PFOA 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) # for colors  
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/PFOA\_1cpt\_v8

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

Set up MCSim file

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

## The mod.exe had been created.

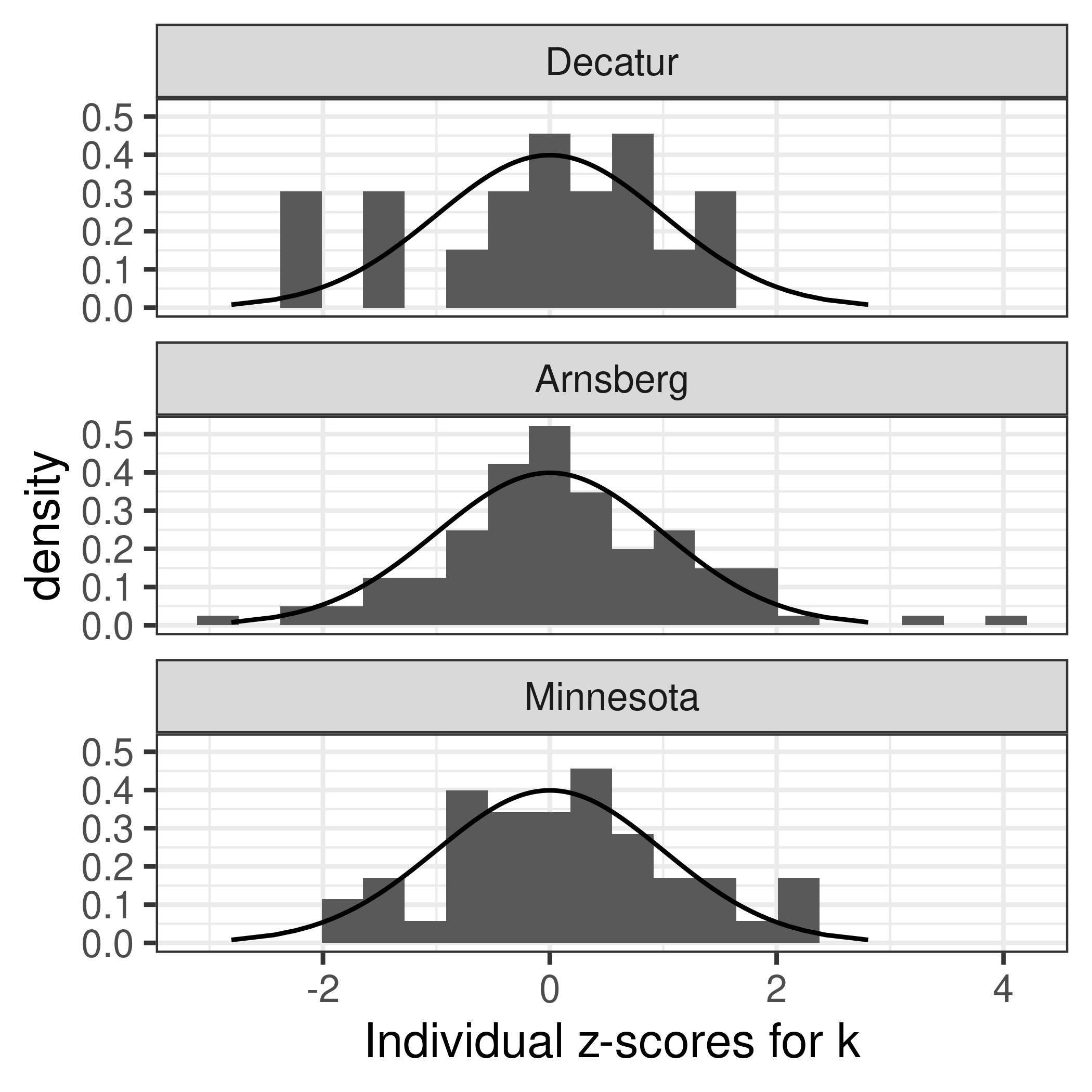
## Set filenames and load data

## Set up dataset

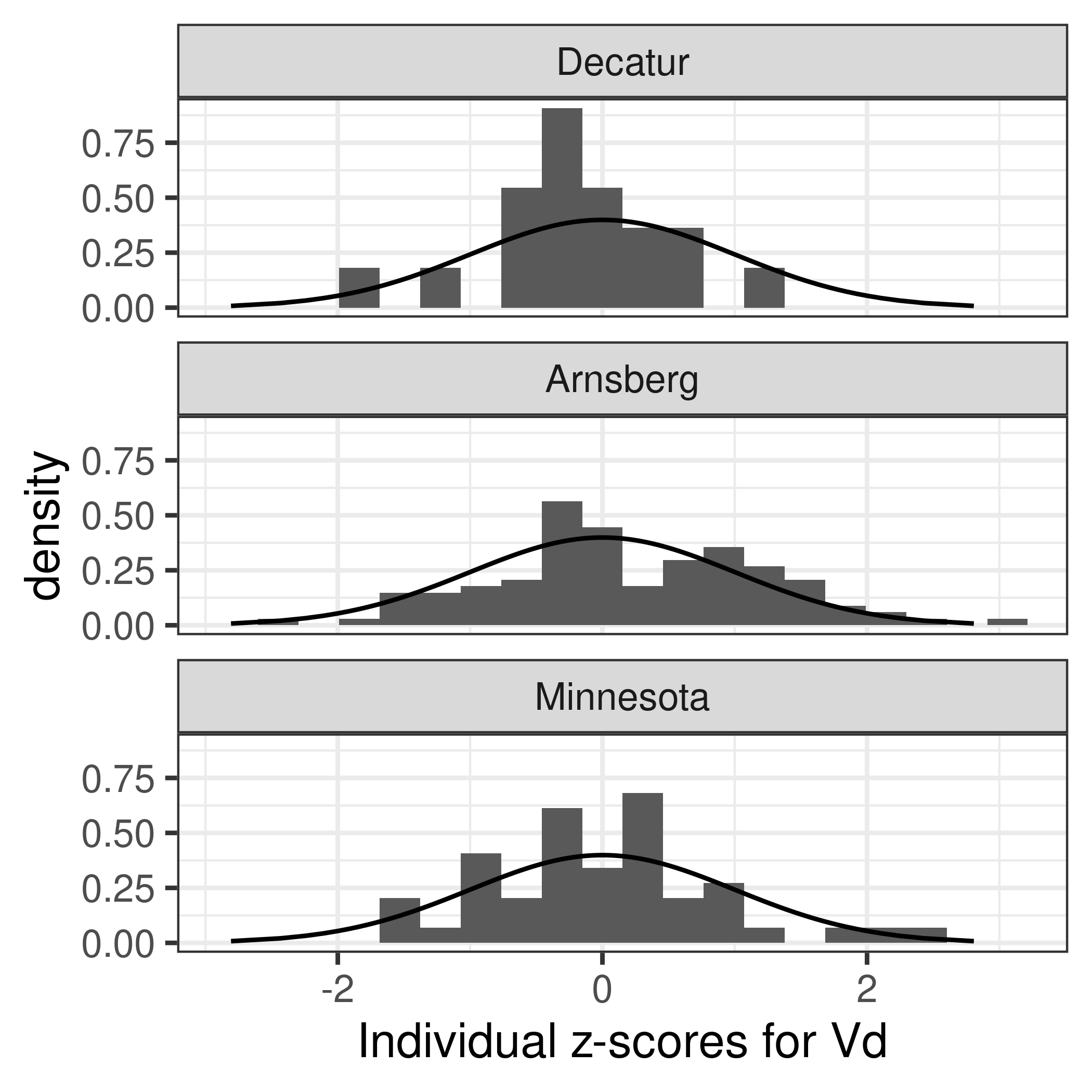
id\_lut <- multicheck$df\_check %>% select(Level) %>% unique () %>%  
 mutate(dataset = c(   
 rep("Decatur M Train", 9),  
 rep("Decatur F Train", 9),  
 rep("Arnsberg M Train", 41),  
 rep("Arnsberg F Train", 69),  
 rep("Decatur M Test", 9),  
 rep("Decatur F Test", 10),  
 rep("Arnsberg M Test",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

## 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\_PFOA.pdf")),iplotk,dpi=600)

## Saving 3.5 x 3.5 in image

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

## Saving 3.5 x 3.5 in image

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

## Saving 3.5 x 3.5 in image

ggsave(file.path("output-plots",  
 paste0( sa,"Indiv\_zscores\_Vd\_PFOA.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 make sure “City” appeared.

nrow(multicheck$df\_check)

## [1] 312000

nrow(id\_lut)

## [1] 361

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

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

## [1] 312000

names(multicheck$df\_check)

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

multicheck2 <- multicheck$df\_check %>%   
 left\_join(id\_lut, by = c("Level", "Simulation"))%>%   
 group\_by\_at ( vars(-Prediction)) %>%   
 summarise(Prediction = median(Prediction)) %>%  
 ungroup() %>%  
 group\_by(City) %>%   
 mutate(Train\_Test = factor(Train\_Test, levels = c("Train", "Test")),  
 `City (datatype)` = case\_when(datatype == 'Individual' ~ paste0('\n', City, "\n(", datatype, ")") ,  
 datatype == 'Summary' & grepl('-', as.character(City)) ~ paste0(gsub('-', '\n', City),"" ),  
 TRUE ~ as.character(City)),  
 `City (datatype)` = factor ( `City (datatype)`),  
 label = case\_when(Train\_Test=="Train" ~ "A: PFOA Train",  
 Train\_Test=="Test" ~ "B: PFOA 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` %in%  
 c("Lubeck-Bartell", "Little Hocking-Bartell", "Little Hocking-Emmett") ~ 0,  
 datatype == "Summary" & `City` == "Paulsboro" ~ 1,  
 TRUE ~ 18 ),   
 size = if\_else(datatype =="Individual", 1.75, 2.5 ) )

## `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 ) +   
 theme(  
 legend.text = element\_text(  
 margin = margin(t = 2, b = 2, unit = "pt")) )

## Loading required package: scales

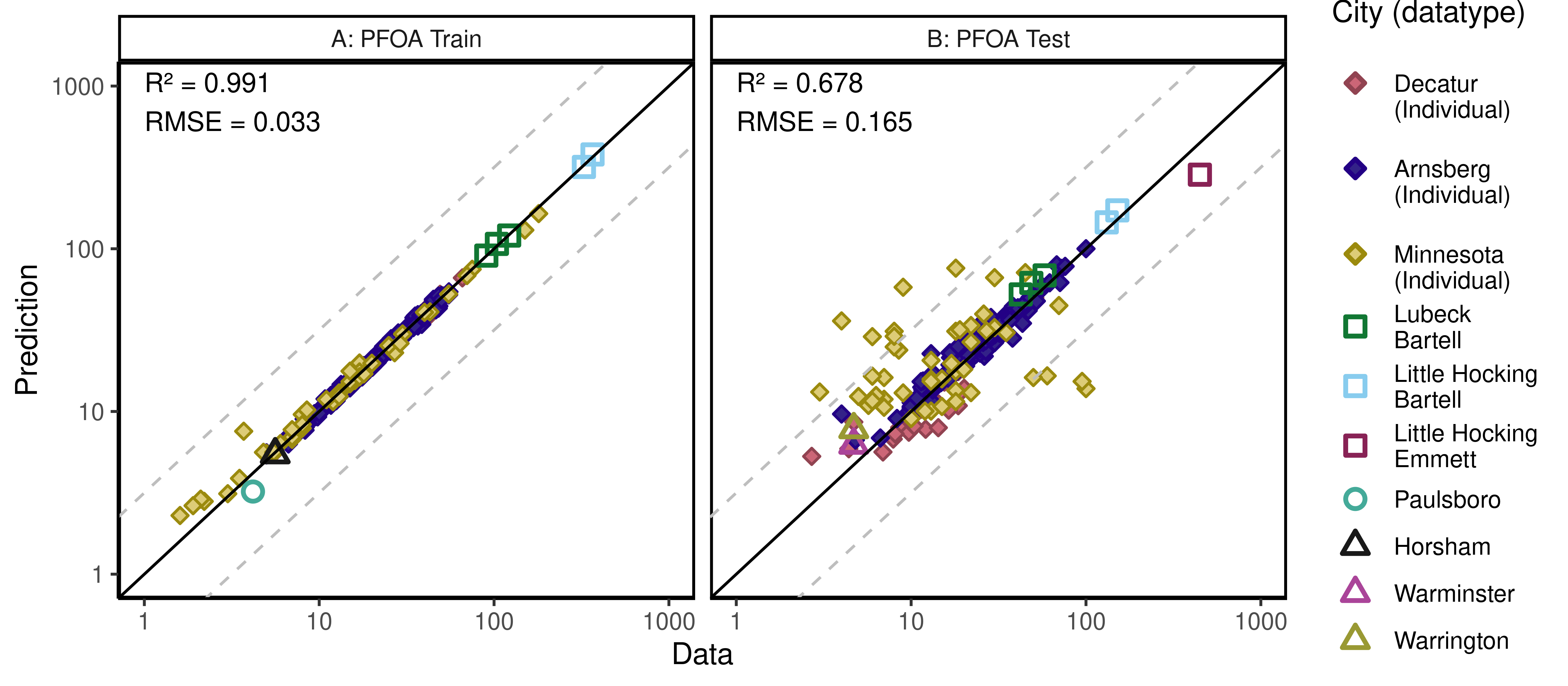
##   
## Attaching package: 'scales'

