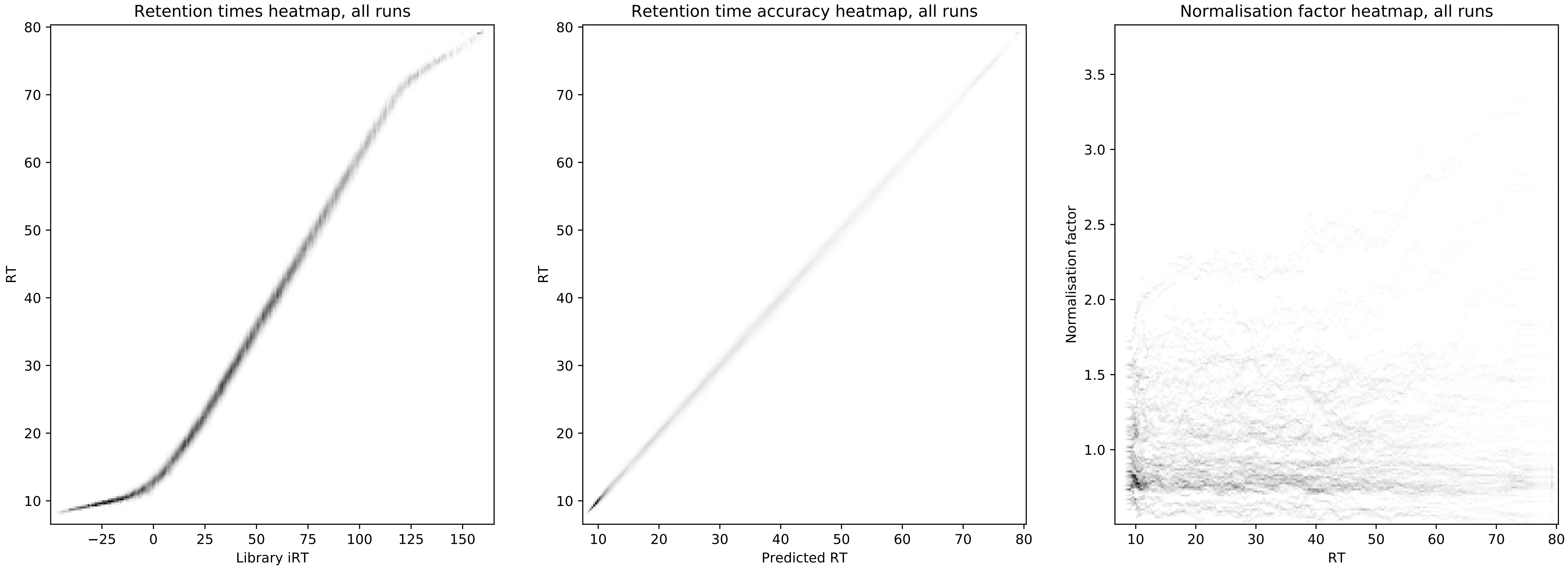
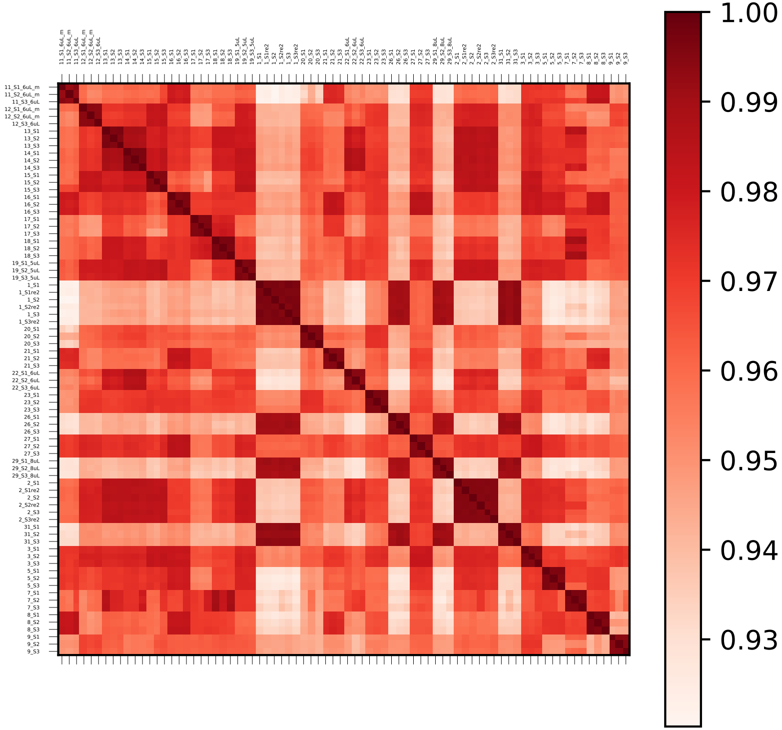
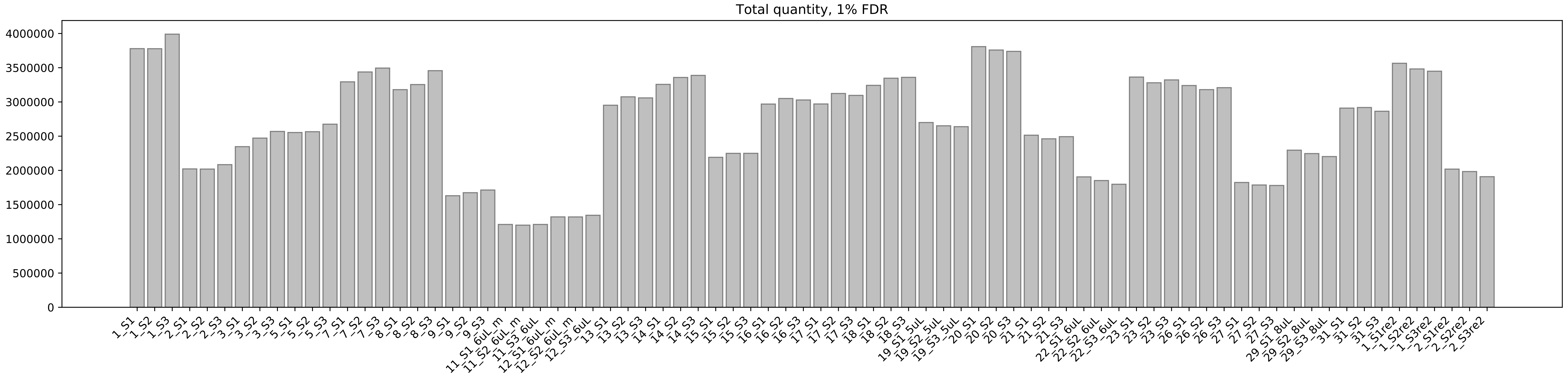
