Discovering Associations - Model 1

Count data of rose vase life days.

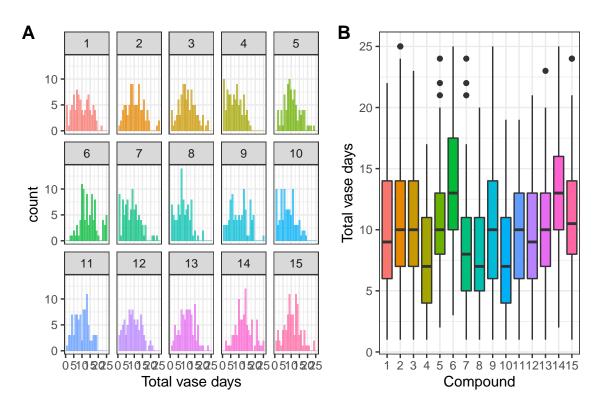
Poisson-mixed effects modelling.

Out of 1440 datapoints, we have 60 missing outcomes (total vase days), which is 4.1% of the data. More data description, can copy some from simulation description.

Checking the distribution of the Vase Days of the count data. It looks like there is a larger degree of overdispersion than the poisson model currently accounts for (nope, it's just conditional on the compound: the goodfit should be done per compound).

```
p1<-ggplot(d, aes(x=tot.vase.days, fill=compound))+geom_histogram(alpha=0.7, bins=25)+facet_wrap(~compo
p2<-ggplot(d, aes(x=compound,y=tot.vase.days, fill=compound))+geom_boxplot()+theme_bw()+
    theme(legend.position = "none")+ylab("Total vase days")+xlab("Compound")

cowplot::plot_grid(p1,p2, rel_widths = c(0.4,0.33), labels = c("A","B"), scale = 0.97)</pre>
```



```
ggsave("figures/mod1_overview.pdf", height=4, width=10)
```

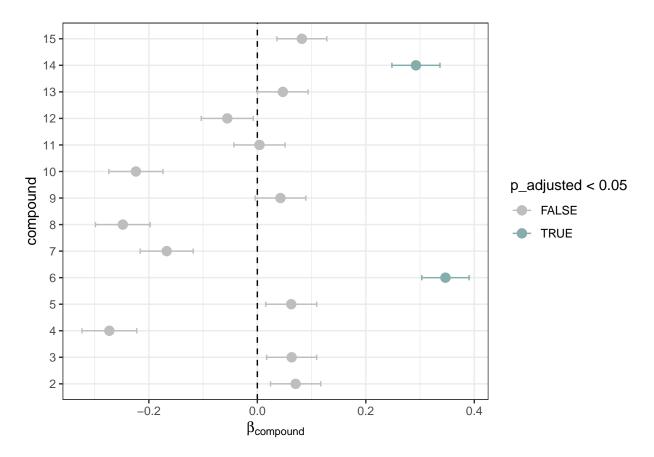
```
#gf <- goodfit(d$tot.vase.days[d$compound==1], "poisson")
#summary(qf)
#plot(gf, type="standing", scale="raw") #I guess the fit would be better if we did it per compound
Initial Model (Model 0).
\#https://bbolker.github.io/mixedmodels-misc/glmmFAQ.html\#overdispersion
overdisp_fun <- function(model) {</pre>
rdf <- df.residual(model)</pre>
rp <- residuals(model,type="pearson")</pre>
Pearson.chisq <- sum(rp^2)</pre>
prat <- Pearson.chisq/rdf #pearson residuals over the residual degrees of freedom
pval <- pchisq(Pearson.chisq, df=rdf, lower.tail=FALSE)</pre>
c(chisq=Pearson.chisq,ratio=prat,rdf=rdf,p=pval)
#inspired by the first answer here for nested data formulation https://stats.stackexchange.com/question
glmer_out <- glmer(tot.vase.days ~ compound + species + garden + (1|rater) + (1|subplotID/bushID), fami</pre>
summary(glmer_out)
## Generalized linear mixed model fit by maximum likelihood (Laplace
     Approximation) [glmerMod]
  Family: poisson (log)
## Formula: tot.vase.days ~ compound + species + garden + (1 | rater) + (1 |
##
       subplotID/bushID)
##
      Data: d
##
##
        AIC
                       logLik deviance df.resid
##
     7222.6
              7327.2 -3591.3
                                7182.6
                                           1360
##
## Scaled residuals:
                1Q Median
       Min
                                3Q
## -2.7555 -0.7878 -0.0460 0.6249
##
## Random effects:
## Groups
                     Name
                                 Variance Std.Dev.
## bushID:subplotID (Intercept) 0.01129 0.1062
## subplotID
                     (Intercept) 0.05483 0.2342
                     (Intercept) 0.12488 0.3534
## rater
## Number of obs: 1380, groups: bushID:subplotID, 96; subplotID, 16; rater, 6
##
## Fixed effects:
##
                Estimate Std. Error z value Pr(>|z|)
## (Intercept) 2.135109 0.171292 12.465 < 2e-16 ***
## compound2
                0.070573
                           0.046365
                                     1.522 0.127983
## compound3
                0.063235
                           0.046126
                                     1.371 0.170402
## compound4
               -0.272908
                           0.050428 -5.412 6.24e-08 ***
## compound5
                           0.046941
                                    1.331 0.183275
               0.062466
## compound6
                0.346817
                           0.043616
                                     7.952 1.84e-15 ***
                           0.048947 -3.415 0.000638 ***
## compound7
               -0.167142
               -0.248027
                           0.050442 -4.917 8.79e-07 ***
## compound8
## compound9
                0.042656
                           0.046612 0.915 0.360130
## compound10 -0.223922
                           0.049918 -4.486 7.26e-06 ***
```

