MS-DAP: Mass Spectrometry Downstream Analysis Pipeline

version: beta 0.2.8.1 https://github.com/ftwkoopmans/msdap/

Contents

1 Quality control **2**

1.1 DIA confidence score distributions 2

1.2 number of peptides and proteins 26

1.3 data completeness 34

1.4 abundance distributions 36

1.5 retention time 45

1.6 variation among replicates 152

1.7 PCA 175

2 Differential abundance analysis **191**

2.1 control_Berlin vs AD_Berlin 191

2.2 control_Magdeburg vs AD_Magdeburg 197

2.3 control_Sweden vs AD_Sweden 203

2.4 control_Berlin,control_Magdeburg... vs AD_Berlin,AD_Magdeburg,AD_Sweden 209

3 Summary of differential testing **215**

4 log **216**

5 R command history **218**

6 R session info **220**

1 Quality control

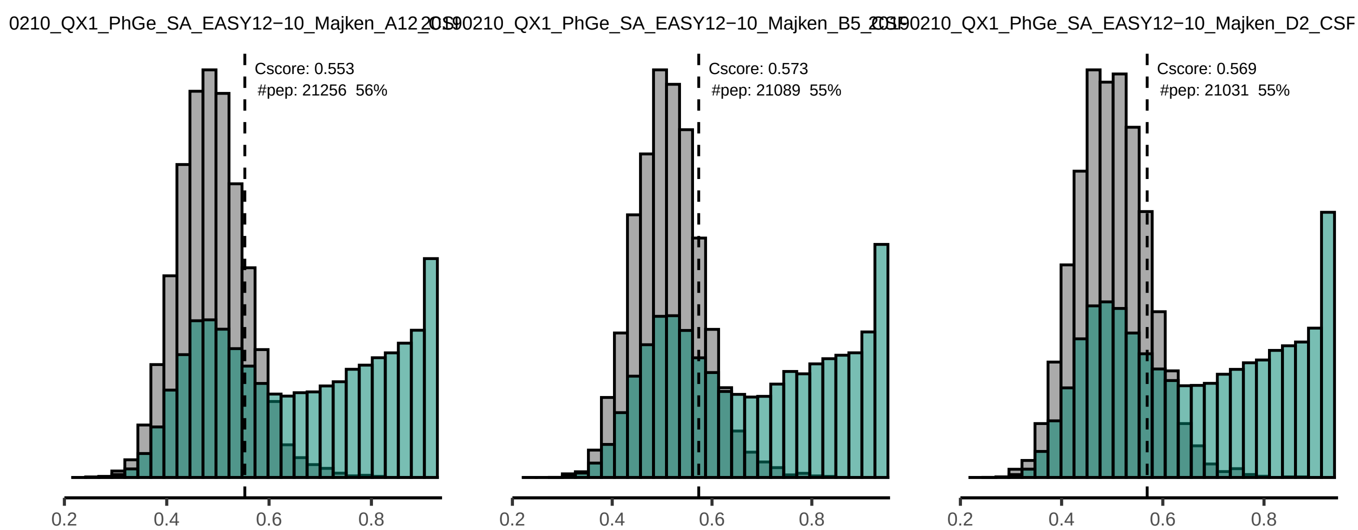
The quality control figures in this section enable you to investigate reproducibility and global clustering of samples by visualizing:

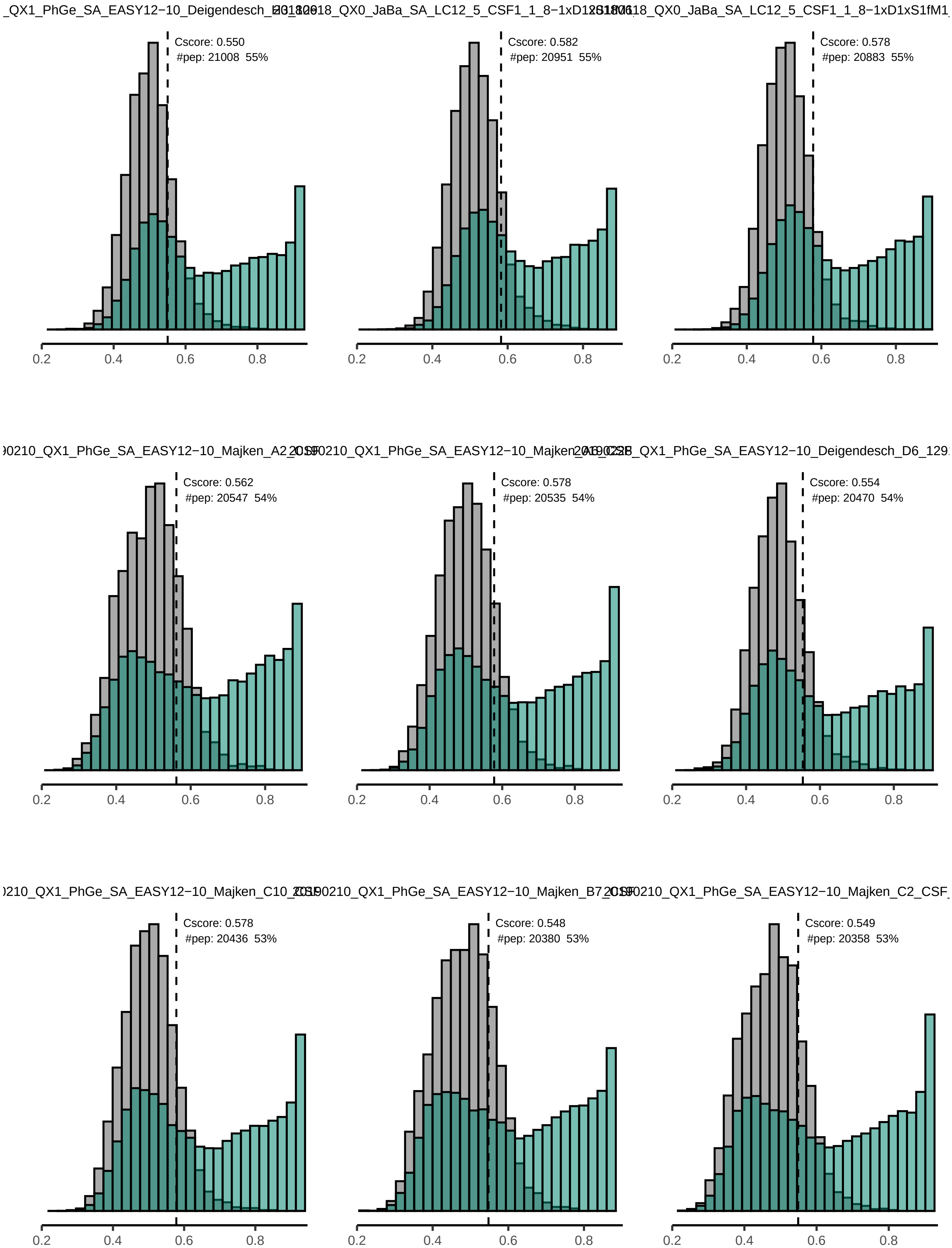
- number of peptides/proteins detected in each sample
- dataset completeness
- local effects in HPLC peptide retention time per sample
- reproducibility of peptide quantification among replicates
- PCA of all samples to visualize clustering

The first set of quality control figures describes individual samples, thereafter group-level quality metrics are described and finally sample clustering is used to highlight structure in the entire dataset.

1.1 DIA confidence score distributions

DIA data was used as input for this analysis. Below histograms visualize both target (green) and decoy (grey) cscores in each sample, indicating how confident the input software was in the identification of peptides from the spectral library in the raw DIA data. Samples are ordered by the number of precursors quantified at q-value confidence threshold 0.01. At this threshold, the respective cscore and number of peptides is shown.





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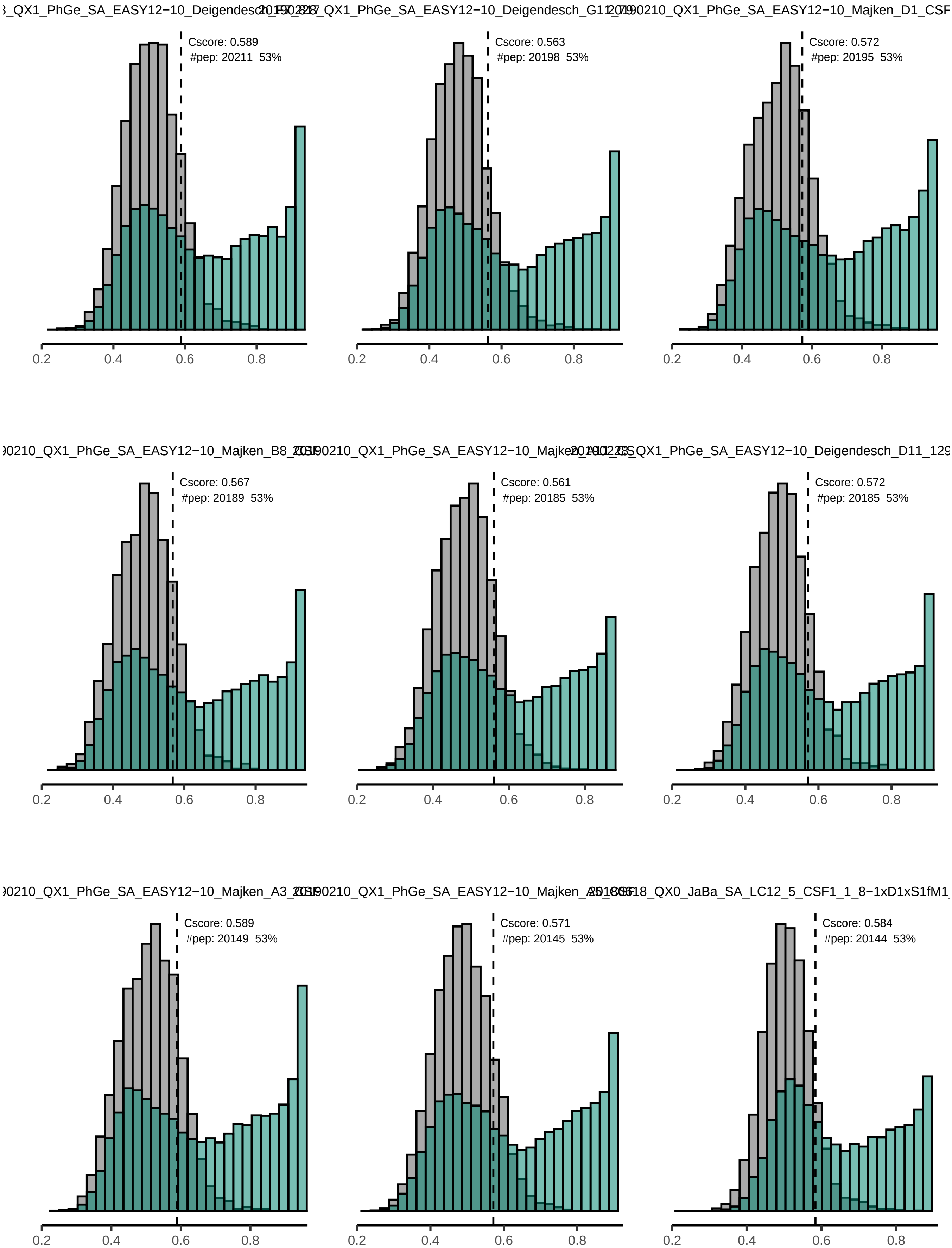
20181018_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
Cscore: 0.550
#pep: 21008 55%
Cscore: 0.582
#pep: 20951 55%
Cscore: 0.578
#pep: 20883 55%
0.2
0.4
0.6
0.8
)0210_QX1_PhGe_SA_EASY12−10_Majken_A2
20190210_QX1_PhGe_SA_EASY12−10_Majken_A6
20190226_QX1_PhGe_SA_EASY12−10_Deigendesch_D6_129
Cscore: 0.562
#pep: 20547 54%
Cscore: 0.578
#pep: 20535 54%
Cscore: 0.554
#pep: 20470 54%
)210_QX1_PhGe_SA_EASY12−10_Majken_C10
20190210_QX1_PhGe_SA_EASY12−10_Majken_B7
20190210_QX1_PhGe_SA_EASY12−10_Majken_C2_CSF
Cscore: 0.578
#pep: 20436 53%
Cscore: 0.548
#pep: 20380 53%
Cscore: 0.549
#pep: 20358 53%


Cscore: 0.589
#pep: 20211 53%
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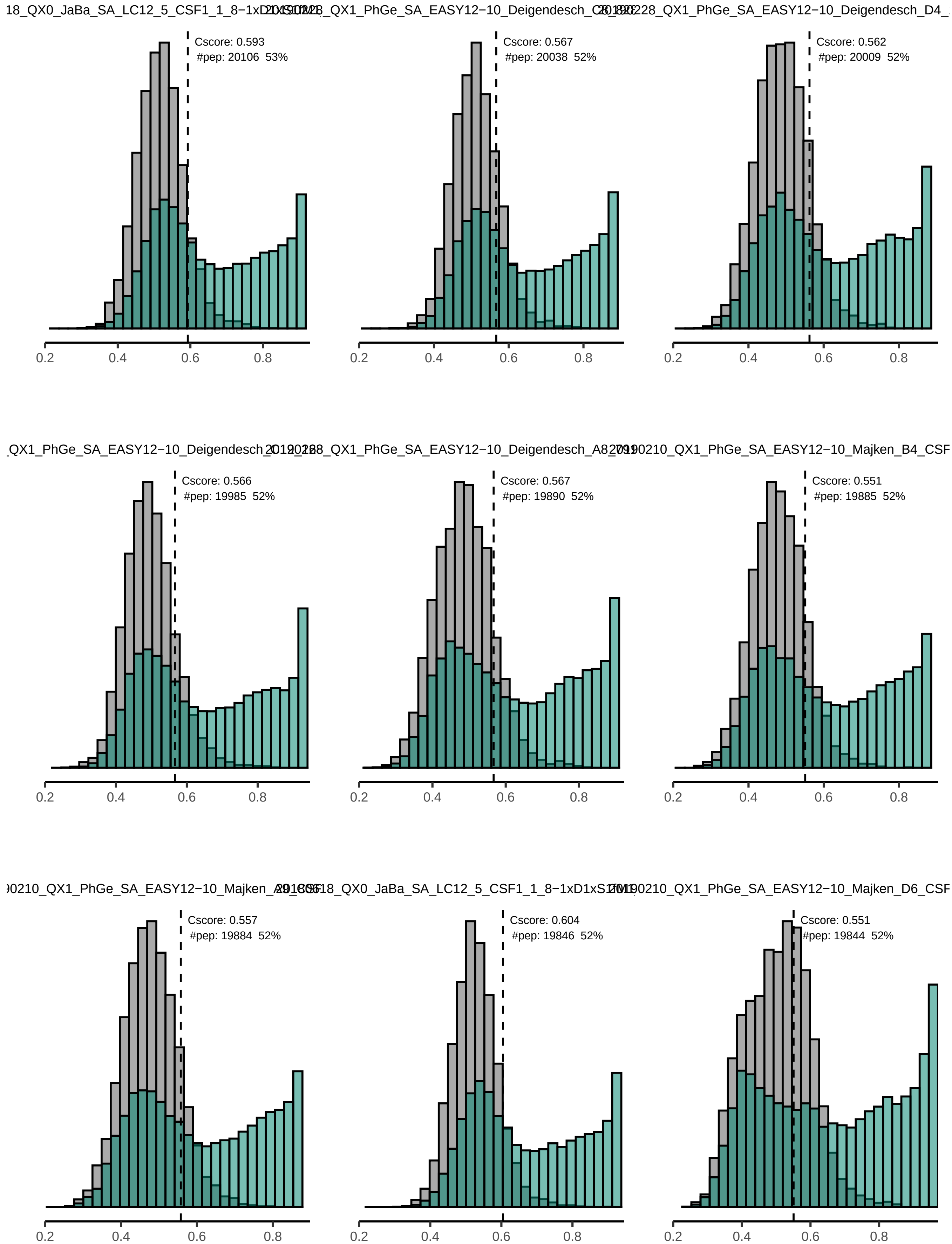
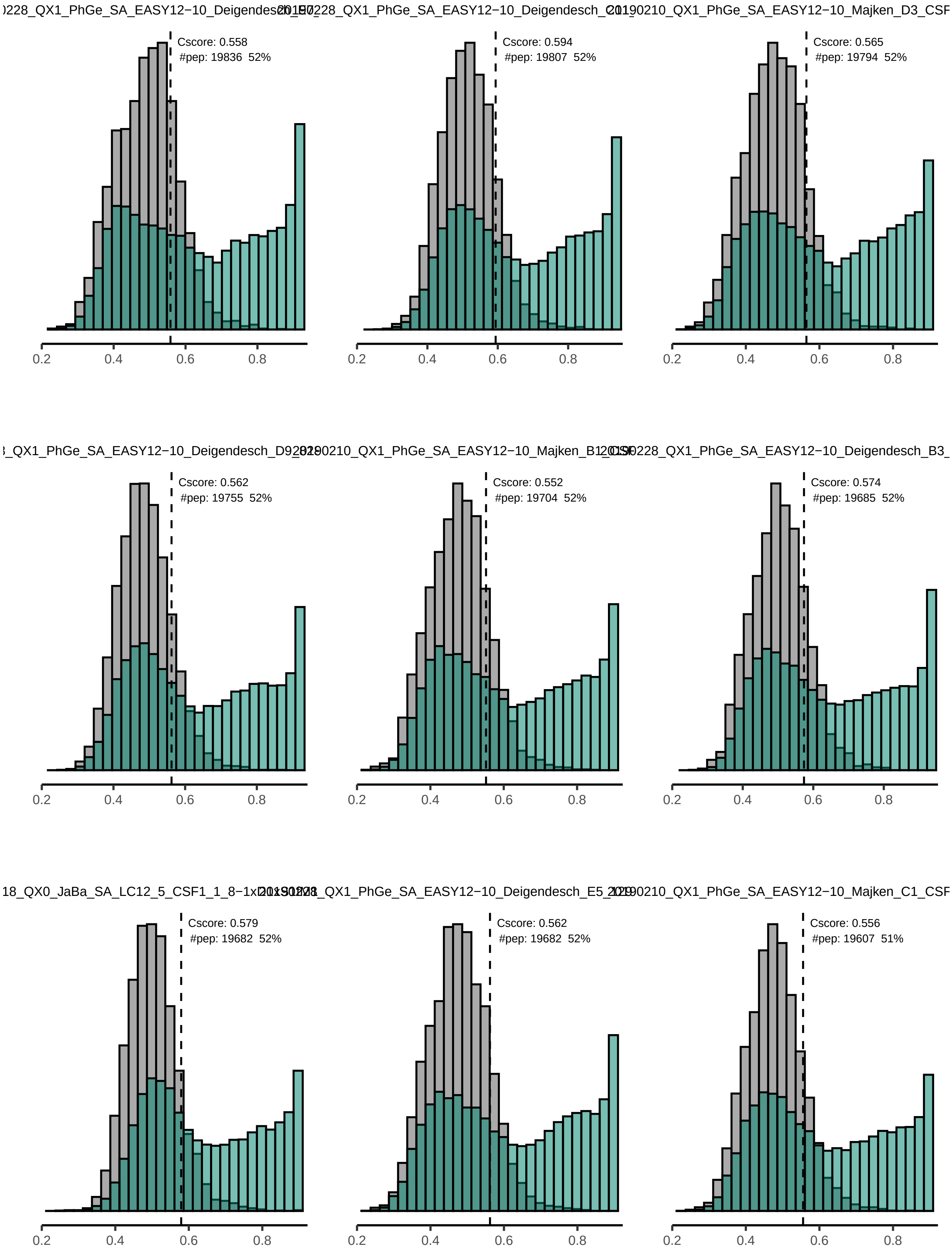
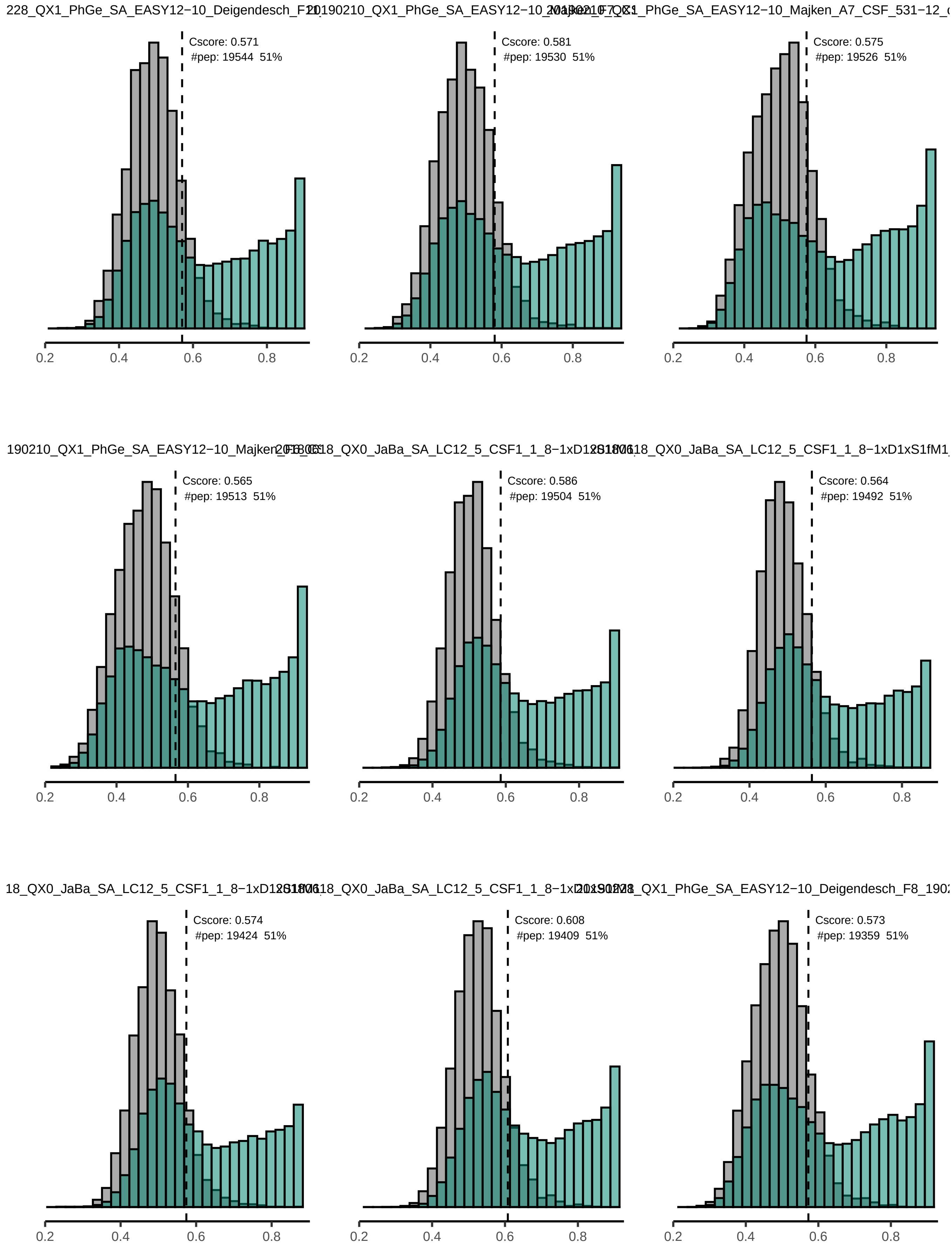
#pep: 20198 53%
Cscore: 0.572
#pep: 20195 53%
Cscore: 0.567
#pep: 20189 53%
Cscore: 0.561
#pep: 20185 53%
Cscore: 0.572
#pep: 20185 53%
Cscore: 0.589
#pep: 20149 53%
Cscore: 0.571
#pep: 20145 53%
Cscore: 0.584
#pep: 20144 53%
0.2
0.4
0.6
0.8



Cscore: 0.593
#pep: 20106 53%
Cscore: 0.567
#pep: 20038 52%
Cscore: 0.562
#pep: 20009 52%
Cscore: 0.566
#pep: 19985 52%
Cscore: 0.567
#pep: 19890 52%
Cscore: 0.551
#pep: 19885 52%
Cscore: 0.557
#pep: 19884 52%
Cscore: 0.604
#pep: 19846 52%
Cscore: 0.551
#pep: 19844 52%


Cscore: 0.558
#pep: 19836 52%
Cscore: 0.594
#pep: 19807 52%
Cscore: 0.565
#pep: 19794 52%
Cscore: 0.562
#pep: 19755 52%
Cscore: 0.552
#pep: 19704 52%
Cscore: 0.574
#pep: 19685 52%
Cscore: 0.579
#pep: 19682 52%
Cscore: 0.562
#pep: 19682 52%
Cscore: 0.556
#pep: 19607 51%


228_QX1_PhGe_SA_EASY12−10_Deigendesch_F11
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20190210_QX1_PhGe_SA_EASY12−10_Majken_A7_CSF_531−12_c
Cscore: 0.571
#pep: 19544 51%
Cscore: 0.581
#pep: 19530 51%
Cscore: 0.575
#pep: 19526 51%
190210_QX1_PhGe_SA_EASY12−10_Majken_F8_C1
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.565
#pep: 19513 51%
Cscore: 0.586
#pep: 19504 51%
Cscore: 0.564
#pep: 19492 51%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_F8_1902
Cscore: 0.574
#pep: 19424 51%
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#pep: 19409 51%
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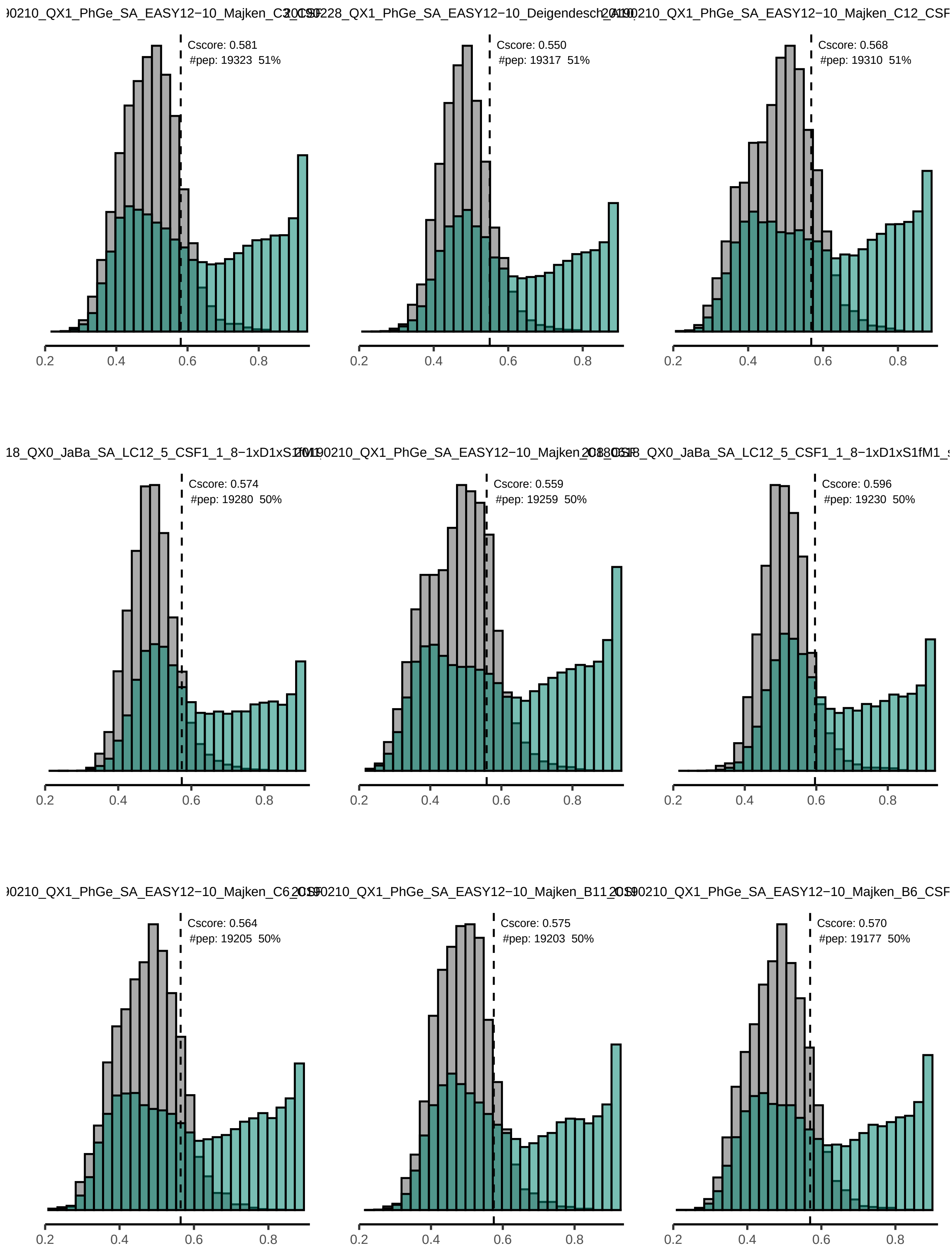
#pep: 19359 51%
0.2
0.4
0.6
0.8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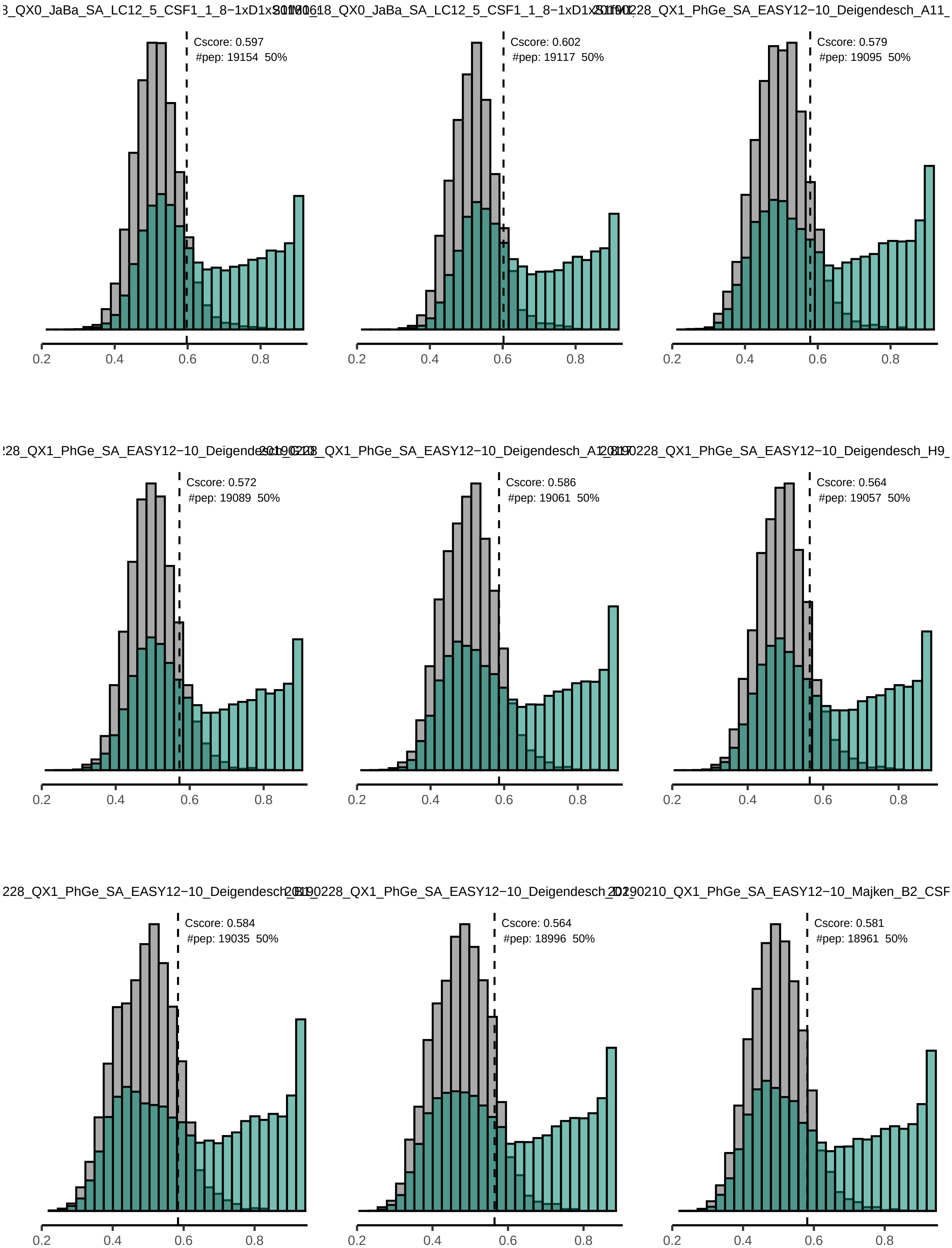
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_A10
Cscore: 0.550
#pep: 19317 51%
20190210_QX1_PhGe_SA_EASY12−10_Majken_C12_CSF
Cscore: 0.568
#pep: 19310 51%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
Cscore: 0.574
#pep: 19280 50%
20190210_QX1_PhGe_SA_EASY12−10_Majken_C8_CSF
Cscore: 0.559
#pep: 19259 50%
20180518_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_s
Cscore: 0.596
#pep: 19230 50%
)0210_QX1_PhGe_SA_EASY12−10_Majken_C6_CSF
Cscore: 0.564
#pep: 19205 50%
20190210_QX1_PhGe_SA_EASY12−10_Majken_B11_CSF
Cscore: 0.575
#pep: 19203 50%
20190210_QX1_PhGe_SA_EASY12−10_Majken_B6_CSF
Cscore: 0.570
#pep: 19177 50%
0.2
0.4
0.6
0.8


3_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1x201806_18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1x201902 20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_A11_
Cscore: 0.597
#pep: 19154 50%
Cscore: 0.602
#pep: 19117 50%
Cscore: 0.579
#pep: 19095 50%
0.2
0.4
0.6
0.8
'28_QX1_PhGe_SA_EASY12−10_Deigendesch 20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_A12 20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_H9_
Cscore: 0.572
#pep: 19089 50%
Cscore: 0.586
#pep: 19061 50%
Cscore: 0.564
#pep: 19057 50%
228_QX1_PhGe_SA_EASY12−10_Deigendesch_B 20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_D 20190210_QX1_PhGe_SA_EASY12−10_Majken_B2_CSF
Cscore: 0.584
#pep: 19035 50%
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#pep: 18996 50%
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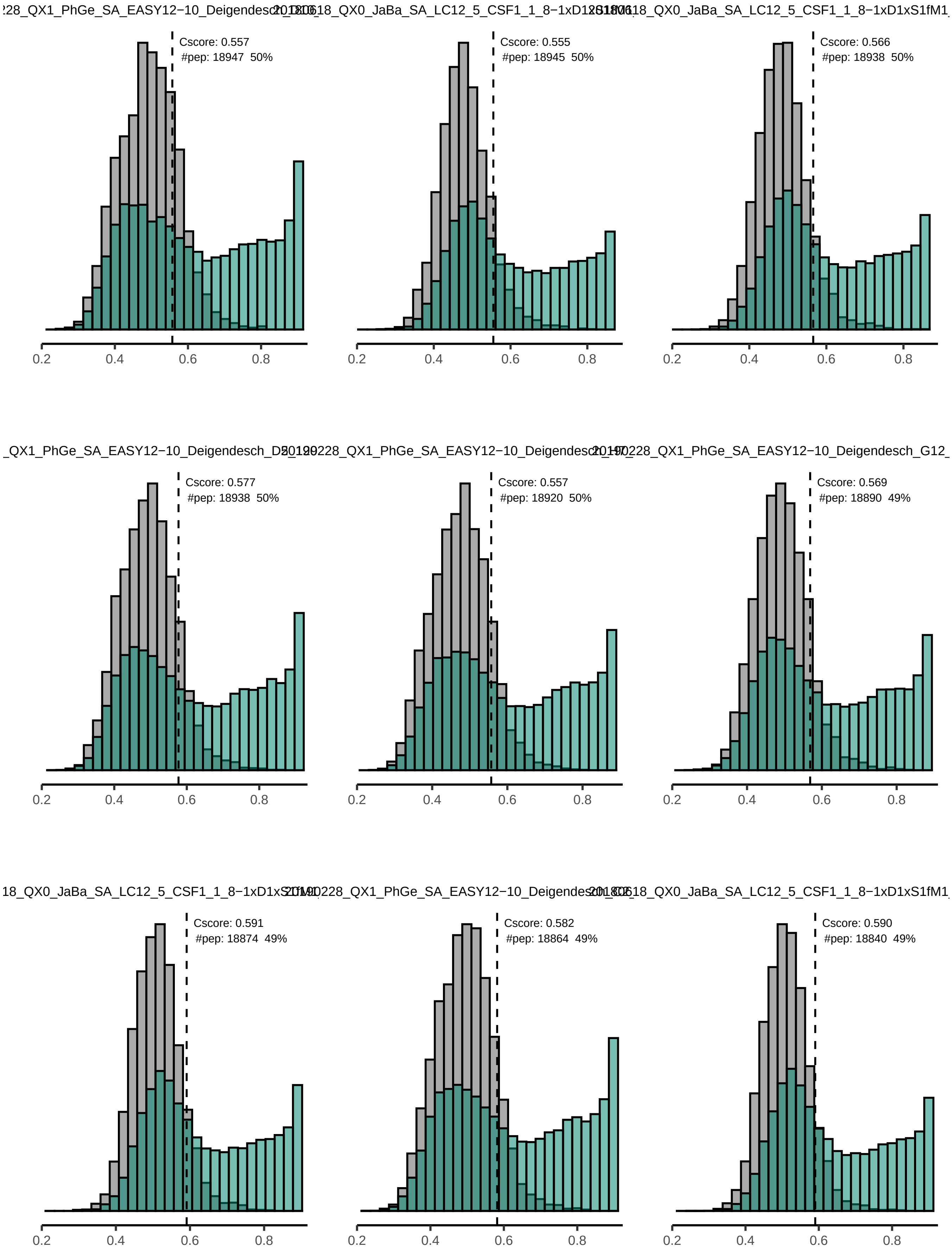
#pep: 18961 50%


Cscore: 0.557
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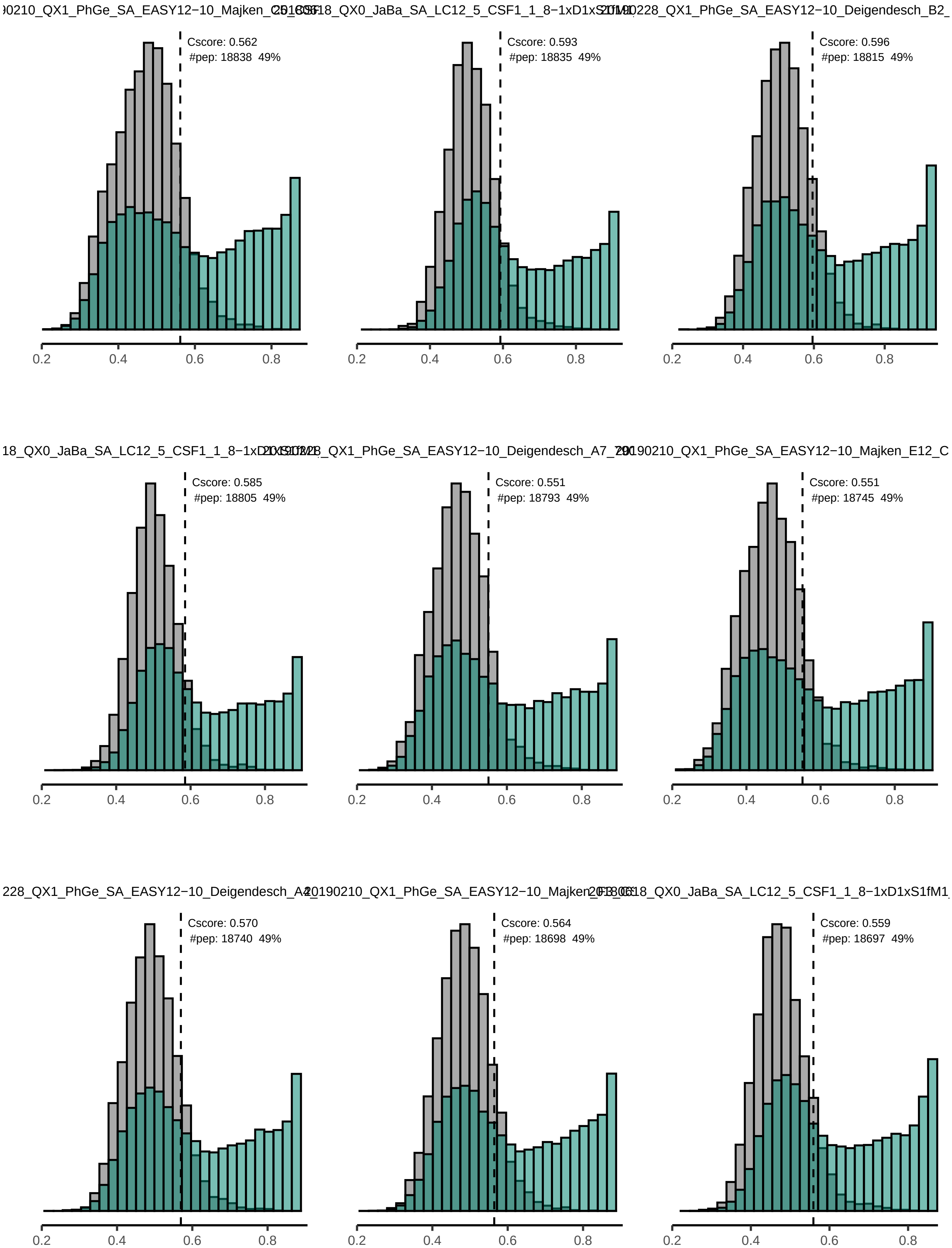
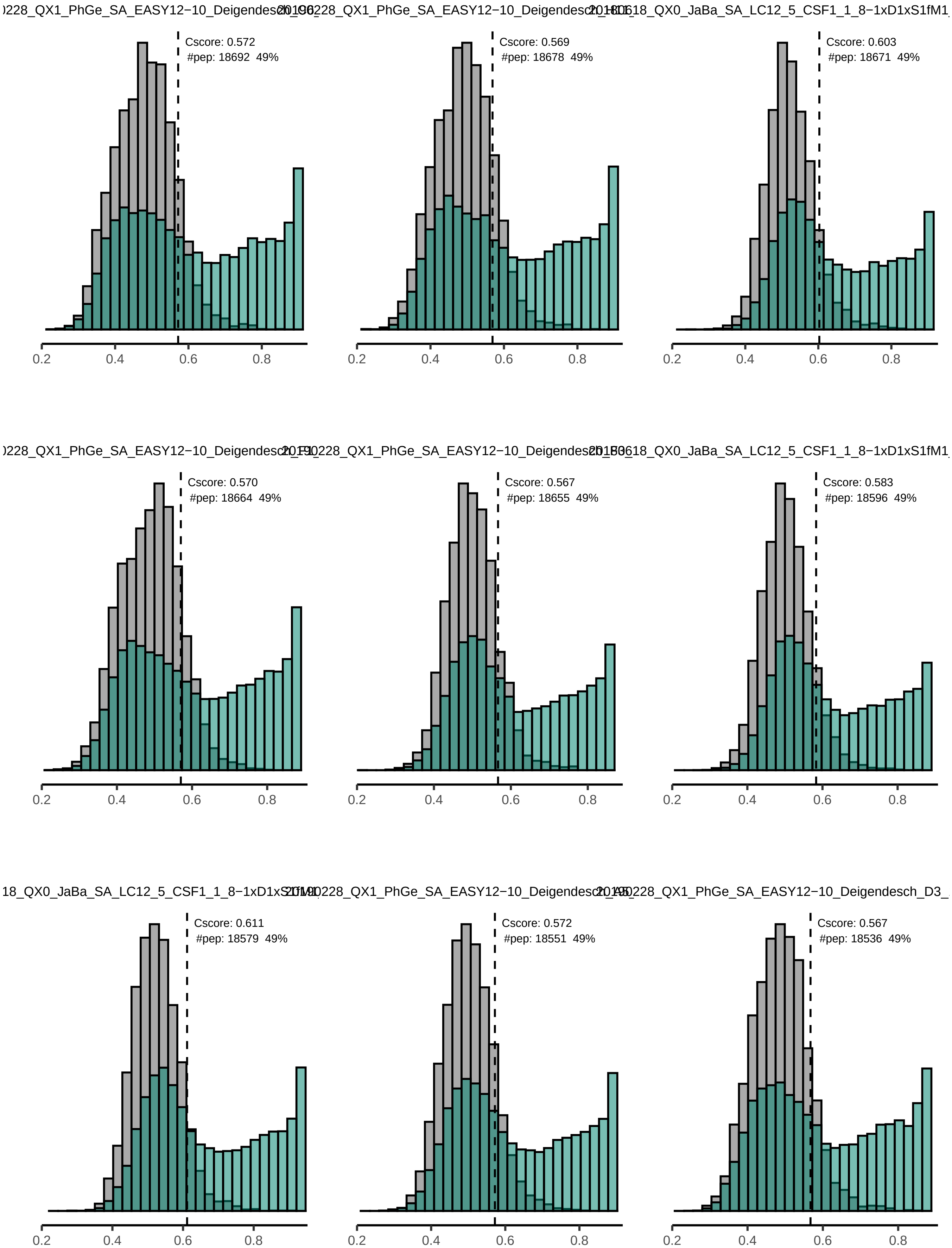
Cscore: 0.555
#pep: 18945 50%
Cscore: 0.566
#pep: 18938 50%
Cscore: 0.577
#pep: 18938 50%
Cscore: 0.557
#pep: 18920 50%
Cscore: 0.569
#pep: 18890 49%
Cscore: 0.591
#pep: 18874 49%
Cscore: 0.582
#pep: 18864 49%
Cscore: 0.590
#pep: 18840 49%
0.2
0.4
0.6
0.8


Cscore: 0.562
#pep: 18838 49%
Cscore: 0.593
#pep: 18835 49%
Cscore: 0.596
#pep: 18815 49%
Cscore: 0.585
#pep: 18805 49%
Cscore: 0.551
#pep: 18793 49%
Cscore: 0.551
#pep: 18745 49%
Cscore: 0.570
#pep: 18740 49%
Cscore: 0.564
#pep: 18698 49%
Cscore: 0.559
#pep: 18697 49%
0.2
0.4
0.6
0.8



)228_QX1_PhGe_SA_EASY12−10_Deigendesch_D6
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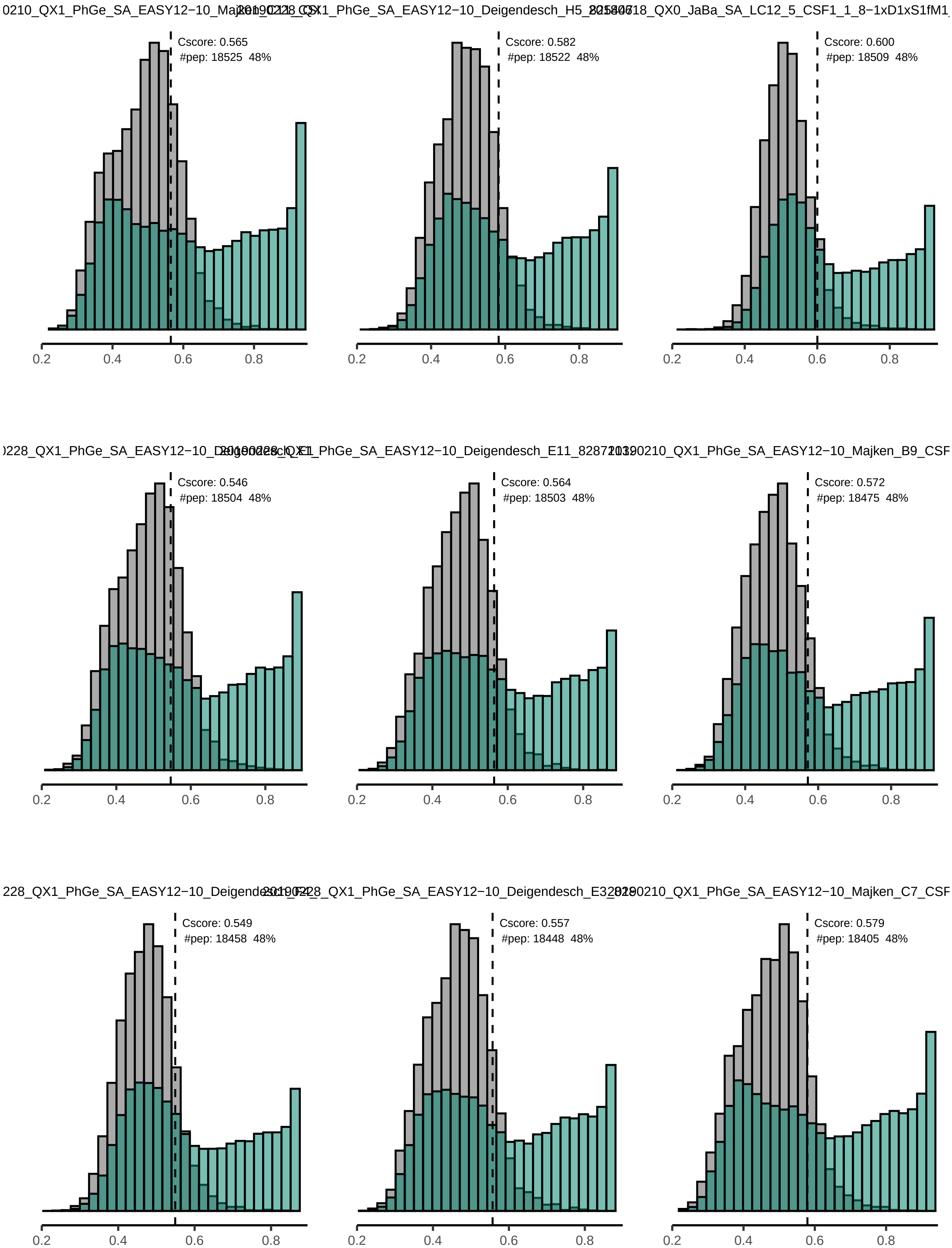
Cscore: 0.572
#pep: 18692 49%
Cscore: 0.569
#pep: 18678 49%
Cscore: 0.603
#pep: 18671 49%
)228_QX1_PhGe_SA_EASY12−10_Deigendesch_F1
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_B6
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.570
#pep: 18664 49%
Cscore: 0.567
#pep: 18655 49%
Cscore: 0.583
#pep: 18596 49%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_A5
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_D3_
Cscore: 0.611
#pep: 18579 49%
Cscore: 0.572
#pep: 18551 49%
Cscore: 0.567
#pep: 18536 49%
0.2
0.4
0.6
0.8


Cscore: 0.565
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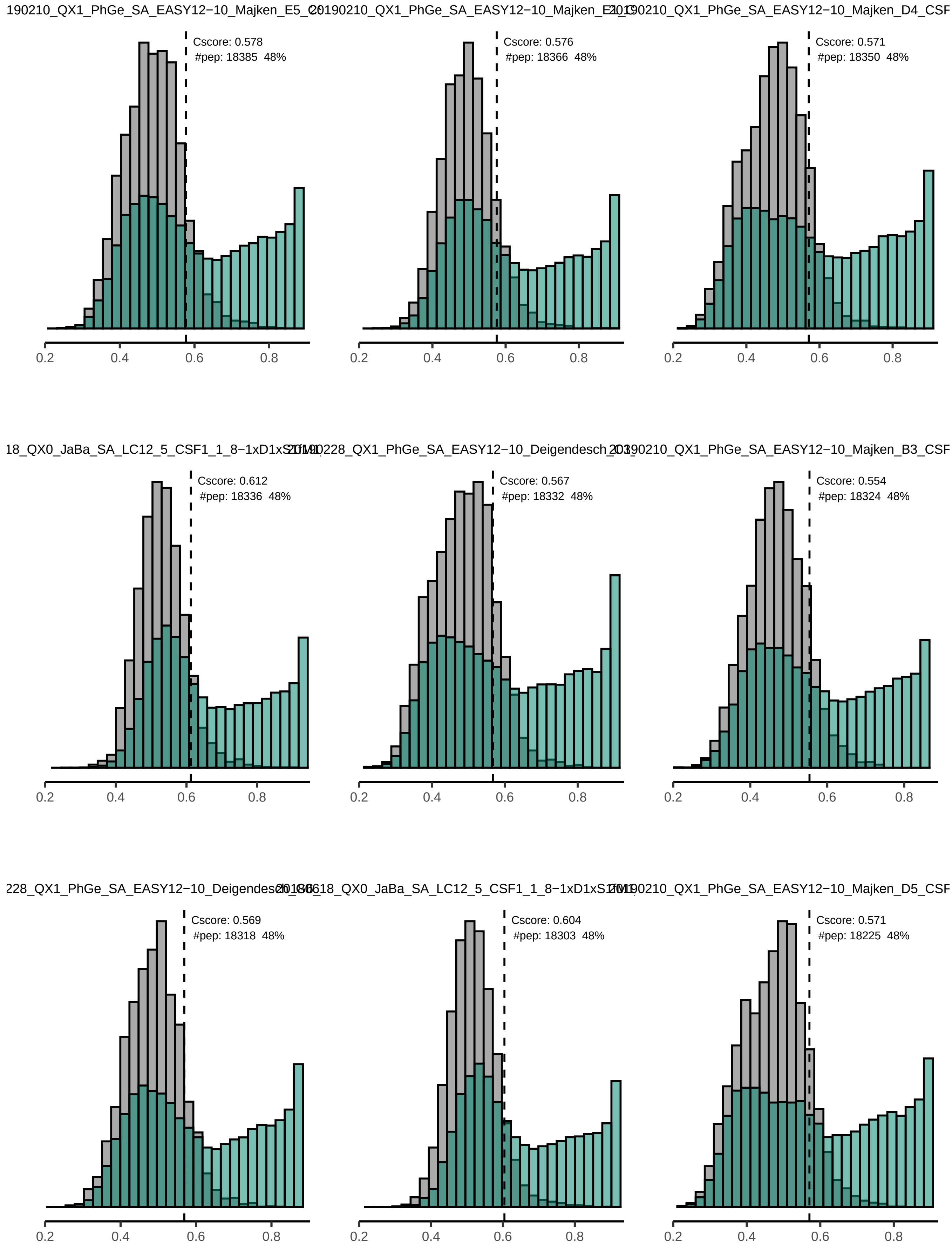
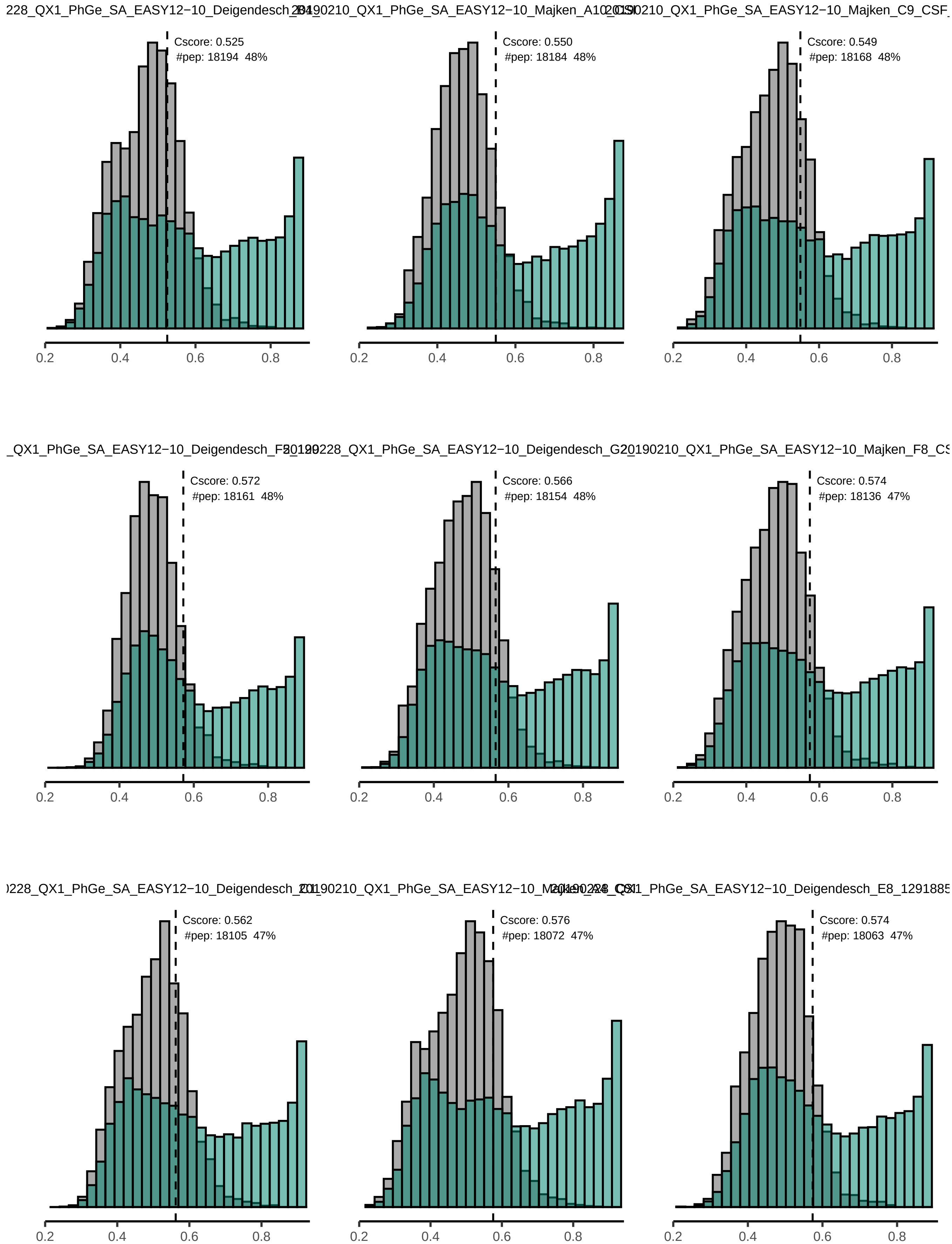
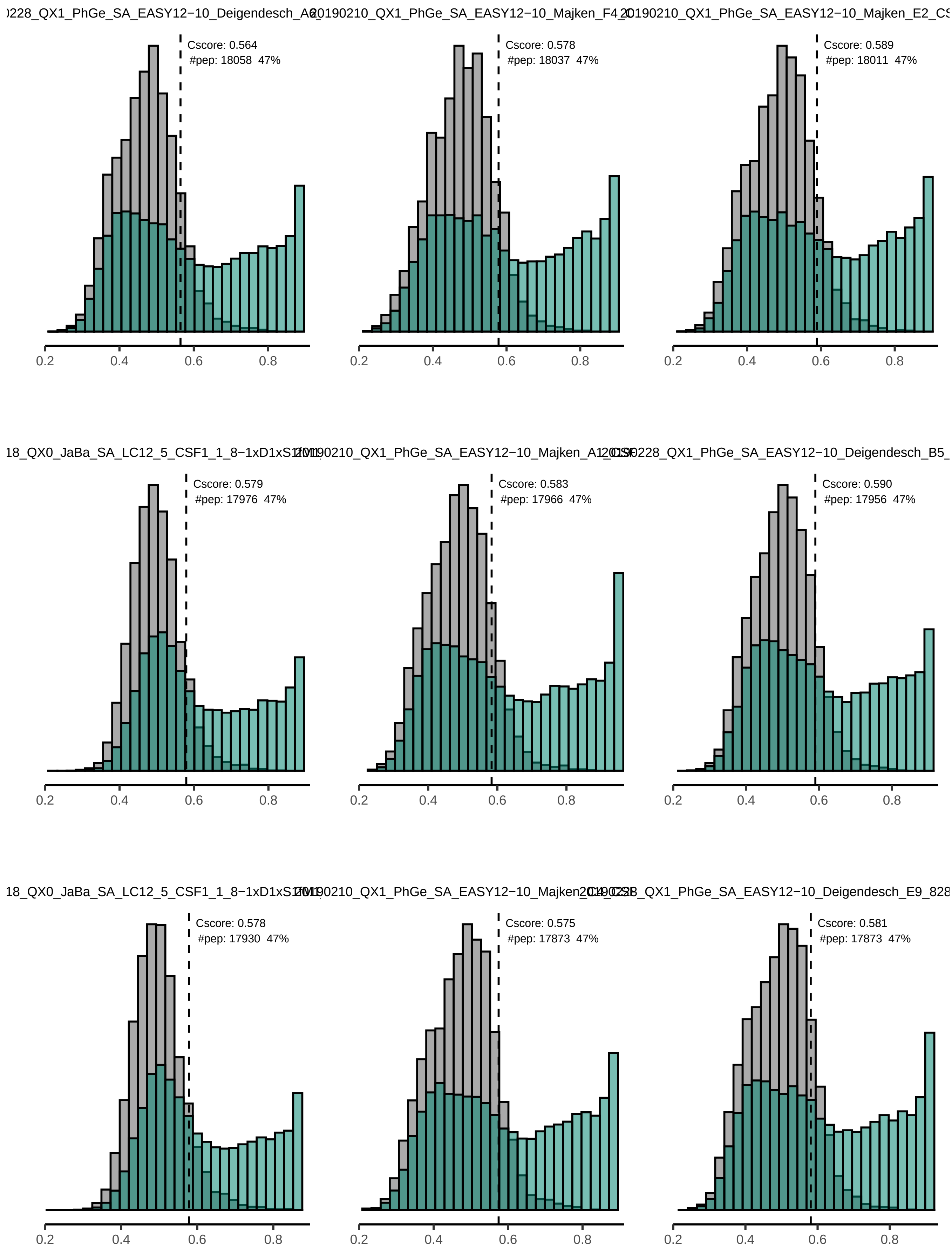
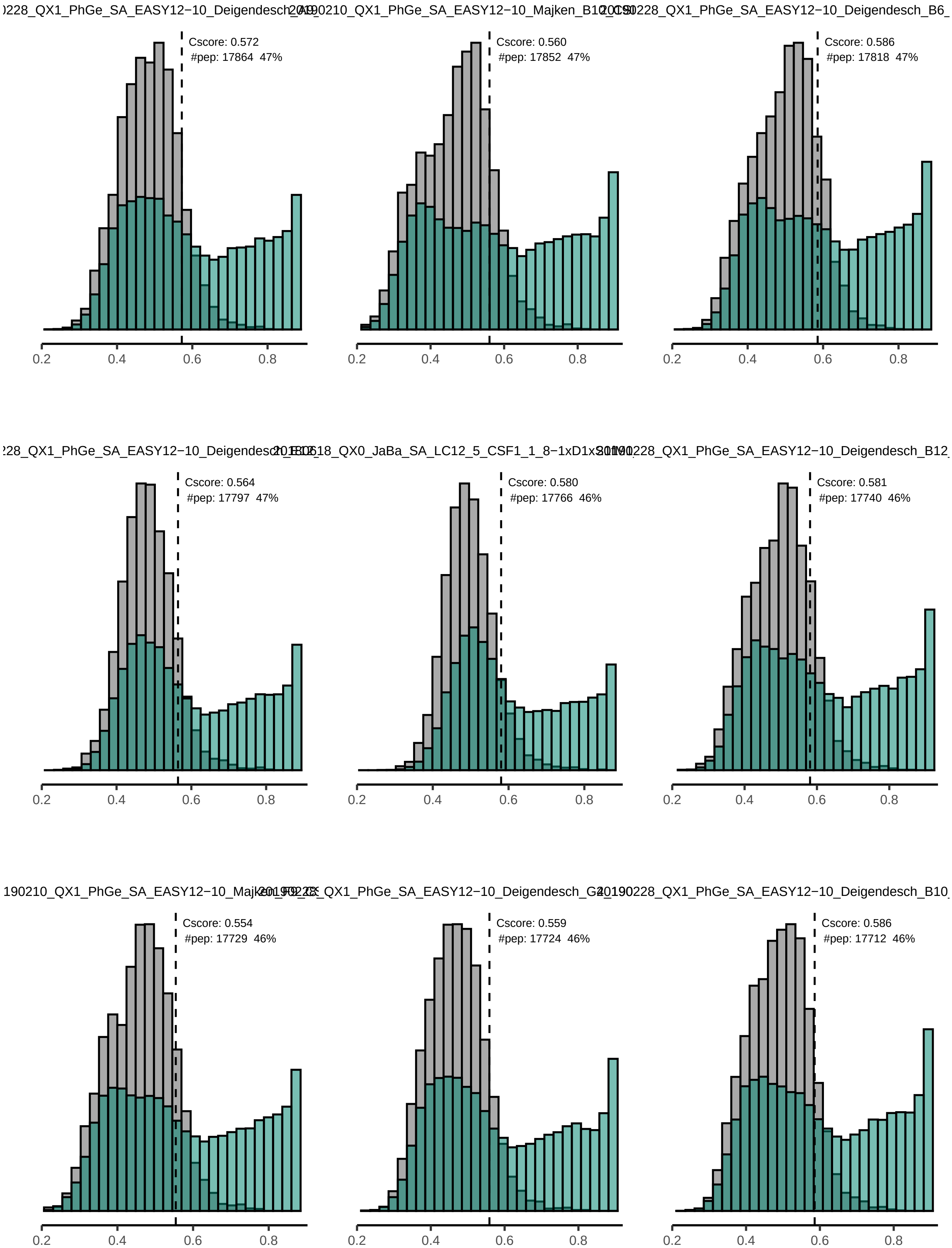
Cscore: 0.582
#pep: 18522 48%
Cscore: 0.600
#pep: 18509 48%
Cscore: 0.546
#pep: 18504 48%
Cscore: 0.564
#pep: 18503 48%
Cscore: 0.572
#pep: 18475 48%
Cscore: 0.549
#pep: 18458 48%
Cscore: 0.557
#pep: 18448 48%
Cscore: 0.579
#pep: 18405 48%
0.2
0.4
0.6
0.8

