

xCELLanalyzer - Data Analysis

Processing and analysis of the impedance data generated for *xCellAnalyze: A Framework for the Analysis of Cellular Impedance Measurements for Mode of Action Discovery*

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N.B.: Datasets 1 to 10 were generated on xCelligence machine A and datasets 11 to 16 were generated on xCelligence machine B

Load libraries

```
library("tidyverse")
library("stringr")
library("knitr")
library("gtools")
library("gplots")
library("dendsort")
library("pheatmap")
library("RColorBrewer")
```

Source the xCELLanalyzer functions:

- **read_xcell:** This function reads the tab-delimited data exported from the RTCA Software Version 1.2. If the naming conventions are followed, only the global `my_filepath` variable and the experiment ID are used as arguments to the function. The cryptic column names generated by the export from the RTCA Software are fixed to only contain the well identifier (of the E-plate). To match the well labels with the compound IDs an `_anno.txt` is read containing the annotation of the wells for the appropriate experiment. The column names are then replaced with the corresponding compound IDs.
- **edit_df:** This function takes the dataframe generated by the `read_xcell`-function and the experiment ID as arguments. In the first row of the raw data file the time point of the last measurement before compound addition was pasted in manually. The function takes this value and creates a tibble that only includes the last measurement before and 800 measurements after compound addition.
- **normalize_xcell:** This function performs a global normalization by dividing each cell index value recorded after compound addition by the last cell index recorded before compound addition.
- **do_median_polish:** This function applies the median polish algorithm on the technical replicates and returns a dataframe with three columns giving the range of the residuals, the column effect and the sum of the residuals. Additionally, a pdf- file is generated that plots the normalized cell index over time for each set of replicates.
- **calculate_median_curves:** This function calculates median normalized cell index values for each set of technical replicates. A dataframe with the normalized, median TCRPs is returned.
- **normalize_dms:** This function performs a local normalization of each median compound TCRP by subtracting the normalized cell index of the DMSO control at each time point. This is done for each independent experiment to make them more comparable and to address potential batch effects.
- **remove_dms:** This function removes the DMSO control from the dataset after local normalization.
- **score1.function:** This function takes the dataframe with basis spline coefficients for each compound as an argument and calculates a distance matrix. The distance measure can be provided as argument to the function. The distance matrix is sorted and for each replicate a rank sum is calculated. A normalized score is calculated by division of the ideal score of a set of replicates by the obtained score. The closer

this value is to 1 the better the reproducibility. The function returns a list with the compound names, number of replicates per group, score and normalized score.

```
source("xCell_functions.R")
```

Process the 12 xCelligence runs with the xcell_process_data.R script.

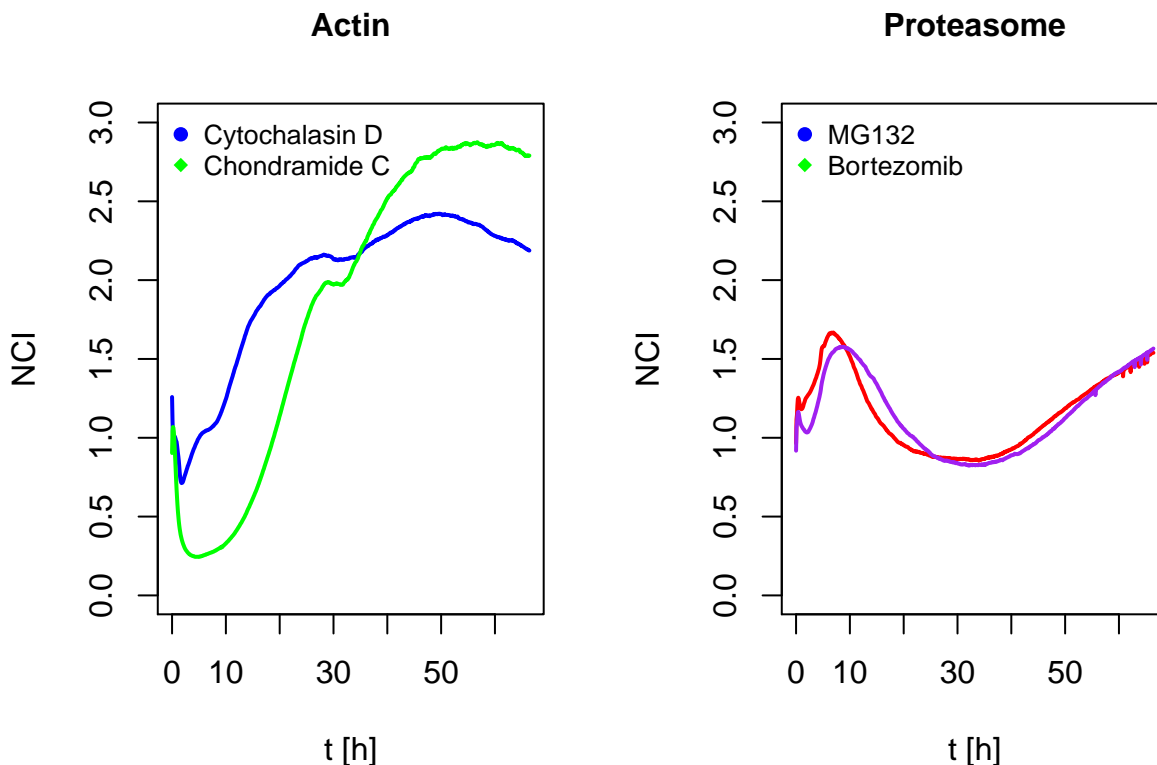
The xcell_process_data.R script processes the 12 datasets in the following manner: The raw data are read and the dataframe is edited to contain only the last measurement before compound addition and 800 measurements after compound addition. Then the global normalization is performed and the do_median_polish function is applied to identify outliers. Outliers with absolute residual sum of greater than 90 are removed. Median TCRPs are calculated and normalized locally by subtracting the DMSO control TCRP. A dataframe without normalization with the DMSO control is also generated for comparisons.

Plot figure 2

```
par(mfrow = c(1,2))

plot(x=rownames(xcell_median_7), y=xcell_median_7[, "7_CytochalasinD"], type="l", col="blue", lwd = 2,
     main = "Actin", cex.main=1, ylim=c(0,3), ylab="NCI", xlab="t [h]")
lines(x=rownames(xcell_median_7), y=xcell_median_7[, "7_ChondramidC"], type="l", col="green", lwd = 2)
legend("topleft", legend=c("Cytochalasin D", "Chondramide C"),
      col= c("blue", "green"), pch=c(16,18), bty="n", ncol=1, cex=0.8, pt.cex=1)

plot(x=rownames(xcell_median_7), y=xcell_median_7[, "7_MG132"], type="l", col="red", lwd = 2,
     main = "Proteasome", cex.main=1, ylim=c(0,3), ylab="NCI", xlab="t [h]")
lines(x=rownames(xcell_median_7), y=xcell_median_7[, "7_Bortezomib"], type="l", col="purple", lwd = 2)
legend("topleft", legend=c("MG132", "Bortezomib"),
      col= c("blue", "green"), pch=c(16,18), bty="n", ncol=1, cex=0.8, pt.cex=1)
```



Combine all matrices containing the normalized median TCRP data from each run in one big matrix and reorder the column names alphabetically

```
median.combined <- cbind(xcell_median_norm_1, xcell_median_norm_2, xcell_median_norm_3,
                        xcell_median_norm_4, xcell_median_norm_5, xcell_median_norm_6,
                        xcell_median_norm_7, xcell_median_norm_8, xcell_median_norm_9,
                        xcell_median_norm_10, xcell_median_norm_11, xcell_median_norm_12,
                        xcell_median_norm_13, xcell_median_norm_14, xcell_median_norm_15,
                        xcell_median_norm_16)

for (i in 1 : length(median.combined[1,])){
  temp <- unlist(strsplit(toString(colnames(median.combined)[i]), "_"))
  colnames(median.combined)[i] <- paste(temp[2], temp[1], sep="_")
}

median.combined.ordered <- median.combined[,mixedorder(colnames(median.combined))]
```

Generate an analogous matrix without the DMSO normalization

```
median.combined_notnorm <- cbind(
  xcell_median_notnorm_1, xcell_median_notnorm_2, xcell_median_notnorm_3,
  xcell_median_notnorm_4, xcell_median_notnorm_5, xcell_median_notnorm_6,
  xcell_median_notnorm_7, xcell_median_notnorm_8, xcell_median_notnorm_9,
  xcell_median_notnorm_10, xcell_median_notnorm_11, xcell_median_notnorm_12,
  xcell_median_notnorm_13, xcell_median_notnorm_14, xcell_median_notnorm_15,
  xcell_median_notnorm_16)

for (i in 1 : length(median.combined_notnorm[1,])){
  temp <- unlist(strsplit(toString(colnames(median.combined_notnorm)[i]), "_"))
  colnames(median.combined_notnorm)[i] <- paste(temp[2], temp[1], sep="_")
}

median.combined_notnorm.ordered <-
  median.combined_notnorm[,mixedorder(colnames(median.combined_notnorm))]
```

Calculate smoothing splines

```
newrownames <- read.delim("newrownames.txt", header=F, stringsAsFactors = FALSE)

#smoothing splines with new rownames
median.sp<-matrix(ncol=22, nrow=219)
row.names(median.sp)<-newrownames$V1
t<-rownames(median.combined.ordered)
t<-as.numeric(t)

i<-0
repeat{
  i<-i+1
  temp<-smooth.spline(x=t, y= median.combined.ordered[,i], nknots=20)
  median.sp[i,]<-temp$fit$coef
  if (i==219) break
}
```

```

#analogous for the data without local normalization
median.sp.notnorm<-matrix(ncol=22, nrow=219)
row.names(median.sp.notnorm)<-newrownames$V1
t<-rownames(median.combined_notnorm.ordered)
t<-as.numeric(t)

i<-0
repeat{
  i<-i+1
  temp<-smooth.spline(x=t, y= median.combined_notnorm.ordered[,i], nknots=20)
  median.sp.notnorm[i,]<-temp$fit$coef
  if (i==219) break
}

```

Calculate score for biological replicates

The goal is to evaluate reproducibility for each compound and to judge which compounds are well reproducible and which not so much. For this purpose a rank-based score is calculated for each compound, the closer to one the better. In addition an overall score is calculated, which is a single number to judge how the experiments and the data analysis overall performed. Again it is a rank-based score, the closer to one the better.

Here we also want to optimize certain parameters for the data analysis, namely the distance measure and data scaling / centering.

Distance measures (source: <https://stat.ethz.ch/R-manual/R-devel/library/stats/html/dist.html>) compared are (written for two vectors x and y):

euclidean: Usual distance between the two vectors (2 norm aka L_2), $\sqrt{\sum((x_i - y_i)^2)}$.

maximum: Maximum distance between two components of x and y (supremum norm)

manhattan: Absolute distance between the two vectors (1 norm aka L_1).

Scaling and Centering of the matrices using the scale function of R base: R documentation: “The value of center determines how column centering is performed. If center is a numeric vector with length equal to the number of columns of x, then each column of x has the corresponding value from center subtracted from it. If center is TRUE then centering is done by subtracting the column means of x from their corresponding columns, and if center is FALSE, no centering is done.

The value of scale determines how column scaling is performed (after centering). If scale is a numeric vector with length equal to the number of columns of x, then each column of x is divided by the corresponding value from scale. If scale is TRUE then scaling is done by dividing the (centered) columns of x by their root-mean-square, and if scale is FALSE, no scaling is done.

The root-mean-square for a column is obtained by computing the square-root of the sum-of-squares of the non-missing values in the column divided by the number of non-missing values minus one.”

```

#criterion how the overall procedure scored
res <- score1.function(median.sp, "euclidean")
euclidean <- sum(res$normscore)/i

median.sp.scaled <- scale(median.sp, center = FALSE, scale = TRUE)
res <- score1.function(median.sp.scaled, "euclidean")
euclidean.scaled <- sum(res$normscore)/i

median.sp.centered.scaled <- scale(median.sp, center = TRUE, scale = TRUE)

```

```

res <- score1.function(median.sp.centered.scaled, "euclidean")
euclidean.centered.scaled <- sum(res$normscore)/i
###

res <- score1.function(median.sp, "maximum")
maximum <- sum(res$normscore)/i

res <- score1.function(median.sp.scaled, "maximum")
maximum.scaled <- sum(res$normscore)/i

res <- score1.function(median.sp.centered.scaled, "maximum")
maximum.centered.scaled <- sum(res$normscore)/i
###

res <- score1.function(median.sp, "manhattan")
manhattan <- sum(res$normscore)/i

res <- score1.function(median.sp.scaled, "manhattan")
manhattan.scaled <- sum(res$normscore)/i

res <- score1.function(median.sp.centered.scaled, "manhattan")
manhattan.centered.scaled <- sum(res$normscore)/i
###

not_scaled <- c(euclidean, maximum, manhattan)
scaled <- c(euclidean.scaled, maximum.scaled, manhattan.scaled)
cent_scaled <- c(euclidean.centered.scaled, maximum.centered.scaled, manhattan.centered.scaled)

tab1 <- rbind(not_scaled, scaled, cent_scaled)
colnames(tab1) <- c("euclidean", "maximum", "manhattan")
tab1 <- as.data.frame(tab1)

#grid.table(round(tab1, 3))
kable(round(tab1, 3), caption = "scores for 5 distance measures +/- scaling and centering")

```

Table 1: scores for 5 distance measures +/- scaling and centering

	euclidean	maximum	manhattan
not_scaled	0.378	0.404	0.342
scaled	0.479	0.473	0.412
cent_scaled	0.479	0.473	0.410

*Result: Euclidean distance with scaled (not centred) data performed best.

Now we want to investigate if the local normalization with the TCRP from DMSO treated cells for each run lead to an improvement of reproducibility.

```

median.sp.notnorm.scaled <- scale(median.sp.notnorm, center = FALSE, scale = TRUE)
res <- score1.function(median.sp.notnorm.scaled, "euclidean")
euclidean.scaled.notnorm <- sum(res$normscore)/i

median.sp.scaled <- scale(median.sp, center = FALSE, scale = TRUE)
res <- score1.function(median.sp.scaled, "euclidean")

```

```
euclidean.scaled <- sum(res$normscore)/i
cat(paste0("without local normalization: ", round(euclidean.scaled.notnorm, 3),
"\nwith local normalization: ", round(euclidean.scaled,3)))
```

```
## without local normalization: 0.274
## with local normalization: 0.479
```

Clearly the local normalization has lead to a strong improvement: 0.479 >> 0.274.

Evaluate reproducibility of biological replicates group-wise, calculate a score for each group of replicates

```
res <- score1.function(median.sp, "euclidean")
groupmatch <- read.delim("groupmatch.txt", header=F)$V1
group.score <- c()

for(i in 1:length(groupmatch)){

  ma <- grep(groupmatch[i], res$rep)
  gscore <- sum(res$normscore[ma])/length(ma)
  group.score <- c(group.score, gscore)

}
group.result <- data.frame(groupmatch,group.score)
group.result <- group.result[order(-group.result$group.score),]
kable(group.result)
```

	groupmatch	group.score
15	Chelerythrine	1.0000000
28	H89	1.0000000
48	SaframycinMx1	1.0000000
54	Staurosporine	1.0000000
60	Wortmannin	1.0000000
19	Cycloheximide	0.9250000
14	Cerulenin	0.9166667
7	Apicidin	0.8333333
57	TubulysinB	0.7857143
2	ActinomycinD	0.7555556
5	Anisomycin	0.6807359
32	Mevastatin	0.6750000
45	Rapamycin	0.6427947
47	Rhizopodin	0.5454259
21	Cytochalasin	0.5416667
23	Emetine	0.5000000
41	PD169316	0.4908789
20	CyclosporinA	0.4810458
16	ChondramidC	0.4530303
33	MG132	0.4431241
44	PurvalanolA	0.4395161
4	Amanitin	0.4377358
42	Podophyllotoxin	0.4328454
11	Bortezomib	0.4243003
58	Vinblastin	0.4202786
43	Puromycin	0.4164809
29	Indirubin3monoxime	0.3968689
17	Colchicine	0.3932894

	groupmatch	group.score
3	Alsterpaullone	0.3887535
1	A23187	0.3631470
8	Apicularen	0.3248723
34	Myriaporone	0.2915516
35	MyxothiazolA	0.2776854
50	SB203580	0.2615083
51	Scriptaid	0.2605042
56	Trichostatin	0.2388983
37	Nocodazol	0.2386498
59	Vioprolide	0.2304310
25	Etoposide	0.1995340
27	Griseofulvin	0.1931039
13	CCCP	0.1835840
49	SB202190	0.1775103
53	Soraphen	0.1771044
10	ArgyriaA	0.1745614
6	Aphidicolin	0.1530034
52	Simvastatin	0.1428155
24	EpothiloneB	0.1351025
26	GephyronicAcidA	0.1312164
38	OkadaicAcid	0.1064823
31	Methotrexate	0.1038177
12	Camptothecin	0.1002997
46	RatjadonC	0.0859606
55	Taxol	0.0708859
30	LY294002	0.0632620
22	Doxorubicin	0.0558336
18	CruentarenA	0.0545505
39	Oligomycin	0.0538105
40	Oxamflatin	0.0514741
36	Neopeltolide	0.0459717
9	ArchazolidB	0.0348333

```
write.csv2(group.result, file = "group_results.csv")
```

What we can do now is to use the score calculated for each biological replicate and define a threshold to remove replicates which are outliers. And then calculate the groupwise scores and the overall score again to check the improvement.

```
#Filter reference set
#normalized score < 0.1 is defined as outlier
res <- score1.function(median.sp, "euclidean")

my_hitlist <- res$rep[res$normscore < 0.1]
my_outliers <- c()

for (i in 1: length(my_hitlist)) {
  temp <- unlist(strsplit(toString(my_hitlist[i]), "_"))
  new_name <- paste0(temp[2], "_", temp[3])
  my_outliers <- c(my_outliers, new_name)
}
```

```
print(my_outliers)
```

```
## [1] "Apiculare_n_1"      "ArchazolidB_3"      "ArchazolidB_6"
## [4] "ArchazolidB_13"     "Argyria_4"          "Bortezomib_9"
## [7] "Camptothecin_4"     "Camptothecin_12"    "Colchicine_16"
## [10] "Cruentare_n_4"      "Cruentare_n_7"      "Cruentare_n_14"
## [13] "Doxorubicin_2"      "Doxorubicin_9"      "Doxorubicin_10"
## [16] "Doxorubicin_11"     "Doxorubicin_12"     "EpothiloneB_13"
## [19] "Etoposide_3"        "Etoposide_15"       "GephyronicAcidA_9"
## [22] "GephyronicAcidA_10" "GephyronicAcidA_13" "Indirubin3monoxime_3"
## [25] "LY294002_2"         "LY294002_5"         "LY294002_11"
## [28] "LY294002_13"        "Methotrexate_1"      "Myriaporone_16"
## [31] "Neopeltolide_2"     "Neopeltolide_6"     "Neopeltolide_16"
## [34] "Nocodazole_15"      "OkadaicAcid_2"      "Oligomycin_1"
## [37] "Oligomycin_7"       "Oligomycin_15"      "Oligomycin_16"
## [40] "Oxamflatin_4"       "Oxamflatin_8"       "Oxamflatin_16"
## [43] "PD169316_9"         "RatjadonC_2"        "RatjadonC_9"
## [46] "RatjadonC_11"       "RatjadonC_12"       "Simvastatin_9"
## [49] "Taxol_1"            "Taxol_6"            "Taxol_7"
## [52] "Taxol_13"           "Taxol_14"           "Vioprolide_10"
```

Plot the biological replicates of each compound (generated by the medians of the technical replicates on each E-plate) with and without local normalization.

```
#pdf(file = "median_TCRP.pdf", paper = "a4")
```

```
par(mfrow = c(1,2))
i<-0
repeat{
  i<-i+1

  ma<-grep(groupmatch[i], colnames(median.combined_notnorm.ordered))
  z<-median.combined_notnorm.ordered[,ma]
  z<-as.data.frame(z)
  z<-z[,mixedorder(names(z))]

  plot(x=rownames(z), y=z[,1], type="l", col="blue", main = "not normalized",
        cex.main=0.8, ylim=c(0,3), ylab="NCI", xlab="t [h]")

  myC <- length(ma)
  myColor <- c("green", "red", "black", "orange")

  for (n in 1:(myC-1))
  {
    lines(x=rownames(z), y=z[,n+1], type="l", col=myColor[n])
  }
  legend("topleft", legend=colnames(z),
        col= c("blue", myColor), pch=c(16,18), bty="n", ncol=1, cex=0.6, pt.cex=0.7)

  z<-median.combined.ordered[,ma]
  z<-as.data.frame(z)
```



```

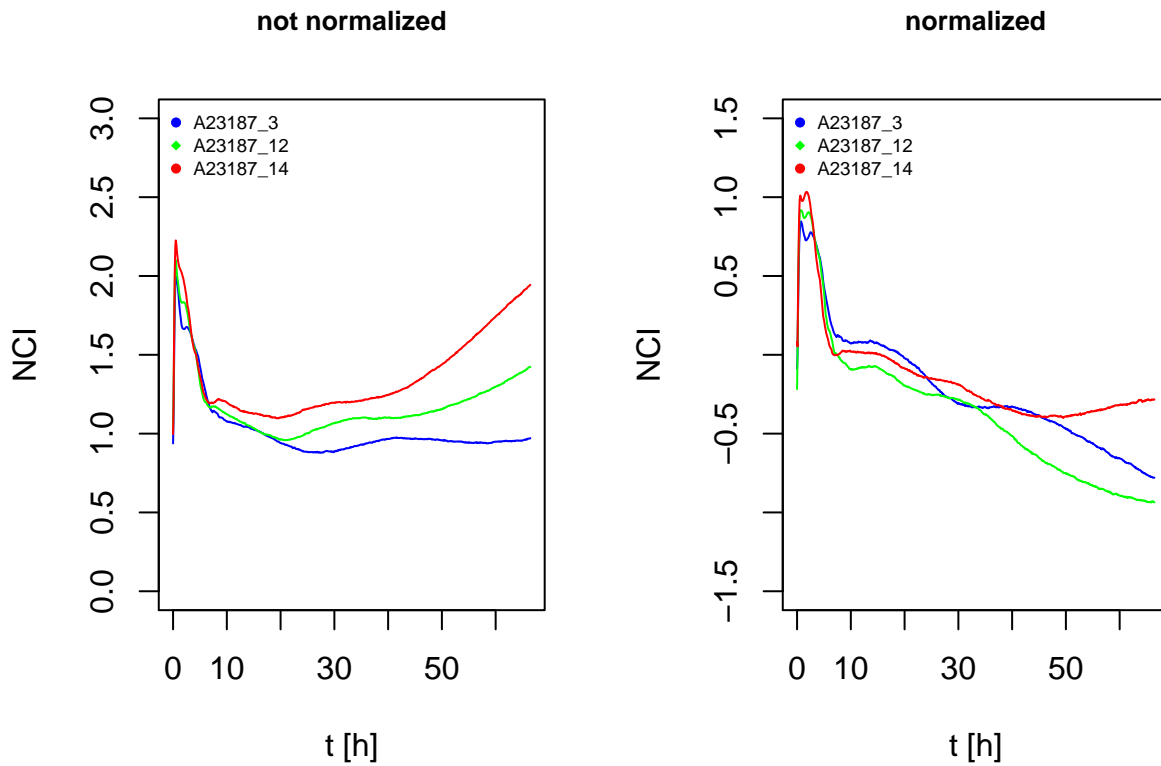
z<-z[,mixedorder(names(z))]

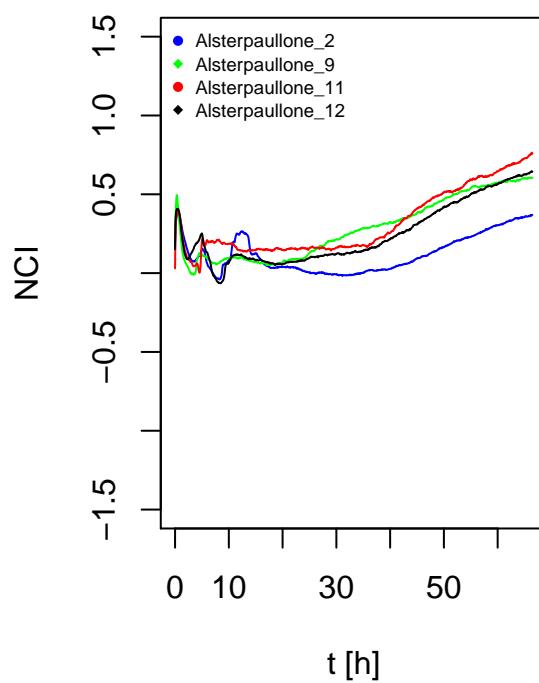
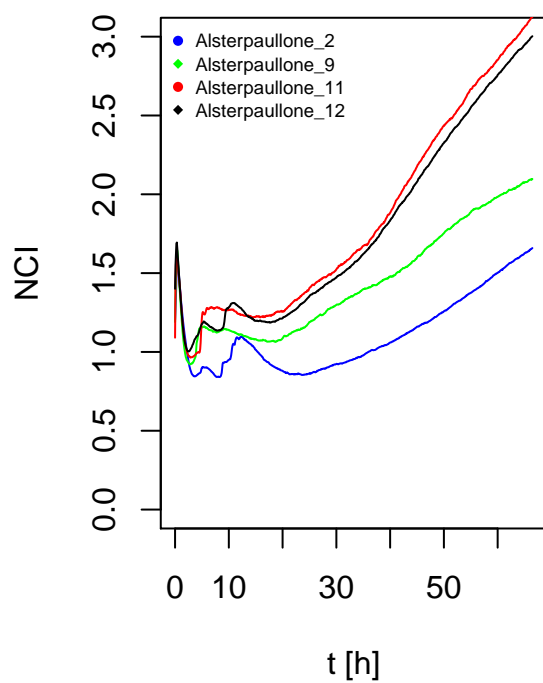
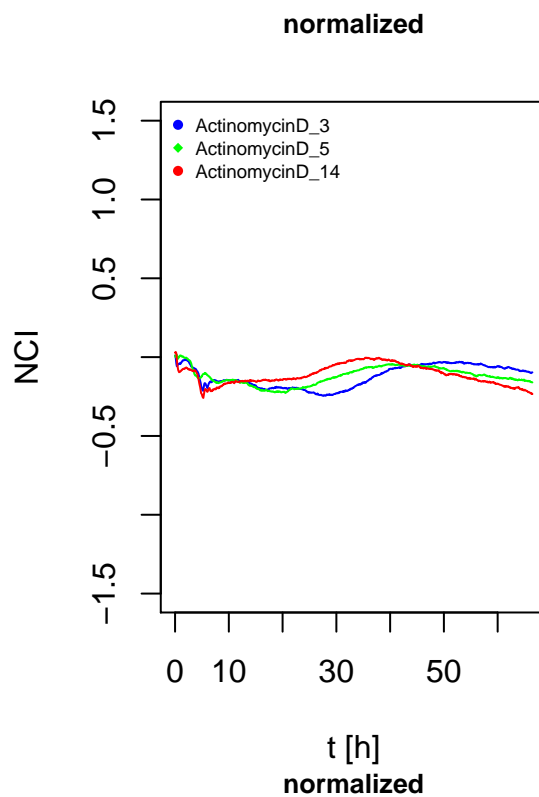
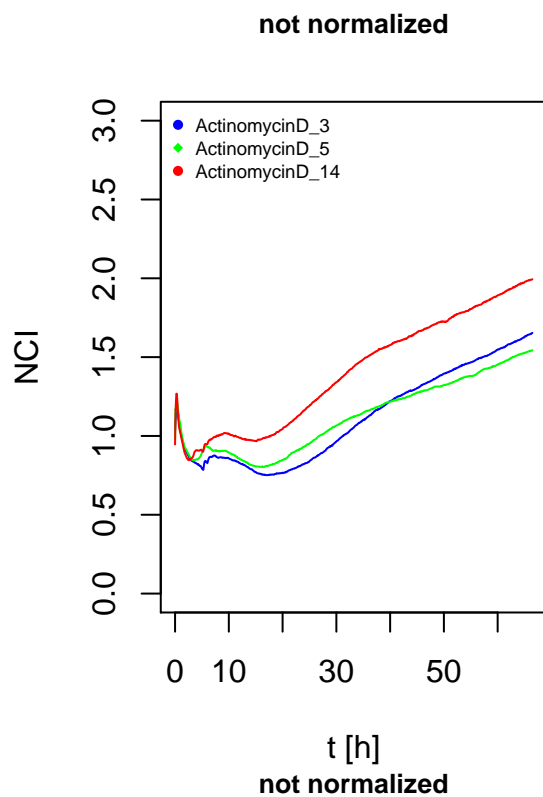
plot(x=rownames(z), y=z[,1], type="l", col="blue", main = "normalized",
     cex.main=0.8, ylim=c(-1.5,1.5), ylab="NCI", xlab="t [h]")

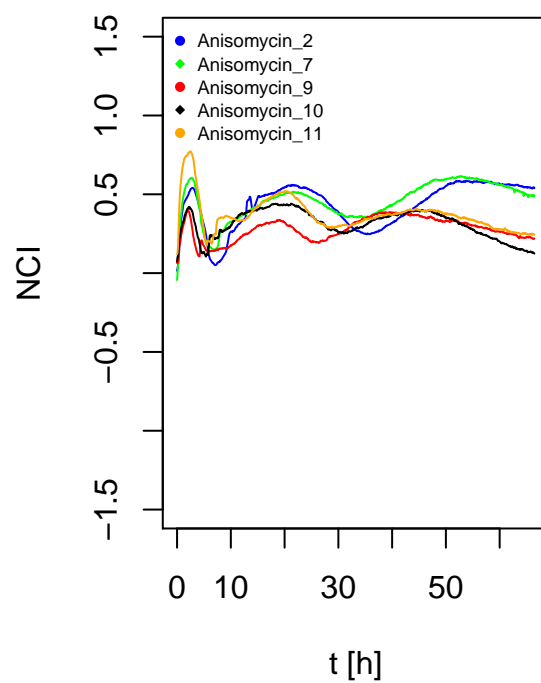
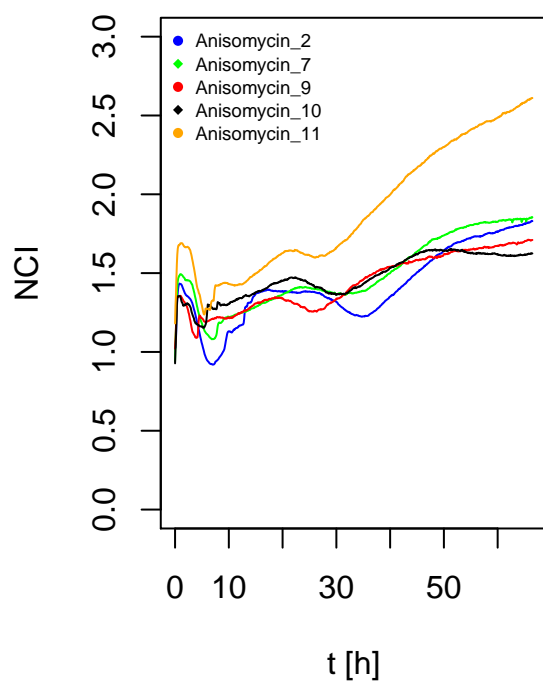
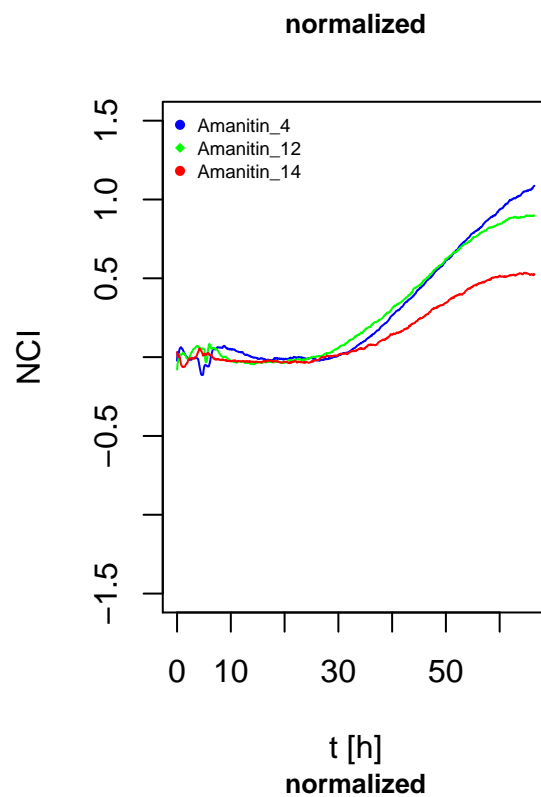
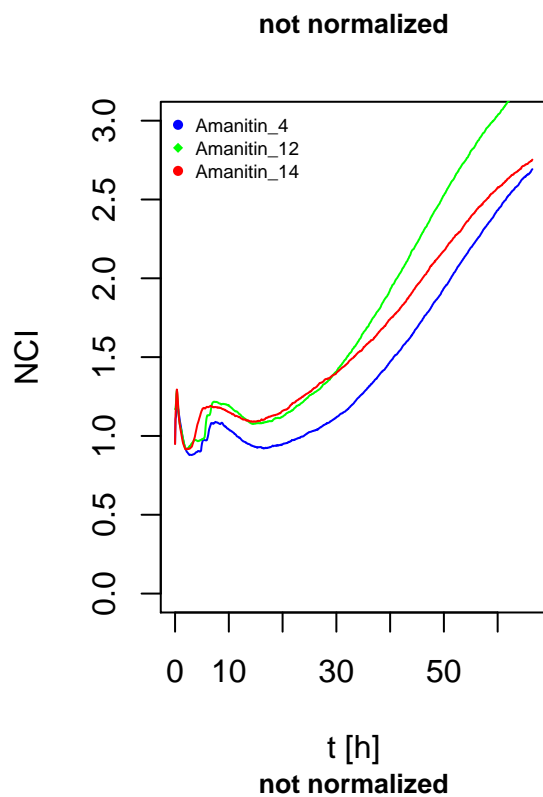
for (n in 1:(myC-1))
{
  lines(x=rownames(z), y=z[,n+1], type="l", col=myColor[n])
}
legend("topleft",legend=colnames(z),
      col= c("blue", myColor),pch=c(16,18),bty="n",ncol=1,cex=0.6,pt.cex=0.7)

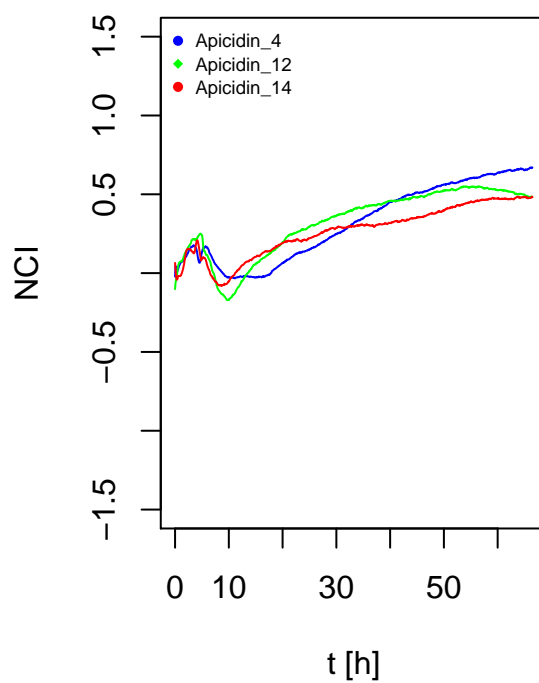
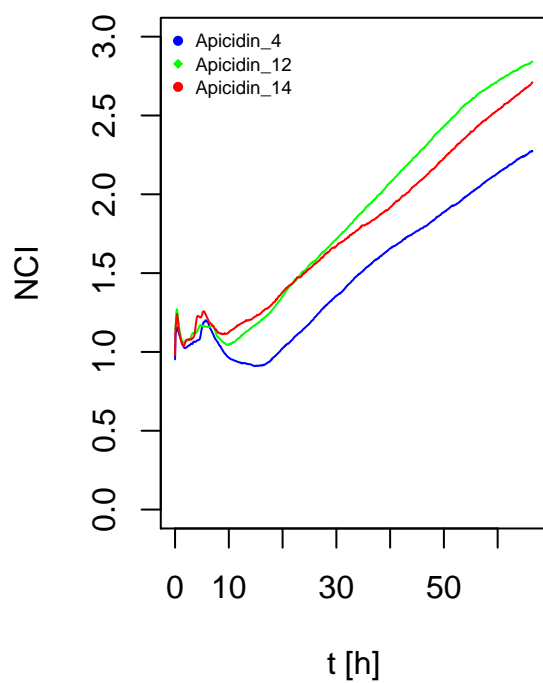
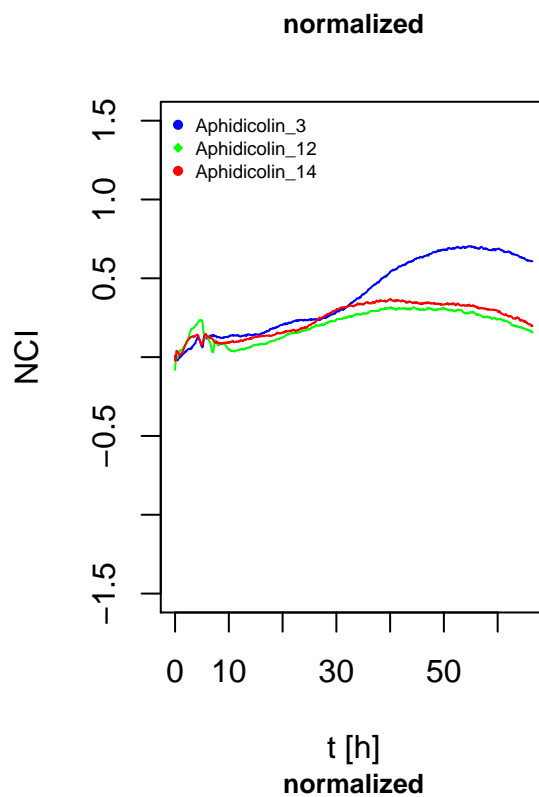
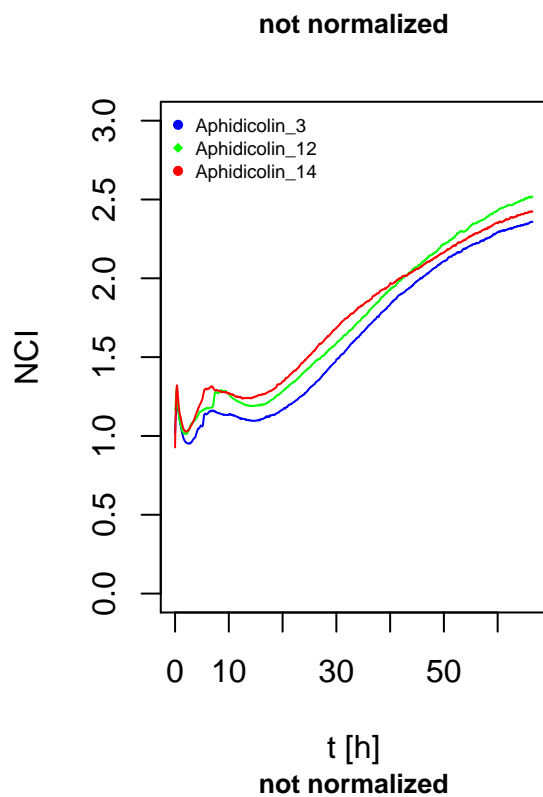
if (i==60) break
}

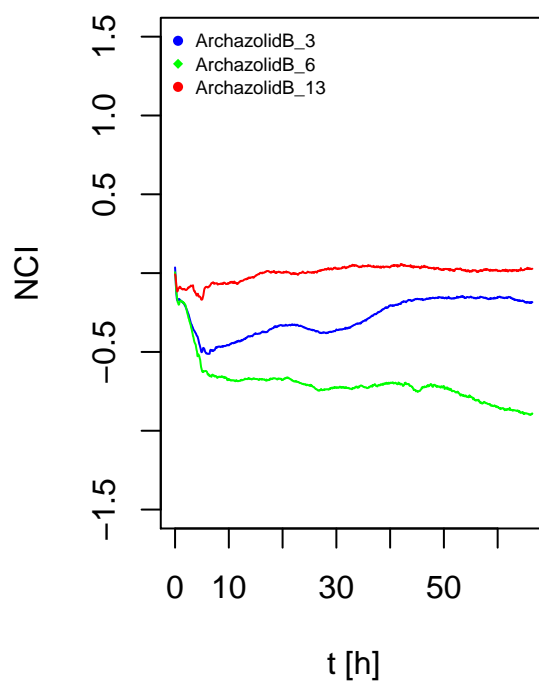
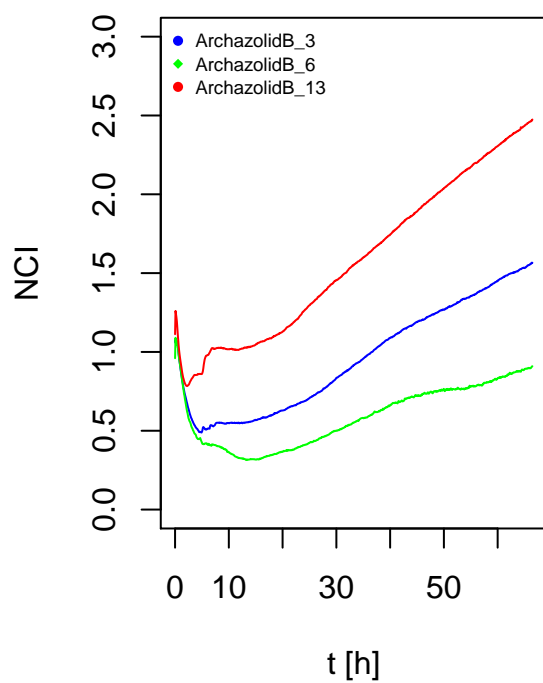
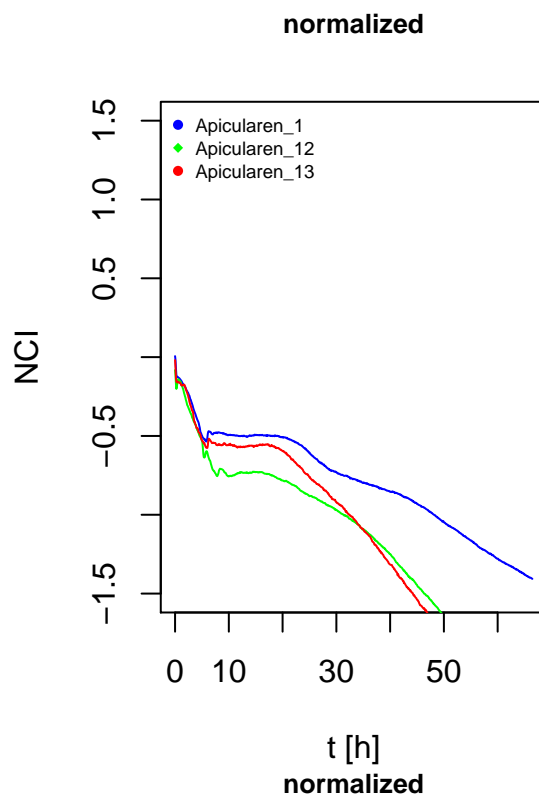
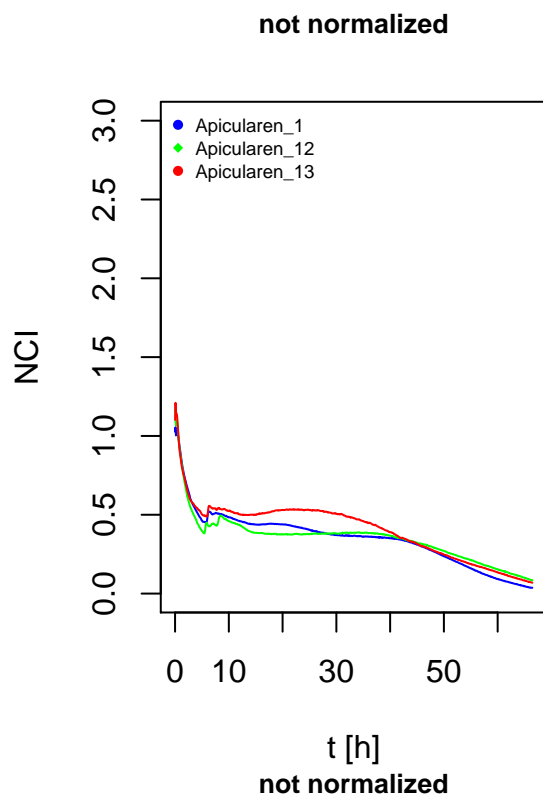
```

