PFHxS 1 compartment Plots (v8)

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library(coda)  
library(bayesplot)

## This is bayesplot version 1.8.0

## - 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 1.3.1 ──

## ✓ tibble 3.1.6 ✓ dplyr 1.0.7  
## ✓ tidyr 1.1.4 ✓ stringr 1.4.0  
## ✓ readr 2.1.1 ✓ forcats 0.5.1  
## ✓ purrr 0.3.4

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

library(reshape2)

##   
## Attaching package: 'reshape2'

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

library(yardstick) # for quick rmse

## For binary classification, the first factor level is assumed to be the event.  
## Use the argument `event\_level = "second"` to alter this as needed.

##   
## Attaching package: 'yardstick'

## The following object is masked from 'package:readr':  
##   
## spec

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.

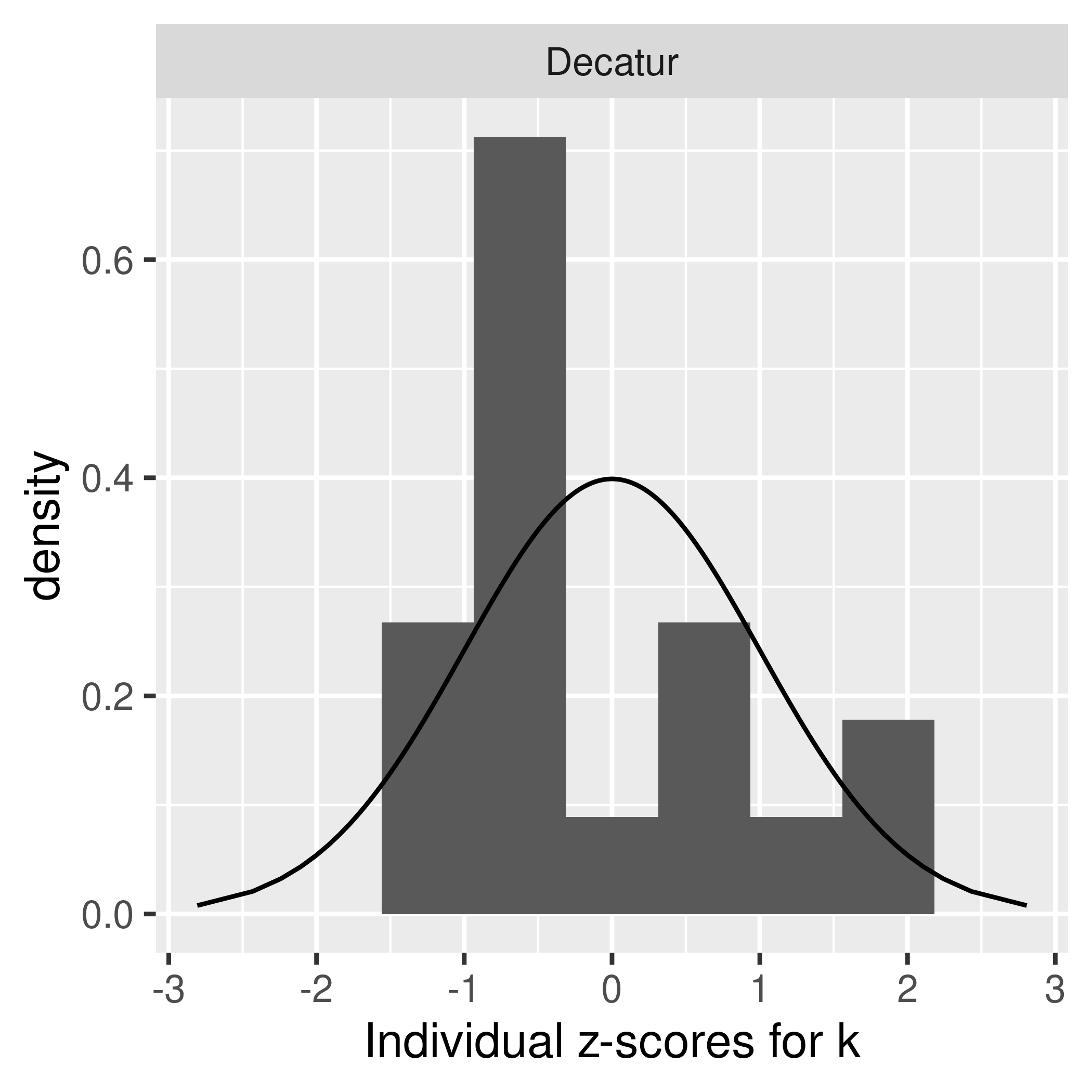
## Set filenames and load data

## Set up dataset

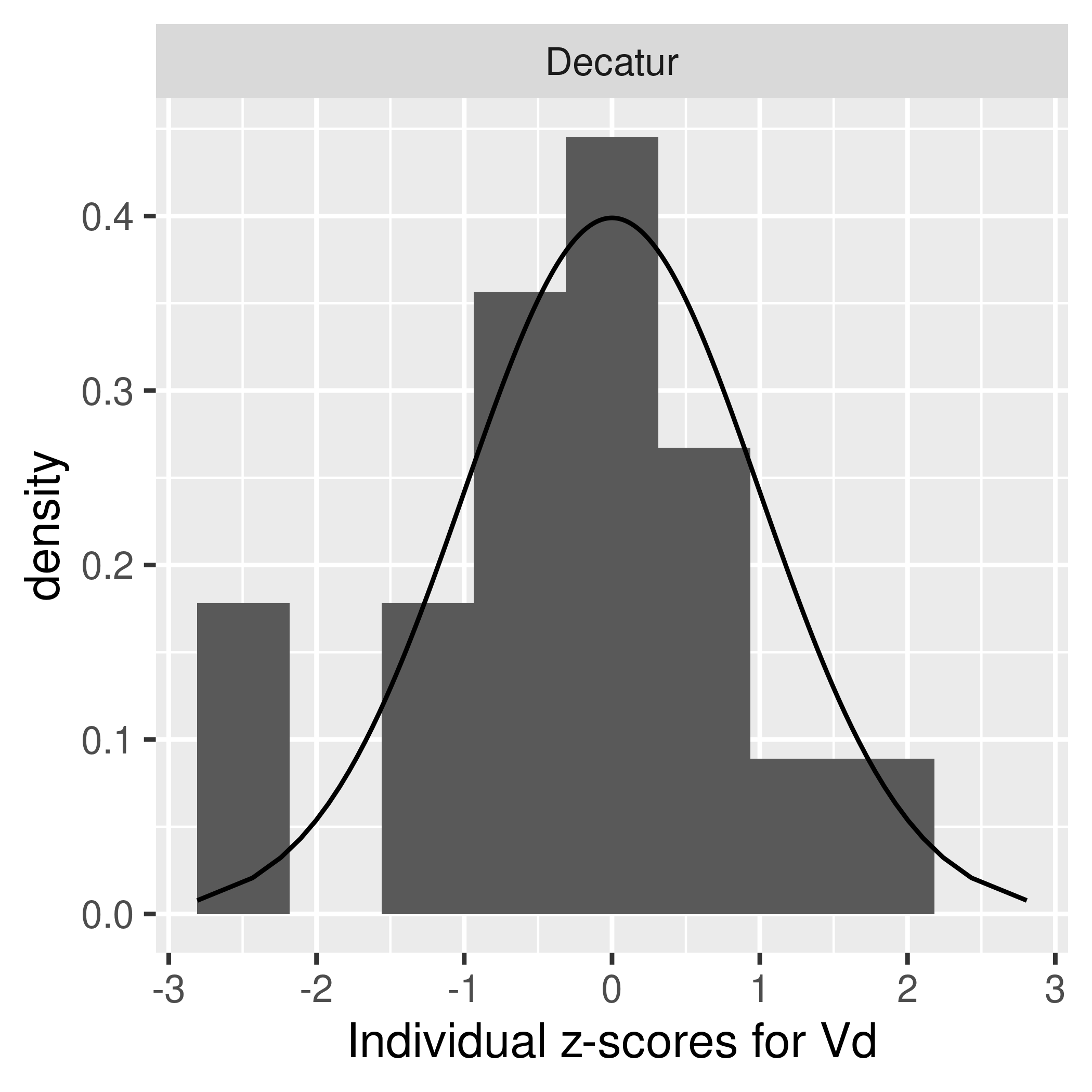
id\_lut <- multicheck$df\_check %>% select(Level) %>% unique () %>%  
 mutate(dataset = c(   
 rep("Decatur M Train", 9),  
 rep("Decatur F Train", 9),  
 rep("Decatur M Test", 9),  
 rep("Decatur F Test", 10),  
 'Paulsboro-Train','Horsham-Train',  
 'Warminster-Test','Warrington-Train'),   
 Sex = 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)

## Individual parameters

set.seed(314159)  
  
indiv\_parms <- indiv\_lut  
lnkparmnames <- paste("ln\_k.",gsub("\_",".",indiv\_parms$Level),".",sep="")  
lnVdparmnames <- paste("ln\_Vd.",gsub("\_",".",indiv\_parms$Level),".",sep="")  
  
parmsamp <- apply(multicheck$parms.samp,2,sample,1)  
  
## Random z-score estimate of each parameter  
indiv\_parms$ln\_k.z.samp <- parmsamp[lnkparmnames]  
indiv\_parms$ln\_Vd.z.samp <- parmsamp[lnVdparmnames]  
  
normd <- data.frame(x=qnorm(ppoints(200)))  
normd$y <- dnorm(normd$x)  
  
iplotk<-  
 ggplot(subset(indiv\_parms,Train\_Test=="Train"))+  
 geom\_histogram(aes(x=ln\_k.z.samp,after\_stat(density)),bins=10)+facet\_wrap(~City,ncol=1)+  
 geom\_line(aes(x=x,y=y),data=normd)+  
 xlab("Individual z-scores for k")  
  
iplotVd<-  
 ggplot(subset(indiv\_parms,Train\_Test=="Train"))+  
 geom\_histogram(aes(x=ln\_Vd.z.samp,after\_stat(density)),bins=10)+facet\_wrap(~City,ncol=1)+  
 geom\_line(aes(x=x,y=y),data=normd)+  
 xlab("Individual z-scores for Vd")  
  
print(iplotk)



print(iplotVd)



ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_k\_PFHxS.pdf")),iplotk,dpi=600)

## Saving 3.5 x 3.5 in image

ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_k\_PFHxS.png")),iplotk,dpi=600)

## Saving 3.5 x 3.5 in image

ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_Vd\_PFHxS.pdf")),iplotVd,dpi=600)

## Saving 3.5 x 3.5 in image

ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_Vd\_PFHxS.png")),iplotVd,dpi=600)

## Saving 3.5 x 3.5 in image

## 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 ~ ""))

## `summarise()` has grouped output by 'Level', 'Simulation', 'Output\_Var', 'Time', 'Data', 'dataset', 'Sex', 'City', 'Train\_Test', 'datatype'. You can override using the `.groups` argument.

#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 ) )

## `summarise()` has grouped output by 'City', 'datatype'. You can override using the `.groups` argument.

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 )

## Loading required package: scales

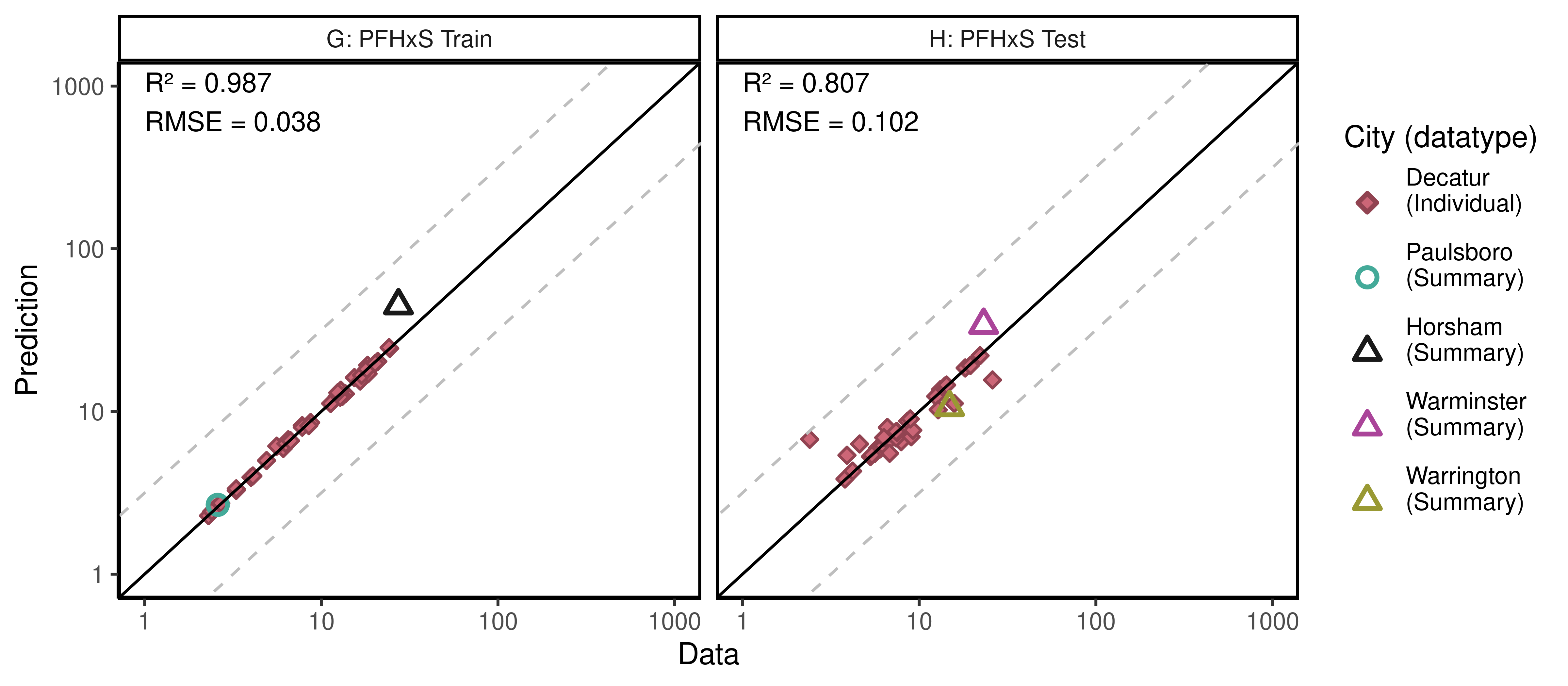
##   
## Attaching package: 'scales'

## The following object is masked from 'package:purrr':  
##   
## discard

## The following object is masked from 'package:readr':  
##   
## col\_factor

## Joining, by = "facet\_label"

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

ggsave(here ("output-plots", paste0( sa,"multicheckplot\_", pfas\_name,  
 ".png")),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))