0.047305 0.084 0.933398

compound11

0.003953

```
## compound12 -0.055445
                       0.047967 -1.156 0.247726
## compound13 0.046949 0.046541 1.009 0.313081
## compound14
            0.292410 0.044307 6.600 4.12e-11 ***
            ## compound15
## species2
             -0.033621
                       0.028069 -1.198 0.231002
## garden2
             0.186685
                       0.120431 1.550 0.121109
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Correlation matrix not shown by default, as p = 17 > 12.
## Use print(x, correlation=TRUE) or
      vcov(x)
                   if you need it
-2*logLik(glmer_out)
## 'log Lik.' 7182.625 (df=20)
AIC(glmer_out)
## [1] 7222.625
BIC(glmer_out)
## [1] 7327.222
overdisp_fun(glmer_out) #quite oki! no significance, yey. i think this might be more relevant than good
        chisq
                    ratio
                                 rdf
## 1416.6181038
                1.0416310 1360.0000000
                                       0.1392638
drop1(glmer_out, test = "Chi")
## Single term deletions
##
## Model:
## tot.vase.days ~ compound + species + garden + (1 | rater) + (1 |
      subplotID/bushID)
##
                       LRT Pr(Chi)
##
          npar
                 AIC
               7222.6
## <none>
           14 7615.7 421.07 <2e-16 ***
## compound
            1 7222.1 1.43 0.2315
## species
             1 7222.9
                      2.23 0.1356
## garden
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```



Conclusion: compounds 6 and 14 significantly increase rose vase days (mention estimates +- sd error, also backcalculated in days, alpha, one-sided Wald test, maybe the exact z and p-values, correction Holm).

Models comparison.

Model 1. Dropping Compounds.

