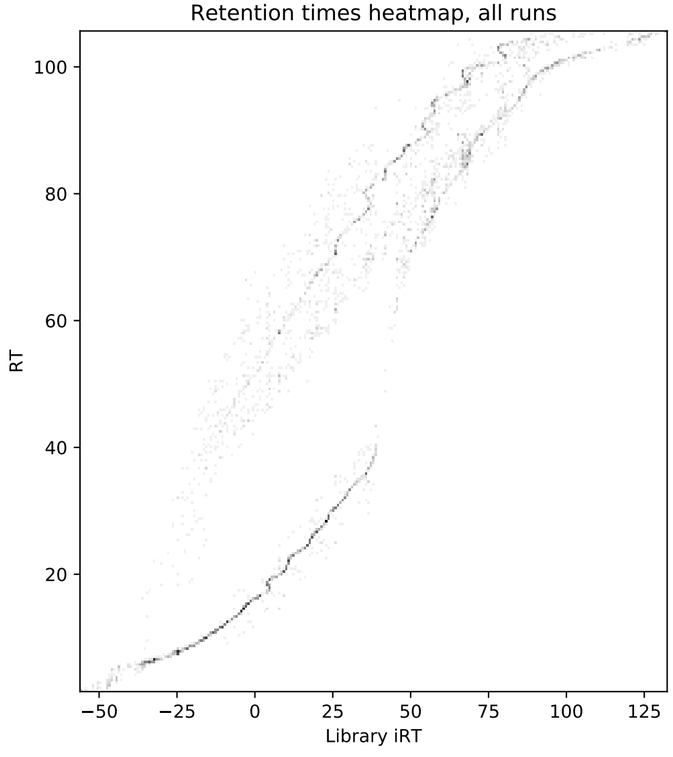
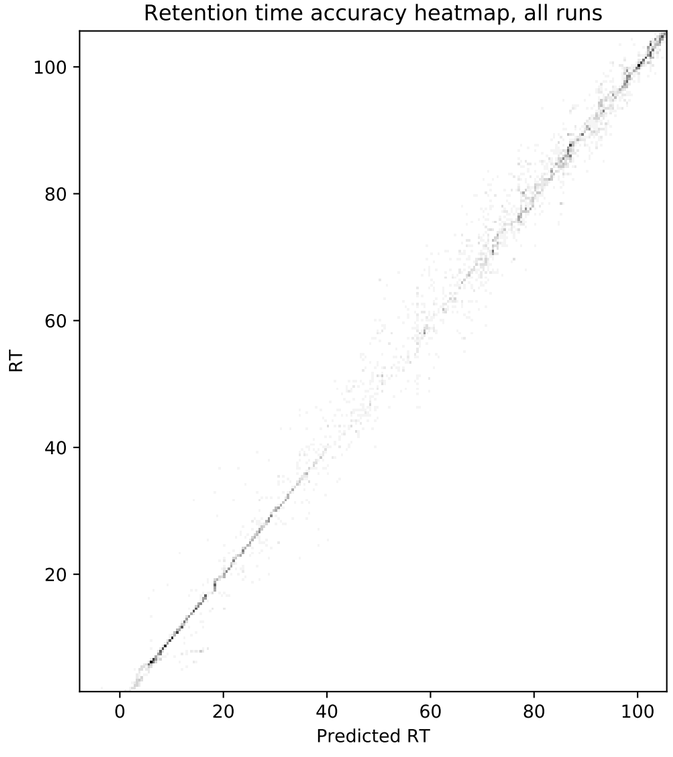
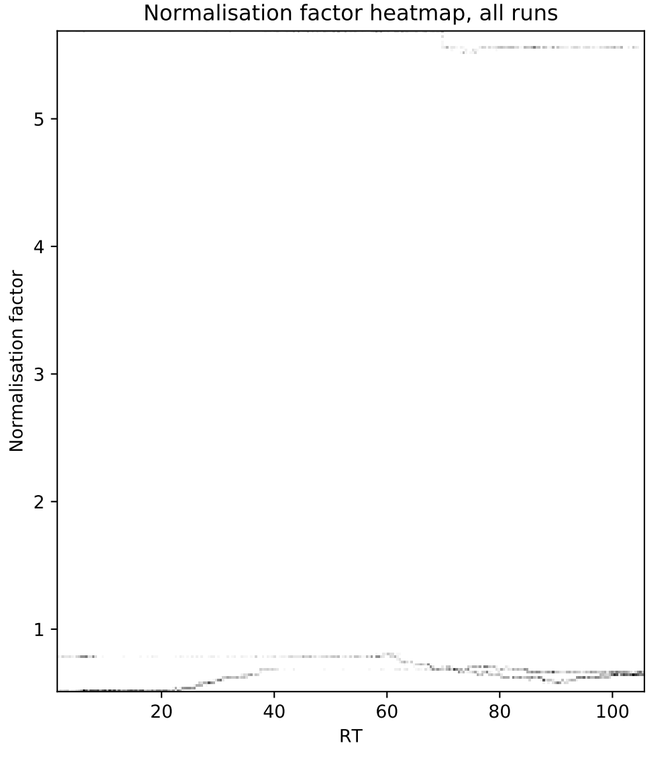