## New names:  
## \* Level -> Level...1  
## \* Level -> Level...2

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

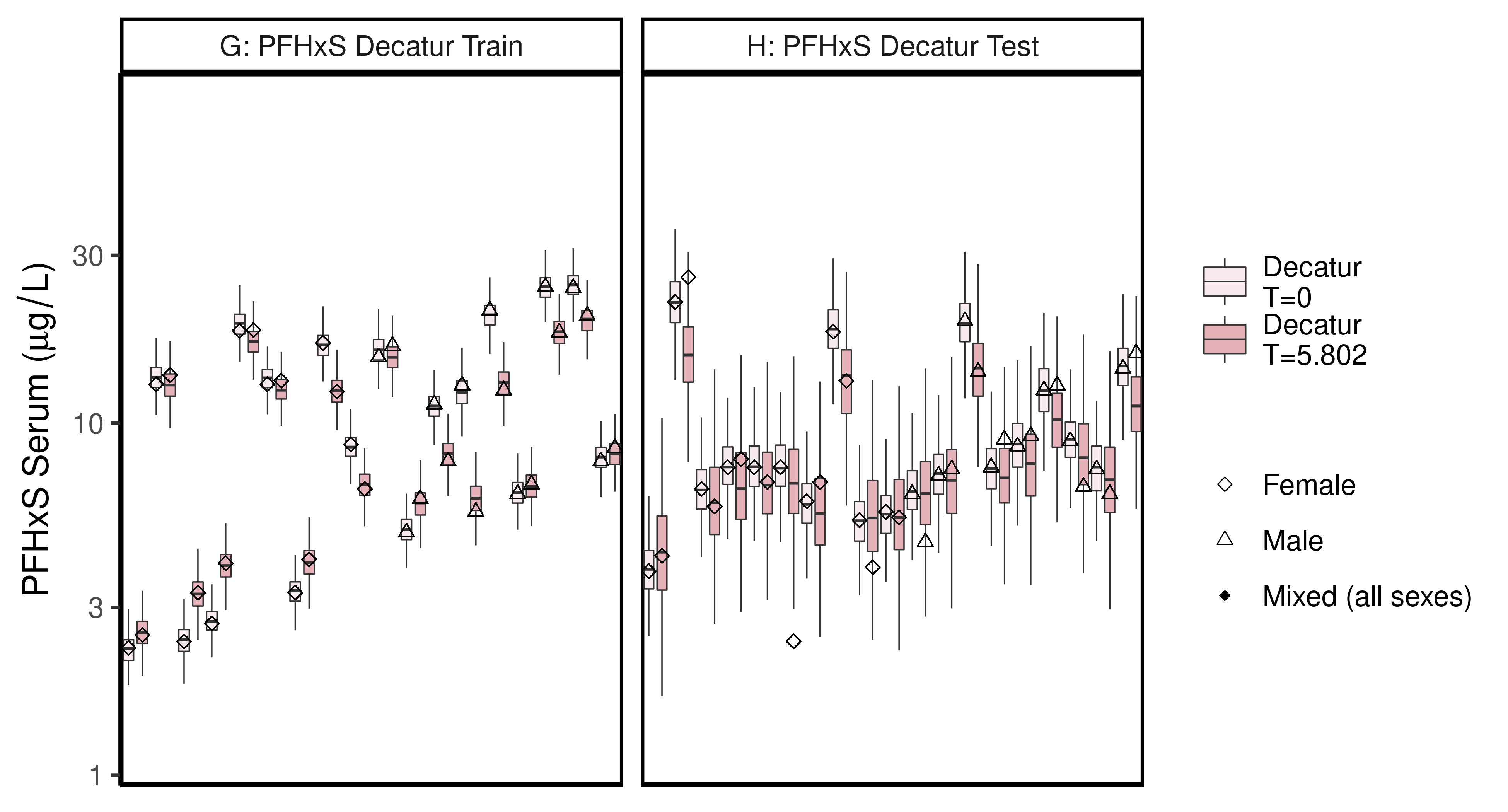
Modify aesthetics lookup table for boxplots

## 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

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

## Saving 6.5 x 3.5 in image

## All boxplots

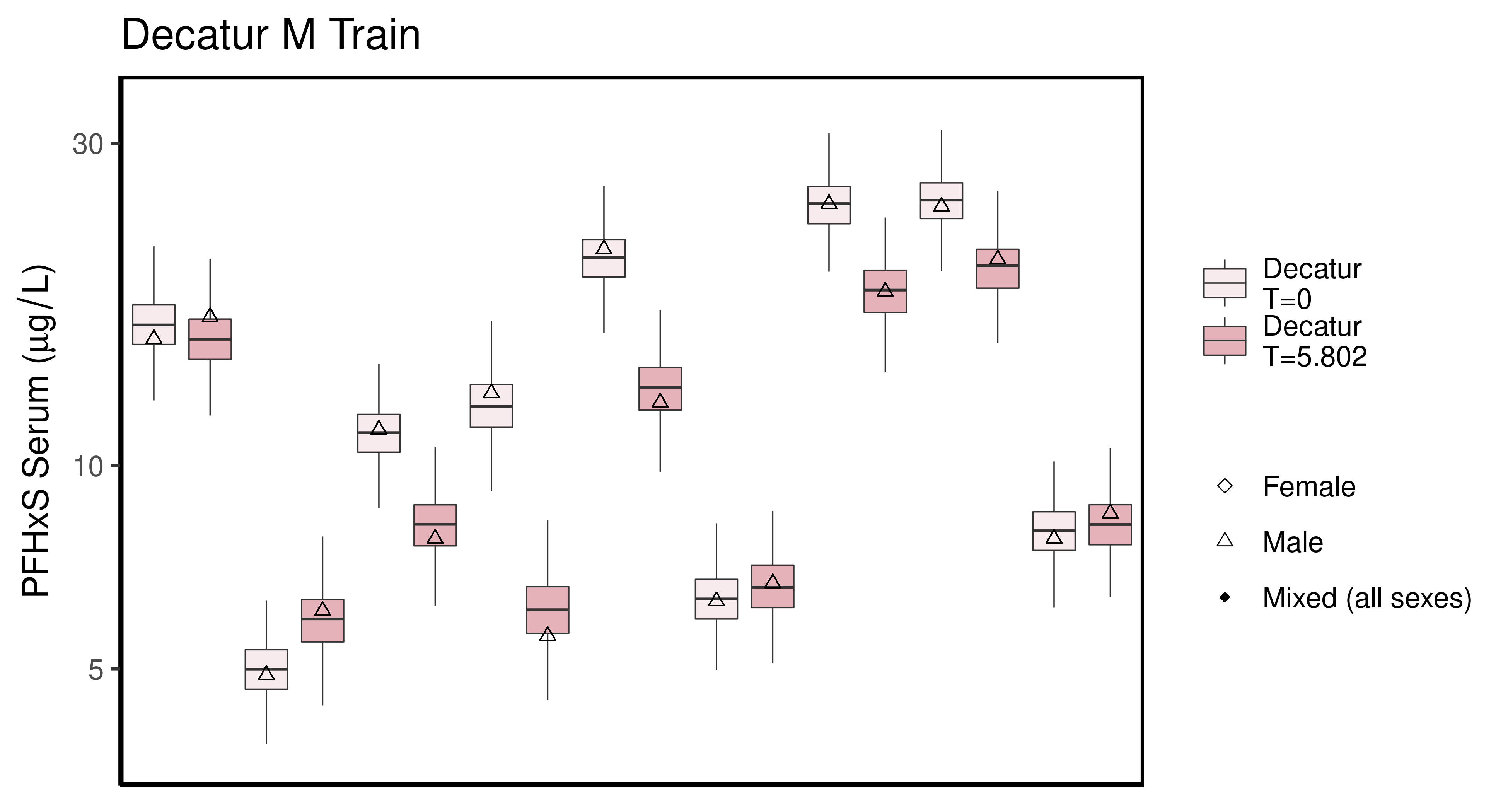
Changed grey start to 1 instead of 0.8, end at 0.6 instead of 0.4. Added shapes and fills to data points.

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)  
   
 ggsave(here ("output-plots",  
 paste0( sa, d,"-boxplot-",   
 pfas\_name,".png")) ,  
 plt,dpi=600)  
  
}

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

## Saving 6.5 x 3.5 in image  
## Saving 6.5 x 3.5 in image

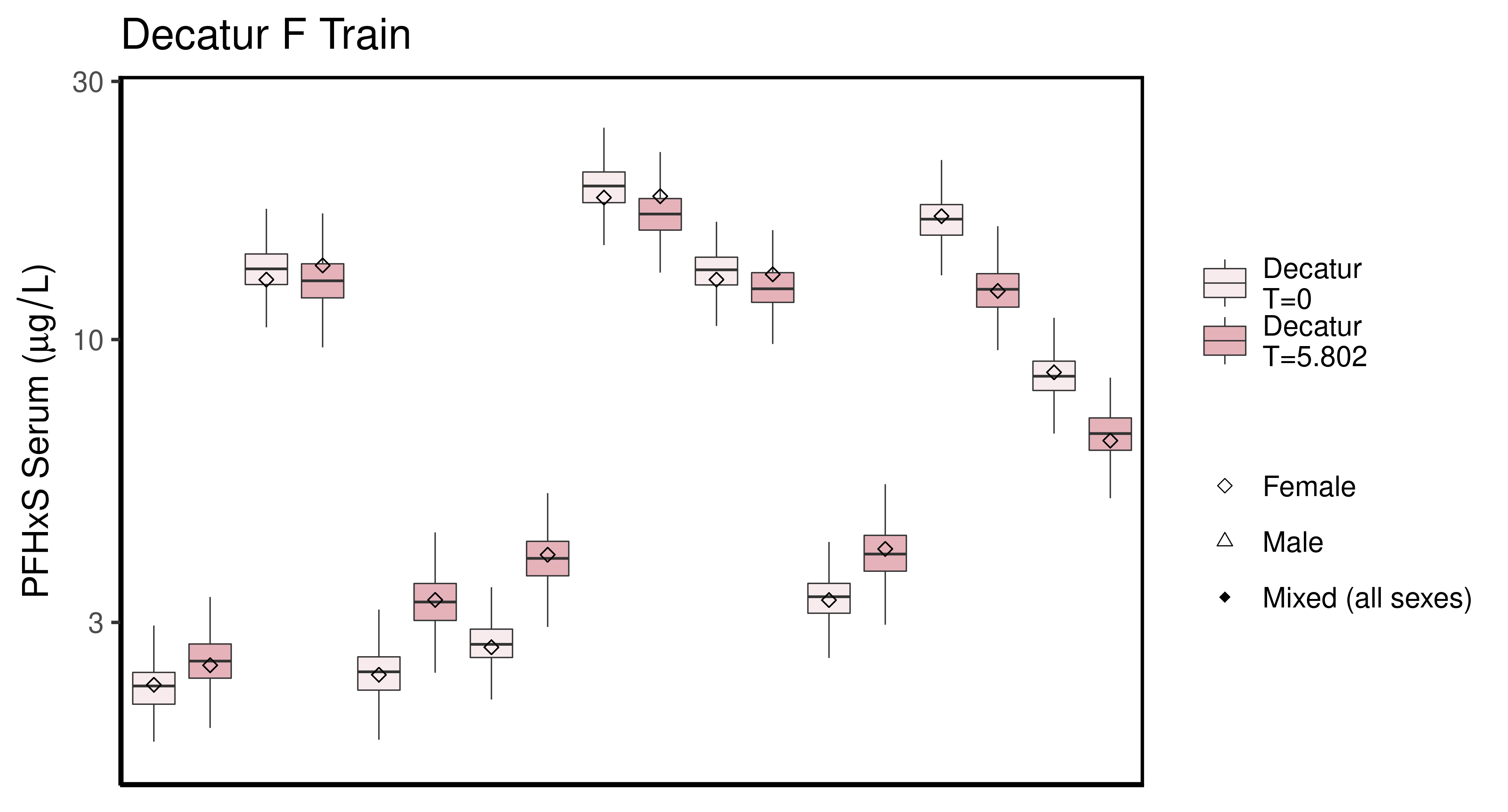
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

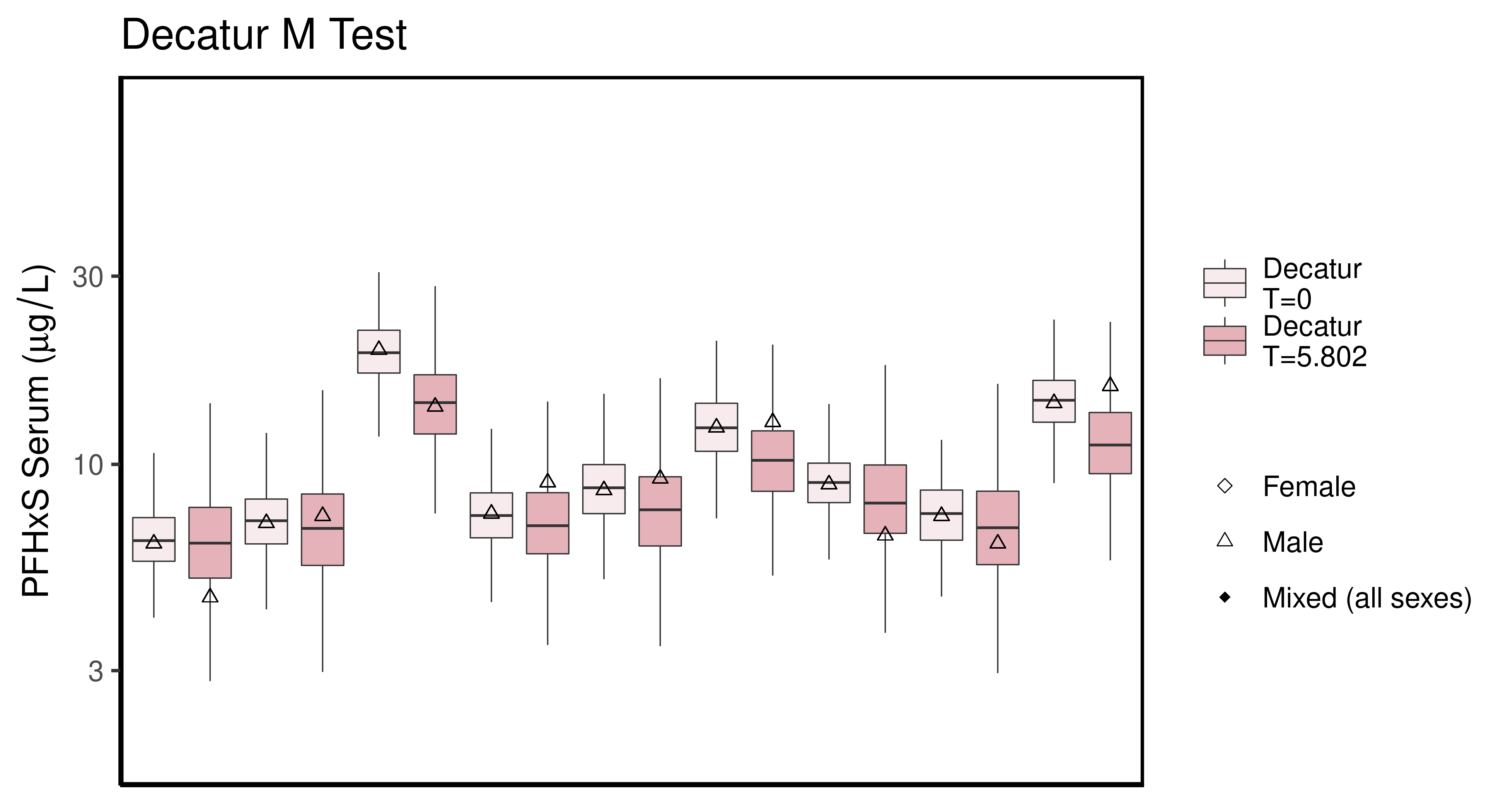
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

