

rpx: an *R* interface to the ProteomeXchange repository

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1 Introduction

The goal of the *rpx* package is to provide programmatic access to proteomics data from *R*, in particular to the ProteomeXchange¹ (PX) central repository (see <http://www.proteomexchange.org/> and <http://central.proteomexchange.org/>). Additional repositories are likely to be added in the future.

2 The *rpx* package

PXDataset objects

The central object that handles data access is the `PXDataset` class. Such an instance can be generated by passing a valid PX experiment identifier to the `PXDataset` constructor.

```
library("rpx")
id <- "PXD000001"
px <- PXDataset(id)
px

## Object of class "PXDataset"
## Id: PXD000001 with 12 files
## [1] 'F063721.dat' ... [12] 'generated'
## Use 'pxfiles(.)' to see all files.
```

*<http://cpu.sysbiol.cam.ac.uk>

¹ Vizcaino J.A. et al. *ProteomeXchange: globally co-ordinated proteomics data submission and dissemination*, Nature Biotechnology 2014, 32, 223 – 226, doi:10.1038/nbt.2839.

Data and meta-data

Several attributes can be extracted from an PXDataset instance, as described below.

The experiment identifier, that was originally used to create the PXDataset instance can be extracted with the pxid method:

```
pxid(px)
## [1] "PXD0000001"
```

The file transfer url where the data files can be accessed can be queried with the pxurl method:

```
pxurl(px)
## [1] "ftp://ftp.pride.ebi.ac.uk/pride/data/archive/2012/03/PXD0000001"
```

The species the data has been generated the data can be obtain calling the pxtax function:

```
pxtax(px)
## [1] "Erwinia carotovora"
```

Relevant bibliographic references can be queried with the pxref method:

```
strwrap(pxref(px))
## [1] "Gatto L, Christoforou A. Using R and Bioconductor for proteomics data analysis."
## [2] "Biochim Biophys Acta. 2014 Jan;1844(1 Pt A):42-51. Review"
```

All files available for the PX experiment can be obtained with the pxfiles method:

```
pxfiles(px)
## [1] "F063721.dat"
## [2] "F063721.dat-mztab.txt"
## [3] "PRIDE_Exp_Complete_Ac_22134.xml.gz"
## [4] "PRIDE_Exp_mzData_Ac_22134.xml.gz"
## [5] "PXD0000001-mztab.txt"
## [6] "README.txt"
## [7] "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01-20141210.mzML"
## [8] "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01-20141210.mzXML"
## [9] "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzXML"
## [10] "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.raw"
## [11] "erwinia_carotovora.fasta"
## [12] "generated"
```

The complete or partial data set can be downloaded with the pxget function. The function takes an instance of class PXDataset as first mandatory argument.

The next argument, list, specifies what files to download. If missing, a menu is printed and the user can select a file. If set to "all", all files of the experiment are downloaded in the working directory.

Alternatively, numerics or logicals can also be used to subset the relevant files to be downloaded based on the `pxfiles(.)` output.

The last argument, `force`, can be set to `TRUE` to force the download of files that already exists in the working directory.

```
pxget(px, "erwinia_carotovora.fasta")
## Downloading 1 file
dir(pattern = "fasta")
## [1] "erwinia_carotovora.fasta"
```

By default, `pxget` will not download and overwrite a file if already available. The last argument of `pxget`, `force`, can be set to `TRUE` to force the download of files that already exists in the working directory.

```
(i <- grep("fasta", pxfiles(px)))
## [1] 11
pxget(px, i) ## same as above
## Downloading 1 file
## erwinia_carotovora.fasta already present.
```

Finally, a list of recent PX additions and updates can be obtained using the `pxannounced()` function:

```
pxannounced()
## 15 new ProteomeXchange announcements
```

	Data.Set	Publication.Data	Message
## 1	PXD004959	2017-03-31 13:21:40	New
## 2	PXD004818	2017-03-31 11:27:32	New
## 3	PXD004911	2017-03-31 08:21:34	New
## 4	PXD005080	2017-03-31 08:17:41	New
## 5	PXD004962	2017-03-31 08:16:03	New
## 6	PXD005946	2017-03-31 07:31:04	New
## 7	PXD005173	2017-03-31 07:20:21	Updated information
## 8	PXD005172	2017-03-31 07:19:24	Updated information
## 9	PXD005176	2017-03-31 07:18:34	Updated information
## 10	PXD005174	2017-03-31 07:16:49	Updated information
## 11	PXD005177	2017-03-31 07:15:52	Updated information
## 12	PXD005171	2017-03-31 07:14:09	Updated information
## 13	PXD005175	2017-03-31 07:13:11	Updated information
## 14	PXD005163	2017-03-31 07:12:20	Updated information
## 15	PXD005159	2017-03-31 07:09:04	Updated information