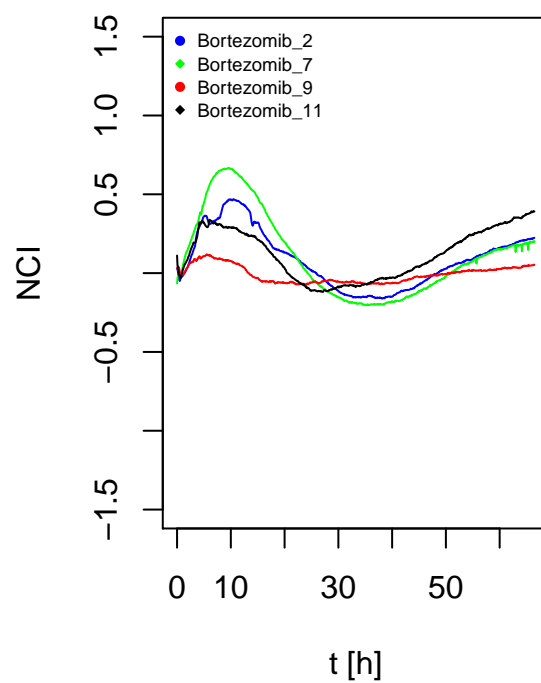
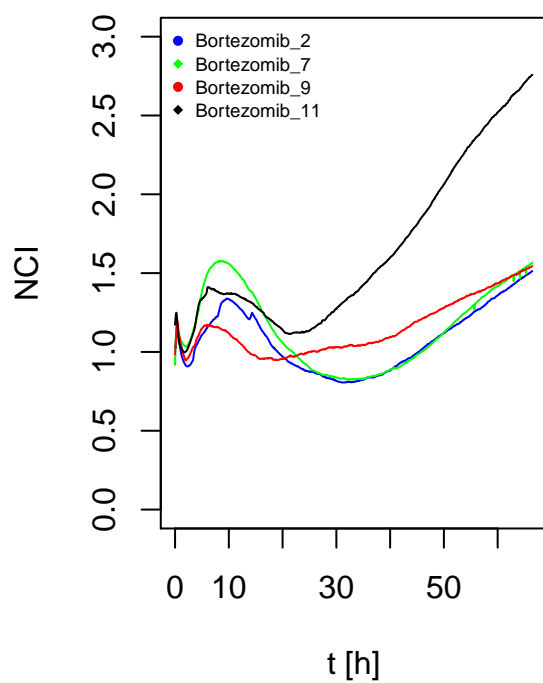
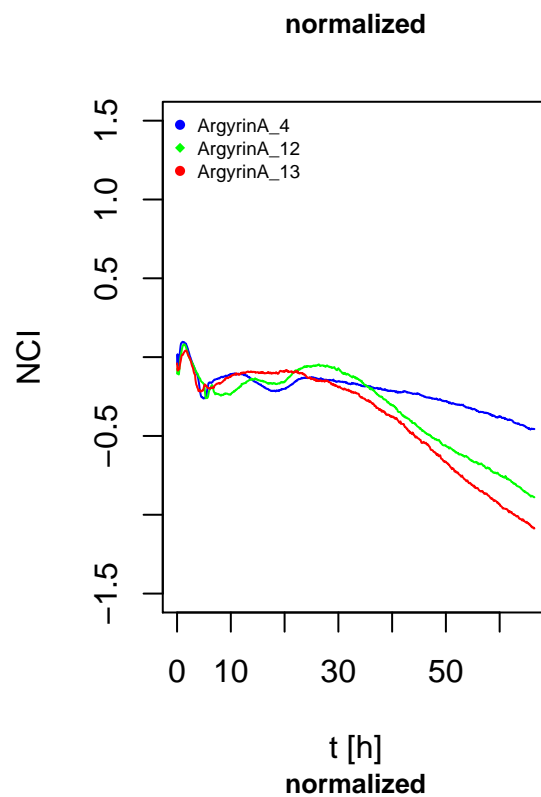
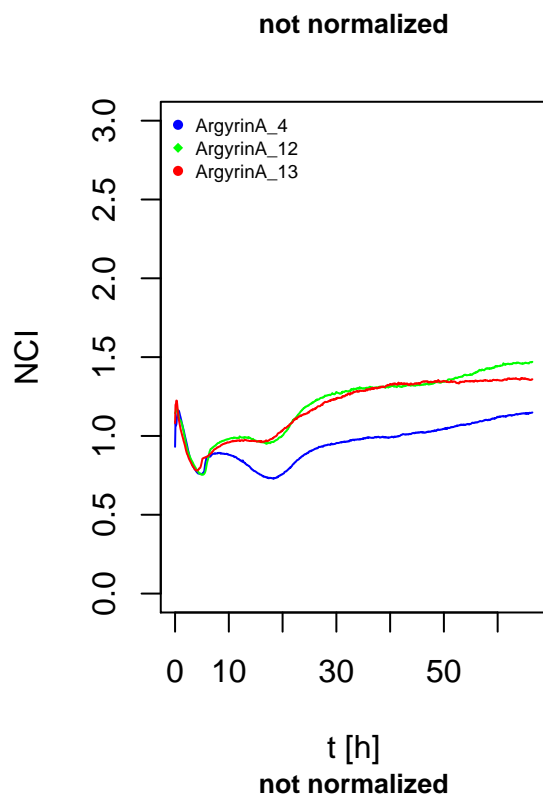


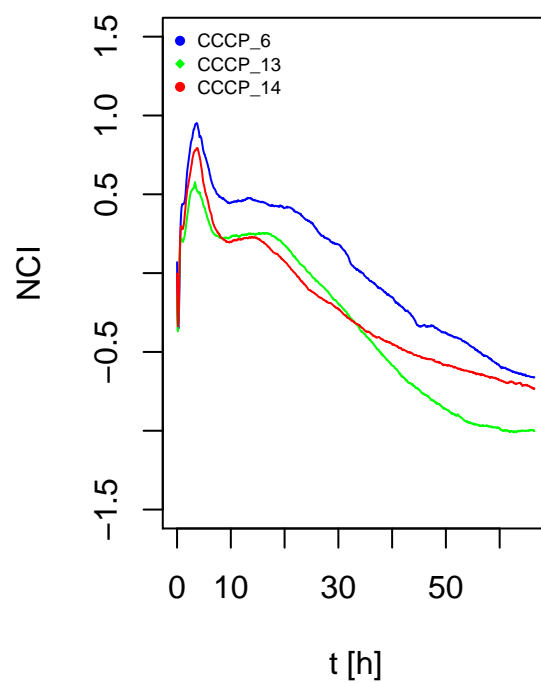
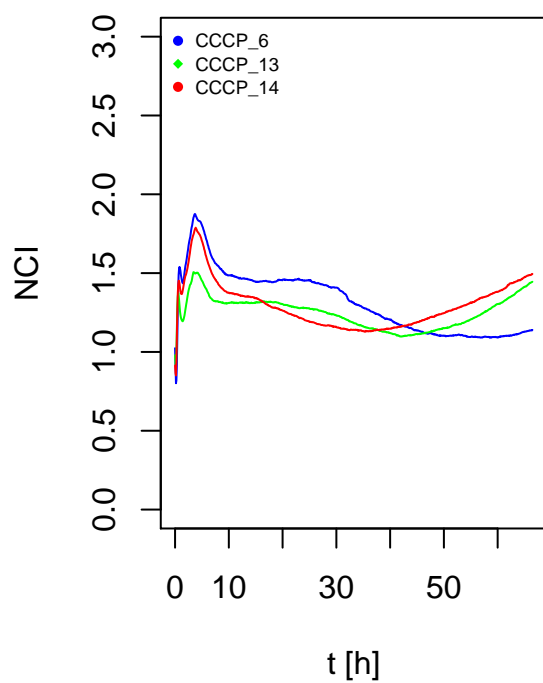
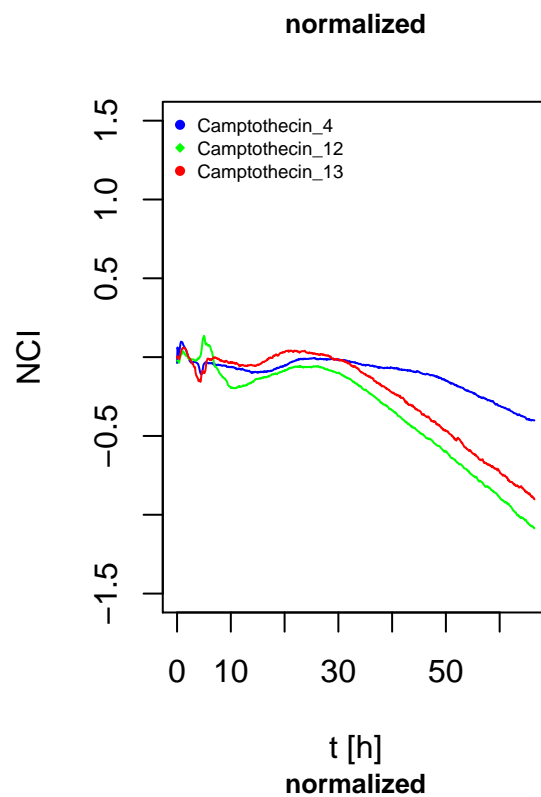
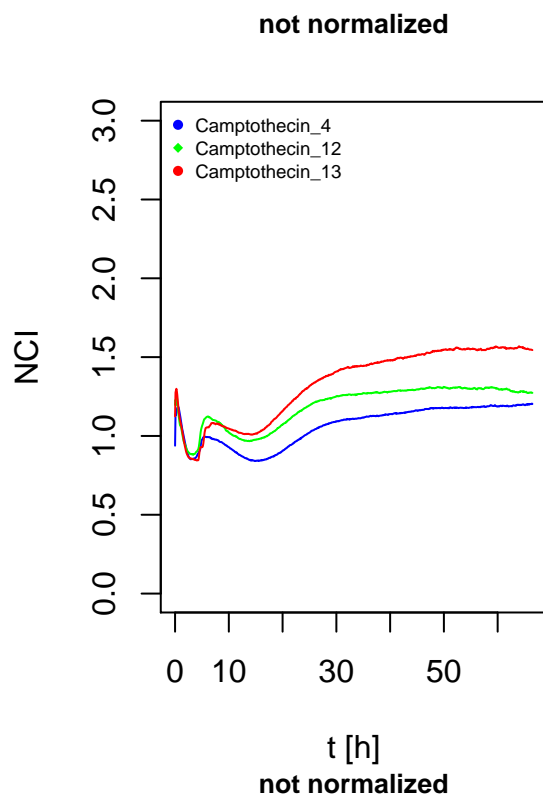


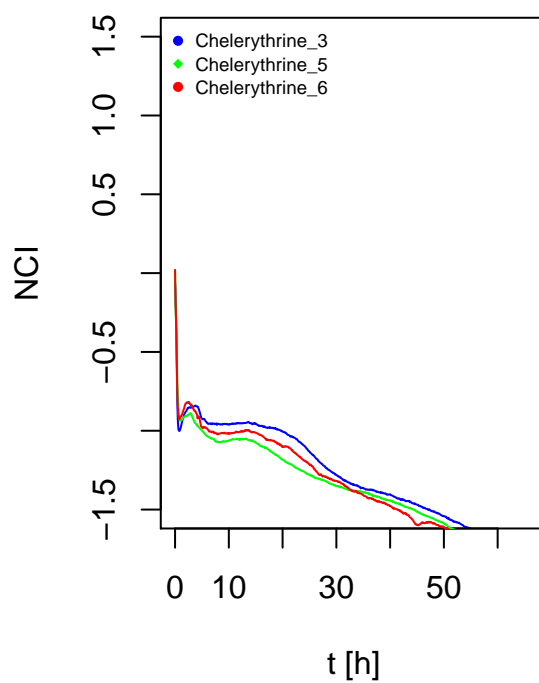
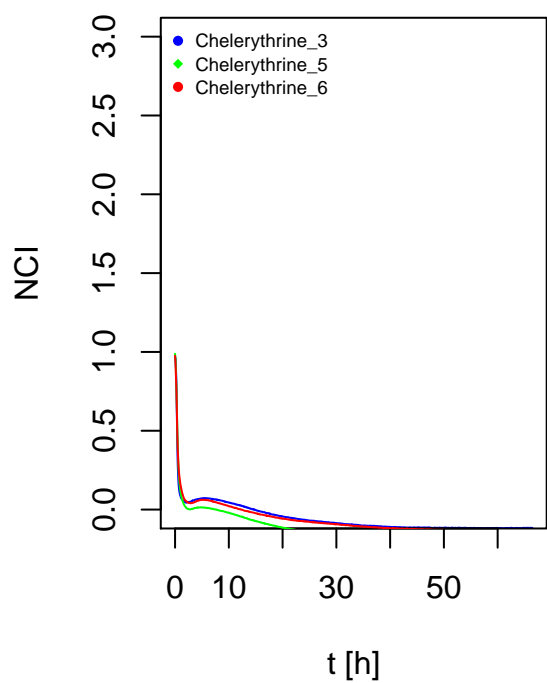
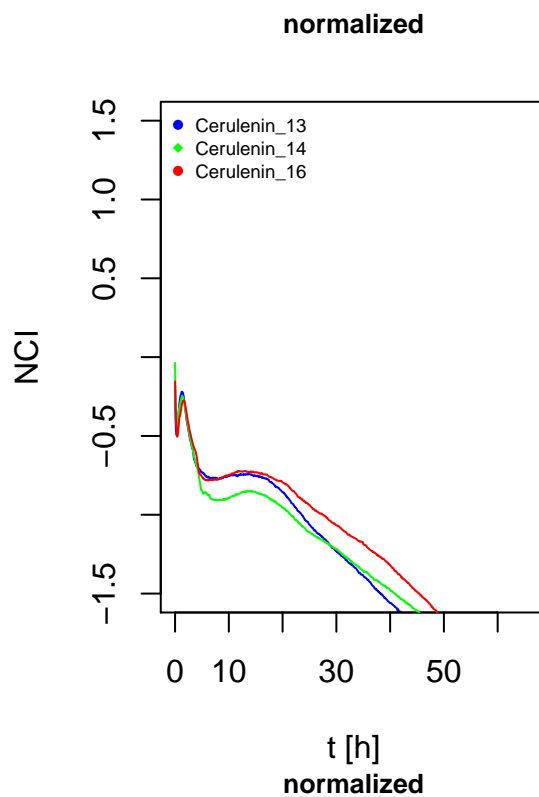
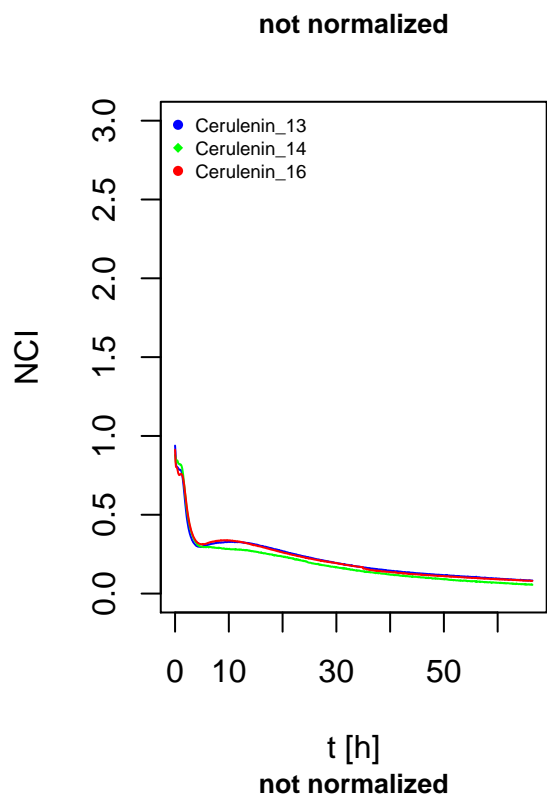


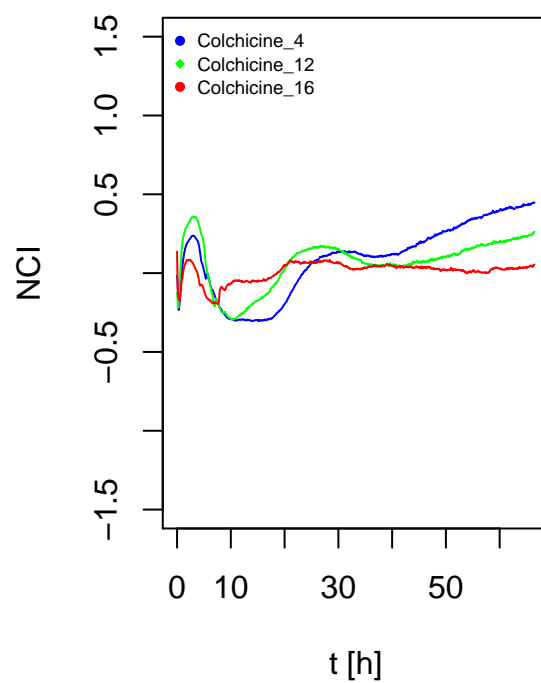
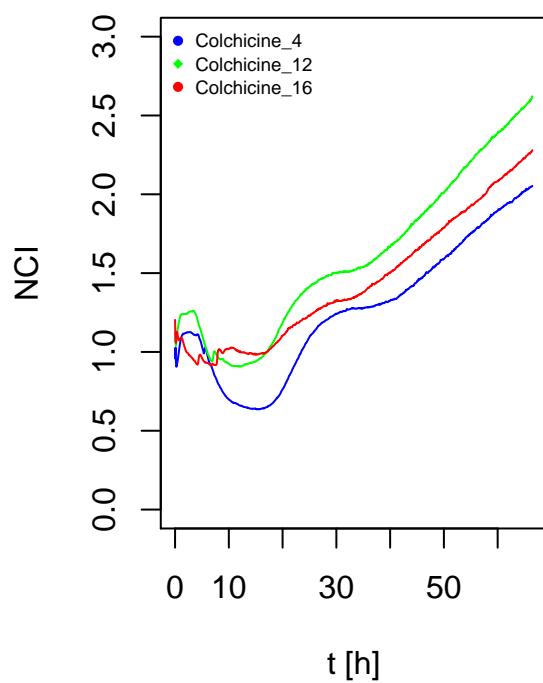
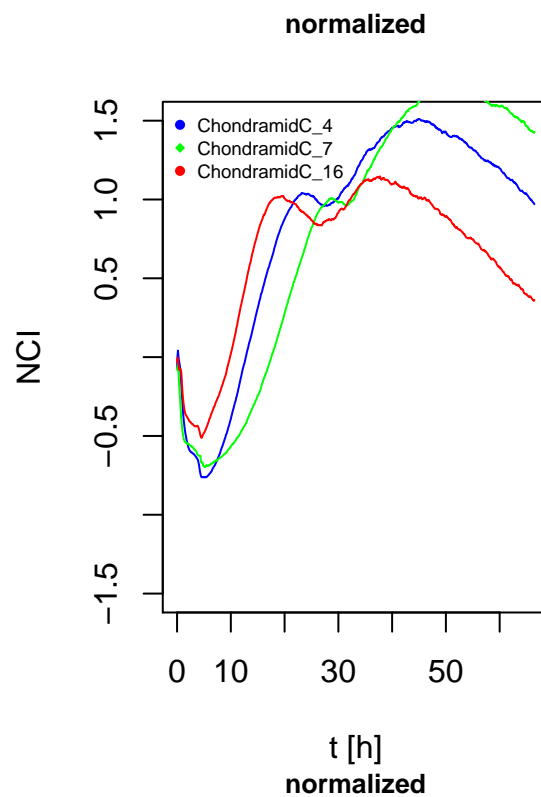
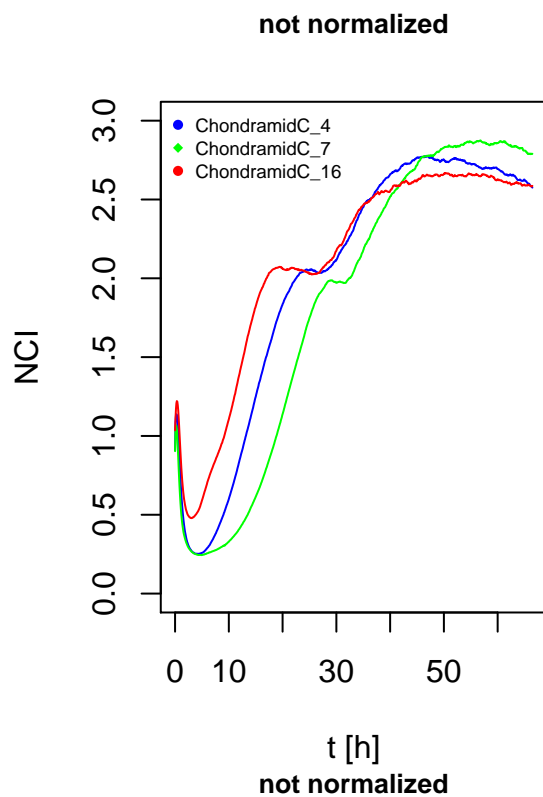


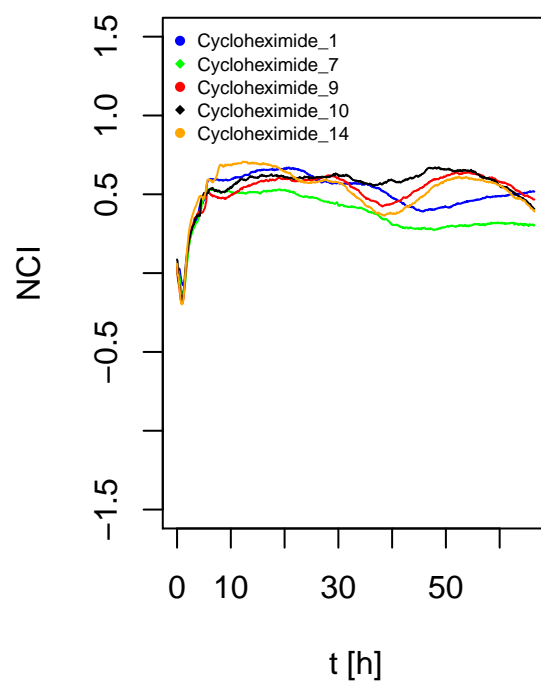
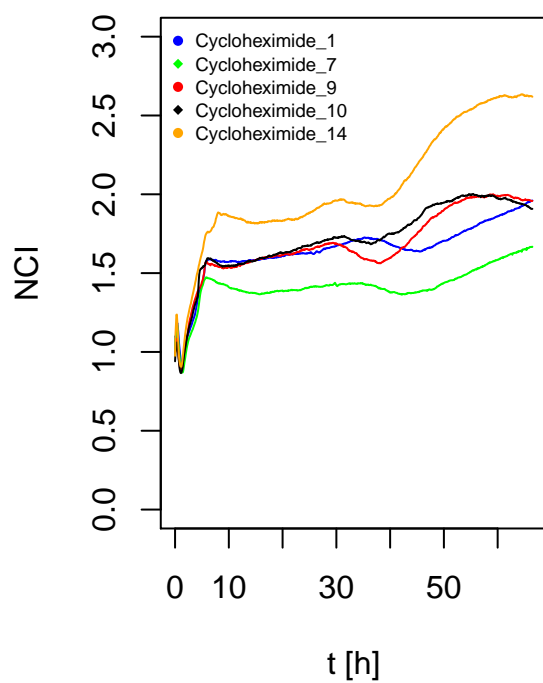
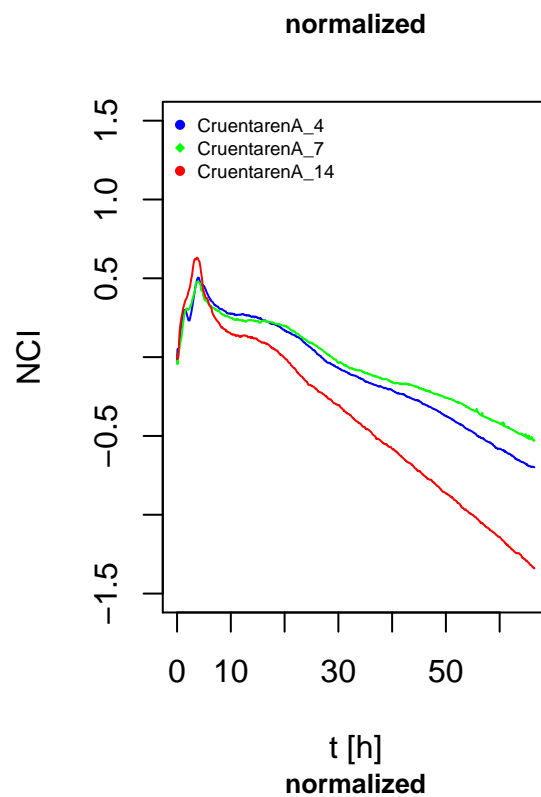
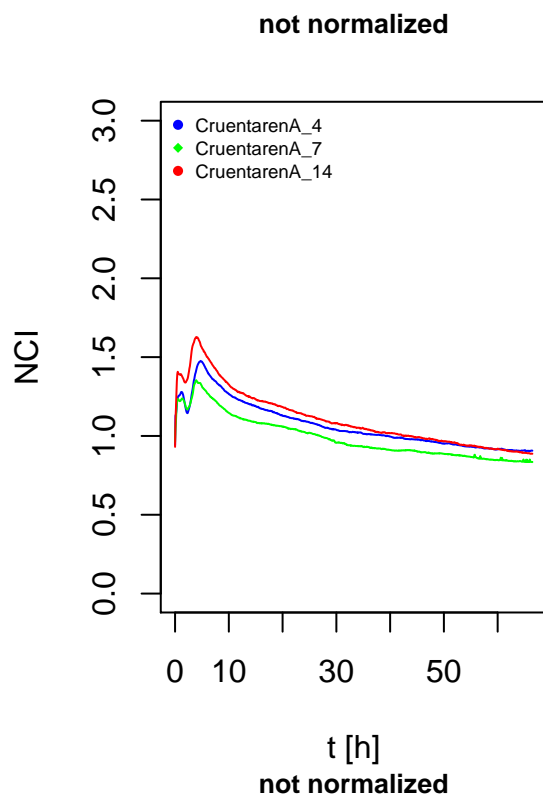


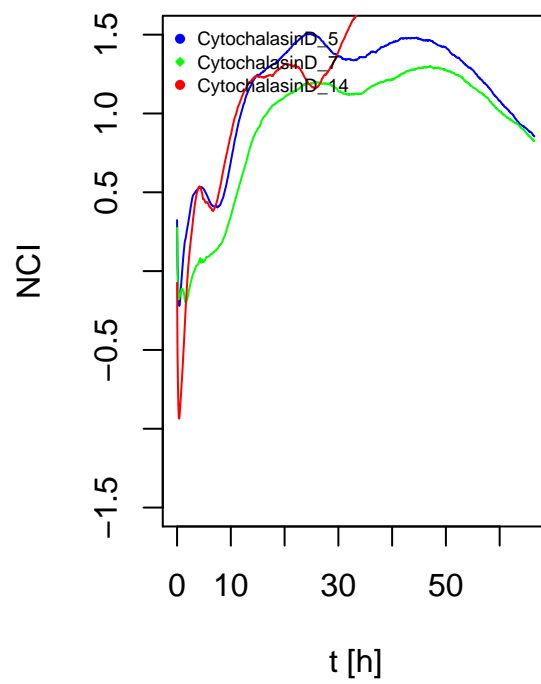
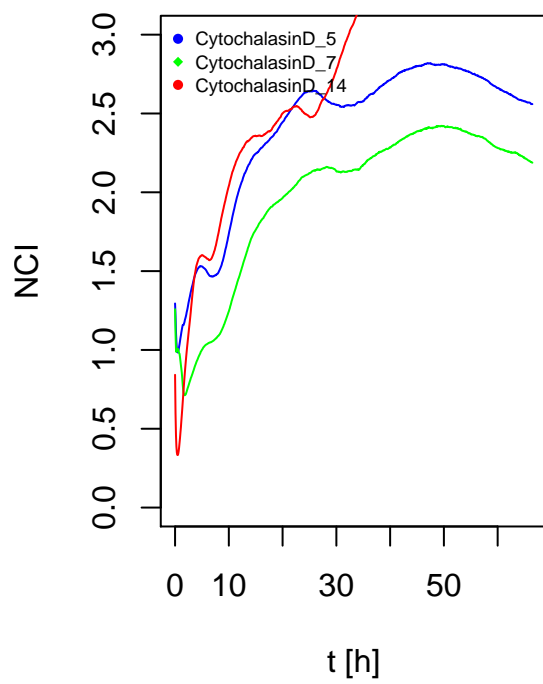
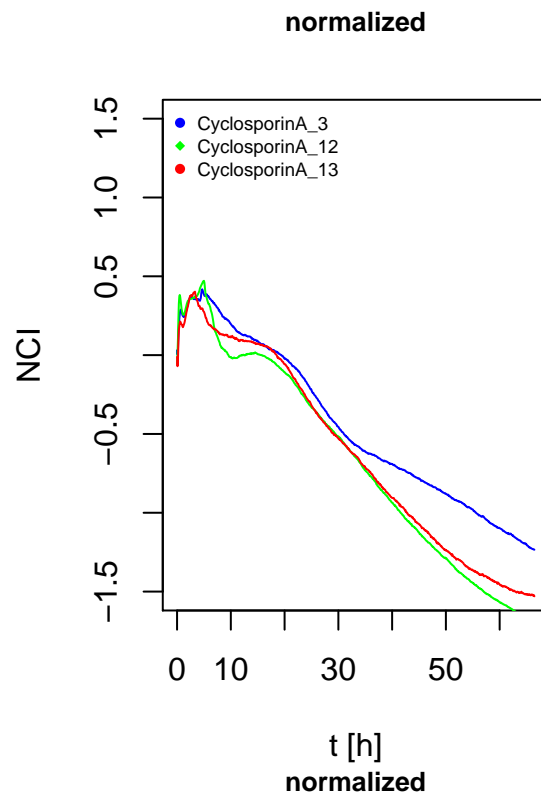
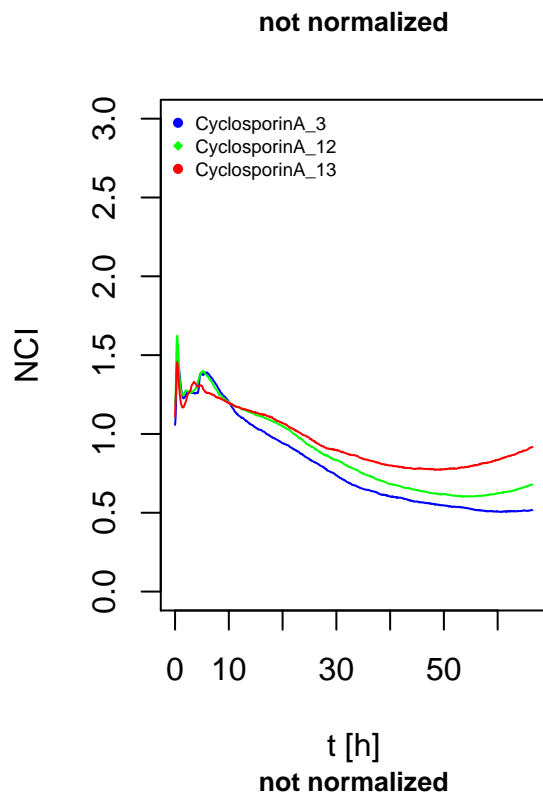


