Package 'bibliospec'

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Type Package

Title Reading Mass Spectrometric Search Results

Version 0.0.4

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Depends R (>= 3.2), methods, DBI, RSQLite

Suggests testthat,parallel

Description R class to access 'sqlite', 'BiblioSpec' generated, mass spectrometry search result files, containing detailed information about peptide spectra matches.
Convert 'Mascot' '.dat' or e.g. 'comet' '.pep.xml' files with 'BiblioSpec' into 'sqlite' files and than access them with the 'CRAN' 'bibliospec' package to analyse with the R-packages 'specL' to generate
spectra libraries, 'protViz' to annotate spectra, or 'prozor' for false discovery rate estimation and protein inference.

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URL https://github.com/protViz/bibliospec

BugReports https://github.com/protViz/bibliospec/issues

Repository CRAN

Collate bibliospec.R zzz.R

NeedsCompilation no

RoxygenNote 5.0.1

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R topics documented:

`Bibliospec-class` *R access to Bibliospec File*

Description

This class implements an R referenz class for BiblioSpec generated sqlite files and can return the data contained as data.frames or as list of tandem mass spectra peptide assignments objects (psm).

Details

The function performs a SQL query on the SQLite files generated by BiblioSpec using the RSQLite package.

BiblioSpec files are generated by using Skyline or the BiblioSpec command line tool available from protwiz.

Fields

`dbfile` database file location

Methods

`getNrPSM()` Get number of psm's in database.

`getPeaks(asList = FALSE)` Get peaks - mz and intensity and spectra id as data.frame.

`getPsmSet()` get class psmSet S3 (list of psm objects). psm objects can be viewed by using the peakplot method of package protViz.

`getSpectraMeta()` Get spectra meta information - retention time , file name, num peaks as data.frame

`getSpectraWithMeta()` Get peaks with all the meta information as data.frame

`summary()` summary of bibliospec file

Author(s)

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References

- UNIT 13.7 Using BiblioSpec for Creating and Searching Tandem MS, Peptide Libraries. Barbara Frewen, Michael J. MacCoss. Current Protocols in Bioinformatics Current Protocols in Bioinformatics. http://dx.doi.org/10.1002/0471250953.bi1307s20.
- The predecessor of the method `getPsmSet` was implemented in the bioconductor package specL:

  Panse C, Trachsel C, Grossmann J and Schlapbach R. (2015). specL - An R/Bioconductor package to prepare peptide spectrum matches for use in targeted proteomics. Bioinformatics. http://dx.doi.org/10.1093/bioinformatics/btv105.

See Also

- https://skyline.gs.washington.edu/labkey/project/home/software/Skyline/begin.view
- https://skyline.gs.washington.edu/labkey/project/home/software/BiblioSpec/begin.view

Examples

```
library(bibliospec)

# use the sqlite file provided in the package
dbfile <- file.path(path.package("bibliospec"),
 "extdata/peptideStd.sqlite")

# call constructor
BS <- Bibliospec(dbfile=dbfile)

# test; should return TRUE
BS$getNrPSM() == 137

S <- BS$getPsmSet()

## Not run:
 library(specL)
 print(S)
 lapply(S[1:10], plot)

## End(Not run)

peaks <- BS$getPeaks()

print(BS$summary())
head(peaks)

colnames(peaks)

spectrMet <- BS$getSpectraMeta()

dim(spectrMet)
alldata <- BS$getSpectraWithMeta()
alldata<- merge(spectrMet, peaks)

modification <- BS$getModification()

head(modification)

table(table(modification$RefSpectraID))
```

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