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data<-read_excel(wefile1,sheet=wesheet1)
d2<-filter(data,data$Assay %in% c("Draize eye","Vitrigel","Acute eye
irritation/corrosion"))
d2[, 'na']<-ifelse((d2$Assay=="Draize eye" & d2$Endpoint=="Draize Score")
|
                (d2$Assay=="Vitrigel" & d2$Endpoint=="Call") |
                d2$Assay=="Acute eye irritation/corrosion",1,0)
d2[, 'nq']<-ifelse((d2$Assay=="Draize eye" & grepl( "Classification",
d2$Endpoint, fixed = TRUE)) |
                d2$Assay=="Acute eye irritation/corrosion",1,0)

n<- d2 %>% group_by(d2$CASRN,d2[,8]) %>%
  summarize(na=max(na),nq=max(nq))
n2a<- n %>% group_by(n[,1]) %>%
  summarize(na=sum(na),nq=sum(nq))
colnames(n2a)<-c('CAS','na','nq')

n<- d2 %>% group_by(d2$CASRN,d2[,8]) %>%
  summarize(na=max(na),nq=max(nq))
n2b<- n %>% group_by(n[,1]) %>%
  summarize(na=sum(na),nq=sum(nq))
colnames(n2b)<-c('Inchikey','na','nq')

all1<-left_join(filter(tlist,!is.na(tlist$CAS)),n2a,by='CAS')
all2<-left_join(filter(tlist,is.na(tlist$CAS)),n2b,by='Inchikey')
all<-rbind(all1,all2)

all<-all[order(all$CID,all$CAS,na.last=FALSE),]
for (i in 1:dim(all)[1]) {
  all$animal[i]<-all$na[i]
  all$a_irr[i]<-all$na[i]
  all$qual[i]<-all$nq[i]
  all$ql_irr[i]<-all$nq[i]}
all[,5:ncol][is.na(all[,5:ncol])] <- 0

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

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