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data1<-read_excel(cfile1,sheet=csheet1,col_types="text")
data<-inner_join(tlist,data1,by="CAS")

d3<-filter(data,`Hazard Name` %notin% c("Acute Aquatic Toxicity","Chronic
Aquatic Toxicity",

"Bioaccumulation","Persistence")
      & (`Authority` != "QSAR Model" | Score != 'I'))

for (i in 1:dim(d3)[1]) {
  if(d3$`Hazard Name`[i] %in% c("Acute Mammalian Toxicity Dermal",
                                "Acute Mammalian Toxicity Inhalation",
                                "Acute Mammalian Toxicity Oral")){

    if(!is.na(d3$Score[i])){
      d3$qual[i]<-1
      d3$ql_acute[i]<-1}
    if(d3$Score[i] %in% c('N/A','I') & !is.na(d3$'Value Mass'[i])){
      d3$animal[i]<-1
      d3$a_acute[i]<-1
      d3$quan[i]<-1
      d3$qn_acute[i]<-1}
    if(!is.na(d3$Score[i]) & d3$Score[i] %notin% c('N/A','I')){
      d3$animal[i]<-1
      d3$a_acute[i]<-1
      d3$quan[i]<-1
      d3$qn_acute[i]<-1}}
    if(d3$`Hazard Name`[i]=="Carcinogenicity"){
      if(!is.na(d3$Score[i])){
        d3$qual[i]<-1
        d3$ql_carc[i]<-1}
      if(!is.na(d3$Score[i]) & d3$Score[i] %notin% c('N/A','I')){
        d3$animal[i]<-1
        d3$a_carc[i]<-1}
      if(d3$Score[i] %in% c('N/A','I') & (grepl("rat",d3$Note[i]) |
grepl("mice",d3$Note[i]))){
        d3$animal[i]<-1
        d3$a_carc[i]<-1}
      if(!is.na(d3$'Value Mass'[i])){
        d3$quan[i]<-1
        d3$qn_carc[i]<-1}}
    if(d3$`Hazard Name`[i] %in% c("Developmental","Reproductive")){
      if(!is.na(d3$Score[i])){
        d3$qual[i]<-1
        d3$ql_repro[i]<-1}
      if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){
        d3$animal[i]<-1
        d3$a_repro[i]<-1}
      if(d3$Score[i]=='N/A' & grepl("rat",d3$Note[i])){
        d3$animal[i]<-1
        d3$a_repro[i]<-1}
      if(!is.na(d3$'Value Mass'[i])){
        d3$animal[i]<-1
        d3$a_repro[i]<-1
        d3$quan[i]<-1

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    d3$qn_repro[i]<-1}}
if(d3$`Hazard Name`[i]=="Endocrine Disruption"){
  if(!is.na(d3$Score[i])){
    d3$qual[i]<-1
    d3$ql_endo[i]<-1}}
if(d3$`Hazard Name`[i] %in% c("Eye Irritation","Skin Irritation")){
  if(!is.na(d3$Score[i])){
    d3$qual[i]<-1
    d3$ql_irr[i]<-1}
  if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){
    d3$animal[i]<-1
    d3$a_irr[i]<-1}
  if(d3$Score[i]=='N/A' & (grepl("rabbit",d3$Note[i]) |
grepl("rat",d3$Note[i]))){
    d3$animal[i]<-1
    d3$a_irr[i]<-1}}
if(d3$`Hazard Name`[i]=="Genotoxicity Mutagenicity"){
  d3$qual[i]<-1
  d3$ql_muta[i]<-1
  if(d3$Score[i] != 'N/A' | grepl('in vivo',d3$Note[i]) | grepl('in
vitro',d3$Note[i])){
    d3$animal[i]<-1
    d3$a_muta[i]<-1}}
if(d3$`Hazard Name`[i] %in% c("Neurotoxicity Repeat
Exposure","Neurotoxicity Single Exposure")){
  if(!is.na(d3$Score[i])){
    d3$qual[i]<-1
    d3$ql_neuro[i]<-1}
  if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){
    d3$animal[i]<-1
    d3$a_neuro[i]<-1}
  if(d3$Score[i]=='N/A' & grepl("rat",d3$Note[i])){
    d3$animal[i]<-1
    d3$a_neuro[i]<-1}
  if(!is.na(d3$`Value Mass`[i])){
    d3$animal[i]<-1
    d3$a_neuro[i]<-1
    d3$quan[i]<-1
    d3$qn_neuro[i]<-1}}
if(d3$`Hazard Name`[i]=="Skin Sensitization"){
  if(!is.na(d3$Score[i])){
    d3$qual[i]<-1
    d3$ql_sens[i]<-1}
  if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){
    d3$animal[i]<-1
    d3$a_sens[i]<-1}
  if(d3$Score[i]=='N/A' & grepl("guinea pig",d3$Note[i])){
    d3$animal[i]<-1
    d3$a_sens[i]<-1}}
if(d3$`Hazard Name`[i]=="Systemic Toxicity Repeat Exposure"){
  if(!is.na(d3$Score[i])){
    d3$qual[i]<-1
    d3$ql_syst[i]<-1}
  if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){

