Package 'drugTargetInteractions'

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Type Package

Title Drug-Target Interactions

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Description Provides utilities for identifying drug-target interactions for sets of small molecule or gene/protein identifiers. The required drug-target interaction information is obained from a local SQLite instance of the ChEMBL database. ChEMBL has been chosen for this purpose, because it provides one of the most comprehensive and best annotatated knowledge resources for drug-target information available in the public domain.

Depends methods, R (>= 4.1)

Imports utils, RSQLite, UniProt.ws, biomaRt,ensembldb, BiocFileCache,dplyr,rappdirs, AnnotationFilter, S4Vectors

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`drugTargetInteractions-package`
Drug-Target Interactions

Description

The drugTargetInteractions package provides utilities for identifying drug-target interactions for sets of small molecule or gene/protein identifiers. The required drug-target interaction information is obained from a local SQLite instance of the ChEMBL database.

Details

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Author(s)

Thomas Girke [cre, aut]

Maintainer: Thomas Girke <thomas.girke@ucr.edu>

cmpIdMapping *cmpIdMapping*

Description

Function to generate compound ID mappings UniChem.

This function requires the ID mapping files "src1src2.txt.gz", "src1src22.txt.gz", and "src1src7.txt.gz" to exist in a directory called "downloads" before being run. These can be generated with the `downloadUniChem` function.

It will do some processing on these files and output an RDS file at `outfile`. This file can then be used in other functions, such as `drugTargetAnnot`.

Usage

```
cmpIdMapping(outfile=file.path(config$resultsPath,"cmp_ids.rds"), rerun=TRUE,config=genConfig())
```

Arguments

`outfile`	Path to output file.
`rerun`	If true, runs processing, otherwise does nothing.
`config`	General configuration. See `genConfig`.

Value

Generates an RDS file at `outfile`.

Author(s)

Thomas Girke

See Also

`downloadUniChem`

Examples

```
cmpIdMapping("cmp_ids.rds",rerun=FALSE)
```

downloadChemblDb *downloadChemblDb*

Description

Download ChEMBL sqlite db for use by several other functions in the package.

Usage

```
downloadChemblDb(version,rerun=TRUE,config=genConfig())
```

Arguments

version	The ChEMBL version to download.
rerun	If TRUE, the file will be downloaded, otherwise do nothing.
config	The configuration object. This gives the location to put the downloaded chembl db.

Value

No return value.

Author(s)

Kevin Horan

Examples

```
downloadChemblDb(27)
```

downloadUniChem *downloadUniChem*

Description

Downloads UniChem compound ID mappings from https://www.ebi.ac.uk/unichem/ucquery/listSources. Mappings are downloaded for DrugBank, PubChem, and ChEBI.

Usage

```
downloadUniChem(rerun=TRUE, config=genConfig())
```

Arguments

rerun	If true, downloads the files, else does nothing.
config	General configuration. See genConfig.

Value

Generates the following output files: "src1src2.txt.gz", "src1src22.txt.gz", and "src1src7.txt.gz". These correspond to mappings from ChEMBL to DrugBank, PubChem, and ChEBI, respectivly.

Author(s)

Thomas Girke

References

https://www.ebi.ac.uk/unichem/ucquery/listSources

See Also

drugTargetAnnotTable

Examples

```
downloadUniChem(rerun=TRUE)
```

---

drugTargetAnnot *drugTargetAnnot*

Description

Function to query known drug-target annotations.

Usage

```
drugTargetAnnot(queryBy=list(molType=NULL, idType=NULL, ids=NULL), cmpid_file=file.path(config$resul
```

Arguments

queryBy	A list defining the query, as described in queryBy.
cmpid_file	Path to a compound ID mapping file, generated by cmpIdMapping.
config	General configuration. See genConfig.

Value

Returns the query results as a data frame.

Author(s)

Thomas Girke

See Also

queryBy cmpIdMapping

Examples

```
# Tthese are just sample files included in the package.
# You should use your own data files.
config = genConfig(chemblDbPath=
        system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"),
        resultsPath =
        system.file("extdata", "results", package="drugTargetInteractions"))

queryBy <- list(molType="cmp", idType="chembl_id", ids=c("CHEMBL1233058", "CHEMBL1200916", "CHEMBL437765"))
qresult <- drugTargetAnnot(queryBy, config=config)
```

---

drugTargetAnnotTable *drugTargetAnnotTable*

Description

Generates a drug target annotation TSV file. This file includes target information from ChEMBL, drugbank, pubchem, and chembi.

