

Example of data preprocessing

Functional Genomics Center Zurich

15 September, 2018

```
## X      Sample.Name      Protein.Name Peptide.Sequence
## 1 1 highG_p02_day06    sp|P04406|G3P_HUMAN  GALQNIIPASTGAAK
## 2 2 highG_p02_day06    sp|P04406|G3P_HUMAN  GALQNIIPASTGAAK
## 3 3 highG_p02_day06    sp|P04406|G3P_HUMAN  GALQNIIPASTGAAK
## 4 4 highG_p02_day06    sp|P04406|G3P_HUMAN  GALQNIIPASTGAAK
## 5 5 highG_p02_day06    sp|P04406|G3P_HUMAN  GALQNIIPASTGAAK
## 6 6 highG_p02_day06    sp|O95477|ABCA1_HUMAN  FVSPLSWDLVGR
##
##      Replicate.Name Precursor.Charge Product.Charge
## 1 13_S172857_highG_p02_day06_hP_dil10      2      1
## 2 13_S172857_highG_p02_day06_hP_dil10      2      1
## 3 13_S172857_highG_p02_day06_hP_dil10      2      1
## 4 13_S172857_highG_p02_day06_hP_dil10      2      1
## 5 13_S172857_highG_p02_day06_hP_dil10      2      1
## 6 13_S172857_highG_p02_day06_hP_dil10      2      1
##
##      Fragment.Ion annotation_QValue Isotope.Label Precursor.Mz Product.Mz
## 1      y11      0.0293      light      706.3988 1042.5891
## 2      y9      0.0293      light      706.3988 815.4621
## 3      y8      0.0293      light      706.3988 702.3781
## 4      y10     0.0293      light      706.3988 928.5462
## 5      y6      0.0293      light      706.3988 534.2882
## 6      y9      0.0293      heavy      693.3762 1052.5763
##
##      Retention.Time      Area Background Condition2 time day Condition
## 1      36.73 128593424      1405325      highG p02 day06 Group 2
## 2      36.73 370520032      4936271      highG p02 day06 Group 2
## 3      36.73 716306944      8070486      highG p02 day06 Group 2
## 4      36.73 90900808      1061179      highG p02 day06 Group 2
## 5      36.73 60684092      656052      highG p02 day06 Group 2
## 6      51.90 2432844      0      highG p02 day06 Group 2
```

Example how to report all proteins.

Rendering the SRMReport

Computing L to Heavy fold changes

```
## [1] "Isotope.Label"
## [1] "log2L_log2H"
##      [1]      NA      NA      NA -10.551477      NA      NA
##      [7]      NA      NA      NA      NA      NA      NA
##     [13]      NA      NA      NA      NA      NA      NA
##     [19]      NA      NA      NA      NA      NA      NA
##     [25] -7.056852      NA      NA      NA      NA      NA
##     [31]      NA      NA      NA      NA -8.396103 -7.948856
##     [37]      NA -7.259949 -8.392739      NA -7.406683      NA
##     [43] -8.921608 -5.935360      NA      NA      NA      NA
##     [49]      NA      NA      NA      NA      NA      NA
##     [55]      NA      NA      NA      NA      NA      NA
##     [61] -5.549133      NA -2.960325 -3.335274 -5.585745 -6.563938
```

