Analysing MaxQuant Output with R

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30 September 2015

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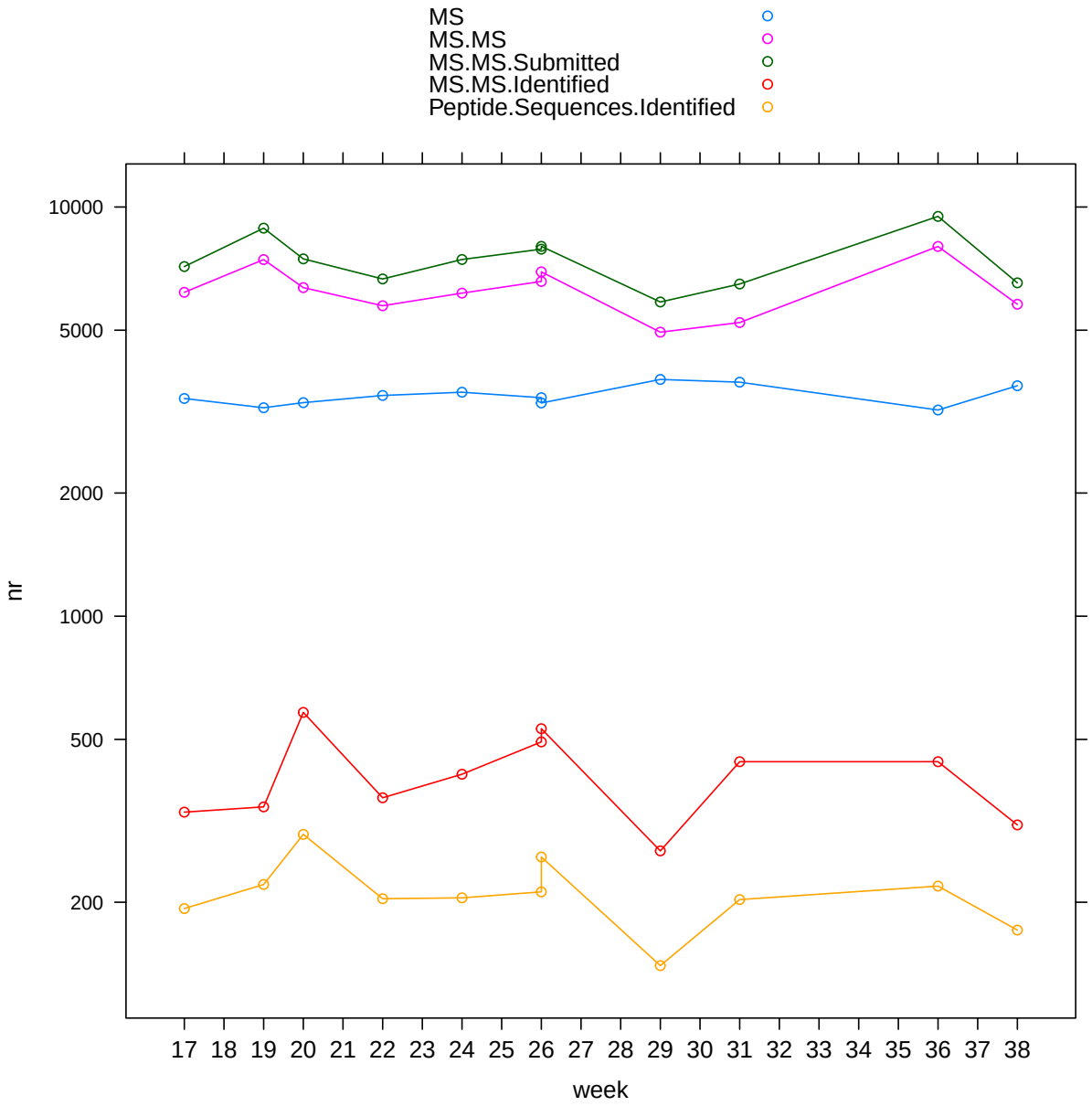
Prepare mrm table

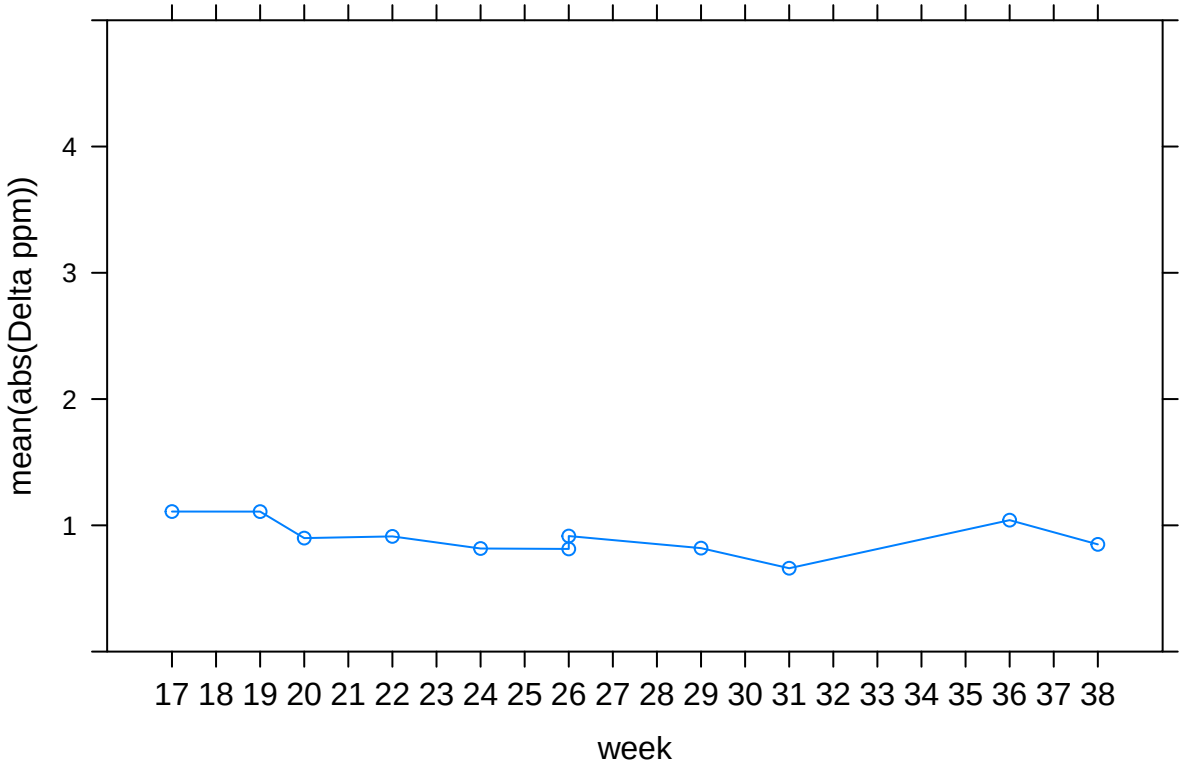
