Gene identifiers and pathway annotation

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Intro

This markdown aims to collect entrez ids, ensemble protein ids and gene symbols in a single table

```
library(readr)
library(tidyr)
library(dplyr)
library(tidylog)
library(magrittr)
```

Neurotransmitter pathways annotation

Defining selected pathways

Genes to pathways relationships

Downloading table containing all genes and pathways relationships

```
if (!file.exists("entrez_to_pathway.tsv")) {
 download.file("http://rest.kegg.jp/link/pathway/hsa","entrez_to_pathway.tsv")
}
entrez_to_pathway <- read.table(</pre>
  "entrez_to_pathway.tsv"
  ,header = F
  ,stringsAsFactors = F
  ,col.names = c("entrez_id", "pathway_id")
  ,sep="\t"
# removing hsa prefix
entrez_to_pathway[, "entrez_id"] %<>% substring(5)
# exporting for package use
usethis::use_data(entrez_to_pathway, overwrite = TRUE)
## <U+2714> Setting active project to 'C:/R/neurotransmission'
## <U+2714> Saving 'entrez_to_pathway' to 'data/entrez_to_pathway.rda'
Filtering for genes in the selected pathways
gene_pathways <- inner_join(entrez_to_pathway, pathways) %>%
  mutate(n = 1) \%
  pivot_wider(
    id_cols = entrez_id,
    names_from = pathway_name,
    values_from = n,
   values_fn = list(n = length),
   values_fill = list(n = 0)
  ) %>%
  # filling 1's in all systems for synaptic vesicle genes
  mutate_at(pathways[["pathway_name"]], ~ ifelse(vesicle == 1, 1L, .)) %>%
  # neurotransmitter systems count for each gene (>=1, <= 5)</pre>
  mutate(system_count = rowSums(select(., -entrez_id, -vesicle)))
## Joining, by = "pathway_id"
## inner_join: added one column (pathway_name)
##
               > rows only in x (31,062)
##
               > rows only in y (
                                        0)
##
               > matched rows
                                      639
##
                                 =======
```

```
> rows total
                                     639
##
## mutate: new variable 'n' with one unique value and 0\% NA
## mutate_at: changed 69 values (18%) of 'glutamatergic' (0 new NA)
              changed 75 values (20%) of 'cholinergic' (0 new NA)
##
              changed 73 values (19%) of 'serotonergic' (0 new NA)
##
              changed 70 values (18%) of 'gabaergic' (0 new NA)
##
##
              changed 73 values (19%) of 'dopaminergic' (0 new NA)
## select: dropped 2 variables (entrez_id, vesicle)
## mutate: new variable 'system_count' with 5 unique values and 0% NA
usethis::use_data(gene_pathways, overwrite = TRUE)
## <U+2714> Saving 'gene_pathways' to 'data/gene_pathways.rda'
gene_pathways
## # / +ibbla: 382 ▼ 8
```

##	# 1	A tibble:	382 x 8					
##		entrez_i	d vesicle	glutamatergic	cholinergic	${\tt serotonergic}$	gabaergic	
##		<chr></chr>	<int></int>	<int></int>	<int></int>	<int></int>	<int></int>	
##	1	10312	1	1	1	1	1	
##	2	10497	1	1	1	1	1	
##	3	10814	1	1	1	1	1	
##	4	10815	1	1	1	1	1	
##	5	112755	1	1	1	1	1	
##	6	1173	1	1	1	1	1	
##	7	1175	1	1	1	1	1	
##	8	1211	1	1	1	1	1	
##	9	1212	1	1	1	1	1	
##	10	1213	1	1	1	1	1	
##	# .	with	372 more 1	rows, and 2 mor	re variables	: dopaminergio	c <int>,</int>	
##	# # system_count <dbl></dbl>							