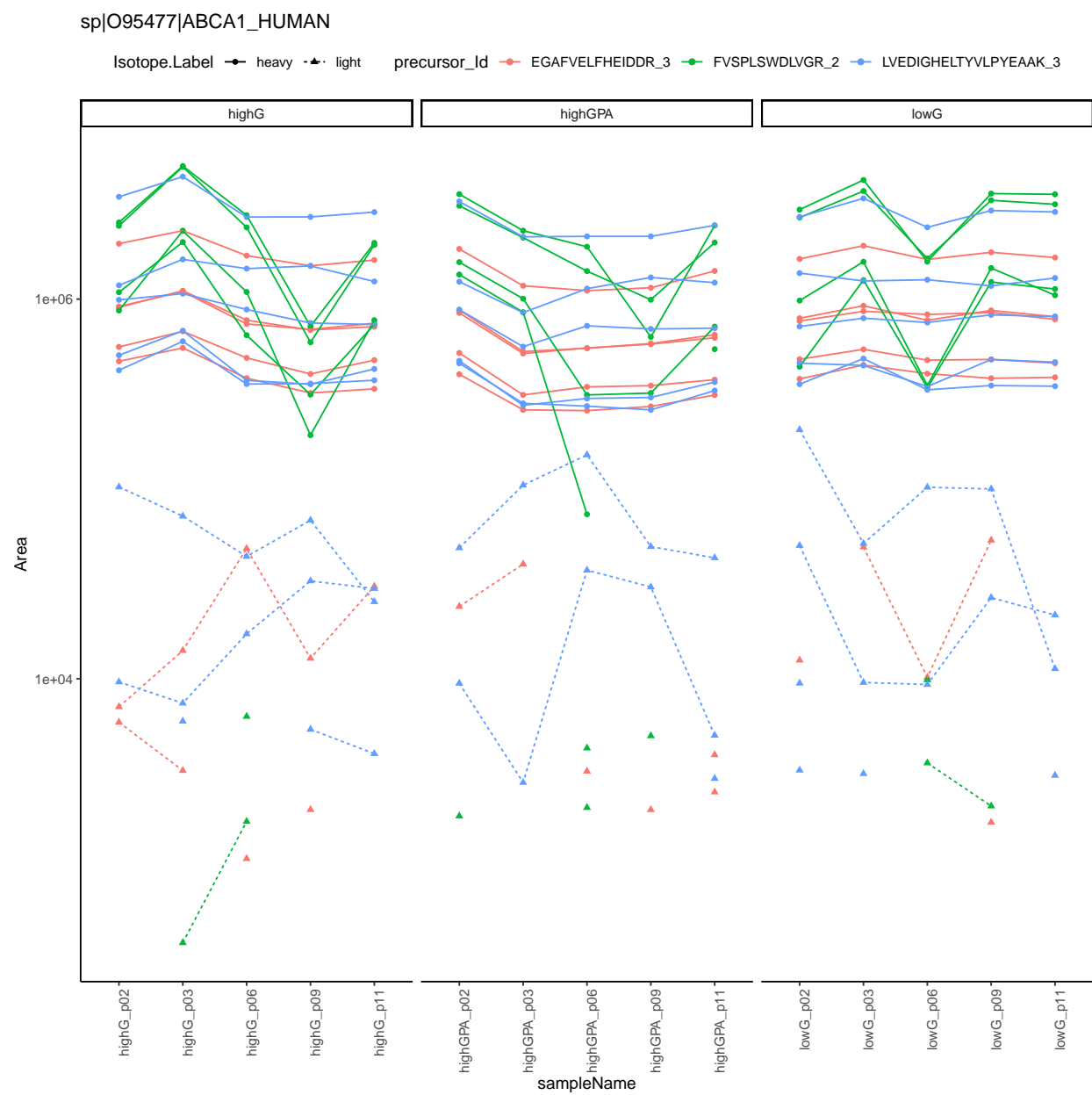


Figure 1: transitions in one plot.