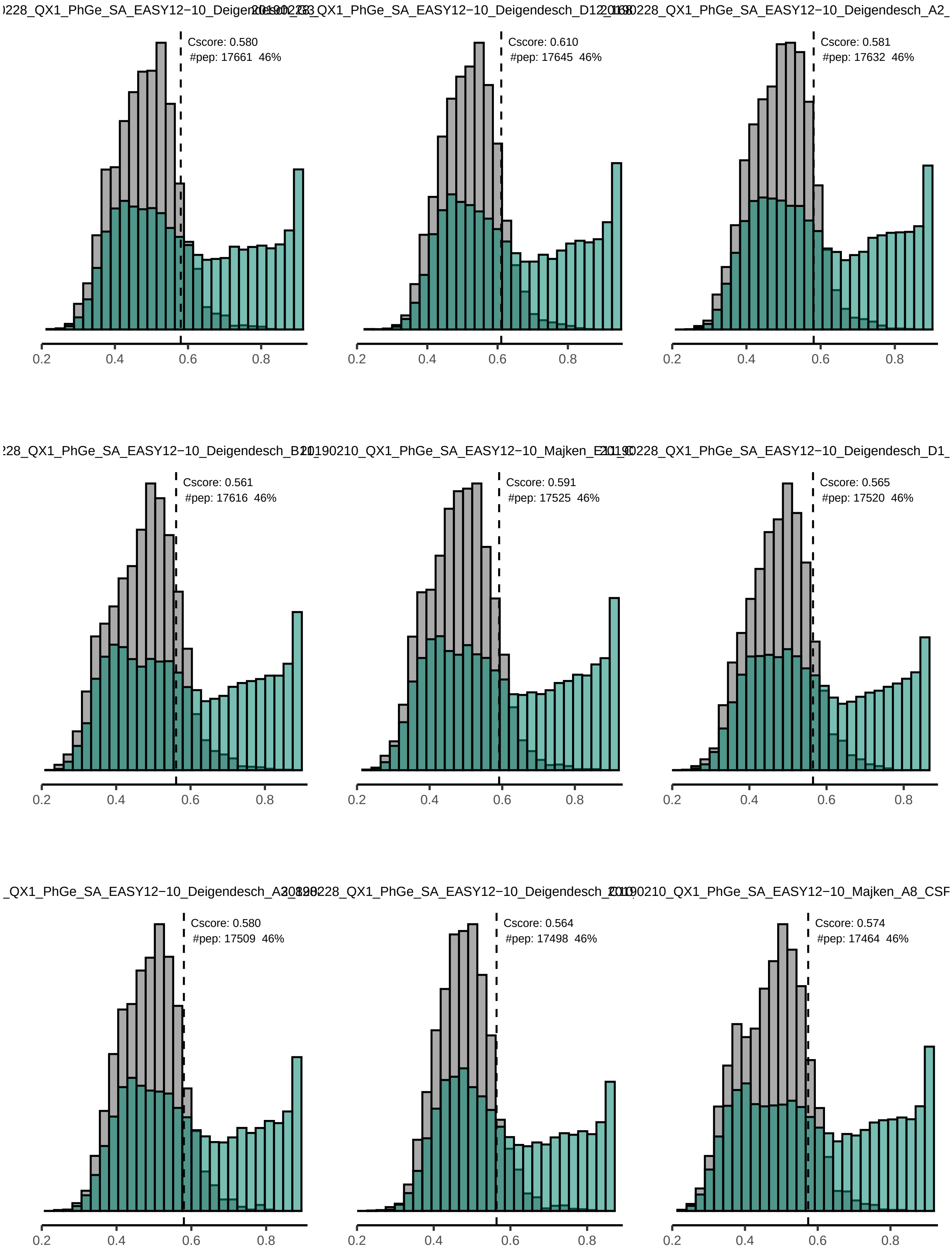

190210_QX1_PhGe_SA_EASY12−10_Majken_E5_C
Cscore: 0.578
#pep: 18385 48%
20190210_QX1_PhGe_SA_EASY12−10_Majken_E1_C
Cscore: 0.576
#pep: 18366 48%
20190210_QX1_PhGe_SA_EASY12−10_Majken_D4_CSF
Cscore: 0.571
#pep: 18350 48%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1M1
Cscore: 0.612
#pep: 18336 48%
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_03
Cscore: 0.567
#pep: 18332 48%
20190210_QX1_PhGe_SA_EASY12−10_Majken_B3_CSF
Cscore: 0.554
#pep: 18324 48%
228_QX1_PhGe_SA_EASY12−10_Deigendesch_06
Cscore: 0.569
#pep: 18318 48%
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1M1
Cscore: 0.604
#pep: 18303 48%
20190210_QX1_PhGe_SA_EASY12−10_Majken_D5_CSF
Cscore: 0.571
#pep: 18225 48%
0.2
0.4
0.6
0.8


Cscore: 0.525
#pep: 18194 48%
Cscore: 0.550
#pep: 18184 48%
Cscore: 0.549
#pep: 18168 48%
Cscore: 0.572
#pep: 18161 48%
Cscore: 0.566
#pep: 18154 48%
Cscore: 0.574
#pep: 18136 47%
Cscore: 0.562
#pep: 18105 47%
Cscore: 0.576
#pep: 18072 47%
Cscore: 0.574
#pep: 18063 47%
0.2
0.4
0.6
0.8

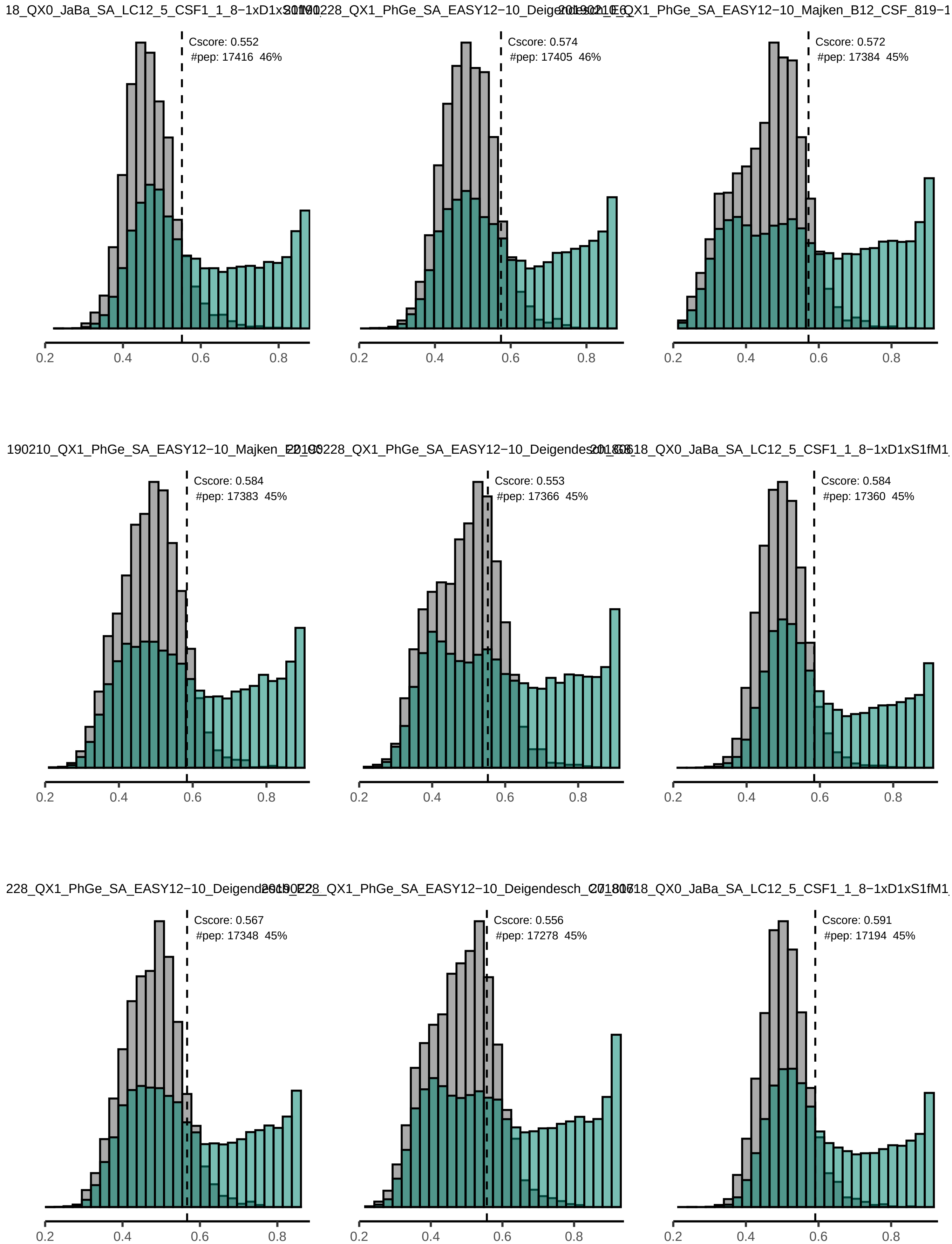

)228_QX1_PhGe_SA_EASY12−10_Deigendesch_A6
20190210_QX1_PhGe_SA_EASY12−10_Majken_F4_
20190210_QX1_PhGe_SA_EASY12−10_Majken_E2_CS
Cscore: 0.564
#pep: 18058 47%
Cscore: 0.578
#pep: 18037 47%
Cscore: 0.589
#pep: 18011 47%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20190210_QX1_PhGe_SA_EASY12−10_Majken_A12_CS
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_B5_
Cscore: 0.579
#pep: 17976 47%
Cscore: 0.583
#pep: 17966 47%
Cscore: 0.590
#pep: 17956 47%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20190210_QX1_PhGe_SA_EASY12−10_Majken_C4_CS
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_E9_828
Cscore: 0.578
#pep: 17930 47%
Cscore: 0.575
#pep: 17873 47%
Cscore: 0.581
#pep: 17873 47%
0.2
0.4
0.6
0.8

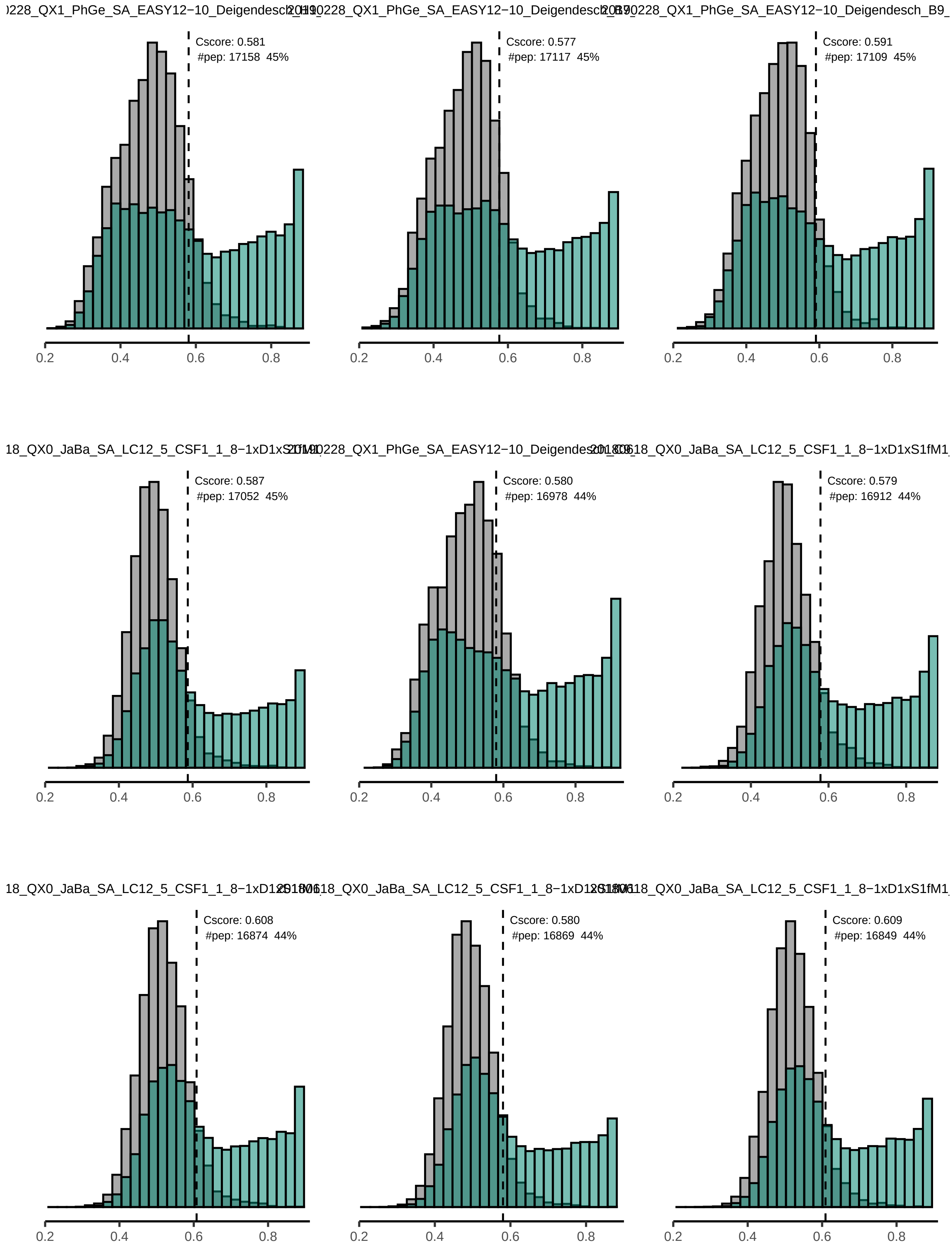


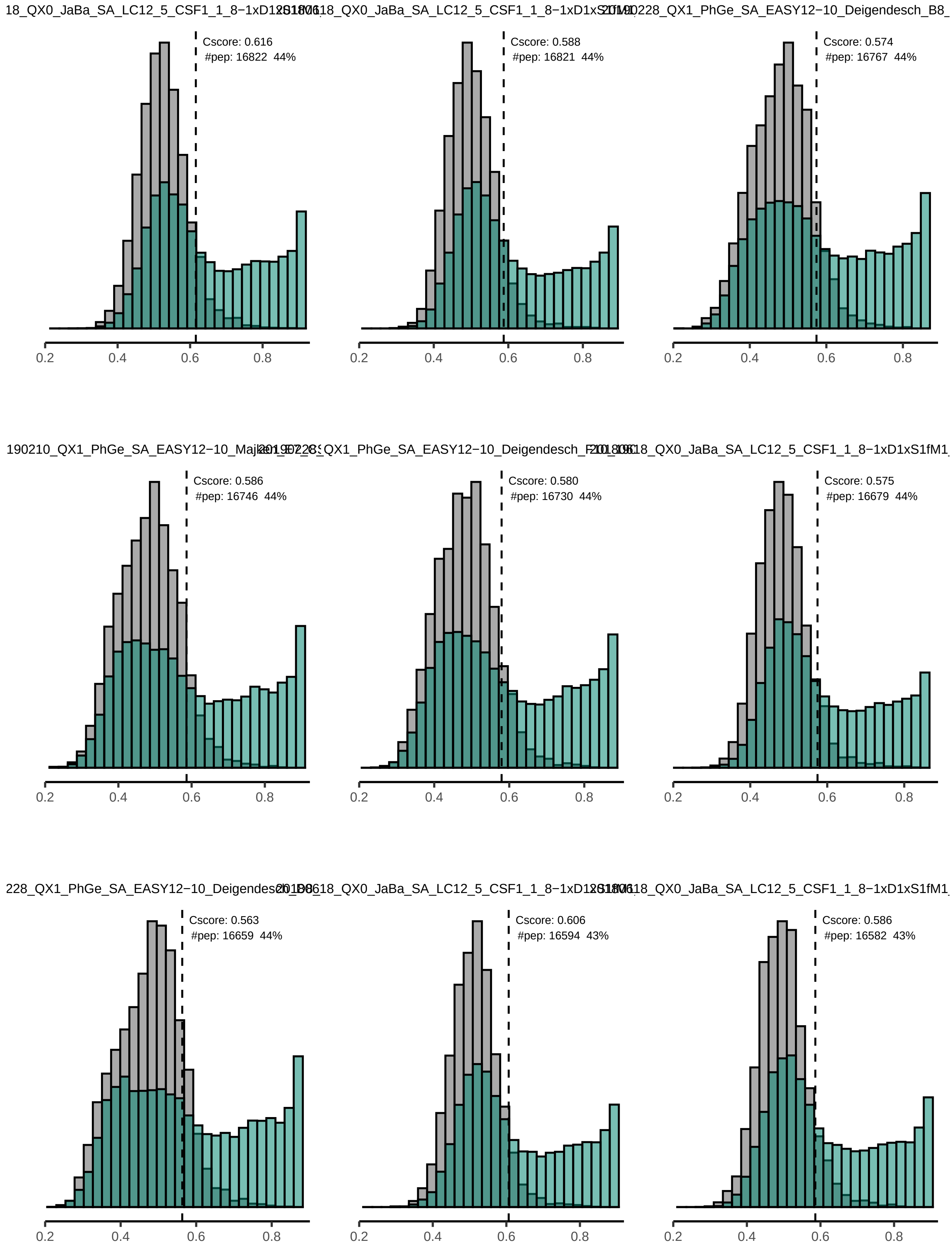
Cscore: 0.572
#pep: 17864 47%
Cscore: 0.560
#pep: 17852 47%
Cscore: 0.586
#pep: 17818 47%
Cscore: 0.564
#pep: 17797 47%
Cscore: 0.580
#pep: 17766 46%
Cscore: 0.581
#pep: 17740 46%
Cscore: 0.554
#pep: 17729 46%
Cscore: 0.559
#pep: 17724 46%
Cscore: 0.586
#pep: 17712 46%
0.2
0.4
0.6
0.8



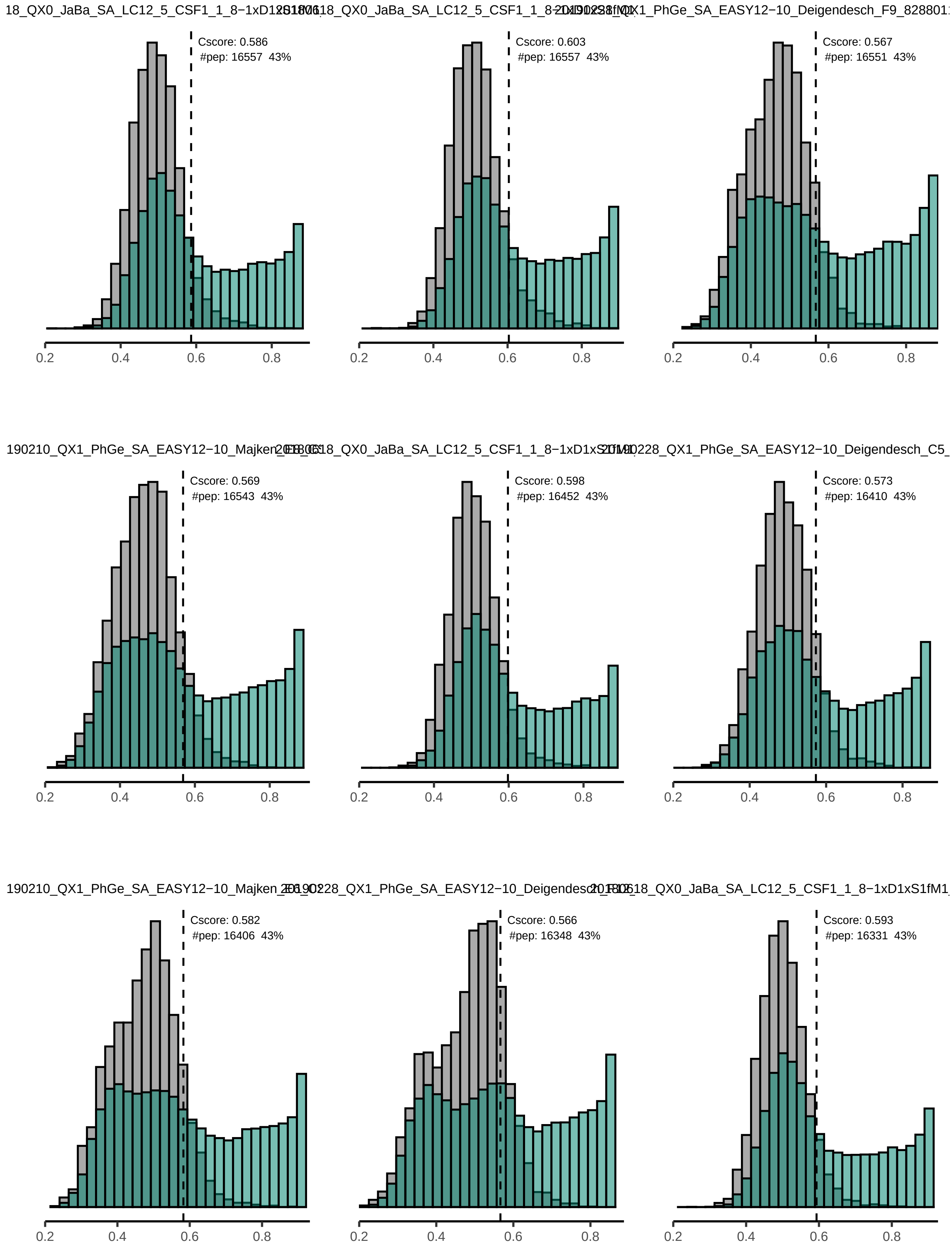
Cscore: 0.580
#pep: 17661 46%
Cscore: 0.610
#pep: 17645 46%
Cscore: 0.581
#pep: 17632 46%
Cscore: 0.561
#pep: 17616 46%
Cscore: 0.591
#pep: 17525 46%
Cscore: 0.565
#pep: 17520 46%
Cscore: 0.580
#pep: 17509 46%
Cscore: 0.564
#pep: 17498 46%
Cscore: 0.574
#pep: 17464 46%
0.2
0.4
0.6
0.8


18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS20190228_QX1_PhGe_SA_EASY12−10_Deige20190210_QX1_PhGe_SA_EASY12−10_Majken_B12_CSF_819−1
Cscore: 0.552
#pep: 17416 46%
Cscore: 0.574
#pep: 17405 46%
Cscore: 0.572
#pep: 17384 45%
0.2
0.4
0.6
0.8
190210_QX1_PhGe_SA_EASY12−10_Majken_B20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.584
#pep: 17383 45%
Cscore: 0.553
#pep: 17366 45%
Cscore: 0.584
#pep: 17360 45%
228_QX1_PhGe_SA_EASY12−10_Deigendesch20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_C20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.567
#pep: 17348 45%
Cscore: 0.556
#pep: 17278 45%
Cscore: 0.591
#pep: 17194 45%

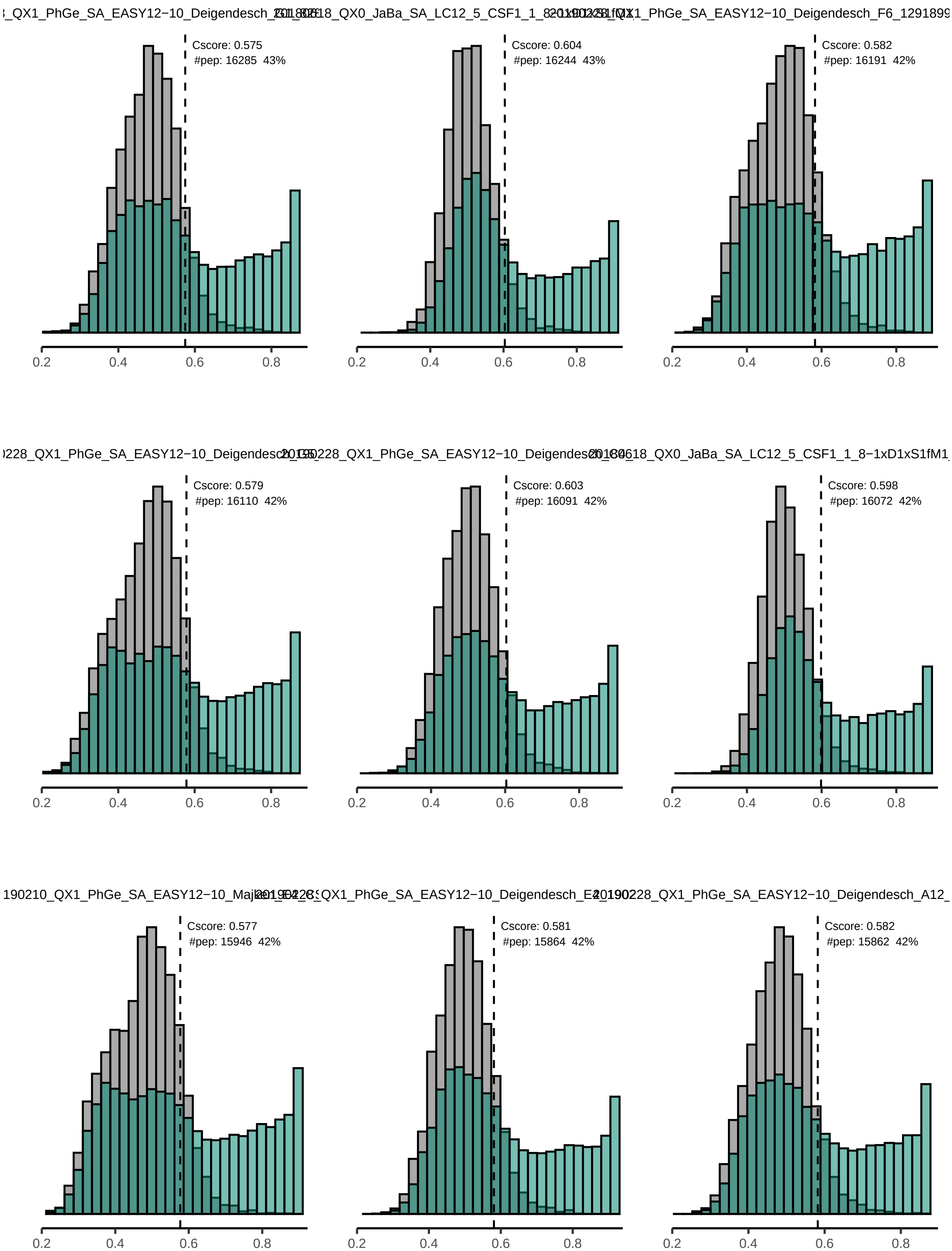

)228_QX1_PhGe_SA_EASY12−10_Deigendesch_H1
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_B9
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_B9_
Cscore: 0.581
#pep: 17158 45%
Cscore: 0.577
#pep: 17117 45%
Cscore: 0.591
#pep: 17109 45%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_C6
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.587
#pep: 17052 45%
Cscore: 0.580
#pep: 16978 44%
Cscore: 0.579
#pep: 16912 44%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
20180618_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1_
Cscore: 0.608
#pep: 16874 44%
Cscore: 0.580
#pep: 16869 44%
Cscore: 0.609
#pep: 16849 44%
0.2
0.4
0.6
0.8



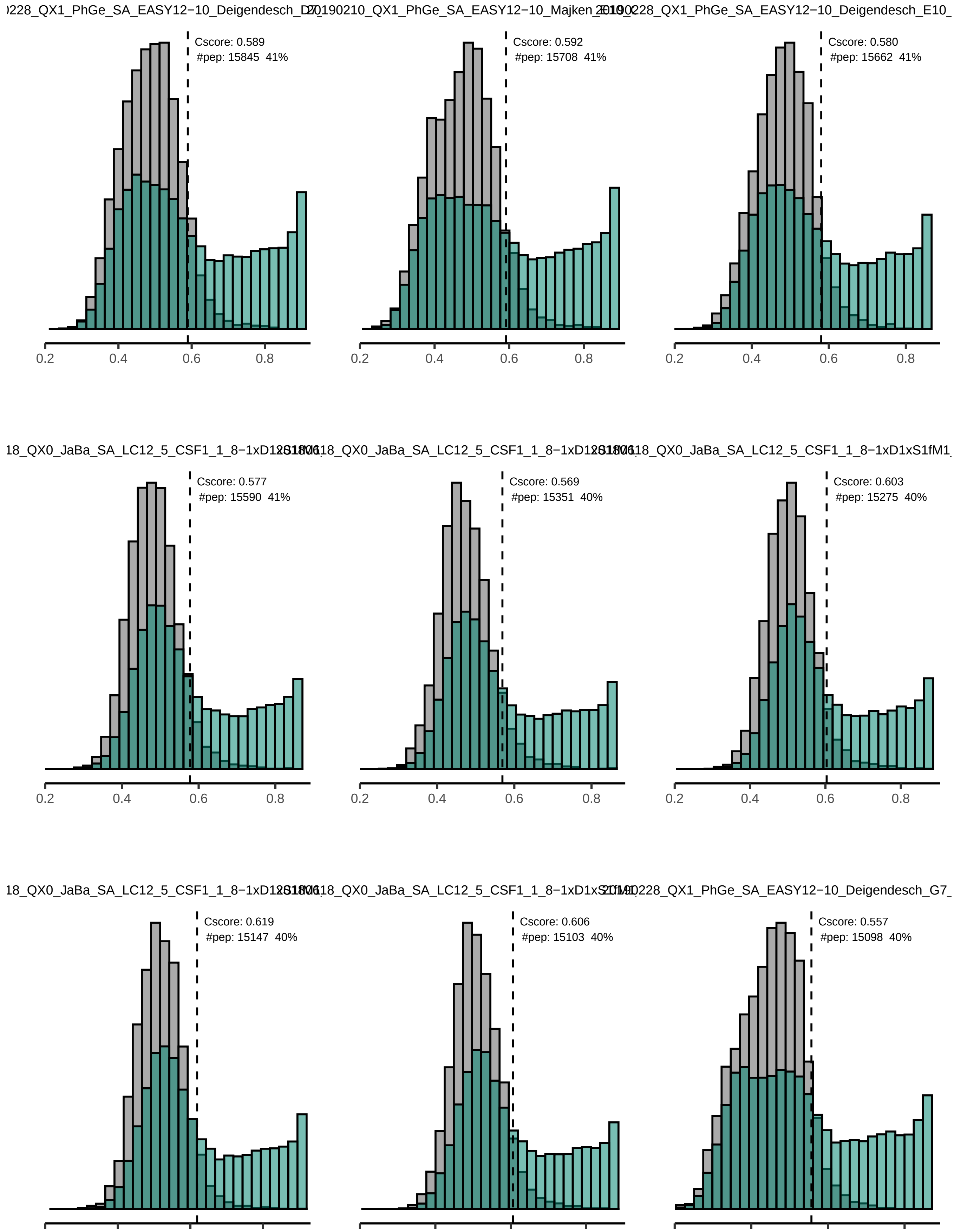
Cscore: 0.616
#pep: 16822 44%
Cscore: 0.588
#pep: 16821 44%
Cscore: 0.574
#pep: 16767 44%
Cscore: 0.586
#pep: 16746 44%
Cscore: 0.580
#pep: 16730 44%
Cscore: 0.575
#pep: 16679 44%
Cscore: 0.563
#pep: 16659 44%
Cscore: 0.606
#pep: 16594 43%
Cscore: 0.586
#pep: 16582 43%
0.2
0.4
0.6
0.8



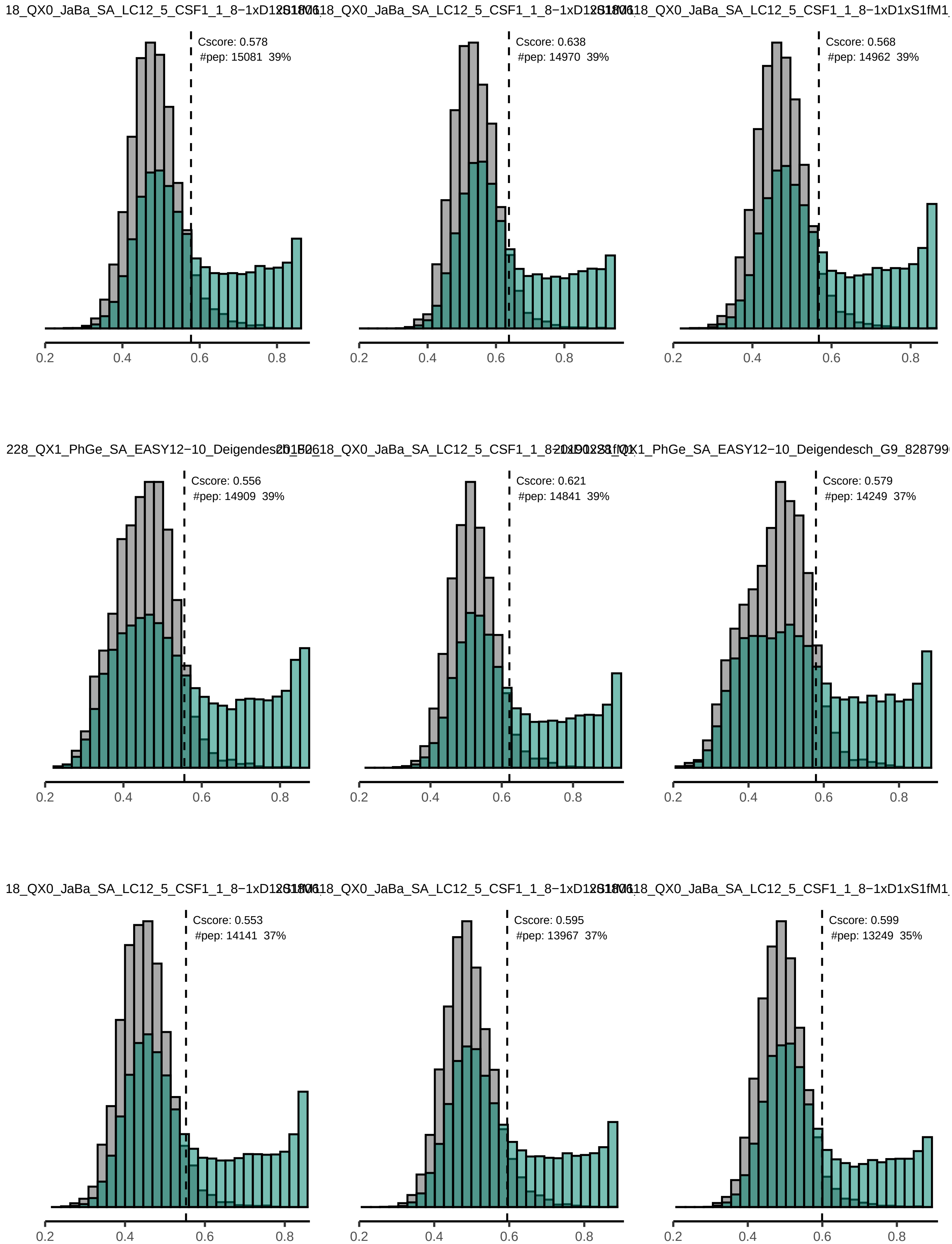
Cscore: 0.586
#pep: 16557 43%
Cscore: 0.603
#pep: 16557 43%
Cscore: 0.567
#pep: 16551 43%
Cscore: 0.569
#pep: 16543 43%
Cscore: 0.598
#pep: 16452 43%
Cscore: 0.573
#pep: 16410 43%
Cscore: 0.582
#pep: 16406 43%
Cscore: 0.566
#pep: 16348 43%
Cscore: 0.593
#pep: 16331 43%



Cscore: 0.575
#pep: 16285 43%
Cscore: 0.604
#pep: 16244 43%
Cscore: 0.582
#pep: 16191 42%
Cscore: 0.579
#pep: 16110 42%
Cscore: 0.603
#pep: 16091 42%
Cscore: 0.598
#pep: 16072 42%
Cscore: 0.577
#pep: 15946 42%
Cscore: 0.581
#pep: 15864 42%
Cscore: 0.582
#pep: 15862 42%



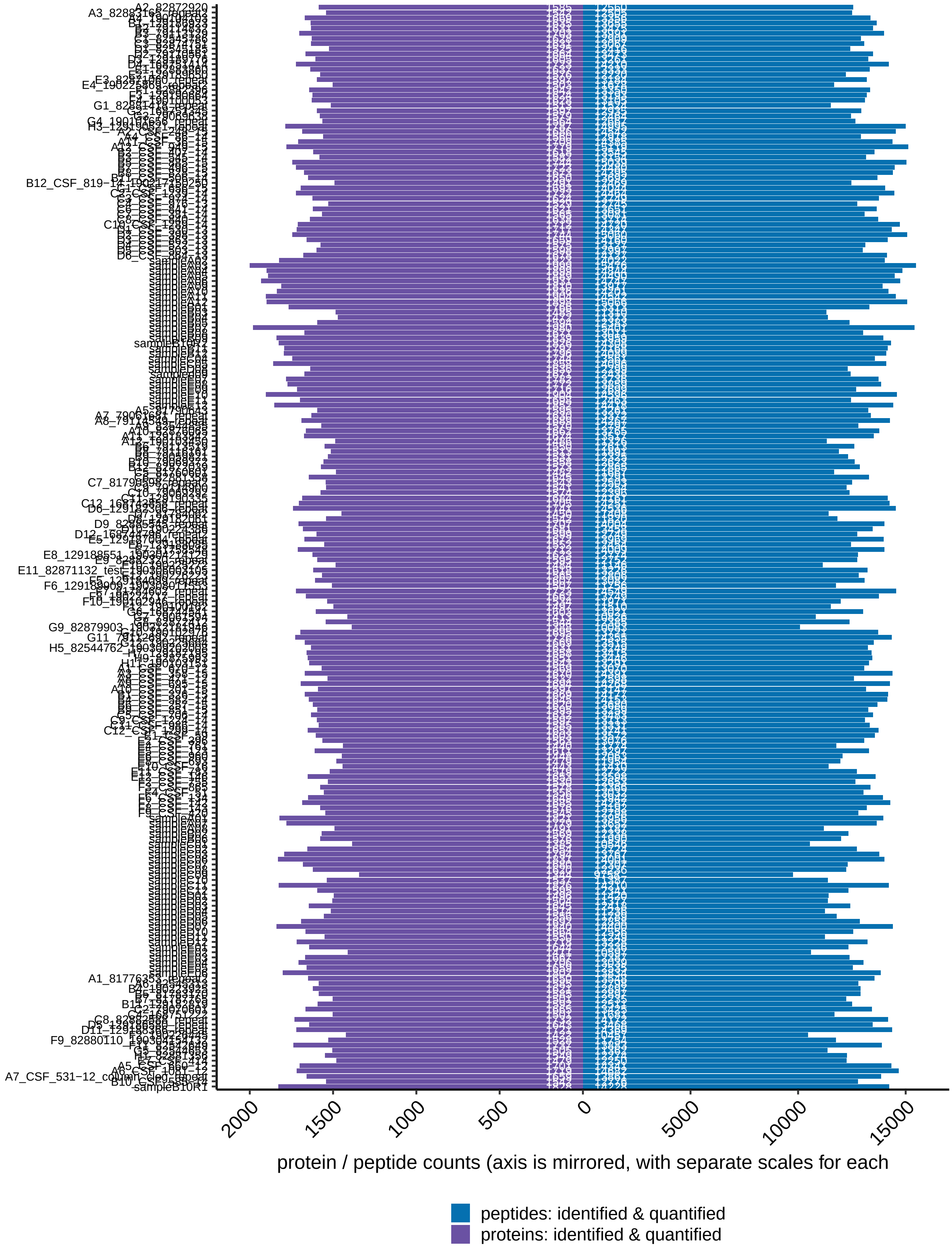
)228_QX1_PhGe_SA_EASY12−10_Deigendesch_D7
20190210_QX1_PhGe_SA_EASY12−10_Majken_E10
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_E10_
Cscore: 0.589
#pep: 15845 41%
Cscore: 0.592
#pep: 15708 41%
Cscore: 0.580
#pep: 15662 41%
18_QX0_JaBa_SA_LC12_5_CSF1_1_8−1xD1xS1fM1
Cscore: 0.577
#pep: 15590 41%
Cscore: 0.569
#pep: 15351 40%
Cscore: 0.603
#pep: 15275 40%
Cscore: 0.619
#pep: 15147 40%
Cscore: 0.606
#pep: 15103 40%
Cscore: 0.557
#pep: 15098 40%
20190228_QX1_PhGe_SA_EASY12−10_Deigendesch_G7_
0.2
0.4
0.6
0.8


Cscore: 0.578
#pep: 15081 39%
Cscore: 0.638
#pep: 14970 39%
Cscore: 0.568
#pep: 14962 39%
Cscore: 0.556
#pep: 14909 39%
Cscore: 0.621
#pep: 14841 39%
Cscore: 0.579
#pep: 14249 37%
Cscore: 0.553
#pep: 14141 37%
Cscore: 0.595
#pep: 13967 37%
Cscore: 0.599
#pep: 13249 35%
0.2
0.4
0.6
0.8

1.2 number of peptides and proteins

These plots show the number of (target) peptides that are 'detected' per sample. For DDA, 'detected' implies the peptide has a MS/MS identification. Peptides quantified through match-between-runs (MBR) are quantified but not detected/identified. In case of DDA, we also show the number of peptides quantified through MBR. For DIA, we refer to a peptide as 'detected' if the confidence score (for identification) is <= 0.01.

Samples in this plot are sorted by their experimental group, and then ordered and by their name within each group. This data is also available in the output table 'samples.xlsx'.

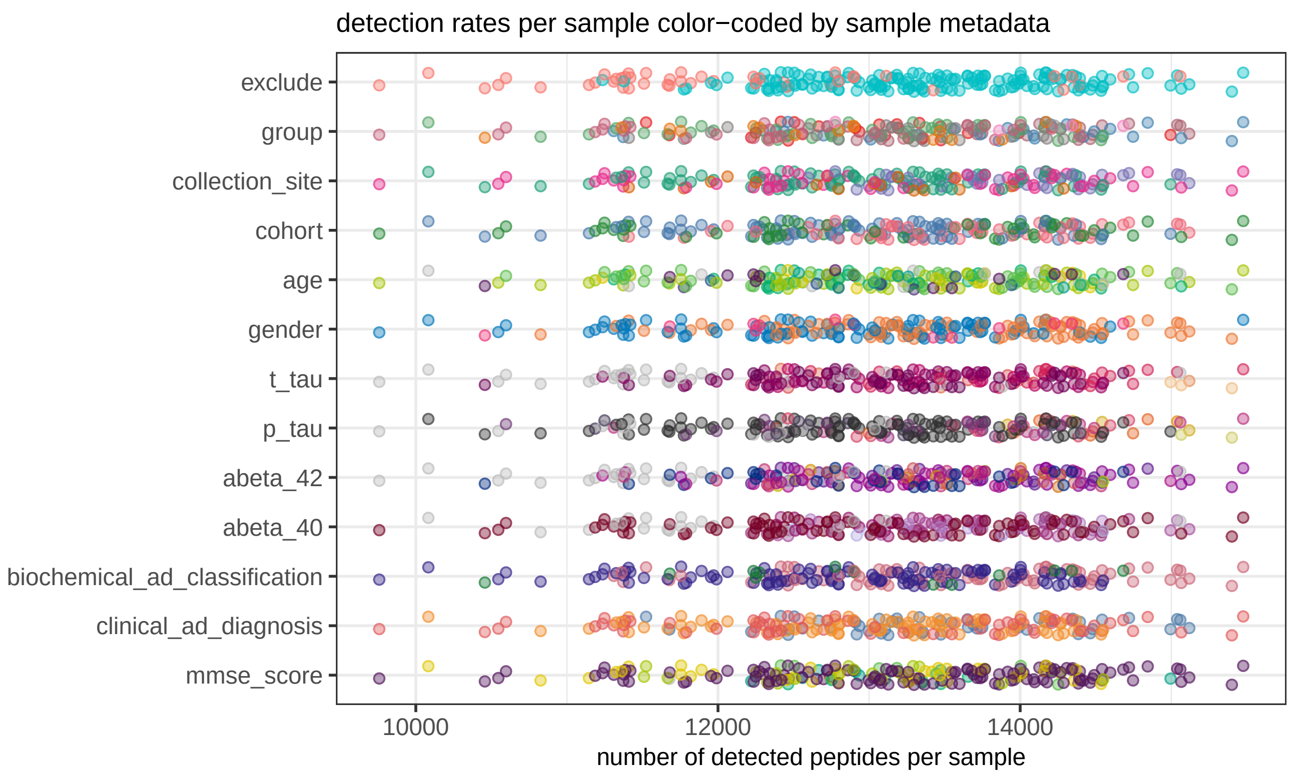

2000
1500
1000
500
0
5000
10000
15000
protein / peptide counts (axis is mirrored, with separate scales for each
peptides: identified & quantified
proteins: identified & quantified

1.2.1 color-coding sample metadata

The number of detected peptides in a sample, as compared to other samples within a dataset, can be used as a measure for sample quality. Color-coding individual samples for metadata that you provided as input (e.g. experiment batch, sample handling order, gel lanes, etc.) allows visual inspection as to whether these relate to the rate of successful peptide detection.

The figure below provides an overview of all sample metadata at a first glance. On each row all samples in the dataset are shown as a data point, each color-coded by the respective property shown on the y-axis (with minor vertical jitter for visual clarity). If any of these metadata coincide with a major effect on the number of detected peptides, this should become apparent by a clustering of samples by color-code. Hereafter, an additional set of figures will further expand this overview into detailed figures for each sample property.

Note that the visualization of sample metadata in this report depends on user-provided input; each column in the metadata input table (besides sample names) that contains more than 1 unique value is automatically used as a factor for color-coding all figures in this section. All information shown in these figures is also available in the output table 'samples.xlsx'.



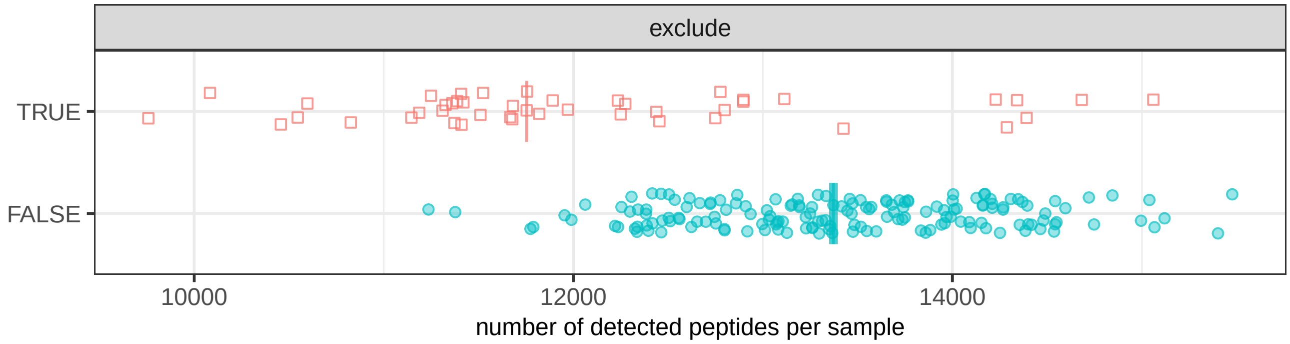
color-coding sample metadata, expanded

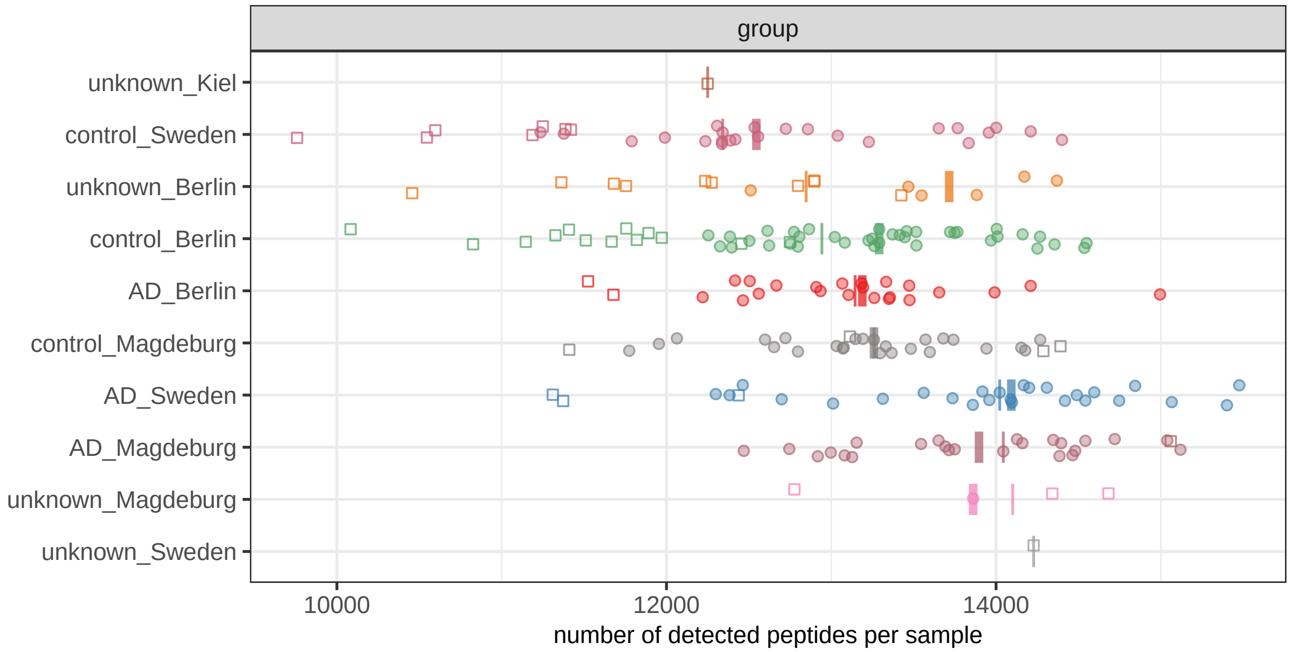
To further detail each sample property, each row in the above figure is now split into separate plots. Thus, a figure is generated for each property in the user-provided metadata (column in the samples table, its name shown in the plot title).

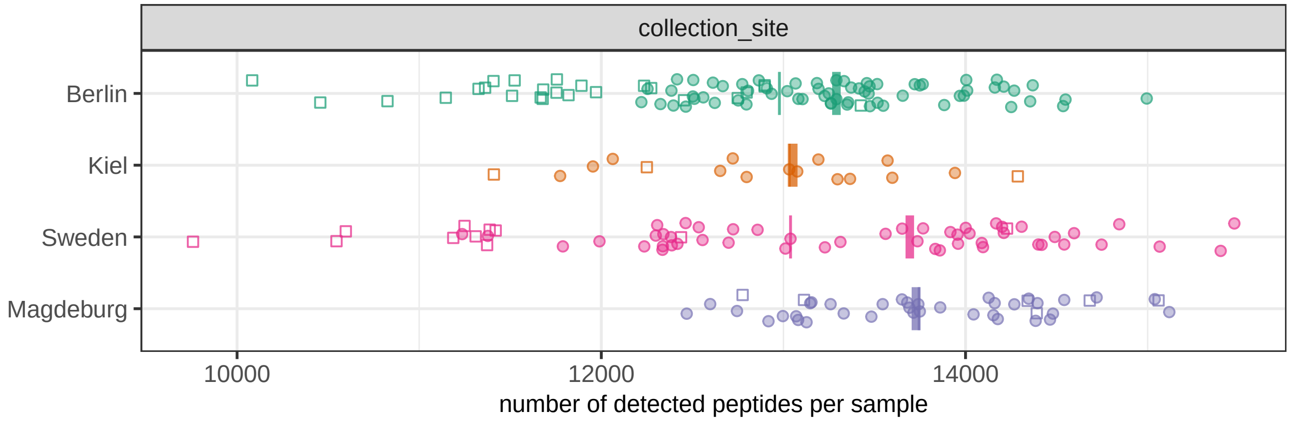
For categorical variables, a scatterplot shows on the y-axis all unique variables while the x-axis depicts the number of detected peptides. Colors are consistent with the above plot. *exclude* samples, if any, are depicted as squares. The median value is shown as a vertical line (thin line = median over all samples, wider line = median while discarding *exclude* samples). For continuous variables, a scatterplot without (left panel) and with Loess fit is shown (right panel, visualized as blue line if data was successfully fitted).

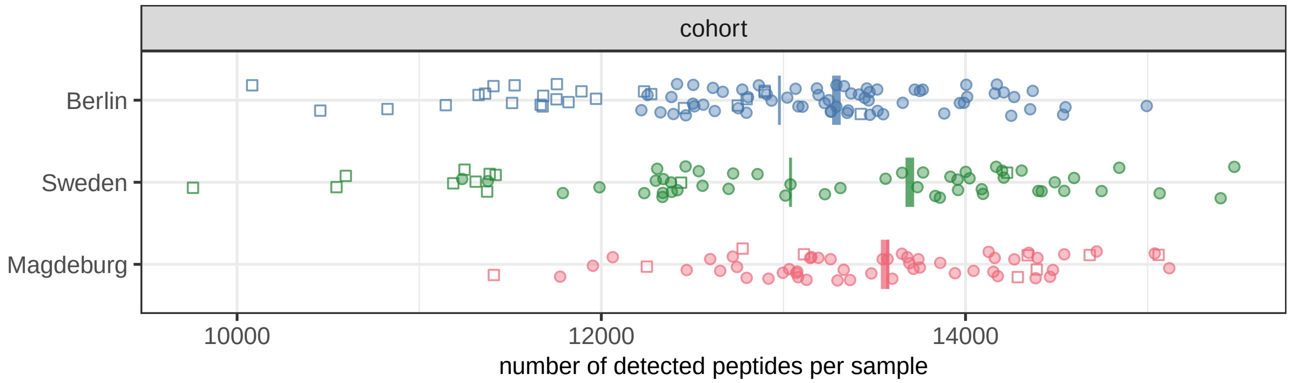
Note that samples flagged as *exclude* are user-provided in the sample metadata table. These are included in data visualizations but excluded from downstream statistical analysis (later part of the report).

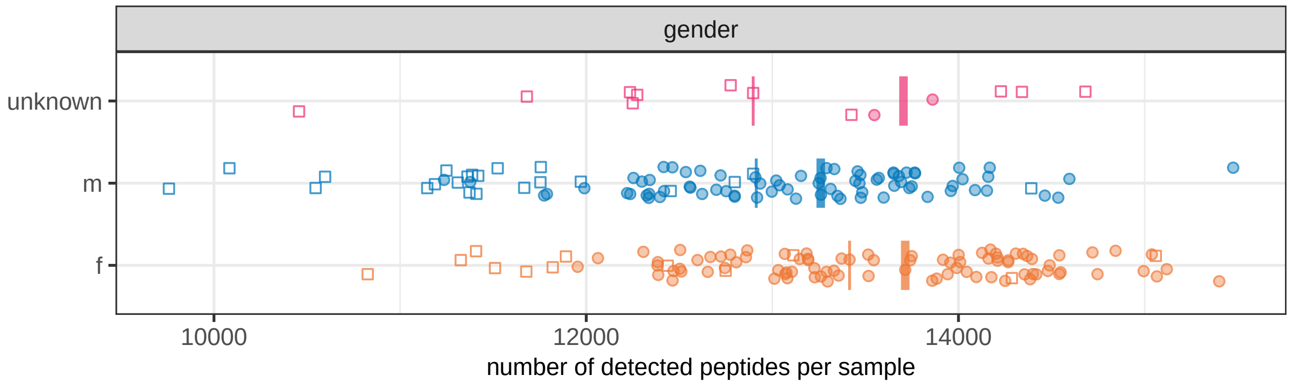
For example: the first plot shows color-coding by the 'group' property, so each row represents a sample group. If samples in a particular group systematically yield fewer peptides than another group, a clear pattern will be visible.