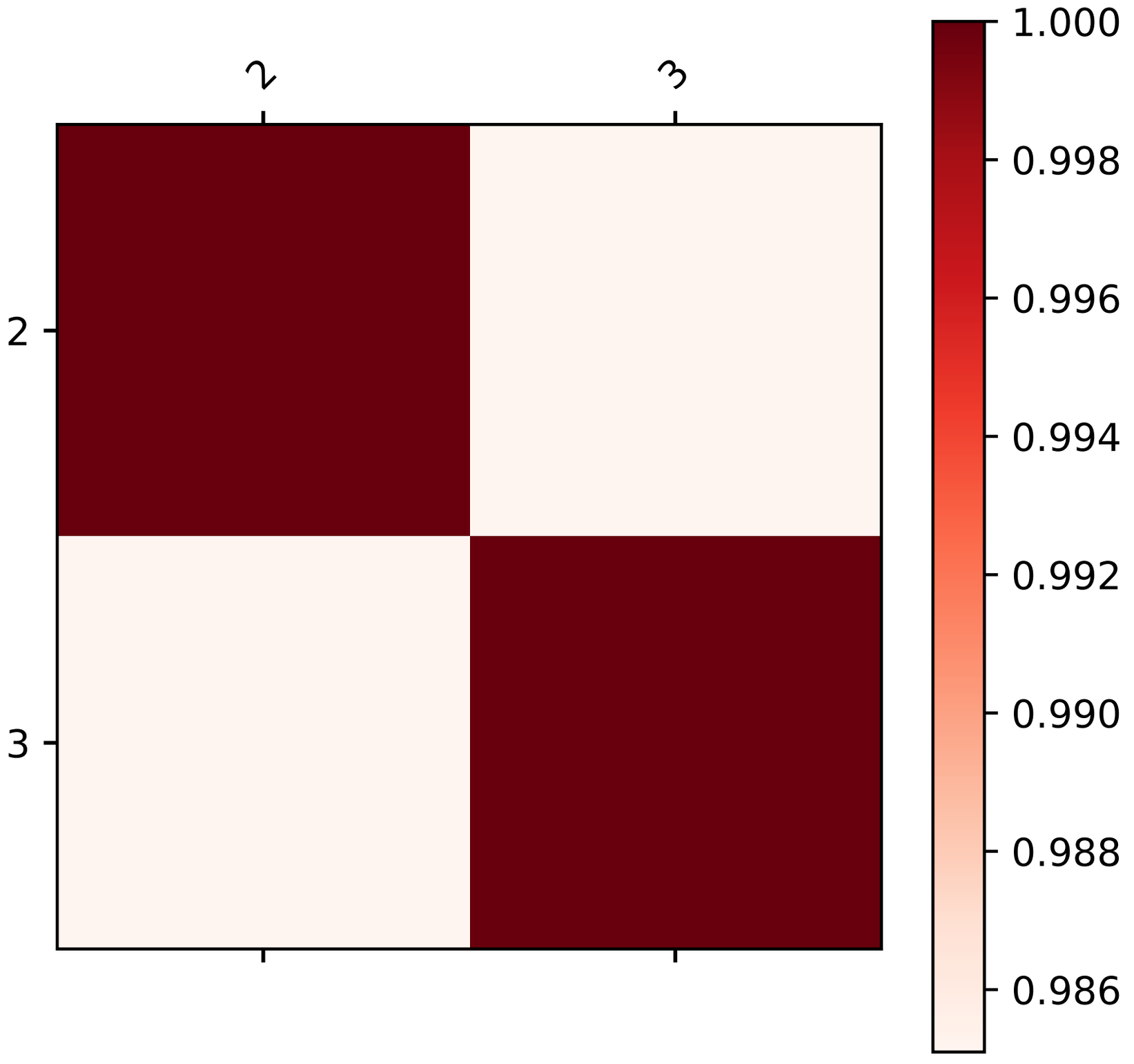
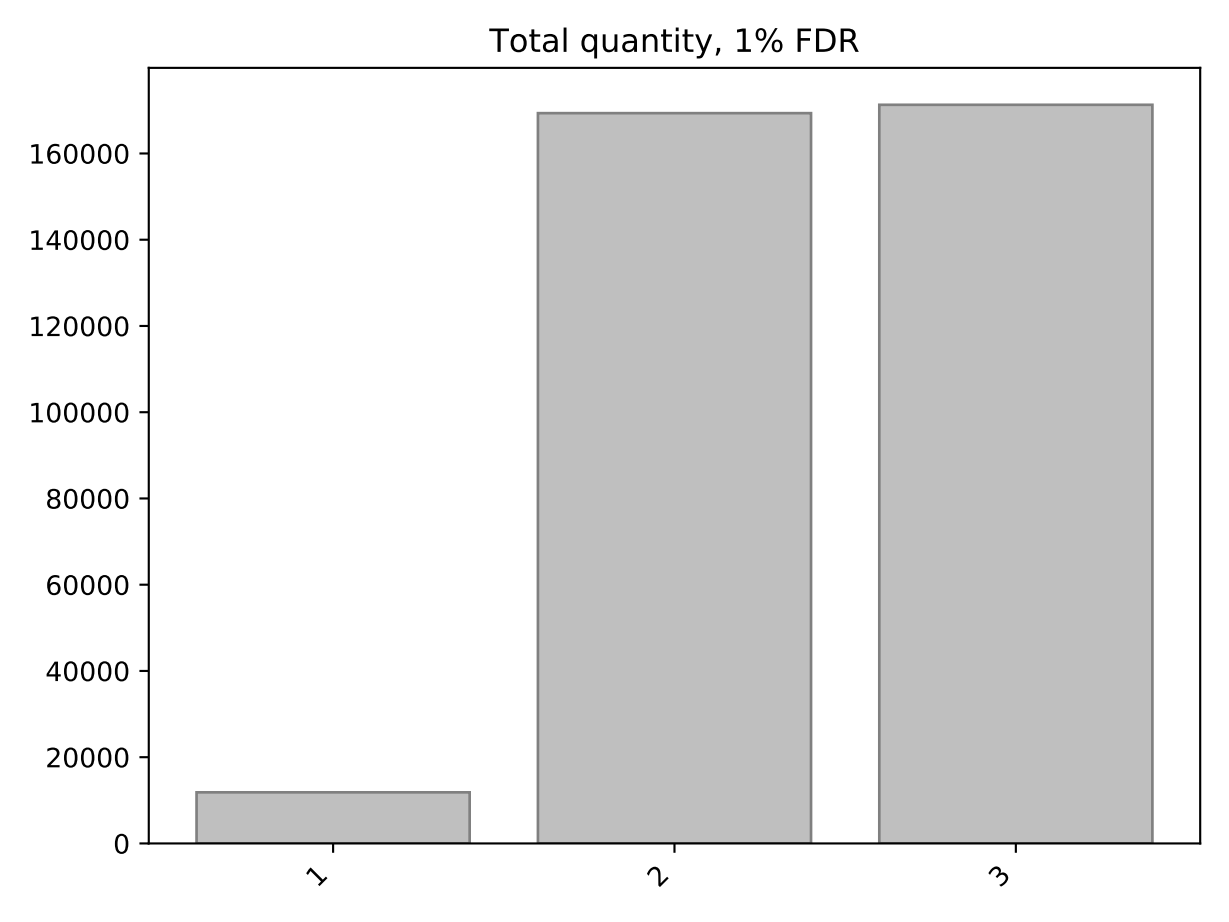
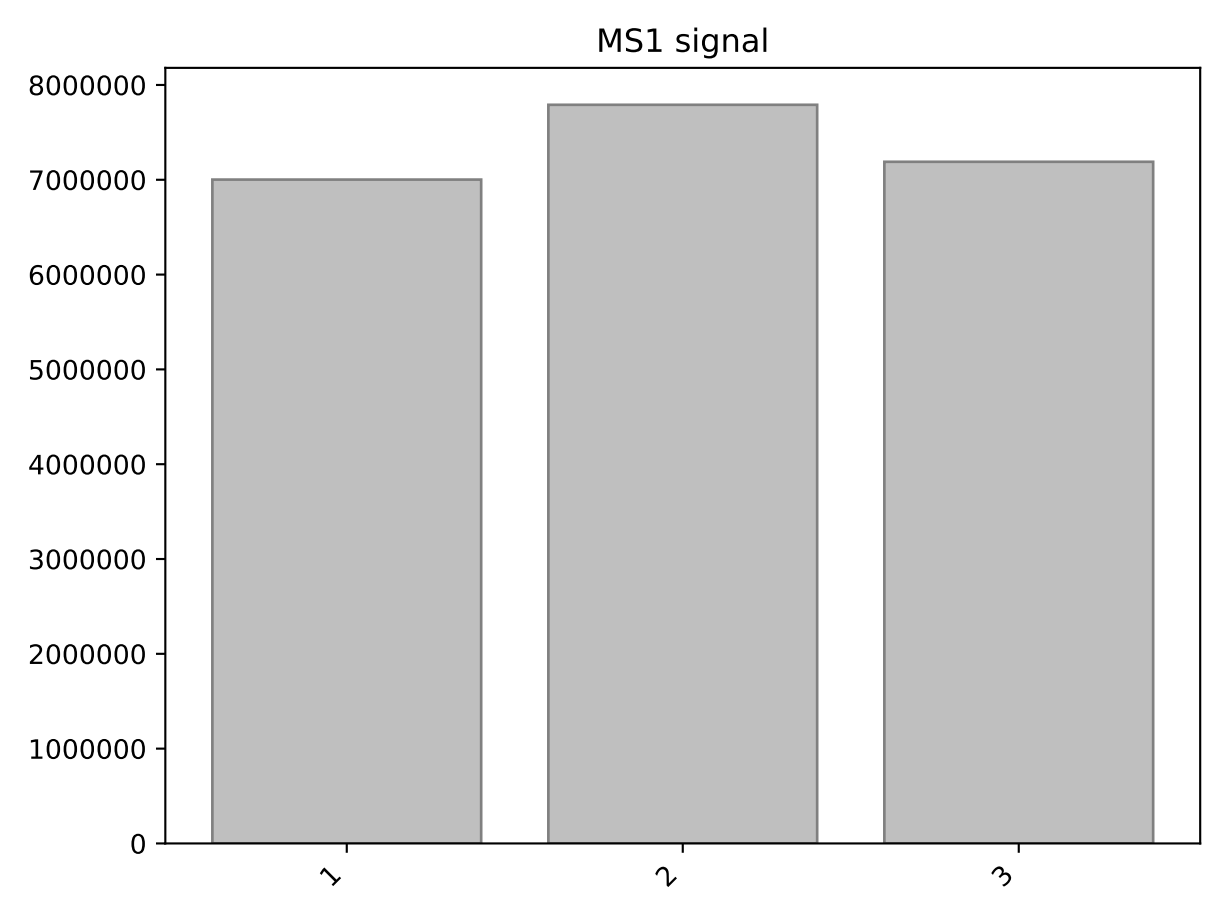