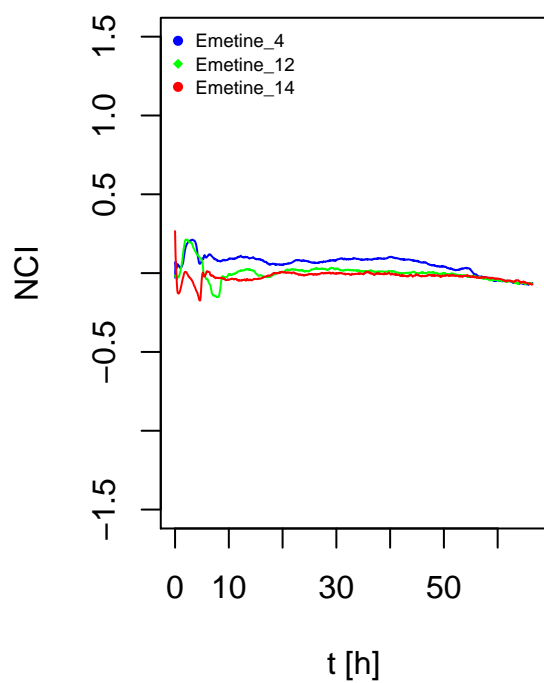
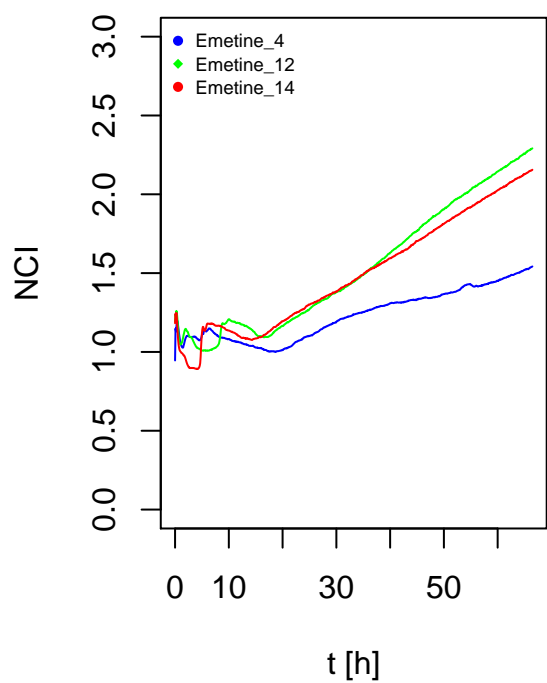
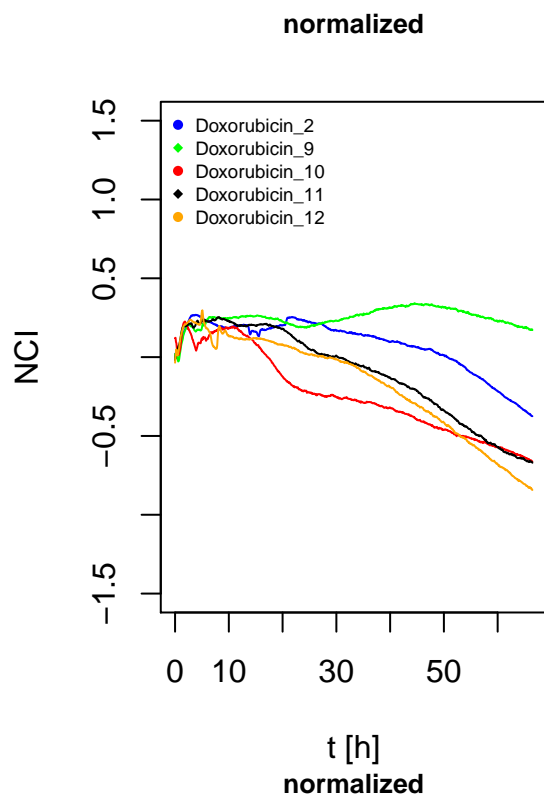
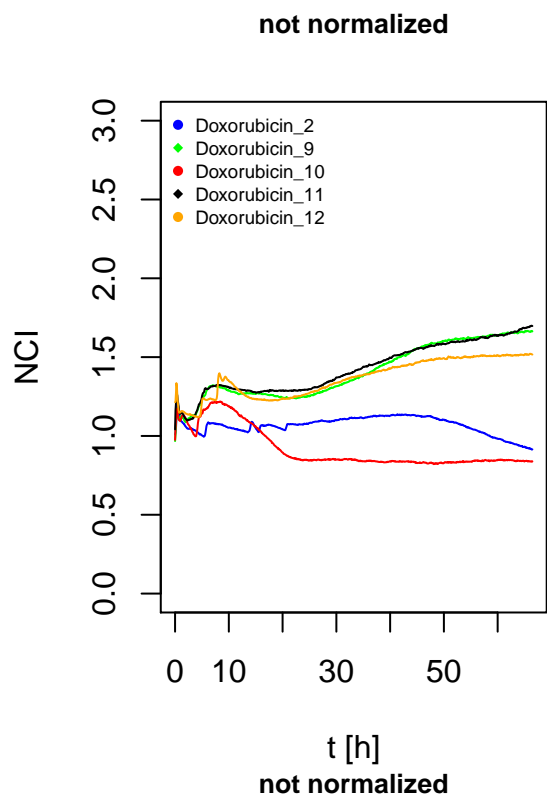


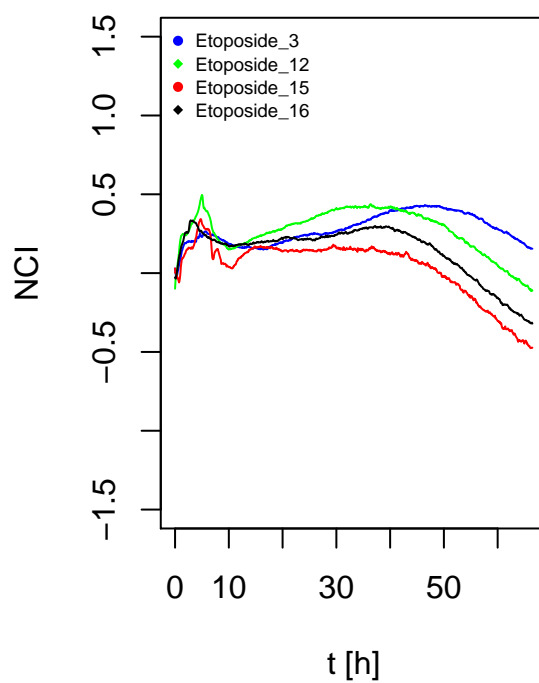
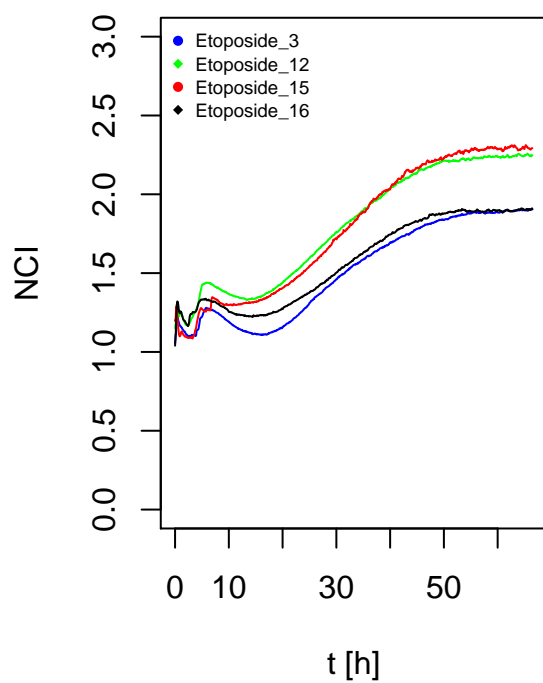
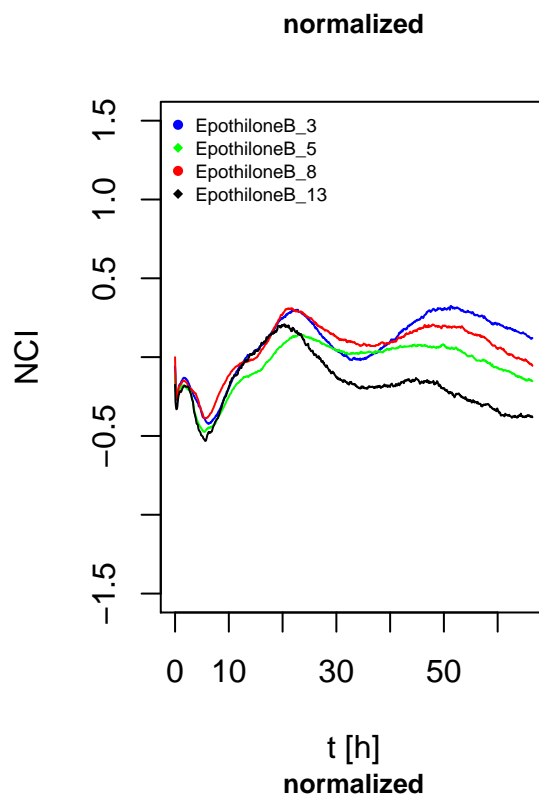
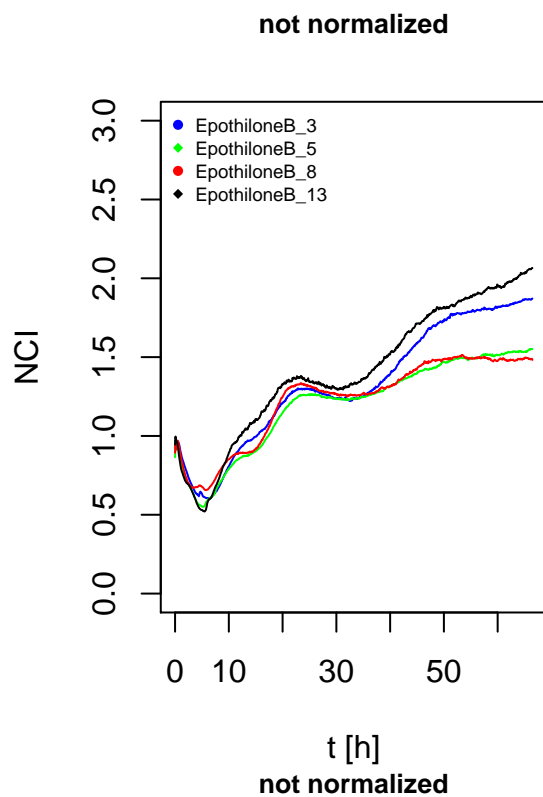


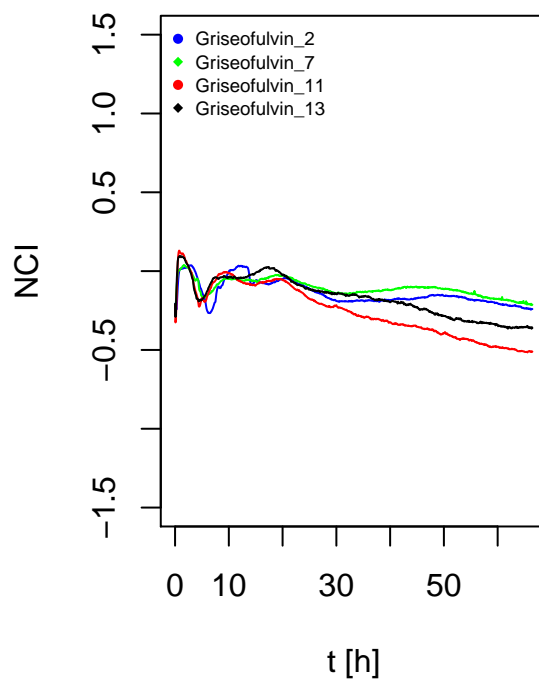
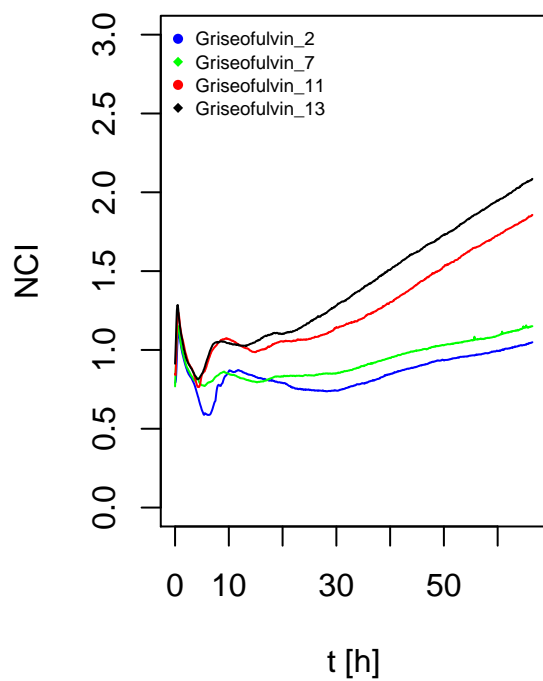
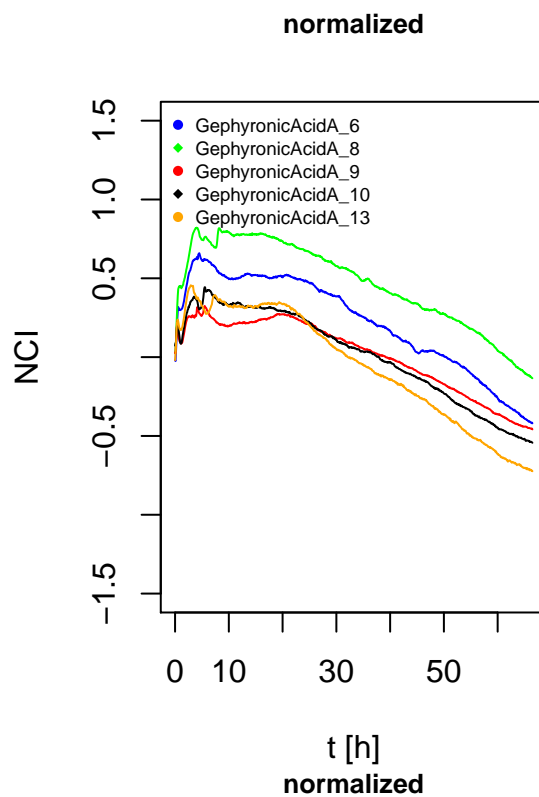
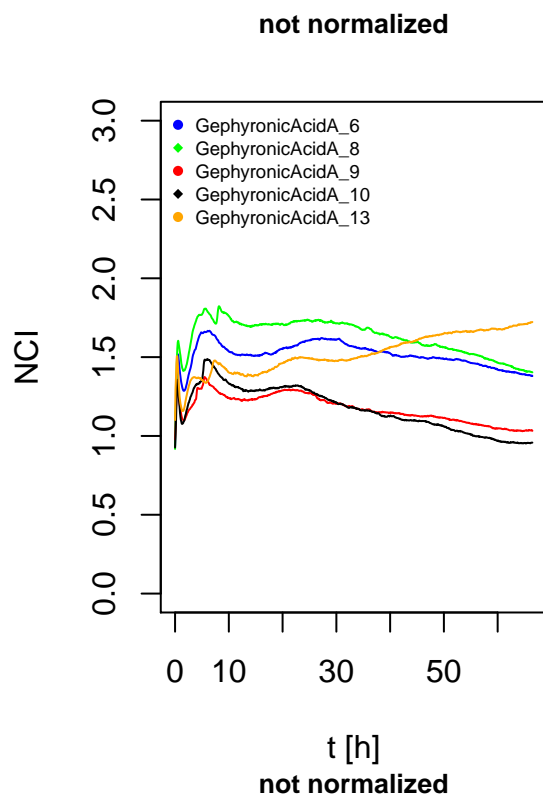


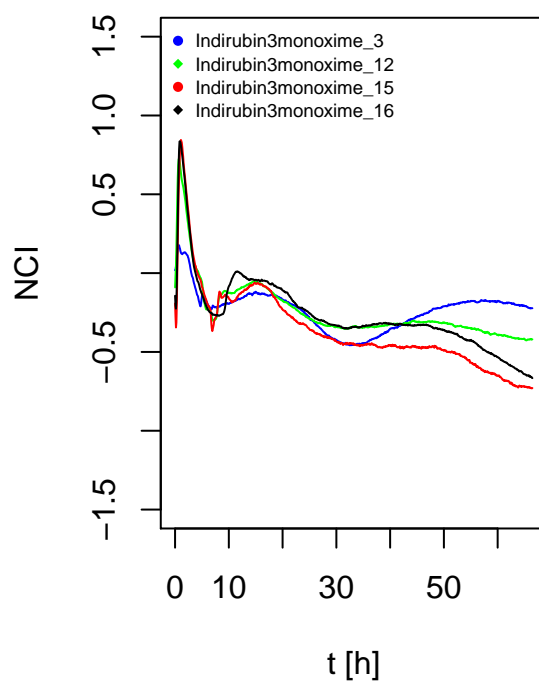
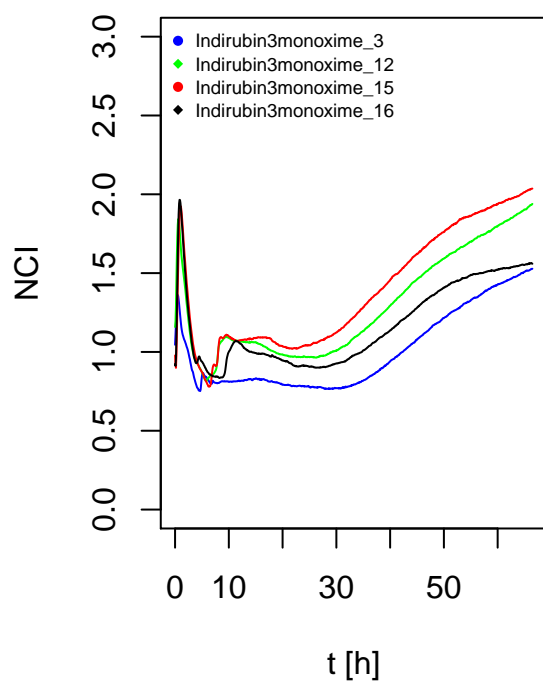
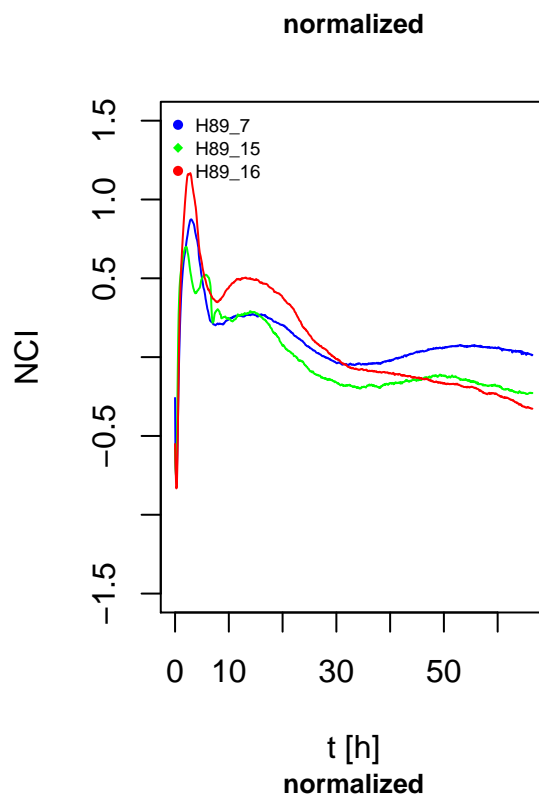
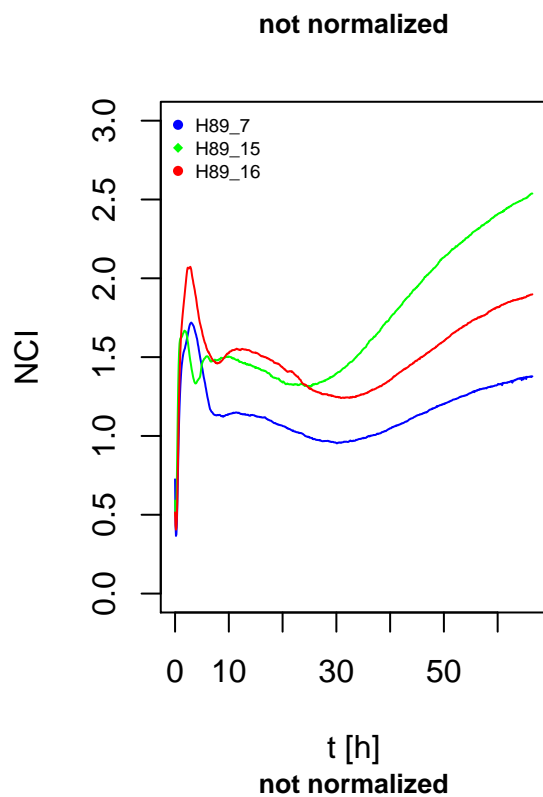


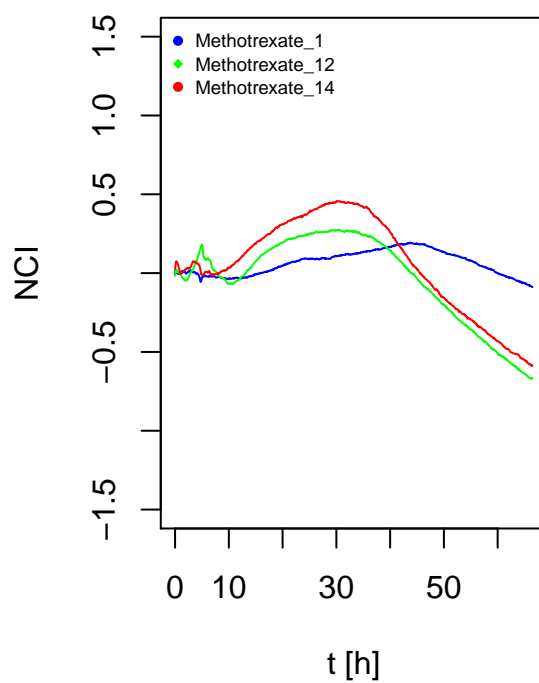
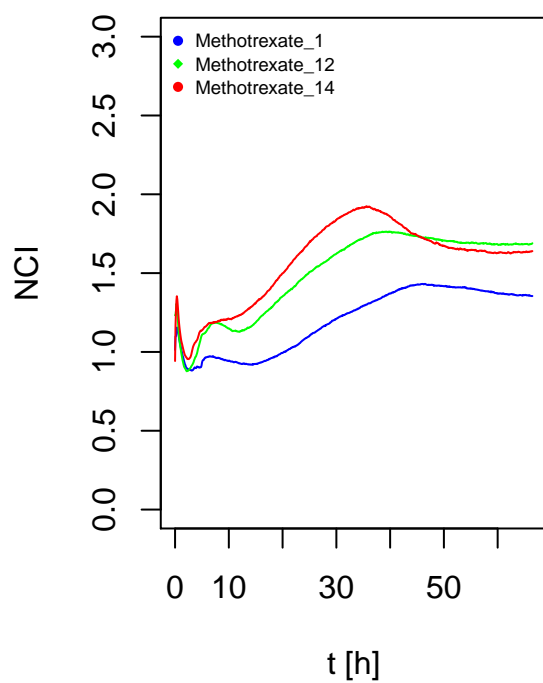
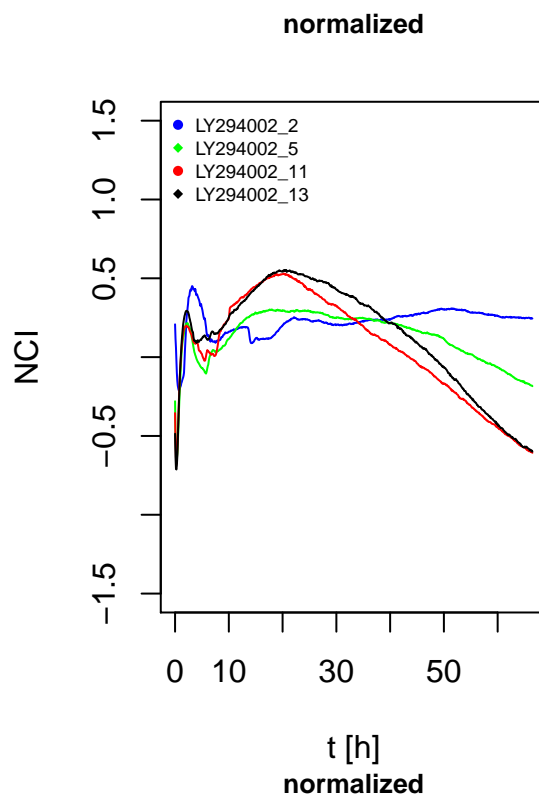
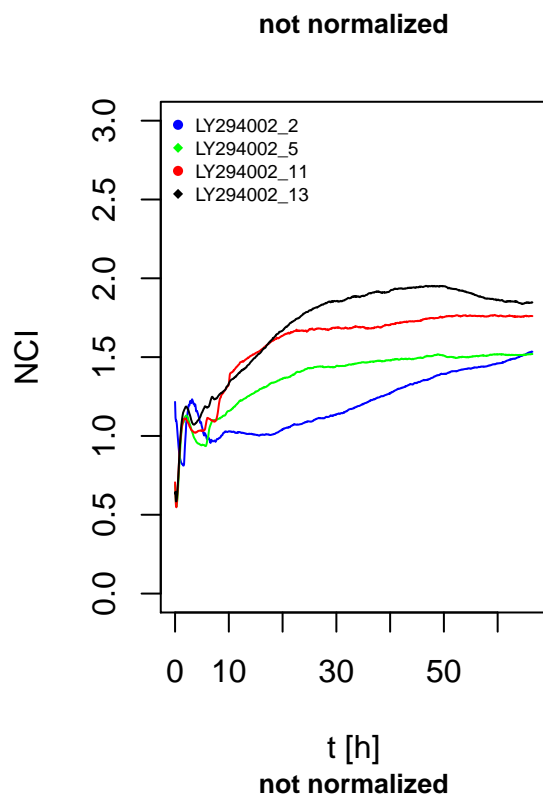


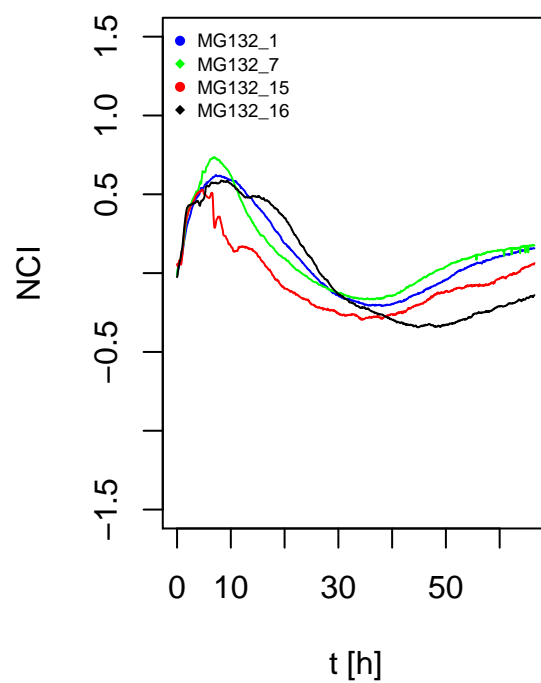
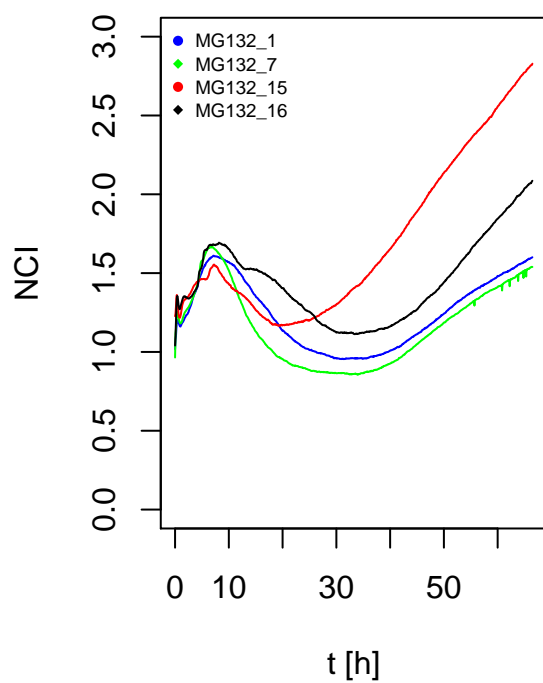
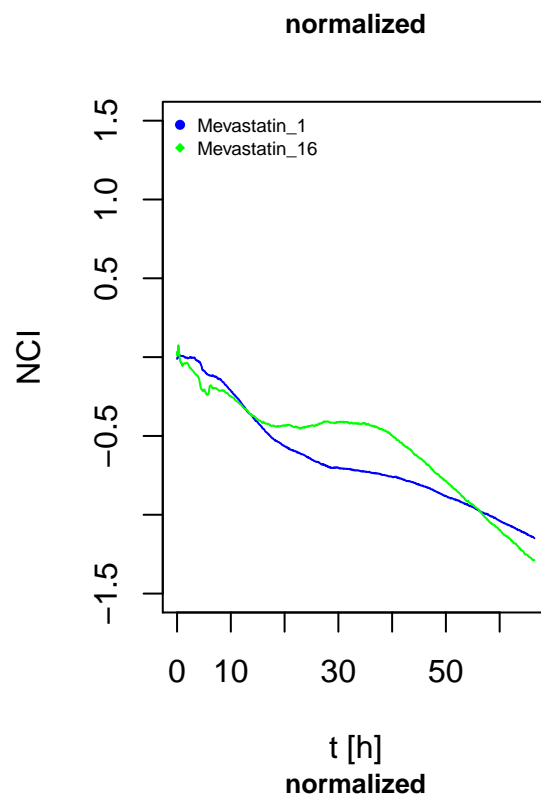
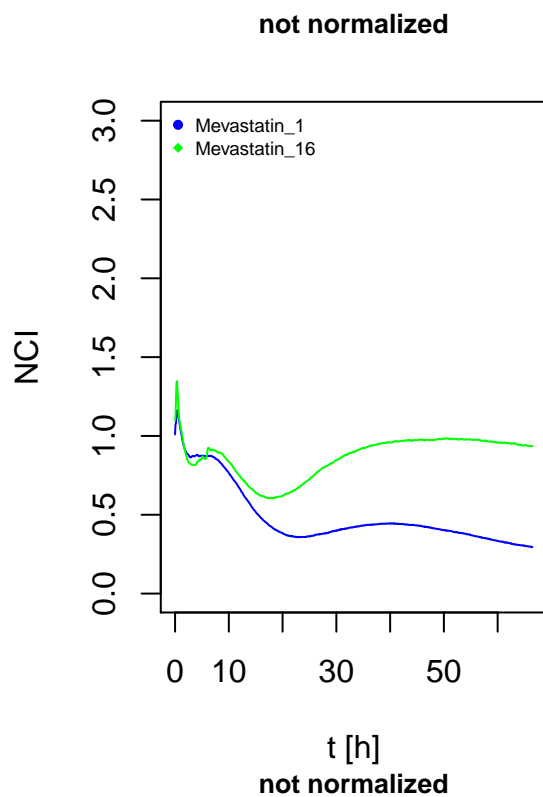


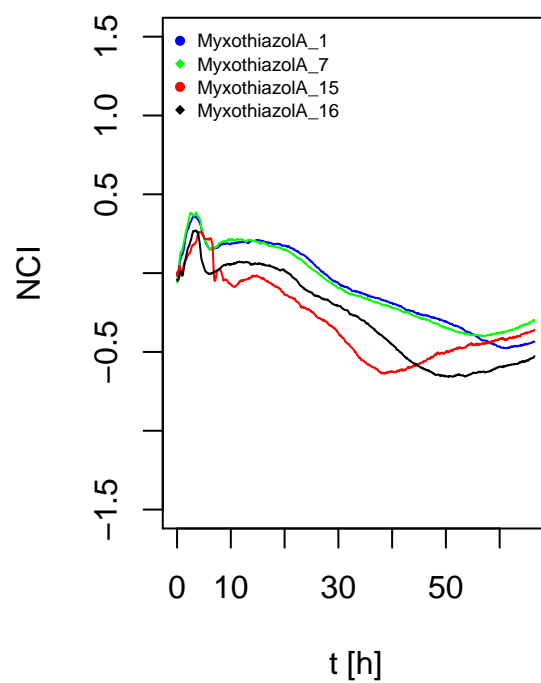
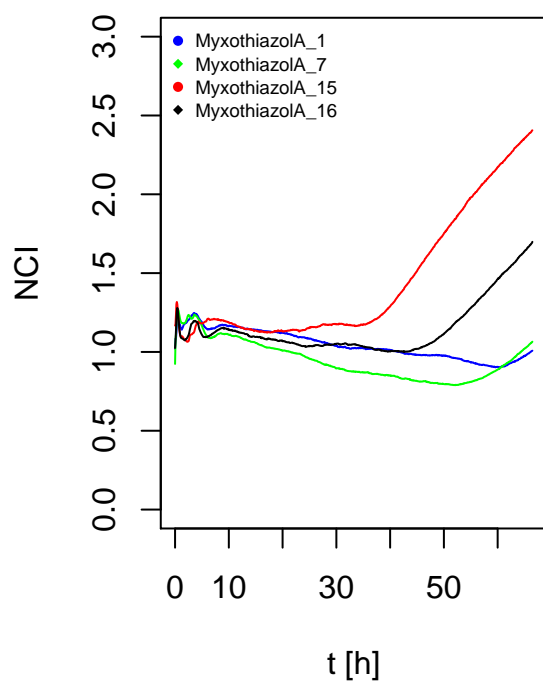
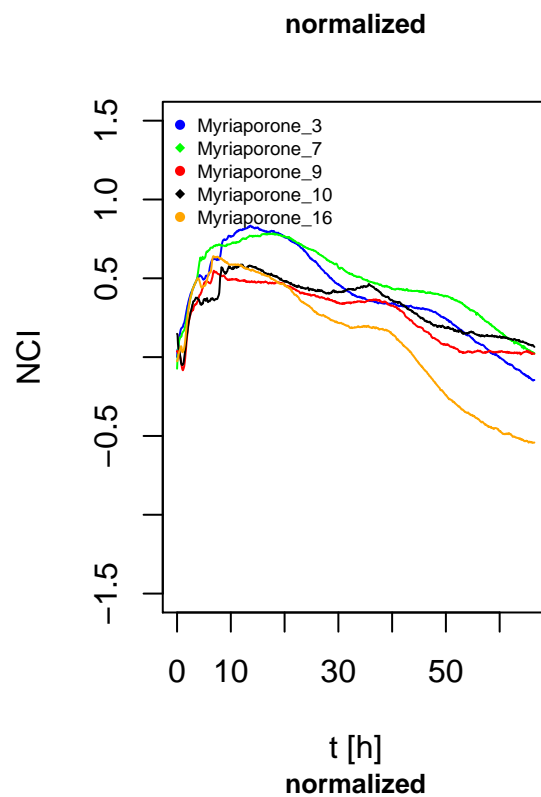
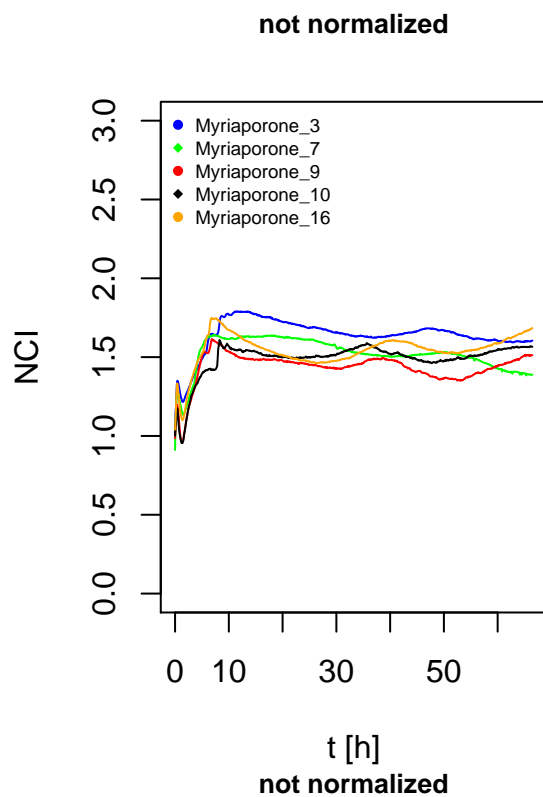