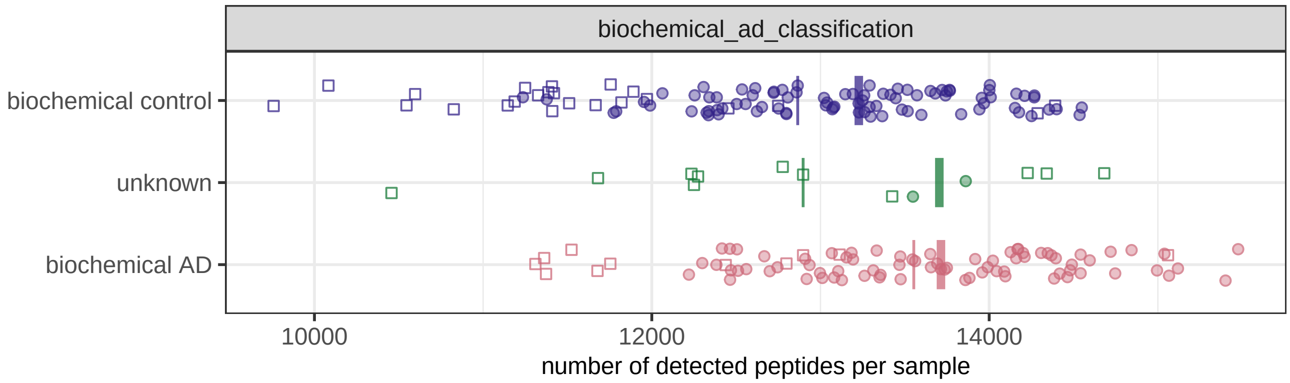


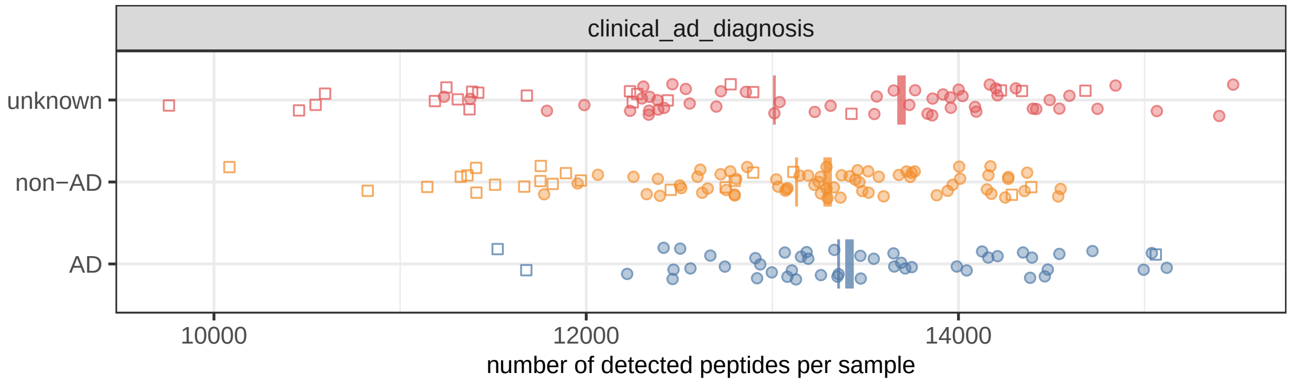


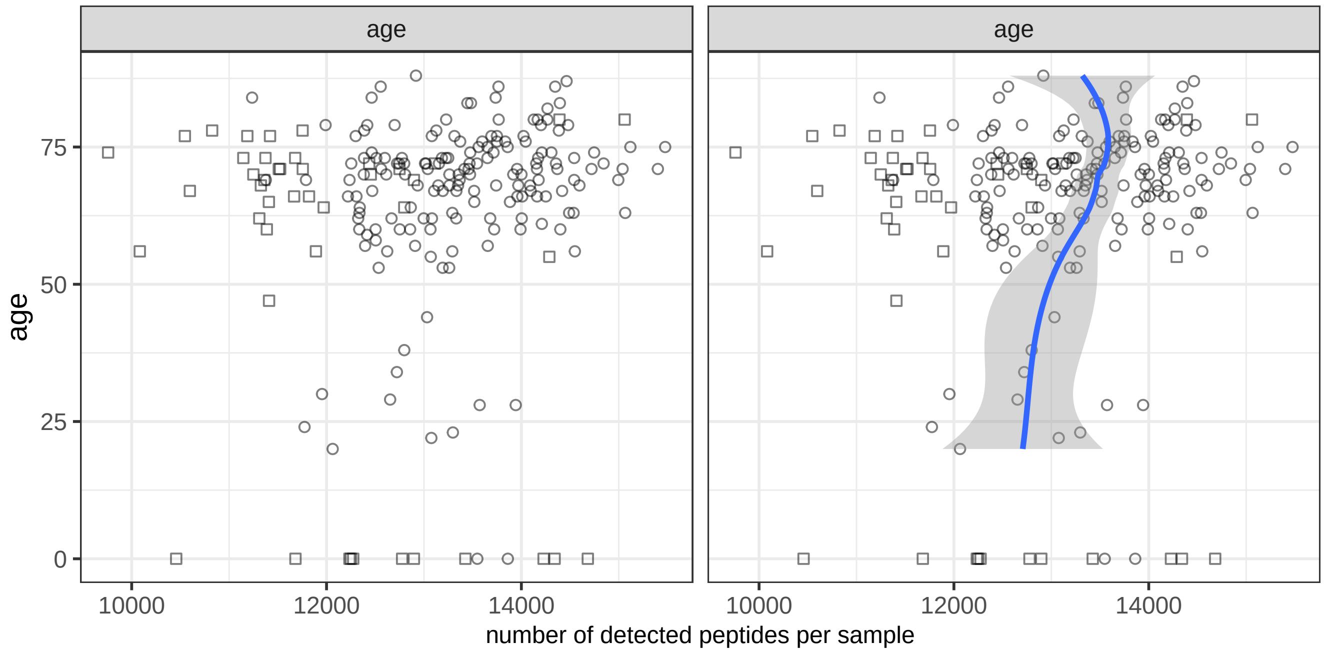


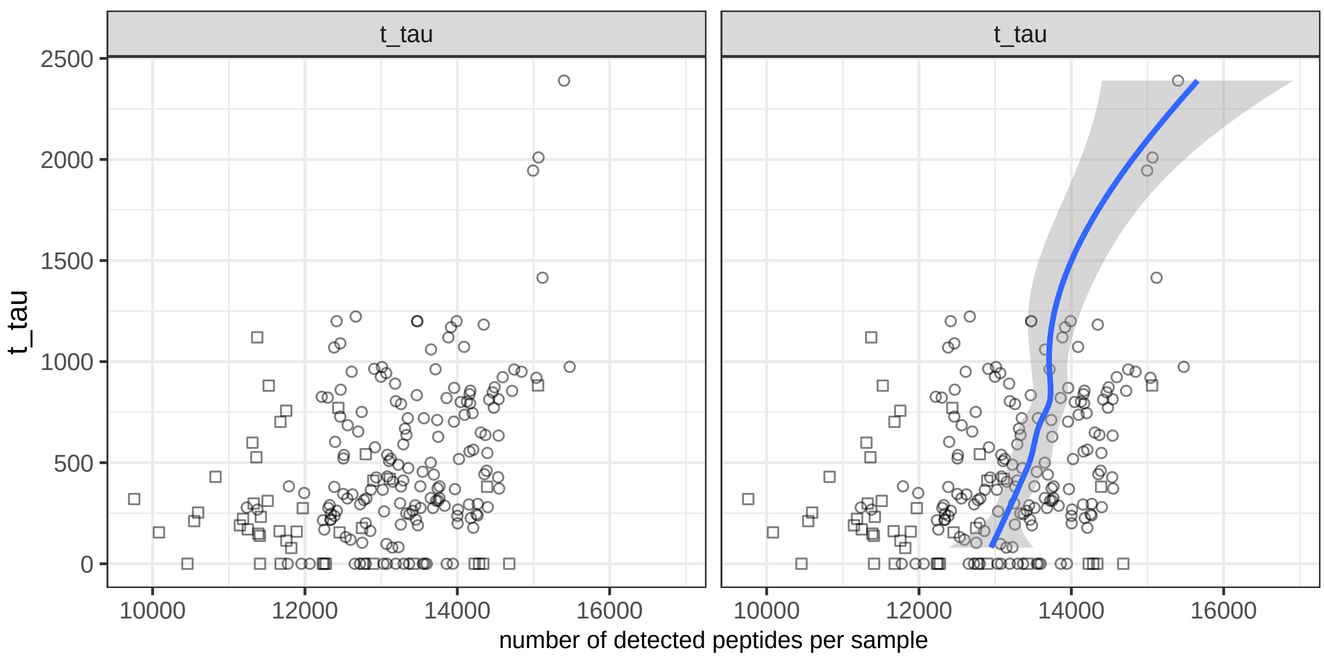

cohort
Berlin
Sweden
Magdeburg
10000
12000
14000
number of detected peptides per sample

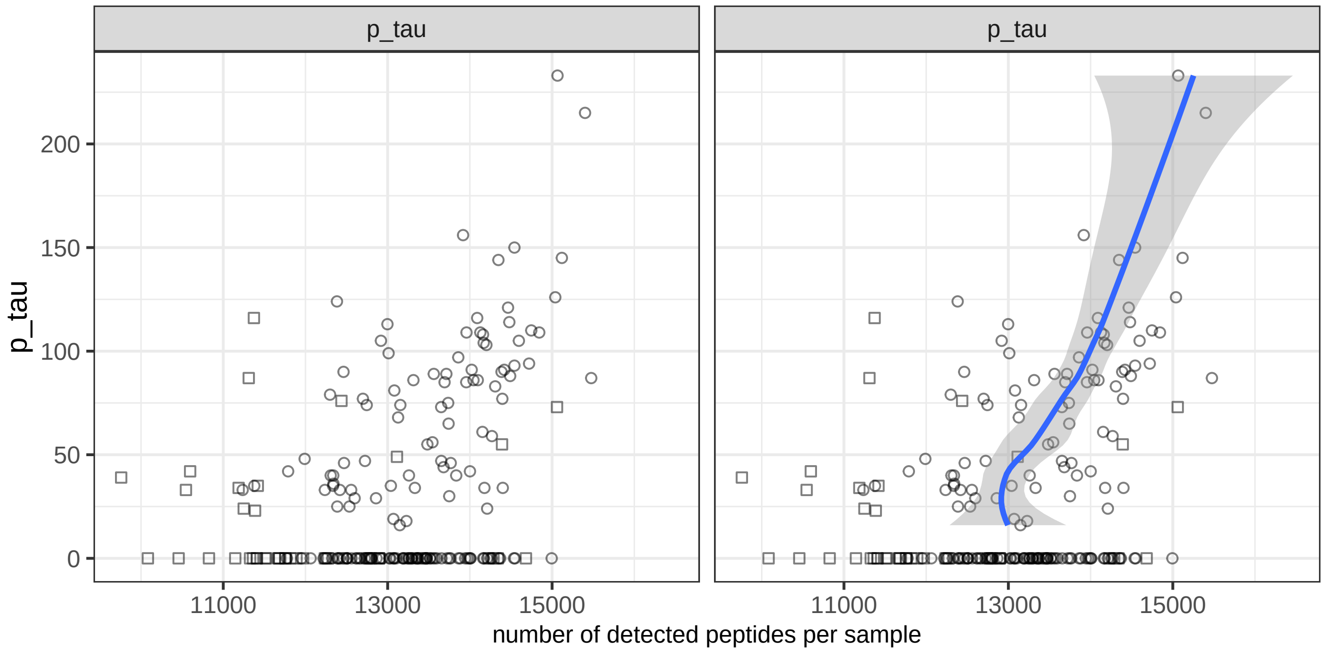

gender
unknown
m
f
10000
12000
14000
number of detected peptides per sample

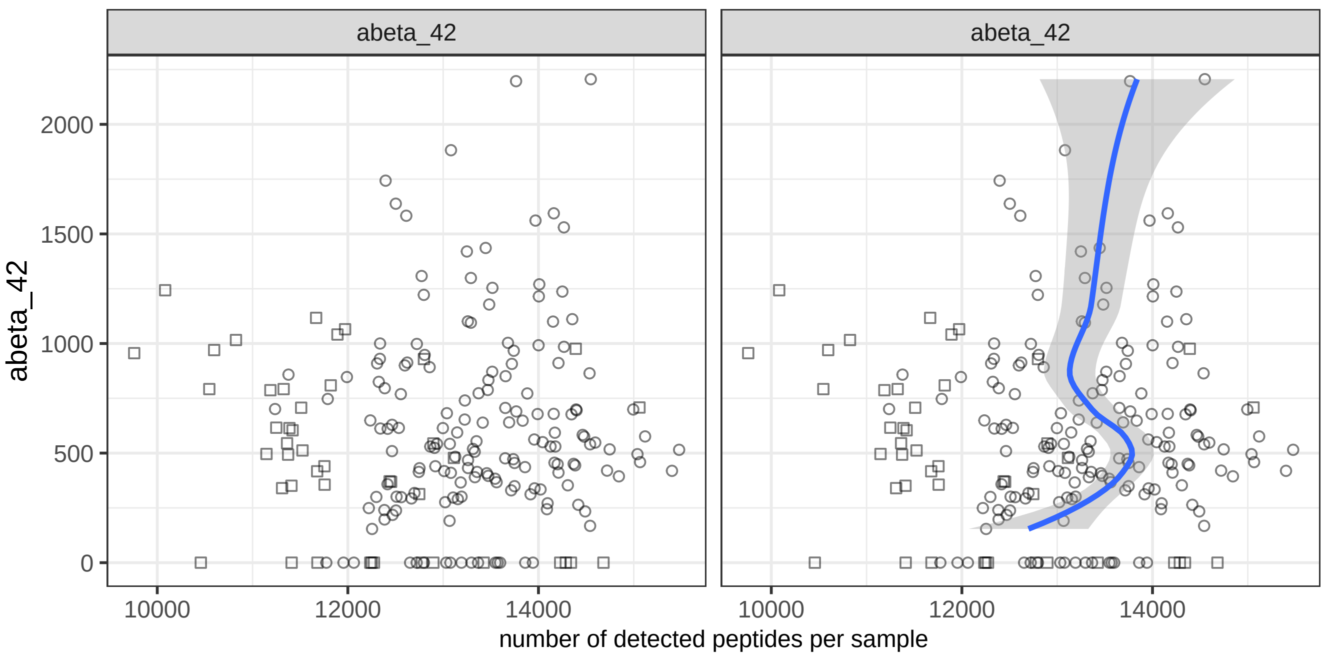

biochemical_ad_classification
biochemical control
unknown
biochemical AD
10000
12000
14000
number of detected peptides per sample

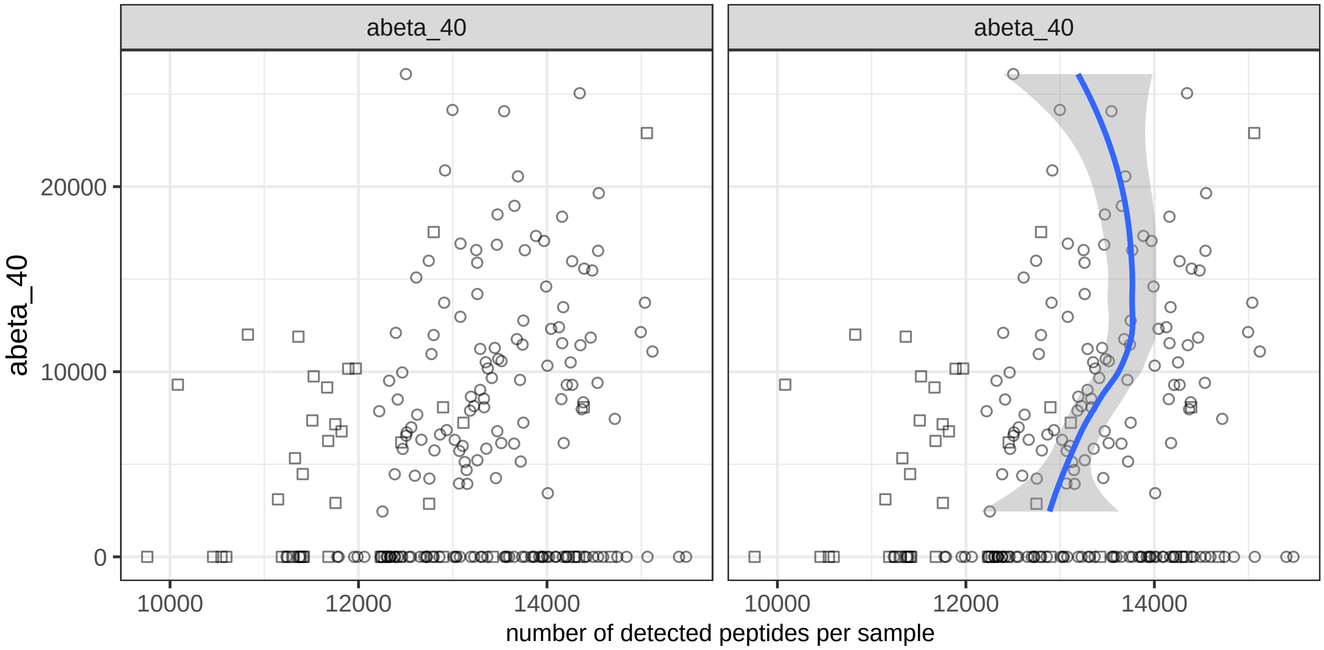

clinical_ad_diagnosis
unknown
non−AD
AD
10000
12000
14000
number of detected peptides per sample

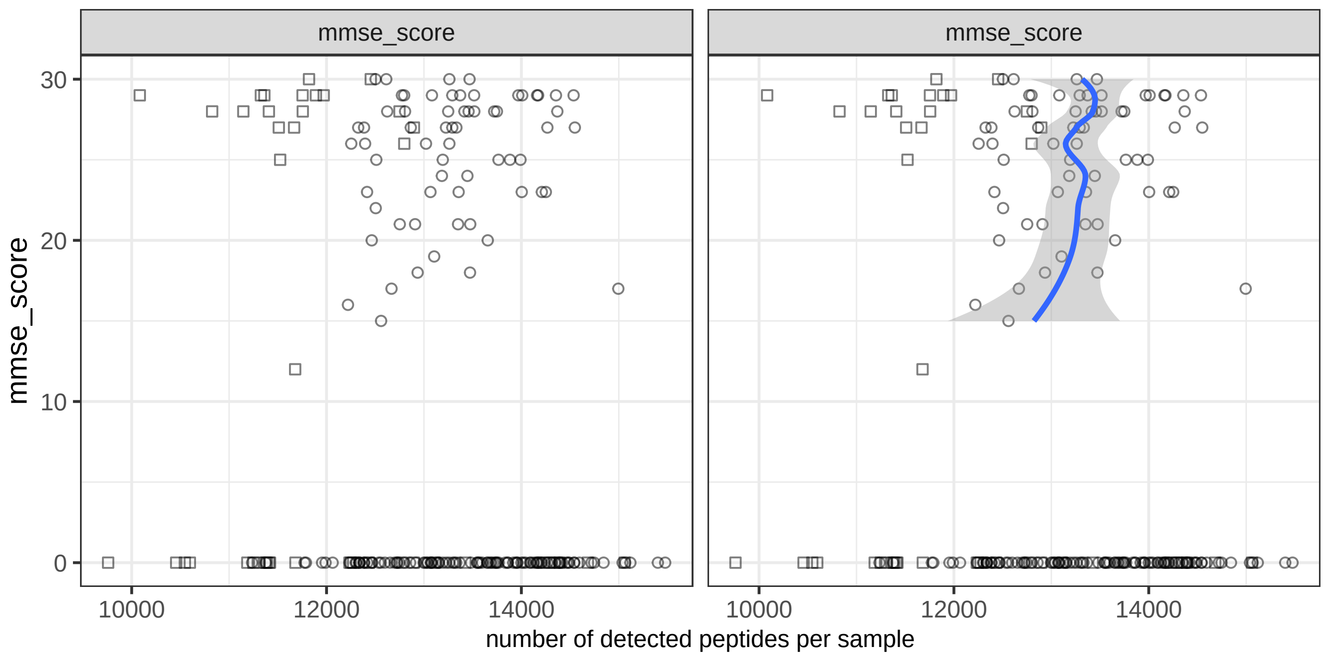

age
age
75
50
25
0
10000
12000
14000
number of detected peptides per sample


t_tau
t_tau
2500
2000
1500
1000
500
0
10000
12000
14000
16000
number of detected peptides per sample


p_tau
p_tau
200
150
100
50
0
p_tau
11000
13000
15000
11000
13000
15000
number of detected peptides per sample


abeta_42
abeta_42
2000
1500
1000
500
0
abeta_42
10000
12000
14000
10000
12000
14000
number of detected peptides per sample

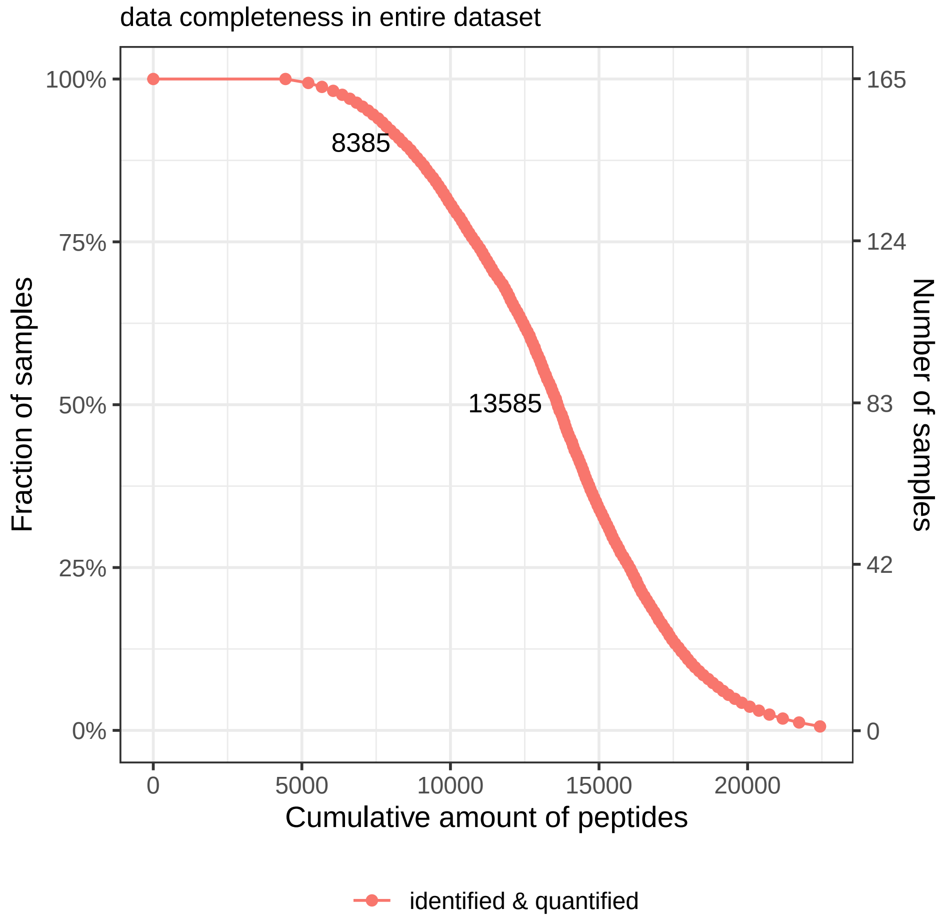

abeta_40
abeta_40
abeta_40
20000
10000
0
10000
12000
14000
10000
12000
14000
number of detected peptides per sample


mmse_score
mmse_score
mmse_score
30
20
10
0
10000
12000
14000
10000
12000
14000
number of detected peptides per sample

1.3 data completeness

To visualize how many peptides are consistently identified in multiple samples, the first figure summarizes how common missing values are in the entire dataset. Optimally, most peptides are identified in 100% of samples and this curve slowly falls of. The following figure shows for each sample whether its peptides are also present in other samples in the dataset or whether these are unique to a (minor) subset of samples. You can use this mark of experimental consistency to compare datasets generated by similar protocols and mass-spec acquisition.

1.3.1 cumulative distribution

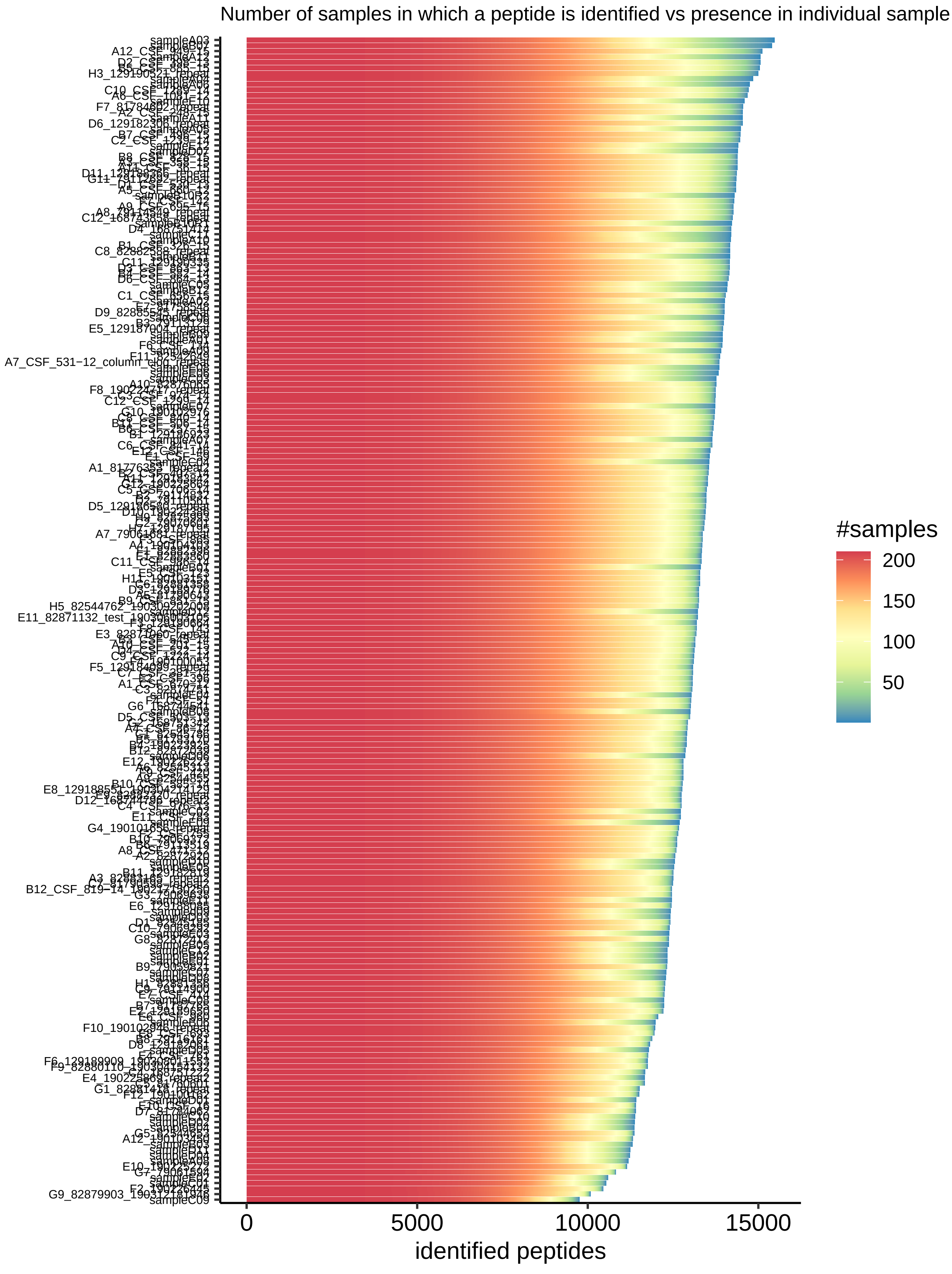


Samples flagged as 'exclude' (by user) are not taken into account in this figure. Exact values are shown for data points matching 90% and 50% of samples to convenience comparison between analyses (e.g. before/after configuring 'exclude' samples, or comparing between experiments of similar protocol).

1.3.2 peptide detection frequency

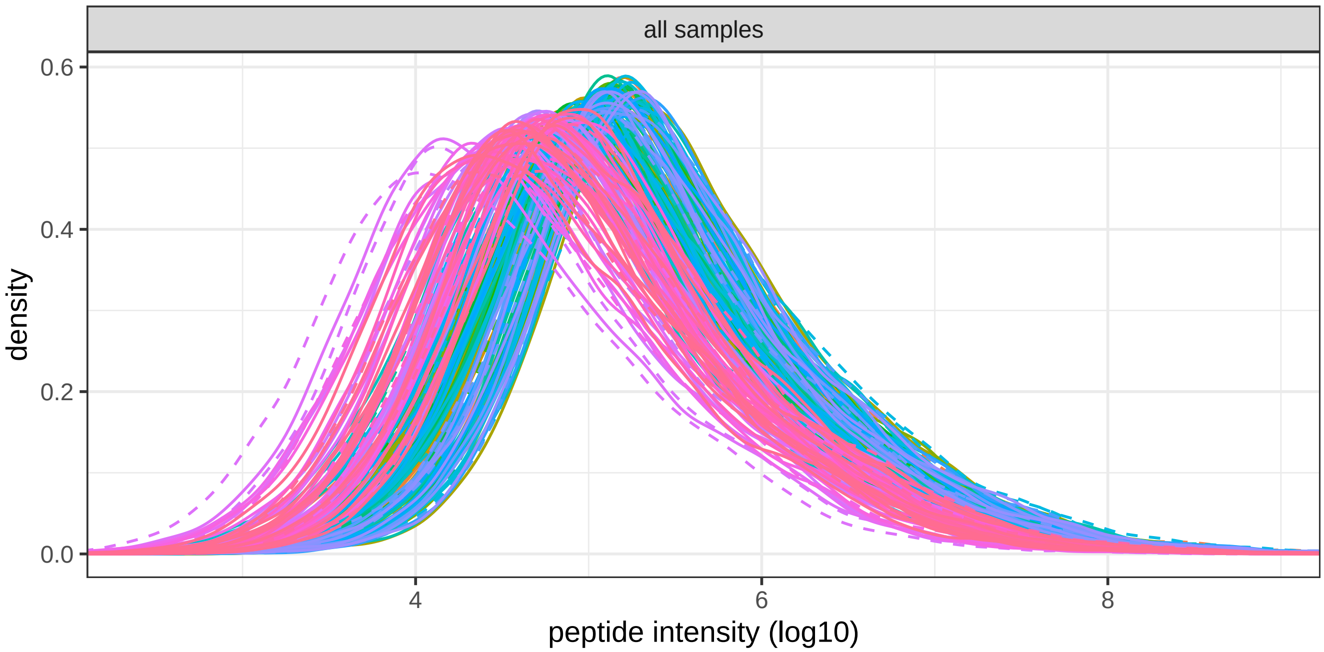
Each identified peptide in a sample is classified and color-coded by the number of other samples where the same peptide is present. Visualization of the amount of peptides that overlap with other samples in the dataset, from peptides identified in most samples (red) to one-hit-wonders (blue), helps identify uncommon samples (more blue/green than other samples).

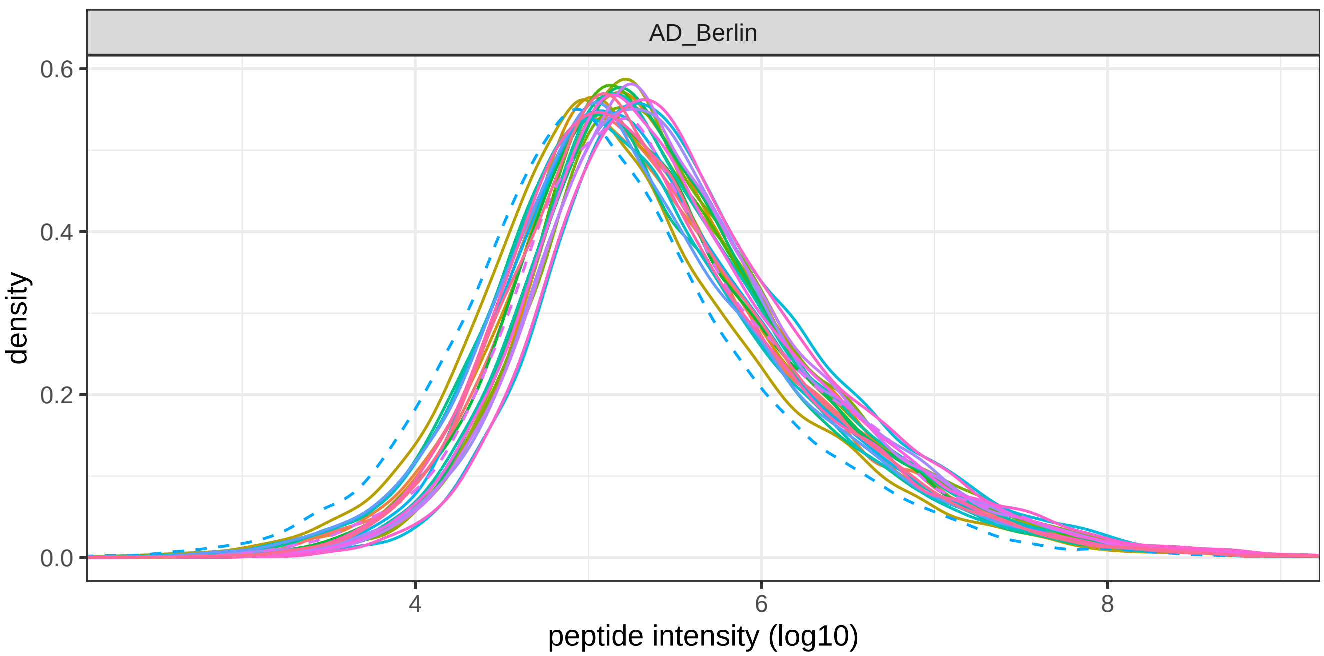
Optimally, the majority of peptides in each sample are red~orange with relatively few uniquely identified peptides (blue~green). Samples are sorted by the total amount of detected peptides.

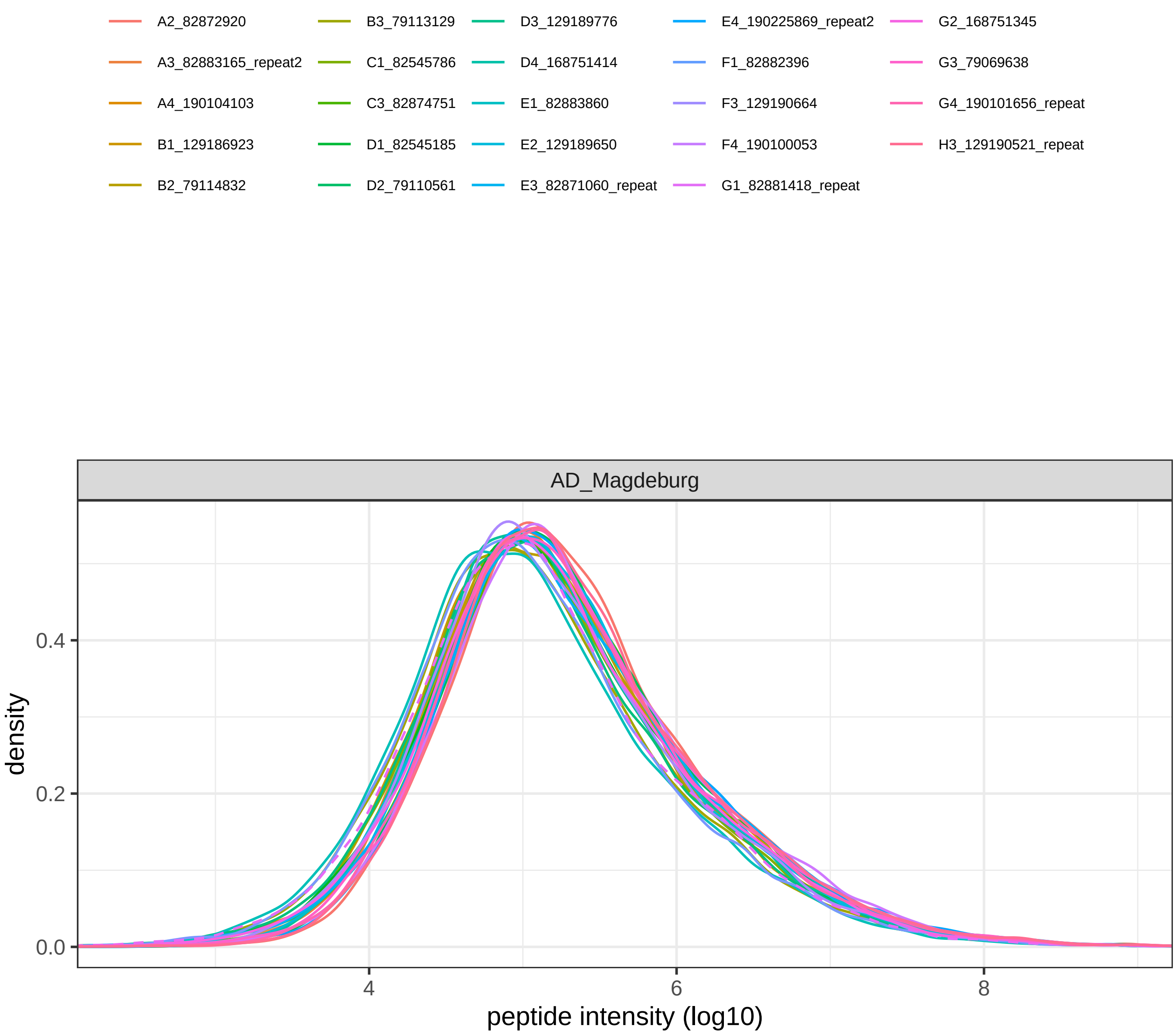

Number of samples in which a peptide is identified vs presence in individual sample
0
5000
10000
15000
identified peptides
#samples
200
150
100
50

1.4 abundance distributions

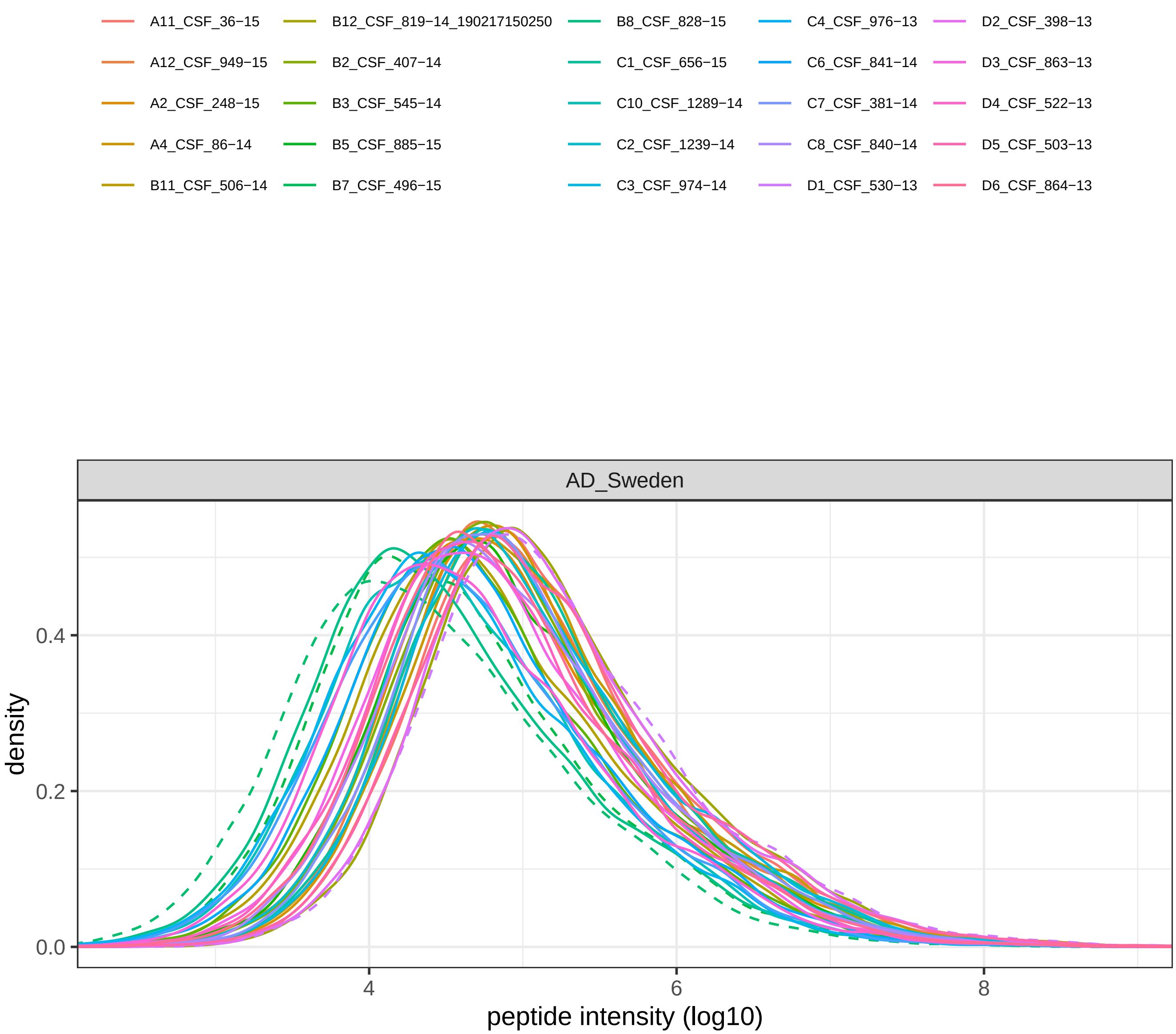
The figures in this subsection are used to identify unexpected mass-spec sensitivity or sample loading differences. Peptide data is shown as provided in input files, so peptide filtering nor intensity normalization has been applied yet (for proper QC, make sure the software that generated the input data did not apply normalization prior). If the dataset is DDA, match-between-runs (MBR) peptides are included in these distributions whereas for DIA only 'detected' peptides (based on confidence score threshold) are included.

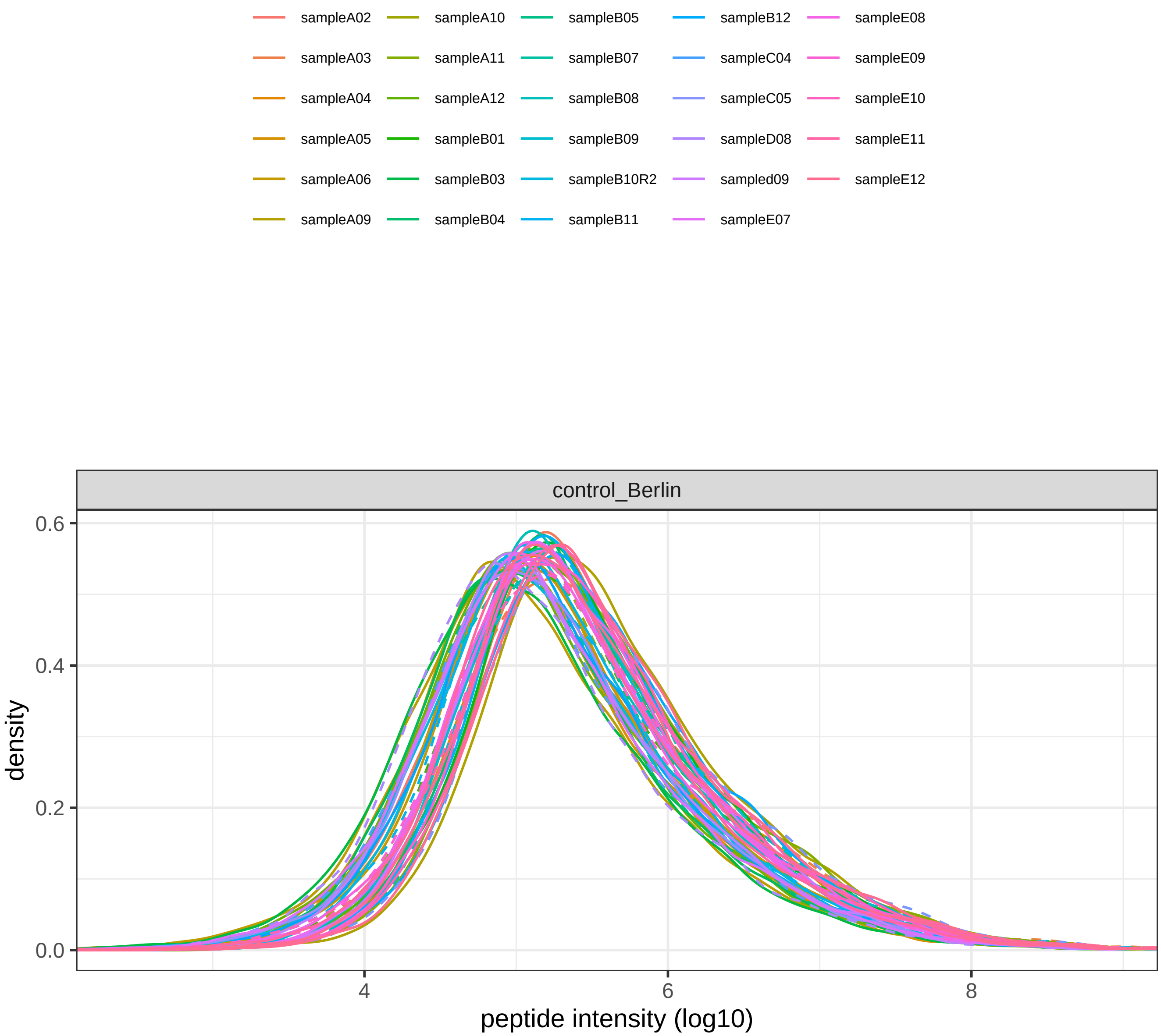




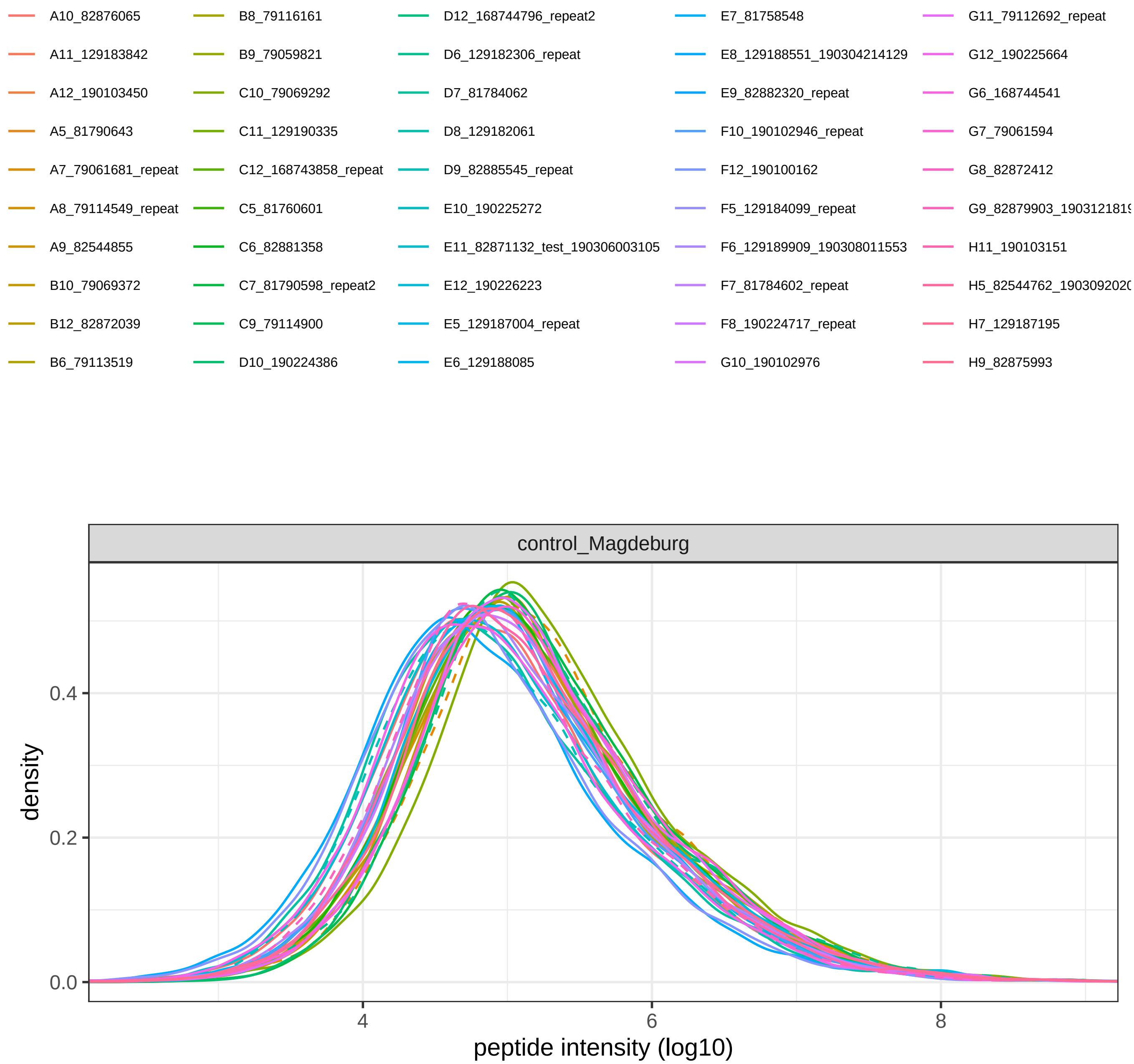


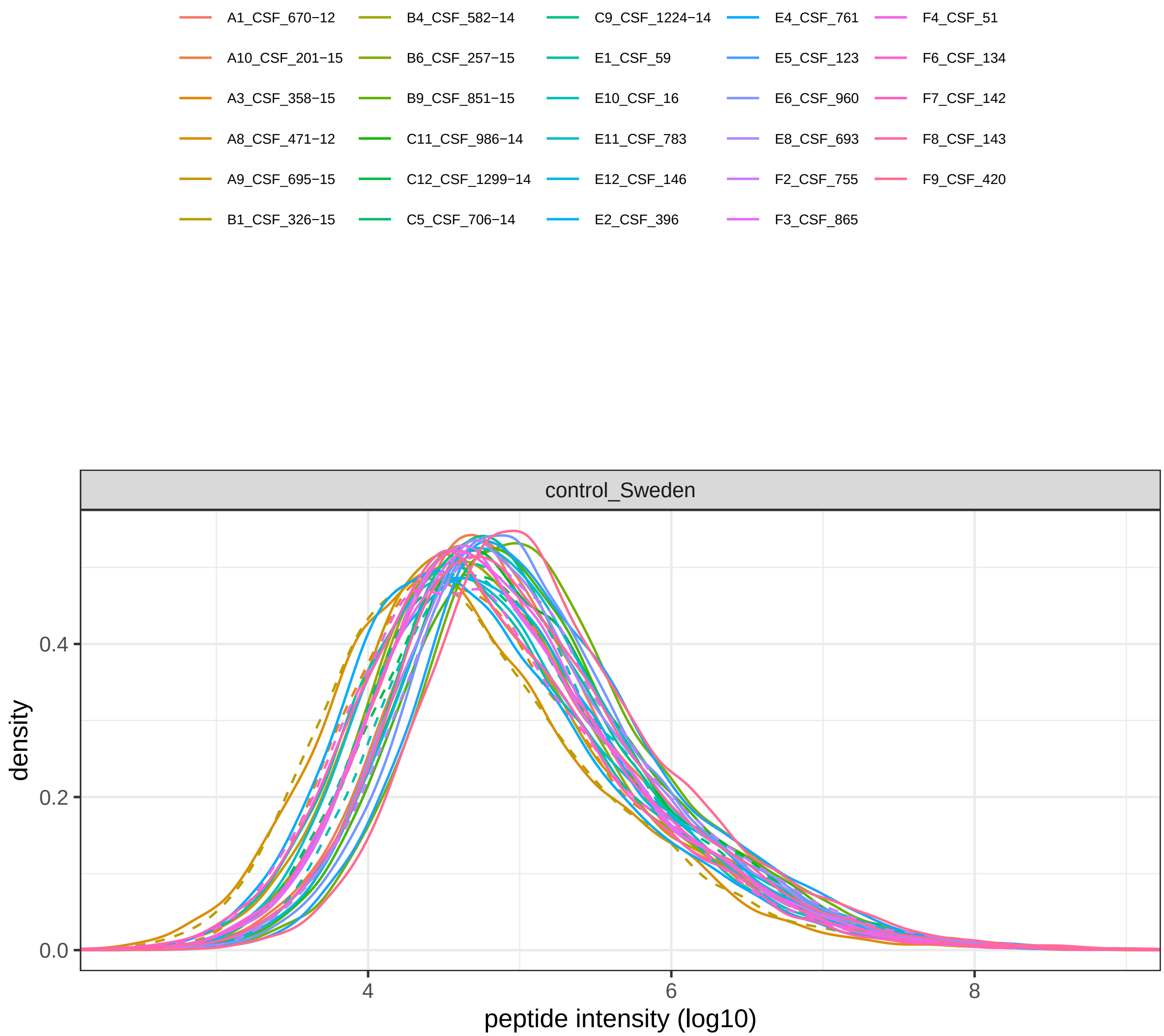
A2_82872920
A3_82883165_repeat2
A4_190104103
B1_129186923
B2_79114832
B3_79113129
C1_82545786
C3_82874751
D1_82545185
D2_79110561
D3_129189776
D4_168751414
E1_82883860
E2_129189650
E3_82871060_repeat
E4_190225869_repeat2
F1_82882396
F3_129190664
F4_190100053
G1_82881418_repeat
G2_168751345
G3_79069638
G4_190101656_repeat
H3_129190521_repeat
AD_Magdeburg
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)


A11_CSF_36−15
A12_CSF_949−15
A2_CSF_248−15
A4_CSF_86−14
B11_CSF_506−14
B12_CSF_819−14_190217150250
B2_CSF_407−14
B3_CSF_545−14
B5_CSF_885−15
B7_CSF_496−15
B8_CSF_828−15
C1_CSF_656−15
C10_CSF_1289−14
C2_CSF_1239−14
C3_CSF_974−14
C4_CSF_976−13
C6_CSF_841−14
C7_CSF_381−14
C8_CSF_840−14
D1_CSF_530−13
D2_CSF_398−13
D3_CSF_863−13
D4_CSF_522−13
D5_CSF_503−13
D6_CSF_864−13
AD_Sweden
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)

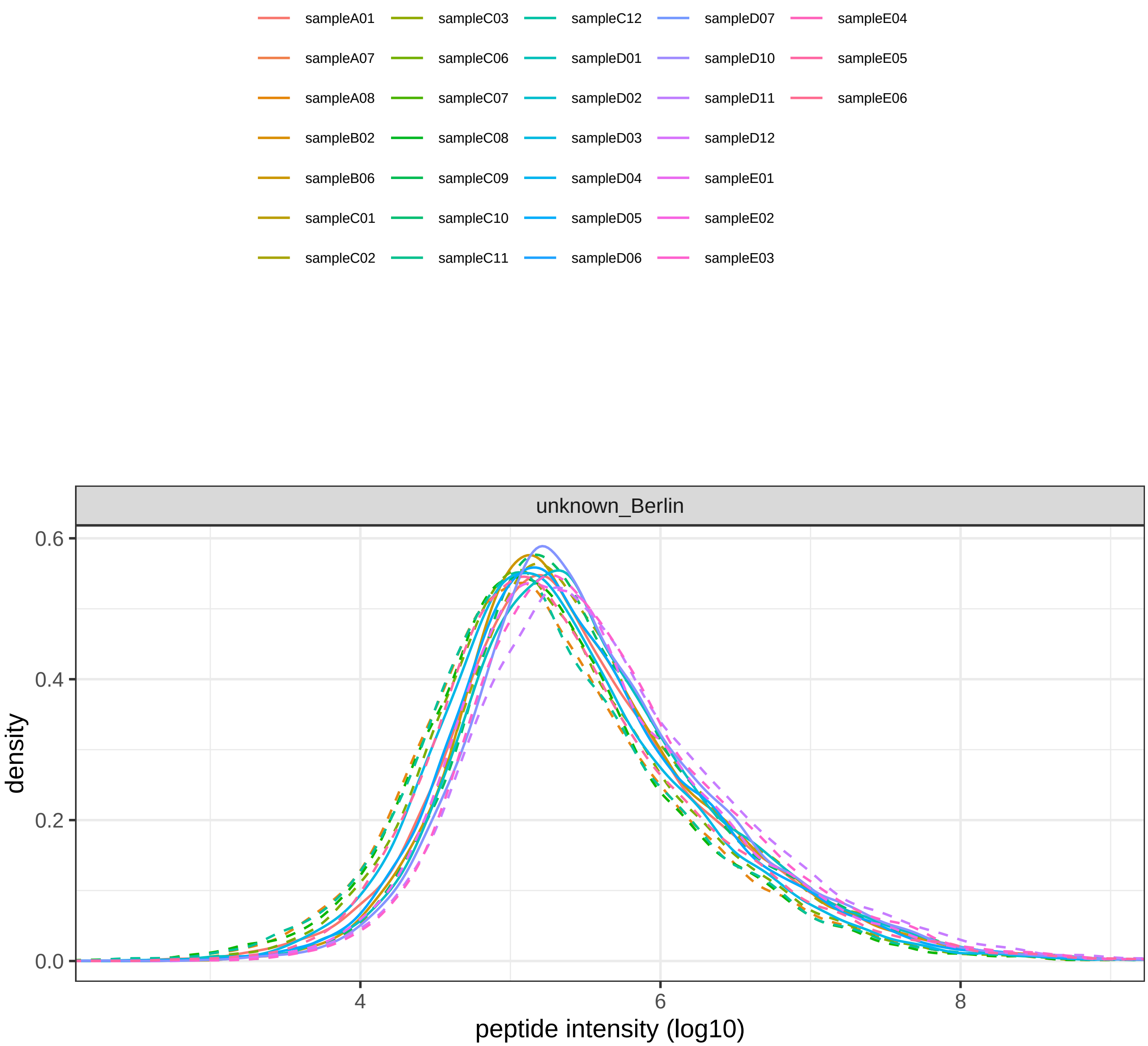


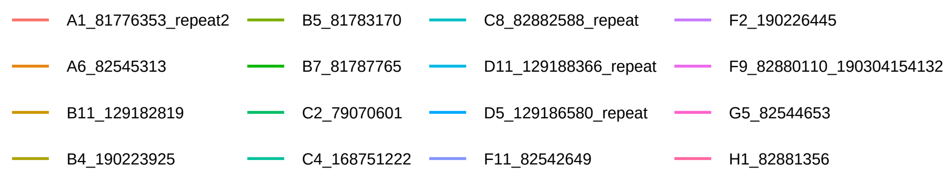
sampleA02
sampleA03
sampleA04
sampleA05
sampleA06
sampleA09
sampleA10
sampleA11
sampleA12
sampleB01
sampleB03
sampleB04
sampleB05
sampleB07
sampleB08
sampleB09
sampleB10R2
sampleB11
sampleB12
sampleC04
sampleC05
sampleD08
sampled09
sampleE07
sampleE08
sampleE09
sampleE10
sampleE11
sampleE12
control_Berlin
0.6
0.4
0.2
0.0
density
4
6
8
peptide intensity (log10)

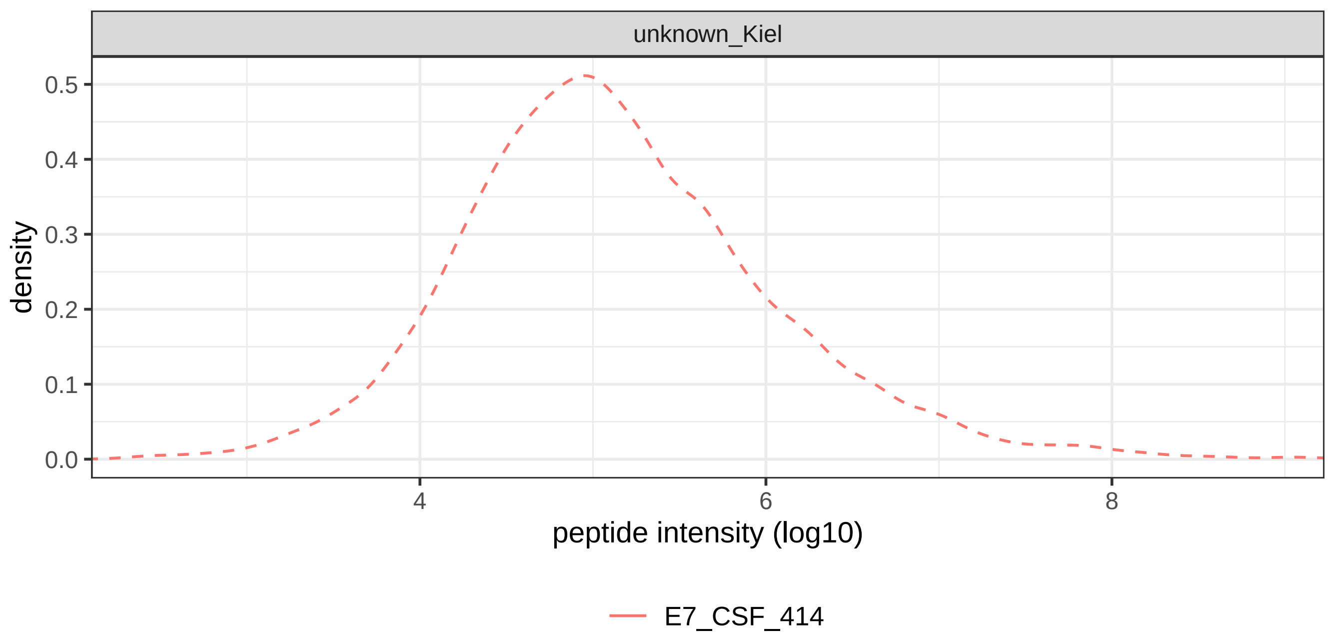

A10_82876065
A11_129183842
A12_190103450
A5_81790643
A7_79061681_repeat
A8_79114549_repeat
A9_82544855
B10_79069372
B12_82872039
B6_79113519
B8_79116161
B9_79059821
C10_79069292
C11_129190335
C12_168743858_repeat
C5_81760601
C6_82881358
C7_81790598_repeat2
C9_79114900
D10_190224386
D12_168744796_repeat2
D6_129182306_repeat
D7_81784062
D8_129182061
D9_82885545_repeat
E10_190225272
E11_82871132_test_190306003105
E12_190226223
E5_129187004_repeat
E6_129188085
E7_81758548
E8_129188551_190304214129
E9_82882320_repeat
F10_190102946_repeat
F12_190100162
F5_129184099_repeat
F6_129189909_190308011553
F7_81784602_repeat
F8_190224717_repeat
G10_190102976
G11_79112692_repeat
G12_190225664
G6_168744541
G7_79061594
G8_82872412
H11_190103151
H7_129187195
H9_82875993
control_Magdeburg
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)

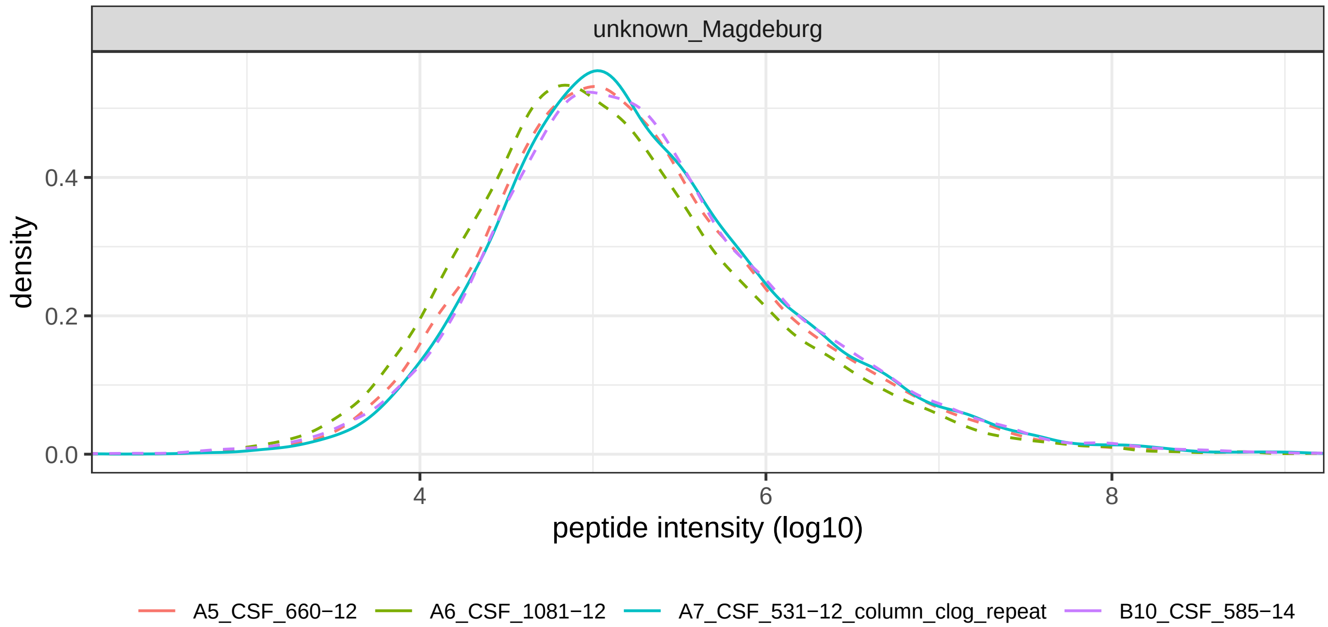


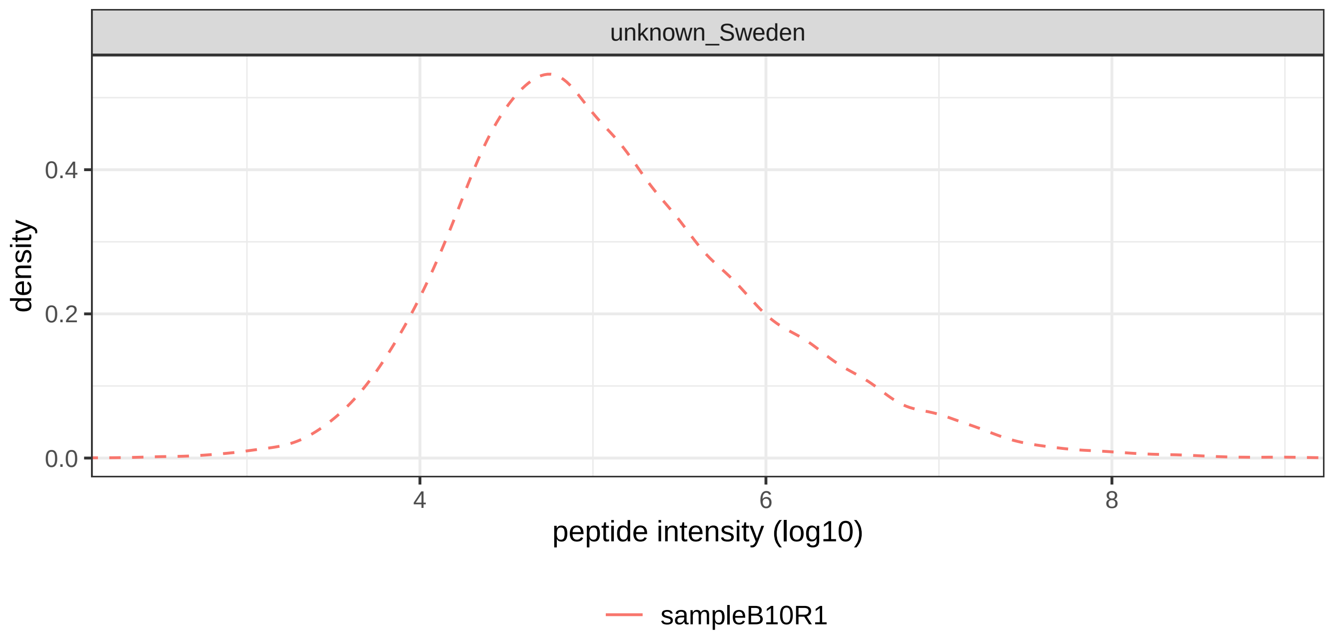
A1_CSF_670−12
A10_CSF_201−15
A3_CSF_358−15
A8_CSF_471−12
A9_CSF_695−15
B1_CSF_326−15
B4_CSF_582−14
B6_CSF_257−15
B9_CSF_851−15
C11_CSF_986−14
C12_CSF_1299−14
C5_CSF_706−14
C9_CSF_1224−14
E1_CSF_59
E10_CSF_16
E11_CSF_783
E12_CSF_146
E2_CSF_396
E4_CSF_761
E5_CSF_123
E6_CSF_960
E8_CSF_693
F2_CSF_755
F3_CSF_865
F4_CSF_51
F6_CSF_134
F7_CSF_142
F8_CSF_143
F9_CSF_420
control_Sweden
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)


sampleA01
sampleA07
sampleA08
sampleB02
sampleB06
sampleC01
sampleC02
sampleC03
sampleC06
sampleC07
sampleC08
sampleC09
sampleC10
sampleC11
sampleC12
sampleD01
sampleD02
sampleD03
sampleD04
sampleD05
sampleD06
sampleD07
sampleD10
sampleD11
sampleD12
sampleE01
sampleE02
sampleE03
sampleE04
sampleE05
sampleE06
unknown_Berlin
0.6
0.4
0.2
0.0
density
4
6
8
peptide intensity (log10)


