

# Calculating Drug Synergy Combinations

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r Sys.Date()

## Instructions

- Ensure all packages are correctly installed.
- Substitute “SynergyFinderTemplate.csv” Under “Load Packages and Data” with the name of a file in the same format, but with your data. This must be in the same folder as the file you’re currently reading.
- Check that the correct data type is entered under “Process Data”. Default is “inhibition”.
- Check that the correct synergy calculation method is entered under “Calculate and Visualise Synergy Scores”. Default is “Bliss”.
- Run code from a .Rmd document using “Ctrl + Enter” on the line or a highlighted block of text. Alternatively hit “Run All” under “Run” in the top right of RStudio, to run the whole document.

## Required Packages

```
# Run these lines if the relevant package is not installed (remove the "#" first though)  
  
## dplyr  
# install.packages("dplyr")  
  
## openxlsx  
# install.packages("openxlsx", dependencies = TRUE)  
  
## synergyfinder  
# if (!requireNamespace("BiocManager", quietly = TRUE))  
#   install.packages("BiocManager")  
# BiocManager::install("synergyfinder")
```

## Load Packages and Data

```
# Load packages  
library(dplyr)
```

```
## Warning: package 'dplyr' was built under R version 3.6.3
```

```
##  
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':  
##  
##   filter, lag
```

```
## The following objects are masked from 'package:base':  
##  
##   intersect, setdiff, setequal, union
```

```
library(openxlsx)
```

```
## Warning: package 'openxlsx' was built under R version 3.6.3
```

```
library(synergyfinder)
```

```
## Warning: package 'synergyfinder' was built under R version 3.6.3
```

```
# Load combination data for any number of correctly indexed drug combinations (see the template file for details)  
# replace filename with a .csv file generated from the excel template  
SynFrame <- read.table(file = "SynergyFinderRTemplate.csv", header = TRUE, sep = ";", fileEncoding = "UTF-8")
```

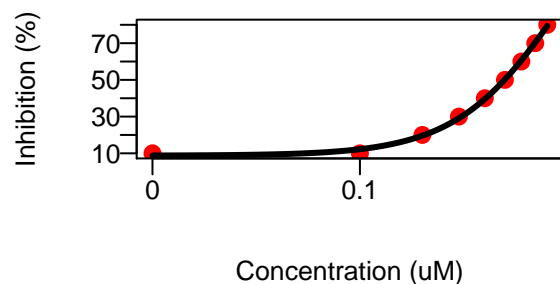
## Process Data

```
# Set the random seed so results are reproducible  
set.seed(42)  
  
# Process the synergy data (check that data.type is correct for your data, accepts "inhibition" or "viability")  
dose.response.mat <- ReshapeData(SynFrame,  
                                data.type = "inhibition",  
                                impute = TRUE,  
                                noise = TRUE,  
                                correction = "non")
```

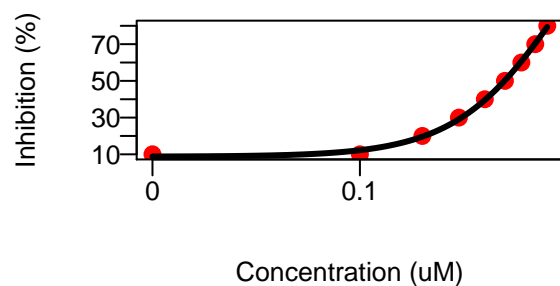
## Plot Dose Response Curves

```
# Plots curves within RStudio and the generated markdown document, but also saves a PDF in the current working directory  
PlotDoseResponse(dose.response.mat, save.file = TRUE)
```

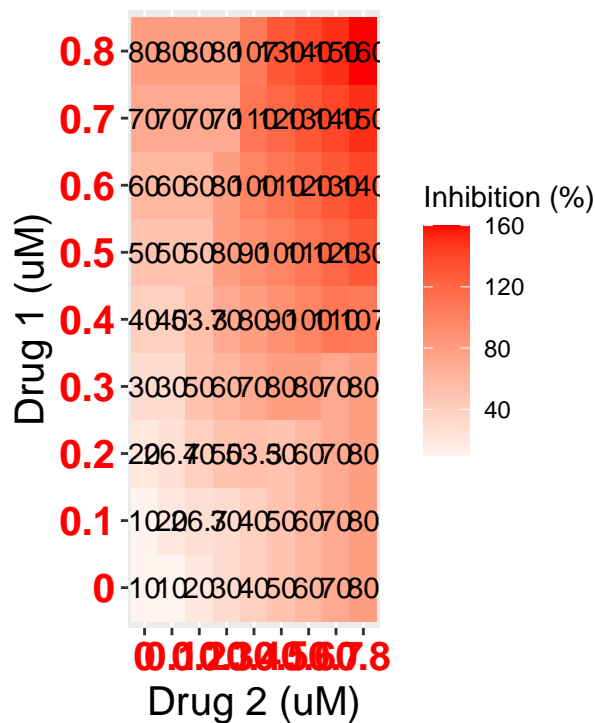
Dose-response curve for drug: Drug 1 in Block