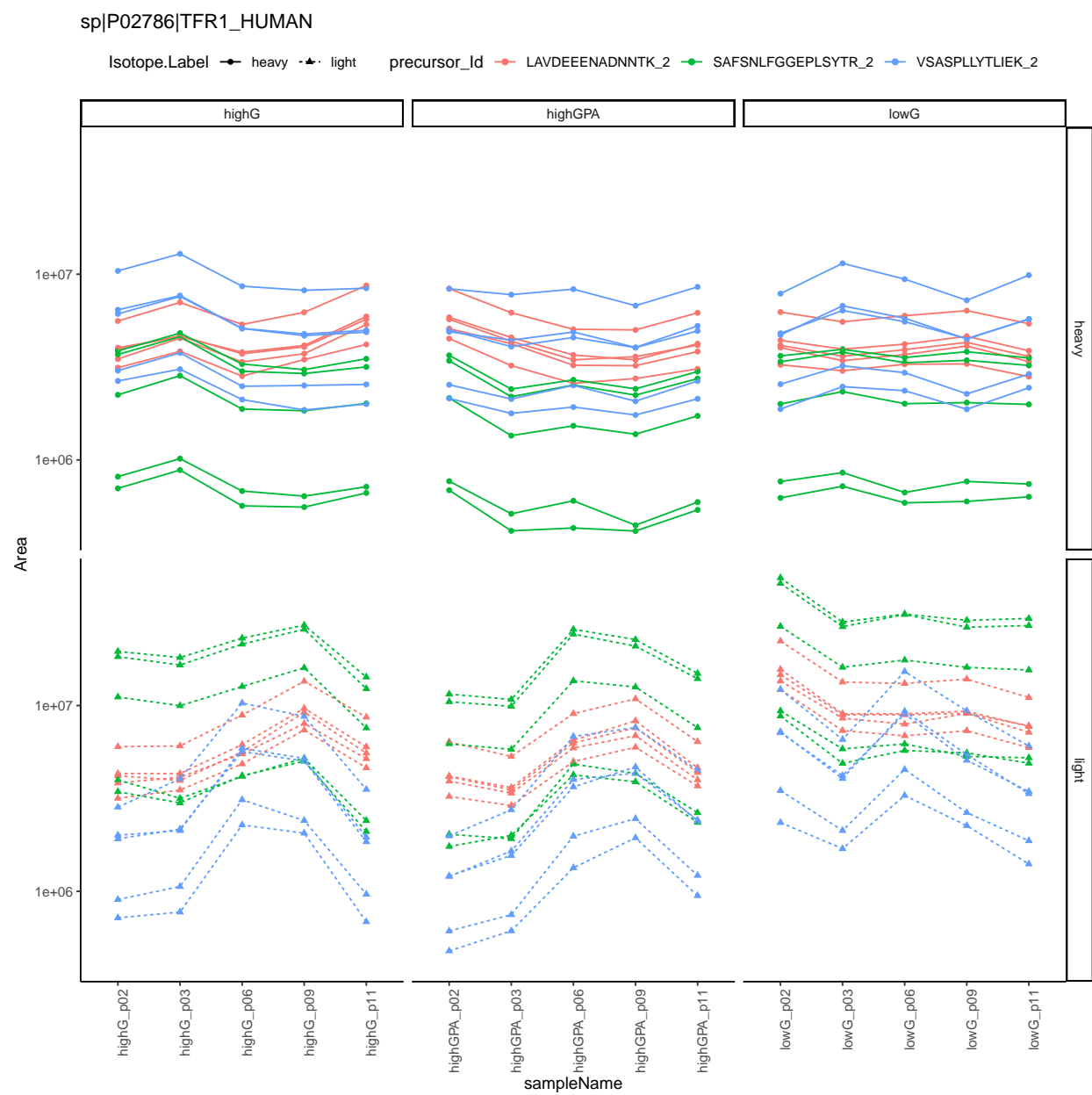
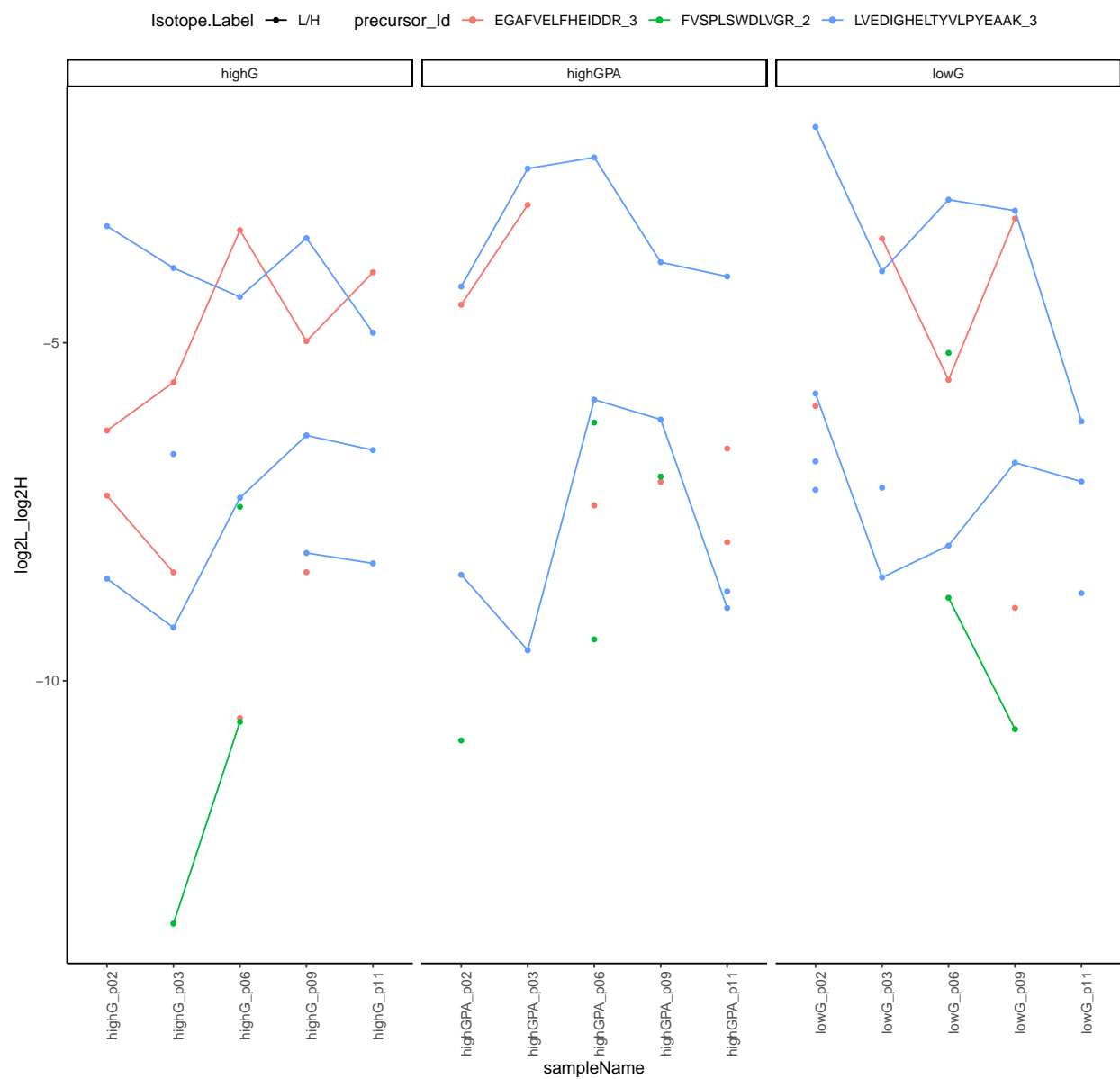