## 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"

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

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

## Level Simulation Output\_Var Time Data Level...1 Level...2  
## 1 1\_1\_1 1 Cserum\_t 0.000000 41.000 1\_1\_1 1\_1\_1  
## 2 1\_1\_1 1 Cserum\_t 5.802000 29.300 1\_1\_1 1\_1\_1  
## 3 1\_1\_2 2 Cserum\_t 0.000000 13.100 1\_1\_2 1\_1\_2  
## 4 1\_1\_2 2 Cserum\_t 5.802000 10.300 1\_1\_2 1\_1\_2  
## 5 1\_1\_3 3 Cserum\_t 0.000000 25.700 1\_1\_3 1\_1\_3  
## 6 1\_1\_3 3 Cserum\_t 5.802000 10.100 1\_1\_3 1\_1\_3  
## 7 1\_1\_4 4 Cserum\_t 0.000000 47.700 1\_1\_4 1\_1\_4  
## 8 1\_1\_4 4 Cserum\_t 5.802000 11.300 1\_1\_4 1\_1\_4  
## 9 1\_1\_5 5 Cserum\_t 0.000000 51.200 1\_1\_5 1\_1\_5  
## 10 1\_1\_5 5 Cserum\_t 5.802000 19.300 1\_1\_5 1\_1\_5  
## 11 1\_1\_6 6 Cserum\_t 0.000000 12.600 1\_1\_6 1\_1\_6  
## 12 1\_1\_6 6 Cserum\_t 5.802000 9.800 1\_1\_6 1\_1\_6  
## 13 1\_1\_7 7 Cserum\_t 0.000000 44.300 1\_1\_7 1\_1\_7  
## 14 1\_1\_7 7 Cserum\_t 5.802000 12.700 1\_1\_7 1\_1\_7  
## 15 1\_1\_8 8 Cserum\_t 0.000000 47.400 1\_1\_8 1\_1\_8  
## 16 1\_1\_8 8 Cserum\_t 5.802000 15.600 1\_1\_8 1\_1\_8  
## 17 1\_1\_9 9 Cserum\_t 0.000000 19.600 1\_1\_9 1\_1\_9  
## 18 1\_1\_9 9 Cserum\_t 5.802000 12.700 1\_1\_9 1\_1\_9  
## 19 1\_1\_10 10 Cserum\_t 0.000000 7.600 1\_1\_10 1\_1\_10  
## 20 1\_1\_10 10 Cserum\_t 5.802000 5.500 1\_1\_10 1\_1\_10  
## 21 1\_1\_11 11 Cserum\_t 0.000000 46.100 1\_1\_11 1\_1\_11  
## 22 1\_1\_11 11 Cserum\_t 5.802000 30.900 1\_1\_11 1\_1\_11  
## 23 1\_1\_12 12 Cserum\_t 0.000000 10.900 1\_1\_12 1\_1\_12  
## 24 1\_1\_12 12 Cserum\_t 5.802000 9.800 1\_1\_12 1\_1\_12  
## 25 1\_1\_13 13 Cserum\_t 0.000000 6.700 1\_1\_13 1\_1\_13  
## 26 1\_1\_13 13 Cserum\_t 5.802000 7.300 1\_1\_13 1\_1\_13  
## 27 1\_1\_14 14 Cserum\_t 0.000000 65.900 1\_1\_14 1\_1\_14  
## 28 1\_1\_14 14 Cserum\_t 5.802000 31.500 1\_1\_14 1\_1\_14  
## 29 1\_1\_15 15 Cserum\_t 0.000000 49.100 1\_1\_15 1\_1\_15  
## 30 1\_1\_15 15 Cserum\_t 5.802000 42.400 1\_1\_15 1\_1\_15  
## 31 1\_1\_16 16 Cserum\_t 0.000000 13.000 1\_1\_16 1\_1\_16  
## 32 1\_1\_16 16 Cserum\_t 5.802000 8.500 1\_1\_16 1\_1\_16  
## 33 1\_1\_17 17 Cserum\_t 0.000000 45.500 1\_1\_17 1\_1\_17  
## 34 1\_1\_17 17 Cserum\_t 5.802000 17.700 1\_1\_17 1\_1\_17  
## 35 1\_1\_18 18 Cserum\_t 0.000000 34.300 1\_1\_18 1\_1\_18  
## 36 1\_1\_18 18 Cserum\_t 5.802000 15.000 1\_1\_18 1\_1\_18  
## 37 1\_2\_1 19 Cserum\_t 0.000000 15.700 1\_2\_1 1\_2\_1  
## 38 1\_2\_1 19 Cserum\_t 0.982900 16.000 1\_2\_1 1\_2\_1  
## 39 1\_2\_2 20 Cserum\_t 0.000000 14.300 1\_2\_2 1\_2\_2  
## 40 1\_2\_2 20 Cserum\_t 0.982900 15.000 1\_2\_2 1\_2\_2  
## 41 1\_2\_3 21 Cserum\_t 0.000000 40.500 1\_2\_3 1\_2\_3  
## 42 1\_2\_3 21 Cserum\_t 0.982900 32.000 1\_2\_3 1\_2\_3  
## 43 1\_2\_4 22 Cserum\_t 0.000000 45.000 1\_2\_4 1\_2\_4  
## 44 1\_2\_4 22 Cserum\_t 0.982900 48.000 1\_2\_4 1\_2\_4  
## 45 1\_2\_5 23 Cserum\_t 0.000000 38.330 1\_2\_5 1\_2\_5  
## 46 1\_2\_5 23 Cserum\_t 0.982900 32.000 1\_2\_5 1\_2\_5  
## 47 1\_2\_6 24 Cserum\_t 0.000000 16.500 1\_2\_6 1\_2\_6  
## 48 1\_2\_6 24 Cserum\_t 0.982900 13.600 1\_2\_6 1\_2\_6  
## 49 1\_2\_7 25 Cserum\_t 0.000000 40.200 1\_2\_7 1\_2\_7  
## 50 1\_2\_7 25 Cserum\_t 0.982900 35.700 1\_2\_7 1\_2\_7  
## 51 1\_2\_8 26 Cserum\_t 0.000000 21.400 1\_2\_8 1\_2\_8  
## 52 1\_2\_8 26 Cserum\_t 0.982900 16.300 1\_2\_8 1\_2\_8  
## 53 1\_2\_9 27 Cserum\_t 0.000000 45.000 1\_2\_9 1\_2\_9  
## 54 1\_2\_9 27 Cserum\_t 0.982900 46.500 1\_2\_9 1\_2\_9  
## 55 1\_2\_10 28 Cserum\_t 0.000000 11.670 1\_2\_10 1\_2\_10  
## 56 1\_2\_10 28 Cserum\_t 0.982900 8.200 1\_2\_10 1\_2\_10  
## 57 1\_2\_11 29 Cserum\_t 0.000000 21.300 1\_2\_11 1\_2\_11  
## 58 1\_2\_11 29 Cserum\_t 0.982900 20.000 1\_2\_11 1\_2\_11  
## 59 1\_2\_12 30 Cserum\_t 0.000000 21.500 1\_2\_12 1\_2\_12  
## 60 1\_2\_12 30 Cserum\_t 0.982900 16.000 1\_2\_12 1\_2\_12  
## 61 1\_2\_13 31 Cserum\_t 0.000000 26.900 1\_2\_13 1\_2\_13  
## 62 1\_2\_13 31 Cserum\_t 0.982900 20.300 1\_2\_13 1\_2\_13  
## 63 1\_2\_14 32 Cserum\_t 0.000000 13.300 1\_2\_14 1\_2\_14  
## 64 1\_2\_14 32 Cserum\_t 0.982900 11.670 1\_2\_14 1\_2\_14  
## 65 1\_2\_15 33 Cserum\_t 0.000000 23.330 1\_2\_15 1\_2\_15  
## 66 1\_2\_15 33 Cserum\_t 0.982900 18.330 1\_2\_15 1\_2\_15  
## 67 1\_2\_16 34 Cserum\_t 0.000000 50.000 1\_2\_16 1\_2\_16  
## 68 1\_2\_16 34 Cserum\_t 0.982900 46.800 1\_2\_16 1\_2\_16  
## 69 1\_2\_17 35 Cserum\_t 0.000000 31.500 1\_2\_17 1\_2\_17  
## 70 1\_2\_17 35 Cserum\_t 0.982900 30.000 1\_2\_17 1\_2\_17  
## 71 1\_2\_18 36 Cserum\_t 0.000000 7.500 1\_2\_18 1\_2\_18  
## 72 1\_2\_18 36 Cserum\_t 0.982900 7.500 1\_2\_18 1\_2\_18  
## 73 1\_2\_19 37 Cserum\_t 0.000000 9.500 1\_2\_19 1\_2\_19  
## 74 1\_2\_19 37 Cserum\_t 0.982900 8.000 1\_2\_19 1\_2\_19  
## 75 1\_2\_20 38 Cserum\_t 0.000000 26.670 1\_2\_20 1\_2\_20  
## 76 1\_2\_20 38 Cserum\_t 0.982900 23.330 1\_2\_20 1\_2\_20  
## 77 1\_2\_21 39 Cserum\_t 0.000000 11.670 1\_2\_21 1\_2\_21  
## 78 1\_2\_21 39 Cserum\_t 0.982900 10.000 1\_2\_21 1\_2\_21  
## 79 1\_2\_22 40 Cserum\_t 0.000000 15.000 1\_2\_22 1\_2\_22  
## 80 1\_2\_22 40 Cserum\_t 0.982900 13.330 1\_2\_22 1\_2\_22  
## 81 1\_2\_23 41 Cserum\_t 0.000000 9.400 1\_2\_23 1\_2\_23  
## 82 1\_2\_23 41 Cserum\_t 0.982900 9.800 1\_2\_23 1\_2\_23  
## 83 1\_2\_24 42 Cserum\_t 0.000000 41.670 1\_2\_24 1\_2\_24  
## 84 1\_2\_24 42 Cserum\_t 0.982900 38.000 1\_2\_24 1\_2\_24  
## 85 1\_2\_25 43 Cserum\_t 0.000000 45.000 1\_2\_25 1\_2\_25  
## 86 1\_2\_25 43 Cserum\_t 0.982900 46.500 1\_2\_25 1\_2\_25  
## 87 1\_2\_26 44 Cserum\_t 0.000000 13.500 1\_2\_26 1\_2\_26  
## 88 1\_2\_26 44 Cserum\_t 0.982900 11.670 1\_2\_26 1\_2\_26  
## 89 1\_2\_27 45 Cserum\_t 0.000000 30.000 1\_2\_27 1\_2\_27  
## 90 1\_2\_27 45 Cserum\_t 0.982900 26.500 1\_2\_27 1\_2\_27  
## 91 1\_2\_28 46 Cserum\_t 0.000000 31.300 1\_2\_28 1\_2\_28  
## 92 1\_2\_28 46 Cserum\_t 0.982900 28.300 1\_2\_28 1\_2\_28  
## 93 1\_2\_29 47 Cserum\_t 0.000000 21.300 1\_2\_29 1\_2\_29  
## 94 1\_2\_29 47 Cserum\_t 0.982900 20.500 1\_2\_29 1\_2\_29  
## 95 1\_2\_30 48 Cserum\_t 0.000000 45.000 1\_2\_30 1\_2\_30  
## 96 1\_2\_30 48 Cserum\_t 0.982900 40.500 1\_2\_30 1\_2\_30  
## 97 1\_2\_31 49 Cserum\_t 0.000000 38.330 1\_2\_31 1\_2\_31  
## 98 1\_2\_31 49 Cserum\_t 0.982900 36.500 1\_2\_31 1\_2\_31  
## 99 1\_2\_32 50 Cserum\_t 0.000000 18.000 1\_2\_32 1\_2\_32  
## 100 1\_2\_32 50 Cserum\_t 0.982900 16.670 1\_2\_32 1\_2\_32  
## 101 1\_2\_33 51 Cserum\_t 0.000000 36.700 1\_2\_33 1\_2\_33  
## 102 1\_2\_33 51 Cserum\_t 0.982900 33.500 1\_2\_33 1\_2\_33  
## 103 1\_2\_34 52 Cserum\_t 0.000000 34.800 1\_2\_34 1\_2\_34  
## 104 1\_2\_34 52 Cserum\_t 0.982900 36.670 1\_2\_34 1\_2\_34  
## 105 1\_2\_35 53 Cserum\_t 0.000000 38.600 1\_2\_35 1\_2\_35  
## 106 1\_2\_35 53 Cserum\_t 0.982900 36.300 1\_2\_35 1\_2\_35  
## 107 1\_2\_36 54 Cserum\_t 0.000000 6.670 1\_2\_36 1\_2\_36  
## 108 1\_2\_36 54 Cserum\_t 0.982900 6.670 1\_2\_36 1\_2\_36  
## 109 1\_2\_37 55 Cserum\_t 0.000000 45.200 1\_2\_37 1\_2\_37  
## 110 1\_2\_37 55 Cserum\_t 0.982900 46.700 1\_2\_37 1\_2\_37  
## 111 1\_2\_38 56 Cserum\_t 0.000000 15.000 1\_2\_38 1\_2\_38  
## 112 1\_2\_38 56 Cserum\_t 0.982900 14.700 1\_2\_38 1\_2\_38  
## 113 1\_2\_39 57 Cserum\_t 0.000000 22.000 1\_2\_39 1\_2\_39  
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## 613 1\_8\_1 354 M\_Cserum 0.000000 58.000 1\_8\_1 1\_8\_1  
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## 618 1\_10\_1 356 M\_Cserum 0.000000 151.110 1\_10\_1 1\_10\_1  
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## 622 1\_13\_1 359 M\_Cbgd\_Css 2.000000 5.604 1\_13\_1 1\_13\_1  
## 623 1\_14\_1 360 M\_Cbgd\_Css 2.000000 4.696 1\_14\_1 1\_14\_1  
## 624 1\_15\_1 361 M\_Cbgd\_Css 2.000000 4.696 1\_15\_1 1\_15\_1  
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## 612 Lubeck-Bartell-Train Mixed (all sexes) Lubeck-Bartell  
## 613 Lubeck-Bartell-Test Mixed (all sexes) Lubeck-Bartell  
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## 620 Little Hocking-Emmett-Test Mixed (all sexes) Little Hocking-Emmett  
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## 622 Horsham-Train Mixed (all sexes) Horsham  
## 623 Warminster-Test Mixed (all sexes) Warminster  
## 624 Warrington-Train Mixed (all sexes) Warrington  
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## 383 Arnsberg F Test 192.T=0  
## 384 Arnsberg F Test 192.T=0.9829  
## 385 Arnsberg F Test 193.T=0  
## 386 Arnsberg F Test 193.T=0.9829  
## 387 Arnsberg F Test 194.T=0  
## 388 Arnsberg F Test 194.T=0.9829  
## 389 Arnsberg F Test 195.T=0  
## 390 Arnsberg F Test 195.T=0.9829  
## 391 Arnsberg F Test 196.T=0  
## 392 Arnsberg F Test 196.T=0.9829  
## 393 Arnsberg F Test 197.T=0  
## 394 Arnsberg F Test 197.T=0.9829  
## 395 Arnsberg F Test 198.T=0  
## 396 Arnsberg F Test 198.T=0.9829  
## 397 Arnsberg F Test 199.T=0  
## 398 Arnsberg F Test 199.T=0.9829  
## 399 Arnsberg F Test 200.T=0  
## 400 Arnsberg F Test 200.T=0.9829  
## 401 Arnsberg F Test 201.T=0  
## 402 Arnsberg F Test 201.T=0.9829  
## 403 Arnsberg F Test 202.T=0  
## 404 Arnsberg F Test 202.T=0.9829  
## 405 Arnsberg F Test 203.T=0  
## 406 Arnsberg F Test 203.T=0.9829  
## 407 Arnsberg F Test 204.T=0  
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## 411 Arnsberg F Test 206.T=0  
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## 419 Arnsberg F Test 210.T=0  
## 420 Arnsberg F Test 210.T=0.9829  
## 421 Arnsberg F Test 211.T=0  
## 422 Arnsberg F Test 211.T=0.9829  
## 423 Arnsberg F Test 212.T=0  
## 424 Arnsberg F Test 212.T=0.9829  
## 425 Arnsberg F Test 213.T=0  
## 426 Arnsberg F Test 213.T=0.9829  
## 427 Arnsberg F Test 214.T=0  
## 428 Arnsberg F Test 214.T=0.9829  
## 429 Arnsberg F Test 215.T=0  
## 430 Arnsberg F Test 215.T=0.9829  
## 431 Arnsberg F Test 216.T=0  
## 432 Arnsberg F Test 216.T=0.9829  
## 433 Arnsberg F Test 217.T=0  
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## 435 Arnsberg F Test 218.T=0  
## 436 Arnsberg F Test 218.T=0.9829  
## 437 Arnsberg F Test 219.T=0  
## 438 Arnsberg F Test 219.T=0.9829  
## 439 Arnsberg F Test 220.T=0  
## 440 Arnsberg F Test 220.T=0.9829  
## 441 Arnsberg F Test 221.T=0  
## 442 Arnsberg F Test 221.T=0.9829  
## 443 Arnsberg F Test 222.T=0  
## 444 Arnsberg F Test 222.T=0.9829  
## 445 Arnsberg F Test 223.T=0  
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## 447 Arnsberg F Test 224.T=0  
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## 450 Arnsberg F Test 225.T=0.9829  
## 451 Arnsberg F Test 226.T=0  
## 452 Arnsberg F Test 226.T=0.9829  
## 453 Arnsberg F Test 227.T=0  
## 454 Arnsberg F Test 227.T=0.9829  
## 455 Arnsberg F Test 228.T=0  
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## 459 Arnsberg F Test 230.T=0  
## 460 Arnsberg F Test 230.T=0.9829  
## 461 Arnsberg F Test 231.T=0  
## 462 Arnsberg F Test 231.T=0.9829  
## 463 Arnsberg F Test 232.T=0  
## 464 Arnsberg F Test 232.T=0.9829  
## 465 Arnsberg F Test 233.T=0  
## 466 Arnsberg F Test 233.T=0.9829  
## 467 Arnsberg F Test 234.T=0  
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## 469 Arnsberg F Test 235.T=0  
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## 472 Arnsberg F Test 236.T=0.9829  
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## 474 Arnsberg F Test 237.T=0.9829  
## 475 Arnsberg F Test 238.T=0  
## 476 Arnsberg F Test 238.T=0.9829  
## 477 Arnsberg F Test 239.T=0  
## 478 Arnsberg F Test 239.T=0.9829  
## 479 Arnsberg F Test 240.T=0  
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## 481 Arnsberg F Test 241.T=0  
## 482 Arnsberg F Test 241.T=0.9829  
## 483 Arnsberg F Test 242.T=0  
## 484 Arnsberg F Test 242.T=0.9829  
## 485 Arnsberg F Test 243.T=0  
## 486 Arnsberg F Test 243.T=0.9829  
## 487 Arnsberg F Test 244.T=0  
## 488 Arnsberg F Test 244.T=0.9829  
## 489 Arnsberg F Test 245.T=0  
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## 497 Arnsberg F Test 249.T=0  
## 498 Arnsberg F Test 249.T=0.9829  
## 499 Arnsberg F Test 250.T=0  
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## 505 Arnsberg F Test 253.T=0  
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## 509 Arnsberg F Test 255.T=0  
## 510 Arnsberg F Test 255.T=0.9829  
## 511 Arnsberg F Test 256.T=0  
## 512 Arnsberg F Test 256.T=0.9829  
## 513 Arnsberg F Test 257.T=0  
## 514 Arnsberg F Test 257.T=0.9829  
## 515 Minnesota Train 258.SteadyState  
## 516 Minnesota Train 259.SteadyState  
## 517 Minnesota Train 260.SteadyState  
## 518 Minnesota Train 261.SteadyState  
## 519 Minnesota Train 262.SteadyState  
## 520 Minnesota Train 263.SteadyState  
## 521 Minnesota Train 264.SteadyState  
## 522 Minnesota Train 265.SteadyState  
## 523 Minnesota Train 266.SteadyState  
## 524 Minnesota Train 267.SteadyState  
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## 526 Minnesota Train 269.SteadyState  
## 527 Minnesota Train 270.SteadyState  
## 528 Minnesota Train 271.SteadyState  
## 529 Minnesota Train 272.SteadyState  
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## 531 Minnesota Train 274.SteadyState  
## 532 Minnesota Train 275.SteadyState  
## 533 Minnesota Train 276.SteadyState  
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## 535 Minnesota Train 278.SteadyState  
## 536 Minnesota Train 279.SteadyState  
## 537 Minnesota Train 280.SteadyState  
## 538 Minnesota Train 281.SteadyState  
## 539 Minnesota Train 282.SteadyState  
## 540 Minnesota Train 283.SteadyState  
## 541 Minnesota Train 284.SteadyState  
## 542 Minnesota Train 285.SteadyState  
## 543 Minnesota Train 286.SteadyState  
## 544 Minnesota Train 287.SteadyState  
## 545 Minnesota Train 288.SteadyState  
## 546 Minnesota Train 289.SteadyState  
## 547 Minnesota Train 290.SteadyState  
## 548 Minnesota Train 291.SteadyState  
## 549 Minnesota Train 292.SteadyState  
## 550 Minnesota Train 293.SteadyState  
## 551 Minnesota Train 294.SteadyState  
## 552 Minnesota Train 295.SteadyState  
## 553 Minnesota Train 296.SteadyState  
## 554 Minnesota Train 297.SteadyState  
## 555 Minnesota Train 298.SteadyState  
## 556 Minnesota Train 299.SteadyState  
## 557 Minnesota Train 300.SteadyState  
## 558 Minnesota Train 301.SteadyState  
## 559 Minnesota Train 302.SteadyState  
## 560 Minnesota Train 303.SteadyState  
## 561 Minnesota Train 304.SteadyState  
## 562 Minnesota Train 305.SteadyState  
## 563 Minnesota Test 306.SteadyState  
## 564 Minnesota Test 307.SteadyState  
## 565 Minnesota Test 308.SteadyState  
## 566 Minnesota Test 309.SteadyState  
## 567 Minnesota Test 310.SteadyState  
## 568 Minnesota Test 311.SteadyState  
## 569 Minnesota Test 312.SteadyState  
## 570 Minnesota Test 313.SteadyState  
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## 579 Minnesota Test 322.SteadyState  
## 580 Minnesota Test 323.SteadyState  
## 581 Minnesota Test 324.SteadyState  
## 582 Minnesota Test 325.SteadyState  
## 583 Minnesota Test 326.SteadyState  
## 584 Minnesota Test 327.SteadyState  
## 585 Minnesota Test 328.SteadyState  
## 586 Minnesota Test 329.SteadyState  
## 587 Minnesota Test 330.SteadyState  
## 588 Minnesota Test 331.SteadyState  
## 589 Minnesota Test 332.SteadyState  
## 590 Minnesota Test 333.SteadyState  
## 591 Minnesota Test 334.SteadyState  
## 592 Minnesota Test 335.SteadyState  
## 593 Minnesota Test 336.SteadyState  
## 594 Minnesota Test 337.SteadyState  
## 595 Minnesota Test 338.SteadyState  
## 596 Minnesota Test 339.SteadyState  
## 597 Minnesota Test 340.SteadyState  
## 598 Minnesota Test 341.SteadyState  
## 599 Minnesota Test 342.SteadyState  
## 600 Minnesota Test 343.SteadyState  
## 601 Minnesota Test 344.SteadyState  
## 602 Minnesota Test 345.SteadyState  
## 603 Minnesota Test 346.SteadyState  
## 604 Minnesota Test 347.SteadyState  
## 605 Minnesota Test 348.SteadyState  
## 606 Minnesota Test 349.SteadyState  
## 607 Minnesota Test 350.SteadyState  
## 608 Minnesota Test 351.SteadyState  
## 609 Minnesota Test 352.SteadyState  
## 610 Lubeck-Bartell-Train 353.T=0  
## 611 Lubeck-Bartell-Train 353.T=0.5  
## 612 Lubeck-Bartell-Train 353.T=1.25  
## 613 Lubeck-Bartell-Test 354.T=0  
## 614 Lubeck-Bartell-Test 354.T=0.5  
## 615 Lubeck-Bartell-Test 354.T=1.25  
## 616 Little Hocking-Bartell-Train 355.T=0  
## 617 Little Hocking-Bartell-Train 355.T=0.75  
## 618 Little Hocking-Bartell-Test 356.T=0  
## 619 Little Hocking-Bartell-Test 356.T=0.75  
## 620 Little Hocking-Emmett-Test 357.SteadyState  
## 621 Paulsboro-Train 358.T=2.2  
## 622 Horsham-Train 359.T=2  
## 623 Warminster-Test 360.T=2  
## 624 Warrington-Train 361.T=2

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

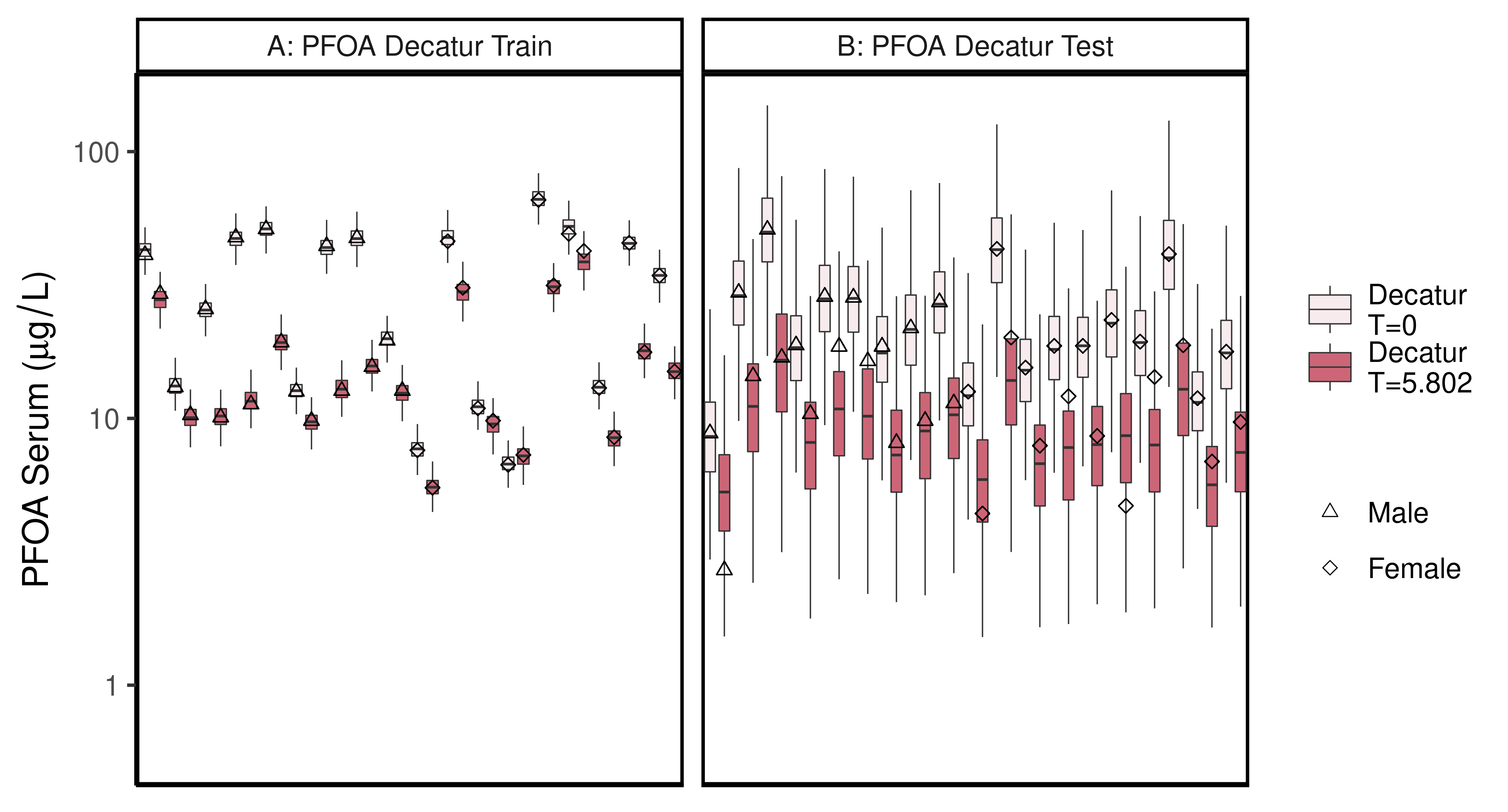
Modify aesthetics lookup table for boxplots

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

## Decatur boxplots

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

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



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

## Saving 6.5 x 3.5 in image

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.

print(pfas\_name)

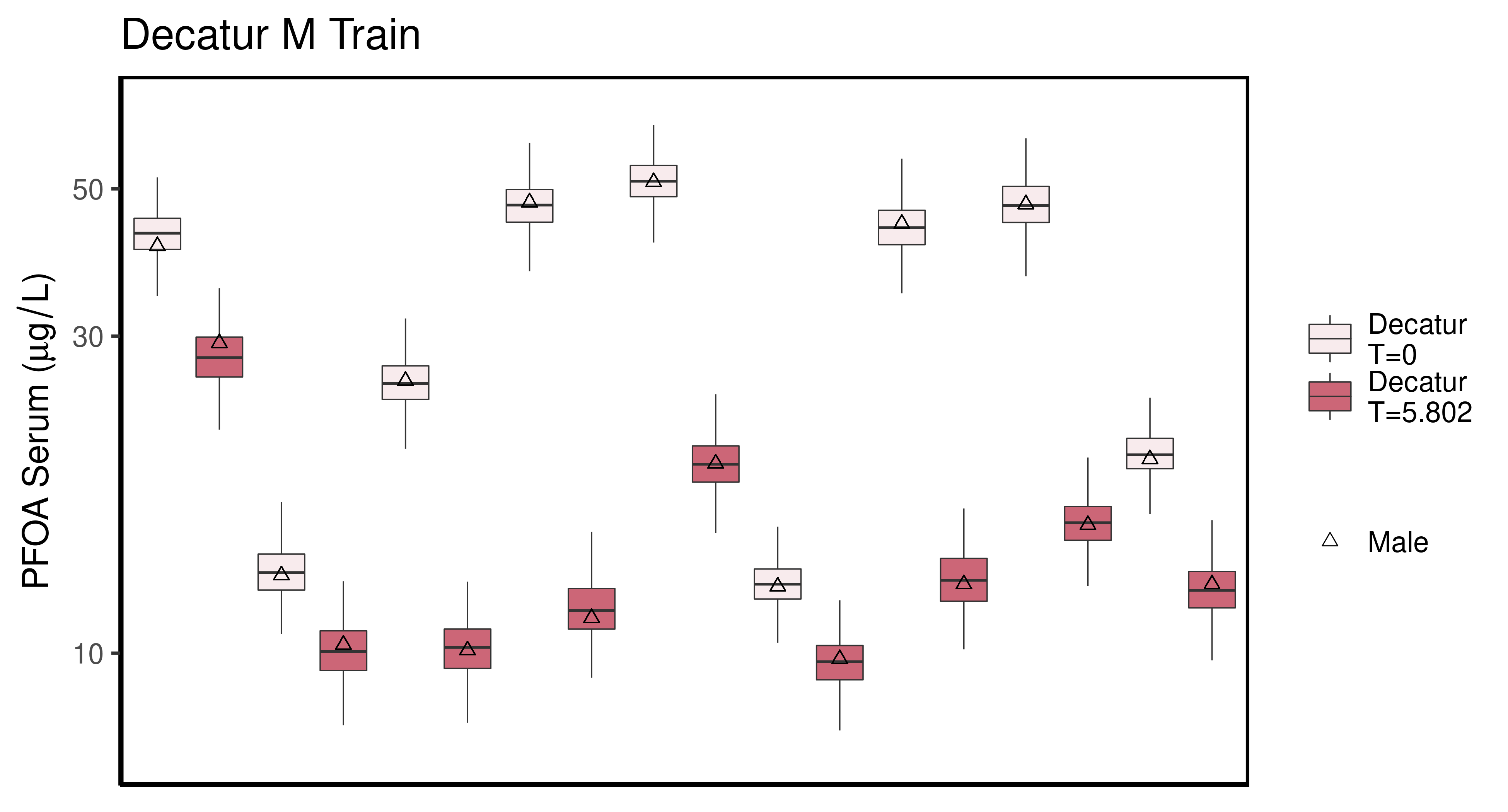
## [1] "PFOA"

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

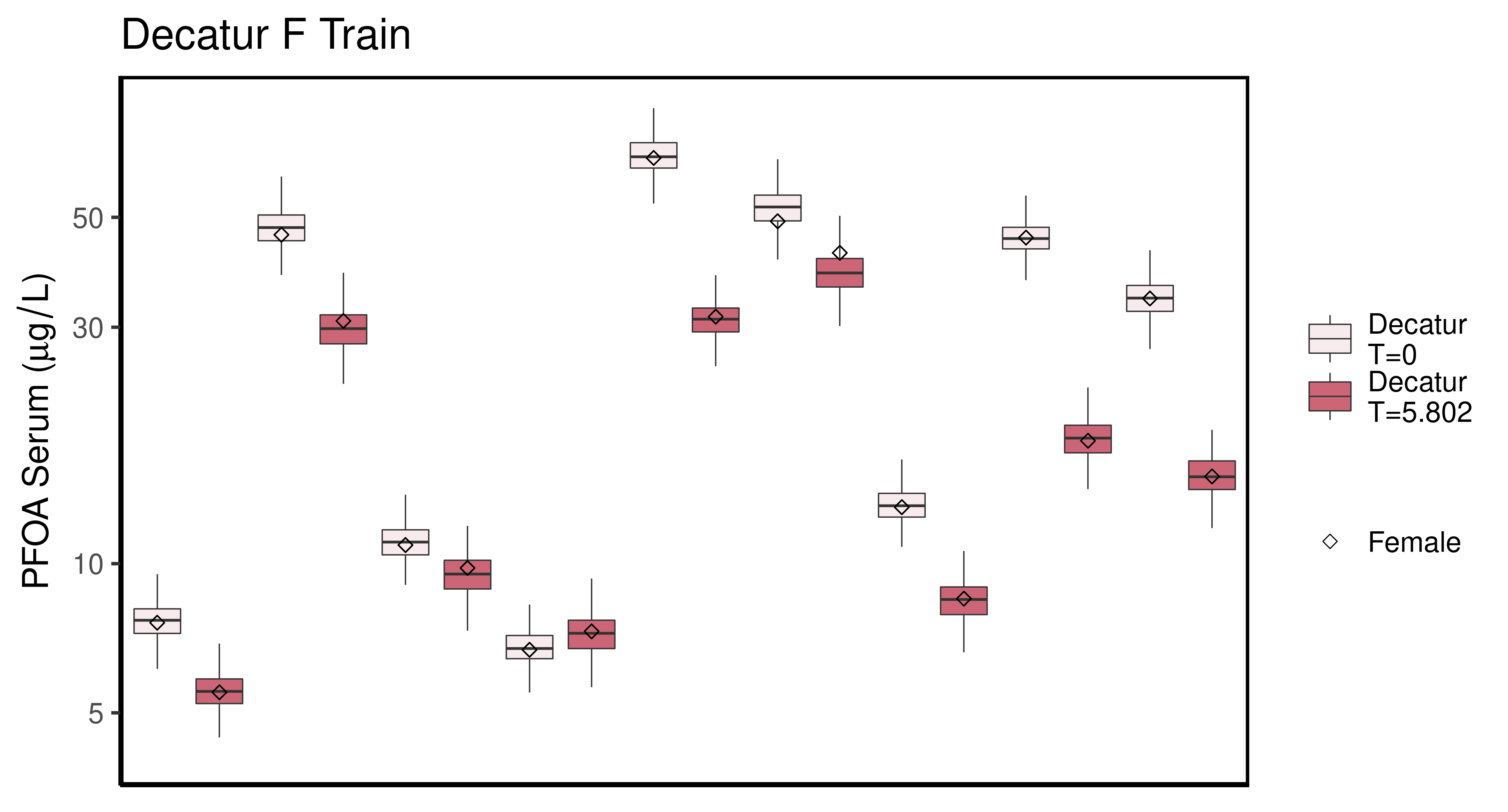
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

