```
data<-read_excel(wsnfile1,sheet=wsnsheet1)
names(data)[names(data) == 'CASRN'] <- "CAS"
names(data)[names(data) == 'Record ID'] <- "Record"
names(data)[names(data) == 'QSAR Ready ID'] <- "Inchikey"
all<-tlist

d2<-inner_join(filter(tlist,!is.na(tlist$CAS)),data,by="CAS")
a<-filter(d2,d2$Assay %in% c('Human Maximization Test','Human Repeat
Insult Patch Test',
                             'Guinea Pig
Maximization/Buehler','LLNA'))
b<-filter(d2,d2$Assay %in% c('DPRA','mMUSST','SENS-IS','U-
SENS','KeratinoSens',
                       'LuSens','hCLAT'))

a$h<-ifelse(a$Assay %in% c('Human Maximization Test','Human Repeat Insult
Patch Test'),1,0)
a$a<-ifelse(a$Assay %in% c('Guinea Pig Maximization/Buehler','LLNA'),1,0)
a$q<-ifelse(a$Assay %in% c('Guinea Pig Maximization/Buehler','LLNA') &
              grepl('Classification',a$Endpoint),1,0)
b$d<-ifelse(b$Assay=='DPRA',1,0)
b$k<-ifelse(b$Assay=='KeratinoSens',1,0)
b$l<-ifelse(b$Assay=='LuSens',1,0)
b$m<-ifelse(b$Assay=='mMUSST',1,0)
b$s<-ifelse(b$Assay=='SENS-IS',1,0)
b$u<-ifelse(b$Assay=='U-SENS',1,0)
b$h<-ifelse(b$Assay=='hCLAT',1,0)
if(nrow(a)!=0){
na<- a %>% group_by(CAS,Record) %>%
  summarize(h=max(h),a=max(a),q=max(q))
na2<- na %>% group_by(CAS) %>%
  summarize(h=sum(h),a=sum(a),q=sum(q))
if(nrow(na2)>0){all<-left_join(all, na2, by= 'CAS')}}
if(nrow(b)!=0){
nb<- b %>% group_by(CAS,Record) %>%

summarize(h=max(h),d=max(d),k=max(k),l=max(l),m=max(m),u=max(u),s=max(s))
nb2<- nb %>% group_by(CAS) %>%

summarize(h=sum(h),d=sum(d),k=sum(k),l=sum(l),m=sum(m),u=sum(u),s=sum(s))
nb2$c1<-ifelse(nb2$d>0,1,0)
nb2$c2<-ifelse(nb2$k>0 | nb2$l>0,1,0)
nb2$c3<-ifelse(nb2$h>0 | nb2$m>0,1,0)
nb2$sum<-nb2$c1+nb2$c2+nb2$c3
nb2$a2<-0
nb2$e2<-0
for (i in 1:dim(nb2)[1]) {
  if(nb2$sum[i] >= 2){
    nb2$a2[i]<-1
    nb2$e2[i]<-nb2$s[i]+nb2$u[i]}
  else{nb2$e2[i]<-
nb2$k[i]+nb2$l[i]+nb2$d[i]+nb2$h[i]+nb2$s[i]+nb2$u[i]+nb2$m[i]}}
if(nrow(nb2)>0){all<-left_join(all, nb2, by= 'CAS')}}
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```
d2<-inner_join(filter(tlist,is.na(tlist$CAS)),data,by="Inchikey")
a<-filter(d2,d2$Assay %in% c('Human Maximization Test','Human Repeat
Insult Patch Test',
                             'Guinea Pig Maximization/Buehler','LLNA'))
b<-filter(d2,d2$Assay %in% c('DPRA','mMUSST','SENS-IS','U-
SENS','KeratinoSens',
                             'LuSens','hCLAT'))

a$h<-ifelse(a$Assay %in% c('Human Maximization Test','Human Repeat Insult
Patch Test'),1,0)
a$a<-ifelse(a$Assay %in% c('Guinea Pig Maximization/Buehler','LLNA'),1,0)
a$q<-ifelse(a$Assay %in% c('Guinea Pig Maximization/Buehler','LLNA') &
              grepl('Classification',a$Endpoint),1,0)
b$d<-ifelse(b$Assay=='DPRA',1,0)
b$k<-ifelse(b$Assay=='KeratinoSens',1,0)
b$l<-ifelse(b$Assay=='LuSens',1,0)
b$m<-ifelse(b$Assay=='mMUSST',1,0)
b$s<-ifelse(b$Assay=='SENS-IS',1,0)
b$u<-ifelse(b$Assay=='U-SENS',1,0)
b$h<-ifelse(b$Assay=='hCLAT',1,0)
if(nrow(a)!=0){
  na<- a %>% group_by(Inchikey,Record) %>%
    summarize(h=max(h),a=max(a),q=max(q))
  na2<- na %>% group_by(Inchikey) %>%
    summarize(h=sum(h),a=sum(a),q=sum(q))
  if(nrow(na2)>0){all<-left_join(all, na2, by= 'Inchikey')}}
if(nrow(b)!=0){
  nb<- b %>% group_by(Inchikey,Record) %>%

summarize(h=max(h),d=max(d),k=max(k),l=max(l),m=max(m),u=max(u),s=max(s))
  nb2<- nb %>% group_by(Inchikey) %>%

summarize(h=sum(h),d=sum(d),k=sum(k),l=sum(l),m=sum(m),u=sum(u),s=sum(s))
  nb2$c1<-ifelse(nb2$d>0,1,0)
  nb2$c2<-ifelse(nb2$k>0 | nb2$l>0,1,0)
  nb2$c3<-ifelse(nb2$h>0 | nb2$m>0,1,0)
  nb2$sum<-nb2$c1+nb2$c2+nb2$c3
  nb2$a2<-0
  nb2$e2<-0
  for (i in 1:dim(nb2)[1]) {
    if(nb2$sum[i] >= 2){
      nb2$a2[i]<-1
      nb2$e2[i]<-nb2$s[i]+nb2$u[i]}
    else{nb2$e2[i]<-
nb2$k[i]+nb2$l[i]+nb2$d[i]+nb2$h[i]+nb2$s[i]+nb2$u[i]+nb2$m[i]}}
  if(nrow(nb2)>0){all<-left_join(all, nb2, by= 'Inchikey')}}

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

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

for (i in 1:dim(all)[1]) {
  all$animal[i]<-sum(all$a[i],all$a2[i],na.rm=TRUE)
  all$a_sens[i]<-sum(all$a[i],all$a2[i],na.rm=TRUE)
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  all$human[i]<-sum(all$h[i],na.rm=TRUE)
  all$h_sens[i]<-sum(all$h[i],na.rm=TRUE)
  all$exp[i]<-sum(all$e2[i],na.rm=TRUE)
  all$e_conn[i]<-sum(all$e2[i],na.rm=TRUE)}

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