This function requires the ID mapping files "src1src2.txt.gz", "src1src22.txt.gz", and "src1src7.txt.gz" to exist in a directory called "downloads" before being run. These can be generated with the downloadUniChem function.

Usage

```
drugTargetAnnotTable(outfile, rerun=TRUE,config=genConfig())
```

Arguments

outfile	The name of the output file to write the results to.
rerun	If true, download and generate output file. Otherwise do nothing.
config	General configuration. See genConfig.

Value

Writes output file to outfile.

Author(s)

Thomas Girke

See Also

downloadUniChem

Examples

```
config = genConfig(chemblDbPath=
    system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"))
drugTargetAnnotTable(outfile="drugTargetAnnot.xls", config=config)
```

---

drugTargetBioactivity *drugTargetBioactivity*

Description

Function to query bioactivity data by target or compound ids

Usage

```
drugTargetBioactivity( queryBy=list(molType=NULL, idType=NULL, ids=NULL), cmpid_file=file.path(config
```

Arguments

queryBy	A list defining the query, as described in queryBy.
cmpid_file	Path to a compound ID mapping file, generated by cmpIdMapping.
config	General configuration. See genConfig.

Value

Returns results as a data frame.

Author(s)

Thomas Girke

See Also

queryBy cmpIdMapping

Examples

```
 config = genConfig(chemblDbPath=
        system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"),
        resultsPath =
        system.file("extdata", "results", package="drugTargetInteractions"))

queryBy <- list(molType="protein", idType="uniprot", ids=c("P05979", "P35354", "P33033", "Q8VCT3", "P29475", "P
 qresult <- drugTargetBioactivity( queryBy, config=config)

queryBy <- list(molType="cmp", idType="molregno", ids=c("101036", "101137", "1384464"))
 qresult <- drugTargetBioactivity( queryBy, config=config)

queryBy <- list(molType="cmp", idType="DrugBank_ID", ids=c("DB00945", "DB00316", "DB01050"))
 qresult <- drugTargetBioactivity(queryBy, config=config)

 queryBy <- list(molType="cmp", idType="PubChem_ID", ids=c("2244", "3672", "1983"))
 qresult <- drugTargetBioactivity(queryBy, config=config)
```

---

genConfig *genConfig*

Description

Create a default configuration object.

Usage

```
genConfig( chemblDbPath = "chembldb.db", downloadPath = "downloads", resultsPath = "results" )
```

Arguments

chemblDbPath	Path or filename of ChEMBL SQLite db file.
downloadPath	The name of a directory to put downloaded files in.
resultsPath	The name of a directory to put output files in.

Value

A config object that can be passed to ther functions.

Author(s)

Kevin Horan

Examples

```
config = genConfig()
```

getDrugTarget *getDrugTarget*

Description

This function allows you to query a subset of the data fetched by drugTargetAnnotTable.

Usage

```
getDrugTarget(dt_file=file.path(config$resultsPath,"drugTargetAnnot.xls"), queryBy=list(molType=NULL
      id_mapping=c(chembl="chembl_id", pubchem="PubChem_ID", uniprot="UniProt_ID"), columns,config=g
```

Arguments

dt_file	The drug target annotation file. This can be generated with drugTargetAnnotTable.
queryBy	A list defining the query, as described in queryBy.
id_mapping	A list providing the id columns for ChEMBL, PubChem, and UniProt. It should contain the fields "chembl", "pubchem", and "uniprot", each wit the column name of the respective id number in the drug target annotation file. See default value above for an example.
columns	A list of column indexes to select as a subset of the final result set.
config	General configuration. See genConfig.

Value

Returns the query result as a data frame.