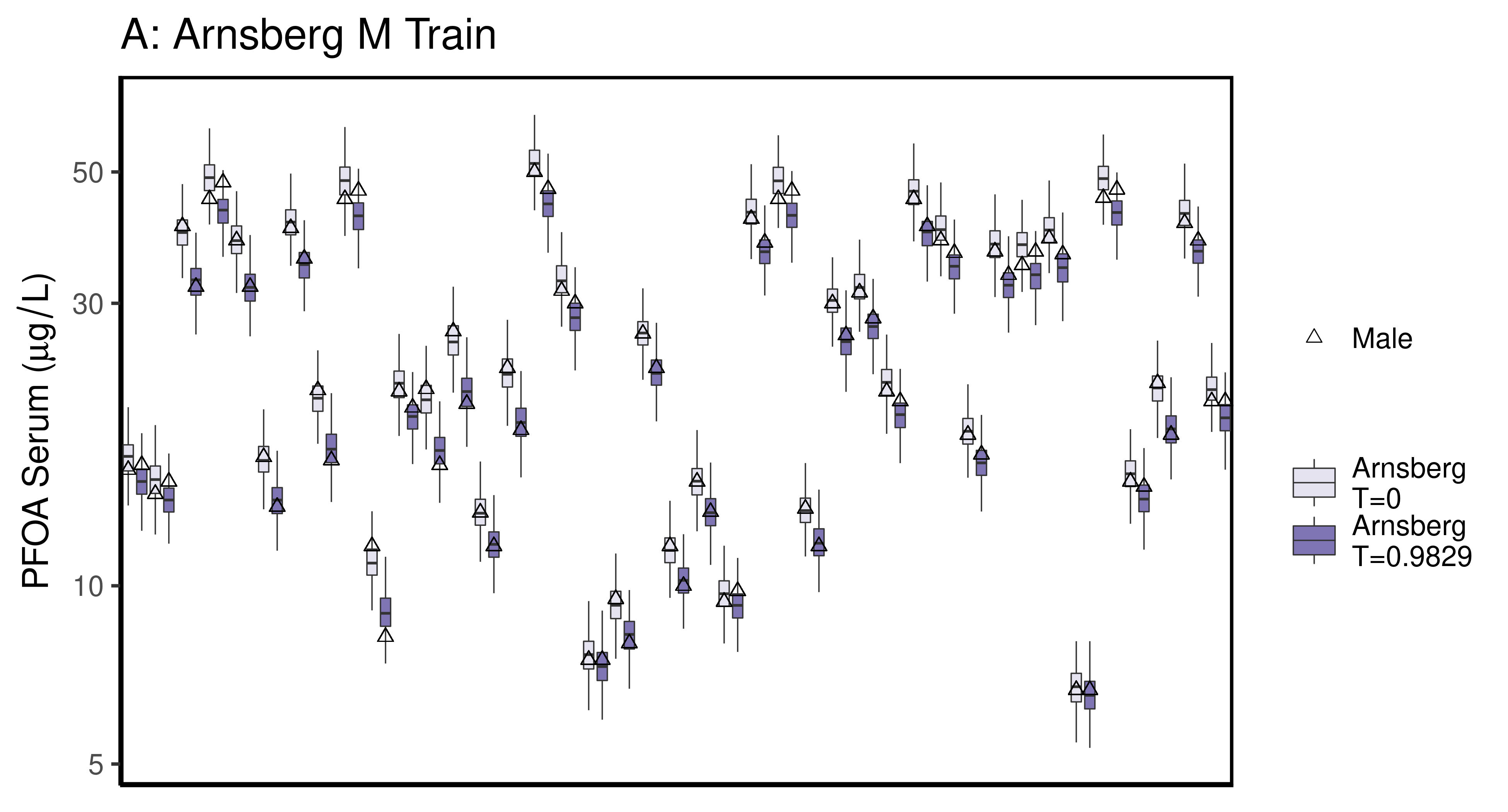
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

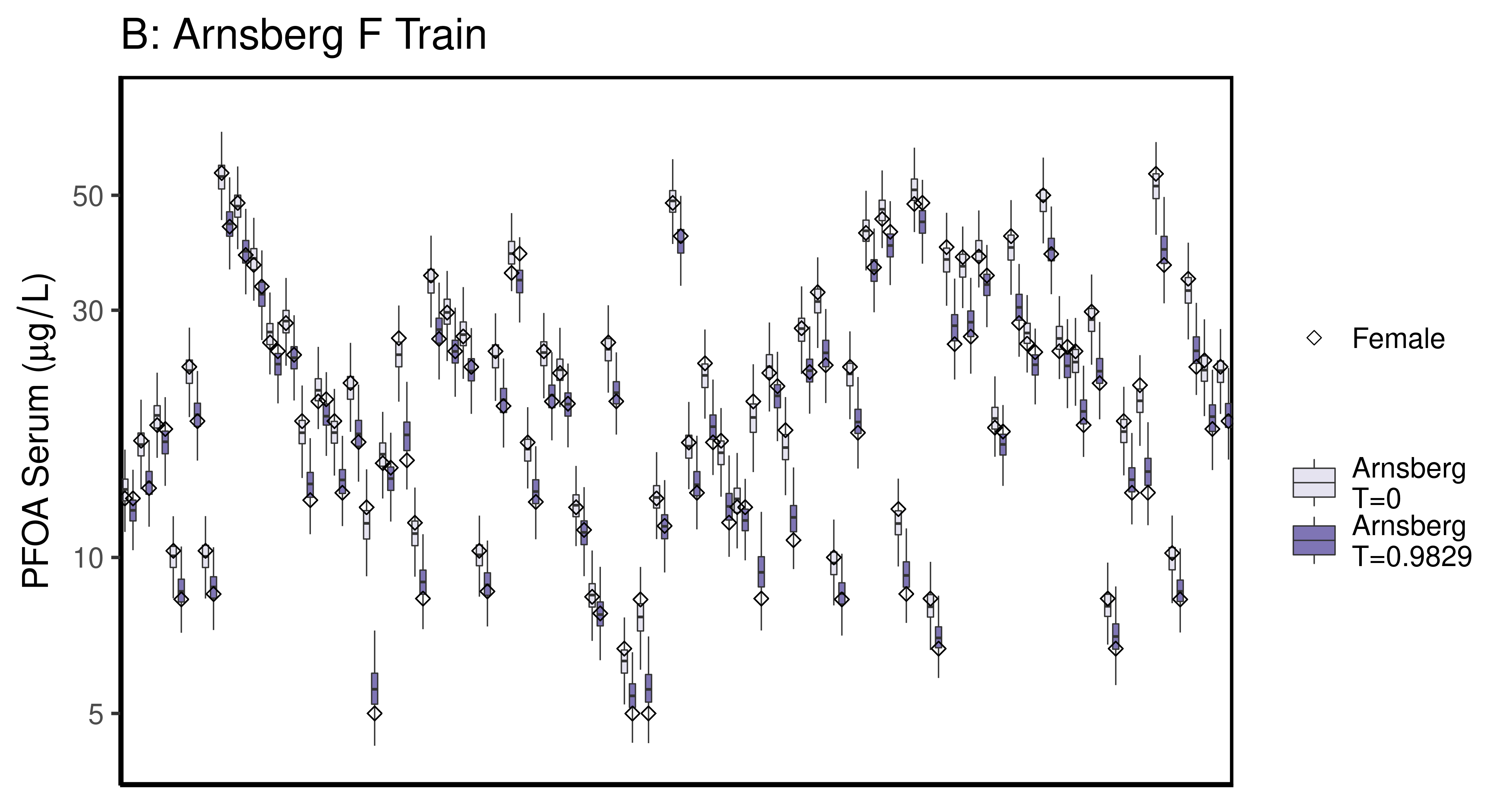
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

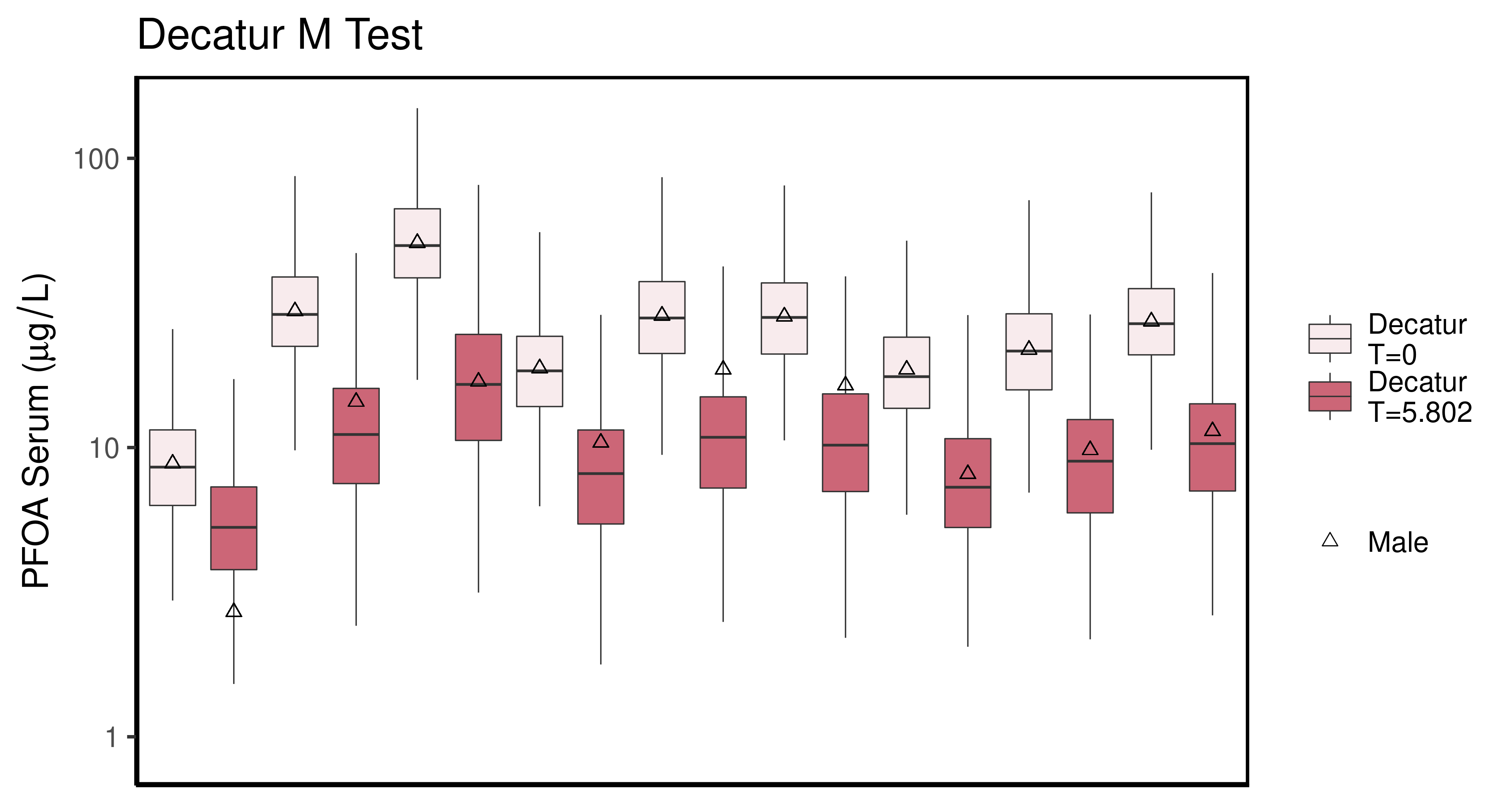
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## 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

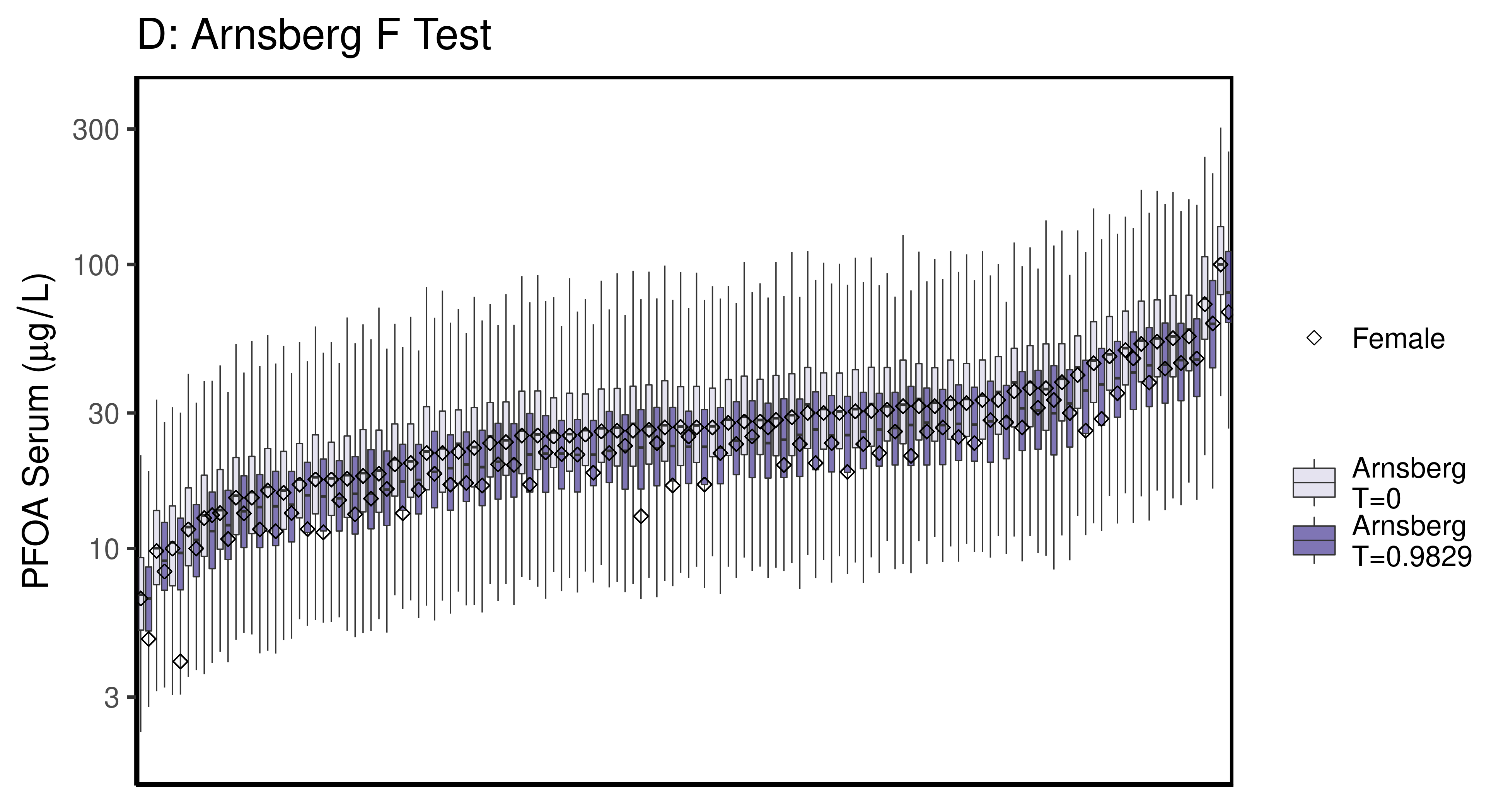
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

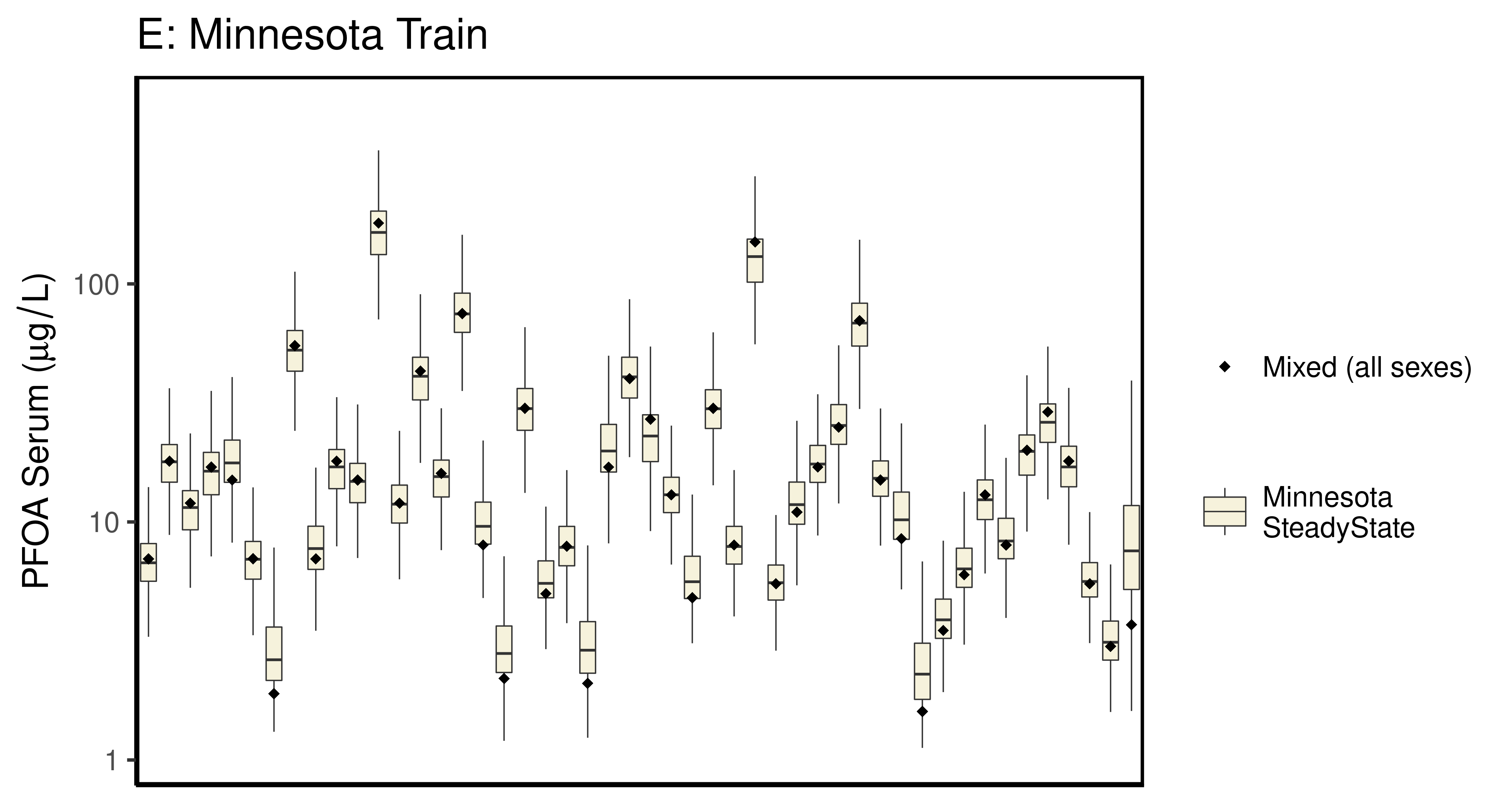
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

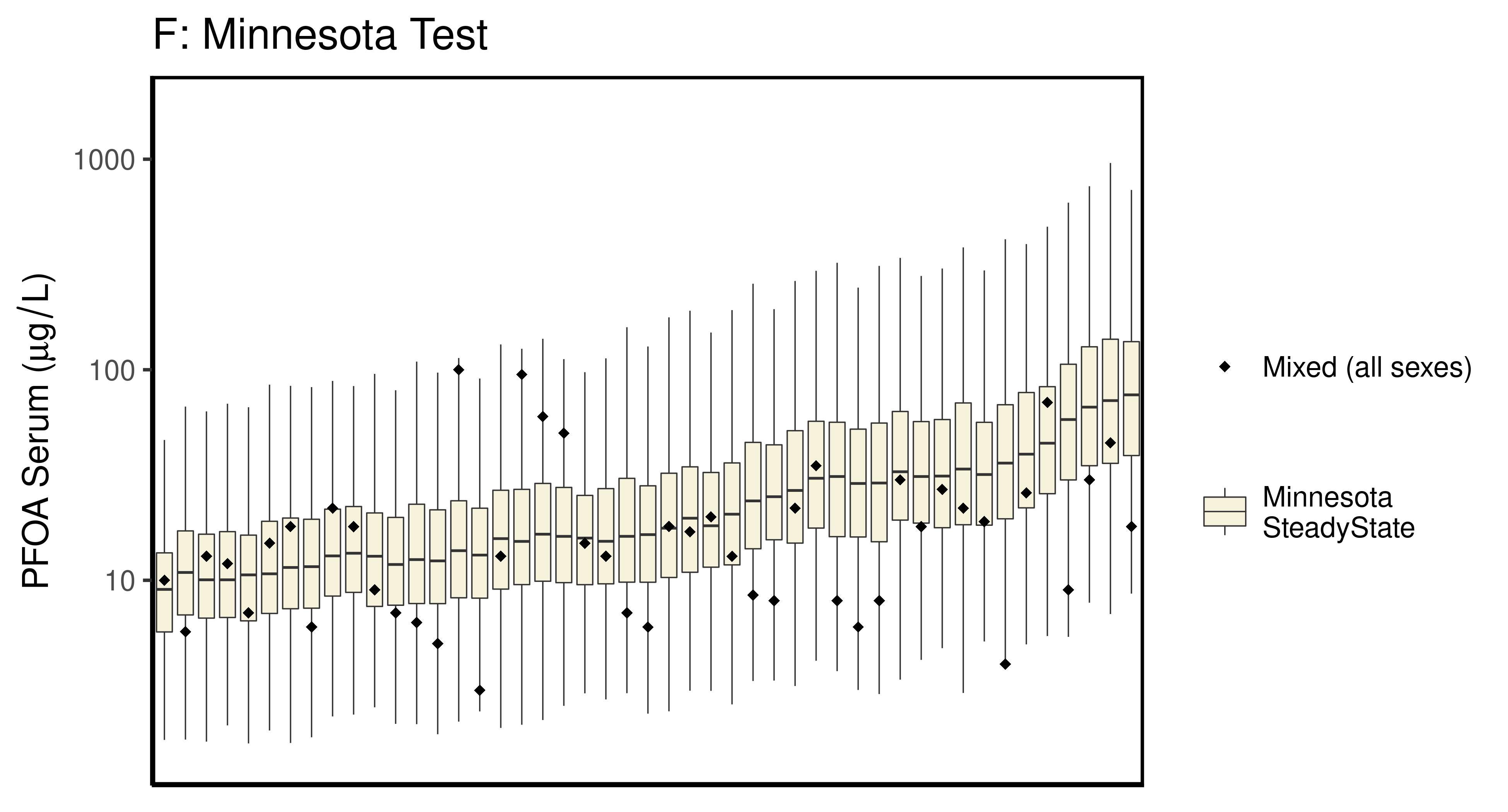
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

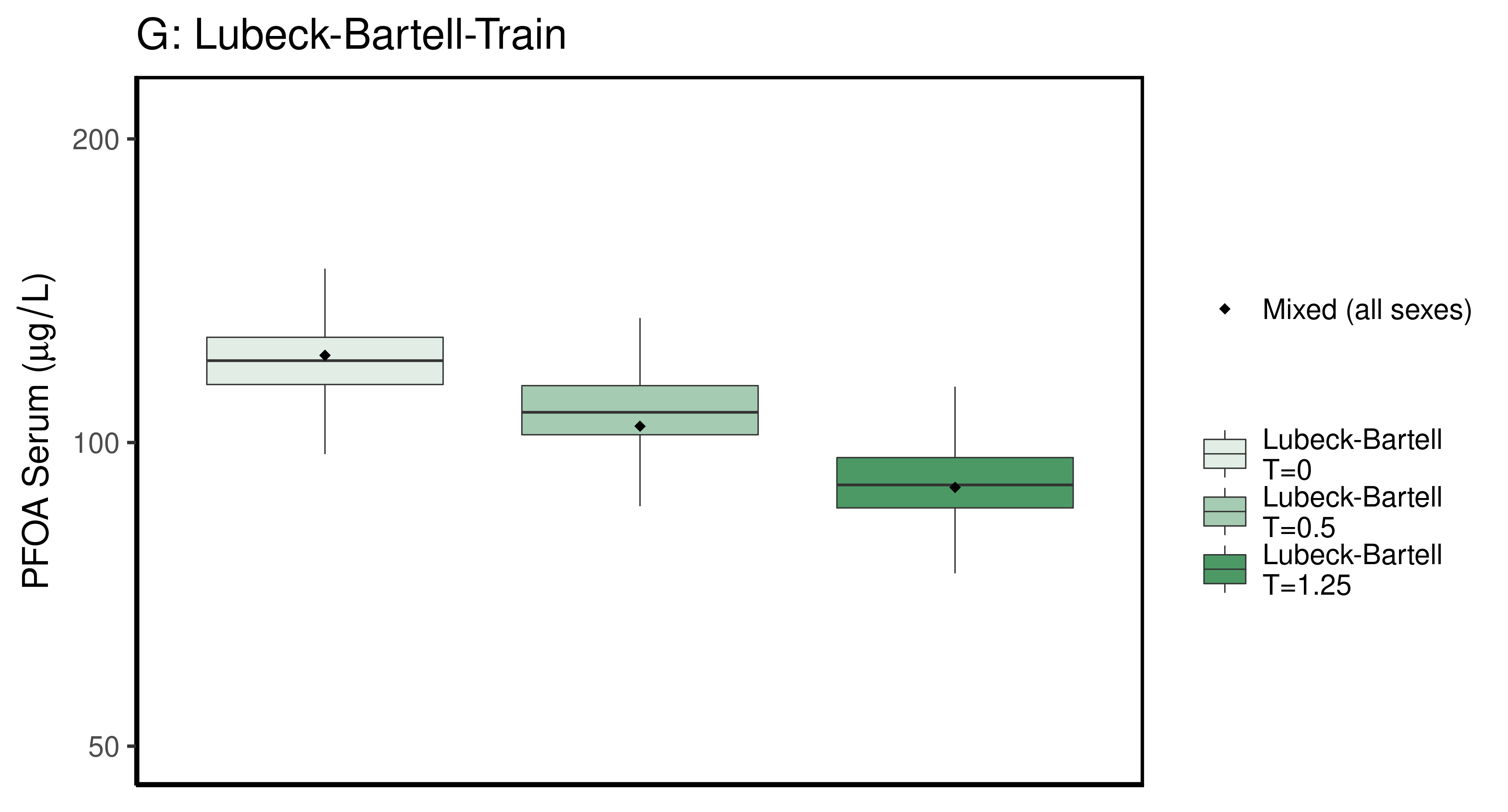
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

