```
Wetmore_Css <-
function(chem.name=NULL,chem.CAS=NULL,daily.dose=1,which.quantile=0.95,species="Human",cleara
nce.assay.conc=NULL,units="mgperL")
{
  if (!(which.quantile %in% c(0.05,0.5, 0.95))) stop("Wetmore papers only includes 5%, 50%, and 95%
quantiles.")
  if (!(units %in% c("mgperL","uM"))) stop("Wetmore papers only includes mgperL and uM values for Css")
  if (is.null(chem.CAS) & is.null(chem.name))
  {
    stop("Must specifiy compound name or CAS.\n")
  } else if ((!is.null(chem.CAS) & !any(Wetmore.data[,"CASRN"]==chem.CAS)) & (!is.null(chem.name) &
!any(Wetmore.data[,"Compound"]==chem.name)))
  {
    stop("Compound not found.\n")
  } else {
    if (!is.null(chem.CAS)) chem.name <-
Wetmore.data[Wetmore.data[,"CASRN"]==chem.CAS,"Compound"][1]
    else chem.CAS <- Wetmore.data[Wetmore.data[,"Compound"]==chem.name,"CASRN"][1]
    this.data <-
subset(Wetmore.data,Wetmore.data[,"CASRN"]==chem.CAS&toupper(Wetmore.data[,"Species"])==toup
per(species))
    if (!is.null(clearance.assay.conc))
    {
      this.data <- subset(this.data,Wetmore.data[,"Concentration..uM."]==clearance.assay.conc)
      if (dim(this.data)[1]!=1) stop(paste("No",clearance.assay.conc,"uM clearance assay data
for",chem.name,"in",species))
    } else {
      this.data <- this.data[1,]
    }
    if (units=="mgperL")
    {
      if (which.quantile==0.05) return(daily.dose*this.data[,"Css_lower_5th_perc.mg.L."])
      else if (which.quantile==0.5) return(daily.dose*this.data[,"Css_median_perc.mg.L."])
      else return(daily.dose*this.data[,"Css_upper_95th_perc.mg.L."])
    } else {
      if (which.quantile==0.05) return(daily.dose*this.data[,"Css_lower_5th_perc.uM."])
      else if (which.quantile==0.5) return(daily.dose*this.data[,"Css_median_perc.uM."])
      else return(daily.dose*this.data[,"Css_upper_95th_perc.uM."])
    }
  }
}
```