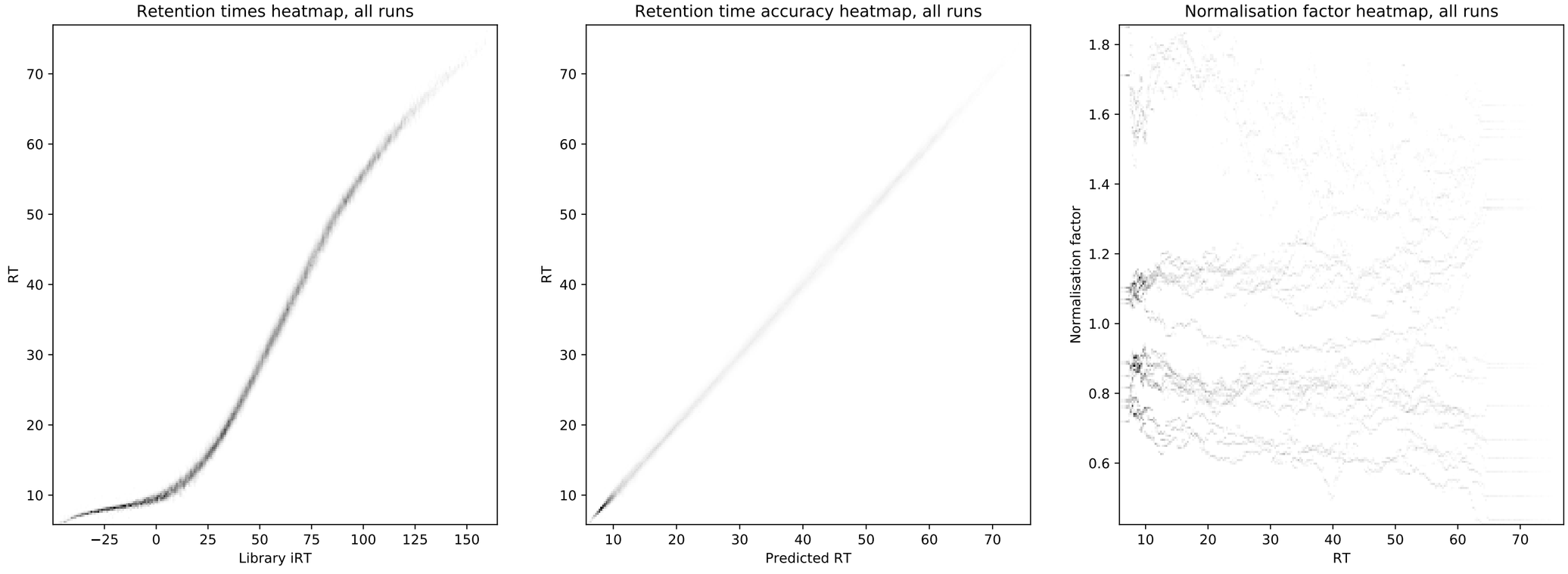
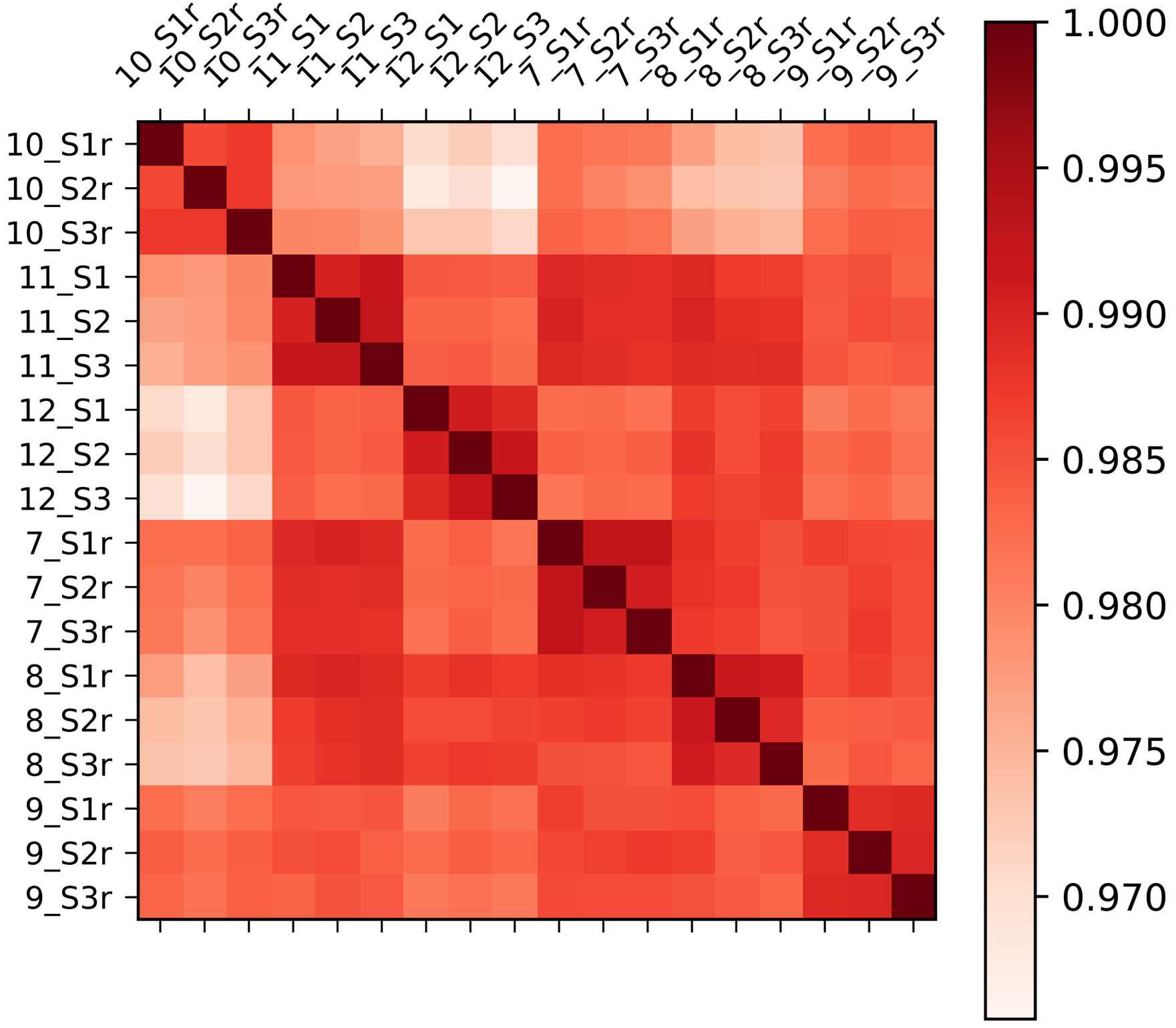
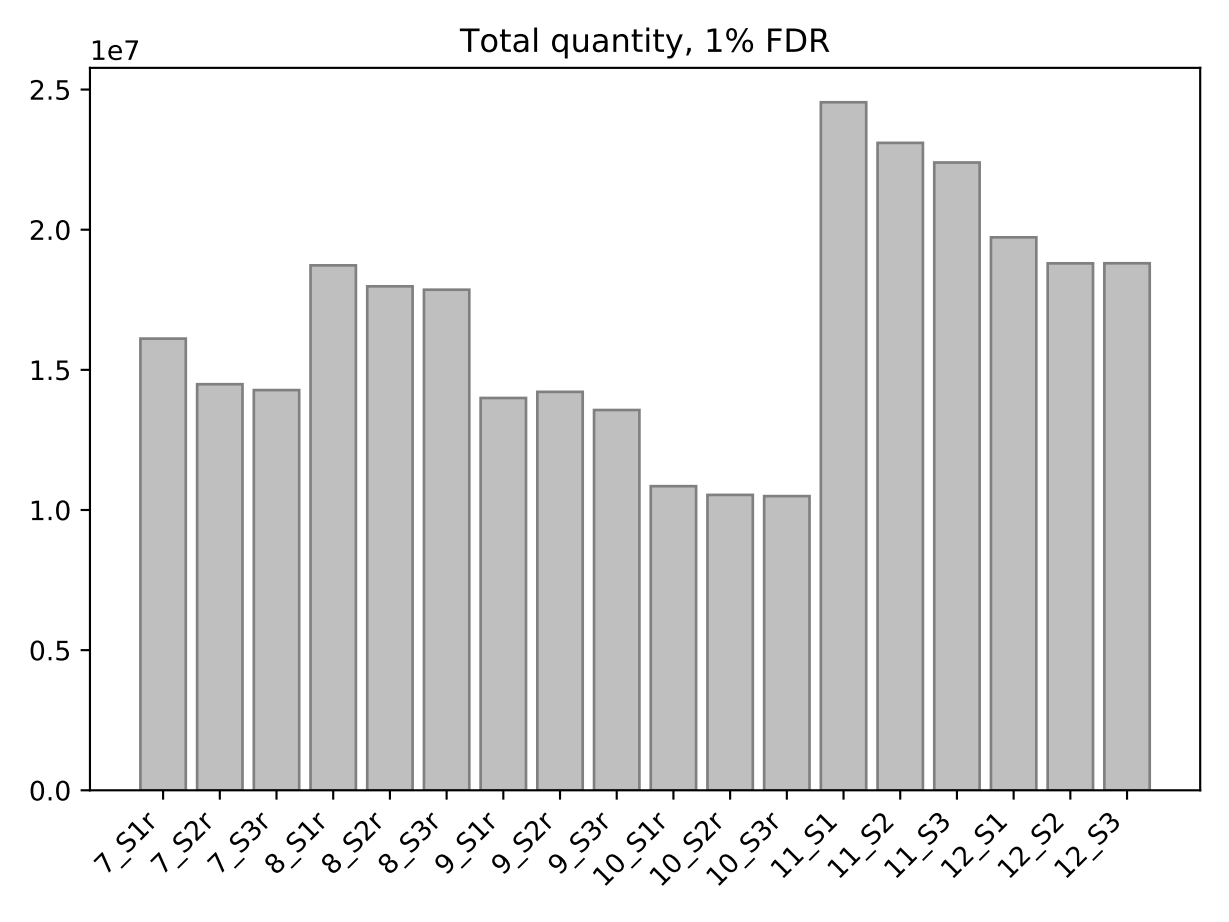