Retention times heatmap, all runs
RT
Library iRT
100
80
60
40
20
−50
−25
0
25
50
75
100
125

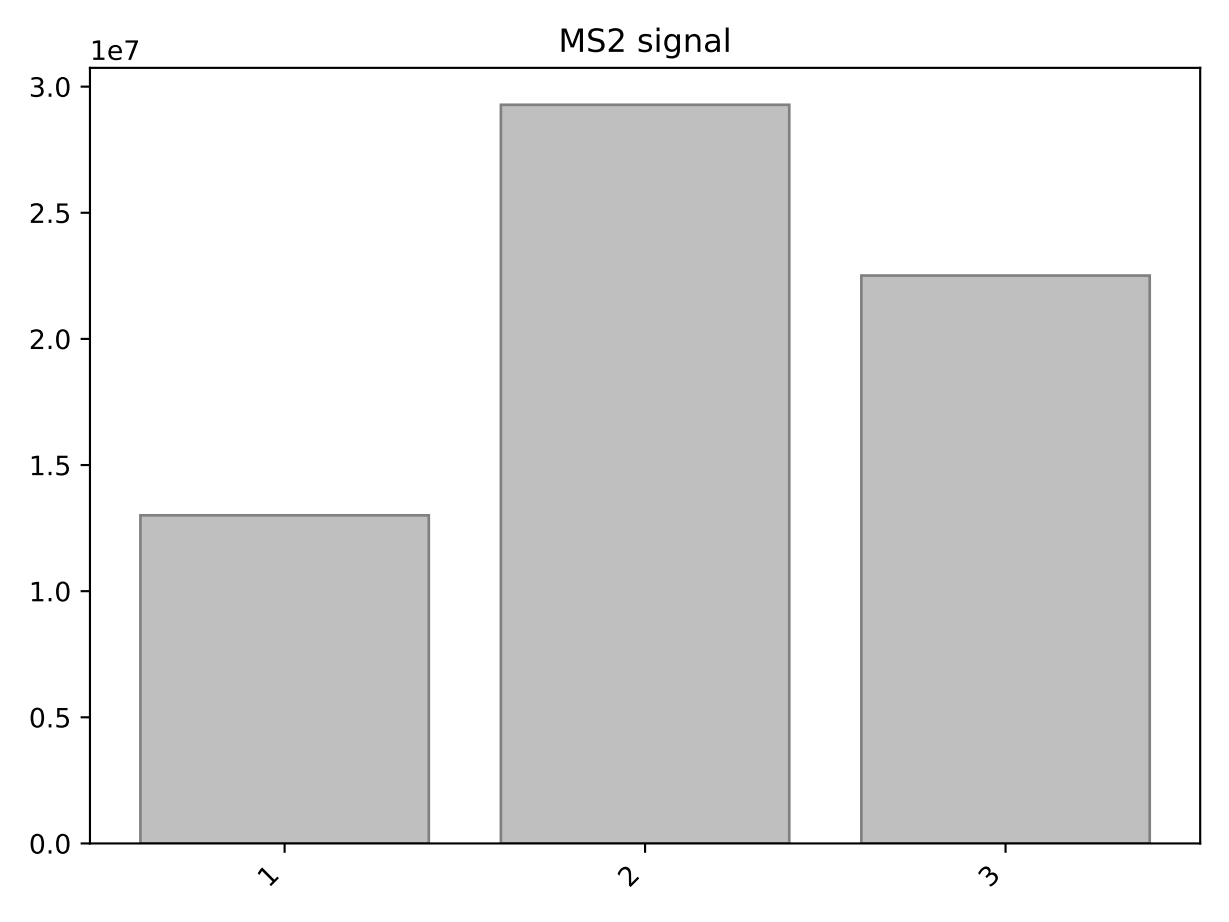

Retention time accuracy heatmap, all runs
RT
Predicted RT
100
80
60
40
20
0
20
40
60
80
100

