```
setwd("L:/Lab/NCCT_vLiver/projects/v-Liver-Sim/vLiverPBPK/R/dev")
library(gdata)
pkdata <- read.xls("pkdata-020413.xlsx",sheet=2,stringsAsFactors=FALSE)
averagetissue <- read.xls("pkdata-020413.xlsx",sheet=3,stringsAsFactors=FALSE)
tissuedata <- read.xls("pkdata-020413.xlsx",sheet=1,stringsAsFactors=FALSE,skip=1)[1:13,]
colnames(tissuedata) <-
c("Tissue","Fcell","Fint","FWc","FLc","FPc","Fn_Lc","Fn_PLc","Fa_PLc","pH","Mouse Vol (L/kg)","Rat Vol
(L/kg)","Dog Vol (L/kg)","Human Vol (L/kg)","Mouse Flow (mL/min/kg)","Rat Flow (mL/min/kg)","Dog Flow
(mL/min/kg)","Human Flow (mL/min/kg)")
tissuedata[,2] <- as.numeric(tissuedata[,2])
tissuedata[,3] <- as.numeric(tissuedata[,3])

tissuelist <- list(Liver=c("Liver"),Kidney=c("Kidneys"),Lung=c("Lung"),Skin=c("Skin"))
chem.prop <- read.xls("vLiver-Chem-Prop-073013.xlsx",stringsAsFactors=FALSE,skip=2)
chem.prop <- chem.prop[,c(1:2,8:24,35:39)]

in.vivo.data <- read.xls("HT-PBPK compounds-020413.xlsx",stringsAsFactors=FALSE,sheet=3)
#in.vivo.data[is.na(in.vivo.data)] <- ""
in.vivo.data[in.vivo.data==" "] <- ""
for (this.col in (1:length(colnames(in.vivo.data))))
  if (is.na(in.vivo.data[1,this.col]))
  {
    this.row <- 1
    while (is.na(in.vivo.data[this.row,this.col]))
    {
      in.vivo.data[this.row,this.col] <- ""
      this.row <- this.row + 1
    }
    this.row <- dim(in.vivo.data)[1]
    while (is.na(in.vivo.data[this.row,this.col]))
    {
      in.vivo.data[this.row,this.col] <- ""
      this.row <- this.row - 1
    }
  }

PK.data.in.vivo <- NULL
this.col <- 1
this.chem <- NA
for (this.col in (1:length(colnames(in.vivo.data)))[in.vivo.data[1,]!=""])
{
  this.CAS <- NA
  this.species <- NA
  this.reference <- NA
  this.weight <- NA
  this.weight.units <- NA
  this.time <- NA
  this.time.units <- NA
  this.media <- NA
  this.media.units <- NA
  this.dose <- NA
  this.dose.units <- NA
  this.value <- NA
  print(paste(this.col))
  if (in.vivo.data[1,this.col]!="")
  {
```

```
  if (regexpr("X\\.",colnames(in.vivo.data)[this.col])==-1) this.chem <- colnames(in.vivo.data)[this.col]
  this.chem <- gsub("\\."," ",this.chem)
  this.chem <- gsub("^ .", "", this.chem)
  this.chem <- gsub(" $", "", this.chem)
  if (any(chem.prop[,1]==this.chem)) this.CAS <- chem.prop[chem.prop[,1]==this.chem,2]
  if (in.vivo.data[2,this.col]!="") this.species <- in.vivo.data[2,this.col]
  if (in.vivo.data[1,this.col]!="") this.reference <- in.vivo.data[1,this.col]
  if (in.vivo.data[3,this.col]!="") this.weight <- in.vivo.data[3,this.col]
  if (in.vivo.data[4,this.col]!="") this.weight.units <- in.vivo.data[4,this.col]
  if (in.vivo.data[6,this.col]!="") this.time.units <- in.vivo.data[6,this.col]
  this.first.col <- this.col
  this.col <- this.col + 1
  while (in.vivo.data[1,this.col]=="")
  {
    this.row.index <- 8
    while(is.na(in.vivo.data[this.row.index,this.col]))
    {
      this.row.index <- this.row.index + 1