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    d3$animal[i]<-1
    d3$a_syst[i]<-1}
  if(d3$Score[i]=='N/A' & grepl("rat",d3$Note[i])){
    d3$animal[i]<-1
    d3$a_syst[i]<-1}
  if(!is.na(d3$'Value Mass'[i])){
    d3$animal[i]<-1
    d3$a_syst[i]<-1
    d3$quan[i]<-1
    d3$qn_syst[i]<-1}}
  if(d3$`Hazard Name`[i]=="Systemic Toxicity Single Exposure"){
    if(!is.na(d3$Score[i])){
      d3$qual[i]<-1
      d3$ql_acute[i]<-1}
    if(!is.na(d3$Score[i]) & d3$Score[i] != 'N/A'){
      d3$animal[i]<-1
      d3$a_acute[i]<-1}
    if(d3$Score[i]=='N/A' & grepl("rat",d3$Note[i])){
      d3$animal[i]<-1
      d3$a_acute[i]<-1}}
  if(d3$`Authority`[i] == "QSAR Model"){
    d3$qsar[i]<-1
    if(d3$a_acute[i]==1 | d3$ql_acute[i]==1 |
d3$qn_acute[i]==1){d3$qs_acute[i]<-1}
    if(d3$a_carc[i]==1 | d3$ql_carc[i]==1 |
d3$qn_carc[i]==1){d3$qs_carc[i]<-1}
    if(d3$a_repro[i]==1 | d3$ql_repro[i]==1 |
d3$qn_repro[i]==1){d3$qs_repro[i]<-1}
    if(d3$a_neuro[i]==1 | d3$ql_neuro[i]==1 |
d3$qn_neuro[i]==1){d3$qs_neuro[i]<-1}
    if(d3$a_endo[i]==1 | d3$ql_endo[i]==1 |
d3$qn_endo[i]==1){d3$qs_endo[i]<-1}
    if(d3$a_syst[i]==1 | d3$ql_syst[i]==1 |
d3$qn_syst[i]==1){d3$qs_syst[i]<-1}
    if(d3$a_irr[i]==1 | d3$ql_irr[i]==1){d3$qs_irr[i]<-1}
    if(d3$a_sens[i]==1 | d3$ql_sens[i]==1 |
d3$qn_sens[i]==1){d3$qs_sens[i]<-1}
    if(d3$a_muta[i]==1 | d3$ql_muta[i]==1){d3$qs_muta[i]<-1}
    d3[i,c(5:35,46:ncolt)]<-0}
}

d4<-d3[,c(2,5:ncolt)]
n<- d4 %>% group_by(CAS) %>%
  summarise_all(sum)

all<-merge(n,tlist,all.y=TRUE,by="CAS")
commonNames <- names(n)[which(colnames(n) %in% colnames(tlist))]
commonNames <- commonNames[commonNames %notin% c("CAS")]
for(i in commonNames){
  left <- paste(i, ".x", sep="")
  right <- paste(i, ".y", sep="")
  all[is.na(all[left]),left] <- all[is.na(all[left]),right]
  all[right]<- NULL
  colnames(all)[colnames(all) == left] <- i

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}  
  
all<-all[order(all$CID,all$CAS,na.last=FALSE),]  
  
all<-all[,c(ncolt-2,1,(ncolt-1):ncolt,2:(ncolt-3))]  
  
wb <- loadWorkbook(outfile)  
writeData(wb, sheet = "Comptox", all[1:ncolt], colNames = F,startRow=3)  
saveWorkbook(wb,outfile,overwrite = T)
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