PFOS 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 1.3.0 ──

## ✓ tibble 3.1.0 ✓ dplyr 1.0.5  
## ✓ tidyr 1.1.3 ✓ stringr 1.4.0  
## ✓ readr 1.4.0 ✓ 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 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/PFOS\_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.

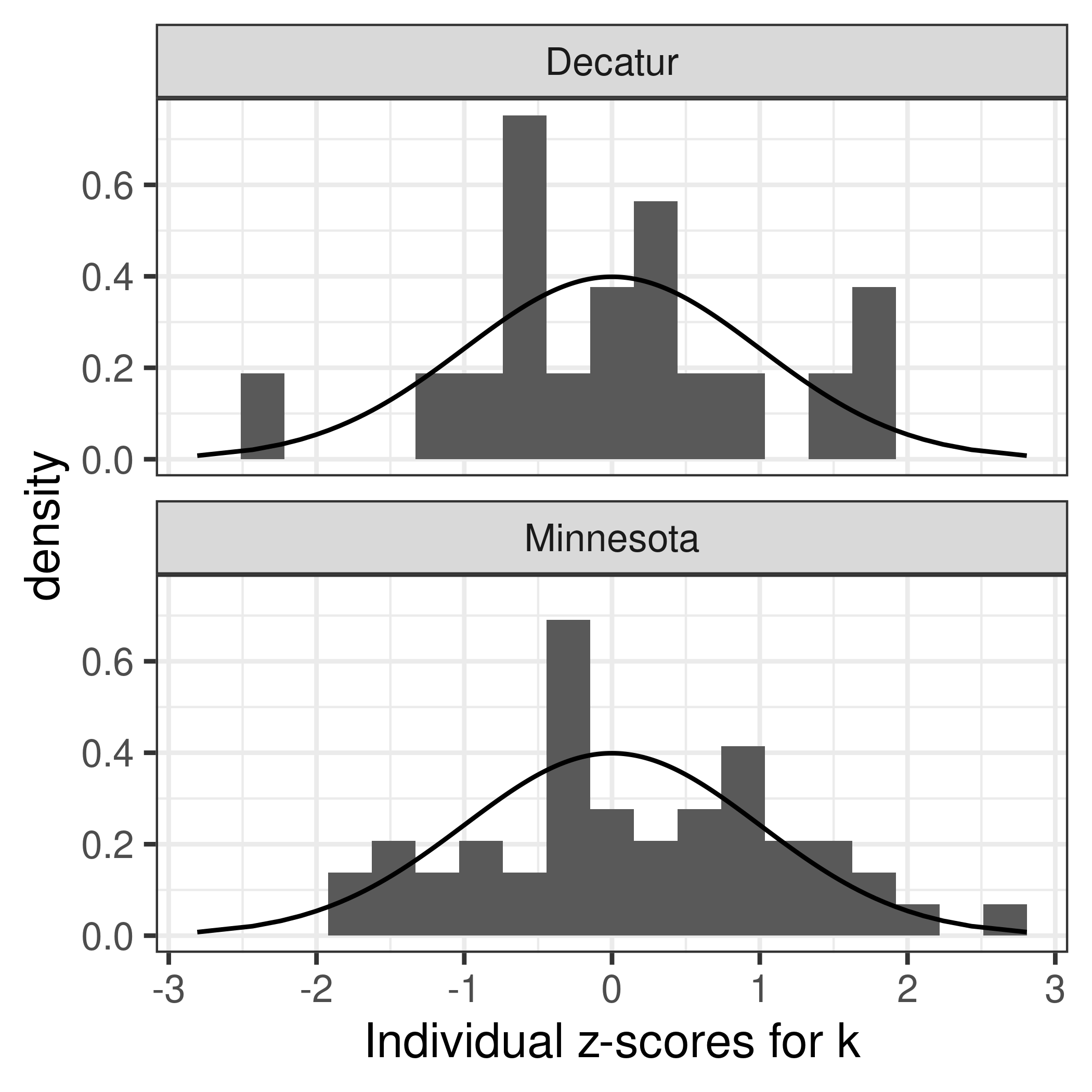
## Set filenames and load data

## Set up dataset

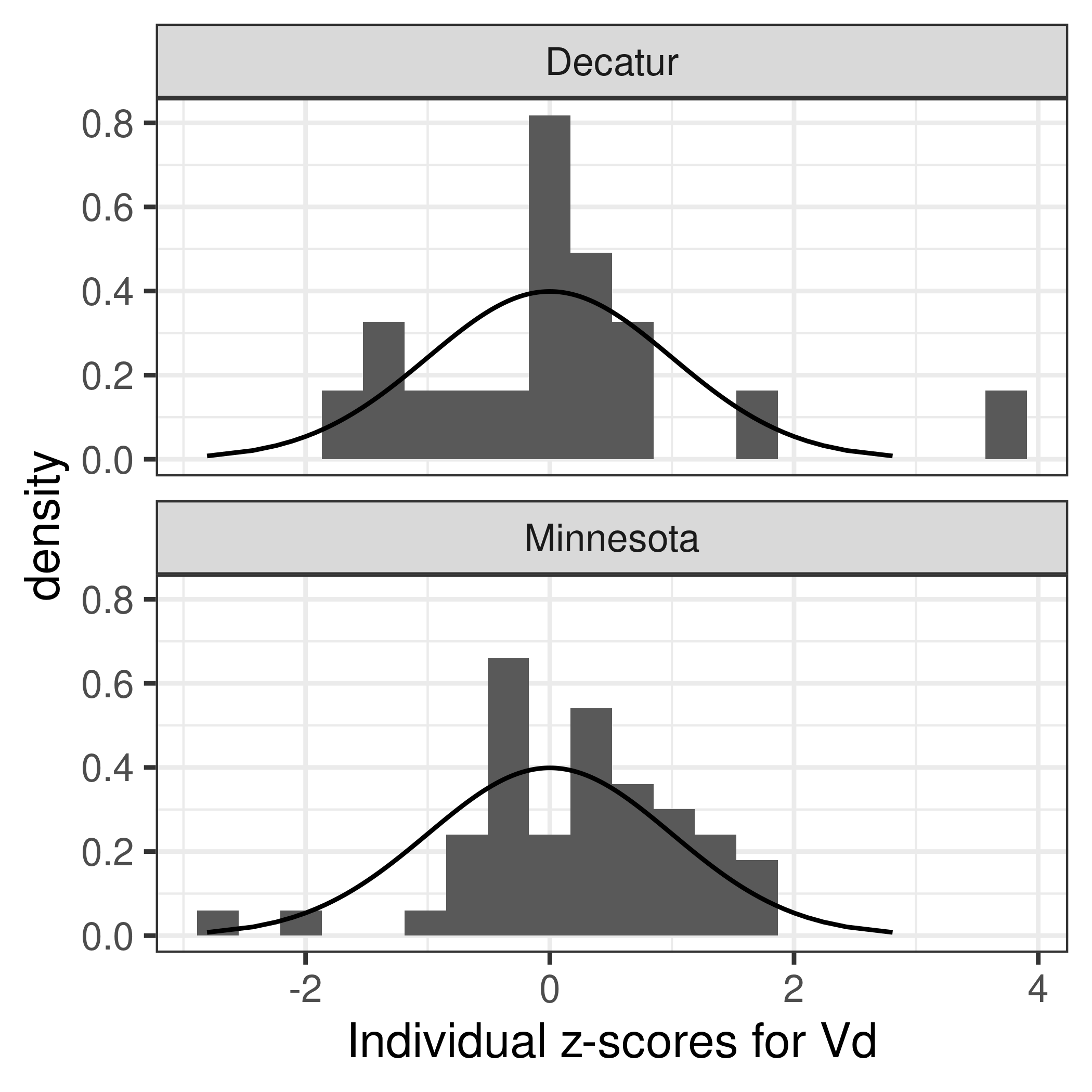
id\_lut <- multicheck$df\_check %>% select(Level) %>% unique () %>%  
 mutate(dataset = c(   
 rep("Decatur M Train", 9),  
 rep("Decatur F Train", 9),  
 rep("Decatur M Test", 9),  
 rep("Decatur F Test", 10),  
 rep("Minnesota Train", 49),  
 rep("Minnesota Test", 49),  
 'Paulsboro-Train','Horsham-Train',  
 'Warminster-Test','Warrington-Train'),   
 Sex = c(   
 rep("M", 9),  
 rep("F", 9),  
 rep("M", 9),  
 rep("F", 10),  
 rep("Mixed", 49),  
 rep("Mixed", 49),   
 rep("Mixed", 4)),  
 City = c(   
 rep("Decatur", 18),  
 rep("Decatur", 19),  
 rep("Minnesota", 98),  
 'Paulsboro','Horsham','Warminster','Warrington'),   
 Train\_Test = c(   
 rep("Train", 9),  
 rep("Train", 9),  
 rep("Test", 9),  
 rep("Test", 10),  
 rep("Train", 49),  
 rep("Test", 49),  
 'Train','Train',  
 'Test','Test'),  
 datatype = c(  
 rep("Individual",9+9+9+10+49+49),  
 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", "Minnesota")) %>%  
 mutate( dataset = as.factor(dataset))  
  
nv <- data.frame(dataset =unique(indiv\_lut$dataset),   
 variable= rep("Pop GM", 6),  
 type= rep("Pop GM", 6), 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=20)+facet\_wrap(~City,ncol=1)+  
 geom\_line(aes(x=x,y=y),data=normd)+  
 xlab("Individual z-scores for k") + theme\_bw()  
  
iplotVd<-  
 ggplot(subset(indiv\_parms,Train\_Test=="Train"))+  
 geom\_histogram(aes(x=ln\_Vd.z.samp,after\_stat(density)),bins=20)+facet\_wrap(~City,ncol=1)+  
 geom\_line(aes(x=x,y=y),data=normd)+  
 xlab("Individual z-scores for Vd") + theme\_bw()  
  
print(iplotk)



print(iplotVd)



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

## Saving 3.5 x 3.5 in image

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

## Saving 3.5 x 3.5 in image

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

## Saving 3.5 x 3.5 in image

ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_Vd\_PFOS.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] 88000

nrow(id\_lut)

## [1] 139

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

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

## [1] 88000

names(multicheck$df\_check)

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

multicheck2 <- multicheck$df\_check %>% left\_join(id\_lut)%>%   
 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("\n", City, "\n(", datatype, ")\n") ),  
 label = case\_when(Train\_Test=="Train" ~ "C: PFOS Train",  
 Train\_Test=="Test" ~"D: PFOS Test",  
 TRUE ~ ""))

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

## `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(1,3, 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

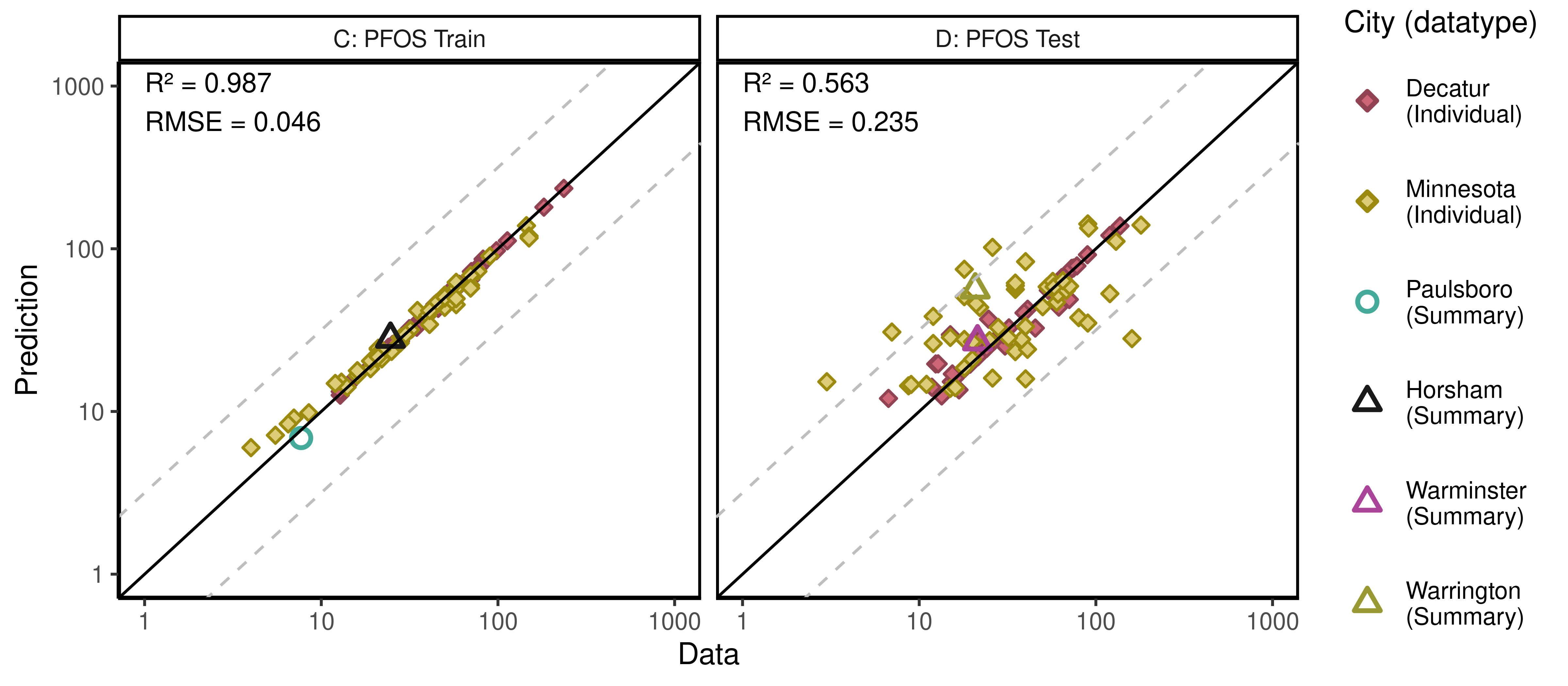
##   
## Attaching package: 'scales'

