Package ‘msqc1’

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Title Sigma mix MSQC1 data

Version 1.8.0

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Depends R (>= 3.2), lattice, stats, utils

Suggests BiocStyle, knitr, testthat, specL

Description The data set contains an eight technical replicate data set and a three replicate dilution series of the MS Qual/Quant QC Mix standard sample (Sigma-Aldrich, Buchs, Switzerland) measured on five different mass spec platforms at the Functional Genomics Center Zurich.

License GPL

LazyData true

VignetteBuilder knitr

NeedsCompilation no

biocViews ExperimentData, MassSpectrometryData, ReproducibleResearch

URL `https://panoramaweb.org/labkey/MSQC1.url`,
`http://fgcz-bfabric.uzh.ch/bfabric/project.html?projectId=1959`

git_url https://git.bioconductor.org/packages/msqc1

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R topics documented:

`msqc1-package` *Sigma mix MSQC1 data*

Description

The data set contains an eight technical replicate data set and a three replicate dilution series of the MS Qual/Quant QC Mix standard sample (Sigma-Aldrich, Buchs, Switzerland) measured on five different mass spec platforms at the Functional Genomics Center Zurich.

Details

To obtain the MSQC1 stock solution, MS Qual/Quant QC Mix (Catalog #: MSQC1, Lot # 081M6281) was purchased from SigmaLAldrich (Buchs, Switzerland).

The first sample `msqc1_8rep` is based on eight techniqal replicates. To derive a complex sample matrix, 10 mul of MSQC1 working solution was mixed with 10mul (approx 10 mug) tryptic yeast digest (Saccharomyces cerevisiae), 1mul iRT peptide stock solution (Biognosys, Schlieren, Switzerland), and 19 mul 0.1% FA. This sample is denoted as standard sample.

The `msqc1_dil` sample was derived from a six point dilution series containing relative MSQC1 amounts of 0.025, 0.05, 0.2, 1, 2, and 5 with respect to the standard sample. The amount of yeast digest and iRT peptides was kept constant across all dilution steps. The reference L:H ratio vs. the on column amount of SIL peptide can be found in the data set `peptides`.

Both samples were meassured on five mass spectrometers. The mass spectrometers and operation modes are:

- `QTRAP` (ABSciex, Concord, Canada) - SRM mode
- `TSQvantage` (ThermoScientific, Bremen, Germany) - SRM mode
- `Qexactive` (ThermoScientific, Bremen, Germany) - PRM mode
- `QExactiveHF` (ThermoScientific, Bremen, Germany) - DIA mode
- `TRIPLETOF` 5600 (ABSciex, Concord, Canada) - SWATH and MS1 mode

All Raw LC-MS data from all platforms were imported into Skyline 3.1 (doi: 10.1093/bioinformatics/btq054). A single expert user adjusted the automatic peak group selection and integration border positioning (skyline legacy peak scoring).

The data were exported from skyline as csv files and included in this package as `data.frame` in RData files.

Author(s)

Tobias Kockmann, Christian Trachsel, Christian Panse

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References

- `www.sigmaLaldrich.com`
- skyline software - doi: 10.1093/bioinformatics/btq054
- peptide mix `http://www.sigmaaldrich.com/life-science/proteomics/mass-spectrometry/ms-qual-quant-qc-mix.html`, 2014

- Functional Genomic Center Zurich data repository (internal project p1959) `http://fgcz-bfabric.uzh.ch/bfabric/userlab/show-project.html?projectId=1959` - contains all mass spectrometer generated raw files. access for registered users.
- `https://panoramaweb.org/labkey/project/PanoramaPublic/` search for msqc1 (not published yet) - contains all skyline files and the export template

Examples

```
 # Have Fun!
browseVignettes('msqc1')
```

`msqc1_8rep` *MSQC1 8 technical replicates*

Description

The data set contains a 8 technical replicates meassured on five mass spec devices.

Usage

```
data("msqc1_8rep")
```

Format

A data frame with 6272 observations on the following 16 variables.

