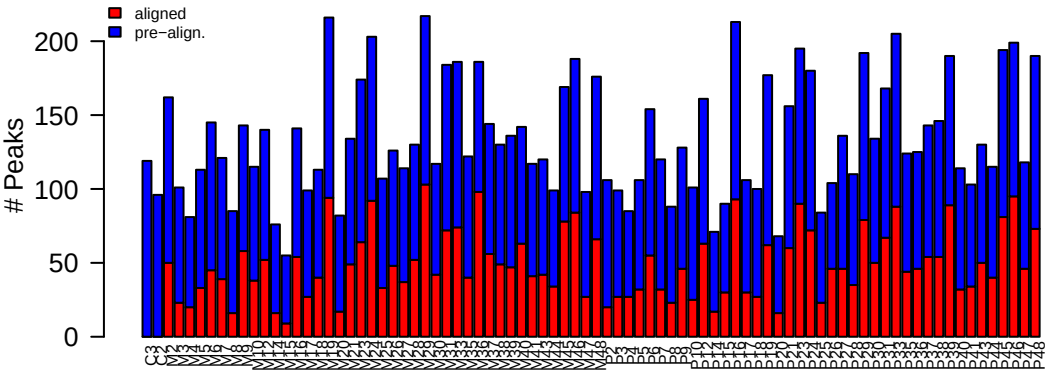
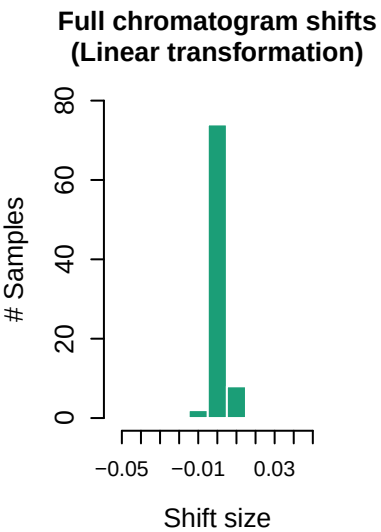
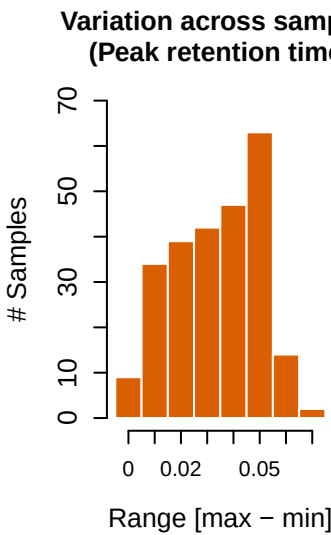
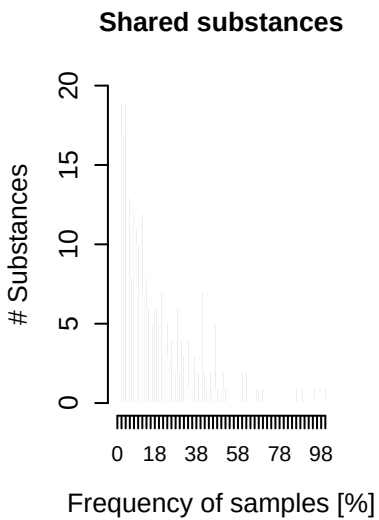

aligned
pre−align.
Peaks
0
50
100
150
200


Full chromatogram shifts
(Linear transformation)
Samples
0
20
40
60
80
−0.05
−0.01
0.03
Shift size


Variation across samples
(Peak retention time)
Samples
0
10
30
50
70
0
0.02
0.05
Range [max − min]


Shared substances
Substances
0
5
10
15
20
0
18
38
58
78
98
Frequency of samples [%]