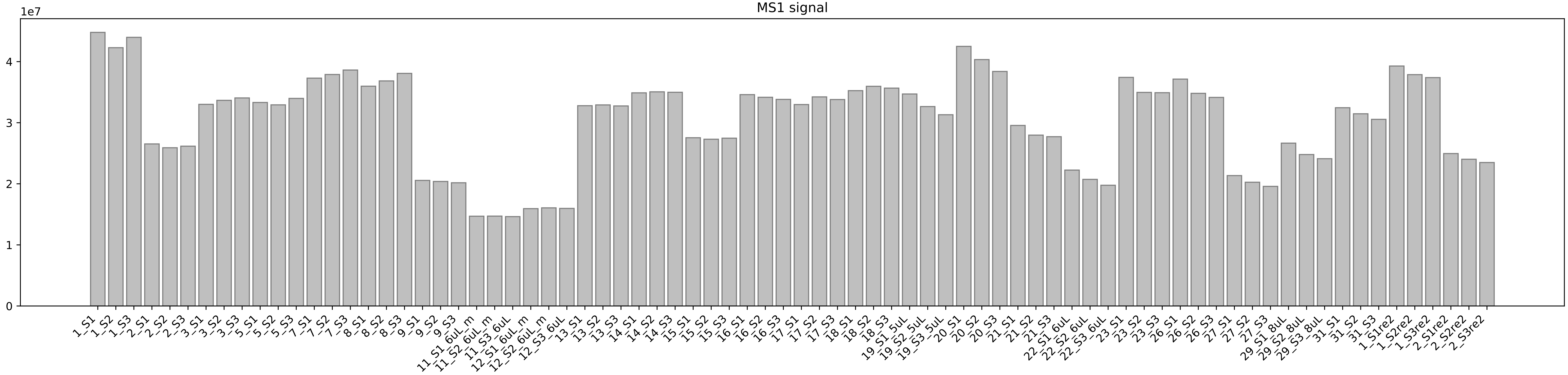
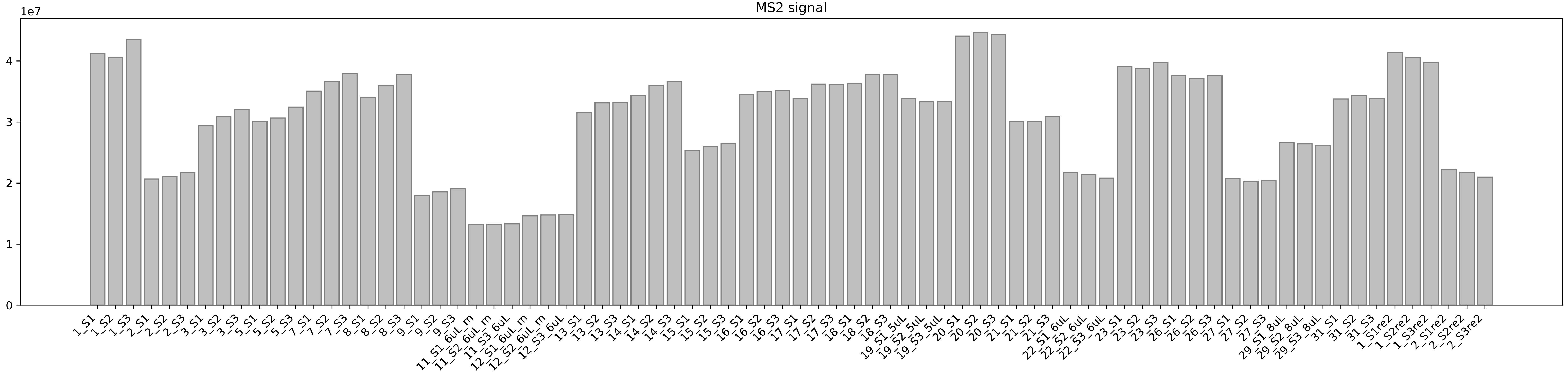
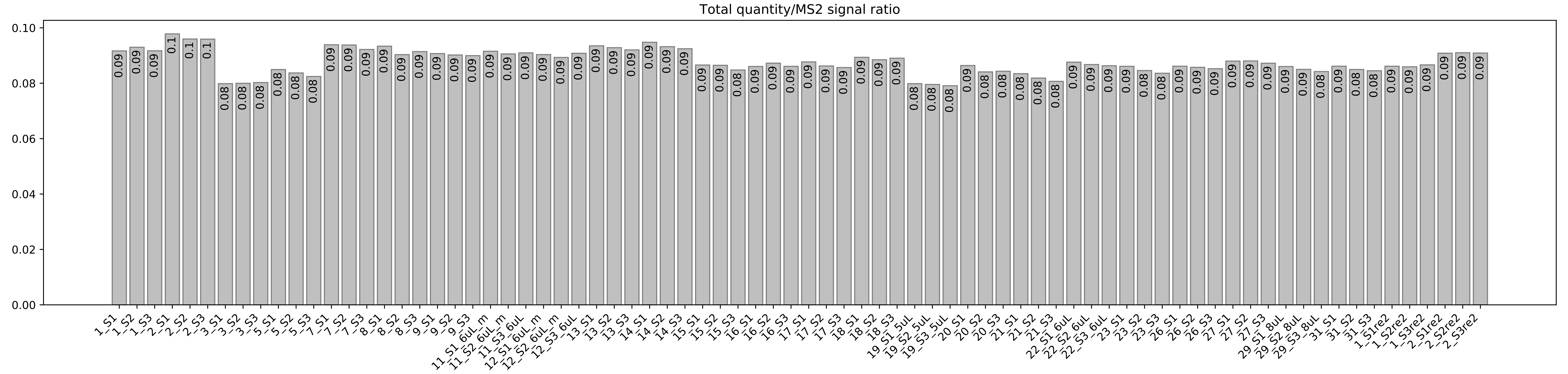

