\_density(aes(halflife\_GSD, color = "Prior"),data=PFHxS\_priors,geom="line", size=2)+  
 stat\_density(aes(PFHxS\_halflife\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("H: PFHxS"~T[1/2]~"Population GSD"),   
 subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_hl\_gsd\_med," (",  
 PFHxS\_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)

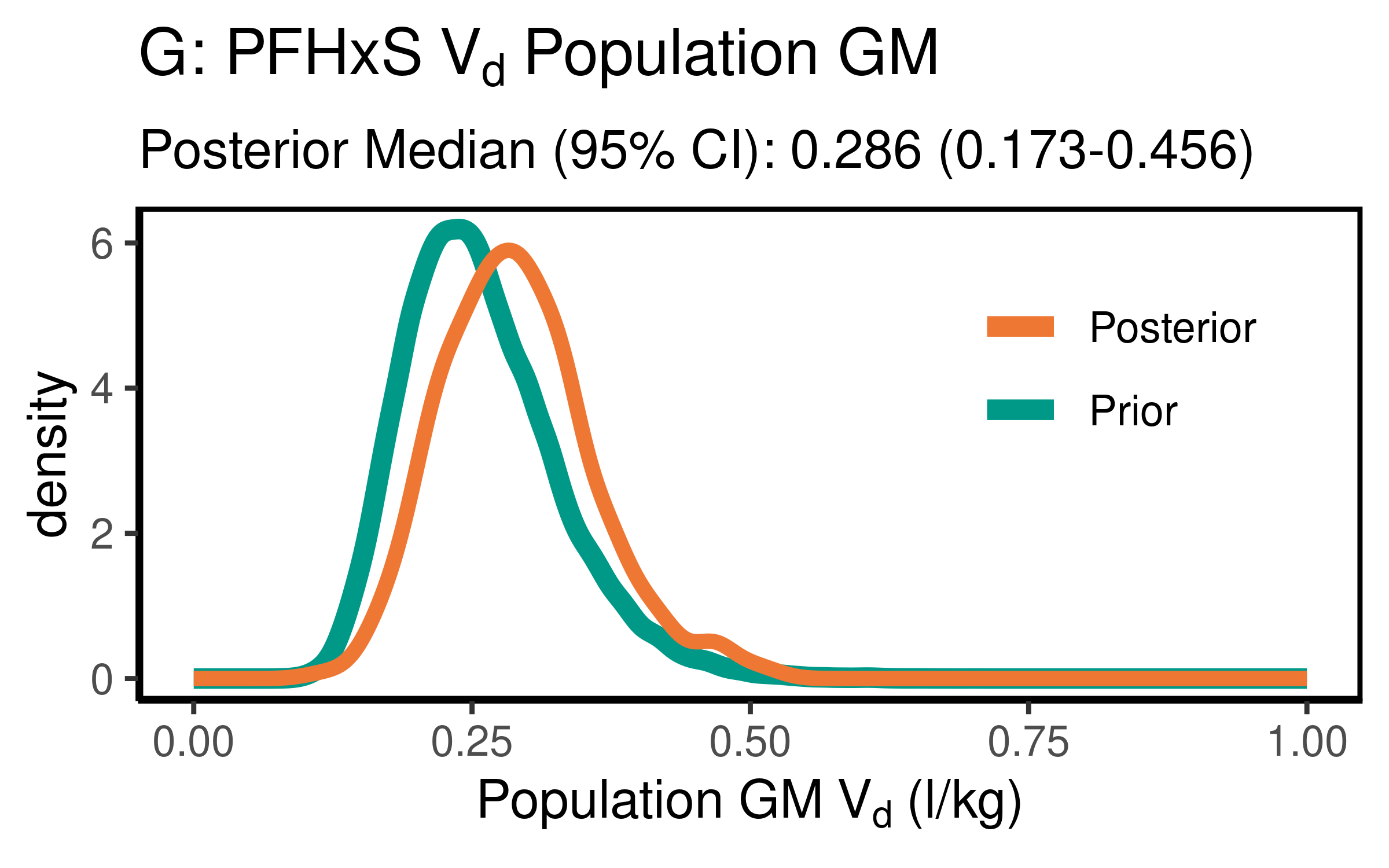


ggsave(here ("output-plots",paste0( sa, "PFHxS\_hl\_gsd.pdf")) ,p,dpi=600)