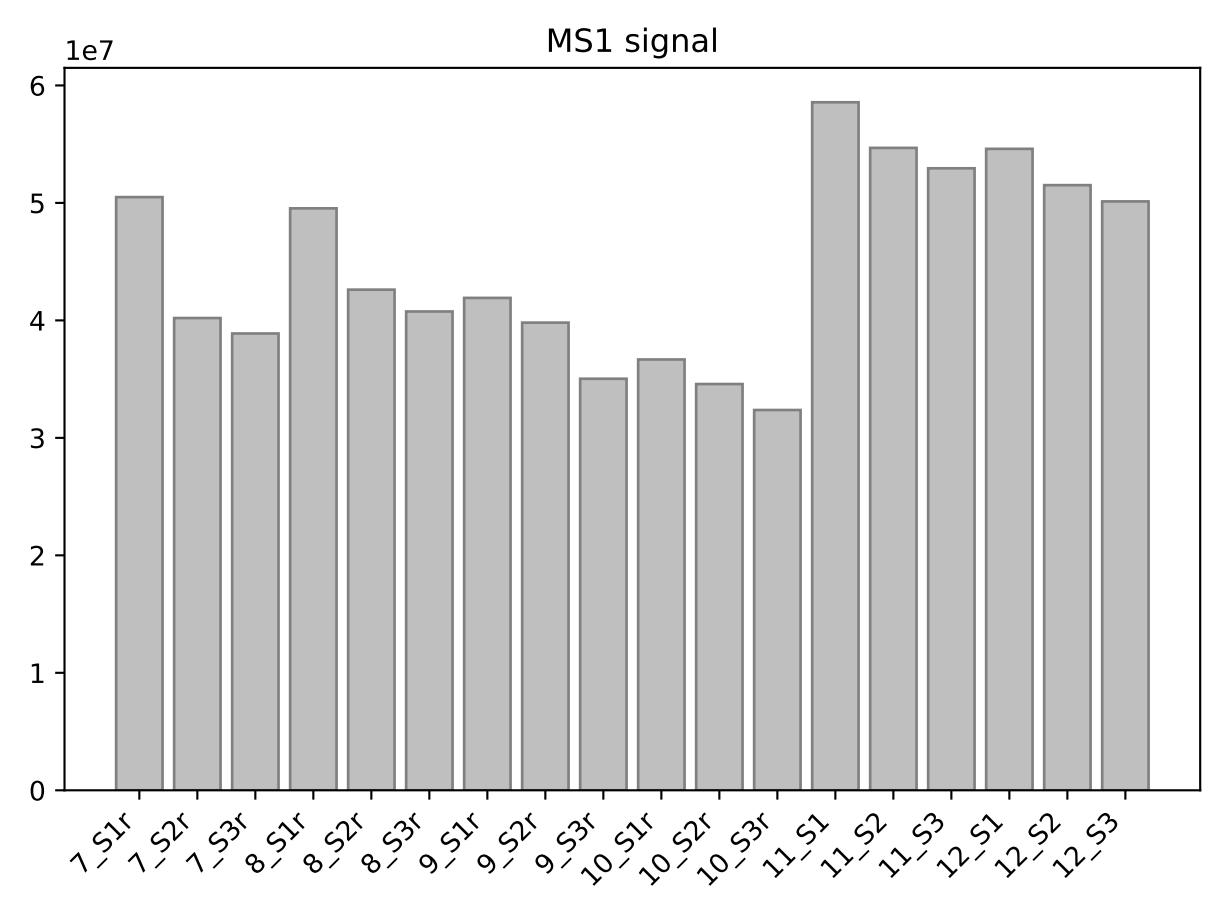
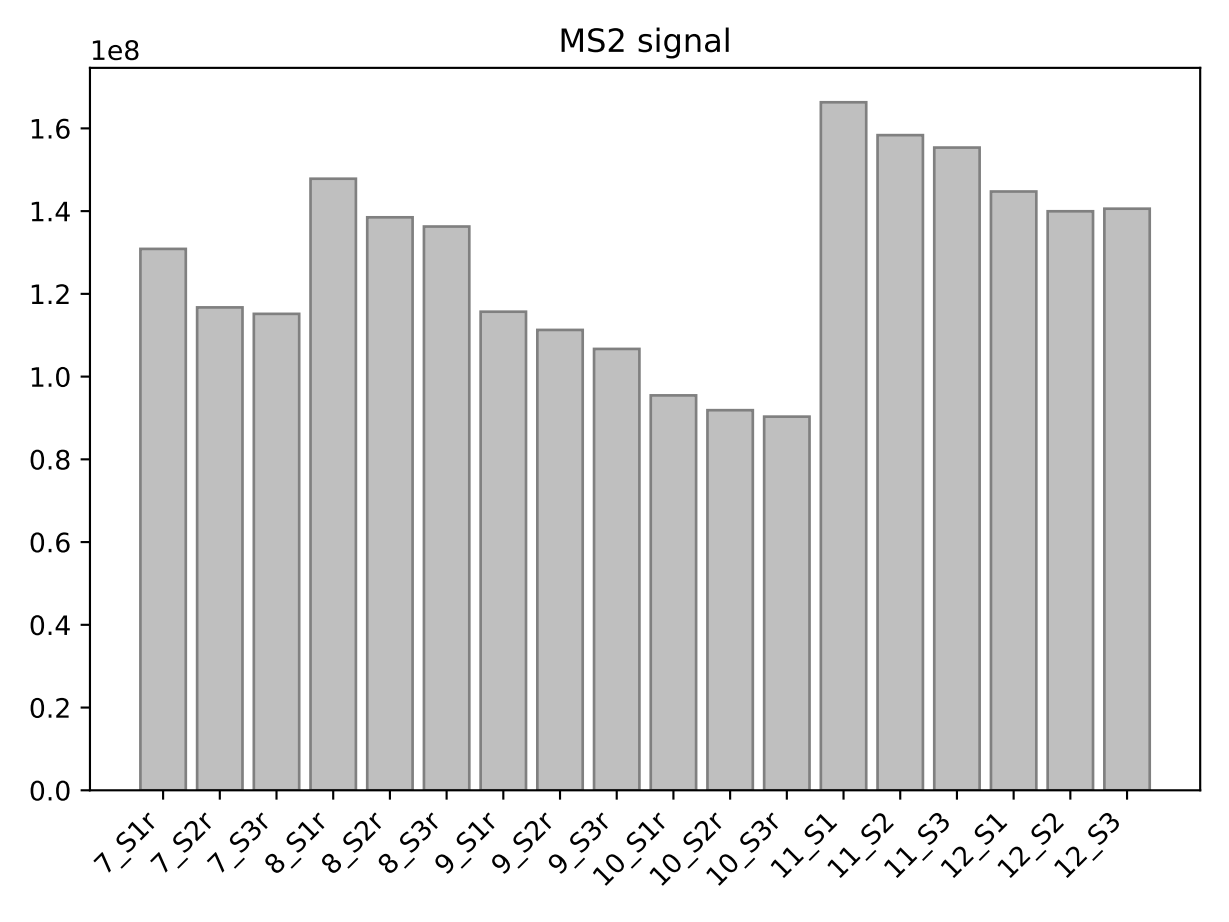
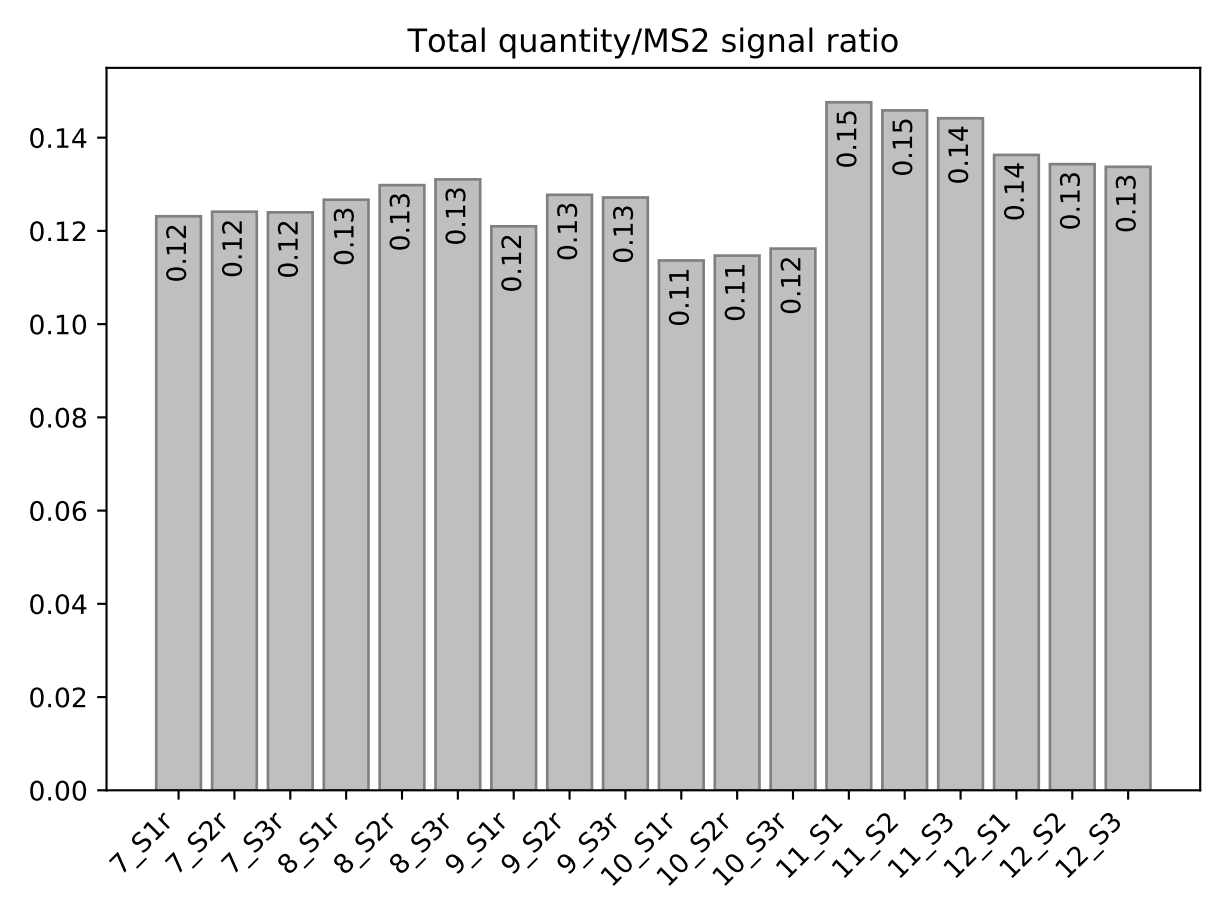