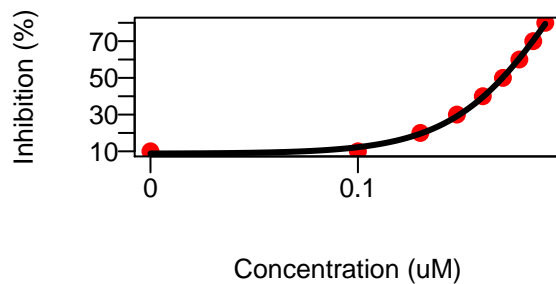
Dose-response curve for drug: Drug 2 in Block



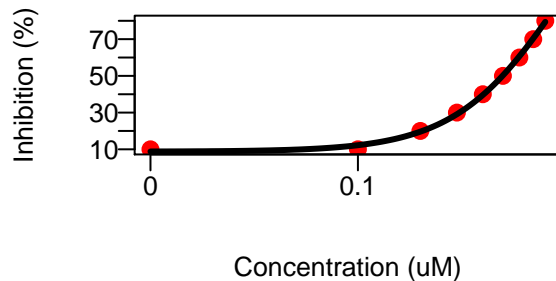
Dose-response matrix  
BlockID: 1



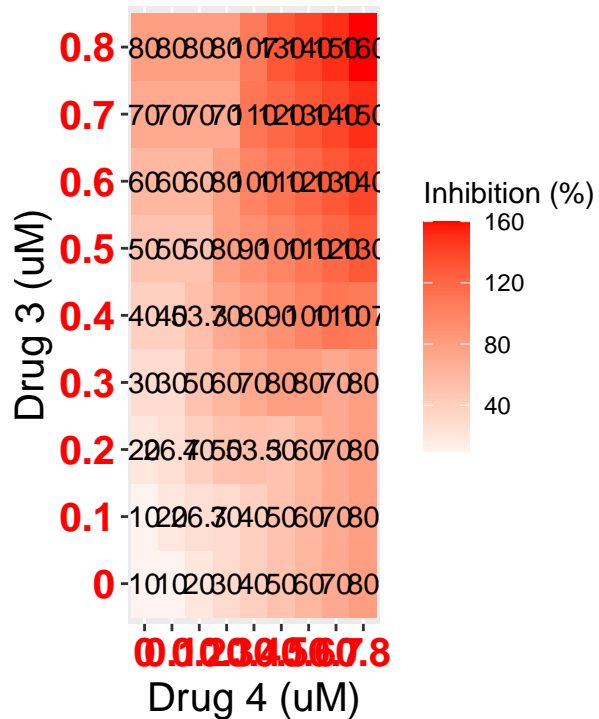
Dose-response curve for drug: Drug 3 in Block



Dose-response curve for drug: Drug 4 in Block



Dose-response matrix  
BlockID: 2

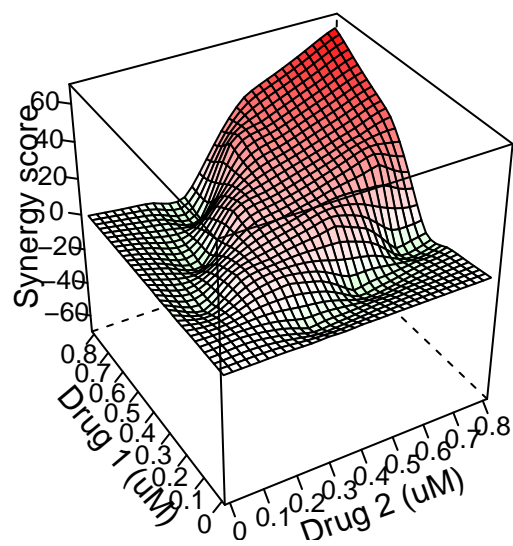
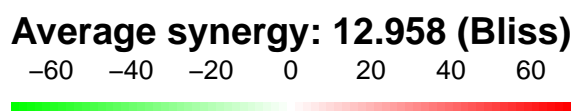
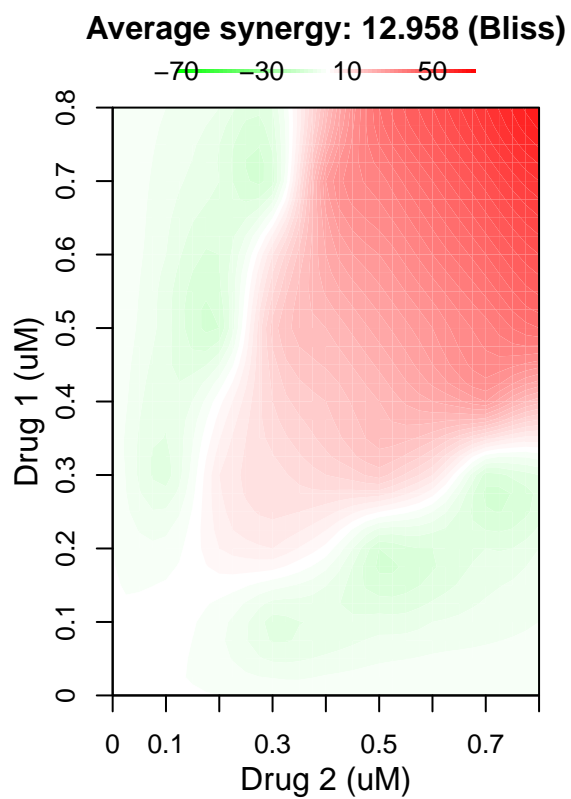