`Replicate.Name` a factor with levels `04_MSQC1_in_yd_incl_iRT_1in40_rep1` `05_MSQC1_in_yd_incl_iRT_1in40_r`
`06_MSQC1_in_yd_incl_iRT_1in40_rep3` `07_MSQC1_in_yd_incl_iRT_1in40_rep4` `08_MSQC1_in_yd_incl_iRT`
`09_MSQC1_in_yd_incl_iRT_1in40_rep6` `10_MSQC1_in_yd_incl_iRT_1in40_rep7` `11_MSQC1_in_yd_incl_iRT`
`20131204_001_HS_yeast` `20131204_002_HS_yeast` `20131204_003_HS_yeast` `20131204_003_HS_yeast_01`
`20131204_004_HS_yeast` `20131204_004_HS_yeast_02` `20131204_005_HS_yeast` `20131204_005_HS_yeast_03`
`20131204_006_HS_yeast` `20131204_006_HS_yeast_04` `20131204_007_HS_yeast` `20131204_008_HS_yeast`
`20131204_008_HS_yeast_05` `20131204_009_HS_yeast_06` `20131204_010_HS_yeast_07` `20131204_011_HS_ye`
`20140212_006_MSQC1_QTrap_01` `20140212_007_MSQC1_QTrap_02` `20140212_008_MSQC1_QTrap_03`
`20140212_009_MSQC1_QTrap_04` `20140212_011_MSQC1_QTrap_05` `20140212_012_MSQC1_QTrap_06`
`20140212_013_MSQC1_QTrap_07` `20140212_014_MSQC1_QTrap_08` `20140326_01_MSQC1_Yeast_iRT_12MS2_1e`
`20140326_02_MSQC1_Yeast_iRT_12MS2_1e5_70k` `20140326_03_MSQC1_Yeast_iRT_12MS2_1e5_70k`
`20140326_04_MSQC1_Yeast_iRT_12MS2_1e5_70k` `20140326_05_MSQC1_Yeast_iRT_12MS2_1e5_70k`
`20140326_06_MSQC1_Yeast_iRT_12MS2_1e5_70k` `20140326_07_MSQC1_Yeast_iRT_12MS2_1e5_70k`
`20140326_08_MSQC1_Yeast_iRT_12MS2_1e5_70k`

`File.Name` a factor with levels `20131204_001_HS_yeast.wiff` `20131204_002_HS_yeast.wiff`
`20131204_003_HS_yeast_01.raw` `20131204_003_HS_yeast.wiff` `20131204_004_HS_yeast_02.raw`
`20131204_004_HS_yeast.wiff` `20131204_005_HS_yeast_03.raw` `20131204_005_HS_yeast.wiff`
`20131204_006_HS_yeast_04.raw` `20131204_006_HS_yeast.wiff` `20131204_007_HS_yeast.wiff`
`20131204_008_HS_yeast_05.raw` `20131204_008_HS_yeast.wiff` `20131204_009_HS_yeast_06.raw`
`20131204_010_HS_yeast_07.raw` `20131204_011_HS_yeast_08.raw` `20140212_006_MSQC1_QTrap_01.wiff`
`20140212_007_MSQC1_QTrap_02.wiff` `20140212_008_MSQC1_QTrap_03.wiff` `20140212_009_MSQC1_QTrap_0`
`20140212_011_MSQC1_QTrap_05.wiff` `20140212_012_MSQC1_QTrap_06.wiff` `20140212_013_MSQC1_QTrap_0`
`20140212_014_MSQC1_QTrap_08.wiff` `20140326_01_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw`
`20140326_02_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw` `20140326_03_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw`
`20140326_04_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw` `20140326_05_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw`

`20140326_06_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw` `20140326_07_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw` `20140326_08_MSQC1_Yeast_iRT_12MS2_1e5_70k.raw` `20150526_04_MSQC1_in_yd_incl_iRT_1in40_rep1.ra` `20150526_05_MSQC1_in_yd_incl_iRT_1in40_rep2.raw` `20150526_06_MSQC1_in_yd_incl_iRT_1in40_rep3.` `20150526_07_MSQC1_in_yd_incl_iRT_1in40_rep4.raw` `20150526_08_MSQC1_in_yd_incl_iRT_1in40_rep5.` `20150526_09_MSQC1_in_yd_incl_iRT_1in40_rep6.raw` `20150526_10_MSQC1_in_yd_incl_iRT_1in40_rep7.` `20150526_11_MSQC1_in_yd_incl_iRT_1in40_rep8.raw`

`Protein.Name` a factor with levels `CAH1/P00915` `CAH2/P00918` `Catalase/P04040` `CRP/P02741` `DT-Diaphorase(NQO1)/P15559` `iRT-C18 Standard Peptides` `PPIA/Q13427`

`Peptide.Sequence` a factor with levels `ADVTPADFSEWSK` `ALIVLAHSER` `AVQQPDGLAVLGIFLK` `DGLDAASYYAPVR` `EGHLSPDIVAEQK` `ESDTSYVSLK` `FEDENFILK` `FSTVAGESGSADTVR` `GAGAFGYFEVTHDITK` `GAGSSEPVTGLDAK` `GGPFSDSYR` `GTFIIDPAAVIR` `GTFIIDPGGVIR` `GYSIFSYATK` `LFLQFGAQGSPFLK` `LGGNEQVTR` `NLSVEDAAR` `SADFTNFDPR` `TAENFR` `TPVISGGPYEYR` `TPVITGAPYEYR` `VEATFGVDESNAK` `VLDALQAIK` `VSFELFADK` `YILAGVENSK`

`Isotope.Label.Type` a factor with levels `heavy` `light`

`Precursor.Mz` a numeric vector

`Precursor.Charge` a numeric vector

`Product.Mz` a numeric vector

`Product.Charge` a numeric vector

`Fragment.Ion` a factor with levels `b8` `precursor` `precursor [M+1]` `precursor [M+2]` `y10` `y11` `y12` `y4` `y5` `y6` `y7` `y8` `y9`

`Retention.Time` a numeric vector

`Area` a numeric vector

`Background` a numeric vector

`relative.amount` a numeric vector

`instrument` a factor with levels `QExactive` `QExactiveHF` `QTRAP` `TRIPLETOF` `TSQVantage`

`File.Name.Id` a numeric vector

Value

A `data.frame` and `msqc1` S3 object.