A1_81776353_repeat2
A6_82545313
B11_129182819
B4_190223925
B5_81783170
B7_81787765
C2_79070601
C4_168751222
C8_82882588_repeat
D11_129188366_repeat
D5_129186580_repeat
F11_82542649
F2_190226445
F9_82880110_190304154132
G5_82544653
H1_82881356


unknown_Kiel
density
0.0
0.1
0.2
0.3
0.4
0.5
4
6
8
peptide intensity (log10)
E7_CSF_414


unknown_Magdeburg
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)
A5_CSF_660−12
A6_CSF_1081−12
A7_CSF_531−12_column_clog_repeat
B10_CSF_585−14

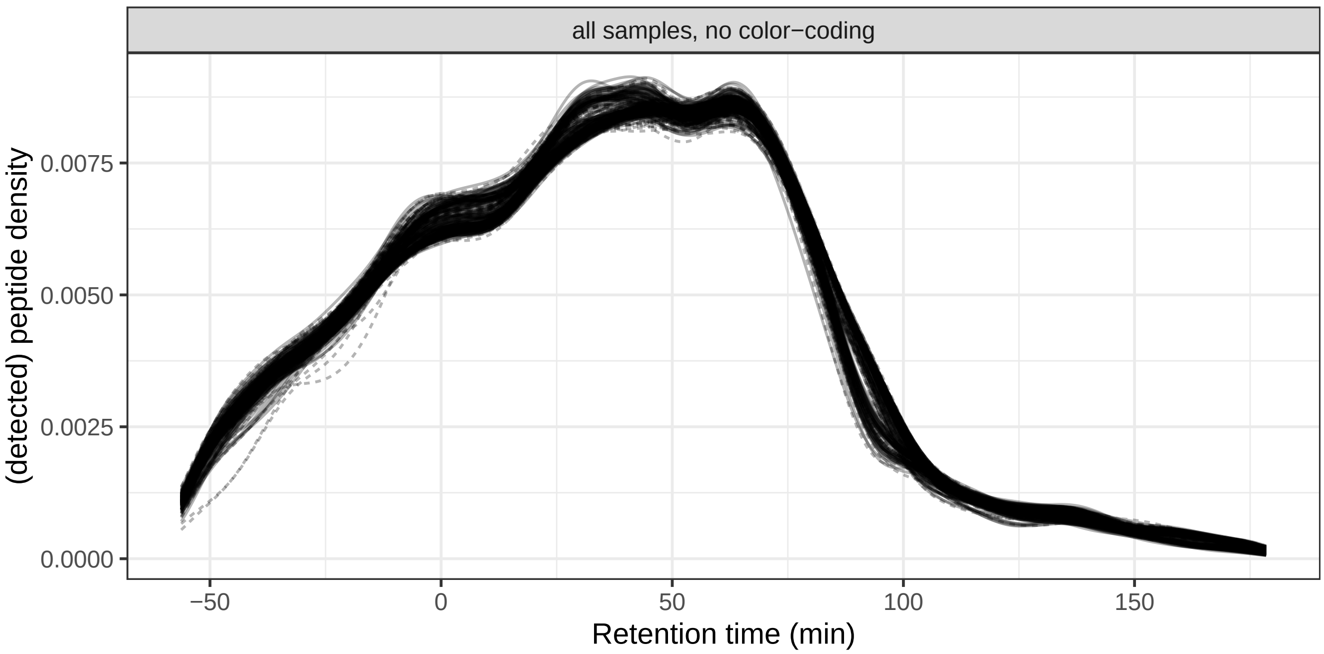

unknown_Sweden
density
0.0
0.2
0.4
4
6
8
peptide intensity (log10)
sampleB10R1

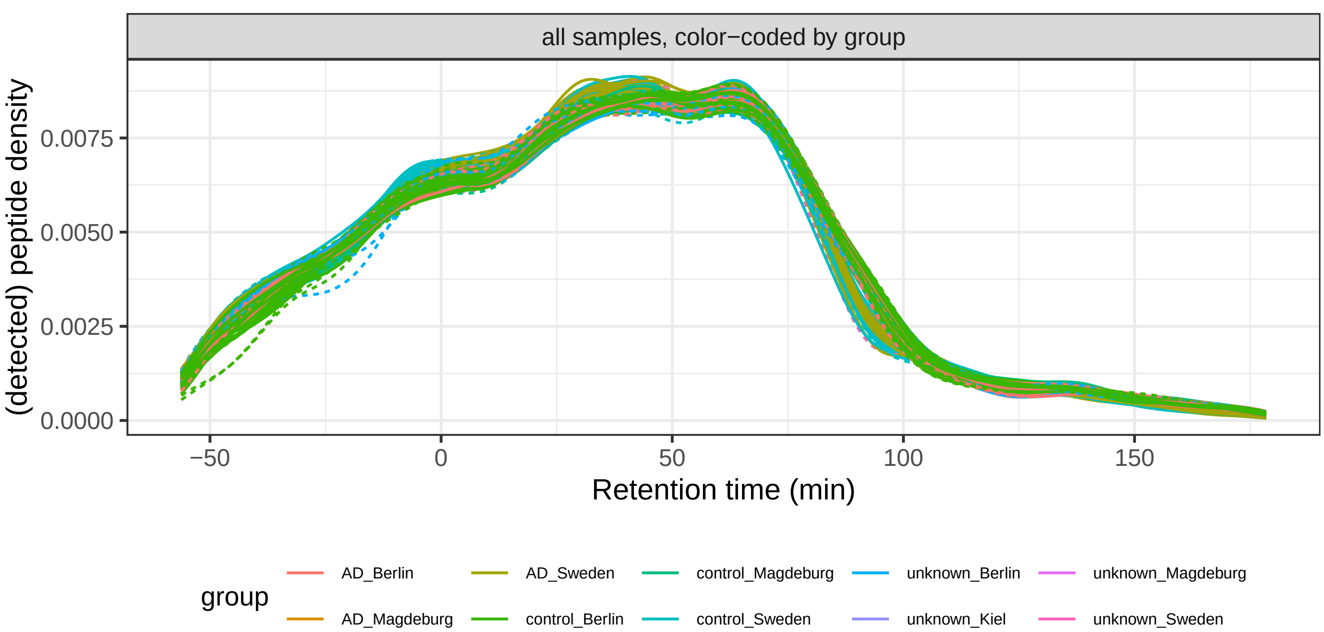
1.5 retention time

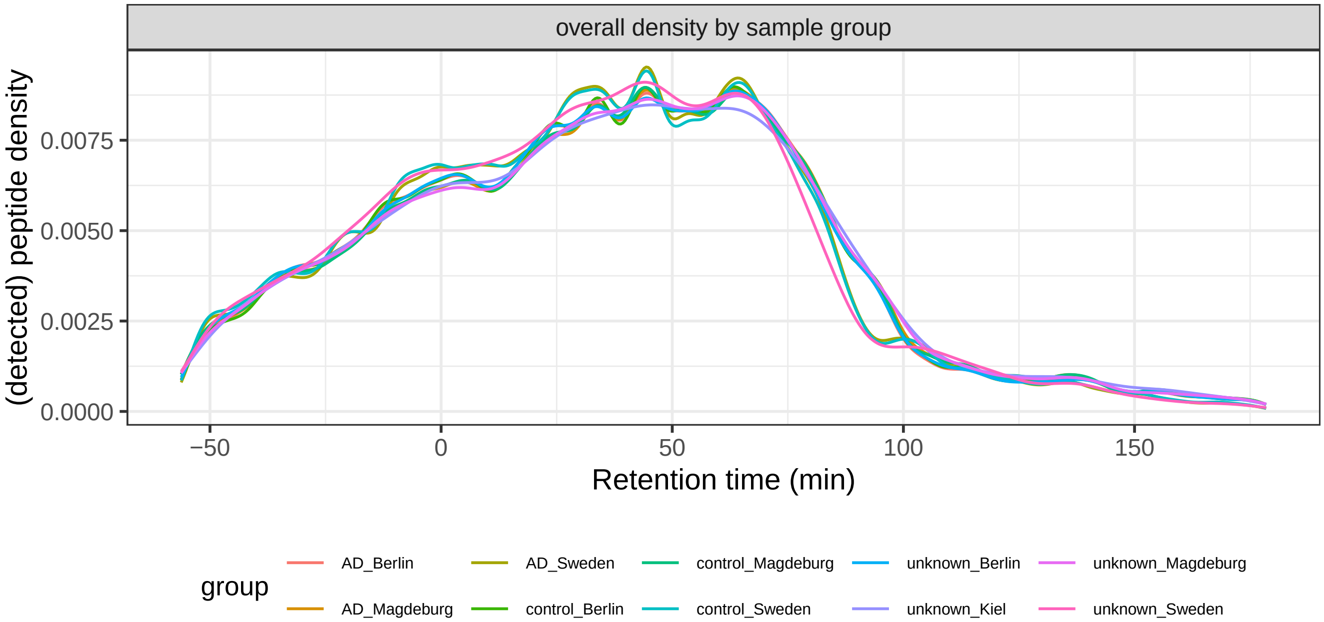
The figures in this section allow you to identify potential problems during HPLC elution, such as a temporarily blocking column, failing ionization spray or decreasing sensitivity over time. For each sample, all peptides that are also observed in a replicate (such that there is a point of reference available) are visualized.

1.5.1 retention time distributions

The density of the number of peptides eluting at each point in time. The figure below presents an overview of all samples that allows for the identification of outlier samples that follow distinct elution patterns. The following section shows details for each sample. Samples marked as 'exclude' in the provided sample metadata table are visualized as dashed lines.





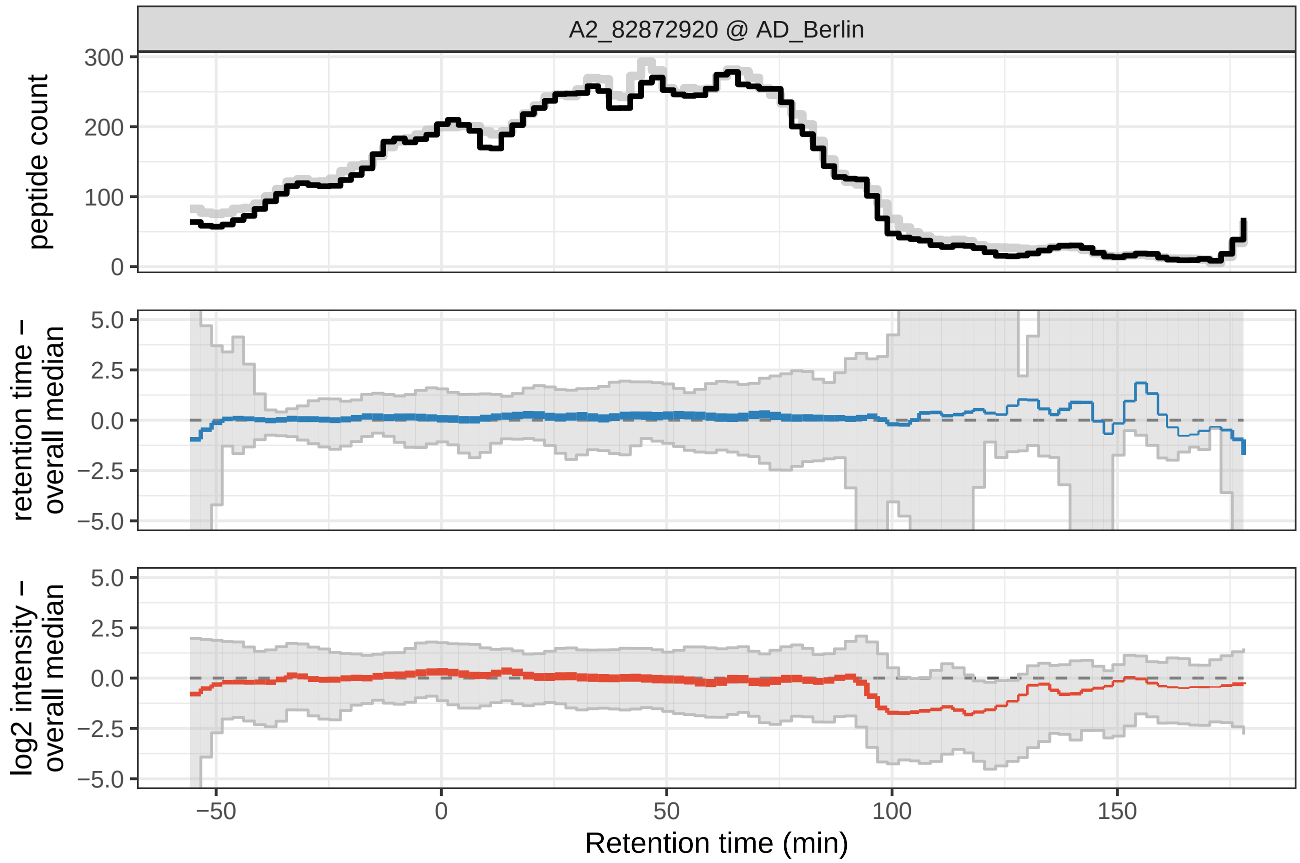


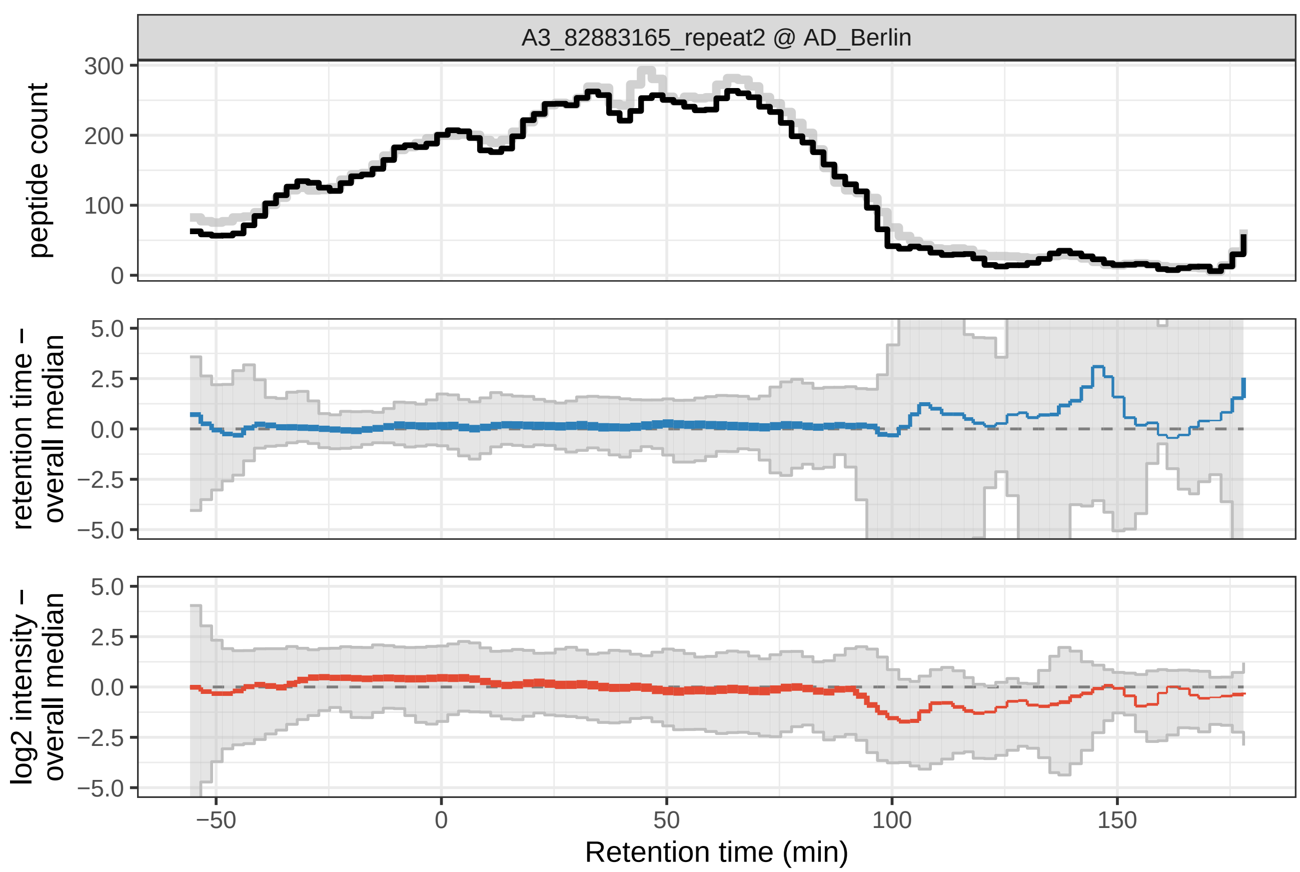
1.5.2 retention time local effects

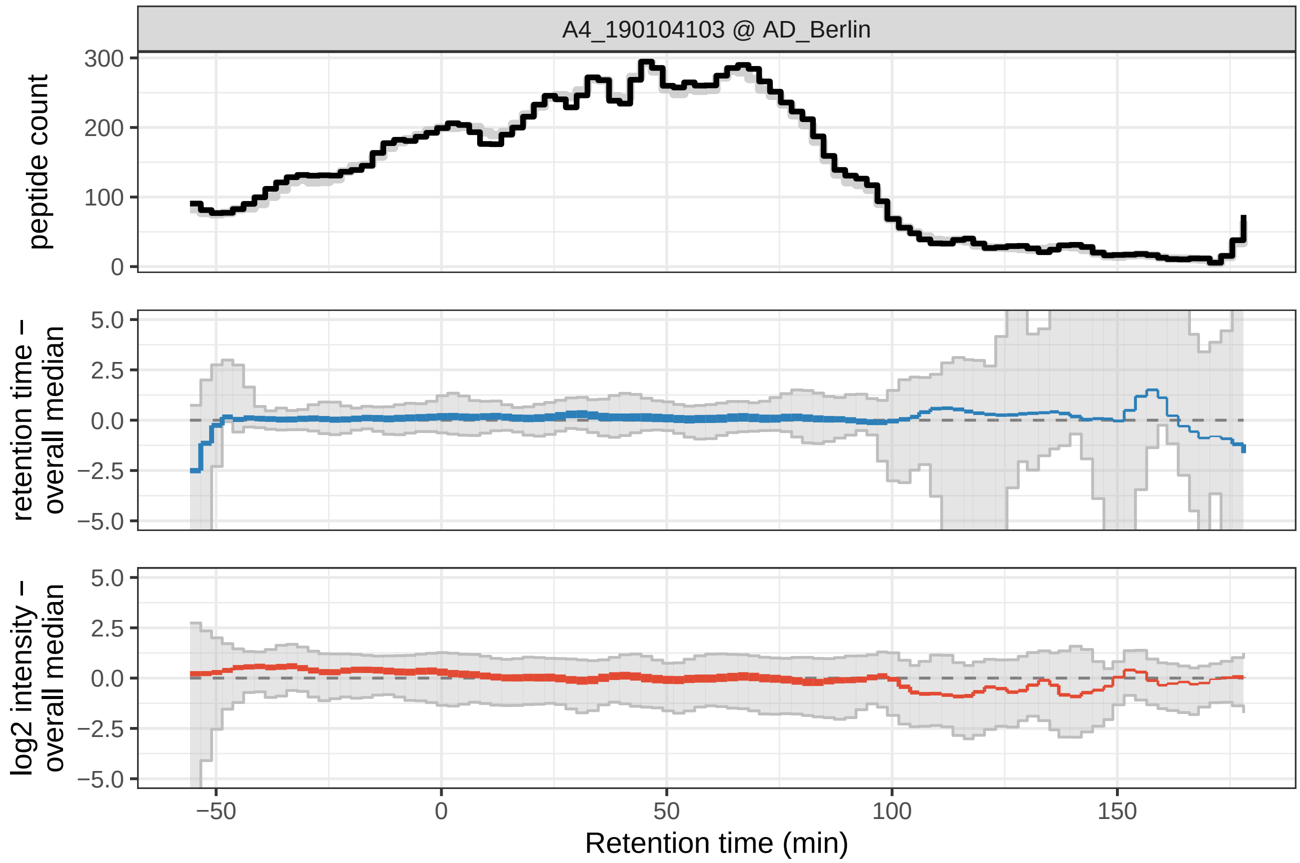
To investigate how each measurement differs from others, we visualize each sample as a 3 panel figure. First, the data is binned across the retention time dimension (x-axis). If a samples was marked as 'exclude' in the provided sample metadata, this is indicated in the plot title.

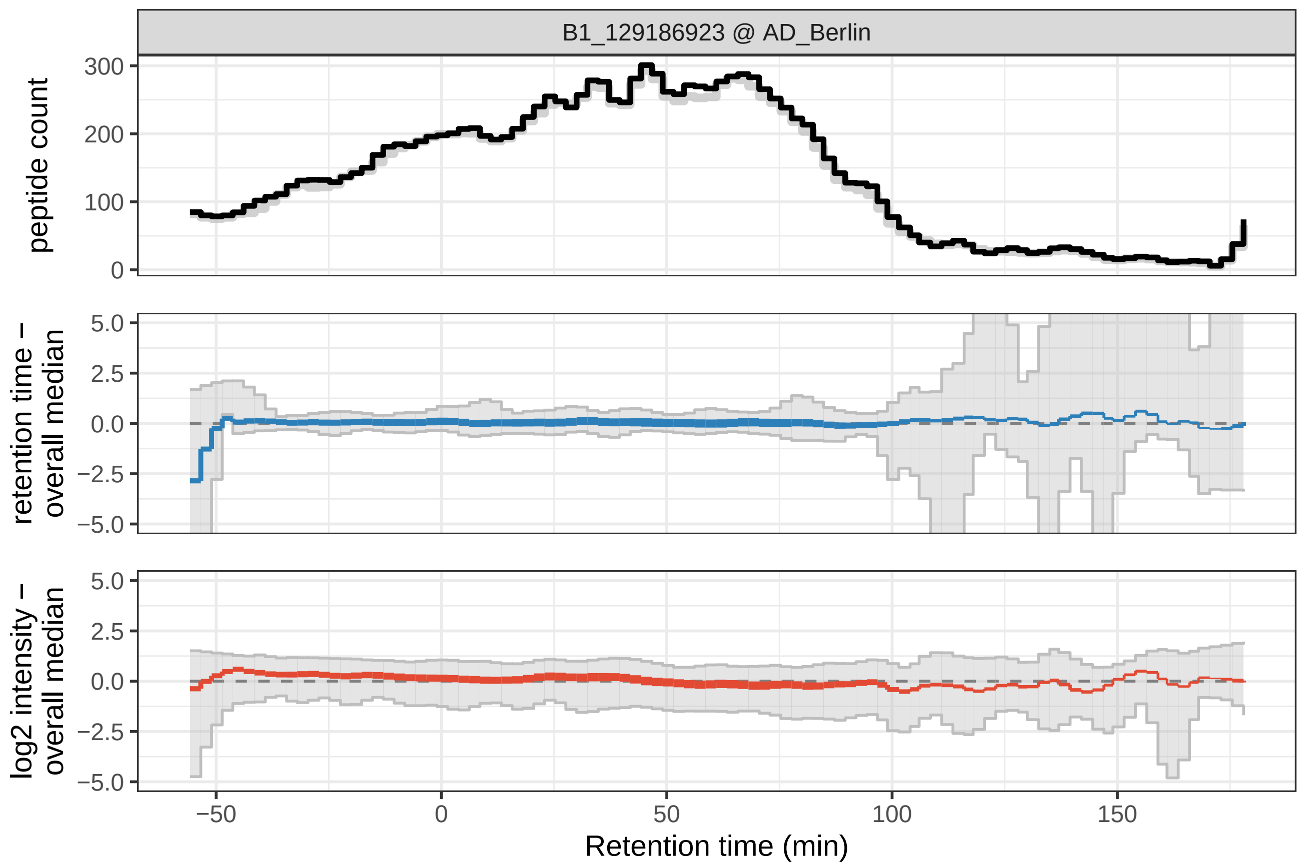
The top panel shows the number of peptides in the input data, e.g. as recognized by the software that generated input for this pipeline, over time (black line). For reference, the grey line shows the median amount over all samples (note; if this is the exact same in all samples, the grey line may not be visible as it falls behind the black line).

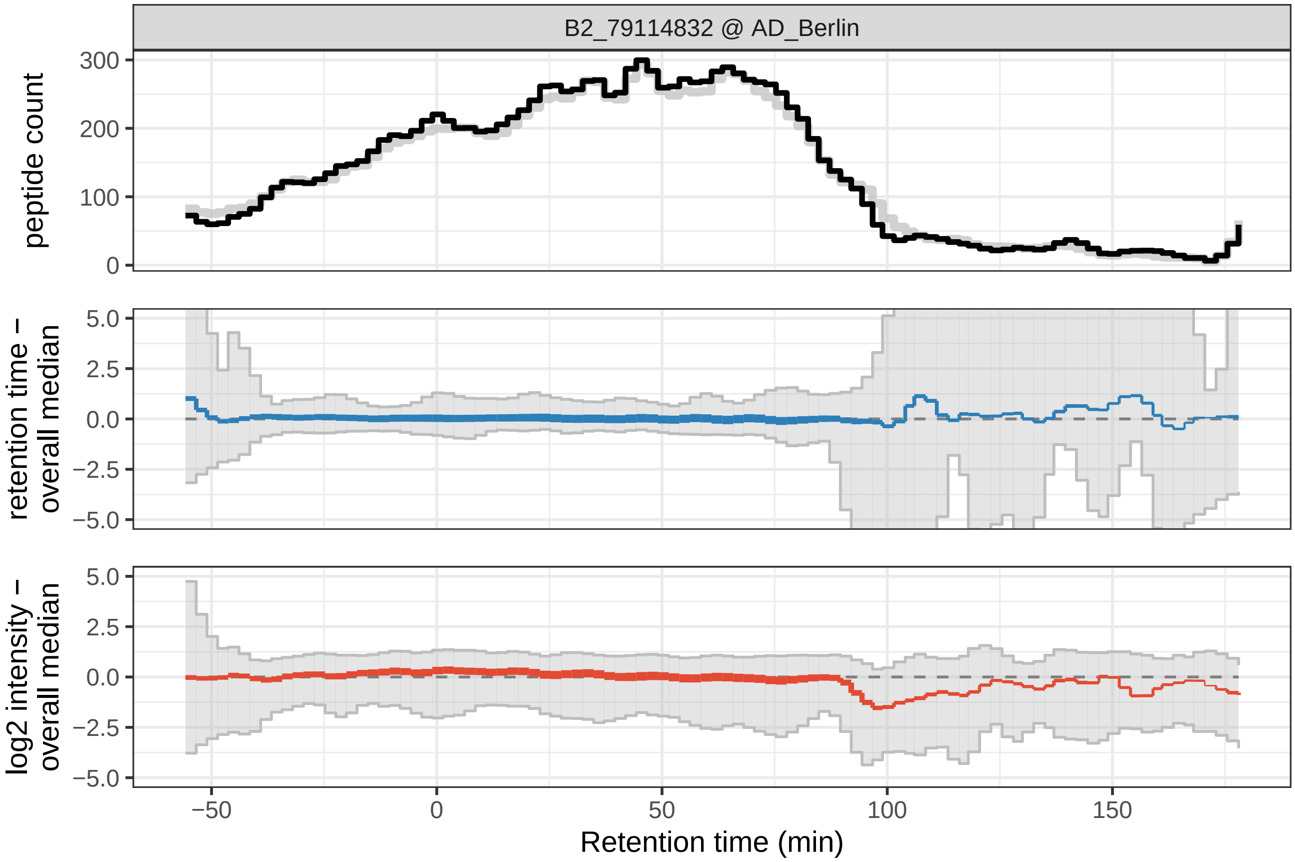
The middle panel indicates whether peptide retention times deviate from their median over all samples (blue line). The grey area depicts the 5% and 95% quantiles, respectively. The line width corresponds to the number of peptides eluting at that time (data from first panel). Analogously, the bottom panel shows the deviation in peptide abundance as compared to the median over all samples (red line).

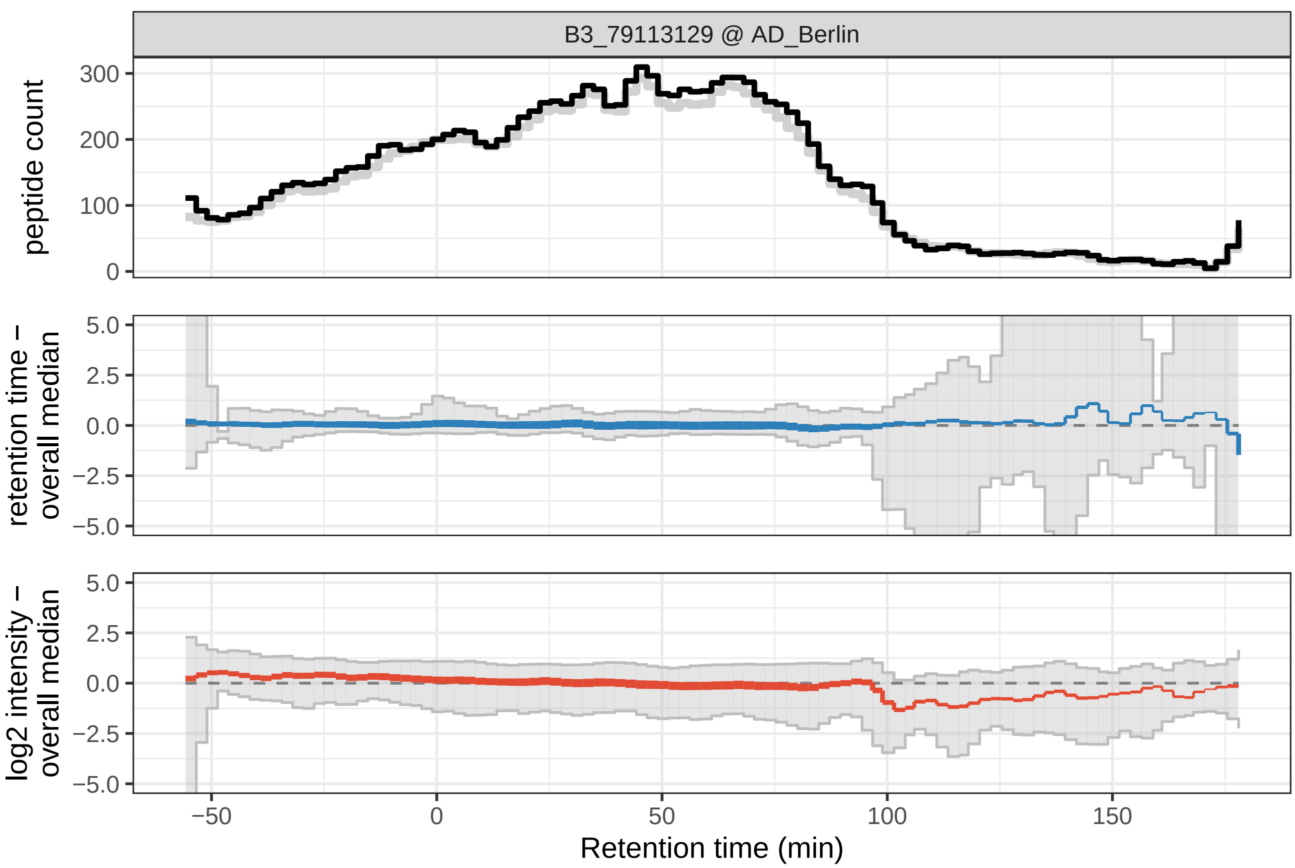

A2_82872920 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

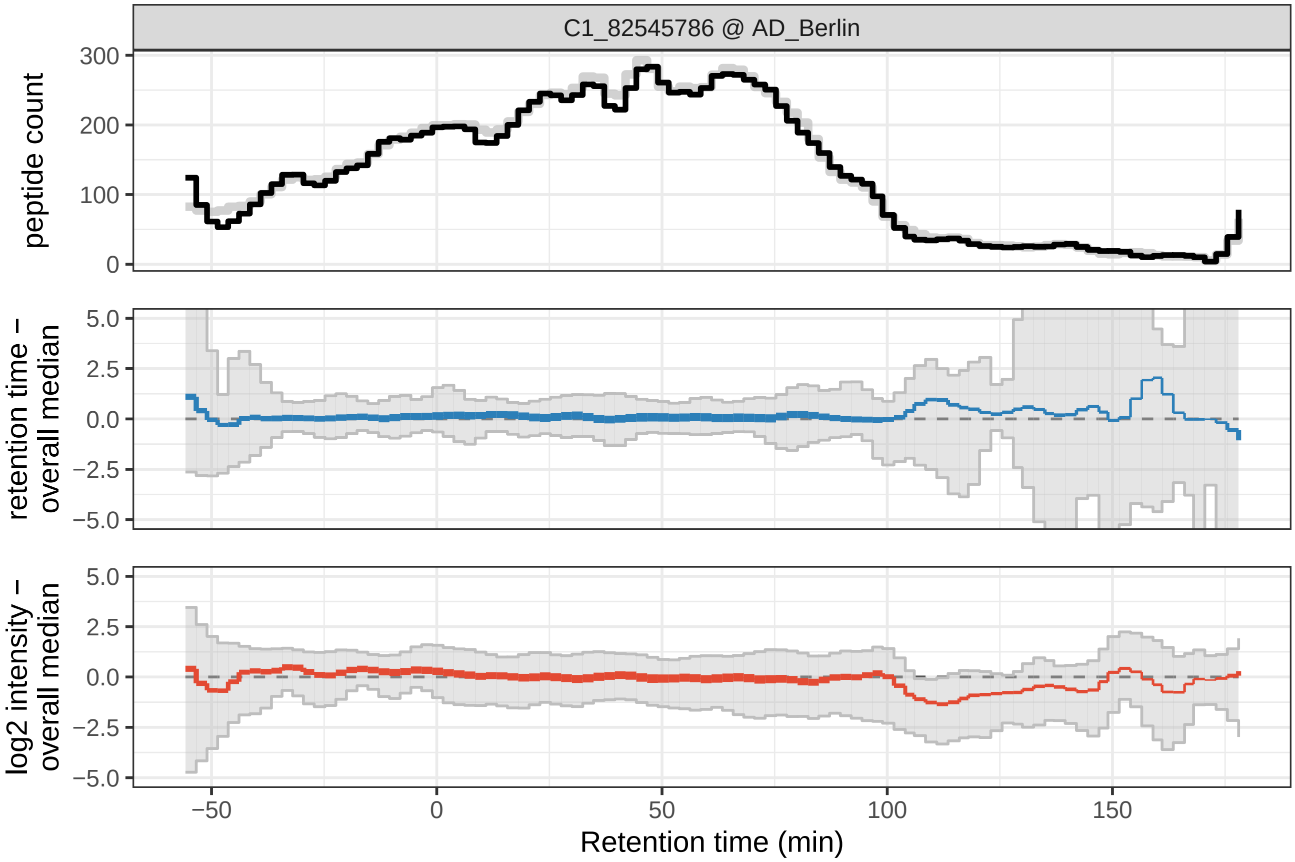

A3_82883165_repeat2 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

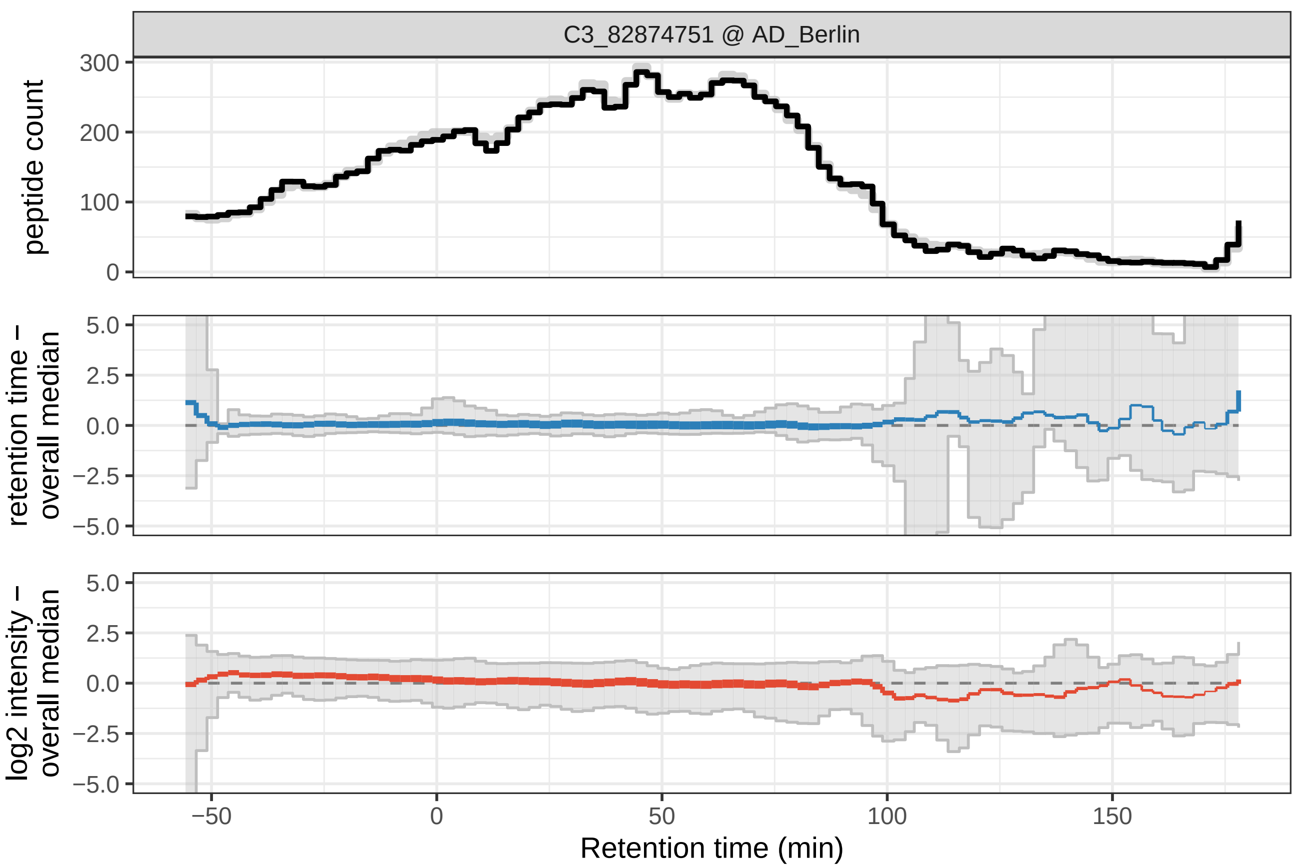

A4_190104103 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

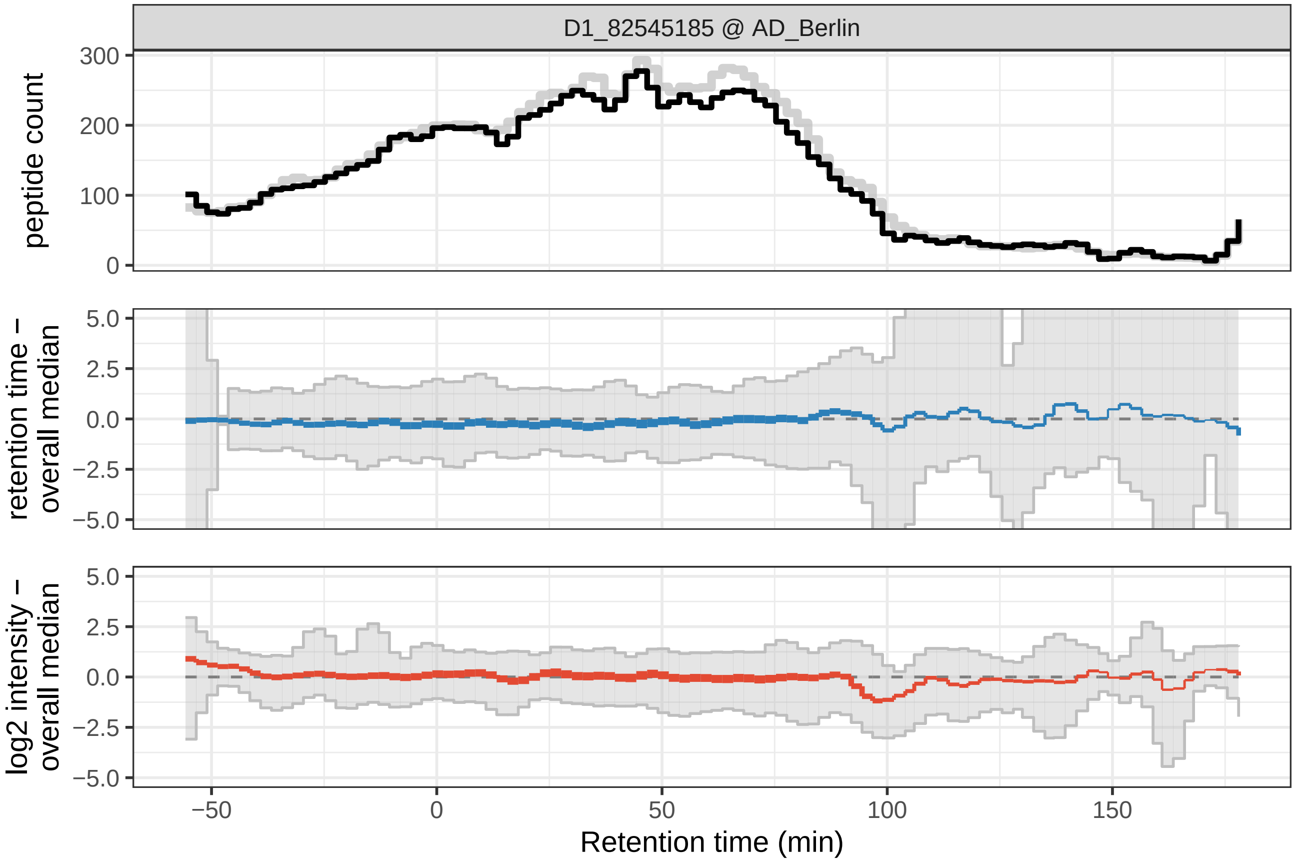

B1_129186923 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

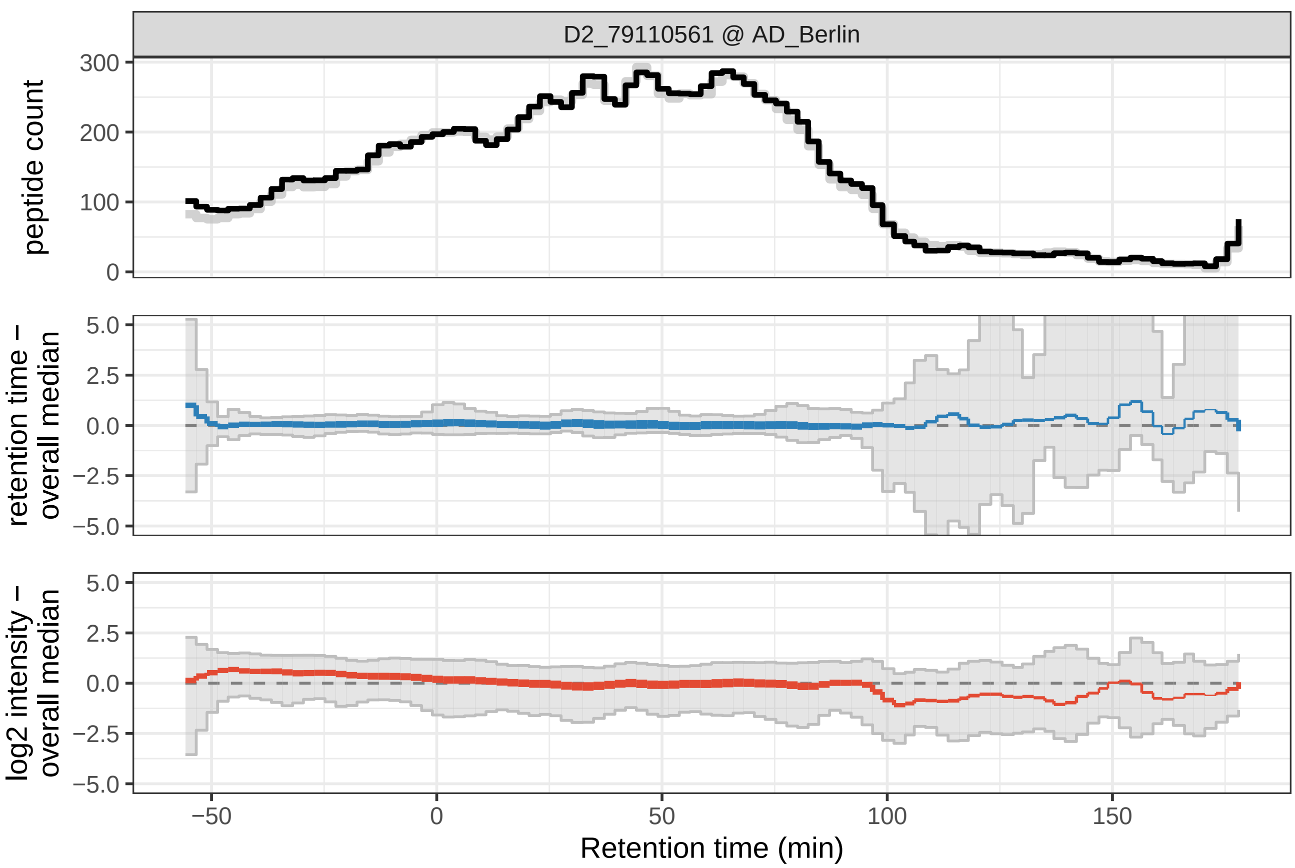

B2_79114832 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

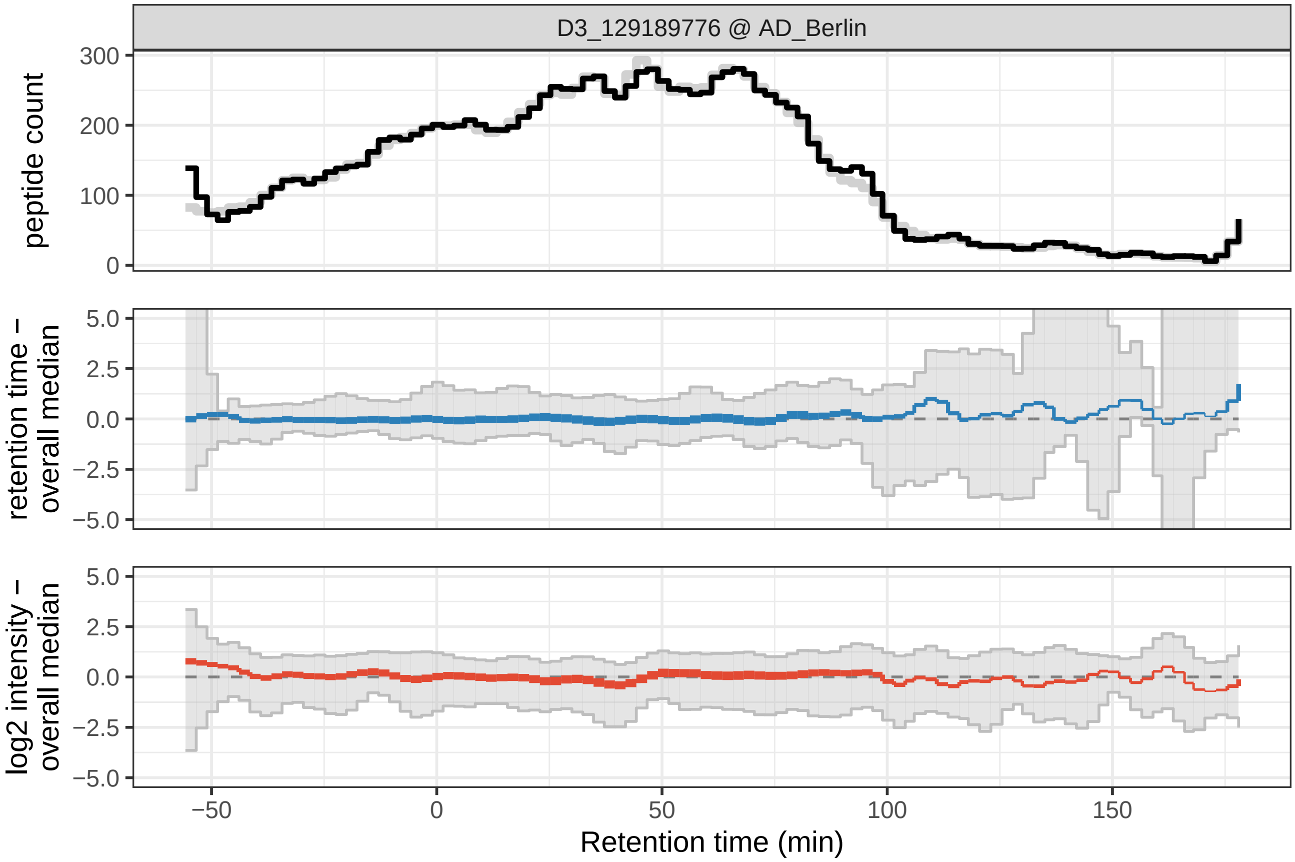

B3_79113129 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


C1_82545786 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

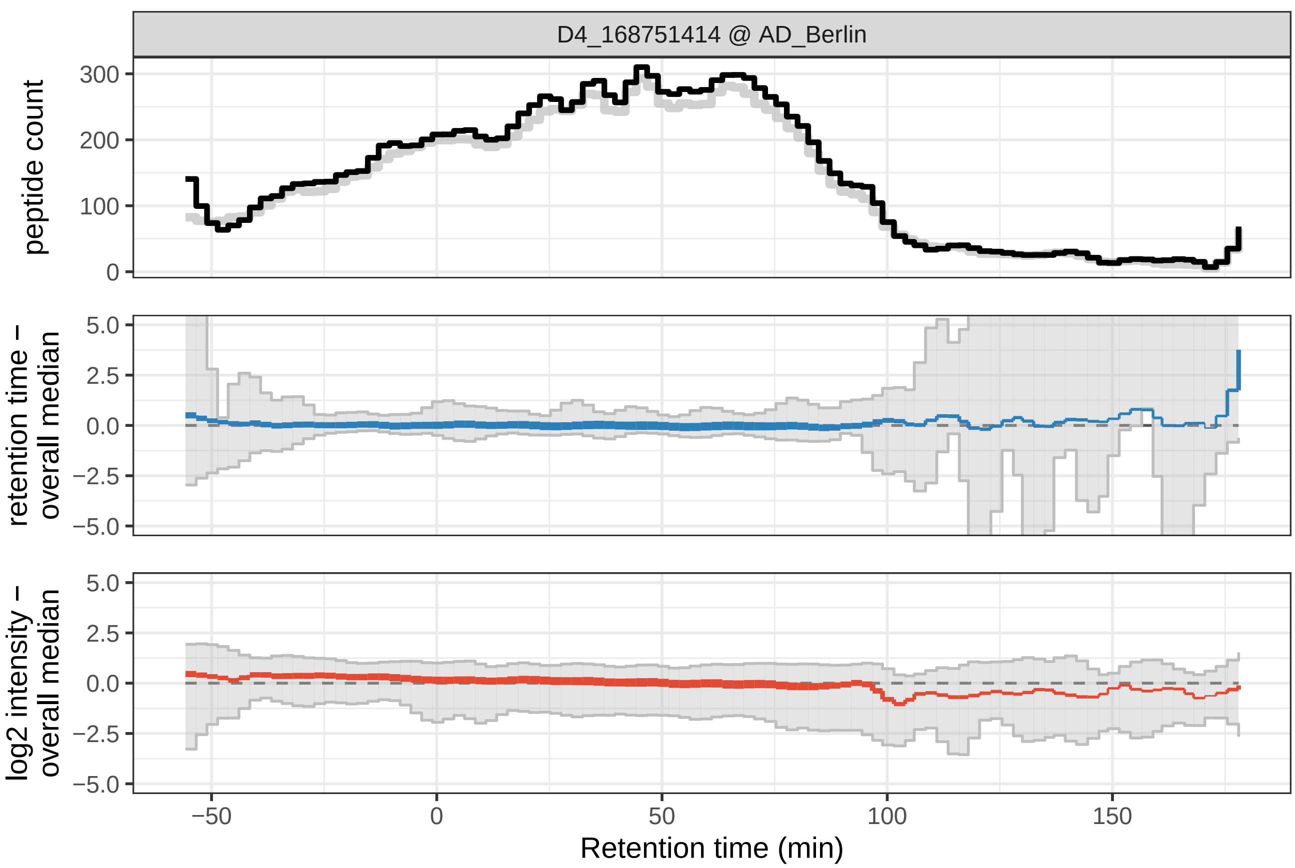

C3_82874751 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


D1_82545185 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

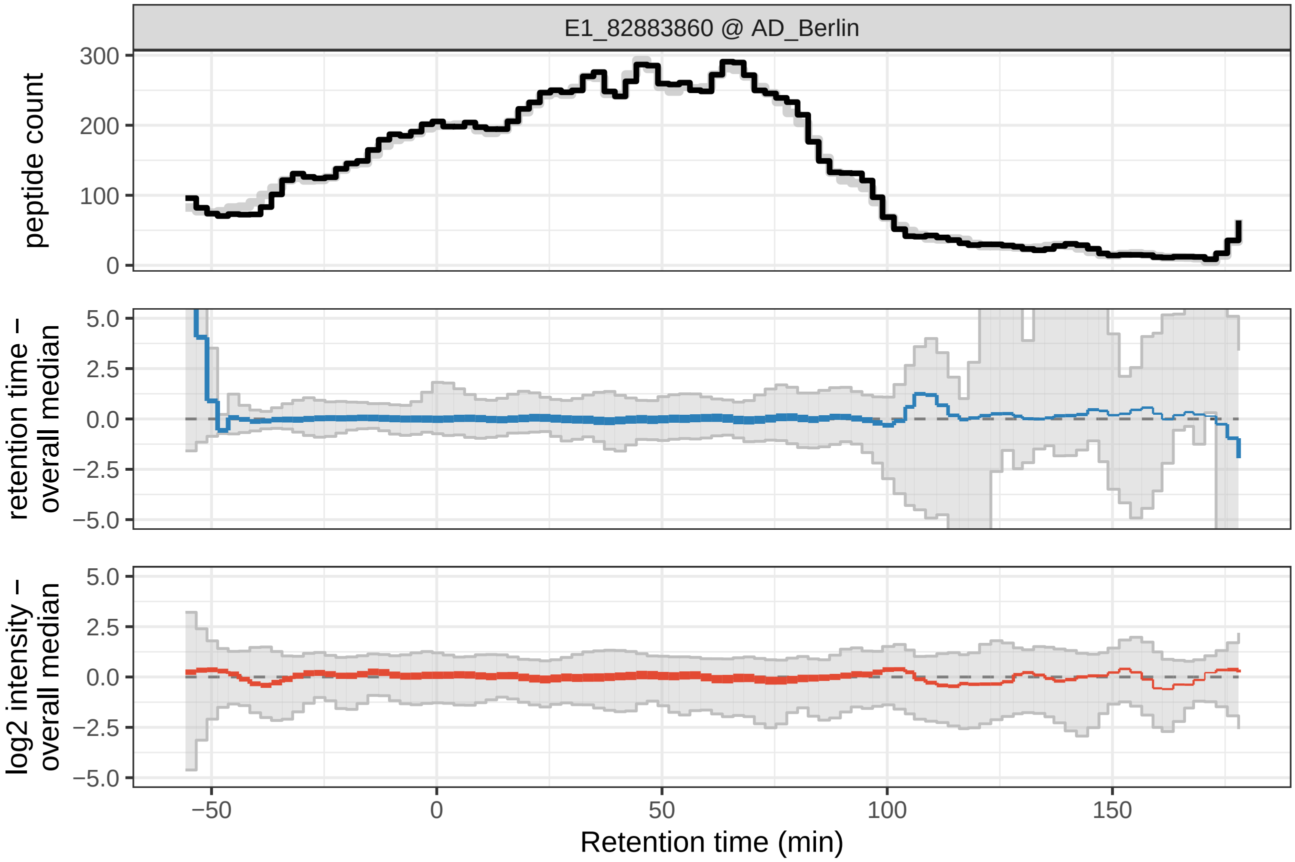

D2_79110561 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

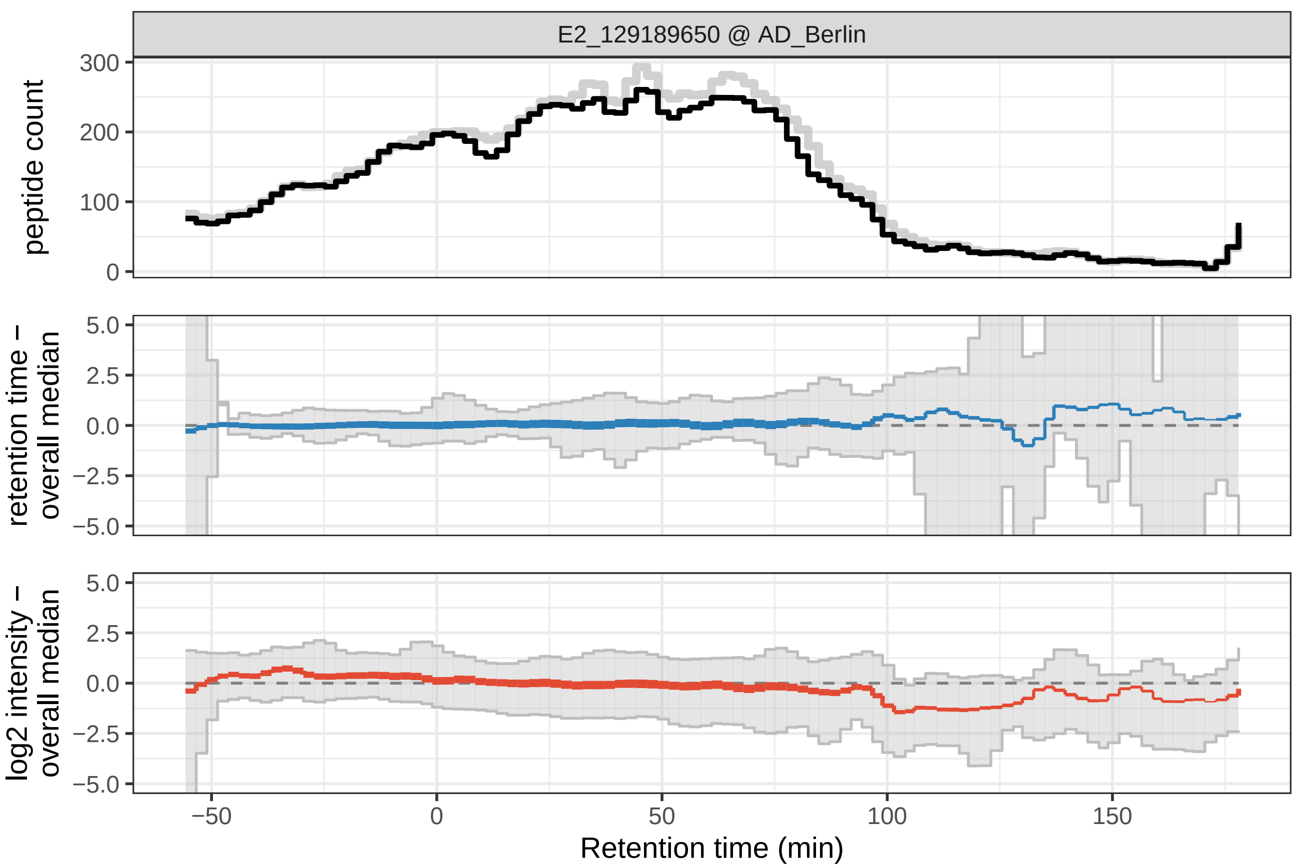


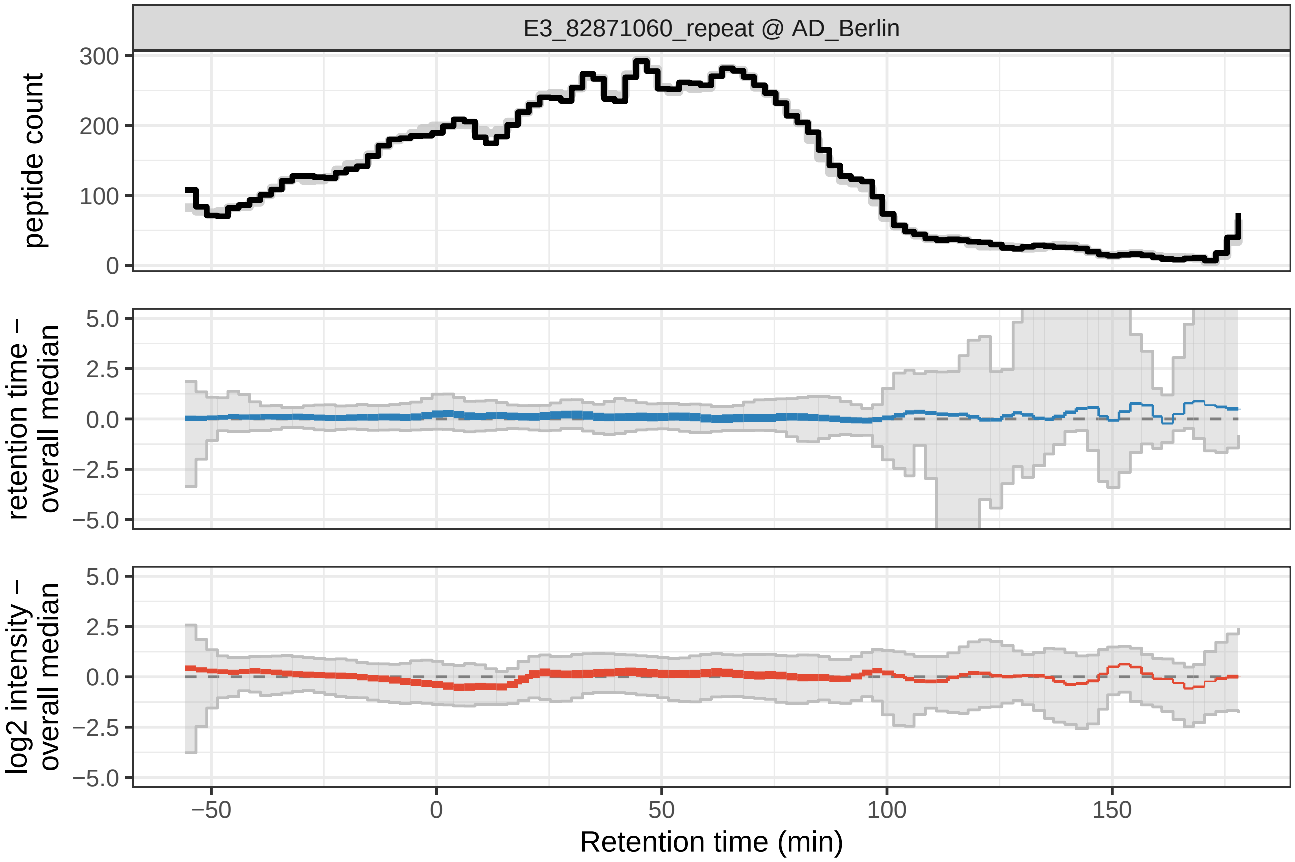
D3_129189776 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