## NULL

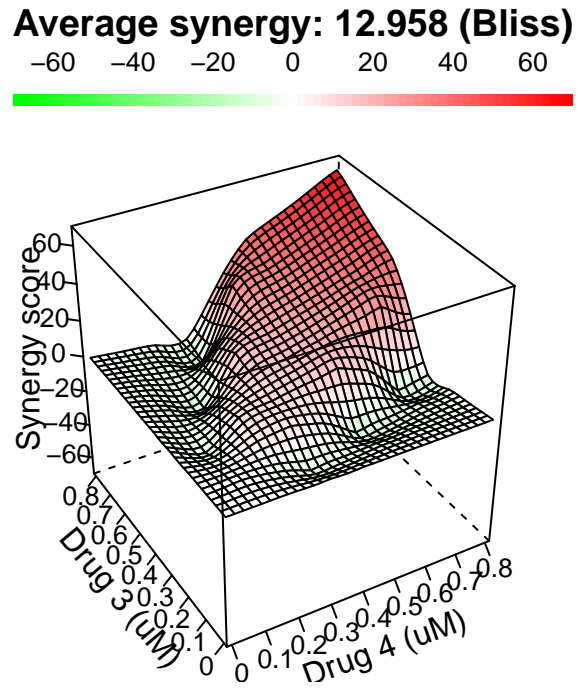
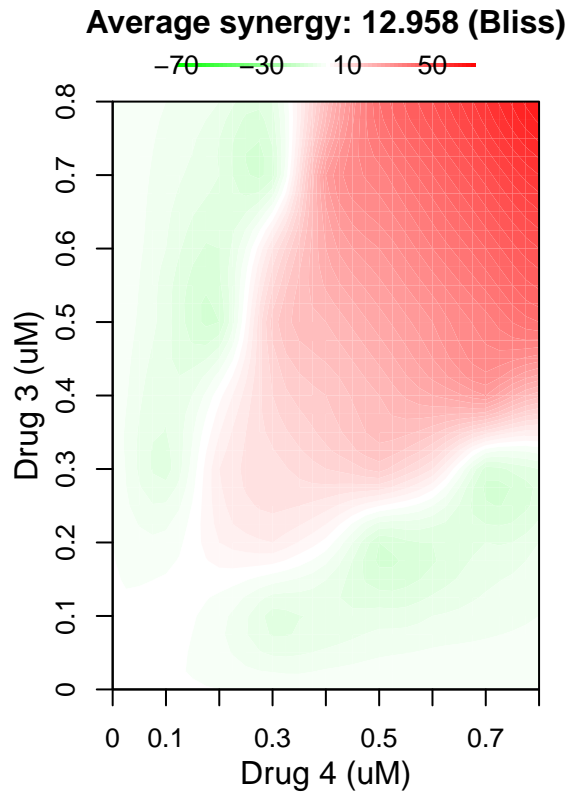
## Calculate and Visualise Synergy Scores

```
# Calculate synergy scores (method accepts "HSA", "Loewe", "Bliss", "ZIP")
synergy.score <- CalculateSynergy(data = dose.response.mat,
                                  method = "Bliss")

# Visualise synergy scores, providing an average value and a visual indication of where synergy is high
# Plots scores within RStudio and the generated markdown document, but also saves a PDF in the current directory
PlotSynergy(synergy.score, type = "all", save.file = TRUE)
```



## [1] 12.958



Find the Synergy Scores for Different Concentration Combinations

```
# Isolate the synergy values for each concentration combination, and ensure that the column names are c
scores <- as.data.frame(synergy.score$scores)
colnames(scores) <- colnames(scores) %>% gsub("X1.", "", .)

# Save it as an excel table to the current working directory. Columns are drug_col, Rows are drug_row
write.xlsx(scores, file = "SynergyScores.xlsx", asTable = TRUE, col.names = TRUE, row.names = TRUE)
```