Examples

```
data(msqc1_8rep)
## maybe str(msqc1_8rep) ; plot(msqc1_8rep) ...
```

`msqc1_8rep_QEXACTIVEHF_assayDevel`

QEXACTIVEHF peptide signal response.

Description

This data set contains peptide signal response for the QEXACTIVEHF mass spec device. The peptide level signals as measured by DIA.

Usage

```
data("msqc1_8rep_QEXACTIVEHF_assayDevel")
```

Format

A data frame with 1864 observations on the following 16 variables.

`Replicate.Name` a factor with levels `04_MSQC1_in_yd_incl_iRT_1in40_rep1` `05_MSQC1_in_yd_incl_iRT_1in40_r` `06_MSQC1_in_yd_incl_iRT_1in40_rep3` `07_MSQC1_in_yd_incl_iRT_1in40_rep4` `08_MSQC1_in_yd_incl_iRT` `09_MSQC1_in_yd_incl_iRT_1in40_rep6` `10_MSQC1_in_yd_incl_iRT_1in40_rep7` `11_MSQC1_in_yd_incl_iRT`

`File.Name` a factor with levels `20150526_04_MSQC1_in_yd_incl_iRT_1in40_rep1.raw` `20150526_05_MSQC1_in_yd` `20150526_06_MSQC1_in_yd_incl_iRT_1in40_rep3.raw` `20150526_07_MSQC1_in_yd_incl_iRT_1in40_rep4.` `20150526_08_MSQC1_in_yd_incl_iRT_1in40_rep5.raw` `20150526_09_MSQC1_in_yd_incl_iRT_1in40_rep6.` `20150526_10_MSQC1_in_yd_incl_iRT_1in40_rep7.raw` `20150526_11_MSQC1_in_yd_incl_iRT_1in40_rep8.`

`Protein.Name` a factor with levels `CAH1/P00915` `CAH2/P00918` `Catalase/P04040` `CRP/P02741` `DT-Diaphorase(NQO1)/P15559` `iRT-C18 Standard Peptides` `P00915MSQC1|CAH1_HUMAN_MSQC1` `P00918MSQC1|CAH2_HUMAN_MSQC1` `P02741MSQC1|CRP_HUMAN_MSQC1` `P04040MSQC1|CATA_HUMAN_MSQC1` `P15559MSQC1|NQO1_HUMAN_MSQC1` `P62937MSQC1|PPIA_HUMAN_MSQC1` `PPIA/Q13427`

`Peptide.Sequence` a factor with levels `ADVLTTGAGNPVGDK` `ADVTPADFSEWSK` `AFYVNVLNEEQR` `ALIVLAHSER` `APLTKPLK` `AVQQPDGLAVLGIFLK` `DAQIFIQK` `DGLDAASYYAPVR` `DLFNAIATGK` `DPANFQYPAESVLAYK` `DPILFPSFIHSQK` `DYPLIPVGK` `EGHLSPDIVAEQK` `EIINVGHSFHVNFEDNDNR` `EPISVSSEQVLK` `ESDTSYVSLK` `ESISVSSEQLAQFR` `FEDENFILK` `FGLSVGHHLGK` `FNTANDDNVTQVR` `FSTVAGESGSADTVR` `GAGAFGYFEVTHDITK` `GAGSSEPVTGLDAK` `GGPFSDSYR` `GGPLDGTYR` `GTFIIDPAAVIR` `GTFIIDPGGVIR` `GYSIFSYATK` `HDTSLKPISVSYNPATAK` `HNGPEHWHK` `ILNNGHAFNVEFDDSQDK` `IQILEGWK` `LCENIAGHLK` `LFAYPDTHR` `LFLQFGAQGSPFLK` `LFQFHFHWGSTNEHGSEHTVD` `LGGNEQVTR` `LGPNYLHIPVNCPYR` `LIQFHFHWGSLDGQGSEHTVDK` `LNVITVGPR` `LSQEDPDYGIR` `LVNANGEAVYCK` `LYPIANGNNQSPVDIK` `NAIHTFVQSGSHLAAR` `NGPEQWSK` `NLSVEDAAR` `QDNEILIFWSK` `QSPVDIDTHTAK` `SADFTNFDPR` `SIPTDNQIK` `TEWLDGK` `TPVISGGPYEYR` `TPVITGAPYEYR` `VEATFGVDESNAK` `VFEHIGK` `VGSAKPGLQK` `VLDALQAIK` `VSFELFADK` `VVDVLDSIK` `YAAELHLVHWNTK` `YDPSLKPLSVSYDQATSLR` `YEVQGEVFTKPQLWP` `YILAGVENSK` `YNAEKPK` `YSAELHVAHWNSAK` `YSSLAEAASK`