Author(s)

Thomas Girke

See Also

drugTargetAnnotTable

Examples

```
 config = genConfig(chemblDbPath=
       system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"),
       resultsPath =
       system.file("extdata", "results", package="drugTargetInteractions"))
id_mapping <- c(chembl="chembl_id", pubchem="PubChem_ID", uniprot="UniProt_ID", drugbank="DrugBank_ID")

 queryBy <- list(molType="cmp", idType="chembl", ids=c("CHEMBL25", "CHEMBL1742471"))
 getDrugTarget(queryBy=queryBy, id_mapping=id_mapping,
       columns=c(1,5,8,16,17),config=config)
```

```
queryBy <- list(molType="cmp", idType="pubchem", ids=c("2244", "65869", "2244"))
getDrugTarget(queryBy=queryBy, id_mapping=id_mapping,
      columns=c(1,5,8,16,17),config=config)

queryBy <- list(molType="protein", idType="uniprot", ids=c("P43166", "P00915", "P43166"))
getDrugTarget(queryBy=queryBy, id_mapping=id_mapping,
      columns=c(1,5,8,16,17),config=config)
```

---

getParalogs *getParalogs*

Description

Using biomaRt, obtain for query genes the corresponding UniProt IDs as well as paralogs. Query genes can be Gene Names or ENSEMBL Gene IDs from H sapiens. The result is similar to IDMs and SSNNs from getUniprotIDs function, but instead of UNIREF clusters, biomaRt's paralogs are used to obtain SSNNs.

Usage

```
getParalogs(queryBy)
```

Arguments

queryBy	A list defining the query, as described in queryBy.

Value

Returns a list with the paralogs for the given genes.

Author(s)

Thomas Girke

See Also

getUniprotIDs queryBy

Examples

```
queryBy <- list(molType="gene", idType="external_gene_name", ids=c("ZPBP", "MAPK1", "EGFR"))

#requires network connection and is slow
result <- getParalogs(queryBy)
```

getSymEnsUp *Gene to Protein ID Mappings*

Description

The getSymEnsUp function returns for a query of gene or protein IDs a mapping table containing: ENSEMBL Gene IDs, Gene Names/Symbols, UniProt IDs and ENSEMBL Protein IDs. Subsequent slots contain the corresponding named character vectors. Internally, the function uses the ensembldb package.

Usage

```
getSymEnsUp(EnsDb = "EnsDb.Hsapiens.v86", ids, idtype)
```

Arguments

EnsDb	EnsDb instance of ensembldb package
ids	Character vector with IDs matching the type specified under idtype
idtype	Character vector of length one containing one of: GENE_NAME, ENSEMBL_GENE_ID or UNIPROT_ID

Value

List object with following components:

idDF	ID mapping data.frame
ens_gene_id	named character vector
up_ens_id	named character vector
up_gene_id	named character vector

Author(s)

Thomas Girke

Examples

```
gene_name <- c("CA7", "CFTR")
getSymEnsUp(EnsDb="EnsDb.Hsapiens.v86", ids=gene_name, idtype="GENE_NAME")
```

getUniprotIDs *Retrieve UniProt IDs via ID and Cluster Mappings*

Description

The following returns for a set of query IDs (e.g. Ensembl gene IDs) the corresponding UniProt IDs based on two independent approaches: ID mappings (IDMs) and sequence similarity nearest neighbors (SSNNs) using UNIREF clusters. Note, the 'keys' or query IDs (e.g. ENSEMBL genes) can only be reliably maintained in the SSNN results when 'chunksize=1' since batch queries for protein clusters with 'UnitProt.ws' will often drop the query IDs. To address this, the query result contains an extra 'QueryID' column when 'chunksize=1', but not when it is set to a different value than 1.

The `getParalogs` function is similar but it uses biomaRt's paralogs instead of UNIREF clusters.

Usage

```
getUniprotIDs(taxId = 9606, kt = "ENSEMBL", keys, seq_cluster = "UNIREF90", chunksize=20)
```

Arguments

`taxId`	An NCBI taxonomy ID
`kt`	Should be either "ENSEMBL" or "UNIPROTKB".
`keys`	Query IDs.
`seq_cluster`	Which cluster to use. Should be one of 'UNIREF100', 'UNIREF90', 'UNIREF50'.
`chunksize`	Queries are done in batches, this parameter sets the size of each batch.

Value

Returns a list of data.