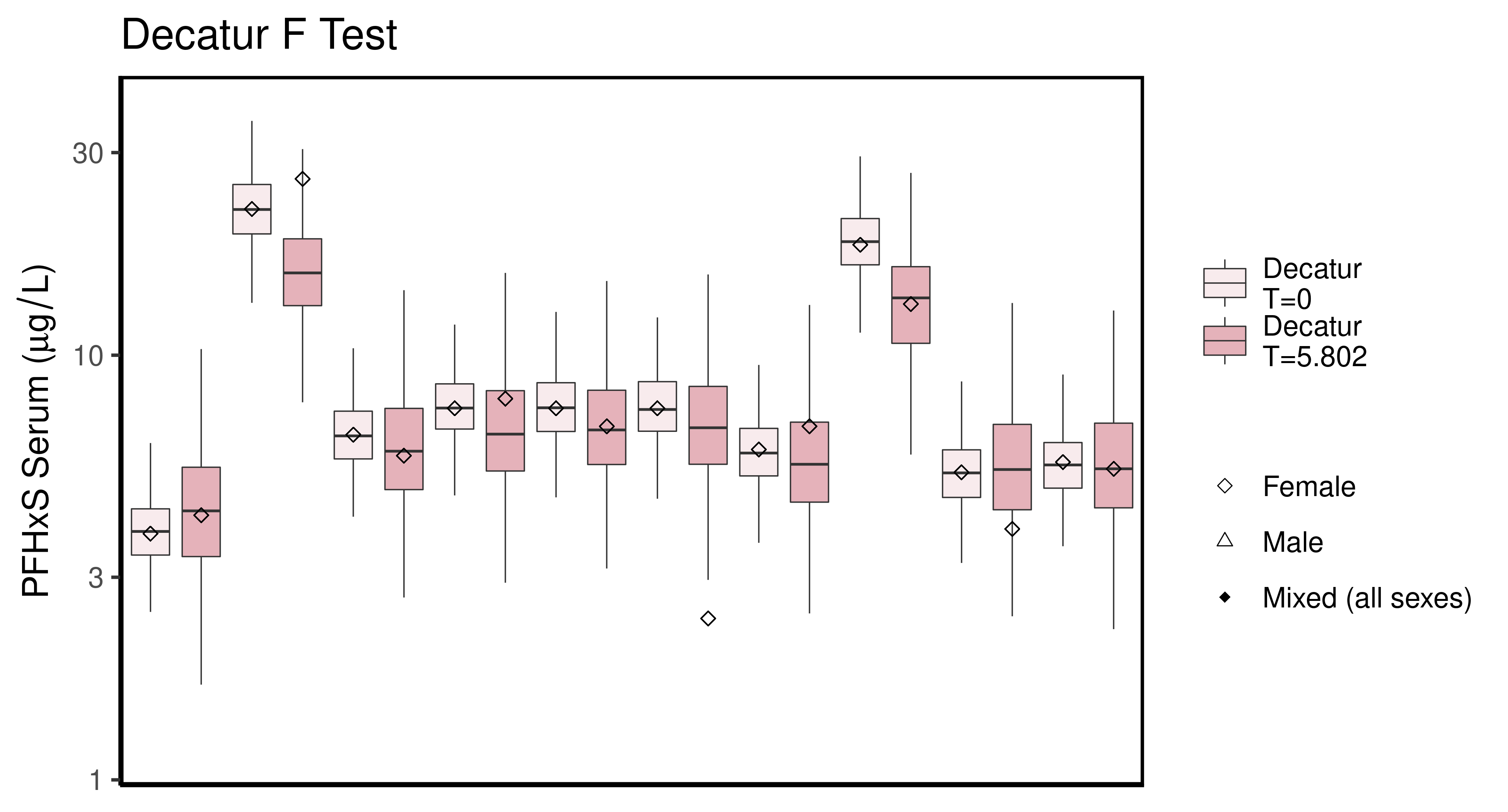
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

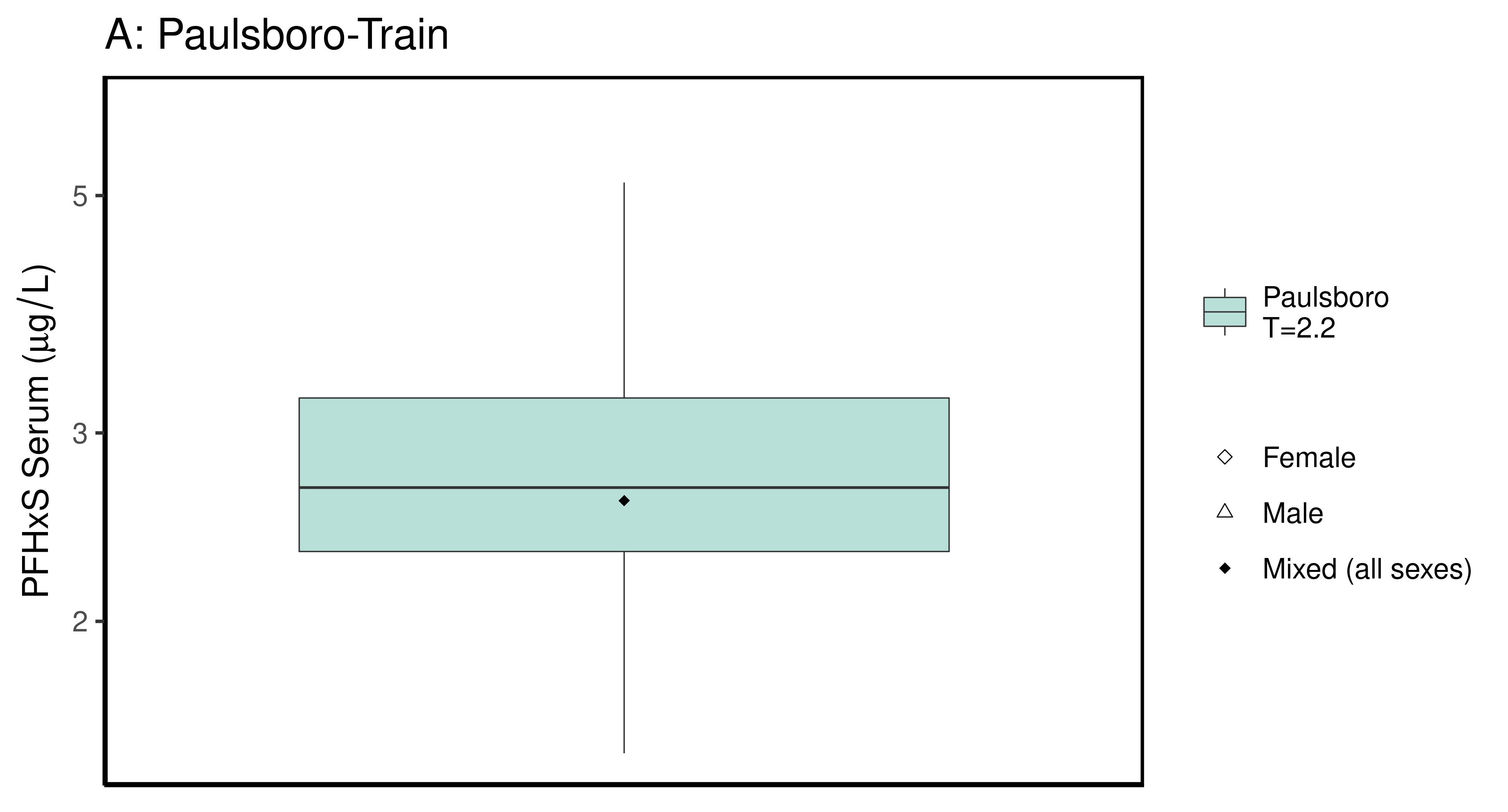
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

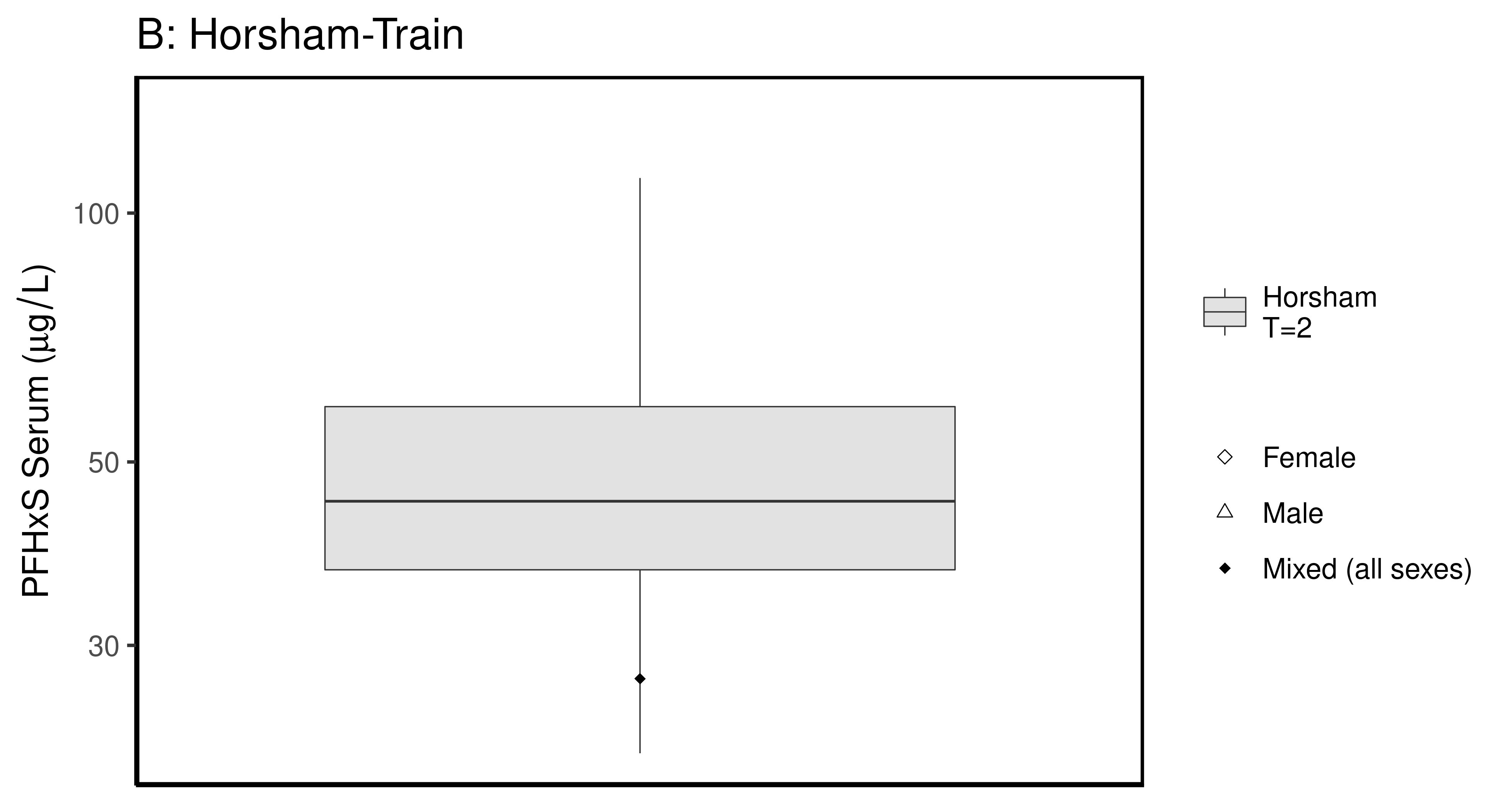
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

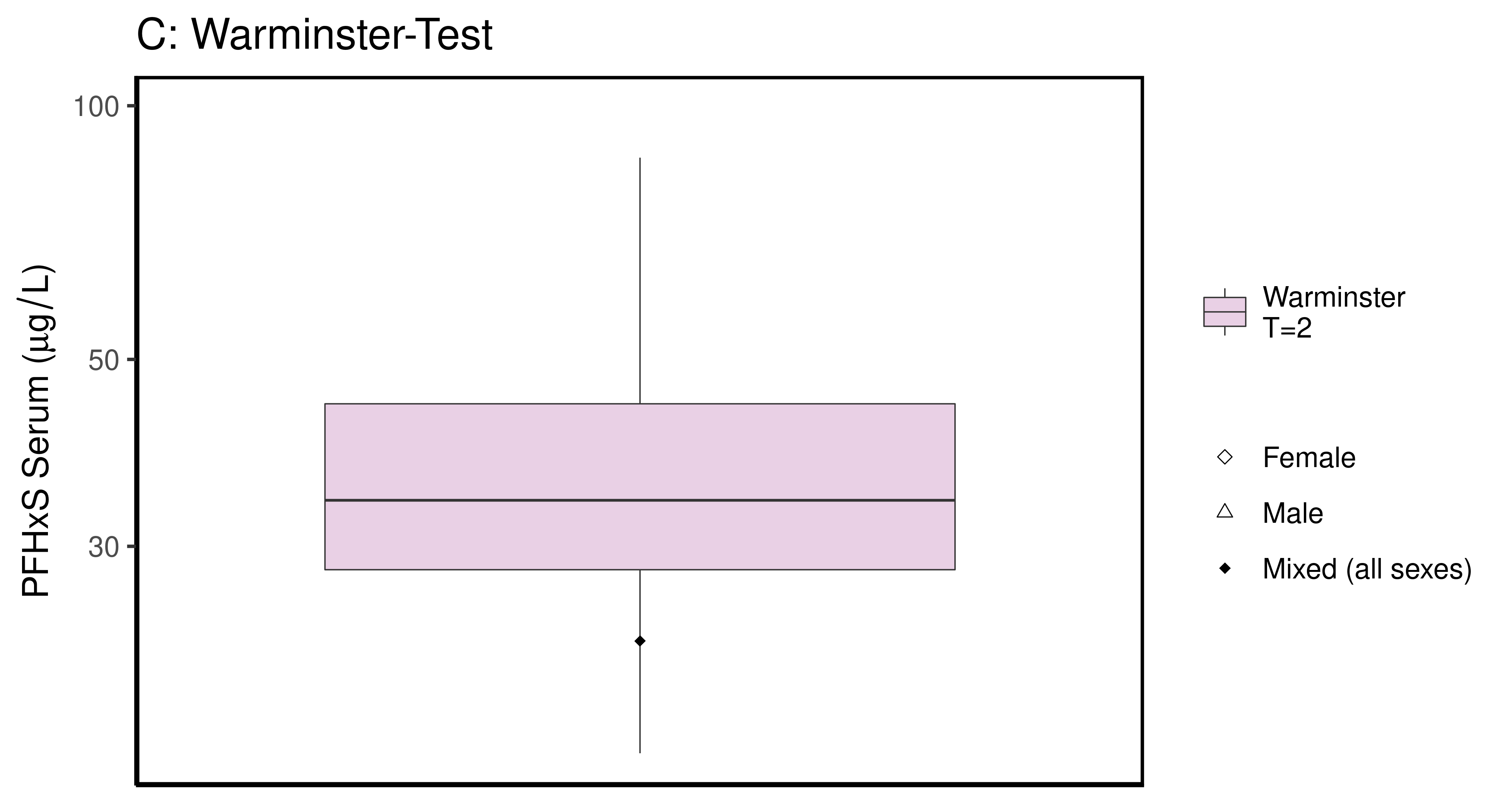
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