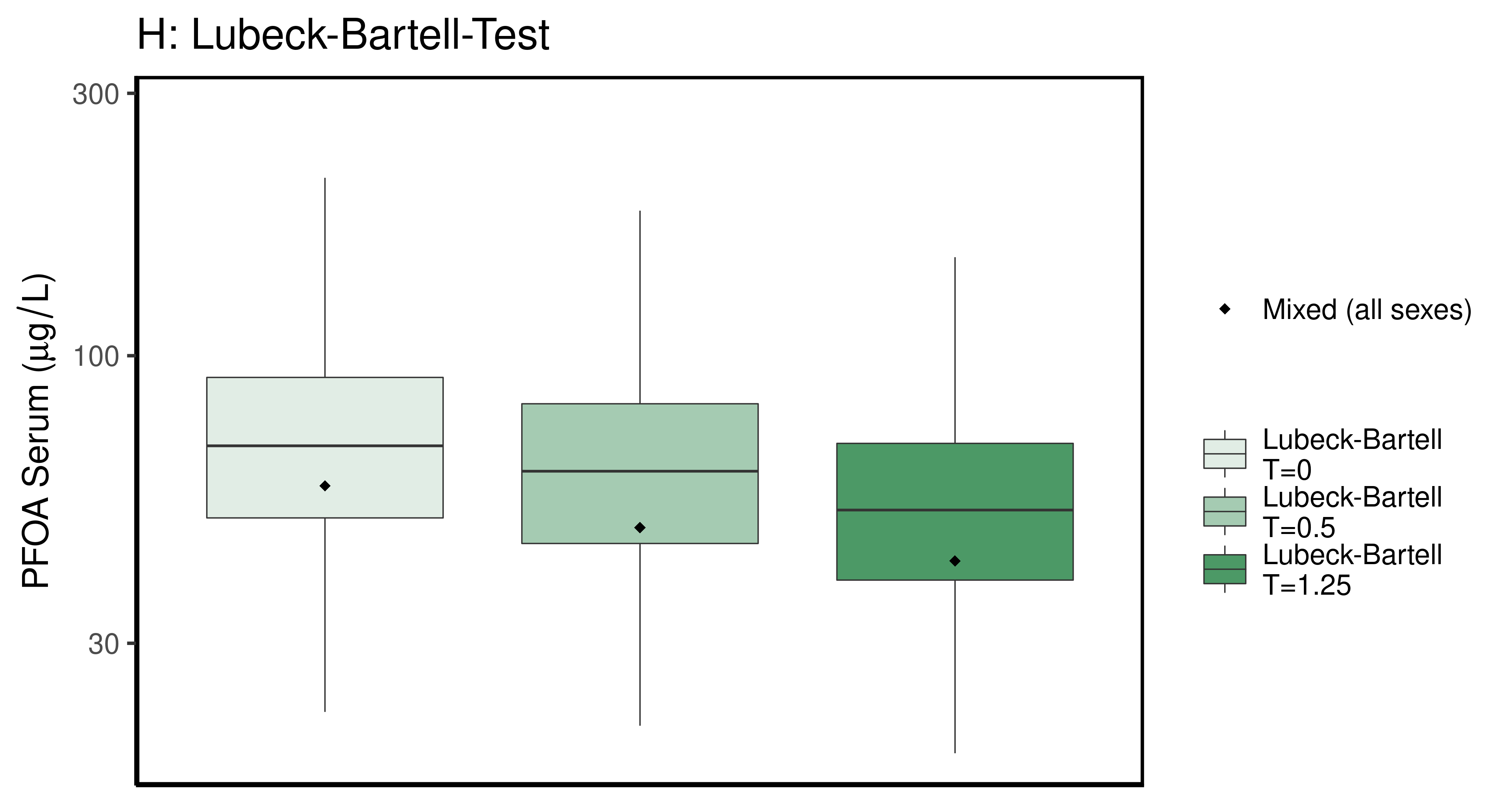
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

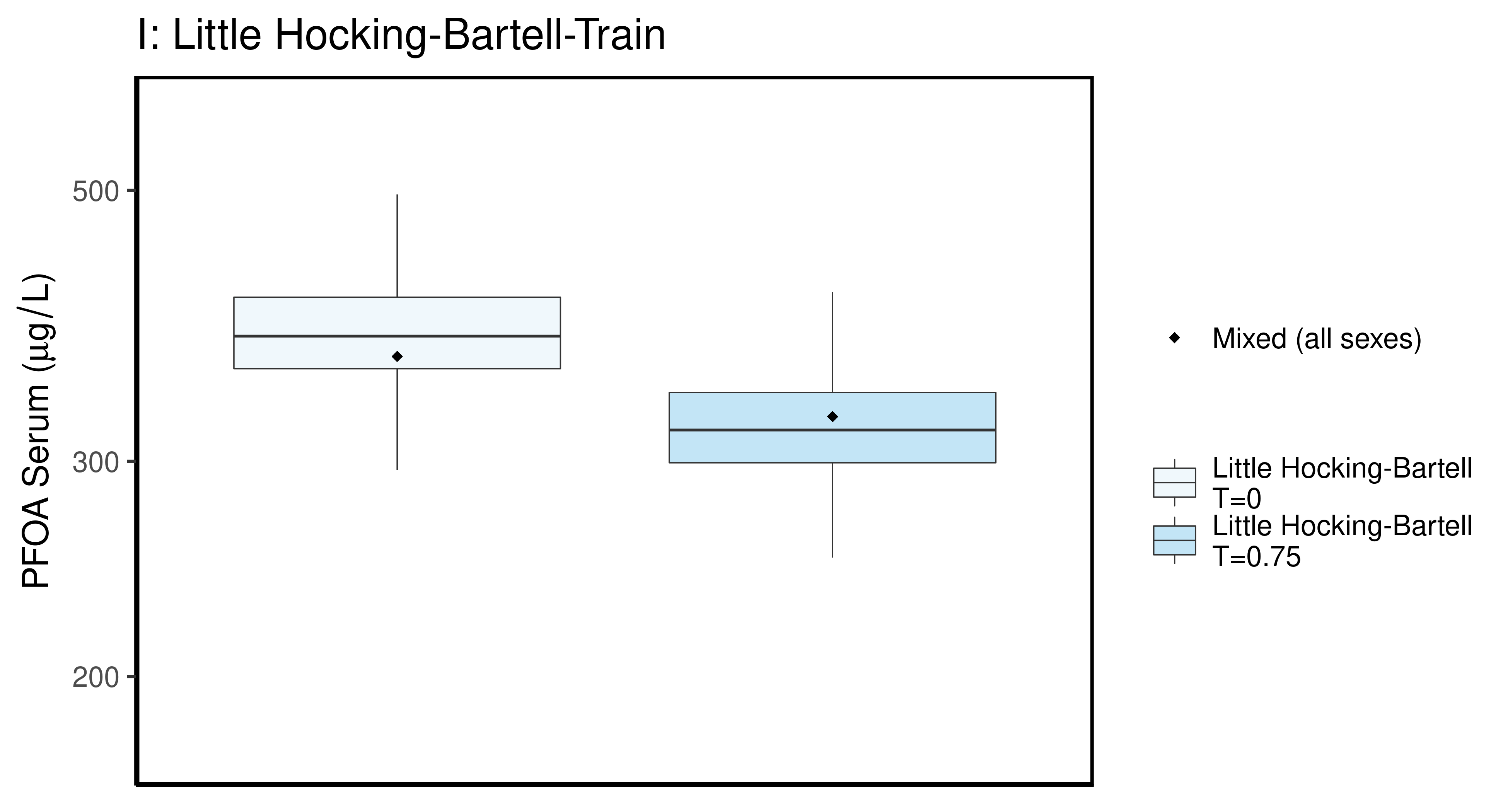
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

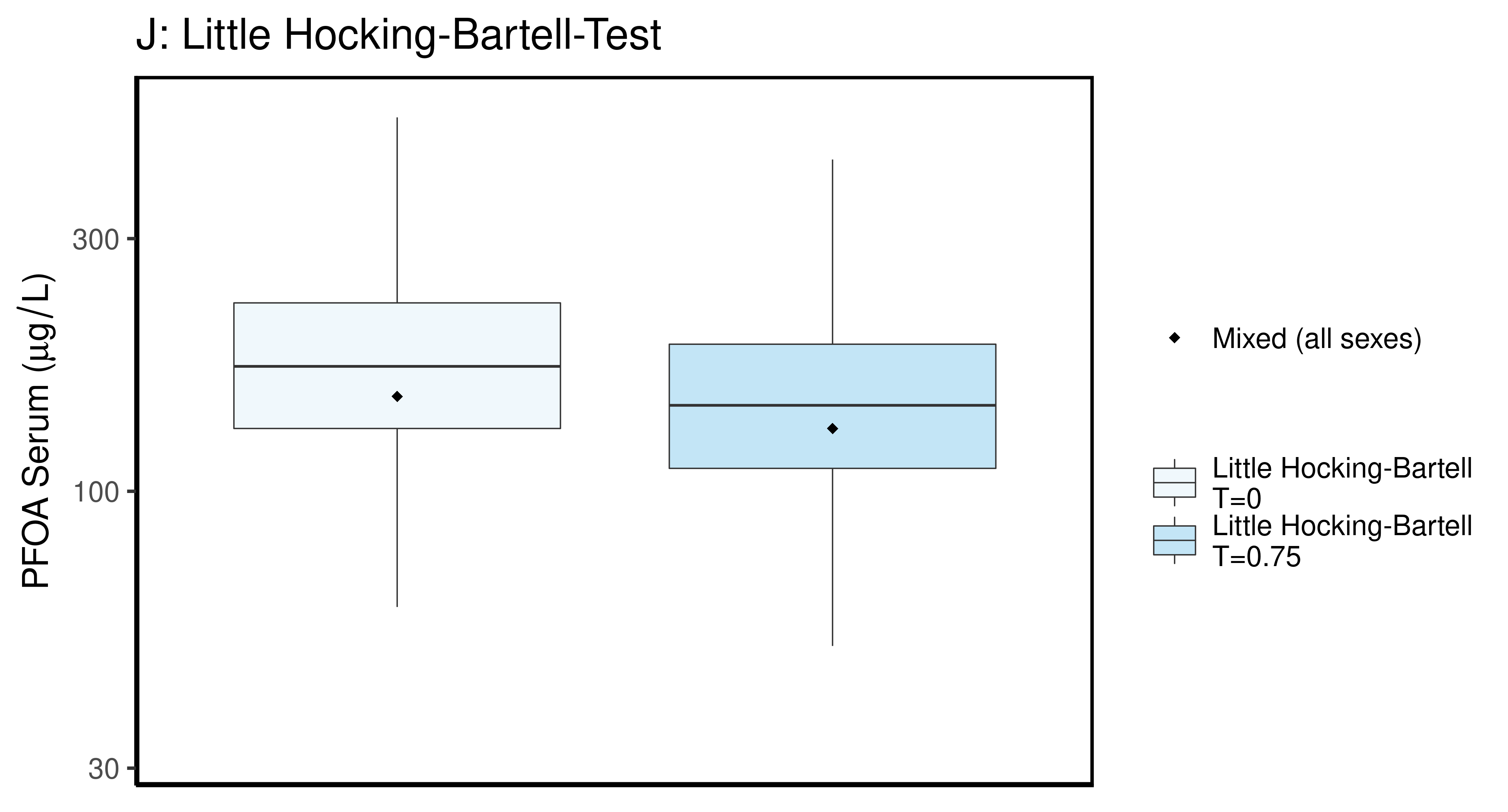
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

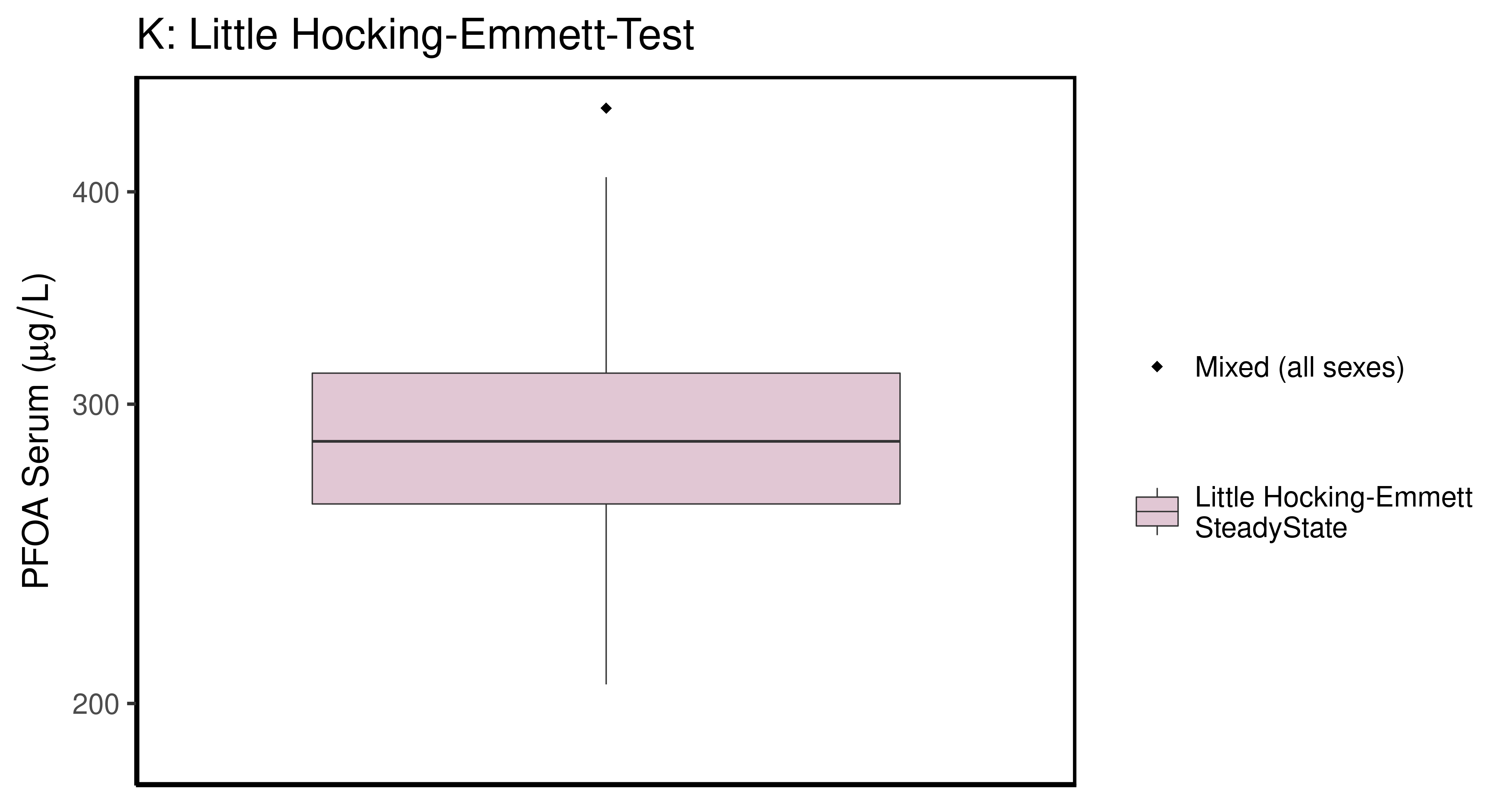
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

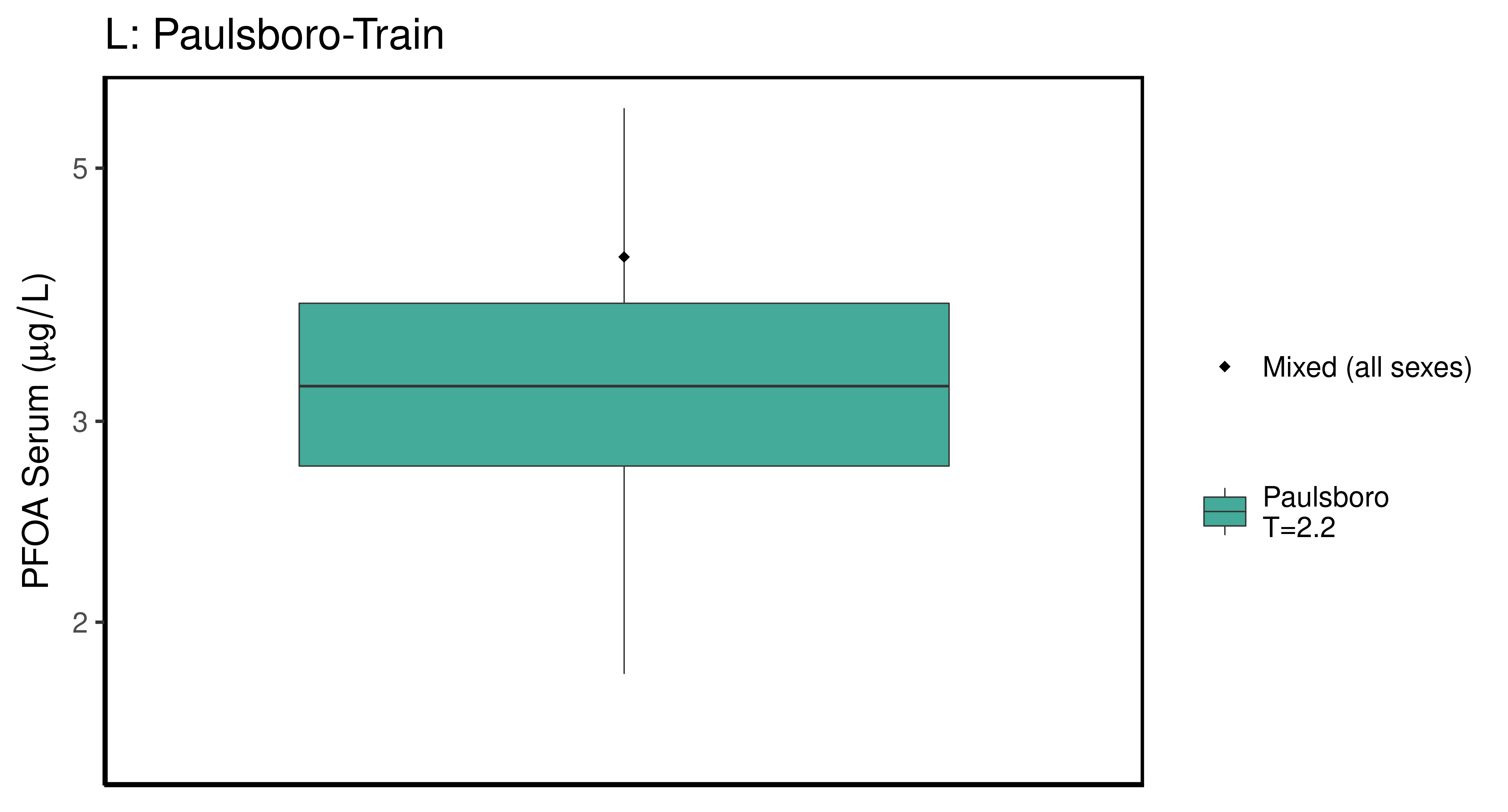
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

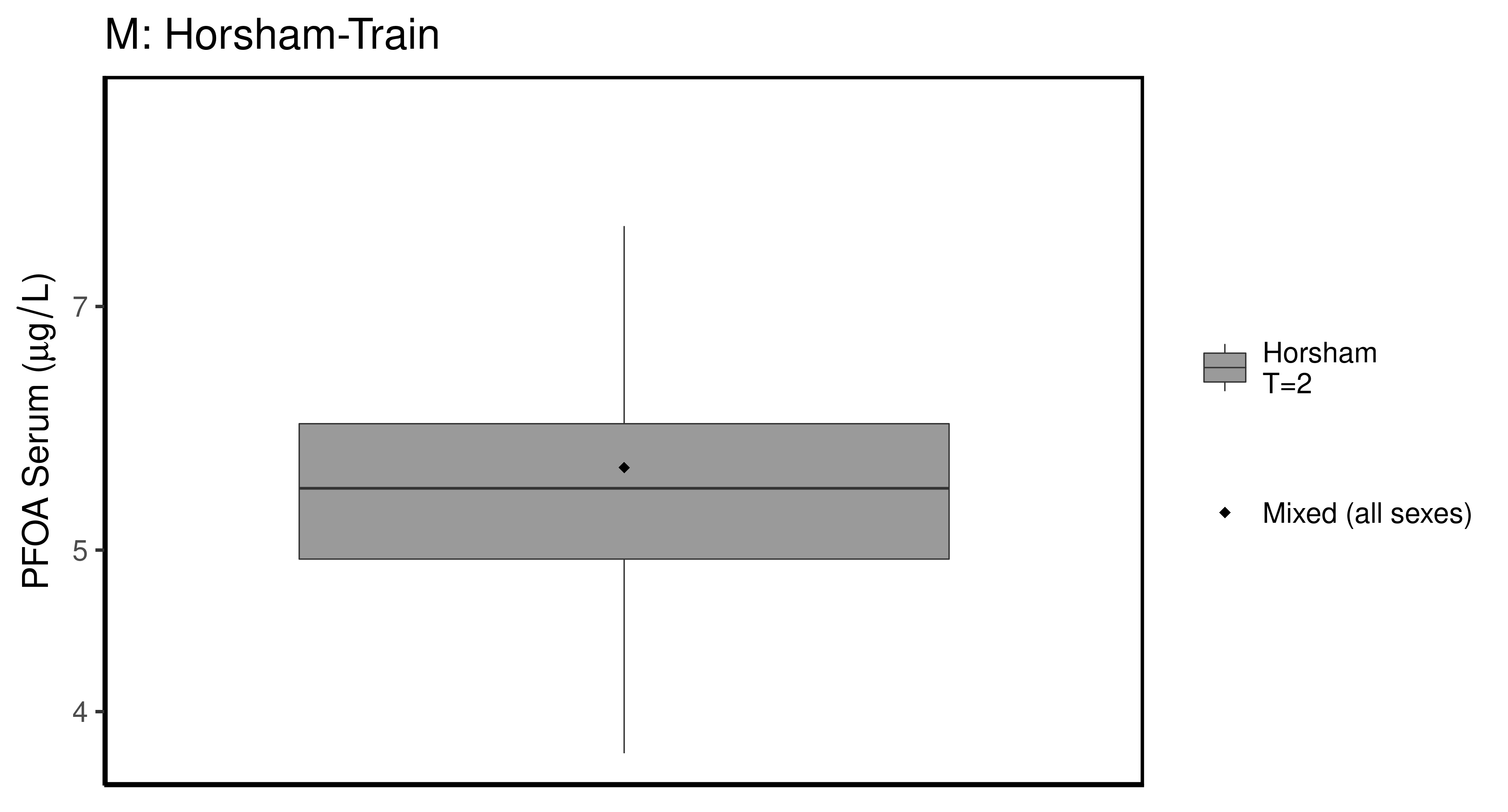
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