A simple use-case

Below, we show how to automate the extraction of files of interest (fasta and mzTab files), download them and read them using appropriate Bioconductor infrastructure. (Note that we read version 0.9 of the MzTab format below. For recent data, the version argument would be omitted.)

```
(mzt <- grep("F0.+mztab", pxfiles(px), value = TRUE))
## [1] "F063721.dat-mztab.txt"

(fas <- grep("fasta", pxfiles(px), value = TRUE))
## [1] "erwinia_carotovora.fasta"

pxget(px, c(mzt, fas))

## Downloading 2 files
## erwinia_carotovora.fasta already present.

library("Biostrings")
readAAStringSet(fas)

## A AAStringSet instance of length 4499
##      width seq                                     names
## [1] 148 MADITLISGSTLGSAEYVAEHLAEELLE...IDITQHQIPEDPAEEWLGSWVNLLK
##      ECA0001 putative ...
## [2] 154 VAEIYQIDNLDRGILSALMENARTPYA...QTIDEIQSTETLISLQNPIMRTIAP
##      ECA0002 AsnC-fami...
## [3] 331 MKKQYIEKQQQISFVKSSFSSQLEQLL...QLPHIGVQCGVWPQPLRESVSGLL
##      ECA0003 putative ...
## [4] 493 MITLESLEMLLSIDENELLDLVVTLM...FDHIWRFDTGLKSRLMRRWQH GKAY
##      ECA0004 conserved...
## [5] 500 MRQTAALAERISRLSHALEHGLYERQH...SEWLAKIEASLQQVAEQIQQSEQQD
##      ECA0005 conserved...
## ... ..
## [4495] 645 MSDKIIHLTDDSFDTDVLKADGAILVD...WISVRRKVDPLRVFASDMARRLELL
##      trx-rv3790 trx-rv...
## [4496] 95 MTKMNNKARRTARELKHLGASIQTTSL...PALYREL RDEFPMGYLG DYKDDDDK
##      TimBlower TimBlower

## [4497] 315 MFSNLSKRWAQRTLKSFYSTATGAAS...WVKKFKWAGIKTRKF
##      VFNPPKPRK
##      sp|P07143|CY1_YEA...
## [4498] 235 FPTDDDDKIVGGYTCAANSIPYQVSLN...QKNKPGVYTKVCNYVNWIIQQTIAAN
##      sp|P00761|TRYP_PI...
## [4499] 271 GVSGSCNIDVVCPEGNGHRDVIRSVAA...LSDWLDAAGTGAQFIDGLDSTGTPPV sp|Q7M135|LYSC_LY...

library("MSnbase")
(x <- readMzTabData(mzt, "PEP", version = "0.9"))
```

```
## Detected a metadata section
## Detected a peptide section
## MSnSet (storageMode: lockedEnvironment)
## assayData: 1528 features, 6 samples
##   element names: exprs
## protocolData: none
## phenoData
##   sampleNames: sub[1] sub[2] ... sub[6] (6 total)
##   varLabels: abundance
##   varMetadata: labelDescription
## featureData
##   featureNames: 1 2 ... 1528 (1528 total)
##   fvarLabels: sequence accession ... uri (14 total)
##   fvarMetadata: labelDescription
## experimentData: use 'experimentData(object)'
## Annotation:
## - - - Processing information - - -
## mzTab read: Fri Mar 31 19:38:55 2017
## MSnbase version: 2.0.2

head(exprs(x))

##      sub[1]   sub[2]   sub[3]   sub[4]   sub[5]   sub[6]
## 1 10630132 11238708 12424917 10997763  9928972 10398534
## 2 11105690 12403253 13160903 12229367 11061660 10131218
## 3  1183431  1322371  1599088  1243715  1306602  1159064
## 4  5384959  5508454  6883086  6136023  5626680  5213771
## 5 18033537 17926487 21052620 19810368 17381162 17268329
## 6  9873585 10299931 11142071 10258214  9664315  9518271

head(fData(x)[, 1:2])

##      sequence accession
## 1    DGVSVAR    ECA0625
## 2    NVVLDK    ECA0625
## 3 VEDALHATR    ECA0625
## 4 LAGGVAVIK    ECA0625
## 5  LIAEAMEK    ECA0625
## 6  SFGAPTITK    ECA0625
```

3 Session information

- R version 3.3.3 (2017-03-06), x86_64-w64-mingw32

- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, stats4, utils
- Other packages: Biobase 2.34.0, BiocGenerics 0.20.0, BiocParallel 1.8.1, Biostrings 2.42.1, IRanges 2.8.2, MSnbase 2.0.2, ProtGenerics 1.6.0, Rcpp 0.12.10, S4Vectors 0.12.2, XVector 0.14.1, mzR 2.8.1, rpx 1.10.2
- Loaded via a namespace (and not attached): BiocInstaller 1.24.0, BiocStyle 2.2.1, MALDIquant 1.16.1, RCurl 1.95-4.8, XML 3.98-1.5, affy 1.52.0, affyio 1.44.0, assertthat 0.1, bitops 1.0-6, codetools 0.2-15, colorspace 1.3-2, digest 0.6.12, doParallel 1.0.10, evaluate 0.10, foreach 1.4.3, ggplot2 2.2.1, grid 3.3.3, gtable 0.2.0, highr 0.6, impute 1.48.0, iterators 1.0.8, knitr 1.15.1, lattice 0.20-35, lazyeval 0.2.0, limma 3.30.13, magrittr 1.5, munsell 0.4.3, mzID 1.12.0, pcaMethods 1.66.0, plyr 1.8.4, preprocessCore 1.36.0, reshape2 1.4.2, scales 0.4.1, stringi 1.1.3, stringr 1.2.0, tibble 1.2, tools 3.3.3, vsn 3.42.3, zlibbioc 1.20.0