Base ID lookup table

Entrez to STRING

 $Downloading\ entrez\ to\ string\ mapping\ table\ directly\ from\ STRING\ https://string-db.org/mapping_files/entrez/$

```
if (!file.exists("human.entrez_2_string.2018.tsv.gz")) {
  download.file(
    "https://string-db.org/mapping_files/entrez/human.entrez_2_string.2018.tsv.gz",
    "human.entrez_2_string.2018.tsv.gz"
  )
}
entrez_to_string <- read_tsv(</pre>
  gzfile("human.entrez_2_string.2018.tsv.gz"),
  skip = 1,
  col_names = c("entrez_id", "string_id"),
  col_types = cols_only("-", "c", "c")
gene_ids <- gene_pathways %>% select(entrez_id) %>% left_join(entrez_to_string)
## select: dropped 7 variables (vesicle, glutamatergic, cholinergic, serotonergic, gabaergic, ...)
## Joining, by = "entrez_id"
## left_join: added one column (string_id)
##
              > rows only in x
                                     11
              > rows only in y (18,222)
##
              > matched rows
##
                                    371
##
                                =======
              > rows total
                                    382
##
gene_ids
## # A tibble: 382 x 2
##
      entrez_id string_id
##
      <chr>
                <chr>>
   1 10312
                9606.ENSP00000265686
##
## 2 10497
                9606.ENSP00000367756
## 3 10814
                9606.ENSP00000352544
## 4 10815
                9606.ENSP00000305613
## 5 112755
                9606.ENSP00000215095
## 6 1173
                9606.ENSP00000292807
## 7 1175
                9606.ENSP00000263270
## 8 1211
                9606.ENSP00000242285
## 9 1212
                9606.ENSP00000309415
## 10 1213
                9606.ENSP00000479606
## # ... with 372 more rows
```

STRING names

9 1212

10 1213

... with 372 more rows

Downloading string names mapping table directly from STRING https://string-db.org/mapping_files/entrez/

```
if (!file.exists("human.name 2 string.tsv.gz")) {
  download.file(
    "https://string-db.org/mapping_files/STRING_display_names/human.name_2_string.tsv.gz",
    "human.name 2 string.tsv.gz"
 )
}
string_names <- read_tsv(</pre>
  gzfile("human.name_2_string.tsv.gz"),
 skip = 1,
 col_names = c("string_name", "string_id"),
  col_types = cols_only("-", "c", "c")
gene_ids %<>% left_join(string_names)
## Joining, by = "string_id"
## left_join: added one column (string_name)
##
              > rows only in x
                                     11
              > rows only in y (18,724)
##
##
              > matched rows
                                     371
##
                                =======
##
              > rows total
                                    382
gene_ids
## # A tibble: 382 x 3
##
      entrez_id string_id
                                     string_name
##
               <chr>
      <chr>
                                     <chr>>
   1 10312
                9606.ENSP00000265686 TCIRG1
##
## 2 10497
                9606.ENSP00000367756 UNC13B
## 3 10814
                9606.ENSP00000352544 CPLX2
## 4 10815
                9606.ENSP00000305613 CPLX1
## 5 112755
                9606.ENSP00000215095 STX1B
## 6 1173
                9606.ENSP00000292807 AP2M1
## 7 1175
                9606.ENSP00000263270 AP2S1
## 8 1211
                9606.ENSP00000242285 CLTA
```