`Isotope.Label.Type` a factor with levels `light`

`Precursor.Mz` a numeric vector

`Precursor.Charge` a numeric vector

`Product.Mz` a numeric vector

`Product.Charge` a numeric vector

`Fragment.Ion` a factor with levels `b3` `b4` `b5` `b6` `b7` `b8` `y10` `y11` `y12` `y3` `y4` `y5` `y6` `y7` `y8` `y9`

`Retention.Time` a numeric vector

`Area` a numeric vector

`Background` a numeric vector

`relative.amount` a numeric vector

`QEXACTIVEHF` a factor with levels `QEXACTIVEHF`

`File.Name.Id` a numeric vector

Value

A `data.frame` and `msqc1` S3 object.

Examples

```
data(msqc1_8rep_QEXACTIVEHF_assayDevel)
## maybe str(msqc1_8rep_QEXACTIVEHF_assayDevel) ; plot(msqc1_8rep_QEXACTIVEHF_assayDevel) ...
```

`msqc1_8rep_tripleTOF5600_assayDevel`
tripleTOF5600 peptide signal response

Description

This data set contains peptide signal response for the tripleTOF5600 mass spec device. The peptide level signals were measured in SWATH-MS mode.

Usage

```
data("msqc1_8rep_tripleTOF5600_assayDevel")
```

Format

A data frame with 1616 observations on the following 17 variables.

`Replicate.Name` a factor with levels `20131204_001_HS_yeast` `20131204_002_HS_yeast` `20131204_003_HS_yeast` `20131204_004_HS_yeast` `20131204_005_HS_yeast` `20131204_006_HS_yeast` `20131204_007_HS_yeast` `20131204_008_HS_yeast`

`File.Name` a factor with levels `20131204_001_HS_yeast.wiff` `20131204_002_HS_yeast.wiff` `20131204_003_HS_yeast.wiff` `20131204_004_HS_yeast.wiff` `20131204_005_HS_yeast.wiff` `20131204_006_HS_yeast.wiff` `20131204_007_HS_yeast.wiff` `20131204_008_HS_yeast.wiff`

`Protein.Name` a factor with levels `CAH1/P00915` `CAH2/P00918` `Catalase/P04040` `CRP/P02741` `DT-Diaphorase(NQO1)/P15559` `iRT-C18 Standard Peptides` `P00915MSQC1|CAH1_HUMAN_MSQC1` `P00918MSQC1|CAH2_HUMAN_MSQC1` `P02741MSQC1|CRP_HUMAN_MSQC1` `P04040MSQC1|CATA_HUMAN_MSQC1` `P15559MSQC1|NQO1_HUMAN_MSQC1` `P62937MSQC1|PPIA_HUMAN_MSQC1` `PPIA/Q13427`

`Peptide.Sequence` a factor with levels `ADGLAVIGVLMK` `ADVLTTGAGNPVGDK` `ADVTPADFSEWSK` `AFYVNVLNEEQR` `ALIVLAHSER` `APLTKPLK` `AVQQPDGLAVLGIFLK` `DAQIFIQK` `DGLDAASYYAPVR` `DLFNAIATGK` `DPILFPSFIHSQK` `DYPLIPVGK` `EGHLSPDIVAEQK` `EGMNIVEAMER` `EPISVSSEQVLK` `ESDTSYVSLK` `ESISVSSEQLAQFR` `FEDENFILK` `FGLSVGHHLGK` `FNTANDDNVTQVR` `FSTVAGESGSADTVR` `GAGAFGYFEVTHDITK` `GAGSSEPVTGLDAK` `GGPFSDSYR` `GGPLDGTYR` `GTFIIDPAAVIR` `GTFIIDPGGVIR` `GYSIFSYATK` `HDTSLKPISVSYNPATAK` `ILNNGHAFNVEFDDSQDK` `IQILEGWK` `LFAYPDTHR` `LFLQFGAQGSPFLK` `LGGNEQVTR` `LNVITVGPR` `LSQEDPDYGIR` `LYPIANGNNQSPVDIK` `NAIHTFVQSGSHLAAR` `NGPEQWSK` `NLSVEDAAR` `QSPVDIDTHTAK` `SADFTNFDPR` `TEWLDGK` `TPVISGGPYEYR` `TPVITGAPYEYR` `TSFNYAMK` `VEATFGVDESNAK` `VGSAKPGLQK` `VLDALQAIK` `VSFELFADK` `VVDVLDSIK` `YAAELHLVHWNTK` `YDPSLKPLSVSYDQATSLR` `YILAGVENSK` `YSAELHVAHWNSAK` `YSSLAEAASK`

`Isotope.Label.Type` a factor with levels `light`

`Precursor.Mz` a numeric vector

`Precursor.Charge` a numeric vector

`Product.Mz` a numeric vector

`Product.Charge` a numeric vector

`Fragment.Ion` a factor with levels `b2` `b3` `b7` `b8` `precursor` `precursor [M+1]` `precursor [M+2]` `y10` `y11` `y12` `y13` `y14` `y2` `y3` `y4` `y5` `y6` `y7` `y8` `y9`

`Retention.Time` a numeric vector

`Area` a numeric vector

`Background` a numeric vector

`relative.amount` a numeric vector

`flag` a factor with levels `False` `True`

`instrument` a factor with levels `TRIPLETOF`

`File.Name.Id` a numeric vector

Details

The signal response of the peptide *TAENF[R]* was not measured due to the lower m/z limit used by the DIA/SWATH-MS methods.