Retention times heatmap, all runs
RT
80
70
60
50
40
30
20
10
Library iRT
−25
0
25
50
75
100
125
150
Retention time accuracy heatmap, all runs
RT
80
70
60
50
40
30
20
10
Predicted RT
10
20
30
40
50
60
70
80
Normalisation factor heatmap, all runs
Normalisation factor
3.5
3.0
2.5
2.0
1.5
1.0
RT
10
20
30
40
50
60
70
80


11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
1_S1
1_S1re2
1_S2
1_S2re2
1_S3
1_S3re2
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
2_S1
2_S1re2
2_S2
2_S2re2
2_S3
2_S3re2
31_S1
31_S2
31_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93


Total quantity, 1% FDR
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2


MS1 signal
1e7
0
1
2
3
4
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2


MS2 signal
1e7
0
1
2
3
4
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2


Total quantity/MS2 signal ratio
0.10
0.08
0.06
0.04
0.02
0.00
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2
0.09
0.09
0.09
0.1
0.1
0.1
0.08
0.08
0.08
0.08
0.08
0.08
0.09
0.09
0.09
0.09
0.09
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0.09
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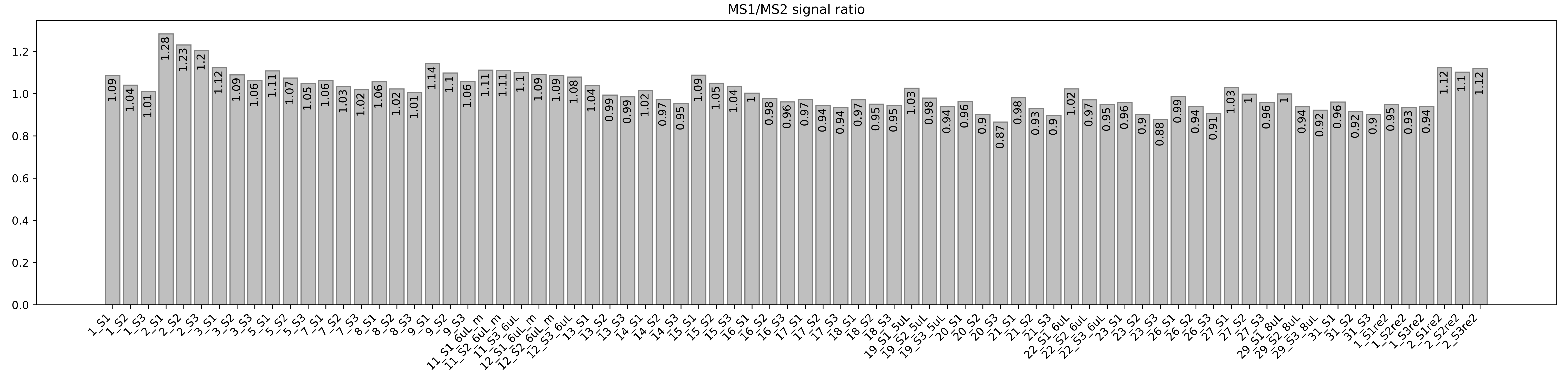
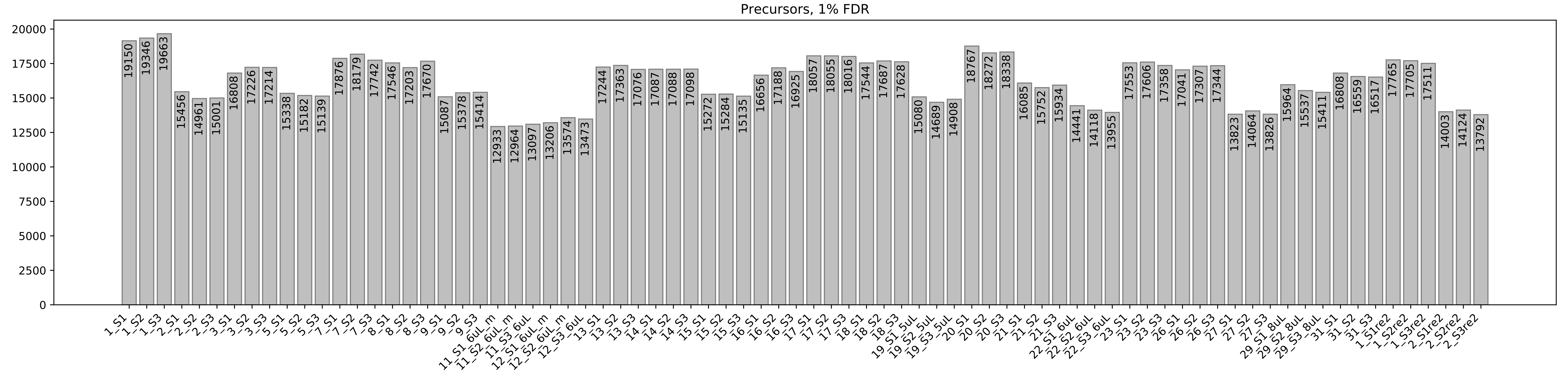
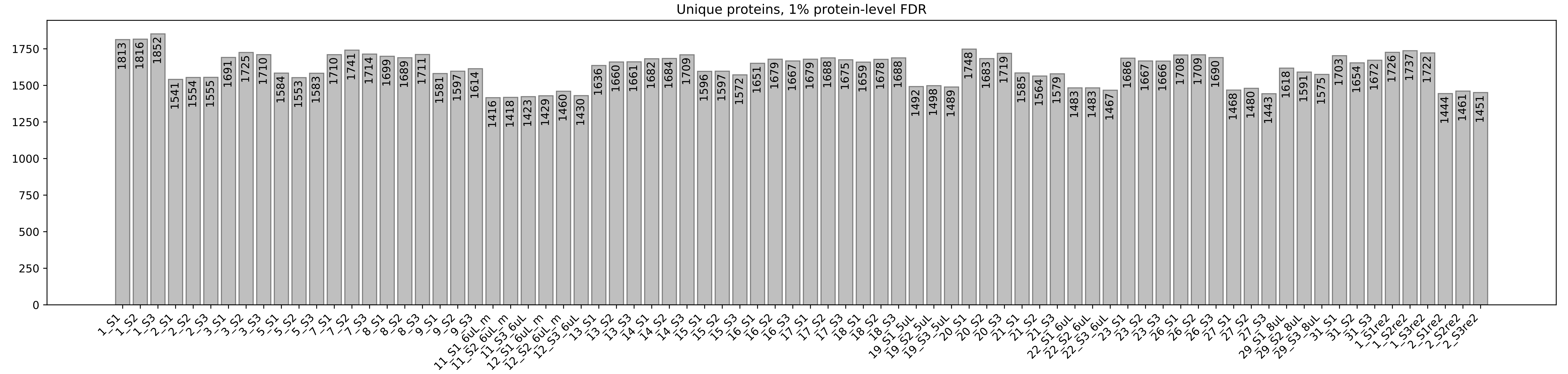
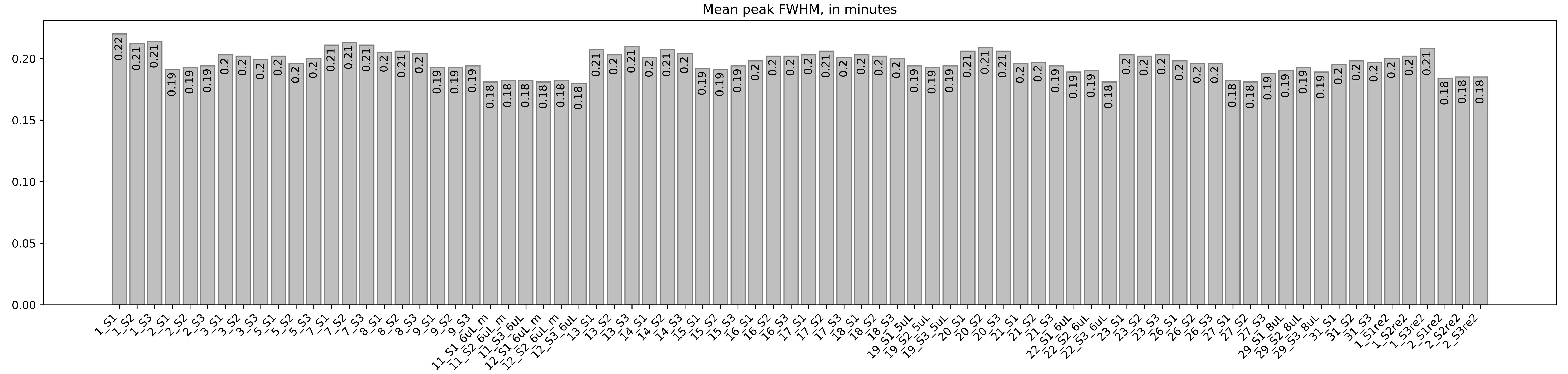
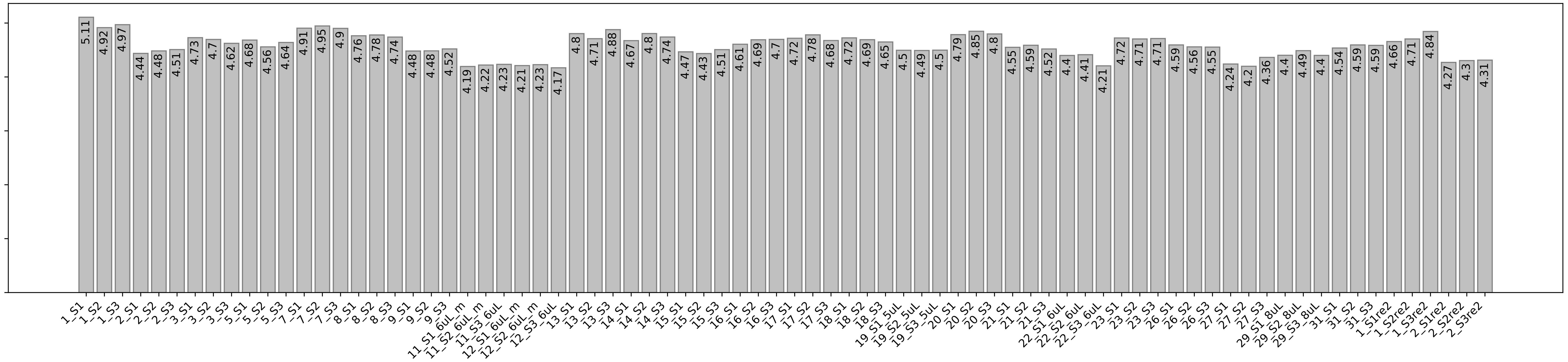
0.08
0.09
0.09
0.09
0.09
0.09
0.09