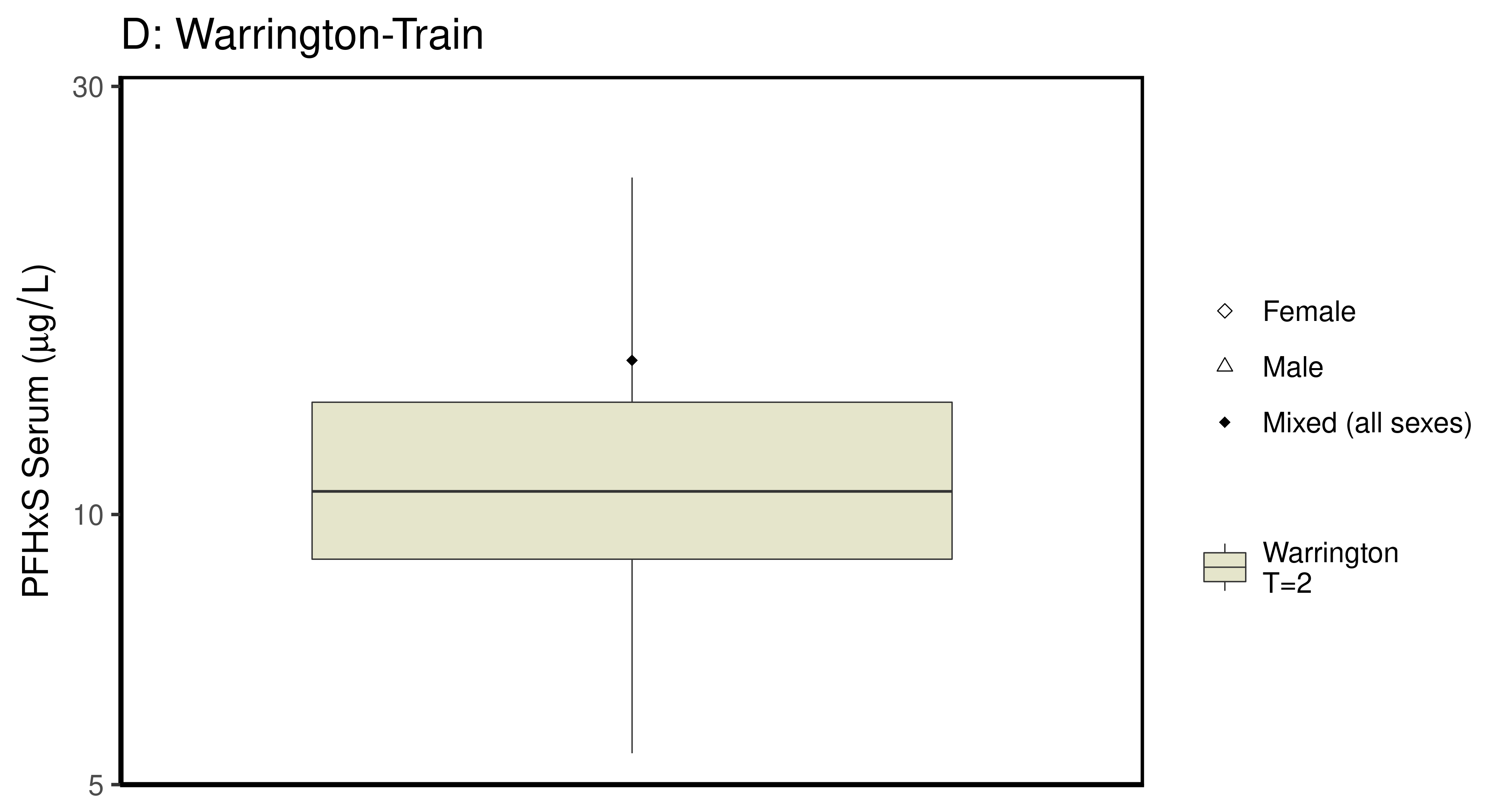
## Saving 6.5 x 3.5 in image

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



## Saving 6.5 x 3.5 in image

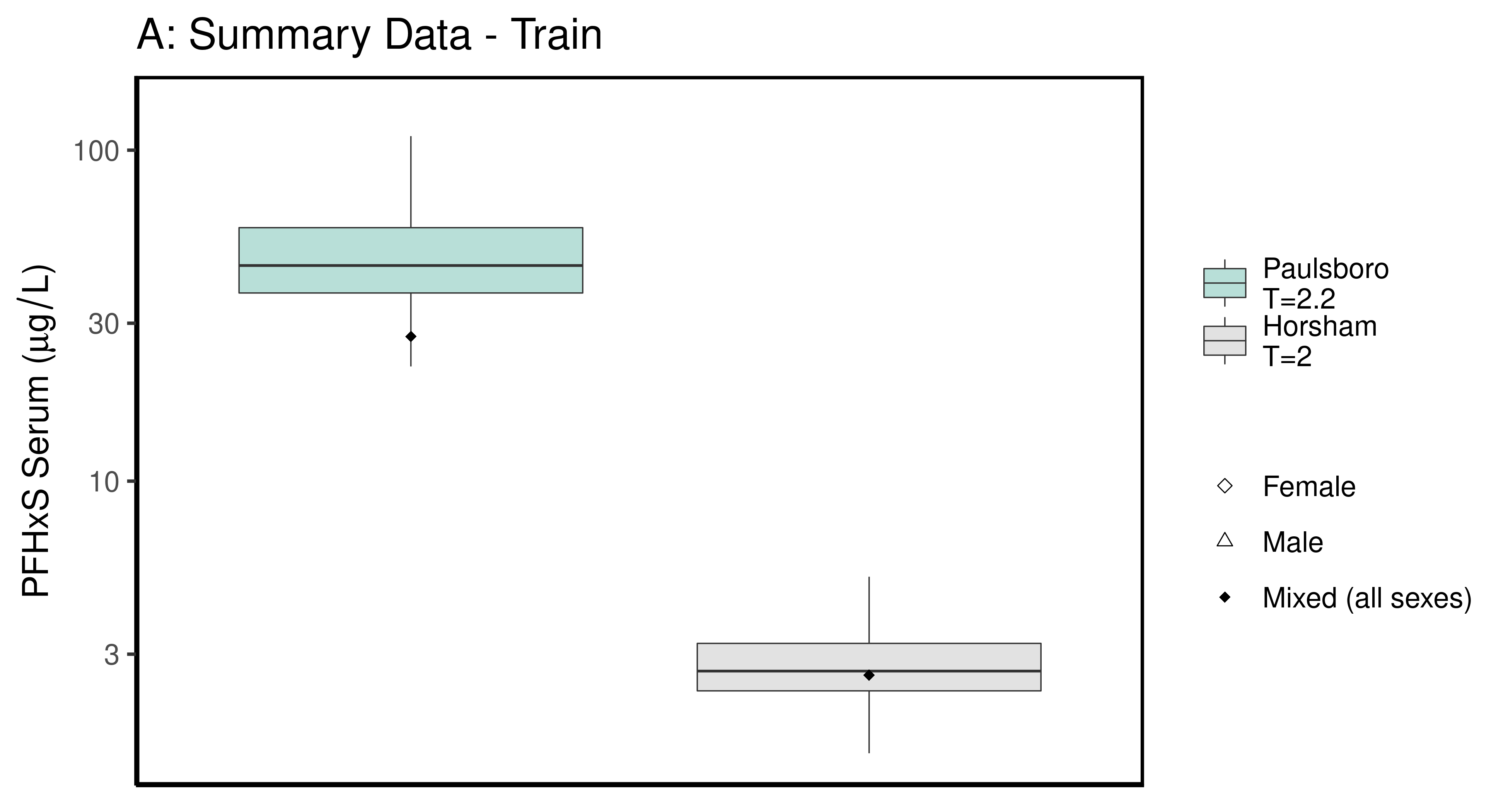
## Saving 6.5 x 3.5 in image



### 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

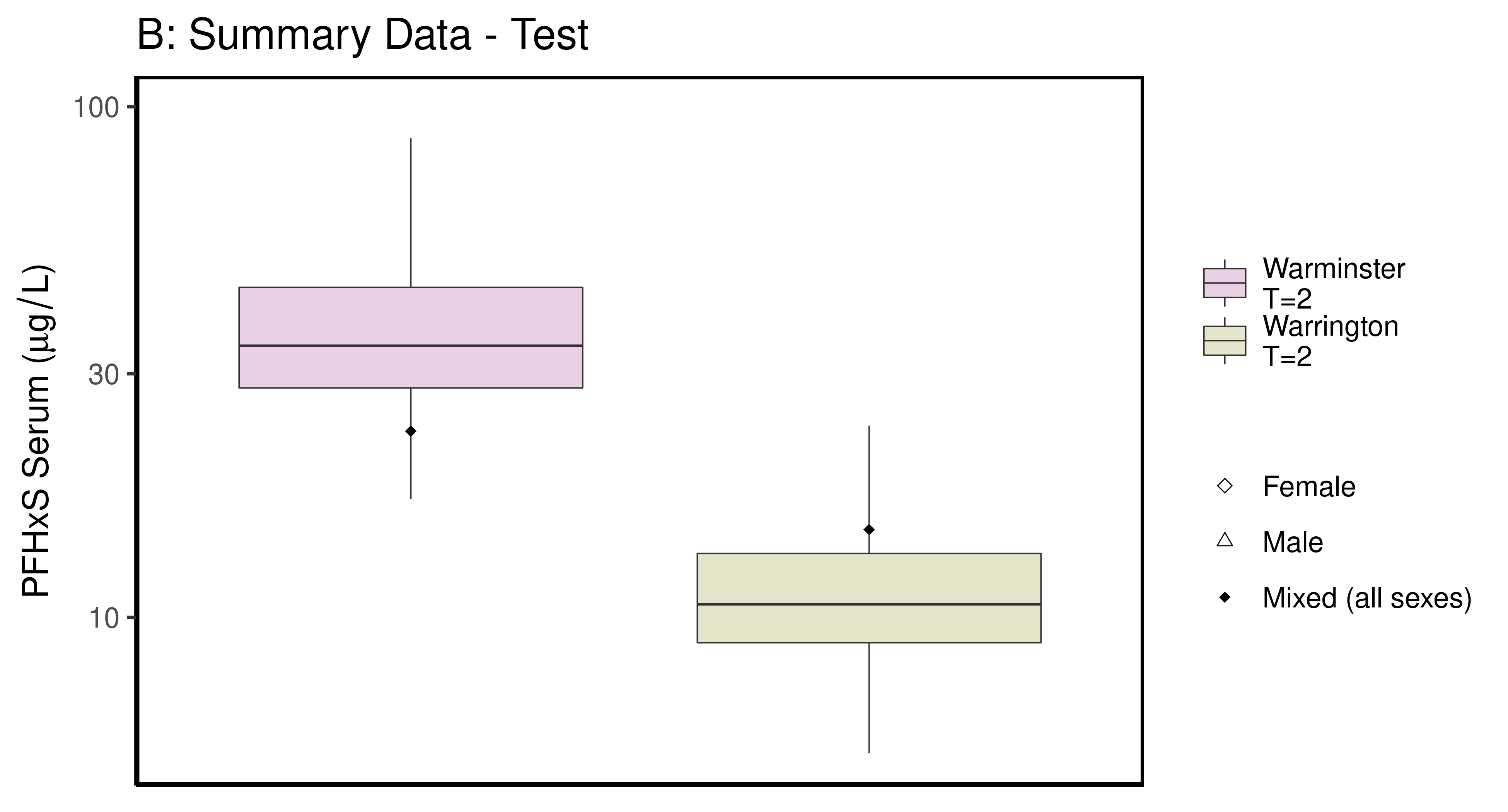
ggsave(here ("output-plots", paste0( sa, "SummaryTrainDataboxplot", pfas\_name,".png")), plt\_train,dpi=600)