## 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("Female", "Male", "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 Cserum\_t 0.000000 82.400 1\_1\_1 1\_1\_1  
## 2 1\_1\_1 1 Cserum\_t 5.802000 70.300 1\_1\_1 1\_1\_1  
## 3 1\_1\_2 2 Cserum\_t 0.000000 32.600 1\_1\_2 1\_1\_2  
## 4 1\_1\_2 2 Cserum\_t 5.802000 14.200 1\_1\_2 1\_1\_2  
## 5 1\_1\_3 3 Cserum\_t 0.000000 236.000 1\_1\_3 1\_1\_3  
## 6 1\_1\_3 3 Cserum\_t 5.802000 75.400 1\_1\_3 1\_1\_3  
## 7 1\_1\_4 4 Cserum\_t 0.000000 61.000 1\_1\_4 1\_1\_4  
## 8 1\_1\_4 4 Cserum\_t 5.802000 12.800 1\_1\_4 1\_1\_4  
## 9 1\_1\_5 5 Cserum\_t 0.000000 182.000 1\_1\_5 1\_1\_5  
## 10 1\_1\_5 5 Cserum\_t 5.802000 43.900 1\_1\_5 1\_1\_5  
## 11 1\_1\_6 6 Cserum\_t 0.000000 25.300 1\_1\_6 1\_1\_6  
## 12 1\_1\_6 6 Cserum\_t 5.802000 18.800 1\_1\_6 1\_1\_6  
## 13 1\_1\_7 7 Cserum\_t 0.000000 113.000 1\_1\_7 1\_1\_7  
## 14 1\_1\_7 7 Cserum\_t 5.802000 24.000 1\_1\_7 1\_1\_7  
## 15 1\_1\_8 8 Cserum\_t 0.000000 78.200 1\_1\_8 1\_1\_8  
## 16 1\_1\_8 8 Cserum\_t 5.802000 26.400 1\_1\_8 1\_1\_8  
## 17 1\_1\_9 9 Cserum\_t 0.000000 54.400 1\_1\_9 1\_1\_9  
## 18 1\_1\_9 9 Cserum\_t 5.802000 26.500 1\_1\_9 1\_1\_9  
## 19 1\_1\_10 10 Cserum\_t 0.000000 81.200 1\_1\_10 1\_1\_10  
## 20 1\_1\_10 10 Cserum\_t 5.802000 31.500 1\_1\_10 1\_1\_10  
## 21 1\_1\_11 11 Cserum\_t 0.000000 70.700 1\_1\_11 1\_1\_11  
## 22 1\_1\_11 11 Cserum\_t 5.802000 50.200 1\_1\_11 1\_1\_11  
## 23 1\_1\_12 12 Cserum\_t 0.000000 13.700 1\_1\_12 1\_1\_12  
## 24 1\_1\_12 12 Cserum\_t 5.802000 12.800 1\_1\_12 1\_1\_12  
## 25 1\_1\_13 13 Cserum\_t 0.000000 42.000 1\_1\_13 1\_1\_13  
## 26 1\_1\_13 13 Cserum\_t 5.802000 28.100 1\_1\_13 1\_1\_13  
## 27 1\_1\_14 14 Cserum\_t 0.000000 98.000 1\_1\_14 1\_1\_14  
## 28 1\_1\_14 14 Cserum\_t 5.802000 35.100 1\_1\_14 1\_1\_14  
## 29 1\_1\_15 15 Cserum\_t 0.000000 56.900 1\_1\_15 1\_1\_15  
## 30 1\_1\_15 15 Cserum\_t 5.802000 45.900 1\_1\_15 1\_1\_15  
## 31 1\_1\_16 16 Cserum\_t 0.000000 32.500 1\_1\_16 1\_1\_16  
## 32 1\_1\_16 16 Cserum\_t 5.802000 13.300 1\_1\_16 1\_1\_16  
## 33 1\_1\_17 17 Cserum\_t 0.000000 60.500 1\_1\_17 1\_1\_17  
## 34 1\_1\_17 17 Cserum\_t 5.802000 27.600 1\_1\_17 1\_1\_17  
## 35 1\_1\_18 18 Cserum\_t 0.000000 43.800 1\_1\_18 1\_1\_18  
## 36 1\_1\_18 18 Cserum\_t 5.802000 34.700 1\_1\_18 1\_1\_18  
## 37 1\_2\_1 19 Cserum\_t 0.000000 64.100 1\_2\_1 1\_2\_1  
## 38 1\_2\_1 19 Cserum\_t 5.802000 15.000 1\_2\_1 1\_2\_1  
## 39 1\_2\_2 20 Cserum\_t 0.000000 89.600 1\_2\_2 1\_2\_2  
## 40 1\_2\_2 20 Cserum\_t 5.802000 24.700 1\_2\_2 1\_2\_2  
## 41 1\_2\_3 21 Cserum\_t 0.000000 74.700 1\_2\_3 1\_2\_3  
## 42 1\_2\_3 21 Cserum\_t 5.802000 39.800 1\_2\_3 1\_2\_3  
## 43 1\_2\_4 22 Cserum\_t 0.000000 68.400 1\_2\_4 1\_2\_4  
## 44 1\_2\_4 22 Cserum\_t 5.802000 30.000 1\_2\_4 1\_2\_4  
## 45 1\_2\_5 23 Cserum\_t 0.000000 72.900 1\_2\_5 1\_2\_5  
## 46 1\_2\_5 23 Cserum\_t 5.802000 32.200 1\_2\_5 1\_2\_5  
## 47 1\_2\_6 24 Cserum\_t 0.000000 78.100 1\_2\_6 1\_2\_6  
## 48 1\_2\_6 24 Cserum\_t 5.802000 45.400 1\_2\_6 1\_2\_6  
## 49 1\_2\_7 25 Cserum\_t 0.000000 24.100 1\_2\_7 1\_2\_7  
## 50 1\_2\_7 25 Cserum\_t 5.802000 15.400 1\_2\_7 1\_2\_7  
## 51 1\_2\_8 26 Cserum\_t 0.000000 60.900 1\_2\_8 1\_2\_8  
## 52 1\_2\_8 26 Cserum\_t 5.802000 22.000 1\_2\_8 1\_2\_8  
## 53 1\_2\_9 27 Cserum\_t 0.000000 137.000 1\_2\_9 1\_2\_9  
## 54 1\_2\_9 27 Cserum\_t 5.802000 70.700 1\_2\_9 1\_2\_9  
## 55 1\_2\_10 28 Cserum\_t 0.000000 26.600 1\_2\_10 1\_2\_10  
## 56 1\_2\_10 28 Cserum\_t 5.802000 15.200 1\_2\_10 1\_2\_10  
## 57 1\_2\_11 29 Cserum\_t 0.000000 120.000 1\_2\_11 1\_2\_11  
## 58 1\_2\_11 29 Cserum\_t 5.802000 61.700 1\_2\_11 1\_2\_11  
## 59 1\_2\_12 30 Cserum\_t 0.000000 60.900 1\_2\_12 1\_2\_12  
## 60 1\_2\_12 30 Cserum\_t 5.802000 22.500 1\_2\_12 1\_2\_12  
## 61 1\_2\_13 31 Cserum\_t 0.000000 41.100 1\_2\_13 1\_2\_13  
## 62 1\_2\_13 31 Cserum\_t 5.802000 12.400 1\_2\_13 1\_2\_13  
## 63 1\_2\_14 32 Cserum\_t 0.000000 39.200 1\_2\_14 1\_2\_14  
## 64 1\_2\_14 32 Cserum\_t 5.802000 12.800 1\_2\_14 1\_2\_14  
## 65 1\_2\_15 33 Cserum\_t 0.000000 18.100 1\_2\_15 1\_2\_15  
## 66 1\_2\_15 33 Cserum\_t 5.802000 13.400 1\_2\_15 1\_2\_15  
## 67 1\_2\_16 34 Cserum\_t 0.000000 19.400 1\_2\_16 1\_2\_16  
## 68 1\_2\_16 34 Cserum\_t 5.802000 16.800 1\_2\_16 1\_2\_16  
## 69 1\_2\_17 35 Cserum\_t 0.000000 21.500 1\_2\_17 1\_2\_17  
## 70 1\_2\_17 35 Cserum\_t 5.802000 11.800 1\_2\_17 1\_2\_17  
## 71 1\_2\_18 36 Cserum\_t 0.000000 53.800 1\_2\_18 1\_2\_18  
## 72 1\_2\_18 36 Cserum\_t 5.802000 30.600 1\_2\_18 1\_2\_18  
## 73 1\_2\_19 37 Cserum\_t 0.000000 16.000 1\_2\_19 1\_2\_19  
## 74 1\_2\_19 37 Cserum\_t 5.802000 6.700 1\_2\_19 1\_2\_19  
## 75 1\_3\_1 38 Cbgd\_Css 0.000001 13.000 1\_3\_1 1\_3\_1  
## 76 1\_3\_2 39 Cbgd\_Css 0.000001 50.000 1\_3\_2 1\_3\_2  
## 77 1\_3\_3 40 Cbgd\_Css 0.000001 45.000 1\_3\_3 1\_3\_3  
## 78 1\_3\_4 41 Cbgd\_Css 0.000001 55.000 1\_3\_4 1\_3\_4  
## 79 1\_3\_5 42 Cbgd\_Css 0.000001 58.000 1\_3\_5 1\_3\_5  
## 80 1\_3\_6 43 Cbgd\_Css 0.000001 50.000 1\_3\_6 1\_3\_6  
## 81 1\_3\_7 44 Cbgd\_Css 0.000001 150.000 1\_3\_7 1\_3\_7  
## 82 1\_3\_8 45 Cbgd\_Css 0.000001 12.000 1\_3\_8 1\_3\_8  
## 83 1\_3\_9 46 Cbgd\_Css 0.000001 58.000 1\_3\_9 1\_3\_9  
## 84 1\_3\_10 47 Cbgd\_Css 0.000001 21.000 1\_3\_10 1\_3\_10  
## 85 1\_3\_11 48 Cbgd\_Css 0.000001 19.000 1\_3\_11 1\_3\_11  
## 86 1\_3\_12 49 Cbgd\_Css 0.000001 25.000 1\_3\_12 1\_3\_12  
## 87 1\_3\_13 50 Cbgd\_Css 0.000001 4.000 1\_3\_13 1\_3\_13  
## 88 1\_3\_14 51 Cbgd\_Css 0.000001 32.000 1\_3\_14 1\_3\_14  
## 89 1\_3\_15 52 Cbgd\_Css 0.000001 58.000 1\_3\_15 1\_3\_15  
## 90 1\_3\_16 53 Cbgd\_Css 0.000001 8.500 1\_3\_16 1\_3\_16  
## 91 1\_3\_17 54 Cbgd\_Css 0.000001 5.500 1\_3\_17 1\_3\_17  
## 92 1\_3\_18 55 Cbgd\_Css 0.000001 58.000 1\_3\_18 1\_3\_18  
## 93 1\_3\_19 56 Cbgd\_Css 0.000001 50.000 1\_3\_19 1\_3\_19  
## 94 1\_3\_20 57 Cbgd\_Css 0.000001 145.000 1\_3\_20 1\_3\_20  
## 95 1\_3\_21 58 Cbgd\_Css 0.000001 77.000 1\_3\_21 1\_3\_21  
## 96 1\_3\_22 59 Cbgd\_Css 0.000001 50.000 1\_3\_22 1\_3\_22  
## 97 1\_3\_23 60 Cbgd\_Css 0.000001 90.000 1\_3\_23 1\_3\_23  
## 98 1\_3\_24 61 Cbgd\_Css 0.000001 14.000 1\_3\_24 1\_3\_24  
## 99 1\_3\_25 62 Cbgd\_Css 0.000001 21.000 1\_3\_25 1\_3\_25  
## 100 1\_3\_26 63 Cbgd\_Css 0.000001 35.000 1\_3\_26 1\_3\_26  
## 101 1\_3\_27 64 Cbgd\_Css 0.000001 28.000 1\_3\_27 1\_3\_27  
## 102 1\_3\_28 65 Cbgd\_Css 0.000001 7.000 1\_3\_28 1\_3\_28  
## 103 1\_3\_29 66 Cbgd\_Css 0.000001 150.000 1\_3\_29 1\_3\_29  
## 104 1\_3\_30 67 Cbgd\_Css 0.000001 50.000 1\_3\_30 1\_3\_30  
## 105 1\_3\_31 68 Cbgd\_Css 0.000001 50.000 1\_3\_31 1\_3\_31  
## 106 1\_3\_32 69 Cbgd\_Css 0.000001 70.000 1\_3\_32 1\_3\_32  
## 107 1\_3\_33 70 Cbgd\_Css 0.000001 21.000 1\_3\_33 1\_3\_33  
## 108 1\_3\_34 71 Cbgd\_Css 0.000001 19.000 1\_3\_34 1\_3\_34  
## 109 1\_3\_35 72 Cbgd\_Css 0.000001 40.000 1\_3\_35 1\_3\_35  
## 110 1\_3\_36 73 Cbgd\_Css 0.000001 70.000 1\_3\_36 1\_3\_36  
## 111 1\_3\_37 74 Cbgd\_Css 0.000001 45.000 1\_3\_37 1\_3\_37  
## 112 1\_3\_38 75 Cbgd\_Css 0.000001 22.000 1\_3\_38 1\_3\_38  
## 113 1\_3\_39 76 Cbgd\_Css 0.000001 29.000 1\_3\_39 1\_3\_39  
## 114 1\_3\_40 77 Cbgd\_Css 0.000001 28.000 1\_3\_40 1\_3\_40  
## 115 1\_3\_41 78 Cbgd\_Css 0.000001 6.500 1\_3\_41 1\_3\_41  
## 116 1\_3\_42 79 Cbgd\_Css 0.000001 22.000 1\_3\_42 1\_3\_42  
## 117 1\_3\_43 80 Cbgd\_Css 0.000001 21.000 1\_3\_43 1\_3\_43  
## 118 1\_3\_44 81 Cbgd\_Css 0.000001 41.000 1\_3\_44 1\_3\_44  
## 119 1\_3\_45 82 Cbgd\_Css 0.000001 41.000 1\_3\_45 1\_3\_45  
## 120 1\_3\_46 83 Cbgd\_Css 0.000001 16.000 1\_3\_46 1\_3\_46  
## 121 1\_3\_47 84 Cbgd\_Css 0.000001 70.000 1\_3\_47 1\_3\_47  
## 122 1\_3\_48 85 Cbgd\_Css 0.000001 16.000 1\_3\_48 1\_3\_48  
## 123 1\_3\_49 86 Cbgd\_Css 0.000001 30.000 1\_3\_49 1\_3\_49  
## 124 1\_4\_1 87 Cbgd\_Css 0.000001 3.000 1\_4\_1 1\_4\_1  
## 125 1\_4\_2 88 Cbgd\_Css 0.000001 8.700 1\_4\_2 1\_4\_2  
## 126 1\_4\_3 89 Cbgd\_Css 0.000001 9.000 1\_4\_3 1\_4\_3  
## 127 1\_4\_4 90 Cbgd\_Css 0.000001 11.000 1\_4\_4 1\_4\_4  
## 128 1\_4\_5 91 Cbgd\_Css 0.000001 15.000 1\_4\_5 1\_4\_5  
## 129 1\_4\_6 92 Cbgd\_Css 0.000001 16.000 1\_4\_6 1\_4\_6  
## 130 1\_4\_7 93 Cbgd\_Css 0.000001 40.000 1\_4\_7 1\_4\_7  
## 131 1\_4\_8 94 Cbgd\_Css 0.000001 26.000 1\_4\_8 1\_4\_8  
## 132 1\_4\_9 95 Cbgd\_Css 0.000001 18.000 1\_4\_9 1\_4\_9  
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## 134 1\_4\_11 97 Cbgd\_Css 0.000001 35.000 1\_4\_11 1\_4\_11  
## 135 1\_4\_12 98 Cbgd\_Css 0.000001 41.000 1\_4\_12 1\_4\_12  
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## 141 1\_4\_18 104 Cbgd\_Css 0.000001 38.000 1\_4\_18 1\_4\_18  
## 142 1\_4\_19 105 Cbgd\_Css 0.000001 160.000 1\_4\_19 1\_4\_19  
## 143 1\_4\_20 106 Cbgd\_Css 0.000001 32.000 1\_4\_20 1\_4\_20  
## 144 1\_4\_21 107 Cbgd\_Css 0.000001 7.000 1\_4\_21 1\_4\_21  
## 145 1\_4\_22 108 Cbgd\_Css 0.000001 28.000 1\_4\_22 1\_4\_22  
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## 174 1\_6\_1 137 M\_Cbgd\_Css 2.000000 24.639 1\_6\_1 1\_6\_1  
## 175 1\_7\_1 138 M\_Cbgd\_Css 2.000000 21.378 1\_7\_1 1\_7\_1  
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## 67 Decatur F Test 34.T=0  
## 68 Decatur F Test 34.T=5.802  
## 69 Decatur F Test 35.T=0  
## 70 Decatur F Test 35.T=5.802  
## 71 Decatur F Test 36.T=0  
## 72 Decatur F Test 36.T=5.802  
## 73 Decatur F Test 37.T=0  
## 74 Decatur F Test 37.T=5.802  
## 75 Minnesota Train 38.SteadyState  
## 76 Minnesota Train 39.SteadyState  
## 77 Minnesota Train 40.SteadyState  
## 78 Minnesota Train 41.SteadyState  
## 79 Minnesota Train 42.SteadyState  
## 80 Minnesota Train 43.SteadyState  
## 81 Minnesota Train 44.SteadyState  
## 82 Minnesota Train 45.SteadyState  
## 83 Minnesota Train 46.SteadyState  
## 84 Minnesota Train 47.SteadyState  
## 85 Minnesota Train 48.SteadyState  
## 86 Minnesota Train 49.SteadyState  
## 87 Minnesota Train 50.SteadyState  
## 88 Minnesota Train 51.SteadyState  
## 89 Minnesota Train 52.SteadyState  
## 90 Minnesota Train 53.SteadyState  
## 91 Minnesota Train 54.SteadyState  
## 92 Minnesota Train 55.SteadyState  
## 93 Minnesota Train 56.SteadyState  
## 94 Minnesota Train 57.SteadyState  
## 95 Minnesota Train 58.SteadyState  
## 96 Minnesota Train 59.SteadyState  
## 97 Minnesota Train 60.SteadyState  
## 98 Minnesota Train 61.SteadyState  
## 99 Minnesota Train 62.SteadyState  
## 100 Minnesota Train 63.SteadyState  
## 101 Minnesota Train 64.SteadyState  
## 102 Minnesota Train 65.SteadyState  
## 103 Minnesota Train 66.SteadyState  
## 104 Minnesota Train 67.SteadyState  
## 105 Minnesota Train 68.SteadyState  
## 106 Minnesota Train 69.SteadyState  
## 107 Minnesota Train 70.SteadyState  
## 108 Minnesota Train 71.SteadyState  
## 109 Minnesota Train 72.SteadyState  
## 110 Minnesota Train 73.SteadyState  
## 111 Minnesota Train 74.SteadyState  
## 112 Minnesota Train 75.SteadyState  
## 113 Minnesota Train 76.SteadyState  
## 114 Minnesota Train 77.SteadyState  
## 115 Minnesota Train 78.SteadyState  
## 116 Minnesota Train 79.SteadyState  
## 117 Minnesota Train 80.SteadyState  
## 118 Minnesota Train 81.SteadyState  
## 119 Minnesota Train 82.SteadyState  
## 120 Minnesota Train 83.SteadyState  
## 121 Minnesota Train 84.SteadyState  
## 122 Minnesota Train 85.SteadyState  
## 123 Minnesota Train 86.SteadyState  
## 124 Minnesota Test 87.SteadyState  
## 125 Minnesota Test 88.SteadyState  
## 126 Minnesota Test 89.SteadyState  
## 127 Minnesota Test 90.SteadyState  
## 128 Minnesota Test 91.SteadyState  
## 129 Minnesota Test 92.SteadyState  
## 130 Minnesota Test 93.SteadyState  
## 131 Minnesota Test 94.SteadyState  
## 132 Minnesota Test 95.SteadyState  
## 133 Minnesota Test 96.SteadyState  
## 134 Minnesota Test 97.SteadyState  
## 135 Minnesota Test 98.SteadyState  
## 136 Minnesota Test 99.SteadyState  
## 137 Minnesota Test 100.SteadyState  
## 138 Minnesota Test 101.SteadyState  
## 139 Minnesota Test 102.SteadyState  
## 140 Minnesota Test 103.SteadyState  
## 141 Minnesota Test 104.SteadyState  
## 142 Minnesota Test 105.SteadyState  
## 143 Minnesota Test 106.SteadyState  
## 144 Minnesota Test 107.SteadyState  
## 145 Minnesota Test 108.SteadyState  
## 146 Minnesota Test 109.SteadyState  
## 147 Minnesota Test 110.SteadyState  
## 148 Minnesota Test 111.SteadyState  
## 149 Minnesota Test 112.SteadyState  
## 150 Minnesota Test 113.SteadyState  
## 151 Minnesota Test 114.SteadyState  
## 152 Minnesota Test 115.SteadyState  
## 153 Minnesota Test 116.SteadyState  
## 154 Minnesota Test 117.SteadyState  
## 155 Minnesota Test 118.SteadyState  
## 156 Minnesota Test 119.SteadyState  
## 157 Minnesota Test 120.SteadyState  
## 158 Minnesota Test 121.SteadyState  
## 159 Minnesota Test 122.SteadyState  
## 160 Minnesota Test 123.SteadyState  
## 161 Minnesota Test 124.SteadyState  
## 162 Minnesota Test 125.SteadyState  
## 163 Minnesota Test 126.SteadyState  
## 164 Minnesota Test 127.SteadyState  
## 165 Minnesota Test 128.SteadyState  
## 166 Minnesota Test 129.SteadyState  
## 167 Minnesota Test 130.SteadyState  
## 168 Minnesota Test 131.SteadyState  
## 169 Minnesota Test 132.SteadyState  
## 170 Minnesota Test 133.SteadyState  
## 171 Minnesota Test 134.SteadyState  
## 172 Minnesota Test 135.SteadyState  
## 173 Paulsboro-Train 136.T=2.2  
## 174 Horsham-Train 137.T=2  
## 175 Warminster-Test 138.T=2  
## 176 Warrington-Train 139.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"

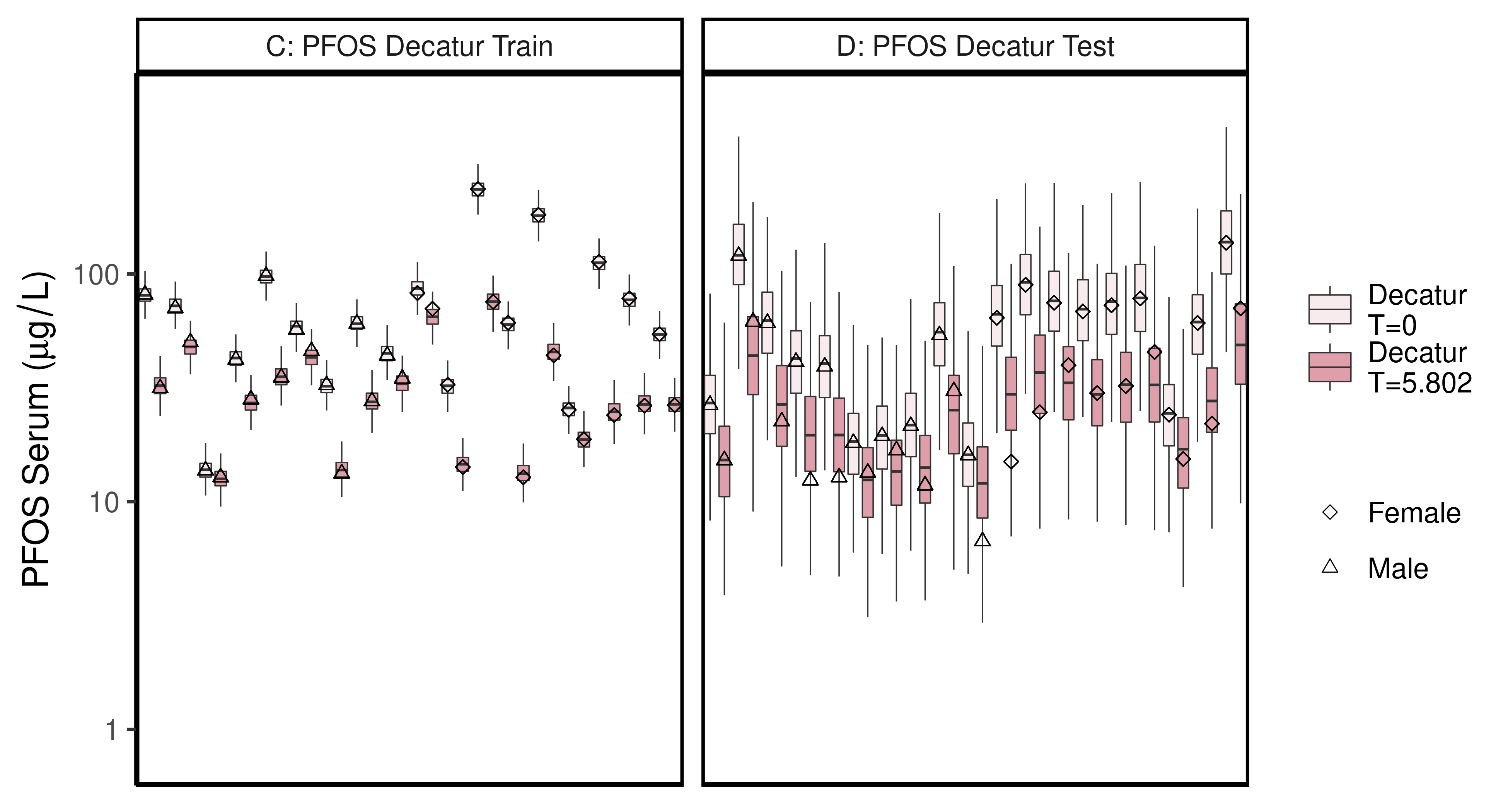
Modify aesthetics lookup table for boxplots