- nr of assigned spectra (MS2) / versus total spectra
- How many H/L target peptides are identified
- Ratio among H/L of the target peptides
- Intensity of heavy or light over the runs

Analysed Dataset is jennifergarcia_20150923_firstBatchFromCRG.sqlite3

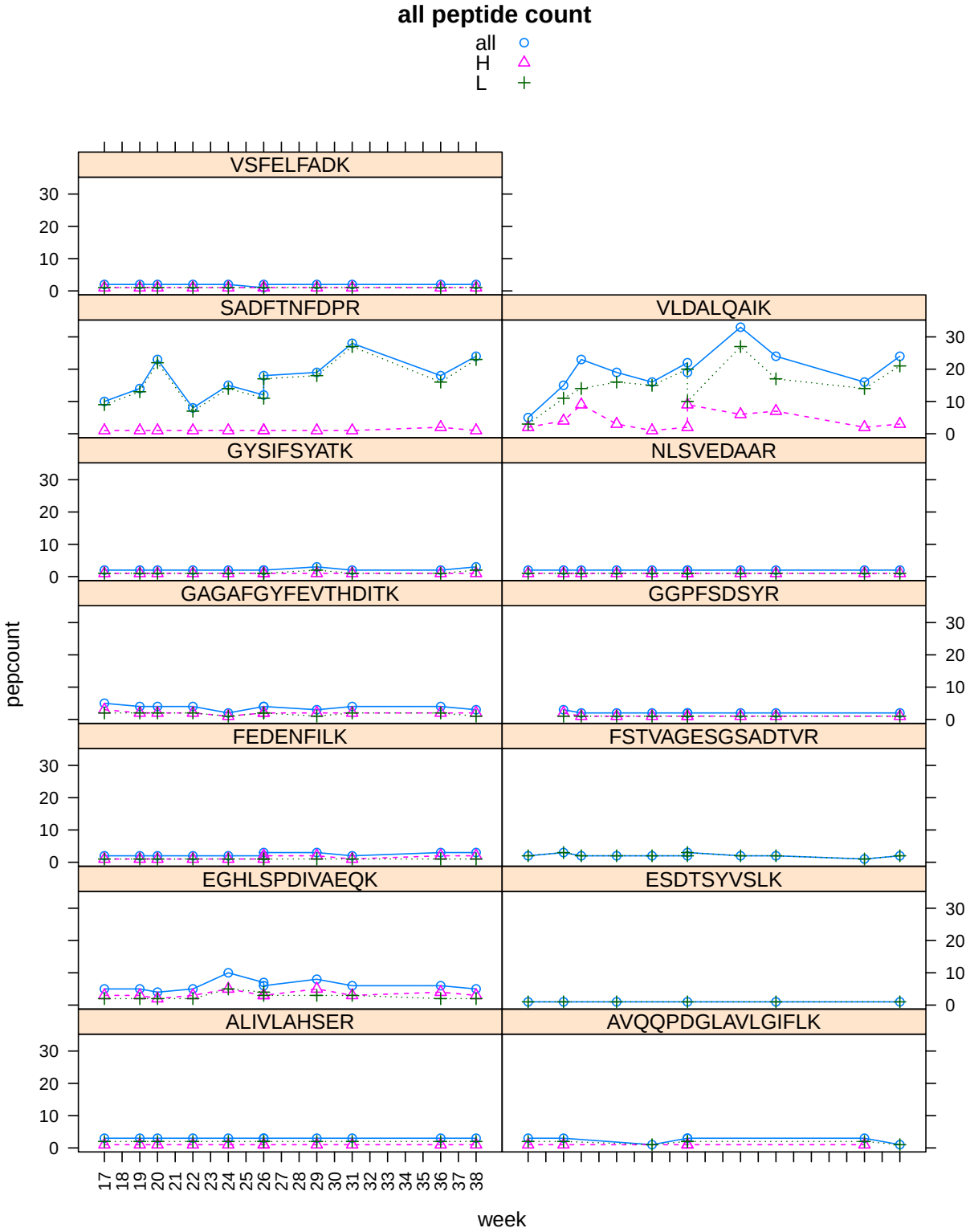
Number of spectra, spectra peptide matches, and unique peptides



Looking at measurement error



Looking at MSQC 1 peptide counts



Look at Intensities (by species)

