

# Package ‘DeepTarget’

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**Type** Package

**Title** Deep characterization of cancer drugs

**Version** 1.2.0

**Description** This package predicts a drug’s primary target(s) or secondary target(s) by integrating large-scale genetic and drug screens from the Cancer Dependency Map project run by the Broad Institute. It further investigates whether the drug specifically targets the wild-type or mutated target forms. To show how to use this package in practice, we provided sample data along with step-by-step example.

**License** GPL-2

**Encoding** UTF-8

**biocViews** GeneTarget, GenePrediction, Pathways, GeneExpression, RNASeq, ImmunOncology, DifferentialExpression, GeneSetEnrichment, ReportWriting, CRISPR

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|            |                                                                           |
|------------|---------------------------------------------------------------------------|
| computeCor | <i>Compute a correlation between the every gene vs each drug response</i> |
|------------|---------------------------------------------------------------------------|

---

Description

Compute correlations between the viability of cell lines after CRISPR Knock Out of each gene and of the same cell lines after drug treatment.

Usage

```
computeCor(DrugName, DRS, GES)
```

Arguments

|          |                                                          |
|----------|----------------------------------------------------------|
| DrugName | Drug Name                                                |
| DRS      | Drug's response scores                                   |
| GES      | Gene effect scores from Knock-out method such as CRISPR. |

Value

a list of matrices for the interesting drugs, where each matrix containing gene names with the correlation values and P values associated with response scores from a given drug ID.

Author(s)

sanjushinha7, Trinh Nguyen

**Examples**

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
sim.out <- bplapply(S.Drugs, function(x) computeCor(x, sec.prism, KO.GES))
names(sim.out) <- S.Drugs
head(sim.out)
```

---

|                   |                                                                                            |
|-------------------|--------------------------------------------------------------------------------------------|
| Depmap2DeepTarget | <i>Retrieval and preparation of input data required from Depmap to Deeptarget package.</i> |
|-------------------|--------------------------------------------------------------------------------------------|

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**Description**

Retrieve gene expression, Cripr, mutation data from KO method, and drug matrix and then preparation the matrix compatible as input for Deeptarget.

**Usage**

```
Depmap2DeepTarget(FileN, version)
```

**Arguments**

|         |                                                                                                                                                                               |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| FileN   | File Named used as input for DeepTarget: "CCLE_expression.csv", "CRISPRGeneEffect.csv", "OmicsSomaticMutations.csv", or "secondary-screen-dose-response-curve-parameters.csv" |
| version | Version of data                                                                                                                                                               |

**Value**

a data frame for each required input data

**Author(s)**

Trinh Nguyen, Ying Hu, and sanju

**Examples**

```
library(readr)
library(depmap)
# expression
CCLE.exp <- Depmap2DeepTarget("CCLE_expression.csv", "19Q4")
```

DMB

*Predicting Drug Mutant Binding for mutant or non-mutant form***Description**

Predicting whether the drug is likely bind to mutant or non-mutant form and also generates the plot for visualization.

**Usage**

```
DMB(DrugName,GOI,Pred,Mutant,DRS,GES,plot=TRUE)
```

**Arguments**

|          |                                                                                                                                         |
|----------|-----------------------------------------------------------------------------------------------------------------------------------------|
| DrugName | Drug of interest                                                                                                                        |
| GOI      | Gene of interest                                                                                                                        |
| Pred     | Prediction object resulting from both PredTarget and PredMaxSim functions to predict whether it is a primary target or secondary target |
| Mutant   | Mutant matrix                                                                                                                           |
| DRS      | Drug response matrix                                                                                                                    |
| GES      | Gene Effect Scores                                                                                                                      |
| plot     | Default is TRUE for plotting                                                                                                            |

**Value**

The plot of viability after KO as the X-axis vs drug response in a mutant target as the Y-axis.

**Author(s)**

sanjushinha7, Trinh Nguyen

**Examples**

```
library(BiocParallel)
data (OntargetM)
S.Drugs <- c('K70301465','K09951645')
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
d.mt <- OntargetM$mutations_mat
sim.out <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim.out,Meta.data)
Drug.Gene.max.sim <- PredMaxSim(sim.out,Meta.data)
identical ( DrugTargetSim[,1],Drug.Gene.max.sim[,1])
Pred.d <-cbind (DrugTargetSim,Drug.Gene.max.sim)
DOI = 'dabrafenib'
```