## 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.

#CD  
 # 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("C: PFOS Decatur Train", "D: PFOS 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

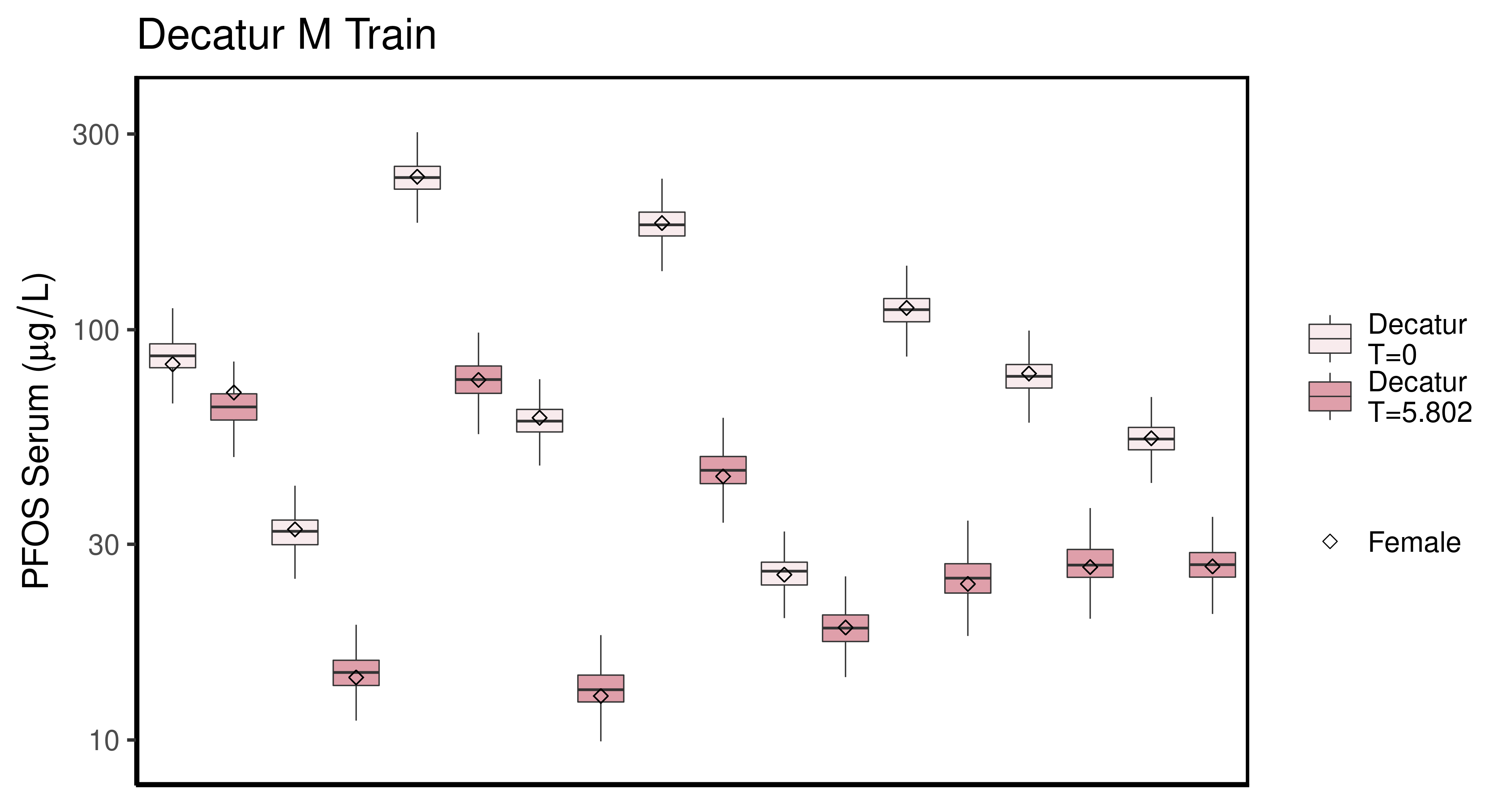
Changed grey start to 1 instead of 0.8, end at 0.6 instead of 0.4. Added shapes and fills to data points.

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

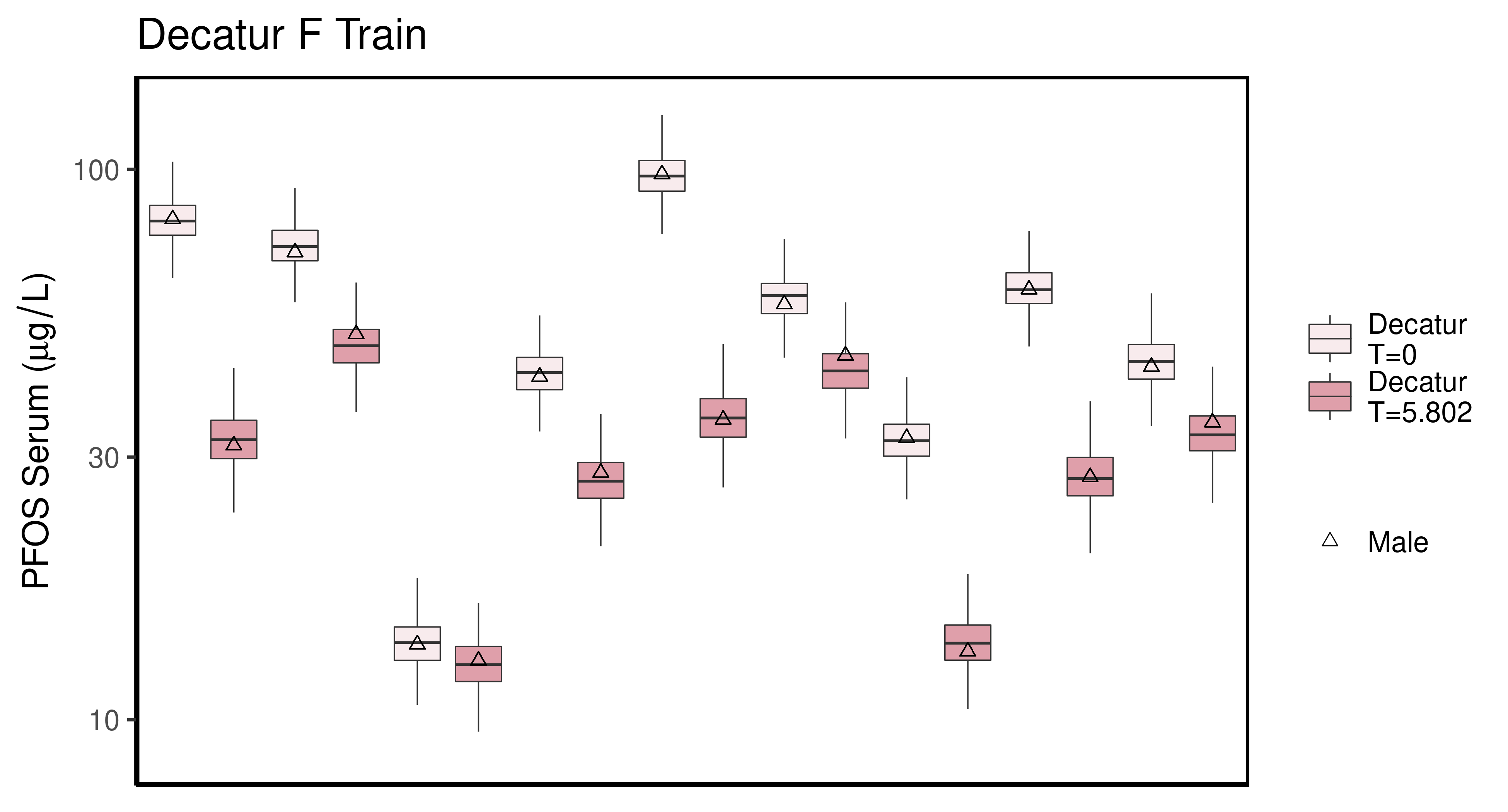
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

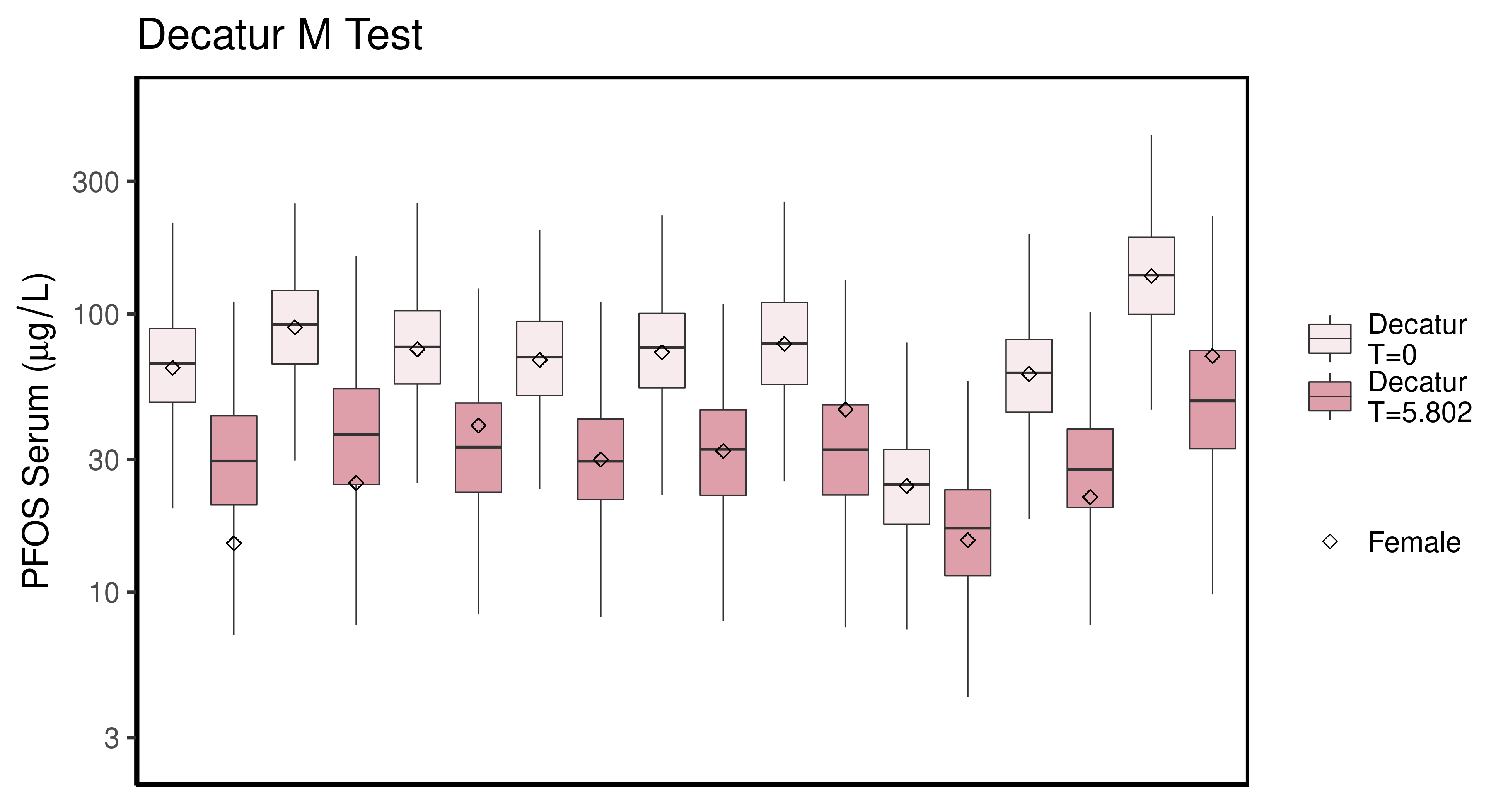
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

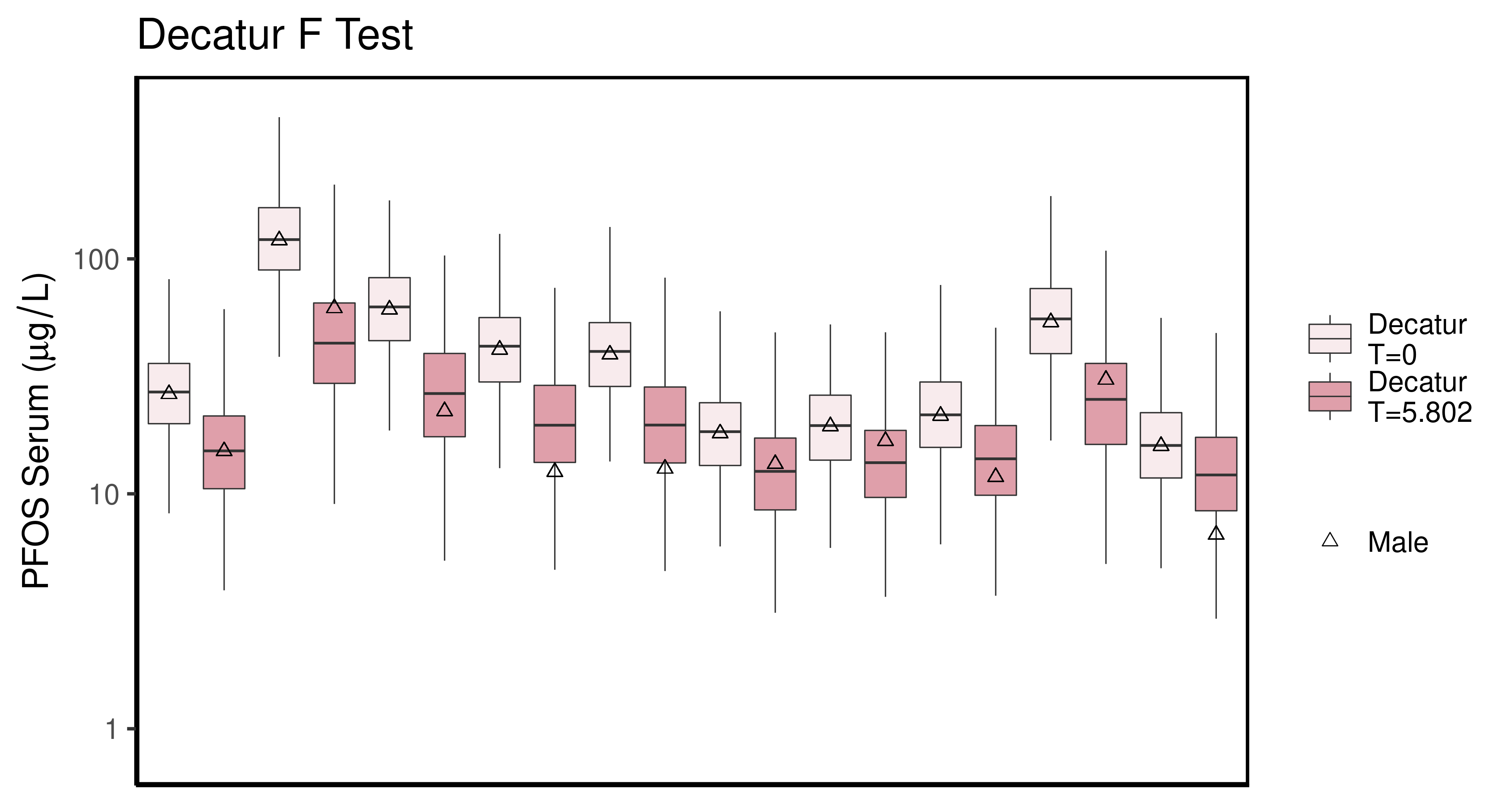
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

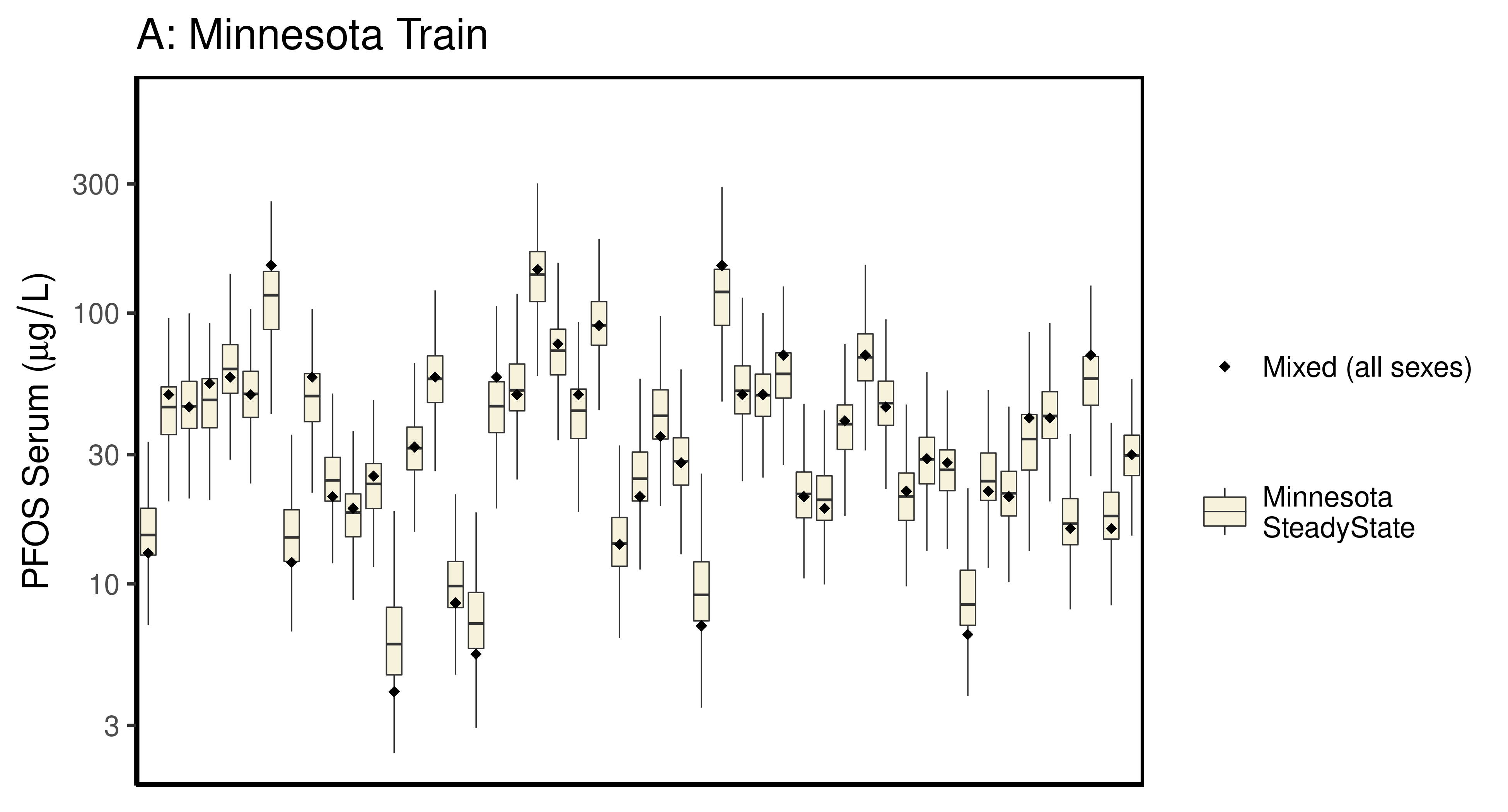
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