```
glmer_out1 <- glmer(tot.vase.days ~ species + garden + (1|rater) + (1|subplotID/bushID), family=poisson
# -2*logLik(qlmer_out1)
# AIC(qlmer_out1)
# BIC(qlmer_out1)
# LRT.1=2*(logLik(qlmer_out)-logLik(qlmer_out1))
# c(LRT.1,1-pchisq(LRT.1,1))
mod1<-as.data.frame(anova(glmer out1,glmer out, test="LRT")) %>%
  mutate(Model=c("Model 1", "Full model"),
         dropped_predictor=c("Compound","-"))%>%
  relocate(c(Model, dropped_predictor))
Model 2. Dropping species.
glmer_out2 <- glmer(tot.vase.days ~ compound + garden + (1|rater) + (1|subplotID/bushID), family=poisson</pre>
mod2<-as.data.frame(anova(glmer_out2,glmer_out, test="LRT")) %>%
  mutate(Model=c("Model 2", "Full model"),
         dropped_predictor=c("Species","-"))%>%
  relocate(c(Model, dropped_predictor))
Model 3. Dropping garden.
glmer_out3 <- glmer(tot.vase.days ~ compound + species + (1|rater) + (1|subplotID/bushID), family=poiss</pre>
mod3<-as.data.frame(anova(glmer_out3,glmer_out, test="LRT")) %>%
  mutate(Model=c("Model 3", "Full model"),
         dropped predictor=c("Garden","-"))%>%
  relocate(c(Model, dropped_predictor))
Model 4.1 - Dropping bushID random effect.
glmer_out4 <- glmer(tot.vase.days ~ compound + garden + species + (1|rater) + (1|subplotID), family=poi</pre>
mod4<-as.data.frame(anova(glmer_out4,glmer_out, test="LRT")) %>%
  mutate(Model=c("Model 4", "Full model"),
         dropped predictor=c("BushID","-"))%>%
 relocate(c(Model, dropped predictor))
Model 4.2 - Dropping subplotID random effect
glmer_out5 <- glmer(tot.vase.days ~ compound + garden + species + (1|rater) + (1|bushID), family=poisson
mod5<-as.data.frame(anova(glmer_out5,glmer_out, test="LRT")) %>%
  mutate(Model=c("Model 5", "Full model"),
         dropped_predictor=c("subplotID","-"))%>%
  relocate(c(Model, dropped predictor))
```

Dropping rater as random effect.

Model 7 (dropping Species and Garden) is generated and compared to models 2 (dropping Species) and 3 (dropping Garden).

```
glmer_out7 <- glmer(tot.vase.days ~ compound + (1|subplotID/bushID) + (1|rater), family=poisson(link =</pre>
# -2*logLik(qlmer_out6)
# AIC(qlmer_out6)
# BIC(qlmer_out6)
# LRT.6.2=2*(logLik(glmer_out2)-logLik(glmer_out6))
# c(LRT.6.2,1-pchisq(LRT.6.2,1))
# LRT.6.3=2*(logLik(glmer_out3)-logLik(glmer_out6))
# c(LRT.6.3,1-pchisq(LRT.6.3,1))
mod7.1<-as.data.frame(anova(glmer_out7,glmer_out2, test="LRT")) %>%
  mutate(Model=c("Model 7", "Model 2"),
         dropped_predictor=c("Species, Garden", "Species")) %>%
  relocate(c(Model, dropped_predictor))
mod7.2<-as.data.frame(anova(glmer_out7,glmer_out3, test="LRT")) %>%
  mutate(Model=c("Model 7", "Model 3"),
         dropped_predictor=c("Species, Garden", "Garden")) %>%
  relocate(c(Model, dropped_predictor))
```

Model 7 is compared with models lacking any of the random effects. Model 8 without subplotID

Model 9 without bushID.

```
glmer_out9 <- glmer(tot.vase.days ~ compound + (1|subplotID) + (1|rater), family=poisson(link = "log"),
# -2*logLik(glmer_out8)
# AIC(glmer_out8)
# BIC(glmer_out8)
# LRT.8=2*(logLik(glmer_out6)-logLik(glmer_out8))</pre>
```

Model 10 without rater.