### Volume of distribution

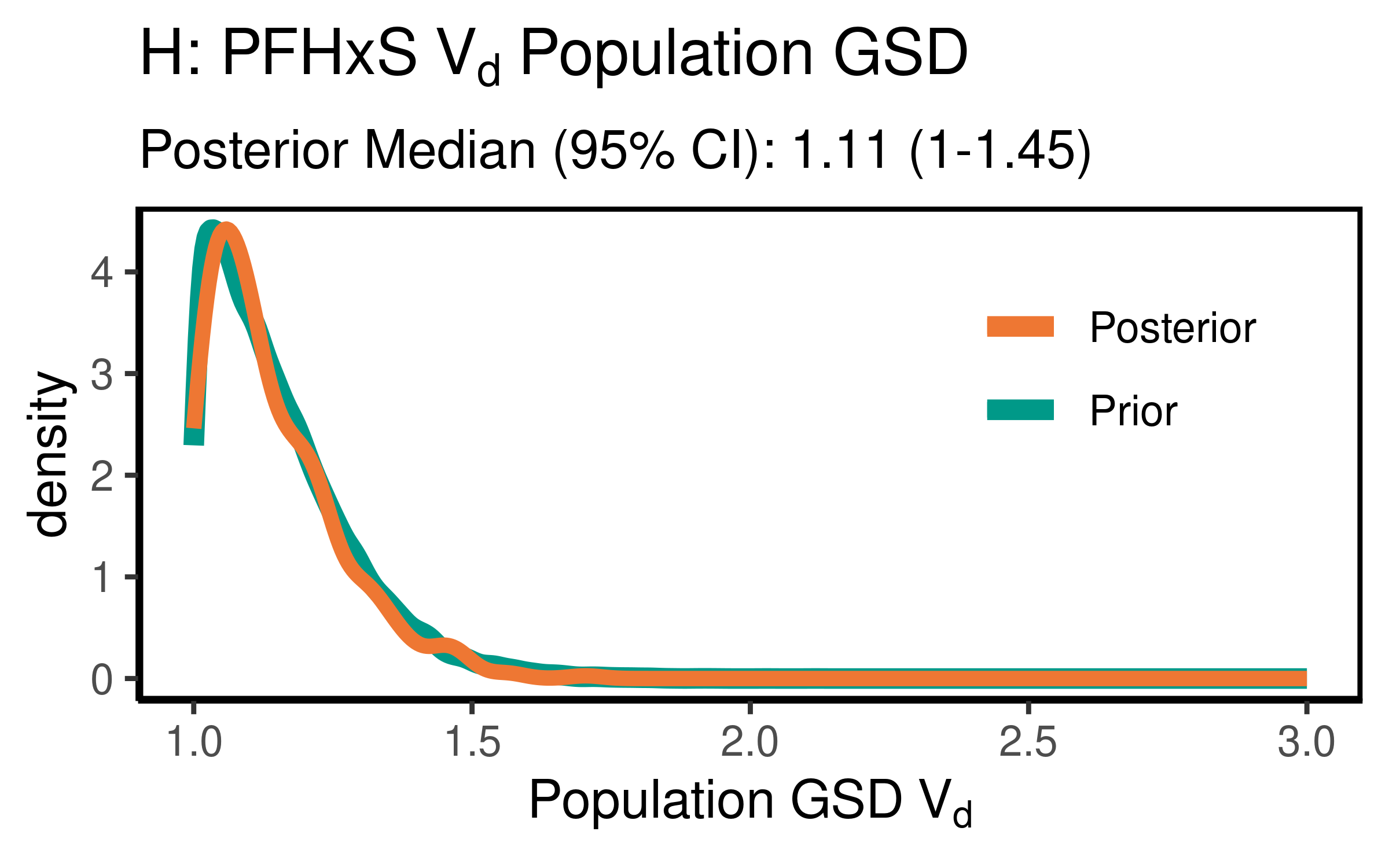
For PFHxS, the data were not particularly informative, but slightly increased the estimate of the median to 0.308(0.223-0.548) slightly compared to the case where Cbgd was considered to be entirely from non-drinking water sources. They were not informative as to the population GSD, with the posterior distributions essentially unchanged from the priors.