      if (this.row.index > dim(in.vivo.data)[1]) break()
    }
    if (this.row.index > dim(in.vivo.data)[1]) break()
    if (in.vivo.data[3,this.col]!="") this.dose <- in.vivo.data[3,this.col]
    if (in.vivo.data[4,this.col]!="") this.dose.units <- in.vivo.data[4,this.col]
    if (in.vivo.data[5,this.col]!="") this.media <- in.vivo.data[5,this.col]
    if (in.vivo.data[6,this.col]!="") this.media.units <- in.vivo.data[6,this.col]
    this.row.stub <- data.frame(this.chem,stringsAsFactors=FALSE)
    this.row.stub <- cbind(this.row.stub,data.frame(this.CAS,stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(this.reference,stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(this.species,stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(as.numeric(this.weight),stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(this.weight.units,stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(as.numeric(this.dose),stringsAsFactors=FALSE))
    this.row.stub <- cbind(this.row.stub,data.frame(this.dose.units,stringsAsFactors=FALSE))
    while (in.vivo.data[this.row.index,this.col] != "")
    {
      this.time <- in.vivo.data[this.row.index,this.first.col]
      this.value <- in.vivo.data[this.row.index,this.col]
      this.row <- cbind(this.row.stub,data.frame(as.numeric(this.time),stringsAsFactors=FALSE))
      this.row <- cbind(this.row,data.frame(this.time.units,stringsAsFactors=FALSE))
      this.row <- cbind(this.row,data.frame(this.media,stringsAsFactors=FALSE))
      this.row <- cbind(this.row,data.frame(this.media.units,stringsAsFactors=FALSE))
      this.row <- cbind(this.row,data.frame(as.numeric(this.value),stringsAsFactors=FALSE))
      colnames(this.row) <- c("Compound","CAS","Reference","Species","Species Weight","Species
Weight Units","Dose","Dose Units and Type","Time","Time Units","Media","Media Units","Value")
      PK.data.in.vivo <- rbind(PK.data.in.vivo,this.row)
      print(paste(this.row.index,this.col))
      this.row.index <- this.row.index + 1
      while(is.na(in.vivo.data[this.row.index,this.col]))
      {
        this.row.index <- this.row.index + 1
        if (this.row.index > dim(in.vivo.data)[1]) break()
#         browser()
      }
      if (this.row.index > dim(in.vivo.data)[1]) break()
    }
    this.col <- this.col + 1
```

```
    if (this.col > dim(in.vivo.data)[2]) break()
  }
 }
}

#Check for Chemicals missing CAS numbers:
unique(PK.data.in.vivo$Compound[is.na(PK.data.in.vivo$CAS)])


chem.physical_and_invitro.data <- chem.prop
chem.invivo.PK.data <- PK.data.in.vivo
PK.physiology.data <- pkdata
tissue.data <- tissuedata
average.tissue <- averagetissue



Wetmore.data <-
read.xls("Supp_Table_8_SimCyp_IVIVE_input_output_083011.xls",stringsAsFactors=F,skip=1)
Wetmore.data.1 <- Wetmore.data[Wetmore.data[,"Concentration..uM."]==1,]
Wetmore.data.10 <- Wetmore.data[Wetmore.data[,"Concentration..uM."]==10,]