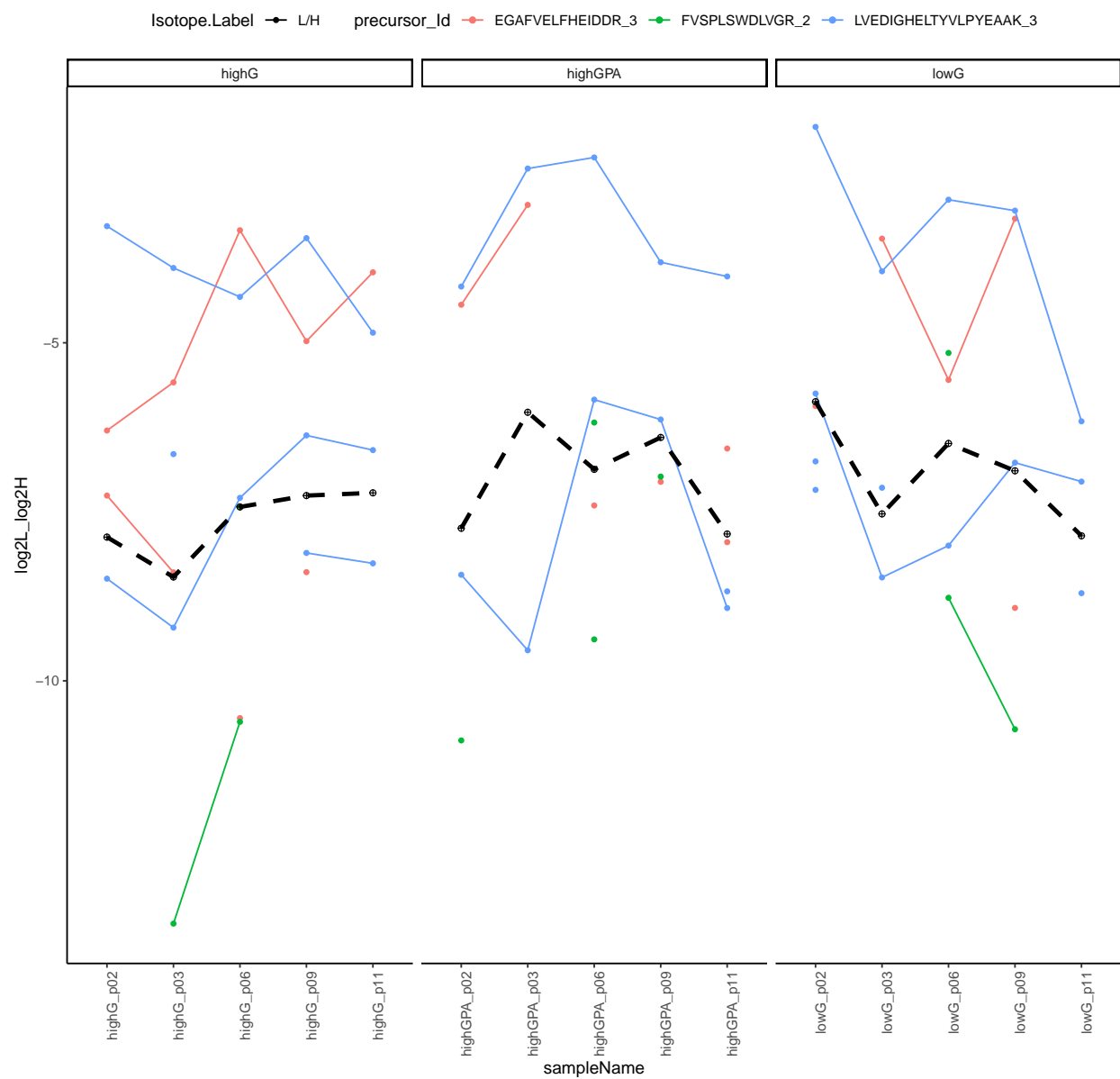
Figure 2: transitions in separate plot.