PFHxS\_priors$Vd\_GM <- rlnorm(50000,  
 meanlog=-1.38629,  
 sdlog=0.2624)  
PFHxS\_Vd\_GM <- exp(dat$`M\_ln\_Vd(1)`)  
  
   
  
PFHxS\_vd\_gm\_pr\_med <- signif(median(PFHxS\_priors$Vd\_GM,3))  
PFHxS\_vd\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFHxS\_priors$Vd\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
PFHxS\_vd\_gm\_med <- signif(median(PFHxS\_Vd\_GM),3)  
PFHxS\_vd\_gm\_med\_95ci <- paste(signif(quantile(PFHxS\_Vd\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(Vd\_GM, color = "Prior"),data=PFHxS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFHxS\_Vd\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,1)+labs(title = bquote("G: PFHxS"~V[d]~"Population GM"),  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_vd\_gm\_med," (",   
 PFHxS\_vd\_gm\_med\_95ci,")",sep=""))+  
 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, "PFHxS\_vd\_gm.pdf")) ,p,dpi=600)

PFHxS\_priors$Vd\_GSD = exp(abs(rnorm(50000,sd=0.17)))  
PFHxS\_Vd\_GSD <- exp(dat$`SD\_ln\_Vd(1)`)  
  
PFHxS\_vd\_gsd\_pr\_med <- signif(median(PFHxS\_priors$Vd\_GSD,3))  
PFHxS\_vd\_gsd\_pr\_med\_95ci <- paste(signif(quantile(PFHxS\_priors$Vd\_GSD,  
 prob=c(0.025,0.975)), 3), collapse="-")  
  
PFHxS\_vd\_gsd\_med <- signif(median(PFHxS\_Vd\_GSD),3)  
PFHxS\_vd\_gsd\_med\_95ci <- paste(signif(quantile(PFHxS\_Vd\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(Vd\_GSD, color = "Prior"),data=PFHxS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFHxS\_Vd\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("H: PFHxS"~V[d]~"Population GSD "),  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_vd\_gsd\_med," (",  
 PFHxS\_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)