Wetmore.data.abridged <- NULL
Wetmore.data.1.CASlist <- unique(Wetmore.data.1[,"CASRN"])
Wetmore.data.10.CASlist <- unique(Wetmore.data.10[,"CASRN"])
good.cols <- c(1:19)
for (this.CAS in unique(Wetmore.data[,"CASRN"]))
{
 if (this.CAS %in% Wetmore.data.1.CASlist) Wetmore.data.abridged <-
rbind(Wetmore.data.abridged,Wetmore.data.1[Wetmore.data.1[,"CASRN"]==this.CAS,good.cols][1,])
 if (this.CAS %in% Wetmore.data.10.CASlist) Wetmore.data.abridged <-
rbind(Wetmore.data.abridged,Wetmore.data.10[Wetmore.data.10[,"CASRN"]==this.CAS,good.cols][1,])
}
Wetmore.data.abridged <- cbind(Wetmore.data.abridged,"Human")
colnames(Wetmore.data.abridged)[20] <- "Species"



Wetmore.rat.data <- read.xls("toxsci_12_0787_File012.xls",skip=2,stringsAsFactors=F)
Wetmore.rat.data.1 <- Wetmore.rat.data[Wetmore.rat.data[,"Conc.uM."]==1,]
Wetmore.rat.data.10 <- Wetmore.rat.data[Wetmore.rat.data[,"Conc.uM."]==10,]
Wetmore.rat.data.abridged <- NULL
Wetmore.rat.data.1.CASlist <- unique(Wetmore.rat.data.1[,"CASRN"])
Wetmore.rat.data.10.CASlist <- unique(Wetmore.rat.data.10[,"CASRN"])
good.cols <- c(1,2,3,4,9,9,5,10,6,11,7,8,12,15,16)
for (this.CAS in unique(Wetmore.rat.data[,"CASRN"]))
{
 if (this.CAS %in% Wetmore.rat.data.1.CASlist) Wetmore.rat.data.abridged <-
rbind(Wetmore.rat.data.abridged,Wetmore.rat.data.1[Wetmore.rat.data.1[,"CASRN"]==this.CAS,good.col
s][1,])
 if (this.CAS %in% Wetmore.rat.data.10.CASlist) Wetmore.rat.data.abridged <-
rbind(Wetmore.rat.data.abridged,Wetmore.rat.data.10[Wetmore.rat.data.10[,"CASRN"]==this.CAS,good.c
ols][1,])
}

Wetmore.rat.data.abridged[,5] <- Wetmore.rat.data.abridged[,5]*100
Wetmore.rat.data.abridged <- cbind(Wetmore.rat.data.abridged,NA)
```

```
Wetmore.rat.data.abridged <- cbind(Wetmore.rat.data.abridged,NA)
Wetmore.rat.data.abridged <- cbind(Wetmore.rat.data.abridged,NA)
Wetmore.rat.data.abridged <- cbind(Wetmore.rat.data.abridged,NA)
Wetmore.rat.data.abridged <- cbind(Wetmore.rat.data.abridged,"Rat")
Wetmore.rat.data.abridged[,18] <- Wetmore.rat.data.abridged[,15]
Wetmore.rat.data.abridged[,15] <- Wetmore.rat.data.abridged[,14]
Wetmore.rat.data.abridged[,14] <- NA
colnames(Wetmore.rat.data.abridged) <- colnames(Wetmore.data.abridged)

Wetmore.data <- rbind(Wetmore.data.abridged,Wetmore.rat.data.abridged)

save(average.tissue,chem.invivo.PK.data,chem.physical_and_invitro.data,PK.physiology.data,tissue.data
,tissuelist,Wetmore.data,file="L:\\Lab\\NCCT_vLiver\\projects\\v-Liver-
Sim\\vLiverPBPK\\data\\Tables.RData")


Wetmore.Human.CASlist <- unique(subset(Wetmore.data,Species=="Human")$CASRN)
Wetmore.Rat.CASlist <- unique(subset(Wetmore.data,Species=="Rat")$CASRN)
vLiver.Human.CASlist <-
unique(chem.physical_and_invitro.data[chem.physical_and_invitro.data$Human=="Y","CAS"])
vLiver.Rat.CASlist <-
unique(chem.physical_and_invitro.data[chem.physical_and_invitro.data$Rat=="Y","CAS"])
```