```
GOI = 'BRAF'
DMB (DOI,GOI,Pred.d,d.mt,sec.prism,KO.GES)
```

DoInteractExp

*Compute the interaction between the drug and KO expression***Description**

Computes interaction between the drug and KO expression in term of lower vs higher expression using linear model.

**Usage**

```
DoInteractExp(Predtargets,Exp,DRS, GES,CutOff=3)
```

**Arguments**

|             |                                                                                         |
|-------------|-----------------------------------------------------------------------------------------|
| Predtargets | a dataframe of drugs information and their most targeted gene with stats of correlation |
| Exp         | Expression matrix                                                                       |
| DRS         | Drug scores matrix                                                                      |
| GES         | Gene effect scores matrix from KO method                                                |
| CutOff      | desired cut-off for low expression                                                      |

**Value**

A list of drug names with their interaction values from two groups low and high expression based on the desired cut-off.

|       |                                                            |
|-------|------------------------------------------------------------|
| drug1 | interaction with estimate and P vals from the linear model |
| drug2 | interaction with estimate and P vals from the linear model |
| drugN | interaction with estimate and P vals from the linear model |

**Author(s)**

sanjushin7, Trinh Nguyen

**Examples**

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[,"broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
sim.out <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
```

```
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim.out,D.M = Meta.data)
d.expr <- OntargetM$expression_20Q4
ExpInteract <- DoInteractExp (DrugTargetSim,d.expr,sec.prism,KO.GES,CutOff = 2)
```

---

|                  |                                                                                               |
|------------------|-----------------------------------------------------------------------------------------------|
| DoInteractMutant | <i>Compute interaction between the drug and KO expression in term of mutant vs non-mutant</i> |
|------------------|-----------------------------------------------------------------------------------------------|

---

## Description

Compute interaction between the drug and KO expression in term of mutant vs non-mutant

## Usage

```
DoInteractMutant(Predtargets,Mutant,DRS,GES)
```

## Arguments

|             |                                                                                         |
|-------------|-----------------------------------------------------------------------------------------|
| Predtargets | a dataframe of drugs information and their most targeted gene with stats of correlation |
| Mutant      | Mutant matrix                                                                           |
| DRS         | Drug scores matrix                                                                      |
| GES         | Gene effect scores matrix from KO method                                                |

## Value

A list of drug names with their interaction values from two groups mutant and non-mutant

|       |                                                            |
|-------|------------------------------------------------------------|
| drug1 | interaction with estimate and P vals from the linear model |
| drug2 | interaction with estimate and P vals from the linear model |
| drugN | interaction with estimate and P vals from the linear model |

## Author(s)

sanjushinha7, Trinh Nguyen

## Examples

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
sim <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
```

```

names(sim) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim,Meta.data)
d.mt <- OntargetM$mutations_mat
MutantInteract <- DoInteractMutant (DrugTargetSim,d.mt,sec.prism,KO.GES)

```

---

|       |                                                                                                            |
|-------|------------------------------------------------------------------------------------------------------------|
| DoPWY | <i>Provide a probability score for each pathway for the primary of mechanism of action (MOA) of a drug</i> |
|-------|------------------------------------------------------------------------------------------------------------|

---

## Description

Predicts a Primary Target at a pathway Level. It next finds the pathways that are most enriched in the genes with high DKS scores. It does this by performing a pathway enrichment test on the ranked gene list by DKS score. The output is a data frame of pathway-level probabilities for each drug to be the primary of mechanism of action.

## Usage

```
DoPWY(Sim.GES.DRS,D.M)
```

## Arguments

|             |                                            |
|-------------|--------------------------------------------|
| Sim.GES.DRS | The list of result from "GetSim" function. |
| D.M         | meta data from drug                        |

## Value

a list of drugs, where each of them is data frame containing the pathway level probability to be a primary of mechanism of action.

|       |                                                                       |
|-------|-----------------------------------------------------------------------|
| drug1 | a dataframe contain the pathway level probability to be a primary MOA |
| drug2 | a dataframe contain the pathway level probability to be a primary MOA |
| drugN | a dataframe contain the pathway level probability to be a primary MOA |

## Author(s)

sanjushinha7, Trinh Nguyen

## Examples

```

library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism

```

```
sim <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
names(sim) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
Pwy.Enr <- DoPWY(sim,Meta.data)
```

---

|     |                                                                               |
|-----|-------------------------------------------------------------------------------|
| DTR | <i>Predicting Drug Target Response (DTR) for primary or secondary targets</i> |
|-----|-------------------------------------------------------------------------------|

---

### Description

Predicting whether the drug is likely response to primary or secondary targets and also generates the plot for visualization.

### Usage

