14 ExpoBioLink module

14.1 Application domain

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.

14.2 Theory

14.3 Work pipeline

Users can easily get the modeling results and their visualization plots of high quality by following the detailed instructions in each step. The biological relationships between exposures and health outcome are interpreted from the perspectives of protein-protein interaction (PPI) and gene ontology (GO).

```r
# The following two packages should be installed in advance
# devtools::install_github("ExposomeX/exbiolink", force = TRUE)
# devtools::install_github("ExposomeX/extidy", force = TRUE)

# library(exbiolink)
# library(extidy)
library(tidyverse)

# devtools::install_github("ExposomeX/exposomex", force = TRUE)
library(exposomex)
```

```r
res = InitBioLink()

res1 = LoadBioLink(PID=res$PID,
                   UseExample="example#1")
res1$Expo$Data
```

```
## # A tibble: 221 x 7
##     SerialNo FullName GroupName DiseaseID    ExposureID MetabolomeID ProteomeID
##     <chr>    <chr>    <chr>     <chr>        <chr>      <chr>        <chr>
##  1 Y1       CSNU     disease   OMIM:220100  <NA>       <NA>         <NA>
##  2 Y2       SCZD     disease   OMIM:181500  <NA>       <NA>         <NA>
##  3 Y3       TGCT     disease   OMIM:273300  <NA>       <NA>         <NA>
##  4 Y4       RASJ     disease   OMIM:604302  <NA>       <NA>         <NA>
##  5 Y5       HH3      disease   OMIM:244200  <NA>       <NA>         <NA>
##  6 Y6       DECRD    disease   OMIM:616034  <NA>       <NA>         <NA>
##  7 Y7       PMDS1    disease   OMIM:261550  <NA>       <NA>         <NA>
##  8 Y8       CRMCC2   disease   OMIM:617341  <NA>       <NA>         <NA>
##  9 Y9       FSHD1    disease   OMIM:158900  <NA>       <NA>         <NA>
## 10 Y10      RA       disease   OMIM:180300  <NA>       <NA>         <NA>
## # ... with 211 more rows
```

```r
res2 = ConvToExpoID(PID = res$PID,
                    OutPath = "default")
res2
```

```
## # A tibble: 221 x 8
##     SerialNo FullName GroupName DiseaseID    ExposureID MetabolomeID Prote~1 EX
##     <chr>    <chr>    <chr>     <chr>        <chr>      <chr>        <chr>   <chr>
##  1 Y1       CSNU     disease   OMIM:220100  <NA>       <NA>         <NA>    EX:D~
##  2 Y2       SCZD     disease   OMIM:181500  <NA>       <NA>         <NA>    EX:D~
```

```
##  3 Y3        TGCT    disease   OMIM:273300 <NA>      <NA>      <NA>      EX:D~
##  4 Y4        RASJ    disease   OMIM:604302 <NA>      <NA>      <NA>      EX:D~
##  5 Y5        HH3     disease   OMIM:244200 <NA>      <NA>      <NA>      EX:D~
##  6 Y6        DECRD   disease   OMIM:616034 <NA>      <NA>      <NA>      EX:D~
##  7 Y7        PMDS1   disease   OMIM:261550 <NA>      <NA>      <NA>      EX:D~
##  8 Y8        CRMCC2  disease   OMIM:617341 <NA>      <NA>      <NA>      EX:D~
##  9 Y9        FSHD1   disease   OMIM:158900 <NA>      <NA>      <NA>      EX:D~
## 10 Y10       RA      disease   OMIM:180300 <NA>      <NA>      <NA>      EX:D~
## # ... with 211 more rows, and abbreviated variable name 1: ProteomeID
```