Value

A `data.frame` and `msqc1` S3 object.

Examples

```
data(msqc1_8rep_tripleTOF5600_assayDevel)

#filter <- !(msqc1_8rep_tripleTOF5600_assayDevel$Protein.Name %in% peptides$Protein.Name)

#msqc1:::.signal_response_ident_plot(msqc1_8rep_tripleTOF5600_assayDevel[filter, ],
#  instrument="tripleTOF560",
#  prot="P02741")
```

`msqc1_dil` *msqc1 dilution series*

Description

MSQC1 3 technical replicates dilution series meassured on five mass spec devices.

Usage

```
data("msqc1_dil")
```

Format

A data frame with 15300 observations on the following 15 variables.

`Replicate.Name` a factor with levels `20140807_01_MSQC1_1_40dil_1_140808162146` `20140807_02_MSQC1_1_40dil`
`20140807_02_MSQC1_1_40dil_2_140808175142` `20140807_03_MSQC1_1_40dil_3_140808192115`
`20140807_04_MSQC1_1_20dil_1_140808214050` `20140807_05_MSQC1_1_20dil_2_140808231024`
`20140807_06_MSQC1_1_20dil_3_140809004002` `20140807_07_MSQC1_1_5dil_1_140809025941`
`20140807_08_MSQC1_1_5dil_2_140809051908` `20140807_09_MSQC1_1_5dil_3` `20140807_10_MSQC1_nodil_1`
`20140807_11_MSQC1_nodil_2` `20140807_12_MSQC1_nodil_3` `20140807_13_MSQC1_x2_1` `20140807_14_MSQC1_`
`20140807_15_MSQC1_x2_3` `20140807_16_MSQC1_x5_1` `20140807_17_MSQC1_x5_2` `20140807_18_MSQC1_x5_3`
`20140808_02_MSQC1_1_40dil_2_140808175141` `20140812_004_QC_dil1_40_1` `20140812_005_QC_dil1_40_2`
`20140812_006_QC_dil1_40_3` `20140812_008_QC_dil1_20_1` `20140812_009_QC_dil1_20_2`
`20140812_010_QC_dil1_20_3` `20140812_012_QC_dil1_5_1_re` `20140812_013_QC_dil1_5_2_re`
`20140812_014_QC_dil1_5_3` `20140812_016_QC_nodil_1` `20140812_017_QC_nodil_2` `20140812_018_QC_nodi`
`20140812_020_QC_conc2_1` `20140812_021_QC_conc2_2` `20140812_022_QC_conc_2_3` `20140812_024_QC_conc`
`20140812_025_QC_conc5_2` `20140812_026_QC_conc5_3` `20140818_003_MSQC1_1_40dil_1`

20140818_004_MSQC1_1_40dil_1 20140818_005_MSQC1_1_40dil_3 20140818_007_MSQC1_1_20dil_1 20140818_008_MSQC1_1_20dil_2 20140818_009_MSQC1_1_20dil_3 20140818_011_MSQC1_NoDil_1 20140818_013_MSQC1_NoDil_2 20140818_015_MSQC1_NoDil_3 20140818_017_MSQC1_x2_1 20140818_019_MSQC1_x2_2 20140818_021_MSQC1_x2_3 20140818_023_MSQC1_x5_1 20140818_025_MSQC1_x5_
20140818_027_MSQC1_x5_3 20140818_030_MSQC1_1_5dil_1 20140818_032_MSQC1_1_5dil_2 20140818_034_MSQC1_1_5dil_3 20150526_16_MSCQ1_40xdil_rep1 20150526_17_MSCQ1_40xdil_rep2 20150526_18_MSCQ1_40xdil_rep3 20150526_20_MSCQ1_20xdil_rep1 20150526_21_MSCQ1_20xdil_rep2 20150526_22_MSCQ1_20xdil_rep3 20150526_24_MSCQ1_5xdil_rep1 20150526_25_MSCQ1_5xdil_rep2 20150526_26_MSCQ1_5xdil_rep3 20150526_28_MSCQ1_nodil_rep1 20150526_29_MSCQ1_nodil_rep2 20150526_30_MSCQ1_nodil_rep3 20150526_32_MSCQ1_2x_rep1 20150526_33_MSCQ1_2x_rep2 20150526_34_MSCQ1_2x_rep3 20150526_36_MSCQ1_5x_rep1 20150526_37_MSCQ1_5x_rep2 20150526_38_MSCQ1_5x_rep3 20150601_001_QCdil_40dil_1 20150601_002_QCdil_40dil_2 20150601_003_QCdil_40dil_3 20150601_004_QCdil_20dil_1 20150601_005_QCdil_20dil_2 20150601_006_QCdil_20dil_3 20150601_007_QCdil_5dil_1 20150601_008_QCdil_5dil_2 20150601_009_QCdil_5dil_3 20150601_010_nodil_1 20150601_011_nodil_2 20150601_012_nodil_3 20150601_013_2conc_1_re 20150601_014_2conc_2_re 20150601_015_2conc_3 20150601_016_5conc_1 20150601_017_5conc_2 20150601_018_5conc_3