##	[67]	-3.459113	-6.297851	-4.975770	NA	NA	-4.437000
##	[73]	-3.163649	NA	-3.957385	-8.772215	NA	NA
##	[79]	-10.607116	-13.591488	NA	NA	NA	NA
##	[85]	-6.979330	NA	-10.882085	-10.716845	NA	NA
##	[91]	NA	NA	NA	NA	NA	NA
##	[97]	NA	NA	NA	NA	NA	NA
##	[103]	NA	NA	NA	-5.150000	NA	NA
##	[109]	-7.426682	NA	NA	NA	NA	NA
##	[115]	NA	-6.179531	NA	NA	NA	NA
##	[121]	NA	NA	NA	NA	NA	NA
##	[127]	NA	NA	NA	NA	-9.387400	NA
##	[133]	NA	NA	NA	NA	NA	NA
##	[139]	NA	-6.646594	NA	NA	NA	NA
##	[145]	NA	NA	NA	NA	-6.754770	NA
##	[151]	NA	NA	NA	NA	NA	NA
##	[157]	-7.143938	NA	NA	NA	NA	NA
##	[163]	NA	NA	NA	-2.883584	-6.161626	-2.422533
##	[169]	-4.321249	-3.893215	-4.018760	-3.942126	-3.274540	-3.451653
##	[175]	-3.808598	-2.258144	-4.167787	-3.045330	-1.806327	-4.850652
##	[181]	-8.000091	-7.053558	-9.548436	-7.293350	-9.212809	-8.923240
##	[187]	-8.470963	-8.489043	-6.369571	-6.134781	-5.840968	-8.431795
##	[193]	-6.773117	-5.750571	-6.587164	NA	-8.703663	NA
##	[199]	NA	NA	-8.676629	NA	NA	-8.108589
##	[205]	NA	NA	NA	NA	-7.175805	-8.262446