```
DTR(DN,GN,Pred,Exp,DRS,GES,CutOff= 3,plot = TRUE)
```

### Arguments

|        |                                                                                                        |
|--------|--------------------------------------------------------------------------------------------------------|
| DN     | Drug of interest                                                                                       |
| GN     | Gene of interest                                                                                       |
| Pred   | Prediction object, an output result from prediction whether it is a primary target or secondary target |
| Exp    | Expression matrix                                                                                      |
| DRS    | Drug response matrix                                                                                   |
| GES    | Gene Effect Scores                                                                                     |
| plot   | whether users want to plot, default is true                                                            |
| CutOff | cutoff value for gene expression of gene of interest high or low                                       |

### Value

vialbility after KO vs drug response of gene of interest low vs high cut-off values set by users

### Author(s)

sanjushinha7, Trinh Nguyen

### Examples

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
S.Drugs <- c('K70301465', 'K09951645')
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
```

```
d.expr <- OntargetM$expression_20Q4
sim.out <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim.out,Meta.data)
Drug.Gene.max.sim <- PredMaxSim(sim.out,Meta.data)
identical ( DrugTargetSim[,1],Drug.Gene.max.sim[,1] )
Pred.d <-cbind (DrugTargetSim,Drug.Gene.max.sim )
DOI = 'ibrutinib'
GOI = 'BTK'
DTR(DOI,GOI,Pred.d,d.expr,sec.prism,KO.GES,CutOff= 2)
```

---

|           |                                                                                                                                                                        |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| OntargetM | <i>An object containing a small part of the data from the Cancer Dependency Map (<a href="http://depmap.org">depmap.org</a>) to demonstrate in DeepTarget pipeline</i> |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

An object containing Viability matrix after CRISPR-KO; Viability after Drug Treatment; Drug metadata from Broad, mutation matrix, and expression matrix with common cell-lines and common drugs. This is a subset of the total data due to memory constraints, full data can be downloaded from [depmap.org/portal](http://depmap.org/portal).

## Usage

```
data("OntargetM")
```

## Format

A list of one dataframe and 4 matrices

**DrugMetadata** a dataframe containing 11 unique drugs as rownames with their associated information: **broad\_id\_trimmed** as ID of the drug, **name**, **target**, **drug\_category**, and **moa** as columns

**secondary\_prism** a viability scores matrix (after Drug Treatment) with 16 drugs as row names across 392 unique celllines as column names

**avana\_CRISPR** a Gene effect scores (after CRISPR-KO) matrix for 487 genes as row names across 392 unique celllines as column names

**mutations\_mat** Mutation binary matrix for 476 genes as row names across 392 unique cell lines as column names; 0 is WT; 1 is mutated

**expression\_20Q4** Expression matrix for 550 genes as row names across 392 unique celllines as column names

## Details

For a full list data used in the paper, please use the link below to download data

**Source**

DrugMetadata: Please download full data from this link [https://depmap.org/repurposing/#:~:text=Corseello\\_supplemental\\_tables.xlsx](https://depmap.org/repurposing/#:~:text=Corseello_supplemental_tables.xlsx)

Secondary prism: please download full data from this link <https://depmap.org/portal/download/all/?releasename=PRISM+Repurposing+19Q4&filename=secondary-screen-dose-response-curve-parameters.csv>

avana\_CRISPR: please download full data from this link <https://depmap.org/portal/download/all/?releasename=DepMap+Public+22Q4&filename=CRISPRGeneEffect.csv>

mutations\_mat: Please download full data from this link <https://depmap.org/portal/download/all/?releasename=DepMap+Public+22Q4&filename=OmicsSomaticMutations.csv>

expression\_20Q4: Please download full data of file named "CCLE\_expression.csv" from this link <https://depmap.org/portal/download/all/>

**Examples**

```
data(OntargetM)
```

---

plotCor

*Plot the correlation*

---

**Description**

Plot the correlation of a predicted target

**Usage**

```
plotCor(DN,GN,Pred,DRS,GES,plot=TRUE)
```

**Arguments**

|      |                               |
|------|-------------------------------|
| DN   | Drug Name                     |
| GN   | Gene Name                     |
| Pred | Output from prediction object |
| DRS  | Drug response score           |
| GES  | Gene Effect scores            |
| plot | default is plot=TRUE          |