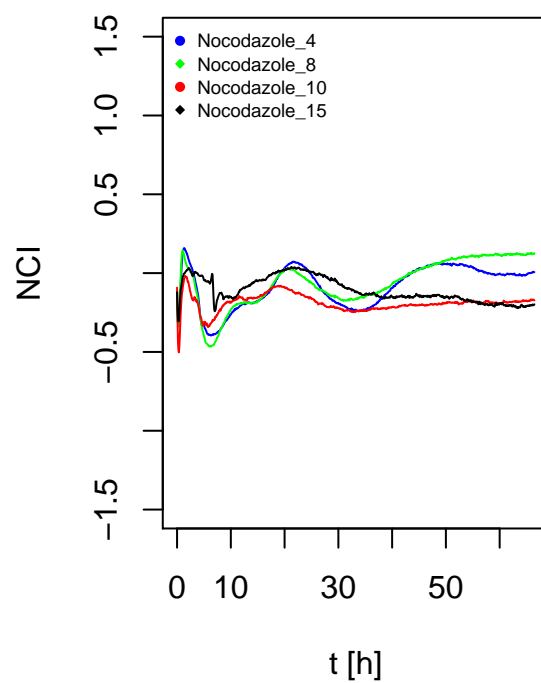
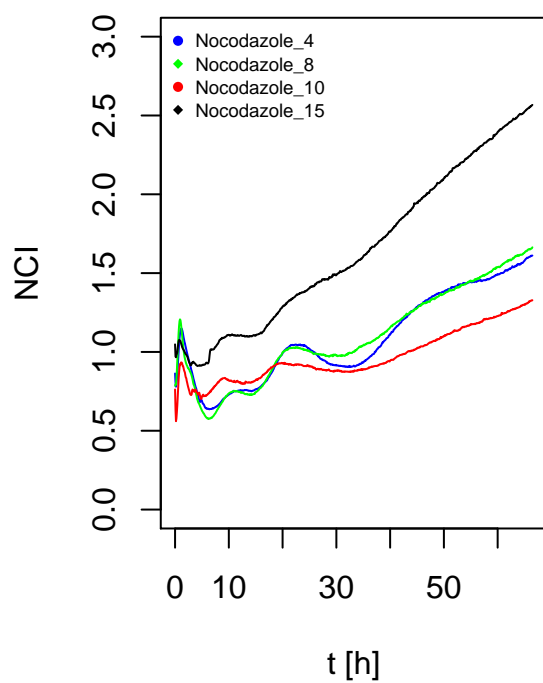
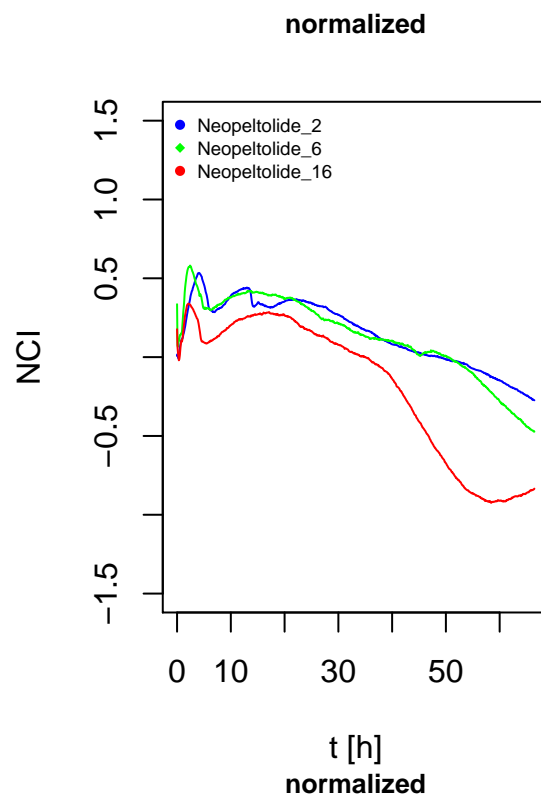
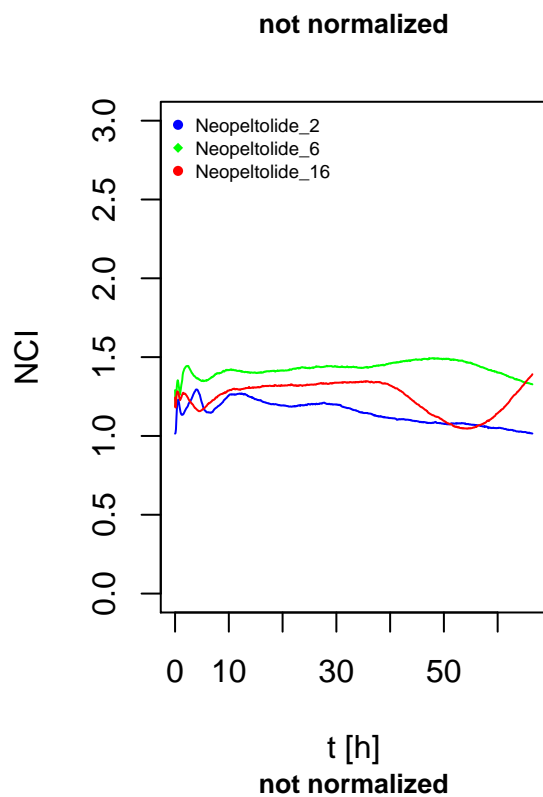


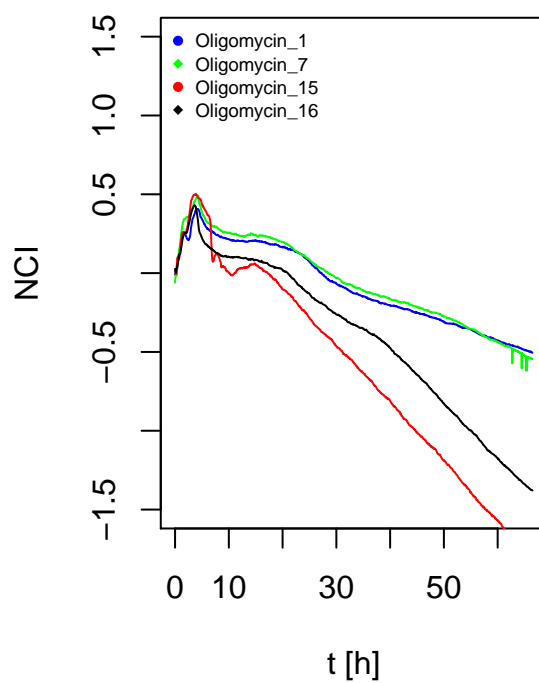
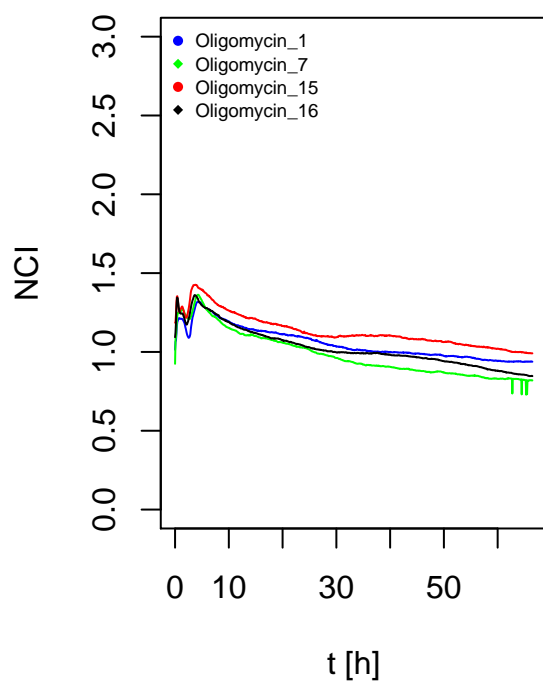
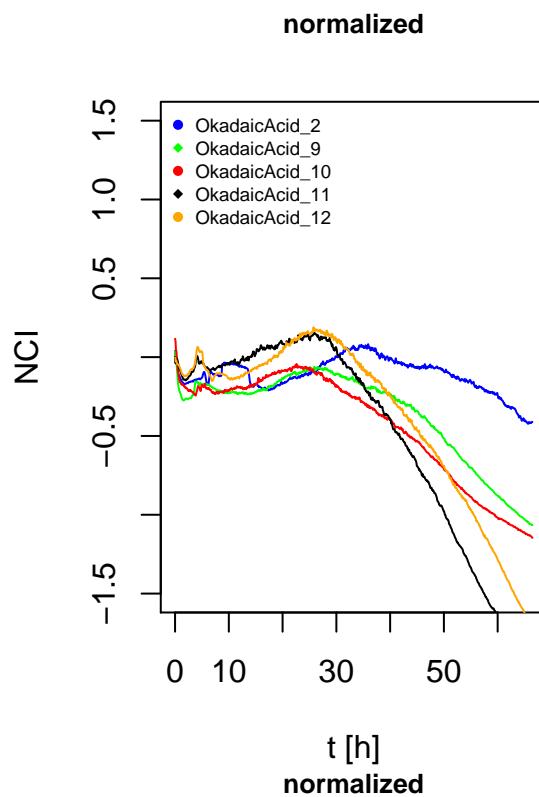
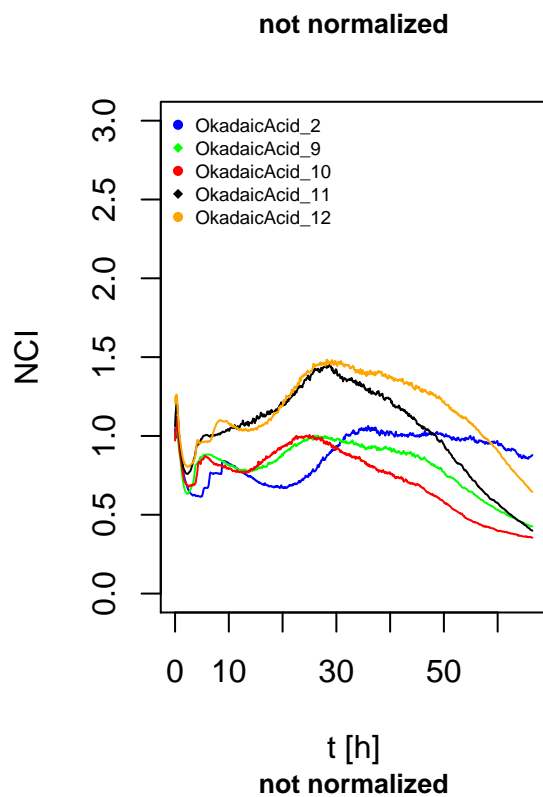


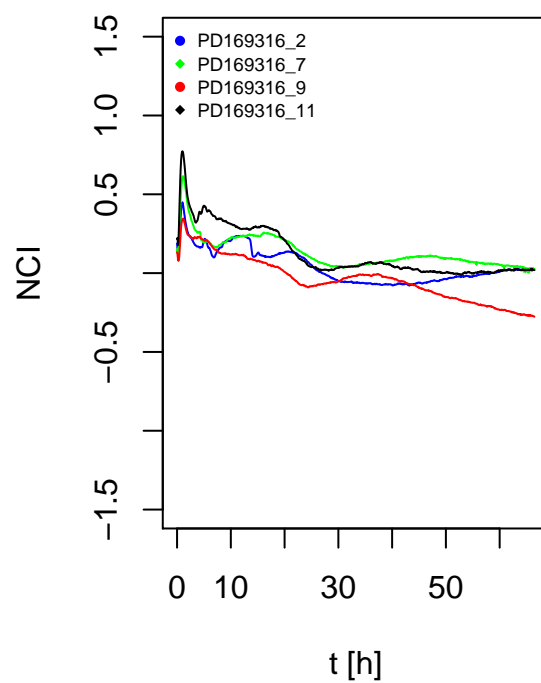
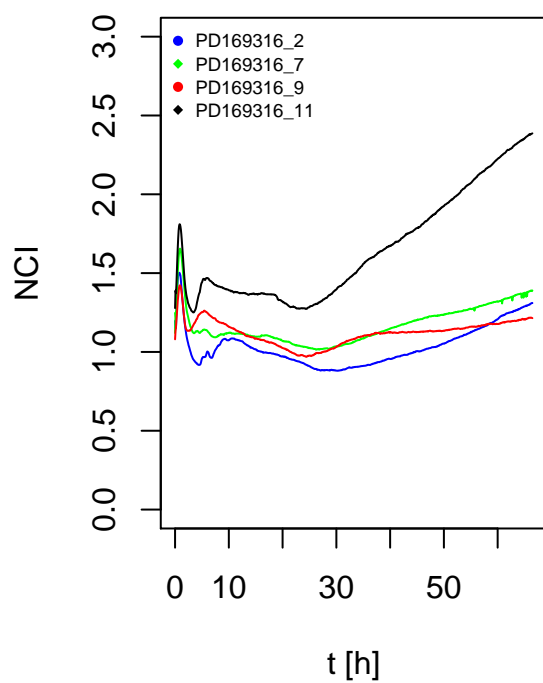
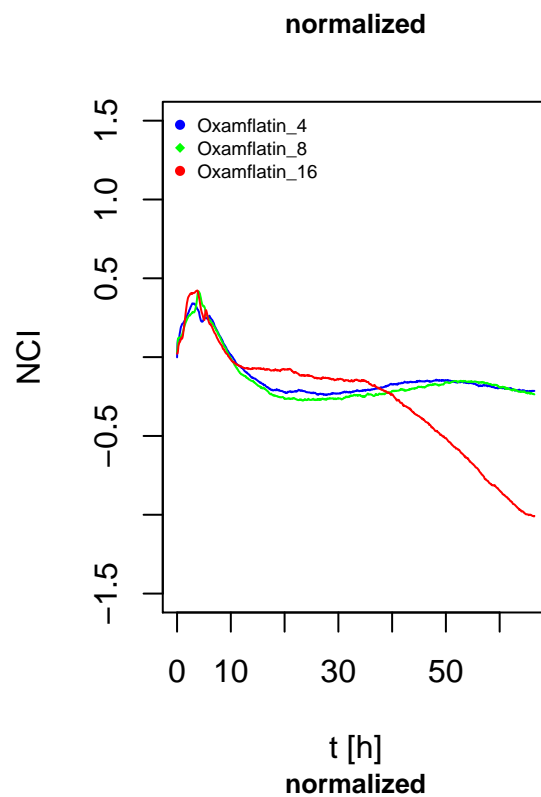
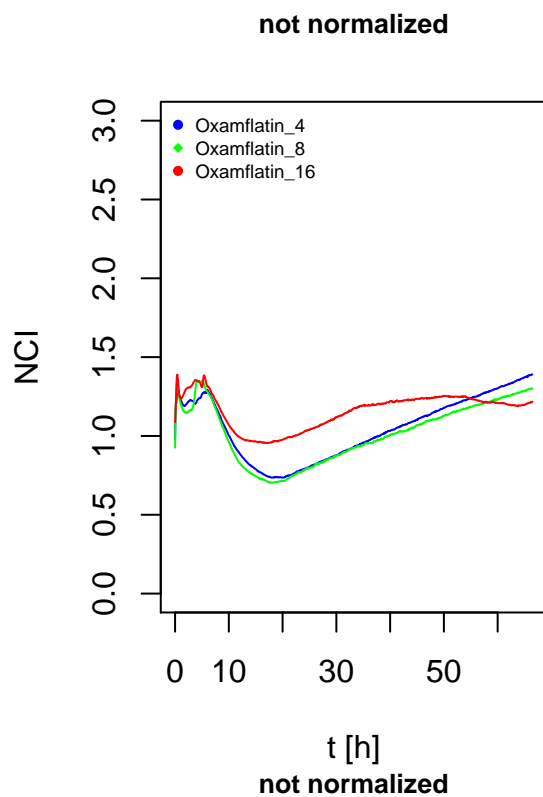


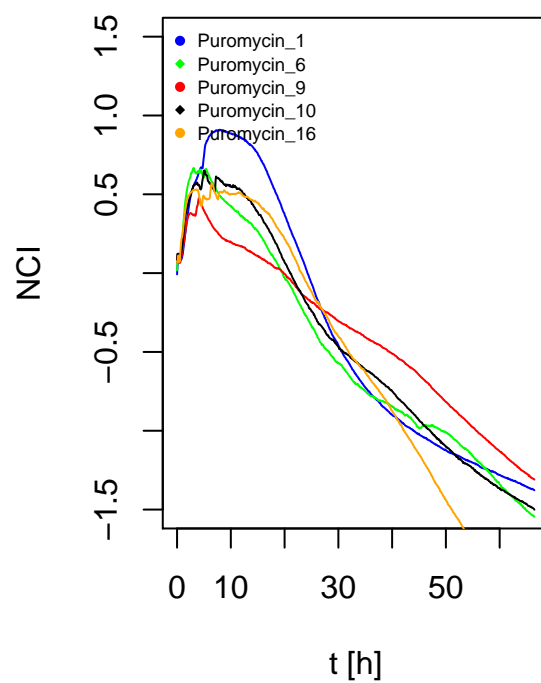
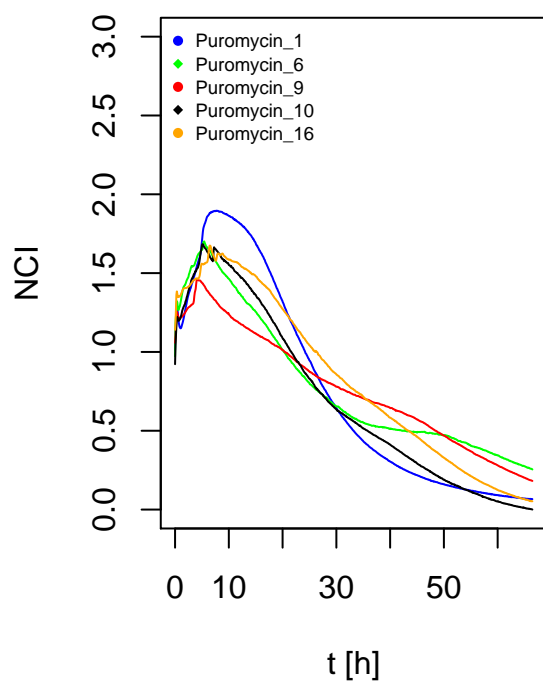
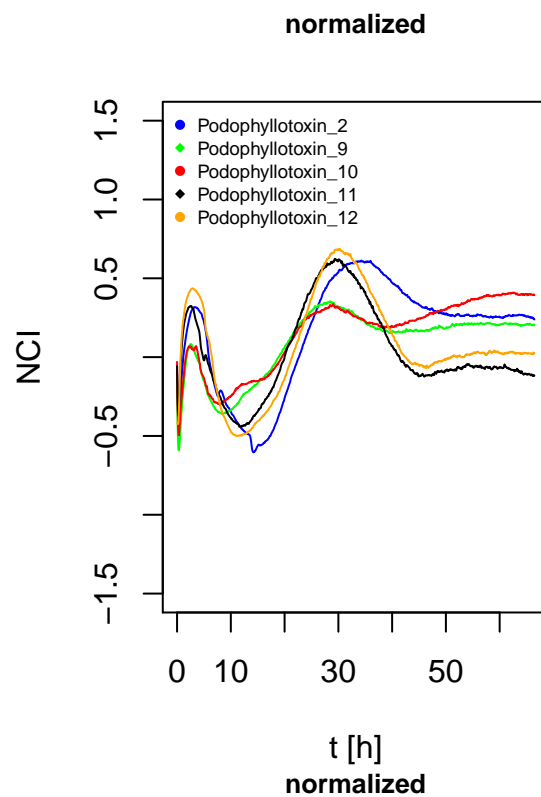
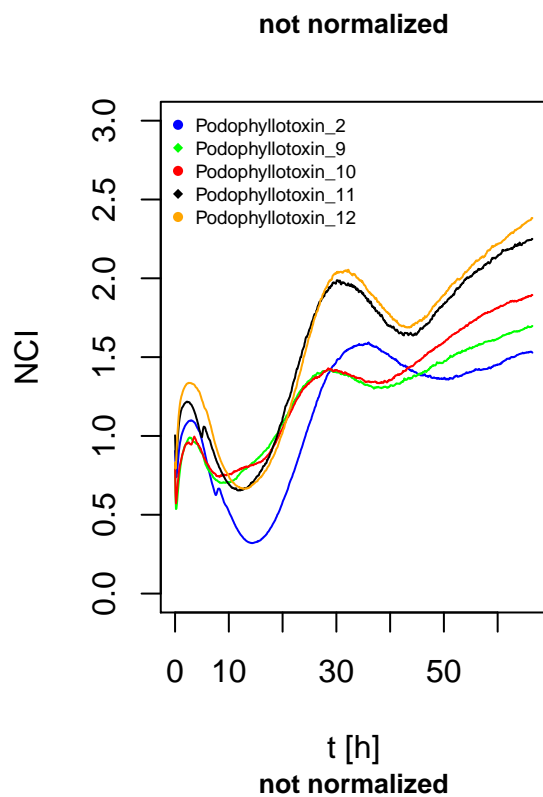


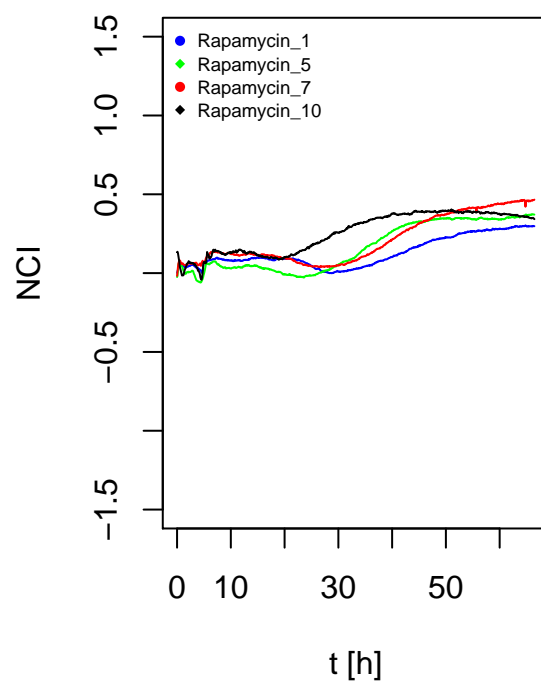
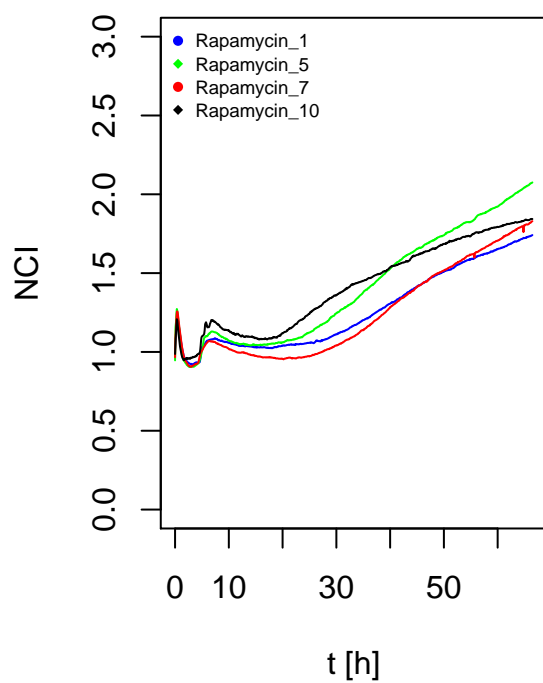
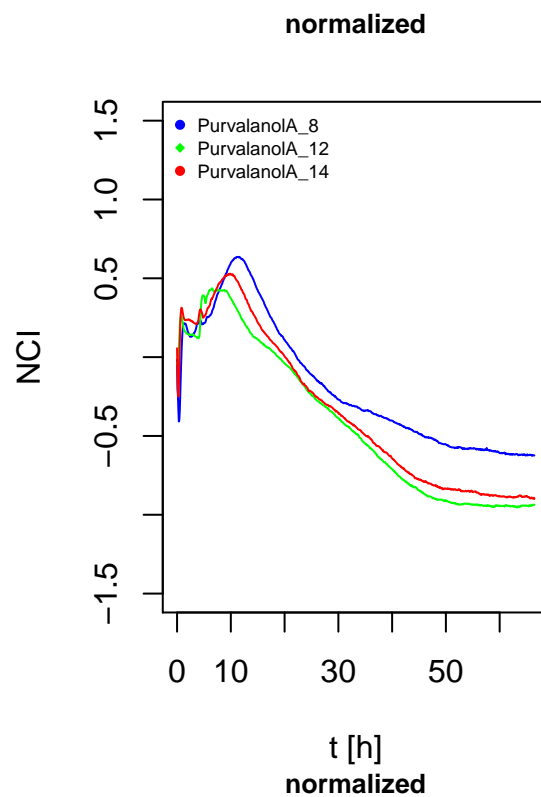
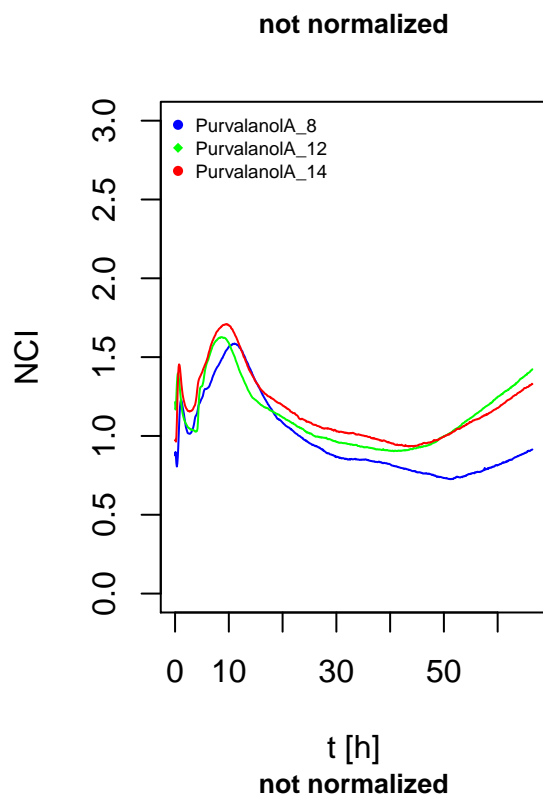


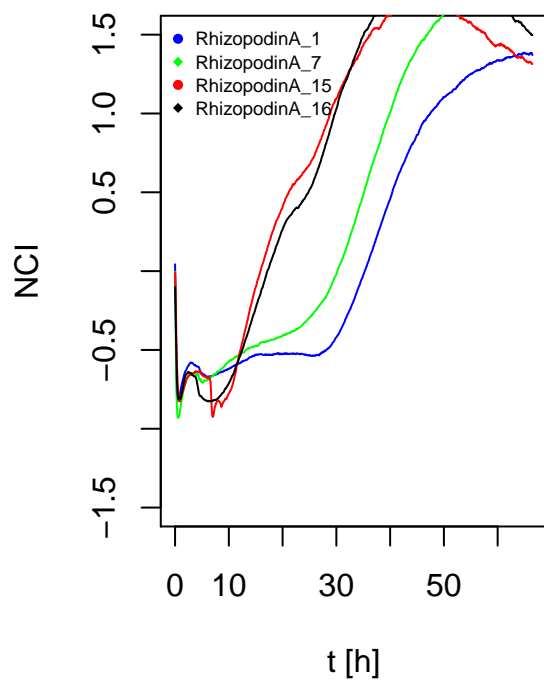
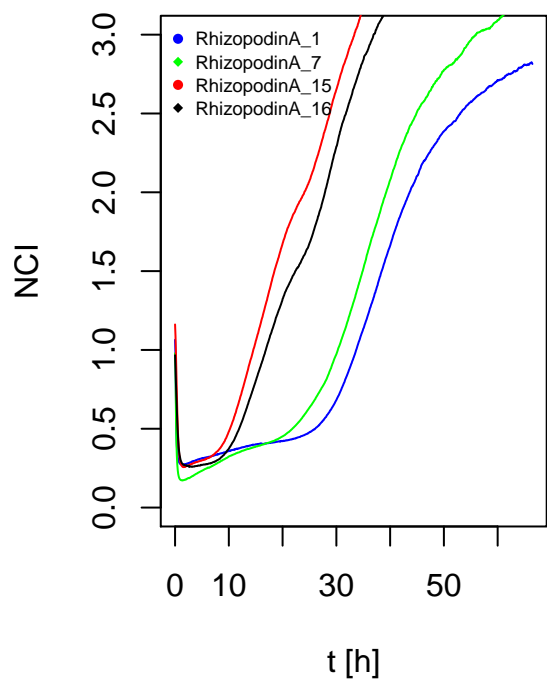
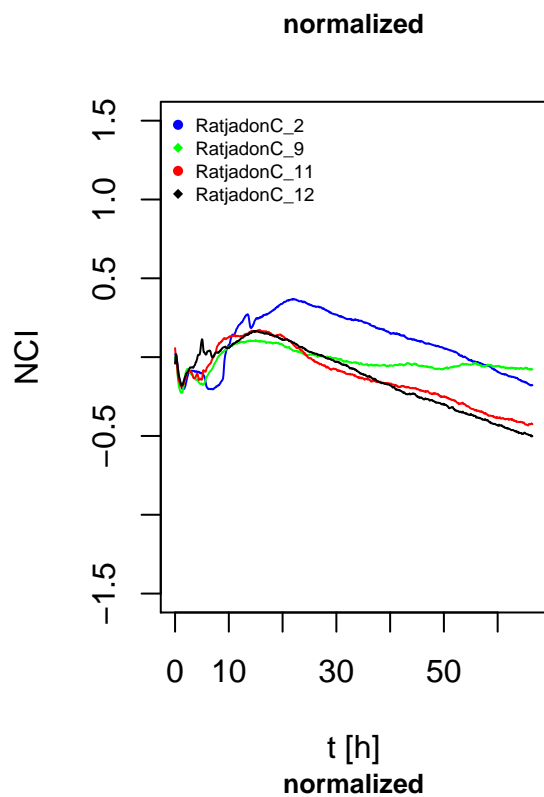
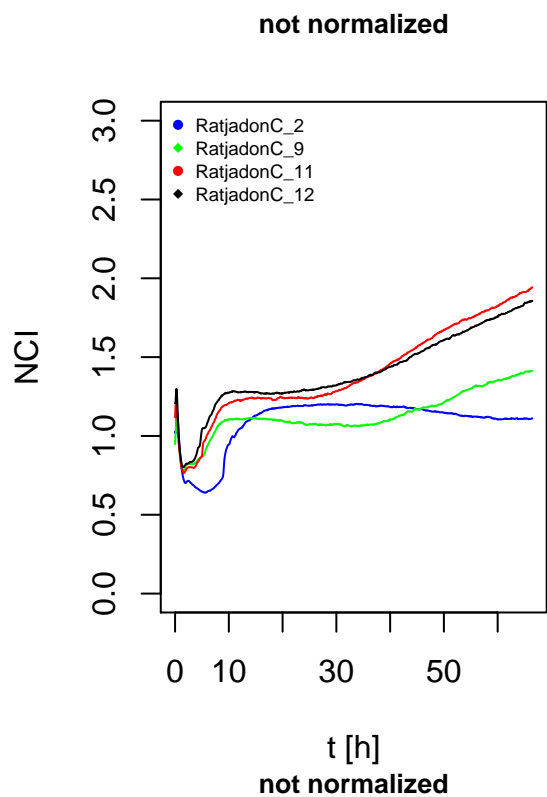


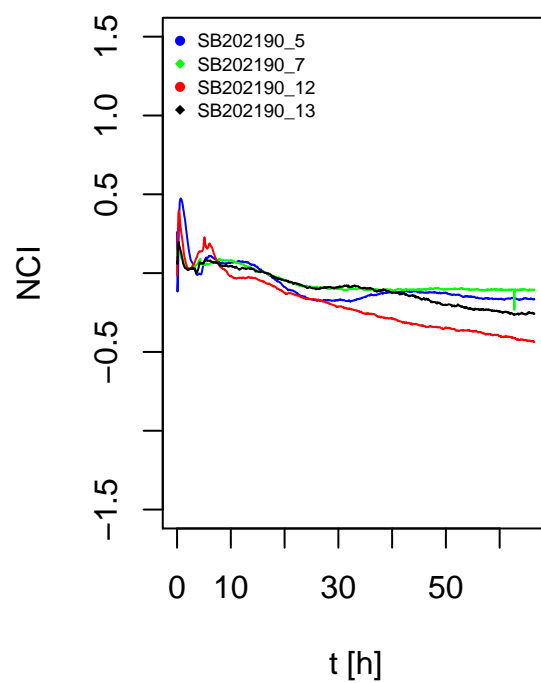
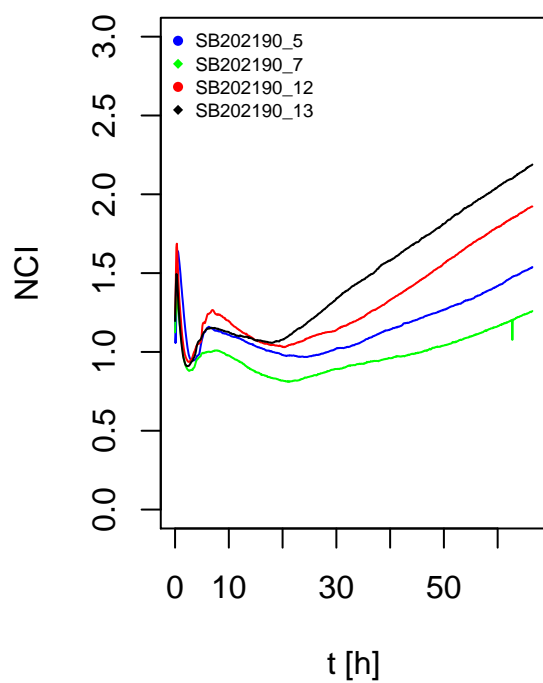
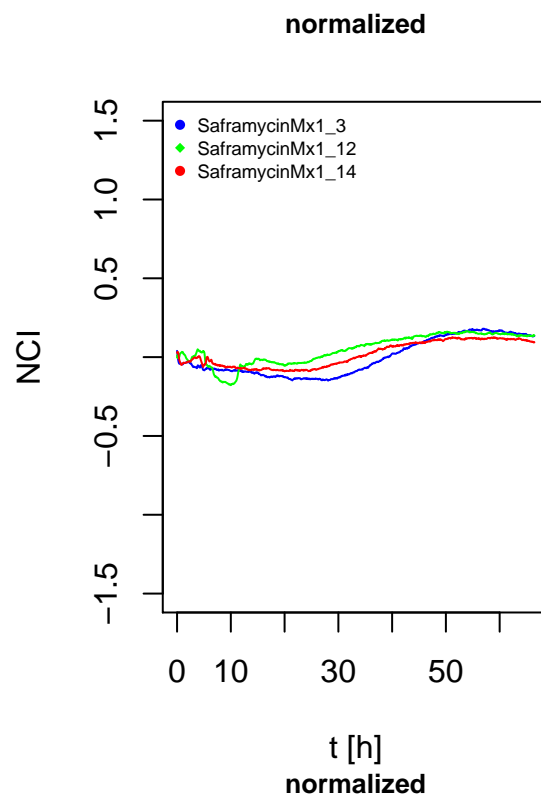
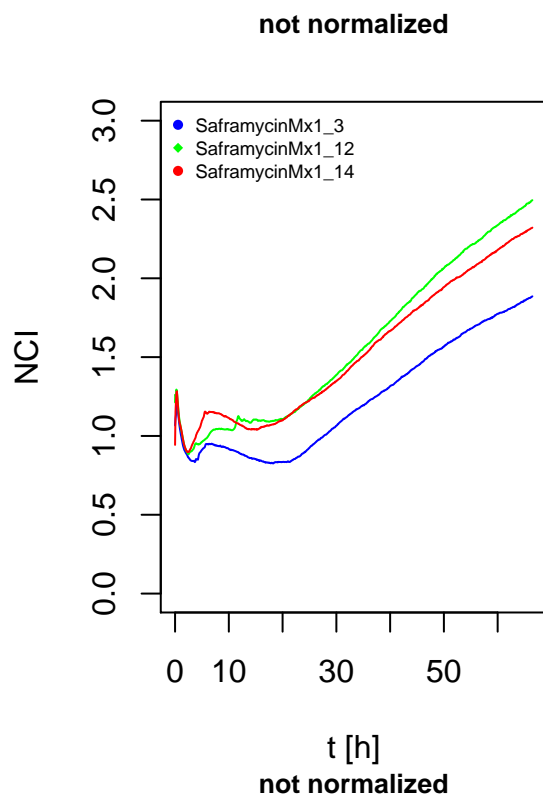


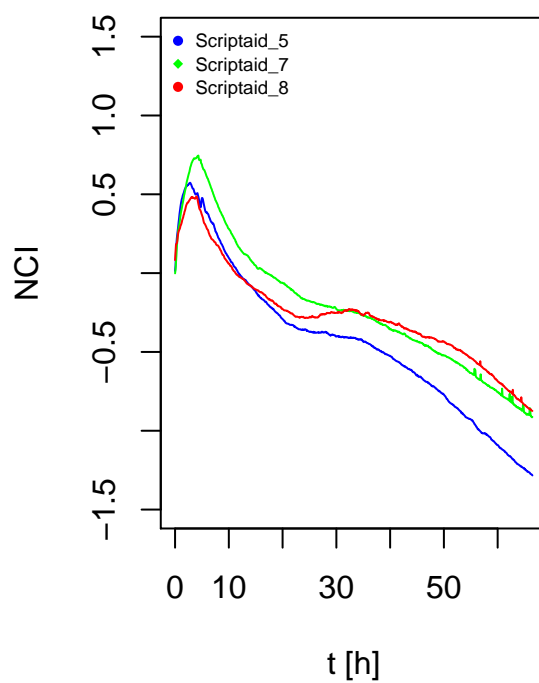
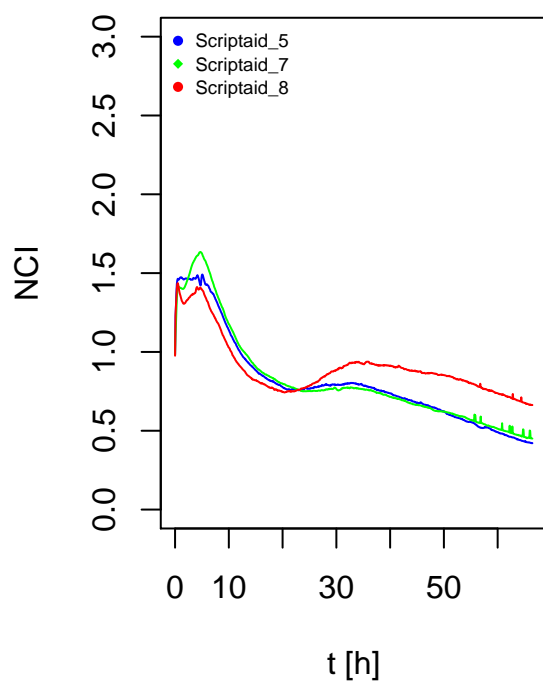
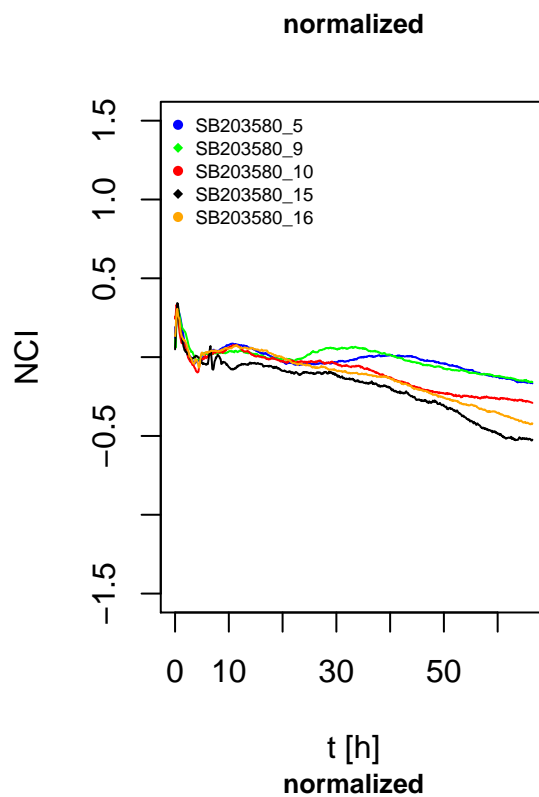
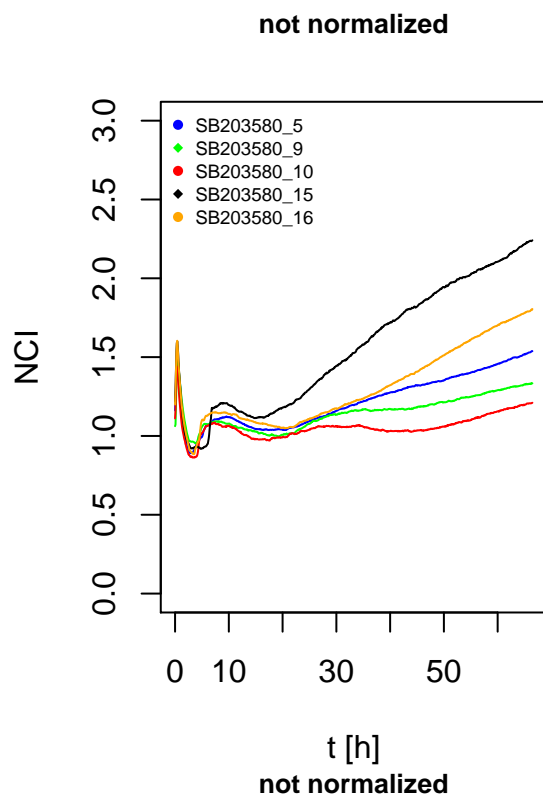