Retention times heatmap, all runs
RT
Library iRT
Retention time accuracy heatmap, all runs
RT
Predicted RT
Normalisation factor heatmap, all runs
Normalisation factor
RT

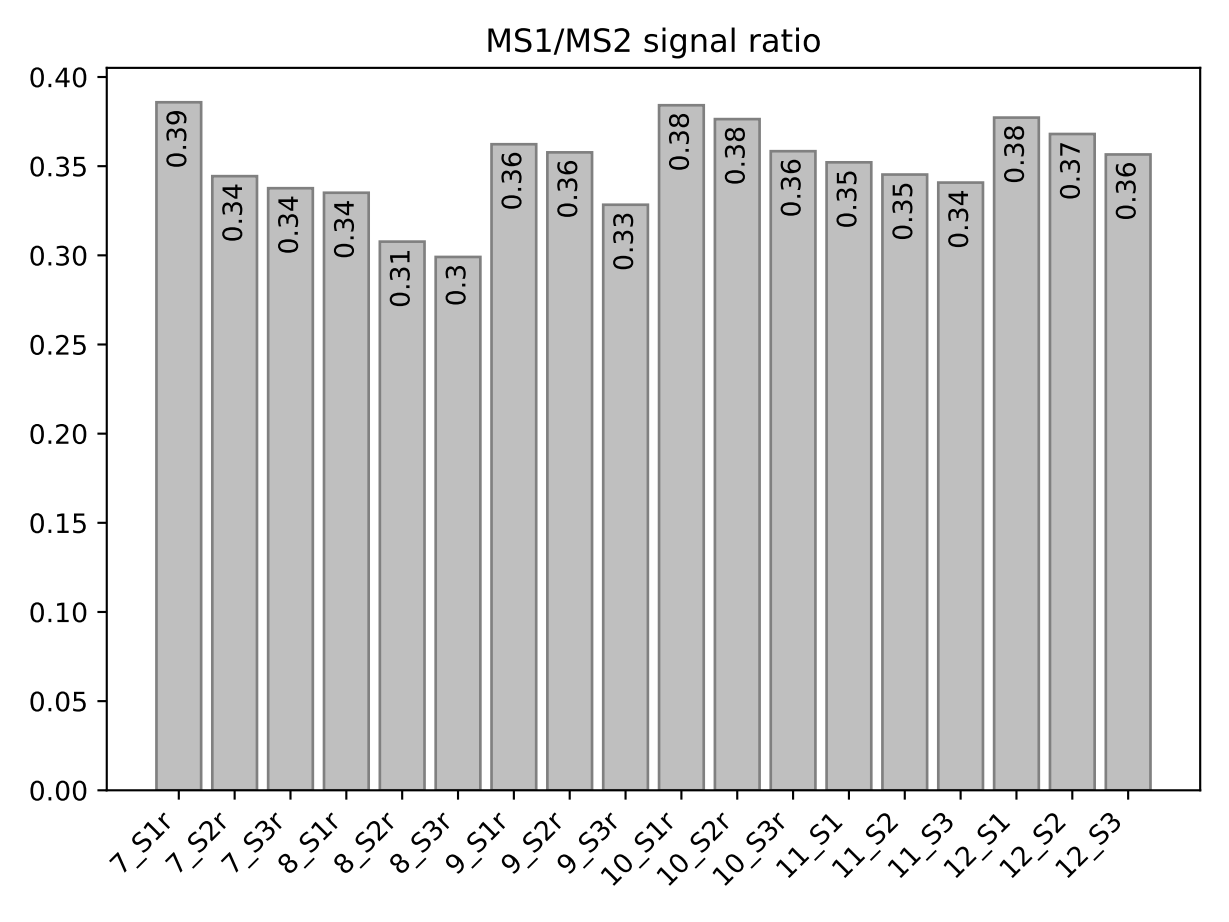

10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
1.000
0.995
0.990
0.985
0.980
0.975
0.970

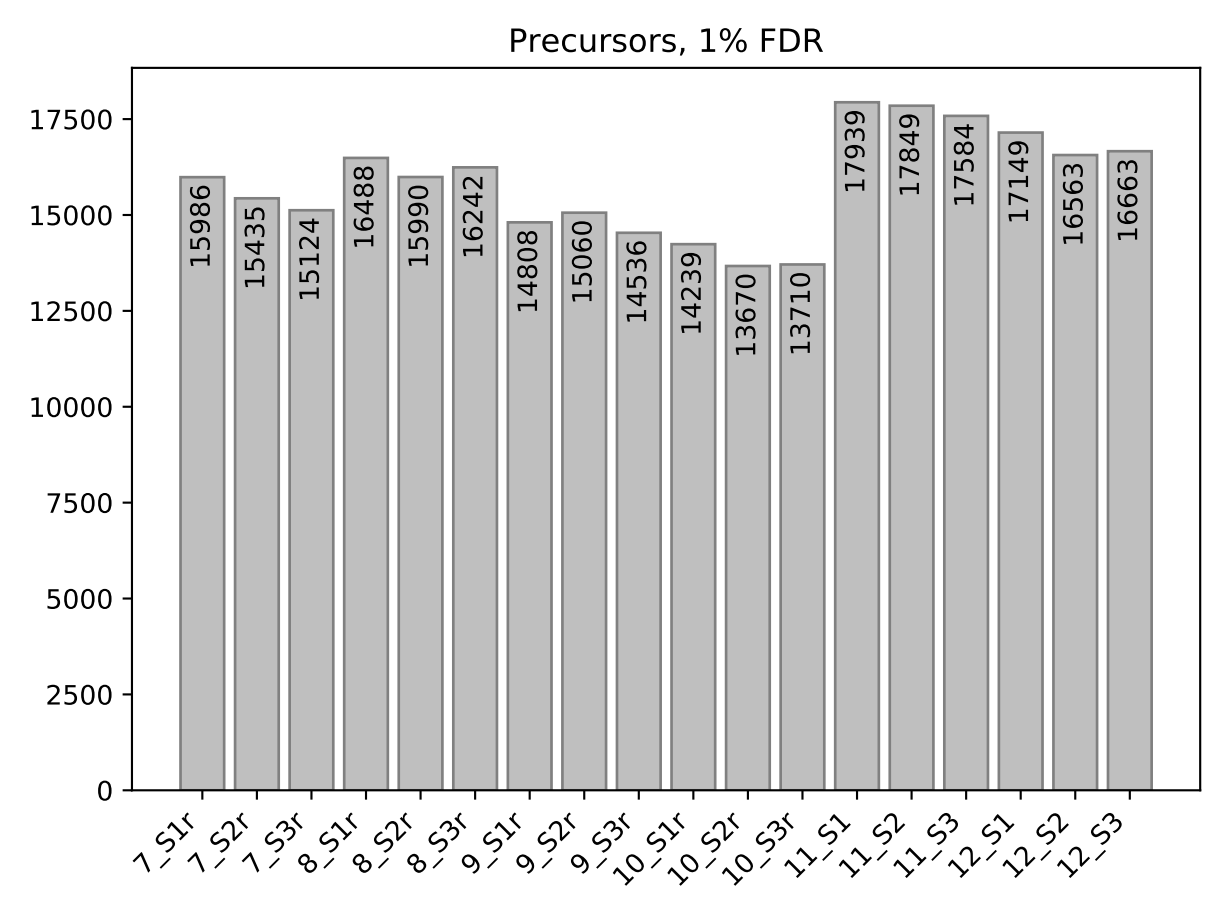

Total quantity, 1% FDR
1e7
2.5
2.0
1.5
1.0
0.5
0.0
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