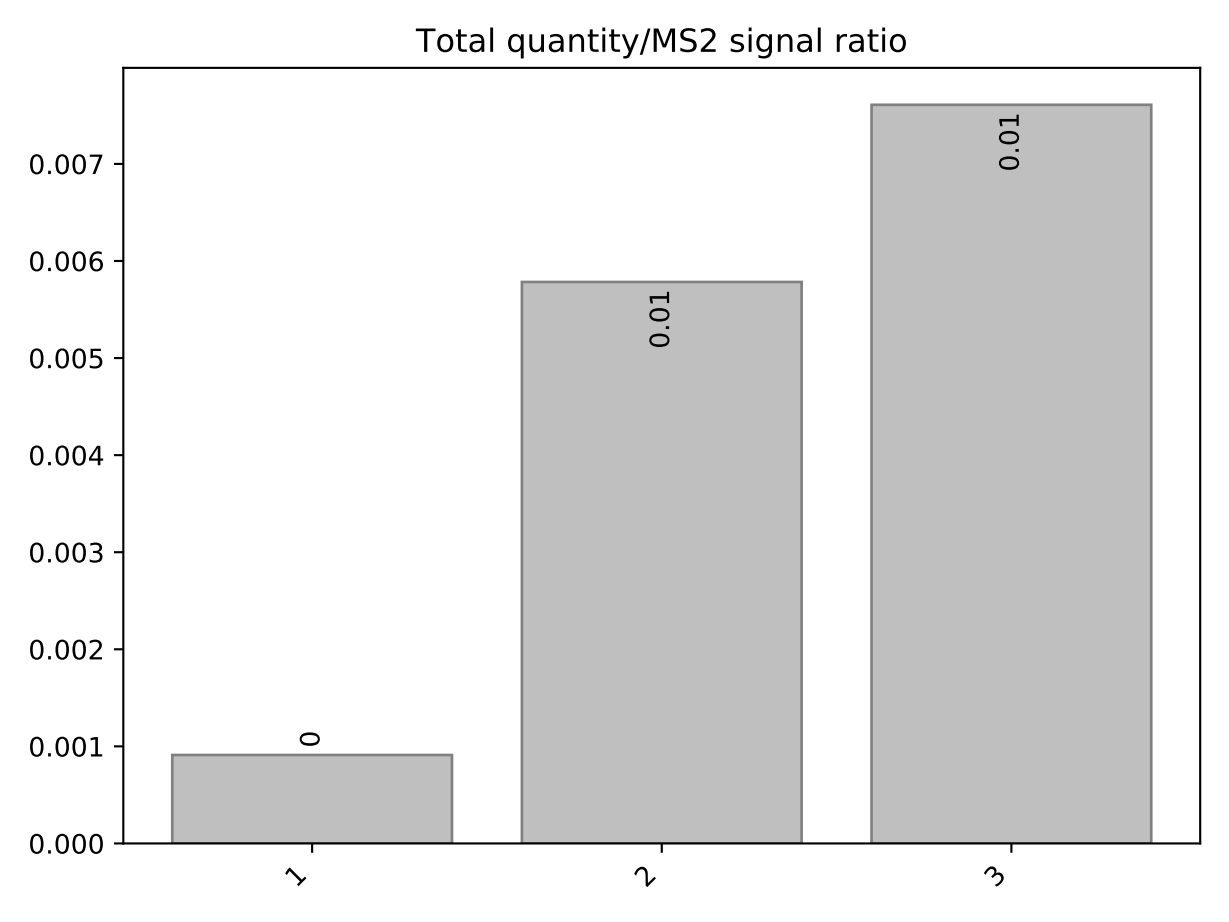

Normalisation factor heatmap, all runs
Normalisation factor
RT
5
4
3
2
1
20
40
60
80
100