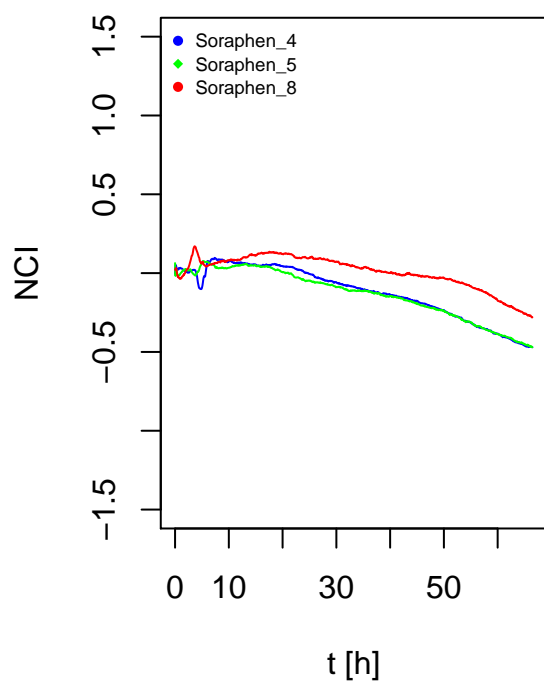
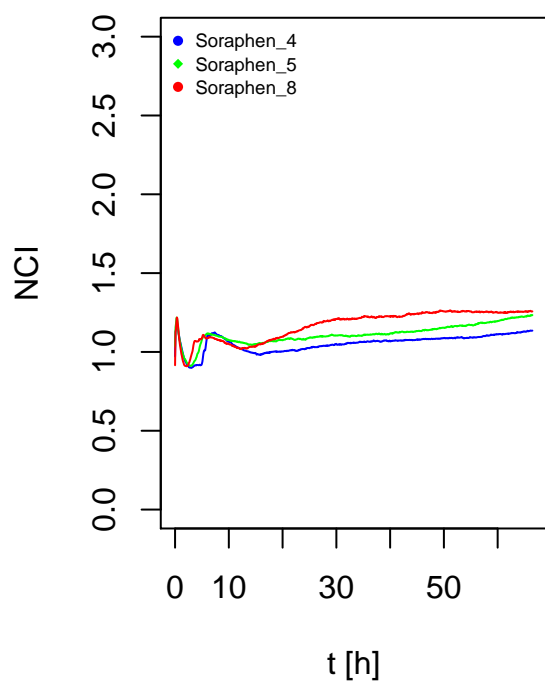
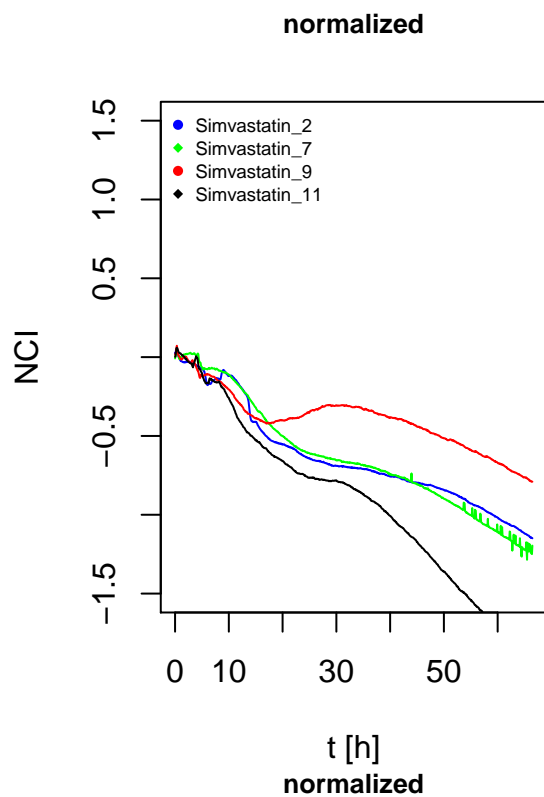
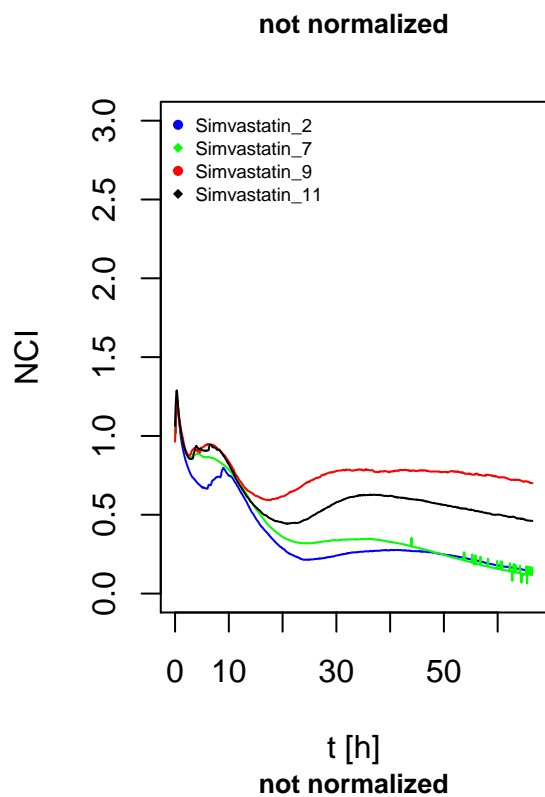


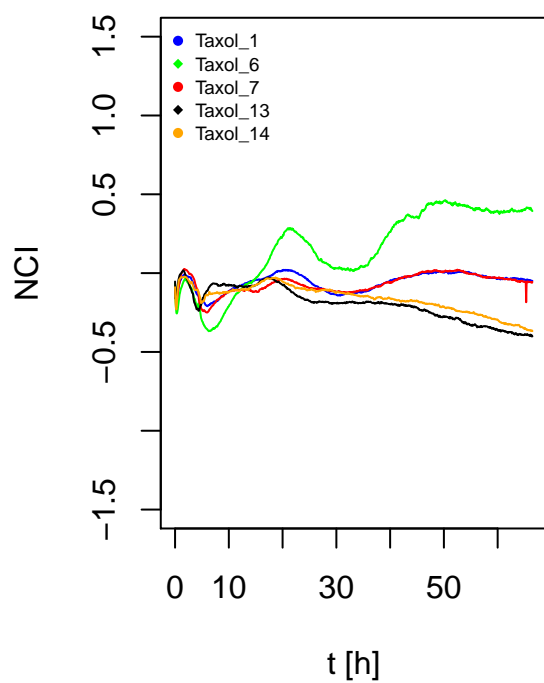
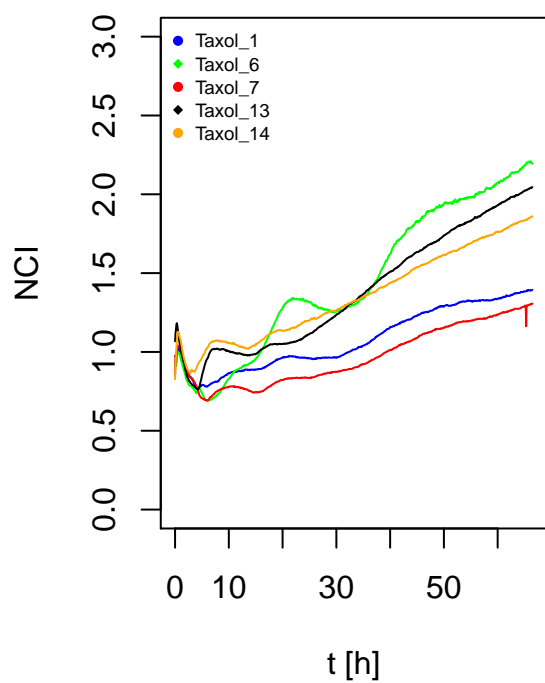
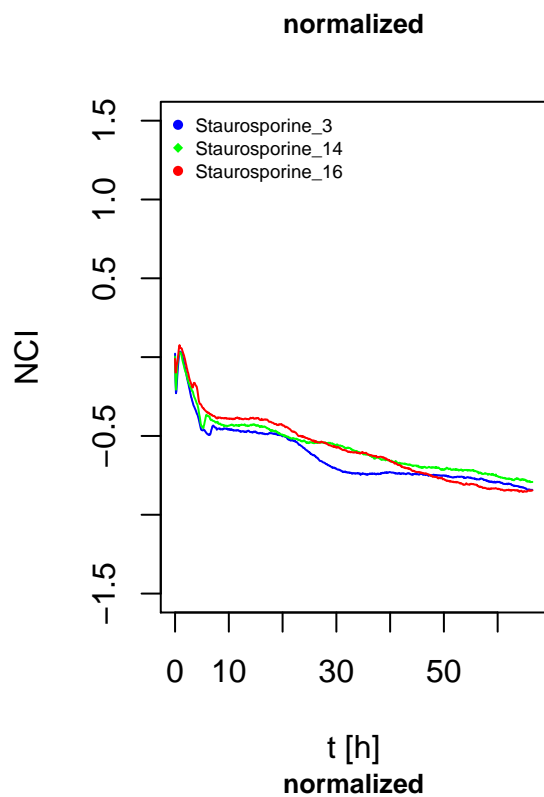
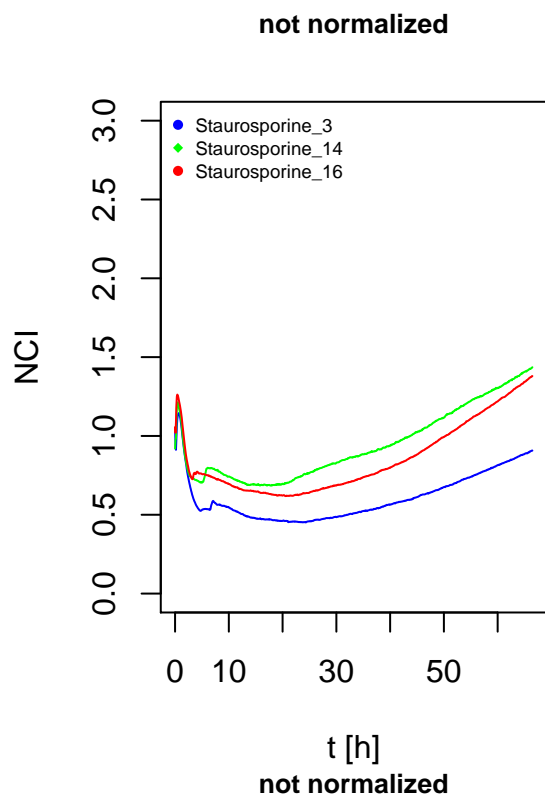


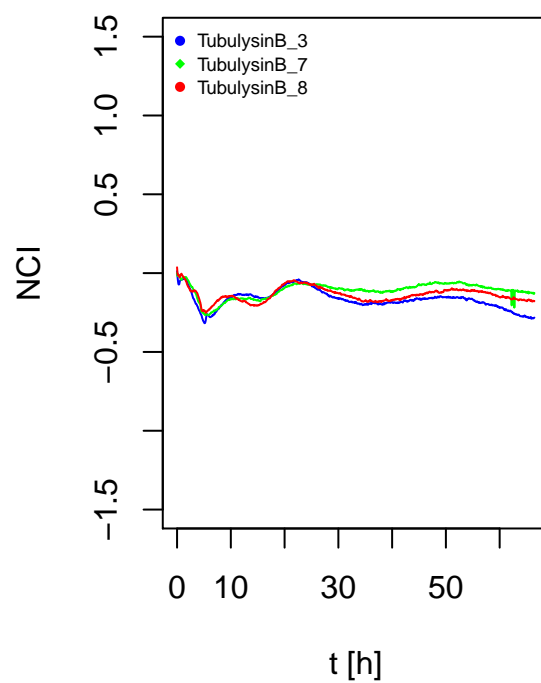
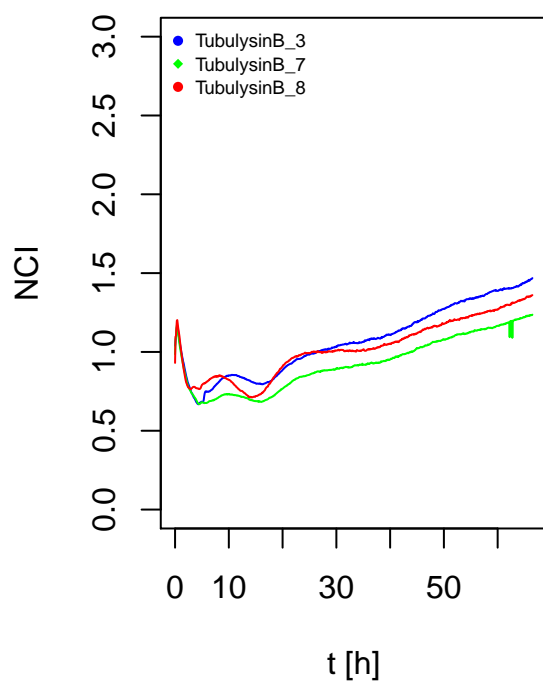
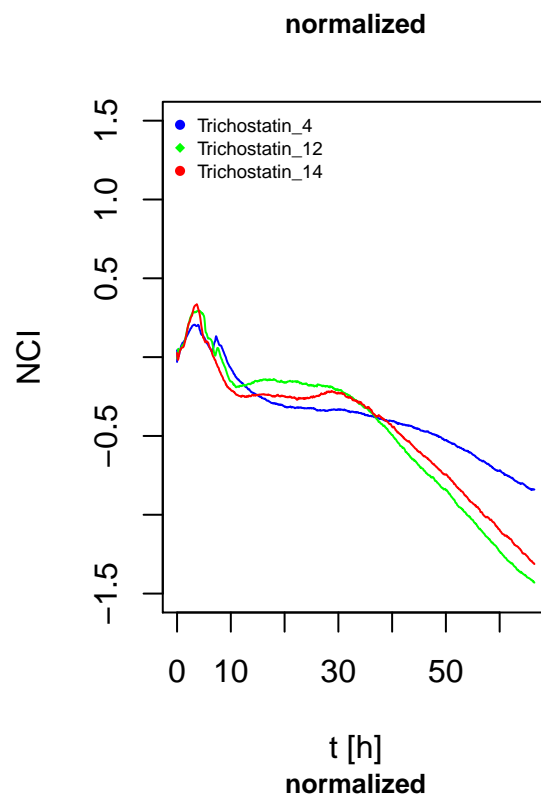
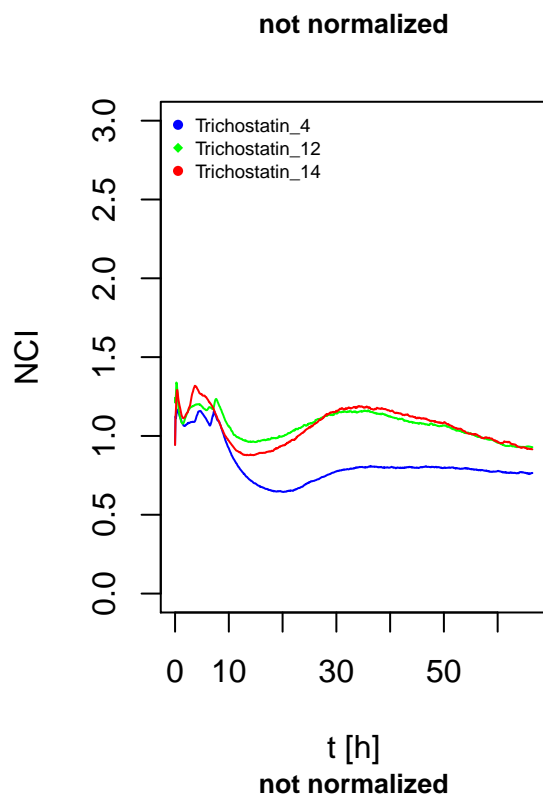


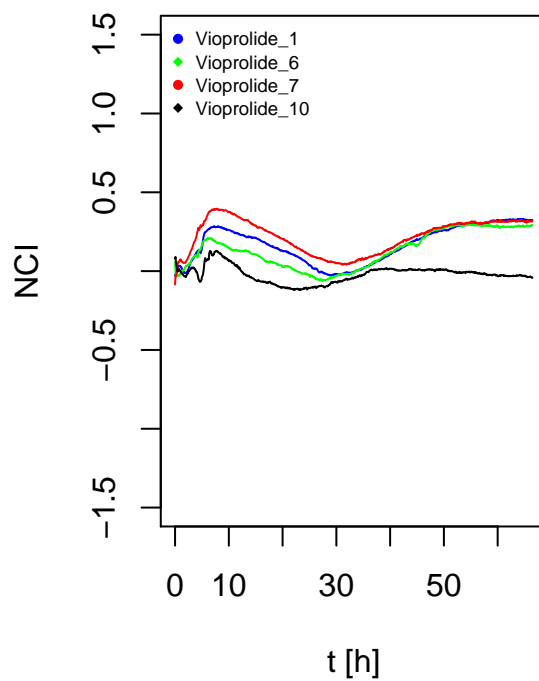
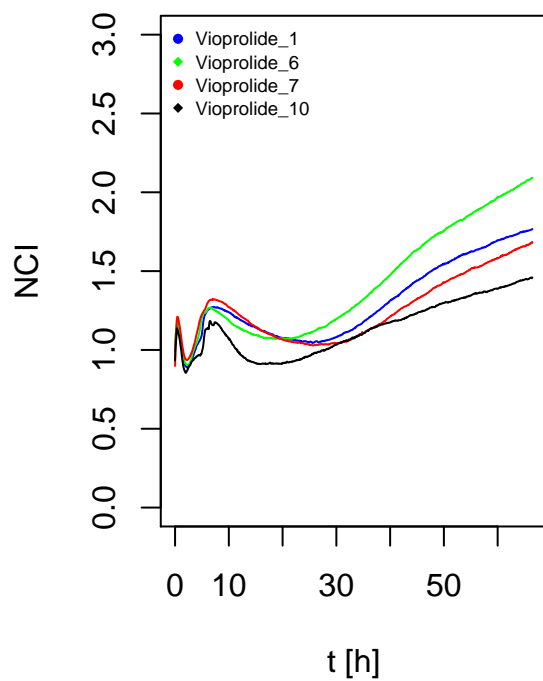
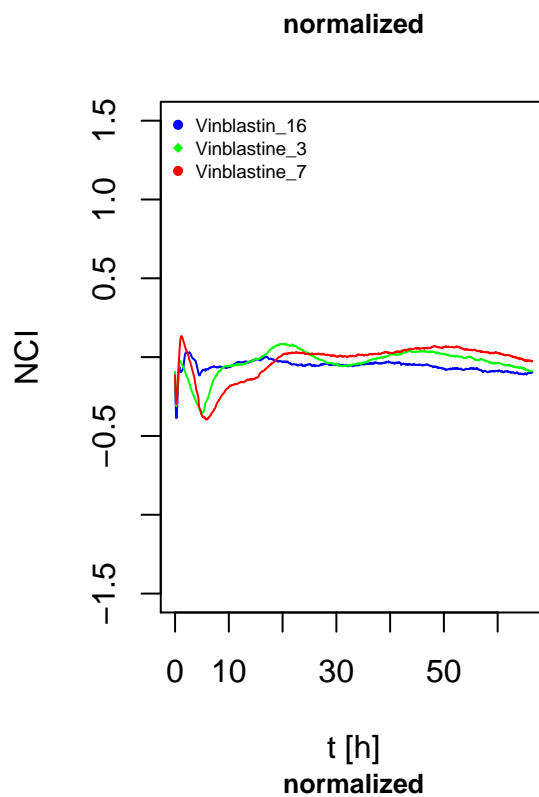
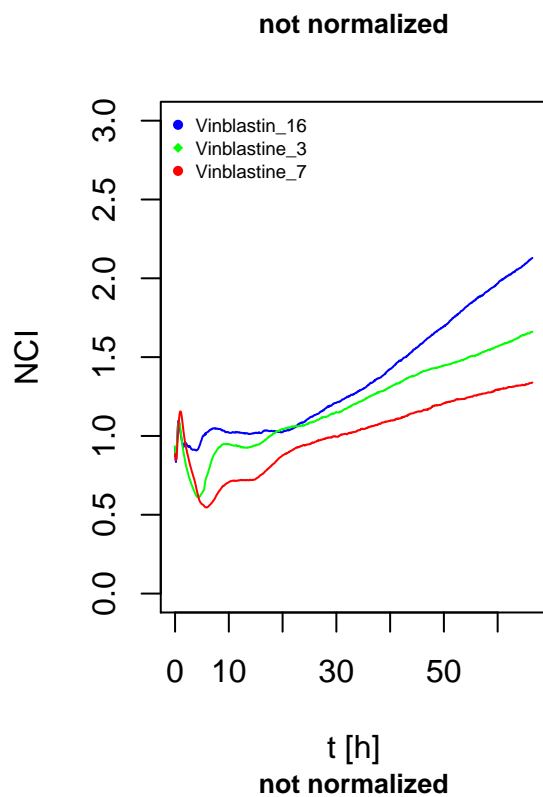


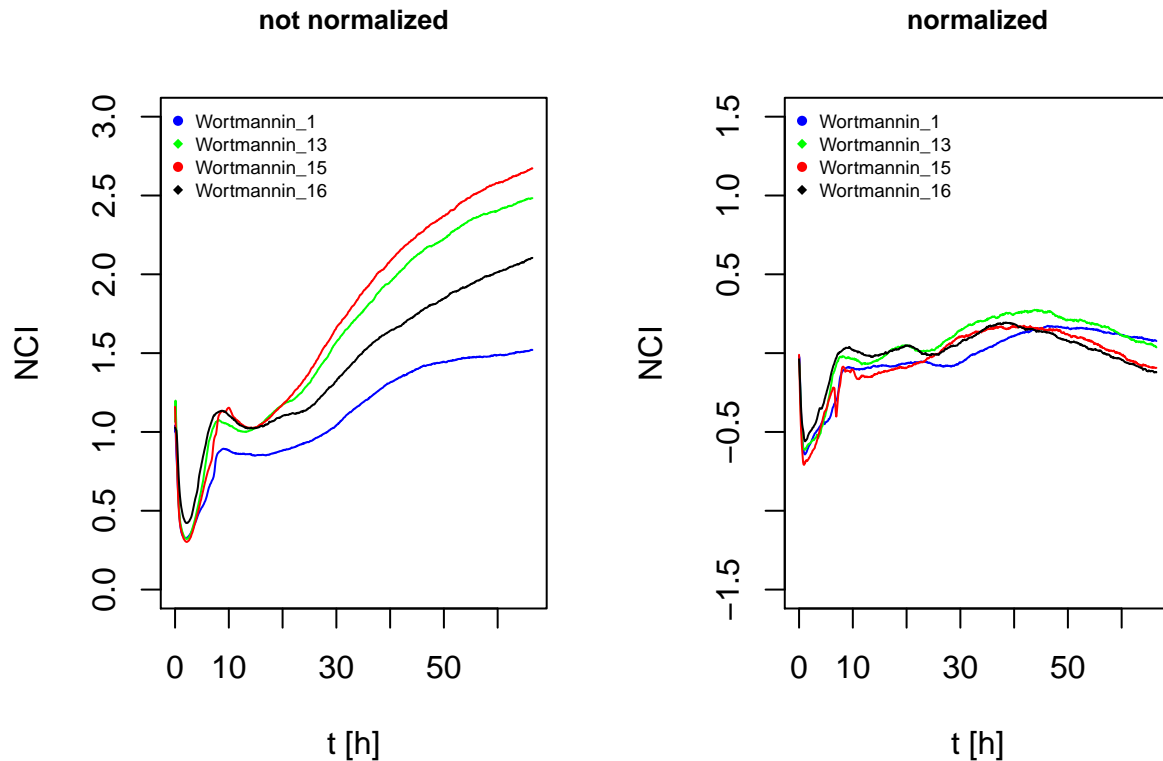












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#dev.off()
```

In the case where more than one biological replicate or one compound was found to be below the threshold, the one that deviates the most is removed from the data.

```
my_outliers_selected <- c("Apiculaire_1", "ArchazolidB_13", "Argyria_4", "Camptothecin_4", "Colchicine_4")
```

```
ma <- match(my_outliers_selected, colnames(median.combined.ordered))
median.combined.edited <- median.combined.ordered[, -ma]
```

```
#calculate cubic smoothing splines
```

```
median.sp.edited<-matrix(ncol=22, nrow=192)
row.names(median.sp.edited)<-newrownames$V1[-ma]
t<-rownames(median.combined.edited)
t<-as.numeric(t)

i<-0
repeat{
  i<-i+1
  temp<-smooth.spline(x=t, y= median.combined.edited[,i], nknots=20)
  median.sp.edited[i,]<-temp$fit$coef
  if (i==192) break
}
```

```
median.sp.edited.scaled <- scale(median.sp.edited, center = FALSE, scale = TRUE)
res <- score1.function(median.sp.edited.scaled, "euclidean")
```

```

euclidean.scaled <- sum(res$normscore)/i
cat(paste0("Euclidean.scaled after removal of outliers: ", round(euclidean.scaled, 3)))

## Euclidean.scaled after removal of outliers: 0.647

group.score <- c()

for(i in 1:length(groupmatch)){

  ma <- grep(groupmatch[i], res$rep)
  gscore <- sum(res$normscore[ma])/length(ma)
  group.score <- c(group.score, gscore)

}

group.result <- data.frame(groupmatch,group.score)
group.result <- group.result[order(-group.result$group.score),]
kable(group.result)

```

	groupmatch	group.score
8	Apicularen	1.0000000
10	ArgyriaA	1.0000000
14	Cerulein	1.0000000
15	Chelerythrine	1.0000000
17	Colchicine	1.0000000
28	H89	1.0000000
30	LY294002	1.0000000
31	Methotrexate	1.0000000
36	Neopeltolide	1.0000000
40	Oxamflatin	1.0000000
48	SaframycinMx1	1.0000000
54	Staurosporine	1.0000000
56	Trichostatin	1.0000000
57	TubulysinB	1.0000000
60	Wortmannin	1.0000000
1	A23187	0.9523810
24	EpothiloneB	0.9523810
19	Cycloheximide	0.9304348
29	Indirubin3monoxime	0.8484848
41	PD169316	0.8484848
2	ActinomycinD	0.8333333
59	Vioprolide	0.8333333
5	Anisomycin	0.8320261
7	Apicidin	0.8055556
20	CyclosporinA	0.7777778
21	Cytochalasin	0.7619048
4	Amanitin	0.7023810
45	Rapamycin	0.6944444
3	Alsterpaullone	0.6835017
42	Podophyllotoxin	0.6631485
51	Scriptaid	0.6395604
50	SB203580	0.6392857
18	CruentarenA	0.6250000
43	Puromycin	0.6110276
16	ChondramidC	0.5865801

	groupmatch	group.score
52	Simvastatin	0.5578866
11	Bortezomib	0.5544890
32	Mevastatin	0.5500000
37	Nocodazol	0.5454981
58	Vinblastin	0.5440476
44	PurvalanolA	0.5438596
38	OkadaicAcid	0.5435235
23	Emetine	0.5158730
12	Camptothecin	0.5142857
47	Rhizopodin	0.4989508
25	Etoposide	0.4779202
33	MG132	0.4687747
49	SB202190	0.3631785
6	Aphidicolin	0.3492424
27	Griseofulvin	0.3425232
53	Soraphen	0.3399933
34	Myriaporone	0.3336412
55	Taxol	0.3334500
35	MyxothiazolA	0.2868851
13	CCCP	0.2359447
22	Doxorubicin	0.1784604
9	ArchazolidB	0.1758621
26	GephyronicAcidA	0.1675484
46	RatjadonC	0.1181932
39	Oligomycin	0.0831636

```
write.csv2(group.result, "group_result_filter.csv")
```

With the improved data the medians of the biological replicates is calculated.

```
#Calculate medians of medians
median.combined.median<-matrix(ncol=60, nrow=800)
colnames(median.combined.median)<-groupmatch
rownames(median.combined.median)<-row.names(median.combined.edited)
i<-0
repeat{
  i<-i+1

  name<-groupmatch[i]
  ma<-grep(groupmatch[i], colnames(median.combined.edited))
  z<-median.combined.edited[,ma]
  median.combined.median[,i]<-apply(z, 1, median)

  if (i==60) break
}

#smoothing splines for median.combined
xmedian.combined<-matrix(ncol=22, nrow=60)
row.names(xmedian.combined)<-colnames(median.combined.median)
t<-rownames(median.combined.median)
t<-as.numeric(t)
```

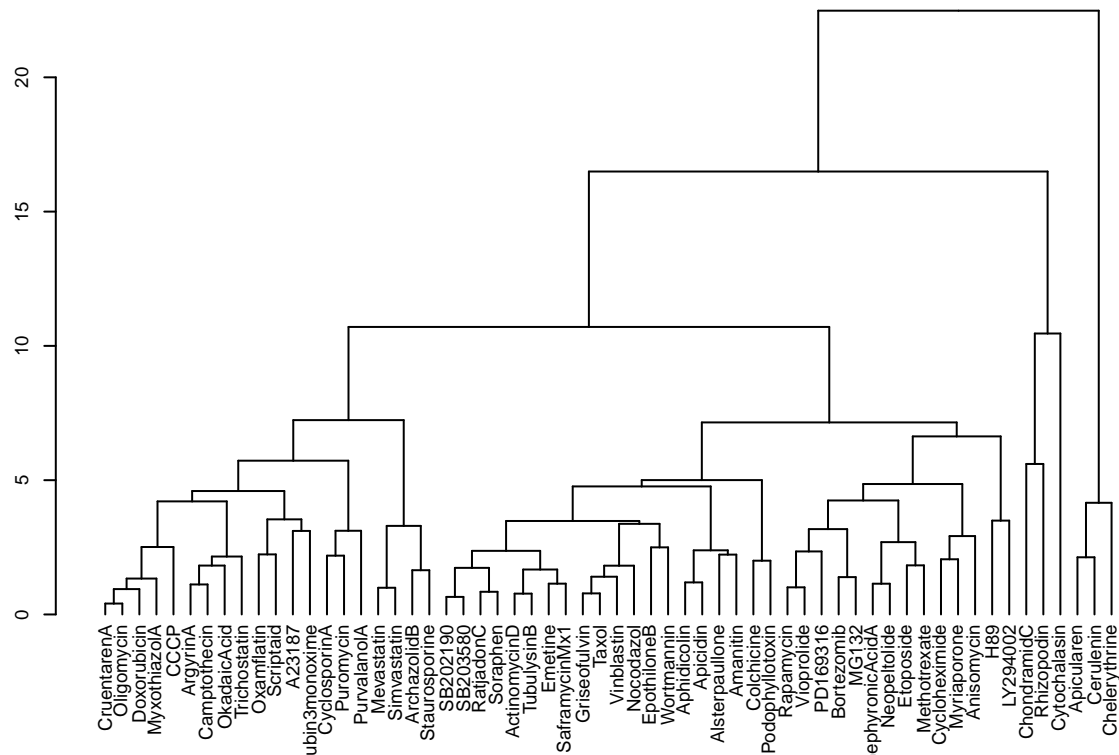
```

i<-0
repeat{
  i<-i+1
  temp<-smooth.spline(x=t, y= median.combined.median[,i], nknots=20)
  xmedian.combined[i,<-temp$fit$coef
  if (i==60) break
}

#Scaling
xmedian.combined.scaled <- scale(xmedian.combined, scale = TRUE, center = FALSE)
colnames(xmedian.combined.scaled) <- c("c1", "c2", "c3", "c4", "c5", "c6", "c7", "c8", "c9",
                                         "c10", "c11", "c12", "c13", "c14", "c15", "c16", "c17",
                                         "c18", "c19", "c20", "c21", "c22")

##distmat and hierarchical clustering
xmedian.combined.distmat <- dist(xmedian.combined.scaled, method = "euclidean")
xmedian.hclust.sorted <- dendsort(hclust(xmedian.combined.distmat, method = "complete"))
par(cex = 0.6)
plot(as.dendrogram(xmedian.hclust.sorted))

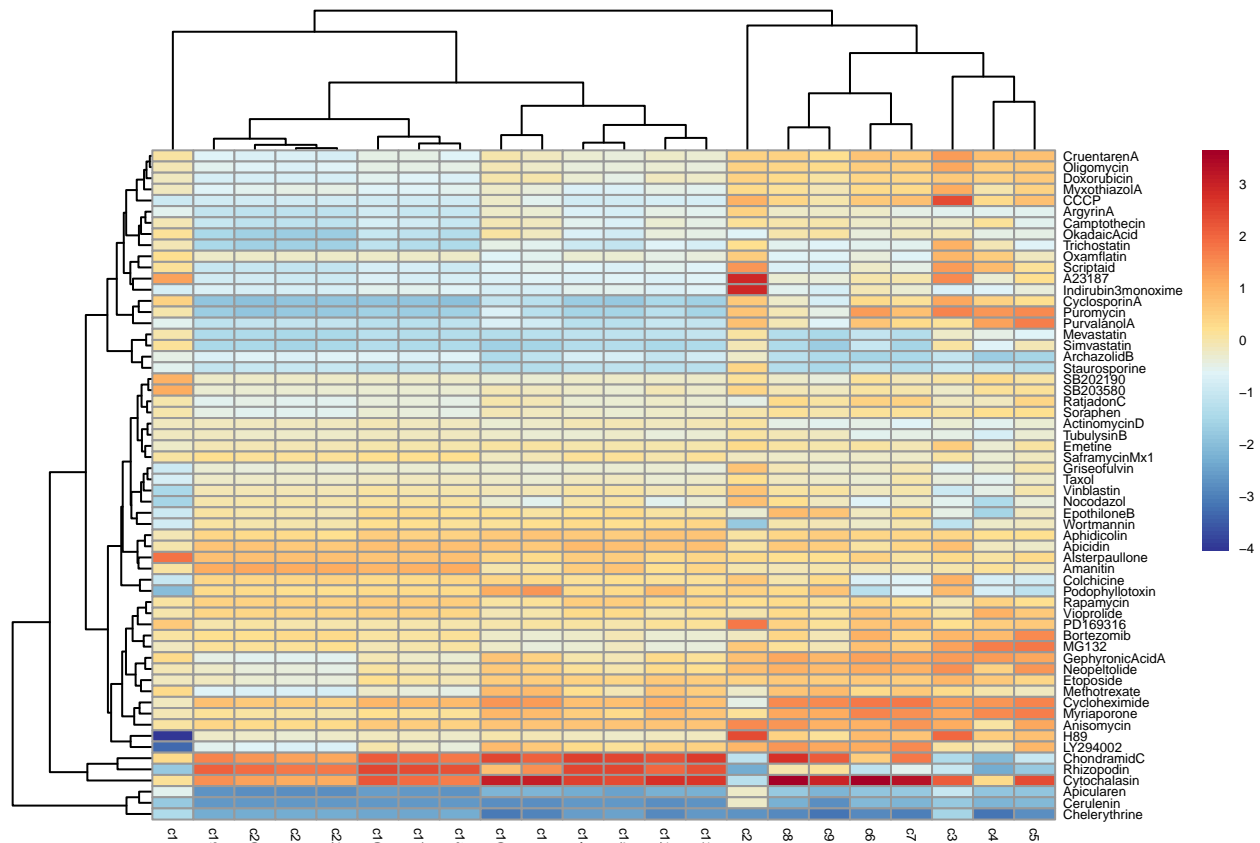
```



```

#heatmap
my_color = colorRampPalette(rev(brewer.pal(n = 10, name = "RdYlBu")))(100)
pheatmap(xmedian.combined.scaled, cluster_rows = xmedian.hclust.sorted, cluster_cols = TRUE,
         color = my_color, fontsize = 5.0)

```



Rank-based MoA prediction

