

UniProt.ws: A package for retrieving data from the UniProt web service

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1 Configuring `uniport.ws`

The *UniProt.ws* package provides a `select` interface to the UniProt web service.

```
suppressPackageStartupMessages({
  library(UniProt.ws)
})
up <- UniProt.ws(taxId=9606)
```

If you already know about the `select` interface, you can immediately learn about the various methods for this object by just looking at its help page.

```
help("UniProt.ws")
```

When you load the *UniProt.ws* package, it creates a `UniProt.ws` object. If you look at the object you will see some helpful information about it.

```
up
## "UniProt.ws" object:
## An interface object for UniProt web services
## Current Taxonomy ID:
## 9606
## Current Species name:
## Homo sapiens
## To change Species see: help('availableUniprotSpecies')
```

By default, you can see that the `UniProt.ws` object is set to retrieve records from *Homo sapiens*. But you can change that of course. In order to change it, you first need to look up the appropriate taxonomy ID for the species that you are interested in. UniProt provides support for over 20 thousand species, so there are a few to choose from! In order to make this easier, we have provided the helper function `availableUniprotSpecies` which will list all the supported species along with their taxonomy ids. When you call the `availableUniprotSpecies` function, it's recommended that you make use of the `pattern` argument to limit your queries like this:

```
availableUniprotSpecies(pattern="musculus")
##   taxon ID      Species name
## 1   520121      Anthocoris musculus
## 2   208057      Anthoscopus musculus
```

UniProt.ws: A package for retrieving data from the UniProt web service

```
## 3 238007 Apomys musculus
## 4 213557 Baiomys musculus
## 5 9771 Balaenoptera musculus
## 6 197864 Blepharisma musculus
## 7 10090 Mus musculus
## 8 35531 Mus musculus bactrianus
## 9 10091 Mus musculus castaneus
## 10 57486 Mus musculus molossinus
## 11 1891730 Mus musculus polyomavirus 1
```

Once you have learned the taxonomy ID for the species of interest, you can then change the taxonomy id for the `UniProt.ws` object using `taxId` setter or by calling the constructor for `UniProt.ws`

```
mouseUp <- UniProt.ws(10090)
mouseUp
## "UniProt.ws" object:
## An interface object for UniProt web services
## Current Taxonomy ID:
## 10090
## Current Species name:
## Mus musculus
## To change Species see: help('availableUniprotSpecies')
```

As you can see the species is different for the `mouseUp` new object.

2 Using UniProt.ws

Once you are satisfied that you have an `uniprot.ws` that is using the appropriate organisms, you can make use of the standard set of methods in a `select` interface. Specifically: `columns`, `keytypes`, `keys` and `select`.

You will probably notice that there are a large number of columns that can be retrieved.

```
head(keytypes(up))
## [1] "AARHUS/GHENT-2DPAGE" "AGD" "ALLERGOME"
## [4] "ARACHNOSERVER" "BIOCYC" "CGD"
```

And most (but not all) of these fields can also be used as keytypes.

```
head(columns(up))
## [1] "3D" "AARHUS/GHENT-2DPAGE" "AGD"
## [4] "ALLERGOME" "ARACHNOSERVER" "BIOCYC"
```

If necessary you can also look up the keys of a given type. But please be warned that the web service is slow at this particular kind of lookup. So if you really want to do this kind of operation you are probably going to want to save the result to your R session.

UniProt.ws: A package for retrieving data from the UniProt web service

```
egs = keys(up, "ENTREZ_GENE")
```

Finally, you can loop up whatever combinations of columns, keytypes and keys that you need when using `select`.

```
keys <- c("1", "2")
columns <- c("PDB", "HGNC", "SEQUENCE")
kt <- "ENTREZ_GENE"
res <- select(up, keys, columns, kt)

## Getting mapping data for 1 ... and ACC
## Getting mapping data for P04217 ... and PDB_ID
## Getting mapping data for P04217 ... and HGNC_ID
## Getting extra data for P04217, V9HWD8, P01023
## 'select()' returned 1:many mapping between keys and columns

res

##  ENTREZ_GENE  PDB  HGNC
## 1           1 <NA> HGNC:5
## 2           1 <NA> <NA>
## 3           2 1BV8 HGNC:7
## 4           2 2P9R HGNC:7
## 5           2 4ACQ HGNC:7
##
## 1
## 2
## 3 MGKNKLLHPSLVLLLLLVLLPTDASVSGKPQYMLVPSLLHTTETTEKGCVLLSYLNETVTVSASLESVRGNRSLFTDLEAENDVLHCVAFAVPKSSSNEEVMFL
## 4 MGKNKLLHPSLVLLLLLVLLPTDASVSGKPQYMLVPSLLHTTETTEKGCVLLSYLNETVTVSASLESVRGNRSLFTDLEAENDVLHCVAFAVPKSSSNEEVMFL
## 5 MGKNKLLHPSLVLLLLLVLLPTDASVSGKPQYMLVPSLLHTTETTEKGCVLLSYLNETVTVSASLESVRGNRSLFTDLEAENDVLHCVAFAVPKSSSNEEVMFL
```

sessionInfo()

```
sessionInfo()

## R version 4.0.3 (2020-10-10)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Ubuntu 18.04.5 LTS
##
## Matrix products: default
## BLAS: /home/biocbuild/bbs-3.12-bioc/R/lib/libRblas.so
## LAPACK: /home/biocbuild/bbs-3.12-bioc/R/lib/libRlapack.so
##
## locale:
## [1] LC_CTYPE=en_US.UTF-8 LC_NUMERIC=C
## [3] LC_TIME=en_US.UTF-8 LC_COLLATE=C
## [5] LC_MONETARY=en_US.UTF-8 LC_MESSAGES=en_US.UTF-8
## [7] LC_PAPER=en_US.UTF-8 LC_NAME=C
```

UniProt.ws: A package for retrieving data from the UniProt web service

```
## [9] LC_ADDRESS=C          LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] parallel stats graphics grDevices utils datasets methods
## [8] base
##
## other attached packages:
## [1] UniProt.ws_2.30.0 BiocGenerics_0.36.0 RCurl_1.98-1.2
## [4] RSQLite_2.2.1
##
## loaded via a namespace (and not attached):
## [1] Rcpp_1.0.5          highr_0.8           compiler_4.0.3
## [4] pillar_1.4.6       BiocManager_1.30.10 dbplyr_1.4.4
## [7] bitops_1.0-6       tools_4.0.3         digest_0.6.27
## [10] bit_4.0.4          evaluate_0.14       memoise_1.1.0
## [13] BiocFileCache_1.14.0 tibble_3.0.4        lifecycle_0.2.0
## [16] pkgconfig_2.0.3    rlang_0.4.8         DBI_1.1.0
## [19] curl_4.3           yaml_2.2.1          xfun_0.19
## [22] httr_1.4.2         dplyr_1.0.2         stringr_1.4.0
## [25] knitr_1.30         rappdirs_0.3.1     generics_0.1.0
## [28] vctrs_0.3.4       S4Vectors_0.28.0   IRanges_2.24.0
## [31] tidyselect_1.1.0   stats4_4.0.3        bit64_4.0.5
## [34] glue_1.4.2         Biobase_2.50.0      R6_2.5.0
## [37] AnnotationDbi_1.52.0 rmarkdown_2.5       purrr_0.3.4
## [40] blob_1.2.1         magrittr_1.5        htmltools_0.5.0
## [43] ellipsis_0.3.1    assertthat_0.2.1   BiocStyle_2.18.0
## [46] stringi_1.5.3      crayon_1.3.4
```