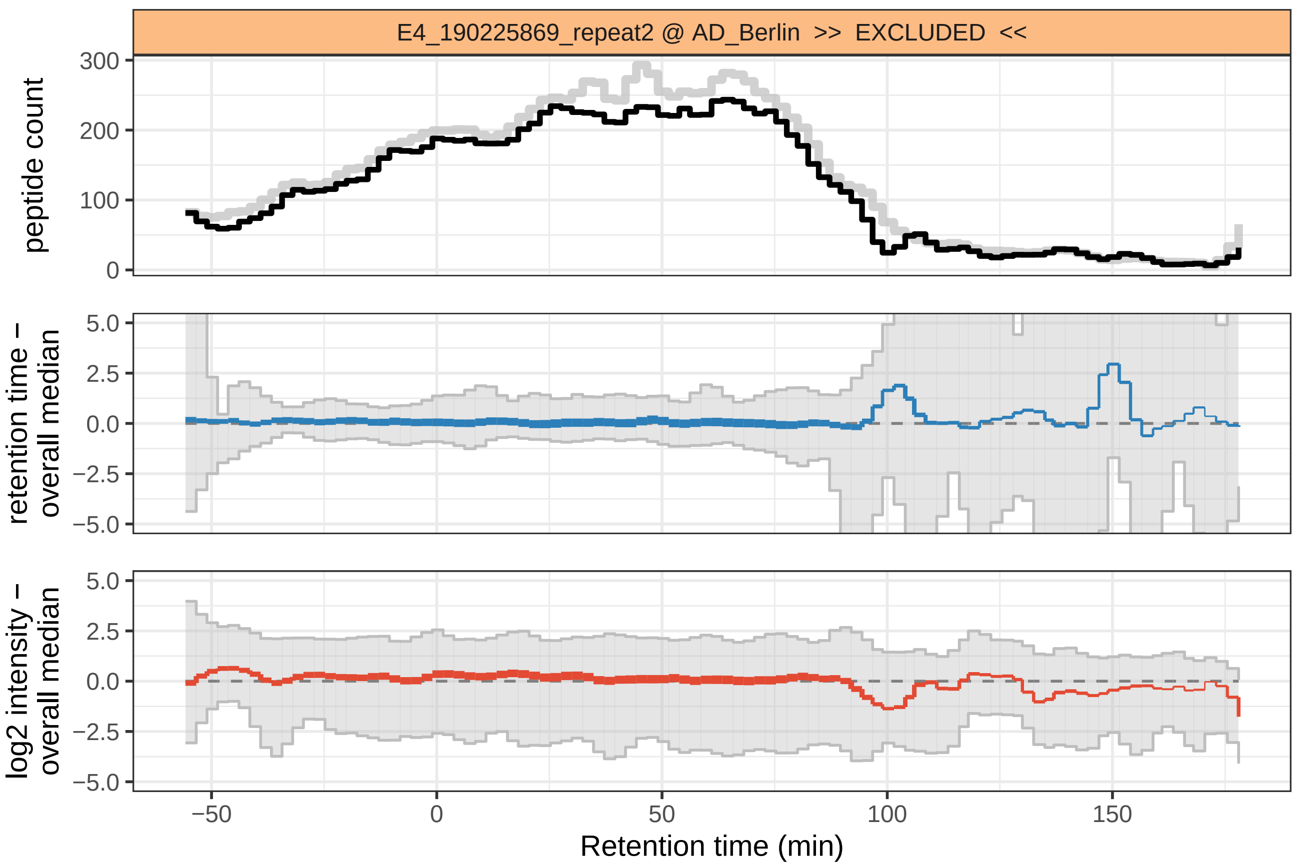


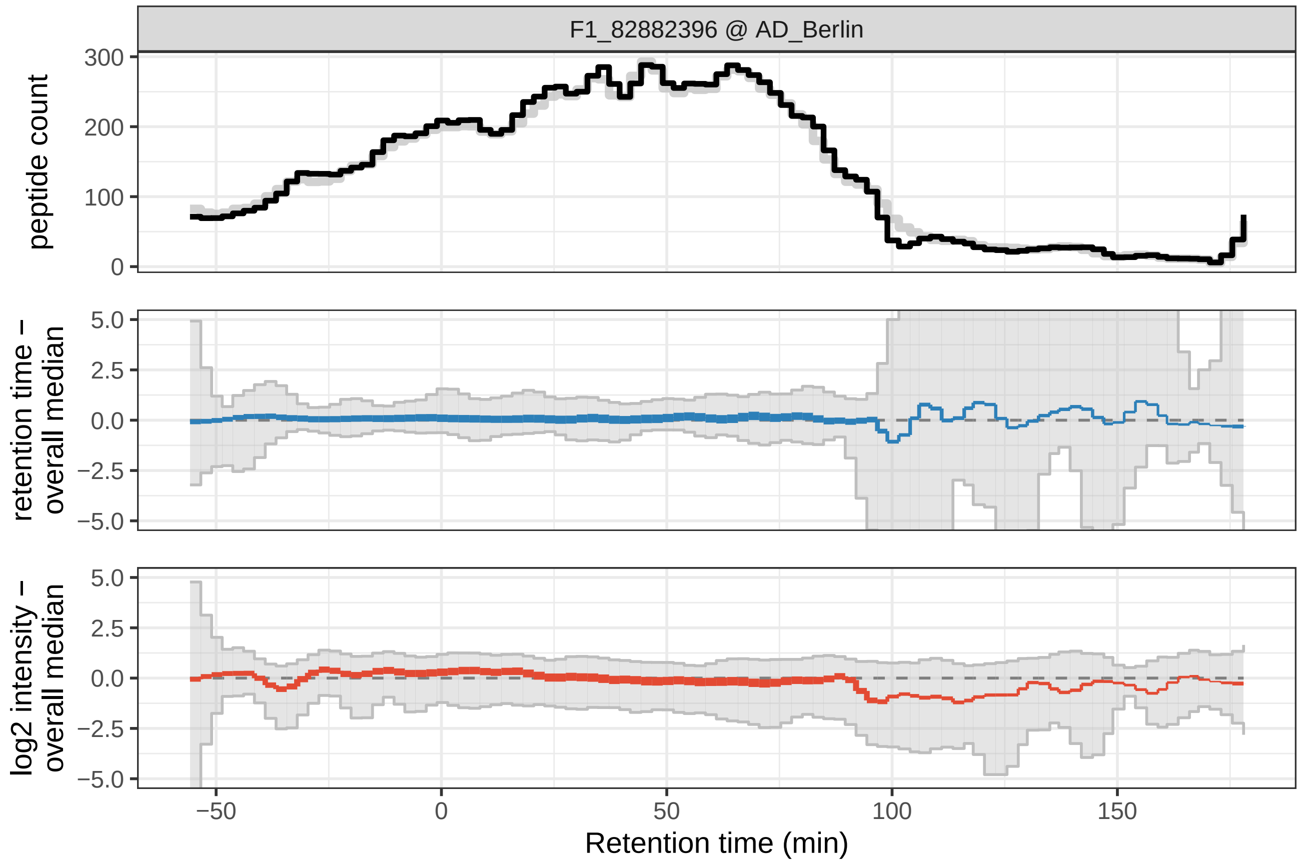
D4_168751414 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