```
glmer_out10 <- glmer(tot.vase.days ~ compound + (1|subplotID/bushID), family=poisson(link = "log"), dat</pre>
# -2*logLik(qlmer_out9)
# AIC(qlmer_out9)
# BIC(qlmer_out9)
# LRT.9=2*(logLik(glmer_out6)-logLik(glmer_out9))
# c(LRT.9,1-pchisq(LRT.9,1))
mod10<-as.data.frame(anova(glmer_out10,glmer_out7, test="LRT")) %>%
  mutate(Model=c("Model 10", "Model 7"),
         dropped_predictor=c("Species, Garden, Rater", "Species, Garden")) %>%
  relocate(c(Model, dropped_predictor))
modselection<-bind_rows(mod1,mod2,mod3,mod4,mod5,mod6,mod7.1,mod7.2,mod8,mod9,mod10) %>%
  dplyr::rename("Dropped predictor"=dropped_predictor) %>%
  mutate(npar=as.factor(npar),
         Df = as.factor(Df))
print(xtable(modselection, digits=c(1,1,1,1,1,1,1,1,1,2,1,3)),
      include.rownames=FALSE, file="output_xtables/modelselection1.tex") #only added additional hlines
```

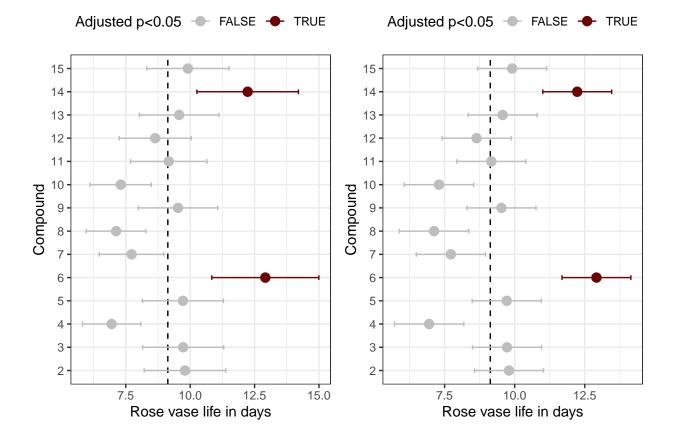
Results using model 7

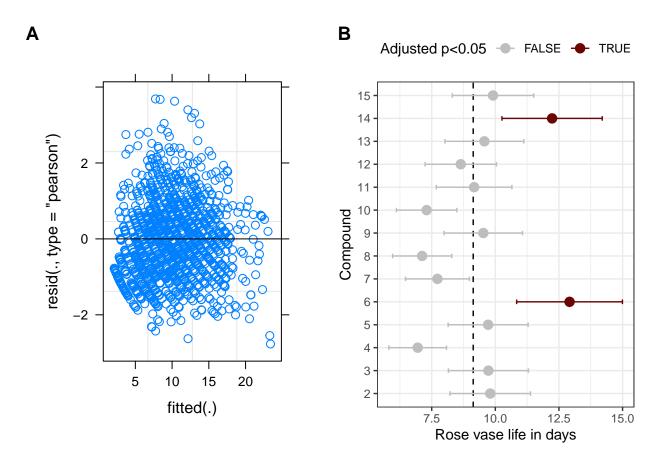
p3<-plot(glmer_out7)

```
summary(glmer_out7)
## Generalized linear mixed model fit by maximum likelihood (Laplace
     Approximation) [glmerMod]
## Family: poisson ( log )
## Formula: tot.vase.days ~ compound + (1 | subplotID/bushID) + (1 | rater)
##
     Data: d
##
##
       ATC
                BIC logLik deviance df.resid
##
     7222.3
             7316.4 -3593.1
                               7186.3
                                           1362
##
## Scaled residuals:
               1Q Median
                                ЗQ
##
      Min
                                       Max
## -2.7683 -0.7958 -0.0394 0.6268 3.6864
##
## Random effects:
## Groups
                     Name
                                 Variance Std.Dev.
## bushID:subplotID (Intercept) 0.01157 0.1076
```

```
## subplotID
                    (Intercept) 0.06436 0.2537
                    (Intercept) 0.12580 0.3547
## rater
## Number of obs: 1380, groups: bushID:subplotID, 96; subplotID, 16; rater, 6
## Fixed effects:
##
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) 2.211664 0.162032 13.650 < 2e-16 ***
               0.070518 0.046365
                                   1.521 0.128280
## compound2
                                   1.371 0.170255
## compound3
               0.063256 0.046126
## compound4
             ## compound5
              0.062239
                          0.046941 1.326 0.184866
                          0.043616 7.953 1.82e-15 ***
              0.346864
## compound6
              -0.167281
## compound7
                          0.048947 -3.418 0.000632 ***
## compound8
              -0.248209 0.050442 -4.921 8.62e-07 ***
## compound9
              0.042485
                          0.046612 0.911 0.362052
## compound10
             -0.223806
                          0.049917 -4.484 7.34e-06 ***
## compound11
              0.003961
                          0.047305 0.084 0.933272
## compound12
             -0.055097
                          0.047966 -1.149 0.250693
              0.046986
## compound13
                          0.046541 1.010 0.312699
                          0.044307 6.597 4.20e-11 ***
## compound14
              0.292286
## compound15
              0.081856
                          0.045998 1.780 0.075147 .
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Correlation matrix not shown by default, as p = 15 > 12.
## Use print(x, correlation=TRUE) or
      vcov(x)
##
                     if you need it
#this is where emmeans package comes in
glmer1.rg <- ref_grid(glmer_out7)</pre>
glmer1.emm.s <- emmeans(glmer1.rg, "compound")</pre>
backcalc<-confint(glmer1.emm.s, level = .9, type = "response") %>%
 mutate(predictor=paste0("compound",compound))
# ctrl<-exp(summary(glmer_out)$coeff)[1,1]</pre>
# comp6<-exp(summary(glmer_out)$coeff)[6,1]</pre>
# comp14<-exp(summary(glmer_out)$coeff)[14,1]</pre>
# ctrl*comp6-ctrl
# ctrl*comp14-ctrl
ctrl1_noExp<-summary(glmer_out7)$coeff[1,1]</pre>
ctrl1<-exp(summary(glmer_out7)$coeff)[1,1]</pre>
ctrl1_stderr<-exp(summary(glmer_out7)$coeff)[1,2]</pre>
glmer_coefficients<-as.data.frame(summary(glmer_out7)$coeff) %>%
 rownames_to_column("predictor") %>%
 filter(grepl("compound",predictor)) %>%
 dplyr::rename(pval=`Pr(>|z|)`) %>%
 #we want to have p-adjusted (Holm) values for one-sided test H.alt: lambda(compound)>lambda(water)
 dplyr::mutate(one sided pval=ifelse(`z value`>0, pval/2, (1-pval/2)),
        p_adjusted=p.adjust(one_sided_pval, method="holm"),
```