## Saving 6.5 x 3.5 in image

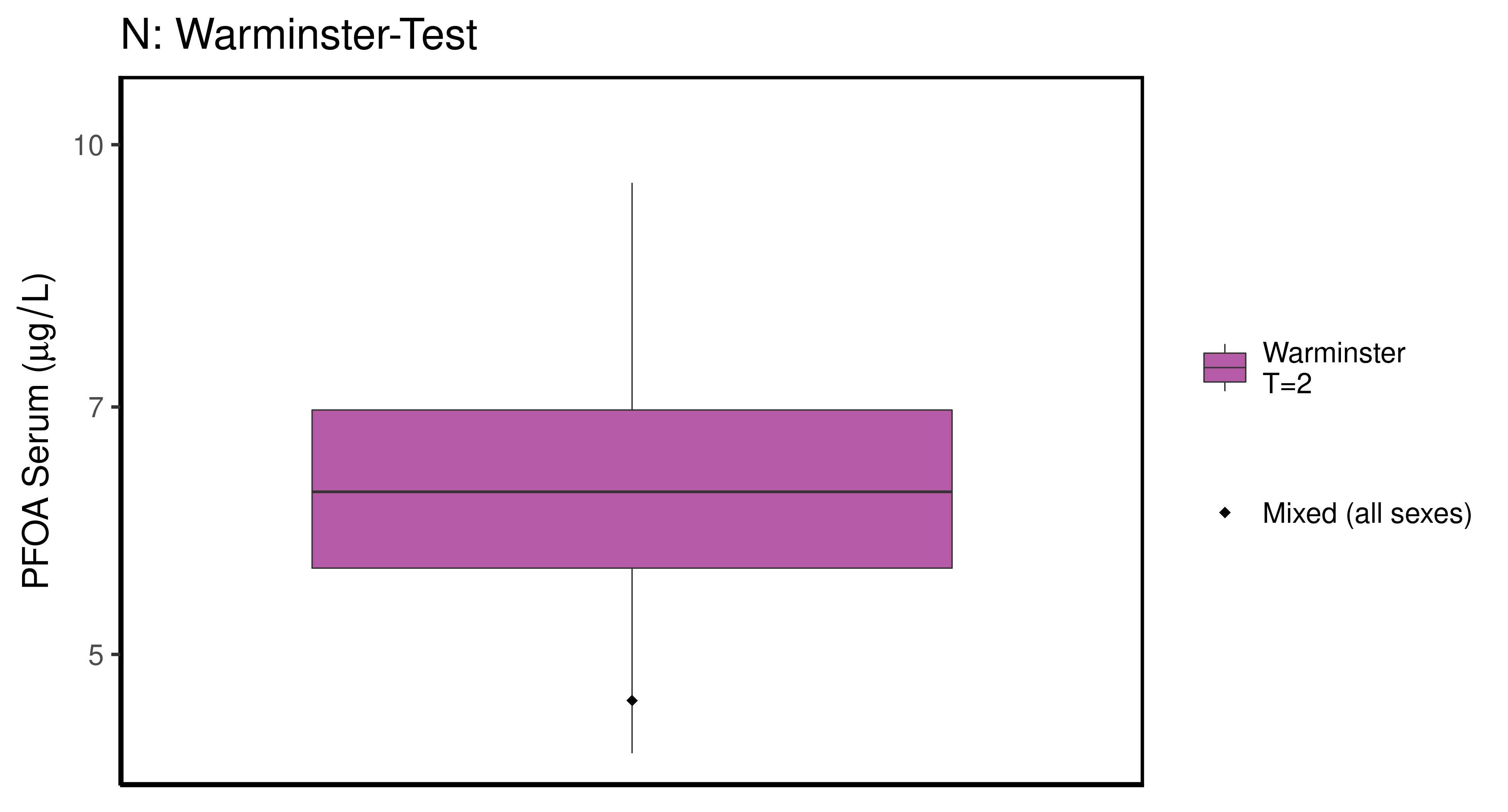
## Joining, by = c("legend\_label", "City", "Train\_Test", "datatype", "Time.desc")



## Saving 6.5 x 3.5 in image

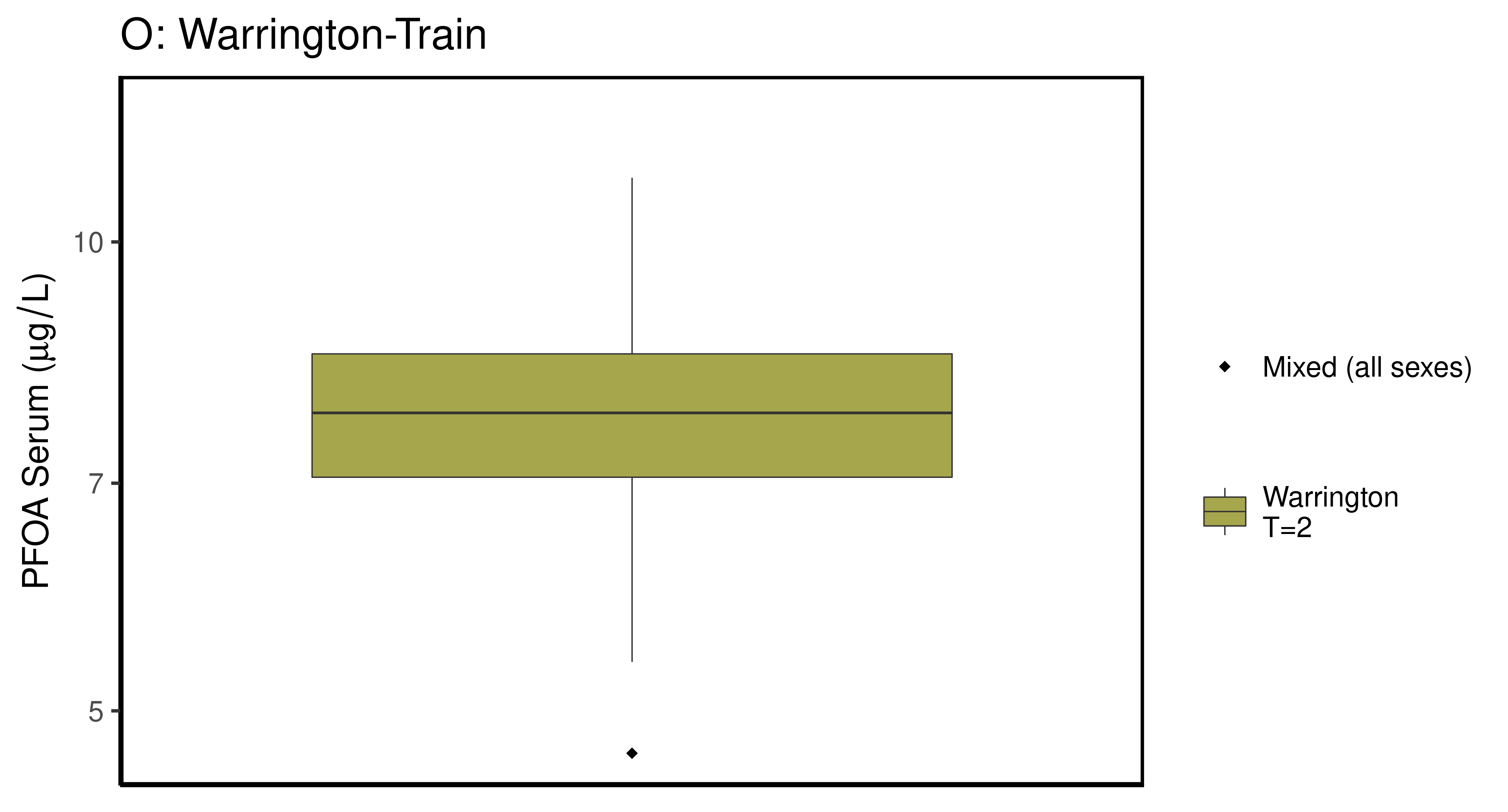
## Saving 6.5 x 3.5 in image

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



## Saving 6.5 x 3.5 in image

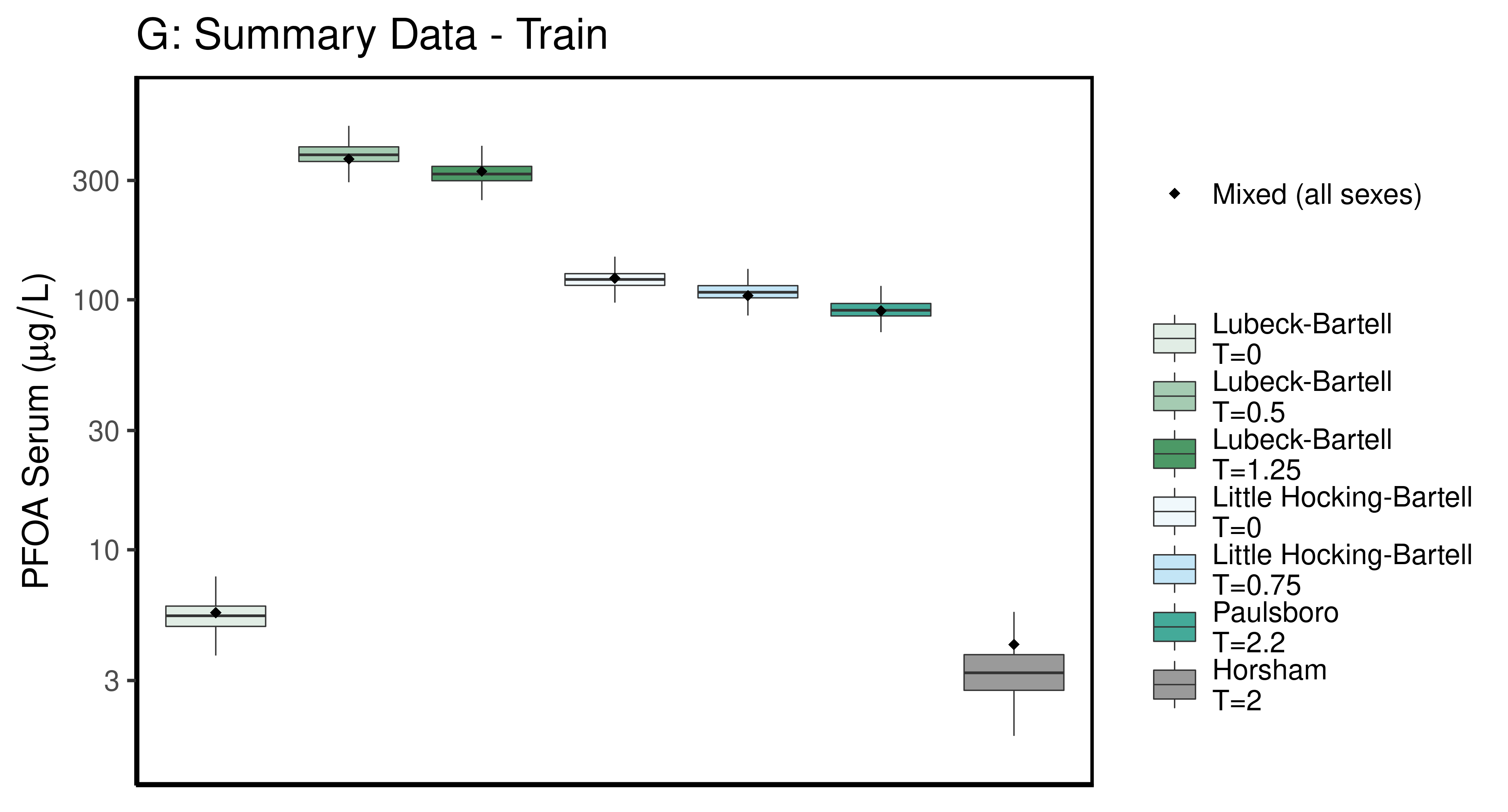
## Saving 6.5 x 3.5 in image



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



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

## Saving 6.5 x 3.5 in image

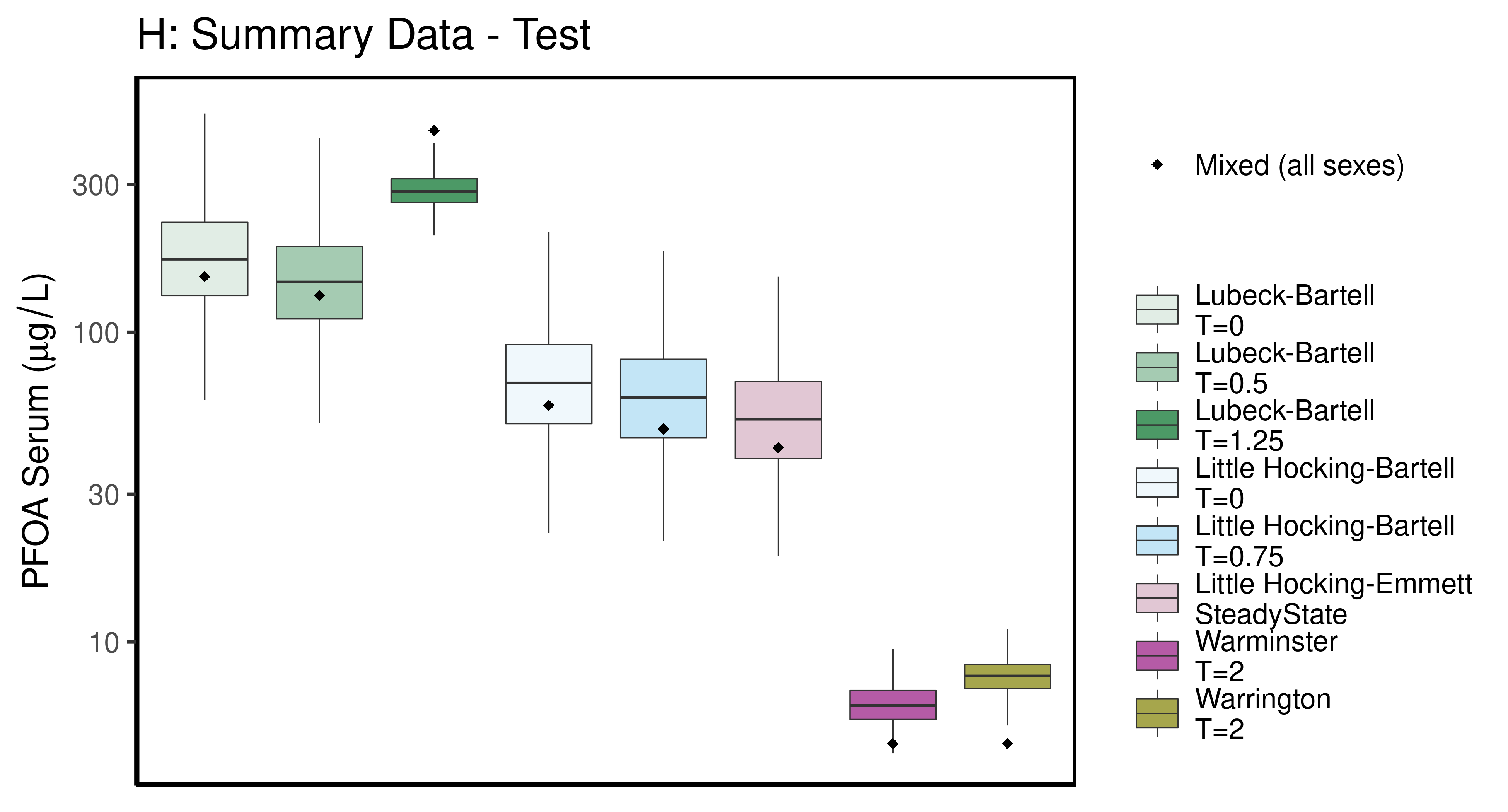
ggsave(here ("output-plots", paste0( sa, "SummaryTrainDataboxplot",pfas\_name,".png")), plt\_train,dpi=600)

## 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="H: Summary Data - Test", facets = FALSE,   
 pfas\_nom = pfas\_name)  
 print(plt\_test)



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

## Saving 6.5 x 3.5 in image

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

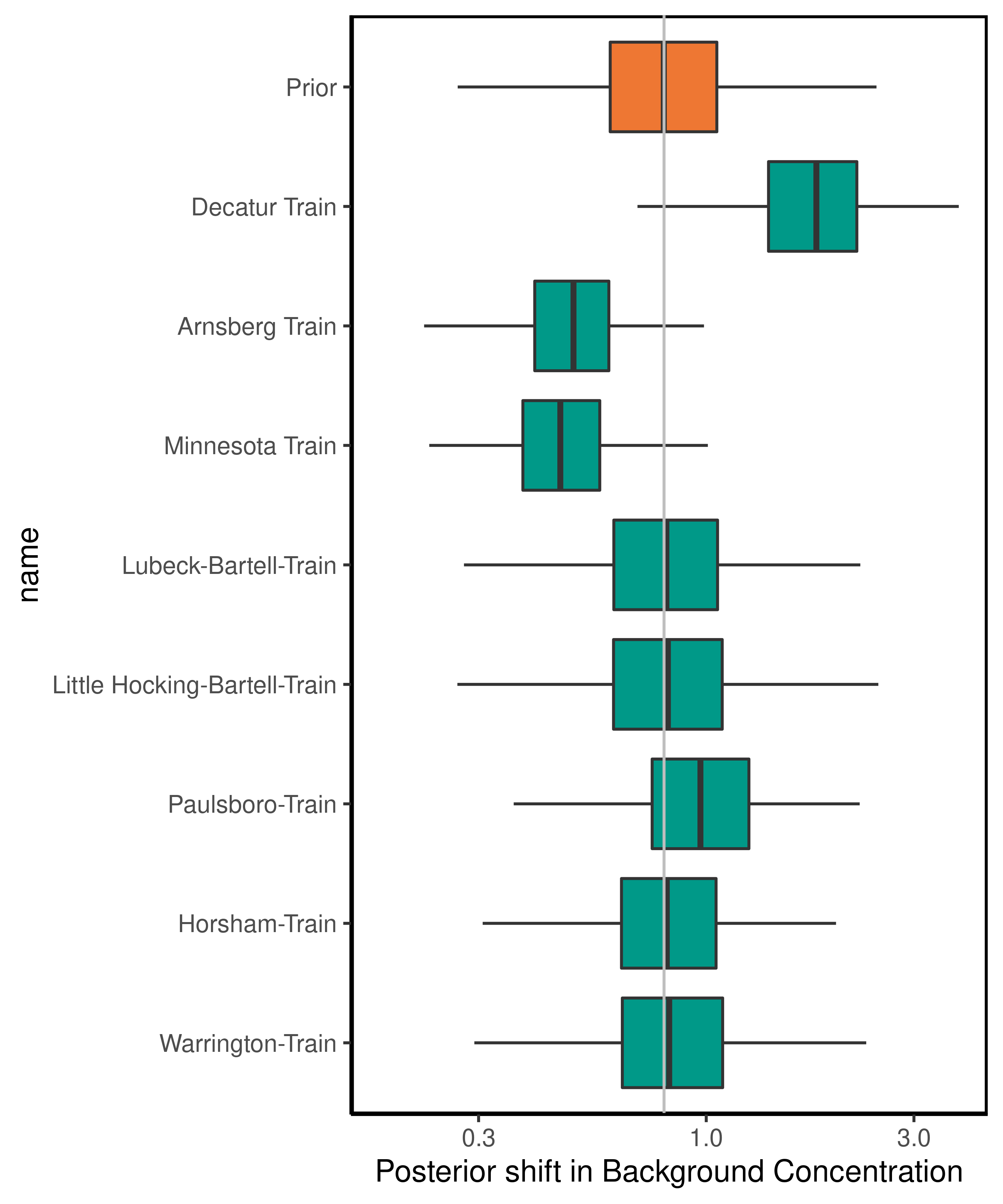
## Saving 6.5 x 3.5 in image

## PFOA

### Background posteriors

Shows shift in background estimate.

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



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

## Saving 5 x 6 in image

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

## Saving 5 x 6 in image

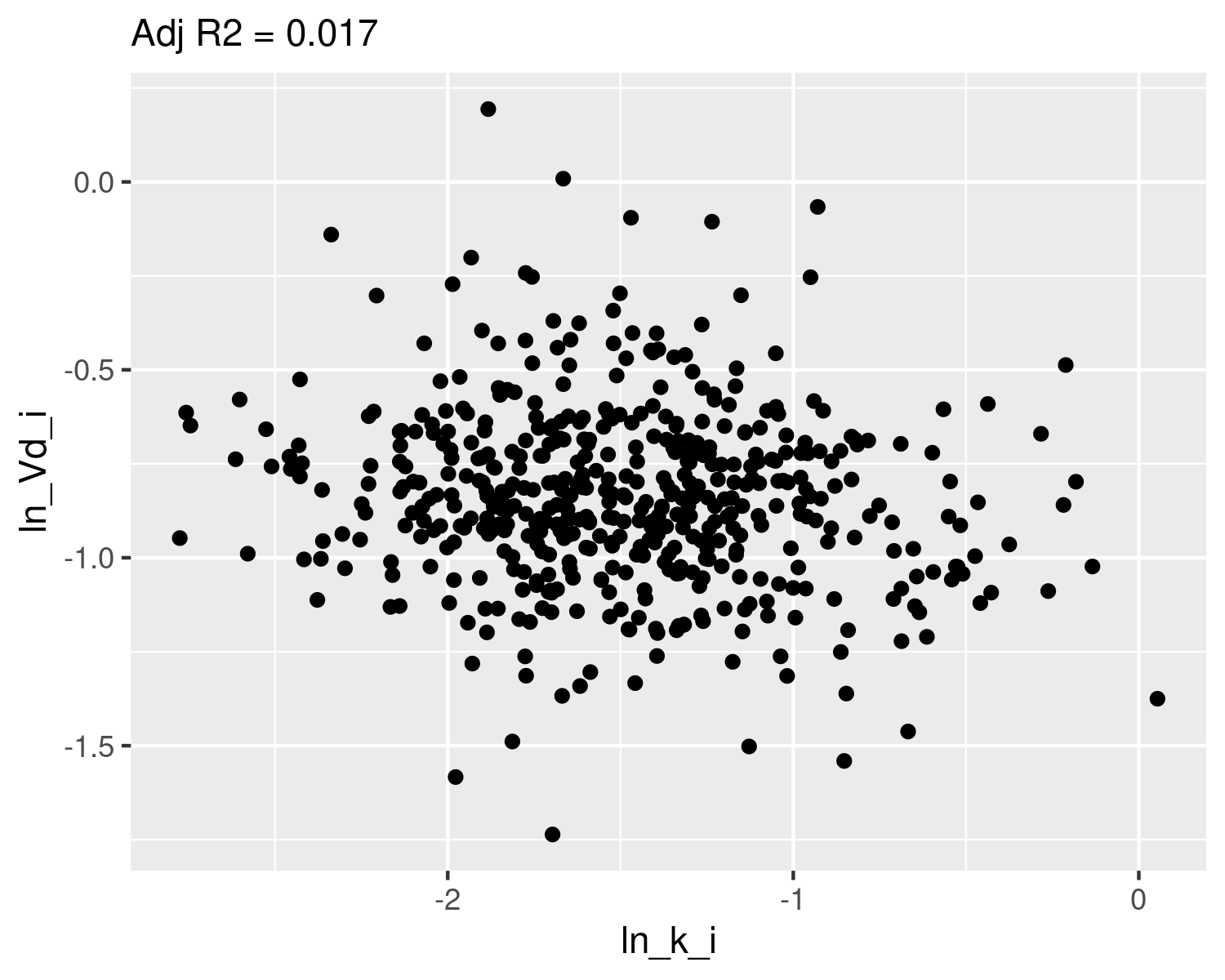
### Half-life

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.