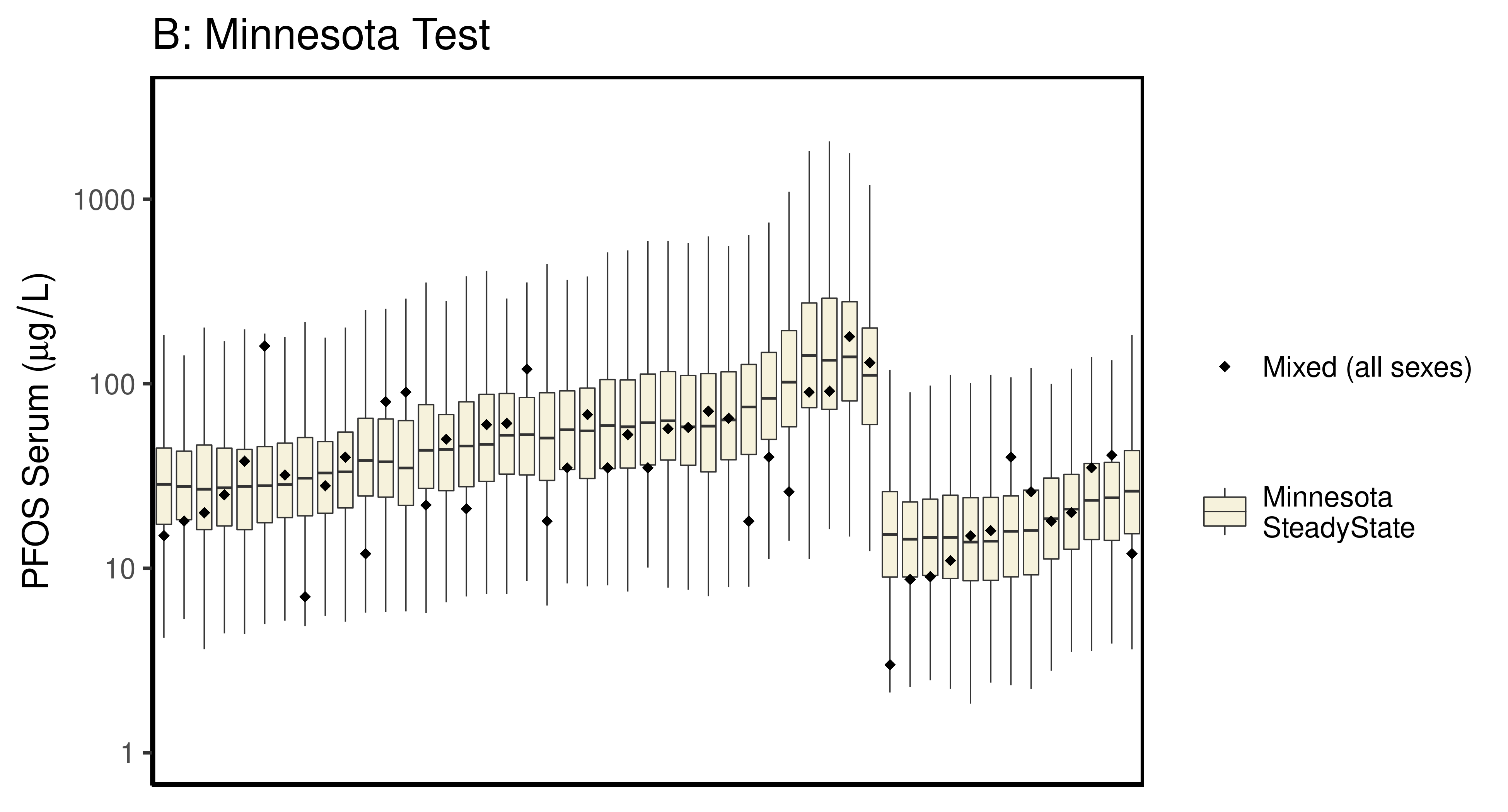
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

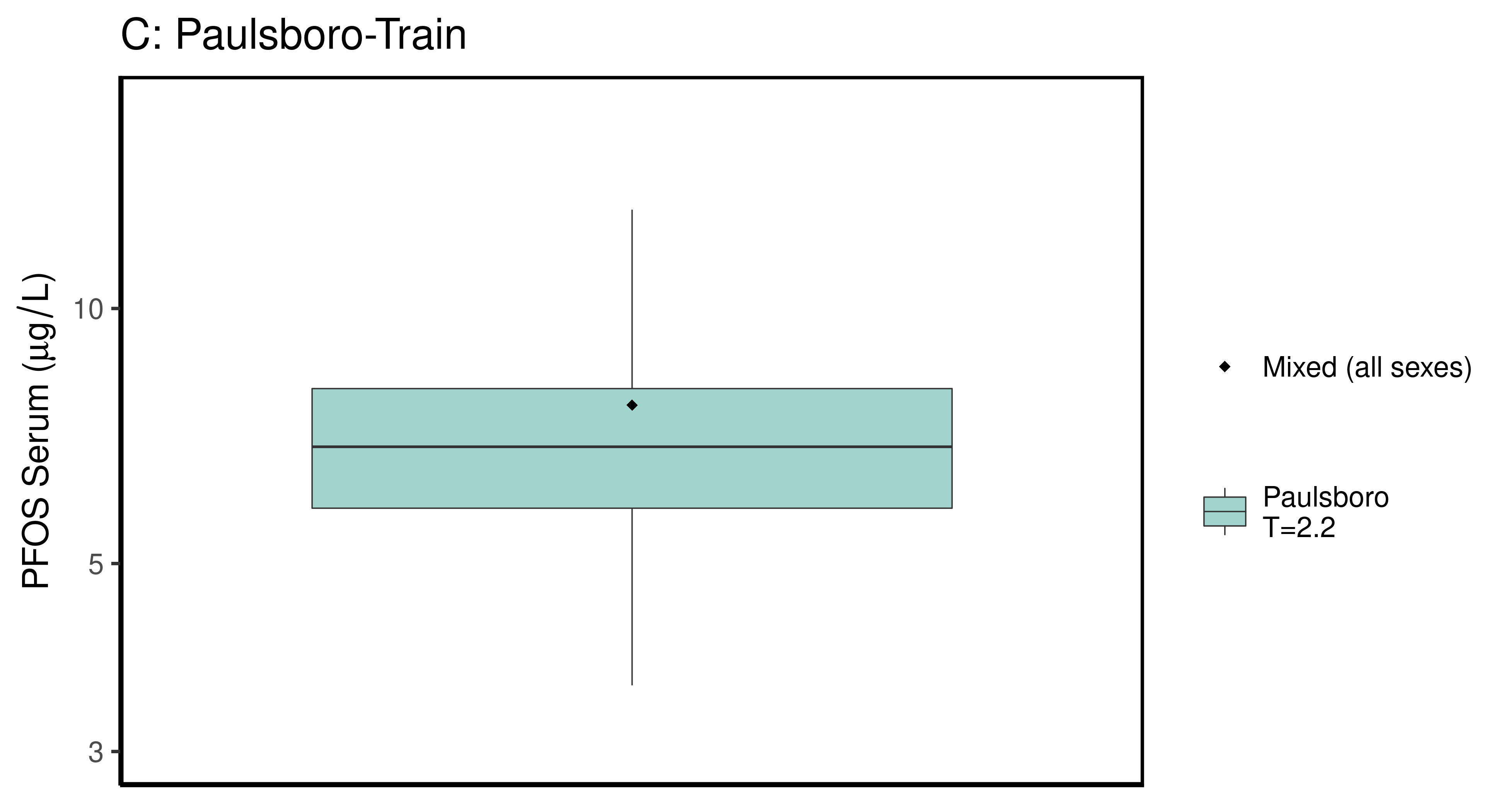
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

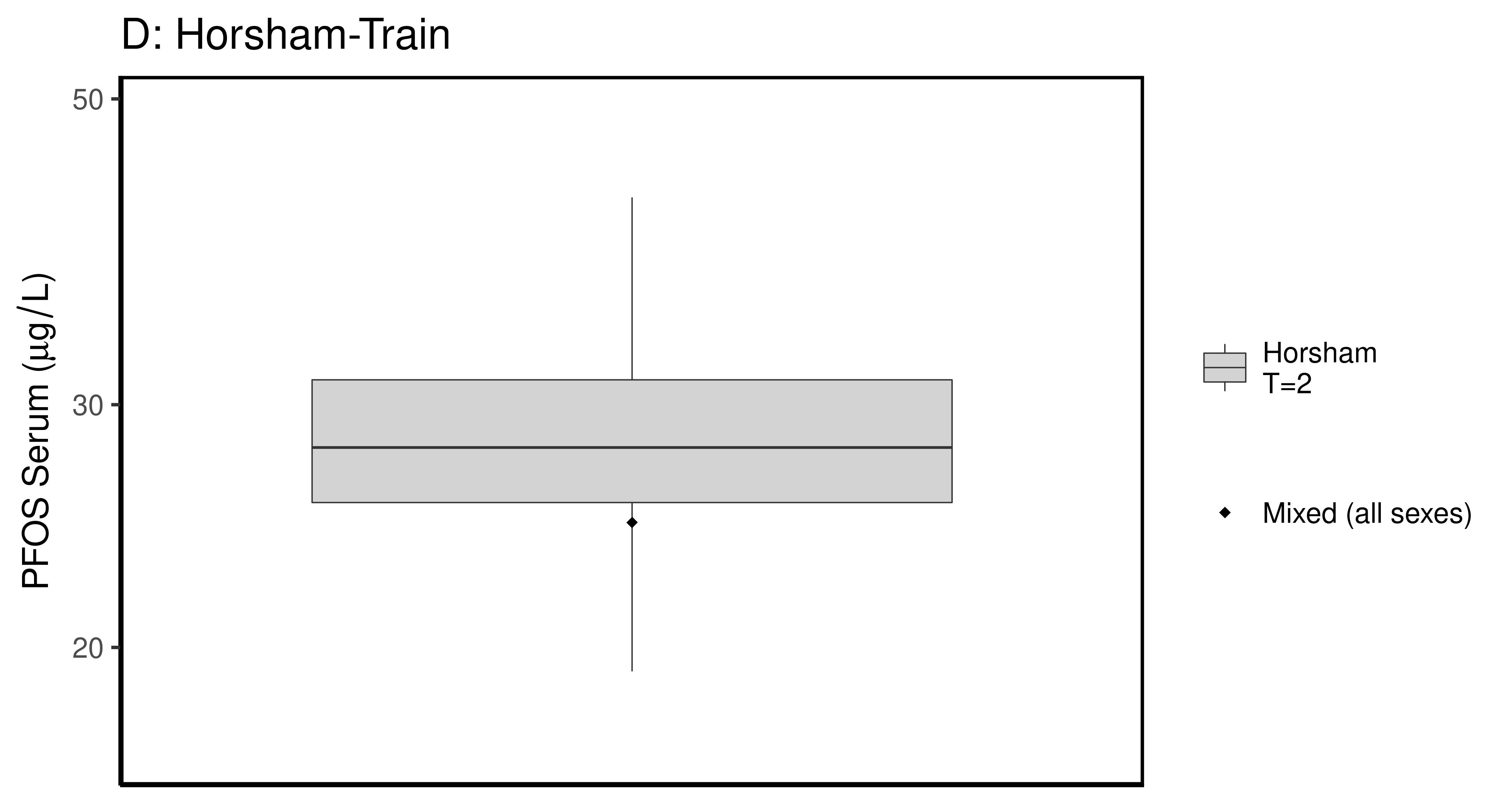
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

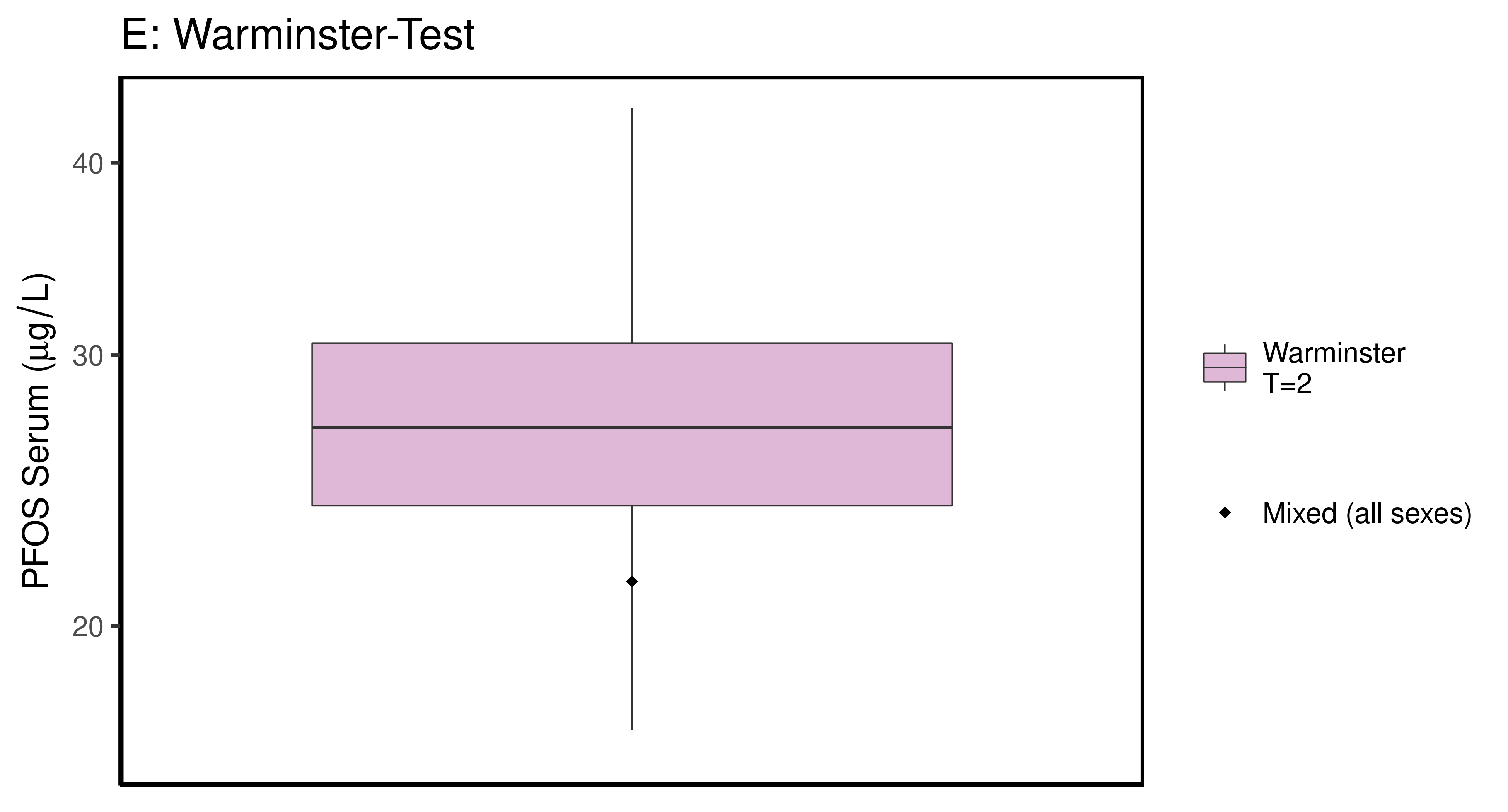
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