```r
res3 = BioLink(PID = res$PID,
               OutPath = "default",
               Mode = "PPI",
               ChemCas = "default",
               ChemInchikey = "default",
               DiseaseID = "default",
               MetabolomeID = "default",
               MetBiospec = "blood",
               ProteomeID = "default")
res3$Edges
```

```
## # A tibble: 310 x 9
##     source    target     intera~1 sourc~2 targe~3 datab~4 edge_~5 sourc~6 targe~7
##     <chr>     <chr>      <chr>    <chr>   <chr>   <chr>     <dbl> <chr>   <chr>
##  1 EX:E00321 EX:P000667 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
##  2 EX:E00321 EX:P000608 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
##  3 EX:E00321 EX:P000493 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
##  4 EX:E00321 EX:P000687 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
##  5 EX:E03544 EX:P000608 Active   chemic~ protein toxcast       1 EX:E03~ EX:P00~
##  6 EX:E00321 EX:P000420 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
##  7 EX:E47866 EX:P000466 Active   chemic~ protein toxcast       1 EX:E47~ EX:P00~
##  8 EX:E04534 EX:P000298 Active   chemic~ protein toxcast       1 EX:E04~ EX:P00~
##  9 EX:E04534 EX:P166812 Active   chemic~ protein toxcast       1 EX:E04~ EX:P16~
## 10 EX:E00321 EX:P000153 Active   chemic~ protein toxcast       1 EX:E00~ EX:P00~
## # ... with 300 more rows, and abbreviated variable names 1: interaction,
## #   2: source.class, 3: target.class, 4: database, 5: edge_type,
## #   6: source.label, 7: target.label
```

```r
res3$Nodes
```

```
## # A tibble: 126 x 3
##    id        label group
##    <chr>     <chr> <chr>
##  1 EX:E00321 Hg    exposure
##  2 EX:P000667 CCL2 ppi
##  3 EX:P000608 PAI  ppi
##  4 EX:P000493 TPA  ppi
##  5 EX:P000687 T10  ppi
##  6 EX:E03544 Tcdd  exposure
##  7 EX:P000420 EPA  ppi
##  8 EX:E47866 Zmp   exposure
##  9 EX:P000466 NET  ppi
## 10 EX:E04534 Tg    exposure
## # ... with 116 more rows
```

```
res4 = VizBioLink(PID = res$PID,
                  OutPath = "default",
                  Mode = 'PPI',
                  Layout = "force-directed",
                  Brightness = "light",
                  Palette = "default1")
res4
```
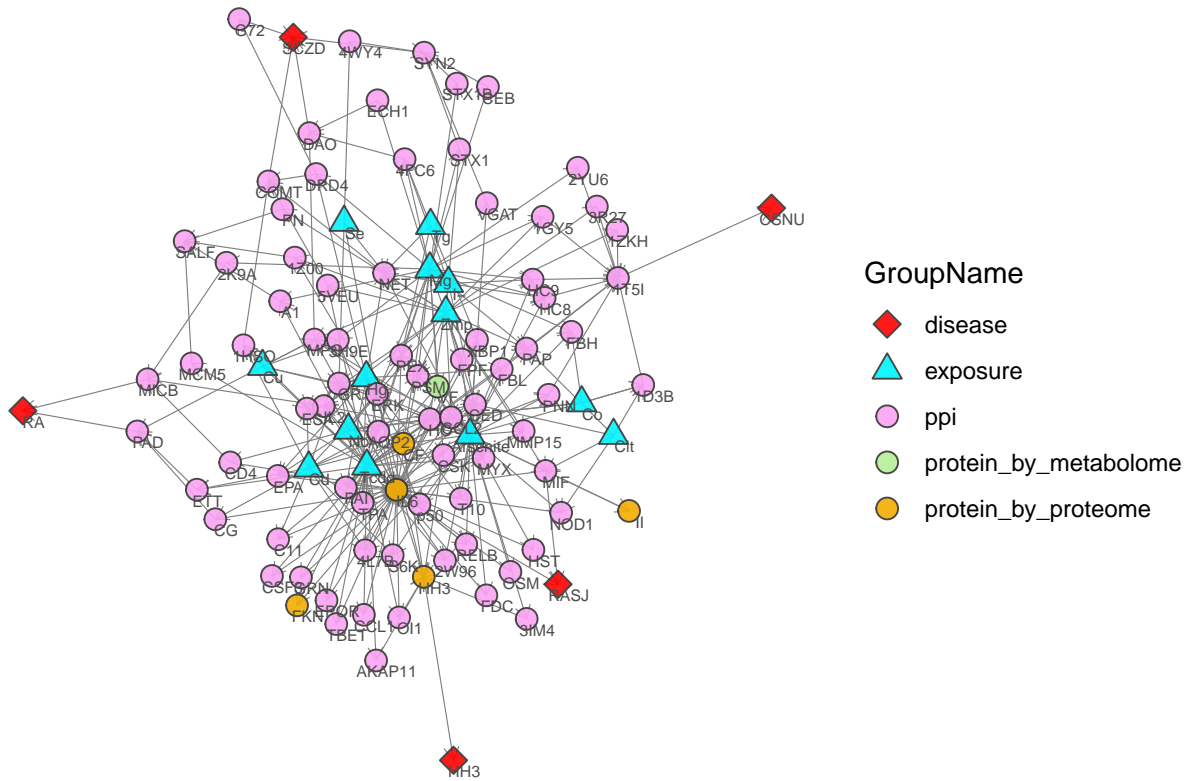


```
res5 = BioLink(PID = res$PID,
               OutPath = "default",
               Mode = "GO",
               ChemCas = "default",
               ChemInchikey = "default",