File.Name a factor with levels 20140807_01_MSQC1_1_40dil_1_140808162146.raw 20140807_02_MSQC1_1_40dil_
20140807_03_MSQC1_1_40dil_3_140808192115.raw 20140807_04_MSQC1_1_20dil_1_140808214050.raw 20140807_05_MSQC1_1_20dil_2_140808231024.raw 20140807_06_MSQC1_1_20dil_3_140809004002.raw 20140807_07_MSQC1_1_5dil_1_140809025941.raw 20140807_08_MSQC1_1_5dil_2_140809051908.raw 20140807_09_MSQC1_1_5dil_3.raw 20140807_10_MSQC1_nodil_1.raw 20140807_11_MSQC1_nodil_2.raw 20140807_12_MSQC1_nodil_3.raw 20140807_13_MSQC1_x2_1.raw 20140807_14_MSQC1_x2_2.raw 20140807_15_MSQC1_x2_3.raw 20140807_16_MSQC1_x5_1.raw 20140807_17_MSQC1_x5_2.raw 20140807_18_MSQC1_x5_3.raw 20140812_004_QC_dil1_40_1.raw 20140812_005_QC_dil1_40_2.raw 20140812_006_QC_dil1_40_3.raw 20140812_008_QC_dil1_20_1.raw 20140812_009_QC_dil1_20_2.raw 20140812_010_QC_dil1_20_3.raw 20140812_012_QC_dil1_5_1_re.raw 20140812_013_QC_dil1_5_2_re.raw
20140812_014_QC_dil1_5_3.raw 20140812_016_QC_nodil_1.raw 20140812_017_QC_nodil_2.raw 20140812_018_QC_nodil_3.raw 20140812_020_QC_conc2_1.raw 20140812_021_QC_conc2_2.raw 20140812_022_QC_conc_2_3.raw 20140812_024_QC_conc5_1.raw 20140812_025_QC_conc5_2.raw 20140812_026_QC_conc5_3.raw 20140818_003_MSQC1_1_40dil_1.wiff 20140818_004_MSQC1_1_40dil_1.wi
20140818_005_MSQC1_1_40dil_3.wiff 20140818_007_MSQC1_1_20dil_1.wiff 20140818_008_MSQC1_1_20di
20140818_009_MSQC1_1_20dil_3.wiff 20140818_011_MSQC1_NoDil_1.wiff 20140818_013_MSQC1_NoDil_2.
20140818_015_MSQC1_NoDil_3.wiff 20140818_017_MSQC1_x2_1.wiff 20140818_019_MSQC1_x2_2.wiff 20140818_021_MSQC1_x2_3.wiff 20140818_023_MSQC1_x5_1.wiff 20140818_025_MSQC1_x5_2.wiff 20140818_027_MSQC1_x5_3.wiff 20140818_030_MSQC1_1_5dil_1.wiff 20140818_032_MSQC1_1_5dil_2.wif
20140818_034_MSQC1_1_5dil_3.wiff 20150526_16_MSCQ1_40xdil_rep1.raw 20150526_17_MSCQ1_40xdil_r
20150526_18_MSCQ1_40xdil_rep3.raw 20150526_20_MSCQ1_20xdil_rep1.raw 20150526_21_MSCQ1_20xdil_
20150526_22_MSCQ1_20xdil_rep3.raw 20150526_24_MSCQ1_5xdil_rep1.raw 20150526_25_MSCQ1_5xdil_re
20150526_26_MSCQ1_5xdil_rep3.raw 20150526_28_MSCQ1_nodil_rep1.raw 20150526_29_MSCQ1_nodil_rep
20150526_30_MSCQ1_nodil_rep3.raw 20150526_32_MSCQ1_2x_rep1.raw 20150526_33_MSCQ1_2x_rep2.raw 20150526_34_MSCQ1_2x_rep3.raw 20150526_36_MSCQ1_5x_rep1.raw 20150526_37_MSCQ1_5x_rep2.raw 20150526_38_MSCQ1_5x_rep3.raw 20150601_001_QCdil_40dil_1.wiff 20150601_002_QCdil_40dil_2.wiff
20150601_003_QCdil_40dil_3.wiff 20150601_004_QCdil_20dil_1.wiff 20150601_005_QCdil_20dil_2.wi
20150601_006_QCdil_20dil_3.wiff 20150601_007_QCdil_5dil_1.wiff 20150601_008_QCdil_5dil_2.wiff
20150601_009_QCdil_5dil_3.wiff 20150601_010_nodil_1.wiff 20150601_011_nodil_2.wiff 20150601_012_nodil_3.wiff 20150601_013_2conc_1_re.wiff 20150601_014_2conc_2_re.wiff 20150601_015_2conc_3.wiff 20150601_016_5conc_1.wiff 20150601_017_5conc_2.wiff 20150601_018_5conc_3.wiff