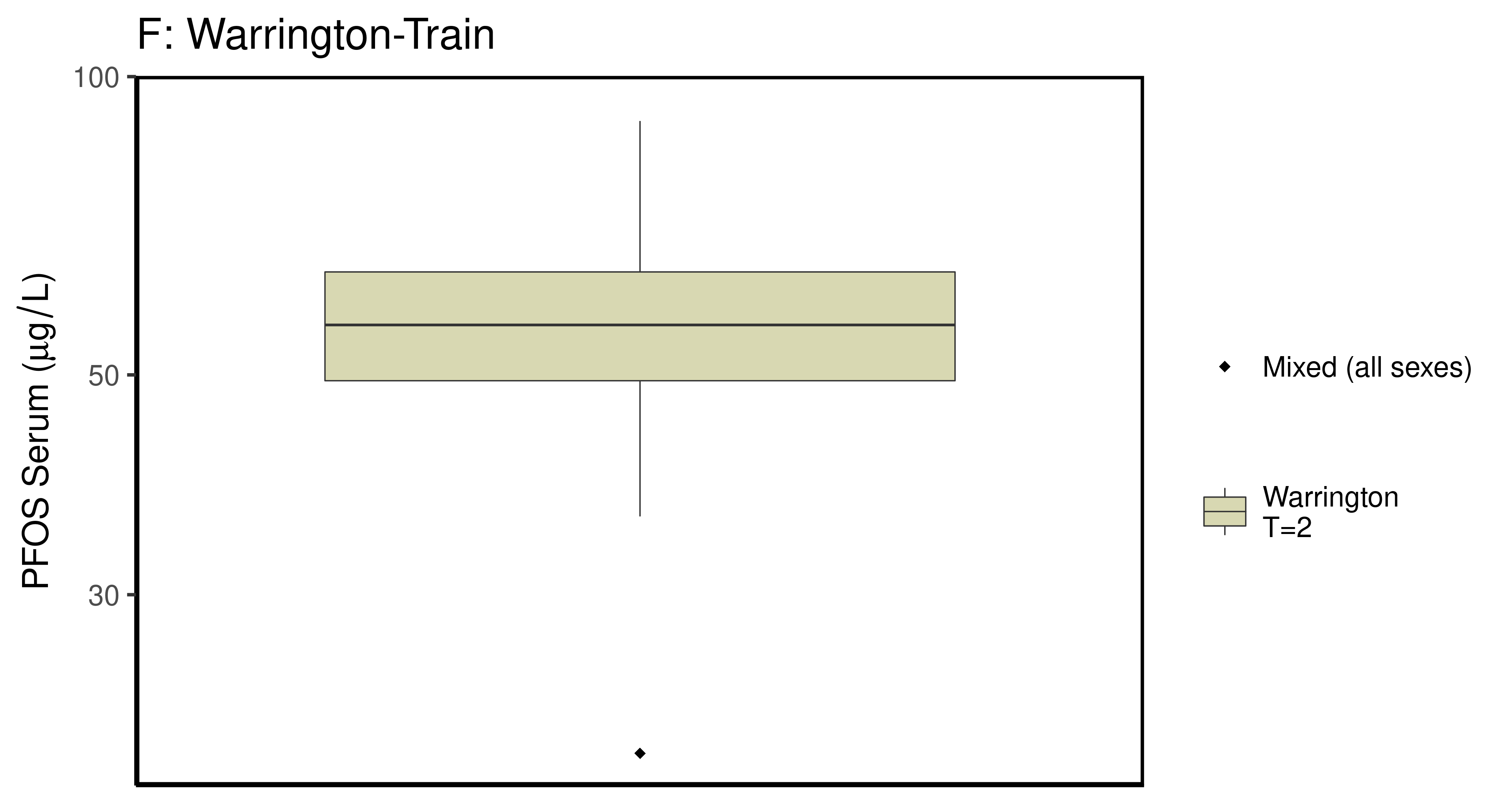
## Saving 6.5 x 3.5 in image

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



## Saving 6.5 x 3.5 in image

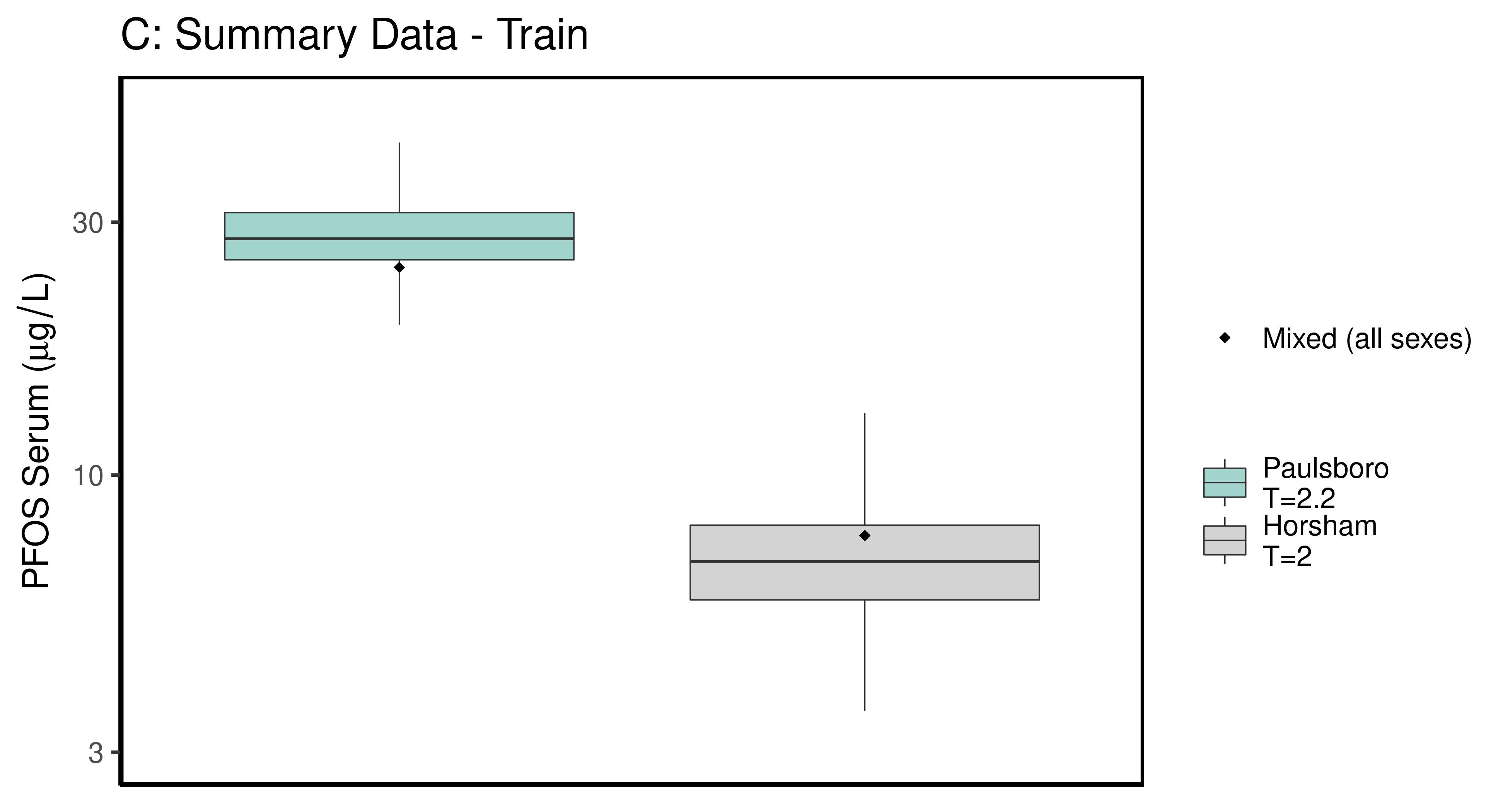
## Saving 6.5 x 3.5 in image



### 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="C: 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

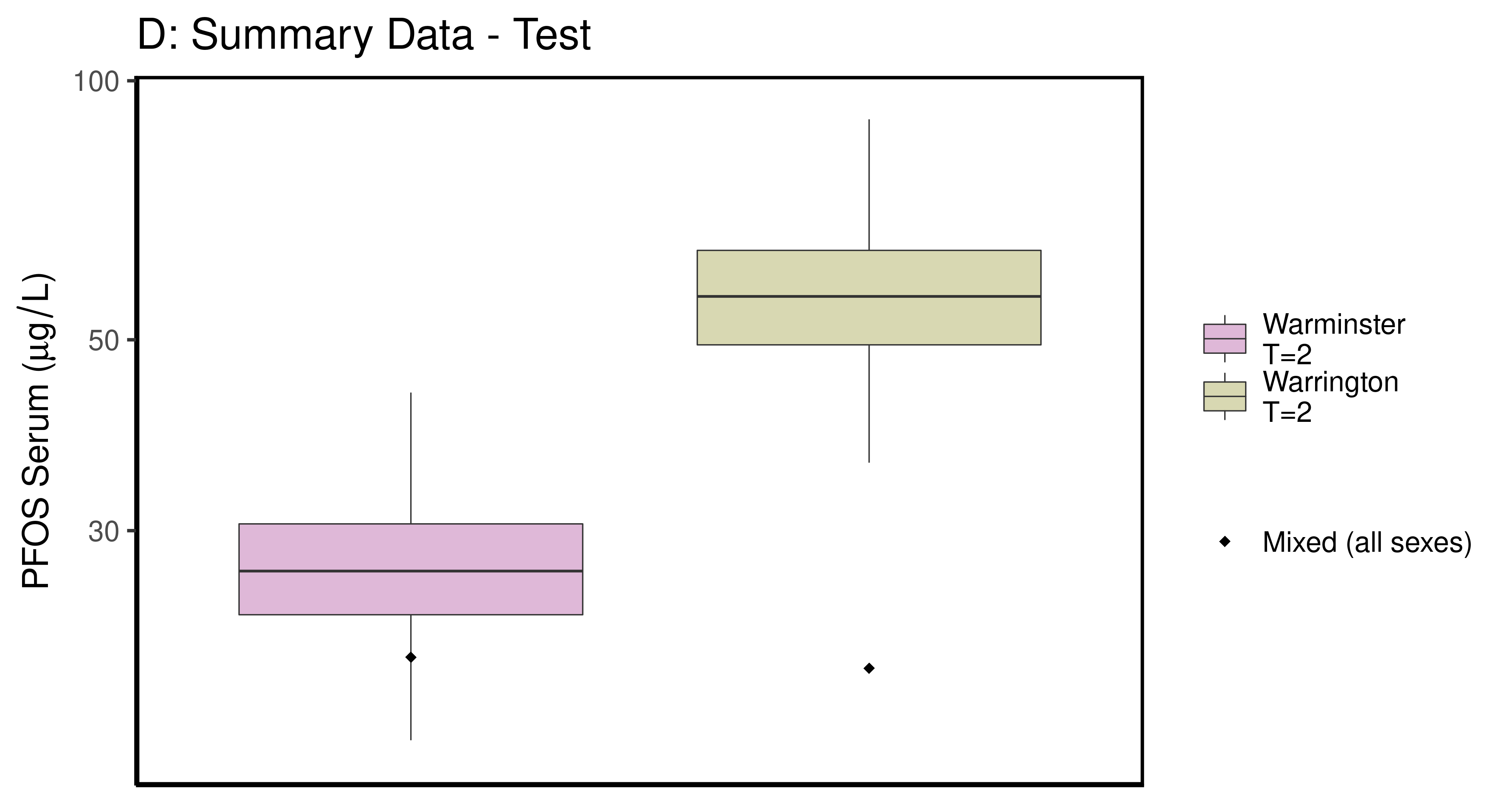
ggsave(here ("output-plots", paste0( sa, "SummaryTrainDataboxplot",pfas\_name,".png")), plt\_train,dpi=600)

## 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="D: 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)

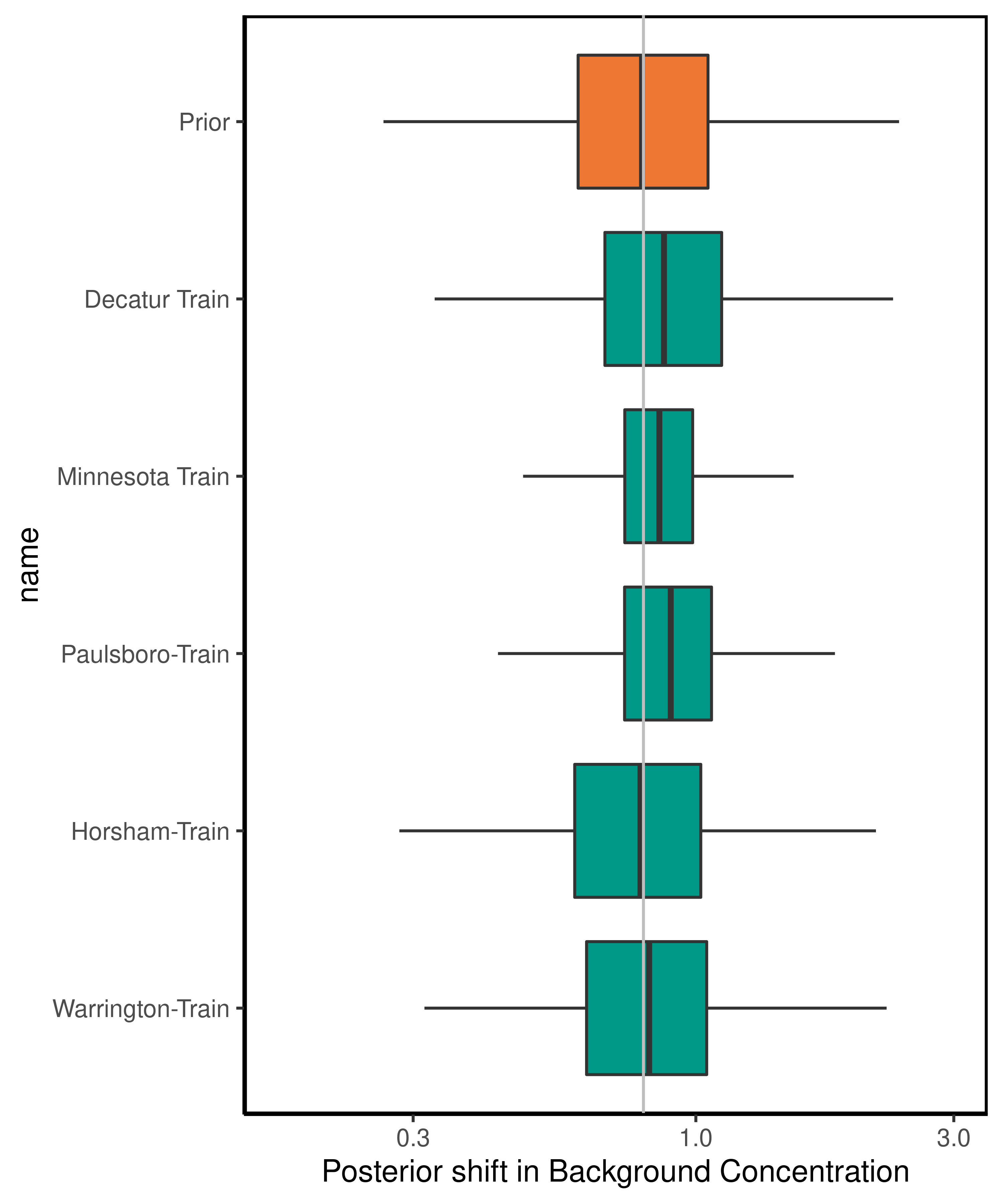
## Saving 6.5 x 3.5 in image

## PFOS

### Background posteriors

Shows shift in background estimate.

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



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

## Saving 5 x 6 in image

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

## Saving 5 x 6 in image

### Half-life

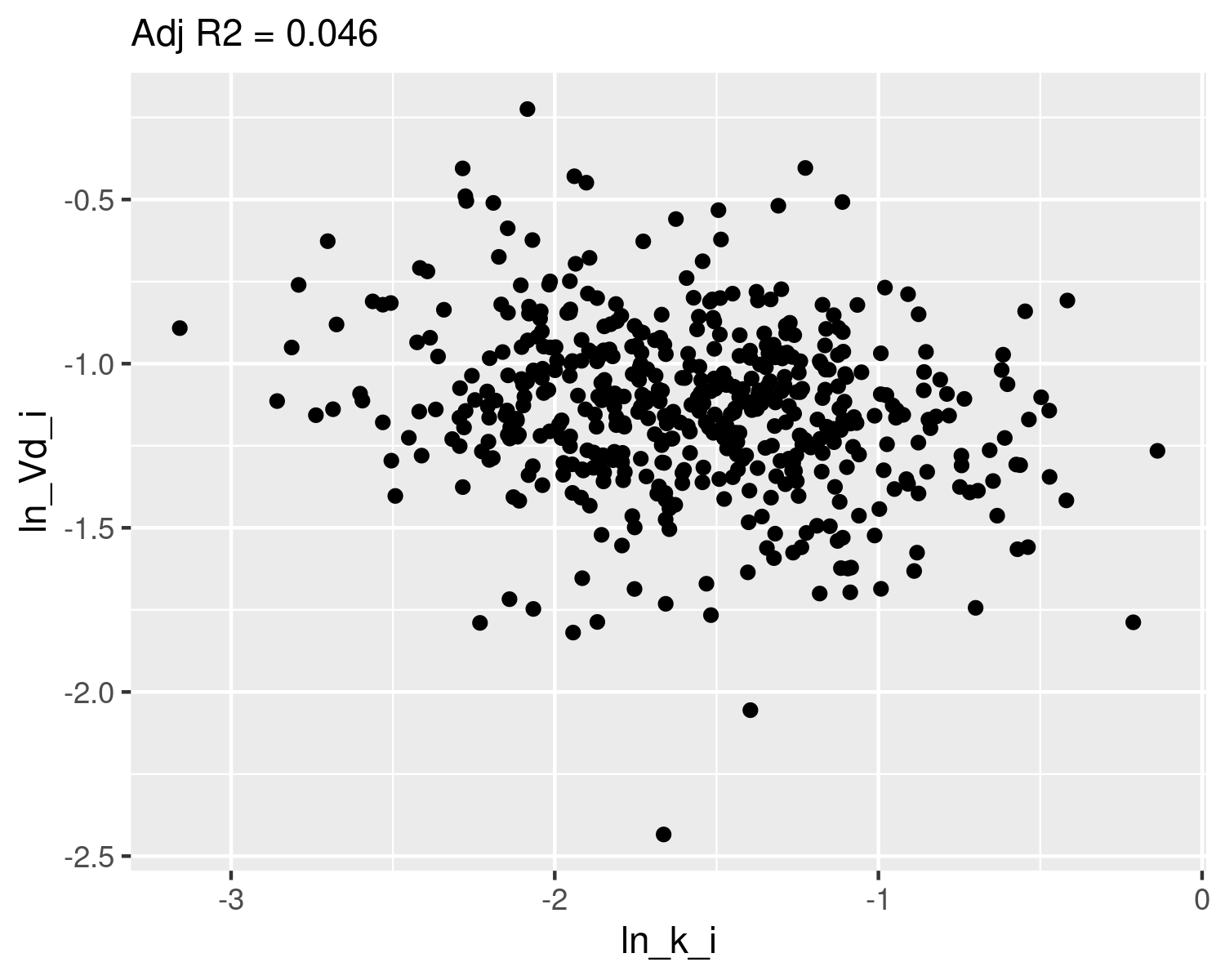
For PFOS, the population GM of the half-life has a posterior distribution that is narrower than the prior, with a posterior median (95% CI) estimate of 3.06 (2.16-4.37) years. The population GSD posterior is larger than the prior at 1.47(1.44-1.75).

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.