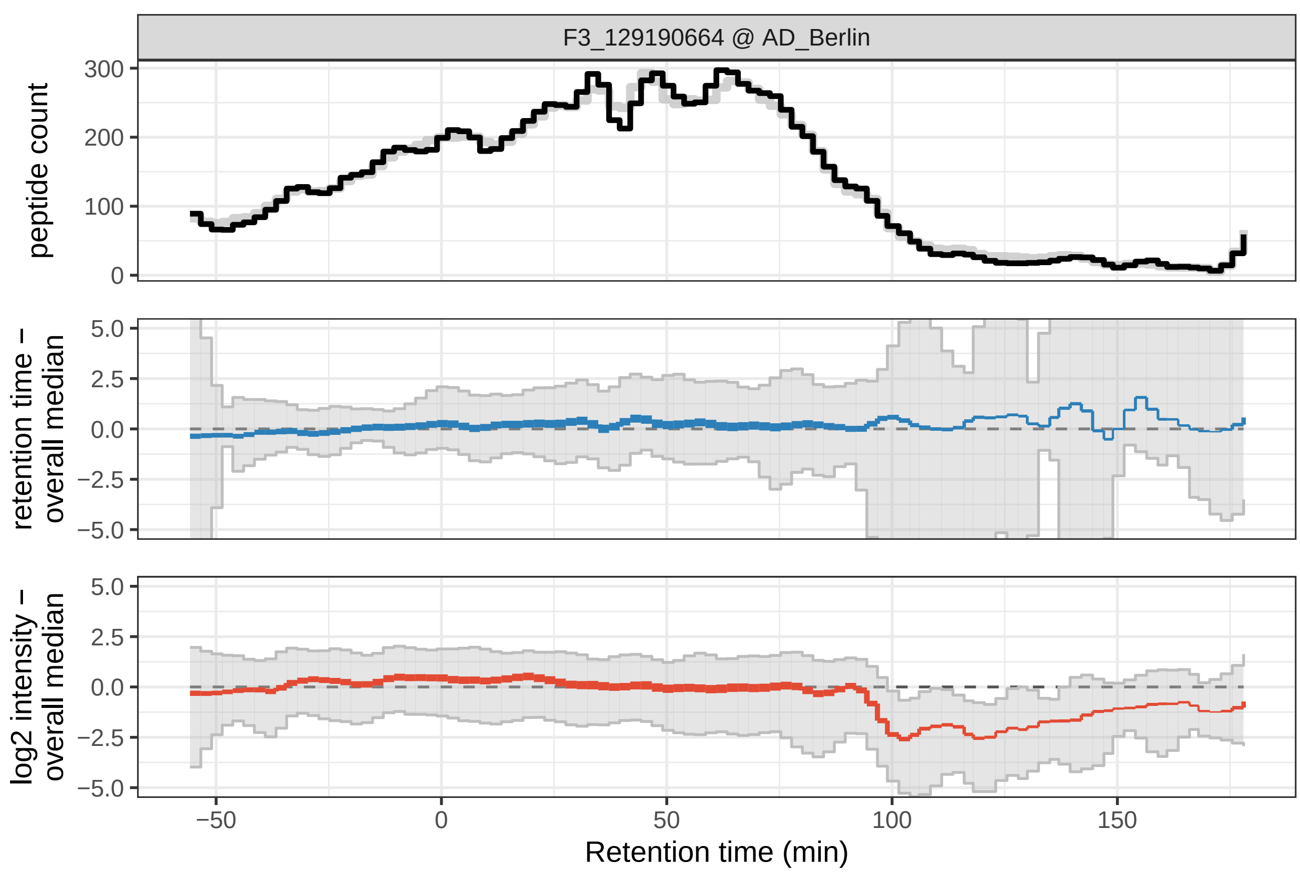

E1_82883860 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

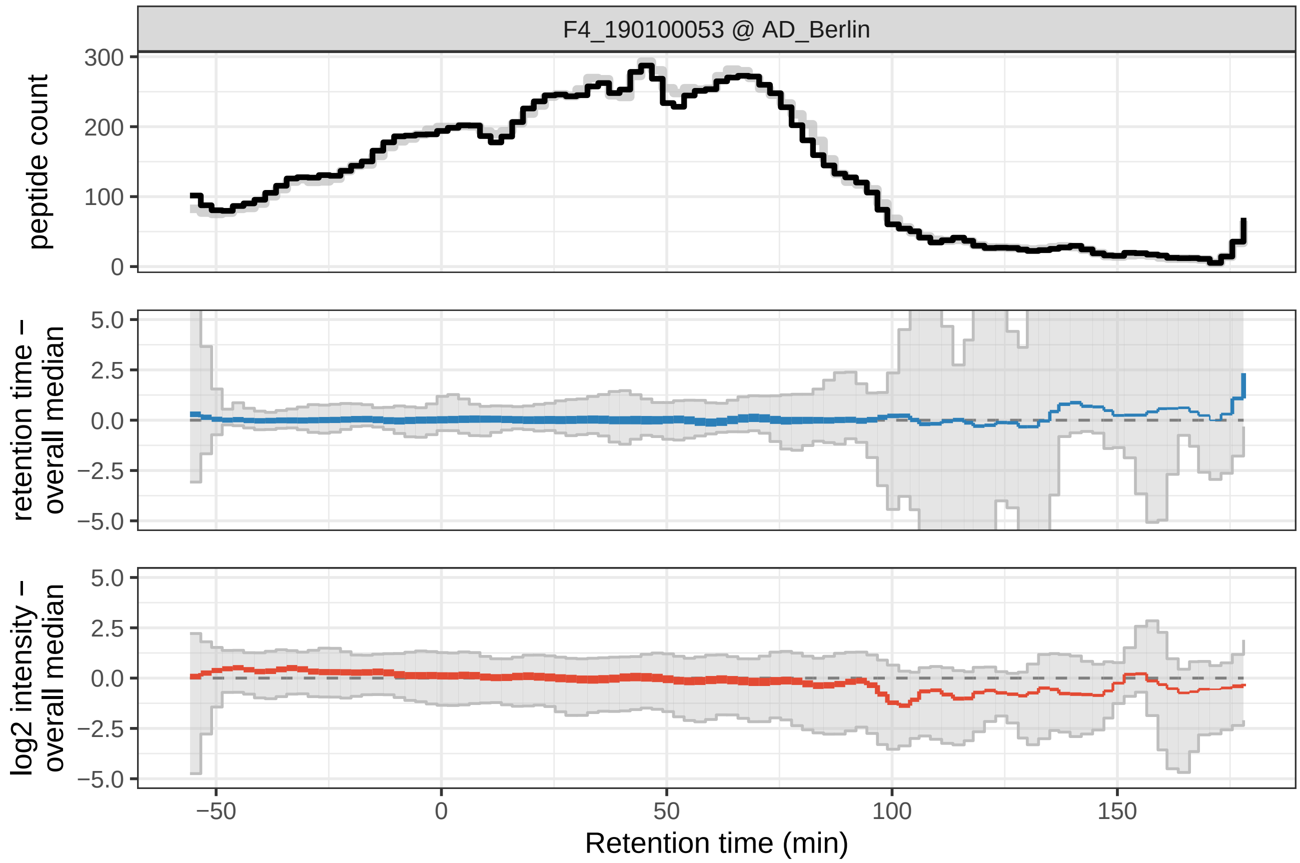

E2_129189650 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

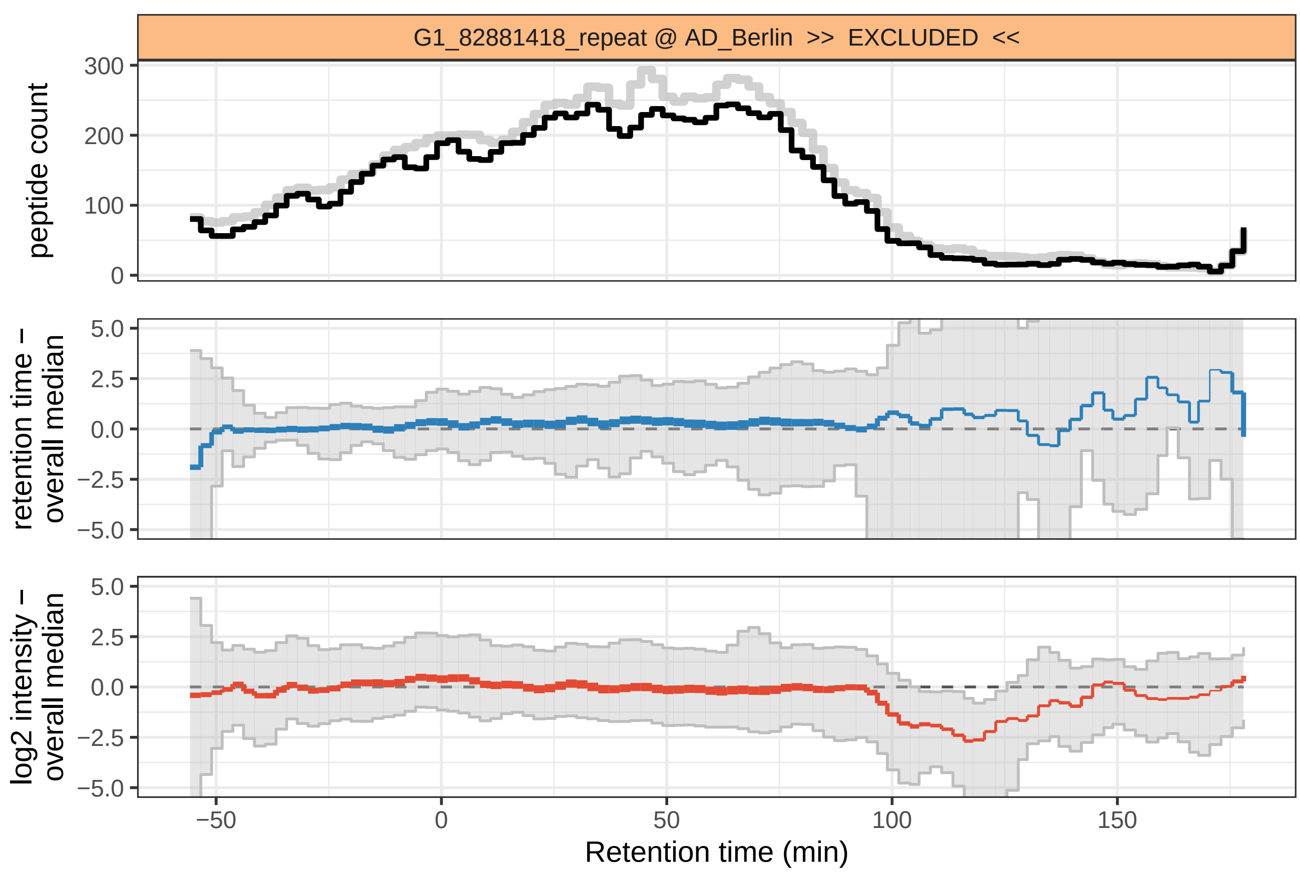

E3_82871060_repeat @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

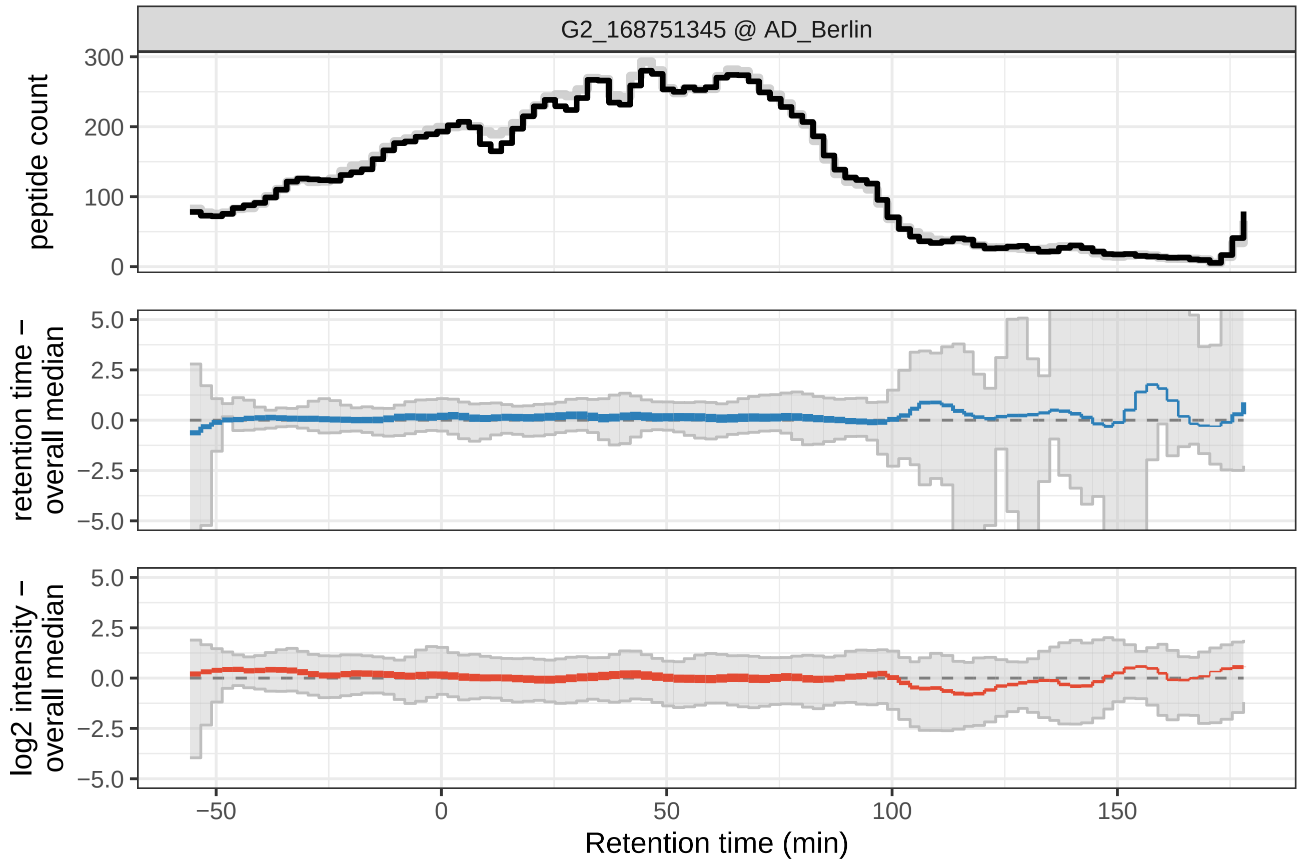

E4_190225869_repeat2 @ AD_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

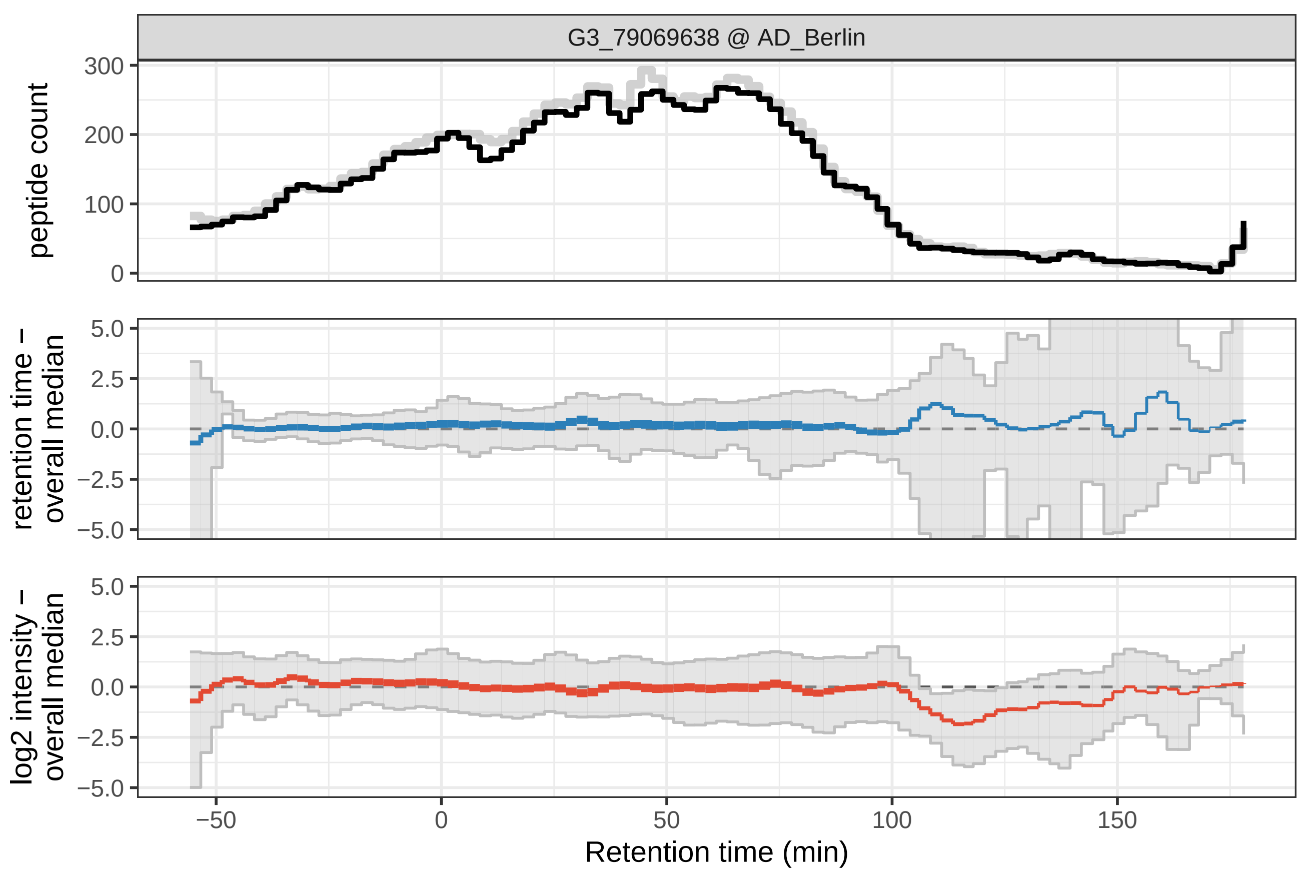

F1_82882396 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

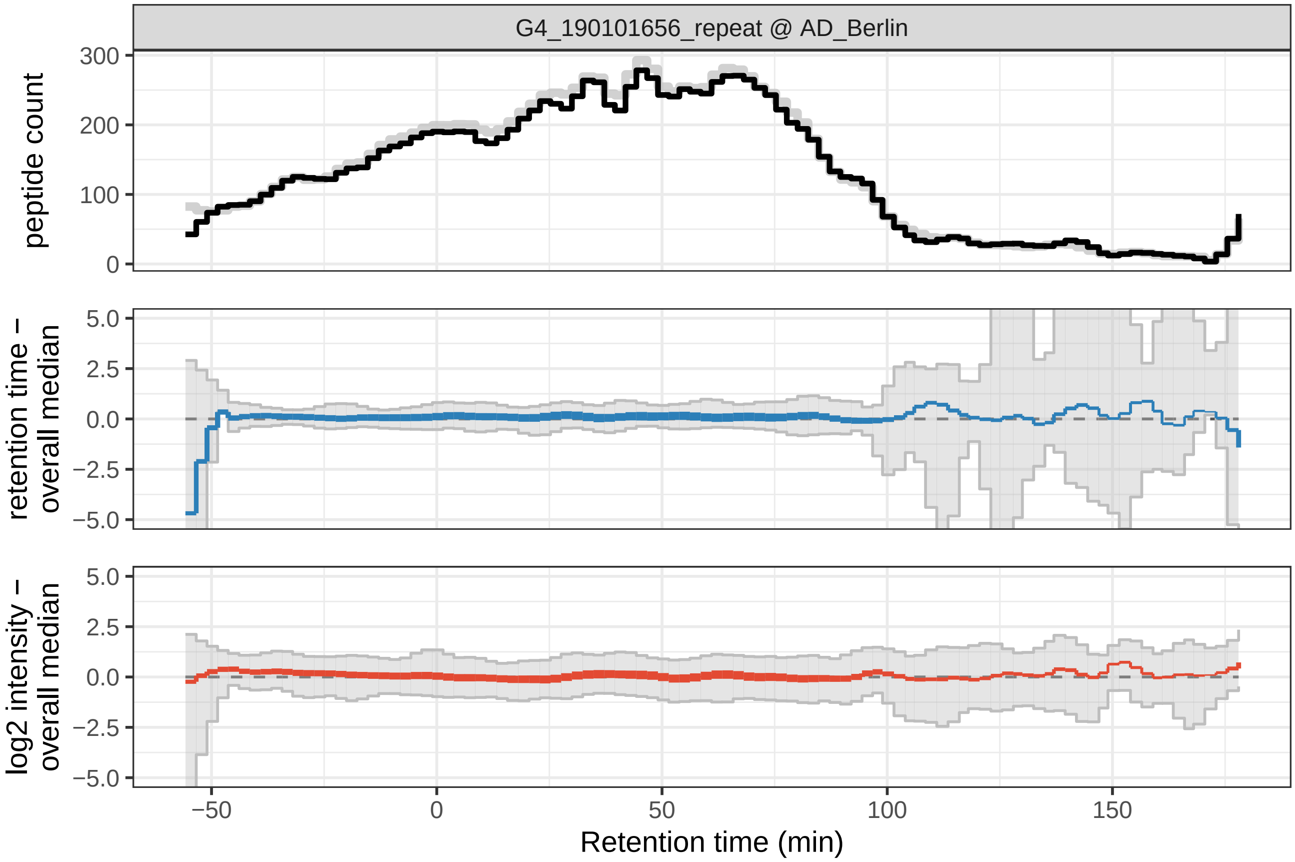

F3_129190664 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

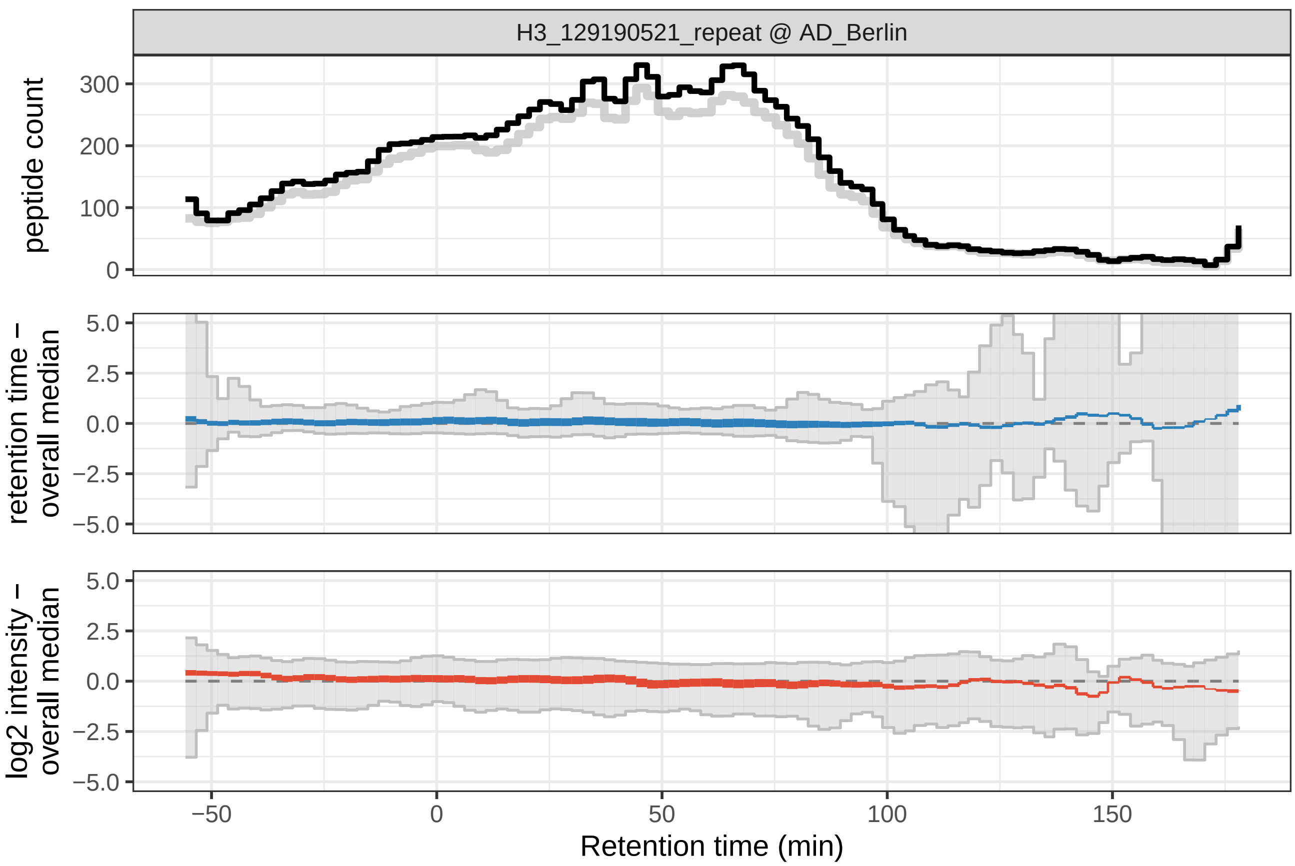

F4_190100053 @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

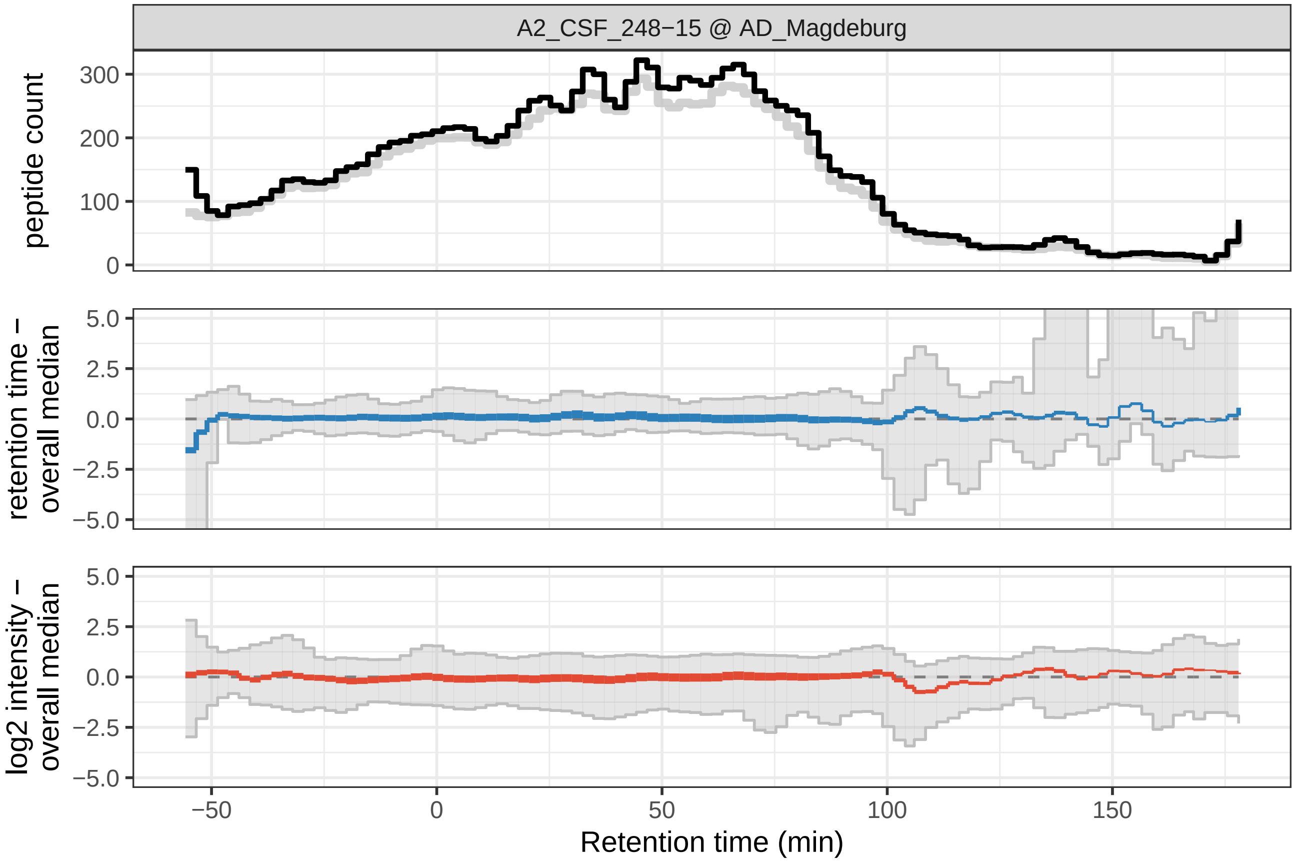

G1_82881418_repeat @ AD_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

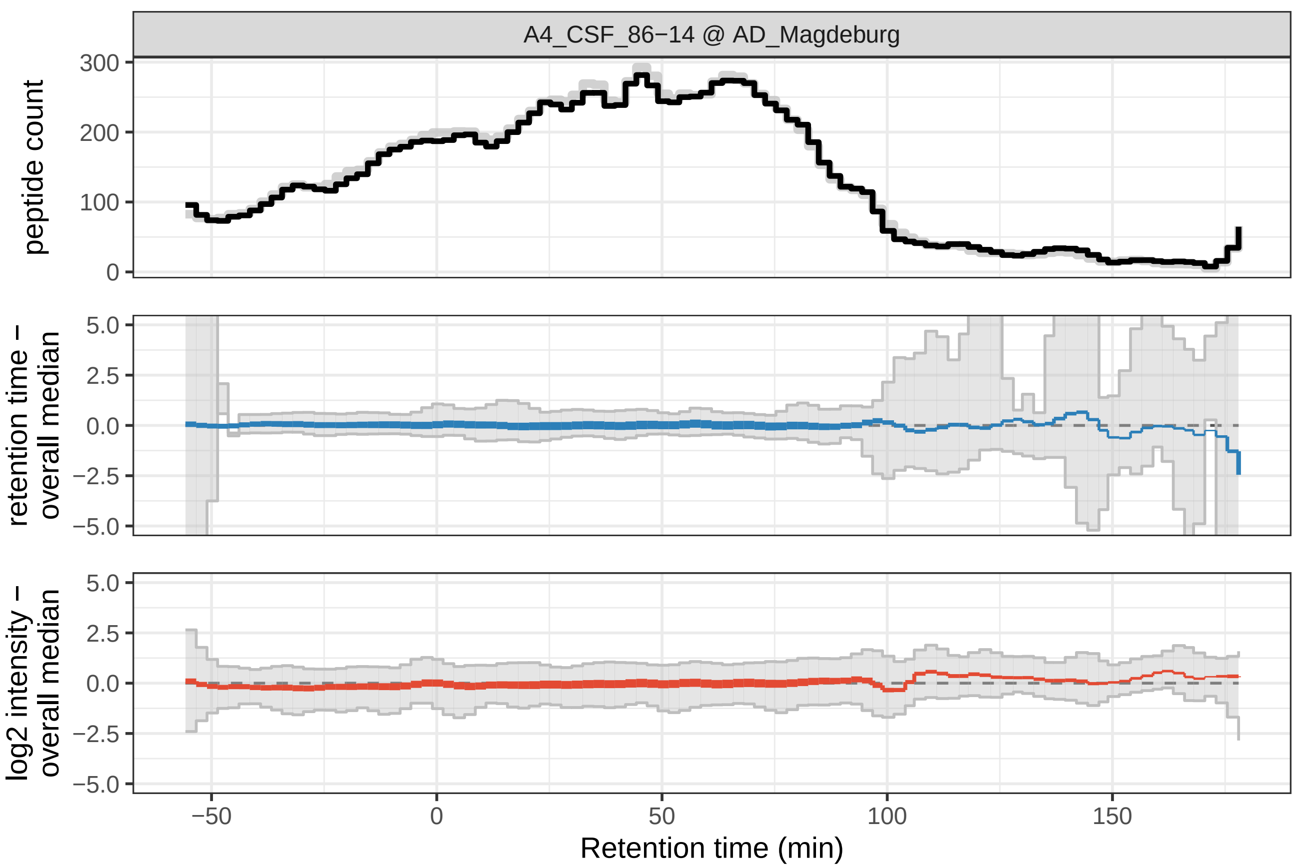

G2_168751345 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

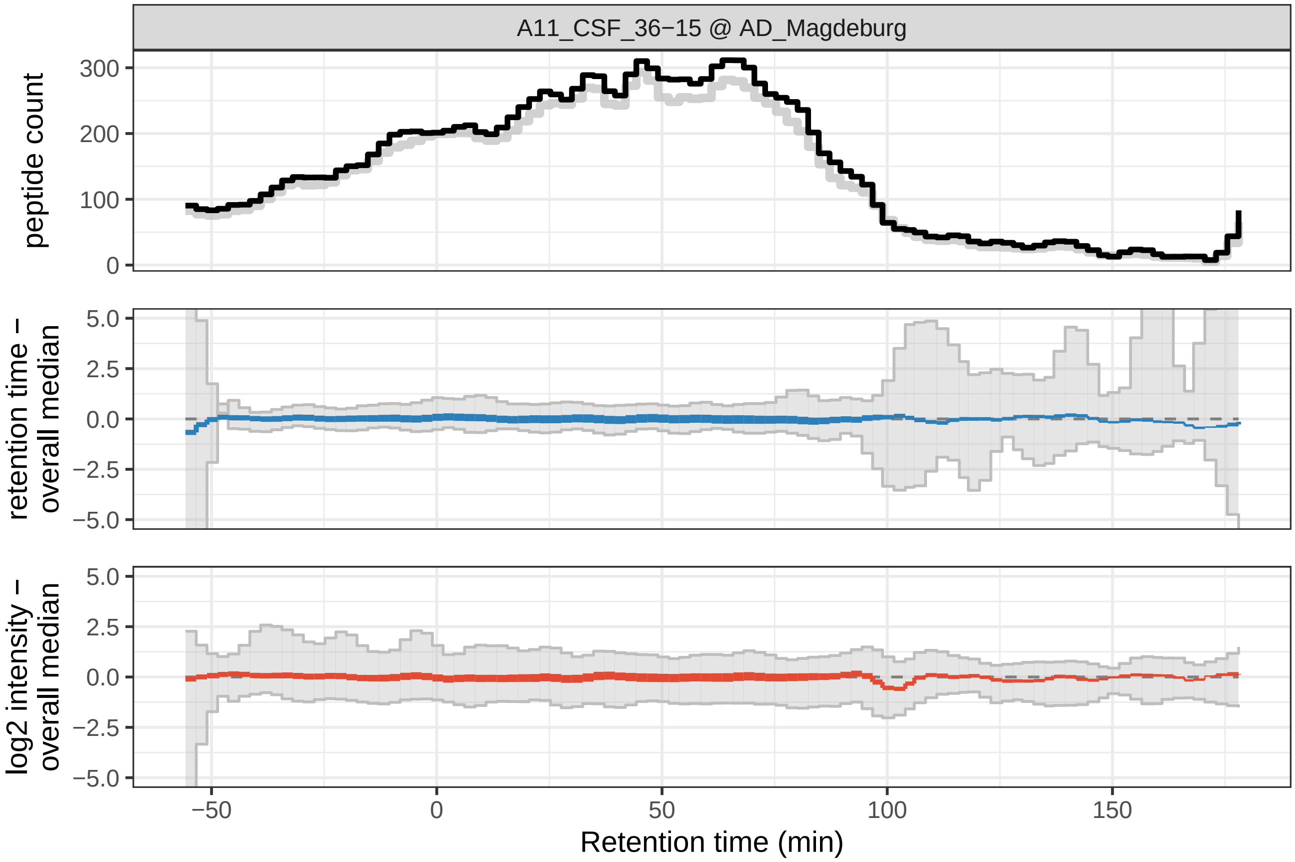

G3_79069638 @ AD_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

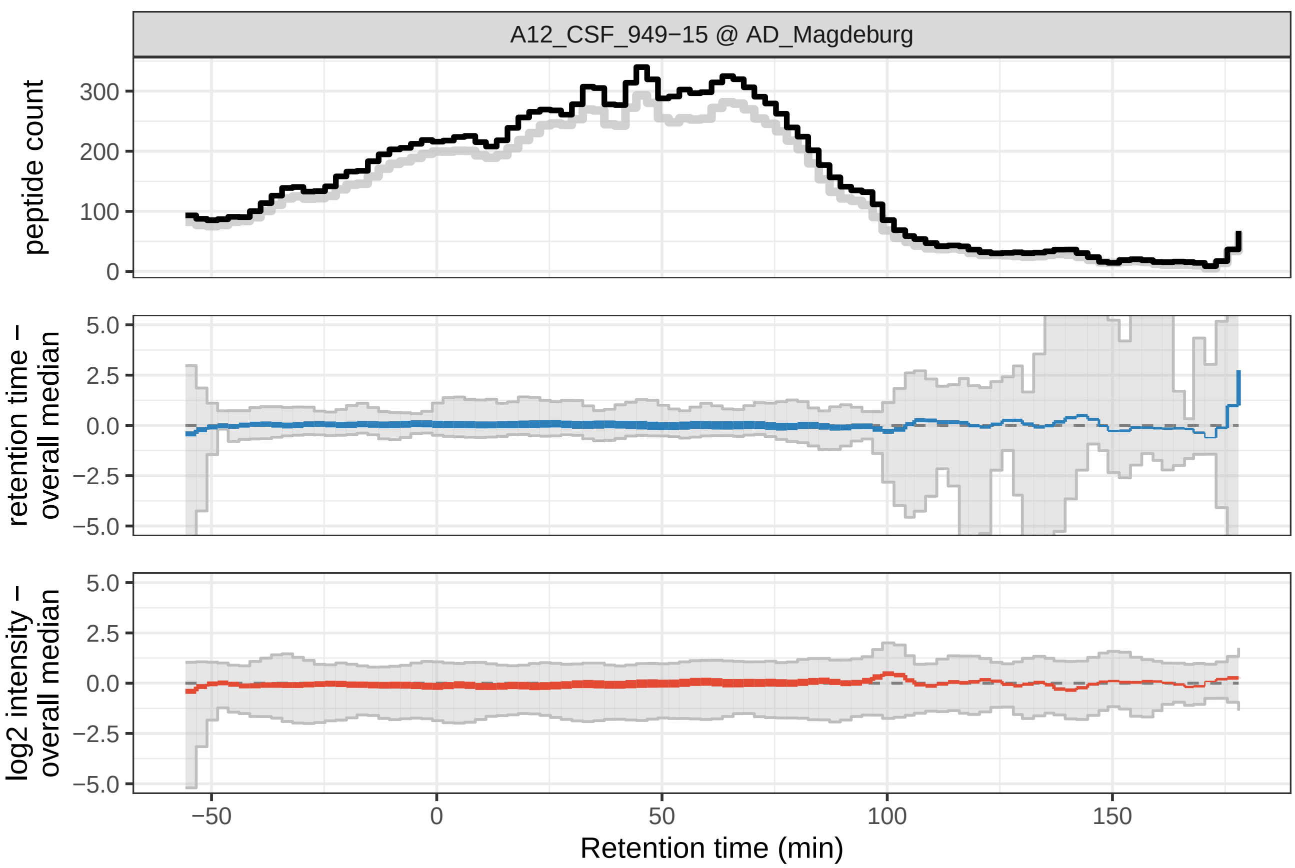

G4_190101656_repeat @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

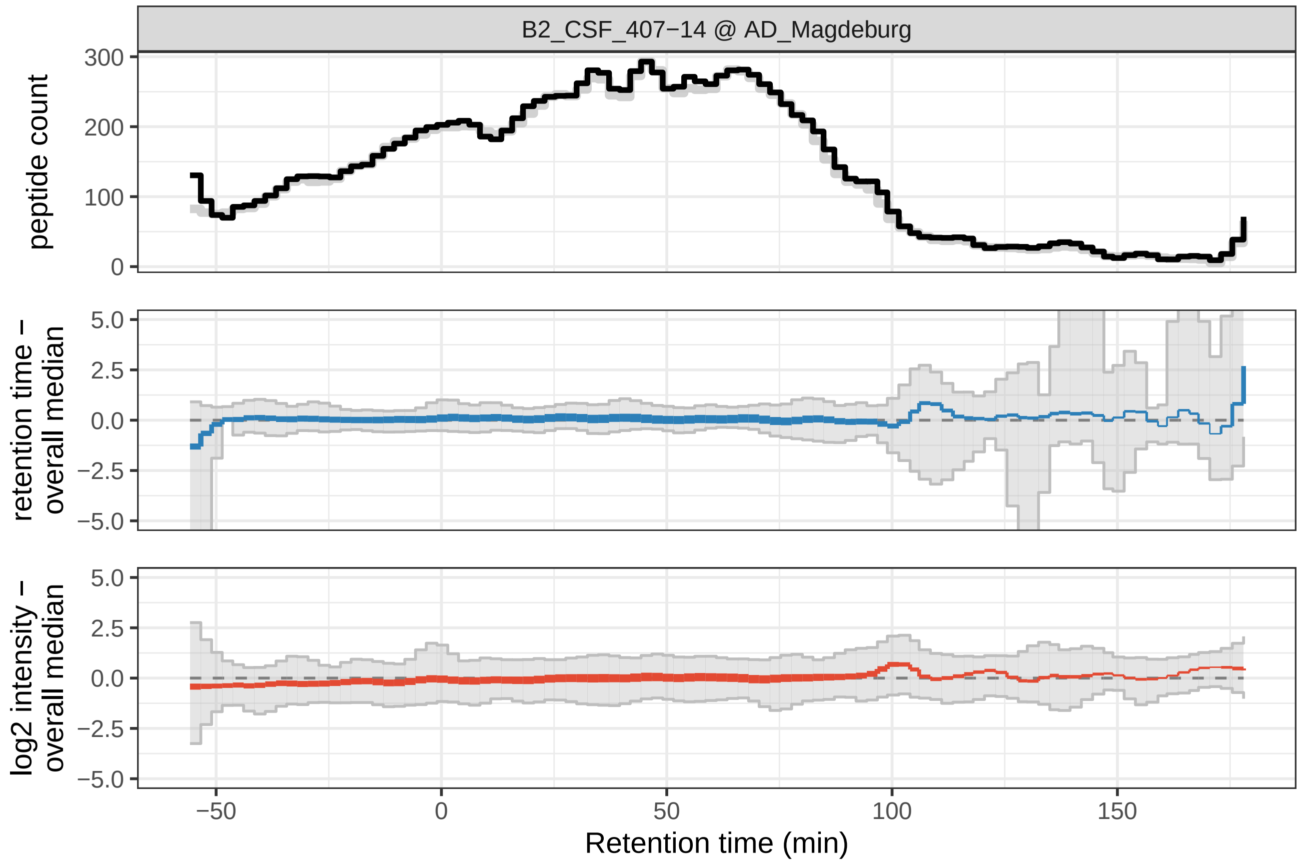

H3_129190521_repeat @ AD_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

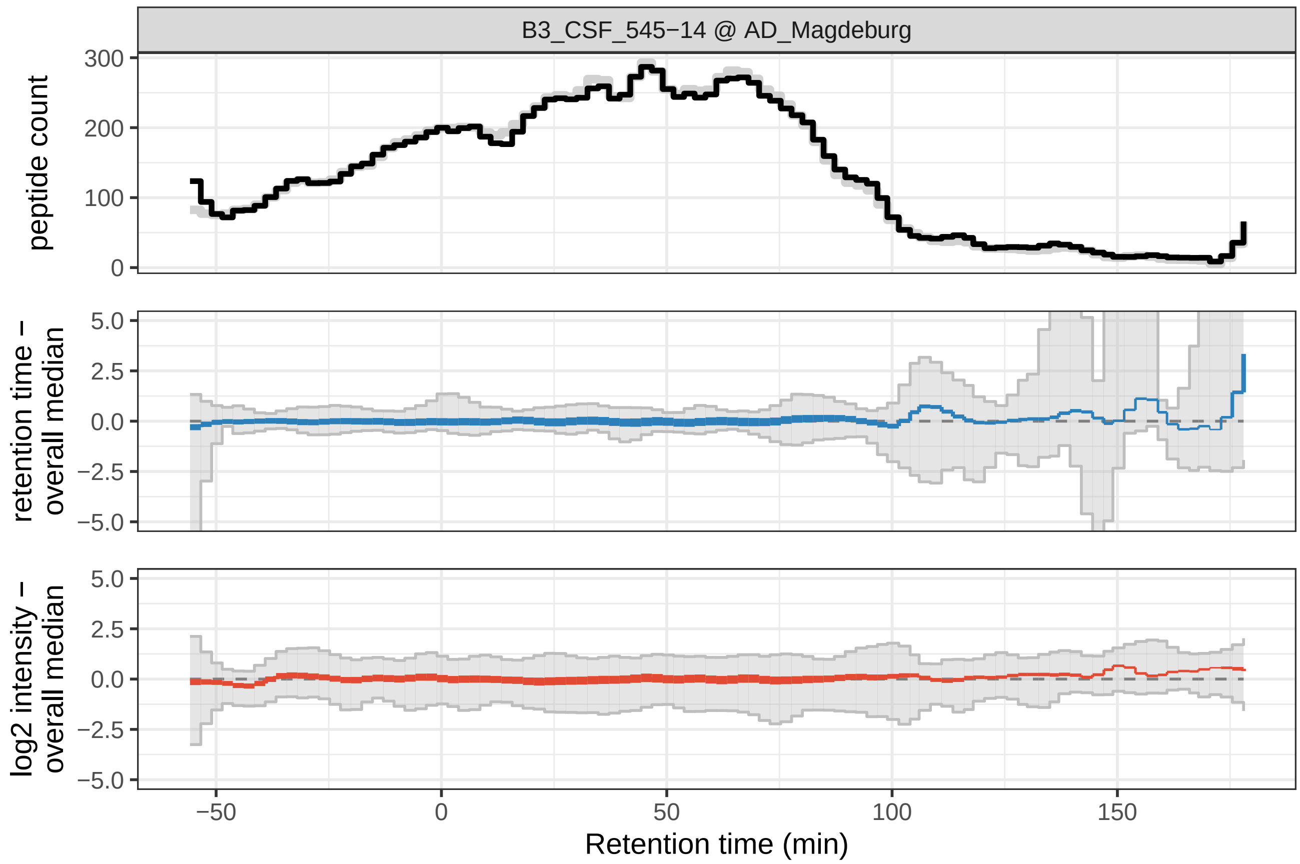

A2_CSF_248−15 @ AD_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

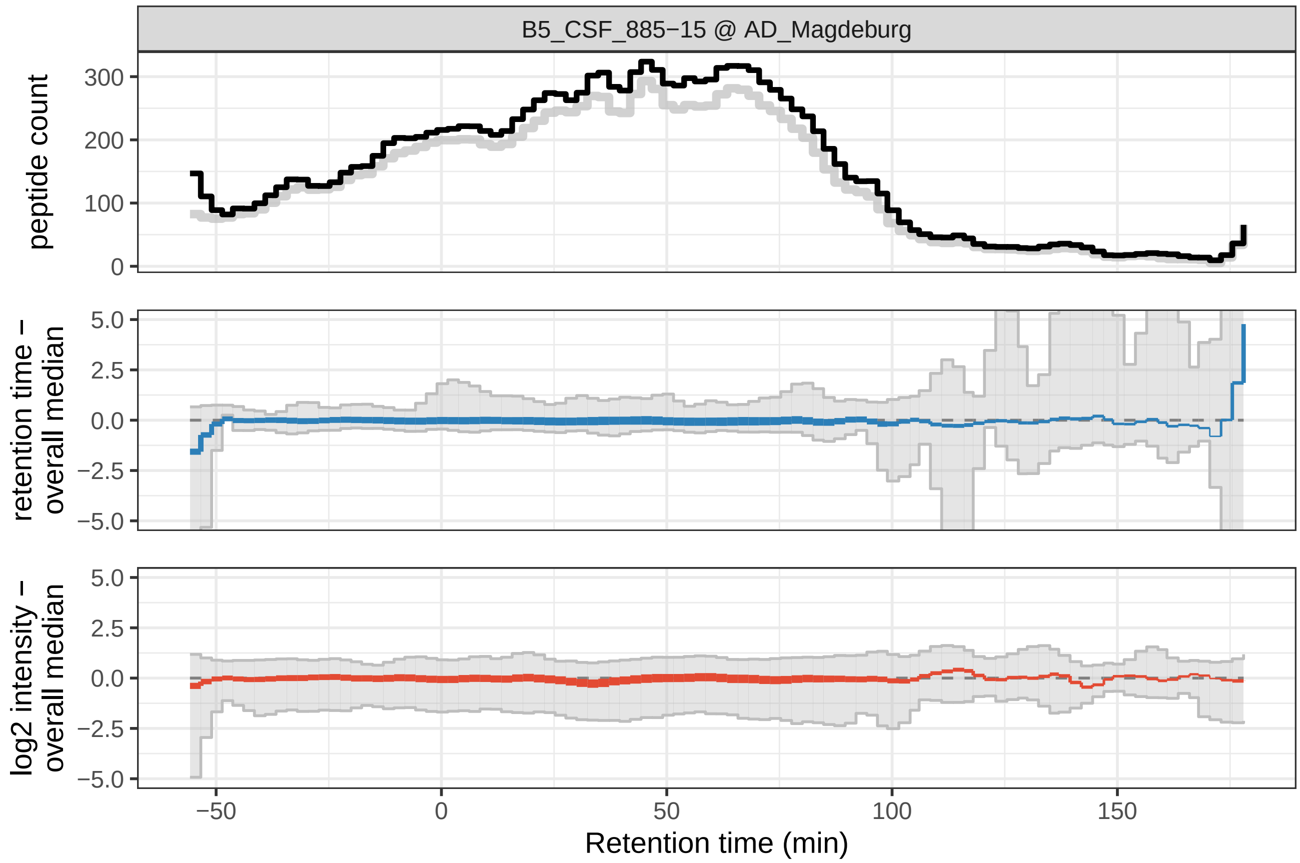

A4_CSF_86−14 @ AD_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

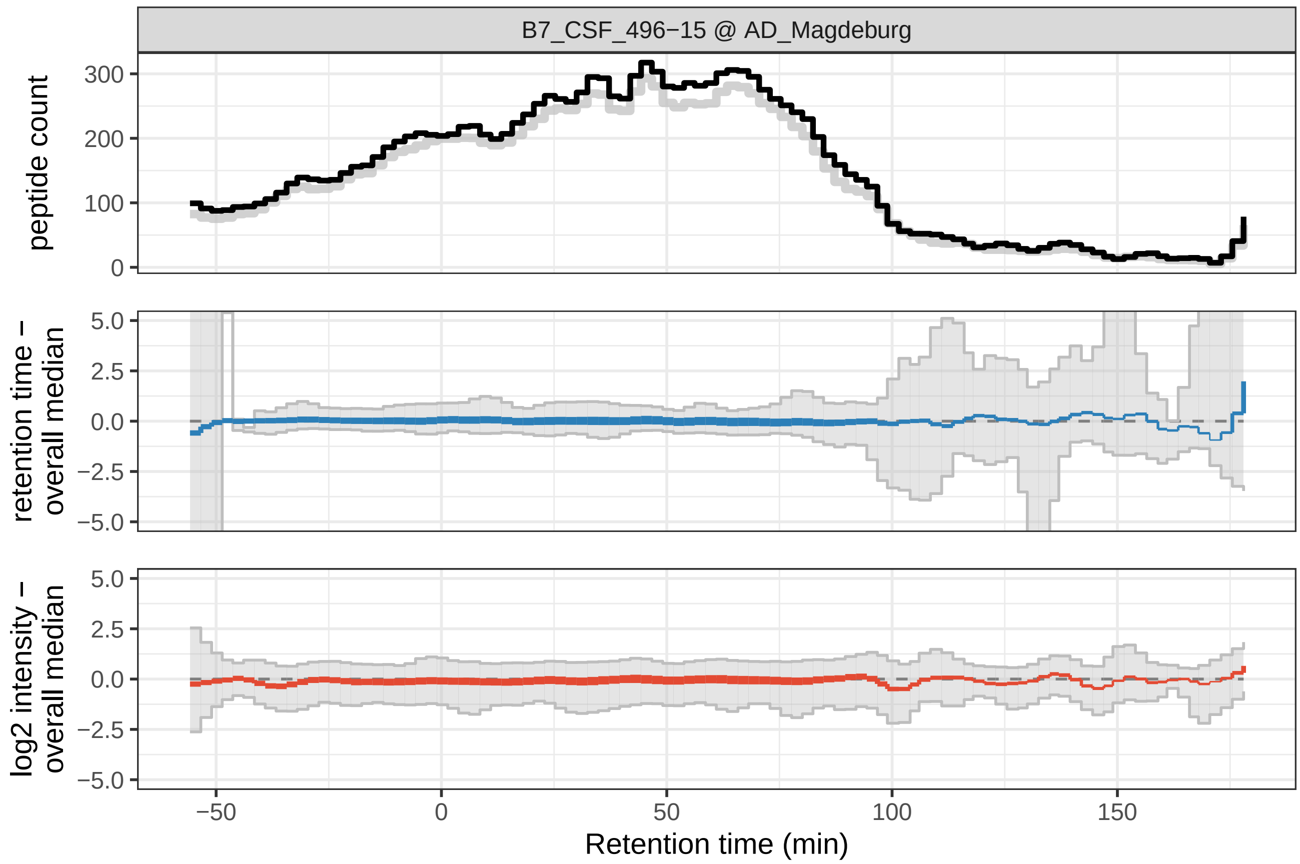

A11_CSF_36−15 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

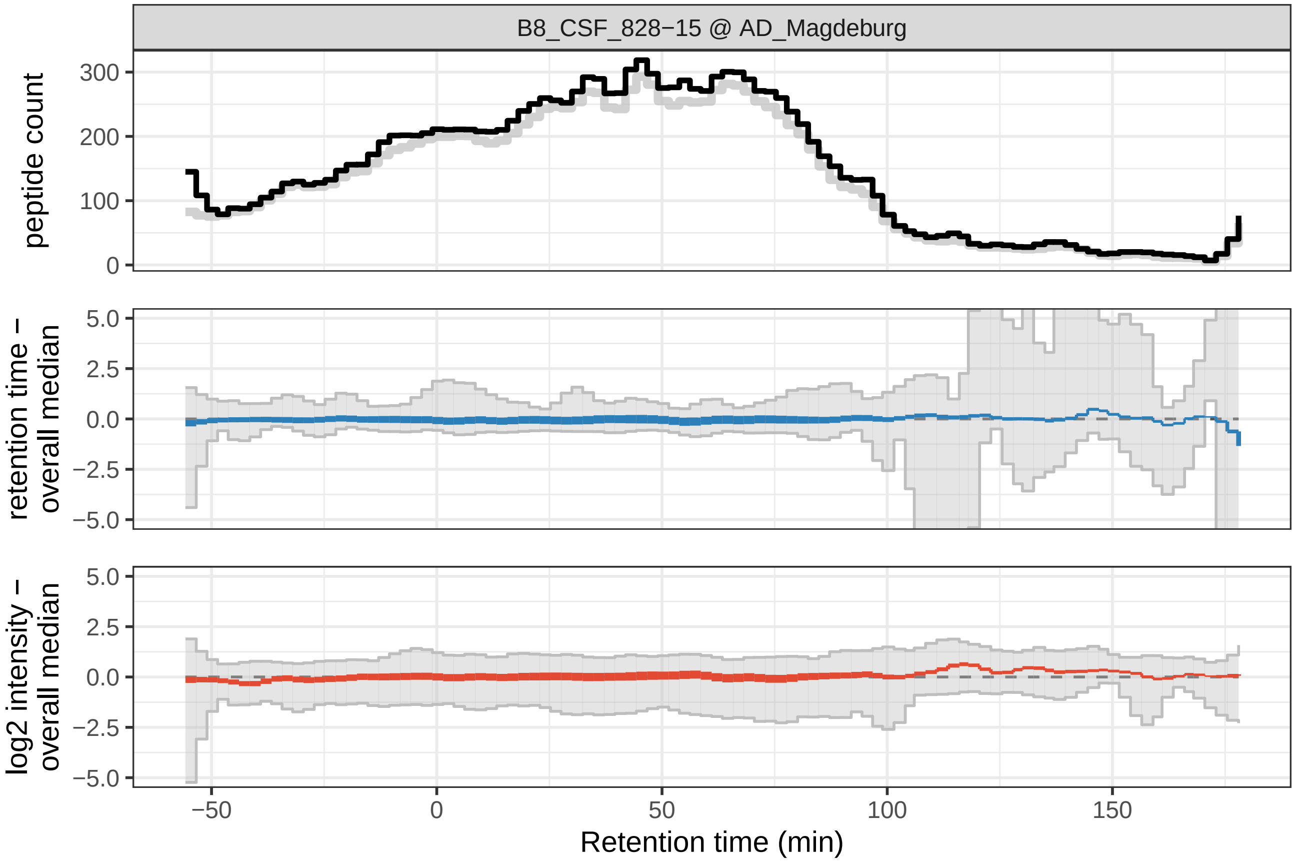

A12_CSF_949−15 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

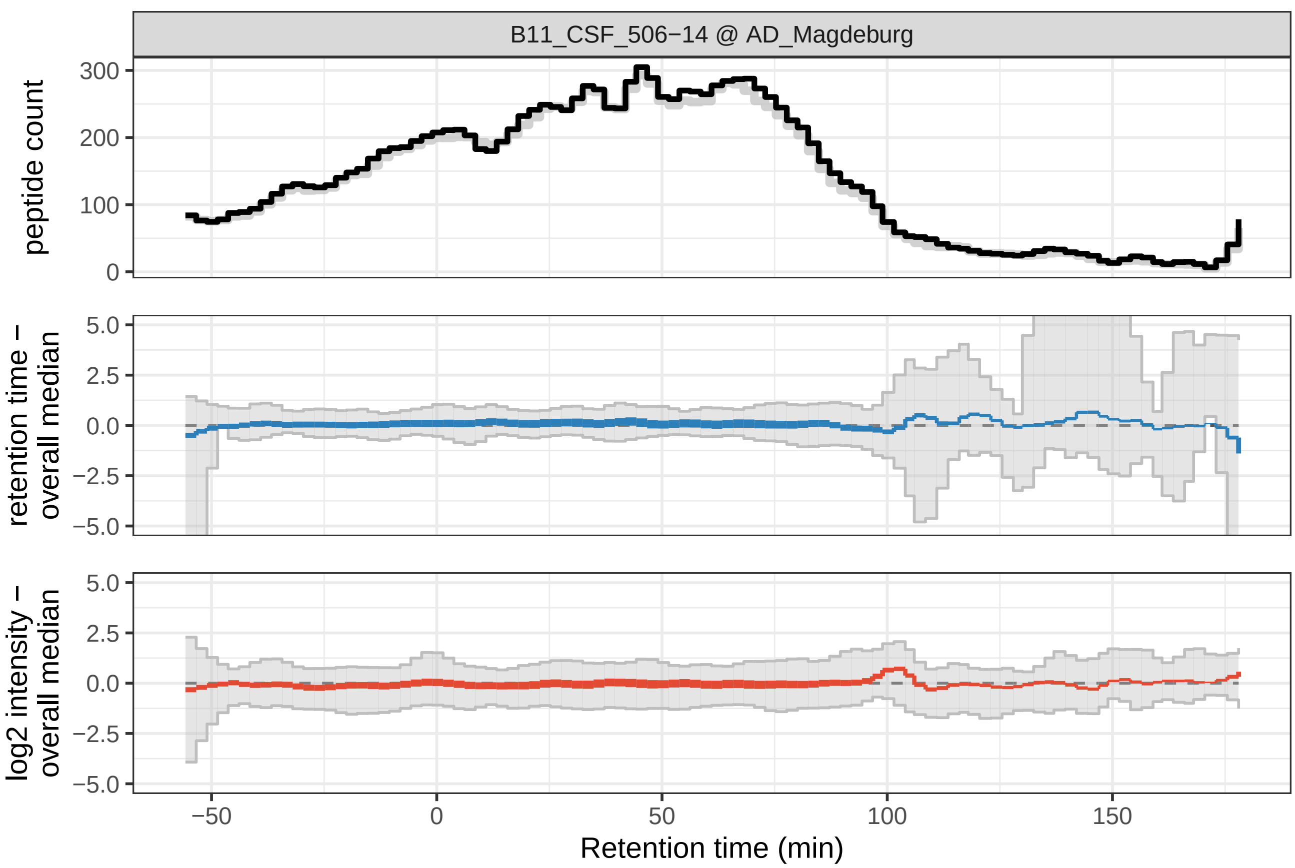

B2_CSF_407−14 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

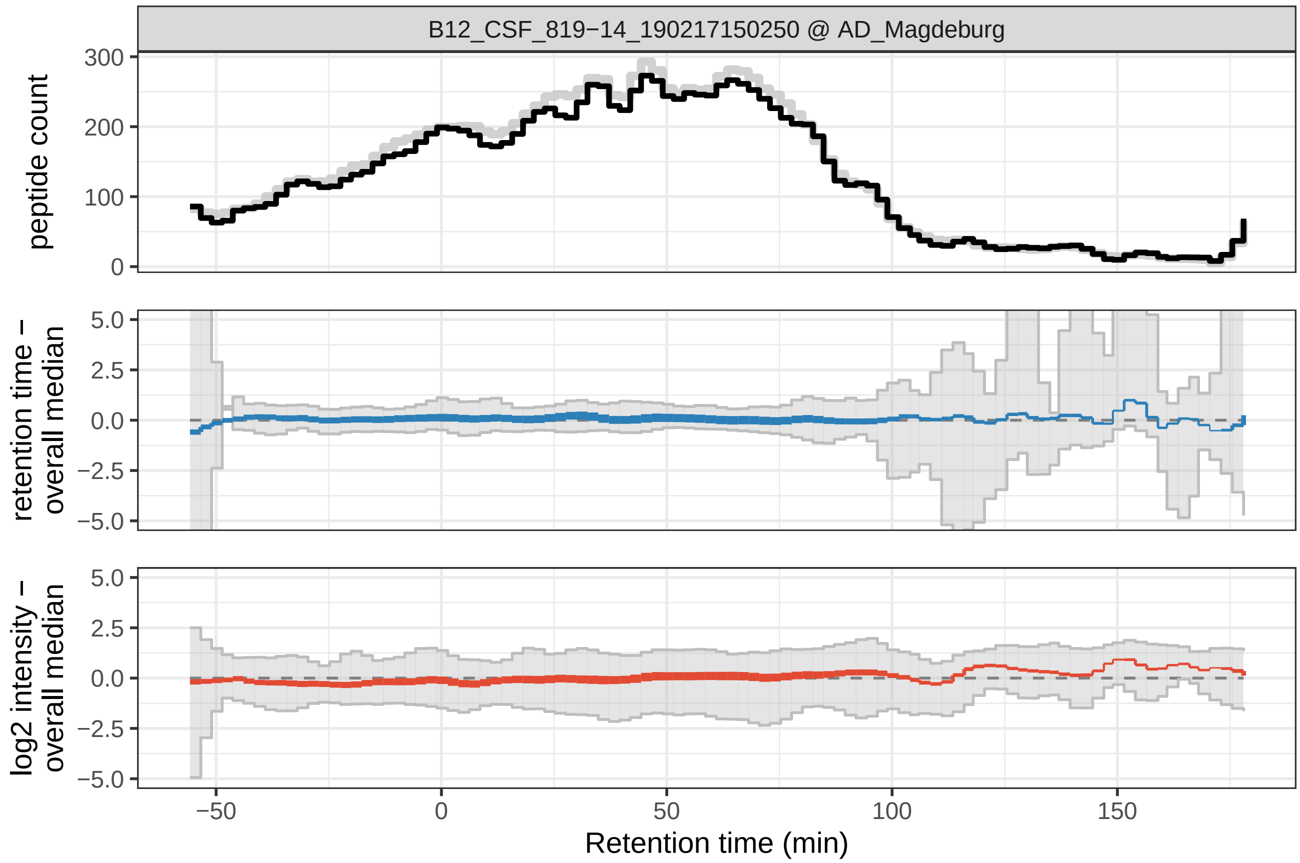

B3_CSF_545−14 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

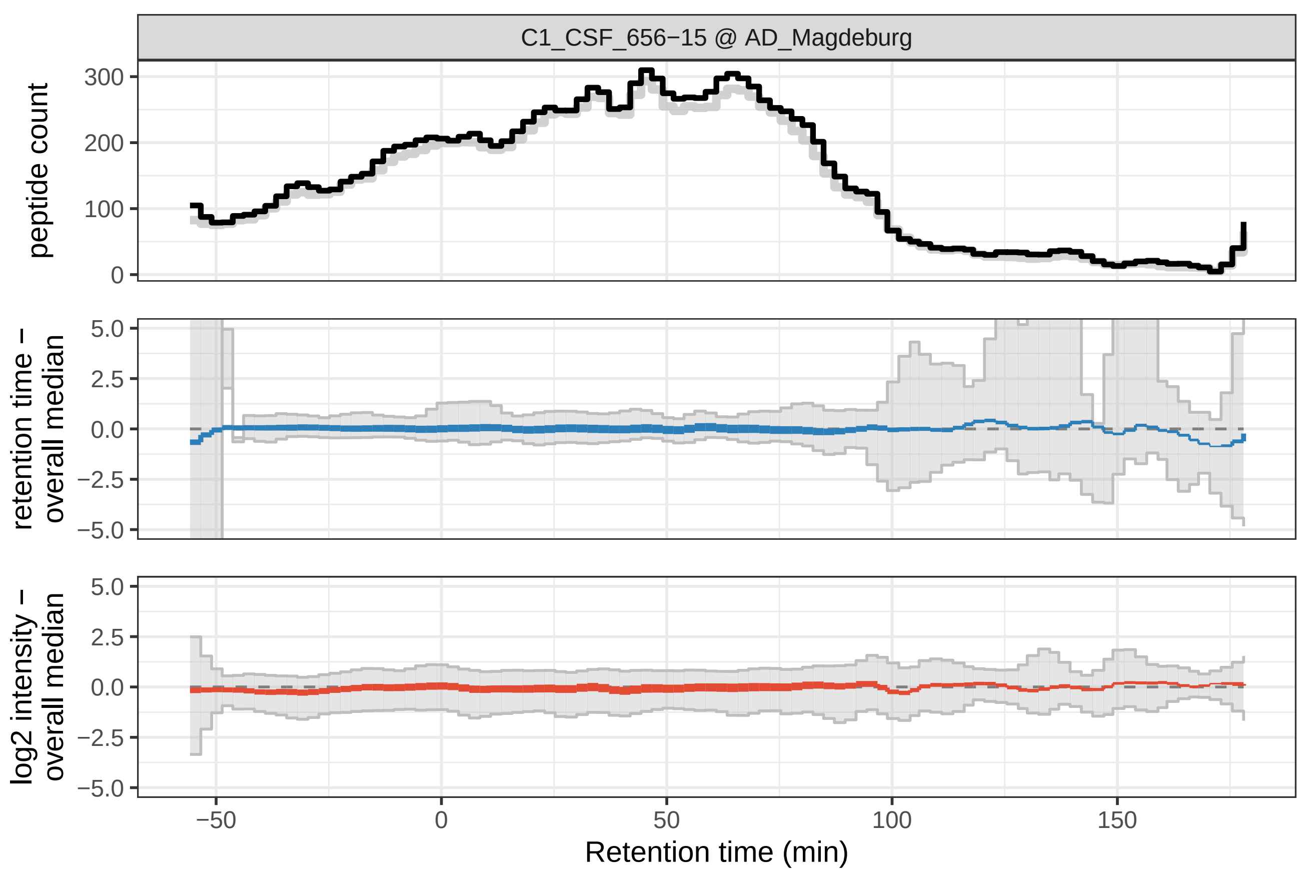

B5_CSF_885−15 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

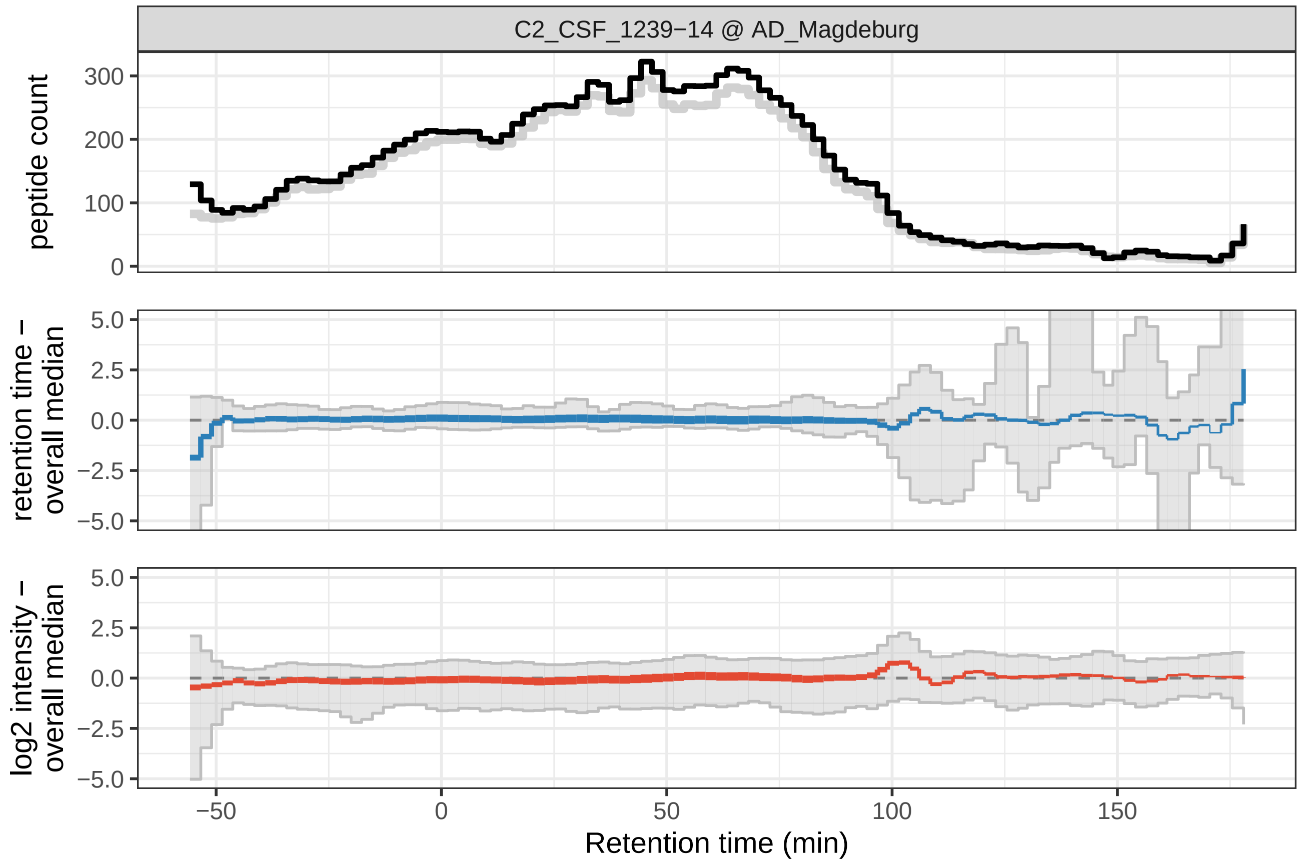

B7_CSF_496−15 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

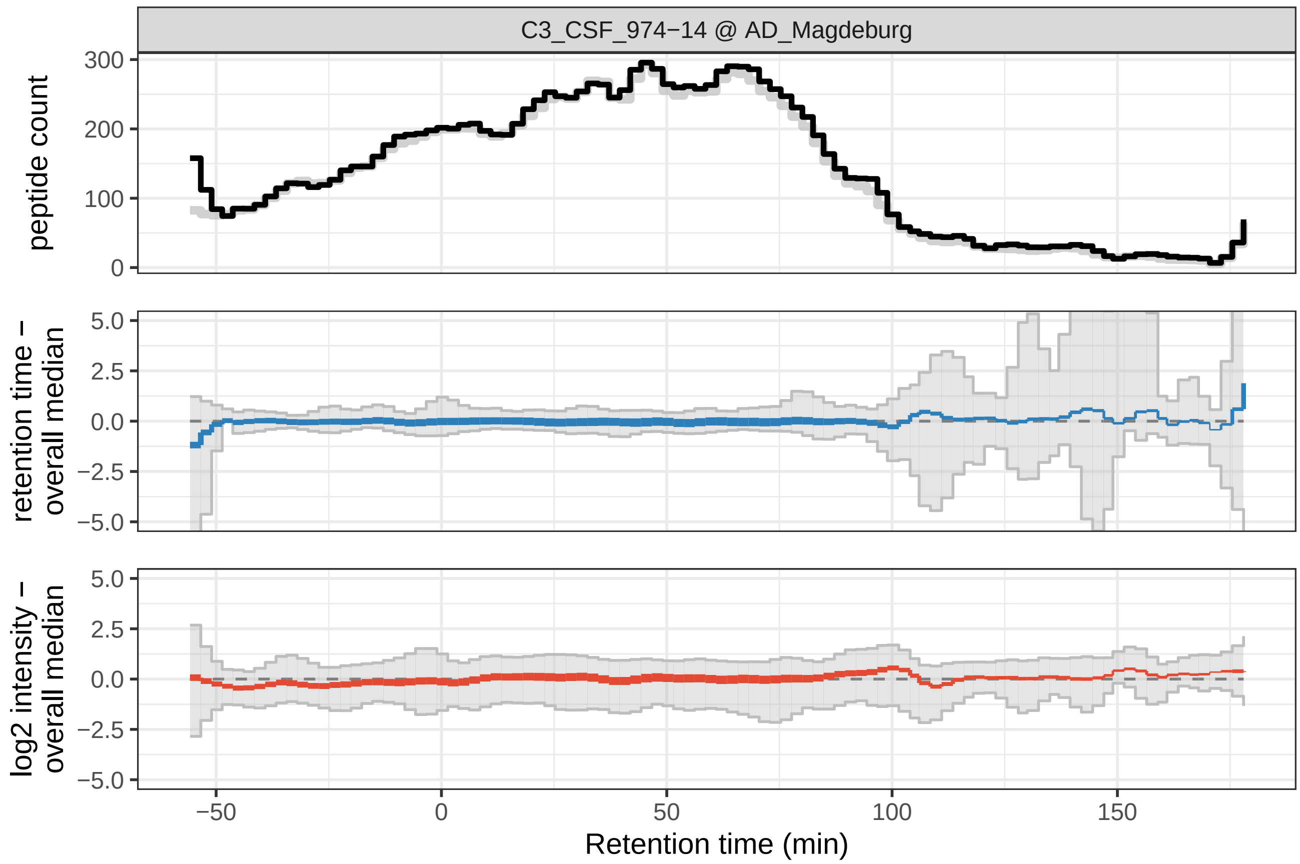

B8_CSF_828−15 @ AD_Magdeburg
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

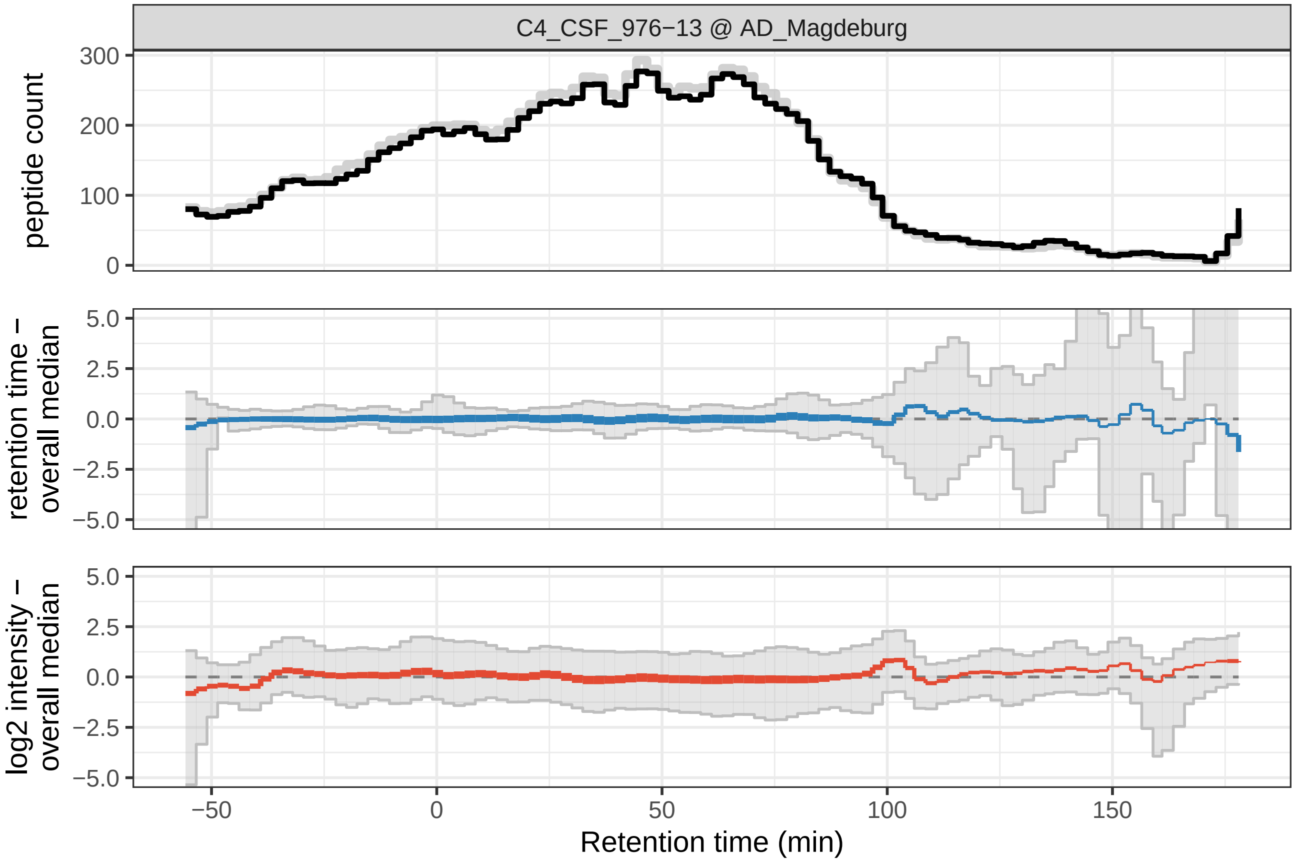

B11_CSF_506−14 @ AD_Magdeburg
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

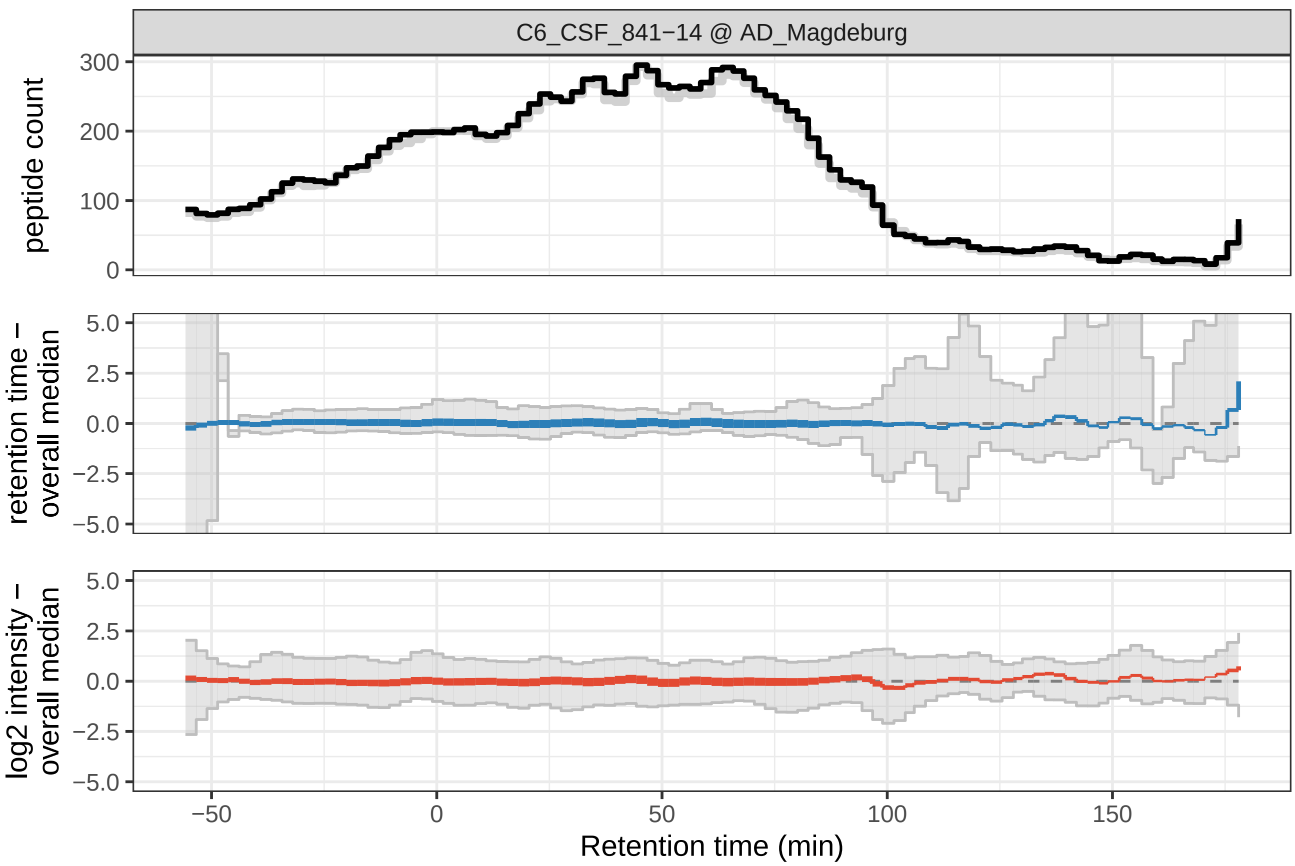

B12_CSF_819−14_190217150250 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

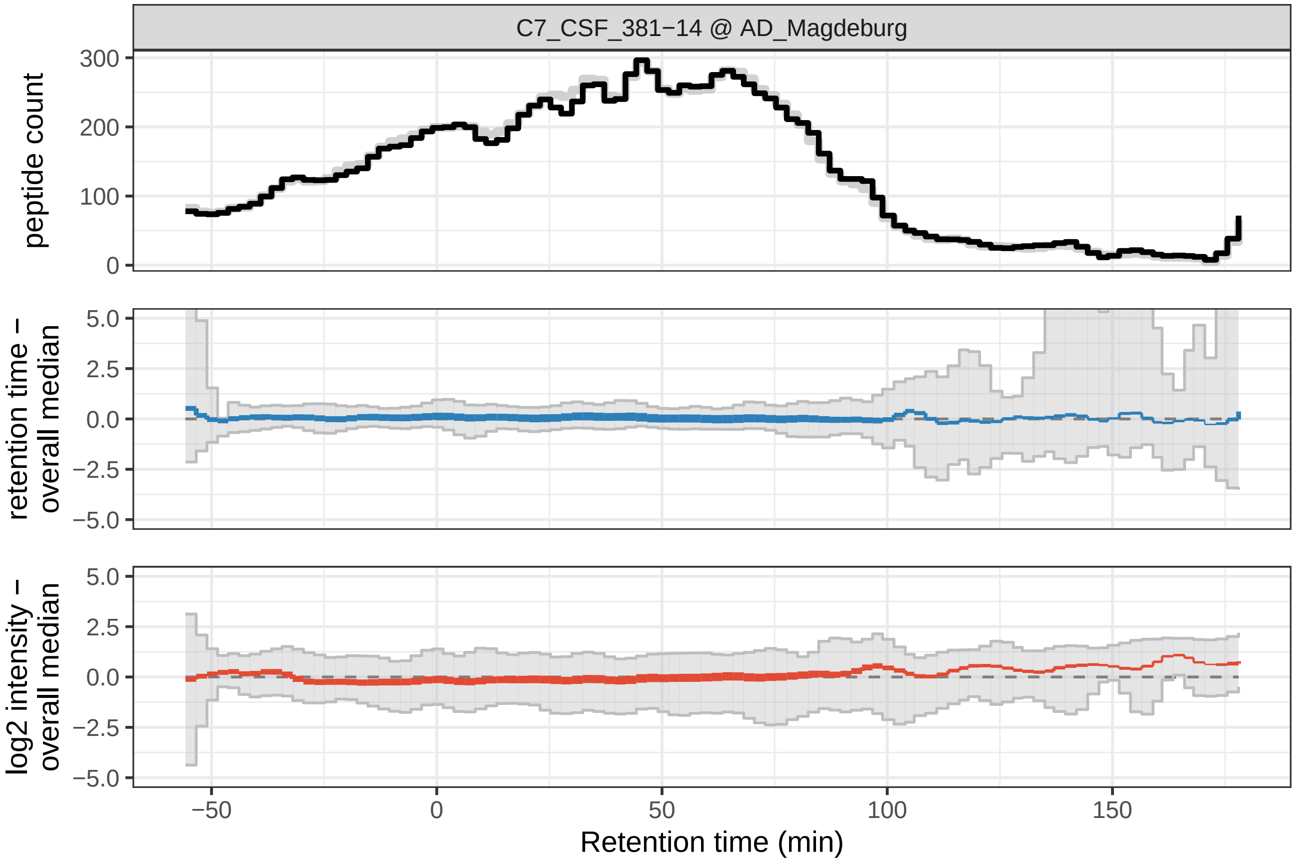

C1_CSF_656−15 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

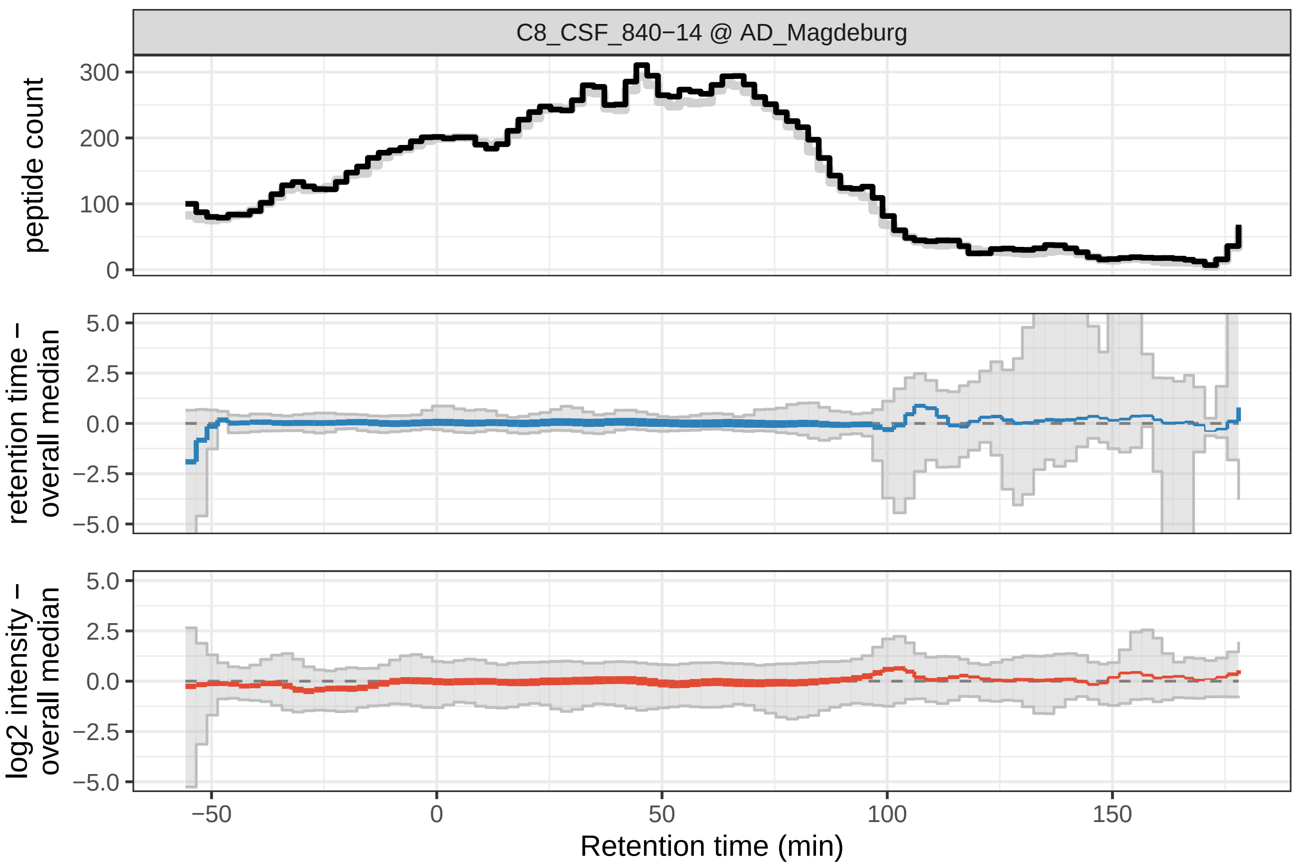

C2_CSF_1239−14 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

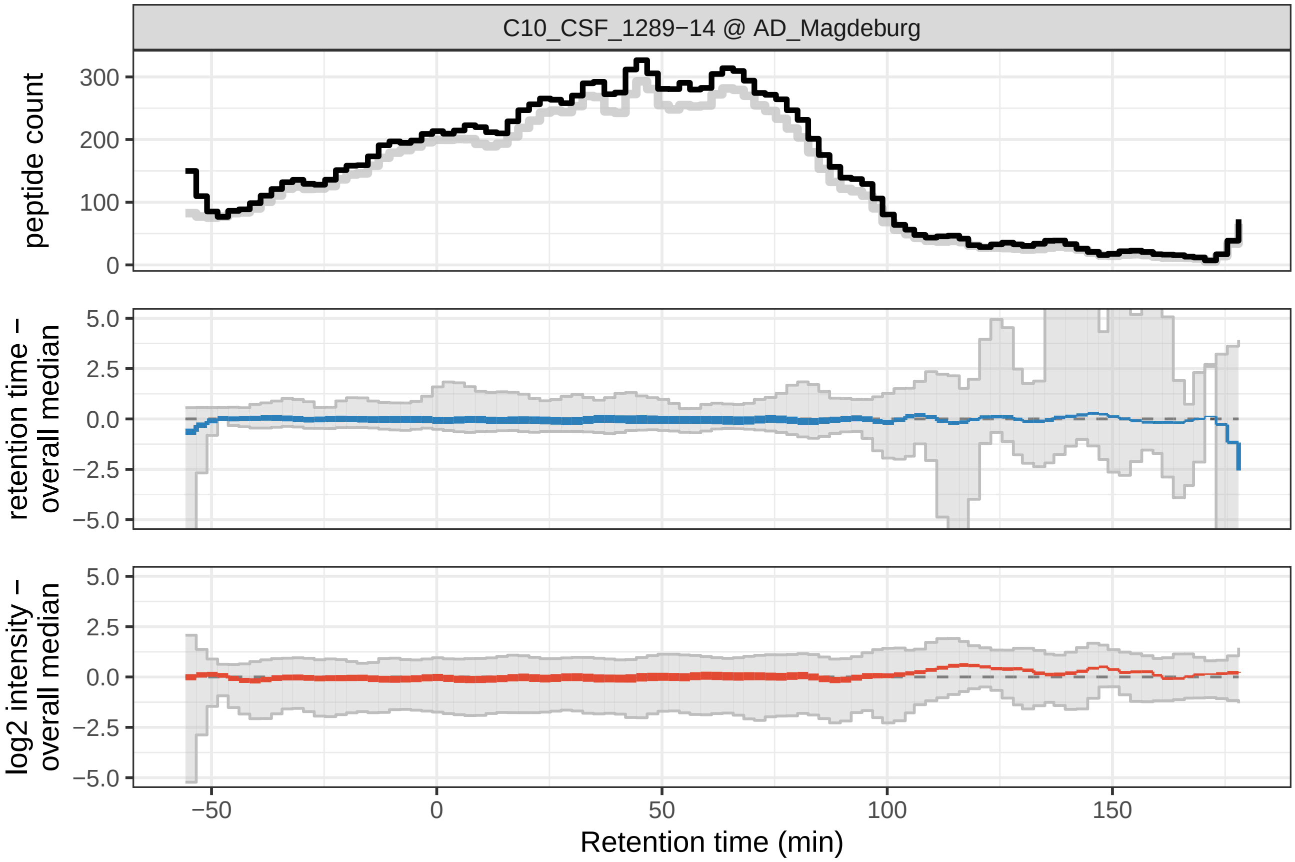

C3_CSF_974−14 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

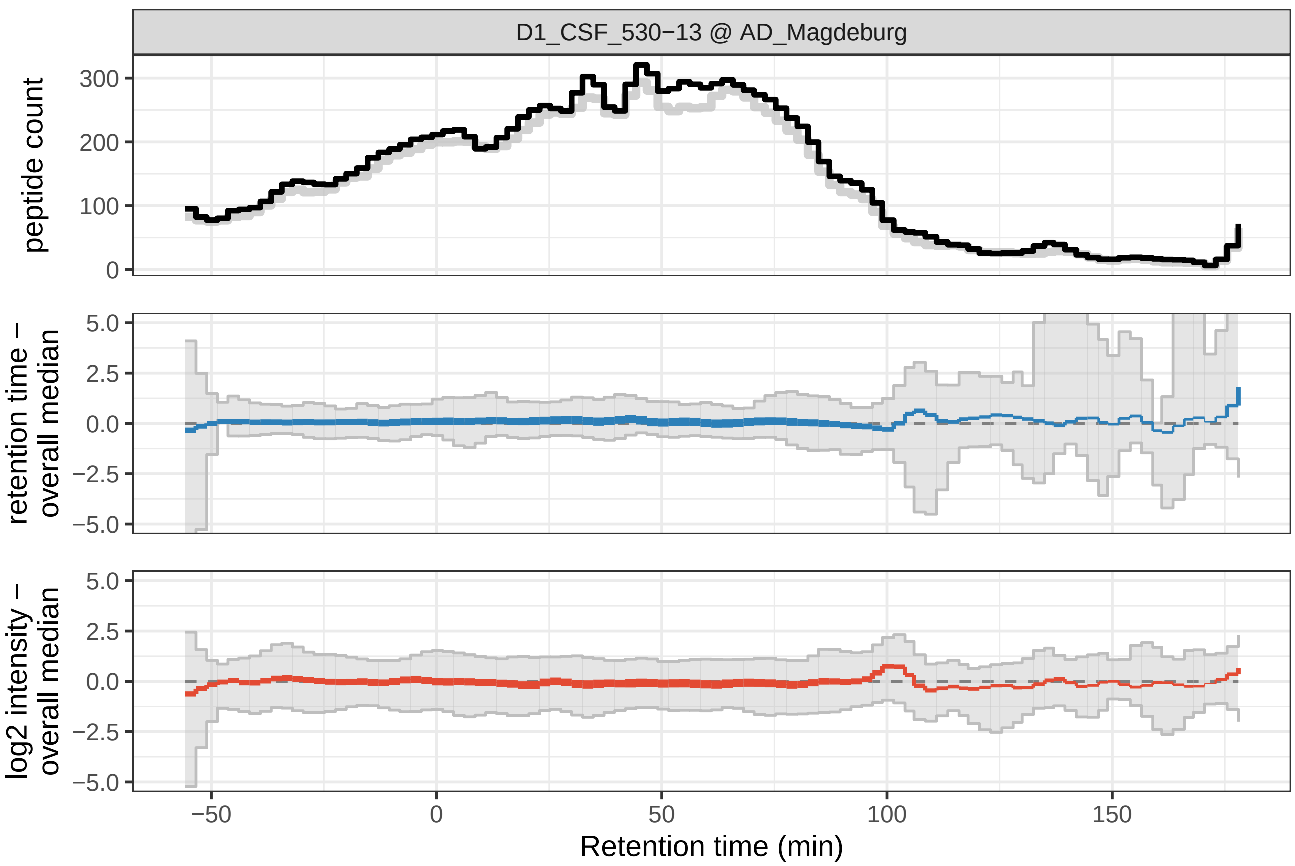

C4_CSF_976−13 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

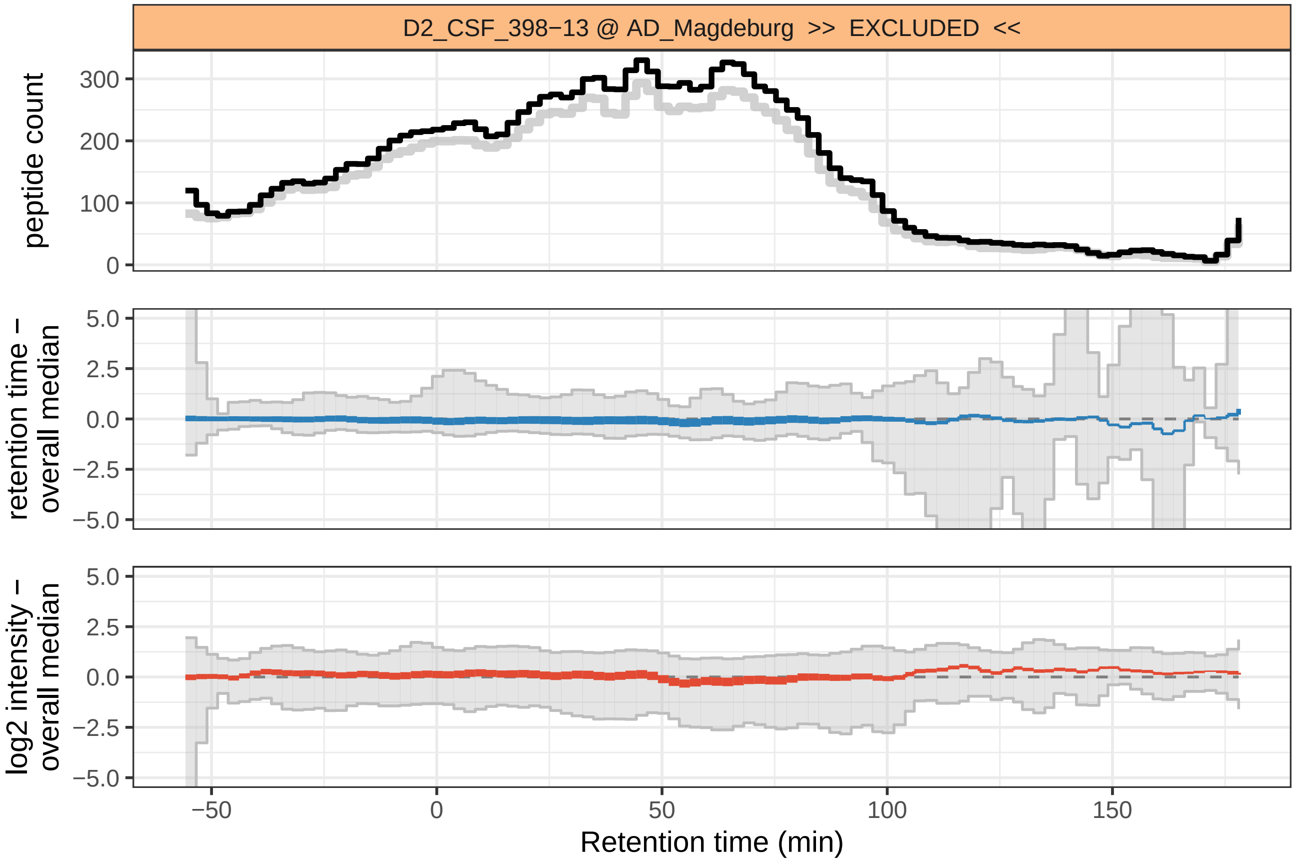

C6_CSF_841−14 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

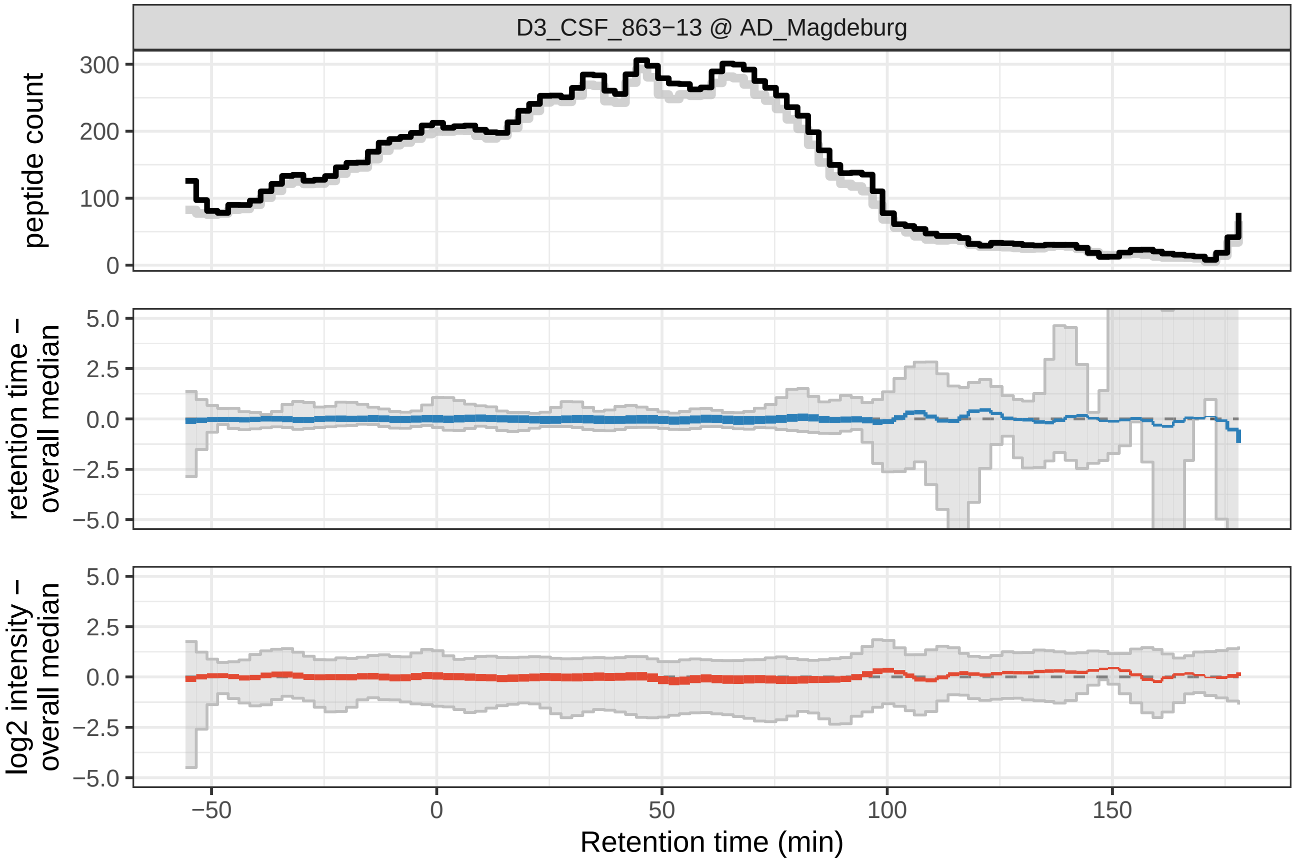

C7_CSF_381−14 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

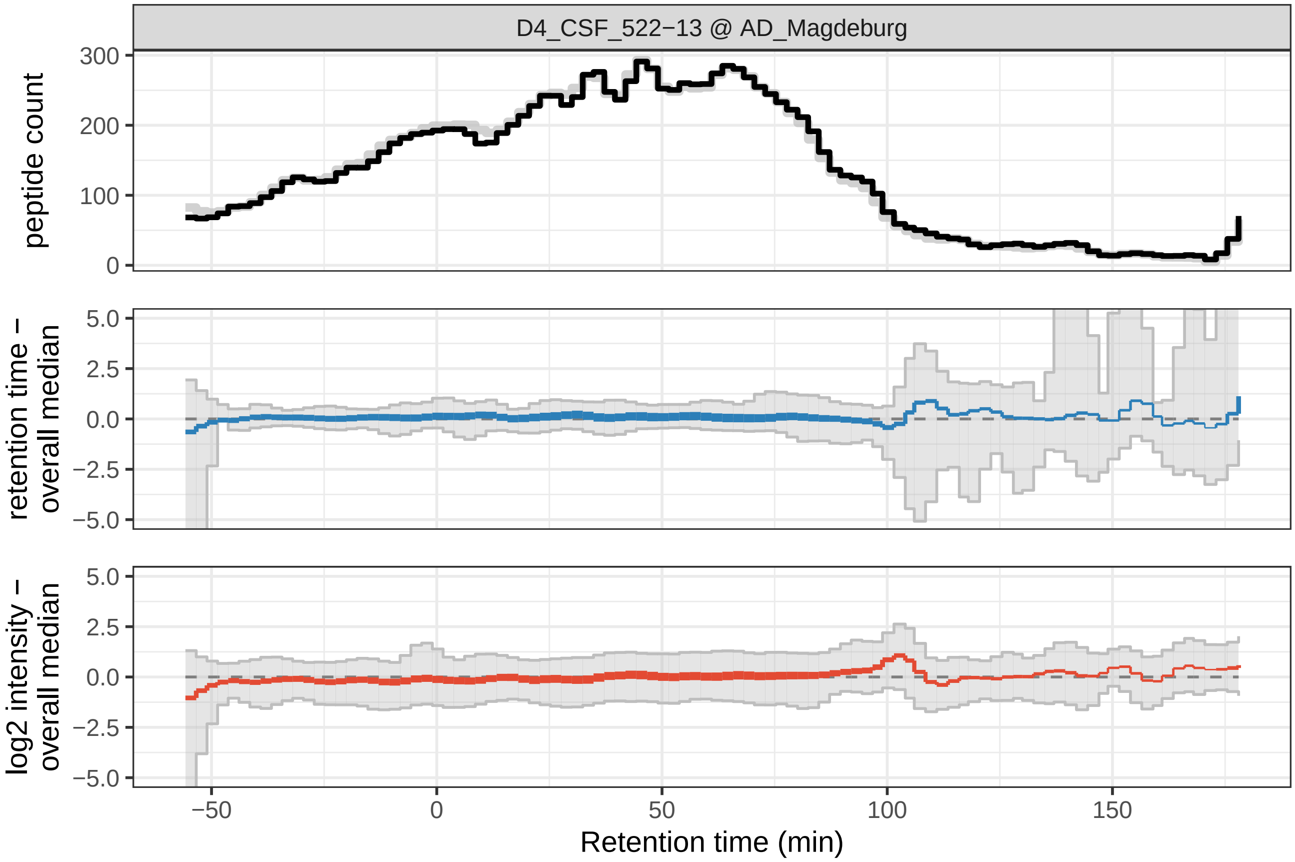

C8_CSF_840−14 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)


C10_CSF_1289−14 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

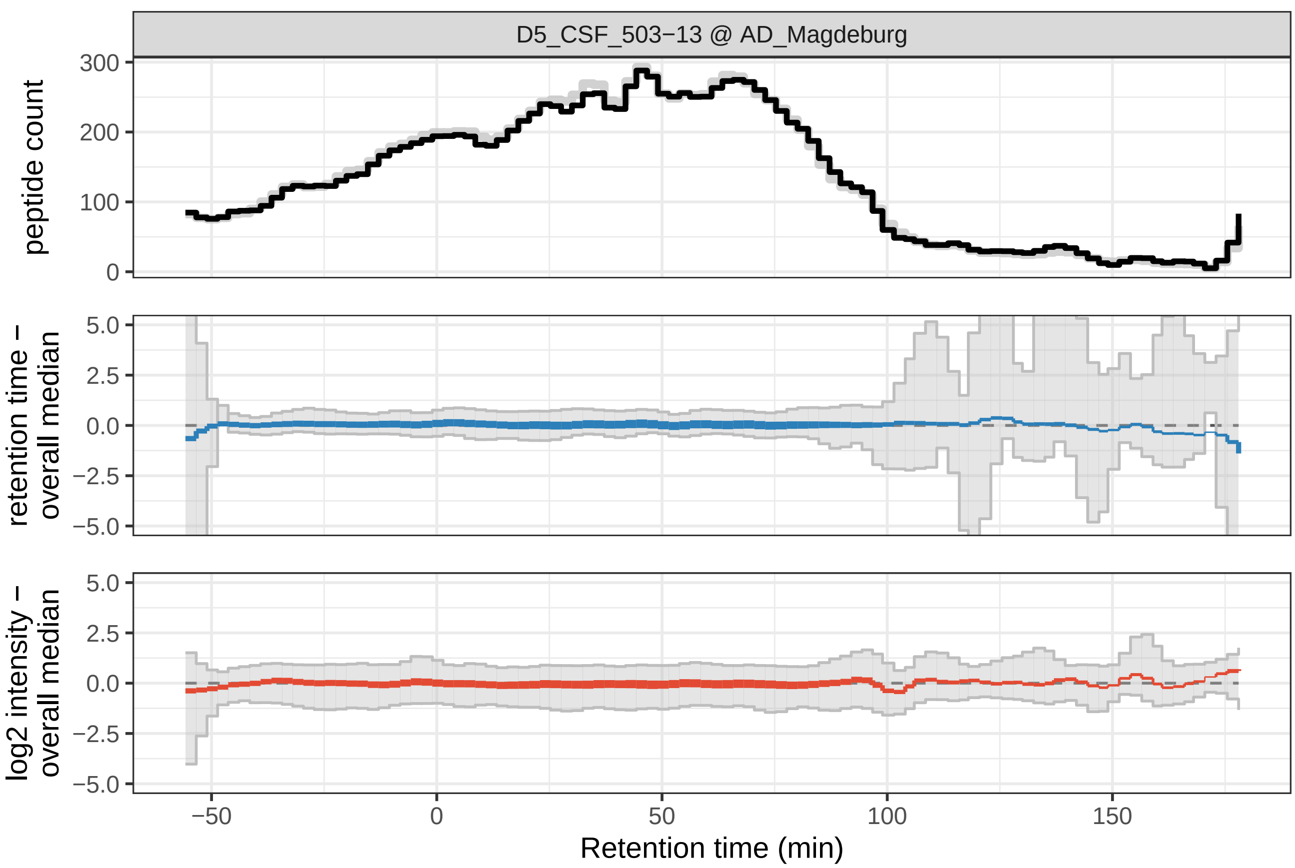

D1_CSF_530−13 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)


D2_CSF_398−13 @ AD_Magdeburg >> EXCLUDED <<
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

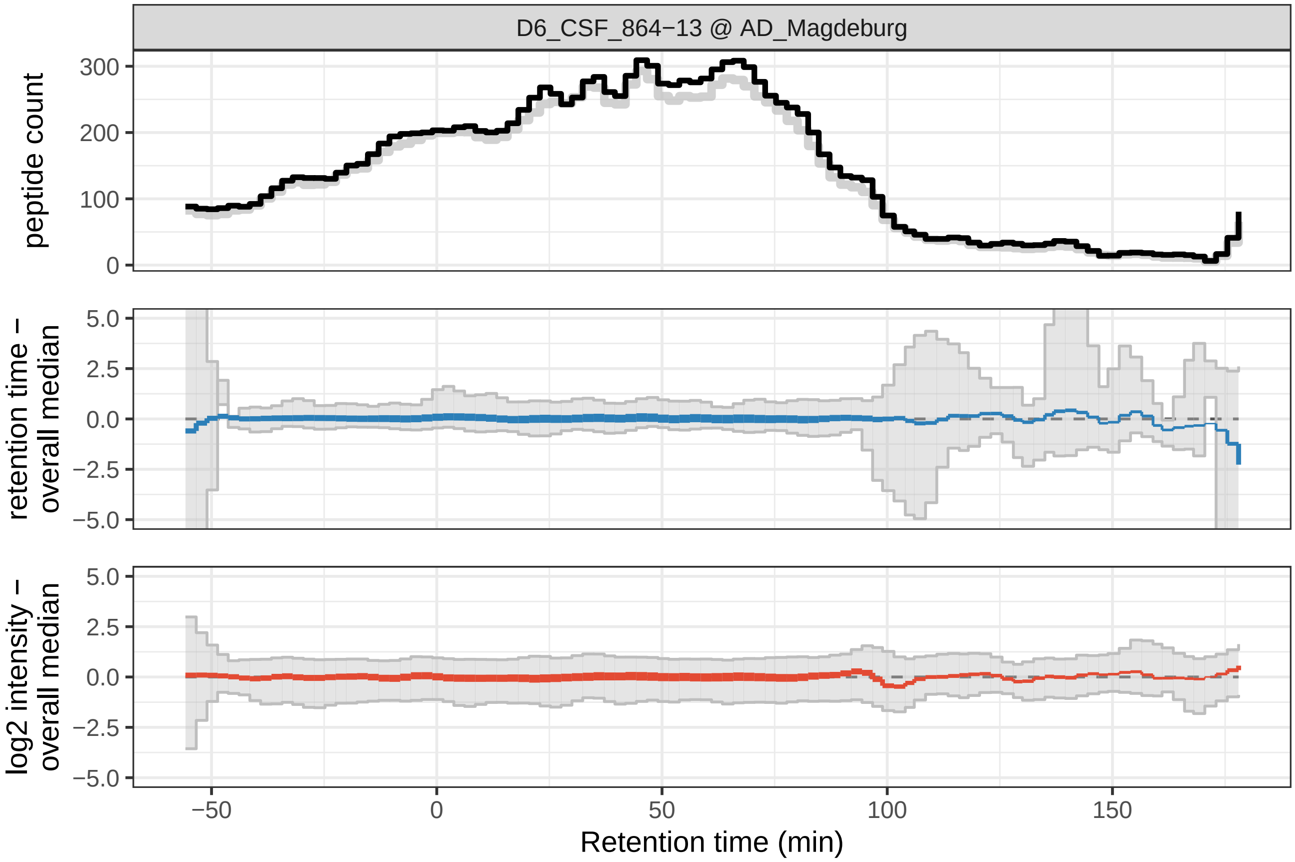

D3_CSF_863−13 @ AD_Magdeburg
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