```
significant_higher=ifelse(p_adjusted<0.05, T, F),</pre>
         Estimate_days=exp(Estimate)*ctrl1,
         Std.Error_days=exp(`Std. Error`)*ctrl1_stderr) %>%
  left_join(backcalc)
## Joining, by = "predictor"
#recheck backcalculation
cor(glmer_coefficients$Estimate_days,glmer_coefficients$rate)
## [1] 1
pCIs<-ggplot(glmer_coefficients %>%
         mutate(compound=factor(gsub("compound","",predictor), levels=2:15)),
       aes(x=compound, y=Estimate days, color=p adjusted<0.05))+
  geom_hline(yintercept=ctrl1, linetype="dashed")+
  geom_errorbar(aes(ymin=asymp.LCL, ymax=asymp.UCL), width=0.2)+geom_point(size=3)+theme_bw()+
  scale_color_manual(values=c("grey", "#6B0504"), name="Adjusted p<0.05")+coord_flip()+
  ylab("Rose vase life in days")+
  xlab("Compound")+
  theme(legend.position = "top")
cowplot::plot_grid(
ggplot(glmer_coefficients %>%
         mutate(compound=factor(gsub("compound","",predictor), levels=2:15)),
       aes(x=compound, y=Estimate_days, color=p_adjusted<0.05))+</pre>
  geom_hline(yintercept=ctrl1, linetype="dashed")+
  geom_errorbar(aes(ymin=Estimate_days - SE, ymax=Estimate_days + SE), width=0.2)+geom_point(size=3)+th
  scale_color_manual(values=c("grey", "#6B0504"), name="Adjusted p<0.05")+coord_flip()+
  ylab("Rose vase life in days")+
  xlab("Compound")+
  theme(legend.position = "top"),
ggplot(glmer_coefficients %>%
         mutate(compound=factor(gsub("compound","",predictor), levels=2:15)),
       aes(x=compound, y=Estimate_days, color=p_adjusted<0.05))+</pre>
  geom_hline(yintercept=ctrl1, linetype="dashed")+
  geom_errorbar(aes(ymin=Estimate_days - Std.Error_days, ymax=Estimate_days + Std.Error_days), width=0.
  scale_color_manual(values=c("grey","#6B0504"), name="Adjusted p<0.05")+coord_flip()+</pre>
  ylab("Rose vase life in days")+
  xlab("Compound")+
  theme(legend.position = "top")
```





```
ggsave("figures/mod1_diagn_outcome.pdf", height=4.8, width=8.3)
ggsave("figures/mod1_diagnostics.pdf",cowplot::plot_grid(p3), height=3, width=4.5)
ggsave("figures/mod1_outcome.pdf",p4, height=5, width=4.5)
```

Contrasts

Now do contrasts of the promising compounds.