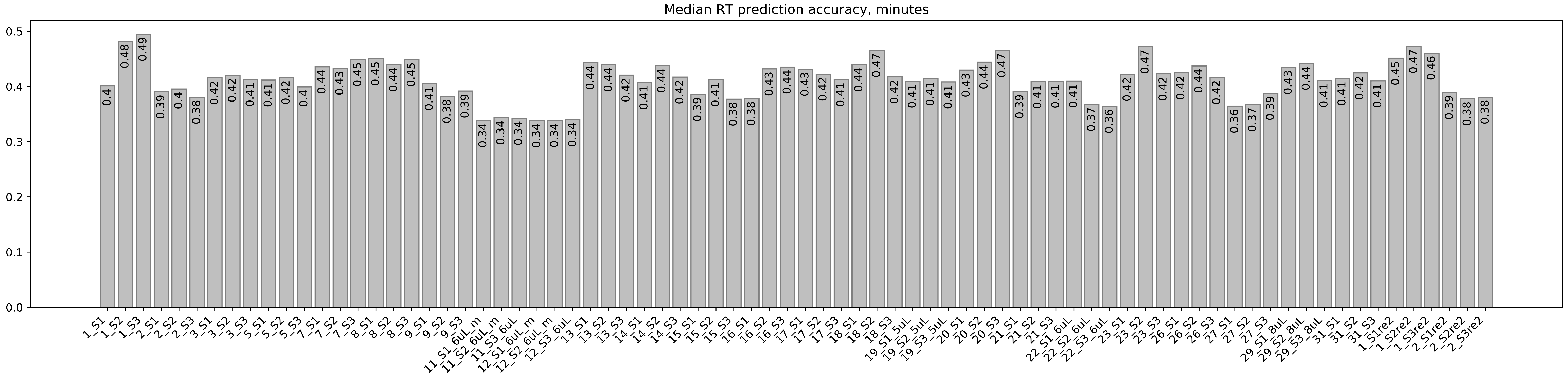

MS1/MS2 signal ratio
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1_S1 1.09
1_S2 1.04
1_S3 1.01
2_S1 1.28
2_S2 1.23
2_S3 1.2
3_S1 1.12
3_S2 1.09
3_S3 1.06
5_S1 1.11
5_S2 1.07
5_S3 1.05
7_S1 1.06
7_S2 1.03
7_S3 1.02
8_S1 1.06
8_S2 1.02
8_S3 1.01
9_S1 1.14
9_S2 1.1
9_S3 1.06
11_S1_6uL_m 1.11
11_S2_6uL_m 1.11
11_S3_6uL 1.1
12_S1_6uL_m 1.09
12_S2_6uL_m 1.09
12_S3_6uL 1.08
13_S1 1.04
13_S2 0.99
13_S3 0.99
14_S1 1.02
14_S2 0.97
14_S3 0.95
15_S1 1.09
15_S2 1.05
15_S3 1.04
16_S1 1
16_S2 0.98
16_S3 0.96
17_S1 0.97
17_S2 0.94
17_S3 0.94
18_S1 0.97
18_S2 0.95
18_S3 0.95
19_S1_5uL 1.03
19_S2_5uL 0.98
19_S3_5uL 0.94
20_S1 0.96
20_S2 0.9
20_S3 0.87
21_S1 0.98
21_S2 0.93
21_S3 0.9
22_S1_6uL 1.02
22_S2_6uL 0.97
22_S3_6uL 0.95
23_S1 0.96
23_S2 0.9
23_S3 0.88
26_S1 0.99
26_S2 0.94
26_S3 0.91
27_S1 1.03
27_S2 1
27_S3 0.96
29_S1_8uL 1
29_S2_8uL 0.94
29_S3_8uL 0.92
31_S1 0.96
31_S2 0.92
31_S3 0.9
1_S1re2 0.95
1_S2re2 0.93
1_S3re2 0.94
2_S1re2 1.12
2_S2re2 1.1
2_S3re2 1.12

