

# Package ‘topdownrdata’

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**Version** 1.31.0

**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

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**BugReports** <https://codeberg.org/sgibb/topdownrdata/issues/>

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

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## 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 |
|---------------------------|-----------------------|-------------------------|-------------------|-------------------|
| horse myoglobin           | P68082                | sigma M1882             | Met-loss          |                   |
| bovine carbonic anhydrase | P00921                | sigma C2522             | Met-loss + Acetyl |                   |
| histone H3.3              | P84243                | NEB M2507S              | Met-loss          |                   |
| histone H4                | P62805                | NEB M2504S              | Met-loss          |                   |
| C3a recombinant protein   | P01024 part (672-748) | recombinantly expressed | carbamidomethyl   |                   |

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 artificial 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 NCBSets (N-/C-terminal/Bidirectional) and plot fragment coverage
fragmentationMap(as(tds, "NCBSets"))

```

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topDownDataPath

*TopDown Proteomic Datasets*


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## 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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