```
xmedian.combined.scaled <- scale(xmedian.combined)
mydistmat <- dist(xmedian.combined.scaled, method = "euclidean")
mydistmat <- as.matrix(mydistmat)
rank.predict <- matrix(ncol=60, nrow=60)
colnames(rank.predict) <- colnames(mydistmat)
rownames(rank.predict) <- c(1:60)

for (i in 1:60){
  mydistmat.ordered <- mydistmat[order(mydistmat[,i]),]
  rank.predict[,i] <- rownames(mydistmat.ordered)
}

rank <- 1:59
rank.predict <- rank.predict[-1,]
rank.predict <- as.data.frame(cbind(rank, rank.predict))

write.csv2(rank.predict, "rankpredict.csv")
rank.predict
```

##	rank	A23187	ActinomycinD	Alsterpauillone
## 2	1	Scriptaid	TubulysinB	Rapamycin
## 3	2	Indirubin3monoxime	Taxol	Amanitin
## 4	3	MyxothiazolA	SaframycinMx1	Apicidin
## 5	4	Oxamflatin	Griseofulvin	Aphidicolin
## 6	5	Oligomycin	Emetine	Vioprolide

## 7	6	CCCP	SB202190	SaframycinMx1
## 8	7	CruentarenA	Soraphen	PD169316
## 9	8	Doxorubicin	Oxamflatin	Emetine
## 10	9	SB203580	SB203580	Bortezomib
## 11	10	Trichostatin	Vinblastin	Anisomycin
## 12	11	SB202190	Nocodazol	SB202190
## 13	12	Camptothecin	RatjadonC	Etoposide
## 14	13	PD169316	Colchicine	SB203580
## 15	14	Soraphen	EpothiloneB	Colchicine
## 16	15	ArgyriaA	MyxothiazolA	ActinomycinD
## 17	16	PurvalanolA	Wortmannin	EpothiloneB
## 18	17	Griseofulvin	Camptothecin	MG132
## 19	18	Emetine	Rapamycin	TubulysinB
## 20	19	CyclosporinA	Doxorubicin	Neopeltolide
## 21	20	TubulysinB	ArgyriaA	Myriaporone
## 22	21	ActinomycinD	Vioprolide	Soraphen
## 23	22	Taxol	Oligomycin	Oxamflatin
## 24	23	RatjadonC	PD169316	Methotrexate
## 25	24	OkadaicAcid	Aphidicolin	RatjadonC
## 26	25	Neopeltolide	Etoposide	Taxol
## 27	26	GephyronicAcidA	Methotrexate	Wortmannin
## 28	27	Puromycin	CruentarenA	Cycloheximide
## 29	28	Mevastatin	Bortezomib	GephyronicAcidA
## 30	29	MG132	ArchazolidB	Vinblastin
## 31	30	Etoposide	Indirubin3monoxime	Oligomycin
## 32	31	SaframycinMx1	Scriptaid	CruentarenA
## 33	32	Methotrexate	Amanitin	Griseofulvin
## 34	33	Simvastatin	Apicidin	MyxothiazolA
## 35	34	Bortezomib	Podophyllotoxin	Doxorubicin
## 36	35	Nocodazol	Alsterpaullone	Nocodazol
## 37	36	Staurosporine	OkadaicAcid	Podophyllotoxin
## 38	37	Vinblastin	MG132	Camptothecin
## 39	38	Colchicine	Staurosporine	A23187
## 40	39	Vioprolide	Trichostatin	Scriptaid
## 41	40	Rapamycin	Neopeltolide	ArgyriaA
## 42	41	ArchazolidB	A23187	Indirubin3monoxime
## 43	42	Anisomycin	Mevastatin	CCCP
## 44	43	EpothiloneB	CCCP	LY294002
## 45	44	Aphidicolin	GephyronicAcidA	OkadaicAcid
## 46	45	Alsterpaullone	PurvalanolA	PurvalanolA
## 47	46	H89	Anisomycin	ArchazolidB
## 48	47	Apicidin	Simvastatin	Trichostatin
## 49	48	Myriaporone	Myriaporone	H89
## 50	49	Podophyllotoxin	LY294002	ChondramidC
## 51	50	LY294002	H89	Staurosporine
## 52	51	Wortmannin	CyclosporinA	Mevastatin
## 53	52	Amanitin	Cycloheximide	Rhizopodin
## 54	53	Cycloheximide	Puromycin	Simvastatin
## 55	54	Apiculin	Rhizopodin	Puromycin
## 56	55	Cerulenin	Apiculin	CyclosporinA
## 57	56	Chelerythrine	ChondramidC	Cytochalasin
## 58	57	ChondramidC	Cerulenin	Apiculin
## 59	58	Rhizopodin	Chelerythrine	Cerulenin
## 60	59	Cytochalasin	Cytochalasin	Chelerythrine

##	Amanitin	Anisomycin	Aphidicolin
## 2	Rapamycin	Neopeltolide	Apicidin
## 3	Apicidin	Myriaporone	Rapamycin
## 4	Alsterpaullone	Aphidicolin	Vioprolide
## 5	Vioprolide	Etoposide	Etoposide
## 6	Aphidicolin	PD169316	Emetine
## 7	SaframycinMx1	Apicidin	SaframycinMx1
## 8	Colchicine	Cycloheximide	Alsterpaullone
## 9	Emetine	Rapamycin	Anisomycin
## 10	EpothiloneB	GephyronicAcidA	Amanitin
## 11	Bortezomib	Vioprolide	PD169316
## 12	Wortmannin	Alsterpaullone	Colchicine
## 13	ActinomycinD	Bortezomib	EpothiloneB
## 14	Vinblastin	Emetine	Neopeltolide
## 15	PD169316	MG132	Methotrexate
## 16	Etoposide	Methotrexate	Bortezomib
## 17	Anisomycin	Amanitin	Myriaporone
## 18	Taxol	EpothiloneB	Vinblastin
## 19	TubulysinB	SaframycinMx1	Wortmannin
## 20	SB202190	Oligomycin	Soraphen
## 21	Nocodazol	Colchicine	Taxol
## 22	Podophyllotoxin	CruentarenA	SB202190
## 23	MG132	Vinblastin	ActinomycinD
## 24	SB203580	Doxorubicin	SB203580
## 25	Oxamflatin	Soraphen	RatjadonC
## 26	Griseofulvin	RatjadonC	GephyronicAcidA
## 27	Soraphen	SB203580	Podophyllotoxin
## 28	RatjadonC	LY294002	TubulysinB
## 29	Cycloheximide	SB202190	Cycloheximide
## 30	Myriaporone	Taxol	MG132
## 31	Neopeltolide	Myxothiazola	Oligomycin
## 32	Methotrexate	Podophyllotoxin	Griseofulvin
## 33	Oligomycin	Griseofulvin	Doxorubicin
## 34	Myxothiazola	TubulysinB	CruentarenA
## 35	Doxorubicin	ActinomycinD	Oxamflatin
## 36	GephyronicAcidA	Nocodazol	Nocodazol
## 37	CruentarenA	Oxamflatin	Myxothiazola
## 38	Camptothecin	Wortmannin	LY294002
## 39	Indirubin3monoxime	H89	Camptothecin
## 40	LY294002	CCCP	ArgyrinA
## 41	ArgyrinA	A23187	Scriptaid
## 42	Scriptaid	Camptothecin	CCCP
## 43	Rhizopodin	Scriptaid	H89
## 44	H89	Indirubin3monoxime	Indirubin3monoxime
## 45	CCCP	ArgyrinA	A23187
## 46	ArchazolidB	Purvalanola	OkadaicAcid
## 47	A23187	OkadaicAcid	Purvalanola
## 48	ChondramidC	Trichostatin	Trichostatin
## 49	OkadaicAcid	ChondramidC	ArchazolidB
## 50	Purvalanola	Cytochalasin	ChondramidC
## 51	Staurosporine	Puromycin	Staurosporine
## 52	Trichostatin	ArchazolidB	Mevastatin
## 53	Mevastatin	Staurosporine	Rhizopodin
## 54	Simvastatin	Mevastatin	Puromycin

## 55	Puromycin	CyclosporinA	Simvastatin
## 56	CyclosporinA	Rhizopodin	CyclosporinA
## 57	Cytochalasin	Simvastatin	Cytochalasin
## 58	Apicularen	Apicularen	Apicularen
## 59	Cerulenin	Cerulenin	Cerulenin
## 60	Chelerythrine	Chelerythrine	Chelerythrine
##	Apicidin	Apicularen	ArchazolidB
## 2	Aphidicolin	Cerulenin	Staurosporine
## 3	Rapamycin	Chelerythrine	Mevastatin
## 4	Amanitin	Simvastatin	Simvastatin
## 5	Alsterpaullone	Mevastatin	ArgyriaA
## 6	Vioprolide	Staurosporine	TubulysinB
## 7	Colchicine	CyclosporinA	ActinomycinD
## 8	SaframycinMx1	Trichostatin	Taxol
## 9	Etoposide	ArchazolidB	Griseofulvin
## 10	Anisomycin	OkadaicAcid	Camptothecin
## 11	Emetine	ArgyriaA	Nocodazol
## 12	EpothiloneB	Camptothecin	Trichostatin
## 13	Podophyllotoxin	Puromycin	Oxamflatin
## 14	PD169316	Scriptaid	Indirubin3monoxime
## 15	Bortezomib	Purvalanola	OkadaicAcid
## 16	Wortmannin	Indirubin3monoxime	SB202190
## 17	Myriaporone	A23187	Soraphen
## 18	Cycloheximide	Griseofulvin	Vinblastin
## 19	Neopeltolide	Myxothiazola	SB203580
## 20	Methotrexate	TubulysinB	SaframycinMx1
## 21	Vinblastin	CCCP	Scriptaid
## 22	ActinomycinD	Oxamflatin	RatjadonC
## 23	Taxol	Soraphen	Myxothiazola
## 24	TubulysinB	ActinomycinD	Emetine
## 25	SB202190	Doxorubicin	Wortmannin
## 26	SB203580	Taxol	EpothiloneB
## 27	Soraphen	RatjadonC	Doxorubicin
## 28	Nocodazol	SB203580	Colchicine
## 29	RatjadonC	SB202190	Oligomycin
## 30	MG132	Oligomycin	A23187
## 31	GephyronicAcidA	Nocodazol	Purvalanola
## 32	Oxamflatin	CruentarenA	CyclosporinA
## 33	Griseofulvin	Vinblastin	CruentarenA
## 34	Oligomycin	Emetine	Methotrexate
## 35	CruentarenA	SaframycinMx1	CCCP
## 36	Doxorubicin	Methotrexate	Rapamycin
## 37	Myxothiazola	Wortmannin	Podophyllotoxin
## 38	LY294002	EpothiloneB	PD169316
## 39	Camptothecin	Colchicine	Vioprolide
## 40	H89	PD169316	Bortezomib
## 41	CCCP	Bortezomib	Apicularen
## 42	ArgyriaA	MG132	Etoposide
## 43	Scriptaid	Etoposide	Aphidicolin
## 44	Indirubin3monoxime	H89	Amanitin
## 45	A23187	GephyronicAcidA	MG132
## 46	ChondramidC	Neopeltolide	Alsterpaullone
## 47	OkadaicAcid	Podophyllotoxin	Apicidin
## 48	Rhizopodin	LY294002	Puromycin

## 49	ArchazolidB	Vioprolide	Cerulenin
## 50	Trichostatin	Rapamycin	Neopeltolide
## 51	Purvalanola	Aphidicolin	GephyronicAcidA
## 52	Staurosporine	Alsterpaullone	Chelerythrine
## 53	Mevastatin	Amanitin	H89
## 54	Cytochalasin	Apicidin	LY294002
## 55	Simvastatin	Myriaporone	Anisomycin
## 56	Puromycin	Anisomycin	Myriaporone
## 57	CyclosporinA	Cycloheximide	Cycloheximide
## 58	Apicularen	Rhizopodin	Rhizopodin
## 59	Cerulenin	ChondramidC	ChondramidC
## 60	Chelerythrine	Cytochalasin	Cytochalasin
##	ArgyriaA	Bortezomib	Camptothecin
## 2	Camptothecin	MG132	ArgyriaA
## 3	OkadaicAcid	Vioprolide	OkadaicAcid
## 4	Trichostatin	Emetine	Soraphen
## 5	Griseofulvin	Rapamycin	Doxorubicin
## 6	Soraphen	Oligomycin	Trichostatin
## 7	Doxorubicin	PD169316	RatjadonC
## 8	Taxol	SB202190	Myxothiazola
## 9	TubulysinB	Neopeltolide	Griseofulvin
## 10	Myxothiazola	CruentarenA	SB203580
## 11	RatjadonC	RatjadonC	Scriptaid
## 12	Scriptaid	Soraphen	Oligomycin
## 13	Mevastatin	Myxothiazola	SB202190
## 14	ActinomycinD	Etoposide	Taxol
## 15	Indirubin3monoxime	SaframycinMx1	TubulysinB
## 16	Staurosporine	Aphidicolin	CruentarenA
## 17	SB203580	SB203580	ActinomycinD
## 18	SB202190	Doxorubicin	Oxamflatin
## 19	Oligomycin	GephyronicAcidA	Methotrexate
## 20	Oxamflatin	Oxamflatin	Emetine
## 21	CruentarenA	Myriaporone	Purvalanola
## 22	Purvalanola	Taxol	Mevastatin
## 23	ArchazolidB	Alsterpaullone	Indirubin3monoxime
## 24	Vinblastin	Griseofulvin	Vinblastin
## 25	Emetine	ActinomycinD	CCCP
## 26	Nocodazol	TubulysinB	Staurosporine
## 27	Simvastatin	Anisomycin	SaframycinMx1
## 28	Methotrexate	Apicidin	Etoposide
## 29	CCCP	Vinblastin	A23187
## 30	A23187	Amanitin	Nocodazol
## 31	SaframycinMx1	Methotrexate	Simvastatin
## 32	CyclosporinA	EpothiloneB	ArchazolidB
## 33	EpothiloneB	Wortmannin	PD169316
## 34	Etoposide	Colchicine	CyclosporinA
## 35	Wortmannin	CCCP	EpothiloneB
## 36	PD169316	Nocodazol	Wortmannin
## 37	Colchicine	Cycloheximide	GephyronicAcidA
## 38	Puromycin	Scriptaid	Neopeltolide
## 39	Neopeltolide	Camptothecin	Bortezomib
## 40	Bortezomib	Purvalanola	Puromycin
## 41	GephyronicAcidA	ArgyriaA	Vioprolide
## 42	Vioprolide	A23187	Colchicine

## 43	Rapamycin	LY294002	MG132
## 44	MG132	Podophyllotoxin	Rapamycin
## 45	Aphidicolin	H89	Aphidicolin
## 46	LY294002	Indirubin3monoxime	LY294002
## 47	Podophyllotoxin	OkadaicAcid	Podophyllotoxin
## 48	H89	Trichostatin	Apicidin
## 49	Apicidin	Puromycin	Alsterpaullone
## 50	Alsterpaullone	ArchazolidB	Myriaporone
## 51	Anisomycin	Mevastatin	Anisomycin
## 52	Myriaporone	Staurosporine	H89
## 53	Amanitin	CyclosporinA	Amanitin
## 54	Apicularen	Simvastatin	Cycloheximide
## 55	Cycloheximide	ChondramidC	Apicularen
## 56	Cerulenin	Rhizopodin	Cerulenin
## 57	Chelerythrine	Cytochalasin	Chelerythrine
## 58	Rhizopodin	Apicularen	ChondramidC
## 59	ChondramidC	Cerulenin	Rhizopodin
## 60	Cytochalasin	Chelerythrine	Cytochalasin
##	CCCP	Cerulenin	Chelerythrine
## 2	Oligomycin	Apicularen	Cerulenin
## 3	Myxothiazola	Chelerythrine	Apicularen
## 4	CruentarenA	Simvastatin	Simvastatin
## 5	Doxorubicin	Staurosporine	Staurosporine
## 6	Scriptaid	Mevastatin	Mevastatin
## 7	Purvalanola	ArchazolidB	ArchazolidB
## 8	Soraphen	CyclosporinA	Trichostatin
## 9	A23187	Trichostatin	CyclosporinA
## 10	Puromycin	ArgyriaA	OkadaicAcid
## 11	Neopeltolide	OkadaicAcid	ArgyriaA
## 12	Trichostatin	Camptothecin	Camptothecin
## 13	Camptothecin	Indirubin3monoxime	Scriptaid
## 14	GephyronicAcidA	Purvalanola	Indirubin3monoxime
## 15	RatjadonC	Puromycin	Purvalanola
## 16	Oxamflatin	Scriptaid	TubulysinB
## 17	MG132	Griseofulvin	Puromycin
## 18	Griseofulvin	TubulysinB	ActinomycinD
## 19	ArgyriaA	A23187	Griseofulvin
## 20	Emetine	Myxothiazola	Taxol
## 21	Bortezomib	Taxol	Oxamflatin
## 22	SB202190	ActinomycinD	Myxothiazola
## 23	Etoposide	Oxamflatin	Nocodazol
## 24	CyclosporinA	CCCP	Soraphen
## 25	Taxol	Soraphen	RatjadonC
## 26	H89	Nocodazol	SB202190
## 27	SB203580	Doxorubicin	A23187
## 28	PD169316	RatjadonC	SB203580
## 29	OkadaicAcid	SB202190	Doxorubicin
## 30	Methotrexate	SB203580	CCCP
## 31	Indirubin3monoxime	Vinblastin	Vinblastin
## 32	TubulysinB	Oligomycin	Wortmannin
## 33	ActinomycinD	CruentarenA	Oligomycin
## 34	Vinblastin	Emetine	SaframycinMx1
## 35	SaframycinMx1	SaframycinMx1	Emetine
## 36	LY294002	Wortmannin	CruentarenA

## 37	Nocodazol	EpothiloneB	EpothiloneB
## 38	Vioprolide	Methotrexate	Colchicine
## 39	Colchicine	Colchicine	Methotrexate
## 40	Mevastatin	H89	Bortezomib
## 41	Myriaporone	Bortezomib	Podophyllotoxin
## 42	EpothiloneB	PD169316	MG132
## 43	Aphidicolin	MG132	PD169316
## 44	Anisomycin	Etoposide	Etoposide
## 45	Simvastatin	Podophyllotoxin	Vioprolide
## 46	Rapamycin	LY294002	Rapamycin
## 47	Staurosporine	Vioprolide	H89
## 48	Podophyllotoxin	Rapamycin	LY294002
## 49	Wortmannin	Neopeltolide	Neopeltolide
## 50	Apicidin	GephyronicAcidA	Aphidicolin
## 51	ArchazolidB	Aphidicolin	GephyronicAcidA
## 52	Alsterpaullone	Amanitin	Amanitin
## 53	Amanitin	Alsterpaullone	Alsterpaullone
## 54	Cycloheximide	Apicidin	Apicidin
## 55	Apicularen	Anisomycin	Myriaporone
## 56	Cerulenin	Myriaporone	Anisomycin
## 57	Chelerythrine	Cycloheximide	Cycloheximide
## 58	ChondramidC	Rhizopodin	Rhizopodin
## 59	Rhizopodin	ChondramidC	ChondramidC
## 60	Cytochalasin	Cytochalasin	Cytochalasin
##	ChondramidC	Colchicine	CruentarenA
## 2	Rhizopodin	Podophyllotoxin	Oligomycin
## 3	Apicidin	Emetine	Doxorubicin
## 4	Cytochalasin	SaframycinMx1	Myxothiazola
## 5	Cycloheximide	Nocodazol	Soraphen
## 6	Aphidicolin	Apicidin	GephyronicAcidA
## 7	Amanitin	EpothiloneB	RatjadonC
## 8	Anisomycin	ActinomycinD	Neopeltolide
## 9	Alsterpaullone	Aphidicolin	CCCP
## 10	EpothiloneB	Taxol	Etoposide
## 11	Rapamycin	Vinblastin	SB202190
## 12	Podophyllotoxin	Rapamycin	SB203580
## 13	Wortmannin	TubulysinB	Emetine
## 14	Myriaporone	Amanitin	MG132
## 15	Vioprolide	Griseofulvin	Scriptaid
## 16	Etoposide	Etoposide	Bortezomib
## 17	Colchicine	Vioprolide	Methotrexate
## 18	SaframycinMx1	Oxamflatin	Oxamflatin
## 19	Methotrexate	Soraphen	PD169316
## 20	Emetine	SB202190	Camptothecin
## 21	Vinblastin	Wortmannin	Griseofulvin
## 22	Neopeltolide	PD169316	Taxol
## 23	PD169316	SB203580	Purvalanola
## 24	LY294002	Alsterpaullone	Vioprolide
## 25	Nocodazol	RatjadonC	TubulysinB
## 26	GephyronicAcidA	Methotrexate	ArgyriaA
## 27	Bortezomib	Myxothiazola	ActinomycinD
## 28	Taxol	Bortezomib	SaframycinMx1
## 29	TubulysinB	Oligomycin	A23187
## 30	ActinomycinD	Anisomycin	Myriaporone

## 31	RatjadonC	Doxorubicin	OkadaicAcid
## 32	SB203580	Neopeltolide	Trichostatin
## 33	SB202190	CruentarenA	Vinblastin
## 34	Soraphen	MG132	Aphidicolin
## 35	Griseofulvin	Camptothecin	Rapamycin
## 36	MG132	ArgyriaA	Anisomycin
## 37	Oligomycin	GephyronicAcidA	EpothiloneB
## 38	Doxorubicin	Indirubin3monoxime	Puromycin
## 39	CruentarenA	Scriptaid	Indirubin3monoxime
## 40	Oxamflatin	Myriaporone	Nocodazol
## 41	MyxothiazolA	H89	Colchicine
## 42	Camptothecin	CCCP	LY294002
## 43	H89	LY294002	Wortmannin
## 44	ArgyriaA	ArchazolidB	Apicidin
## 45	OkadaicAcid	A23187	Alsterpaullone
## 46	Indirubin3monoxime	Cycloheximide	CyclosporinA
## 47	CCCP	OkadaicAcid	H89
## 48	ArchazolidB	Trichostatin	Mevastatin
## 49	A23187	Staurosporine	Podophyllotoxin
## 50	Scriptaid	PurvalanolA	Amanitin
## 51	Trichostatin	Mevastatin	Cycloheximide
## 52	PurvalanolA	Simvastatin	Simvastatin
## 53	Staurosporine	Rhizopodin	Staurosporine
## 54	Mevastatin	CyclosporinA	ArchazolidB
## 55	Simvastatin	Puromycin	Apicularen
## 56	Puromycin	ChondramidC	ChondramidC
## 57	CyclosporinA	Cytochalasin	Rhizopodin
## 58	Apicularen	Apicularen	Cerulenin
## 59	Cerulenin	Cerulenin	Cytochalasin
## 60	Chelerythrine	Chelerythrine	Chelerythrine
##	Cycloheximide	CyclosporinA	Cytochalasin
## 2	Myriaporone	Puromycin	Cycloheximide
## 3	Anisomycin	Trichostatin	ChondramidC
## 4	Aphidicolin	PurvalanolA	Myriaporone
## 5	Apicidin	Simvastatin	Anisomycin
## 6	Neopeltolide	Mevastatin	Apicidin
## 7	Etoposide	Scriptaid	Aphidicolin
## 8	Vioprolide	OkadaicAcid	Neopeltolide
## 9	GephyronicAcidA	Camptothecin	Etoposide
## 10	Rapamycin	ArgyriaA	Alsterpaullone
## 11	Bortezomib	CCCP	GephyronicAcidA
## 12	Alsterpaullone	A23187	Rapamycin
## 13	MG132	MyxothiazolA	Vioprolide
## 14	PD169316	Staurosporine	Amanitin
## 15	Amanitin	Doxorubicin	LY294002
## 16	Methotrexate	CruentarenA	Methotrexate
## 17	Emetine	Oligomycin	Bortezomib
## 18	EpothiloneB	Soraphen	Rhizopodin
## 19	SaframycinMx1	Indirubin3monoxime	EpothiloneB
## 20	LY294002	Oxamflatin	PD169316
## 21	CruentarenA	RatjadonC	Podophyllotoxin
## 22	Oligomycin	SB203580	MG132
## 23	RatjadonC	SB202190	Emetine
## 24	Colchicine	Griseofulvin	Colchicine

## 25	Wortmannin	ArchazolidB	Wortmannin
## 26	Soraphen	Taxol	SaframycinMx1
## 27	Doxorubicin	TubulysinB	CruentarenA
## 28	Podophyllotoxin	Apicularen	Oligomycin
## 29	Vinblastin	ActinomycinD	RatjadonC
## 30	SB202190	Emetine	Vinblastin
## 31	SB203580	Methotrexate	Doxorubicin
## 32	Myxothiazola	GephyronicAcidA	Soraphen
## 33	Cytochalasin	MG132	SB203580
## 34	Taxol	Bortezomib	SB202190
## 35	ActinomycinD	Neopeltolide	H89
## 36	TubulysinB	PD169316	Taxol
## 37	Griseofulvin	Vinblastin	Myxothiazola
## 38	Oxamflatin	Etoposide	ActinomycinD
## 39	H89	Nocodazol	TubulysinB
## 40	Nocodazol	SaframycinMx1	Nocodazol
## 41	CCCP	H89	Griseofulvin
## 42	ChondramidC	Cerulenin	Oxamflatin
## 43	Camptothecin	Vioprolide	CCCP
## 44	Scriptaid	EpothiloneB	Camptothecin
## 45	Purvalanola	Wortmannin	A23187
## 46	ArgyriaA	LY294002	Scriptaid
## 47	A23187	Colchicine	ArgyriaA
## 48	OkadaicAcid	Rapamycin	OkadaicAcid
## 49	Indirubin3monoxime	Aphidicolin	Purvalanola
## 50	Rhizopodin	Myriaporone	Indirubin3monoxime
## 51	Trichostatin	Anisomycin	Trichostatin
## 52	Puromycin	Alsterpaullone	Puromycin
## 53	ArchazolidB	Podophyllotoxin	ArchazolidB
## 54	CyclosporinA	Apicidin	CyclosporinA
## 55	Mevastatin	Chelerythrine	Mevastatin
## 56	Staurosporine	Amanitin	Staurosporine
## 57	Simvastatin	Cycloheximide	Simvastatin
## 58	Apicularen	ChondramidC	Apicularen
## 59	Cerulenin	Rhizopodin	Cerulenin
## 60	Chelerythrine	Cytochalasin	Chelerythrine
##	Doxorubicin	Emetine	EpothiloneB
## 2	Oligomycin	SaframycinMx1	Vinblastin
## 3	CruentarenA	Taxol	Nocodazol
## 4	Soraphen	ActinomycinD	Emetine
## 5	Myxothiazola	Soraphen	Taxol
## 6	RatjadonC	TubulysinB	SaframycinMx1
## 7	Camptothecin	SB202190	TubulysinB
## 8	SB203580	RatjadonC	Wortmannin
## 9	SB202190	Griseofulvin	Colchicine
## 10	Emetine	SB203580	ActinomycinD
## 11	Griseofulvin	Etoposide	Aphidicolin
## 12	Methotrexate	Rapamycin	Rapamycin
## 13	Scriptaid	Vinblastin	RatjadonC
## 14	Etoposide	Oxamflatin	Griseofulvin
## 15	Oxamflatin	Colchicine	Soraphen
## 16	Taxol	Aphidicolin	Apicidin
## 17	Neopeltolide	Vioprolide	Etoposide
## 18	CCCP	Myxothiazola	Methotrexate

## 19	GephyronicAcidA	EpothiloneB	Vioprolide
## 20	ArgyriaA	Oligomycin	Podophyllotoxin
## 21	PD169316	Doxorubicin	SB203580
## 22	TubulysinB	PD169316	SB202190
## 23	ActinomycinD	Bortezomib	Amanitin
## 24	Bortezomib	Nocodazol	PD169316
## 25	PurvalanolaA	Methotrexate	Myxothiazola
## 26	MG132	CruentarenA	Doxorubicin
## 27	OkadaicAcid	Neopeltolide	Bortezomib
## 28	SaframycinMx1	Apicidin	Oligomycin
## 29	Vinblastin	Wortmannin	Neopeltolide
## 30	Trichostatin	MG132	Anisomycin
## 31	Vioprolide	Camptothecin	Oxamflatin
## 32	A23187	Alsterpaullone	Alsterpaullone
## 33	EpothiloneB	Amanitin	CruentarenA
## 34	Aphidicolin	GephyronicAcidA	Camptothecin
## 35	Rapamycin	Podophyllotoxin	ArgyriaA
## 36	Indirubin3monoxime	ArgyriaA	LY294002
## 37	Nocodazol	Anisomycin	GephyronicAcidA
## 38	Myriaporone	Scriptaid	MG132
## 39	Wortmannin	CCCP	Myriaporone
## 40	Colchicine	Myriaporone	Indirubin3monoxime
## 41	LY294002	Indirubin3monoxime	OkadaicAcid
## 42	Anisomycin	A23187	CCCP
## 43	Puromycin	OkadaicAcid	ArchazolidB
## 44	CyclosporinA	LY294002	Cycloheximide
## 45	Apicidin	Trichostatin	Scriptaid
## 46	Mevastatin	PurvalanolaA	H89
## 47	Alsterpaullone	ArchazolidB	Trichostatin
## 48	H89	H89	A23187
## 49	Podophyllotoxin	Cycloheximide	Staurosporine
## 50	Staurosporine	Staurosporine	PurvalanolaA
## 51	Simvastatin	Mevastatin	Mevastatin
## 52	ArchazolidB	Simvastatin	Simvastatin
## 53	Amanitin	Puromycin	CyclosporinA
## 54	Cycloheximide	CyclosporinA	ChondramidC
## 55	Apiculin	Rhizopodin	Puromycin
## 56	ChondramidC	ChondramidC	Rhizopodin
## 57	Cerulenin	Apiculin	Cytochalasin
## 58	Rhizopodin	Cytochalasin	Apiculin
## 59	Cytochalasin	Cerulenin	Cerulenin
## 60	Chelerythrine	Chelerythrine	Chelerythrine
##	Etoposide	GephyronicAcidA	Griseofulvin
## 2	Neopeltolide	Neopeltolide	Taxol
## 3	Aphidicolin	Etoposide	TubulysinB
## 4	Methotrexate	CruentarenA	Vinblastin
## 5	GephyronicAcidA	Myriaporone	ActinomycinD
## 6	Emetine	Oligomycin	Soraphen
## 7	PD169316	Doxorubicin	Nocodazol
## 8	Vioprolide	PD169316	Emetine
## 9	Oligomycin	Methotrexate	RatjadonC
## 10	Rapamycin	MG132	Myxothiazola
## 11	CruentarenA	Bortezomib	SB203580
## 12	Doxorubicin	Anisomycin	SB202190

## 13	Myriaporone	Soraphen	ArgyriaA
## 14	Soraphen	Myxothiazola	Oxamflatin
## 15	Anisomycin	RatjadonC	Doxorubicin
## 16	RatjadonC	Vioprolide	SaframycinMx1
## 17	SaframycinMx1	Emetine	Camptothecin
## 18	Apicidin	Aphidicolin	Oligomycin
## 19	Bortezomib	SB203580	Indirubin3monoxime
## 20	SB203580	SB202190	EpothiloneB
## 21	SB202190	CCCP	CruentareneA
## 22	Myxothiazola	Rapamycin	PD169316
## 23	MG132	Cycloheximide	Colchicine
## 24	Taxol	Oxamflatin	Scriptaid
## 25	EpothiloneB	SaframycinMx1	Wortmannin
## 26	Vinblastin	LY294002	Rapamycin
## 27	Colchicine	Camptothecin	Etoposide
## 28	Griseofulvin	Griseofulvin	Vioprolide
## 29	ActinomycinD	Apicidin	Methotrexate
## 30	Oxamflatin	Taxol	Bortezomib
## 31	TubulysinB	Scriptaid	Aphidicolin
## 32	Alsterpaullone	Alsterpaullone	MG132
## 33	Wortmannin	Vinblastin	OkadaicAcid
## 34	Camptothecin	EpothiloneB	Purvalanola
## 35	LY294002	TubulysinB	ArchazolidB
## 36	Podophyllotoxin	ActinomycinD	CCCP
## 37	Cycloheximide	Purvalanola	Neopeltolide
## 38	Amanitin	A23187	Trichostatin
## 39	Nocodazol	Colchicine	Staurosporine
## 40	CCCP	ArgyriaA	A23187
## 41	Scriptaid	Wortmannin	Podophyllotoxin
## 42	ArgyriaA	OkadaicAcid	GephyronicAcidA
## 43	A23187	H89	Mevastatin
## 44	H89	Nocodazol	Apicidin
## 45	OkadaicAcid	Amanitin	LY294002
## 46	Indirubin3monoxime	Podophyllotoxin	Amanitin
## 47	Purvalanola	Trichostatin	Alsterpaullone
## 48	Trichostatin	Indirubin3monoxime	H89
## 49	Puromycin	Puromycin	Anisomycin
## 50	ArchazolidB	CyclosporinA	Simvastatin
## 51	Mevastatin	Mevastatin	Myriaporone
## 52	Staurosporine	Staurosporine	CyclosporinA
## 53	CyclosporinA	Simvastatin	Puromycin
## 54	Simvastatin	ArchazolidB	Cycloheximide
## 55	ChondramidC	ChondramidC	Apiculin
## 56	Rhizopodin	Cytochalasin	Rhizopodin
## 57	Cytochalasin	Rhizopodin	Cerulenin
## 58	Apiculin	Apiculin	ChondramidC
## 59	Cerulenin	Cerulenin	Chelerythrine
## 60	Chelerythrine	Chelerythrine	Cytochalasin
##	H89	Indirubin3monoxime	LY294002
## 2	LY294002	Griseofulvin	H89
## 3	CCCP	ArgyriaA	Neopeltolide
## 4	Oligomycin	A23187	Etoposide
## 5	Vinblastin	Scriptaid	Vinblastin
## 6	Neopeltolide	Taxol	EpothiloneB

## 7	Cruentarena	Nocodazol	GephyronicAcidA
## 8	MG132	Camptothecin	Methotrexate
## 9	Griseofulvin	TubulysinB	Doxorubicin
## 10	Etoposide	Vinblastin	Myriaporone
## 11	Myxothiazola	ActinomycinD	Oligomycin
## 12	Doxorubicin	Oxamflatin	Anisomycin
## 13	Nocodazol	Soraphen	Griseofulvin
## 14	Emetine	Myxothiazola	Cruentarena
## 15	Taxol	Staurosporine	RatjadonC
## 16	Colchicine	Doxorubicin	Emetine
## 17	GephyronicAcidA	SB203580	Taxol
## 18	Podophyllotoxin	SB202190	Aphidicolin
## 19	PD169316	Emetine	Soraphen
## 20	Bortezomib	Oligomycin	Nocodazol
## 21	Indirubin3monoxime	PD169316	Myxothiazola
## 22	Anisomycin	Trichostatin	Podophyllotoxin
## 23	Soraphen	Purvalanola	PD169316
## 24	Scriptaid	RatjadonC	CCCP
## 25	Vioprolide	Mevastatin	Vioprolide
## 26	Oxamflatin	ArchazolidB	Rapamycin
## 27	RatjadonC	Cruentarena	Bortezomib
## 28	Aphidicolin	CCCP	Colchicine
## 29	Myriaporone	SaframycinMx1	MG132
## 30	EpothiloneB	OkadaicAcid	Wortmannin
## 31	Purvalanola	Simvastatin	Camptothecin
## 32	Rapamycin	Colchicine	TubulysinB
## 33	ActinomycinD	EpothiloneB	SaframycinMx1
## 34	SaframycinMx1	Etoposide	Apicidin
## 35	TubulysinB	Methotrexate	ArgyriaA
## 36	ArgyriaA	MG132	Cycloheximide
## 37	Methotrexate	Rapamycin	ActinomycinD
## 38	Camptothecin	CyclosporinA	SB203580
## 39	A23187	Vioprolide	SB202190
## 40	Apicidin	Bortezomib	Indirubin3monoxime
## 41	SB202190	H89	Purvalanola
## 42	SB203580	Neopeltolide	Oxamflatin
## 43	Trichostatin	GephyronicAcidA	OkadaicAcid
## 44	Wortmannin	Aphidicolin	Scriptaid
## 45	Amanitin	LY294002	Amanitin
## 46	Cycloheximide	Puromycin	Trichostatin
## 47	Puromycin	Wortmannin	A23187
## 48	OkadaicAcid	Podophyllotoxin	Alsterpaullone
## 49	Alsterpaullone	Anisomycin	Puromycin
## 50	Staurosporine	Alsterpaullone	Staurosporine
## 51	CyclosporinA	Apicidin	ArchazolidB
## 52	Mevastatin	Amanitin	CyclosporinA
## 53	ArchazolidB	Myriaporone	Mevastatin
## 54	Simvastatin	Apicularen	Simvastatin
## 55	Rhizopodin	Cycloheximide	ChondramidC
## 56	ChondramidC	Cerulenin	Cytochalasin
## 57	Apicularen	Chelerythrine	Rhizopodin
## 58	Cytochalasin	Rhizopodin	Apicularen
## 59	Cerulenin	ChondramidC	Cerulenin
## 60	Chelerythrine	Cytochalasin	Chelerythrine

##	Methotrexate	Mevastatin	MG132
## 2	Etoposide	Simvastatin	Bortezomib
## 3	RatjadonC	Staurosporine	Vioprolide
## 4	Soraphen	Trichostatin	Oligomycin
## 5	Doxorubicin	ArchazolidB	CruentarenA
## 6	Emetine	ArgyriaA	PD169316
## 7	Neopeltolide	OkadaicAcid	Neopeltolide
## 8	Oligomycin	Camptothecin	GephyronicAcidA
## 9	SB203580	Scriptaid	MyxothiazolA
## 10	CruentarenA	CyclosporinA	Doxorubicin
## 11	GephyronicAcidA	PurvalanolA	Etoposide
## 12	Aphidicolin	Indirubin3monoxime	Emetine
## 13	SB202190	Oxamflatin	SB202190
## 14	Camptothecin	Griseofulvin	Oxamflatin
## 15	MyxothiazolA	MyxothiazolA	Soraphen
## 16	SaframycinMx1	TubulysinB	Rapamycin
## 17	EpothiloneB	ActinomycinD	Myriaporone
## 18	Taxol	Soraphen	SB203580
## 19	PD169316	Taxol	RatjadonC
## 20	TubulysinB	SB202190	Aphidicolin
## 21	ActinomycinD	Doxorubicin	SaframycinMx1
## 22	Griseofulvin	SB203580	CCCP
## 23	Rapamycin	A23187	Griseofulvin
## 24	Vioprolide	RatjadonC	Anisomycin
## 25	Vinblastin	Puromycin	Taxol
## 26	Wortmannin	Apiculanen	ActinomycinD
## 27	Myriaporone	Oligomycin	Vinblastin
## 28	OkadaicAcid	CCCP	Scriptaid
## 29	Apicidin	CruentarenA	Alsterpaullone
## 30	ArgyriaA	Nocodazol	TubulysinB
## 31	Bortezomib	Emetine	PurvalanolA
## 32	Oxamflatin	Vinblastin	Methotrexate
## 33	Anisomycin	SaframycinMx1	Apicidin
## 34	Colchicine	Methotrexate	Amanitin
## 35	Podophyllotoxin	Wortmannin	Colchicine
## 36	Alsterpaullone	Cerulenin	EpothiloneB
## 37	Nocodazol	EpothiloneB	Camptothecin
## 38	MG132	PD169316	Nocodazol
## 39	LY294002	Bortezomib	Cycloheximide
## 40	Scriptaid	Colchicine	A23187
## 41	CCCP	MG132	Wortmannin
## 42	Trichostatin	Etoposide	H89
## 43	Cycloheximide	Vioprolide	ArgyriaA
## 44	Amanitin	Rapamycin	Indirubin3monoxime
## 45	A23187	Neopeltolide	LY294002
## 46	PurvalanolA	GephyronicAcidA	Podophyllotoxin
## 47	Indirubin3monoxime	Chelerythrine	Puromycin
## 48	H89	Aphidicolin	Trichostatin
## 49	Mevastatin	Podophyllotoxin	OkadaicAcid
## 50	ArchazolidB	H89	CyclosporinA
## 51	Puromycin	Alsterpaullone	Mevastatin
## 52	Staurosporine	LY294002	Staurosporine
## 53	CyclosporinA	Amanitin	ArchazolidB
## 54	Simvastatin	Apicidin	Simvastatin

## 55	ChondramidC	Myriaporone	ChondramidC
## 56	Rhizopodin	Anisomycin	Rhizopodin
## 57	Cytochalasin	Cycloheximide	Cytochalasin
## 58	Apicularen	Rhizopodin	Apicularen
## 59	Cerulenin	ChondramidC	Cerulenin
## 60	Chelerythrine	Cytochalasin	Chelerythrine
##	Myriaporone	MyxothiazolA	Neopeltolide
## 2	Neopeltolide	Oligomycin	GephyronicAcidA
## 3	Cycloheximide	Doxorubicin	Etoposide
## 4	GephyronicAcidA	CruentarenA	Myriaporone
## 5	Anisomycin	Soraphen	CruentarenA
## 6	Etoposide	RatjadonC	Oligomycin
## 7	Aphidicolin	SB202190	Anisomycin
## 8	Vioprolide	Oxamflatin	PD169316
## 9	Bortezomib	CCCP	Doxorubicin
## 10	MG132	SB203580	Methotrexate
## 11	PD169316	Emetine	Bortezomib
## 12	Rapamycin	Griseofulvin	MG132
## 13	Methotrexate	Camptothecin	Emetine
## 14	Apicidin	Scriptaid	Aphidicolin
## 15	CruentarenA	Taxol	MyxothiazolA
## 16	Oligomycin	TubulysinB	Vioprolide
## 17	Emetine	ActinomycinD	Soraphen
## 18	Doxorubicin	ArgyriaA	RatjadonC
## 19	Alsterpaullone	Bortezomib	Rapamycin
## 20	RatjadonC	MG132	SB203580
## 21	Soraphen	Neopeltolide	SB202190
## 22	LY294002	Purvalanola	CCCP
## 23	SaframycinMx1	SaframycinMx1	Apicidin
## 24	MyxothiazolA	Etoposide	SaframycinMx1
## 25	SB203580	PD169316	Cycloheximide
## 26	SB202190	Methotrexate	LY294002
## 27	EpothiloneB	GephyronicAcidA	Taxol
## 28	Amanitin	Trichostatin	EpothiloneB
## 29	Vinblastin	Vinblastin	Griseofulvin
## 30	Wortmannin	OkadaicAcid	Oxamflatin
## 31	Taxol	A23187	Vinblastin
## 32	Colchicine	Vioprolide	Alsterpaullone
## 33	Griseofulvin	Nocodazol	Colchicine
## 34	Oxamflatin	EpothiloneB	TubulysinB
## 35	CCCP	Indirubin3monoxime	ActinomycinD
## 36	ActinomycinD	Rapamycin	Camptothecin
## 37	TubulysinB	Colchicine	Scriptaid
## 38	Podophyllotoxin	Aphidicolin	Nocodazol
## 39	H89	Wortmannin	A23187
## 40	Camptothecin	Puromycin	H89
## 41	Nocodazol	Mevastatin	Wortmannin
## 42	Scriptaid	CyclosporinA	Podophyllotoxin
## 43	Purvalanola	Myriaporone	Purvalanola
## 44	ArgyriaA	Anisomycin	Amanitin
## 45	A23187	Staurosporine	ArgyriaA
## 46	OkadaicAcid	Apicidin	OkadaicAcid
## 47	Indirubin3monoxime	Alsterpaullone	Indirubin3monoxime
## 48	Trichostatin	Simvastatin	Trichostatin

## 49	Puromycin	LY294002	Puromycin
## 50	Cytochalasin	ArchazolidB	CyclosporinA
## 51	ChondramidC	H89	Mevastatin
## 52	CyclosporinA	Podophyllotoxin	ArchazolidB
## 53	Mevastatin	Amanitin	Staurosporine
## 54	ArchazolidB	Cycloheximide	Simvastatin
## 55	Staurosporine	Apicularen	ChondramidC
## 56	Simvastatin	Cerulenin	Cytochalasin
## 57	Rhizopodin	ChondramidC	Rhizopodin
## 58	Apicularen	Rhizopodin	Apicularen
## 59	Cerulenin	Chelerythrine	Cerulenin
## 60	Chelerythrine	Cytochalasin	Chelerythrine
##	Nocodazol	OkadaicAcid	Oligomycin
## 2	Vinblastin	Camptothecin	CruentarenA
## 3	Taxol	ArgyriaA	Doxorubicin
## 4	Griseofulvin	Trichostatin	MyxothiazolA
## 5	TubulysinB	Doxorubicin	Soraphen
## 6	ActinomycinD	Soraphen	RatjadonC
## 7	EpothiloneB	RatjadonC	CCCP
## 8	Emetine	Mevastatin	Neopeltolide
## 9	Colchicine	MyxothiazolA	GephyronicAcidA
## 10	SaframycinMx1	Scriptaid	Emetine
## 11	Soraphen	Oligomycin	SB202190
## 12	RatjadonC	SB203580	SB203580
## 13	Oxamflatin	Methotrexate	Etoposide
## 14	Wortmannin	CruentarenA	Oxamflatin
## 15	Rapamycin	Griseofulvin	Bortezomib
## 16	Indirubin3monoxime	TubulysinB	MG132
## 17	SB202190	CyclosporinA	Scriptaid
## 18	SB203580	SB202190	Camptothecin
## 19	Podophyllotoxin	Taxol	PD169316
## 20	MyxothiazolA	Simvastatin	Methotrexate
## 21	ArgyriaA	Staurosporine	Griseofulvin
## 22	Vioprolide	PurvalanolA	Taxol
## 23	Doxorubicin	ActinomycinD	TubulysinB
## 24	Aphidicolin	Oxamflatin	ActinomycinD
## 25	Camptothecin	CCCP	PurvalanolA
## 26	PD169316	Emetine	SaframycinMx1
## 27	Oligomycin	ArchazolidB	Vioprolide
## 28	Etoposide	Indirubin3monoxime	ArgyriaA
## 29	ArchazolidB	Puromycin	Vinblastin
## 30	Amanitin	A23187	A23187
## 31	Apicidin	Vinblastin	Aphidicolin
## 32	Bortezomib	SaframycinMx1	Rapamycin
## 33	Methotrexate	Etoposide	OkadaicAcid
## 34	CruentarenA	Nocodazol	Trichostatin
## 35	Scriptaid	EpothiloneB	Myriaporone
## 36	MG132	Wortmannin	EpothiloneB
## 37	Staurosporine	GephyronicAcidA	Nocodazol
## 38	Neopeltolide	Neopeltolide	Colchicine
## 39	LY294002	PD169316	Indirubin3monoxime
## 40	Alsterpaullone	Bortezomib	Anisomycin
## 41	CCCP	Colchicine	Wortmannin
## 42	OkadaicAcid	Vioprolide	LY294002

## 43	Anisomycin	MG132	Puromycin
## 44	H89	Aphidicolin	Apicidin
## 45	A23187	Rapamycin	Alsterpaullone
## 46	Trichostatin	LY294002	H89
## 47	GephyronicAcidA	Podophyllotoxin	CyclosporinA
## 48	Mevastatin	Myriaporone	Podophyllotoxin
## 49	Purvalanola	Apicidin	Mevastatin
## 50	Myriaporone	Alsterpaullone	Amanitin
## 51	Simvastatin	H89	Staurosporine
## 52	Cycloheximide	Anisomycin	Cycloheximide
## 53	CyclosporinA	Apiculin	Simvastatin
## 54	Puromycin	Amanitin	ArchazolidB
## 55	Rhizopodin	Cycloheximide	Apiculin
## 56	ChondramidC	Cerulenin	ChondramidC
## 57	Apiculin	Chelerythrine	Rhizopodin
## 58	Cerulenin	ChondramidC	Cerulenin
## 59	Chelerythrine	Rhizopodin	Cytochalasin
## 60	Cytochalasin	Cytochalasin	Chelerythrine
##	Oxamflatin	PD169316	Podophyllotoxin
## 2	SB202190	Etoposide	Colchicine
## 3	ActinomycinD	Vioprolide	EpothiloneB
## 4	Soraphen	SB203580	Apicidin
## 5	SB203580	Emetine	Emetine
## 6	Emetine	Rapamycin	Aphidicolin
## 7	Myxothiazola	SB202190	Vinblastin
## 8	TubulysinB	Neopeltolide	Nocodazol
## 9	Taxol	Bortezomib	SaframycinMx1
## 10	SaframycinMx1	Oligomycin	Taxol
## 11	Griseofulvin	MG132	Etoposide
## 12	Scriptaid	GephyronicAcidA	Rapamycin
## 13	Oligomycin	Aphidicolin	ActinomycinD
## 14	Doxorubicin	Soraphen	TubulysinB
## 15	CruentarenA	Anisomycin	Wortmannin
## 16	RatjadonC	CruentarenA	Griseofulvin
## 17	Camptothecin	Doxorubicin	Amanitin
## 18	Bortezomib	SaframycinMx1	Methotrexate
## 19	PD169316	RatjadonC	Vioprolide
## 20	MG132	Myxothiazola	Soraphen
## 21	ArgyriaA	Alsterpaullone	Oxamflatin
## 22	Vioprolide	Oxamflatin	Anisomycin
## 23	Vinblastin	Griseofulvin	RatjadonC
## 24	Colchicine	Taxol	LY294002
## 25	Rapamycin	Methotrexate	Neopeltolide
## 26	Etoposide	Vinblastin	PD169316
## 27	Nocodazol	ActinomycinD	Doxorubicin
## 28	A23187	TubulysinB	SB202190
## 29	Indirubin3monoxime	Myriaporone	SB203580
## 30	CCCP	Apicidin	Oligomycin
## 31	Trichostatin	Colchicine	Myxothiazola
## 32	Methotrexate	EpothiloneB	Alsterpaullone
## 33	Aphidicolin	Amanitin	Bortezomib
## 34	Neopeltolide	Nocodazol	H89
## 35	EpothiloneB	A23187	CruentarenA
## 36	Purvalanola	Scriptaid	Camptothecin

## 37	Wortmannin	Camptothecin	ArgyriaA
## 38	OkadaicAcid	Indirubin3monoxime	GephyronicAcidA
## 39	GephyronicAcidA	CCCP	Myriaporone
## 40	Alsterpaullone	Wortmannin	MG132
## 41	ArchazolidB	ArgyriaA	Indirubin3monoxime
## 42	Mevastatin	Purvalanola	Cycloheximide
## 43	Amanitin	Cycloheximide	CCCP
## 44	Staurosporine	LY294002	Scriptaid
## 45	Apicidin	Podophyllotoxin	OkadaicAcid
## 46	Simvastatin	H89	ArchazolidB
## 47	Podophyllotoxin	OkadaicAcid	Trichostatin
## 48	Anisomycin	Trichostatin	A23187
## 49	Myriaporone	Puromycin	Staurosporine
## 50	CyclosporinA	ArchazolidB	Purvalanola
## 51	H89	Staurosporine	Rhizopodin
## 52	Puromycin	Mevastatin	Mevastatin
## 53	LY294002	CyclosporinA	ChondramidC
## 54	Cycloheximide	Simvastatin	Simvastatin
## 55	Apicularen	ChondramidC	CyclosporinA
## 56	Rhizopodin	Rhizopodin	Puromycin
## 57	Cerulenin	Cytochalasin	Cytochalasin
## 58	ChondramidC	Apicularen	Apicularen
## 59	Chelerythrine	Cerulenin	Cerulenin
## 60	Cytochalasin	Chelerythrine	Chelerythrine
##	Puromycin	Purvalanola	Rapamycin
## 2	CyclosporinA	Puromycin	Vioprolide
## 3	Purvalanola	Scriptaid	Aphidicolin
## 4	CCCP	Doxorubicin	SaframycinMx1
## 5	Scriptaid	Myxothiazola	Apicidin
## 6	Trichostatin	CCCP	Amanitin
## 7	CruentarenA	CruentarenA	Emetine
## 8	Myxothiazola	CyclosporinA	Alsterpaullone
## 9	Doxorubicin	Oligomycin	Etoposide
## 10	Oligomycin	Camptothecin	PD169316
## 11	OkadaicAcid	ArgyriaA	Bortezomib
## 12	Camptothecin	Trichostatin	Colchicine
## 13	A23187	Soraphen	EpothiloneB
## 14	ArgyriaA	RatjadonC	Vinblastin
## 15	Simvastatin	Griseofulvin	SB202190
## 16	Mevastatin	OkadaicAcid	ActinomycinD
## 17	Soraphen	Oxamflatin	Taxol
## 18	RatjadonC	SB203580	SB203580
## 19	Oxamflatin	SB202190	Anisomycin
## 20	GephyronicAcidA	Indirubin3monoxime	Wortmannin
## 21	SB203580	A23187	TubulysinB
## 22	SB202190	MG132	Soraphen
## 23	MG132	Mevastatin	RatjadonC
## 24	Indirubin3monoxime	Simvastatin	MG132
## 25	Griseofulvin	Taxol	Griseofulvin
## 26	Neopeltolide	Bortezomib	Neopeltolide
## 27	Staurosporine	GephyronicAcidA	Oxamflatin
## 28	Bortezomib	TubulysinB	Methotrexate
## 29	Taxol	Emetine	Nocodazol
## 30	Methotrexate	ActinomycinD	Myriaporone

## 31	PD169316	PD169316	Oligomycin
## 32	Emetine	Staurosporine	Doxorubicin
## 33	TubulysinB	Neopeltolide	GephyronicAcidA
## 34	Etoposide	Vinblastin	CruentarenA
## 35	ActinomycinD	Methotrexate	Myxothiazola
## 36	H89	Etoposide	Podophyllotoxin
## 37	Vinblastin	SaframycinMx1	Cycloheximide
## 38	SaframycinMx1	Nocodazol	Camptothecin
## 39	ArchazolidB	Vioprolide	LY294002
## 40	LY294002	H89	ArgyriaA
## 41	Vioprolide	ArchazolidB	Scriptaid
## 42	Nocodazol	LY294002	Indirubin3monoxime
## 43	Myriaporone	Rapamycin	CCCP
## 44	EpothiloneB	EpothiloneB	A23187
## 45	Rapamycin	Wortmannin	H89
## 46	Apicularen	Myriaporone	OkadaicAcid
## 47	Wortmannin	Aphidicolin	Purvalanola
## 48	Aphidicolin	Colchicine	ArchazolidB
## 49	Colchicine	Anisomycin	Trichostatin
## 50	Anisomycin	Alsterpaullone	Staurosporine
## 51	Alsterpaullone	Apicidin	Mevastatin
## 52	Apicidin	Podophyllotoxin	Simvastatin
## 53	Podophyllotoxin	Amanitin	ChondramidC
## 54	Cycloheximide	Cycloheximide	Rhizopodin
## 55	Amanitin	Apicularen	Puromycin
## 56	Cerulenin	Cerulenin	CyclosporinA
## 57	Chelerythrine	Chelerythrine	Cytochalasin
## 58	ChondramidC	ChondramidC	Apicularen
## 59	Cytochalasin	Rhizopodin	Cerulenin
## 60	Rhizopodin	Cytochalasin	Chelerythrine
##	RatjadonC	Rhizopodin	SaframycinMx1
## 2	Soraphen	ChondramidC	Emetine
## 3	Doxorubicin	Amanitin	ActinomycinD
## 4	SB203580	Apicidin	TubulysinB
## 5	Myxothiazola	Podophyllotoxin	Rapamycin
## 6	SB202190	Wortmannin	Taxol
## 7	Oligomycin	Aphidicolin	SB202190
## 8	Emetine	Colchicine	Vioprolide
## 9	Taxol	Rapamycin	Colchicine
## 10	TubulysinB	EpothiloneB	SB203580
## 11	Griseofulvin	Alsterpaullone	Aphidicolin
## 12	CruentarenA	SaframycinMx1	Soraphen
## 13	Methotrexate	Vioprolide	Vinblastin
## 14	Camptothecin	Nocodazol	Oxamflatin
## 15	ActinomycinD	Vinblastin	EpothiloneB
## 16	SaframycinMx1	Cycloheximide	Griseofulvin
## 17	Etoposide	Emetine	Wortmannin
## 18	Vinblastin	Anisomycin	RatjadonC
## 19	Oxamflatin	ActinomycinD	Nocodazol
## 20	Bortezomib	Etoposide	Amanitin
## 21	ArgyriaA	Taxol	Apicidin
## 22	EpothiloneB	TubulysinB	Etoposide
## 23	Wortmannin	Methotrexate	Bortezomib
## 24	Vioprolide	Myriaporone	Alsterpaullone

## 25	PD169316	Bortezomib	PD169316
## 26	Neopeltolide	Griseofulvin	MyxothiazolA
## 27	Rapamycin	PD169316	Methotrexate
## 28	OkadaicAcid	SB202190	Doxorubicin
## 29	GephyronicAcidA	RatjadonC	Oligomycin
## 30	Nocodazol	Soraphen	CruentarenA
## 31	Aphidicolin	SB203580	MG132
## 32	MG132	Oxamflatin	Podophyllotoxin
## 33	Scriptaid	LY294002	Neopeltolide
## 34	CCCP	Neopeltolide	Camptothecin
## 35	PurvalanolA	Cytochalasin	ArgyriaA
## 36	Colchicine	MG132	Anisomycin
## 37	Trichostatin	Oligomycin	GephyronicAcidA
## 38	Indirubin3monoxime	GephyronicAcidA	Scriptaid
## 39	Apicidin	Doxorubicin	Myriaporone
## 40	Myriaporone	MyxothiazolA	Indirubin3monoxime
## 41	Alsterpaullone	ArchazolidB	ArchazolidB
## 42	Anisomycin	CruentarenA	OkadaicAcid
## 43	A23187	H89	CCCP
## 44	LY294002	Camptothecin	A23187
## 45	Amanitin	ArgyriaA	Trichostatin
## 46	Podophyllotoxin	Indirubin3monoxime	LY294002
## 47	ArchazolidB	OkadaicAcid	Cycloheximide
## 48	Mevastatin	Scriptaid	PurvalanolA
## 49	Staurosporine	Staurosporine	Staurosporine
## 50	Puromycin	CCCP	Mevastatin
## 51	Simvastatin	A23187	H89
## 52	CyclosporinA	Trichostatin	Simvastatin
## 53	H89	Mevastatin	CyclosporinA
## 54	Cycloheximide	PurvalanolA	Puromycin
## 55	Apicularen	Simvastatin	Rhizopodin
## 56	ChondramidC	CyclosporinA	ChondramidC
## 57	Rhizopodin	Puromycin	Apicularen
## 58	Cerulenin	Apicularen	Cytochalasin
## 59	Cytochalasin	Chelerythrine	Cerulenin
## 60	Chelerythrine	Cerulenin	Chelerythrine
##	SB202190	SB203580	Scriptaid
## 2	SB203580	SB202190	Trichostatin
## 3	Soraphen	Soraphen	Oxamflatin
## 4	Oxamflatin	RatjadonC	MyxothiazolA
## 5	RatjadonC	TubulysinB	A23187
## 6	ActinomycinD	Emetine	Doxorubicin
## 7	Emetine	ActinomycinD	Camptothecin
## 8	TubulysinB	Oxamflatin	Oligomycin
## 9	SaframycinMx1	Doxorubicin	CruentarenA
## 10	MyxothiazolA	MyxothiazolA	CCCP
## 11	Taxol	SaframycinMx1	ArgyriaA
## 12	Doxorubicin	Taxol	PurvalanolA
## 13	Oligomycin	Griseofulvin	Soraphen
## 14	Griseofulvin	Oligomycin	SB202190
## 15	CruentarenA	PD169316	SB203580
## 16	PD169316	Camptothecin	Griseofulvin
## 17	Bortezomib	CruentarenA	Indirubin3monoxime
## 18	Camptothecin	Methotrexate	OkadaicAcid

## 19	Vioprolide	Etoposide	Mevastatin
## 20	Rapamycin	Vioprolide	RatjadonC
## 21	Etoposide	Bortezomib	CyclosporinA
## 22	Methotrexate	Rapamycin	ActinomycinD
## 23	Vinblastin	ArgyriaA	Taxol
## 24	Scriptaid	Vinblastin	Emetine
## 25	MG132	Scriptaid	TubulysinB
## 26	ArgyriaA	Aphidicolin	Puromycin
## 27	Aphidicolin	MG132	Simvastatin
## 28	Alsterpaullone	Neopeltolide	PD169316
## 29	Wortmannin	EpothiloneB	MG132
## 30	EpothiloneB	GephyronicAcidA	Staurosporine
## 31	Nocodazol	Alsterpaullone	Etoposide
## 32	Neopeltolide	Nocodazol	SaframycinMx1
## 33	GephyronicAcidA	Wortmannin	Methotrexate
## 34	Colchicine	OkadaicAcid	GephyronicAcidA
## 35	A23187	A23187	Bortezomib
## 36	OkadaicAcid	Colchicine	Neopeltolide
## 37	Indirubin3monoxime	Indirubin3monoxime	Vinblastin
## 38	Apicidin	Purvalanola	Nocodazol
## 39	Purvalanola	Trichostatin	ArchazolidB
## 40	Amanitin	Apicidin	Vioprolide
## 41	CCCP	CCCP	Colchicine
## 42	Trichostatin	Amanitin	Rapamycin
## 43	Anisomycin	Anisomycin	Aphidicolin
## 44	Myriaporone	Myriaporone	EpothiloneB
## 45	ArchazolidB	ArchazolidB	H89
## 46	Mevastatin	Mevastatin	Wortmannin
## 47	Staurosporine	Staurosporine	Podophyllotoxin
## 48	Podophyllotoxin	Podophyllotoxin	Myriaporone
## 49	Simvastatin	Simvastatin	Alsterpaullone
## 50	CyclosporinA	CyclosporinA	Anisomycin
## 51	Puromycin	LY294002	LY294002
## 52	LY294002	Puromycin	Apicidin
## 53	Cycloheximide	Cycloheximide	Amanitin
## 54	H89	H89	Cycloheximide
## 55	Apicularen	Apicularen	Apicularen
## 56	ChondramidC	ChondramidC	Cerulenin
## 57	Rhizopodin	Rhizopodin	Chelerythrine
## 58	Cerulenin	Cerulenin	Rhizopodin
## 59	Chelerythrine	Cytochalasin	ChondramidC
## 60	Cytochalasin	Chelerythrine	Cytochalasin
##	Simvastatin	Soraphen	Staurosporine
## 2	Mevastatin	RatjadonC	Mevastatin
## 3	Staurosporine	Doxorubicin	ArchazolidB
## 4	Trichostatin	SB203580	Simvastatin
## 5	ArchazolidB	SB202190	ArgyriaA
## 6	CyclosporinA	Myxothiazola	Trichostatin
## 7	ArgyriaA	Oligomycin	Camptothecin
## 8	Scriptaid	Emetine	Indirubin3monoxime
## 9	OkadaicAcid	Taxol	OkadaicAcid
## 10	Camptothecin	Griseofulvin	Griseofulvin
## 11	Purvalanola	TubulysinB	TubulysinB
## 12	Oxamflatin	CruentarenA	ActinomycinD

## 13	Indirubin3monoxime	ActinomycinD	Scriptaid
## 14	MyxothiazolA	Camptothecin	Taxol
## 15	Apicularen	Oxamflatin	Oxamflatin
## 16	Griseofulvin	SaframycinMx1	CyclosporinA
## 17	Puromycin	Methotrexate	Soraphen
## 18	A23187	ArgyriaA	Nocodazol
## 19	TubulysinB	Etoposide	MyxothiazolA
## 20	ActinomycinD	Vinblastin	SB202190
## 21	Soraphen	PD169316	SB203580
## 22	SB202190	Bortezomib	PurvalanolA
## 23	Doxorubicin	Vioprolide	RatjadonC
## 24	Taxol	Scriptaid	Doxorubicin
## 25	SB203580	EpothiloneB	Vinblastin
## 26	RatjadonC	Neopeltolide	A23187
## 27	CCCP	Rapamycin	Emetine
## 28	Oligomycin	Nocodazol	SaframycinMx1
## 29	CruentarenA	OkadaicAcid	Apicularen
## 30	Nocodazol	GephyronicAcidA	Oligomycin
## 31	Emetine	MG132	CCCP
## 32	Cerulenin	Wortmannin	CruentarenA
## 33	SaframycinMx1	Aphidicolin	Wortmannin
## 34	Vinblastin	CCCP	EpothiloneB
## 35	Methotrexate	PurvalanolA	Puromycin
## 36	Bortezomib	Colchicine	Colchicine
## 37	Wortmannin	Trichostatin	Cerulenin
## 38	MG132	Indirubin3monoxime	Methotrexate
## 39	PD169316	A23187	PD169316
## 40	EpothiloneB	Apicidin	Bortezomib
## 41	Colchicine	Alsterpaullone	Rapamycin
## 42	Chelerythrine	Myriaporone	Etoposide
## 43	Etoposide	Anisomycin	MG132
## 44	Vioprolide	Mevastatin	Vioprolide
## 45	Neopeltolide	Amanitin	Podophyllotoxin
## 46	GephyronicAcidA	Podophyllotoxin	Aphidicolin
## 47	Rapamycin	ArchazolidB	Chelerythrine
## 48	Aphidicolin	LY294002	Neopeltolide
## 49	H89	Staurosporine	GephyronicAcidA
## 50	Podophyllotoxin	Simvastatin	H89
## 51	Alsterpaullone	Puromycin	Amanitin
## 52	LY294002	CyclosporinA	Alsterpaullone
## 53	Amanitin	H89	LY294002
## 54	Apicidin	Cycloheximide	Apicidin
## 55	Myriaporone	Apicularen	Anisomycin
## 56	Anisomycin	ChondramidC	Myriaporone
## 57	Cycloheximide	Rhizopodin	Cycloheximide
## 58	Rhizopodin	Cerulenin	Rhizopodin
## 59	ChondramidC	Chelerythrine	ChondramidC
## 60	Cytochalasin	Cytochalasin	Cytochalasin
##	Taxol	Trichostatin	TubulysinB
## 2	Griseofulvin	OkadaicAcid	ActinomycinD
## 3	TubulysinB	Camptothecin	Taxol
## 4	ActinomycinD	ArgyriaA	Griseofulvin
## 5	Vinblastin	Scriptaid	SaframycinMx1
## 6	Emetine	Mevastatin	Emetine

## 7	Nocodazol	CyclosporinA	Soraphen
## 8	Soraphen	Simvastatin	SB202190
## 9	SaframycinMx1	Myxothiazola	Nocodazol
## 10	RatjadonC	Doxorubicin	SB203580
## 11	SB202190	Staurosporine	Vinblastin
## 12	SB203580	Purvalanola	RatjadonC
## 13	EpothiloneB	CCCP	Oxamflatin
## 14	Oxamflatin	Soraphen	EpothiloneB
## 15	Myxothiazola	Oligomycin	Myxothiazola
## 16	Doxorubicin	Oxamflatin	Camptothecin
## 17	Camptothecin	CruentarenA	ArgyriaA
## 18	ArgyriaA	A23187	Wortmannin
## 19	Colchicine	Puromycin	Doxorubicin
## 20	Wortmannin	RatjadonC	Colchicine
## 21	Oligomycin	Griseofulvin	Rapamycin
## 22	Rapamycin	SB203580	Oligomycin
## 23	Vioprolide	SB202190	Vioprolide
## 24	Etoposide	Indirubin3monoxime	Methotrexate
## 25	CruentarenA	TubulysinB	PD169316
## 26	PD169316	Taxol	CruentarenA
## 27	Methotrexate	ActinomycinD	Etoposide
## 28	Aphidicolin	ArchazolidB	Aphidicolin
## 29	Indirubin3monoxime	Emetine	Bortezomib
## 30	Bortezomib	Methotrexate	ArchazolidB
## 31	Scriptaid	Vinblastin	Indirubin3monoxime
## 32	Podophyllotoxin	SaframycinMx1	Scriptaid
## 33	MG132	Nocodazol	OkadaicAcid
## 34	ArchazolidB	Etoposide	Amanitin
## 35	Neopeltolide	GephyronicAcidA	Apicidin
## 36	OkadaicAcid	Neopeltolide	Podophyllotoxin
## 37	Apicidin	PD169316	Staurosporine
## 38	Amanitin	Bortezomib	Alsterpaullone
## 39	CCCP	MG132	MG132
## 40	Trichostatin	EpothiloneB	Neopeltolide
## 41	Staurosporine	Colchicine	Trichostatin
## 42	GephyronicAcidA	Wortmannin	A23187
## 43	Alsterpaullone	Vioprolide	Mevastatin
## 44	Purvalanola	Rapamycin	CCCP
## 45	A23187	Apicularen	GephyronicAcidA
## 46	LY294002	Aphidicolin	Purvalanola
## 47	Mevastatin	Podophyllotoxin	Anisomycin
## 48	Anisomycin	H89	Simvastatin
## 49	Myriaporone	LY294002	LY294002
## 50	H89	Myriaporone	Myriaporone
## 51	Simvastatin	Apicidin	H89
## 52	CyclosporinA	Alsterpaullone	CyclosporinA
## 53	Cycloheximide	Anisomycin	Puromycin
## 54	Puromycin	Amanitin	Cycloheximide
## 55	Rhizopodin	Cerulenin	Rhizopodin
## 56	Apicularen	Cycloheximide	Apicularen
## 57	ChondramidC	Chelerythrine	ChondramidC
## 58	Cerulenin	Rhizopodin	Cerulenin
## 59	Chelerythrine	ChondramidC	Chelerythrine
## 60	Cytochalasin	Cytochalasin	Cytochalasin

##	Vinblastin	Vioprolide	Wortmannin
## 2	Taxol	Rapamycin	SaframycinMx1
## 3	Nocodazol	Aphidicolin	EpothiloneB
## 4	Griseofulvin	Bortezomib	Taxol
## 5	TubulysinB	SaframycinMx1	ActinomycinD
## 6	ActinomycinD	Emetine	TubulysinB
## 7	Emetine	PD169316	Vinblastin
## 8	EpothiloneB	Etoposide	Emetine
## 9	SaframycinMx1	MG132	RatjadonC
## 10	Soraphen	Amanitin	Rapamycin
## 11	RatjadonC	Apicidin	Aphidicolin
## 12	Colchicine	Alsterpaullone	Soraphen
## 13	Rapamycin	SB202190	Vioprolide
## 14	Wortmannin	Soraphen	Griseofulvin
## 15	Vioprolide	SB203580	Nocodazol
## 16	SB203580	RatjadonC	SB202190
## 17	SB202190	Neopeltolide	Methotrexate
## 18	Aphidicolin	Vinblastin	SB203580
## 19	Etoposide	Taxol	Colchicine
## 20	Doxorubicin	Anisomycin	Apicidin
## 21	PD169316	Myriaporone	Amanitin
## 22	Oxamflatin	ActinomycinD	Etoposide
## 23	Myxothiazola	EpothiloneB	Bortezomib
## 24	Oligomycin	Wortmannin	Oxamflatin
## 25	ArgyriaA	Oligomycin	Podophyllotoxin
## 26	Podophyllotoxin	Oxamflatin	Doxorubicin
## 27	Methotrexate	TubulysinB	Camptothecin
## 28	Camptothecin	Colchicine	Myxothiazola
## 29	Indirubin3monoxime	GephyronicAcidA	Alsterpaullone
## 30	Bortezomib	Griseofulvin	Oligomycin
## 31	Apicidin	CruentarenaA	ArgyriaA
## 32	CruentarenaA	Doxorubicin	PD169316
## 33	Amanitin	Methotrexate	CruentarenaA
## 34	LY294002	Myxothiazola	Neopeltolide
## 35	Neopeltolide	Nocodazol	MG132
## 36	MG132	Cycloheximide	OkadaicAcid
## 37	Anisomycin	Podophyllotoxin	Myriaporone
## 38	Scriptaid	Camptothecin	GephyronicAcidA
## 39	Alsterpaullone	Scriptaid	ArchazolidB
## 40	GephyronicAcidA	LY294002	Anisomycin
## 41	ArchazolidB	CCCP	LY294002
## 42	H89	ArgyriaA	Scriptaid
## 43	CCCP	Indirubin3monoxime	Cycloheximide
## 44	OkadaicAcid	Purvalanola	Indirubin3monoxime
## 45	Myriaporone	H89	Trichostatin
## 46	Purvalanola	A23187	Staurosporine
## 47	Staurosporine	OkadaicAcid	CCCP
## 48	A23187	Trichostatin	Purvalanola
## 49	Trichostatin	ArchazolidB	Mevastatin
## 50	Mevastatin	Staurosporine	H89
## 51	Cycloheximide	Mevastatin	A23187
## 52	Simvastatin	Puromycin	Simvastatin
## 53	CyclosporinA	Simvastatin	Rhizopodin
## 54	Puromycin	CyclosporinA	CyclosporinA

## 55	Rhizopodin	ChondramidC	Puromycin
## 56	ChondramidC	Rhizopodin	ChondramidC
## 57	Apicularen	Cytochalasin	Apicularen
## 58	Cerulenin	Apicularen	Cytochalasin
## 59	Cytochalasin	Cerulenin	Cerulenin
## 60	Chelerythrine	Chelerythrine	Chelerythrine

DMSO pilot test for figure 1