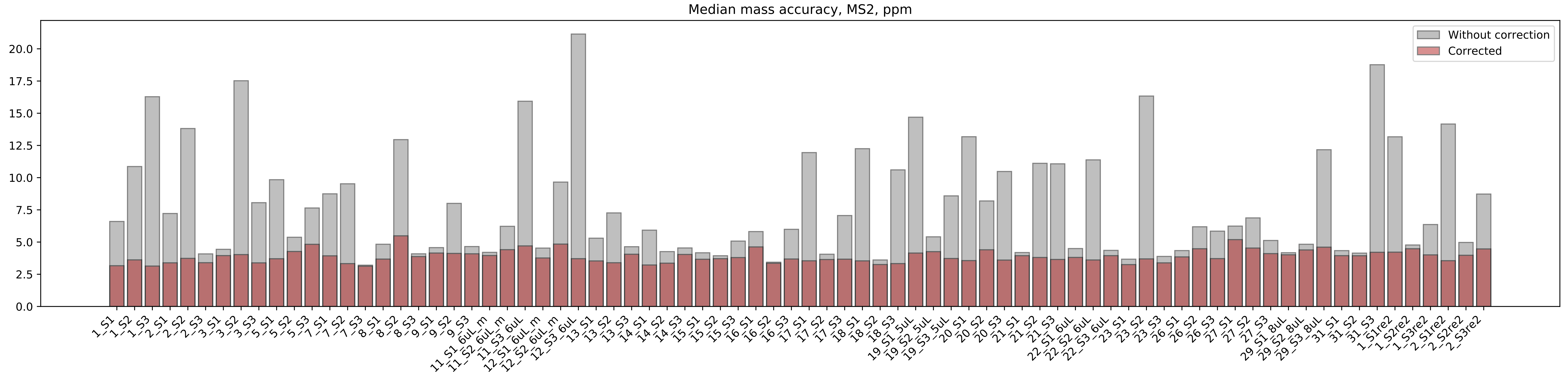

Precursors, 1% FDR
20000
17500
15000
12500
10000
7500
5000
2500
0
1_S1 19150
1_S2 19346
1_S3 19663
2_S1 15456
2_S2 14961
2_S3 15001
3_S1 16808
3_S2 17226
3_S3 17214
5_S1 15338
5_S2 15182
5_S3 15139
7_S1 17876
7_S2 18179
7_S3 17742
8_S1 17546
8_S2 17203
8_S3 17670
9_S1 15087
9_S2 15378
9_S3 15414
11_S1_6uL_m 12933
11_S2_6uL_m 12964
11_S3_6uL 13097
12_S1_6uL_m 13206
12_S2_6uL_m 13574
12_S3_6uL 13473
13_S1 17244
13_S2 17363
13_S3 17076
14_S1 17087
14_S2 17088
14_S3 17098
15_S1 15272
15_S2 15284
15_S3 15135
16_S1 16656
16_S2 17188
16_S3 16925
17_S1 18057
17_S2 18055
17_S3 18016
18_S1 17544
18_S2 17687
18_S3 17628
19_S1_5uL 15080
19_S2_5uL 14689
19_S3_5uL 14908
20_S1 18767
20_S2 18272
20_S3 18338
21_S1 16085
21_S2 15752
21_S3 15934
22_S1_6uL 14441
22_S2_6uL 14118
22_S3_6uL 13955
23_S1 17553
23_S2 17606
23_S3 17358
26_S1 17041
26_S2 17307
26_S3 17344
27_S1 13823
27_S2 14064
27_S3 13826
29_S1_8uL 15964
29_S2_8uL 15537
29_S3_8uL 15411
31_S1 16808
31_S2 16559
31_S3 16517
1_S1re2 17765
1_S2re2 17705
1_S3re2 17511
2_S1re2 14003
2_S2re2 14124
2_S3re2 13792

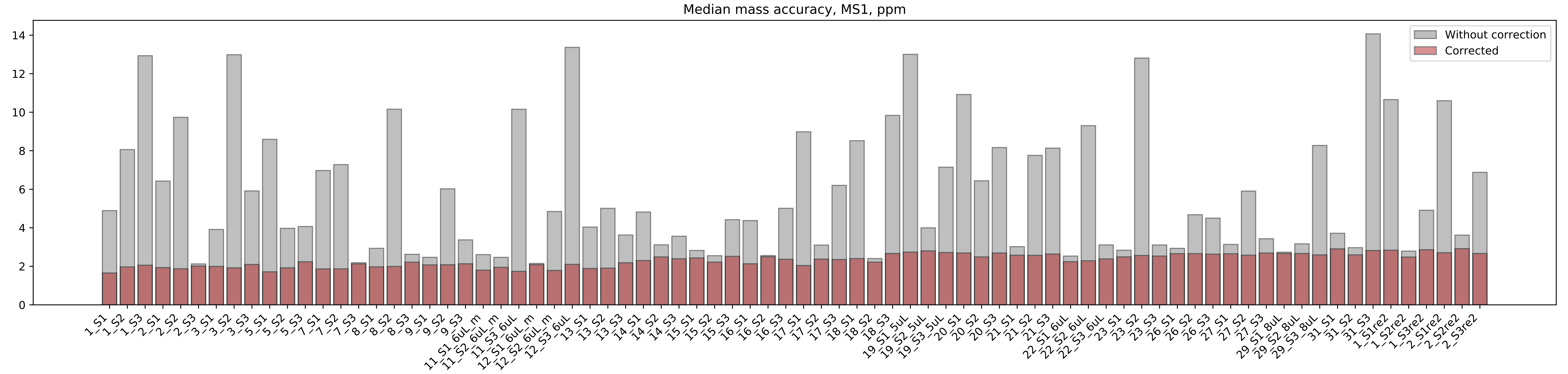

Unique proteins, 1% protein-level FDR
0
250
500
750
1000
1250
1500
1750
1_S1 1813
1_S2 1816
1_S3 1852
2_S1 1541
2_S2 1554
2_S3 1555
3_S1 1691
3_S2 1725
3_S3 1710
5_S1 1584
5_S2 1553
5_S3 1583
7_S1 1710
7_S2 1741
7_S3 1714
8_S1 1699
8_S2 1689
8_S3 1711
9_S1 1581
9_S2 1597
9_S3 1614
11_S1_6uL_m 1416
11_S2_6uL_m 1418
11_S3_6uL 1423
12_S1_6uL_m 1429
12_S2_6uL_m 1460
12_S3_6uL 1430
13_S1 1636
13_S2 1660
13_S3 1661
14_S1 1682
14_S2 1684
14_S3 1709
15_S1 1596
15_S2 1597
15_S3 1572
16_S1 1651
16_S2 1679
16_S3 1667
17_S1 1679
17_S2 1688
17_S3 1675
18_S1 1659
18_S2 1678
18_S3 1688
19_S1_5uL 1492
19_S2_5uL 1498
19_S3_5uL 1489
20_S1 1748
20_S2 1683
20_S3 1719
21_S1 1585
21_S2 1564
21_S3 1579
22_S1_6uL 1483
22_S2_6uL 1483
22_S3_6uL 1467
23_S1 1686
23_S2 1667
23_S3 1666
26_S1 1708
26_S2 1709
26_S3 1690
27_S1 1468
27_S2 1480
27_S3 1443
29_S1_8uL 1618
29_S2_8uL 1591
29_S3_8uL 1575
31_S1 1703
31_S2 1654
31_S3 1672
1_S1re2 1726
1_S2re2 1737
1_S3re2 1722
2_S1re2 1444
2_S2re2 1461
2_S3re2 1451