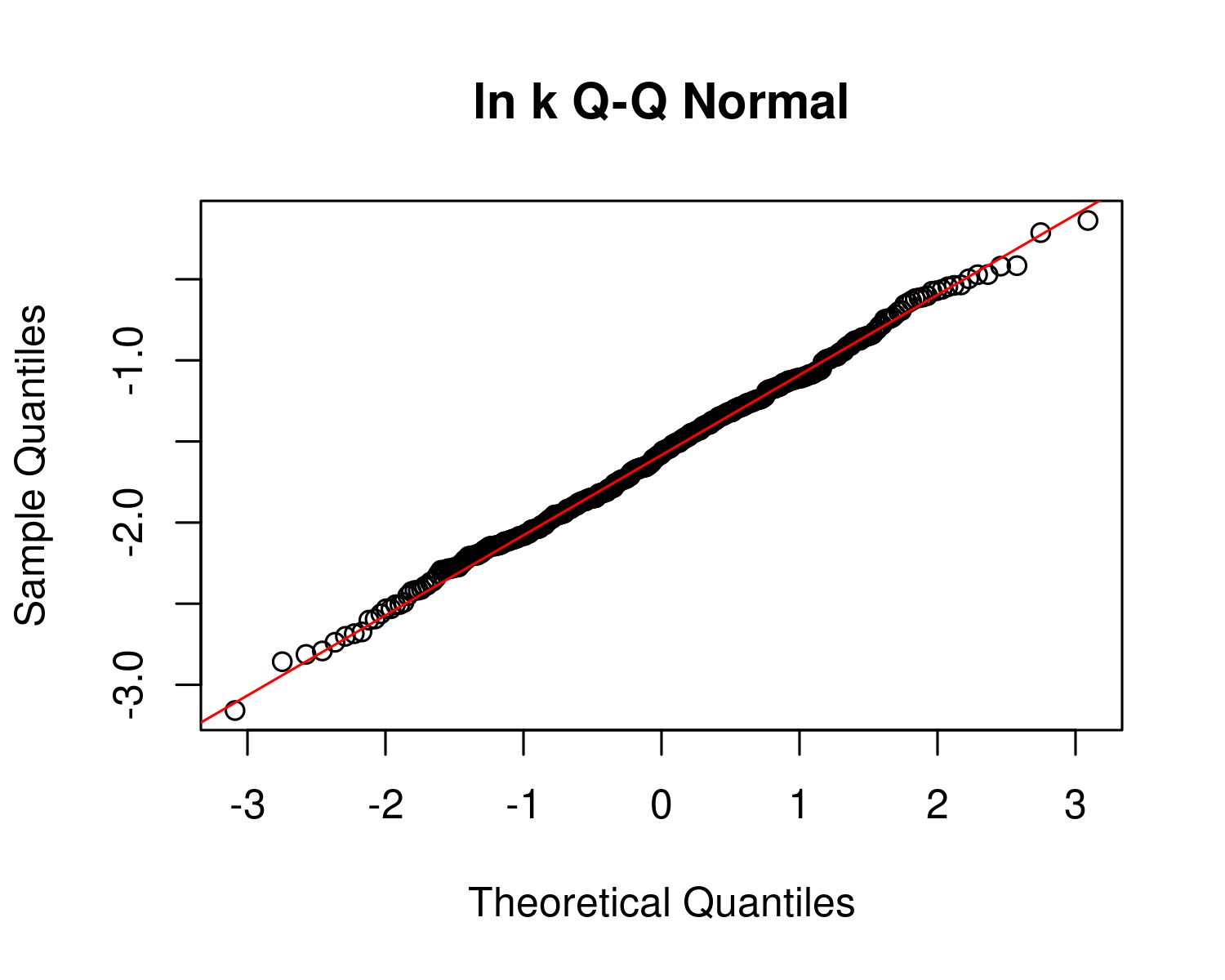
## M\_ln\_k(1) V\_ln\_k(1) M\_ln\_Vd(1) SD\_ln\_Vd(1) z\_ln\_k z\_ln\_Vd  
## 12503 -1.78081 0.285228 -0.952589 0.099030200 -0.961933416 -2.139841913  
## 15901 -1.58629 0.201249 -0.969862 0.117249000 -0.292525723 -1.263479244  
## 17543 -1.51202 0.201935 -0.990878 0.099988900 0.258788216 0.083307969  
## 18721 -1.77048 0.192680 -0.504773 0.079285300 -1.152131886 0.188325130  
## 11662 -1.64655 0.247044 -1.118770 0.155813000 0.195782826 0.189814193  
## 13403 -1.67037 0.204080 -0.987917 0.076863000 0.030123945 0.217615352  
## 13192 -1.48840 0.205743 -1.161630 0.097435400 0.085417732 -0.648814142  
## 15663 -1.73395 0.161690 -0.941647 0.133450000 1.116610213 0.254774383  
## 1246 -1.56178 0.234900 -1.118080 0.083615400 -1.218857416 -0.468830015  
## 16132 -1.47170 0.220846 -1.348210 0.039526200 1.267368722 -1.192510054  
## 10602 -1.66126 0.145580 -1.006460 0.119143000 -0.744781596 0.121228235  
## 10563 -1.55578 0.219351 -0.915973 0.133472000 -1.131218571 -1.035932658  
## 15932 -1.53965 0.225097 -1.212150 0.304727000 -0.716358490 -0.191888295  
## 1114 -1.57212 0.143150 -1.353580 0.060456400 0.252652370 -0.970546336  
## 1699 -1.72310 0.181150 -1.394070 0.002710170 0.152045707 0.057771938  
## 1141 -1.71915 0.235515 -1.115950 0.317802000 -0.307656430 -2.110692675  
## 13383 -1.58035 0.187495 -1.067820 0.078978300 -0.953017331 0.978176274  
## 12832 -1.52325 0.206817 -1.147450 0.080134500 -0.648242811 0.371021737  
## 19552 -1.73858 0.269688 -1.041740 0.014100600 1.224313624 0.720910931  
## 14423 -1.72443 0.244522 -1.020560 0.245251000 0.199811608 1.879594880  
## 12372 -1.88535 0.200824 -0.824227 0.051924500 -0.578483722 -0.396316112  
## 12042 -1.68883 0.222860 -1.231820 0.081923900 -0.942300733 0.110322947  
## 10473 -1.41388 0.260457 -0.974745 0.184174000 -0.203728180 -0.593140881  
## 1509 -1.79090 0.322931 -1.208560 0.122928000 -1.666474840 0.419621770  
## 1552 -1.48118 0.164918 -1.359260 0.026906900 -0.484455109 -0.545738743  
## 19513 -1.71252 0.211311 -0.989702 0.061660400 -0.741072661 1.160921499  
## 17471 -1.74664 0.186104 -1.032350 0.007978960 1.160615779 0.639817834  
## 18092 -1.54205 0.294871 -0.959400 0.073912900 1.012067125 -0.122020443  
## 1613 -1.41711 0.229896 -1.243510 0.174357000 -0.072078474 0.184645026  
## 14383 -1.67568 0.140886 -0.946274 0.006121810 -1.136782298 -0.517806023  
## 14263 -1.60634 0.154418 -1.108690 0.326070000 0.900624729 0.067988352  
## 18291 -1.43525 0.146936 -1.151450 0.108204000 0.851770447 -0.184797156  
## 1945 -1.53114 0.162382 -1.290380 0.191541000 0.727715174 -1.403691615  
## 19613 -1.44761 0.173023 -1.218000 0.010419300 0.736502146 0.229740706  
## 1842 -1.70720 0.161055 -1.071380 0.243799000 -0.352129617 -0.889081301  
## 1873 -1.63256 0.198483 -1.109280 0.055205400 0.705515513 -0.160401177  
## 19423 -1.63666 0.186280 -1.106420 0.231938000 1.300357989 -0.242136794  
## 19352 -1.33777 0.242559 -1.514870 0.101520000 0.038252014 -0.028837196  
## 11812 -1.72255 0.244641 -1.128230 0.005779080 -0.979283770 -0.316215474  
## 14982 -1.74793 0.182659 -1.195730 0.201199000 0.793761231 -0.416160087  
## 11263 -1.63248 0.227020 -1.226210 0.098182600 0.786506872 -1.023895957  
## 1028 -1.44108 0.227241 -1.497500 0.279376000 -0.310463131 1.099495275  
## 1051 -1.37358 0.197145 -1.192990 0.212443000 1.698884846 0.817712470  
## 17222 -1.60673 0.263080 -0.775905 0.156705000 -0.794593709 0.168875510  
## 1747 -1.57055 0.149488 -1.244460 0.152799000 0.348437716 0.038665440  
## 1284 -1.76566 0.205009 -0.927193 0.155017000 -2.265401074 1.078174892  
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## 16502 -1.26098 0.272060 -1.405550 0.027308000 -0.809440902 0.342994219  
## 15103 -1.65713 0.300501 -0.859839 0.003772110 0.267085116 -0.124701883  
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## 19872 -1.52489 0.225053 -1.268170 0.334098000 -0.279741696 -0.437523579  
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## 15553 -1.61085 0.245026 -1.558870 0.209524000 0.188870195 -0.988041784  
## 19433 -1.55771 0.161607 -1.126080 0.002561330 -0.050148494 0.265546446  
## 15642 -1.31965 0.158509 -1.499780 0.211088000 -1.495419632 -0.728186155  
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## 1920 -1.63960 0.256817 -1.109250 0.058825100 -2.403663727 -0.079333090  
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## 18021 -1.34489 0.287951 -1.449690 0.014336100 -1.019179409 1.197547370  
## 17623 -1.63211 0.230542 -0.957265 0.008806150 1.090553483 -0.698130988  
## 1499 -1.70673 0.253401 -1.243180 0.166719000 -1.139469805 0.293604948  
## 18673 -1.65524 0.144727 -0.950627 0.019642400 -0.015725635 0.437297744  
## 1093 -1.58098 0.262768 -0.931401 0.029045400 0.297491282 0.627762573  
## 13553 -1.64468 0.112668 -1.381070 0.158695000 3.200590040 -1.160543514  
## 12592 -1.56243 0.221979 -0.810870 0.017618100 0.089244244 -0.020788418  
## 12912 -1.47563 0.253248 -1.449350 0.267489000 0.570972338 1.044724089  
## 1785 -1.56519 0.234420 -0.961575 0.337497000 0.528685630 1.311594585  
## 14041 -1.55624 0.200230 -1.682980 0.039643900 -0.440904798 -0.082439028  
## 1624 -1.58871 0.206067 -1.067880 0.117994000 -0.672793368 0.919224762  
## 1841 -1.59702 0.242987 -1.157960 0.050034900 2.154313365 -0.243269921  
## 19553 -1.58897 0.176284 -0.974234 0.016211400 0.593852716 0.351094377  
## 12722 -1.52174 0.124294 -1.499270 0.173234000 -0.384063768 -1.340384172  
## 15122 -1.43917 0.225557 -1.345530 0.071023900 0.719783276 0.425846094  
## 1348 -1.58841 0.181888 -1.044740 0.045054800 1.708173402 -0.814353733  
## 15183 -1.65215 0.194633 -1.161910 0.235166000 1.075215667 0.693374081  
## 14432 -1.86349 0.159467 -1.069830 0.085695500 0.777420367 0.705544556  
## 1468 -1.60422 0.172838 -1.233920 0.097173900 0.052200047 0.278350539  
## 17953 -1.64563 0.161398 -1.277810 0.051313600 -1.083698485 -1.202692142  
## 1557 -1.66389 0.208662 -1.326200 0.039139600 -0.008856207 0.642761817  
## 19642 -1.36383 0.151261 -1.230990 0.125808000 2.030643112 -0.605973945  
## 16191 -1.90796 0.183750 -0.794787 0.091698600 -1.113328933 -1.377257613  
## 17011 -1.52187 0.232224 -1.208410 0.040071900 1.138271925 -0.925992687  
## 1820 -1.54997 0.147997 -1.149720 0.087674700 -0.614892642 0.567243857  
## 10851 -1.74327 0.190786 -0.866111 0.092164700 -2.193536615 2.595481260  
## 13483 -1.69765 0.239625 -1.050810 0.098970100 -1.215686372 -0.239984547  
## 13183 -1.42996 0.196183 -1.349920 0.006047990 -0.045326362 0.687536401  
## 18462 -1.78429 0.255510 -1.050510 0.302213000 1.598812624 -0.151788986  
## 15542 -1.36531 0.145370 -1.549210 0.113384000 0.927542200 0.227544260  
## 18752 -1.47846 0.263995 -0.931570 0.141422000 0.829284552 -0.668648038  
## 12081 -1.58205 0.167345 -1.022160 0.129913000 1.024603876 0.030829067  
## 1014 -1.62575 0.146259 -0.873709 0.107367000 -0.476238068 0.028429558  
## 15612 -1.39444 0.170533 -1.357100 0.095935100 1.638868393 -0.365455074  
## 14833 -1.51299 0.153173 -1.247730 0.098087600 -0.632050958 -2.208012195  
## 1639 -1.64404 0.167499 -1.087890 0.010836000 -1.379618576 0.297039427  
## 10353 -1.68356 0.185246 -0.988275 0.062948000 -0.257455748 2.129700659  
## 15011 -1.73574 0.138168 -0.785989 0.210057000 1.679972711 1.325041143  
## 12253 -1.56823 0.192441 -1.132960 0.050170900 -2.545858038 -0.116171447  
## 10793 -1.60612 0.210550 -1.125460 0.134709000 0.012078784 -1.470146221  
## 10103 -1.53976 0.164855 -1.254430 0.067924900 1.960925111 -0.379271835  
## 1903 -1.60294 0.163912 -0.921678 0.075232200 -0.385905481 -1.465005931  
## 1679 -1.57705 0.197029 -1.197260 0.086086800 0.910757548 1.075148263  
## 1795 -1.44186 0.169519 -1.282230 0.071725800 -1.448130794 -1.226124877  
## 1489 -1.70365 0.151234 -1.189020 0.172850000 -1.121614596 -3.056328234  
## 1881 -1.57304 0.259497 -1.020810 0.273858000 -0.973617906 1.450657775  
## 15061 -1.69238 0.285552 -0.977120 0.099873800 -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)))

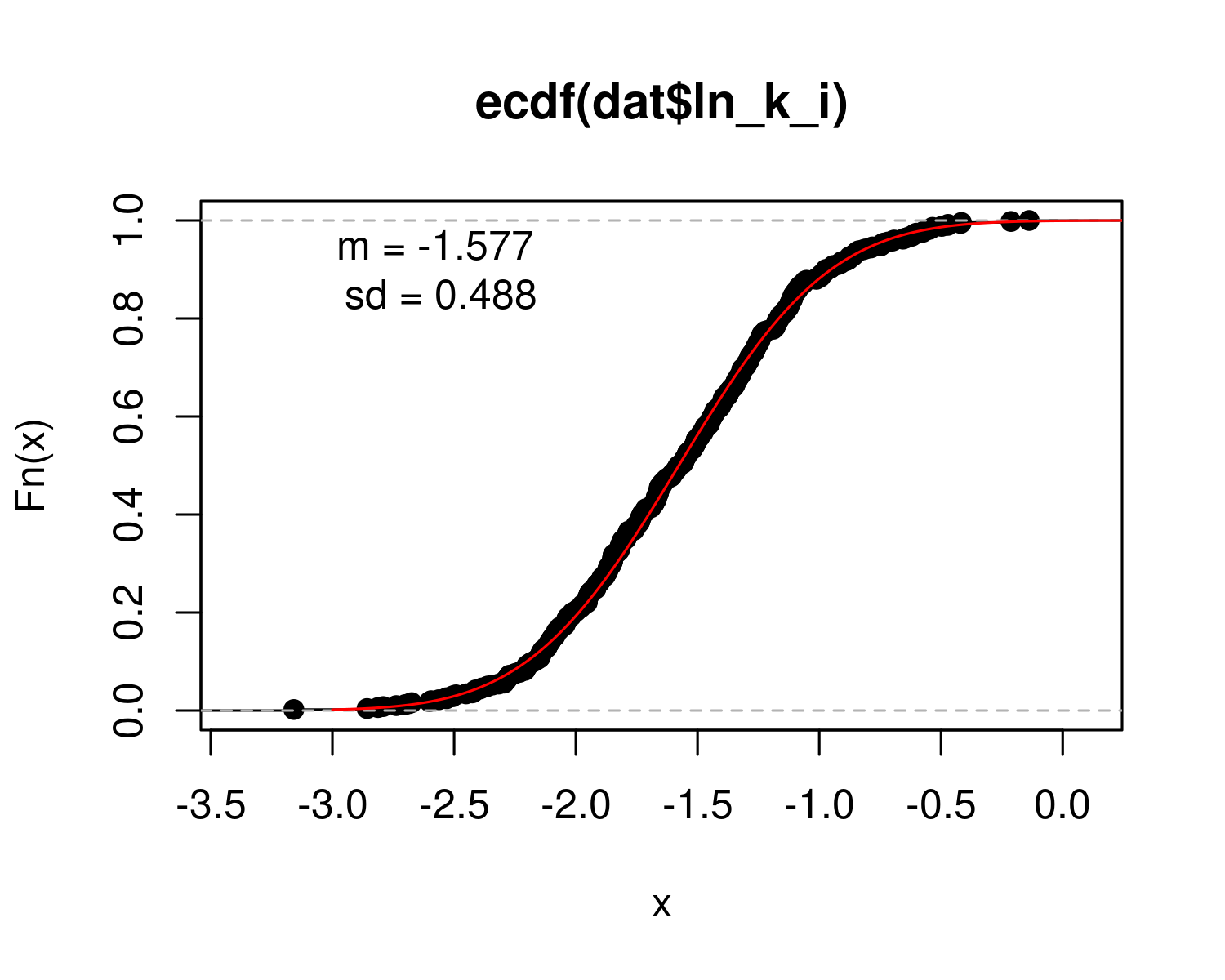


## Check normality

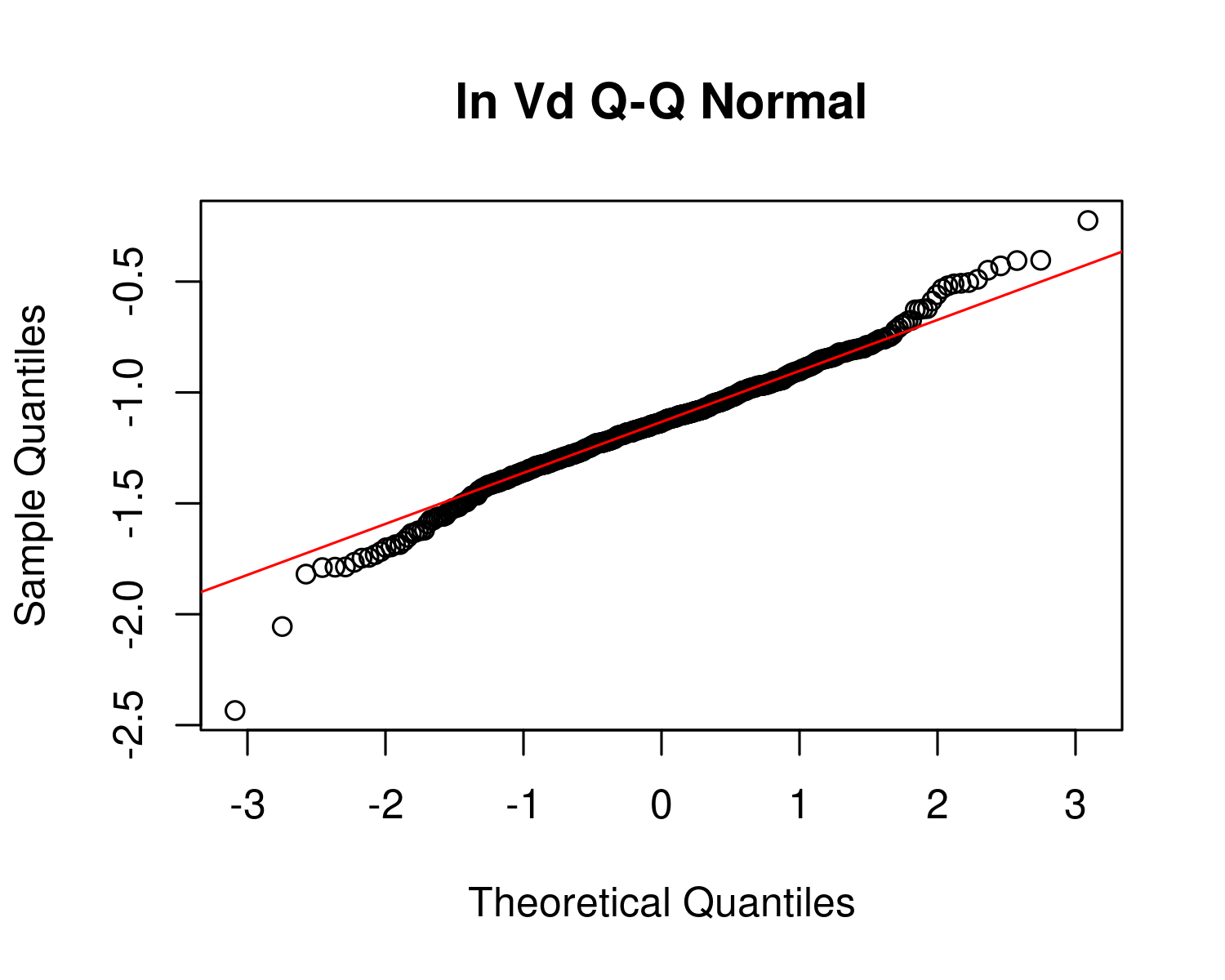
qqnorm(dat$ln\_k\_i,main="ln k Q-Q Normal")  
qqline(dat$ln\_k\_i,col="red")



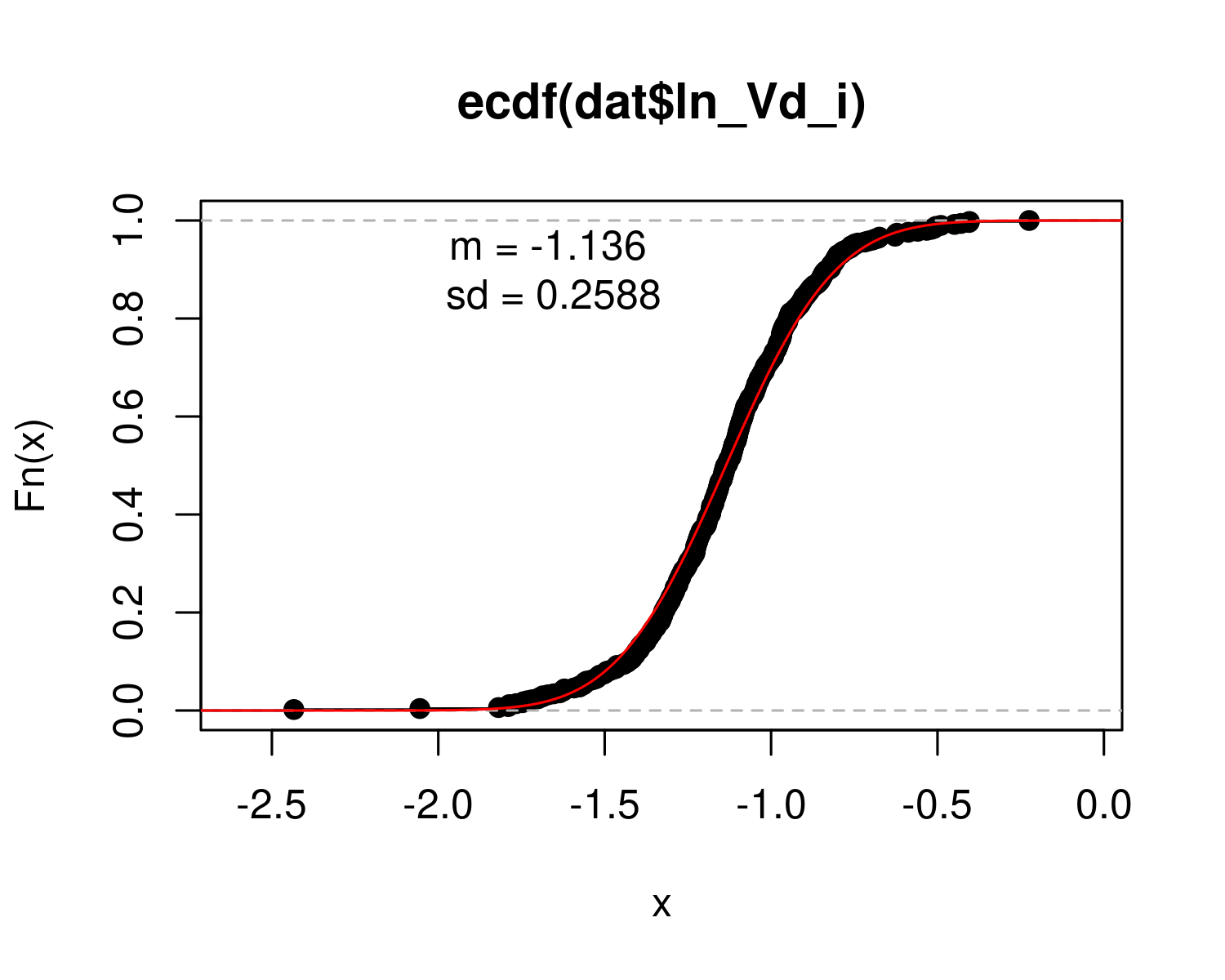
plot(ecdf(dat$ln\_k\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_k\_i <- mean(dat$ln\_k\_i)  
sd\_ln\_k\_i <- sd(dat$ln\_k\_i)  
lines(x,pnorm(x,mean=m\_ln\_k\_i,sd=sd\_ln\_k\_i),col="red")  
text(m\_ln\_k\_i-2\*sd\_ln\_k\_i,0.9,paste("m =",signif(m\_ln\_k\_i,4),"\nsd =",signif(sd\_ln\_k\_i,4)))