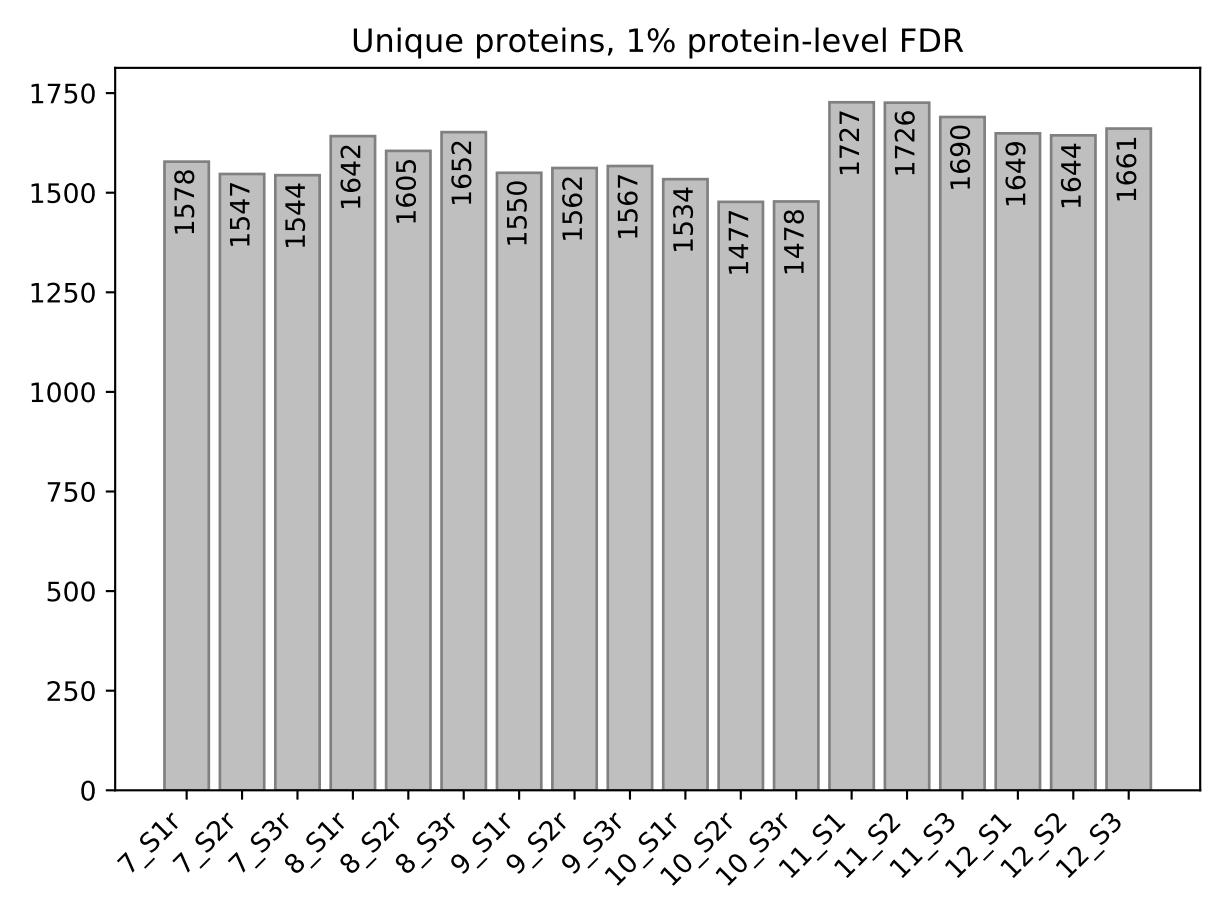

MS1 signal
1e7
6
5
4
3
2
1
0
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