sp|O95477|ABCA1_HUMAN



sp|O95477|ABCA1_HUMAN



Get Protein intensities

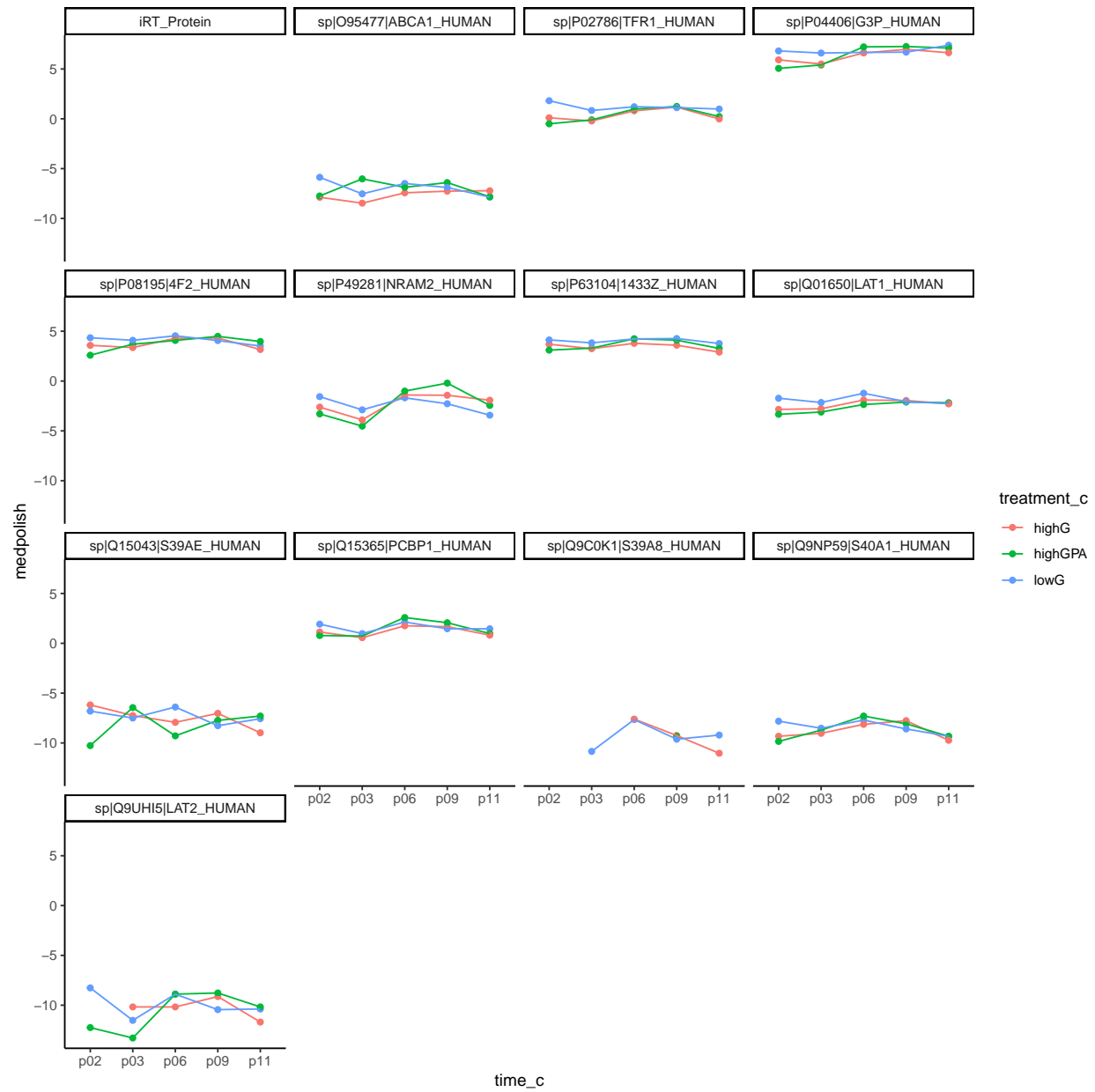


