Package 'topdownrdata'

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Title Example Files for the topdownr R Package

Description Example data for the topdownr package generated on a Thermo Orbitrap Fusion Lumos MS device.

Depends topdownr

biocViews ExperimentData, MassSpectrometryData

License GPL (>= 3)

NeedsCompilation no

URL https://codeberg.org/sgibb/topdownrdata/

BugReports https://codeberg.org/sgibb/topdownrdata/issues/

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topdownrdata-package *Example Data for the topdownr package.*

Description

This package contains example files accompanying the topdownr.

Details

It has just one function topDownDataPath() that returns the file path to the 5 example protein datasets.

Each dataset has four different categories of files:

- One .fasta file containing the protein sequence.
- Multiple .experiments.csv, .txt, and .mzML files (the same number of files for each of the three types):
  - The .experiments.csv files contain the information about the used method and the settings of the mass spectrometer (fragmentation conditions).
  - The .txt scan header files contain (additional) information about the spectra (monoisotopic *m/z*, ion injection time, ...).
  - The .mzML files contain the deconvoluted spectra.

In total this package has 341 files: a .fasta file for each protein (5) and 20 files of each of the three method/spectra information files for every protein except for the *bovine carbonic anhydrase* and *C3a recombinant protein* which have 26 of each.

The topdownr package needs all the four file types. The sequence information of the .fasta file is used to calculate the fragmentation *in-silico*. The theoretical fragments are matched against the experimental seen fragments that are stored in the .mzML files. In the next step the fragmentation data have to be combined with the general information about spectra and the fragmentation condition from the .txt scan header and the .experiments.csv method files, respectively.

In combination these information could be used to investigate fragmentation conditions and to find the one (or more) that maximise the overall fragment coverage. Please see a small example on the end of this manual page and a full featured example analysis in the topdownr analysis vignette: vignette("analysis", package="topdownr").

The .meth files were created with the following command:

```
library("topdownr")

writeMethodXmls(defaultMs1Settings(LastMass=1600),
                defaultMs2Settings(),
                ## mass/z adapted to protein of interest (see table)
                ## z is currently not supported by the Thermo software,
                ## setting to 1.
                mz=cbind(mass=c(745.2, 908.0, 1162.0), z=c(1, 1, 1)),
                groupBy=c("replication", "ETDReactionTime"),
                replications=2,
                pattern="method_CA3_\\%s.xml")
```

General Information:

protein name	uniprot accession	product number	modifications	monoisotopic mass ob
horse myoglobin	P68082	sigma M1882	Met-loss	16
bovine carbonic anhydrase	P00921	sigma C2522	Met-loss + Acetyl	29
histone H3.3	P84243	NEB M2507S	Met-loss	15
histone H4	P62805	NEB M2504S	Met-loss	11
C3a recombinant protein	P01024 part (672-748)	recombinantly expressed	carbamidomethyl	98

All 5 proteins were infused into a Thermo Orbitrap Fusion Lumos at 600 nl/minute in 50 \ FS360-20-10-5-6.35CT emitter.

M/Z used:

protein name	m/z 1	m/z 2	m/z 3
horse myoglobin	707.3/24	893.1/19	1211.7/14
bovine carbonic anhydrase	745.2/39	908.0/32	1162.0/25
histone H3.3	563.8/27	691.8/22	894.9/17
histone H4	562.7/20	703.2/16	937.3/12
C3a recombinant protein	745.2/17	908.0/14	1162.0/11

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References

https://codeberg.org/sgibb/topdownrdata/

See Also

topDownDataPath(), topdownr-package,
Vignettes for the generation `vignette("data-generation", package="topdownr")` and analysis of these data `vignette("analysis", package="topdownr")`.

Examples

```
# List file categories
list.files(topdownrdata::topDownDataPath("myoglobin"))

# List all needed files
list.files(topdownrdata::topDownDataPath("myoglobin"), recursive=TRUE)

# Read files, predict fragments and combine spectra information
tds <- readTopDownFiles(
    path=topDownDataPath("myoglobin"),
    ## Use an artifical pattern to load just the fasta
```

```
    ## file and files from m/z == 1211, ETD reagent
    ## target 1e6 and first replicate to keep runtime
    ## of the example short
    pattern=".*fasta.gz$|1211_.*1e6_1"
)

# Show TopDownSet object
tds

# Filter all intensities that don't have at least 10 % of the highest
# intensity per fragment.
tds <- filterIntensity(tds, threshold=0.1)

# Filter all conditions with a CV above 30 % (across technical replicates)
tds <- filterCv(tds, threshold=30)

# Filter all conditions with a large deviation in injection time
tds <- filterInjectionTime(tds, maxDeviation=log2(3), keepTopN=2)

# Filter all conditions where fragments don't replicate
tds <- filterNonReplicatedFragments(tds)

# Normalise by TIC
tds <- normalize(tds)

# Aggregate technical replicates
tds <- aggregate(tds)

# Coerce to NCBSet (N-/C-terminal/Bidirectional) and plot fragment coverage
fragmentationMap(as(tds, "NCBSet"))
```

`topDownDataPath` *TopDown Proteomic Datasets*

Description

This function returns the path to the example files accompanying the `topdownr`.

Usage

```
topDownDataPath(protein = c("myoglobin", "ca", "h3_3", "h4", "c3a"))
```

Arguments

`protein`	`character`, name of the dataset.

Details

See topdownrdata-package for a description of the datasets.

Value

`character`, path to the directory containing the example files.

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Examples

```
topDownDataPath("myoglobin")
```

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