```
## Warning in FUN(X[[i]], ...): integer overflow - use sum(as.numeric(.))

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```
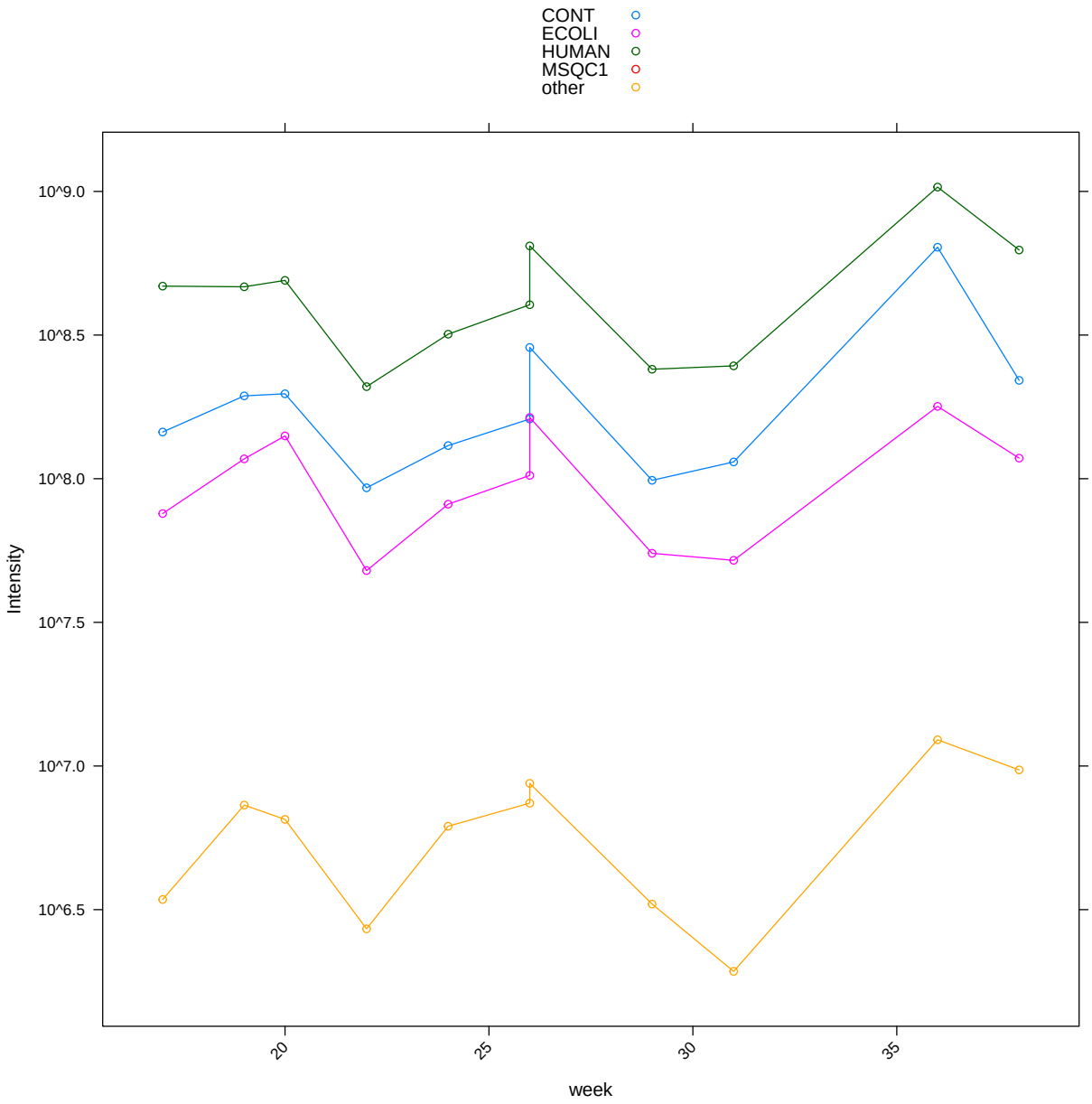
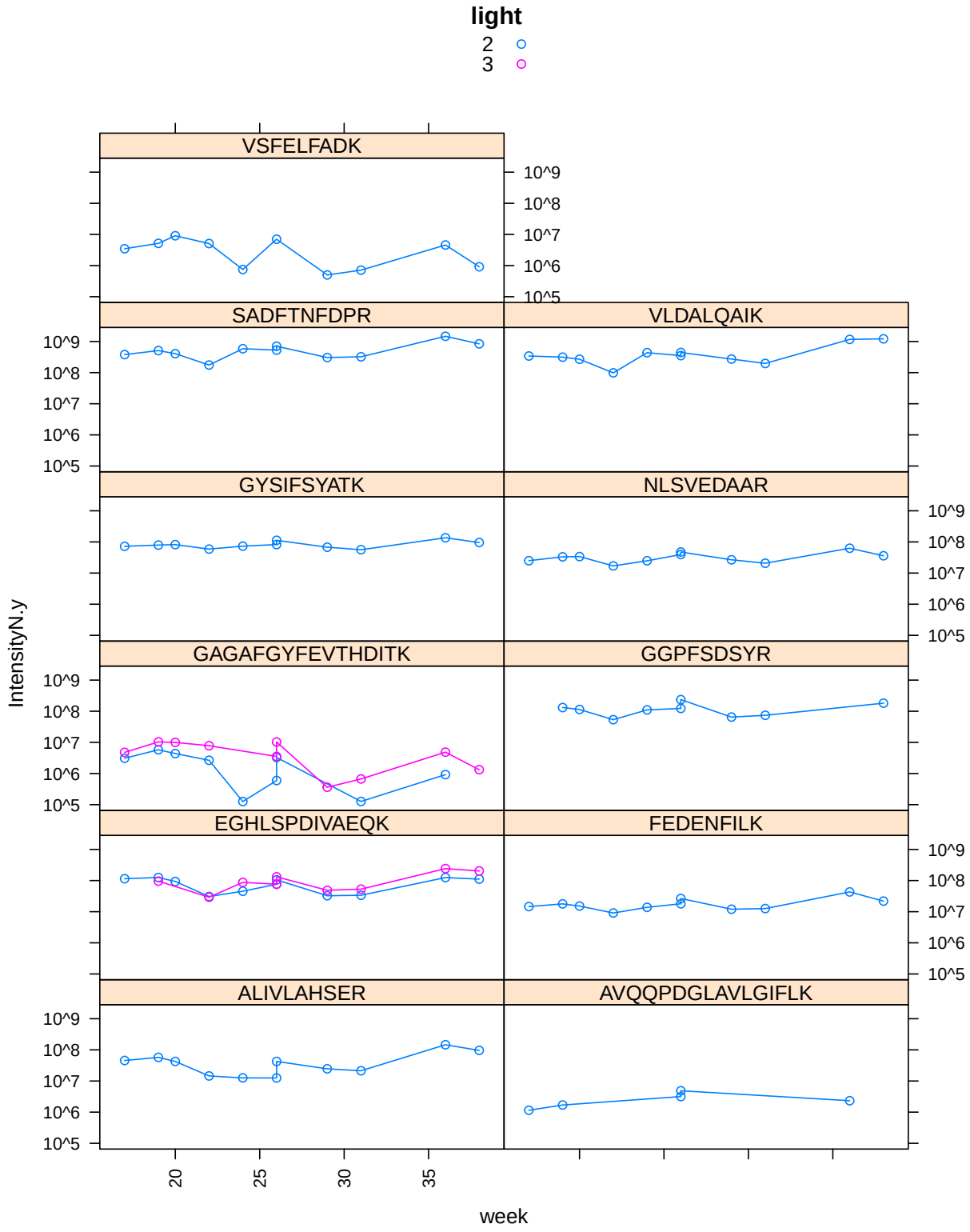
