

Package ‘msqc1’

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Title Sigma mix MSQC1 data

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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>

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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 technical replicates. To derive a complex sample matrix, 10 μ l of MSQC1 working solution was mixed with 10 μ l (approx 10 μ g) tryptic yeast digest (*Saccharomyces cerevisiae*), 1 μ l iRT peptide stock solution (Biognosys, Schlieren, Switzerland), and 19 μ l 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 measured 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](https://doi.org/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](https://doi.org/10.1093/bioinformatics/btq054)
- peptide mix <http://www.sigmalaldrich.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 msvc1 (not published yet) - contains all skyline files and the export template

Examples

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

msqc1_8rep	<i>MSQC1 8 technical replicates</i>
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Description

The data set contains a 8 technical replicates measured 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_1in40_rep5 09_MSQC1_in_yd_incl_iRT_1in40_rep6 10_MSQC1_in_yd_incl_iRT_1in40_rep7 11_MSQC1_in_yd_incl_iRT_1in40_rep8
 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_08
 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_70k
 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.wiff
 20140212_011_MSQC1_QTrap_05.wiff 20140212_012_MSQC1_QTrap_06.wiff 20140212_013_MSQC1_QTrap_07.wiff
 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(NQ01)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIFLK DGLDAASYAPVR
 EGHLSPDIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK
 GGFPSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGNEQVTR NLSVEDAAR
 SADFTNFDPR TAENFR TPVISGGPYEYR TPVITGAPYEYR VEATFGVDESSNAK VLDALQAIK VSFELFADK
 YILAGVENS

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_1in40_rep5 09_MSQC1_in_yd_incl_iRT_1in40_rep6 10_MSQC1_in_yd_incl_iRT_1in40_rep7 11_MSQC1_in_yd_incl_iRT_1in40_rep8

File.Name a factor with levels 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(NQ01)/P15559 iRT-C18 Standard Peptides P00915MSQC1 | CAH1_HUMAN_MSQC1 P00918MSQC1 | CAH2_HUMAN_MSQC1 P02741MSQC1 | CRP_HUMAN_MSQC1 P04040MSQC1 | CATA_HUMAN_MSQC1 P15559MSQC1 | NQ01_HUMAN_MSQC1 P62937MSQC1 | PPIA_HUMAN_MSQC1 PPIA/Q13427

Peptide.Sequence a factor with levels ADVLTTGAGNPVGDK ADVTPADFSEWSK AFYVNVLNNEEQR ALIVLAHSER APLTKPLK AVQQPDGLAVLGIFLK DAQIFIQK DGLDAASYAPVR DLFNAIATGK DPANFQYPAESVLAYK DPILFPSFIHSQK DYPLIPVGK EGHLSPIVAEQK EIINVGHSHFVNFEDNDNR EPISVSSEQVLK ESDTSYVSLK ESISVSSEQLAQFR FEDENFILK FGLSVGHHLGK FNTANDDNVTQVR FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK GGPFSDSYR GGPLDGTYSR GTFIIDPAVIR GTFIIDPGGIVR GYSIFSYATK HDTSLKPISVSYNPATAK HNGPEHWHK ILNNGHAFNVFDDSDQK IQILEGWK LCENIAGHLK LFAYPDTHR LFLQFGAQGSPFLK LQFHFHWGSTNEHGSEHTVD LGGNEQVTR LGPNYLHIPVNCYPYR LIQFHFHWGSLDQGSEHTVDK LNVITVGPYR LSQEDPDYGYR LVNANGEAVYCK LYPIANGNNQSPVDIK NAIHTFVQSGSHLAAR NGPEQWSK NLSVEDAAR QDNEILIFWSK QSPVDIDHTAK SADFTNFDPR SIPTDNQIK TEWLDGK TPVISGGPYEYR TPVITGAPYEYR VEATFGVDESNK VFEHIGK VGSAPGLQK VLDALQAIK VSFELFADK VVDVLDSIK YAAELHLVHWNTK YDPSLKLPSVSYDQATSLR YEYVQGEVFTKPLWP YILAGVENSK YNAEKPK YSAELHVAHWNSAK YSSLAEAAASK

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 msvc1 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(NQ01)/P15559 iRT-C18 Standard Peptides P00915MSQC1 | CAH1_HUMAN_MSQC1 P00918MSQC1 | CAH2_HUMAN_MSQC1 P02741MSQC1 | CRP_HUMAN_MSQC1 P04040MSQC1 | CATA_HUMAN_MSQC1 P15559MSQC1 | NQ01_HUMAN_MSQC1 P62937MSQC1 | PPIA_HUMAN_MSQC1 PPIA/Q13427

Peptide.Sequence a factor with levels ADGLAVIGVLMK ADVLTTGAGNPVGDK ADVTPADFSEWSK AFYVNVLNEEQR ALIVLAHSER APLTKPLK AVQQPDGLAVLGIFLK DAQIFIQK DGLDAASYAPVR DLFNAIATGK DPILFPSFIHSQK DYPLIPVGK EGHLSPDIVAEQK EGMNIVEAMER EPISVSSEQVLK ESDTSYVSLK ESISVSSEQLAQFR FEDENFILK FGLSVGHHLGK FNTANDDNVTQVR FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK GGPFSDSYR GGPLDGTYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK HDTSLKPISVSYNPATAK ILNNGHAFNVEFDDSDQK IQILEGWK LFAYPDTHR LFLQFGAQGSPFLK LGGNEQVTR LNVITVGPR LSQEDPDYGIR LYPIANGNNQSPVDIK NAIHTFVQSGSHLAAR NGPEQWSK NLSVEDAAR QSPVDIDHTAK SADFTNFDPR TEWLDGK TPVISGGPYEYR TPVITGAPYEYR TSFNYAMK VEATFGVDESNK VGSAPGLQK VLDALQAIK VSFELFADK VVDVLDSEIK YAAELHLVHWNTK YDPSLKPLSVSYDQATSLR YILAGVENSK YSAELHVAHWNSAK YSSLAEAAASK

