```
#library(gdata)
library(vLiverPBPK)

#setwd("/Volumes/NCCT_vLiver/projects/v-Liver-Sim/vLiverPBPK/R")

tissuelist <- list(Liver=c("Liver"),Kidney=c("Kidneys"),Lung=c("Lung"),Skin=c("Skin"))

out <- Predict_Ktissue2plasma(0.9,5,6,tissuelist=tissuelist)

Calculate_Hepatic_Clearance(6,0.9,out$flow[["Liver"]])
Calculate_Hepatic_Clearance(6,0.9,out$flow[["Liver"]],model="parallel tube")
Calculate_Hepatic_Clearance(6,0.9,out$flow[["Liver"]],model="dispersion")

chemdata <- read.csv("Unneeded/vLiver-Chem-Prop-072012.csv",stringsAsFactors=FALSE,skip=3)

chemPK <- NULL
for (this.chem in chemdata$Compound.Name)
{
	this.row <- chemdata$Compound.Name==this.chem
	out <-
Predict_Ktissue2plasma(chemdata[this.row,"Fub"],chemdata[this.row,"pKa"],chemdata[this.row,"logP"],tis
suelist=tissuelist)
	new.row <- data.frame(this.chem)
	new.row <- cbind(new.row,data.frame(as.vector(out$Ktissue2plasma)))
	CL_hep <-
Calculate_Hepatic_Clearance(chemdata[this.row,"Clint"],chemdata[this.row,"Fub"],out$flow[["Liver"]])
	new.row <- cbind(new.row,data.frame(CL_hep))
	new.row <- cbind(new.row,data.frame(chemdata[this.row,"Fub"]))
	colnames(new.row)[9] <- "Fub"
	new.row <- cbind(new.row,data.frame(chemdata[this.row,"MW"]))
	colnames(new.row)[10] <- "MW"

	chemPK <- rbind(chemPK,new.row)
}
write.table(chemPK,file="chemPK.txt",sep="\t")



vliver_pbpk(seq(0,10,0.1),list())

Parameterize_vLiverPBPK(as.numeric(chemdata[this.row,"MW"]),as.numeric(chemdata[this.row,"Human.
Clint"]),as.numeric(chemdata[this.row,"Human.Fub"]),as.numeric(chemdata[this.row,"pKa"]),as.numeric(c
hemdata[this.row,"logP"]))

                                        ,1,0.05,5,2)


out <- vliver_pbpk(seq(0,10,0.1),Parameterize_vLiverPBPK(200,1,0.05,5,2))

vliver_pbpk_deriv(out$result[1,2:9],Parameterize_vLiverPBPK(200,1,0.05,5,2))

vliver_pbpk_deriv(out$result[1,2:9],c(Parameterize_vLiverPBPK(200,1,0.05,5,2),UseAmounts=1))


out2 <- vliver_pbpk(seq(0,10,0.1),c(Parameterize_vLiverPBPK(200,1,0.05,5,2),UseAmounts=1))
```

```
out2$result[1:10,"Crest"]/out2$parameters[["Vrest"]]
out$result[1:10,"Crest"]
```