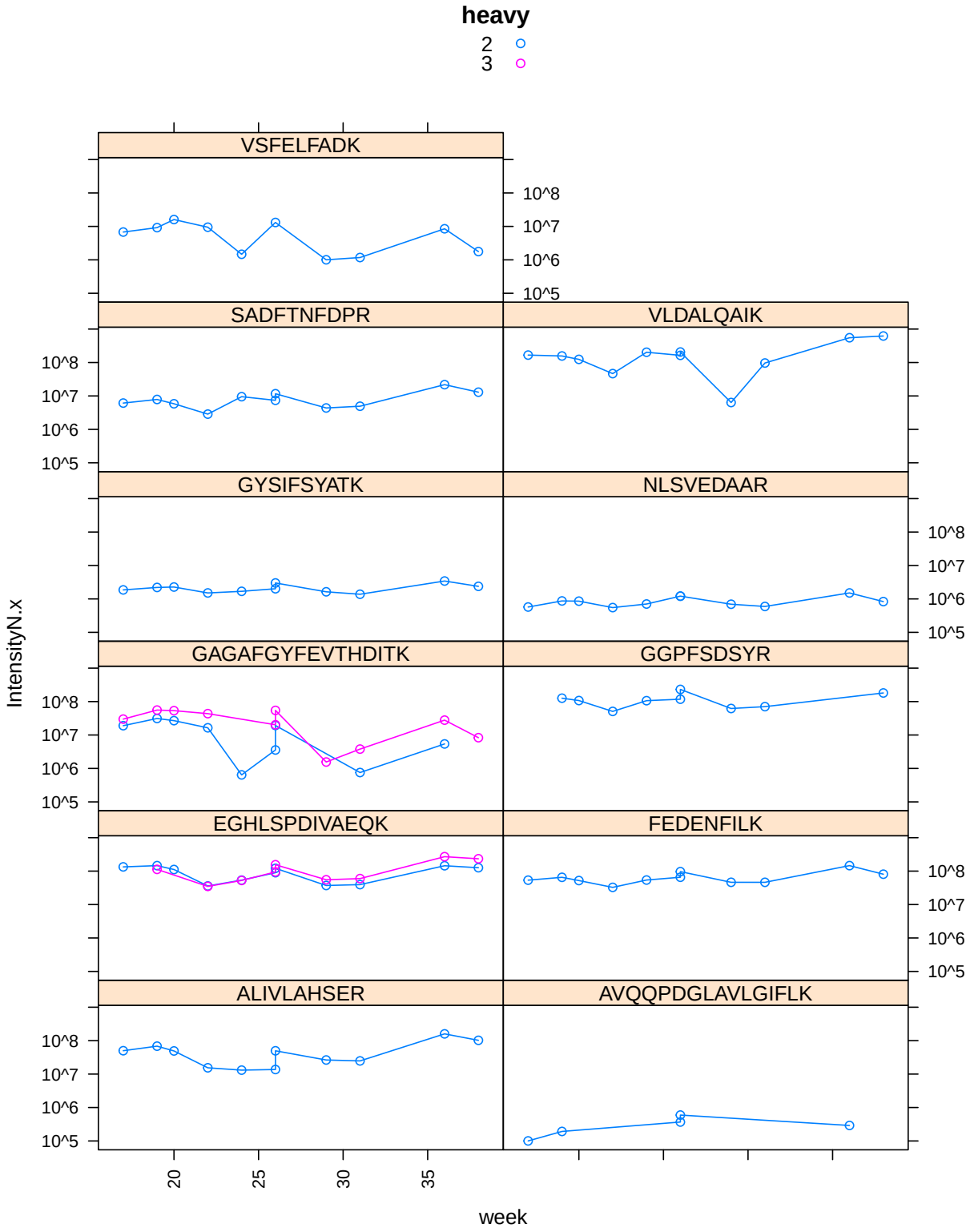
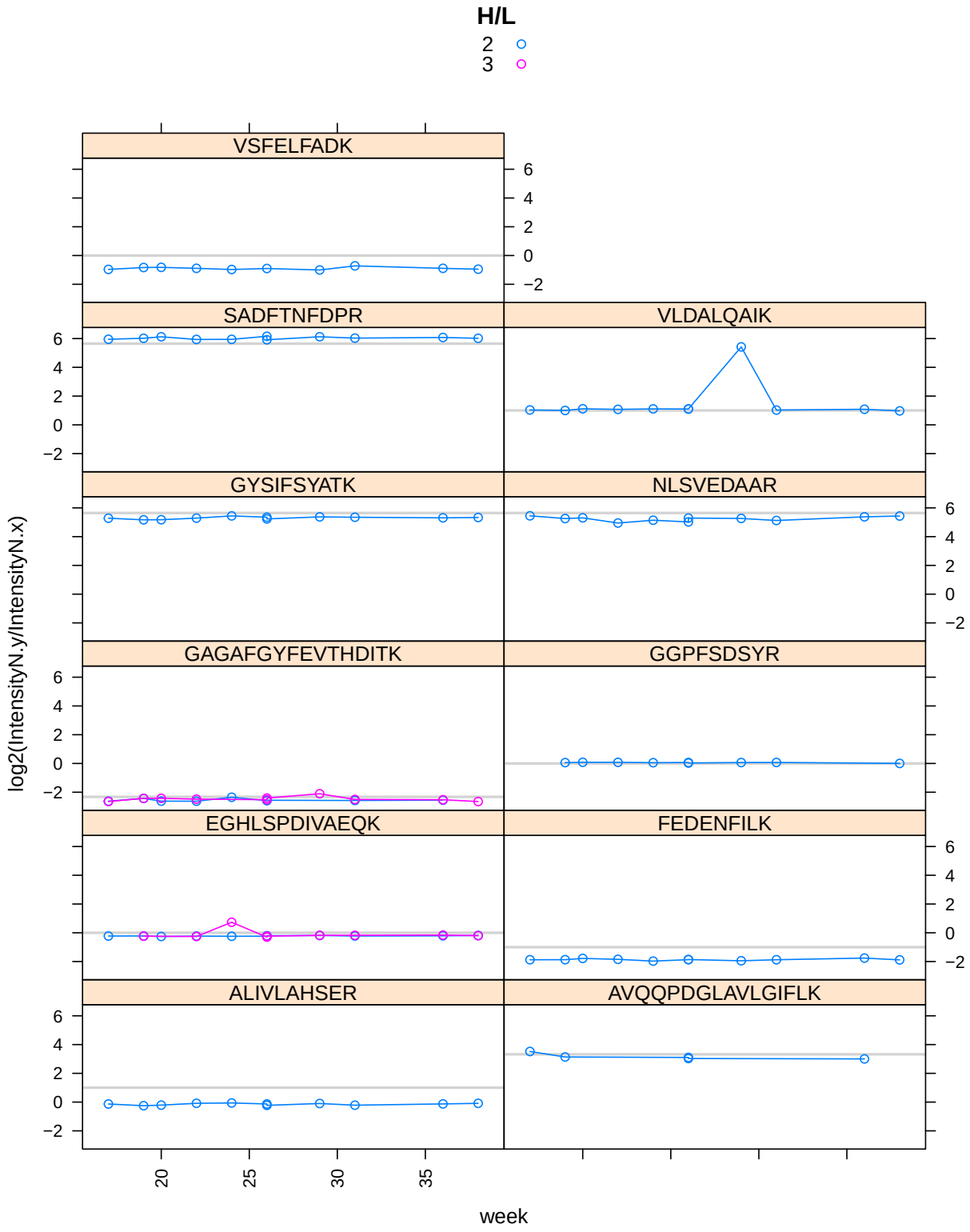


CONT
ECOLI
HUMAN
MSQC1
other
10^9.0
10^8.5
10^8.0
10^7.5
10^7.0
10^6.5
Intensity
20
25
30
35
week

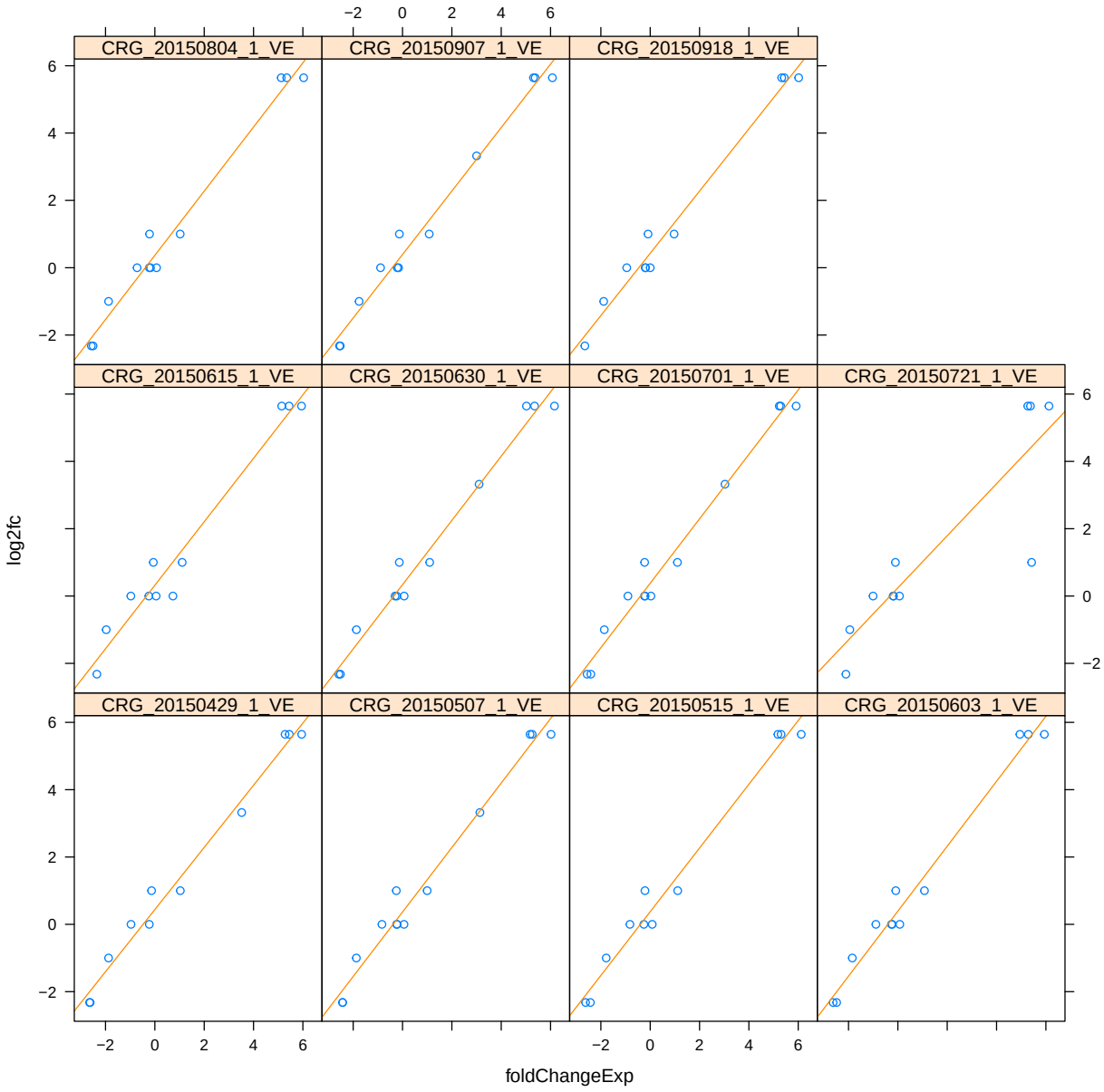
Looking at intensities msqc1