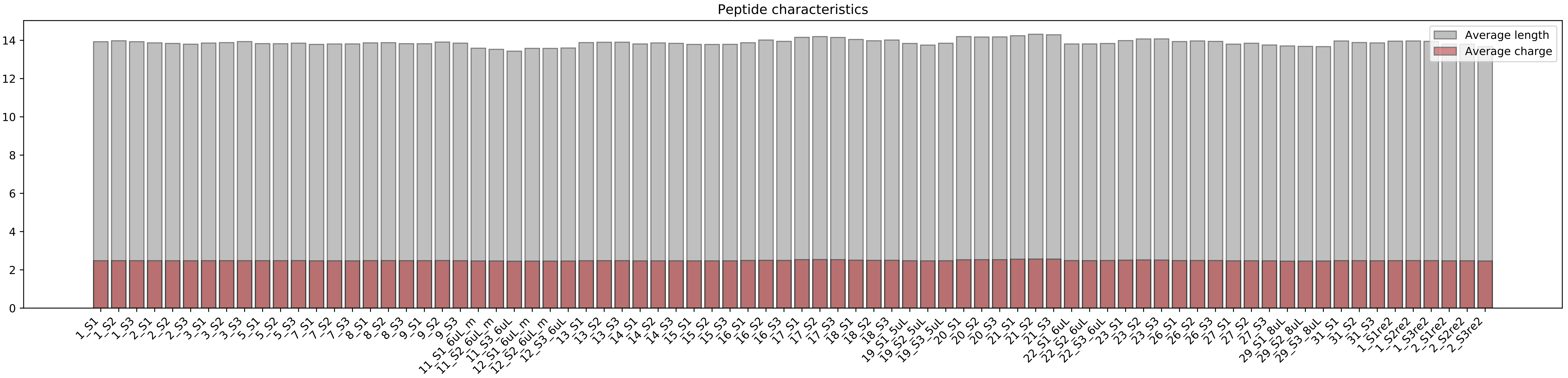

Mean peak FWHM, in minutes
0.00
0.05
0.10
0.15
0.20
1_S1 0.22
1_S2 0.21
1_S3 0.21
2_S1 0.19
2_S2 0.19
2_S3 0.19
3_S1 0.2
3_S2 0.2
3_S3 0.2
5_S1 0.2
5_S2 0.2
5_S3 0.2
7_S1 0.21
7_S2 0.21
7_S3 0.21
8_S1 0.2
8_S2 0.21
8_S3 0.2
9_S1 0.19
9_S2 0.19
9_S3 0.19
11_S1_6uL_m 0.18
11_S2_6uL_m 0.18
11_S3_6uL 0.18
12_S1_6uL_m 0.18
12_S2_6uL_m 0.18
12_S3_6uL 0.18
13_S1 0.21
13_S2 0.2
13_S3 0.21
14_S1 0.2
14_S2 0.21
14_S3 0.2
15_S1 0.19
15_S2 0.19
15_S3 0.19
16_S1 0.2
16_S2 0.2
16_S3 0.2
17_S1 0.2
17_S2 0.21
17_S3 0.2
18_S1 0.2
18_S2 0.2
18_S3 0.2
19_S1_5uL 0.19
19_S2_5uL 0.19
19_S3_5uL 0.19
20_S1 0.21
20_S2 0.21
20_S3 0.21
21_S1 0.2
21_S2 0.2
21_S3 0.19
22_S1_6uL 0.19
22_S2_6uL 0.19
22_S3_6uL 0.18
23_S1 0.2
23_S2 0.2
23_S3 0.2
26_S1 0.2
26_S2 0.2
26_S3 0.2
27_S1 0.18
27_S2 0.18
27_S3 0.19
29_S1_8uL 0.19
29_S2_8uL 0.19
29_S3_8uL 0.19
31_S1 0.2
31_S2 0.2
31_S3 0.2
1_S1re2 0.2
1_S2re2 0.2
1_S3re2 0.21
2_S1re2 0.18
2_S2re2 0.18
2_S3re2 0.18

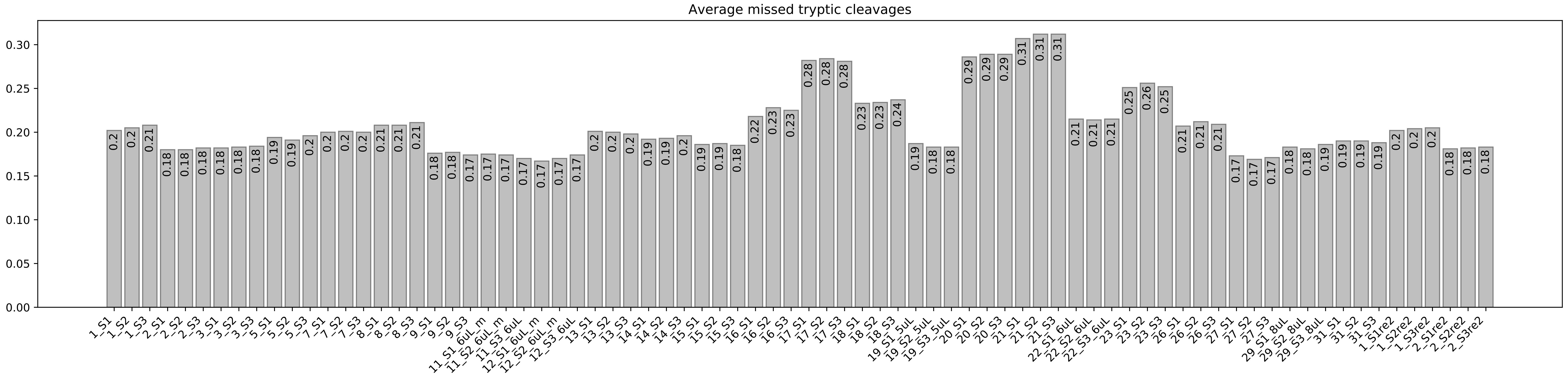

Mean peak FWHM, in MS2 scans

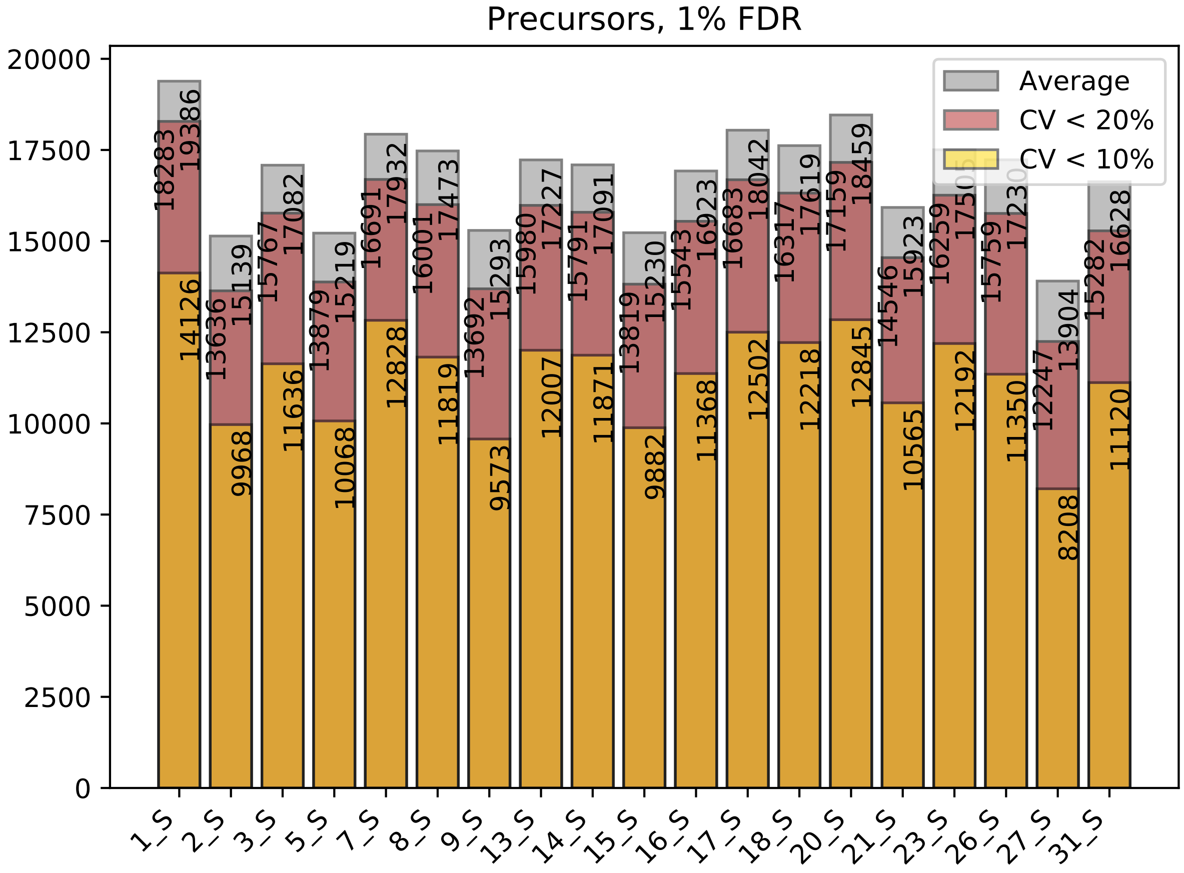

Median RT prediction accuracy, minutes
0.0
0.1
0.2
0.3
0.4
0.5
0.4
0.48
0.49
0.39
0.4
0.38
0.42
0.42
0.41
0.41
0.42
0.4
0.44
0.43
0.45
0.45
0.44
0.45
0.41
0.38
0.39
0.34
0.34
0.34
0.34
0.34
0.34
0.44
0.44
0.42
0.41
0.44
0.42
0.39
0.41
0.38
0.38
0.43
0.44
0.43
0.42
0.41
0.44
0.47
0.42
0.41
0.41
0.41
0.43
0.44
0.47
0.39
0.41
0.41
0.41
0.37
0.36
0.42
0.47
0.42
0.42
0.44
0.42
0.36
0.37
0.39
0.43
0.44
0.41
0.41
0.42
0.41
0.45
0.47
0.46
0.39
0.38
0.38
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2