Protein.Name a factor with levels CAH1/P00915 CAH2/P00918 Catalase/P04040 CRP/P02741 DT-Diaphorase(NQO1)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIFLK DGLDAASYYAPVR

`EGHLSPDIVAEQK` `ESDTSYVSLK` `FEDENFILK` `FSTVAGESGSADTVR` `GAGAFGYFEVTHDITK` `GAGSSEPVTGLDAK` `GGPFSDSYR` `GTFIIDPAAVIR` `GTFIIDPGGVIR` `GYSIFSYATK` `LFLQFGAQGSPFLK` `LGGNEQVTR` `NLSVEDAAR` `SADFTNFDPR` `TAENFR` `TPVISGGPYEYR` `TPVITGAPYEYR` `VEATFGVDESNAK` `VLDALQAIK` `VSFELFADK` `YILAGVENSK`

`Isotope.Label.Type` a factor with levels `heavy` `light`

`Precursor.Mz` a numeric vector

`Precursor.Charge` a numeric vector

`Product.Mz` a numeric vector

`Product.Charge` a numeric vector

`Fragment.Ion` a factor with levels `b8` `precursor` `precursor [M+1]` `precursor [M+2]` `y10` `y11` `y12` `y4` `y5` `y6` `y7` `y8` `y9`

`Retention.Time` a numeric vector

`Area` a numeric vector

`Background` a numeric vector

`relative.amount` a numeric vector

`instrument` a factor with levels `QExactive` `QExactiveHF` `QTRAP` `TRIPLETOF` `TSQVantage`

Value

A `data.frame` and `msqc1` S3 object.

Examples

```
data(msqc1_dil)
## maybe str(msqc1_dil) ; plot(msqc1_dil) ...
```

`msqc1_userstudy` *msqc1 user study*

Description

contains a user study

Usage

```
data("msqc1_userstudy")
```

Format

A data frame with 21204 observations on the following 17 variables.

`Replicate.Name` a factor with levels `01_QCdil_40dil_1` `02_QCdil_40dil_2` `03_MSQC1_1_40dil_1` `03_QCdil_40dil_3` `04_MSQC1_1_40dil_1` `04_QCdil_20dil_1` `05_MSQC1_1_40dil_3` `05_QCdil_20dil_2` `06_QCdil_20dil_3` `07_MSQC1_1_20dil_1` `07_QCdil_5dil_1` `08_MSQC1_1_20dil_2` `08_QCdil_5dil_2` `09_MSQC1_1_20dil_3` `09_QCdil_5dil_3` `10_nodil_1` `11_MSQC1_NoDil_1` `11_nodil_2` `12_nodil_3` `13_2conc_1_re` `13_MSQC1_NoDil_2` `14_2conc_2_re` `15_2conc_3` `15_MSQC1_NoDil_3` `16_5conc_1` `17_5conc_2` `17_MSQC1_x2_1` `18_5conc_3` `19_MSQC1_x2_2` `20140818_003_MSQC1_1_40dil_1` `20140818_004_MSQC1_1_40dil_1` `20140818_005_MSQC1_1_40dil_3` `20140818_007_MSQC1_1_20dil_1` `20140818_008_MSQC1_1_20dil_2` `20140818_009_MSQC1_1_20dil_3` `20140818_011_MSQC1_NoDil_1`

20140818_013_MSQC1_NoDil_2 20140818_015_MSQC1_NoDil_3 20140818_017_MSQC1_x2_1 20140818_019_MSQC1_x2_2 20140818_021_MSQC1_x2_3 20140818_023_MSQC1_x5_1 20140818_025_MSQC1_x5_ 20140818_027_MSQC1_x5_3 20140818_030_MSQC1_1_5dil_1 20140818_032_MSQC1_1_5dil_2 20140818_034_MSQC1_1_5dil_3 20150601_001_QCdil_40dil_1 20150601_002_QCdil_40dil_2 20150601_003_QCdil_40dil_3 20150601_004_QCdil_20dil_1 20150601_005_QCdil_20dil_2 20150601_006_QCdil_20dil_3 20150601_007_QCdil_5dil_1 20150601_008_QCdil_5dil_2 20150601_009_QCdil_5dil_3 20150601_010_nodil_1 20150601_011_nodil_2 20150601_012_nodil_3 20150601_013_2conc_1_re 20150601_014_2conc_2_re 20150601_015_2conc_3 20150601_016_5conc_1 20150601_017_5conc_2 20150601_018_5conc_3 21_MSQC1_x2_3 23_MSQC1_x5_1 25_MSQC1_x5_2 27_MSQC1_x5_3 30_MSQC1_1_5dil_1 32_MSQC1_1_5dil_2 34_MSQC1_1_5dil_3