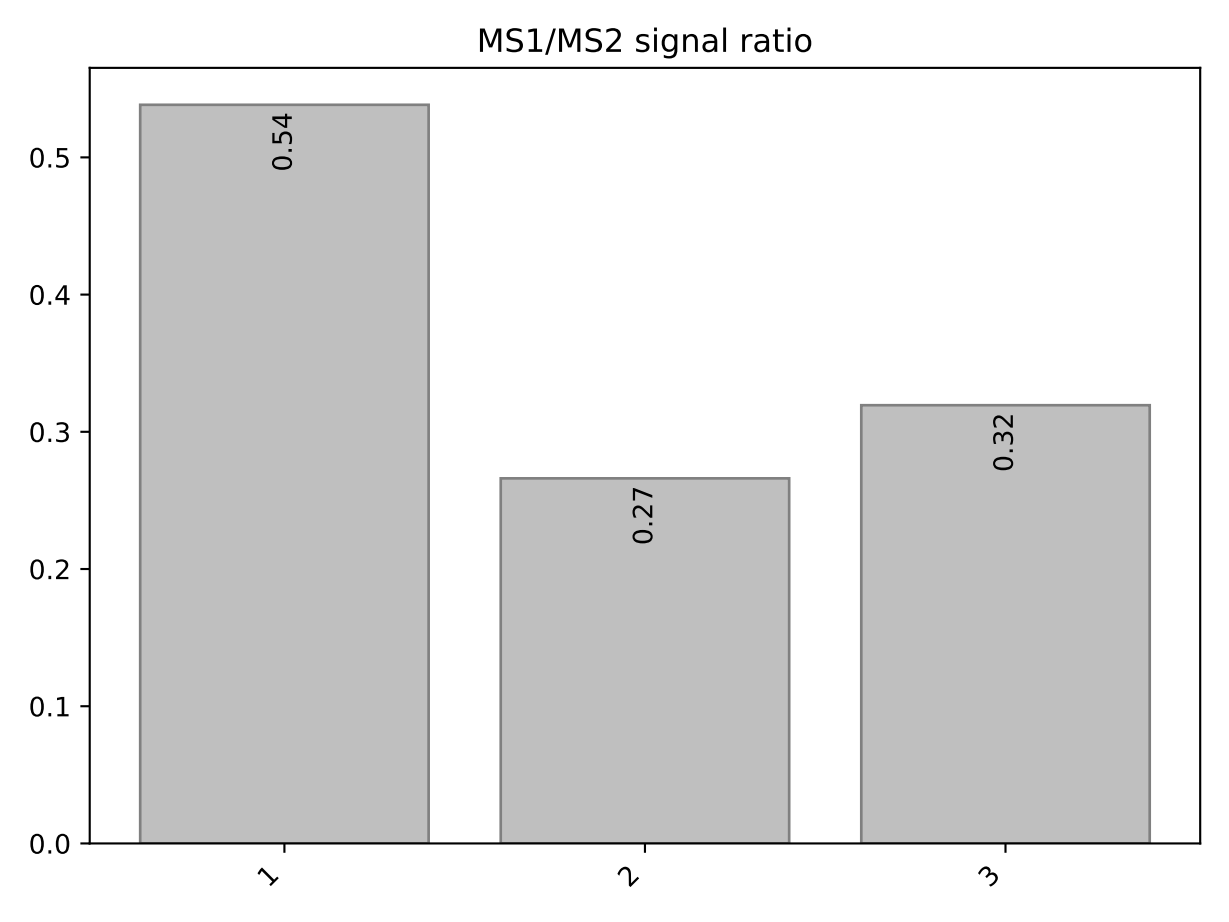

2
3
2
3
1.000
0.998
0.996
0.994
0.992
0.990
0.988
0.986

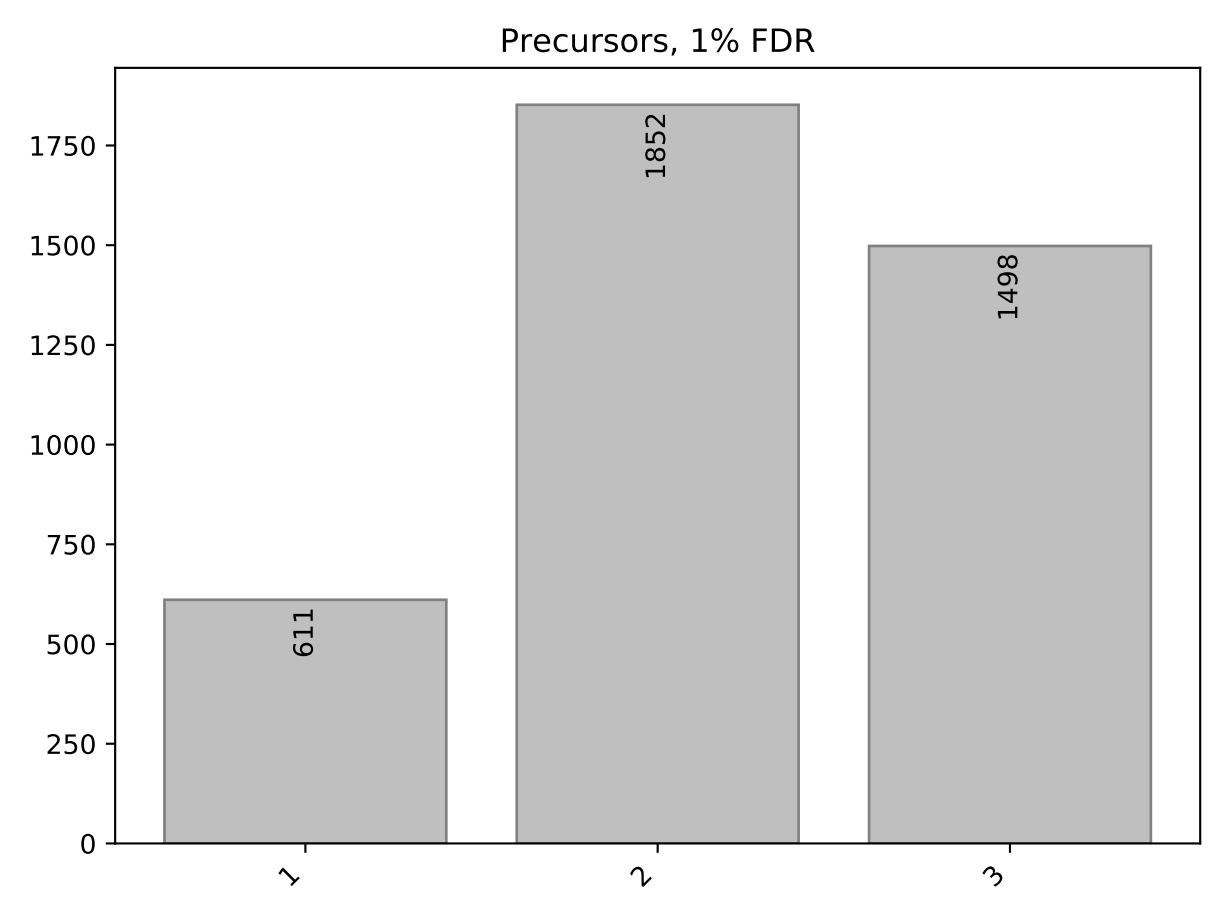

Total quantity, 1% FDR
160000
140000
120000
100000
80000
60000
40000
20000
0
1
2
3