## 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

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

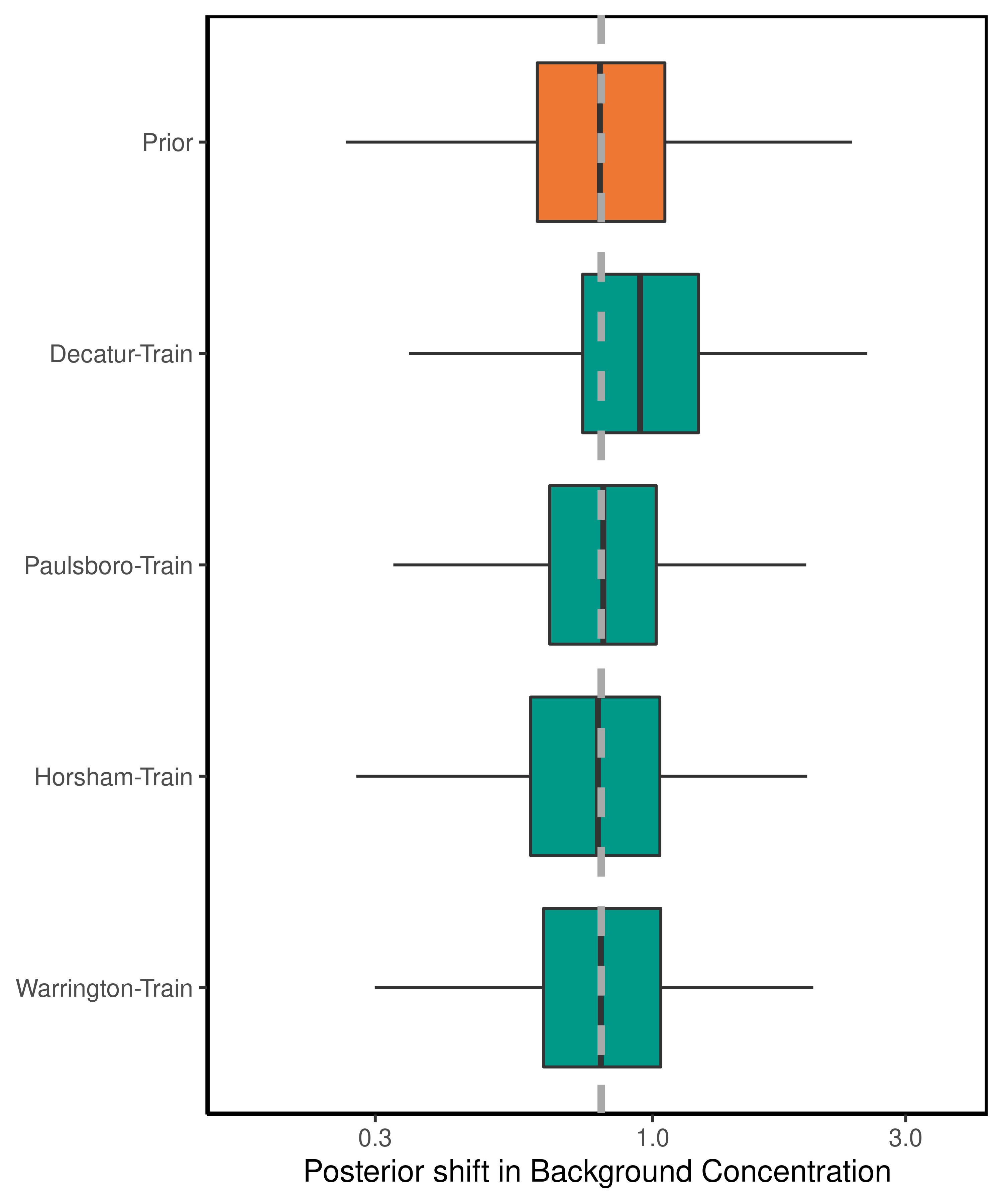
## Saving 6.5 x 3.5 in image

## 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

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

## Saving 5 x 6 in image

### Half-life

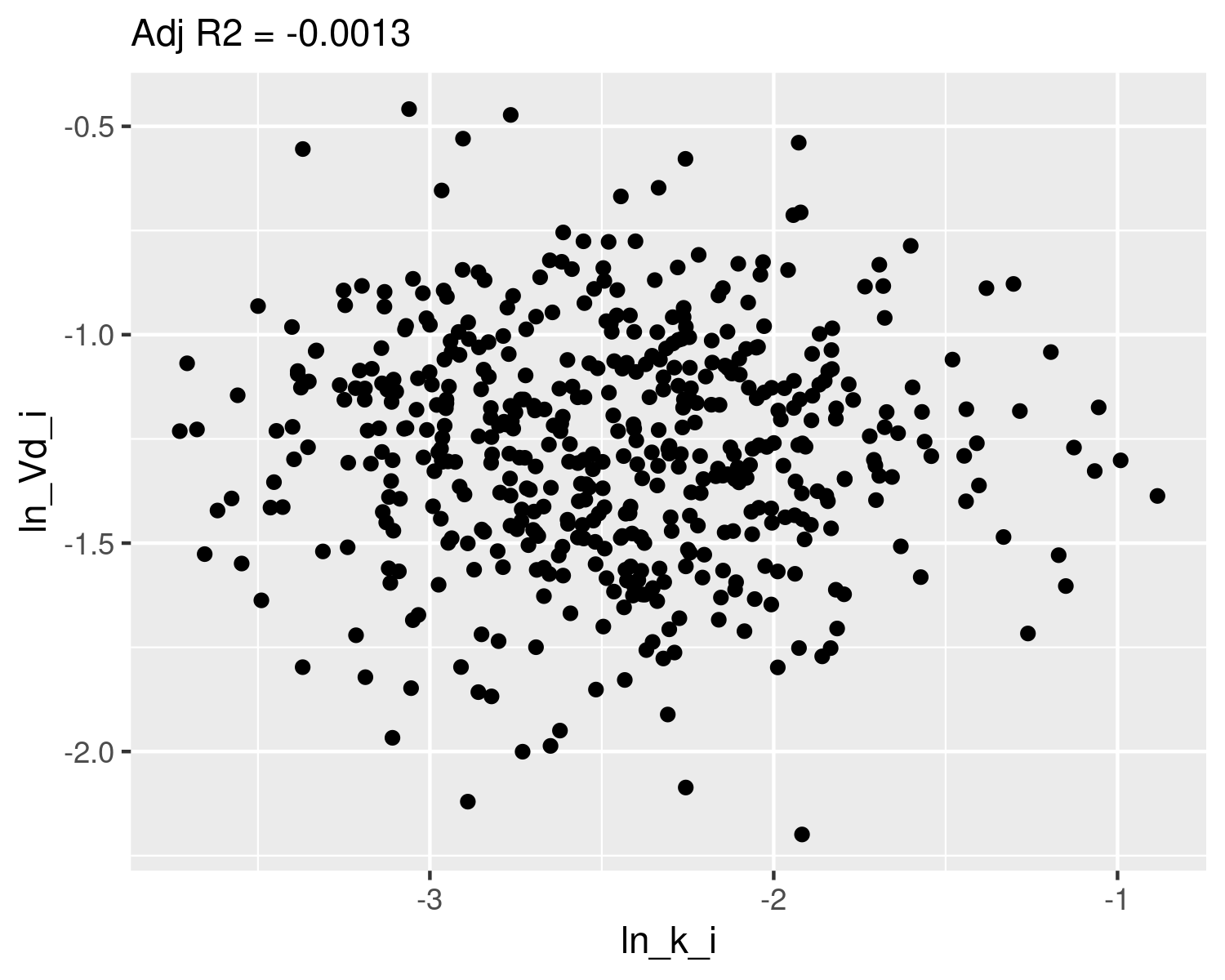
For PFHxS, the population GM of the half-life has a posterior distribution that is narrower than the prior, with a posterior median (95% CI) estimate of 3.06 (2.16-4.37) years. The population GSD posterior is larger than the prior at 1.47(1.44-1.75).

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\_()` was deprecated in dplyr 0.7.0.  
## Please use `rename()` instead.  
## This warning is displayed once every 8 hours.  
## Call `lifecycle::last\_lifecycle\_warnings()` to see where this warning was generated.

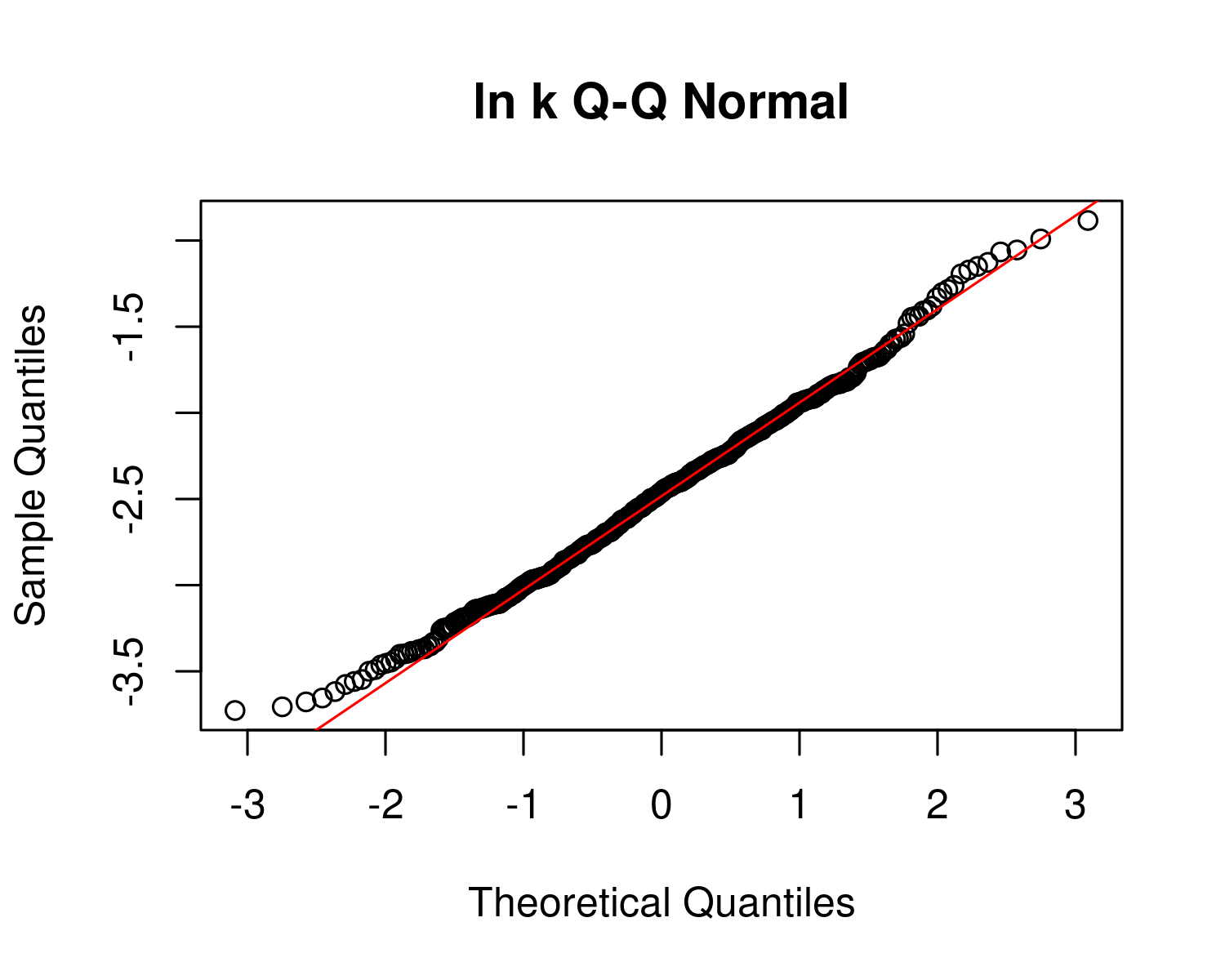
## M\_ln\_k(1) V\_ln\_k(1) M\_ln\_Vd(1) SD\_ln\_Vd(1) z\_ln\_k z\_ln\_Vd  
## 12503 -2.75291 0.2041830 -1.412470 0.191222000 -0.961933416 -2.139841913  
## 15901 -2.72905 0.3388370 -1.262040 0.095982100 -0.292525723 -1.263479244  
## 17543 -2.67035 0.2659090 -1.390400 0.286419000 0.258788216 0.083307969  
## 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  
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## 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  
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## 18382 -2.90847 0.1900410 -1.513860 0.051897200 -0.453551227 0.840642928  
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## 1964 -2.32689 0.1492140 -1.415530 0.006501350 -0.886389751 0.491361149  
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## 15832 -2.10205 0.2009170 -1.533270 0.110261000 -0.650877737 -0.503256667  
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## 12073 -2.38674 0.2187970 -1.414980 0.104553000 -0.390878033 -0.684829990  
## 15683 -2.37177 0.1980320 -1.554080 0.281385000 -0.070586394 -0.221516764  
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## 17573 -2.61984 0.2490640 -1.188020 0.323572000 -0.463031038 0.175989014  
## 19872 -2.25348 0.1875930 -1.510300 0.259134000 -0.279741696 -0.437523579  
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## 15883 -2.73255 0.2387910 -1.224400 0.054648900 1.618766521 0.891044960  
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## 14073 -2.53267 0.1983580 -1.504490 0.126207000 -0.304629836 -0.972329346  
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## 1472 -2.31697 0.1253420 -1.224330 0.004328210 -1.244582466 -0.223544486  
## 17673 -2.49725 0.2248920 -0.953237 0.021532700 -1.205974540 -1.188865752  
## 14023 -2.98113 0.2638230 -0.908168 0.065088700 0.273093950 0.599961163  
## 15453 -2.90986 0.2309110 -1.239930 0.119861000 1.729414034 -0.863306018  
## 16151 -2.57108 0.1473410 -1.136320 0.048124600 -1.064950869 -0.669136112  
## 14392 -2.73386 0.2153710 -1.123620 0.158941000 -0.113736688 0.758080913  
## 1606 -2.71698 0.3049020 -1.202840 0.220314000 -0.643751471 0.977212323  
## 14853 -2.13772 0.2354160 -1.212720 0.221584000 0.940648418 1.486960427  
## 16371 -2.54830 0.1443340 -1.651420 0.048851200 1.918810176 0.809182023  
## 14261 -2.53918 0.3321380 -1.416020 0.025390200 -1.006045550 1.049591298  
## 13171 -2.52621 0.1663700 -0.893134 0.271118000 0.547082630 -1.378317315  
## 10481 -2.41713 0.1124750 -1.124400 0.086692100 0.033847059 -1.166379732  
## 14142 -2.71942 0.1545870 -1.102770 0.042130400 -0.315828929 0.450531663  
## 15372 -2.47209 0.2391330 -1.101620 0.075715300 0.288544593 0.553986739  
## 13811 -2.18047 0.2045900 -1.370160 0.324137000 -0.344392202 0.171533785  
## 1300 -2.67440 0.2350430 -1.102010 0.137870000 0.116631435 -0.806881470  
## 1855 -2.40777 0.2950850 -1.357810 0.011541000 0.542965968 0.978852878  
## 18943 -2.12616 0.1371430 -1.402240 0.004606600 1.143947544 1.171035498  
## 18831 -2.59519 0.1793470 -1.102120 0.057315400 -1.284548845 -0.254750999  
## 1629 -2.83572 0.1805340 -1.441630 0.176029000 0.919811790 -0.261779474  
## 11953 -2.61364 0.2311260 -1.086680 0.137345000 -0.846090161 1.357008537  
## 13562 -2.68224 0.2243340 -1.458800 0.180173000 -1.419304273 1.048195428  
## 18421 -1.92579 0.1908020 -1.629080 0.027536500 -2.665697589 2.228898486  
## 20003 -2.34036 0.1948530 -1.190090 0.084370600 0.835106141 -1.470518812  
## 11401 -2.25904 0.2516890 -1.238840 0.085555000 2.377446549 -1.031250041  
## 1048 -2.56151 0.1372240 -1.522600 0.401672000 0.013969708 0.164813527  
## 12143 -2.50822 0.1877110 -0.970648 0.126705000 -1.633423995 -1.243838156  
## 1075 -2.46098 0.2040470 -1.388510 0.088963900 0.488932473 0.116308174  
## 18021 -2.28623 0.2211310 -1.524870 0.055665500 -1.019179409 1.197547370  
## 17623 -2.79484 0.2085800 -1.296040 0.250570000 1.090553483 -0.698130988  
## 1499 -2.62833 0.1774690 -1.430950 0.442119000 -1.139469805 0.293604948  
## 18673 -2.47243 0.1904210 -1.219440 0.183877000 -0.015725635 0.437297744  
## 1093 -3.22546 0.2556450 -1.293500 0.107878000 0.297491282 0.627762573  
## 13553 -2.20810 0.1711950 -1.279340 0.092635200 3.200590040 -1.160543514  
## 12592 -2.04985 0.2424870 -1.122830 0.219212000 0.089244244 -0.020788418  
## 12912 -2.11565 0.2306120 -1.168590 0.077838100 0.570972338 1.044724089  
## 1785 -2.83093 0.2811680 -1.193550 0.205387000 0.528685630 1.311594585  
## 14041 -2.74332 0.2207640 -0.899848 0.112913000 -0.440904798 -0.082439028  
## 1624 -3.04566 0.2764900 -1.327870 0.116234000 -0.672793368 0.919224762  
## 1841 -2.26703 0.2587430 -1.489040 0.164183000 2.154313365 -0.243269921  
## 19553 -2.19122 0.2239030 -1.503950 0.036649500 0.593852716 0.351094377  
## 12722 -2.03384 0.2361680 -1.159480 0.222747000 -0.384063768 -1.340384172  
## 15122 -2.41409 0.2228960 -0.964277 0.097466900 0.719783276 0.425846094  
## 1348 -2.62948 0.2830370 -1.066280 0.217605000 1.708173402 -0.814353733  
## 15183 -2.83780 0.2155680 -1.139210 0.209466000 1.075215667 0.693374081  
## 14432 -2.58703 0.1585020 -1.086690 0.105126000 0.777420367 0.705544556  
## 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)))