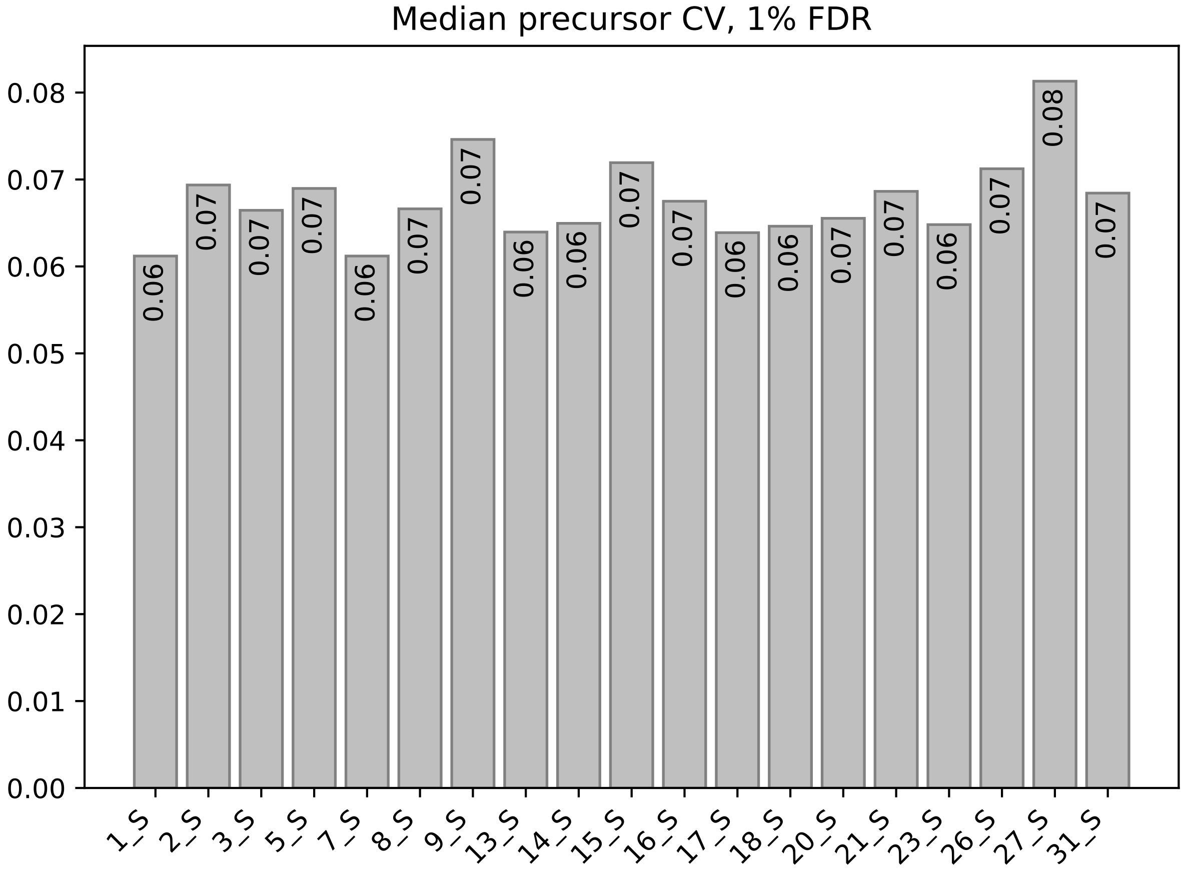

Median mass accuracy, MS2, ppm

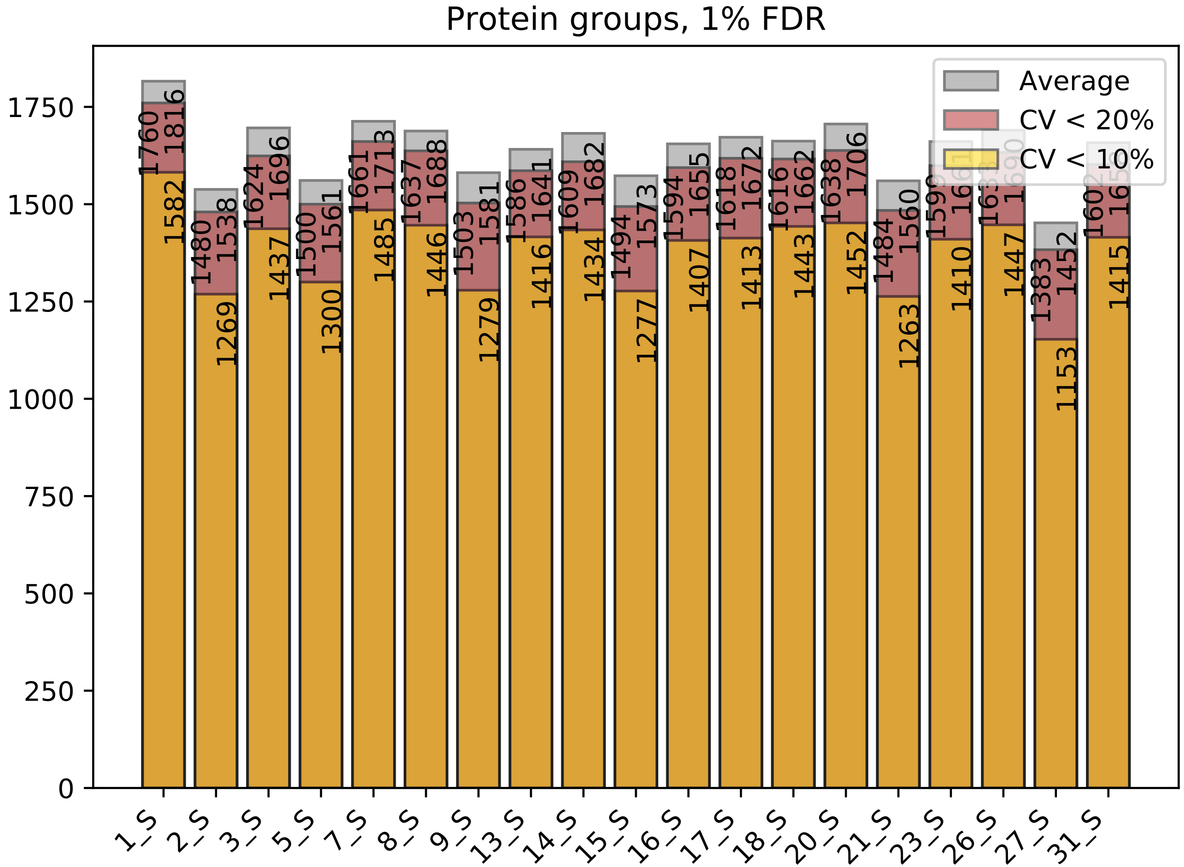

Median mass accuracy, MS1, ppm
Without correction
Corrected
0
2
4
6
8
10
12
14
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2