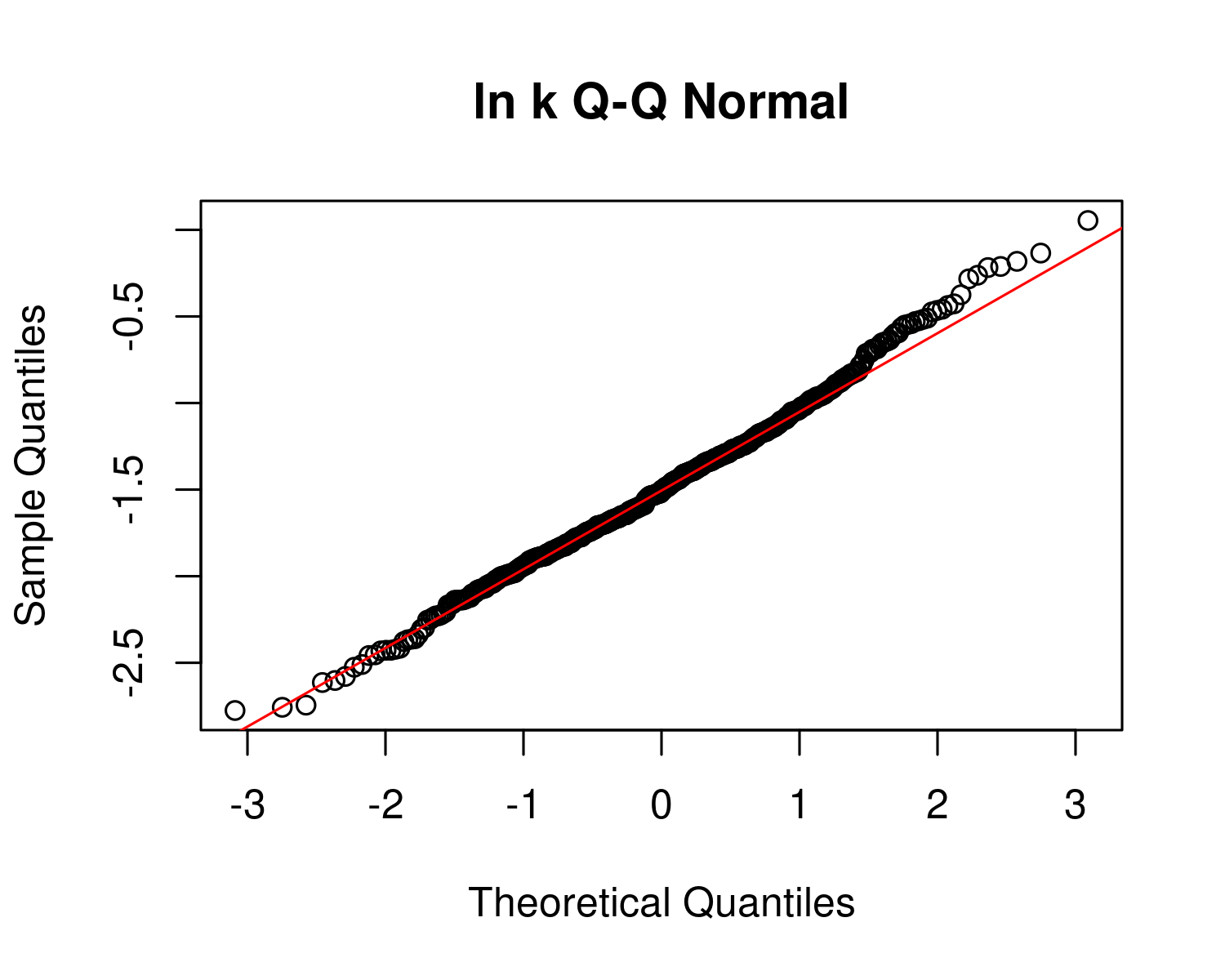
## M\_ln\_k(1) V\_ln\_k(1) M\_ln\_Vd(1) SD\_ln\_Vd(1) z\_ln\_k z\_ln\_Vd  
## 12503 -1.47166 0.2259770 -1.027430 0.11872900 -0.961933416 -2.139841913  
## 15901 -1.57172 0.1917550 -0.981910 0.12890300 -0.292525723 -1.263479244  
## 17543 -1.44315 0.2218600 -0.846605 0.05661850 0.258788216 0.083307969  
## 18721 -1.63377 0.2671930 -0.803807 0.00251033 -1.152131886 0.188325130  
## 11662 -1.63952 0.2442100 -0.641437 0.19616300 0.195782826 0.189814193  
## 13403 -1.50146 0.1316760 -0.912848 0.04207130 0.030123945 0.217615352  
## 13192 -1.52804 0.2576120 -0.836255 0.00522934 0.085417732 -0.648814142  
## 15663 -1.62322 0.2206230 -0.833671 0.12510900 1.116610213 0.254774383  
## 1246 -1.46340 0.1607610 -0.864602 0.11869500 -1.218857416 -0.468830015  
## 16132 -1.35944 0.1421860 -1.046470 0.05301980 1.267368722 -1.192510054  
## 10602 -1.31808 0.1962300 -1.020060 0.07258270 -0.744781596 0.121228235  
## 10563 -1.57564 0.2097090 -0.575507 0.08585640 -1.131218571 -1.035932658  
## 15932 -1.63592 0.2893040 -0.441297 0.46389700 -0.716358490 -0.191888295  
## 1114 -1.50220 0.1654030 -0.812117 0.12570300 0.252652370 -0.970546336  
## 1699 -1.61622 0.1952380 -0.655576 0.06439360 0.152045707 0.057771938  
## 1141 -1.44708 0.0791159 -0.824623 0.03169700 -0.307656430 -2.110692675  
## 13383 -1.53241 0.1373040 -0.898336 0.06439640 -0.953017331 0.978176274  
## 12832 -1.58927 0.2061870 -0.757849 0.09033650 -0.648242811 0.371021737  
## 19552 -1.65200 0.1755320 -0.922508 0.35681400 1.224313624 0.720910931  
## 14423 -1.56912 0.2473010 -0.613524 0.27567500 0.199811608 1.879594880  
## 12372 -1.58129 0.2054630 -0.863814 0.01532240 -0.578483722 -0.396316112  
## 12042 -1.44236 0.2313180 -0.930943 0.08416760 -0.942300733 0.110322947  
## 10473 -1.56596 0.2387790 -0.504892 0.05603230 -0.203728180 -0.593140881  
## 1509 -1.63181 0.2301430 -0.703216 0.00560974 -1.666474840 0.419621770  
## 1552 -1.60037 0.2947500 -0.756522 0.00787158 -0.484455109 -0.545738743  
## 19513 -1.60375 0.2381920 -0.640758 0.10491500 -0.741072661 1.160921499  
## 17471 -1.43266 0.1720730 -0.896787 0.09401620 1.160615779 0.639817834  
## 18092 -1.51021 0.2343130 -0.663190 0.09107450 1.012067125 -0.122020443  
## 1613 -1.42880 0.1599680 -1.366620 0.17959100 -0.072078474 0.184645026  
## 14383 -1.50389 0.3123290 -0.591951 0.14044200 -1.136782298 -0.517806023  
## 14263 -1.48924 0.2104700 -0.621222 0.18017100 0.900624729 0.067988352  
## 18291 -1.63622 0.2309160 -0.890736 0.07126660 0.851770447 -0.184797156  
## 1945 -1.52990 0.3078630 -1.009580 0.08054770 0.727715174 -1.403691615  
## 19613 -1.43231 0.2006660 -0.824693 0.34993200 0.736502146 0.229740706  
## 1842 -1.57472 0.2309900 -0.884116 0.02773450 -0.352129617 -0.889081301  
## 1873 -1.52882 0.1832970 -0.846448 0.09996610 0.705515513 -0.160401177  
## 19423 -1.50740 0.1751370 -0.797601 0.07921920 1.300357989 -0.242136794  
## 19352 -1.51582 0.1875540 -1.128120 0.31836300 0.038252014 -0.028837196  
## 11812 -1.45436 0.1943910 -0.839713 0.17480700 -0.979283770 -0.316215474  
## 14982 -1.54901 0.1428640 -0.848721 0.30714300 0.793761231 -0.416160087  
## 11263 -1.56783 0.2199070 -0.710211 0.41491600 0.786506872 -1.023895957  
## 1028 -1.54302 0.2678610 -0.871150 0.19559700 -0.310463131 1.099495275  
## 1051 -1.46362 0.1975220 -0.995615 0.01698190 1.698884846 0.817712470  
## 17222 -1.62549 0.1728590 -0.610798 0.04805740 -0.794593709 0.168875510  
## 1747 -1.42129 0.1846450 -1.079430 0.10572600 0.348437716 0.038665440  
## 1284 -1.48424 0.2049750 -0.804076 0.04367570 -2.265401074 1.078174892  
## 1564 -1.58495 0.2873960 -0.915255 0.01014360 -0.162205279 0.379427297  
## 18632 -1.54907 0.1614390 -1.054610 0.00165336 1.130864991 -1.078174559  
## 19142 -1.46579 0.2090540 -0.941316 0.07023310 -0.455545976 0.188763468  
## 15793 -1.46362 0.1833740 -0.925623 0.22671500 -0.899166316 1.583133508  
## 1126 -1.47780 0.1995500 -0.867935 0.28911700 0.726838902 -0.250112295  
## 16502 -1.62102 0.1606710 -0.868282 0.25076100 -0.809440902 0.342994219  
## 15103 -1.57576 0.2397400 -0.900027 0.00821699 0.267085116 -0.124701883  
## 11251 -1.49379 0.2818330 -0.843613 0.16180800 -1.737263711 -0.993314763  
## 11732 -1.50231 0.2169980 -0.987321 0.05741900 -1.411425136 -1.021439085  
## 18382 -1.51482 0.2751650 -1.030920 0.25169800 -0.453551227 0.840642928  
## 13433 -1.42797 0.1483210 -0.919814 0.05892850 -1.035491275 0.849573118  
## 16403 -1.49892 0.1997390 -0.983599 0.13235400 1.362142893 0.469618942  
## 11871 -1.50834 0.2055990 -0.802875 0.08667930 0.917456737 -1.269655261  
## 1988 -1.48315 0.1924390 -0.785314 0.08054900 -0.785142161 -1.105120219  
## 1589 -1.51279 0.1841260 -0.923346 0.12130700 0.573518173 -1.897945965  
## 1449 -1.64977 0.2798170 -0.578292 0.16774900 0.918196208 0.491787265  
## 1232 -1.36807 0.3417130 -0.653308 0.19652100 0.256287273 -0.704722317  
## 10171 -1.47809 0.2403040 -0.793030 0.03993560 0.351966556 1.777576130  
## 1259 -1.49576 0.2375770 -0.649087 0.27527200 1.174337357 -0.245389029  
## 18503 -1.47120 0.2198610 -0.999776 0.34880200 -0.480846375 -2.111252318  
## 10801 -1.51003 0.2110390 -0.996705 0.15454600 -0.418829722 -0.585314536  
## 15263 -1.48332 0.1814320 -0.904369 0.40902900 0.955112803 -0.517903726  
## 1042 -1.49419 0.2424220 -0.828952 0.03377570 -1.289006611 0.513919145  
## 18363 -1.51216 0.2052980 -1.039480 0.11045500 0.186197433 -0.626426919  
## 19072 -1.35224 0.2485190 -0.922599 0.03118750 -0.031325502 0.192142595  
## 16632 -1.48603 0.2605770 -0.817629 0.01564830 0.467097310 -1.427277992  
## 1401 -1.54181 0.1358830 -1.034610 0.13711600 1.024197674 0.400991028  
## 14691 -1.43545 0.2440150 -0.910474 0.19227400 0.267358452 1.161564956  
## 17041 -1.48588 0.1928010 -0.966202 0.13837200 0.231826103 0.326346805  
## 19822 -1.61330 0.2439050 -0.588351 0.13230200 0.747592465 -1.014982273  
## 13613 -1.50885 0.2392160 -0.633701 0.24521900 1.217068511 0.101258362  
## 11013 -1.69096 0.2199700 -0.534025 0.01900890 0.383358345 0.991893279  
## 15791 -1.51648 0.1436290 -0.746068 0.09673090 -0.988052822 1.102650759  
## 16531 -1.56947 0.2702700 -0.662266 0.13761300 -0.156852910 0.280375017  
## 1970 -1.40317 0.2466890 -0.987173 0.17438100 1.735535216 -0.406177410  
## 16331 -1.35646 0.2602780 -1.288260 0.43768200 -0.352298306 1.286412690  
## 1242 -1.43832 0.1496560 -0.741701 0.03900760 0.688640044 -0.254030579  
## 15251 -1.52149 0.2075030 -0.881694 0.17508700 1.224406096 -1.144448704  
## 1653 -1.61168 0.1758520 -0.715660 0.08015940 0.794296303 0.266410910  
## 1140 -1.41430 0.1002270 -1.062620 0.17328800 -0.006402398 0.636855748  
## 17771 -1.55676 0.2255080 -0.744089 0.03847910 0.219150635 -1.402115093  
## 18012 -1.38234 0.2666460 -0.838148 0.01181150 -0.886463751 -1.511824827  
## 14062 -1.56862 0.2140640 -0.794915 0.04280680 0.439760291 -0.301192859  
## 1964 -1.30205 0.1852410 -1.111200 0.05588090 -0.886389751 0.491361149  
## 18413 -1.51758 0.1867480 -1.070000 0.14309100 -0.853818454 -0.898156496  
## 13791 -1.47473 0.1167100 -0.950589 0.34175100 -0.989994331 -1.575054814  
## 15832 -1.54427 0.2221950 -0.699935 0.41951700 -0.650877737 -0.503256667  
## 1060 -1.62196 0.2277440 -0.700480 0.14347000 1.053946660 -0.622908441  
## 12073 -1.52741 0.2097110 -0.940174 0.07511050 -0.390878033 -0.684829990  
## 15683 -1.55605 0.2399200 -0.884377 0.09924330 -0.070586394 -0.221516764  
## 1693 -1.44825 0.2611600 -0.998148 0.22416200 -0.462050809 0.388050833  
## 17531 -1.62703 0.1579760 -0.431300 0.02123260 0.540908267 -0.806316456  
## 10311 -1.40523 0.1564300 -1.137370 0.22822500 0.931634971 -0.547213054  
## 18041 -1.45637 0.1471540 -1.050410 0.18772200 -0.209274345 1.213494144  
## 19672 -1.47472 0.1184670 -0.918969 0.32436100 0.617350048 -0.417013230  
## 18351 -1.44541 0.1648200 -0.833319 0.12605100 -0.405077513 0.164593185  
## 13741 -1.49438 0.1397200 -0.858856 0.01891560 1.053103763 -1.569627007  
## 11892 -1.52589 0.1254210 -0.841719 0.26003500 0.602284246 1.466675890  
## 18762 -1.41077 0.1747840 -0.938952 0.05807670 1.017461177 -1.496085449  
## 1808 -1.56318 0.1873870 -0.606047 0.12204600 0.608167318 -1.150289019  
## 15861 -1.58406 0.2683330 -0.911643 0.13762500 0.206735995 -2.023009144  
## 12312 -1.45007 0.1416170 -0.871745 0.20459000 -1.897727292 -0.681652395  
## 13473 -1.36593 0.2800870 -1.076770 0.18433300 -0.682582832 0.507010414  
## 1040 -1.42147 0.2561510 -0.849688 0.01145310 0.481338415 0.747111894  
## 17573 -1.58928 0.1933030 -0.762938 0.00918553 -0.463031038 0.175989014  
## 19872 -1.58679 0.2888820 -0.631627 0.05272770 -0.279741696 -0.437523579  
## 1953 -1.51285 0.2003110 -0.880081 0.24434700 -0.413690145 0.942726154  
## 15883 -1.48029 0.2613290 -1.034740 0.06578180 1.618766521 0.891044960  
## 1663 -1.56782 0.2012710 -0.899684 0.13944800 -0.721055711 -1.691785958  
## 18913 -1.57129 0.2107510 -0.916803 0.16965800 -0.453093157 -0.712147393  
## 1005 -1.44127 0.2417650 -0.965525 0.08648320 0.014257161 -0.332268892  
## 1878 -1.58529 0.2219080 -0.774919 0.31081000 0.215764621 0.983033453  
## 15553 -1.56391 0.2264020 -0.863960 0.33118800 0.188870195 -0.988041784  
## 19433 -1.48263 0.1510180 -0.956022 0.04723680 -0.050148494 0.265546446  
## 15642 -1.68422 0.2677910 -0.668507 0.08586200 -1.495419632 -0.728186155  
## 13873 -1.46777 0.2112260 -1.015750 0.09210150 0.367837753 1.375405013  
## 17882 -1.59235 0.1623460 -0.471441 0.12496900 0.517144022 -0.599264333  
## 1857 -1.50125 0.1826960 -1.078360 0.04547980 -0.484335465 -0.272173202  
## 1103 -1.61380 0.1675800 -0.729922 0.21380000 0.674855616 0.405324773  
## 12581 -1.50950 0.2603350 -0.880965 0.09614510 -0.762448605 0.846734123  
## 1974 -1.36787 0.1572330 -1.005850 0.09913730 0.386073791 0.518125984  
## 13822 -1.50496 0.1704370 -0.853228 0.02475770 -0.664003345 1.579413771  
## 1101 -1.62594 0.2161180 -0.521347 0.03706260 -1.724344195 -0.112951698  
## 1198 -1.45837 0.1568960 -0.948387 0.27207500 1.156319079 -0.484652932  
## 19762 -1.44604 0.2104260 -0.869365 0.26606600 0.693506590 -2.377853826  
## 18271 -1.66192 0.2490240 -0.735196 0.26331900 0.143156356 -0.636048007  
## 18911 -1.51171 0.1493880 -0.912044 0.31328200 1.492813560 0.035663770  
## 19111 -1.50772 0.2341060 -1.005580 0.20565300 -1.632153479 -0.109166877  
## 1374 -1.59652 0.2487760 -0.855533 0.12625500 0.127846023 -1.871305162  
## 1920 -1.58874 0.1819160 -0.719057 0.23716200 -2.403663727 -0.079333090  
## 1504 -1.53211 0.2354720 -0.738271 0.16802500 1.443928256 -0.318596856  
## 16771 -1.53435 0.1623060 -0.837161 0.13471800 -0.878893050 0.118181119  
## 19693 -1.41520 0.1195790 -0.882301 0.03489690 -1.306438327 0.532403631  
## 13331 -1.61075 0.1856270 -0.686037 0.24688400 -0.877198993 -0.197683940  
## 18422 -1.58893 0.2807980 -0.794729 0.29577500 -1.164380459 1.664379027  
## 11663 -1.43399 0.1690300 -0.976866 0.38108400 -1.982347680 0.314495086  
## 13082 -1.61366 0.2640090 -0.827869 0.11757000 -0.989944235 0.601591759  
## 14941 -1.45710 0.1944660 -0.933029 0.02442340 -0.151684601 -1.429557536  
## 1073 -1.52209 0.2753300 -0.570507 0.09962210 0.912506791 -0.472999146  
## 1781 -1.28591 0.1158940 -1.060890 0.27705900 0.407669808 -0.487888829  
## 15091 -1.42076 0.1904500 -0.975126 0.05824720 -1.242184375 1.027388649  
## 13413 -1.50146 0.1286730 -0.908506 0.01943610 -0.642694412 -1.095763686  
## 12463 -1.44975 0.1559780 -1.000420 0.08914800 1.930243689 -0.916445608  
## 11261 -1.47394 0.2629680 -0.820186 0.17317600 0.410199364 1.054094779  
## 10231 -1.44967 0.2333160 -0.822707 0.02827360 -1.291349321 -1.439834035  
## 16911 -1.48570 0.2314710 -0.913189 0.10081700 2.635045375 0.532564109  
## 12011 -1.56731 0.2149610 -0.675284 0.04183570 0.487072288 -1.046928774  
## 14342 -1.55367 0.2719920 -0.759746 0.39567800 0.853892318 0.087385881  
## 1170 -1.27107 0.1558150 -1.177900 0.08436700 1.088442705 -0.174111691  
## 17372 -1.44077 0.2100670 -0.982287 0.11273100 0.226013957 -0.533826331  
## 1839 -1.57173 0.3002830 -0.796230 0.04772850 0.068198838 0.099317747  
## 11531 -1.46929 0.1755490 -0.838876 0.09596460 -0.984815533 -1.020107099  
## 16811 -1.52461 0.1270260 -0.756835 0.10230800 -1.310854422 0.430041832  
## 1825 -1.51603 0.2802960 -0.860012 0.24807500 2.464055335 1.502847759  
## 12443 -1.45651 0.1025680 -0.797462 0.07849340 -0.665428070 -0.270760795  
## 12893 -1.63062 0.1931120 -0.685089 0.13785500 0.912862648 0.871555415  
## 1694 -1.47276 0.2330490 -0.810850 0.13474500 0.964664226 -1.216293810  
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## 14002 -1.56688 0.1681660 -0.513453 0.31571300 -0.505837533 0.858962271  
## 1228 -1.54469 0.2348820 -0.831963 0.13339300 0.406987081 0.934961145  
## 1155 -1.46610 0.1747290 -1.160180 0.06328780 2.040025754 -0.791952504  
## 19331 -1.49767 0.3270680 -0.954200 0.24058200 -0.193935372 1.359486952  
## 1281 -1.50361 0.1570790 -0.891402 0.04977720 1.370222895 0.019649377  
## 17963 -1.52464 0.2377240 -0.892476 0.31192300 -0.515357348 -1.185940292  
## 17163 -1.56248 0.1647450 -0.447016 0.05040710 -0.718232806 0.343632123  
## 15473 -1.52872 0.2643100 -0.571078 0.33333000 -0.177242285 0.585487847  
## 16942 -1.50276 0.1602910 -0.749399 0.13892600 -0.401576463 -1.430200670  
## 13951 -1.49577 0.1391930 -0.978575 0.37831700 0.829883568 1.019029395  
## 17981 -1.49686 0.1400580 -0.740108 0.03130410 -0.785806614 0.320298932  
## 17043 -1.48828 0.1660760 -0.844094 0.16281500 -0.938501217 -0.501576176  
## 19892 -1.59347 0.2888390 -0.613089 0.07798820 0.417806768 -0.141376028  
## 16761 -1.47519 0.1555160 -0.844949 0.19839800 2.098097844 -1.430818217  
## 14713 -1.43092 0.2264300 -0.639910 0.37442800 -0.448862342 0.587857654  
## 12702 -1.43217 0.1576590 -0.916993 0.18215700 -1.095288092 0.868963574  
## 10551 -1.45105 0.1462760 -0.922492 0.11370700 -0.528972750 0.456654992  
## 10322 -1.49708 0.2984920 -1.033020 0.10165300 -0.484793938 -1.355959524  
## 18782 -1.40505 0.2223330 -0.737509 0.42116400 0.127757042 0.643807790  
## 10061 -1.59767 0.1269920 -0.757208 0.16436400 -0.074673107 0.070101188  
## 1083 -1.53817 0.2700500 -0.730248 0.12477900 -0.359162136 0.010391561  
## 14773 -1.36799 0.1743010 -0.924162 0.23427300 -2.048480559 0.721199978  
## 13932 -1.55261 0.2548150 -0.704767 0.11663500 -0.751180021 0.093814902  
## 14413 -1.55739 0.2600260 -0.736536 0.14709100 -1.581383000 -0.564257032  
## 15182 -1.56877 0.2220720 -0.869390 0.14961400 -0.289776058 0.007023682  
## 1371 -1.72882 0.2870550 -0.744408 0.09429150 -0.691954528 -0.561537486  
## 11582 -1.61957 0.1892780 -0.670785 0.17137500 -0.171987946 1.755959697  
## 11852 -1.44274 0.1636890 -0.870505 0.11226300 -0.222564010 0.170426604  
## 11001 -1.63609 0.1830960 -0.730948 0.02373350 0.919241279 1.065195204  
## 1943 -1.46580 0.1855460 -0.916135 0.19941600 -1.110065480 1.504156131  
## 15613 -1.61252 0.2010820 -0.929992 0.20503900 -0.660888997 0.659959697  
## 1793 -1.55676 0.1485310 -0.653115 0.01037830 -0.873774912 -0.838201076  
## 11502 -1.57305 0.3190160 -0.525297 0.09467700 -0.132809701 0.394689060  
## 16553 -1.63116 0.2097070 -0.702170 0.34536600 0.305489104 -0.379625994  
## 11162 -1.37099 0.1863210 -0.795357 0.09894210 2.163842485 2.066779896  
## 13412 -1.47622 0.2095640 -0.751334 0.39108800 0.880378505 -1.029749769  
## 14722 -1.55097 0.2625200 -0.822050 0.05474160 0.505116253 -0.123095504  
## 12323 -1.46704 0.2811320 -0.921961 0.10630700 0.110590205 0.173957707  
## 1722 -1.40051 0.1663530 -0.924951 0.05539080 -0.292858583 0.553190600  
## 1256 -1.45666 0.1526540 -0.954904 0.12622800 0.772319992 -0.759068678  
## 13092 -1.61047 0.2500110 -0.800462 0.09222460 2.128794229 0.035829594  
## 14762 -1.53787 0.2291770 -0.809759 0.12291900 0.547967970 -0.003495063  
## 18661 -1.68894 0.2228650 -0.677324 0.07436910 1.532129229 -0.220190416  
## 1032 -1.41771 0.2025880 -0.853602 0.39076500 1.666430854 -1.557680246  
## 12772 -1.46003 0.2705550 -0.975092 0.29239800 -0.478000049 -0.238045956  
## 1346 -1.52879 0.1768980 -0.938097 0.18542800 -0.368681625 0.424982482  
## 14222 -1.48069 0.1795730 -0.997278 0.21427200 -0.516166127 -0.446779715  
## 1432 -1.49428 0.1559050 -0.882634 0.22123800 0.396937689 -1.401854780  
## 1420 -1.40157 0.1683660 -1.107870 0.08892560 -0.314871760 -0.547414257  
## 15641 -1.57396 0.2303420 -0.750504 0.06893250 -0.684689801 0.247941769  
## 1591 -1.49958 0.2479540 -0.865271 0.26385200 1.632247789 -1.351702539  
## 10181 -1.48432 0.2506910 -0.776539 0.17389700 -0.684533761 1.285374670  
## 15213 -1.52670 0.1975190 -0.825591 0.39785300 -0.313076970 2.096632994  
## 18383 -1.50145 0.1803070 -0.926697 0.35996300 -0.640032652 -1.075716671  
## 17121 -1.52142 0.1405370 -0.834959 0.03218950 0.635304358 0.643818555  
## 11961 -1.69570 0.2928470 -0.603798 0.20059400 0.024848366 0.811107086  
## 1550 -1.72717 0.2859070 -0.679313 0.01462870 0.227622212 -0.373369162  
## 1021 -1.48354 0.2608950 -0.793619 0.07403470 -0.246068246 -0.117755702  
## 13783 -1.54611 0.2746990 -0.723687 0.11083200 0.024223829 0.939509301  
## 1472 -1.59210 0.2498340 -0.576934 0.15238300 -1.244582466 -0.223544486  
## 17673 -1.50497 0.1678060 -0.620597 0.03662980 -1.205974540 -1.188865752  
## 14023 -1.38964 0.1389070 -0.854477 0.02838590 0.273093950 0.599961163  
## 15453 -1.51991 0.2843590 -0.626933 0.10847800 1.729414034 -0.863306018  
## 16151 -1.52944 0.1968600 -0.847476 0.18731000 -1.064950869 -0.669136112  
## 14392 -1.68841 0.2432670 -0.902871 0.36563600 -0.113736688 0.758080913  
## 1606 -1.50807 0.2532860 -1.121310 0.25196000 -0.643751471 0.977212323  
## 14853 -1.49088 0.2196260 -0.875752 0.18648800 0.940648418 1.486960427  
## 16371 -1.42532 0.2203990 -1.061070 0.04566330 1.918810176 0.809182023  
## 14261 -1.57211 0.2171010 -0.880037 0.20193900 -1.006045550 1.049591298  
## 13171 -1.62818 0.3052030 -0.724928 0.21722200 0.547082630 -1.378317315  
## 10481 -1.68060 0.2202700 -0.581894 0.08894920 0.033847059 -1.166379732  
## 14142 -1.50302 0.2039430 -0.982989 0.10057500 -0.315828929 0.450531663  
## 15372 -1.56121 0.2715570 -0.939743 0.04127100 0.288544593 0.553986739  
## 13811 -1.51982 0.1707340 -0.921341 0.36133200 -0.344392202 0.171533785  
## 1300 -1.45299 0.2643750 -1.073200 0.15743700 0.116631435 -0.806881470  
## 1855 -1.45955 0.1588920 -1.149630 0.23371400 0.542965968 0.978852878  
## 18943 -1.48011 0.1918860 -0.800704 0.01223410 1.143947544 1.171035498  
## 18831 -1.45681 0.1715020 -0.823553 0.03793210 -1.284548845 -0.254750999  
## 1629 -1.60269 0.2000120 -0.880358 0.04233730 0.919811790 -0.261779474  
## 11953 -1.52795 0.1493190 -1.203140 0.05004570 -0.846090161 1.357008537  
## 13562 -1.57185 0.2204850 -0.941156 0.05787750 -1.419304273 1.048195428  
## 18421 -1.40577 0.1765290 -0.835779 0.07976180 -2.665697589 2.228898486  
## 20003 -1.35994 0.1678240 -1.022730 0.19834300 0.835106141 -1.470518812  
## 11401 -1.58505 0.1971660 -0.774160 0.24158100 2.377446549 -1.031250041  
## 1048 -1.48919 0.1993050 -0.821110 0.23316200 0.013969708 0.164813527  
## 12143 -1.54976 0.2504290 -0.779318 0.17970800 -1.633423995 -1.243838156  
## 1075 -1.55142 0.2850860 -0.728439 0.01539880 0.488932473 0.116308174  
## 18021 -1.43885 0.1650170 -0.676836 0.10744900 -1.019179409 1.197547370  
## 17623 -1.56458 0.2481620 -0.675031 0.06439390 1.090553483 -0.698130988  
## 1499 -1.47933 0.2354970 -0.842719 0.03511180 -1.139469805 0.293604948  
## 18673 -1.60311 0.1643570 -0.821628 0.09756690 -0.015725635 0.437297744  
## 1093 -1.49444 0.1846610 -0.717872 0.05115940 0.297491282 0.627762573  
## 13553 -1.42957 0.1519730 -0.786311 0.00982651 3.200590040 -1.160543514  
## 12592 -1.47815 0.1860290 -0.869114 0.01620470 0.089244244 -0.020788418  
## 12912 -1.54680 0.1815310 -0.892300 0.02948780 0.570972338 1.044724089  
## 1785 -1.42669 0.2171790 -0.991846 0.08288900 0.528685630 1.311594585  
## 14041 -1.56975 0.2135000 -0.883118 0.00203215 -0.440904798 -0.082439028  
## 1624 -1.46589 0.1993470 -0.957345 0.01713570 -0.672793368 0.919224762  
## 1841 -1.58289 0.2296940 -0.873117 0.07100870 2.154313365 -0.243269921  
## 19553 -1.54739 0.2263010 -0.391179 0.03320420 0.593852716 0.351094377  
## 12722 -1.43217 0.1634400 -0.994116 0.23131900 -0.384063768 -1.340384172  
## 15122 -1.41179 0.1467770 -0.927081 0.28481400 0.719783276 0.425846094  
## 1348 -1.42482 0.1731270 -0.832138 0.09016220 1.708173402 -0.814353733  
## 15183 -1.52820 0.2273670 -0.873265 0.10598700 1.075215667 0.693374081  
## 14432 -1.54149 0.1837410 -0.986642 0.33243600 0.777420367 0.705544556  
## 1468 -1.52714 0.2273480 -0.652243 0.11856900 0.052200047 0.278350539  
## 17953 -1.51122 0.1888740 -0.909895 0.12429800 -1.083698485 -1.202692142  
## 1557 -1.43841 0.1971180 -0.971405 0.00120255 -0.008856207 0.642761817  
## 19642 -1.43905 0.2482490 -0.986455 0.17539200 2.030643112 -0.605973945  
## 16191 -1.52013 0.2185760 -0.769066 0.11450600 -1.113328933 -1.377257613  
## 17011 -1.44545 0.1573750 -1.033650 0.13570000 1.138271925 -0.925992687  
## 1820 -1.52520 0.2170930 -0.880422 0.13424200 -0.614892642 0.567243857  
## 10851 -1.55563 0.2999810 -0.626022 0.00471981 -2.193536615 2.595481260  
## 13483 -1.38049 0.2561920 -1.084550 0.14871900 -1.215686372 -0.239984547  
## 13183 -1.59476 0.2636340 -0.807156 0.24493800 -0.045326362 0.687536401  
## 18462 -1.60507 0.2672580 -0.884388 0.02973600 1.598812624 -0.151788986  
## 15542 -1.61982 0.1783290 -0.602758 0.10187000 0.927542200 0.227544260  
## 18752 -1.41439 0.2021660 -1.021410 0.07233720 0.829284552 -0.668648038  
## 12081 -1.54116 0.1885010 -0.655092 0.03394090 1.024603876 0.030829067  
## 1014 -1.26405 0.1476700 -1.160320 0.03269000 -0.476238068 0.028429558  
## 15612 -1.76674 0.3375280 -0.667801 0.08488970 1.638868393 -0.365455074  
## 14833 -1.47812 0.2484540 -0.867909 0.13378900 -0.632050958 -2.208012195  
## 1639 -1.55076 0.1809390 -0.832294 0.02823040 -1.379618576 0.297039427  
## 10353 -1.46452 0.2528490 -0.771122 0.03499700 -0.257455748 2.129700659  
## 15011 -1.51556 0.1389780 -0.776806 0.02513700 1.679972711 1.325041143  
## 12253 -1.52683 0.1784320 -0.536272 0.36808800 -2.545858038 -0.116171447  
## 10793 -1.40285 0.1793950 -0.935126 0.17230300 0.012078784 -1.470146221  
## 10103 -1.45496 0.1923700 -1.018330 0.05143680 1.960925111 -0.379271835  
## 1903 -1.53717 0.1939060 -0.793830 0.00493727 -0.385905481 -1.465005931  
## 1679 -1.42264 0.1686210 -0.978543 0.10852200 0.910757548 1.075148263  
## 1795 -1.62570 0.1734150 -0.570858 0.04275820 -1.448130794 -1.226124877  
## 1489 -1.43750 0.2315680 -0.742989 0.27496200 -1.121614596 -3.056328234  
## 1881 -1.61298 0.2184480 -0.630581 0.13860100 -0.973617906 1.450657775  
## 15061 -1.32537 0.1226480 -0.867043 0.05831050 -0.067186922 0.717976859