Author(s)

Thomas Girke

See Also

`getParalogs` `UniProt.ws`

Examples

```
keys <- c("ENSG00000145700", "ENSG00000135441", "ENSG00000120071", "ENSG00000120088", "ENSG00000185829", "ENSG0
res_list100 <- getUniprotIDs(taxId=9606, kt="ENSEMBL", keys=keys, seq_cluster="UNIREF100")
```

processDrugage *processDrugage*

Description

Download Drug Age data from genomics.senescence.info/drugs. Process the data and write it out as a TSV spreadsheet.

Usage

```
processDrugage(drugagefile=file.path(config$resultsPath,"drugage_id_mapping.xls"), redownloaddrugage
```

Arguments

drugagefile	The name of the output file.
redownloaddrugage	If true, download the data file. Otherwise assume the file is already downloaded.
config	General configuration. See genConfig.

Value

Output is written to drugagefile.

Author(s)

Thomas Girke

Examples

```
tryCatch({
 config = genConfig(chemblDbPath=
        system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"))
 processDrugage("druage_id_mapping.xls",TRUE,config)
},
error=function(e){
  message("Failed to run processDrugage(), please try again later")
 }
)
```

runDrugTarget_Annot_Bioassay
runDrugTarget_Annot_Bioassay

Description

Meta-function to obtain in one step both drug-target annotation and bioassay data.

Usage

```
runDrugTarget_Annot_Bioassay(res_list, up_col_id="ID", ens_gene_id, cmpid_file=file.path(config$resu
```

Arguments

res_list	Object obtained from getUniprotIDs function.
up_col_id	Column name in data.frames of res_list containing uniprot IDs, usually one of: 'ID', 'ID_up_sp' or 'ID_up_sp_tr'.
ens_gene_id	Named character vector with ENSEMBL gene IDs in name slot and gene symbols or other ID type in value slot
cmpid_file	Path to CMP ID mapping file, often named cmp_ids.rds.
config	General configuration. See genConfig.
...	Slot to pass on additional arguments.

Value

List with two components each containing a data.frame. The first one (Annotation) contains drug-target annotation data, and the second one (Bioassay) contains drug-target bioassay data.

Author(s)

Thomas Girke

References

References to be added...

See Also

See also: drugTargetAnnot and drugTargetBioactivity

Examples

```
config = genConfig(chemblDbPath=
        system.file("extdata", "chembl_sample.db", package="drugTargetInteractions"),
        resultsPath =
        system.file("extdata", "results", package="drugTargetInteractions"))

## (1) Translate gene symbols to ENSEMBL gene IDs
ensembl_gene_id <- c("ENSG00000001626", "ENSG00000168748")
idMap <- getSymEnsUp(EnsDb="EnsDb.Hsapiens.v86", ids=ensembl_gene_id, idtype="ENSEMBL_GENE_ID")
ens_gene_id <- idMap$ens_gene_id


## (2a) Retrieve UniProt IDs with both IDMs and SSNN paralogs
queryBy <- list(molType="gene", idType="ensembl_gene_id", ids=names(ens_gene_id))

 #this function is slow and requires a network connection
 res_list <- getParalogs(queryBy)



## (3) Obtain Drug-Target Annotation and Bioassay Data
drug_target_list <- runDrugTarget_Annot_Bioassay(res_list=res_list,
          up_col_id="ID_up_sp", ens_gene_id,config=config )
```

`transformTTD` *transformTTD*

Description

Integration with Therapeutic Target Database (TTD). This function downloads a data file from idrblab.org and returns it as a data frame.

Usage

```
transformTTD(ttdfile=file.path(config$downloadPath,"TTD_IDs.txt"), redownloadTTD=TRUE,config=genConf
```

Arguments

`ttdfile`	The name of the output file to write the downloaded file to.
`redownloadTTD`	If true, data file will be downloaded again. If false, we assume the file already exists at `ttdfile`.
`config`	General configuration. See `genConfig`.

Value

Returns a data frame with TTD data in it.

Author(s)

Thomas Girke

Examples

```
ttd=tryCatch(
 transformTTD(),
 error=function(e){
  message("Failed to download TTD file, please try again later")
 }
)
```

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