Package 'exdb'

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Title To explore the data, as well as facilitating to find the biological relationship between exposure and diseases from the perspective of bioinformatics.

Version 1.0.0

Description A convenient tool to explore the data, as well as facilitating to find the biological relationship between exposure and diseases from the perspective of bioinformatics. This module adopts the most frequently-used and authoritative databases, e.g., T3DB, CTD, ToxCast, StringDB, STITCH, KEGG, and GO.

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R topics documented:

ExpoAbbr *Explain the abbreviations*

Description

Explain the abbreviations in ExposomeX platform

Usage

```
ExpoAbbr(PID, OutPath = "default", Keys)
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by ExpoDB
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.
Keys	chr. Any keywords to search. "default" means using the values . in the input data file. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "EpiDesign,Cros,Cohort".

Value

A data frame

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   res2 = ExpoAbbr(PID=res$PID, Keys = "default")
   FuncExit(PID = res$PID)
```

ExpoAnno *Annotate the non-targeted features*

Description

Annotate the non-targeted features from high-resolution mass spectrometry

Usage

```
ExpoAnno(PID, OutPath = "default", MassToCharge, AdductPos,
   AdductNeg, Accuracy = 1)
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by ExpoDB
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.
MassToCharge	chr. Mass to charge ratio (m/z). It ranges 50-1000. If "default", the values in the input data file are used. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "150,200,210".
AdductPos	chr. Adducts collected in the positive mode. If "default", the values in the input data file are chosen. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "M+H+Na,M+2ACN+2H,M+DMSO+H". All the positive abducts are M+3ACN+2H,M+ACN+H,M+NH4,M+2ACN+2H,M+2H,M+3H,M+3Na, "M+2Na-H,M+ACN+Na,M+H+Na,M+2K-H,M+H+NH4,2M+K,M+K,2M+NH4,2M+Na,M+2Na,M+D M+2ACN+H,M+IsoProp+Na+H,M+2H+Na,M+ACN+2H,M+H,2M+H,M+CH3OH+H,M+H+2Na,M+N 2M+ACN+H,2M+ACN+Na,M+IsoProp+H,M+H+K"
AdductNeg	chr. Adducts collected in the negative mode. If "default", the values in the input data file are chosen. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "M+Hac-H,M-2H,M-H2O-H". All the negative abducts are "M+FA-H,M+Hac-H,M+Br,3M-H,2M+Hac-H,M+K-2H,2M+FA-H, M-H,M-H2O-H,M+Na-2H,M-2H,M+TFA-H,M+Cl,M-3H,2M-H".
Accuracy	num. Upper limit of accuracy to match the target molecular.

Value

A data frame

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   res6 = ExpoAnno(PID=res$PID, MassToCharge = "default", AdductPos = "all",
   AdductNeg = "all", Accuracy = 5)
   FuncExit(PID = res$PID)
```

ExpoConv *Convert keywords*

Description

Convert the keywords from different sources in ExposomeX platform.

Usage

```
ExpoConv(PID, OutPath = "default", From, To, Keys)
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by ExpoDB
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.
From	chr. Choose the search range of the convert direction for the concerned keywords (from -> to). Options include "chemical" <-> "cas.rn" (Chemical name <-> CAS Registry Number), "inchikey" <-> "chemical" (InChIKey <-> Chemical name), "metabolite" <-> "kegg.entry" (Metabolite name <-> InChIKey), "kegg.entry" <-> "metabolite" (KEGG Entry ID <-> Metabolite name), "protein" <-> "uniprot" (protein name <-> UniProt ID), "uniprot" <-> "ensembl" (UniProt ID <-> Chemical name), "enzyme" <-> "uniprot" (Enzyme name <-> UniProt ID), "disease" <-> "disease.id" (Disease <-> Disease.id)
To	chr. see "from".
Keys	chr. Any keywords belong to the classes of "from" and "to" to search. "default" means using the values in the input data file. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "7440-43-9,OMIM:619217,zinc,GO:0010942".

Value

A data frame

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   res2 = ExpoConv(PID=res$PID, From = "chemical", To = "cas.rn", Keys = "default")
   FuncExit(PID = res$PID)
```

`ExpoDict` *Explain keywords*

Description

Explain the keyword in ExposomeX platform

Usage

```
ExpoDict(PID, OutPath = "default", Class, Keys)
```

Arguments

`PID`	chr. Program ID. It must be the same with the PID generated by ExpoDB
`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.
`Class`	chr. Choose the search range of the concerned keywords. Options include "chemical" (Some exposure factors may be a mixture of chemicals, e.g. PM2.5, tobacco smoking. As chemicals account for the majority, we use "Chemical" for convenience), "metabolite" (the chemicals used for metabolome analysis in the KEGG database), "protein", "enzyme" (referring in particular to the enzymes in the KEGG database), "disease", "GO" (gene ontology), and "ion.adduct" (the ion adducts in the liquid chromatograph-mass spectrometry).
`Keys`	chr. Any keywords to search. "default" means using the values in the input data file. Users can also enter the keywords here. It should be noted that there is fixed format for the entering characters separated with comma and without space, e.g., "7440-43-9,OMIM:619217,zinc,GO:0010942".

Value

A data frame

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   res2 = ExpoDict(PID=res$PID, Class = "GO", Keys = "default")
   FuncExit(PID = res$PID)
```

ExpoNexus *Find the nexuses between keywords*

Description

Find the nexuses between the keywords in ExposomeX platform. Nexus direction from keywords A (class A) to keywords B (class B)

Usage

```
ExpoNexus(PID, OutPath = "default", ClassA, ClassB,
   KeysA = "default", KeysB = "default")
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by ExpoDB
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.
ClassA	chr. Find the nexuses between the keywords in ClassA and ClassB. Options include "chemical" <-> "protein", "chemical" <-> "GO", "protein" <-> "protein", "disease" <-> "GO", "protein" <-> "disease"
ClassB	chr. See "ClassA".
KeysA	chr. The lowercases of name, alias, and ID of chemical, metabolite, protein, and enzyme are all accepted. e.g., "7440-43-9,OMIM:619217,zinc,GO:0010942".
KeysB	chr. See "KeysA".

Value

A data frame

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   res2 = ExpoNexus(PID=res$PID, ClassA = "chemical", ClassB = "protein",
   KeysA = "default", KeysB = "default")
   FuncExit(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 = InitDb()
   res = LoadDb(PID = res$PID, UseExample = "example#1")
   FuncExit(PID = res$PID)
```

InitDb *Initialize ExpoDB module*

Description

Initialize ExpoDB module analysis. It can generate an R6 class object.

Usage

```
InitDb()
```

Details

ExpoDB module is designed as a convenient tool to explore the data, as well as facilitating to find the biological relationship between exposure and diseases from the perspective of bioinformatics. 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)

Bin Wang (corresponding author)

Examples

```
res <- InitDb()
   FuncExit(PID = res$PID)
```

LoadDb *Load data file for ExpoDB module*

Description

Load data file for ExpoDB module

Usage

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

Arguments

PID	chr. Program ID. It must be the same with the PID generated by ExpoDB
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 directory of data file, e.g. "D:/test/eg_data_biolink.xlsx". It should be noted that the slash symbol is "/", not "\".

Value

An R6 class object containing the input data.

Author(s)

Bin Wang

Examples

```
res <- InitDb()
   res1 = LoadDb(PID = res$PID, UseExample = "example#1")
   FuncExit(PID = res$PID)
```

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