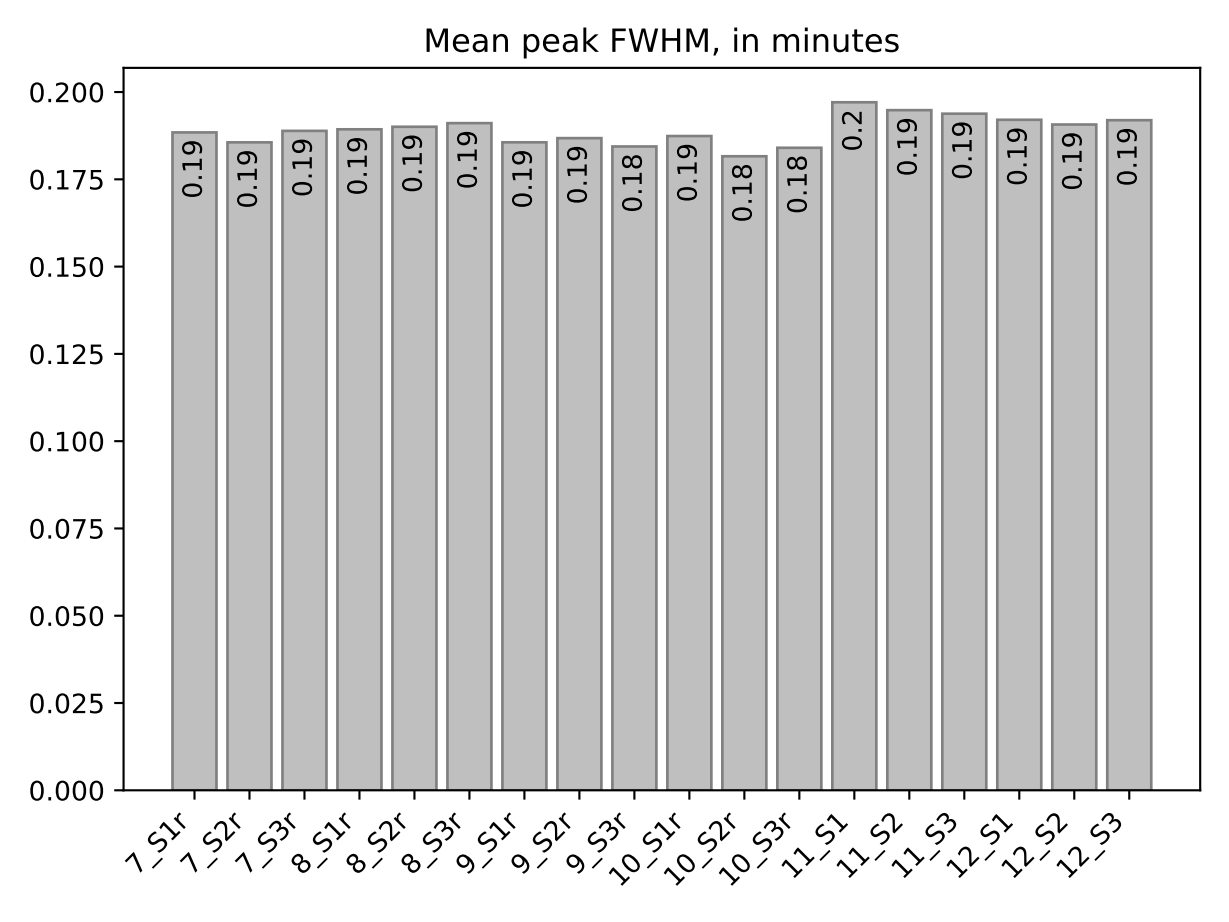

MS2 signal
1e8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

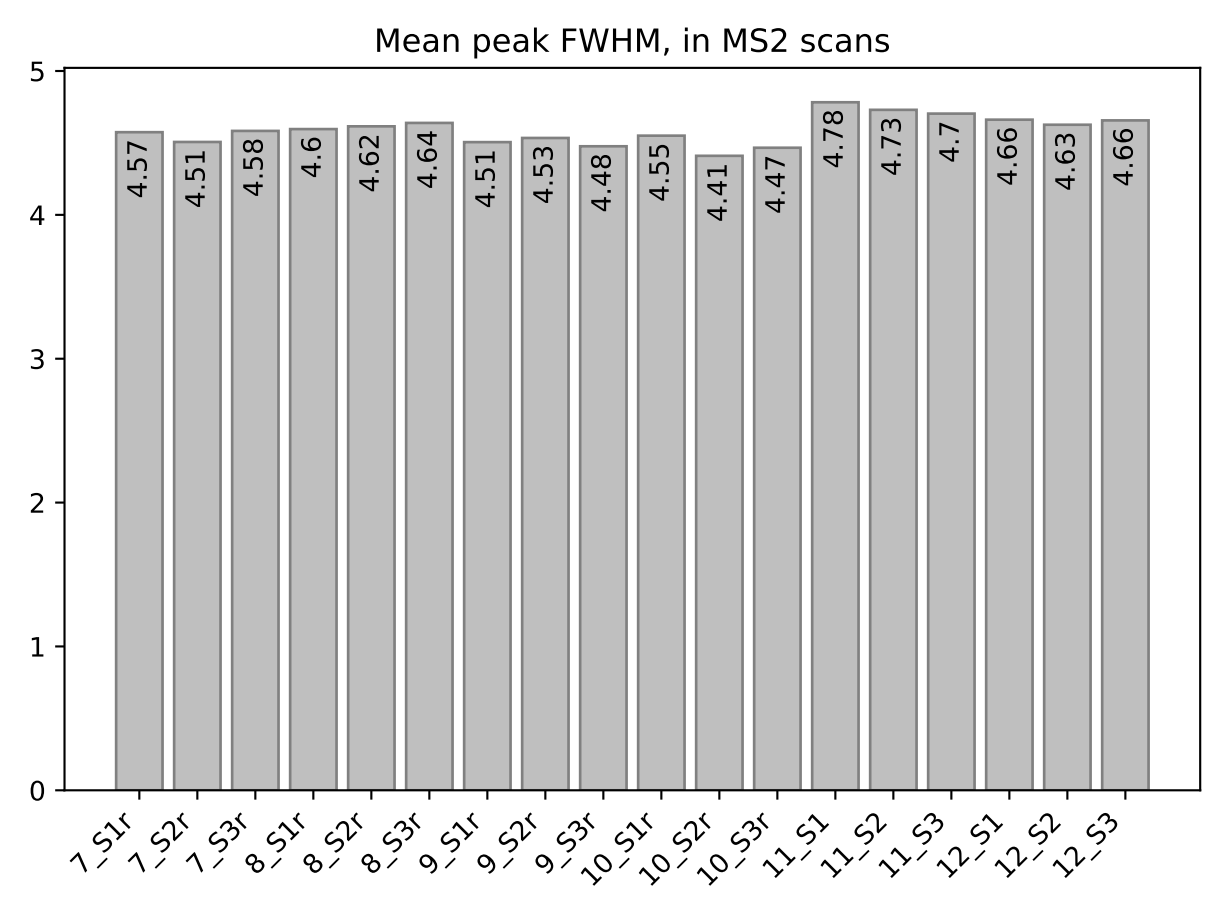

Total quantity/MS2 signal ratio
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.12
0.12
0.12
0.13
0.13
0.13
0.12
0.13
0.13
0.11
0.11
0.12
0.15
0.15
0.14
0.14
0.13
0.13
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

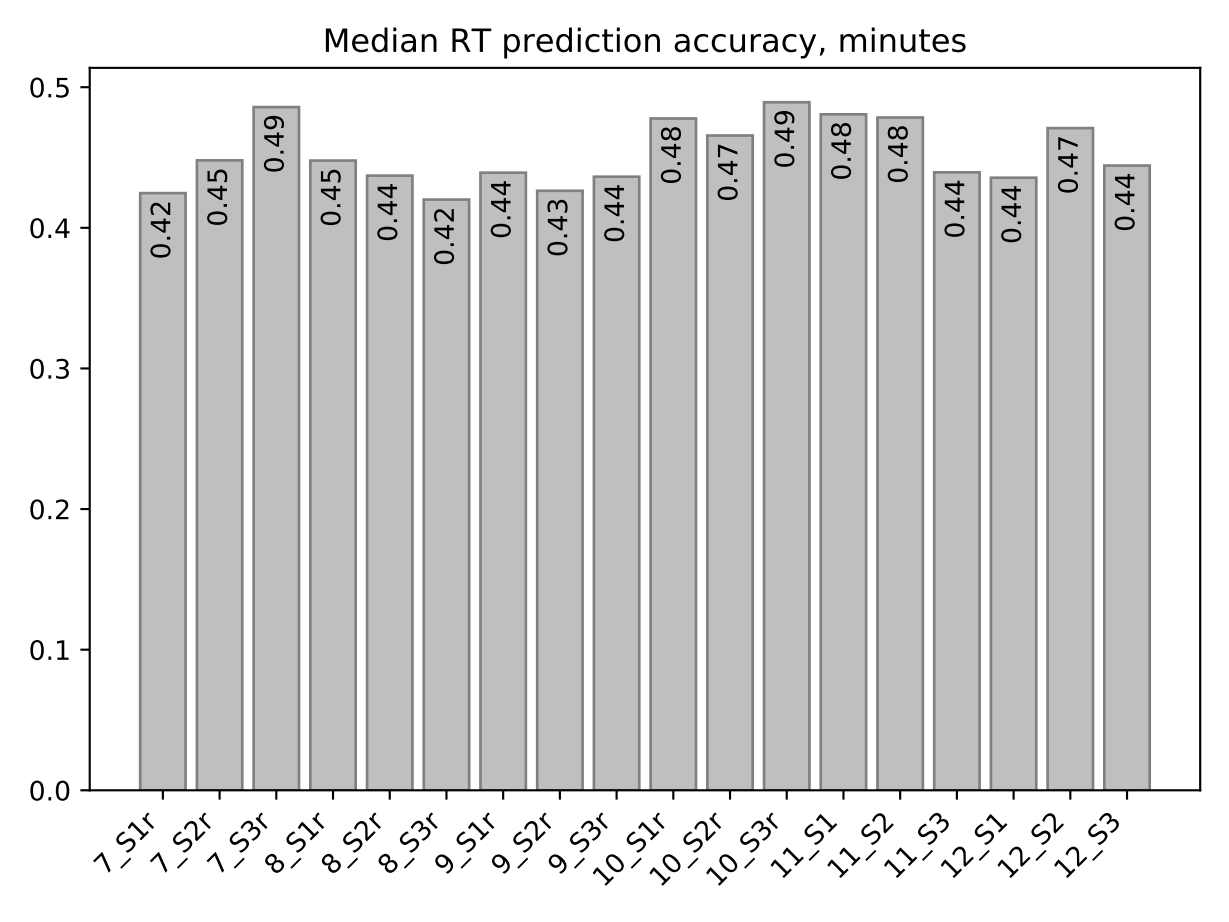

MS1/MS2 signal ratio
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.39
0.34
0.34
0.34
0.31
0.3
0.36
0.36
0.33
0.38
0.38
0.36
0.35
0.35
0.34
0.38
0.37
0.36
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

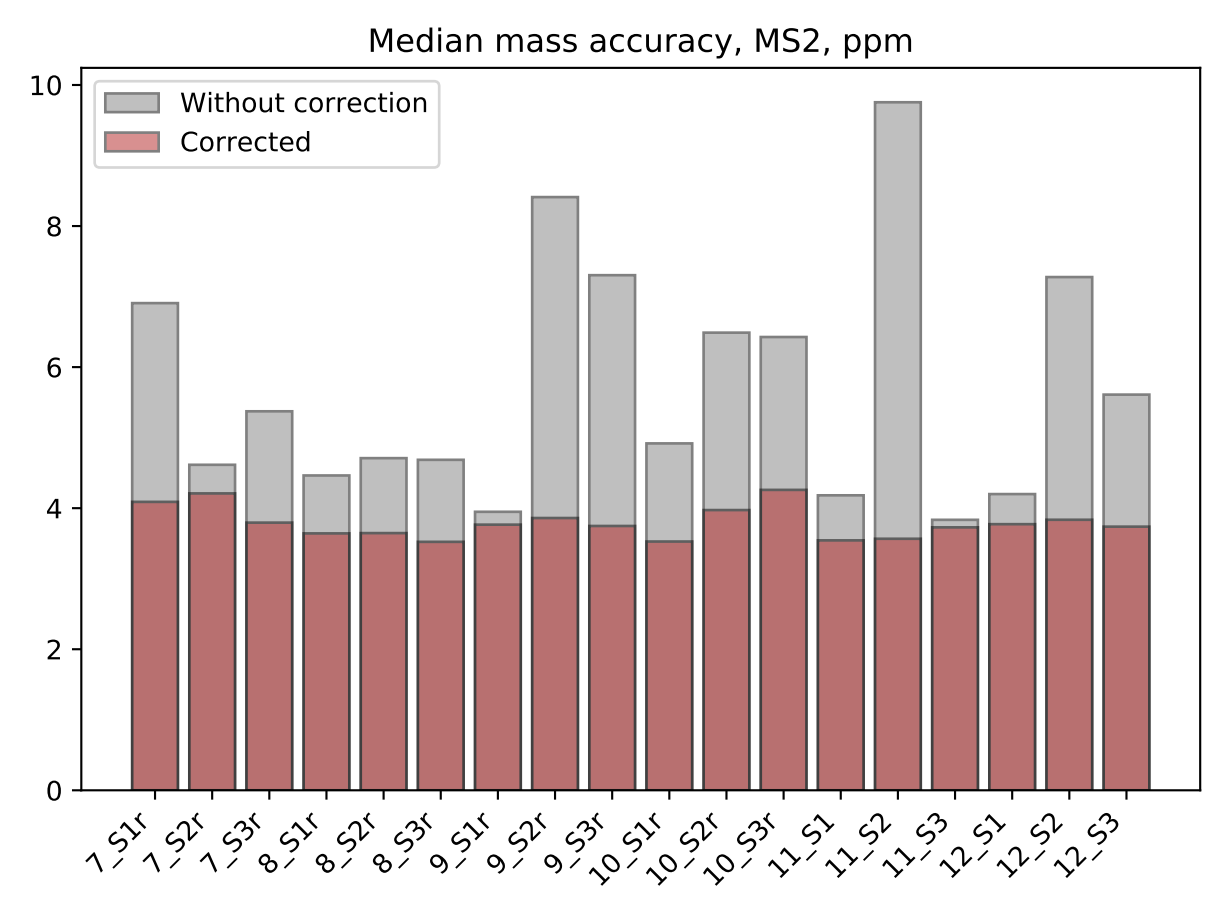

Precursors, 1% FDR
17500
15000
12500
10000
7500
5000
2500
0
15986
15435
15124
16488
15990
16242
14808
15060
14536
14239
13670
13710
17939
17849
17584
17149
16563
16663
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

