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data<-read_excel(wskfile1,sheet=wksheet1)
d2<-filter(data,data$Endpoint %in% c("4h HPT","Corrositex
Classification"))
      grepl( "GHS Classification", data$Endpoint, fixed = TRUE))
d3<-d2[!duplicated(d2[c(2,5,9)]),]
d3[, 'nh']<-ifelse(d3$Endpoint=="4h HPT",1,0)
d3[, 'nc']<-ifelse(d3$Endpoint=="Corrositex Classification",1,0)
d3[, 'ng']<-ifelse(grepl( "GHS Classification", d3$Endpoint, fixed =
TRUE),1,0)

n1<- d3 %>% group_by(d3$CASRN) %>%
  summarize(nh=sum(nh),ng=sum(ng),nc=sum(nc))
colnames(n1)<-c('CAS','nh','ng','nc')

n2<- d3 %>% group_by(d3$'Qsar Ready ID') %>%
  summarize(nh=sum(nh),ng=sum(ng),nc=sum(nc))
colnames(n2)<-c('Inchikey','nh','ng','nc')

all1<-left_join(filter(tlist,!is.na(tlist$CAS)),n1,by='CAS')
all2<-left_join(filter(tlist,is.na(tlist$CAS)),n2,by='Inchikey')
all<-rbind(all1,all2)

all<-all[order(all$CID,all$CAS,na.last=FALSE),]

for (i in 1:dim(all)[1]) {
  all$human[i]<-all$nh[i]
  all$h_irr[i]<-all$nh[i]
  all$qual[i]<-all$ng[i]
  all$ql_irr[i]<-all$ng[i]
  all$animal[i]<-all$ng[i]+all$nc[i]
  all$a_irr[i]<-all$ng[i]+all$nc[i]}

all[,5:ncolt][is.na(all[,5:ncolt])] <- 0

wb <- loadWorkbook(outfile)
writeData(wb, sheet = "Skin", all[1:ncolt], colNames = F,startRow=3)
saveWorkbook(wb,outfile,overwrite = T)

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