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

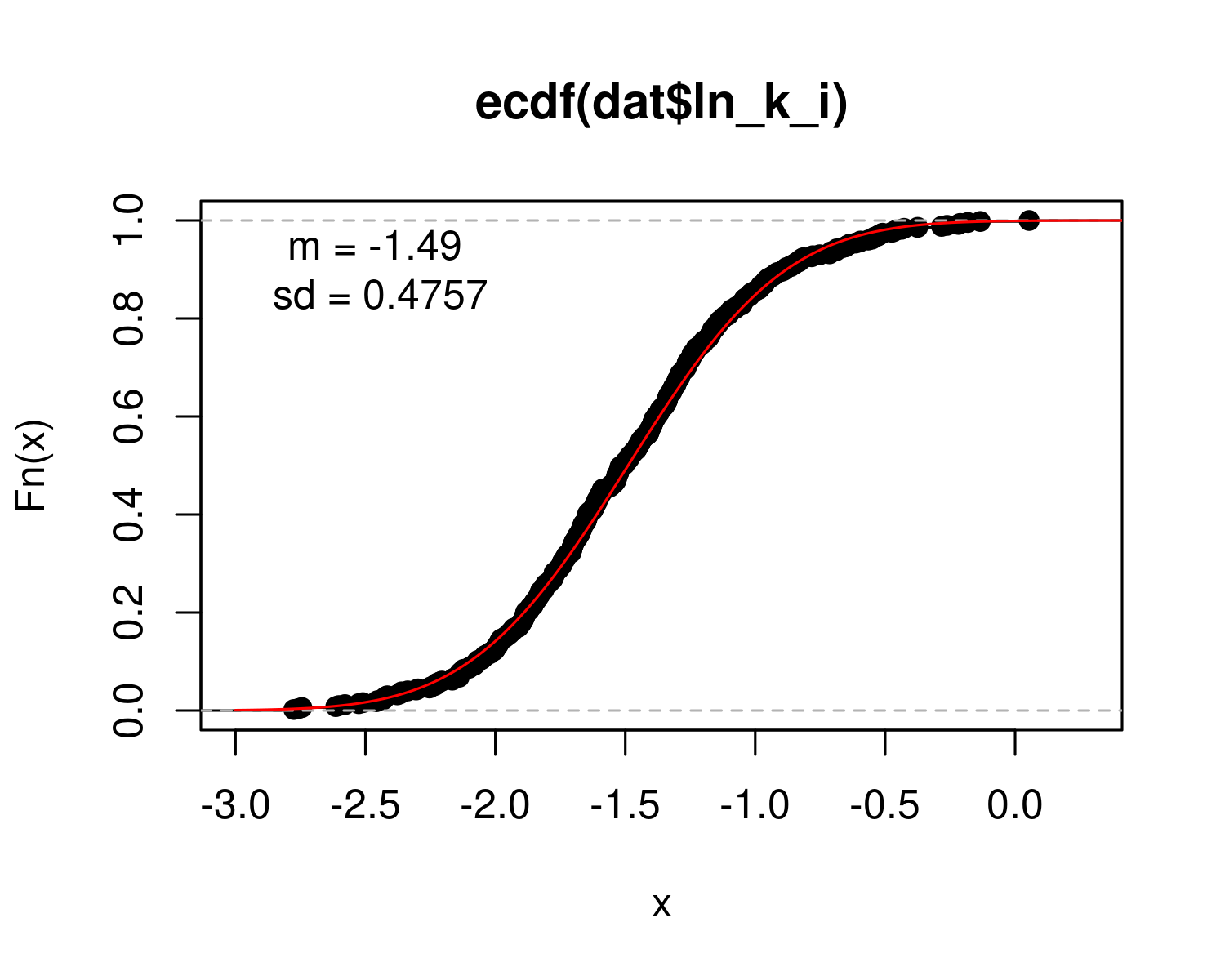


## Check normality

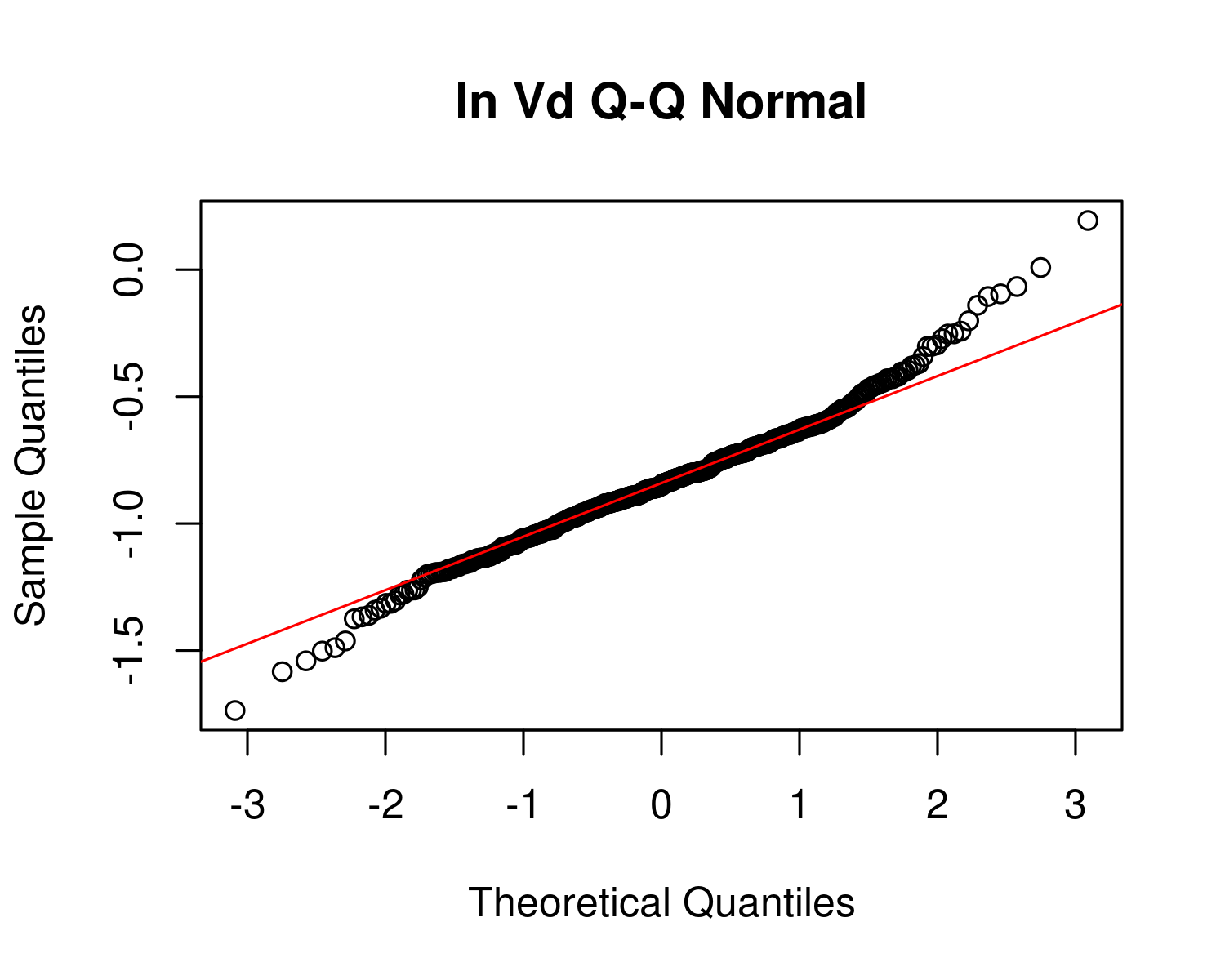
qqnorm(dat$ln\_k\_i,main="ln k Q-Q Normal")  
qqline(dat$ln\_k\_i,col="red")



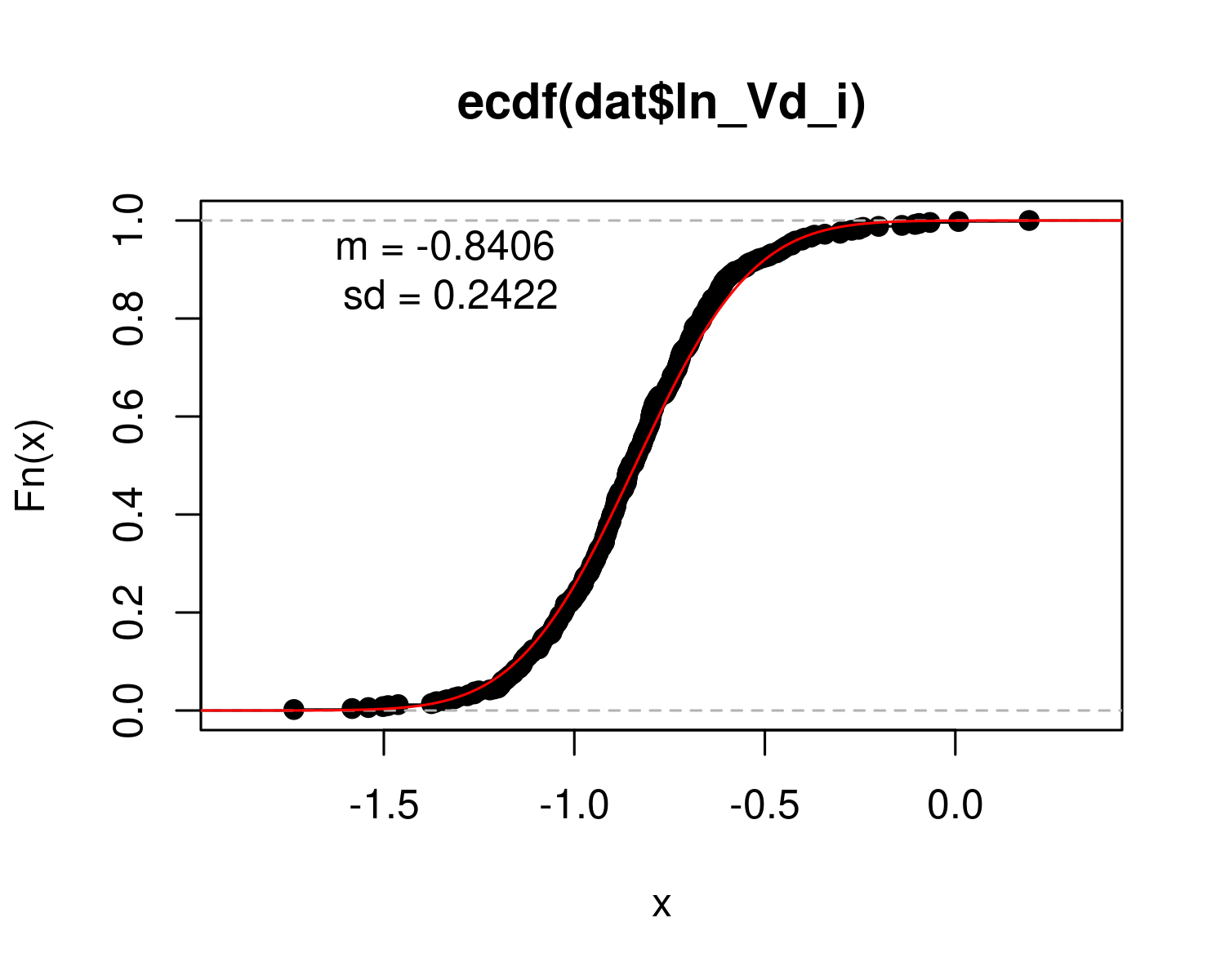
plot(ecdf(dat$ln\_k\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_k\_i <- mean(dat$ln\_k\_i)  
sd\_ln\_k\_i <- sd(dat$ln\_k\_i)  
lines(x,pnorm(x,mean=m\_ln\_k\_i,sd=sd\_ln\_k\_i),col="red")  
text(m\_ln\_k\_i-2\*sd\_ln\_k\_i,0.9,paste("m =",signif(m\_ln\_k\_i,4),"\nsd =",signif(sd\_ln\_k\_i,4)))



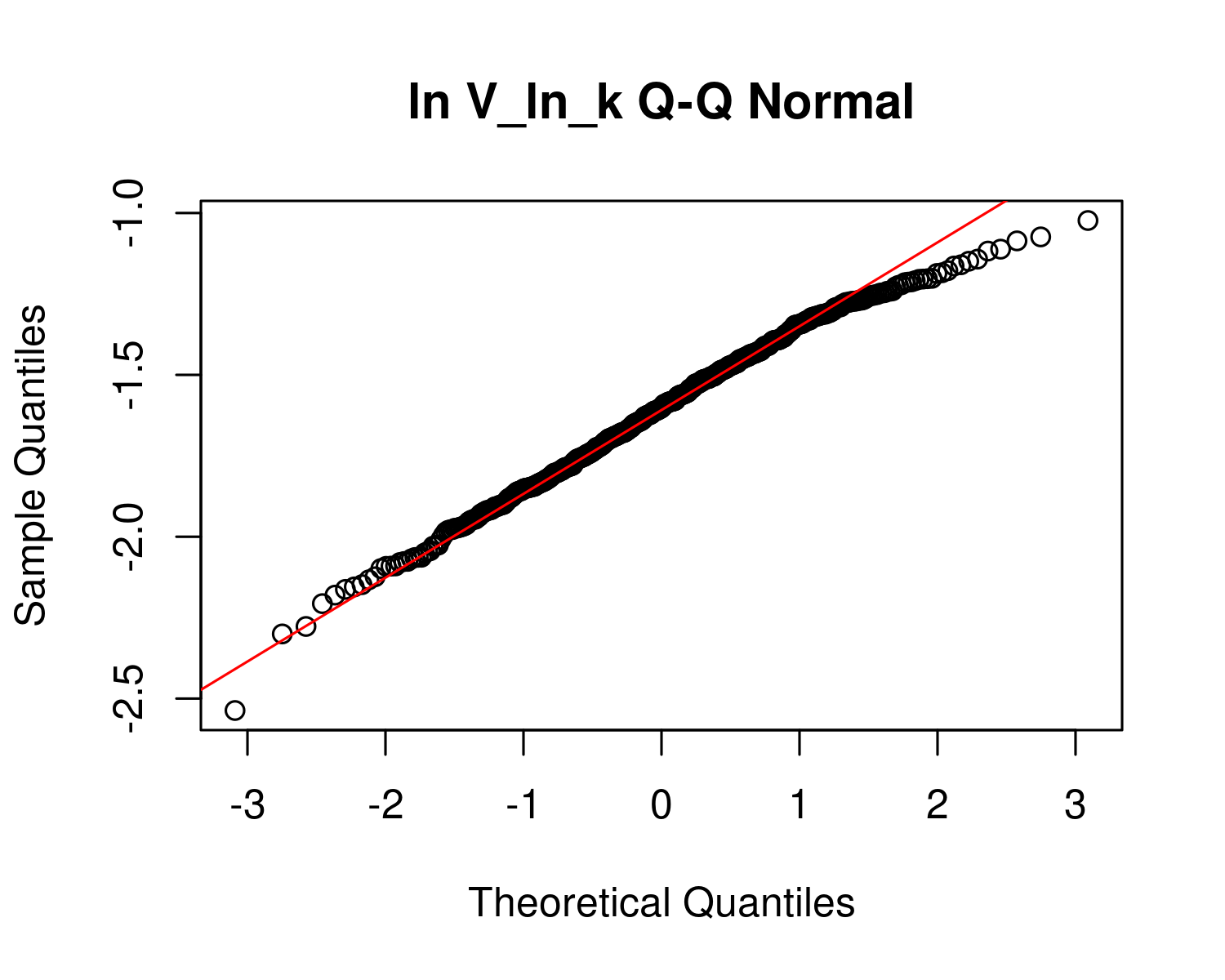
qqnorm(dat$ln\_Vd\_i,main="ln Vd Q-Q Normal")  
qqline(dat$ln\_Vd\_i,col="red")



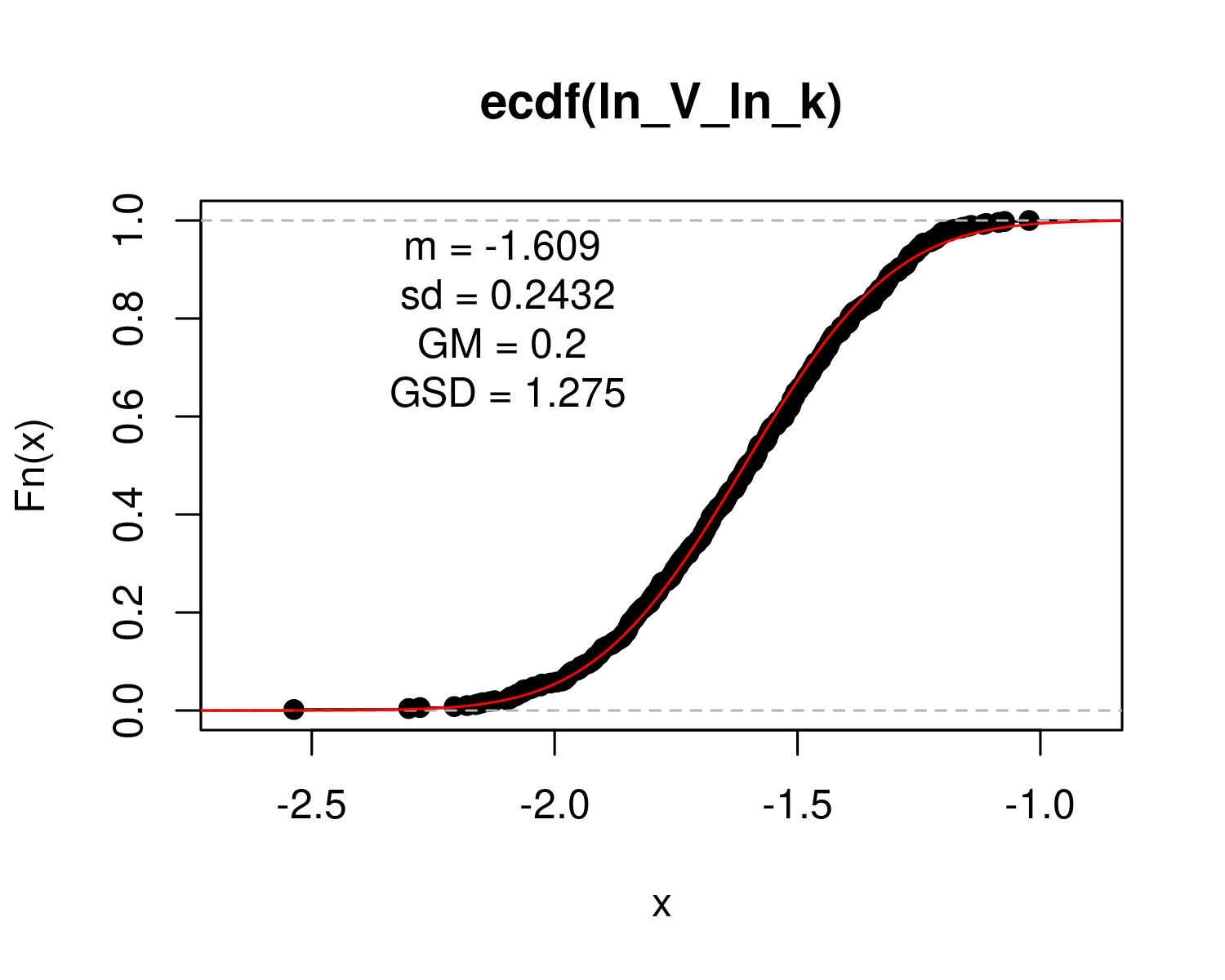
plot(ecdf(dat$ln\_Vd\_i))  
x <- seq(-3,1,0.01)  
m\_ln\_Vd\_i <- mean(dat$ln\_Vd\_i)  
sd\_ln\_Vd\_i <- sd(dat$ln\_Vd\_i)  
  
lines(x,pnorm(x,mean=m\_ln\_Vd\_i,sd=sd\_ln\_Vd\_i),col="red")  
text(m\_ln\_Vd\_i-2\*sd\_ln\_Vd\_i,0.9,paste("m =",signif(m\_ln\_Vd\_i,4),"\nsd =",signif(sd\_ln\_Vd\_i,4)))