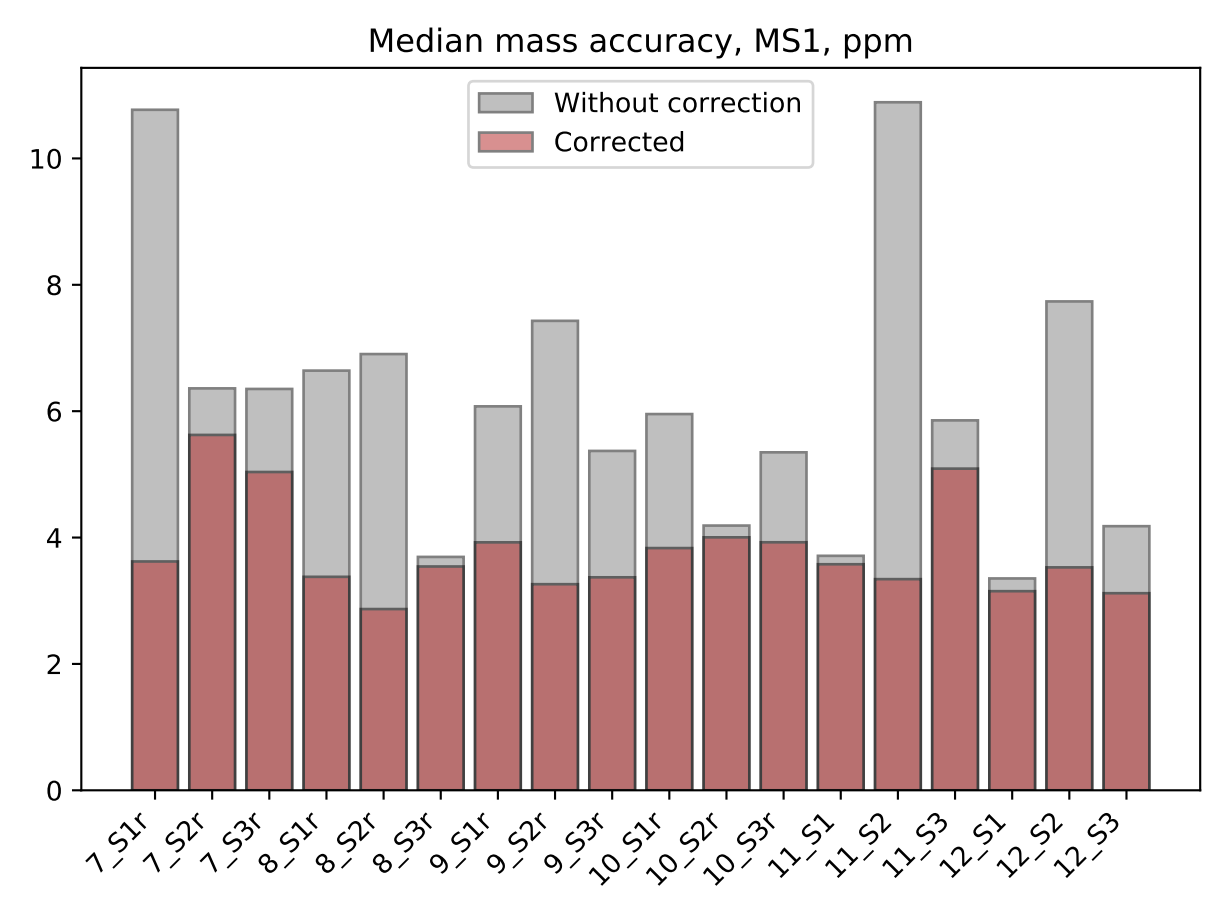

Unique proteins, 1% protein-level FDR
1750
1500
1250
1000
750
500
250
0
1578
1547
1544
1642
1605
1652
1550
1562
1567
1534
1477
1478
1727
1726
1690
1649
1644
1661
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

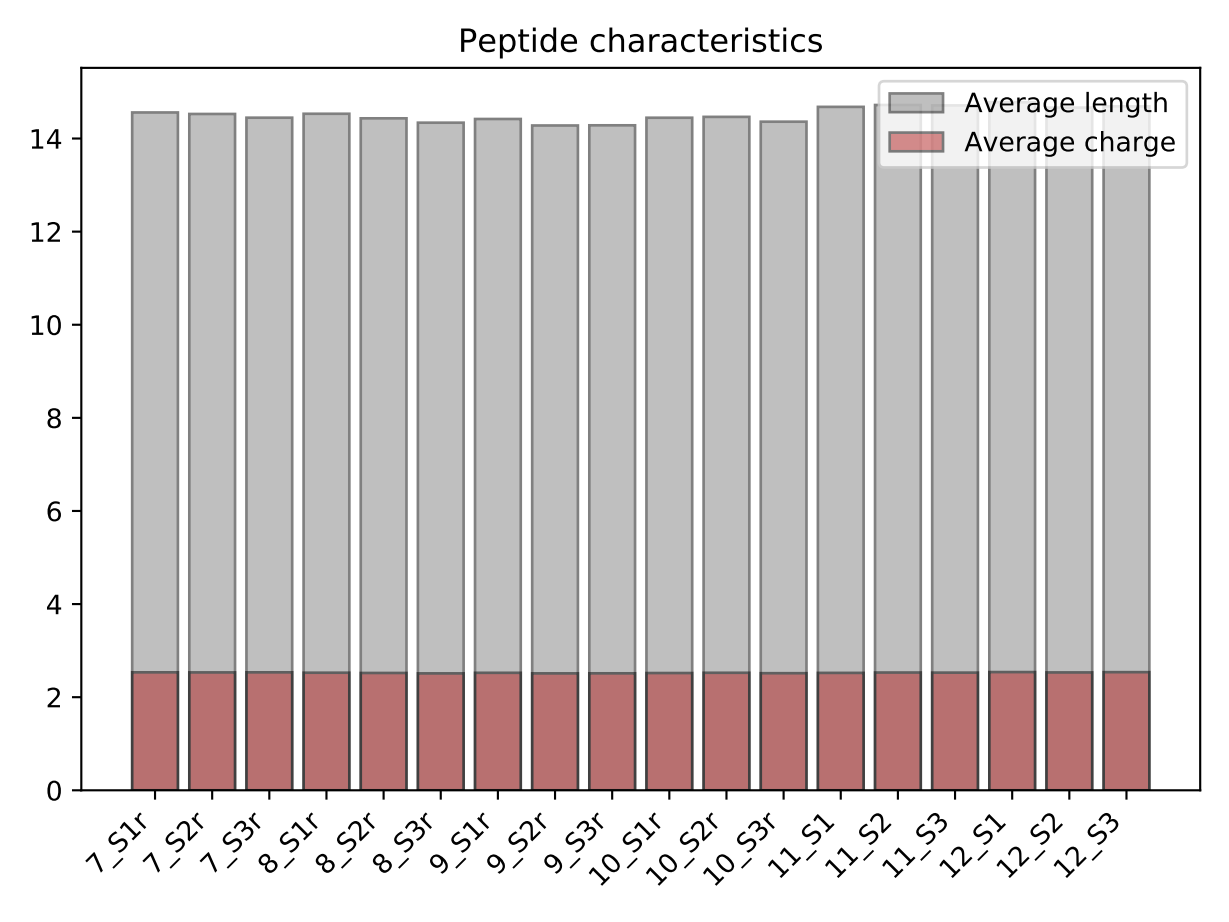

Mean peak FWHM, in minutes
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
0.19
0.19
0.19
0.19
0.19
0.19
0.19
0.19
0.18
0.19
0.18
0.18
0.2
0.19
0.19
0.19
0.19
0.19
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

