Analyse correlation among precursors

Functional Genomics Center Zurich 15 September, 2018

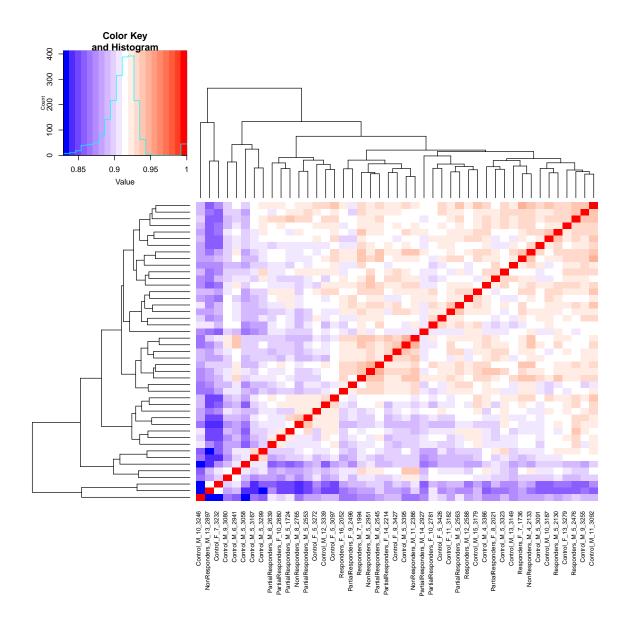
[1] TRUE

QValue Summaries

```
## [1] "precursor_Id" "srm_QValueMin" "srm_QValueNR"
## # A tibble: 16,776 x 7
## # Groups:
               coding, protein_Id, precursor_Id [16,776]
##
      coding protein_Id precursor_Id
                                             Isotope.Label nrReplicates nrNAs
##
      <chr>
              <chr>
                         <chr>>
                                              <chr>
                                                                   <int> <int>
                                                                      23
##
   1 Control P02649
                         _SELEEQLTPVAEETRAR~ Light
                                                                            23
## 2 Control P04264
                         _NKLNDLEDALQQAK__3 Light
                                                                      23
                                                                            23
## 3 Control Q96KN2
                         _VFQ[+1]YIDLHQDEFV~ Light
                                                                      23
                                                                            23
## 4 Control P00450
                         _DIASGLIGPLIIC[+57~ Light
                                                                      23
                                                                            22
## 5 Control P00736
                         _QRPPDLDTSSN[+1]AV~ Light
                                                                      23
                                                                            22
## 6 Control P01023
                         NEDSLVFVQTDK 3
                                                                      23
                                                                            22
## 7 Control P01024
                         _QLANGVDRYISK__3
                                                                      23
                                                                            22
                                             Light
                         _VELLHNPAFC[+57]SL~ Light
## 8 Control P01024
                                                                      23
                                                                            22
                         _VDDGVASFVLNLPSGVT~ Light
                                                                      23
                                                                            22
## 9 Control P01031
## 10 Control P01877
                         _QEPSQGTTTYAVTSILR~ Light
                                                                      23
                                                                            22
## # ... with 16,766 more rows, and 1 more variable: meanArea <dbl>
```

Filter by NA's

```
## # A tibble: 1 x 5
     Isotope.Label protein_Id peptide_Id modPeptide_Id precursor_Id
                                     <int>
                                                                 <int>
##
     <chr>>
                         <int>
                                                   <int>
## 1 Light
                                                    3380
                                                                  4194
                           245
                                      2315
## # A tibble: 1 x 5
     Isotope.Label protein_Id peptide_Id modPeptide_Id precursor_Id
                         <int>
                                     <int>
                                                   <int>
                                                                 <int>
                                                                  3979
## 1 Light
                           245
                                      2208
                                                    3221
## # A tibble: 1 x 5
     Isotope.Label protein_Id peptide_Id modPeptide_Id precursor_Id
     <chr>
                                     <int>
                                                                 <int>
                         <int>
                                                   <int>
## 1 Light
                           237
                                      2058
                                                    2999
                                                                  3671
```

