

# Package ‘msqc1’

February 29, 2024

**Title** Sigma mix MSQC1 data

**Version** 1.30.0

**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

**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	<i>Sigma mix MSQC1 data</i>
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### 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 technical replicates. To derive a complex sample matrix, 10  $\mu$ l of MSQC1 working solution was mixed with 10  $\mu$ l (approx 10  $\mu$ g) tryptic yeast digest (*Saccharomyces cerevisiae*), 1  $\mu$ l iRT peptide stock solution (Biognosys, Schlieren, Switzerland), and 19  $\mu$ 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.

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Maintainer: Christian Panse <cp@fgcz.ethz.ch>

**References**

- [www.sigmaaldrich.com](http://www.sigmaaldrich.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 msvc1 (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 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_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\_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.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(NQ01)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIFLK DGLDAASYYPVR  
 EGHLSPDIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK  
 GGPFSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGGNEQVTR NLSVEDAAR  
 SADFTNFDPR TAENFR TPVISGGPYEYR TPVITGAPYEYR VEATFGVDESNK 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(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 AFYVNVLNNEQR ALIVLAHSER APLTKPLK AVQPPDGLAVLGIFLK DAQIFIQK DGLDAASYAPVR DLFNAIATGK DPANFQYPAESVLAYK DPILFPSFIHSQK DYPLIPVGK EGHLSPDIVAEQK EIINVGHFSFHVNFEDNDNR EPISVSSEQVLK ESDTSYVSLK ESISVSSEQLAQFR FEDENFILK FGLSVGHHLGK FNTANDNDVTQVR FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK GGPFSDSYR GGPLDGTYSR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSATK HDTSLKPISVSNPATAK HNGPEHWHK ILNNGHAFNVFDDSDQK IQILEGWK LCENIAGHLK LFAYPDTHR LFLQFGAQGSPFLK LQFHFHWGSTNEHGSEHTVDGVK LGGNEQVTR LGPNYLHIPPVNCYPYR LIQFHFHWGSLDGQGEHTVDK LNVITVGPYR LSQEDPDYGR LNVANGEAVYCK LYPIANGNNQSPVDIK NAIHTFVQSGSHLAAR NGPEQWSK NLSVEDAAR QDNEILIFWSK QSPVDIDTHTAK SADFTNFDPR SIPTDNQIK TEWLDGK TPVISGGPYEYR TPVITGAPYEYR VEATFGVDESNK VFEHIGK VGSAPGLQK VLDALQAIK VSFELFADK VVDVLDISK YAAELHLVHWNTK YDPSLKPLSVSYDQATSLR YEVQGEVFTKPLWP 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(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 AFYVNVLNNEEQR 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 ILNNGHAFNVEFDDSQDK IQILEGWK LFAYPDTHR LFLQFGAQGSPFLK LGGNEQVTR LNVITVGPR LSQEDPDY GIR LYP IANGNNQSPVDIK NAIHTFVQSGSHLAAR NGPEQWSK NLSVEDAAR QSPVDIDHTAK SADFTNFDPR TEWLDGK TPVISGGPYEYR TPVITGAPYEYR TSFNYAMK VEATFGVDESSNAK VGSAPGLQK VLDALQAIK VSFELFADK VVDVLDSIK YAAELHLVHWNTK YDPSLKPLSVSYDQATSLR YILAGVENS K 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 msvc1 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\_2\_140808162146 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

File.Name a factor with levels 20140807\_01\_MSQC1\_1\_40dil\_1\_140808162146.raw 20140807\_02\_MSQC1\_1\_40dil\_2\_140808162146.raw 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\_conc2\_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.wiff  
20140818\_005\_MSQC1\_1\_40dil\_3.wiff 20140818\_007\_MSQC1\_1\_20dil\_1.wiff 20140818\_008\_MSQC1\_1\_20dil\_2.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 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(NQO1)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIPLK DGLDAASYYPVPR  
EGHLSPIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK  
GGPFSDSYR GTFIIDPAAVIR GTFIIDPGGIVR GYSIFSYATK LFLQFGAQQSPFLK 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 msqc1 S3 object.

**Examples**

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

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msqc1_userstudy	<i>msqc1 user study</i>
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**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.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(NQ01)/P15559 iRT-C18 Standard Peptides PPIA/Q13427

Peptide.Sequence a factor with levels ADVTPADFSEWSK ALIVLAHSER AVQQPDGLAVLGIFLK DGLDAASYAPVR  
 EGHLSPDIVAEQK ESDTSYVSLK FEDENFILK FSTVAGESGSADTVR GAGAFGYFEVTHDITK GAGSSEPVTGLDAK  
 GGPFSDSYR GTFIIDPAAVIR GTFIIDPGGVIR GYSIFSYATK LFLQFGAQGSPFLK LGGNEQVTR 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) ...
```

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peptides	<i>sigma mix peptides</i>
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**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 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(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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