```
return(mtests)
}
summary(glmer_out7)
## Generalized linear mixed model fit by maximum likelihood (Laplace
     Approximation) [glmerMod]
  Family: poisson (log)
## Formula: tot.vase.days ~ compound + (1 | subplotID/bushID) + (1 | rater)
##
      Data: d
##
##
        AIC
                BIC
                      logLik deviance df.resid
##
     7222.3
             7316.4 -3593.1
                               7186.3
                                          1362
##
## Scaled residuals:
##
      Min
               1Q Median
                               3Q
                                      Max
## -2.7683 -0.7958 -0.0394 0.6268 3.6864
##
## Random effects:
## Groups
                    Name
                                Variance Std.Dev.
## bushID:subplotID (Intercept) 0.01157 0.1076
## subplotID
                     (Intercept) 0.06436 0.2537
## rater
                     (Intercept) 0.12580 0.3547
## Number of obs: 1380, groups: bushID:subplotID, 96; subplotID, 16; rater, 6
##
## Fixed effects:
##
                Estimate Std. Error z value Pr(>|z|)
## (Intercept) 2.211664
                          0.162032 13.650 < 2e-16 ***
## compound2
               0.070518
                          0.046365
                                    1.521 0.128280
## compound3
               0.063256
                          0.046126
                                    1.371 0.170255
## compound4
               -0.273139
                          0.050428 -5.416 6.08e-08 ***
                                    1.326 0.184866
## compound5
               0.062239
                          0.046941
## compound6
               0.346864
                          0.043616
                                    7.953 1.82e-15 ***
## compound7
              -0.167281
                          0.048947 -3.418 0.000632 ***
## compound8
               -0.248209
                          0.050442 -4.921 8.62e-07 ***
## compound9
               0.042485
                          0.046612
                                    0.911 0.362052
## compound10
             -0.223806
                          0.049917 -4.484 7.34e-06 ***
## compound11
               0.003961
                          0.047305
                                    0.084 0.933272
## compound12
              -0.055097
                          0.047966 -1.149 0.250693
## compound13
               0.046986
                          0.046541
                                    1.010 0.312699
## compound14
               0.292286
                          0.044307
                                     6.597 4.20e-11 ***
                                    1.780 0.075147 .
## compound15
               0.081856
                          0.045998
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Correlation matrix not shown by default, as p = 15 > 12.
## Use print(x, correlation=TRUE)
       vcov(x)
                     if you need it
##
x<-glht(glmer_out7, linfct=mcp(compound=c("`6` - `14` == 0")))</pre>
mtests1<-wrap_glht_output(x)</pre>
```

```
xtable(mtests1, digits=4)
## \% latex table generated in R 4.1.1 by xtable 1.8-4 package
## % Thu Jun 2 18:56:03 2022
## \begin{table}[ht]
## \centering
## \begin{tabular}{rrrrr}
   \hline
##
## & Estimate & Std. Error & z value & Pr($>$$|$z$|$) \\
     \hline
##
## `6` - `14` & 0.0546 & 0.0401 & 1.3618 & 0.1733 \\
##
      \hline
## \end{tabular}
## \end{table}
print(xtable(mtests1,digits=c(1,2,3,3,4)), file="output_xtables/mod1_contrast_compound6vs14.tex")
rawCI<-confint(glmer1.emm.s, calc = c(n = \text{``wgt.'})) \%
  mutate(Predictor=paste0("compound",compound),
         Predictor=ifelse(compound==1, "(Intercept)", Predictor)) #just for crosschecking
glmer_mainTable<-as.data.frame(summary(glmer_out7)$coeff) %>%
  rownames_to_column("Predictor") %>%
  left_join(rawCI %>% dplyr::select(Predictor,n)) %>%
  mutate(lowerCI=Estimate-qnorm(0.95)*`Std. Error`,
         upperCI=Estimate+qnorm(0.95)*`Std. Error`, #use 0.9 because we are doing a one sided test here
         n=as.factor(n))
## Joining, by = "Predictor"
print(xtable(glmer_mainTable,digits=c(1,1,2,3,3,4,1,3,3)),
      include.rownames=FALSE, file="output_xtables/mod1_mainTable.tex")
#ranef(qlmer out7)
#https://stackoverflow.com/questions/8526681/extract-random-effect-variances-from-lme4-mer-model-object
glmer_randomTable<-as.data.frame(VarCorr(glmer_out7)) %>% dplyr::select(-var2)
print(xtable(glmer_randomTable, digits=c(1,1,1,3,3)),
      include.rownames=FALSE, file="output_xtables/mod1_randomTable.tex")
```