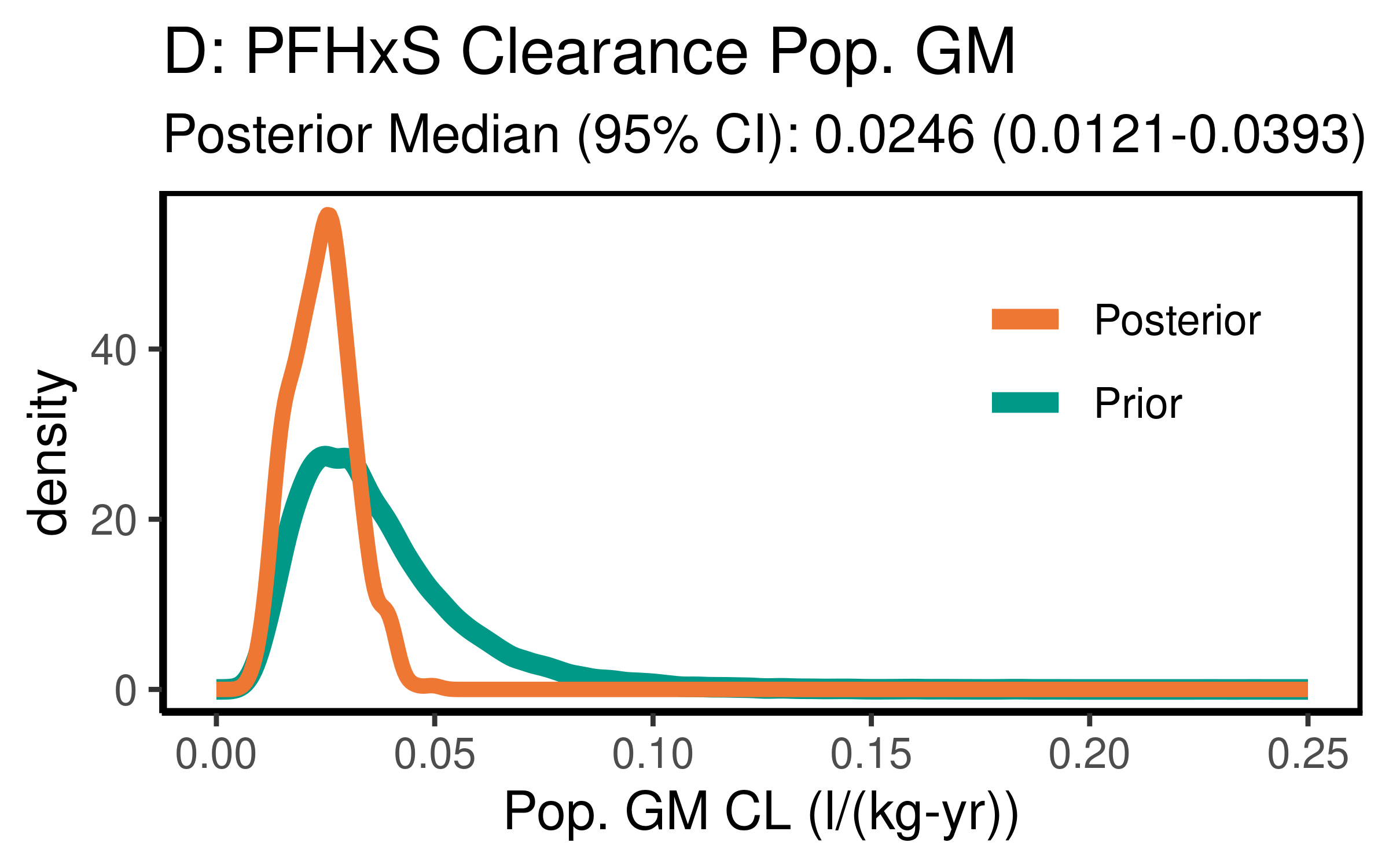


ggsave(here ("output-plots",paste0( sa,"PFHxS\_vd\_gsd.pdf")) ,p,dpi=600)

### Clearance (just pop GM)

Cl is k \* Vd

PFHxS\_priors$CL\_GM <- PFHxS\_priors$Vd\_GM \* (log(2)/PFHxS\_priors$halflife\_GM)  
PFHxS\_CL\_GM <- exp(dat$`M\_ln\_Vd(1)` + dat$`M\_ln\_k(1)`)  
  
PFHxS\_cl\_gm\_pr\_med <- signif(median(PFHxS\_priors$CL\_GM,3))  
PFHxS\_cl\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFHxS\_priors$CL\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
PFHxS\_cl\_gm\_med <- signif(median(PFHxS\_CL\_GM),3)  
PFHxS\_cl\_gm\_med\_95ci <- paste(signif(quantile(PFHxS\_CL\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(CL\_GM, color = "Prior"),data=PFHxS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFHxS\_CL\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,0.25)+labs(title = "D: PFHxS Clearance Pop. GM ",subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_cl\_gm\_med," (",  
 PFHxS\_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, "PFHxS\_CL\_gm.pdf")), p,dpi=600)

## Table significant digit values

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

### Population median estimates [95% CI]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Prior GM | Posterior GM | Prior GSD | Posterior GSD |
| Half-life (years) | 5.29 | 8.3 | 1.56 | 1.57 |
| HL [95% CI] | [2.39-11.8] | [5.38-13.5] | [1.42-1.77] | [1.42-1.77] |
| Volume of distribution | 0.25 | 0.286 | 1.12 | 1.11 |
| [95% CI] | [0.149-0.418] | [0.173-0.456] | [1.01-1.46] | [1-1.45] |
| Clearance | 0.0326 | 0.0246 |  |  |
| [95% CI] | [0.0126-0.0847] | [0.0121-0.0393] | [] | [] |

### Individual Posterior estimates

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | median GM [95% CI] | GM calculator input | GSD individual |
| Half-life (years) | 8.12 [ 2.79-21.6 ] | 8.2 | 1.68 |
| Volume of distribution | 0.281 [ 0.161-0.46 ] | 0.281 | 1.32 |

### Session information

## ─ 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 2021-02-28   
##   
## ─ 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)  
## 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)  
## 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