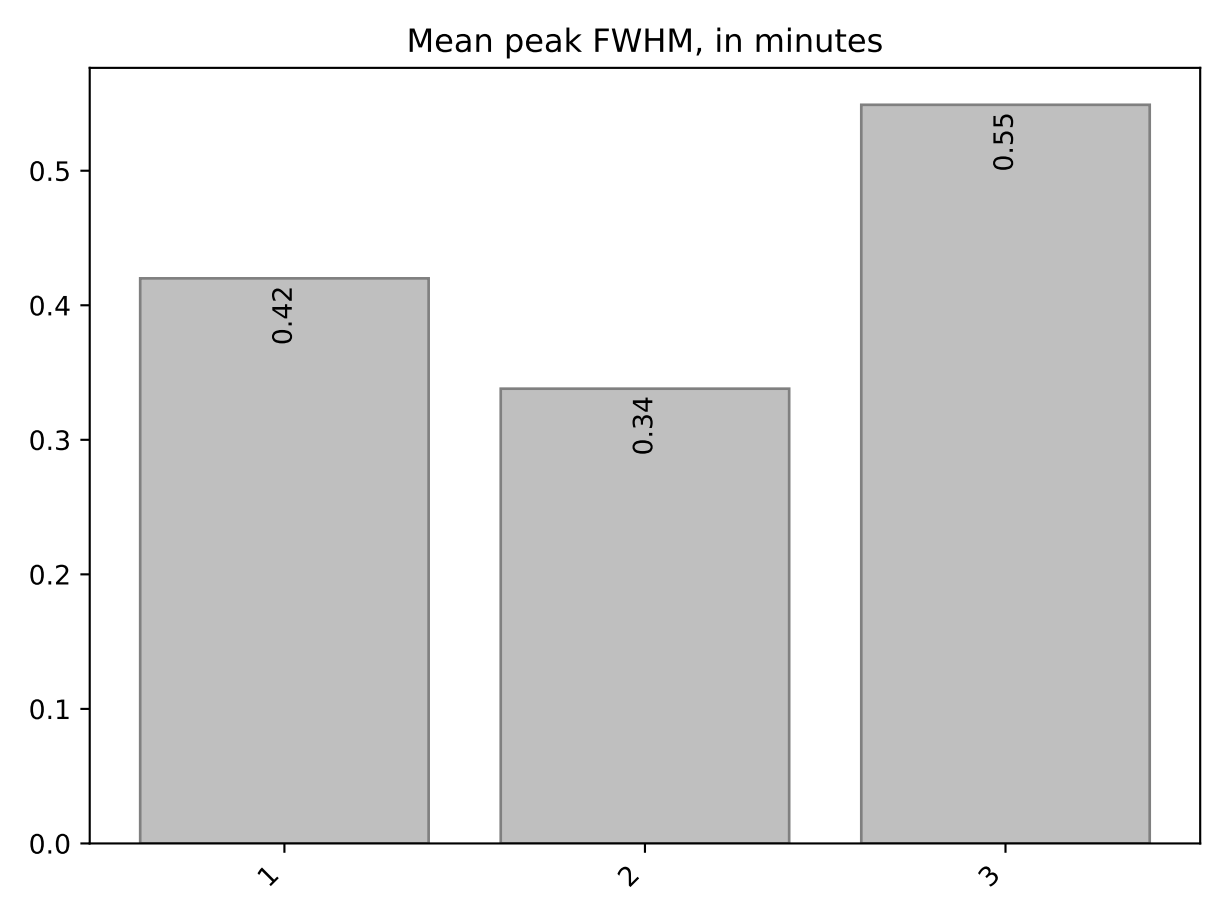

MS1 signal
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
1
2
3

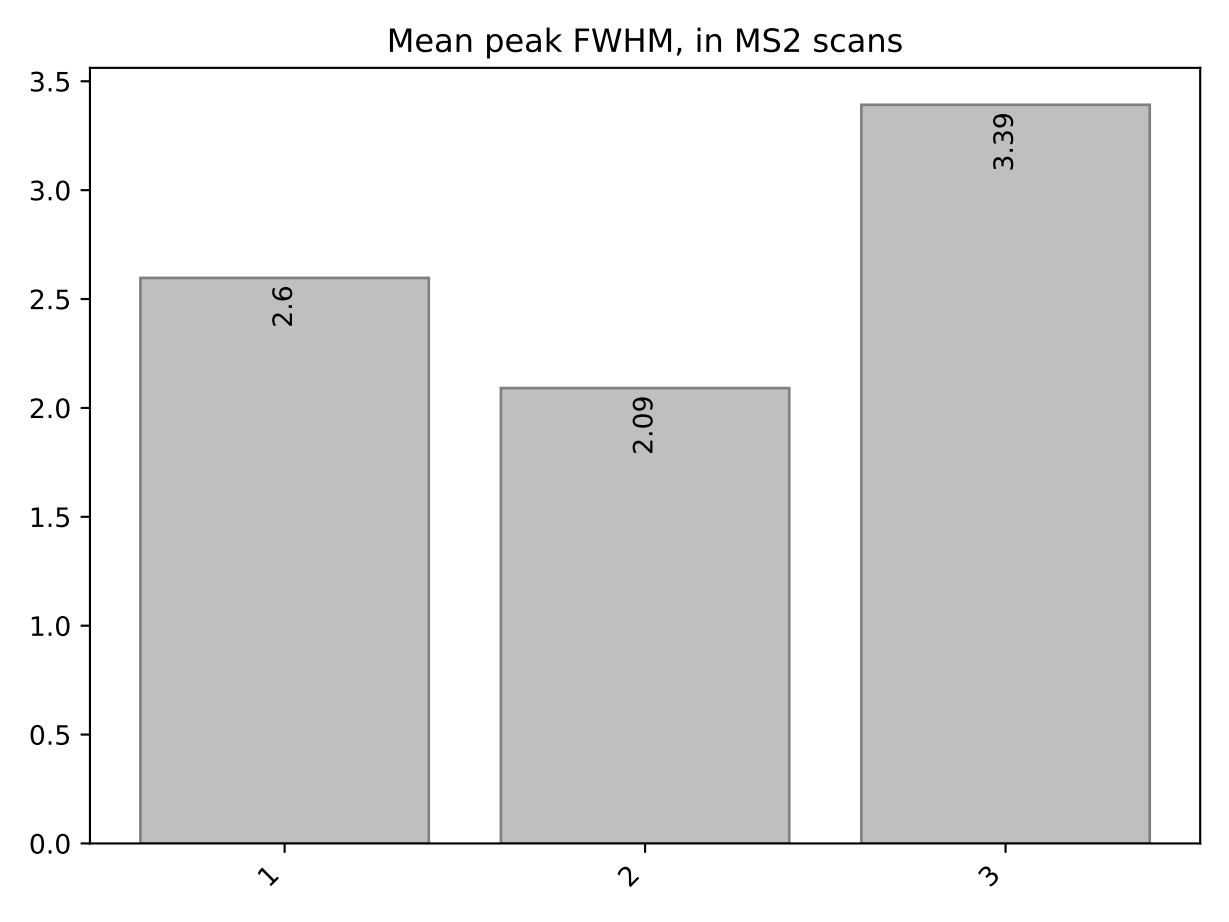

MS2 signal
1e7
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
2
3

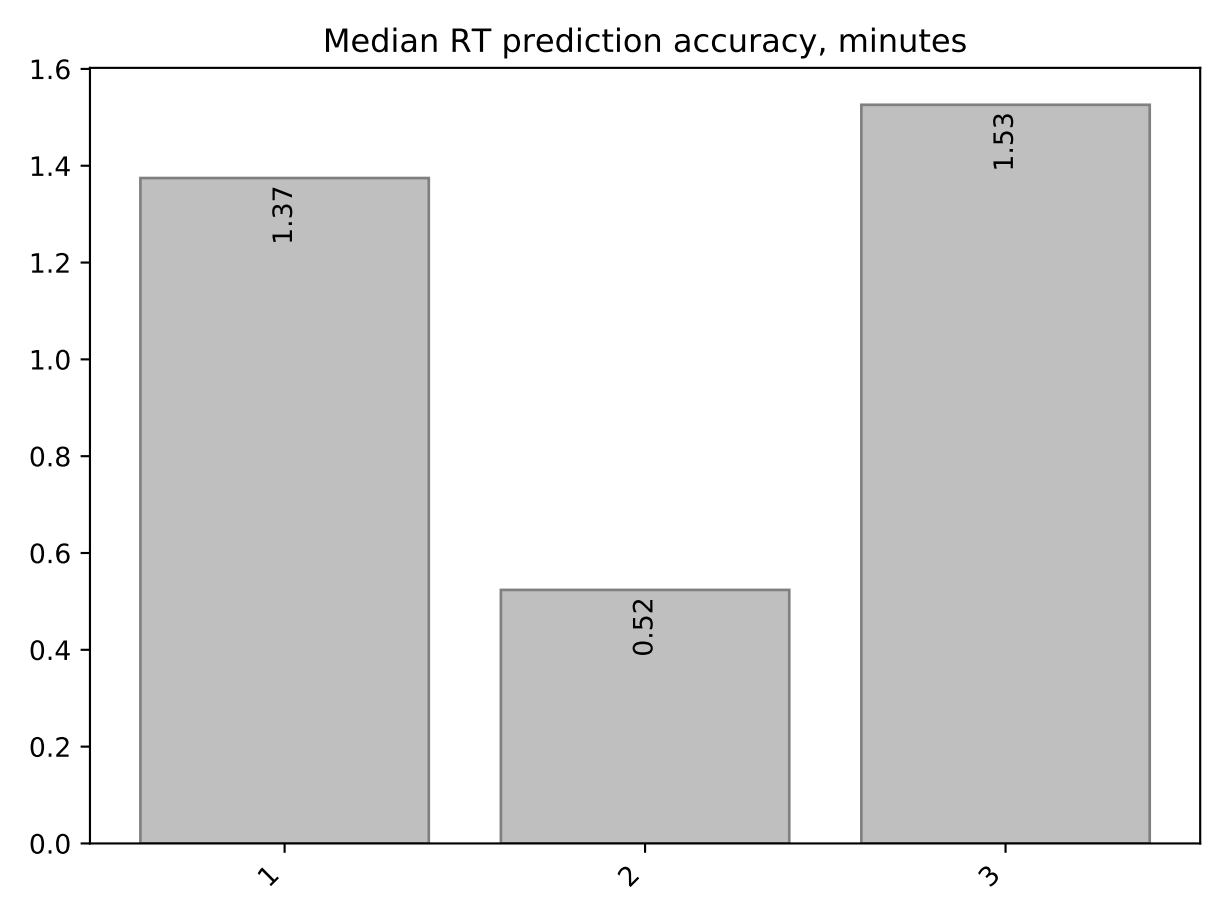

Total quantity/MS2 signal ratio
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
0
0.01
0.01
1
2
3