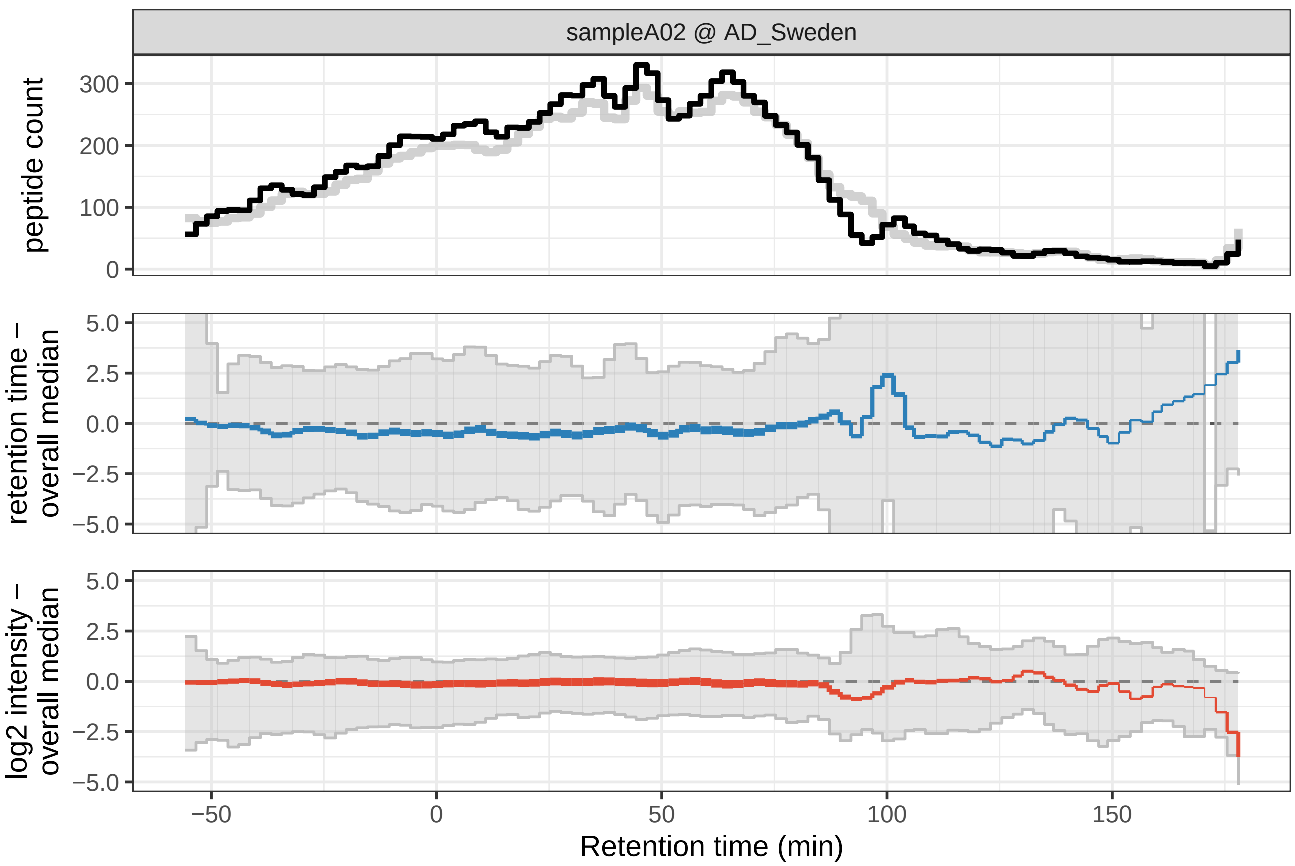


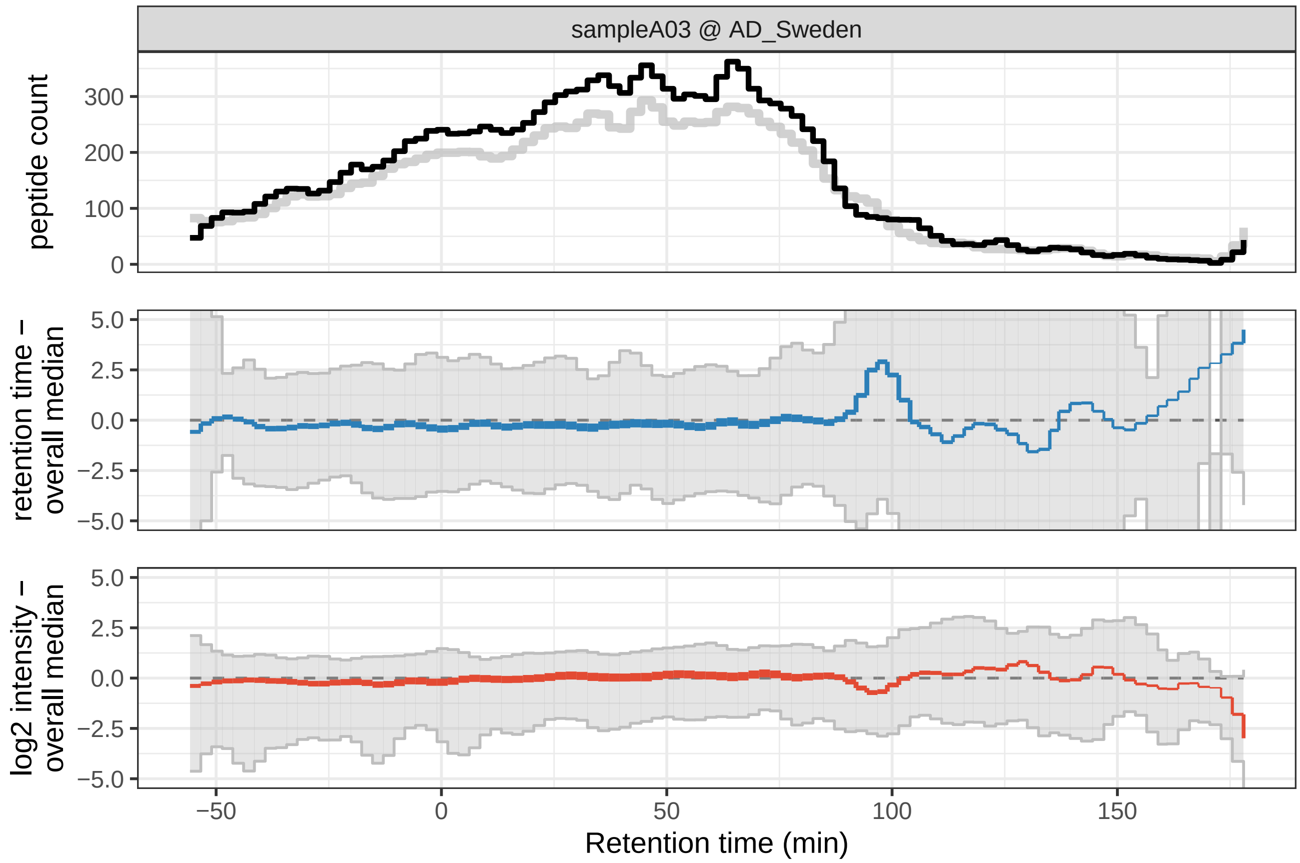
D4_CSF_522−13 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

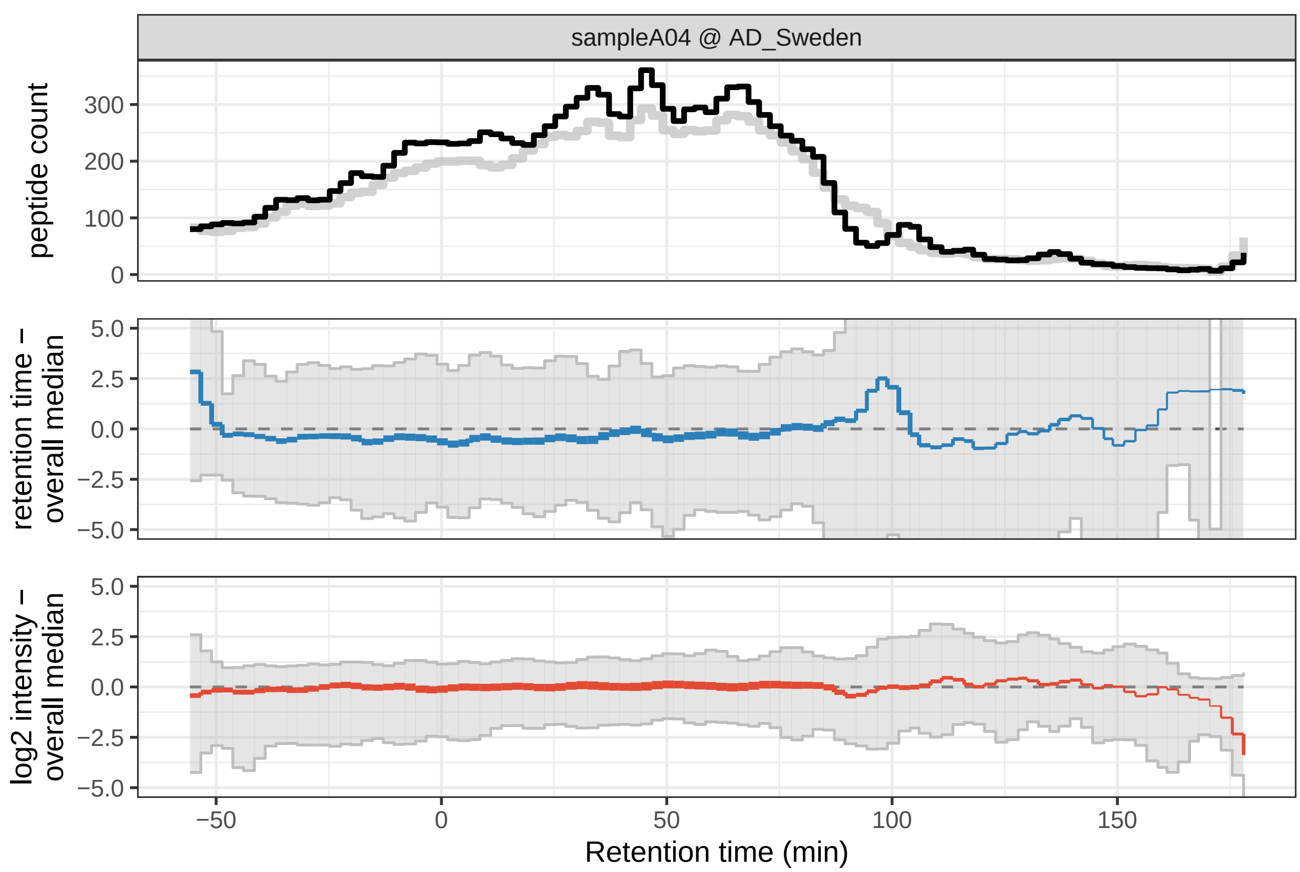


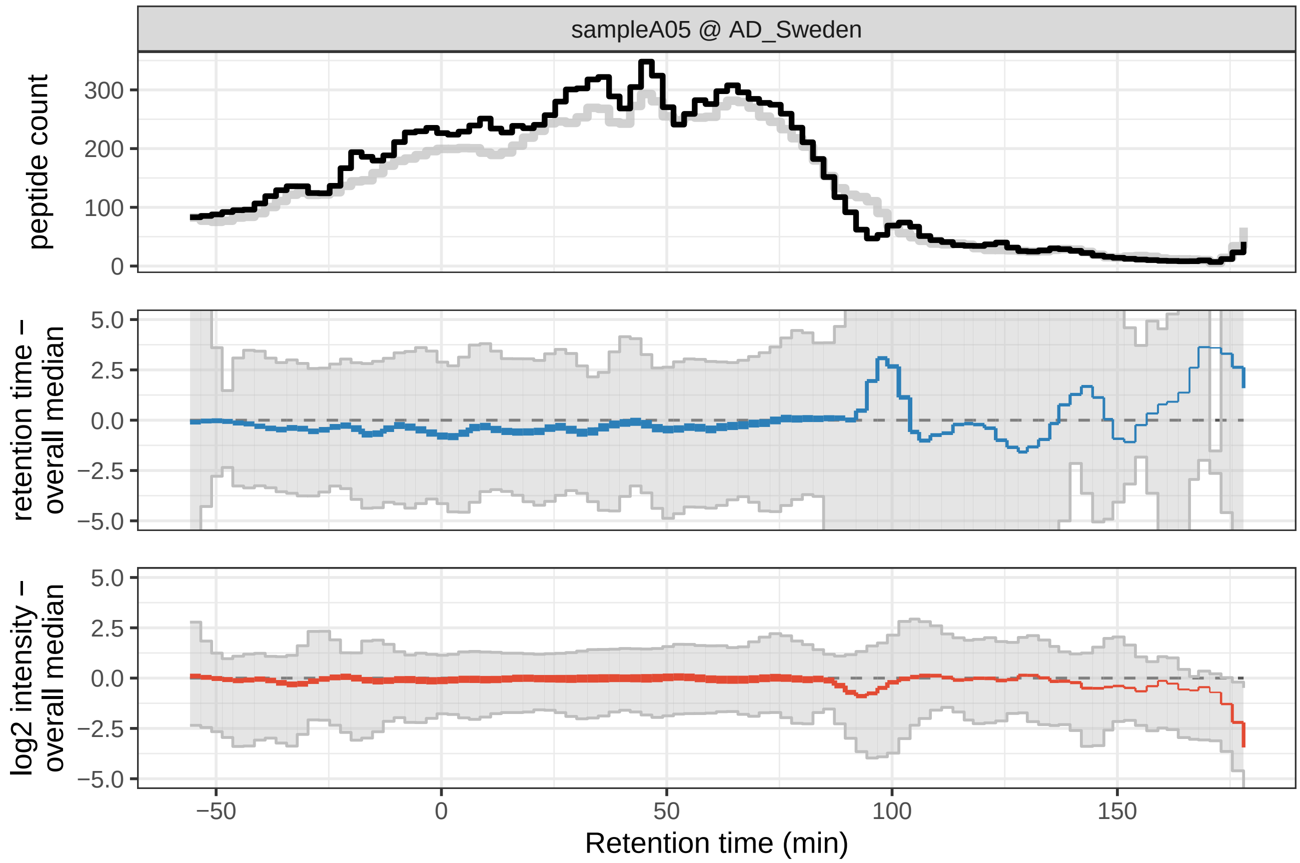
D5_CSF_503−13 @ AD_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