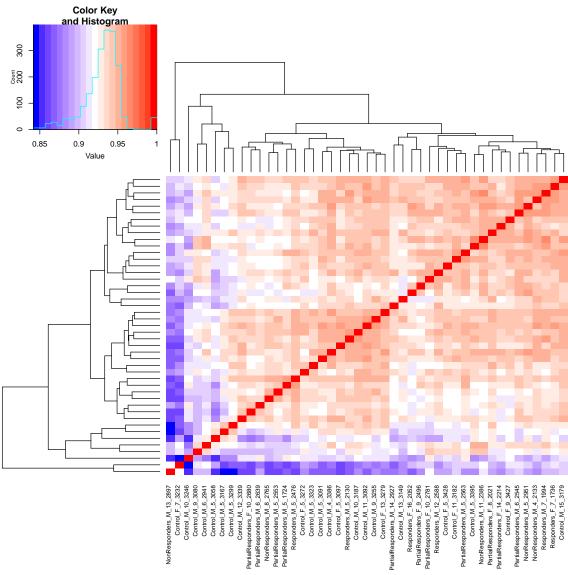


Remove single hit wonders

Correlation Filtering

A tibble: 1 x 5

```
Isotope.Label protein_Id peptide_Id modPeptide_Id precursor_Id
##
     <chr>
                         <int>
                                    <int>
                                                   <int>
                                                                 <int>
## 1 Light
                                     2005
                                                                  3583
                           184
                                                    2927
## # A tibble: 1 x 5
##
     Isotope.Label protein_Id peptide_Id modPeptide_Id precursor_Id
                         <int>
                                    <int>
##
                                                   <int>
                                                                 <int>
## 1 Light
                           145
                                     1455
                                                    2138
                                                                  2619
```