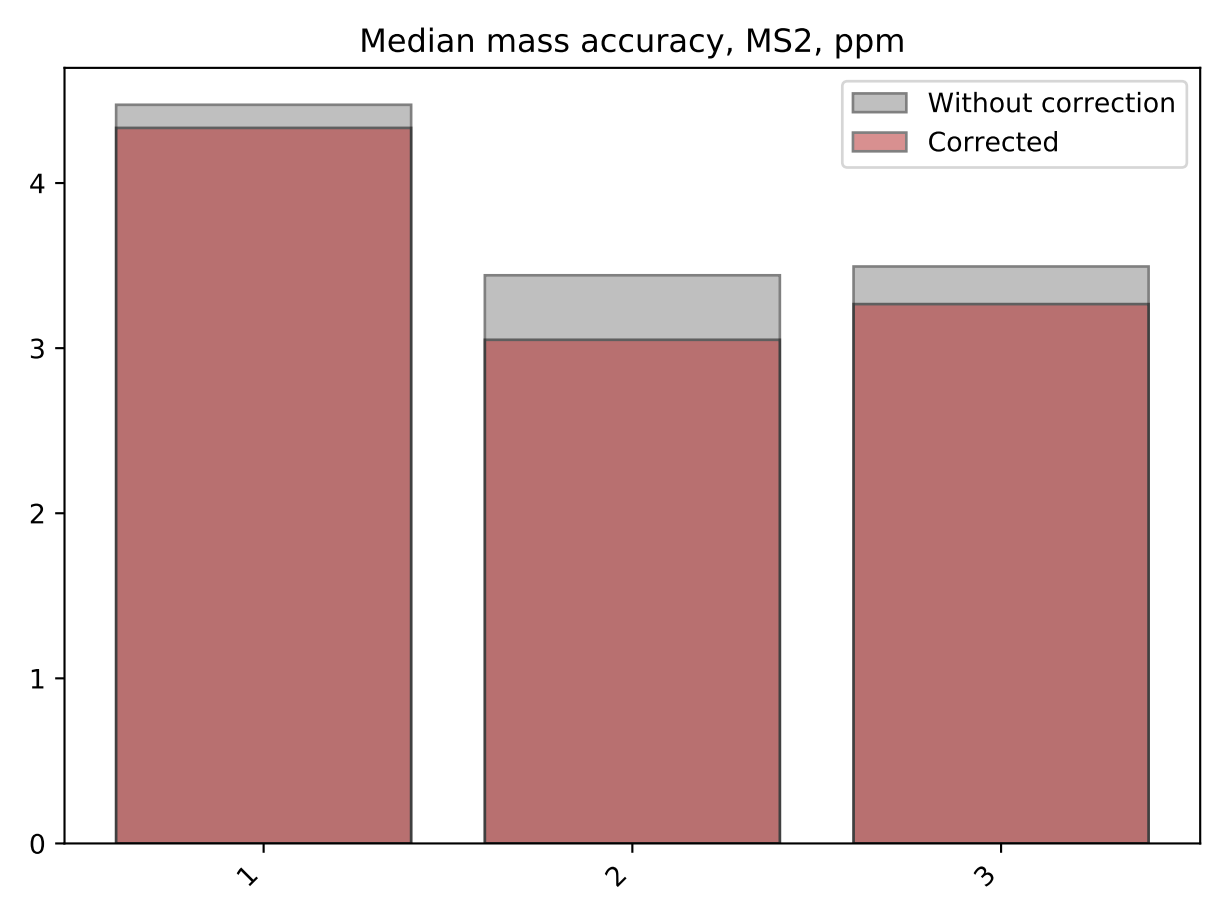

MS1/MS2 signal ratio
0.54
0.27
0.32
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3