```
#working directory
setwd("./DMSO_test/")

#compounds
DMSO_test.raw<-read.csv2(file="DMSO_test_raw.csv", header=T)

#####
#Normalization
x<-as.matrix(DMSO_test.raw[,2:97])
norm<-x[1,]
norm<-as.vector(norm)
DMSO_test.norm<-x/rep(norm, each = nrow(x))
DMSO_test.norm<-DMSO_test.norm[2:163,] #remove first row (last measurement before compound addition)

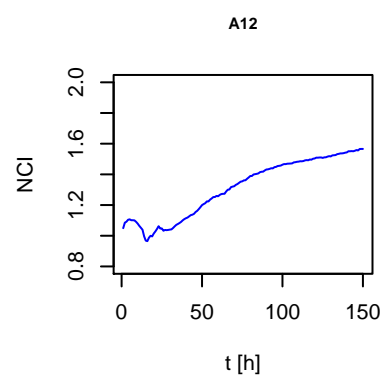
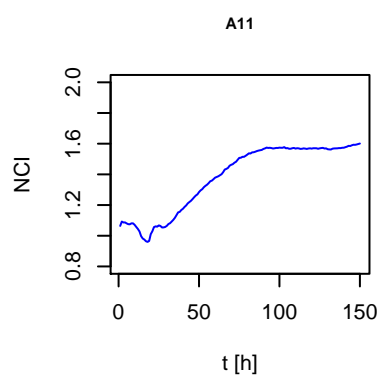
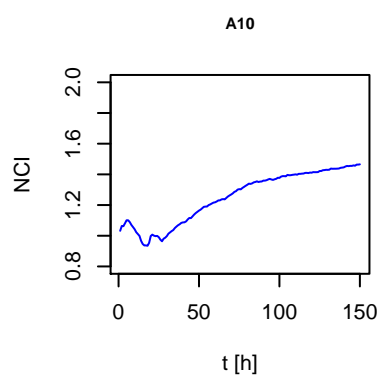
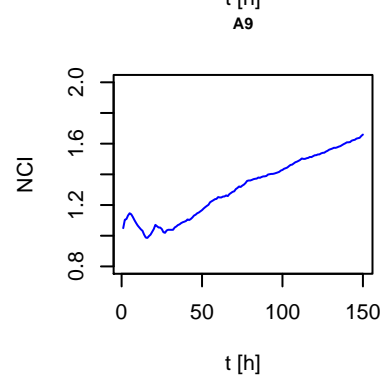
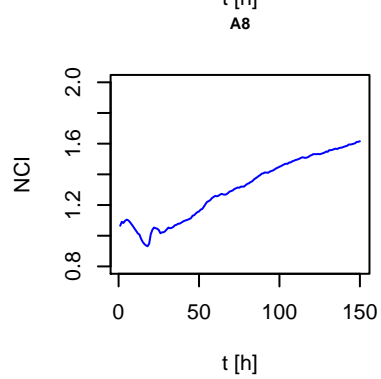
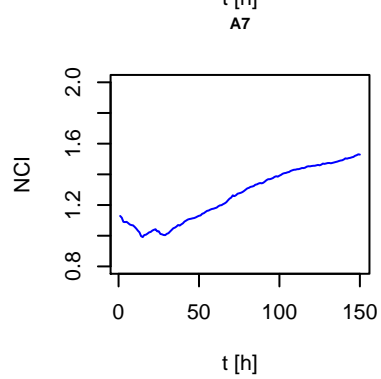
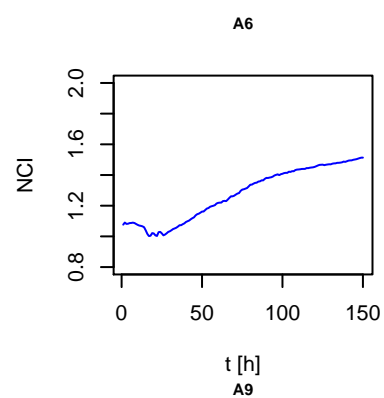
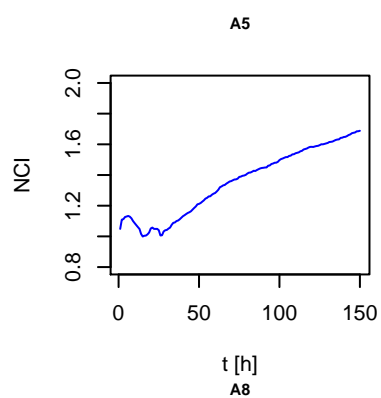
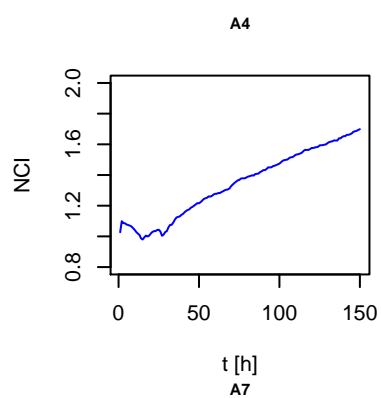
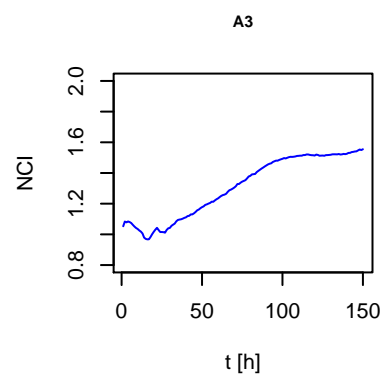
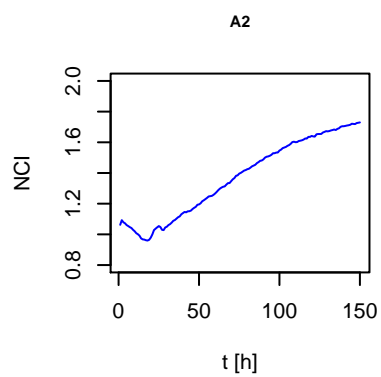
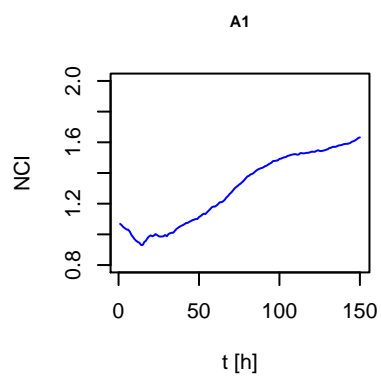
#set measurement
DMSO_test.norm<-DMSO_test.norm[1:150,]
DMSO_test.norm <- as.data.frame(DMSO_test.norm)