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)))

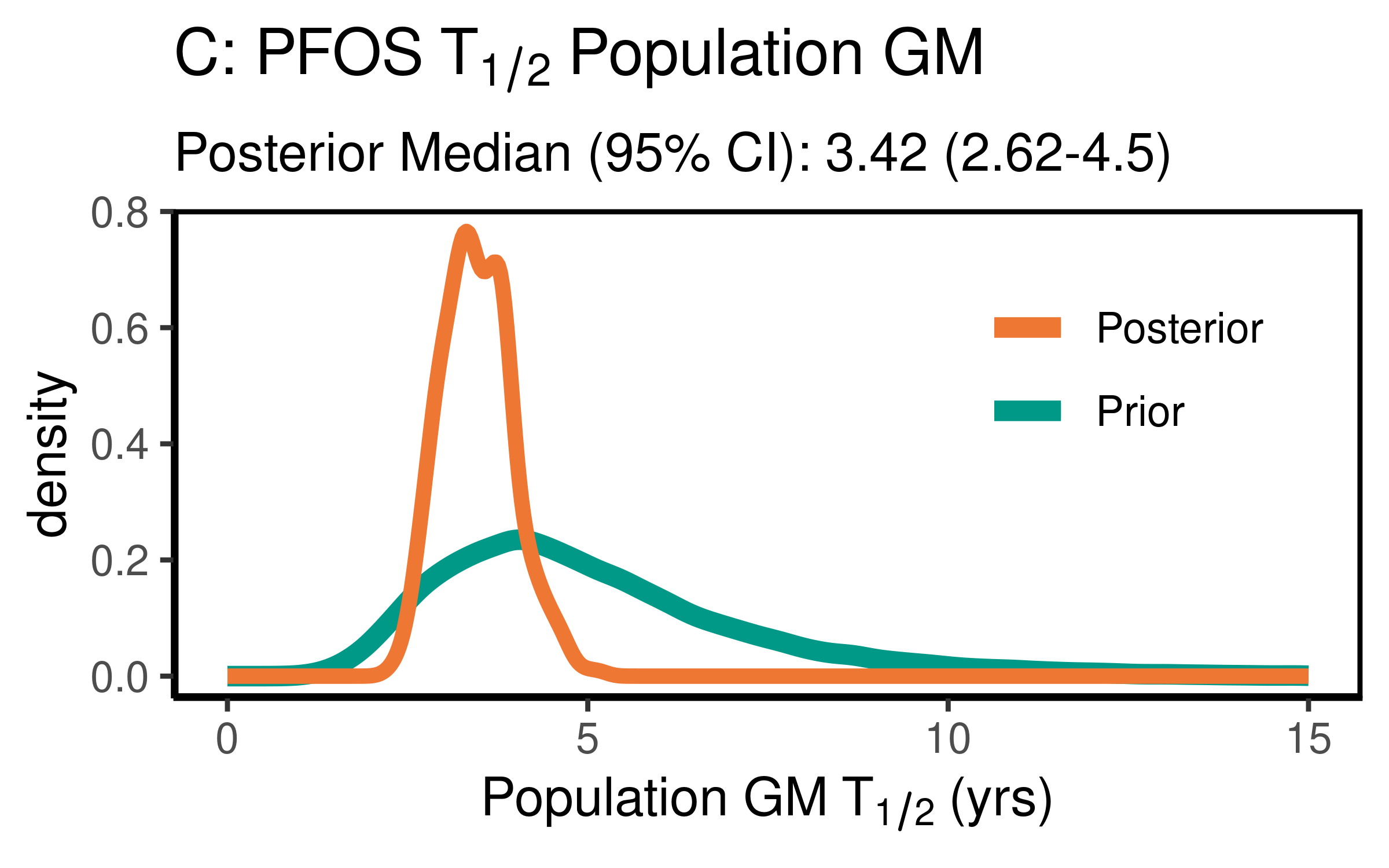


## Calculate table values for individual-level

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  
  
  
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

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

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



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

## Saving 4 x 2.5 in image

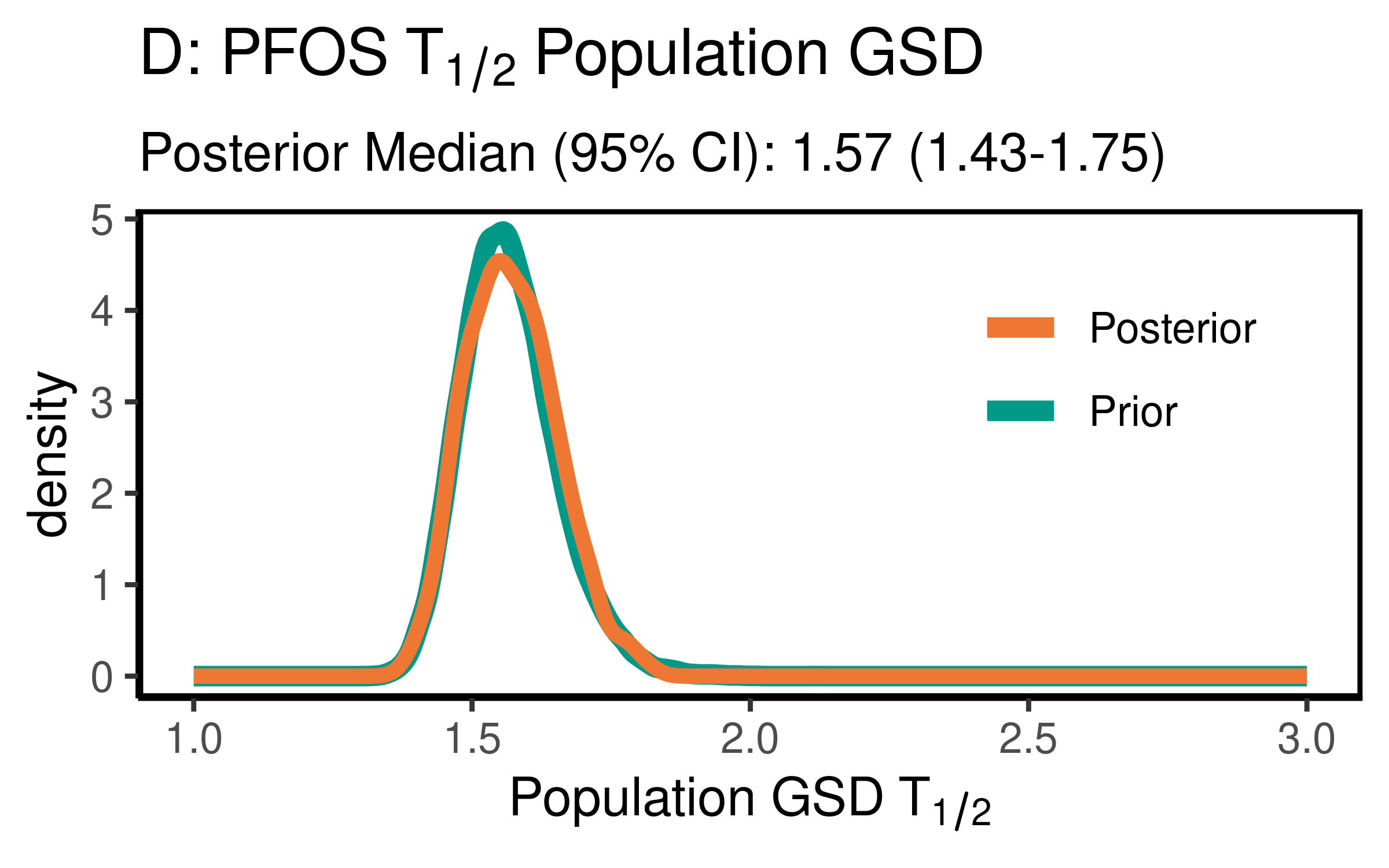
## Warning: Removed 80 rows containing non-finite values (stat\_density).

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

## Saving 4 x 2.5 in image

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

PFOS\_priors$halflife\_GSD = exp(sqrt(exp(rnorm(50000,m=log(0.1987),sd=log(1.267)))))   
PFOS\_halflife\_GSD <- exp(sqrt(dat$`V\_ln\_k(1)`))  
  
PFOS\_hlgsd\_pr\_med <- signif(median(PFOS\_priors$halflife\_GSD,3))  
PFOS\_hlgsd\_pr\_med\_95ci <-paste(signif(quantile(PFOS\_priors$halflife\_GSD,  
 prob=c(0.025,0.975)),  
 3),  
 collapse="-")  
PFOS\_hl\_gsd\_med <- signif(median(PFOS\_halflife\_GSD),3)  
PFOS\_hl\_gsd\_med\_95ci <- paste(signif(quantile(PFOS\_halflife\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
p<-ggplot()+  
 stat\_density(aes(halflife\_GSD, color = "Prior"),data=PFOS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOS\_halflife\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("D: PFOS"~T[1/2]~"Population GSD"),   
 subtitle=paste("Posterior Median (95% CI): ",  
 PFOS\_hl\_gsd\_med," (",  
 PFOS\_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)

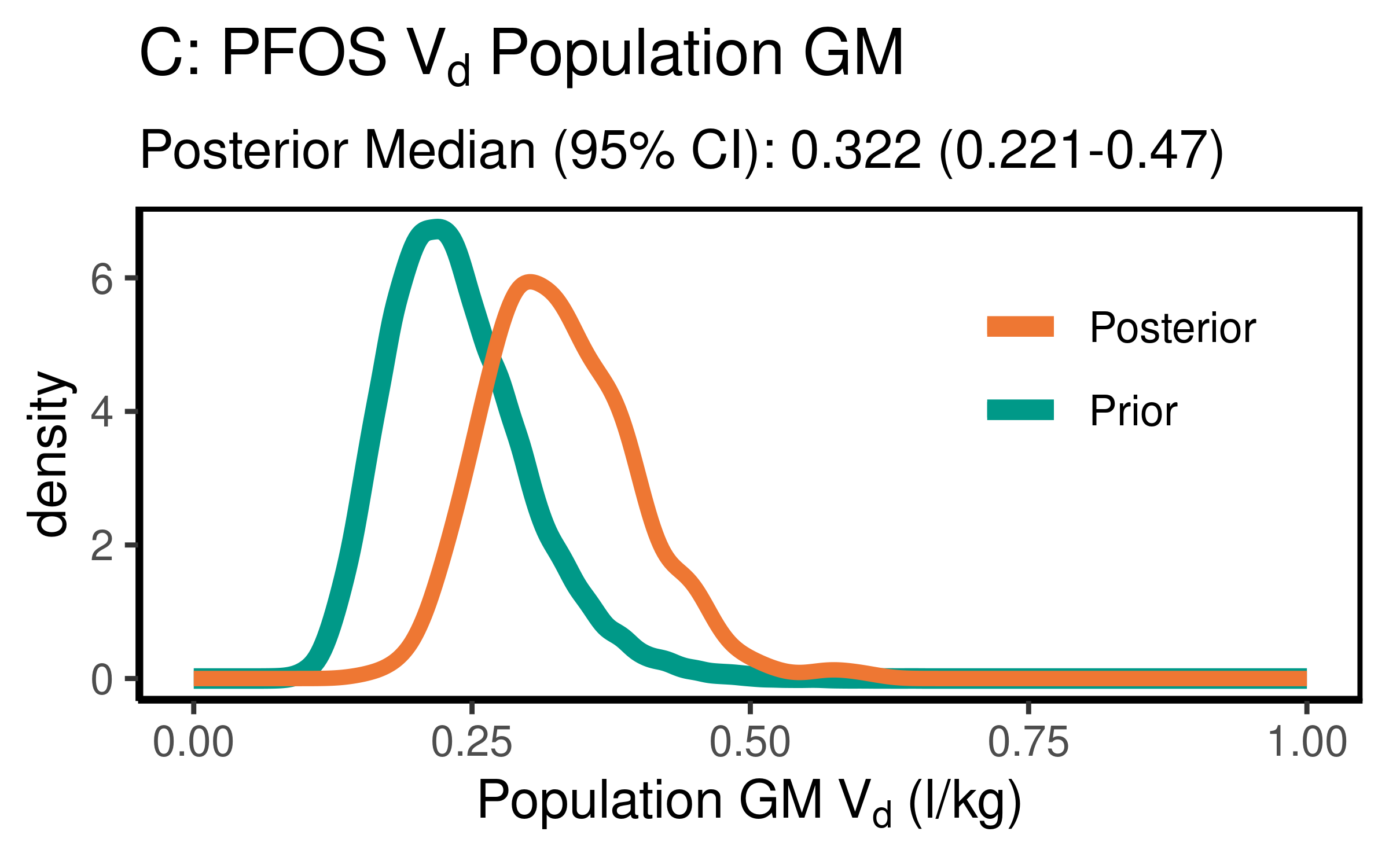


ggsave(here ("output-plots",paste0( sa, "PFOS\_hl\_gsd.pdf")), p, dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFOS\_hl\_gsd.png")), p, dpi=600)

### Distribution Volume

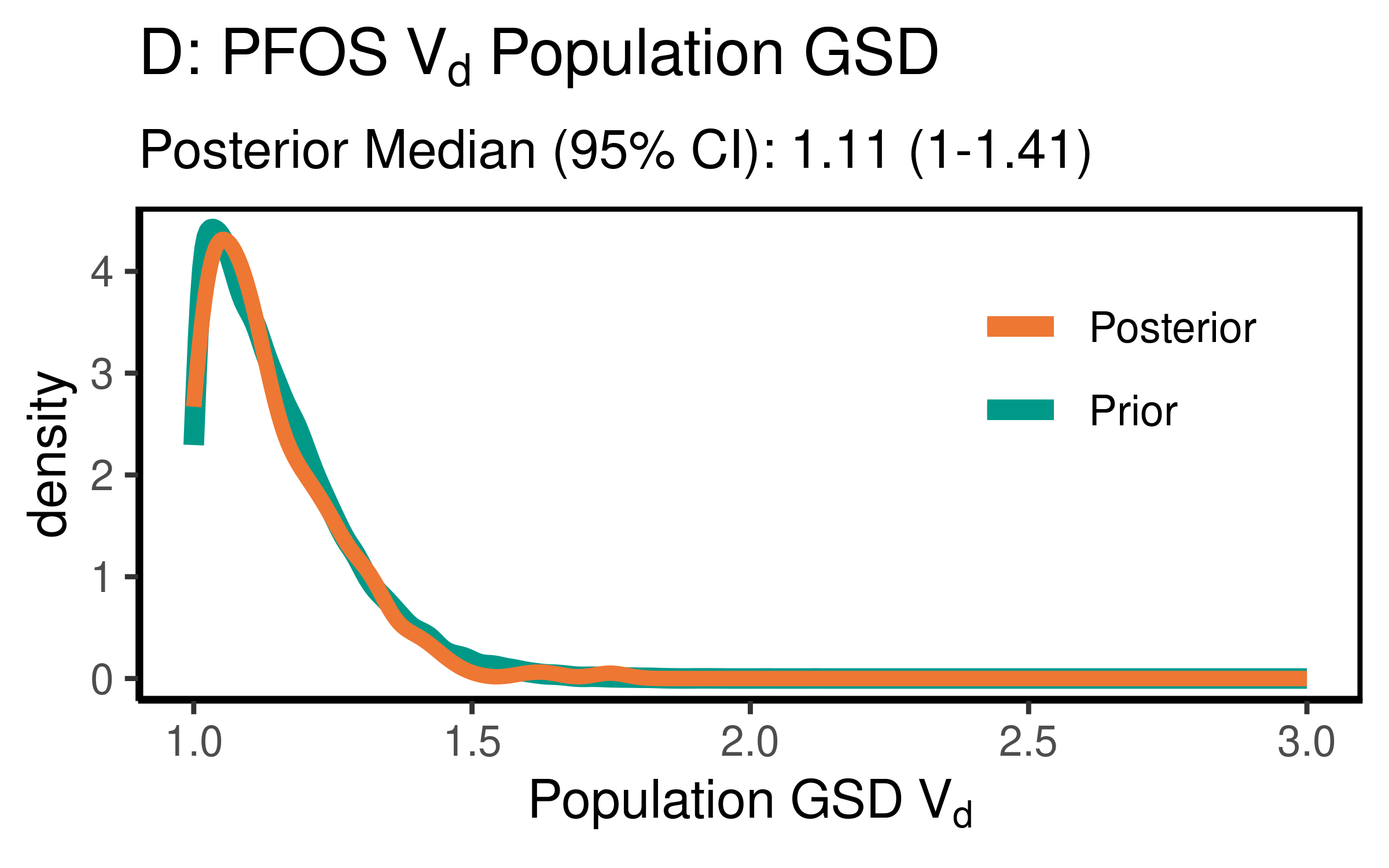
For PFOS, the data were not particularly informative, but slightly increased the estimate of the median to 0.308(0.223-0.548) slightly. They were not informative as to the population GSD, with the posterior distributions essentially unchanged from the priors.

