```
calc_Css <-
function(chem.CAS=NULL,chem.name=NULL,species="Human",dose=1,doses.per.day=NULL)
#,Qh=20.7,QGFR=1.8)
{
  if (is.null(chem.CAS) & is.null(chem.name))
  {
    stop("Must specifiy compound name or CAS.\n")
  } else if ((!is.null(chem.CAS) & !any(chem.invivo.PK.data$CAS==chem.CAS)) & (!is.null(chem.name) &
!any(chem.invivo.PK.data$Compound==chem.name)))
  {
    stop("Compound not found.\n")
  }

  if (!is.null(chem.CAS))
  {
    this.chem.data <- subset(chem.invivo.PK.data,CAS==chem.CAS)
    chem.name <- this.chem.data[1,"Compound"]
  } else {
    this.chem.data <- subset(chem.invivo.PK.data,Compound==chem.name)
    chem.CAS <- this.chem.data[1,"CAS"]
  }
  chem.physical_and_invitro.data.index <- which(chem.physical_and_invitro.data$CAS==chem.CAS)

  if (!(species %in% colnames(PK.physiology.data)))
  {
    if (toupper(species) %in% toupper(colnames(PK.physiology.data)))
    {
      PK.phys.species <-
colnames(PK.physiology.data)[toupper(colnames(PK.physiology.data))==toupper(species)]
      warning(paste(species,"coerced to",PK.phys.species,"for physiological data."))
    } else stop(paste("Physiological PK data for",species,"not found."))
  } else PK.phys.species <- species
  this.phys.data <- PK.physiology.data[,PK.phys.species]
  names(this.phys.data) <- PK.physiology.data[,1]
  #mL/min:
  QGFR <- this.phys.data["GFR"]*this.phys.data["Average BW"]

  if (!(paste(species,"Vol (L/kg)") %in% colnames(tissue.data)))
  {
    if (toupper(paste(species,"Vol (L/kg)")) %in% toupper(colnames(tissue.data)))
    {
      tissue.vols <- tissue.data[,toupper(colnames(tissue.data))==toupper(paste(species,"Vol (L/kg)"))]
      tissue.flows <- tissue.data[,toupper(colnames(tissue.data))==toupper(paste(species,"Flow
(mL/min/kg)"))]
      warning(paste(species,"coerced to",toupper(species),"for physiological data."))
    } else stop(paste("Tissue data for",species,"not found."))
  } else {
    tissue.vols <- tissue.data[,paste(species,"Vol (L/kg)")]
    tissue.flows <- tissue.data[,paste(species,"Flow (mL/min/kg)")]
  }
  names(tissue.vols) <- tissue.data[,1]
  names(tissue.flows) <- tissue.data[,1]
  #mL/min:
  Qh <- (tissue.flows["Liver"]+tissue.flows["Gut"])*this.phys.data["Average BW"]

  if (!(species %in% colnames(chem.physical_and_invitro.data)))
```

```
  {
    if (toupper(species) %in% toupper(colnames(chem.physical_and_invitro.data)))
    {
      chem.main.species <-
colnames(chem.physical_and_invitro.data)[toupper(colnames(chem.physical_and_invitro.data))==toupper
(species)]
      warning(paste(species,"coerced to",chem.main.species,"for chemical specific PK data."))
    } else {
      warning(paste("Chemical specific PK data for",species,"not found, using Human"))
      chem.main.species <- "Human"
    }
  } else chem.main.species <- species

  #Want the units of mL/min/10^6 hepatocytes
  CLint <-
as.numeric(chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,paste(chem.main.speci
es,"Clint",sep=".")])/1000
  fub <-
as.numeric(chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,paste(chem.main.speci
es,"Fub",sep=".")])

  if (chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,species]!="Y")
  {
    if (chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,"Human"]=="Y")
    {
      warning(paste("Chemical specific data for",species,"incomplete, using Human"))
      chem.sub.species <- "Human"
      if (is.na(CLint))
as.numeric(chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,paste(chem.sub.specie
s,"Clint",sep=".")])
      if (is.na(fub))
as.numeric(chem.physical_and_invitro.data[chem.physical_and_invitro.data.index,paste(chem.sub.specie
s,"Fub",sep=".")])
    } else {
      warning("Incomplete chemical specific data, predict=FALSE")
      predict <- FALSE
      if (is.na(CLint) | is.na(fub)) stop()
    }
  } else chem.sub.species <- species


  # Assume dose is in mg/kg BW/day, convert to mg/min to give output in mg/L:
  dose <- dose/24/60*this.phys.data["Average BW"]
  if (is.null(doses.per.day))
  {
    return(1000*dose/(QGFR*fub+calc_Hepatic_Clearance(CLint,fub,Qh=Qh)))
  } else {
    time.interval <- 24/doses.per.day
    dose <- dose/doses.per.day
    PKparams <- Parameterize_vLiverPBPK(200,1,0.05,5,2)
    solve(vliver_pbpk(seq(0,10,0.1),Parameterize_vLiverPBPK(200,1,0.05,5,2))


    )
  }
}
```