Package 'exhep'

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Title This package is to develop a machine learning model of random forest to predict blood concentrations of chemicals and prioritize chemicals of health concern

Version 1.0.0

Description
Quantification of all trace organics in the biological fluids seems impossible and costly, regardless of the high individual exposure variability. We hypothesized that the blood concentration of organic pollutants could be predicted via their exposure and chemical properties. Developing a prediction model on the annotation of chemicals in human blood can provide new insight into the distribution and extent of exposures to a wide range of chemicals in humans. Our objective of this module is to develop a machine learning model (eg., random forest) to predict blood concentrations of chemicals and prioritize chemicals of health concern.

Suggests ggplot2, httr, readxl, vroom, writexl

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R topics documented:

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 InitHEP.
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 = InitHEP()
   res1 = LoadHEP(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 = InitHEP()
   res = LoadHEP(PID = res$PID,UseExample = "example#1")
   FuncExit(PID = res$PID)
```

`InitHEP` *Initialize HExpPridict module*

Description

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

Usage

```
InitHEP()
```

Details

ExpoHExpPredict module is designed to predict blood concentrations of chemicals and prioritize chemicals of health concern.

Value

An R6 class object.

Author(s)

Mingliang Fang, Bin Wang,(corresponding author)

Examples

```
res <- InitHEP()
```

LoadHEP *Load data file for HExpPridict module*

Description

Load data file for HExpPridict module.

Usage

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

Arguments

PID	chr. Program ID. It must be the same with the PID generated by InitHEP.
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_hep.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 <- InitHEP()
   res = LoadHEP(PID = res$PID, UseExample = "example#1")
```

PredBlood *Predict blood concentrations of chemicals*

Description

Predict blood concentrations of chemicals

Usage

```
PredBlood(PID, OutPath="default",MC = "F",N=100)
```

Arguments

PID	chr. Program ID. It must be the same with the PID generated by InitHEP.
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.
MC	lgl. T (or TRUE) and F (or FALSE). Whether to perform Mentocaro simulation.
N	num. Times of Mentocaro simulation.

Value

A list object containing the prediction results.

Author(s)

Mingliang Fang, Bin Wang (corresponding author)

Examples

```
res = InitHEP()
   res1 = LoadHEP(PID = res$PID,UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
   res3 = PredBlood(PID = res$PID, OutPath="default", MC ='F',N=1000)
```

VizPredBlood *Visualize the PredBlood*

Description

Visualize the PredBlood.

Usage

```
VizPredBlood(PID,OutPath="default",Layout="forest",
    Brightness="light",Palette= "default1")
```

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.
Layout	chr. Visualization layout. Available options include "forest" and "boxplot".
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 = InitHEP()
   res1 = LoadHEP(PID = res$PID,UseExample = "example#1")
   res2 = ConvToExpoID(PID = res$PID)
   res3 = PredBlood(PID = res$PID, OutPath="default", MC ='F', N=1000)
   res4 = VizPredBlood(PID = res$PID, OutPath ="default",Layout="forest",
   Brightness="light",Palette= "science" )
```

Index