

# Package ‘octad.db’

November 14, 2024

**Title** Open Cancer TherApeutic Discovery (OCTAD) database

**Version** 1.8.0

**Description** Open Cancer TherApeutic Discovery (OCTAD) package implies sRGES approach for the drug discovery. The essential idea is to identify drugs that reverse the gene expression signature of a disease by tamping down over-expressed genes and stimulating weakly expressed ones. The following package contains all required precomputed data for whole OCTAD pipeline computation.

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**RoxygenNote** 7.2.1

**Depends** R (>= 4.2.0), ExperimentHub

**biocViews** ExperimentData, CancerData, ExperimentHub, SequencingData, ExpressionData

**VignetteBuilder** knitr

**Suggests** knitr, rmarkdown

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## Contents

get_ExperimentHub_data . . . . .	2
octad.db . . . . .	2
<b>Index</b>	<b>4</b>

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get\_ExperimentHub\_data  
*Download file from Experimental Hub*

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### Description

Download file from Experimental Hub.

### Usage

```
get_ExperimentHub_data(file=NULL)
```

### Arguments

file            file id do download it from Experimental Hub archive

### Value

Returns a data.frame object depends on the call

### See Also

[octad.db](#).

### Examples

```
phenoDF=get_ExperimentHub_data("EH7274") #load data.frame with samples included in the OCTAD database.
head(phenoDF)
```

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octad.db            *Open Cancer TherApeutic Discovery (OCTAD) database package*

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### Description

This is a support package for the main package octad which can be obtained [here](#)

## Details

Package includes all required data for drug repurposing OCTAD pipeline. Initialization of the pipeline starts with listing all available samples:

```
phenoDF=.eh[["EH7274"]] #load data.frame with samples included in the OCTAD database. head(phenoDF)
#list all data included within the package
```

Besides, the package includes examples of the output from `diffExp` and `runsRGES` functions from the octad package along with description of the data: `res=octad.db::res_example` #load example res from octad.db `?res_example` `sRGES=octad.db::sRGES_example` #load example sRGES from octad.db `?sRGES_example`

`CCLC.log2.read.count.matrix` log2-transformed matrix containing expression of 56,318 genes in 1,019 cell lines provided in CCLC database `CCLC.overlaps` log2-transformed matrix containing expression of 56,318 genes in 51 cell lines present in both LINCS and CCLC databases `CCLC.sample.meta` data.frame containing cell lines name and tissue of origin from CCLC database `CTRPv2.sensprof` Cancer Therapeutics Response Portal (CTRP) data.frame containing AUC and IC50 for every drug-cell line pair `EncoderDF` a data.frame (64 features by 19127 samples) computed from autoEncoder for every sample in the OCTAD database `cmpd_sets_ChemCluster` list of compounds and their clusters based on chemical structures `cmpd_sets_mesh` list of compounds and their associations with 662 pharmacological MeSH Terms provided in PubChem `fda_drugs` data.frame of FDA approved drugs containing name, target and clinical phase `lincs_sig_info` data.frame for LINCS signatures including experiment id, cell line used in the experiment, perturbation name, perturbation type, dose and time `lincs_signatures` Differential expression of 978 genes in 416,560 experiments `merged_gene_info` data.frame with the annotation of 75,078 genes which could be used for identifier mapping `octad.LINCS.counts` expression matrix of 965 genes and 19127 samples in OCTAD database (965 genes were profiled in LINCS) `phenoDF` data.frame with samples from the OCTAD database including tissue of origin, sample type (tumor-derived or healthy-derived), cancer, original source (e.g. TCGA), mutation and stage data if available `random_gsea_score` pre-computed permuted gsea scores for chemo, mesh and ChemCluster databases that are used for drug enrichment analysis `tsne` 2 dimension tSNE for every sample in the OCTAD database along with sample.id, cancer type and source of the initial data `octad.counts.and.tpm.h5` expression (TPM and raw counts) matrix of 60,498 genes and 19,127 samples

The code can be viewed at the GitHub repository, which also lists the contributor code of conduct:

<https://bioconductor.org/packages/octad> or <https://github.com/Bin-Chen-Lab/octad> for the pipeline package

## References

Zeng, B., Glicksberg, B.S., Newbury, P., Chekalin, E., Xing, J., Liu, K., Wen, A., Chow, C. and Chen, B., 2021. OCTAD: an open workspace for virtually screening therapeutics targeting precise cancer patient groups using gene expression features. *Nature protocols*, 16(2), pp.728-753. <https://www.nature.com/articles/s41596-020-00430-z>

# Index

\* **get\_ExperimentHub\_data**  
    [get\\_ExperimentHub\\_data, 2](#)  
  
[get\\_ExperimentHub\\_data, 2](#)  
  
[octad.db, 2, 2](#)