PFOS\_priors$Vd\_GM <- rlnorm(50000,  
 meanlog=-1.46968,  
 sdlog=0.2624)  
PFOS\_Vd\_GM <- exp(dat$`M\_ln\_Vd(1)`)  
  
   
  
PFOS\_vd\_gm\_pr\_med <- signif(median(PFOS\_priors$Vd\_GM,3))  
PFOS\_vd\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFOS\_priors$Vd\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
PFOS\_vd\_gm\_med <- signif(median(PFOS\_Vd\_GM),3)  
PFOS\_vd\_gm\_med\_95ci <- paste(signif(quantile(PFOS\_Vd\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(Vd\_GM, color = "Prior"),data=PFOS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOS\_Vd\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,1)+labs(title = bquote("C: PFOS"~V[d]~"Population GM"),  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFOS\_vd\_gm\_med," (",   
 PFOS\_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, "PFOS\_vd\_gm.pdf")), p, dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFOS\_vd\_gm.png")), p, dpi=600)

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

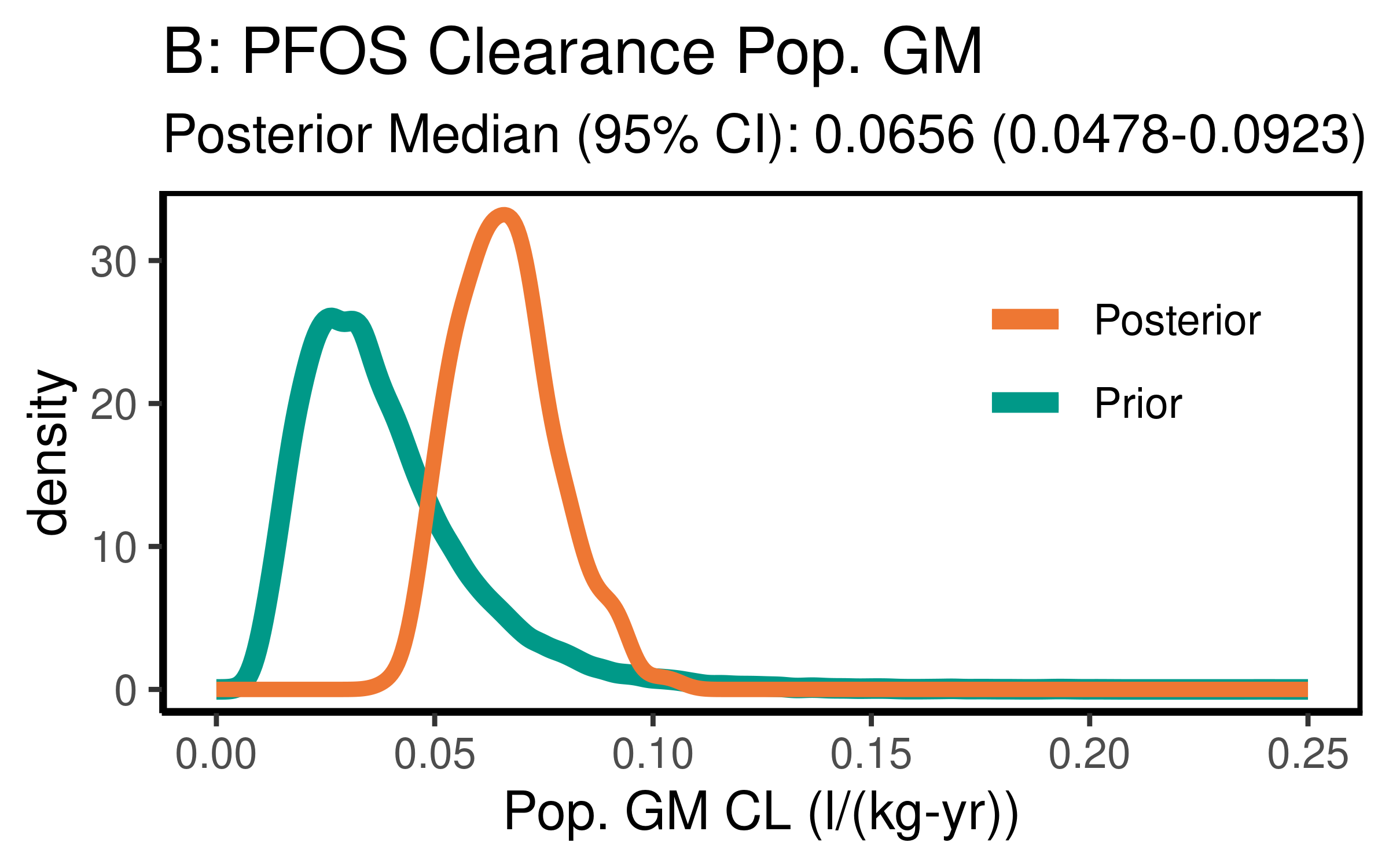


ggsave(here ("output-plots",paste0( sa, "PFOS\_vd\_gsd.pdf")), p, dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFOS\_vd\_gsd.png")), p, dpi=600)

### Clearance

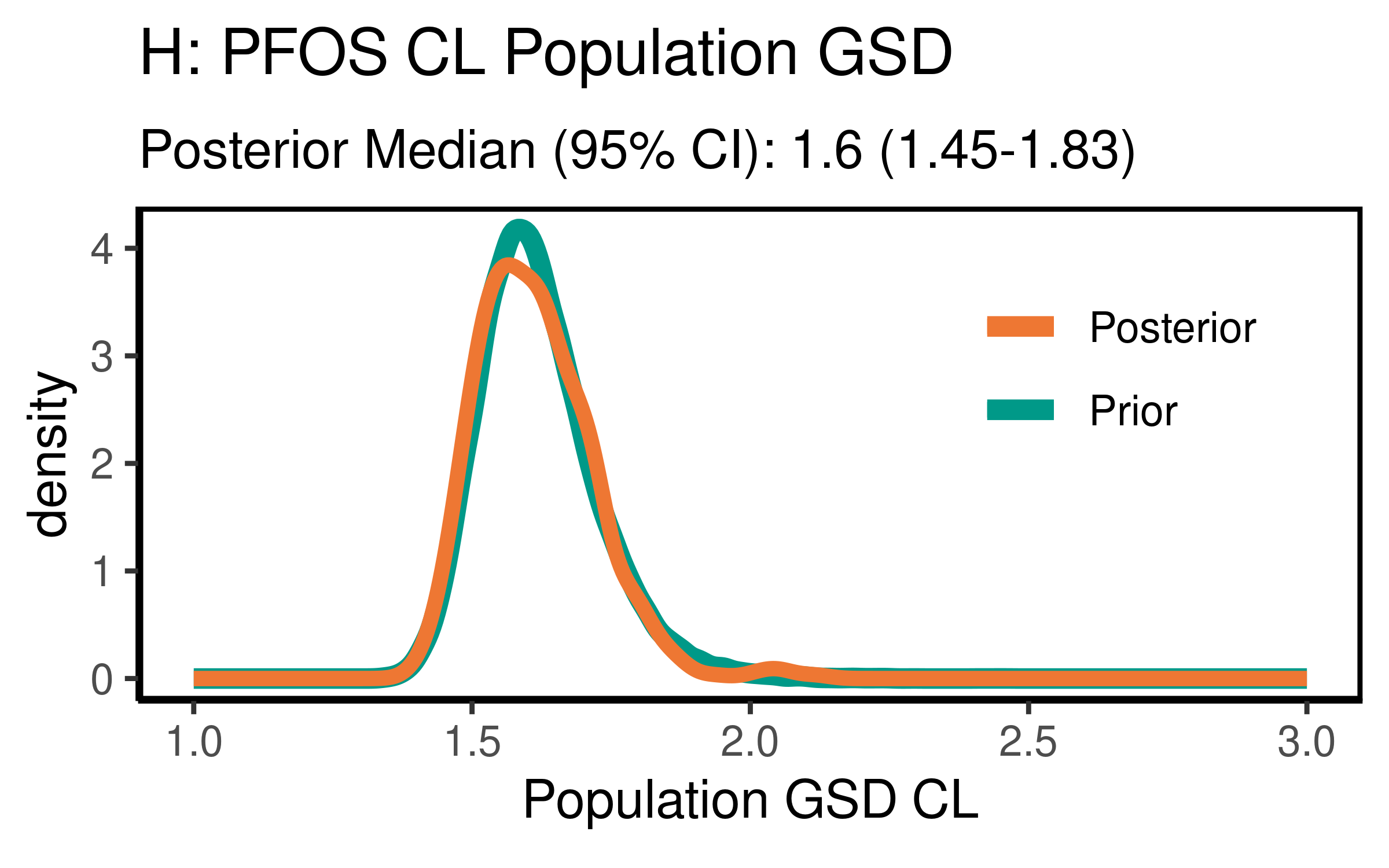
Cl is k \* Vd

PFOS\_priors$CL\_GM <- PFOS\_priors$Vd\_GM \* (log(2)/PFOS\_priors$halflife\_GM)  
PFOS\_CL\_GM <- exp(dat$`M\_ln\_Vd(1)` + dat$`M\_ln\_k(1)`)  
  
PFOS\_cl\_gm\_pr\_med <- signif(median(PFOS\_priors$CL\_GM,3))  
PFOS\_cl\_gm\_pr\_med\_95ci <- paste(signif(quantile(PFOS\_priors$CL\_GM,  
 prob=c(0.025,0.975)), 3), collapse="-")  
PFOS\_cl\_gm\_med <- signif(median(PFOS\_CL\_GM),3)  
PFOS\_cl\_gm\_med\_95ci <- paste(signif(quantile(PFOS\_CL\_GM,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(CL\_GM, color = "Prior"),data=PFOS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOS\_CL\_GM,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(0,0.25)+labs(title = "B: PFOS Clearance Pop. GM ",subtitle=paste("Posterior Median (95% CI): ",  
 PFOS\_cl\_gm\_med," (",  
 PFOS\_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, "PFOS\_CL\_gm.pdf")), p, dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFOS\_CL\_gm.png")), p, dpi=600)

PFOS\_priors$CL\_GSD = exp(sqrt(log(PFOS\_priors$Vd\_GSD)^2 +   
 log(PFOS\_priors$halflife\_GSD)^2))  
PFOS\_CL\_GSD <- exp(sqrt(log(PFOS\_Vd\_GSD)^2 +   
 log(PFOS\_halflife\_GSD)^2))  
  
PFOS\_CL\_gsd\_pr\_med <- signif(median(PFOS\_priors$CL\_GSD,3))  
PFOS\_CL\_gsd\_pr\_med\_95ci <- paste(signif(quantile(PFOS\_priors$CL\_GSD,  
 prob=c(0.025,0.975)), 3), collapse="-")  
  
PFOS\_CL\_gsd\_med <- signif(median(PFOS\_CL\_GSD),3)  
PFOS\_CL\_gsd\_med\_95ci <- paste(signif(quantile(PFOS\_CL\_GSD,  
 prob=c(0.025,0.975)),3),collapse="-")  
  
p<-ggplot()+  
 stat\_density(aes(CL\_GSD, color = "Prior"),data=PFOS\_priors,geom="line",size=2)+  
 stat\_density(aes(PFOS\_CL\_GSD,stat(density), color = "Posterior"),geom="line",size=1.5)+  
 xlim(1,3)+  
 labs(title = bquote("H: PFOS"~CL~"Population GSD "),  
 subtitle=paste("Posterior Median (95% CI): ",  
 PFOS\_CL\_gsd\_med," (",  
 PFOS\_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,"PFOS\_CL\_gsd.pdf")) ,p,dpi=600)  
ggsave(here ("output-plots",paste0( sa,"PFOS\_CL\_gsd.png")) ,p,dpi=600)

## Table significant digit values

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

### Population median estimates [95% CI]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Prior GM | Posterior GM | Prior GSD | Posterior GSD |
| Half-life (years) | 4.62 | 3.42 | 1.56 | 1.57 |
| HL [95% CI] | [2.08-10.3] | [2.62-4.5] | [1.42-1.76] | [1.43-1.75] |
| Volume of distribution | 0.23 | 0.322 | 1.12 | 1.11 |
| [95% CI] | [0.137-0.384] | [0.221-0.47] | [1.01-1.46] | [1-1.41] |
| Clearance | 0.0344 | 0.0656 |  |  |
| [95% CI] | [0.0133-0.0894] | [0.0478-0.0923] | [] | [] |

### Individual Posterior estimates

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | median GM [95% CI] | GM calculator input | GSD individual |
| Half-life (years) | 3.35 [ 1.25-8.61 ] | 3.36 | 1.63 |
| Volume of distribution | 0.322 [ 0.184-0.547 ] | 0.321 | 1.3 |
| Clearance (L/kg-yr) | 0.067 [ 0.0245-0.176 ] [[ 0.0203-0.199 ]] | 0.0664 | 1.65 |

## ─ Session info ───────────────────────────────────────────────────────────────  
## setting value   
## version R version 3.6.3 (2020-02-29)   
## 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 2022-01-23   
##   
## ─ Packages ───────────────────────────────────────────────────────────────────  
## package \* version date lib source   
## assertthat 0.2.1 2019-03-21 [2] CRAN (R 3.6.3)  
## backports 1.2.1 2020-12-09 [2] CRAN (R 3.6.3)  
## bayesplot \* 1.8.0 2021-01-10 [2] CRAN (R 3.6.3)  
## broom 0.7.5 2021-02-19 [2] CRAN (R 3.6.3)  
## cachem 1.0.4 2021-02-13 [2] CRAN (R 3.6.3)  
## callr 3.5.1 2020-10-13 [2] CRAN (R 3.6.3)  
## cellranger 1.1.0 2016-07-27 [2] CRAN (R 3.6.3)  
## cli 2.3.1 2021-02-23 [2] CRAN (R 3.6.3)  
## coda \* 0.19-4 2020-09-30 [2] CRAN (R 3.6.3)  
## colorspace 2.0-0 2020-11-11 [2] CRAN (R 3.6.3)  
## crayon 1.4.1 2021-02-08 [2] CRAN (R 3.6.3)  
## DBI 1.1.1 2021-01-15 [2] CRAN (R 3.6.3)  
## dbplyr 2.1.0 2021-02-03 [2] CRAN (R 3.6.3)  
## debugme 1.1.0 2017-10-22 [2] CRAN (R 3.6.3)  
## desc 1.3.0 2021-03-05 [2] CRAN (R 3.6.3)  
## devtools 2.3.2 2020-09-18 [2] CRAN (R 3.6.3)  
## digest 0.6.27 2020-10-24 [2] CRAN (R 3.6.3)  
## dplyr \* 1.0.5 2021-03-05 [2] CRAN (R 3.6.3)  
## ellipsis 0.3.1 2020-05-15 [2] CRAN (R 3.6.3)  
## evaluate 0.14 2019-05-28 [2] CRAN (R 3.6.3)  
## fansi 0.4.2 2021-01-15 [2] CRAN (R 3.6.3)  
## farver 2.1.0 2021-02-28 [2] CRAN (R 3.6.3)  
## fastmap 1.1.0 2021-01-25 [2] CRAN (R 3.6.3)  
## forcats \* 0.5.1 2021-01-27 [2] CRAN (R 3.6.3)  
## fs 1.5.0 2020-07-31 [2] CRAN (R 3.6.3)  
## generics 0.1.0 2020-10-31 [2] CRAN (R 3.6.3)  
## ggplot2 \* 3.3.3 2020-12-30 [2] CRAN (R 3.6.3)  
## ggridges 0.5.3 2021-01-08 [2] CRAN (R 3.6.3)  
## ggsci \* 2.9 2018-05-14 [2] CRAN (R 3.6.3)  
## glue 1.4.2 2020-08-27 [2] CRAN (R 3.6.3)  
## gtable 0.3.0 2019-03-25 [2] CRAN (R 3.6.3)  
## haven 2.3.1 2020-06-01 [2] CRAN (R 3.6.3)  
## here \* 1.0.1 2020-12-13 [2] CRAN (R 3.6.3)  
## highr 0.8 2019-03-20 [2] CRAN (R 3.6.3)  
## hms 1.0.0 2021-01-13 [2] CRAN (R 3.6.3)  
## htmltools 0.5.1.1 2021-01-22 [2] CRAN (R 3.6.3)  
## httr 1.4.2 2020-07-20 [2] CRAN (R 3.6.3)  
## jsonlite 1.7.2 2020-12-09 [2] CRAN (R 3.6.3)  
## khroma \* 1.7.0 2021-09-02 [1] CRAN (R 3.6.3)  
## knitr 1.31 2021-01-27 [2] CRAN (R 3.6.3)  
## labeling 0.4.2 2020-10-20 [2] CRAN (R 3.6.3)  
## lattice 0.20-41 2020-04-02 [2] CRAN (R 3.6.3)  
## lifecycle 1.0.0 2021-02-15 [2] CRAN (R 3.6.3)  
## lubridate 1.7.10 2021-02-26 [2] CRAN (R 3.6.3)  
## magrittr 2.0.1 2020-11-17 [2] CRAN (R 3.6.3)  
## memoise 2.0.0 2021-01-26 [2] CRAN (R 3.6.3)  
## modelr 0.1.8 2020-05-19 [2] CRAN (R 3.6.3)  
## munsell 0.5.0 2018-06-12 [2] CRAN (R 3.6.3)  
## pillar 1.5.1 2021-03-05 [2] CRAN (R 3.6.3)  
## pkgbuild 1.2.0 2020-12-15 [2] CRAN (R 3.6.3)  
## pkgconfig 2.0.3 2019-09-22 [2] CRAN (R 3.6.3)  
## pkgload 1.2.0 2021-02-23 [2] CRAN (R 3.6.3)  
## plyr 1.8.6 2020-03-03 [2] CRAN (R 3.6.3)  
## prettyunits 1.1.1 2020-01-24 [2] CRAN (R 3.6.3)  
## pROC 1.17.0.1 2021-01-13 [2] CRAN (R 3.6.3)  
## processx 3.4.5 2020-11-30 [2] CRAN (R 3.6.3)  
## ps 1.6.0 2021-02-28 [2] CRAN (R 3.6.3)  
## purrr \* 0.3.4 2020-04-17 [2] CRAN (R 3.6.3)  
## R6 2.5.0 2020-10-28 [2] CRAN (R 3.6.3)  
## Rcpp 1.0.6 2021-01-15 [2] CRAN (R 3.6.3)  
## readr \* 1.4.0 2020-10-05 [2] CRAN (R 3.6.3)  
## readxl 1.3.1 2019-03-13 [2] CRAN (R 3.6.3)  
## remotes 2.2.0 2020-07-21 [2] CRAN (R 3.6.3)  
## reprex 1.0.0 2021-01-27 [2] CRAN (R 3.6.3)  
## reshape2 \* 1.4.4 2020-04-09 [2] CRAN (R 3.6.3)  
## rlang 0.4.10 2020-12-30 [2] CRAN (R 3.6.3)  
## rmarkdown 2.7 2021-02-19 [2] CRAN (R 3.6.3)  
## rprojroot 2.0.2 2020-11-15 [2] CRAN (R 3.6.3)  
## rstudioapi 0.13 2020-11-12 [2] CRAN (R 3.6.3)  
## rvest 1.0.0 2021-03-09 [2] CRAN (R 3.6.3)  
## scales 1.1.1 2020-05-11 [2] CRAN (R 3.6.3)  
## sessioninfo 1.1.1 2018-11-05 [2] CRAN (R 3.6.3)  
## stringi 1.5.3 2020-09-09 [2] CRAN (R 3.6.3)  
## stringr \* 1.4.0 2019-02-10 [2] CRAN (R 3.6.3)  
## testthat 3.0.2 2021-02-14 [2] CRAN (R 3.6.3)  
## tibble \* 3.1.0 2021-02-25 [2] CRAN (R 3.6.3)  
## tidyr \* 1.1.3 2021-03-03 [2] CRAN (R 3.6.3)  
## tidyselect 1.1.0 2020-05-11 [2] CRAN (R 3.6.3)  
## tidyverse \* 1.3.0 2019-11-21 [2] CRAN (R 3.6.3)  
## usethis 2.0.1 2021-02-10 [2] CRAN (R 3.6.3)  
## utf8 1.2.1 2021-03-12 [2] CRAN (R 3.6.3)  
## vctrs 0.3.6 2020-12-17 [2] CRAN (R 3.6.3)  
## withr 2.4.1 2021-01-26 [2] CRAN (R 3.6.3)  
## xfun 0.22 2021-03-11 [2] CRAN (R 3.6.3)  
## xml2 1.3.2 2020-04-23 [2] CRAN (R 3.6.3)  
## yaml 2.2.1 2020-02-01 [2] CRAN (R 3.6.3)  
## yardstick \* 0.0.9 2021-11-22 [1] CRAN (R 3.6.3)  
##   
## [1] /home/ad.abt.local/layc/R/x86\_64-pc-linux-gnu-library/3.6  
## [2] /opt/R/3.6.3/lib64/R/library