Rank precursors by Intensity

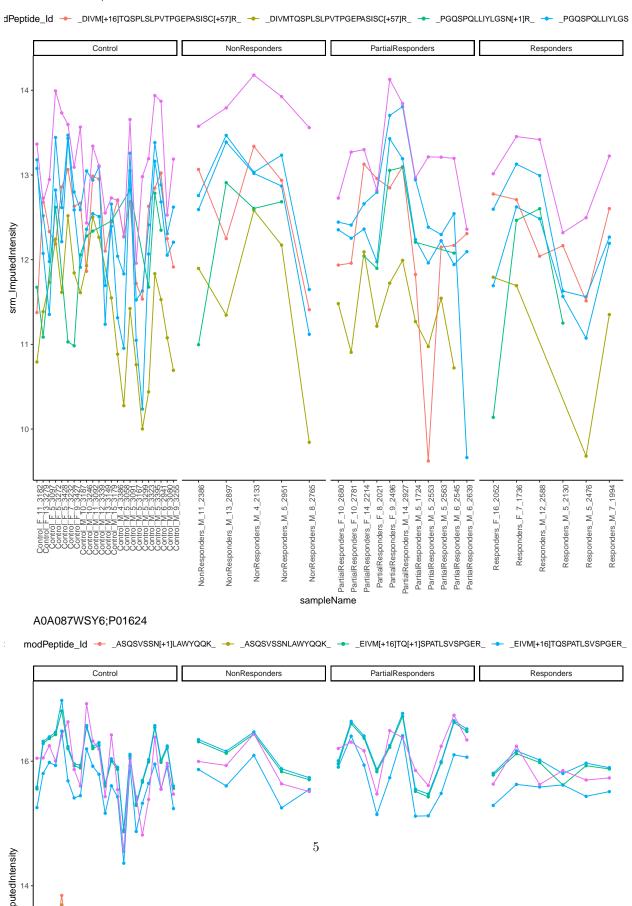
A tibble: 2,619 x 3

protein_Id precursor_Id srm_NrNotNAs ## <chr> <chr> <chr>

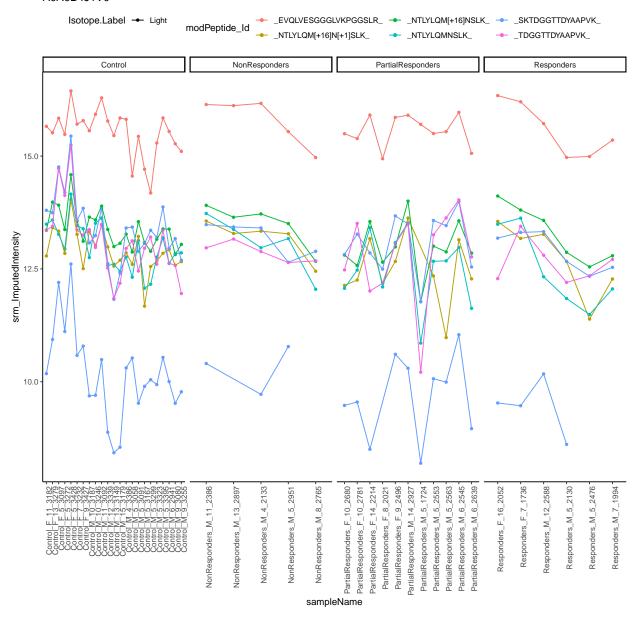
```
1 A0A075B6P5; P01615 _DIVM[+16] TQSPLSLPVTPGEPASISC[+57] R__3
                                                                           45
   2 AOAO75B6P5;P01615 _DIVMTQSPLSLPVTPGEPASISC[+57]R__3
                                                                           41
  3 A0A075B6P5; P01615 PGQSPQLLIYLGSN[+1]R 2
                                                                           27
## 4 AOAO75B6P5;P01615 _PGQSPQLLIYLGSNR__2
                                                                           45
##
   5 AOAO75B6P5; PO1615 _PGQSPQLLIYLGSNR__3
                                                                           45
  6 AOAO75B6P5;P01615 SSQSLLHSNGYNYLDWYLQK 3
                                                                           45
##
  7 A0A075B6S2
                        FSGSGSGTDFTLK 2
                                                                           45
                        _TYLYWYLQK__2
                                                                           22
## 8 A0A075B6S2
## 9 A0A087WSY6; P01624 _ASQSVSSN[+1]LAWYQQK__2
                                                                           45
                                                                           45
## 10 A0A087WSY6; P01624 _ASQSVSSNLAWYQQK__2
## # ... with 2,609 more rows
## [1] "log2 FG.Quantity"
## # A tibble: 2,619 x 9
                                       srm_QValueMin srm_QValueNR srm_NrNotNAs
##
      protein_Id
                   precursor_Id
##
      <chr>
                   <chr>>
                                               <dbl>
                                                            <int>
                                                                          <int>
   1 A0A075B6P5; ~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                                             45
##
                                                               45
   2 AOAO75B6P5;~ DIVMTQSPLSLPVTPG~
                                            6.93e-17
                                                               41
                                                                             41
  3 AOAO75B6P5; ~ _PGQSPQLLIYLGSN[+~
                                                               27
                                                                             27
                                            2.86e- 4
   4 AOAO75B6P5;~ _PGQSPQLLIYLGSNR_~
                                            1.35e-29
                                                               45
                                                                             45
##
  5 AOAO75B6P5;~ _PGQSPQLLIYLGSNR_~
                                            1.19e-63
                                                               45
                                                                             45
  6 AOAO75B6P5; ~ SSQSLLHSNGYNYLDW~
                                                                             45
                                            3.89e-30
                                                               45
                   _FSGSGSGTDFTLK__2
                                                                             45
## 7 A0A075B6S2
                                            3.15e-64
                                                               45
                   _TYLYWYLQK__2
                                                               22
                                                                             22
   8 A0A075B6S2
                                            4.06e-8
                                                                             45
## 9 AOAO87WSY6;~ _ASQSVSSN[+1]LAWY~
                                            1.27e-20
                                                               45
## 10 AOAO87WSY6;~ _ASQSVSSNLAWYQQK_~
                                            1.84e-54
                                                                             45
## # ... with 2,609 more rows, and 4 more variables: srm_NrNotNARank <int>,
      srm_decorelated <lgl>, srm_meanInt <dbl>, srm_meanIntRank <int>
## # A tibble: 110,712 x 10
##
      protein_Id
                                       srm_QValueMin srm_QValueNR srm_NrNotNAs
                   precursor_Id
##
      <chr>
                   <chr>
                                               <dbl>
                                                            <int>
                                                                          <int>
   1 A0A075B6P5;~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                                             45
##
                                                               45
   2 A0A075B6P5; ~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                               45
                                                                             45
   3 A0A075B6P5;~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                                             45
                                                               45
                                                                             45
##
   4 AOAO75B6P5;~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                               45
                                                                            45
## 5 AOAO75B6P5;~ _DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                               45
## 6 A0A075B6P5;~ _DIVM[+16]TQSPLSL~
                                                                             45
                                            2.50e-21
                                                               45
## 7 AOAO75B6P5;~ _DIVM[+16]TQSPLSL~
                                                               45
                                                                             45
                                            2.50e-21
                                            2.50e-21
## 8 AOAO75B6P5;~ _DIVM[+16]TQSPLSL~
                                                               45
                                                                             45
## 9 A0A075B6P5;~ DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                               45
                                                                             45
## 10 A0A075B6P5; ~ DIVM[+16]TQSPLSL~
                                            2.50e-21
                                                               45
                                                                             45
## # ... with 110,702 more rows, and 5 more variables: srm NrNotNARank <int>,
## #
       srm_decorelated <lgl>, srm_meanInt <dbl>, srm_meanIntRank <int>,
## #
       srm_ImputedIntensity <dbl>
```

Aggregation





A0A0B4J1V0



A0A075B6P5;P01615 Control NonResponders PartialResponders Responders 14 srm_ImputedIntensity 10 NonResponders_M_4_2133 PartialResponders_F_9_2496 PartialResponders_M_5_2553 PartialResponders_M_5_2563 PartialResponders_M_6_2545* PartialResponders_M_6_2639* Responders_F_16_2052 Responders_M_12_2588 Responders_M_5_2476 Responders_M_7_1994 NonResponders_M_13_2897 NonResponders_M_8_2765 PartialResponders_F_10_2680 PartialResponders_F_10_2781 PartialResponders_F_14_2214 PartialResponders_F_8_2021 PartialResponders_M_14_2927 PartialResponders_M_5_1724 NonResponders_M_5_2951

Combine all in one function.

sampleName