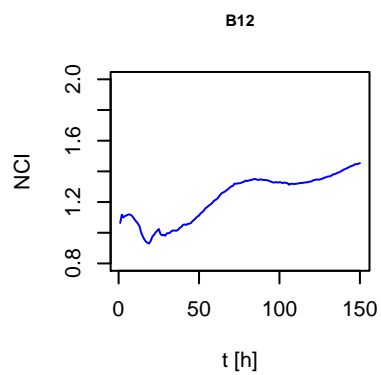
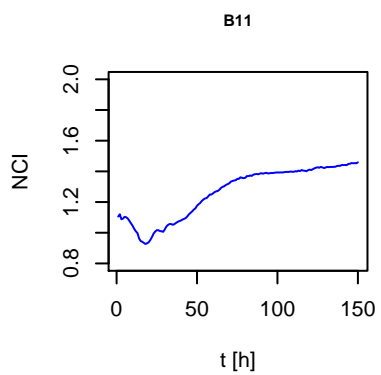
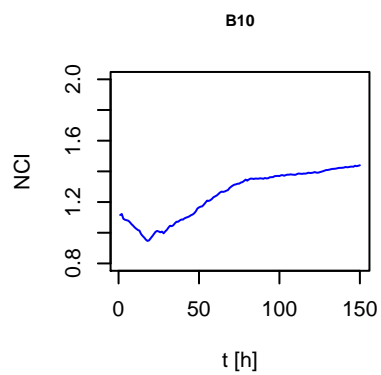
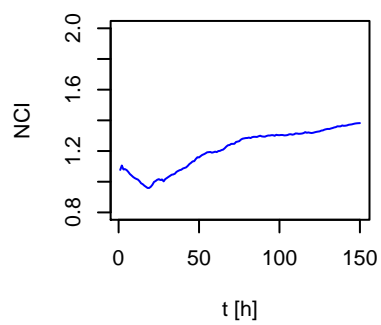
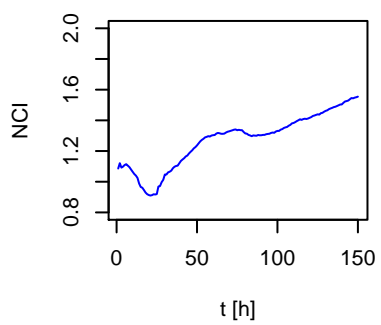
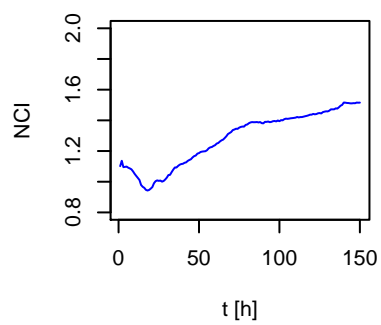
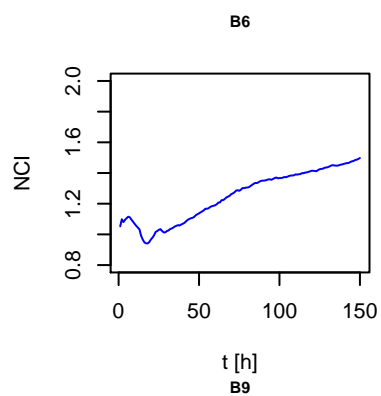
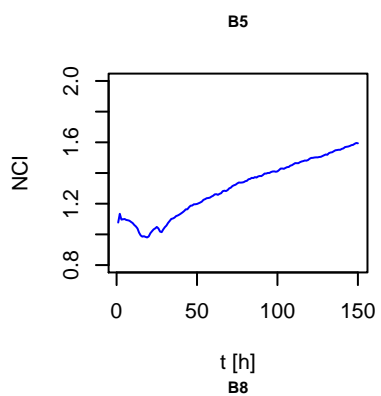
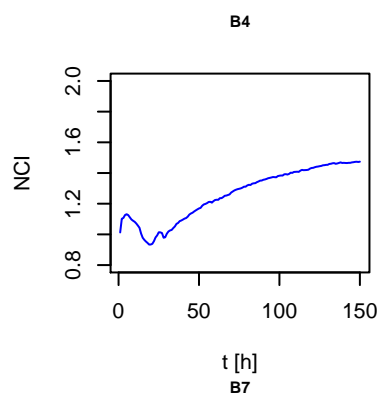
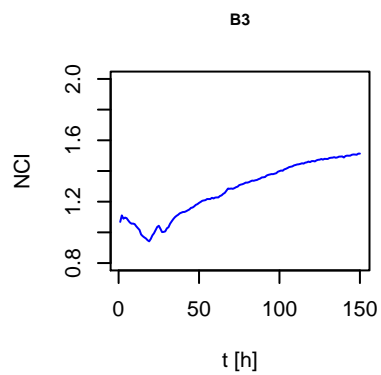
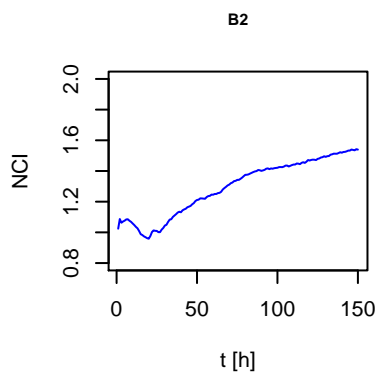
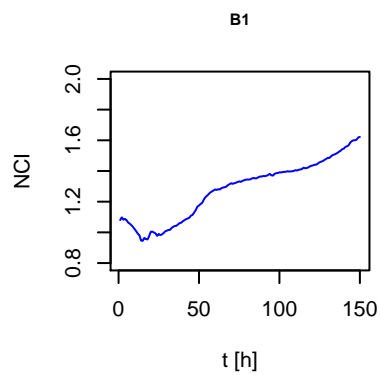
#boxplot
postscript("figure_1.eps", width = 860, height = 600)
par(mar=c(5,3,2,2)+0.1)
boxplot(DMSO_test.norm, ylab = "NCI", xlab = "well position", cex.axis=0.4, las=2, col = "lightgray")
dev.off()

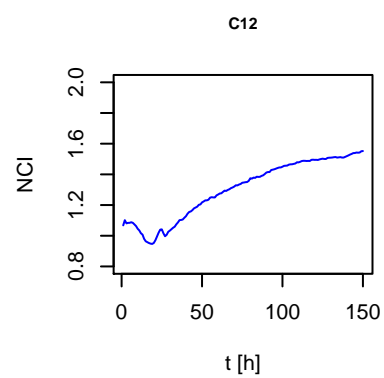
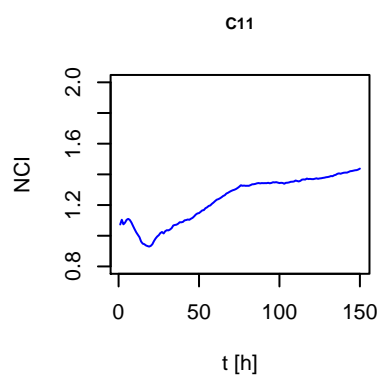
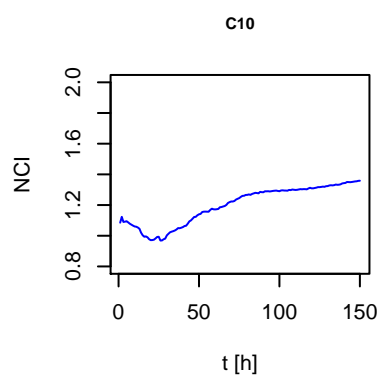
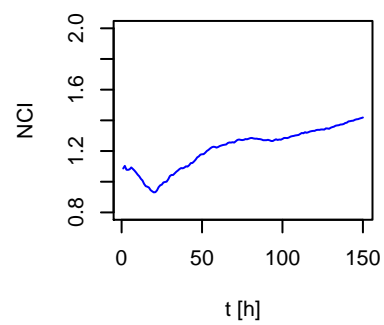
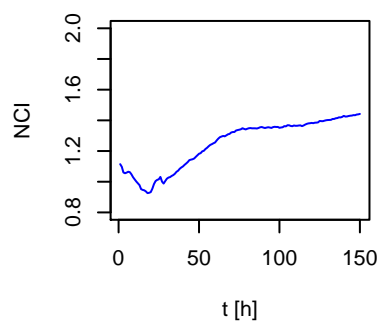
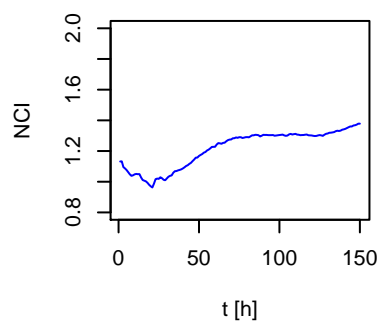
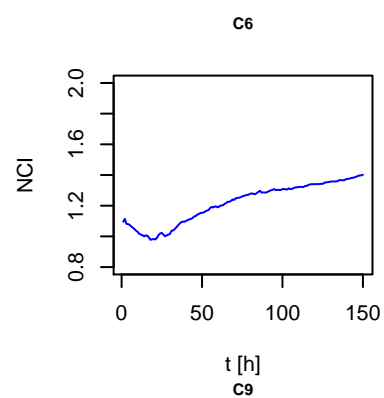
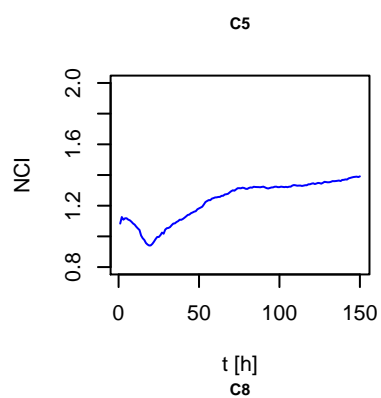
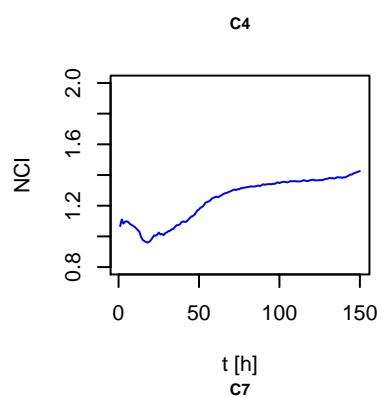
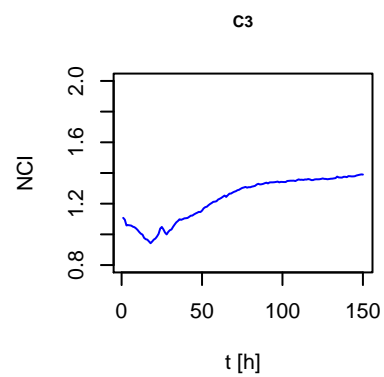
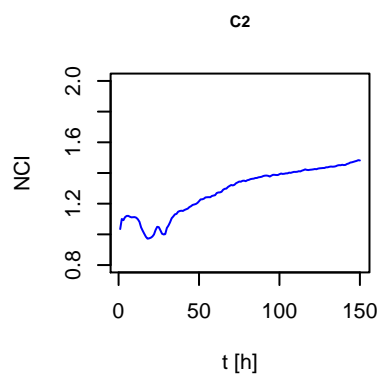
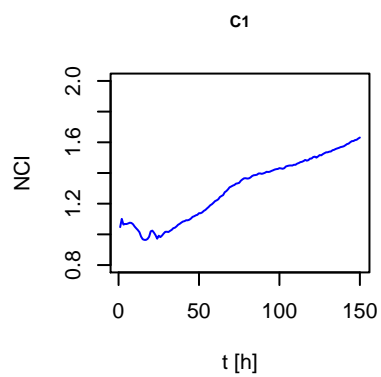
## pdf
## 2

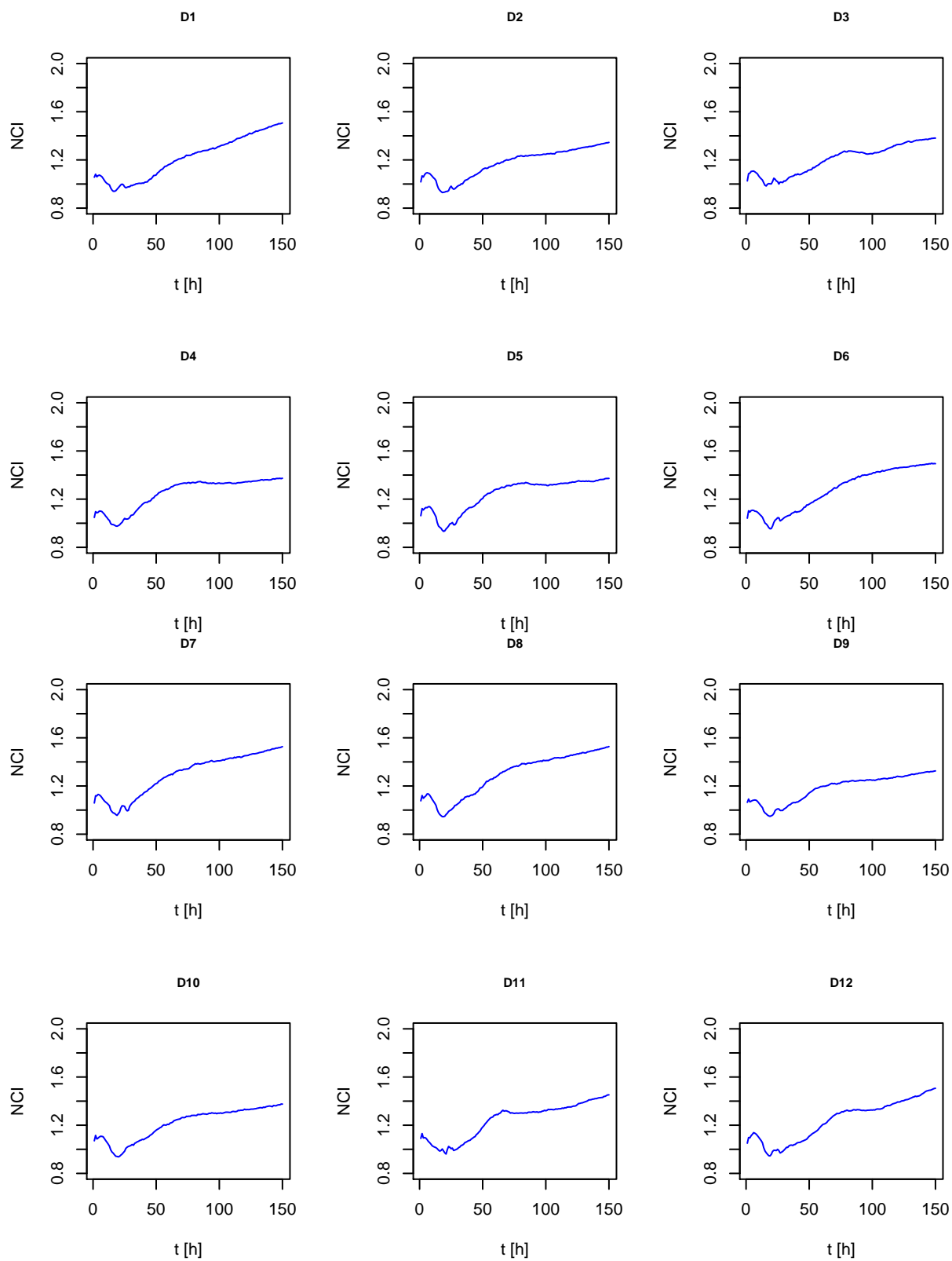
# plot the TCRPs
my_timepoints <- DMSO_test.raw[2:151,]$t - DMSO_test.raw[2,]$t
rownames(DMSO_test.norm) <- my_timepoints

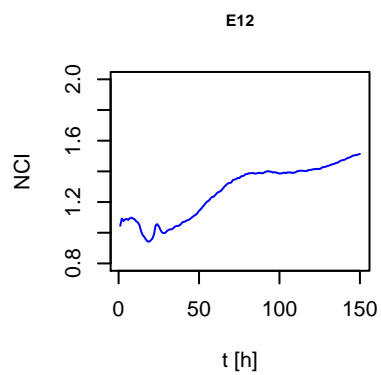
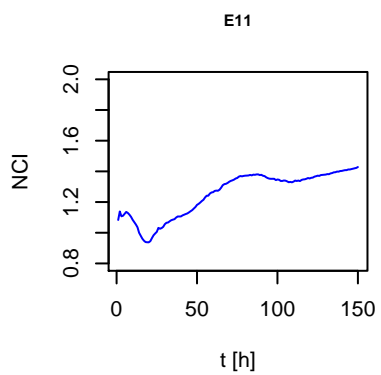
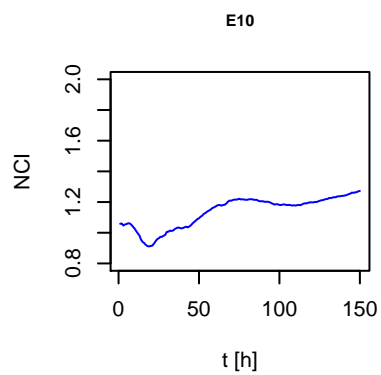
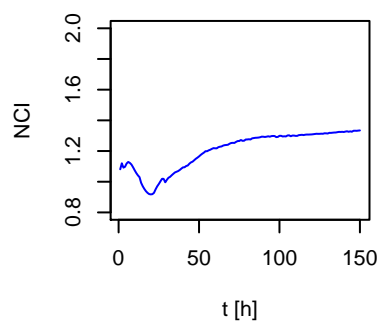
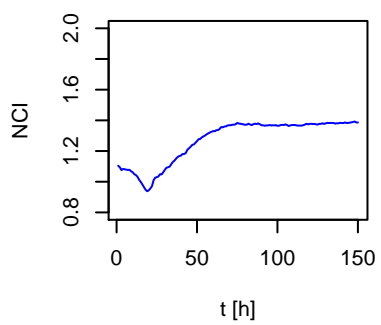
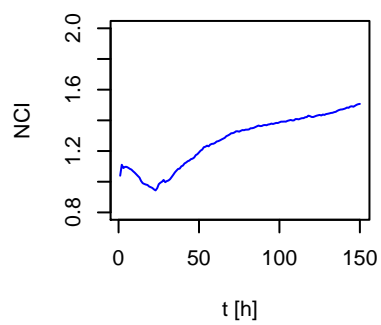
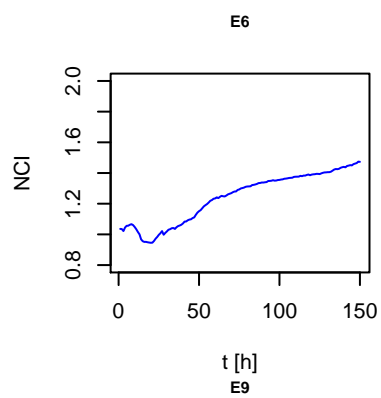
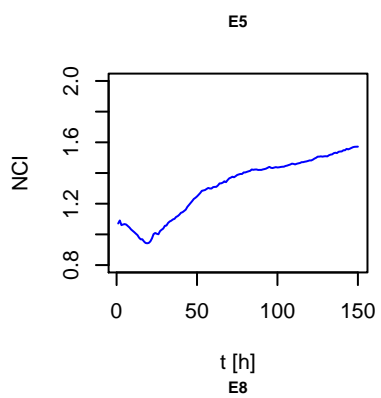
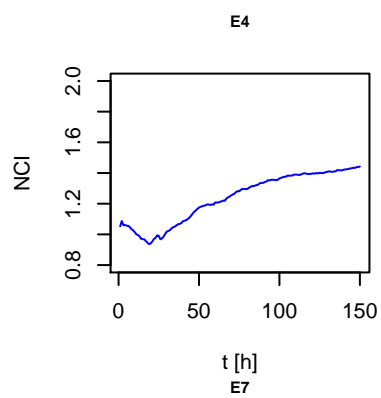
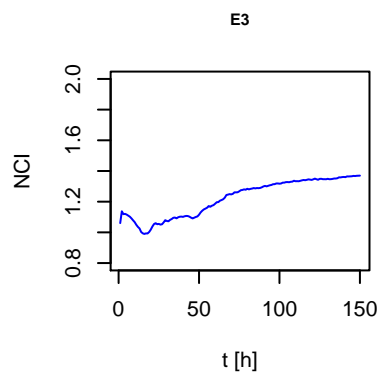
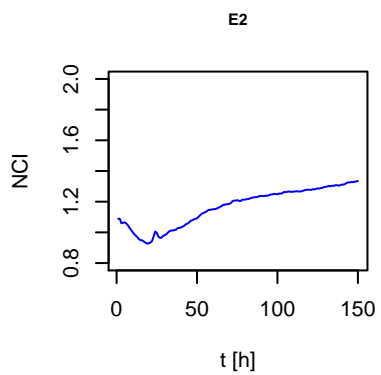
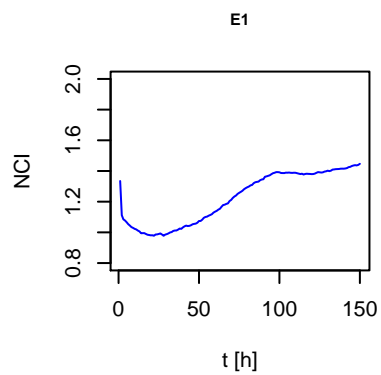
#pdf(file = "DMSO_controls.pdf", paper = "a4r")
par(mfrow = c(2,3))
for (i in 1: ncol(DMSO_test.norm)){
plot(DMSO_test.norm[,i], type="l", col="blue",
      main=colnames(DMSO_test.norm)[i],cex.main=0.8, ylim=c(0.8,2), ylab="NCI", xlab="t [h]")
}
```

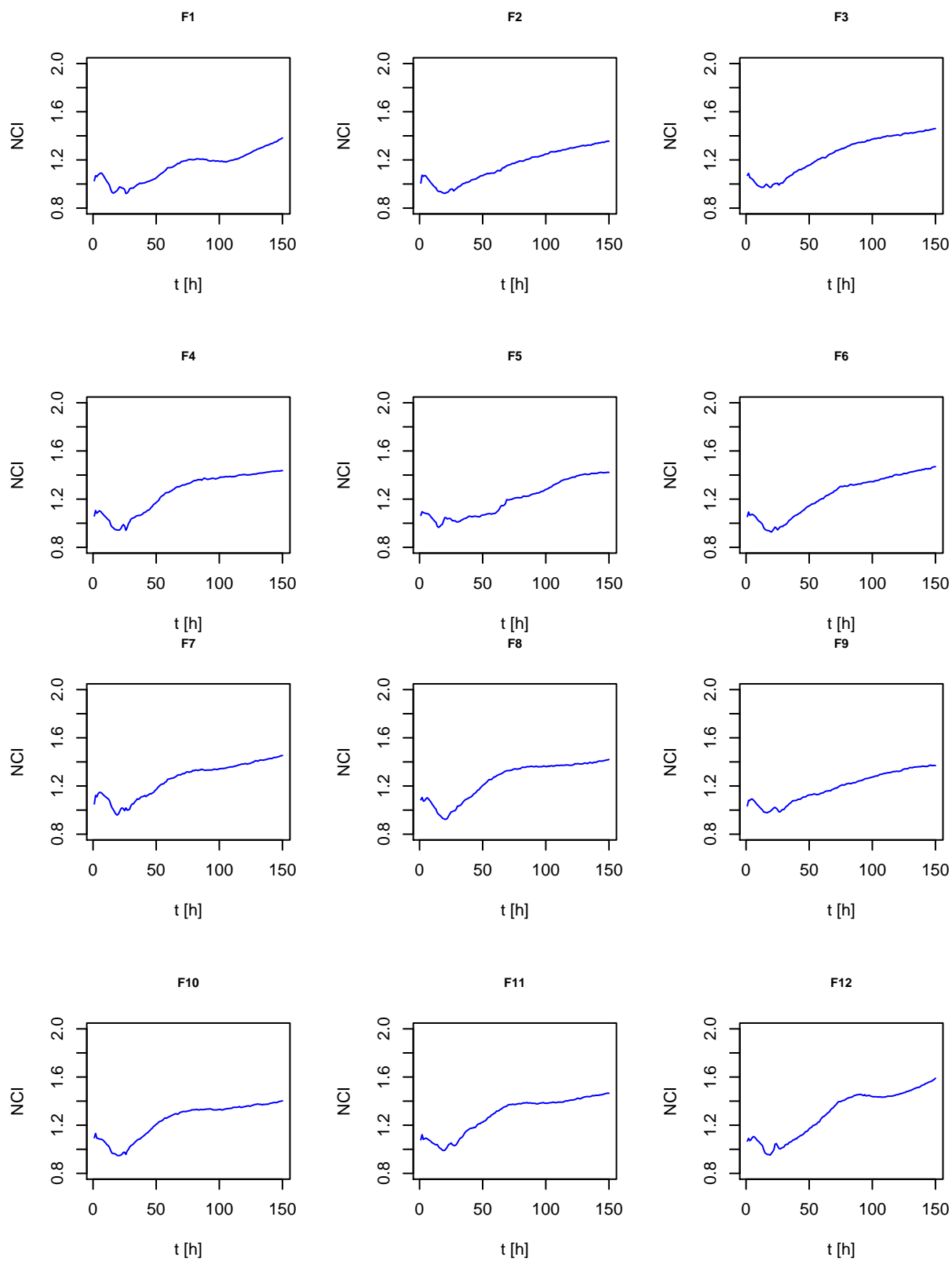


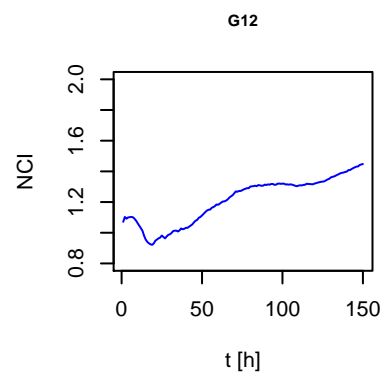
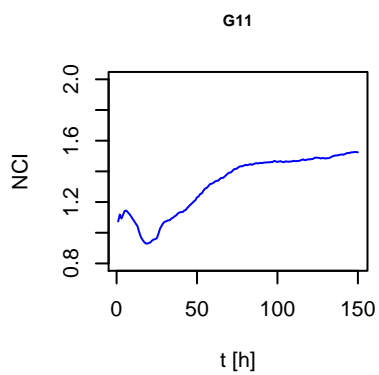
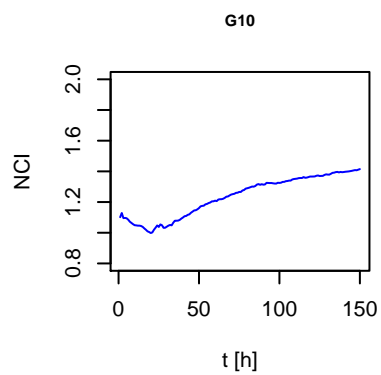
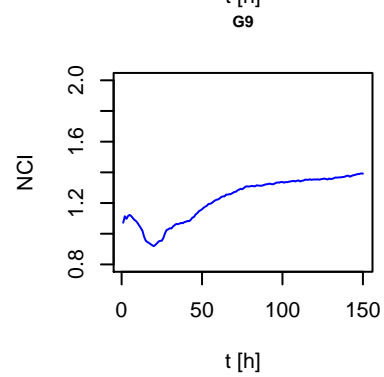
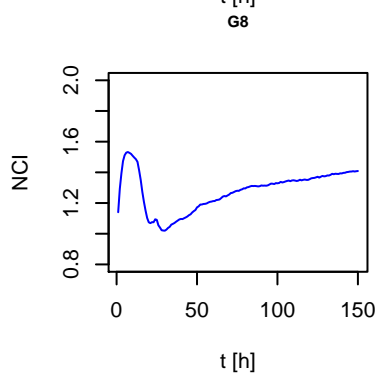
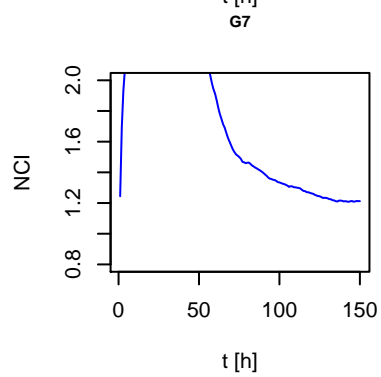
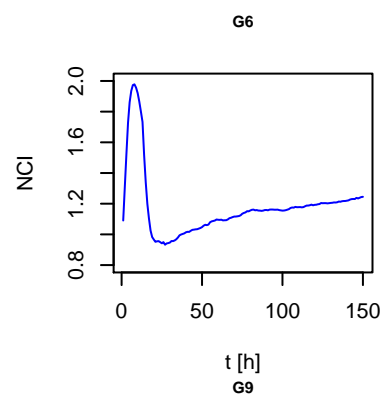
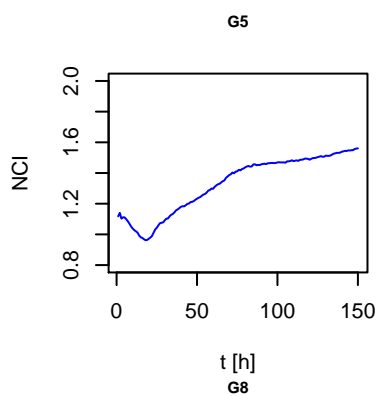
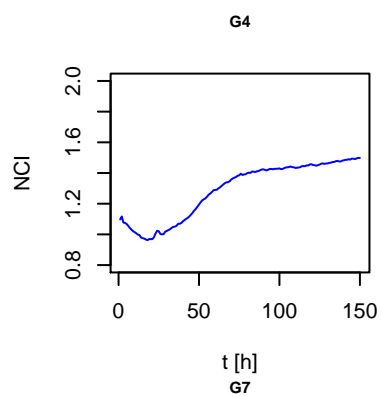
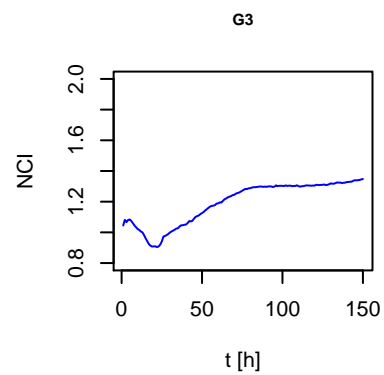
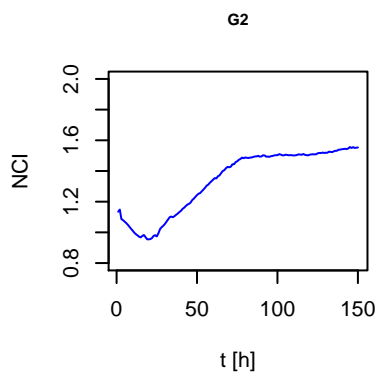
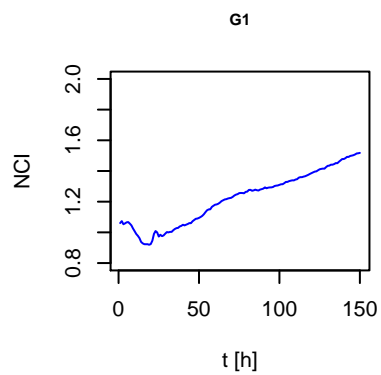


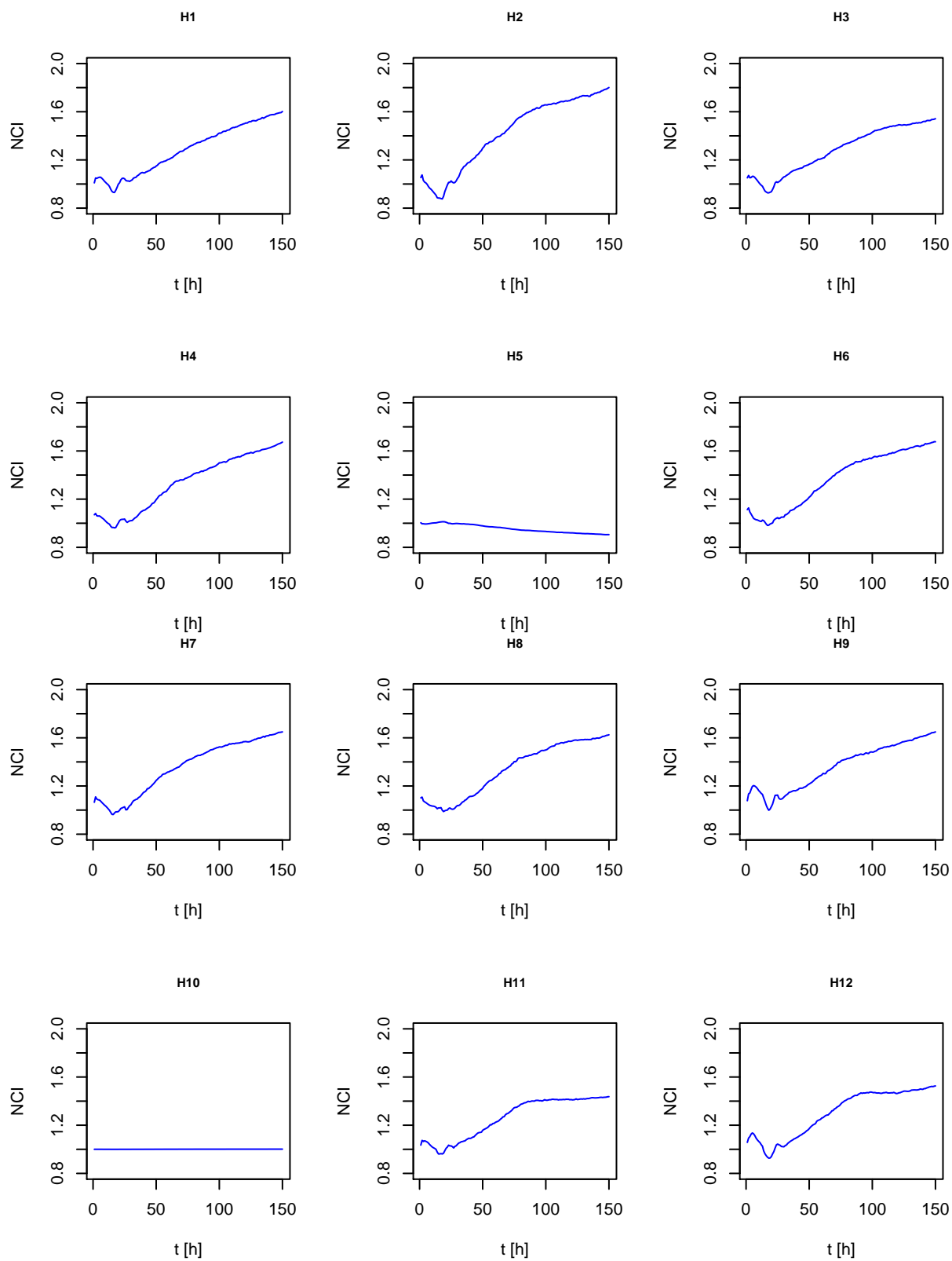












```
#dev.off()
```

```
#calculate medians
```

```

my_matrix <- as.matrix(DMSO_test.norm)
col_medians <- apply(my_matrix, 2, median)

#wilcox test
col_medians["G7"]<- NA
col_medians["H2"] <- NA
col_medians["H5"] <- NA
col_medians["H10"] <- NA

row_A <- col_medians[1:12]
row_B <- col_medians[13:24]
row_C <- col_medians[25:36]
row_D <- col_medians[37:48]
row_E <- col_medians[49:60]
row_F <- col_medians[61:72]
row_G <- col_medians[73:84]
row_G["G6"] <- NA
row_G["G7"] <- NA
row_H <- col_medians[85:96]
row_H["H5"] <- NA
row_H["H10"] <- NA

outer_rows <- c(row_A, row_H)
inner_rows <- c(row_B, row_C, row_D, row_E, row_F, row_G)
median(outer_rows, na.rm = T)

## [1] 1.357712

median(inner_rows, na.rm = T)

## [1] 1.310951

wilcox.test(outer_rows, inner_rows, na.rm = T, alternative = "two.sided")

##
## Wilcoxon rank sum test with continuity correction
##
## data: outer_rows and inner_rows
## W = 1122, p-value = 0.0002719
## alternative hypothesis: true location shift is not equal to 0

```