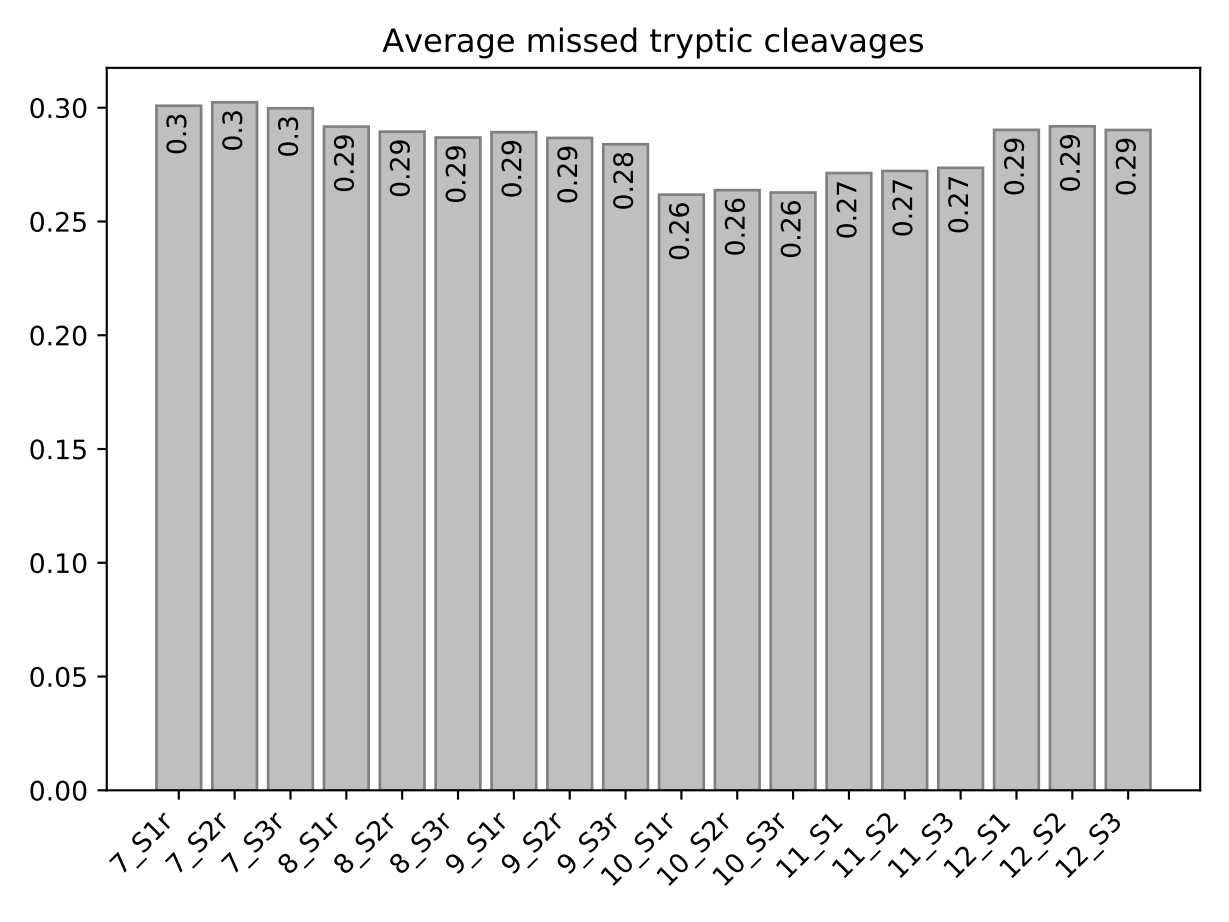

Mean peak FWHM, in MS2 scans
5
4
3
2
1
0
4.57
4.51
4.58
4.6
4.62
4.64
4.51
4.53
4.48
4.55
4.41
4.47
4.78
4.73
4.7
4.66
4.63
4.66
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

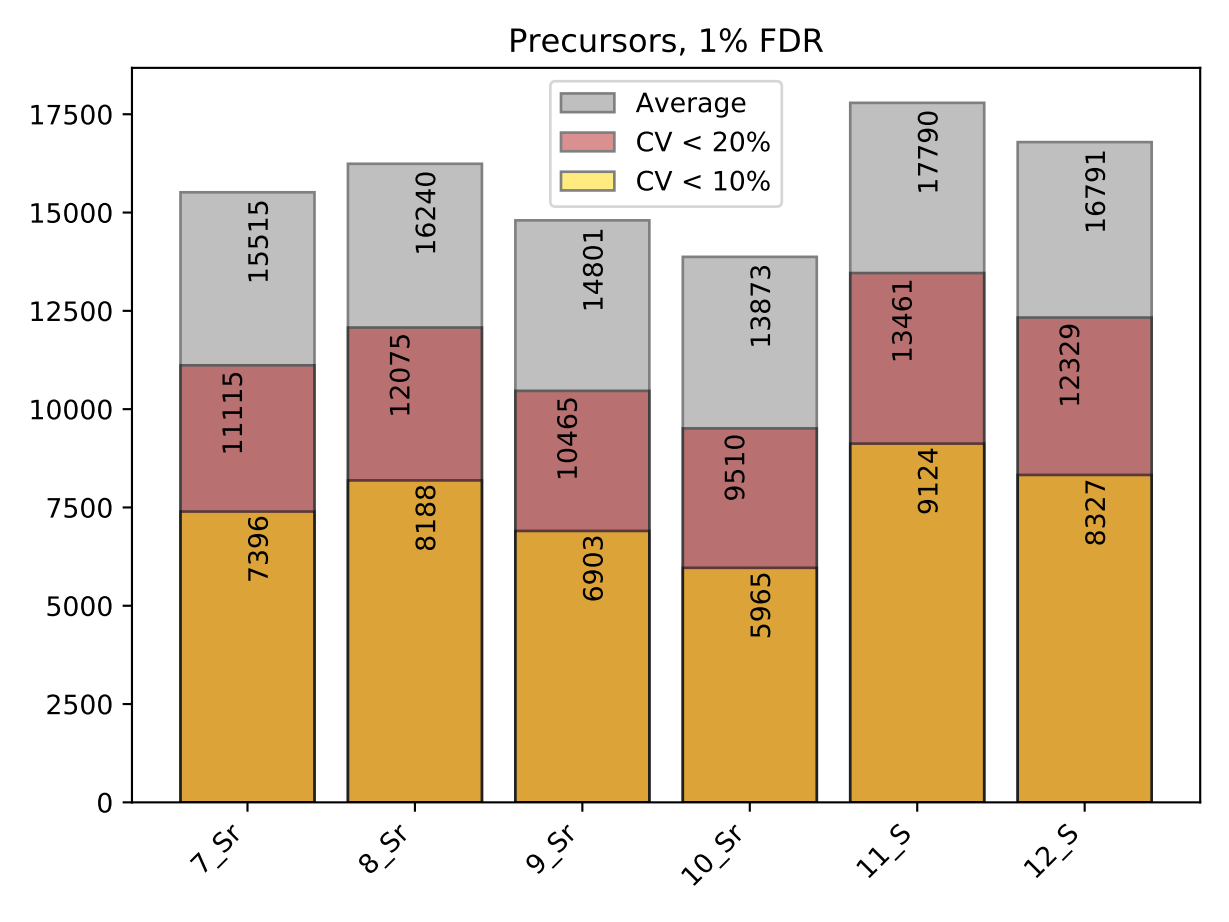

Median RT prediction accuracy, minutes
0.0
0.1
0.2
0.3
0.4
0.5
0.42
0.45
0.49
0.45
0.44
0.42
0.44
0.43
0.44
0.48
0.47
0.49
0.48
0.48
0.44
0.44
0.47
0.44
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

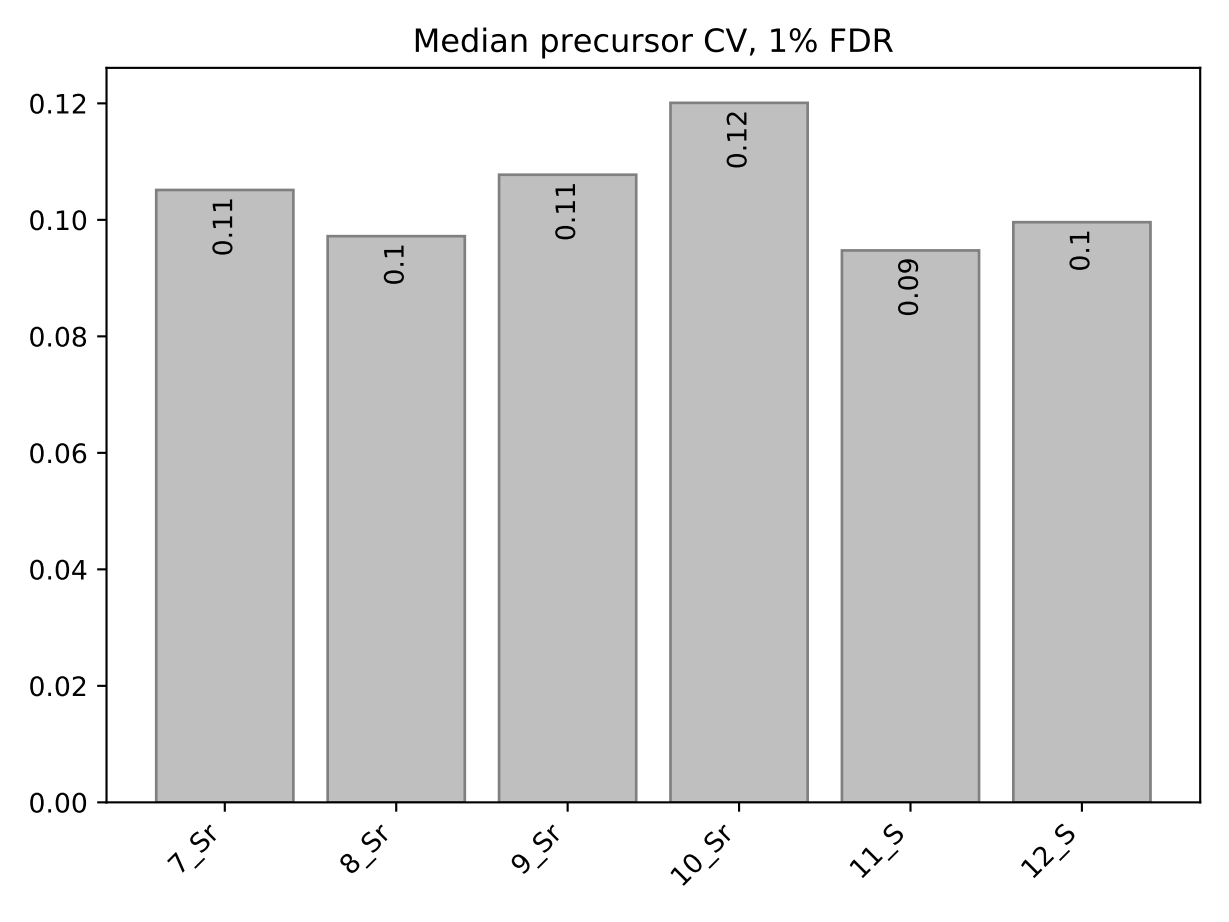

Median mass accuracy, MS2, ppm
Without correction
Corrected
0
2
4
6
8
10
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