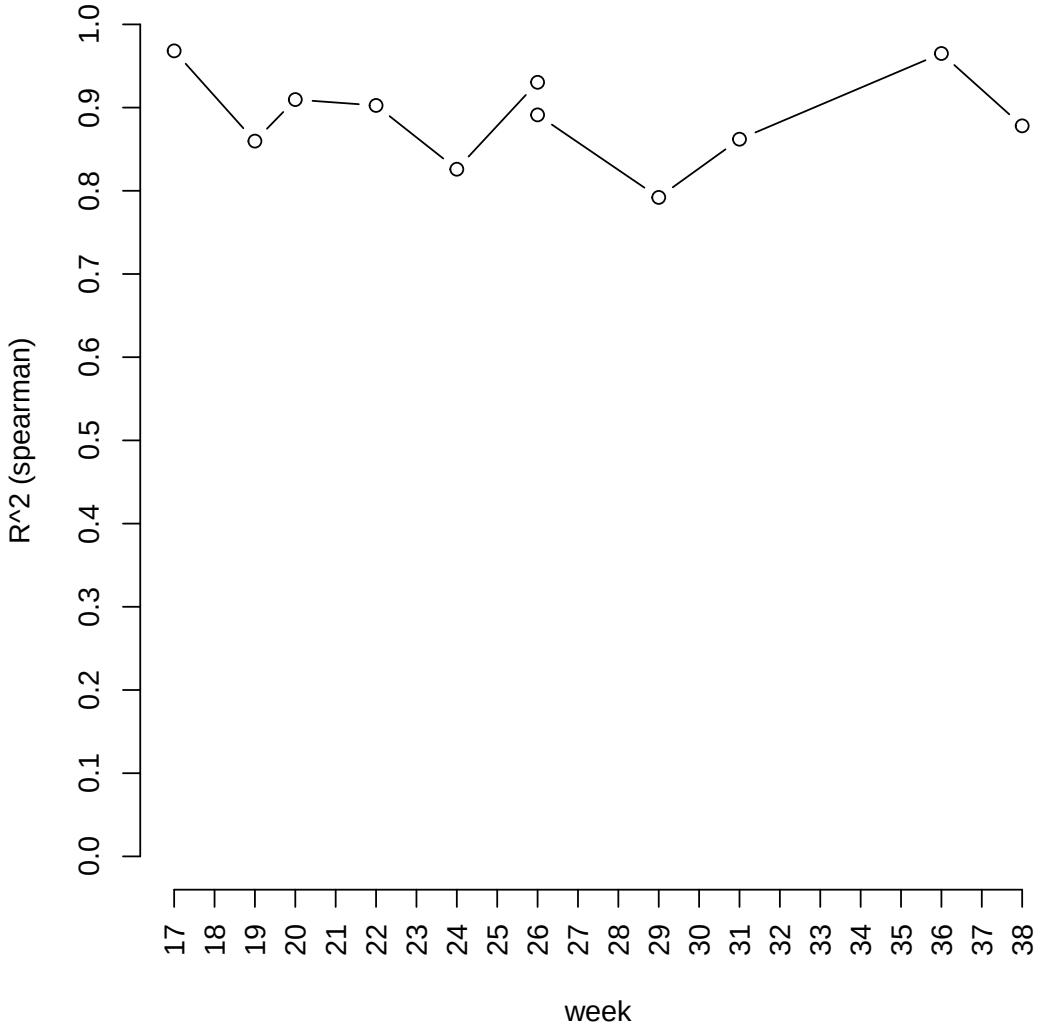



heavy
2
3
VSFELFADK
SADFTNFDPR
VLDALQAIK
GYSIFSYATK
NLSVEDAAR
GAGAFGYFEVTHDITK
GGPFSDSYR
EGHLSPDIVAEQK
FEDENFILK
ALIVLAHSER
AVQQPDGLAVLGIFLK
IntensityN.x
10^8
10^7
10^6
10^5
20
25
30
35
week

Fold change


H/L
2
3
VSFELFADK
SADFTNFDPR
VLDALQAIK
GYSIFSYATK
NLSVEDAAR
GAGAFGYFEVTHDITK
GGPFSDSYR
EGHLSPDIVAEQK
FEDENFILK
ALIVLAHSER
AVQQPDGLAVLGIFLK
log2(IntensityN.y/IntensityN.x)
week


CRG_20150804_1_VE
CRG_20150907_1_VE
CRG_20150918_1_VE
CRG_20150615_1_VE
CRG_20150630_1_VE
CRG_20150701_1_VE
CRG_20150721_1_VE
CRG_20150429_1_VE
CRG_20150507_1_VE
CRG_20150515_1_VE
CRG_20150603_1_VE
log2fc
foldChangeExp


R^2 (spearman)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
week