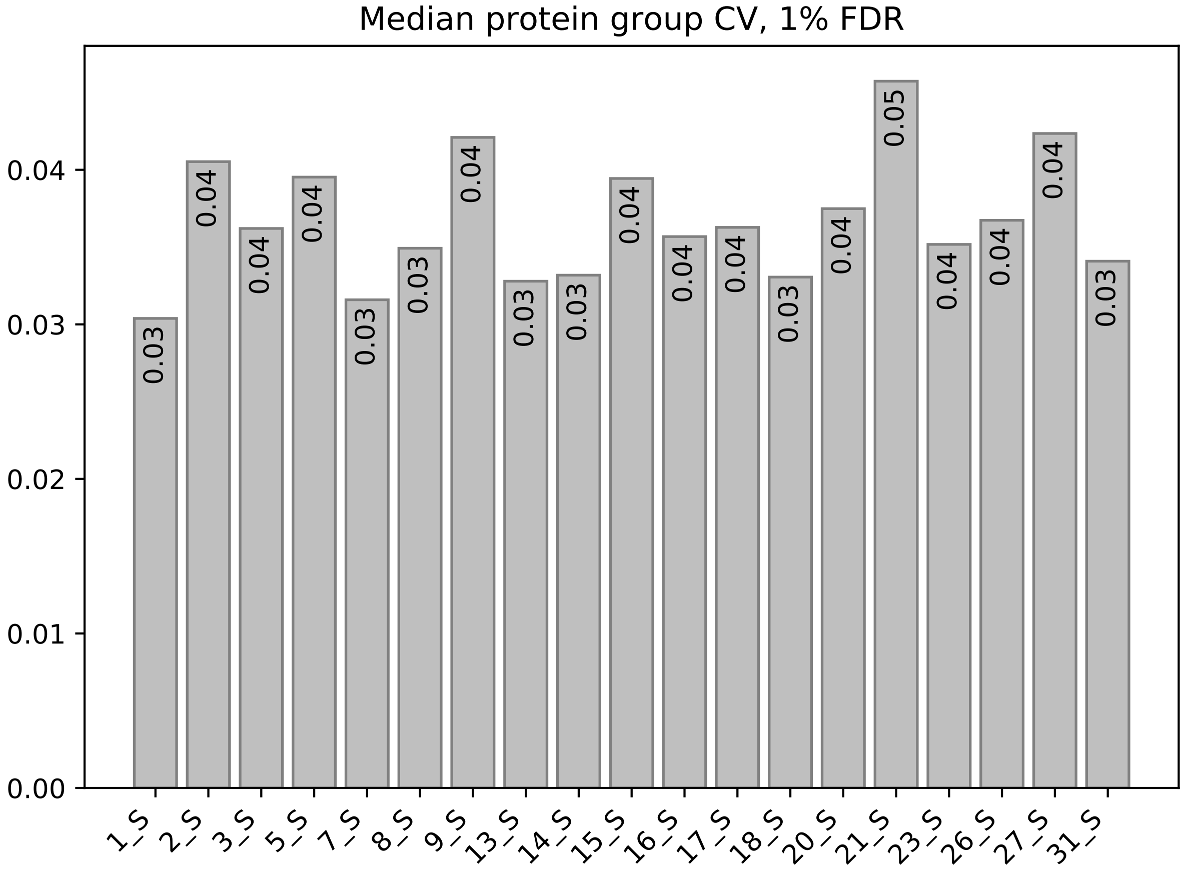

Peptide characteristics
Average length
Average charge
0
2
4
6
8
10
12
14
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2


Average missed tryptic cleavages
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.2
0.2
0.21
0.18
0.18
0.18
0.18
0.18
0.18
0.19
0.19
0.2
0.2
0.2
0.2
0.21
0.21
0.21
0.18
0.18
0.17
0.17
0.17
0.17
0.17
0.17
0.17
0.2
0.2
0.2
0.19
0.19
0.2
0.19
0.19
0.18
0.22
0.23
0.23
0.28
0.28
0.28
0.23
0.23
0.24
0.19
0.18
0.18
0.29
0.29
0.29
0.31
0.31
0.31
0.21
0.21
0.21
0.25
0.26
0.25
0.21
0.21
0.21
0.17
0.17
0.17
0.18
0.18
0.19
0.19
0.19
0.19
0.2
0.2
0.2
0.18
0.18
0.18
1_S1
1_S2
1_S3
2_S1
2_S2
2_S3
3_S1
3_S2
3_S3
5_S1
5_S2
5_S3
7_S1
7_S2
7_S3
8_S1
8_S2
8_S3
9_S1
9_S2
9_S3
11_S1_6uL_m
11_S2_6uL_m
11_S3_6uL
12_S1_6uL_m
12_S2_6uL_m
12_S3_6uL
13_S1
13_S2
13_S3
14_S1
14_S2
14_S3
15_S1
15_S2
15_S3
16_S1
16_S2
16_S3
17_S1
17_S2
17_S3
18_S1
18_S2
18_S3
19_S1_5uL
19_S2_5uL
19_S3_5uL
20_S1
20_S2
20_S3
21_S1
21_S2
21_S3
22_S1_6uL
22_S2_6uL
22_S3_6uL
23_S1
23_S2
23_S3
26_S1
26_S2
26_S3
27_S1
27_S2
27_S3
29_S1_8uL
29_S2_8uL
29_S3_8uL
31_S1
31_S2
31_S3
1_S1re2
1_S2re2
1_S3re2
2_S1re2
2_S2re2
2_S3re2


Precursors, 1% FDR
Average
CV < 20%
CV < 10%
20000
17500
15000
12500
10000
7500
5000
2500
0
1_S
2_S
3_S
5_S
7_S
8_S
9_S
13_S
14_S
15_S
16_S
17_S
18_S
20_S
21_S
23_S
26_S
27_S
31_S
14126
18283
19386
9968
13636
15139
11636
15767
17082
10068
13879
15219
12828
16691
17932
11819
16001
17473
9573
13692
15293
12007
15980
17227
11871
15791
17091
9882
13819
15230
11368
15543
16923
12502
16683
18042
12218
16317
17619
12845
17159
18459
10565
14546
15923
12192
16259
17505
11350
15759
17230
8208
12247
13904
11120
15282
16628


Median precursor CV, 1% FDR
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.06
0.07
0.07
0.07
0.06
0.07
0.07
0.06
0.06
0.07
0.07
0.06
0.06
0.07
0.07
0.06
0.07
0.08
0.07
1_S
2_S
3_S
5_S
7_S
8_S
9_S
13_S
14_S
15_S
16_S
17_S
18_S
20_S
21_S
23_S
26_S
27_S
31_S


Protein groups, 1% FDR
Average
CV < 20%
CV < 10%
0
250
500
750
1000
1250
1500
1750
1_S
2_S
3_S
5_S
7_S
8_S
9_S
13_S
14_S
15_S
16_S
17_S
18_S
20_S
21_S
23_S
26_S
27_S
31_S
1582
1760
1816
1269
1480
1538
1437
1624
1696
1300
1500
1561
1485
1661
1713
1446
1637
1688
1279
1503
1581
1416
1586
1641
1434
1609
1682
1277
1494
1573
1407
1594
1655
1413
1618
1672
1443
1616
1662
1452
1638
1706
1263
1484
1560
1410
1599
1661
1447
1633
1690
1153
1383
1452
1415
1602
1658


Median protein group CV, 1% FDR
0.00
0.01
0.02
0.03
0.04
0.03
0.04
0.04
0.04
0.03
0.03
0.04
0.03
0.03
0.04
0.04
0.04
0.03
0.04
0.05
0.04
0.04
0.04
0.03
1_S
2_S
3_S
5_S
7_S
8_S
9_S
13_S
14_S
15_S
16_S
17_S
18_S
20_S
21_S
23_S
26_S
27_S
31_S