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 mscq1 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 measured 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_MSCQ1_1_40dil_1 20140818_005_MSCQ1_1_40dil_3 20140818_007_MSCQ1_1_20dil_1
 20140818_008_MSCQ1_1_20dil_2 20140818_009_MSCQ1_1_20dil_3 20140818_011_MSCQ1_NoDil_1
 20140818_013_MSCQ1_NoDil_2 20140818_015_MSCQ1_NoDil_3 20140818_017_MSCQ1_x2_1
 20140818_019_MSCQ1_x2_2 20140818_021_MSCQ1_x2_3 20140818_023_MSCQ1_x5_1 20140818_025_MSCQ1_x5_2
 20140818_027_MSCQ1_x5_3 20140818_030_MSCQ1_1_5dil_1 20140818_032_MSCQ1_1_5dil_2
 20140818_034_MSCQ1_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_MSCQ1_1_40dil_1_140808162146.raw 20140807_02_MSCQ1_1_40dil_1_140808162146.raw
 20140807_03_MSCQ1_1_40dil_3_140808192115.raw 20140807_04_MSCQ1_1_20dil_1_140808214050.raw
 20140807_05_MSCQ1_1_20dil_2_140808231024.raw 20140807_06_MSCQ1_1_20dil_3_140809004002.raw
 20140807_07_MSCQ1_1_5dil_1_140809025941.raw 20140807_08_MSCQ1_1_5dil_2_140809051908.raw
 20140807_09_MSCQ1_1_5dil_3.raw 20140807_10_MSCQ1_nodil_1.raw 20140807_11_MSCQ1_nodil_2.raw
 20140807_12_MSCQ1_nodil_3.raw 20140807_13_MSCQ1_x2_1.raw 20140807_14_MSCQ1_x2_2.raw
 20140807_15_MSCQ1_x2_3.raw 20140807_16_MSCQ1_x5_1.raw 20140807_17_MSCQ1_x5_2.raw
 20140807_18_MSCQ1_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_conc2_3.raw 20140812_024_QC_conc5_1.raw 20140812_025_QC_conc5_2.raw
 20140812_026_QC_conc5_3.raw 20140818_003_MSCQ1_1_40dil_1.wiff 20140818_004_MSCQ1_1_40dil_1.wiff
 20140818_005_MSCQ1_1_40dil_3.wiff 20140818_007_MSCQ1_1_20dil_1.wiff 20140818_008_MSCQ1_1_20dil_1.wiff
 20140818_009_MSCQ1_1_20dil_3.wiff 20140818_011_MSCQ1_NoDil_1.wiff 20140818_013_MSCQ1_NoDil_2.wiff
 20140818_015_MSCQ1_NoDil_3.wiff 20140818_017_MSCQ1_x2_1.wiff 20140818_019_MSCQ1_x2_2.wiff
 20140818_021_MSCQ1_x2_3.wiff 20140818_023_MSCQ1_x5_1.wiff 20140818_025_MSCQ1_x5_2.wiff
 20140818_027_MSCQ1_x5_3.wiff 20140818_030_MSCQ1_1_5dil_1.wiff 20140818_032_MSCQ1_1_5dil_2.wiff
 20140818_034_MSCQ1_1_5dil_3.wiff 20150526_16_MSCQ1_40xdil_rep1.raw 20150526_17_MSCQ1_40xdil_rep2.raw
 20150526_18_MSCQ1_40xdil_rep3.raw 20150526_20_MSCQ1_20xdil_rep1.raw 20150526_21_MSCQ1_20xdil_rep2.raw
 20150526_22_MSCQ1_20xdil_rep3.raw 20150526_24_MSCQ1_5xdil_rep1.raw 20150526_25_MSCQ1_5xdil_rep2.raw
 20150526_26_MSCQ1_5xdil_rep3.raw 20150526_28_MSCQ1_nodil_rep1.raw 20150526_29_MSCQ1_nodil_rep2.raw
 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
 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(NQ01)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADPSEWSK ALIVLAHSER AVQPPDGLAVLGIPLK DGLDAASYAPVR

EGHLSPDIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK
 GGPFSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGGNEQVTR NLSVEDAAR
 SADFTNFDPR TAENFR TPVISGGPYEYR TPVITGAPYEYR VEATFGVDESNK 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 mscq1 S3 object.

Examples

```
data(mscq1_dil)
## maybe str(mscq1_dil) ; plot(mscq1_dil) ...
```

mscq1_userstudy	<i>mscq1 user study</i>
-----------------	-------------------------

Description

contains a user study

Usage

```
data("mscq1_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_1.wiff
 20140818_009_MSQC1_1_20dil_3.wiff 20140818_011_MSQC1_NoDil_1.wiff 20140818_013_MSQC1_NoDil_2.wiff
 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 DGLDAASYAPVR
 EGHLSPIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK
 GGFPSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGNEQVTR NLSVEDAAR
 SADFTNFDPR TAENFR TPVISGGPYEYR TPVITGAPYEYR VEATFGVDES#N/AK VLDALQAIK VSFELFADK
 YILAGVENS

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. Therefore 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](https://doi.org/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	<i>sigma mix peptides</i>
----------	---------------------------

Description

This table contains msqc1 peptide properties.

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 GYSIFS YATK NLSVEDAAR SADFTNFDP
 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(NQ01)/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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