Figure 3: Plot protein intensities

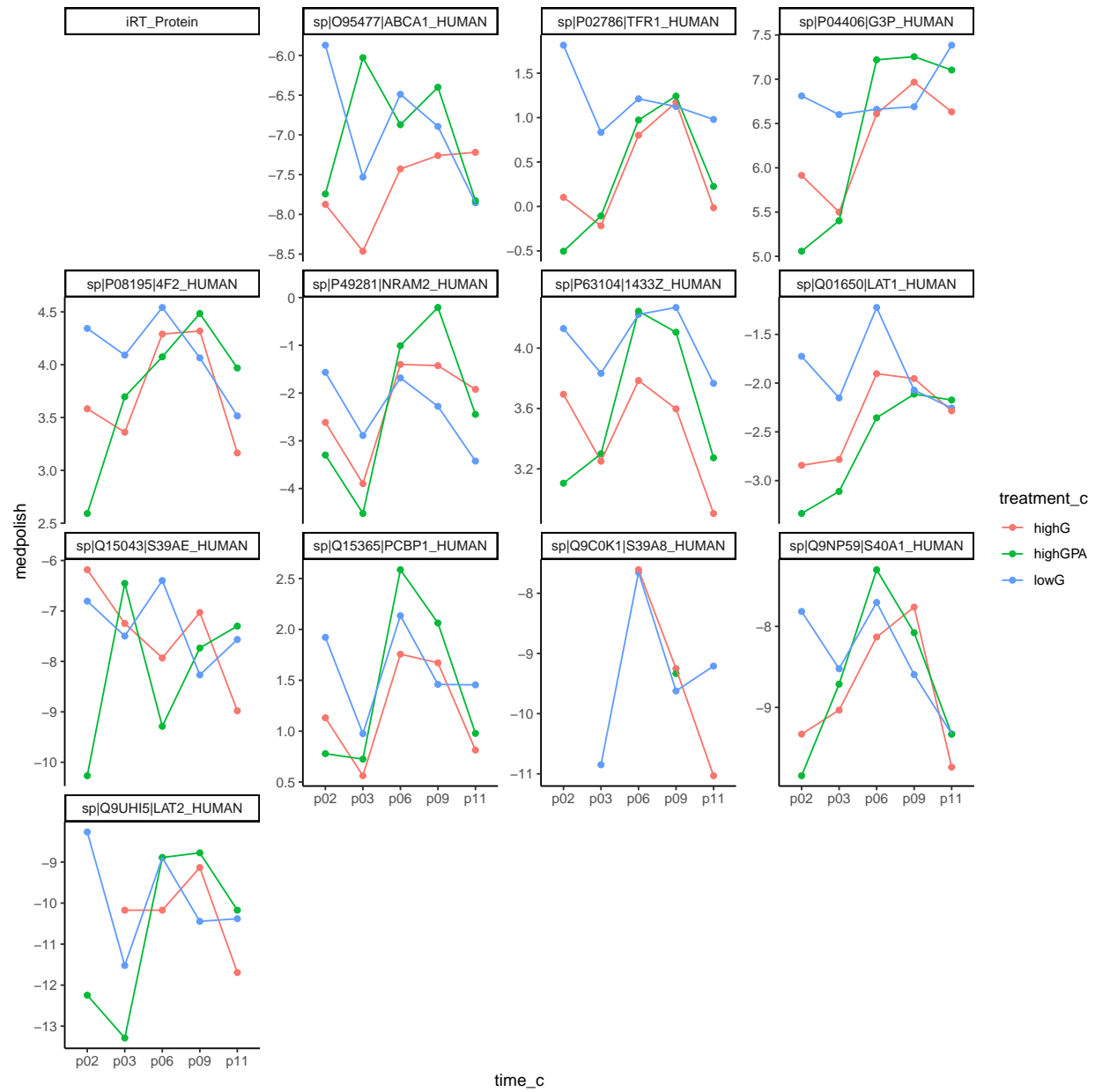


Figure 4: Plot protein intensities