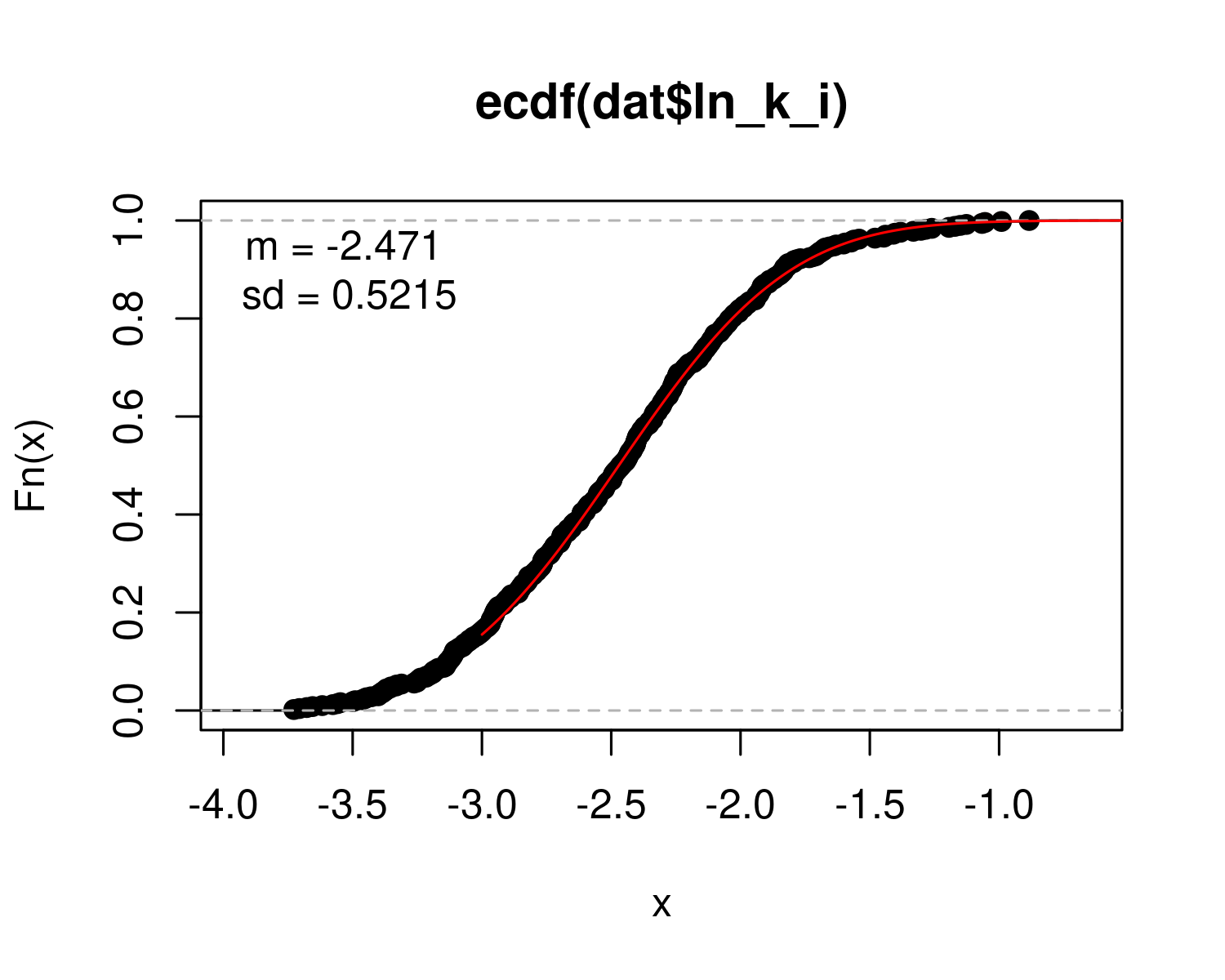


## Check normality

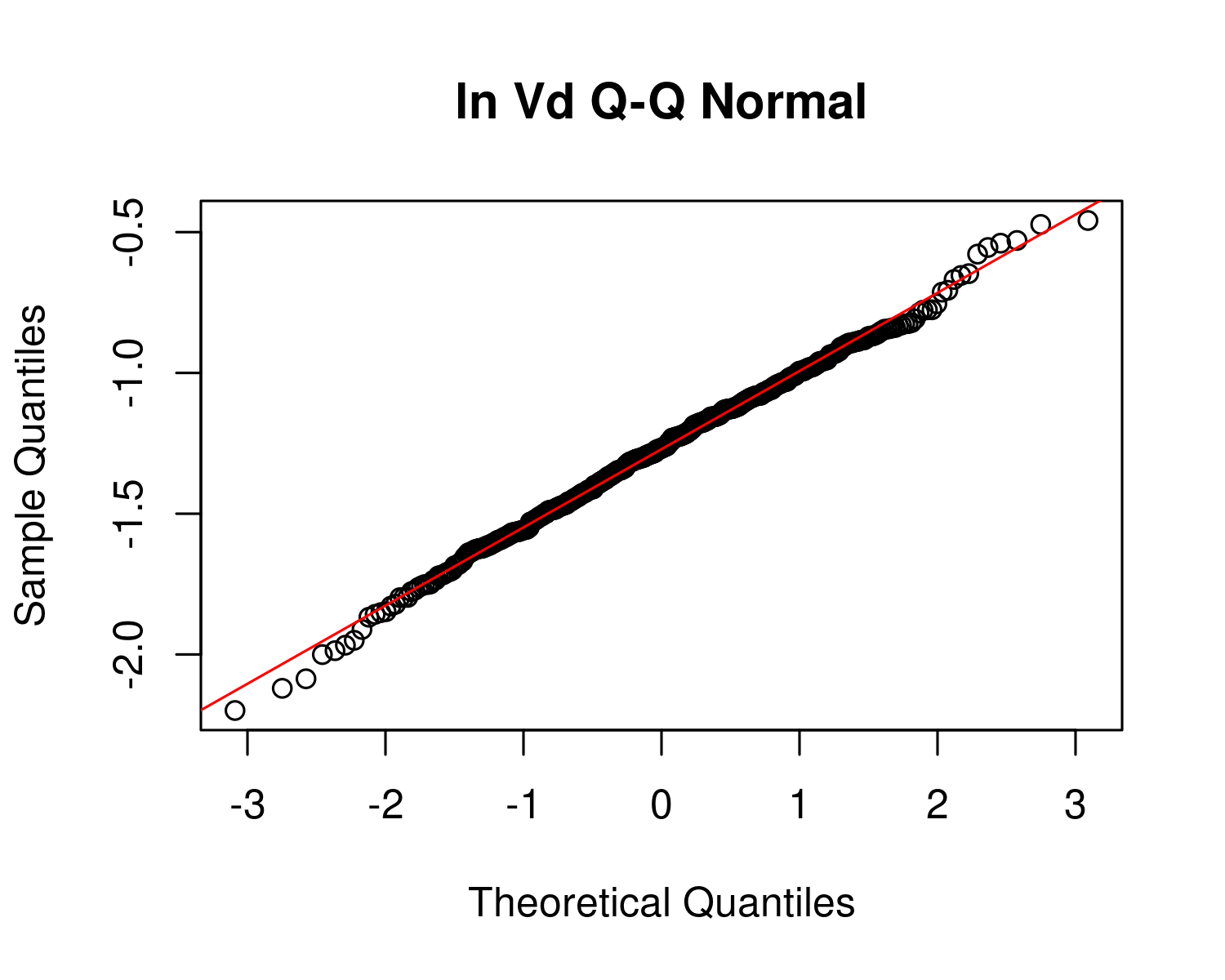
qqnorm(dat$ln\_k\_i,main="ln k Q-Q Normal")  
qqline(dat$ln\_k\_i,col="red")



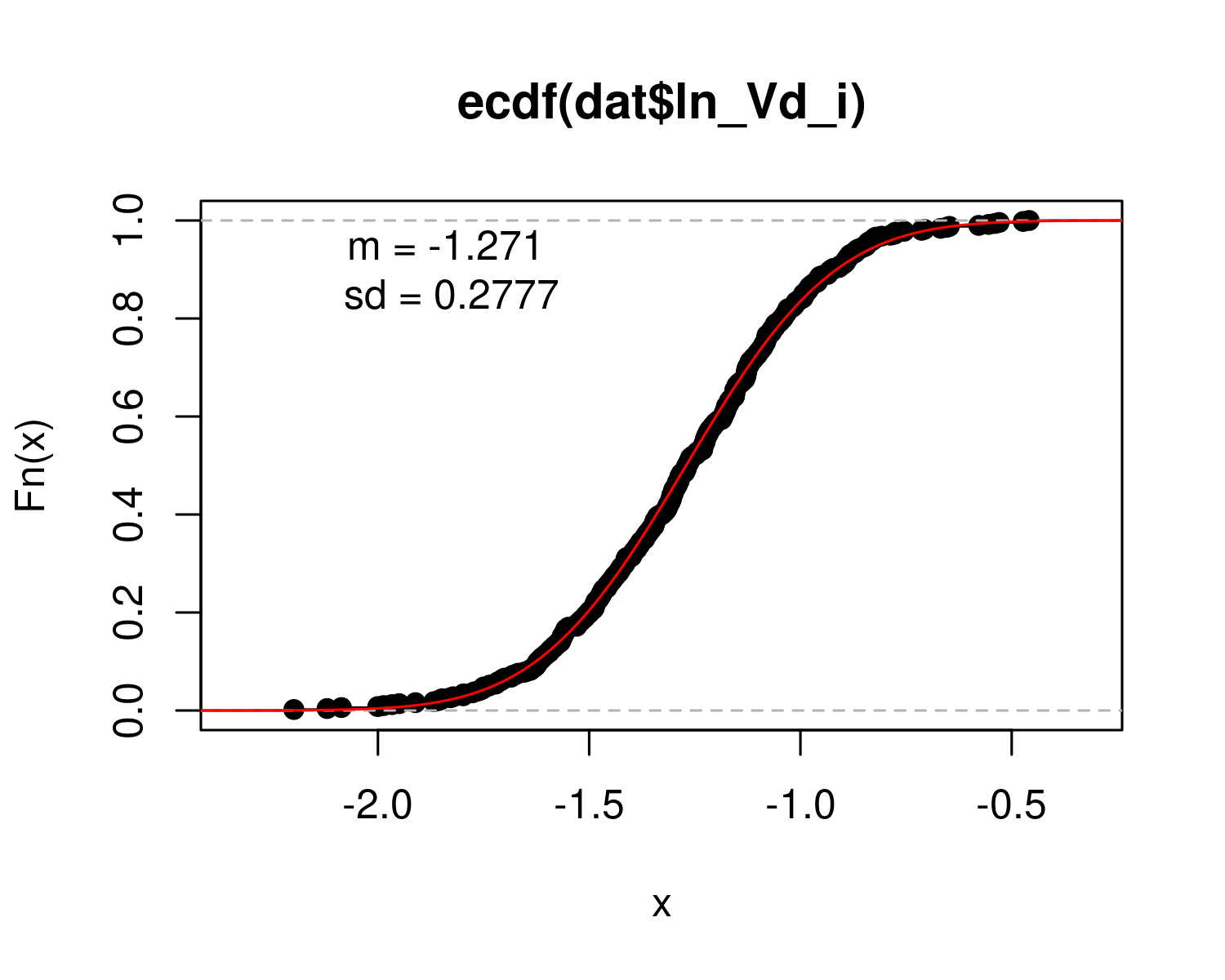
plot(ecdf(dat$ln\_k\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_k\_i <- mean(dat$ln\_k\_i)  
sd\_ln\_k\_i <- sd(dat$ln\_k\_i)  
lines(x,pnorm(x,mean=m\_ln\_k\_i,sd=sd\_ln\_k\_i),col="red")  
text(m\_ln\_k\_i-2\*sd\_ln\_k\_i,0.9,paste("m =",signif(m\_ln\_k\_i,4),"\nsd =",signif(sd\_ln\_k\_i,4)))



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)))



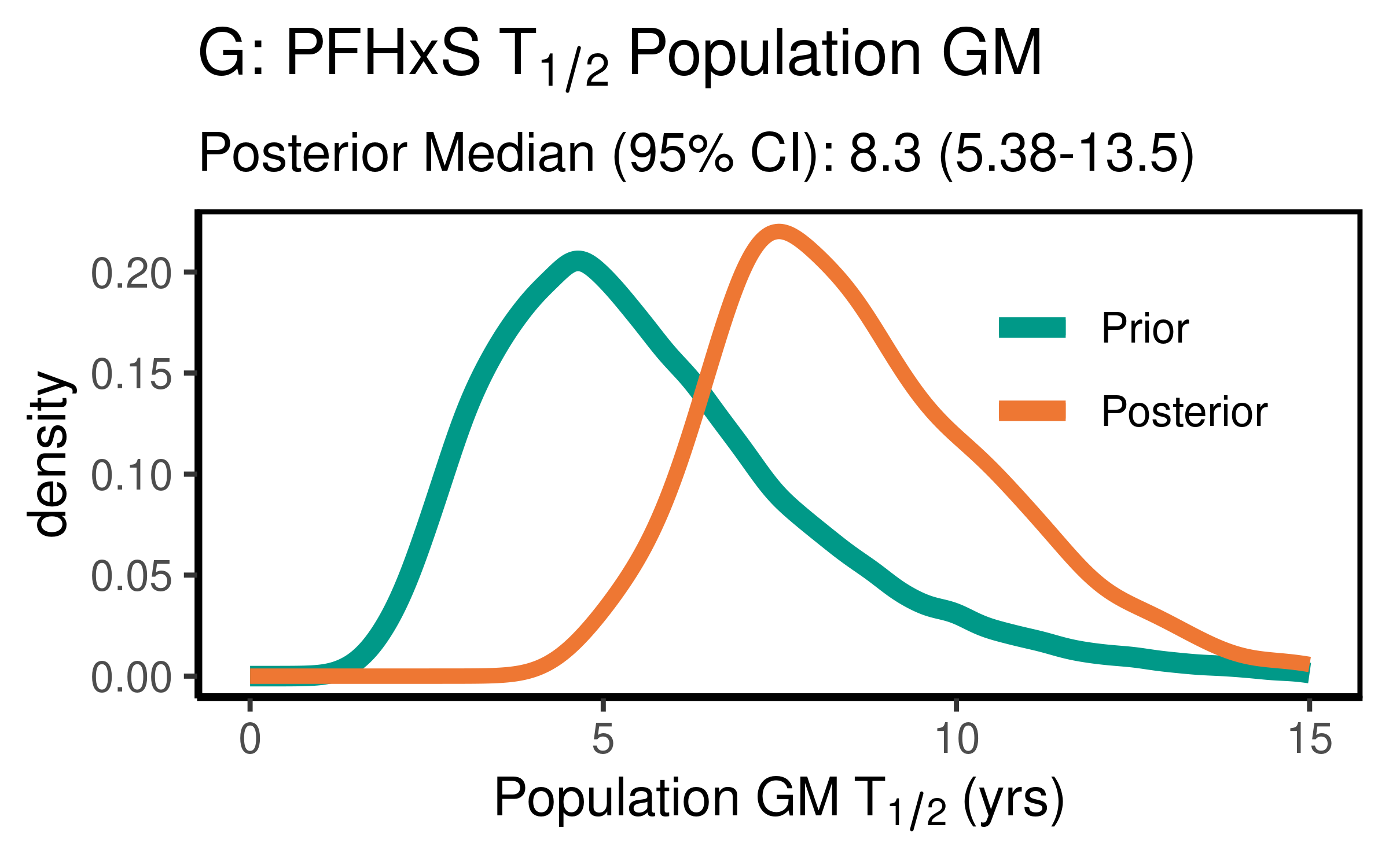
## Calculate table values for individual-level

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  
ci98\_med\_hl\_i <- paste(signif (quantile(hl\_i, prob=c(0.01,0.99)), 3),collapse="-") # 98ci 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  
ci98\_med\_Vd\_i <-paste(signif (quantile(exp(dat$ln\_Vd\_i), prob=c(0.01,0.99)), 3),collapse="-") # 98ci med individual Vd  
gm\_vd\_i <- paste(signif (exp(mean(dat$ln\_Vd\_i)), 3)) # gm (which should be really close)  
gsd\_vd\_i<- paste(signif (exp(sd(dat$ln\_Vd\_i)), 3)) # gsd indiv  
  
med\_CL\_i <- paste(signif (median(exp(dat$ln\_Vd\_i+dat$ln\_k\_i)), 3)) # median individual CL  
ci\_med\_CL\_i <-paste(signif (quantile(exp(dat$ln\_Vd\_i+dat$ln\_k\_i), prob=c(0.025,0.975)), 3),collapse="-") # 95ci med individual CL  
ci98\_med\_CL\_i <-paste(signif (quantile(exp(dat$ln\_Vd\_i+dat$ln\_k\_i), prob=c(0.01,0.99)), 3),collapse="-") # 98ci med individual CL  
gm\_CL\_i <- paste(signif (exp(mean(dat$ln\_Vd\_i+dat$ln\_k\_i)), 3)) # gm (which should be really close)  
gsd\_CL\_i<- paste(signif (exp(sd(dat$ln\_Vd\_i+dat$ln\_k\_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

