Package 'exbiolink'

December 12, 2022

Title ExpoBioLink module is designed to find the biological relationships between exposure factors and health outcome.

Version 1.0.0

Description The module is designed to find the biological relationships between exposure factors and health outcome.
This module adopts the most frequently-used and authoritative databases, e.g., T3DB, CTD, ToxCast, StringDB, STITCH, KEGG, and GO.

License GPL (>= 3)

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NeedsCompilation no

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R topics documented:

`BioLink` *Build the biological link*

Description

Build the biological link between the exposures and diseases

Usage

```
BioLink(PID, OutPath ="default", Mode, ChemCas="default", ChemInchikey= "default",
  DiseaseID= "default", MetabolomeID= "default", MetBiospec= "blood", ProteomeID= "default")
```

Arguments

`PID`	chr. Program ID. It must be the same with the PID generated by InitBioLink.
`OutPath`	chr. Output file directory. e.g. "D:/test". It should be noted that the slash symbol is "/", not "\". If "default", the current working directory will be set.
`Mode`	chr. Method to build the biological link between exposures and diseases. Available options include "PPI" (i.e., protein-protein interaction) and "GO" (i.e., gene ontoloty).
`ChemCas`	chr. CAS Registry Number of chemicals. Default means using the values in the input data file. Users can also copy the part of them by clicking "Available vars". It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "7440-43-9,333-41-5,20461-54-5".
`ChemInchikey`	chr. InChiKey serial number of chemicals. Default means using the values in the input data file. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "WABPQHHGFIMREM-UHFFFAOYSA-N,BTAGRXWGMYTPBY-UHFFFAOYSA-N,IAKOZHOLGAGEJT-UHFFFAOYSA-N".
`DiseaseID`	chr. ID of the concerned diseases. Both IDs from OMIM (e.g., OMIM:220100) and MESH (e.g., MESH:C536409) are accepted. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "OMIM:244200,MESH:C536409,OMIM:181500".
`MetabolomeID`	chr. KEGG entry number of metabolites. Default means using the values in the input data file. Users can also copy the part of them by clicking "Available vars". It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "C00022,C00117,C00794".
`MetBiospec`	chr. Biological sample matrix for the metabolome analysis. Options include "Blood" and "Urine".
`ProteomeID`	chr. Protein ID. Both IDs of Ensembl and UniProt are accepted. Default means using the values in the input data file. Users can also copy the part of them by clicking "Available vars". It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "Q9Y3X0,Q8N5I3,ENSP00000000233,E

Value

A list object containing the edges and nodes of the biological link.

Author(s)

Mingliang Fang, Bin Wang (corresponding author)

Examples

```
res = InitBioLink()
   res1 = LoadBioLink(PID = res$PID, UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
   res3 = BioLink(PID = res$PID, OutPath="default", Mode = "PPI", ChemCas = "default",
   ChemInchikey = "default",DiseaseID = "default",MetabolomeID = "default",
   MetBiospec = "blood", ProteomeID = "default")
```

ConvToExpoID *Convert different IDs to the unified ExposomeX IDs*

Description

Convert the IDs of exposure, chemicals, metabolites, or proteins to the unified ExposomeX ID, i.e., unified identifier in ExposomeX platform

Usage

```
ConvToExpoID(PID, OutPath="default")
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by InitBioLink.
OutPath	chr. Output file directory, e.g. "D:/test". It should be noted that the slash symbol is "/", not "\". If "default", the current working directory will be set

Value

A data frame containing the converted ID information

Author(s)

Mingliang Fang, Weinan Lin, Bin Wang (corresponding author)

Examples

```
res = InitBioLink()
   res1 = LoadBioLink(PID = res$PID, UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
```

FuncExit *End the module analysis*

Description

End the module analysis

Usage

```
FuncExit(PID)
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by any initial functions.

Value

Exit status

Author(s)

Bin Wang (corresponding author)

Examples

```
res = InitBioLink()
   res = LoadBioLink(PID = res$PID,UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
   FuncExit(PID = res$PID)
```

InitBioLink *Initialize ExpoBioLink module*

Description

Initialize ExpoBioLink module analysis. It can generate an R6 class object integrating all the analysis information

Usage

```
InitBioLink()
```

Details

ExpoBioLink module is designed to find the biological relationships between exposure factors and health outcome. This module adopts the most frequently-used and authoritative databases, e.g., T3DB, CTD, ToxCast, StringDB, STITCH, KEGG, and GO.

Value

An R6 class object.

Author(s)

Mingliang Fang, Bin Wang,(corresponding author)

Examples

```
res <- InitBioLink()
```

`LoadBioLink` *Load data file for BioLink module*

Description

Load data file for BioLink module

Usage

```
LoadBioLink(PID, UseExample = "default", DataPath=NULL)
```

Arguments

`PID`	chr. Program ID. It must be the same with the PID generated by InitBioLink.
`UseExample`	chr. Method of uploading data. If "default",user should upload their own data files, or use "example#1" provided by this module.
`DataPath`	chr. Input file directory, e.g. "D:/test/eg_biolink.xlsx". It should be noted that the slash symbol is "/", not "\"

Value

An R6 class object containing the input data.

Author(s)

Mingliang Fang, Bin Wang (corresponding author)

Examples

```
res <- InitBioLink()
   res = LoadBioLink(PID = res$PID, UseExample = "example#1")
```

VizBioLink *Visualize the biological link*

Description

Visualize the biological link. It should be noted that the corresponding link has been built by BioLink function prior to using it

Usage

```
VizBioLink(PID, OutPath="default", Mode, Layout = "force-directed", Brightness = "dark", Palette = "def
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by InitBioLink.
OutPath	chr. Output file directory. e.g. "D:/test". It should be noted that the slash symbol is "/", not "\". If "default", the current working directory will be set.
Mode	chr. Method to build the biological link between exposures and diseases. Available options include "PPI" (i.e., protein-protein interaction) and "GO" (i.e., gene ontoloty).
Layout	chr. Visualization layout. Available options include "force-directed" and "degree-circle".
Brightness	chr. Visualization brightness. Available options include "light" and "dark".
Palette	chr. Visualization palette. Available options include "default1", "default2" and several journal preference styles (i.e., cell, nature, science, lancet, nejm, and jama).

Value

A list object containing the plot of the biological link. This plot can be further processed using ggplot2 package.

Author(s)

Mingliang Fang, Ning Gao, Bin Wang (corresponding author)

Examples

```
res = InitBioLink()
   res1 = LoadBioLink(PID = res$PID,UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
   res3 = BioLink(PID = res$PID, OutPath="default", Mode = "PPI", ChemCas = "default",
   ChemInchikey = "default",DiseaseID = "default",MetabolomeID = "default",
   MetBiospec = "blood", ProteomeID = "default")
   res4 = VizBioLink(PID = res$PID, Mode = 'PPI', Layout = "force-directed",
   Brightness = "dark", Palette = "default1")
```

Index