Package 'msqc1'

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Title Sigma mix MSQC1 data

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Depends R (>= 3.6), lattice, stats, utils

Suggests BiocStyle, knitr, rmarkdown, testthat, specL (>= 1.2)

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

License GPL

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VignetteBuilder knitr

NeedsCompilation no

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http://fgcz-bfabric.uzh.ch/bfabric/project.html?projectId=1959

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`msqc1-package` *Sigma mix MSQC1 data*

Description

contains eight technical replicate data set and a three replicate dilution series of the MS Qual/Quant Quality Control Mix standard sample (Sigma-Aldrich, Buchs, Switzerland) measured on five different mass spectrometer 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.

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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 sklyline 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_rep2` `06_MSQC1_in_yd_incl_iRT_1in40_rep3` `07_MSQC1_in_yd_incl_iRT_1in40_rep4` `08_MSQC1_in_yd_incl_iRT_1i` `09_MSQC1_in_yd_incl_iRT_1in40_rep6` `10_MSQC1_in_yd_incl_iRT_1in40_rep7` `11_MSQC1_in_yd_incl_iRT_1i` `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_yeast_` `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_1e5_70
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_04.wi
20140212_011_MSQC1_QTrap_05.wiff 20140212_012_MSQC1_QTrap_06.wiff 20140212_013_MSQC1_QTrap_07.wi
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.raw
20150526_05_MSQC1_in_yd_incl_iRT_1in40_rep2.raw 20150526_06_MSQC1_in_yd_incl_iRT_1in40_rep3.raw
20150526_07_MSQC1_in_yd_incl_iRT_1in40_rep4.raw 20150526_08_MSQC1_in_yd_incl_iRT_1in40_rep5.raw
20150526_09_MSQC1_in_yd_incl_iRT_1in40_rep6.raw 20150526_10_MSQC1_in_yd_incl_iRT_1in40_rep7.raw
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_rep2` `06_MSQC1_in_yd_incl_iRT_1in40_rep3` `07_MSQC1_in_yd_incl_iRT_1in40_rep4` `08_MSQC1_in_yd_incl_iRT_1i` `09_MSQC1_in_yd_incl_iRT_1in40_rep6` `10_MSQC1_in_yd_incl_iRT_1in40_rep7` `11_MSQC1_in_yd_incl_iRT_1i`

`File.Name` a factor with levels `20150526_04_MSQC1_in_yd_incl_iRT_1in40_rep1.raw` `20150526_05_MSQC1_in_yd_inc` `20150526_06_MSQC1_in_yd_incl_iRT_1in40_rep3.raw` `20150526_07_MSQC1_in_yd_incl_iRT_1in40_rep4.raw` `20150526_08_MSQC1_in_yd_incl_iRT_1in40_rep5.raw` `20150526_09_MSQC1_in_yd_incl_iRT_1in40_rep6.raw` `20150526_10_MSQC1_in_yd_incl_iRT_1in40_rep7.raw` `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` `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` `LFQFHFHWGSTNEHGSEHTVDGVK` `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_2_1`
`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_x2_2`
`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_nodil_3`
`20140812_020_QC_conc2_1` `20140812_021_QC_conc2_2` `20140812_022_QC_conc_2_3` `20140812_024_QC_conc5_1`
`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_2`
`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`

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`20140807_03_MSQC1_1_40dil_3_140808192115.raw` `20140807_04_MSQC1_1_20dil_1_140808214050.raw`

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20140807_07_MSQC1_1_5dil_1_140809025941.raw 20140807_08_MSQC1_1_5dil_2_140809051908.raw
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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
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20140818_034_MSQC1_1_5dil_3.wiff 20150526_16_MSCQ1_40xdil_rep1.raw 20150526_17_MSCQ1_40xdil_rep2
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20150526_26_MSCQ1_5xdil_rep3.raw 20150526_28_MSCQ1_nodil_rep1.raw 20150526_29_MSCQ1_nodil_rep2.r
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.wiff
20150601_006_QCdil_20dil_3.wiff 20150601_007_QCdil_5dil_1.wiff 20150601_008_QCdil_5dil_2.wiff
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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_2 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_20dil_2` `20140818_009_MSQC1_1_20dil_3.wiff` `20140818_011_MSQC1_NoDil_1.wiff` `20140818_013_MSQC1_NoDil_2.wif` `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.wiff` `20140818_034_MSQC1_1_5dil_3.wiff` `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.wiff` `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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