`File.Name` a factor with levels 20140818_003_MSQC1_1_40dil_1.wiff 20140818_004_MSQC1_1_40dil_1.wiff 20140818_005_MSQC1_1_40dil_3.wiff 20140818_007_MSQC1_1_20dil_1.wiff 20140818_008_MSQC1_1_20di 20140818_009_MSQC1_1_20dil_3.wiff 20140818_011_MSQC1_NoDil_1.wiff 20140818_013_MSQC1_NoDil_2. 20140818_015_MSQC1_NoDil_3.wiff 20140818_017_MSQC1_x2_1.wiff 20140818_019_MSQC1_x2_2.wiff 20140818_021_MSQC1_x2_3.wiff 20140818_023_MSQC1_x5_1.wiff 20140818_025_MSQC1_x5_2.wiff 20140818_027_MSQC1_x5_3.wiff 20140818_030_MSQC1_1_5dil_1.wiff 20140818_032_MSQC1_1_5dil_2.wif 20140818_034_MSQC1_1_5dil_3.wiff 20150601_001_QCdil_40dil_1.wiff 20150601_002_QCdil_40dil_2.w 20150601_003_QCdil_40dil_3.wiff 20150601_004_QCdil_20dil_1.wiff 20150601_005_QCdil_20dil_2.wi 20150601_006_QCdil_20dil_3.wiff 20150601_007_QCdil_5dil_1.wiff 20150601_008_QCdil_5dil_2.wiff 20150601_009_QCdil_5dil_3.wiff 20150601_010_nodil_1.wiff 20150601_011_nodil_2.wiff 20150601_012_nodil_3.wiff 20150601_013_2conc_1_re.wiff 20150601_014_2conc_2_re.wiff 20150601_015_2conc_3.wiff 20150601_016_5conc_1.wiff 20150601_017_5conc_2.wiff 20150601_018_5conc_3.wiff

`Protein.Name` a factor with levels CAH1/P00915 CAH2/P00918 Catalase/P04040 CRP/P02741 DT-Diaphorase(NQO1)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

`Peptide.Sequence` a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIFLK DGLDAASYYAPVR EGHLSPDIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK GGPFSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGGNEQVTR NLSVEDAAR SADFTNFDPR TAENFR TPVISGGPYEYR TPVITGAPYEYR VEATFGVDES#N/AK VLDALQAIK VSFELFADK YILAGVENSK

`Isotope.Label.Type` a factor with levels heavy light

`Precursor.Mz` a numeric vector

`Precursor.Charge` a numeric vector

`Product.Mz` a numeric vector

`Product.Charge` a numeric vector

`Fragment.Ion` a factor with levels b8 y10 y11 y12 y4 y5 y6 y7 y8 y9

`Retention.Time` a numeric vector

`Area` a numeric vector

`Background` a numeric vector

`relative.amount` a numeric vector

`instrument` a factor with levels QTRAP TRIPLETOF

`user` a factor with levels algorithm_1 algorithm_2 algorithm_3 user_1 user_2 user_3 user_4 user_5 user_6

`attempt` a factor with levels beginner expert legacy mProphet second_best

Details

The data were derived by a user study. Therfore each individual was given a skyline document containing the dilution series data recorded on the QTRAP and TripleTOF 5600. Starting from skyline legacy results, users curated the data.

In addition, two mProphet doi: 10.1038/nmeth.1584 models (as implemented in skyline) were trained on the 8 replicate data from the same instrument.

Value

A `data.frame` and `msqc1` S3 object.

Examples

```
data(msqc1_userstudy)
## maybe str(msqc1_userstudy) ; plot(msqc1_userstudy) ...
```

`peptides` *sigma mix peptides*

Description

This table contains msqc1 peptide proberties.

Usage

```
data("peptides")
```

Format

A data frame with 14 observations on the following 5 variables.

`Peptide.Sequence` a factor with levels `ALIVLAHSER` `AVQQPDGLAVLGIFLK` `EGHLSPDIVAEQK` `ESDTSYVSLK` `FEDENFILK` `FSTVAGESGSADTVR` `GAGAFGYFEVTHDITK` `GGPFSDSYR` `GYSIFSYATK` `NLSVEDAAR` `SADFTNFDPR` `TAENFR` `VLDALQAIK` `VSFELFADK`

`SIL.peptide.per.vial` a numeric vector

`LH.ratio` a numeric vector

`actual.LH.ratio` a numeric vector

`Protein.Name` a factor with levels `CAH1/P00915` `CAH2/P00918` `Catalase/P04040` `CRP/P02741` `DT-Diaphorase(NQO1)/P15559` `PPIA/Q13427`

Value

A `data.frame`.

Source

`http://www.sigmaaldrich.com/life-science/proteomics/mass-spectrometry/ms-qual-quant-qc-mix.html`, 2014

Examples

```
data(peptides)
## maybe str(peptides) ; plot(peptides) ...
```

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