 ## Fit to posterior for half-life population variability

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



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

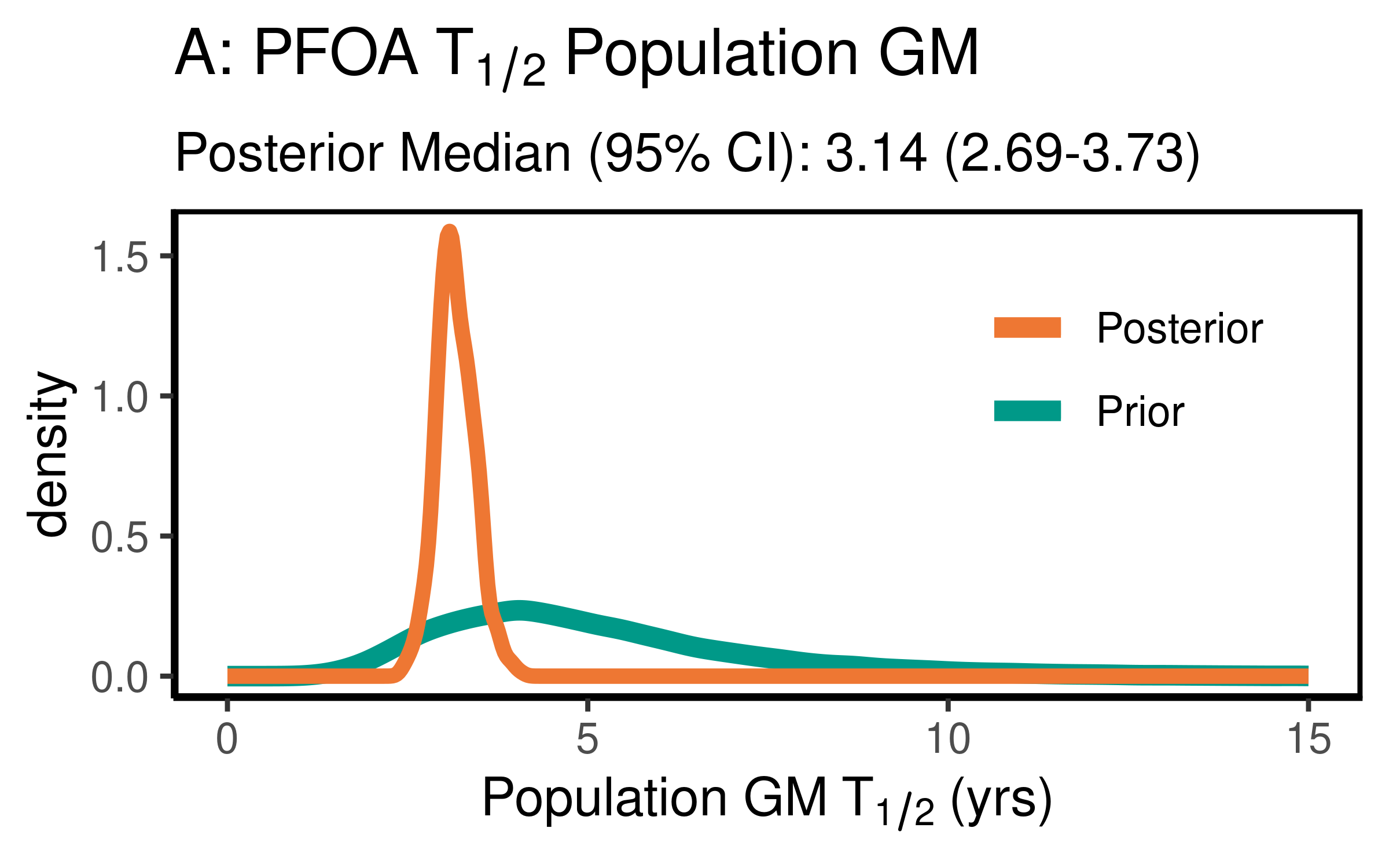


## Calculate table values for individual-level

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

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

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



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

## Saving 4 x 2.5 in image

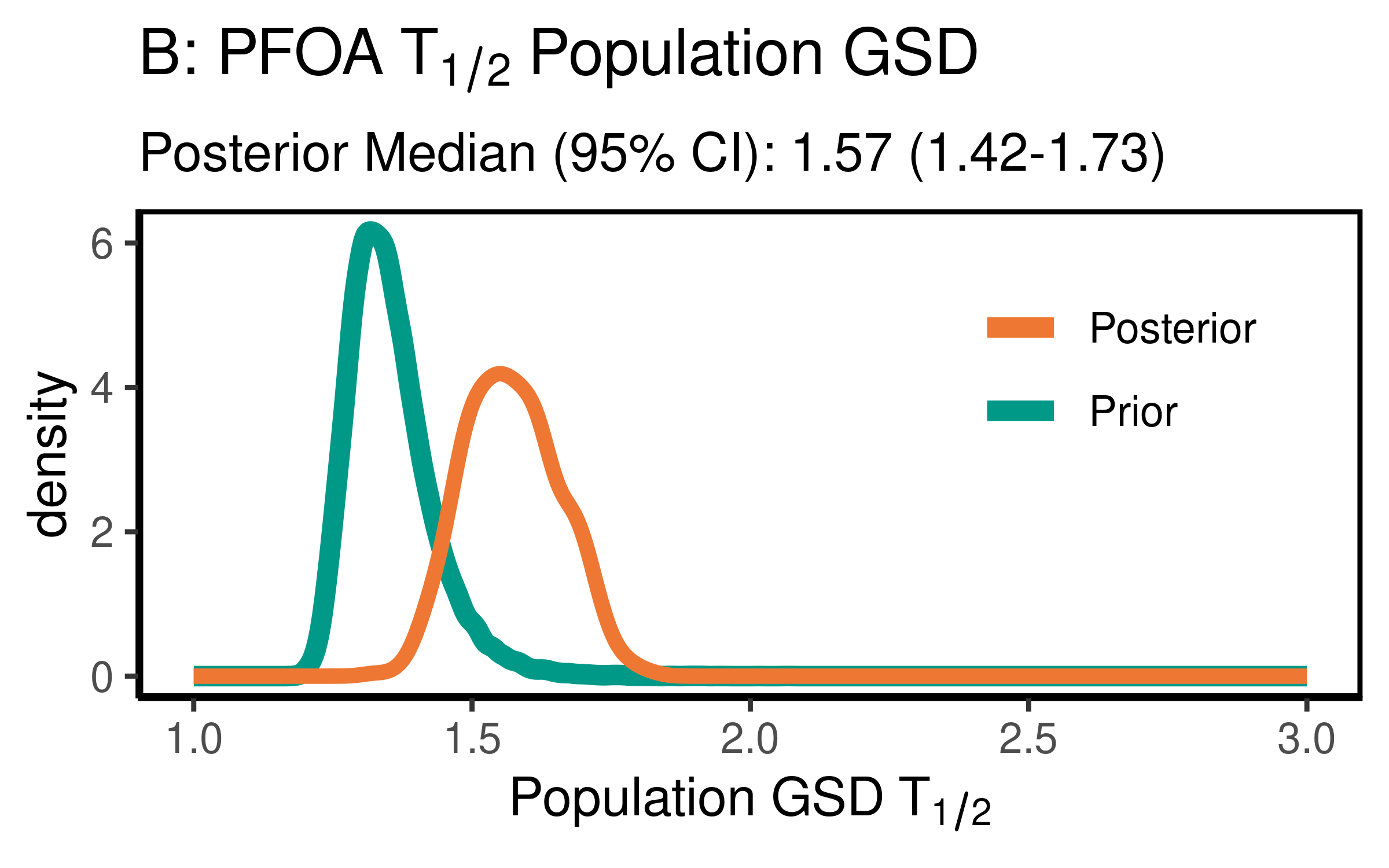
## Warning: Removed 80 rows containing non-finite values (stat\_density).

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

## Saving 4 x 2.5 in image

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

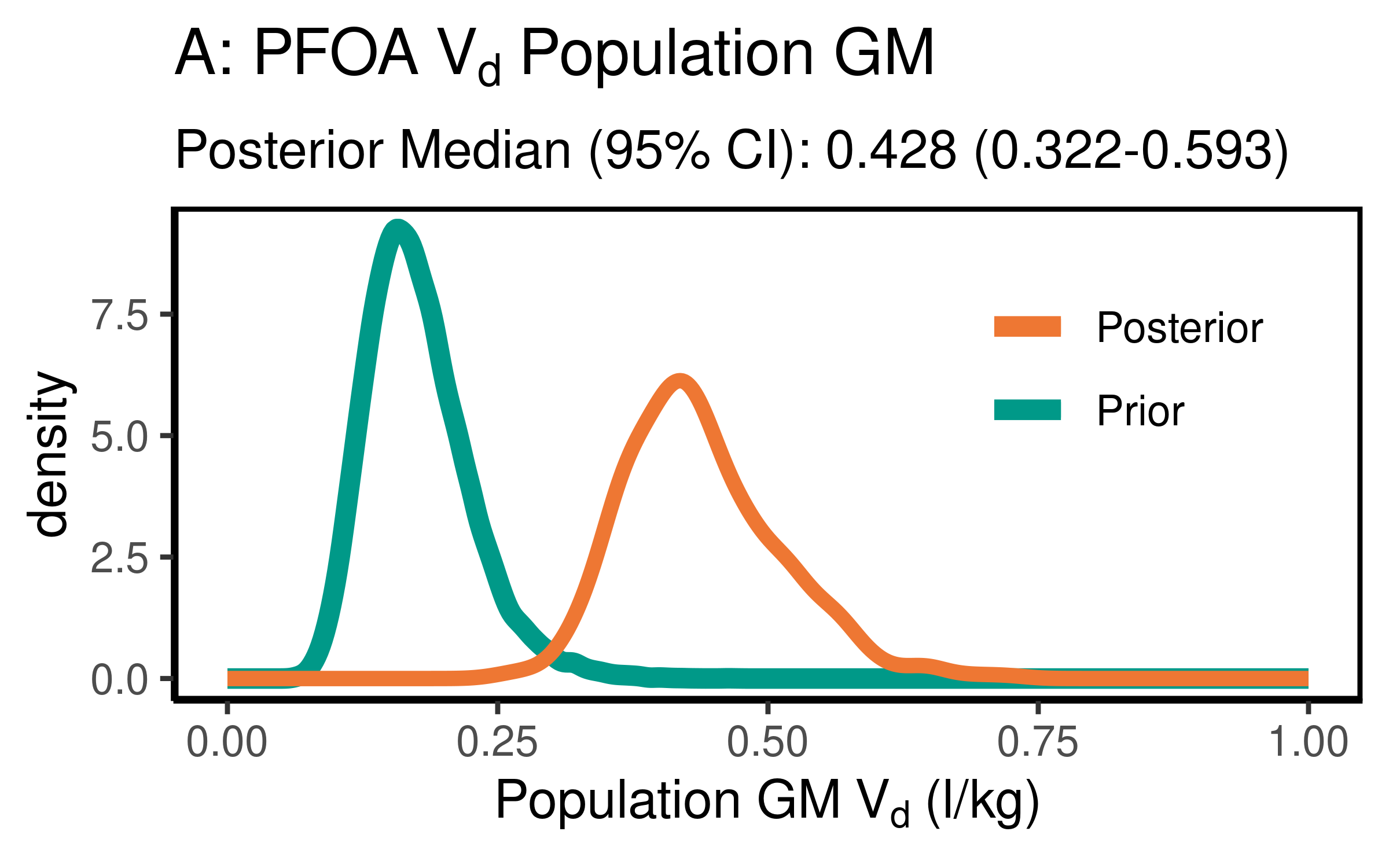
PFOA\_priors$halflife\_GSD = exp(sqrt(1/rgamma(50000,shape=9,rate=0.75))) #inverse gamma for the first trial  
PFOA\_halflife\_GSD <- exp(sqrt(dat$`V\_ln\_k(1)`))  
  
pfoa\_hlgsd\_pr\_med <- signif(median(PFOA\_priors$halflife\_GSD,3))  
pfoa\_hlgsd\_pr\_med\_95ci <-paste(signif(quantile(PFOA\_priors$halflife\_GSD,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



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

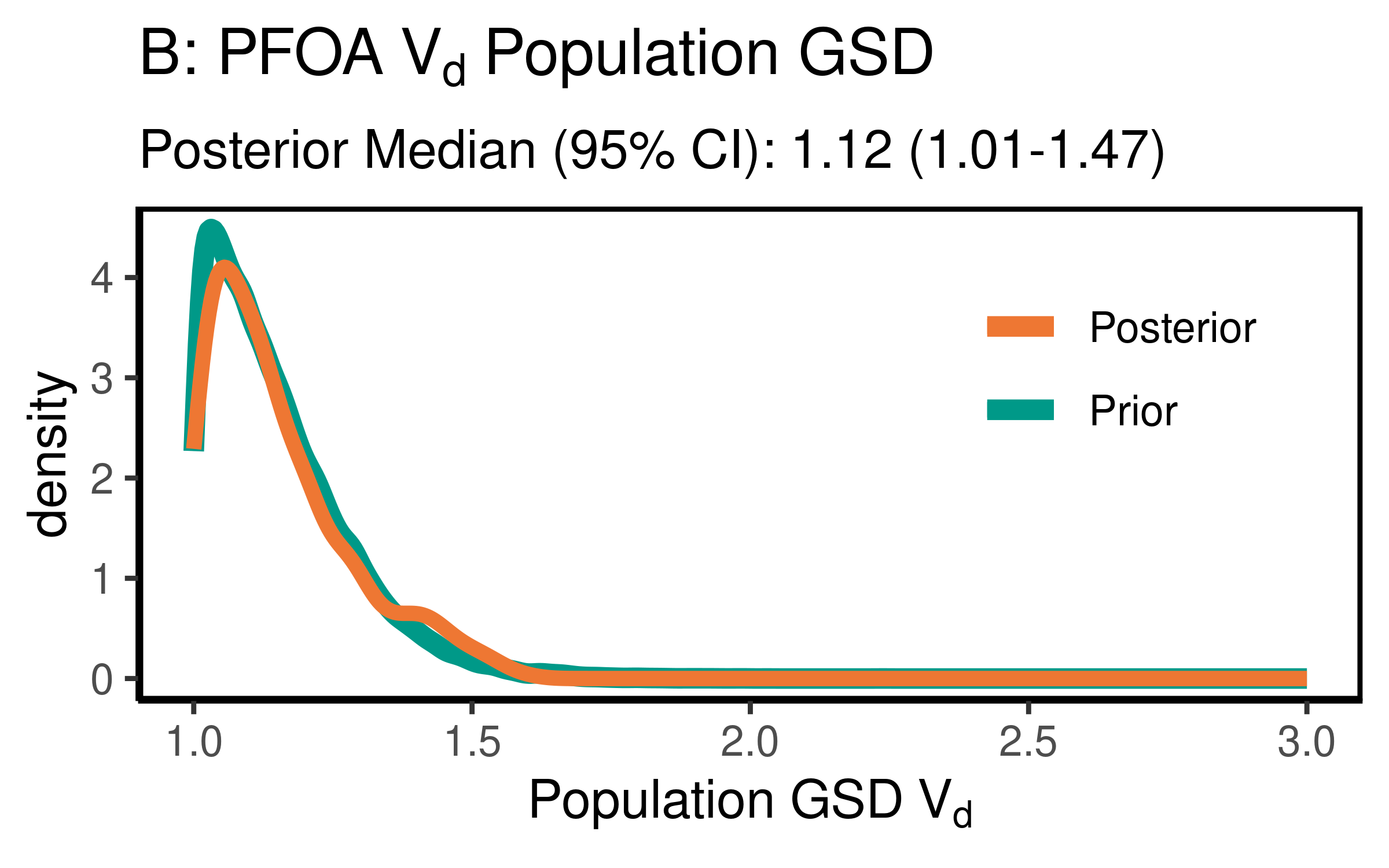
### Distribution Volume

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



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

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

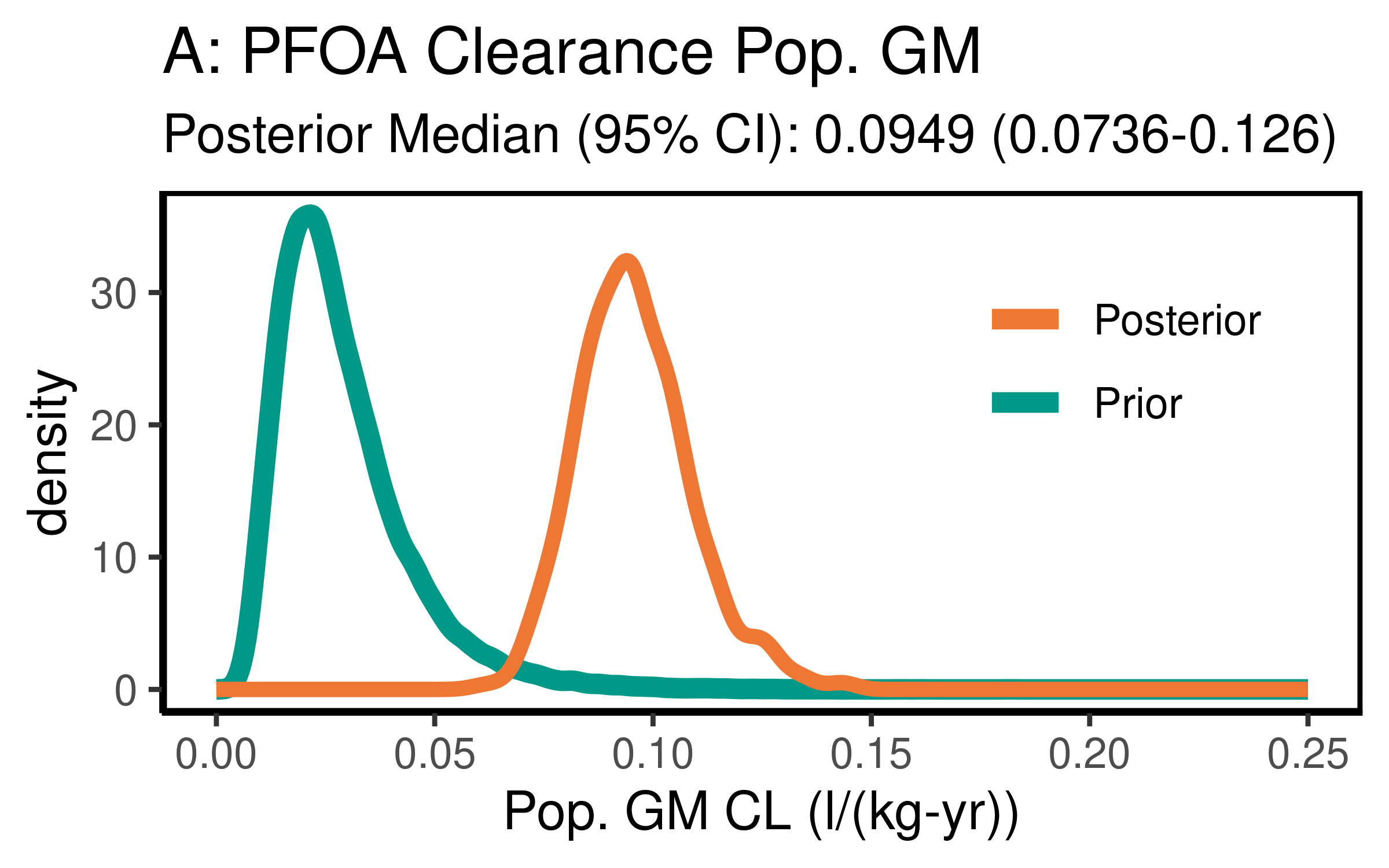


ggsave(here ("output-plots",paste0( sa, "PFOA\_vd\_gsd.pdf")) ,p,dpi=600)  
ggsave(here ("output-plots",paste0( sa, "PFOA\_vd\_gsd.png")) ,p,dpi=600)

### Clearance

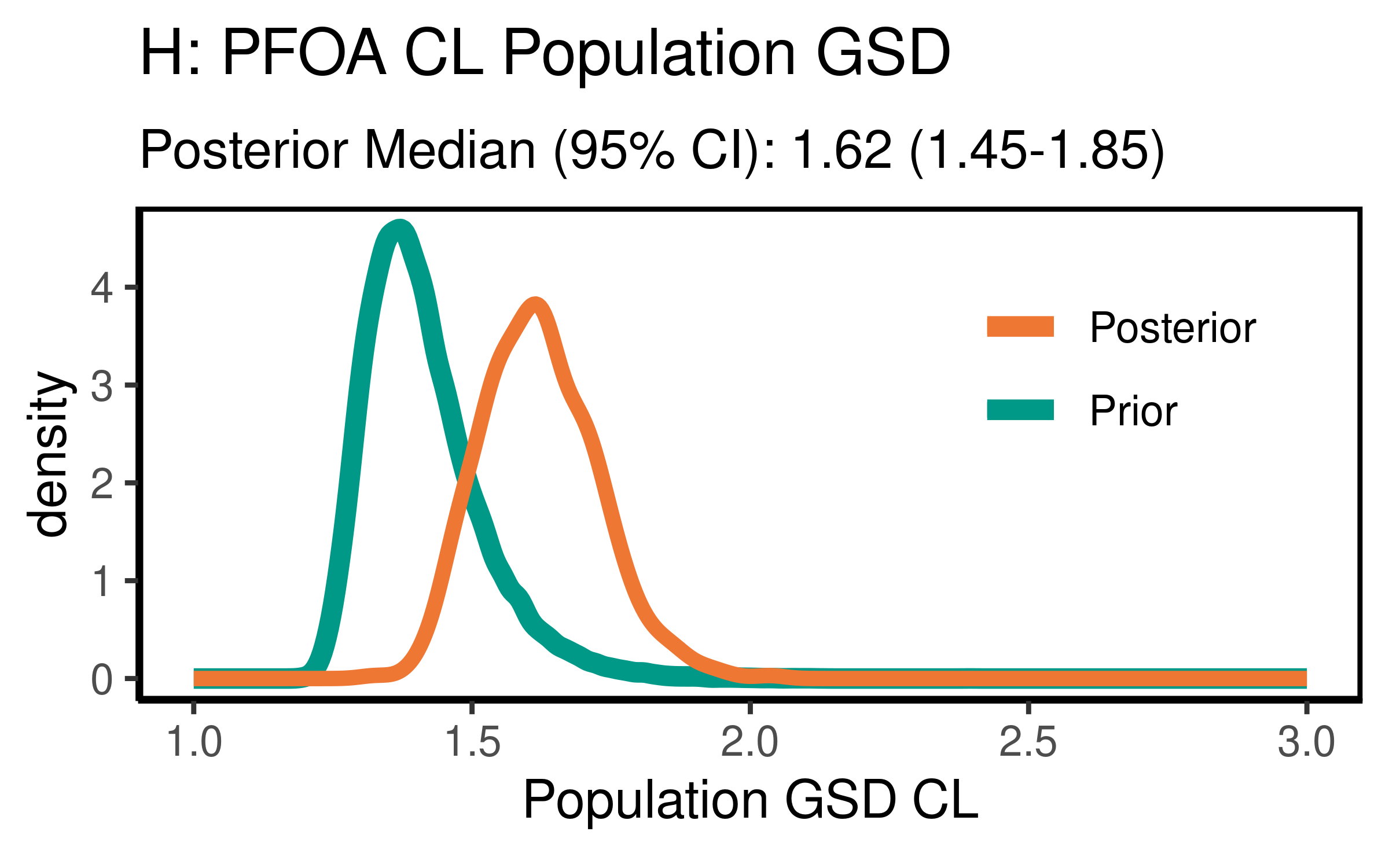
Cl is k \* Vd

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



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

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

## Table significant digit values

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

### Population median estimates [95% CI]

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

### Individual Posterior estimates

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | median GM [95% CI] | GM calculator input | GSD individual |
| Half-life (years) | 3.13 [ 1.13-7.83 ] | 3.07 | 1.61 |
| Volume of distribution | 0.427 [ 0.27-0.739 ] | 0.431 | 1.27 |
| Clearance (L/kg-yr) | 0.0957 [ 0.0369-0.262 ] [[ 0.0327-0.341 ]] | 0.0973 | 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)  
## codetools 0.2-18 2020-11-04 [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