9606.ENSP00000309415 CLTB

9606.ENSP00000479606 CLTC

Entrez names

Downloading gene symbols mapping table directly from NCBI's FTP ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/GENE_INFO/Mammalia/

```
if (!file.exists("Homo_sapiens.gene_info.gz")) {
 download.file(
    "ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/GENE_INFO/Mammalia/Homo_sapiens.gene_info.gz",
    "Homo_sapiens.gene_info.gz"
 )
}
entrez_names <- read_tsv(</pre>
 gzfile("Homo_sapiens.gene_info.gz"),
 skip = 1,
 col_names = c("entrez_id", "entrez_name"),
 col_types = cols_only("-", "c", "c")
)
## Warning: 61645 parsing failures.
## row col expected actual
                                       file
   1 -- 3 columns 16 columns <connection>
   2 -- 3 columns 16 columns <connection>
##
   3 -- 3 columns 16 columns <connection>
    4 -- 3 columns 16 columns <connection>
##
   5 -- 3 columns 16 columns <connection>
## ... ... ... .... ..... .....
## See problems(...) for more details.
gene_ids %<>% left_join(entrez_names)
## Joining, by = "entrez_id"
## left join: added one column (entrez name)
##
             > rows only in x
                                     0
             > rows only in y (61,263)
##
                                   382
##
             > matched rows
##
                                   382
##
             > rows total
gene_ids
## # A tibble: 382 x 4
     entrez_id string_id
                                    string_name entrez_name
     <chr> <chr>
##
                                    <chr>
                                                <chr>
```

```
9606.ENSP00000265686 TCIRG1
  1 10312
                                                 TCIRG1
##
   2 10497
                9606.ENSP00000367756 UNC13B
                                                 UNC13B
##
  3 10814
                9606.ENSP00000352544 CPLX2
                                                 CPLX2
## 4 10815
                9606.ENSP00000305613 CPLX1
                                                 CPLX1
## 5 112755
                9606.ENSP00000215095 STX1B
                                                 STX1B
  6 1173
                9606.ENSP00000292807 AP2M1
                                                 AP2M1
##
   7 1175
                9606.ENSP00000263270 AP2S1
                                                 AP2S1
##
## 8 1211
                9606.ENSP00000242285 CLTA
                                                 CLTA
## 9 1212
                9606.ENSP00000309415 CLTB
                                                 CLTB
## 10 1213
                9606.ENSP00000479606 CLTC
                                                 CLTC
## # ... with 372 more rows
```

Updating missing info

Printing incomplete rows

```
gene_ids[!complete.cases(gene_ids),]
```

```
## # A tibble: 11 x 4
##
      entrez_id string_id string_name entrez_name
##
      <chr>
                <chr>
                           <chr>
                                       <chr>
##
  1 9296
                <NA>
                           <NA>
                                       ATP6V1F
  2 100137049 <NA>
                           <NA>
                                       PLA2G4B
  3 85358
                <NA>
                           <NA>
                                       SHANK3
##
## 4 8681
                <NA>
                           <NA>
                                       JMJD7-PLA2G4B
##
  5 1139
                <NA>
                           <NA>
                                       CHRNA7
  6 107987478 <NA>
                           <NA>
                                       LOC107987478
                                       L0C107987479
  7 107987479 <NA>
                           <NA>
##
                                       CYP2D7
## 8 1564
                <NA>
                           <NA>
## 9 801
                <NA>
                           <NA>
                                       CALM1
## 10 805
                <NA>
                           <NA>
                                       CALM2
## 11 808
                <NA>
                           <NA>
                                       CALM3
```

Incomplete rows are filled manually

```
complete_info <- tribble(</pre>
  ~entrez_id,
                  ~string_id,
                                              ~string_name,
                                                                  ~entrez_name,
   "9296",
                   "9606.ENSP00000417378",
                                               "ATP6V1F",
                                                                   "ATP6V1F",
   "100137049",
                   "9606.ENSP00000396045",
                                               "PLA2G4B",
                                                                   "PLA2G4B",
   "85358",
                                                                   "SHANK3",
                   "9606.ENSP00000371886",
                                               "JMJD7-PLA2G4B",
                                                                   "JMJD7-PLA2G4B",
   "8681",
   "1139",
                   "9606.ENSP00000407546",
                                               "CHRNA7",
                                                                   "CHRNA7",
                                                                   "LOC107987478",
   "107987478",
                   NA,
                                               NA,
   "107987479",
                                                                   "LOC107987479",
                   NA,
                                               NA,
   "1564",
                                               NA,
                                                                   "CYP2D7",
   "801",
                   "9606.ENSP00000349467",
                                               "CALM1",
                                                                   "CALM1",
   "805",
                   "9606.ENSP00000272298",
                                               "CALM2",
                                                                   "CALM2",
                                               "CALM3",
                                                                   "CALM3"
   "808",
                   "9606.ENSP00000291295",
)
# removing incomplete cases and adding updated ones
gene_ids %<>% na.omit %>% bind_rows(complete_info)
```

Exporting base table for package use

```
usethis::use_data(gene_ids, overwrite = TRUE)
```

<U+2714> Saving 'gene_ids' to 'data/gene_ids.rda'