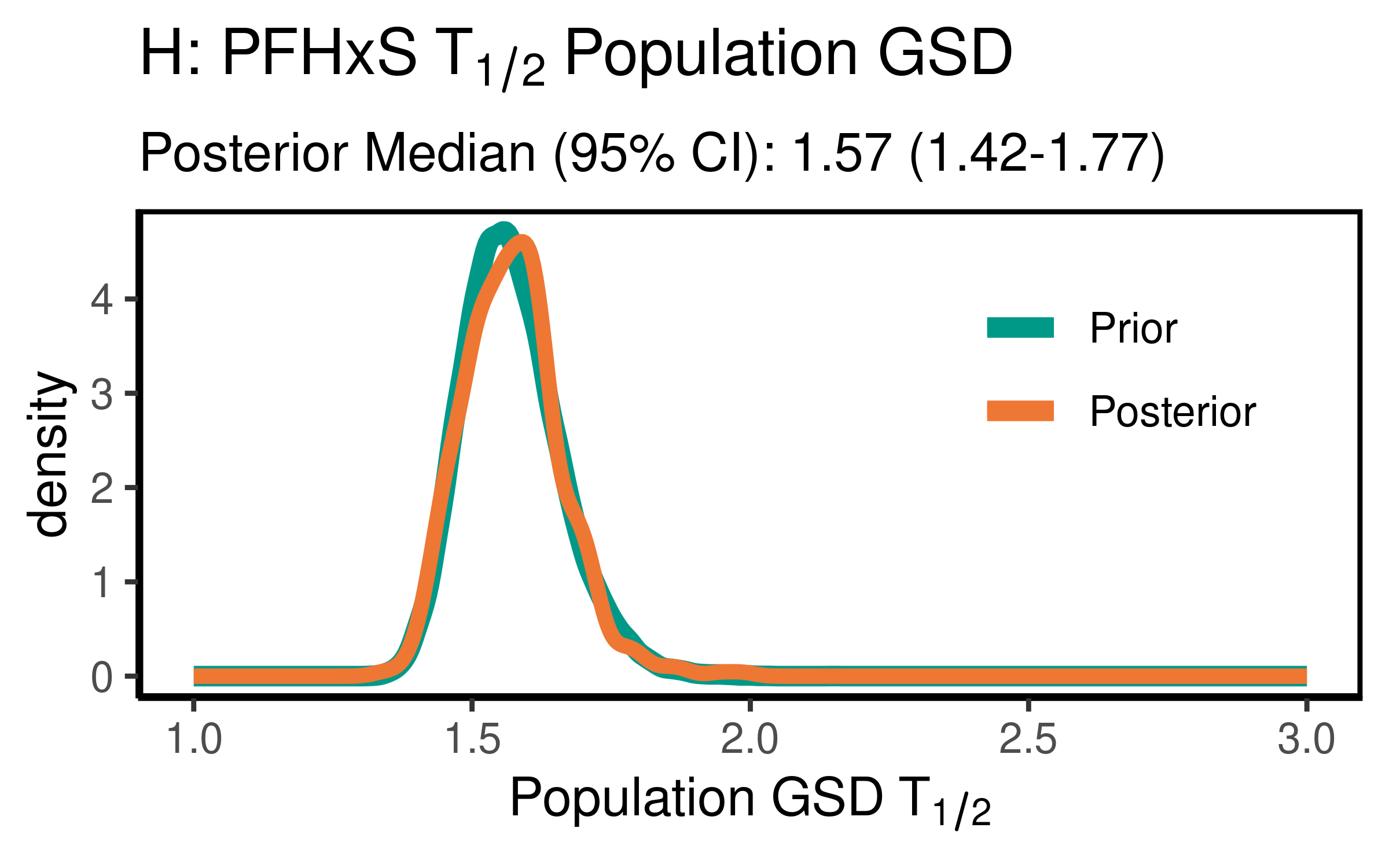
## Warning: Removed 250 rows containing non-finite values (stat\_density).  
  
## Warning: Removed 6 rows containing non-finite values (stat\_density).

ggsave(here ("output-plots",paste0( sa, "PFHxS\_hl\_gm.png")),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)

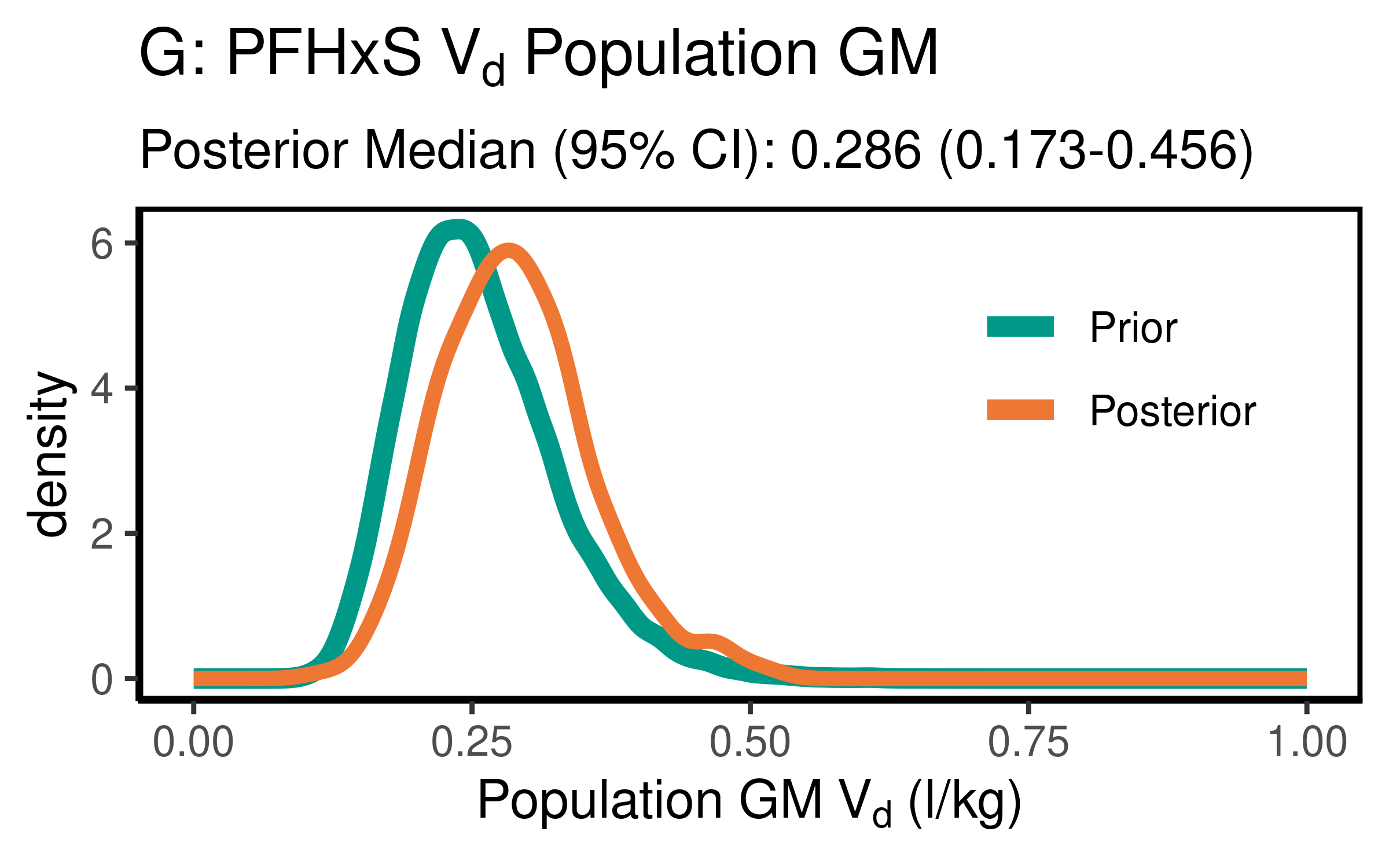


ggsave(here ("output-plots",paste0( sa, "PFHxS\_hl\_gsd.pdf")) ,p,dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFHxS\_hl\_gsd.png")) ,p,dpi=600)

### Volume of distribution

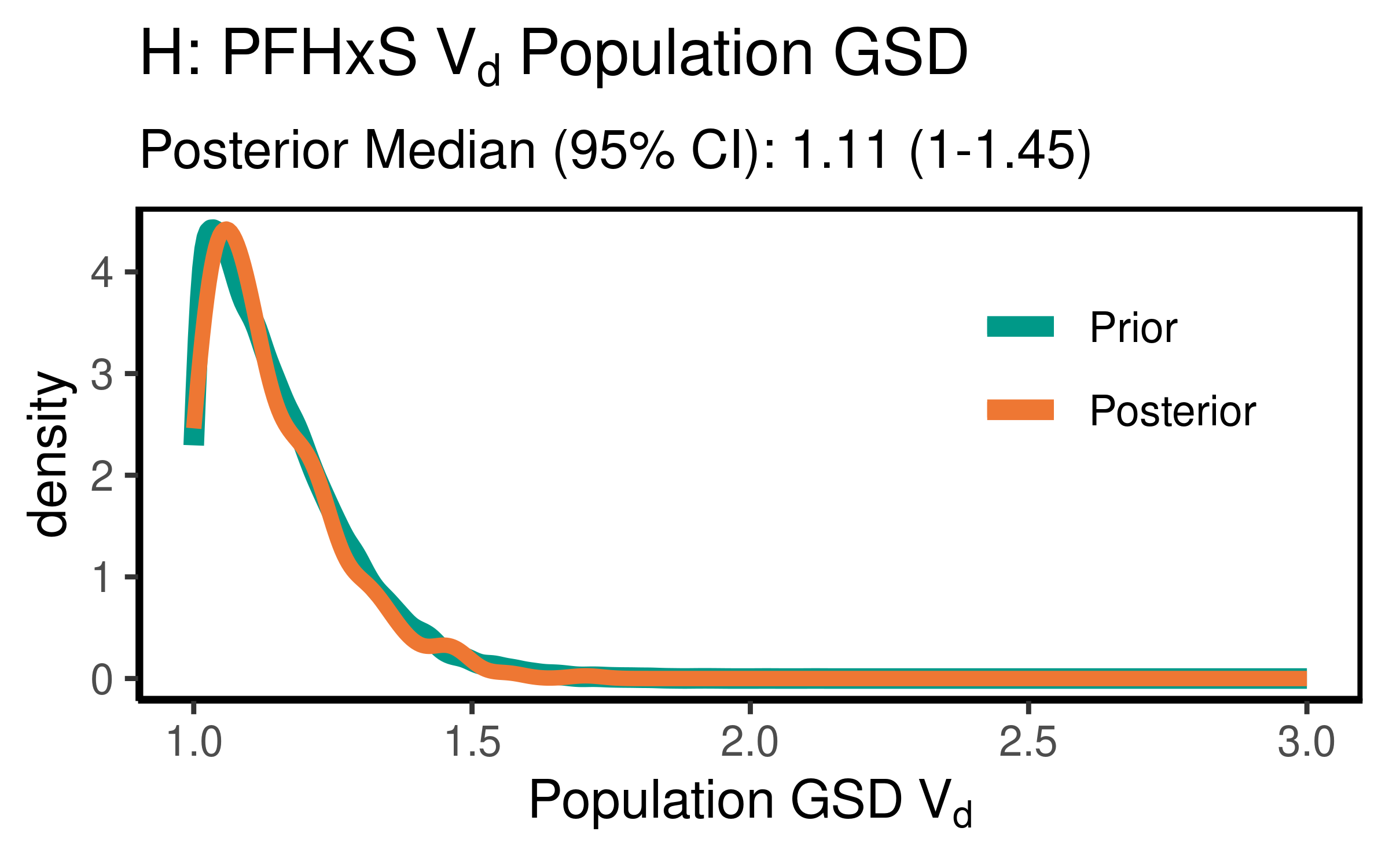
For PFHxS, the data were not particularly informative, but slightly increased the estimate of the median to 0.308(0.223-0.548) slightly compared to the case where Cbgd was considered to be entirely from non-drinking water sources. They were not informative as to the population GSD, with the posterior 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)  
ggsave(here ("output-plots",paste0( sa, "PFHxS\_vd\_gm.png")) ,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)

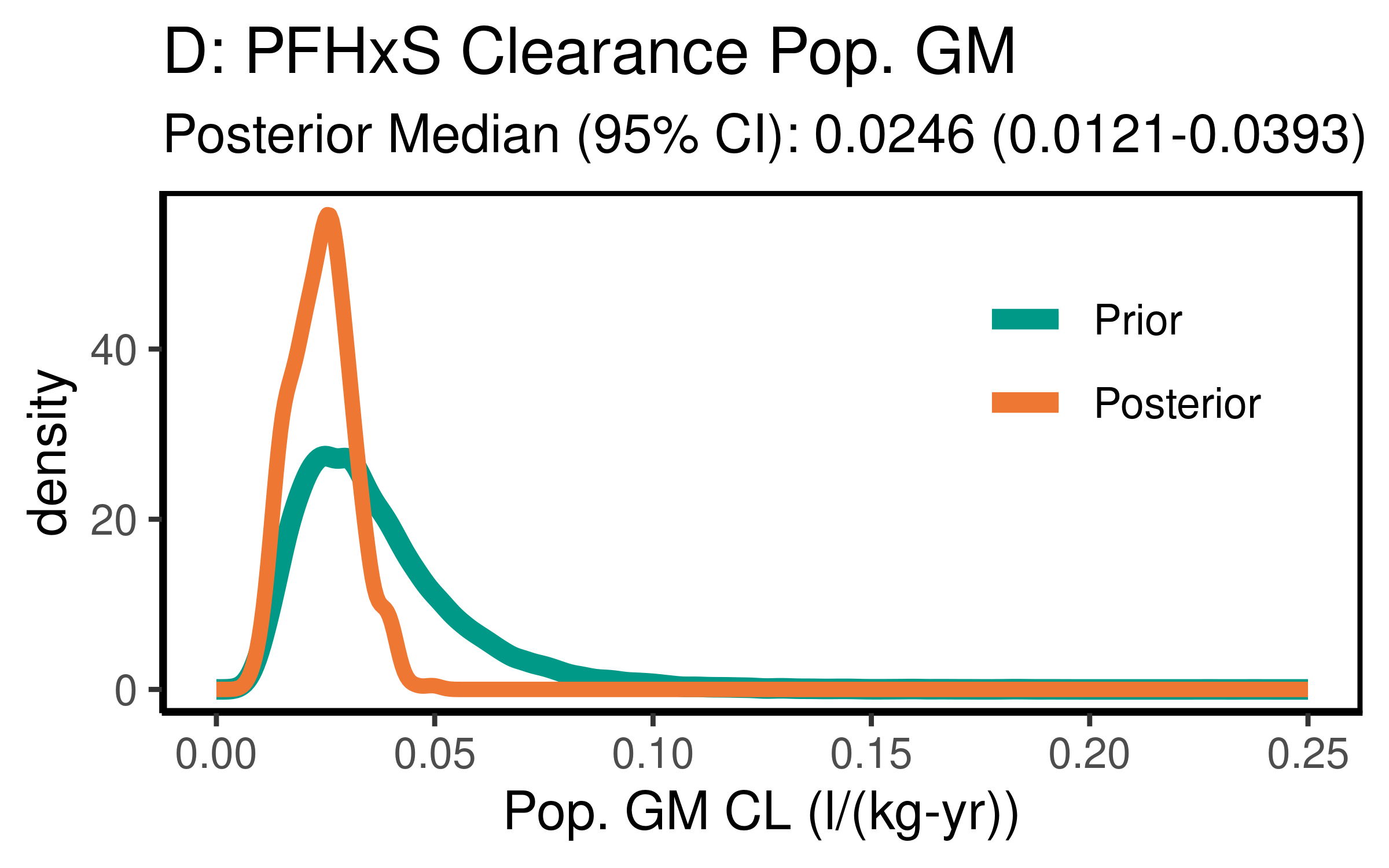


ggsave(here ("output-plots",paste0( sa,"PFHxS\_vd\_gsd.pdf")) ,p,dpi=600)  
ggsave(here ("output-plots",paste0( sa,"PFHxS\_vd\_gsd.png")) ,p,dpi=600)