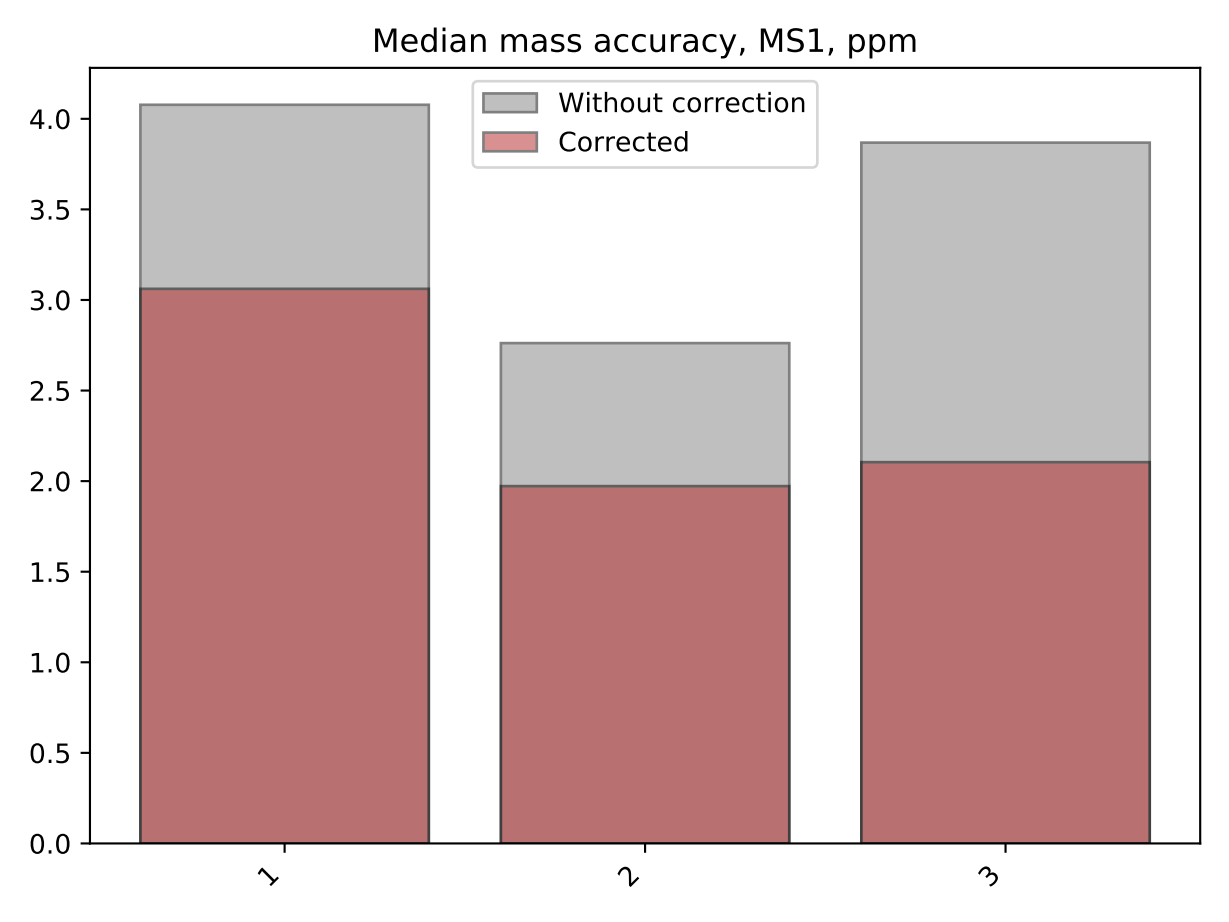

Precursors, 1% FDR
1750
1500
1250
1000
750
500
250
0
611
1852
1498
1
2
3

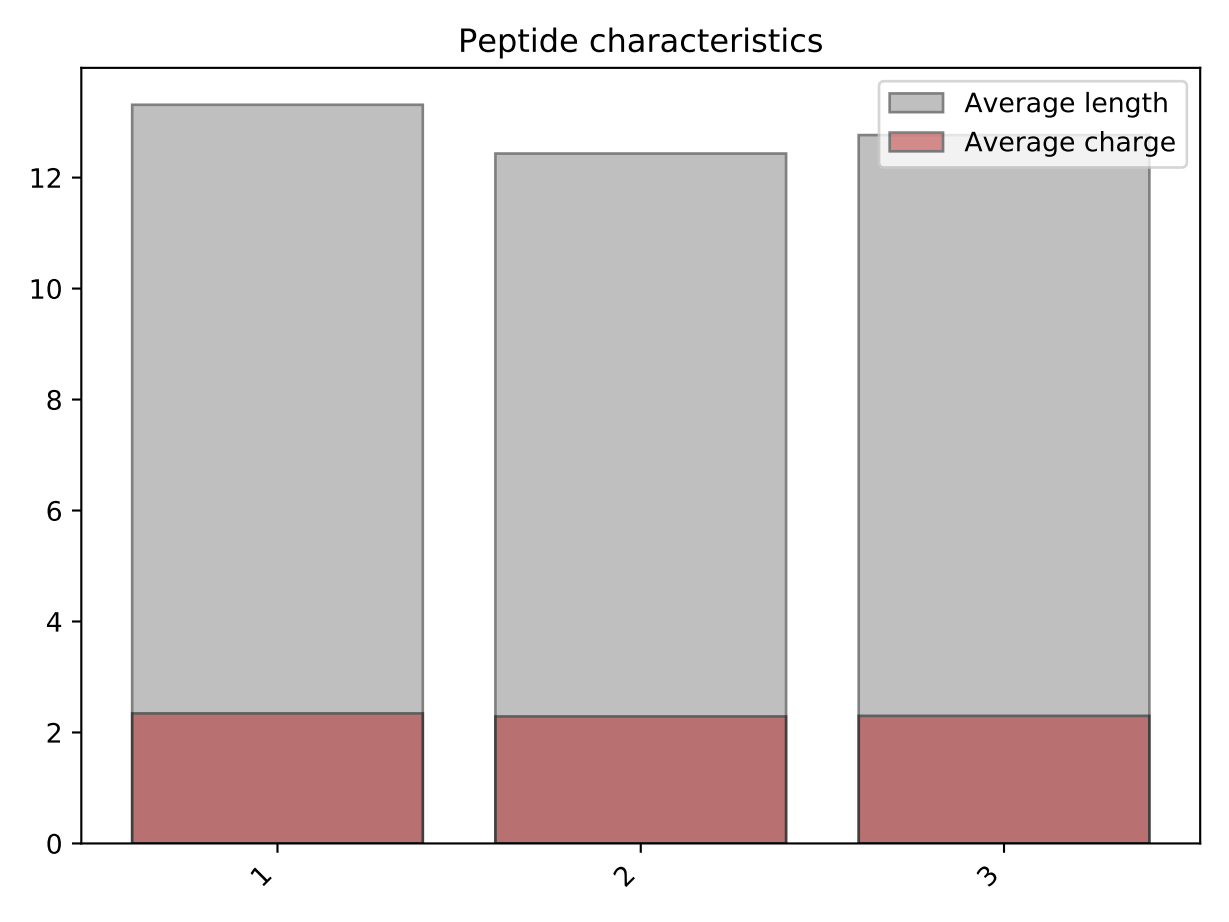

Mean peak FWHM, in minutes
0.0
0.1
0.2
0.3
0.4
0.5
0.42
0.34
0.55
1
2
3

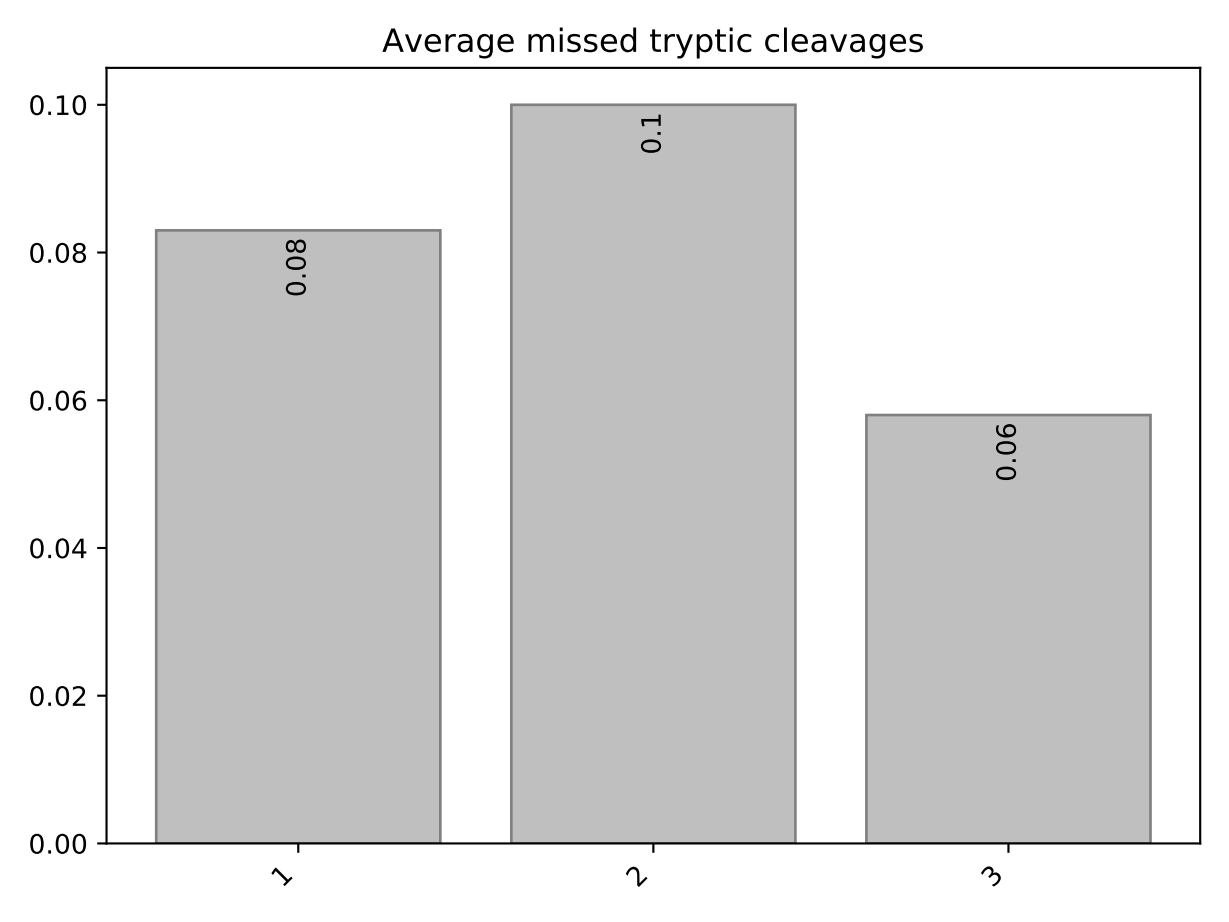

Mean peak FWHM, in MS2 scans
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2.6
2.09
3.39
1
2
3


Median RT prediction accuracy, minutes
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1.37
0.52
1.53
1
2
3


Median mass accuracy, MS2, ppm
Without correction
Corrected
0
1
2
3
4
1
2
3


Median mass accuracy, MS1, ppm
Without correction
Corrected
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
2
3


Peptide characteristics
Average length
Average charge
0
2
4
6
8
10
12
1
2
3


Average missed tryptic cleavages
0.10
0.08
0.06
0.04
0.02
0.00
0.08
0.1
0.06
1
2
3