**Value**

Correlation plot

**Author(s)**

sanjushin7, Trinh Nguyen

**Examples**

```

library(BiocParallel)
data (OntargetM)
set.seed (12345)
S.Drugs <- c('K70301465', 'K09951645')
KO.GES <- OntargetM$savana_CRISPR
sec.prism <- OntargetM$secondary_prism
d.expr <- OntargetM$expression_20Q4
sim.out <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,KO.GES))
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim.out,Meta.data)
Drug.Gene.max.sim <- PredMaxSim(sim.out,Meta.data)
identical ( DrugTargetSim[,1],Drug.Gene.max.sim[,1] )
Pred.d <-cbind (DrugTargetSim,Drug.Gene.max.sim )
DOI = 'ibrutinib'
GOI = 'BTK'
plotCor (DOI,GOI,Pred.d,sec.prism,KO.GES)

```

---

|         |                                                                                                                  |
|---------|------------------------------------------------------------------------------------------------------------------|
| plotSim | <i>Plot the similarity between correlation values and P vals for all genes.<br/>The top 5 genes are labeled.</i> |
|---------|------------------------------------------------------------------------------------------------------------------|

---

**Description**

Plot the similarity between correlation values and P val;

**Usage**

```
plotSim(dx,dy,clr=NULL, plot=TRUE)
```

**Arguments**

|      |                              |
|------|------------------------------|
| dx   | a matrix of p vals           |
| dy   | a matrix of correlation vals |
| clr  | Desired range of color       |
| plot | default plot =TRUE           |

**Value**

a plot of similarity

**Author(s)**

Ying Hu,Trinh Nguyen

## Examples

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
Sample.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
sim.out <- bplapply(Sample.Drugs, function(x) computeCor(x, sec.prism, KO.GES))
names(sim.out) <- Sample.Drugs
P.Values=vapply(sim.out, function(x) x[,1], FUN.VALUE=numeric(nrow(sim.out[[1]])))
estimate.cor.values=vapply(sim.out, function(x) x[,2], FUN.VALUE=numeric(nrow(sim.out[[1]])))
par(mar=c(4,4,5,2), xpd=TRUE, mfrow=c(3,3));
plotSim(dx=P.Values, dy=estimate.cor.values);
```

---

PredMaxSim

*Predict the most similar gene to the drug response*


---

## Description

Predicts the gene that has the most similarity associated with drug's response scores from the set of all genes.

## Usage

```
PredMaxSim (Sim.GES.DRS,D.M)
```

## Arguments

|             |                                                                                                       |
|-------------|-------------------------------------------------------------------------------------------------------|
| Sim.GES.DRS | similarity between Drug's response scores and Gene effect scores from Knock-out method such as CRISPR |
| D.M         | Drug Metadata                                                                                         |

## Value

a dataframe of drug(s) information with the most predicted gene(s) with the max correlation value(s), P value(s), and FDR value(s).

## Author(s)

sanjushin7, Trinh Nguyen

**Examples**

```
library(BiocParallel)
data (OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
sec.prism <- OntargetM$secondary_prism
sim.out <- bplapply(S.Drugs, function(x) computeCor(x, sec.prism, KO.GES))
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
Drug.Gene.max.sim <- PredMaxSim(sim.out, Meta.data)
```

---

PredTarget

---

*Prediction of the most similar known targeted gene.*


---

**Description**

Predicts the gene that has the most similarity to a drug's response scores. This is done based on selecting a gene that has the most correlation across the known targeted genes by their drug.

**Usage**

```
PredTarget(Sim.GES.DRS, D.M)
```

**Arguments**

|             |                                                                                                        |
|-------------|--------------------------------------------------------------------------------------------------------|
| Sim.GES.DRS | similarity between Drug's response scores and Gene effect scores from Knock-out method such as CRISPR. |
| D.M         | Drug Metadata                                                                                          |

**Value**

a dataframe of drug(s) information with the most known predicted gene(s) with the max correlation value(s), P value(s), and FDR value(s).

**Author(s)**

sanjushinha7, Trinh Nguyen

**Examples**

```
library(BiocParallel)
data(OntargetM)
set.seed (12345)
All.Drugs <- OntargetM$DrugMetadata[, "broad_id_trimmed"]
S.Drugs <- sample(All.Drugs, 5)
KO.GES <- OntargetM$avana_CRISPR
```

```
sec.prism <- OntargetM$secondary_prism
sim.out <- bplapply(S.Drugs,function(x) computeCor(x,sec.prism,K0.GES))
names(sim.out) <- S.Drugs
Meta.data <- OntargetM$DrugMetadata
DrugTargetSim <- PredTarget(sim.out,Meta.data)
```

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