### Clearance

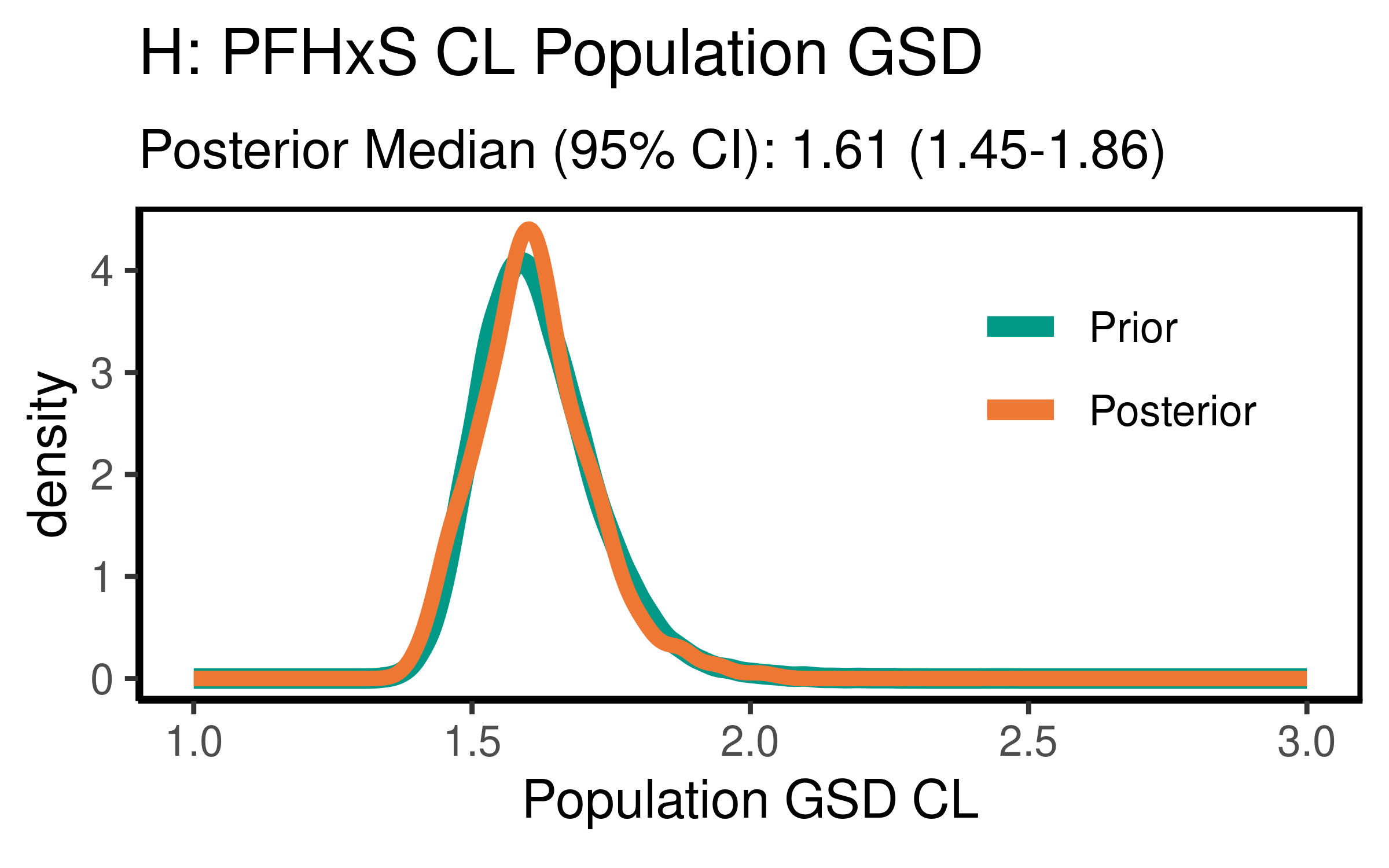
Cl is k \* Vd

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

PFHxS\_priors$CL\_GSD = exp(sqrt(log(PFHxS\_priors$Vd\_GSD)^2 +   
 log(PFHxS\_priors$halflife\_GSD)^2))  
PFHxS\_CL\_GSD <- exp(sqrt(log(PFHxS\_Vd\_GSD)^2 +   
 log(PFHxS\_halflife\_GSD)^2))  
  
PFHxS\_CL\_gsd\_pr\_med <- signif(median(PFHxS\_priors$CL\_GSD,3))  
PFHxS\_CL\_gsd\_pr\_med\_95ci <- paste(signif(quantile(PFHxS\_priors$CL\_GSD,  
 prob=c(0.025,0.975)), 3), collapse="-")  
  
PFHxS\_CL\_gsd\_med <- signif(median(PFHxS\_CL\_GSD),3)  
PFHxS\_CL\_gsd\_med\_95ci <- paste(signif(quantile(PFHxS\_CL\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(CL\_GSD, color = "Prior"),data=PFHxS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFHxS\_CL\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("H: PFHxS"~CL~"Population GSD "),  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFHxS\_CL\_gsd\_med," (",  
 PFHxS\_CL\_gsd\_med\_95ci,  
 ")",sep=""))+  
 xlab(bquote("Population GSD"~CL))+  
 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\_gsd.pdf")) ,p,dpi=600)  
ggsave(here ("output-plots",paste0( sa,"PFHxS\_CL\_gsd.png")) ,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] [[98% CI]] | GM calculator input | GSD individual |
| Half-life (years) | 8.12 [ 2.79-21.6 ] [[ 2.19-24.8 ]] | 8.2 | 1.68 |
| Volume of distribution | 0.281 [ 0.161-0.46 ] [[ 0.14-0.561 ]] | 0.281 | 1.32 |
| Clearance (L/kg-yr) | 0.0224 [ 0.00751-0.078 ] [[ 0.00648-0.101 ]] | 0.0237 | 1.79 |

### Session information

## ─ Session info ───────────────────────────────────────────────────────────────  
## setting value   
## version R version 4.0.5 (2021-03-31)   
## 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 2022-01-22   
##   
## ─ Packages ───────────────────────────────────────────────────────────────────  
## package \* version date lib source   
## assertthat 0.2.1 2019-03-21 [2] CRAN (R 4.0.5)  
## backports 1.4.0 2021-11-23 [1] CRAN (R 4.0.5)  
## bayesplot \* 1.8.0 2021-01-10 [2] CRAN (R 4.0.5)  
## broom 0.7.10 2021-10-31 [1] CRAN (R 4.0.5)  
## cachem 1.0.4 2021-02-13 [2] CRAN (R 4.0.5)  
## callr 3.7.0 2021-04-20 [1] CRAN (R 4.0.5)  
## cellranger 1.1.0 2016-07-27 [2] CRAN (R 4.0.5)  
## cli 3.1.0 2021-10-27 [1] CRAN (R 4.0.5)  
## coda \* 0.19-4 2020-09-30 [2] CRAN (R 4.0.5)  
## codetools 0.2-18 2020-11-04 [2] CRAN (R 4.0.5)  
## colorspace 2.0-2 2021-06-24 [1] CRAN (R 4.0.5)  
## crayon 1.4.2 2021-10-29 [1] CRAN (R 4.0.5)  
## DBI 1.1.1 2021-01-15 [2] CRAN (R 4.0.5)  
## dbplyr 2.1.1 2021-04-06 [1] CRAN (R 4.0.5)  
## desc 1.3.0 2021-03-05 [2] CRAN (R 4.0.5)  
## devtools 2.3.2 2020-09-18 [2] CRAN (R 4.0.5)  
## digest 0.6.29 2021-12-01 [1] CRAN (R 4.0.5)  
## dplyr \* 1.0.7 2021-06-18 [1] CRAN (R 4.0.5)  
## ellipsis 0.3.2 2021-04-29 [1] CRAN (R 4.0.5)  
## evaluate 0.14 2019-05-28 [2] CRAN (R 4.0.5)  
## fansi 0.5.0 2021-05-25 [1] CRAN (R 4.0.5)  
## farver 2.1.0 2021-02-28 [2] CRAN (R 4.0.5)  
## fastmap 1.1.0 2021-01-25 [2] CRAN (R 4.0.5)  
## forcats \* 0.5.1 2021-01-27 [2] CRAN (R 4.0.5)  
## fs 1.5.1 2021-11-30 [1] CRAN (R 4.0.5)  
## generics 0.1.1 2021-10-25 [1] CRAN (R 4.0.5)  
## ggplot2 \* 3.3.5 2021-06-25 [1] CRAN (R 4.0.5)  
## ggridges 0.5.3 2021-01-08 [2] CRAN (R 4.0.5)  
## ggsci \* 2.9 2018-05-14 [2] CRAN (R 4.0.5)  
## glue 1.5.1 2021-11-30 [1] CRAN (R 4.0.5)  
## gtable 0.3.0 2019-03-25 [2] CRAN (R 4.0.5)  
## haven 2.4.3 2021-08-04 [1] CRAN (R 4.0.5)  
## here \* 1.0.1 2020-12-13 [2] CRAN (R 4.0.5)  
## highr 0.9 2021-04-16 [1] CRAN (R 4.0.5)  
## hms 1.1.1 2021-09-26 [1] CRAN (R 4.0.5)  
## htmltools 0.5.2 2021-08-25 [1] CRAN (R 4.0.5)  
## httr 1.4.2 2020-07-20 [2] CRAN (R 4.0.5)  
## jsonlite 1.7.2 2020-12-09 [2] CRAN (R 4.0.5)  
## khroma \* 1.5.0 2021-04-23 [1] CRAN (R 4.0.5)  
## knitr 1.36 2021-09-29 [1] CRAN (R 4.0.5)  
## labeling 0.4.2 2020-10-20 [2] CRAN (R 4.0.5)  
## lattice 0.20-41 2020-04-02 [2] CRAN (R 4.0.5)  
## lifecycle 1.0.1 2021-09-24 [1] CRAN (R 4.0.5)  
## lubridate 1.8.0 2021-10-07 [1] CRAN (R 4.0.5)  
## magrittr 2.0.1 2020-11-17 [2] CRAN (R 4.0.5)  
## memoise 2.0.0 2021-01-26 [2] CRAN (R 4.0.5)  
## modelr 0.1.8 2020-05-19 [2] CRAN (R 4.0.5)  
## munsell 0.5.0 2018-06-12 [2] CRAN (R 4.0.5)  
## pillar 1.6.4 2021-10-18 [1] CRAN (R 4.0.5)  
## pkgbuild 1.2.0 2020-12-15 [2] CRAN (R 4.0.5)  
## pkgconfig 2.0.3 2019-09-22 [2] CRAN (R 4.0.5)  
## pkgload 1.2.0 2021-02-23 [2] CRAN (R 4.0.5)  
## plyr 1.8.6 2020-03-03 [2] CRAN (R 4.0.5)  
## prettyunits 1.1.1 2020-01-24 [2] CRAN (R 4.0.5)  
## pROC 1.18.0 2021-09-03 [1] CRAN (R 4.0.5)  
## processx 3.5.2 2021-04-30 [1] CRAN (R 4.0.5)  
## ps 1.6.0 2021-02-28 [2] CRAN (R 4.0.5)  
## purrr \* 0.3.4 2020-04-17 [2] CRAN (R 4.0.5)  
## R6 2.5.1 2021-08-19 [1] CRAN (R 4.0.5)  
## ragg 1.1.2 2021-03-17 [2] CRAN (R 4.0.5)  
## Rcpp 1.0.7 2021-07-07 [1] CRAN (R 4.0.5)  
## readr \* 2.1.1 2021-11-30 [1] CRAN (R 4.0.5)  
## readxl 1.3.1 2019-03-13 [2] CRAN (R 4.0.5)  
## remotes 2.3.0 2021-04-01 [2] CRAN (R 4.0.5)  
## reprex 2.0.1 2021-08-05 [1] CRAN (R 4.0.5)  
## reshape2 \* 1.4.4 2020-04-09 [2] CRAN (R 4.0.5)  
## rlang 0.4.12 2021-10-18 [1] CRAN (R 4.0.5)  
## rmarkdown 2.11 2021-09-14 [1] CRAN (R 4.0.5)  
## rprojroot 2.0.2 2020-11-15 [2] CRAN (R 4.0.5)  
## rstudioapi 0.13 2020-11-12 [2] CRAN (R 4.0.5)  
## rvest 1.0.2 2021-10-16 [1] CRAN (R 4.0.5)  
## scales \* 1.1.1 2020-05-11 [2] CRAN (R 4.0.5)  
## sessioninfo 1.1.1 2018-11-05 [2] CRAN (R 4.0.5)  
## stringi 1.7.6 2021-11-29 [1] CRAN (R 4.0.5)  
## stringr \* 1.4.0 2019-02-10 [2] CRAN (R 4.0.5)  
## systemfonts 1.0.3 2021-10-13 [1] CRAN (R 4.0.5)  
## testthat 3.0.2 2021-02-14 [2] CRAN (R 4.0.5)  
## textshaping 0.3.3 2021-03-16 [2] CRAN (R 4.0.5)  
## tibble \* 3.1.6 2021-11-07 [1] CRAN (R 4.0.5)  
## tidyr \* 1.1.4 2021-09-27 [1] CRAN (R 4.0.5)  
## tidyselect 1.1.1 2021-04-30 [1] CRAN (R 4.0.5)  
## tidyverse \* 1.3.1 2021-04-15 [1] CRAN (R 4.0.5)  
## tzdb 0.2.0 2021-10-27 [1] CRAN (R 4.0.5)  
## usethis 2.0.1 2021-02-10 [2] CRAN (R 4.0.5)  
## utf8 1.2.2 2021-07-24 [1] CRAN (R 4.0.5)  
## vctrs 0.3.8 2021-04-29 [1] CRAN (R 4.0.5)  
## withr 2.4.3 2021-11-30 [1] CRAN (R 4.0.5)  
## xfun 0.28 2021-11-04 [1] CRAN (R 4.0.5)  
## xml2 1.3.3 2021-11-30 [1] CRAN (R 4.0.5)  
## yaml 2.2.1 2020-02-01 [2] CRAN (R 4.0.5)  
## yardstick \* 0.0.9 2021-11-22 [1] CRAN (R 4.0.5)  
##   
## [1] /home/ad.abt.local/layc/R/x86\_64-pc-linux-gnu-library/4.0  
## [2] /opt/R/4.0.5/lib64/R/library