               DiseaseID = "default",
               MetabolomeID = "default",
               MetBiospec = "blood",
               ProteomeID = "default")
res5$Edges
```

```
## # A tibble: 13 x 7
##    source    target     interaction source.class target.class database edge_t~1
##    <chr>     <chr>      <chr>       <chr>         <chr>        <chr>       <dbl>
## 1 EX:E07343 GO:0006006 association chemical      GO           ctd             1
## 2 EX:E07343 GO:0005977 association chemical      GO           ctd             1
## 3 EX:E26544 GO:0006006 association chemical      GO           ctd             1
## 4 EX:E26544 GO:0006096 association chemical      GO           ctd             1
```

```
##  5 EX:E00033  GO:0043392 association chemical       GO          ctd              1
##  6 EX:E00033  GO:0055114 association chemical       GO          ctd              1
##  7 EX:E38567  GO:0006006 association chemical       GO          ctd              1
##  8 EX:E03544  GO:0006006 association chemical       GO          ctd              1
##  9 GO:0006006 EX:D12164  association GO             disease     ctd              2
## 10 GO:0005977 EX:D12164  association GO             disease     ctd              2
## 11 GO:0006096 EX:D12164  association GO             disease     ctd              2
## 12 GO:0043392 EX:D12164  association GO             disease     ctd              2
## 13 GO:0055114 EX:D12164  association GO             disease     ctd              2
## # ... with abbreviated variable name 1: edge_type
```

```
res5$Nodes
```

```
## # A tibble: 11 x 3
##    id         label                          group
##    <chr>      <chr>                          <chr>
##  1 EX:E07343  Arsenite                       exposure
##  2 GO:0006006 glucose metabolic process      go_by_proteome
##  3 GO:0005977 glycogen metabolic process     go_by_proteome
##  4 EX:E26544  Cd                             exposure
##  5 GO:0006096 glycolytic process             go_by_proteome
##  6 EX:E00033  Cu                             exposure
##  7 GO:0043392 negative regulation of DNA binding go_by_proteome
##  8 GO:0055114 oxidation-reduction process    go_by_proteome
##  9 EX:E38567  Se                             exposure
## 10 EX:E03544  Tcdd                           exposure
## 11 EX:D12164  neural tube defects            disease
```

```
res6 = VizBioLink(PID = res$PID,
                  OutPath = "default",
                  Mode = 'GO',
                  Layout = "force-directed",
                  Brightness = "dark",
                  Palette = "default1")
res6
```
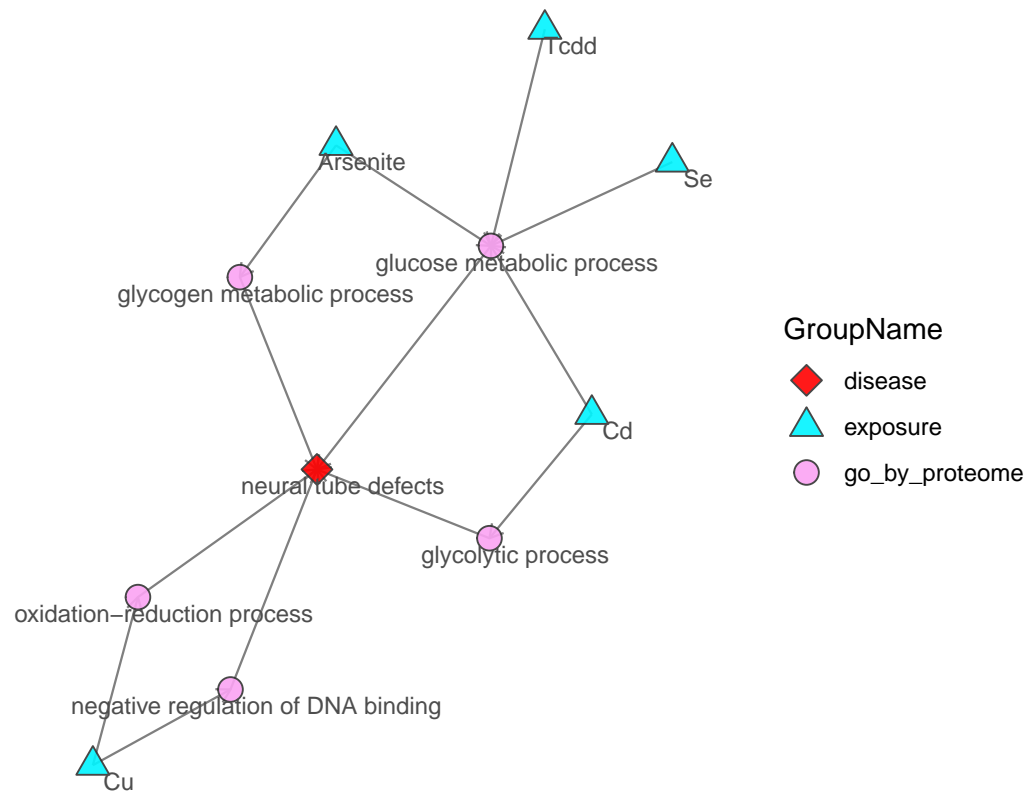
```
FuncExit(PID = res$PID)
```

[1] "Success to exit. Thanks for using ExposomeX platform!"