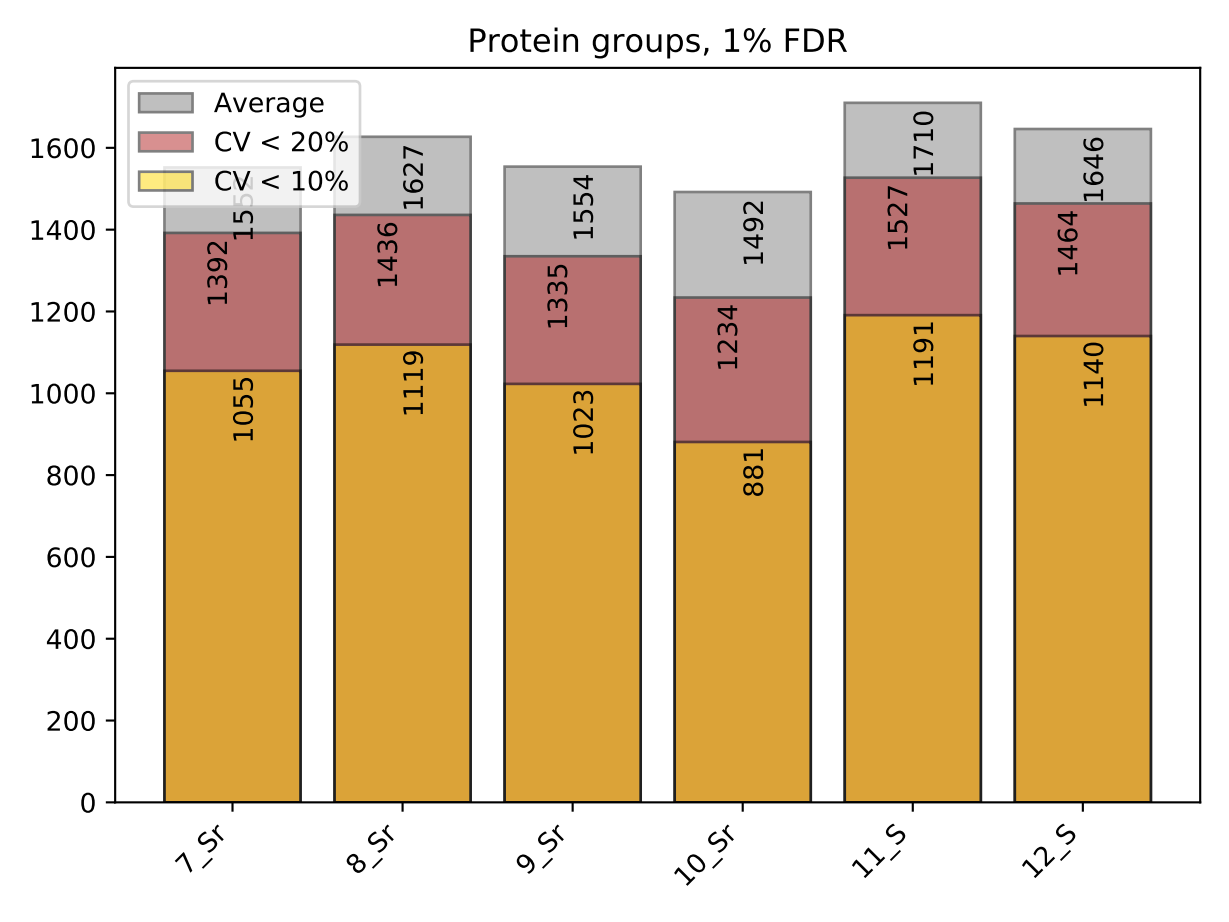

Median mass accuracy, MS1, ppm
Without correction
Corrected
0
2
4
6
8
10
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3

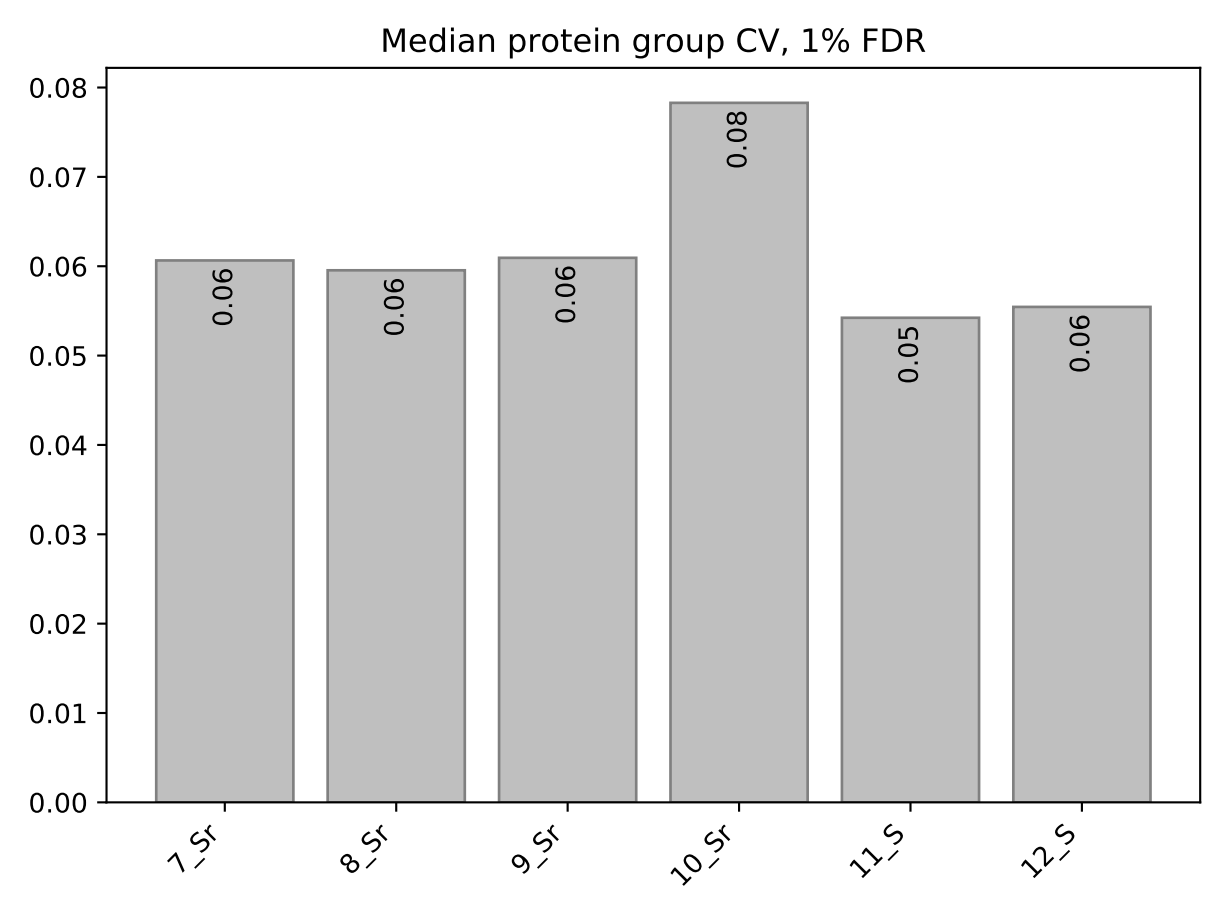

Peptide characteristics
Average length
Average charge
0
2
4
6
8
10
12
14
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3


Average missed tryptic cleavages
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.3
0.3
0.3
0.29
0.29
0.29
0.29
0.29
0.28
0.26
0.26
0.26
0.27
0.27
0.27
0.29
0.29
0.29
7_S1r
7_S2r
7_S3r
8_S1r
8_S2r
8_S3r
9_S1r
9_S2r
9_S3r
10_S1r
10_S2r
10_S3r
11_S1
11_S2
11_S3
12_S1
12_S2
12_S3


Precursors, 1% FDR
Average
CV < 20%
CV < 10%
17500
15000
12500
10000
7500
5000
2500
0
15515
11115
7396
16240
12075
8188
14801
10465
6903
13873
9510
5965
17790
13461
9124
16791
12329
8327
7_Sr
8_Sr
9_Sr
10_Sr
11_S
12_S


Median precursor CV, 1% FDR
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.11
0.1
0.11
0.12
0.09
0.1
7_Sr
8_Sr
9_Sr
10_Sr
11_S
12_S


Protein groups, 1% FDR
Average
CV < 20%
CV < 10%
1600
1400
1200
1000
800
600
400
200
0
1392
1627
1436
1554
1335
1492
1234
1710
1527
1646
1464
1055
1119
1023
881
1191
1140
7_Sr
8_Sr
9_Sr
10_Sr
11_S
12_S


Median protein group CV, 1% FDR
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0.06
0.06
0.06
0.08
0.05
0.06
7_Sr
8_Sr
9_Sr
10_Sr
11_S
12_S