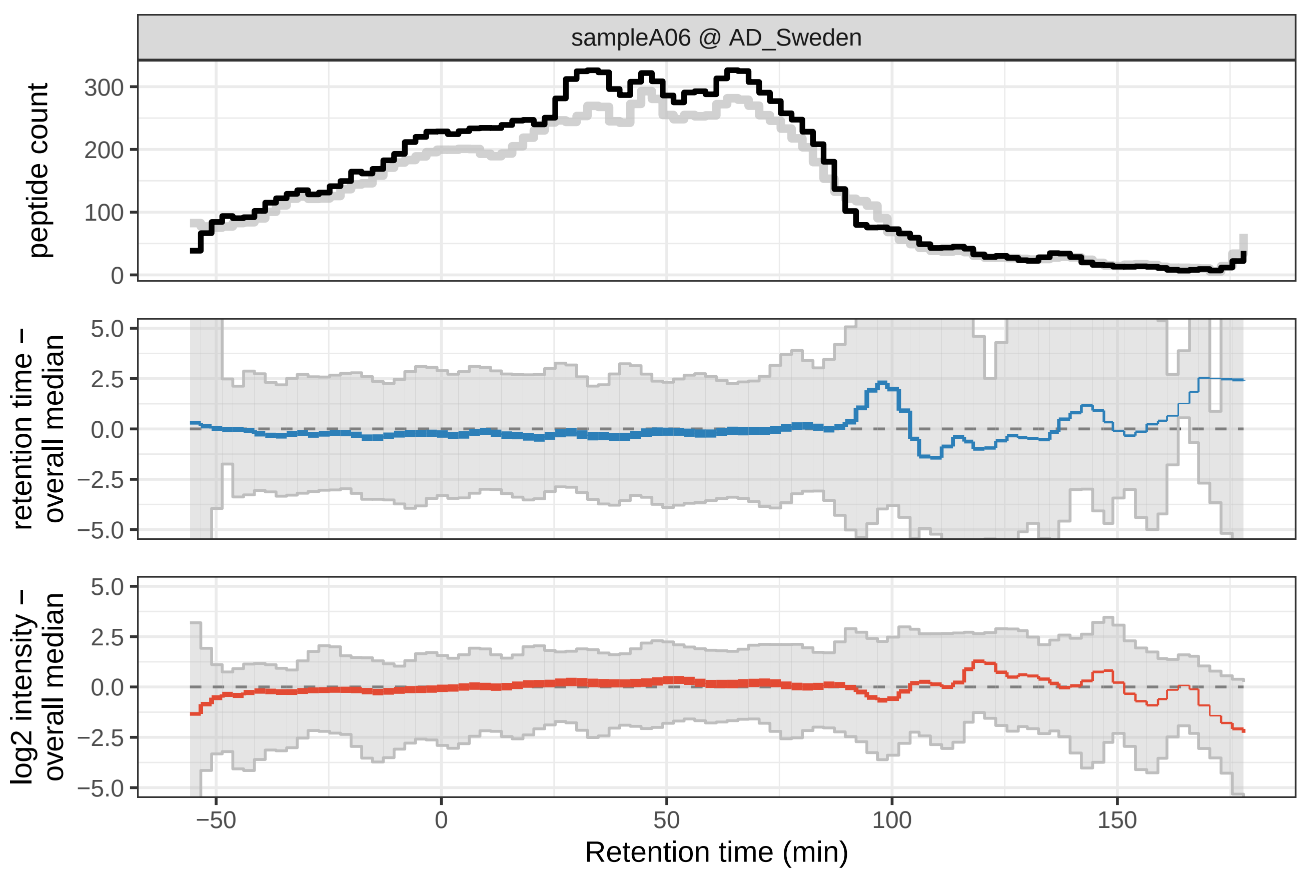

D6_CSF_864−13 @ AD_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

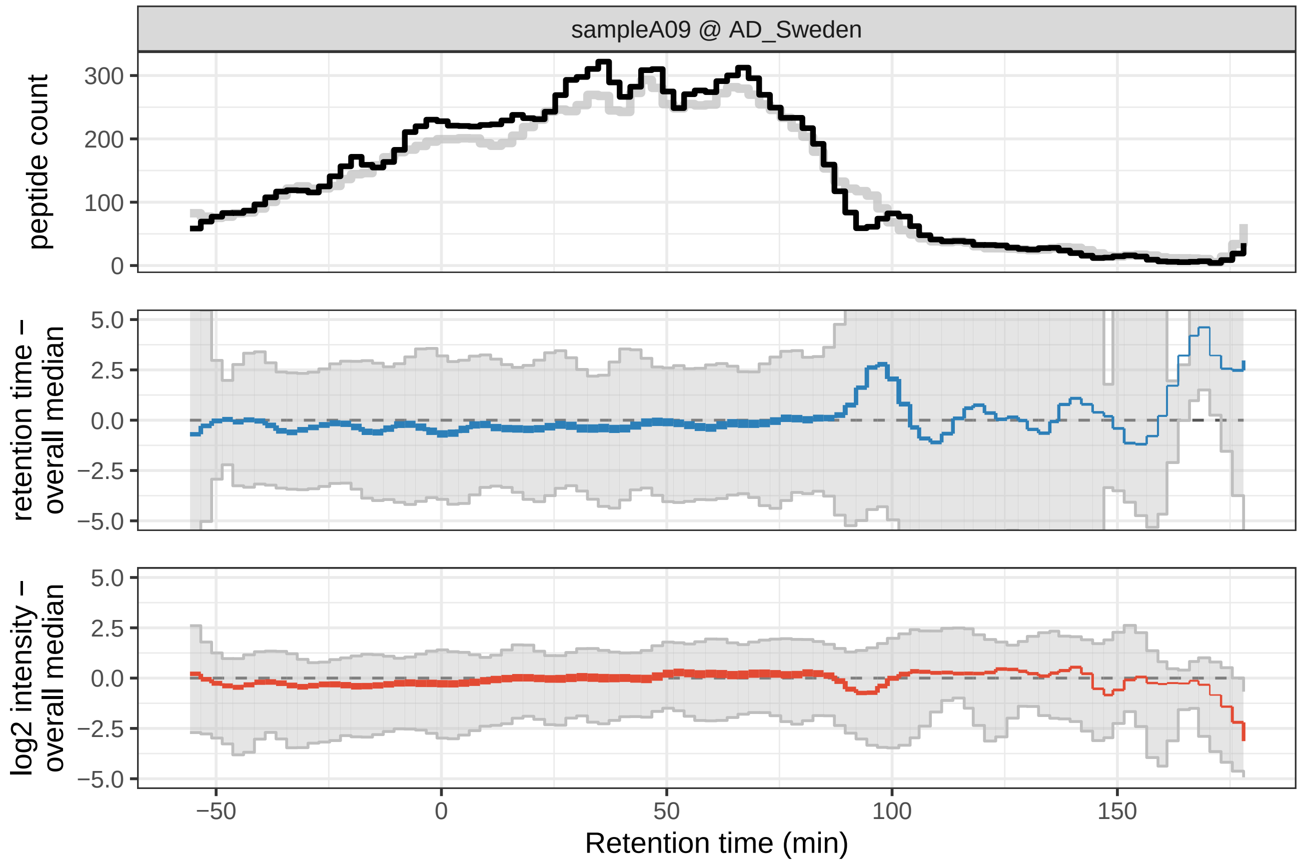

sampleA02 @ AD_Sweden
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

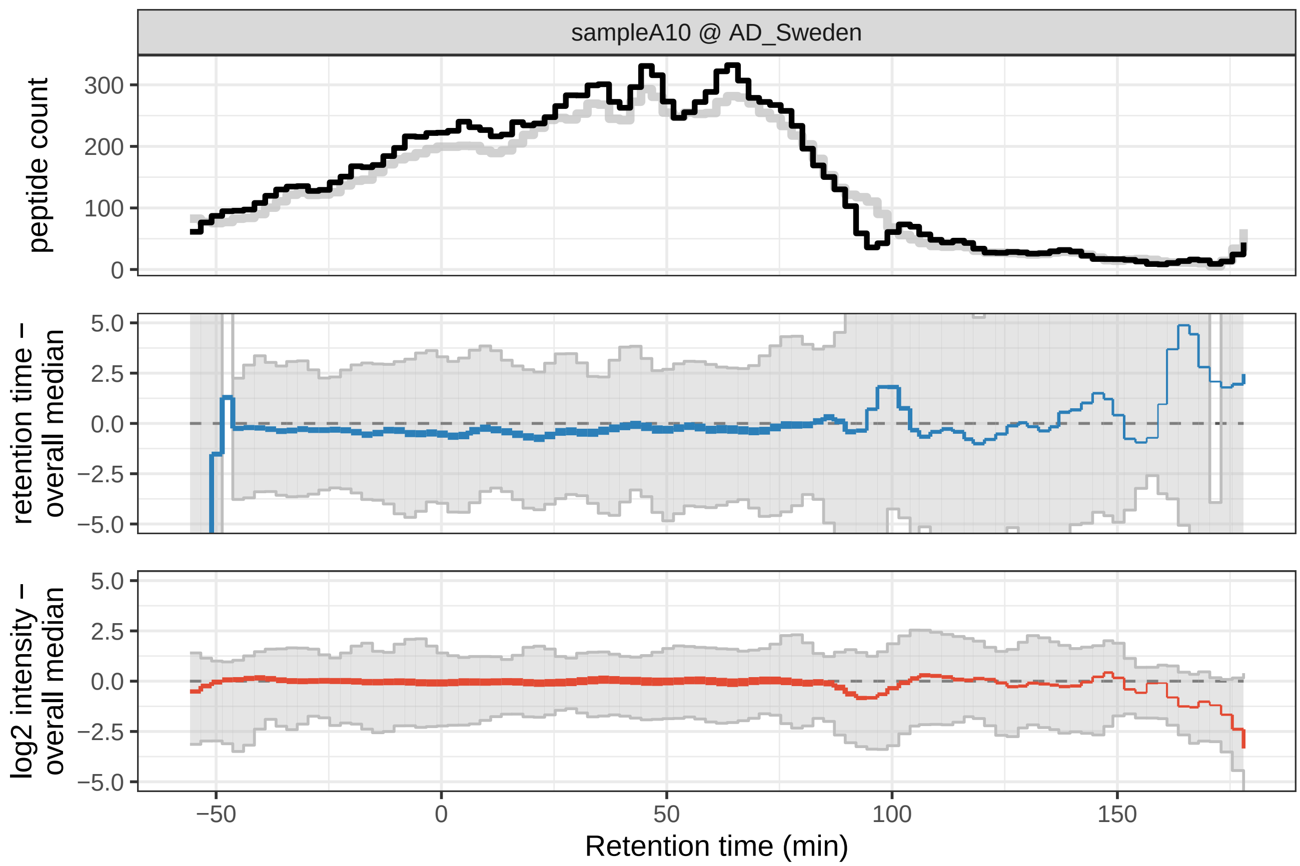

sampleA03 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

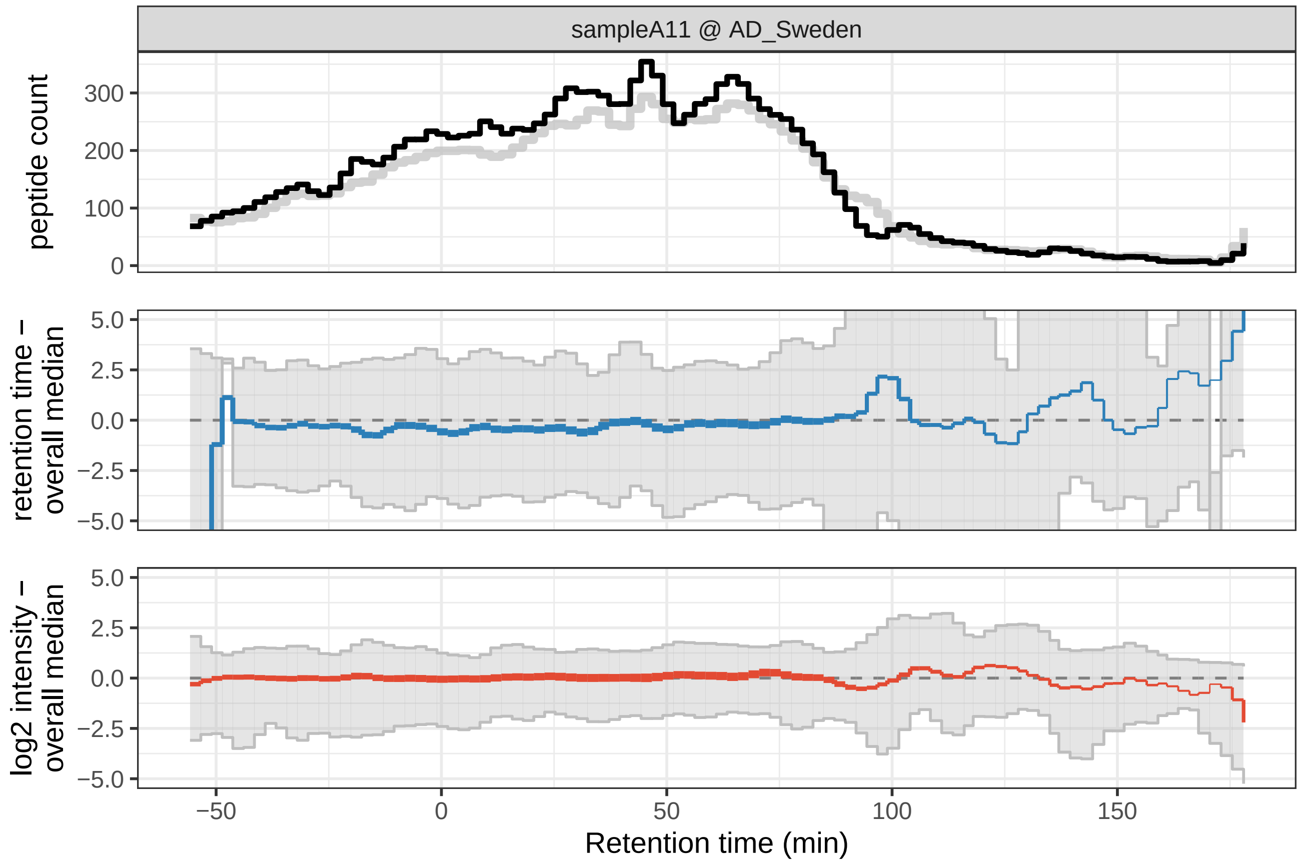

sampleA04 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

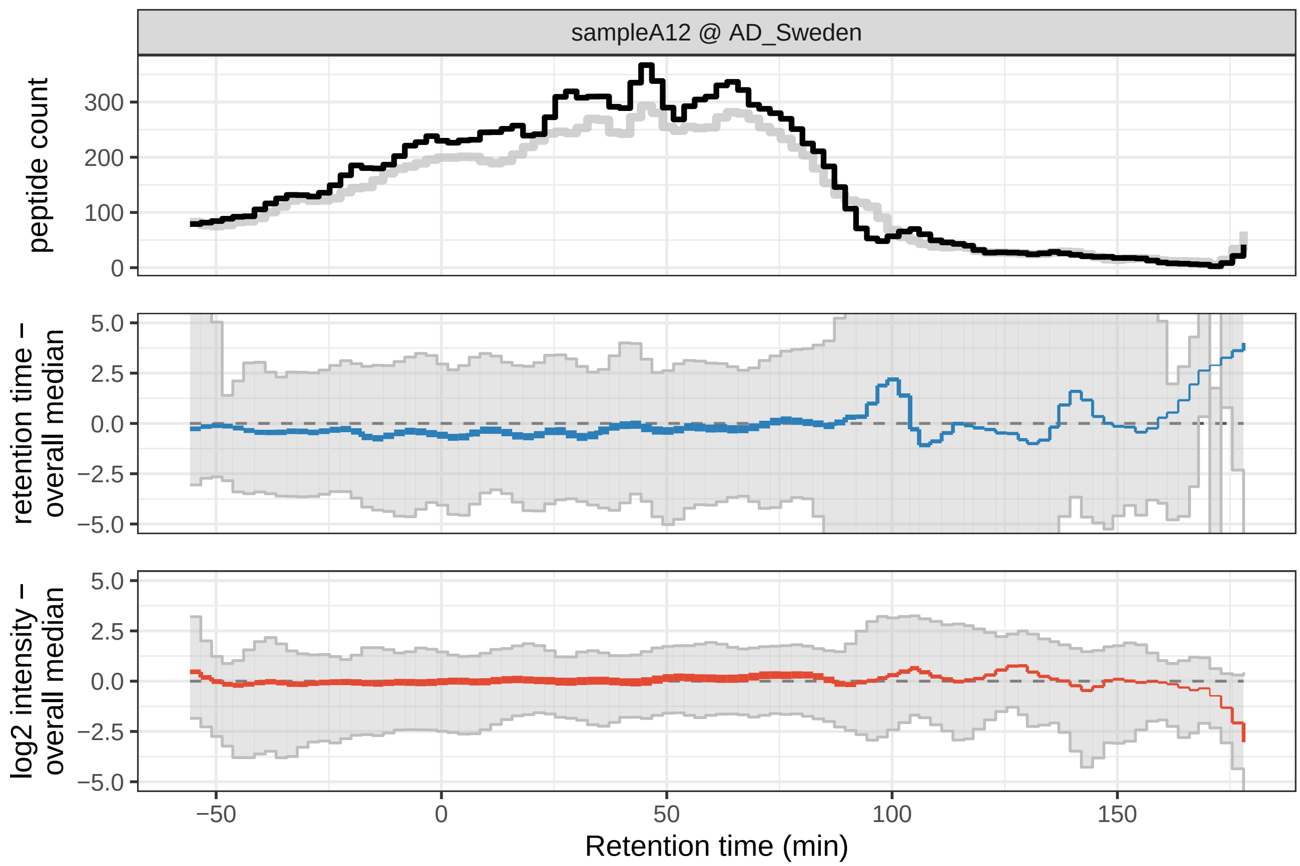

sampleA05 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

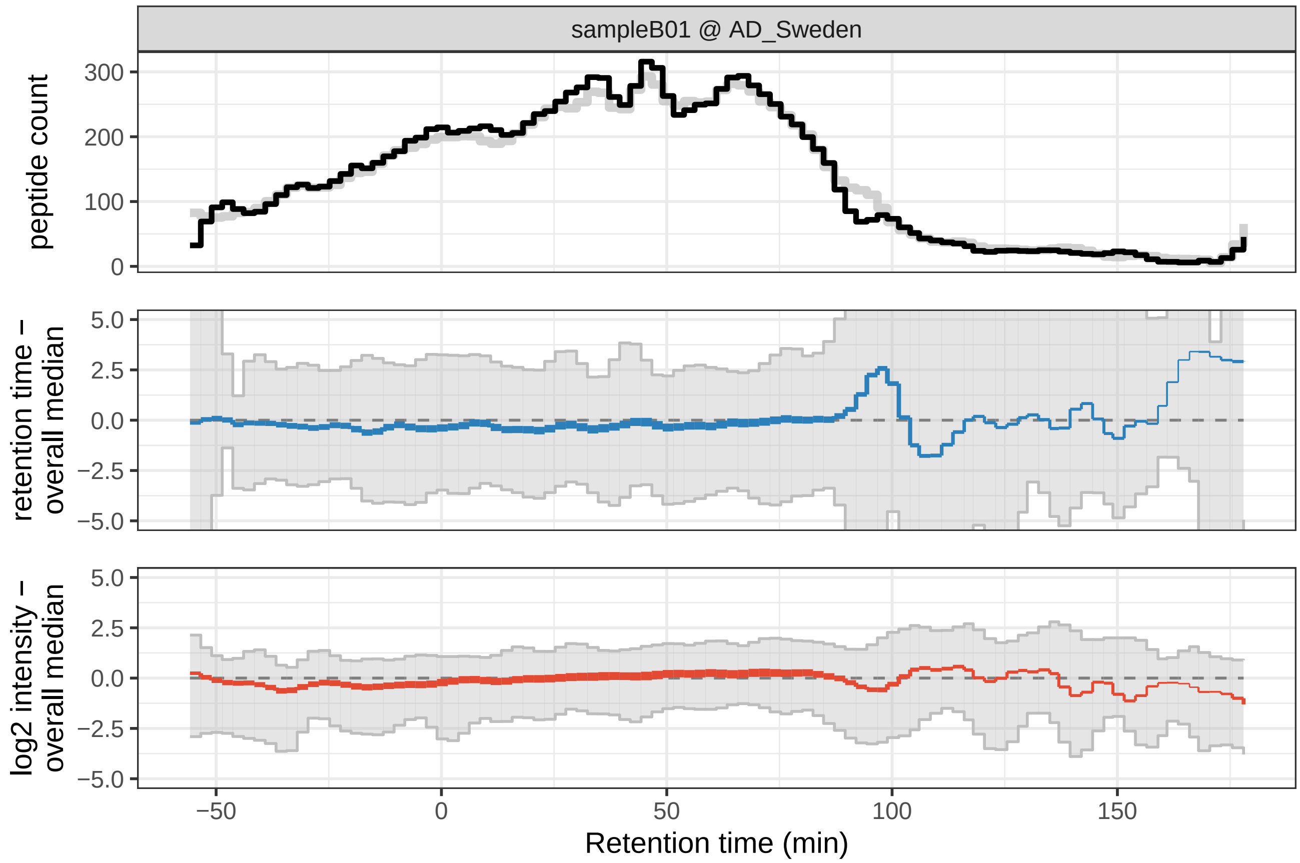

sampleA06 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

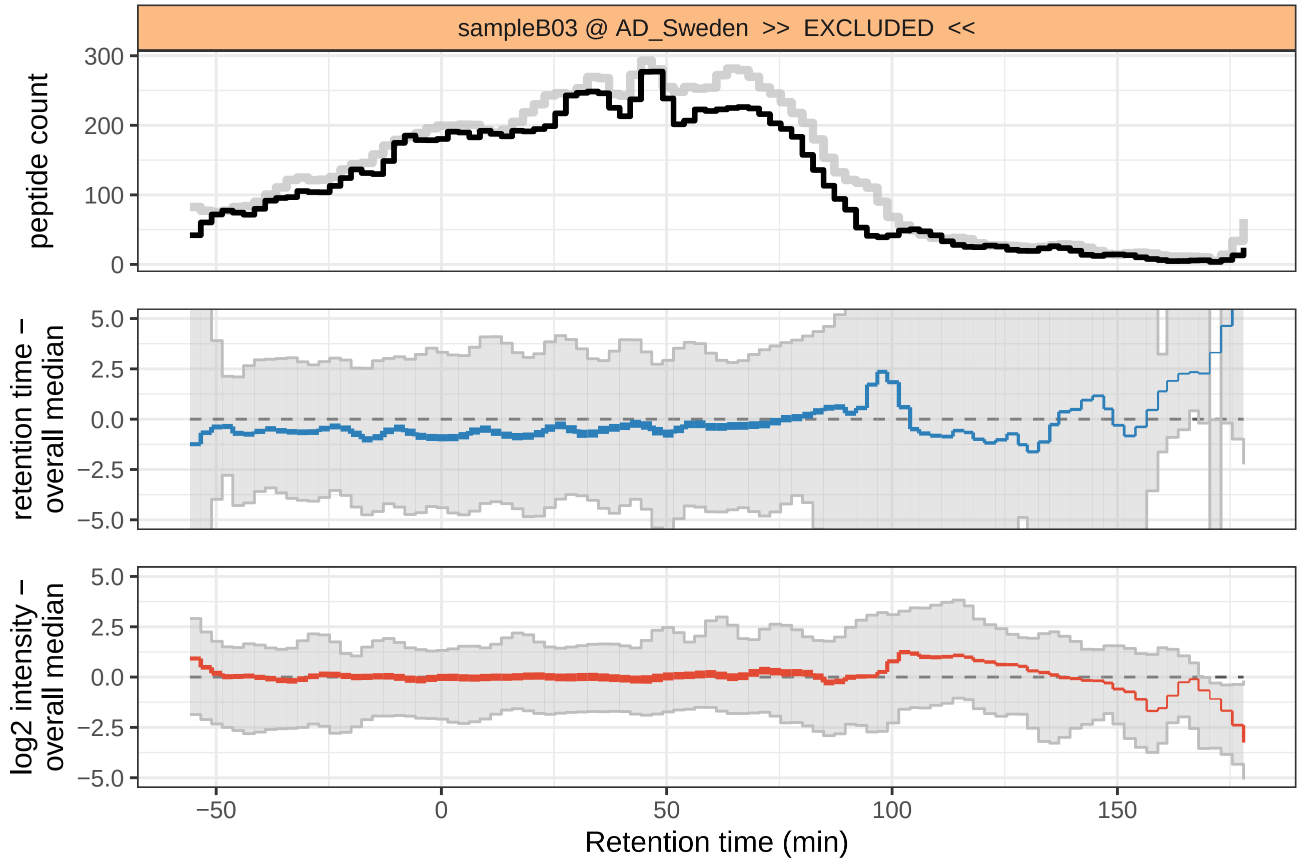

sampleA09 @ AD_Sweden
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

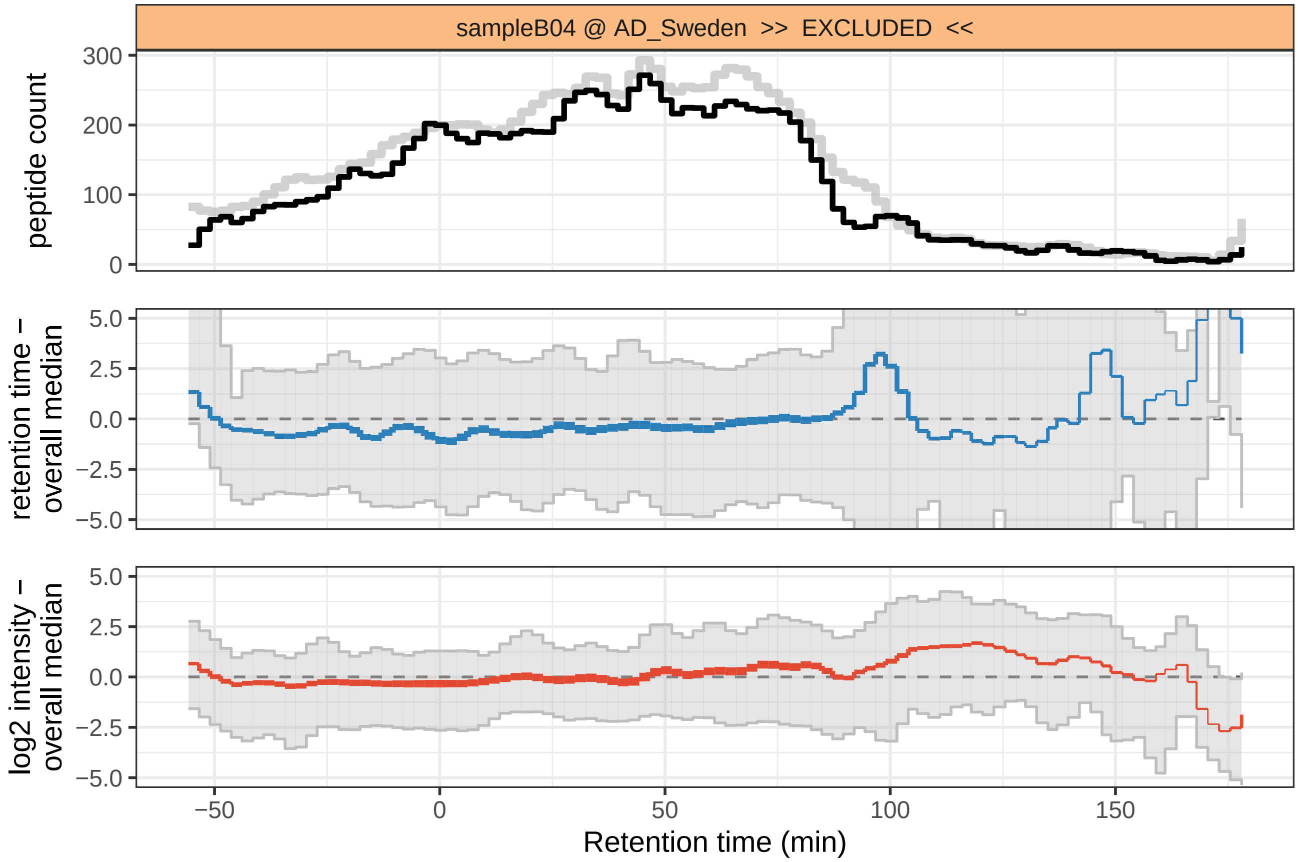

sampleA10 @ AD_Sweden
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

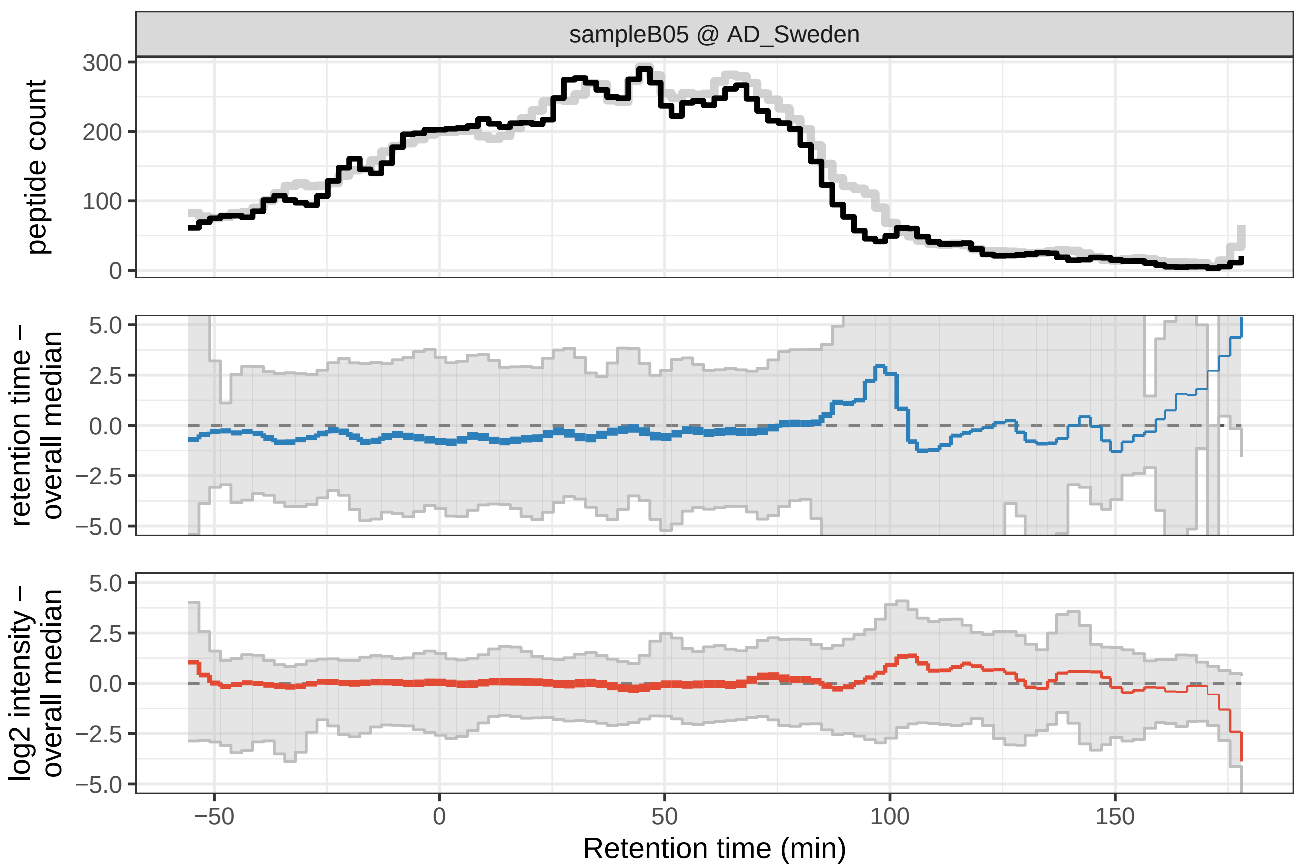

sampleA11 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

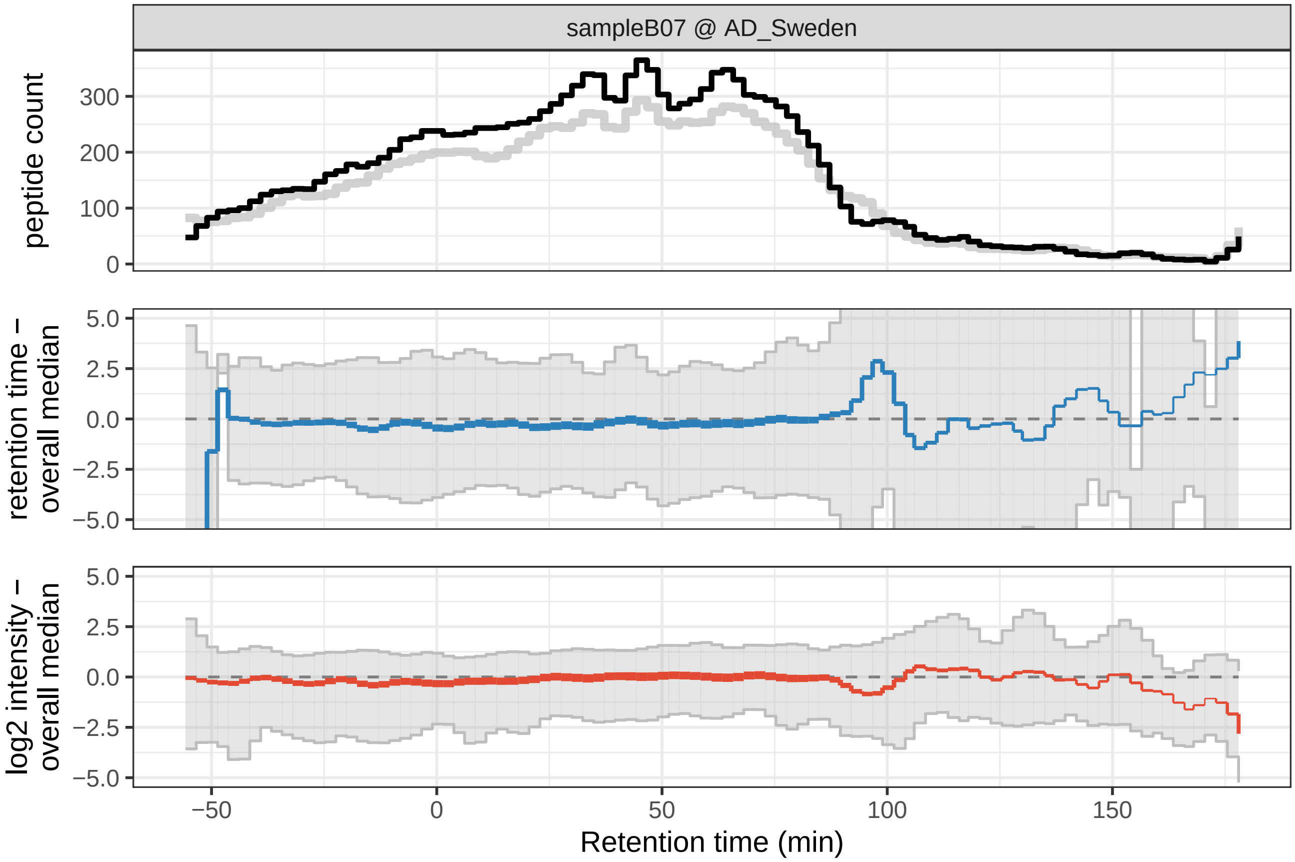

sampleA12 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

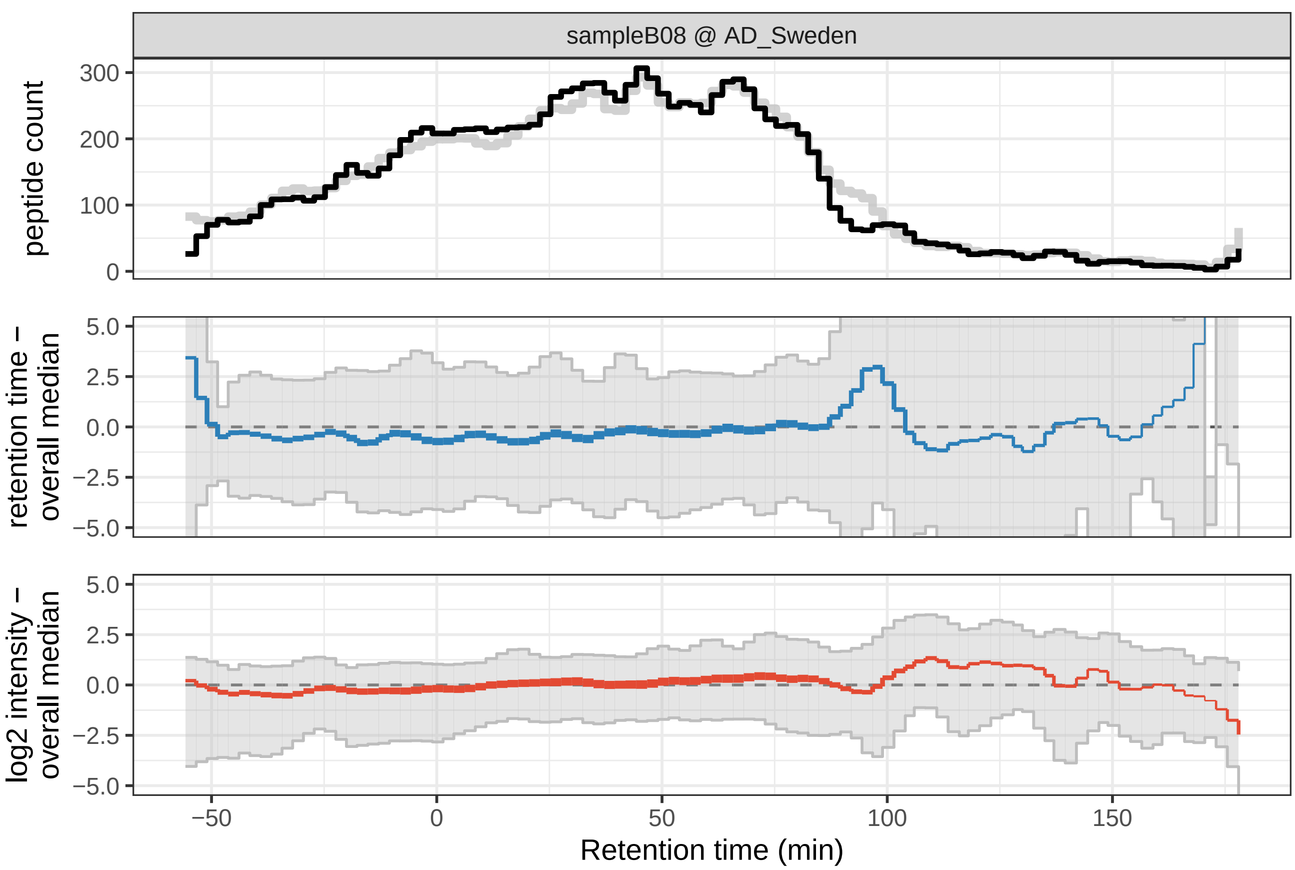

sampleB01 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

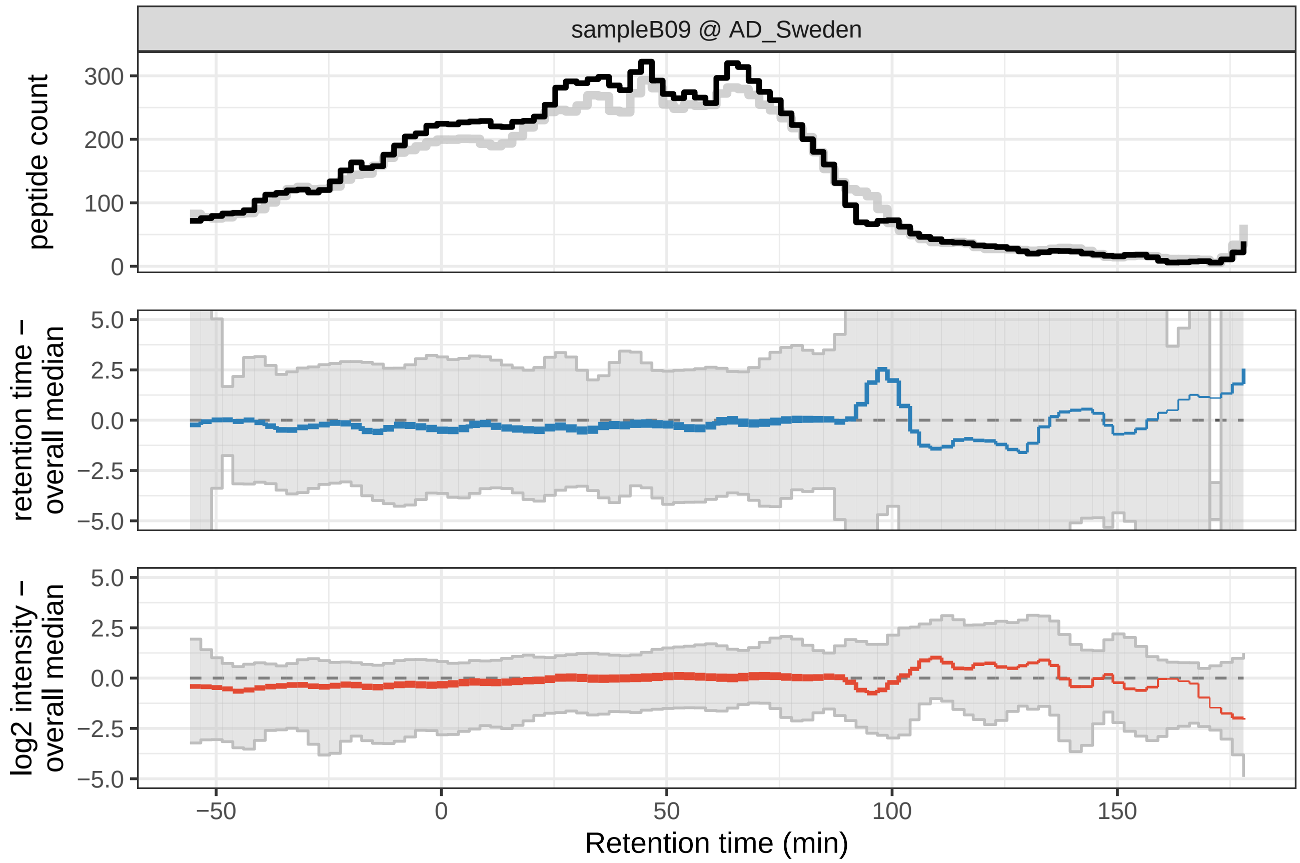

sampleB03 @ AD_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

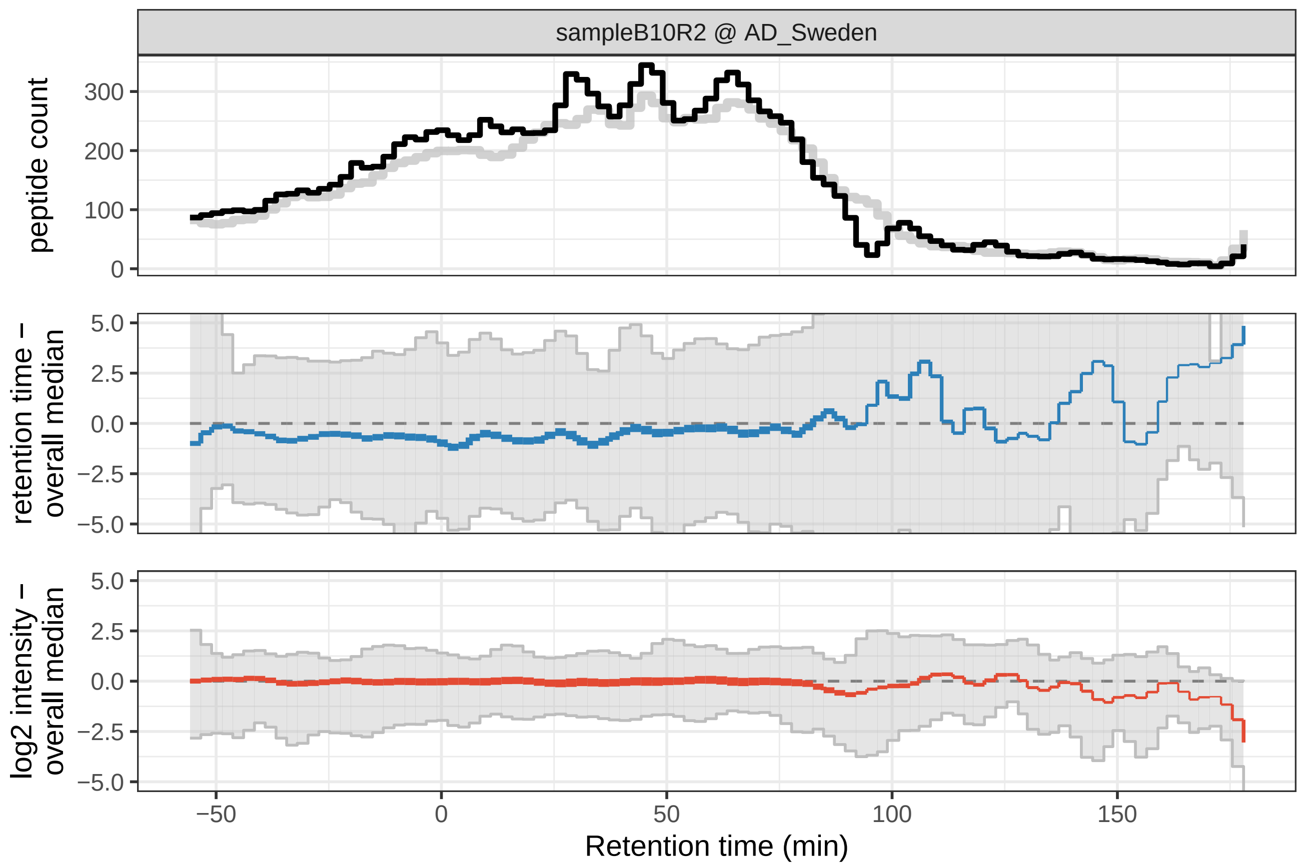

sampleB04 @ AD_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

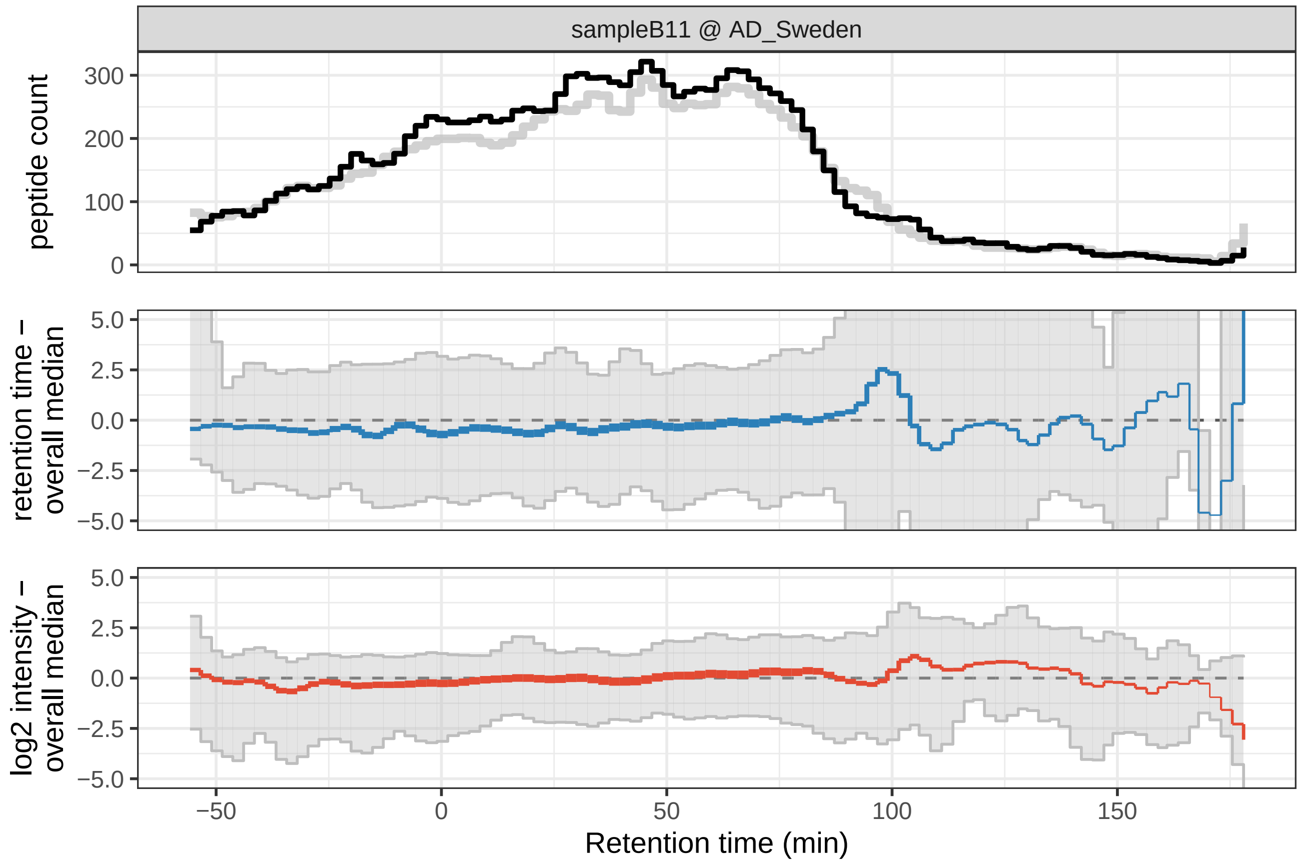

sampleB05 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

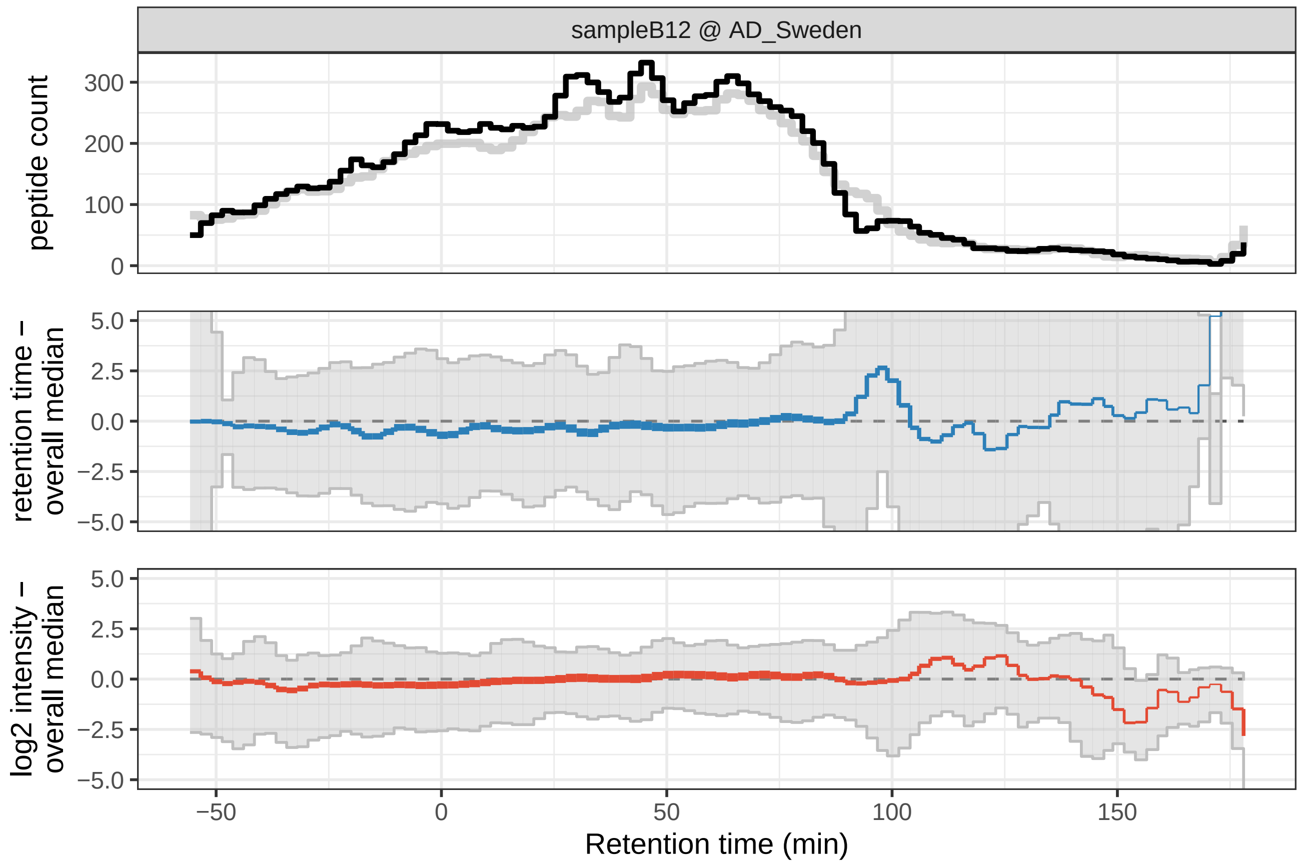

sampleB07 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

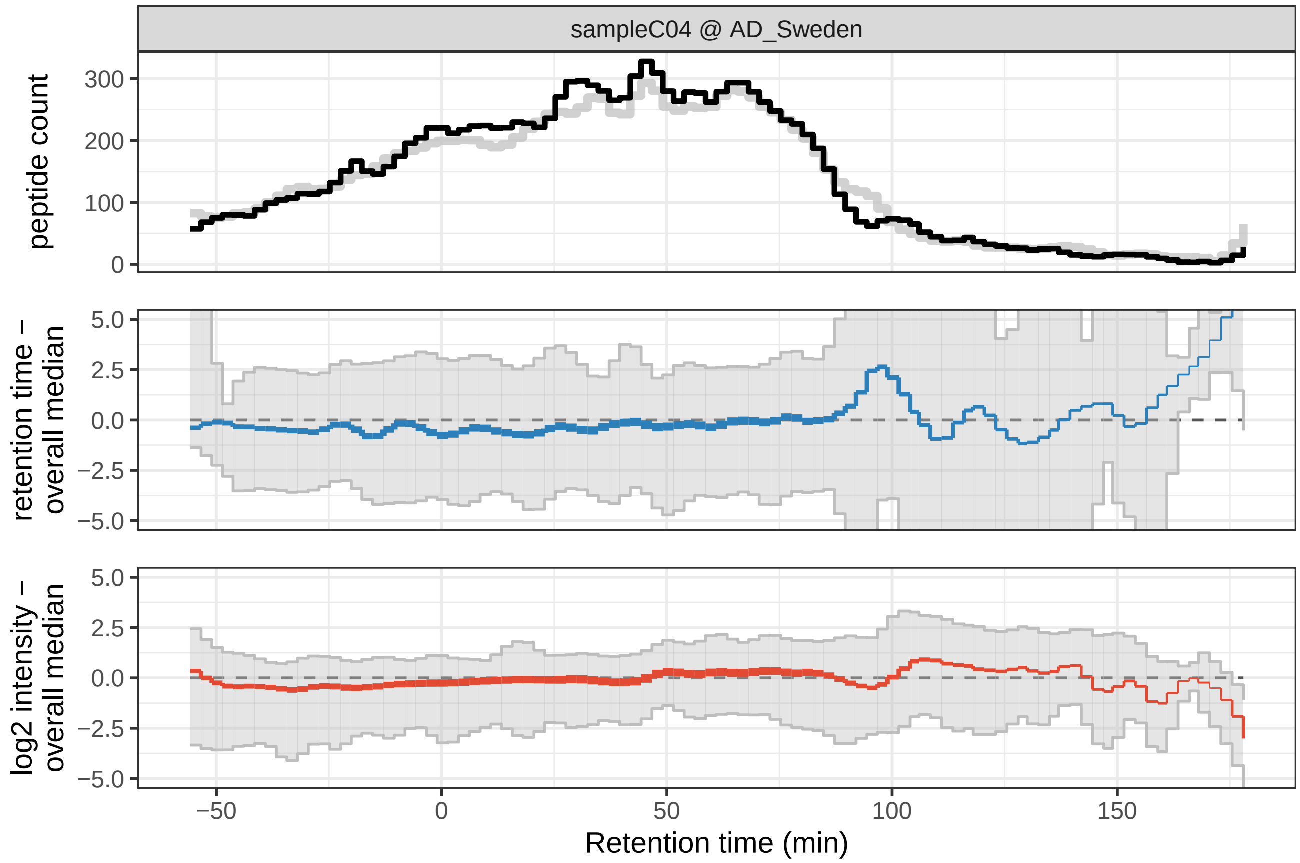

sampleB08 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

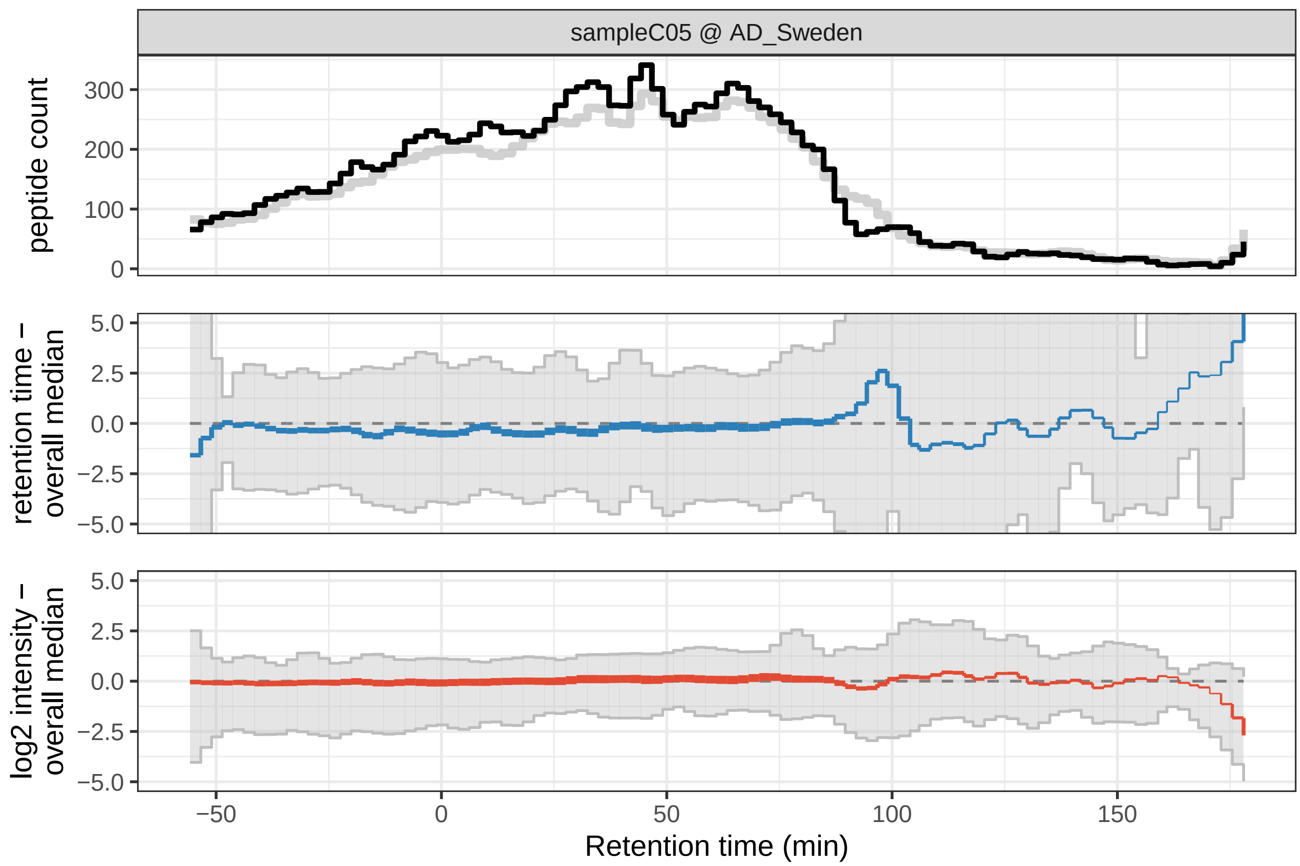

sampleB09 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

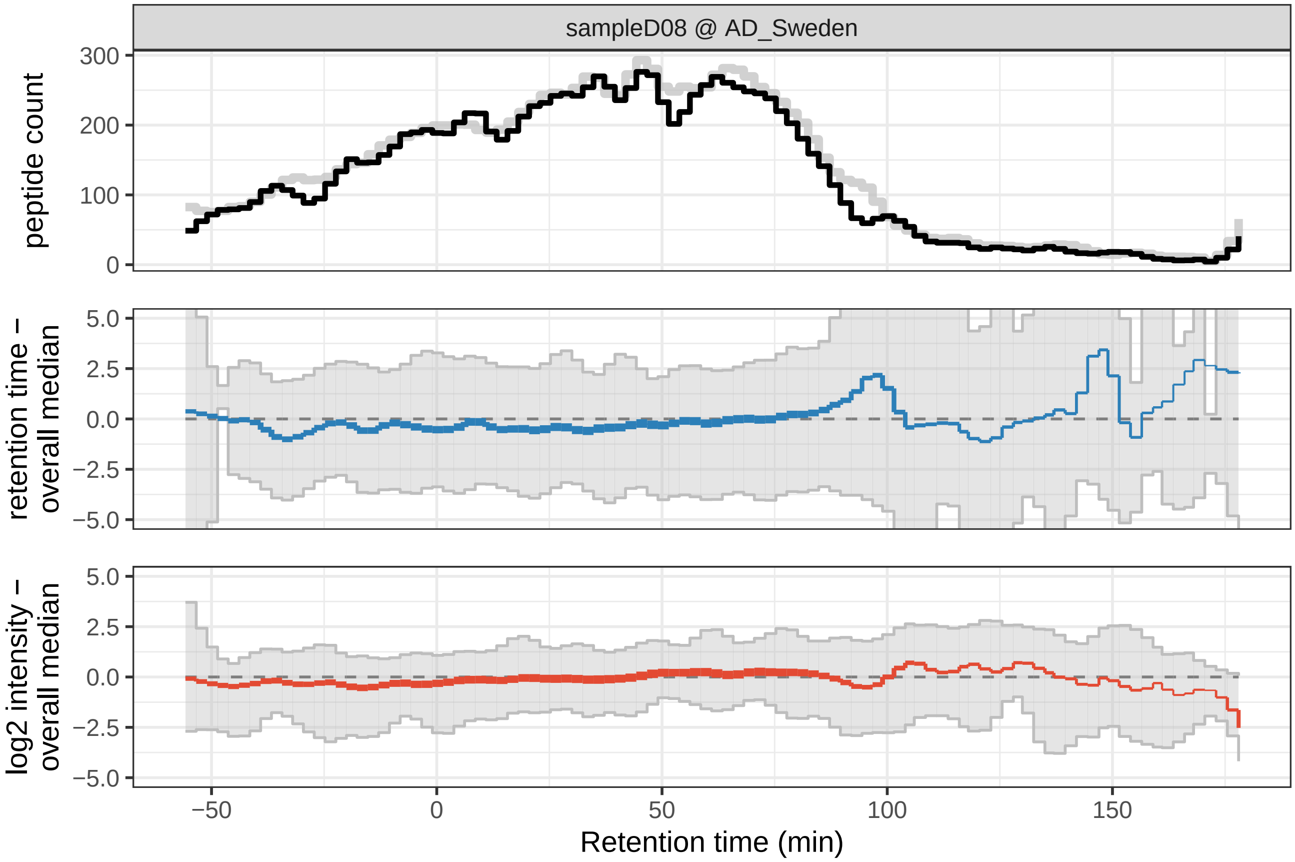

sampleB10R2 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

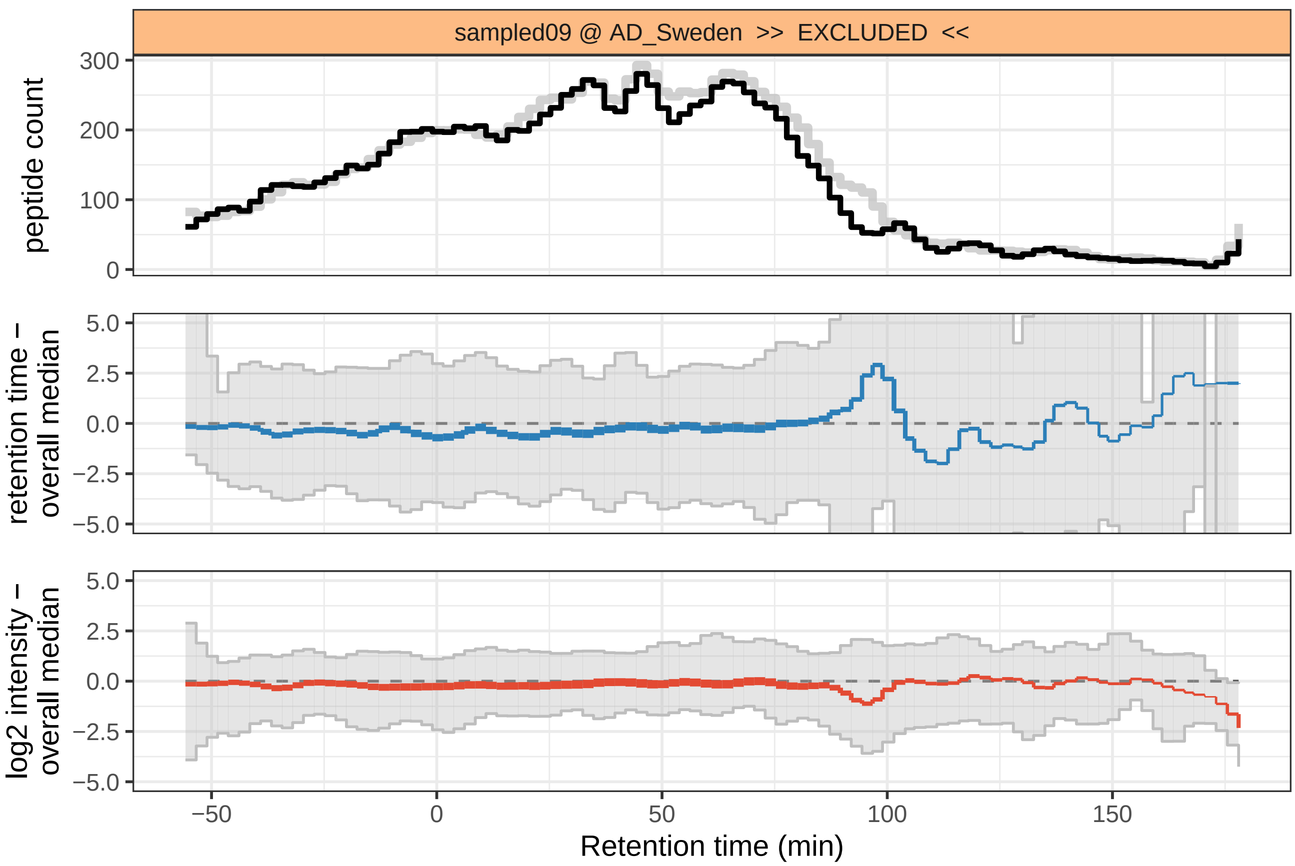

sampleB11 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

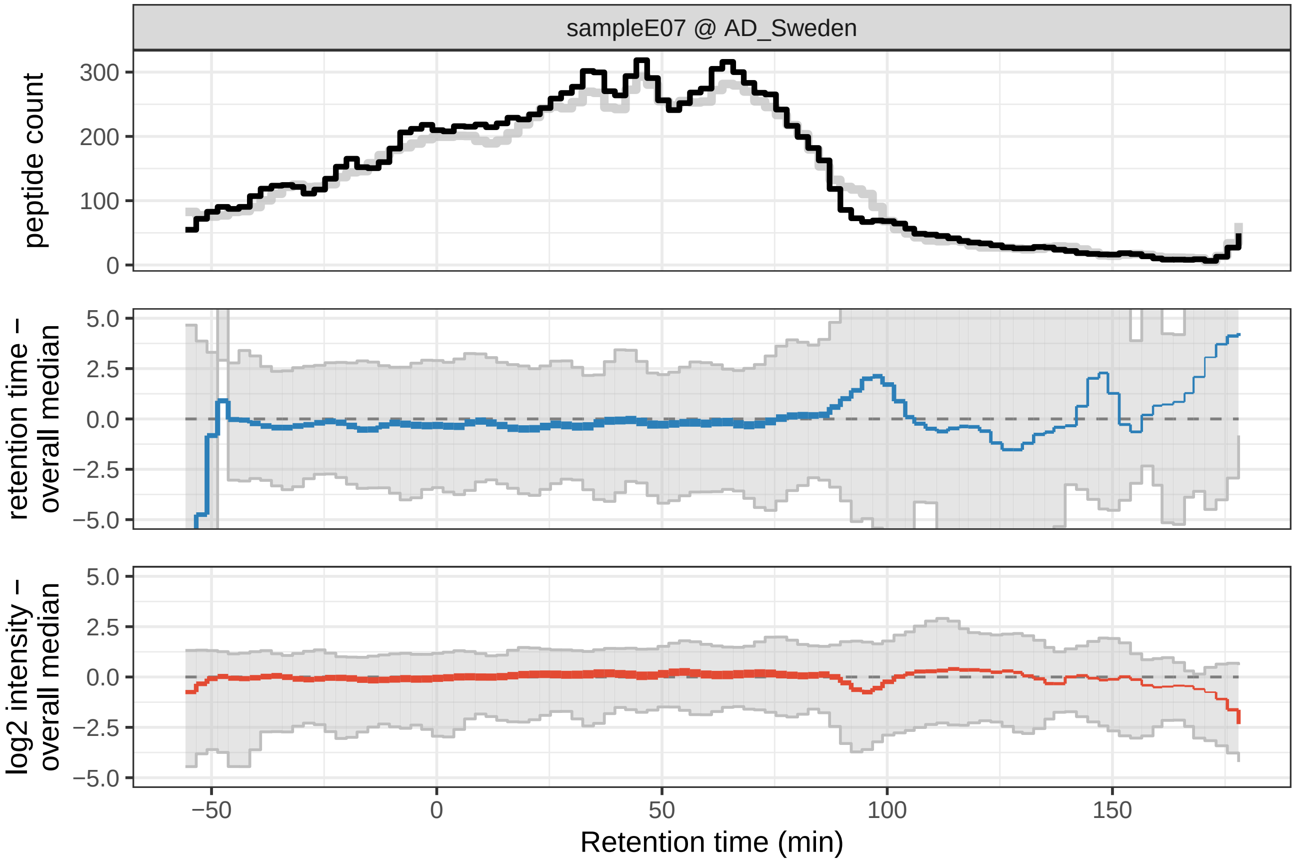

sampleB12 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleC04 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

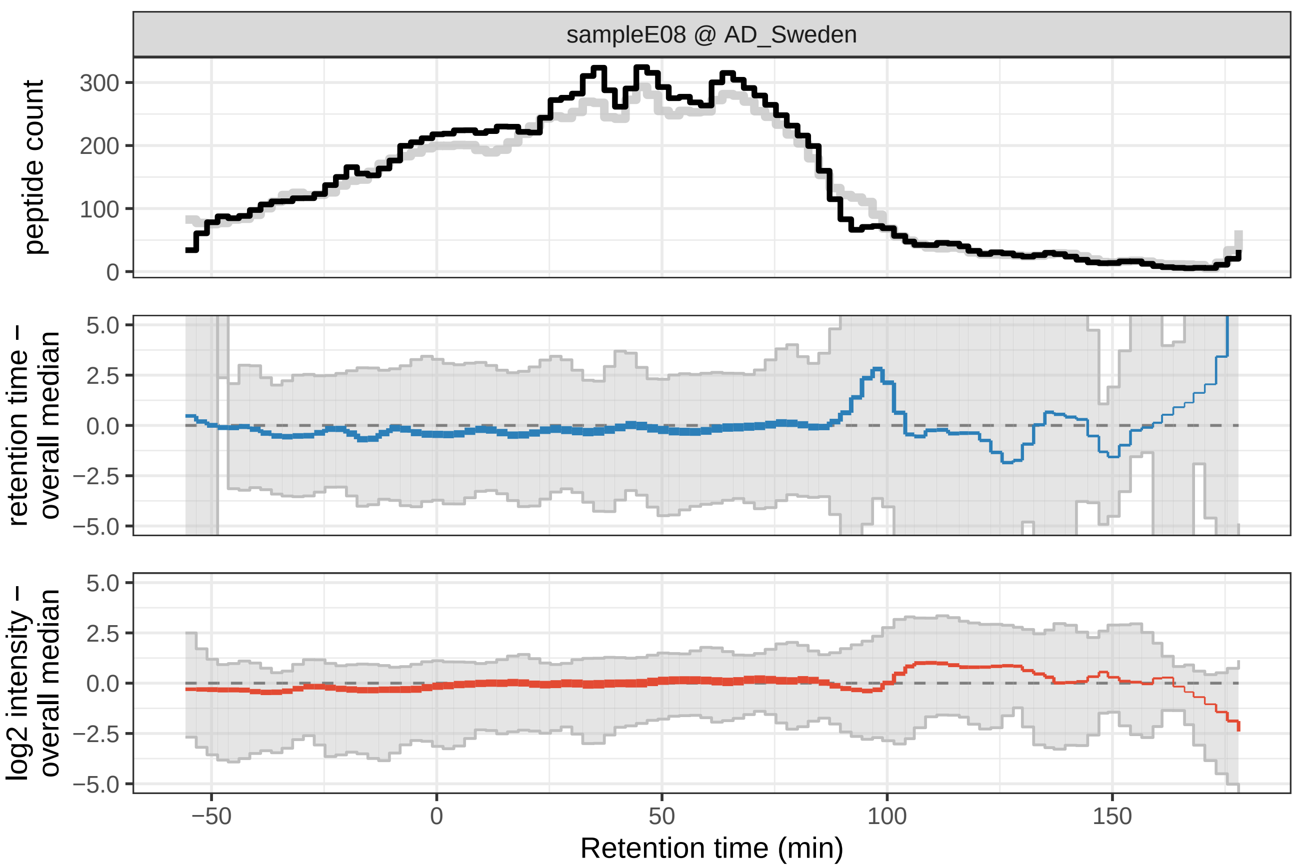

sampleC05 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleD08 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

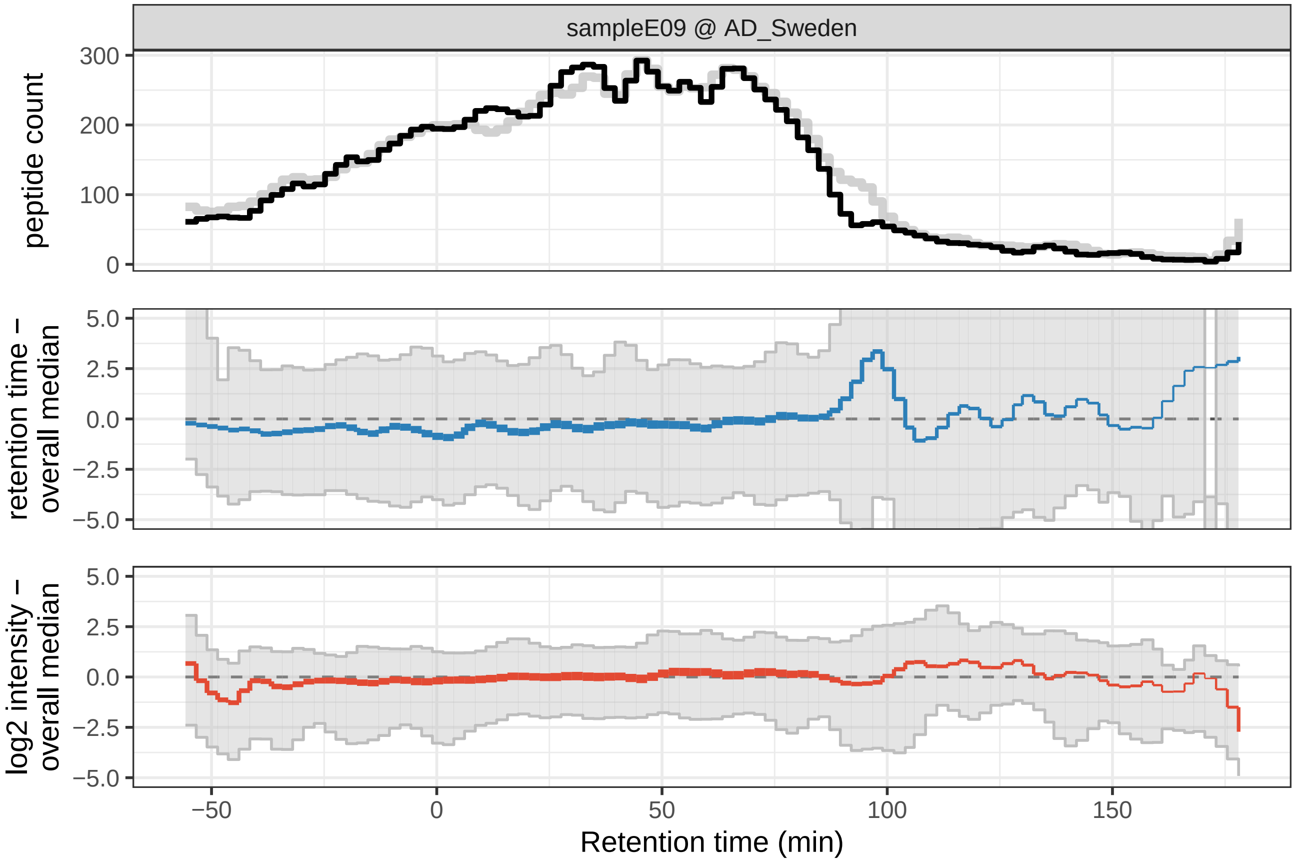

sampled09 @ AD_Sweden >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)



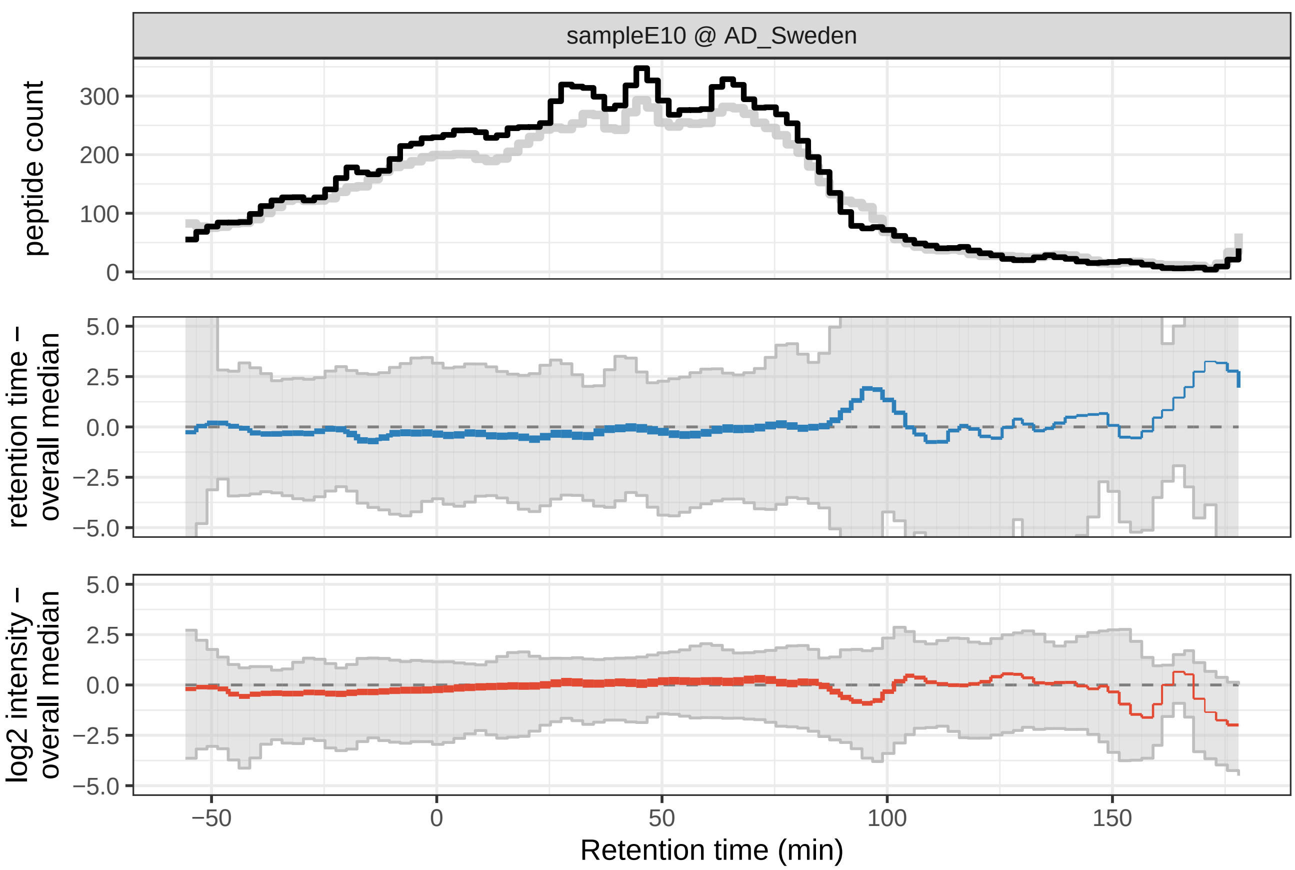
sampleE07 @ AD_Sweden
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)



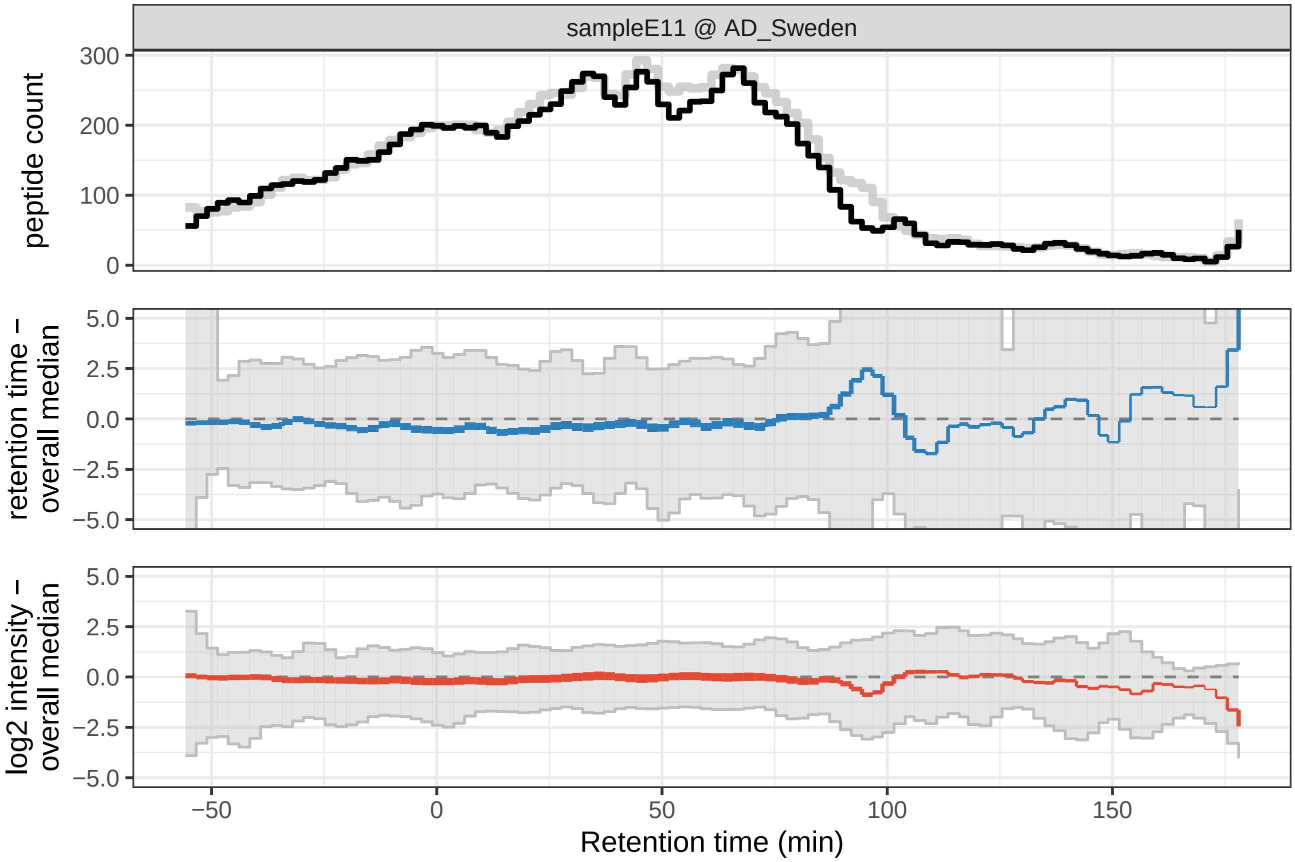
sampleE08 @ AD_Sweden
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

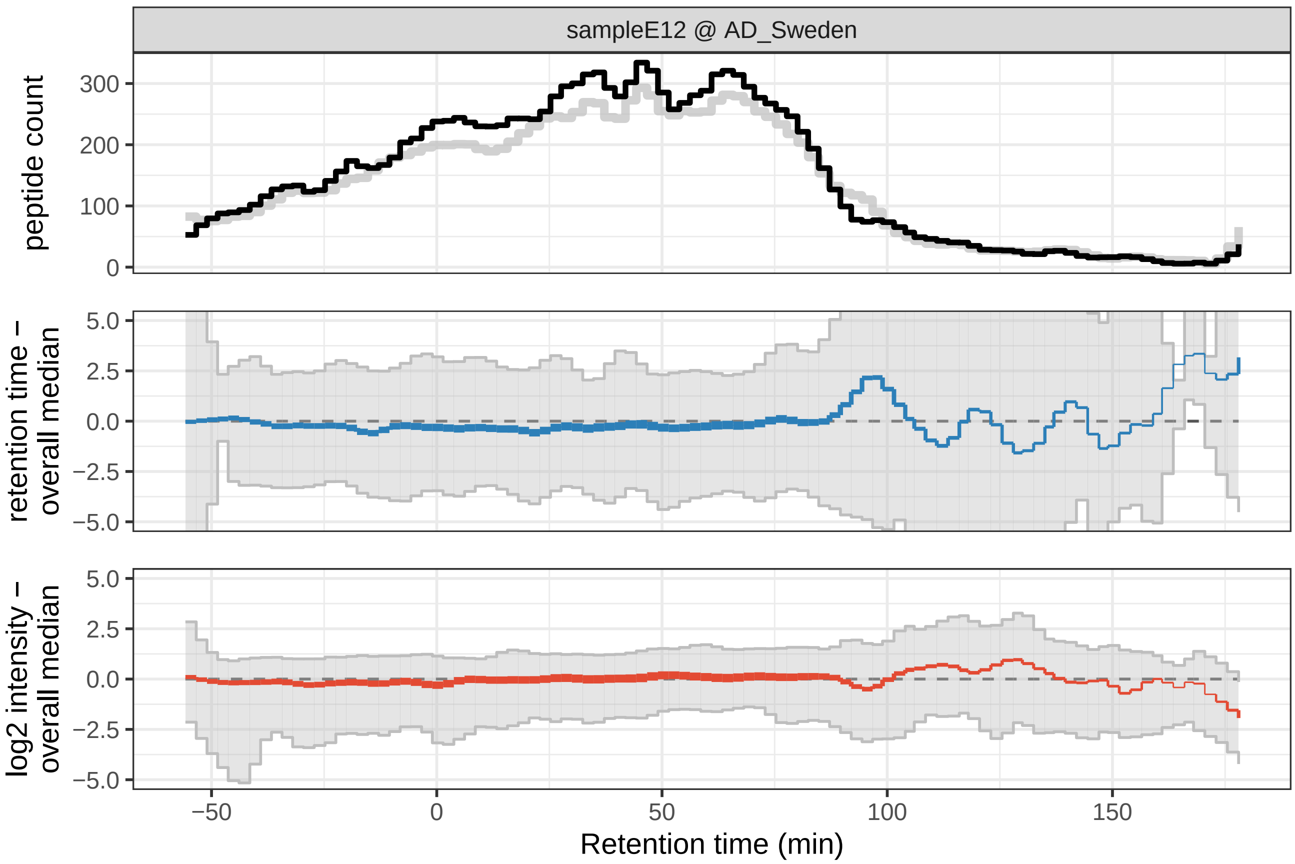


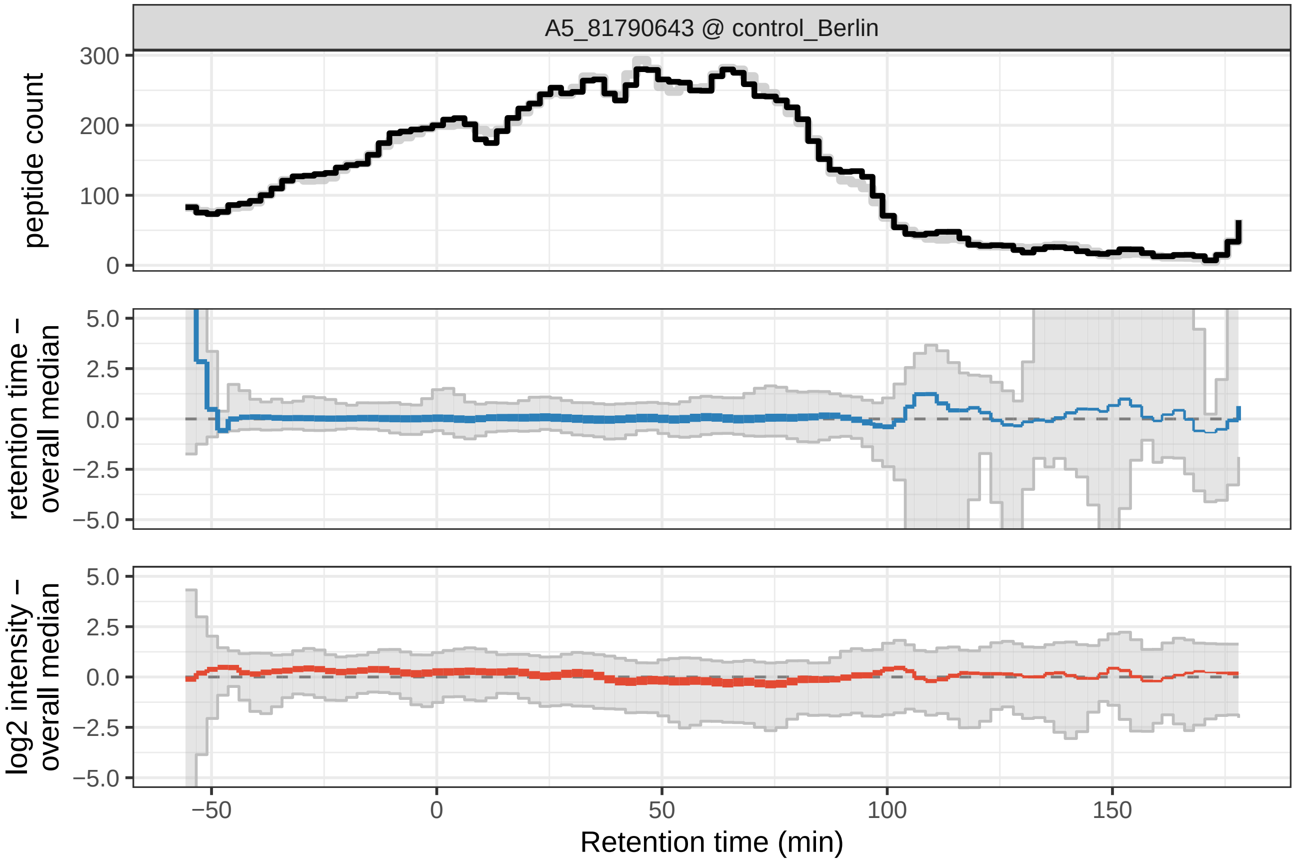
sampleE09 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

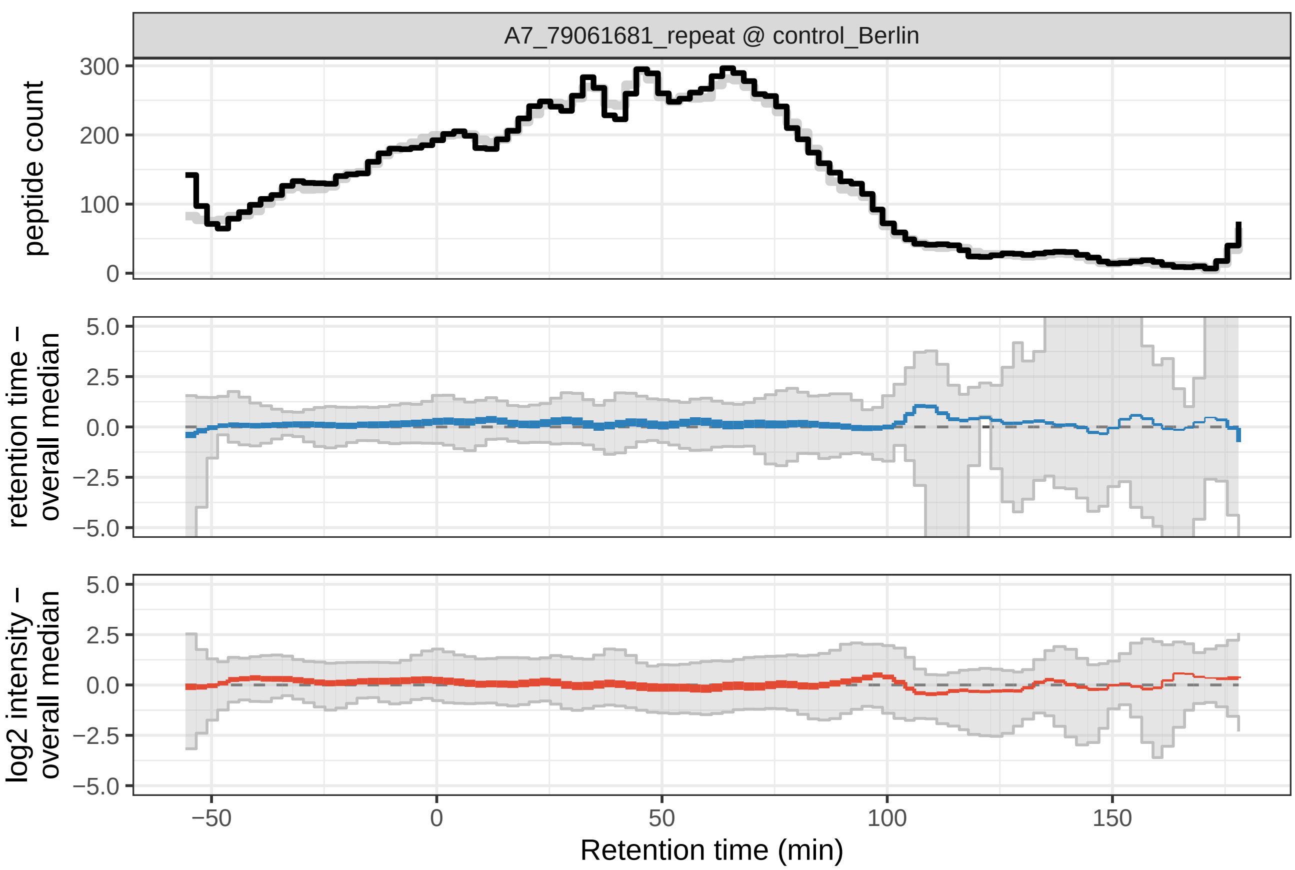


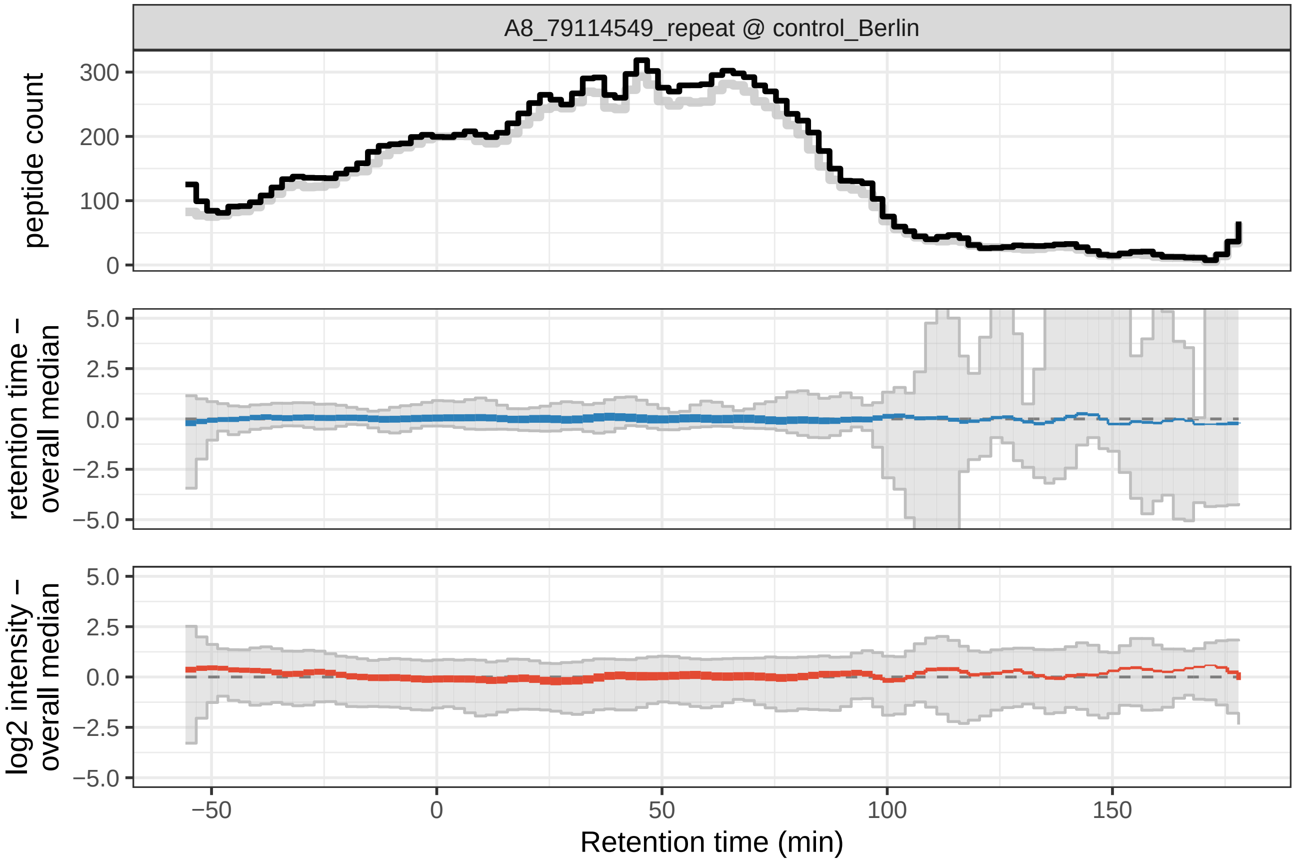
sampleE10 @ AD_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleE11 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


sampleE12 @ AD_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


A5_81790643 @ control_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


A7_79061681_repeat @ control_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


A8_79114549_repeat @ control_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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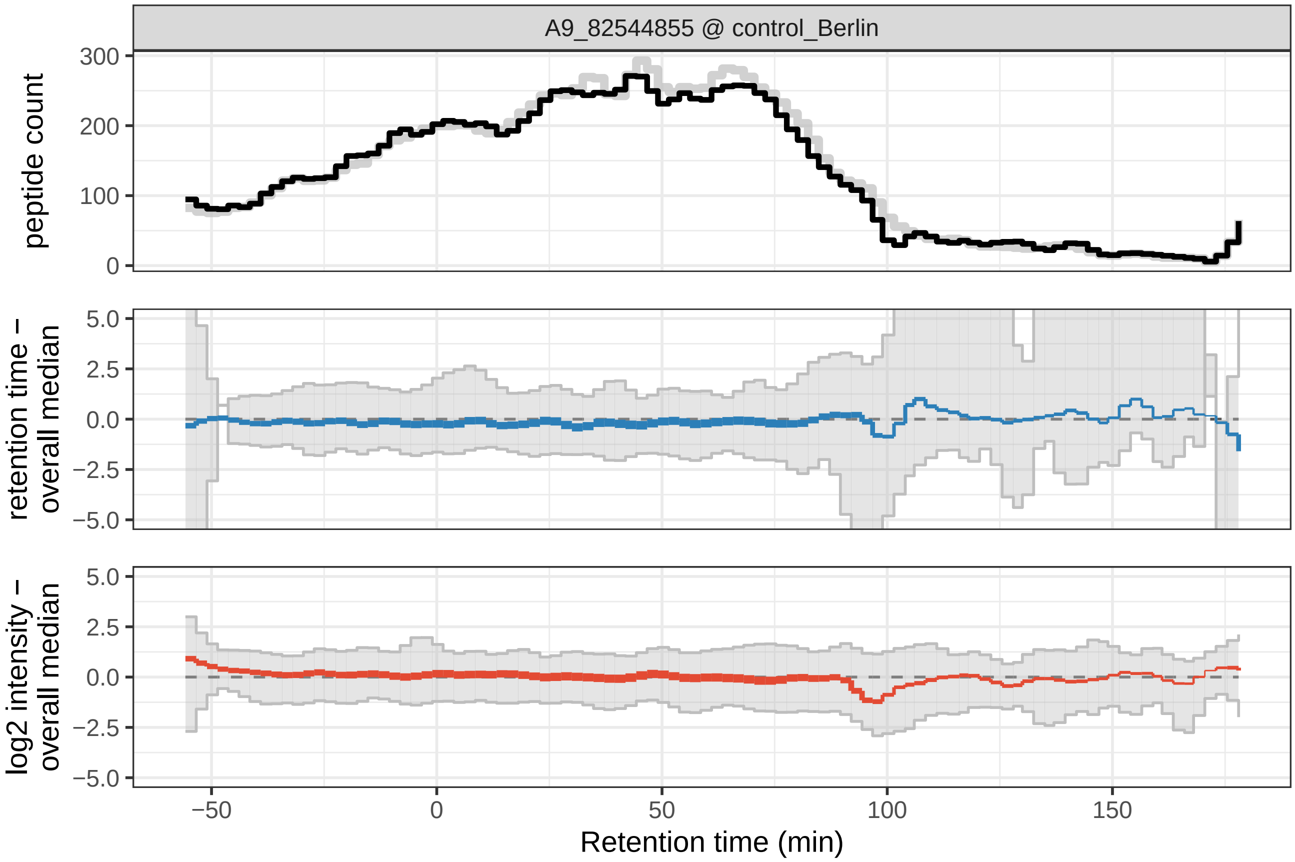
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


A9_82544855 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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−2.5
−5.0
log2 intensity –
overall median
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2.5
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−2.5
−5.0
−50
0
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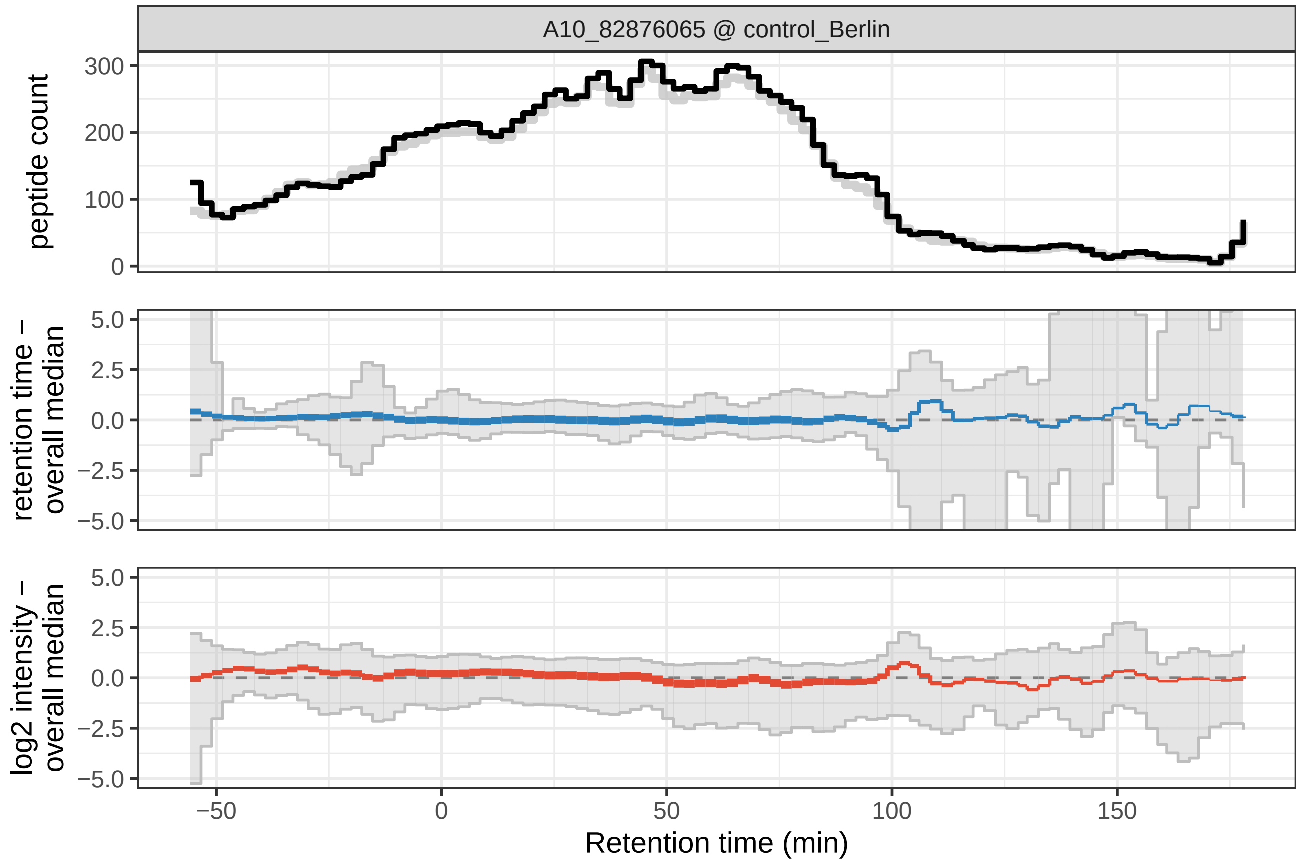
100
150
Retention time (min)


A10_82876065 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
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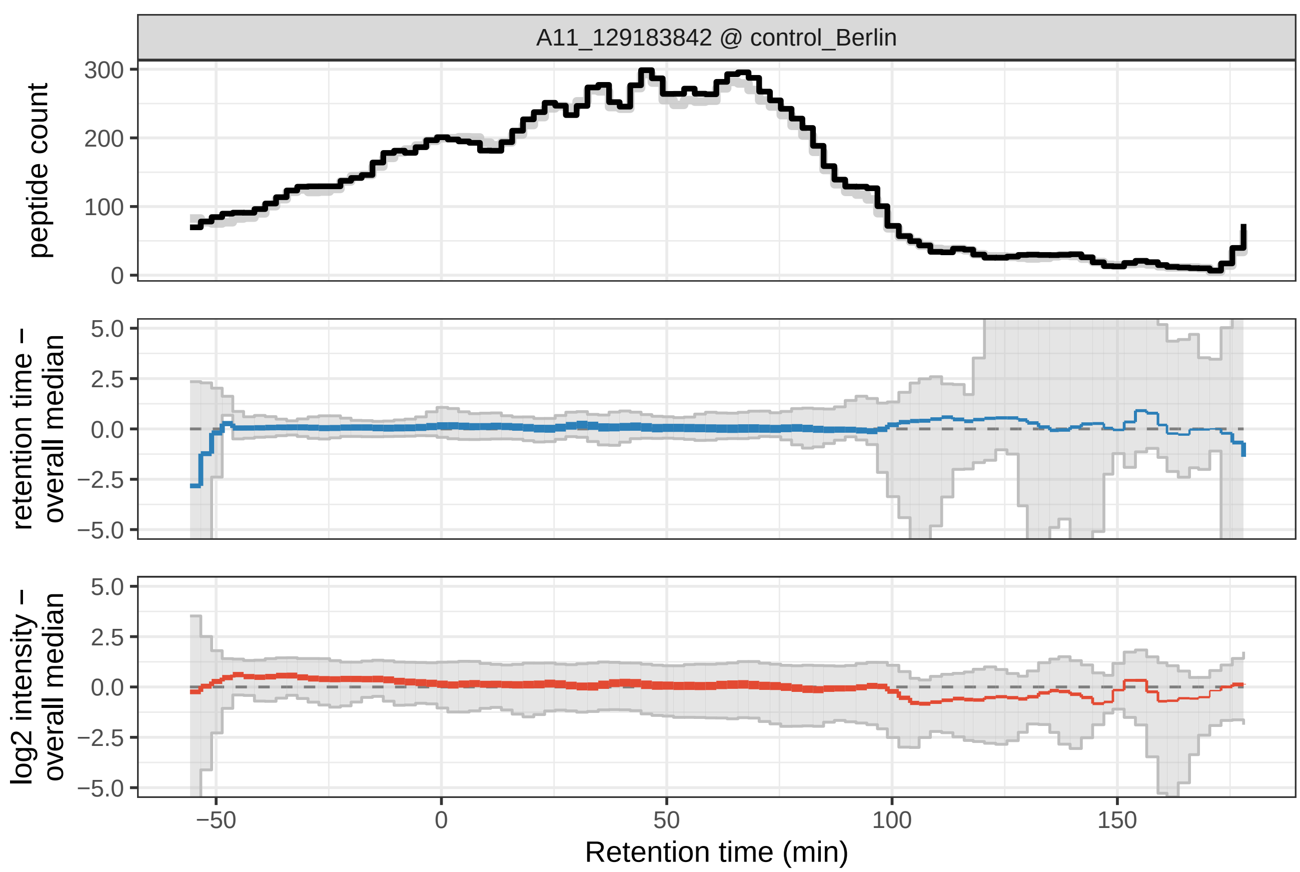
100
150
Retention time (min)


A11_129183842 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
0
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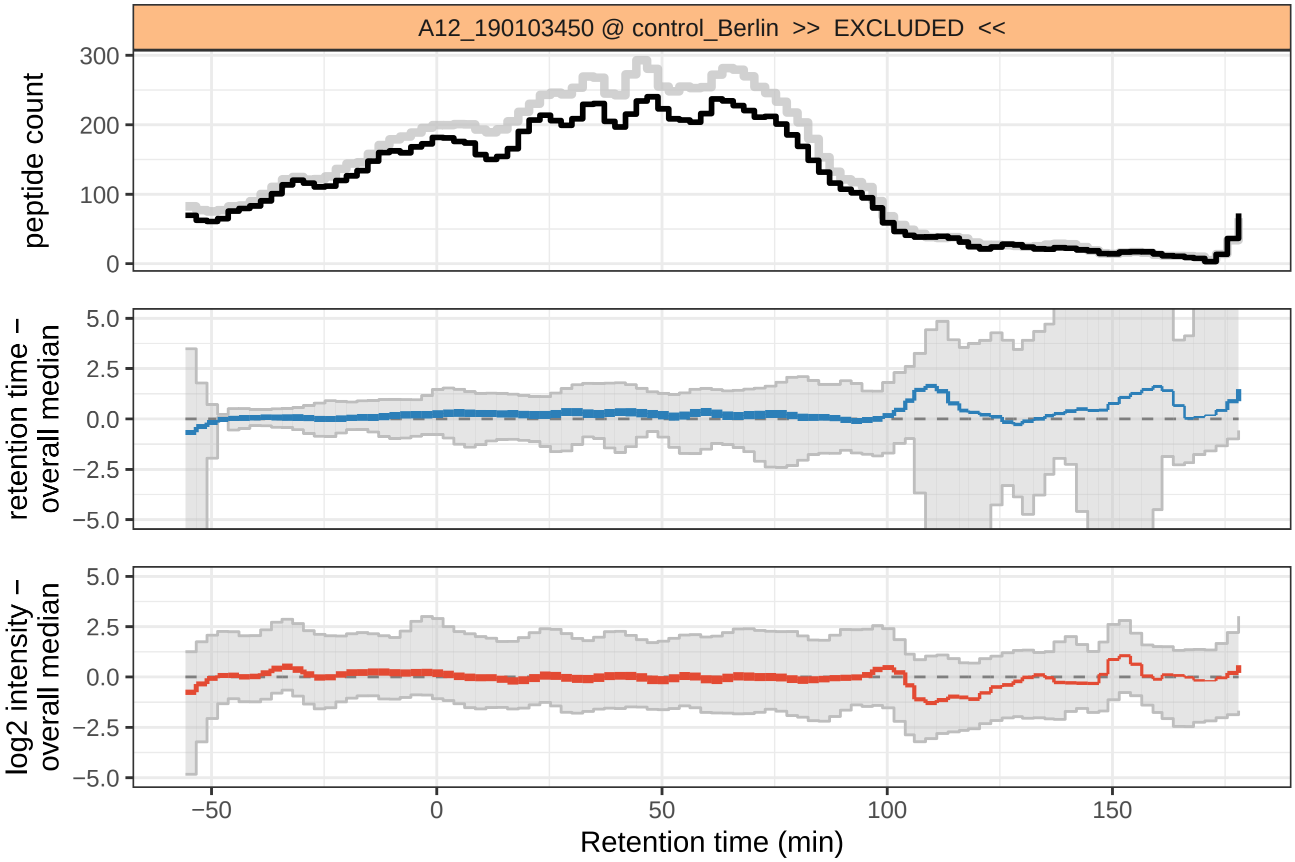
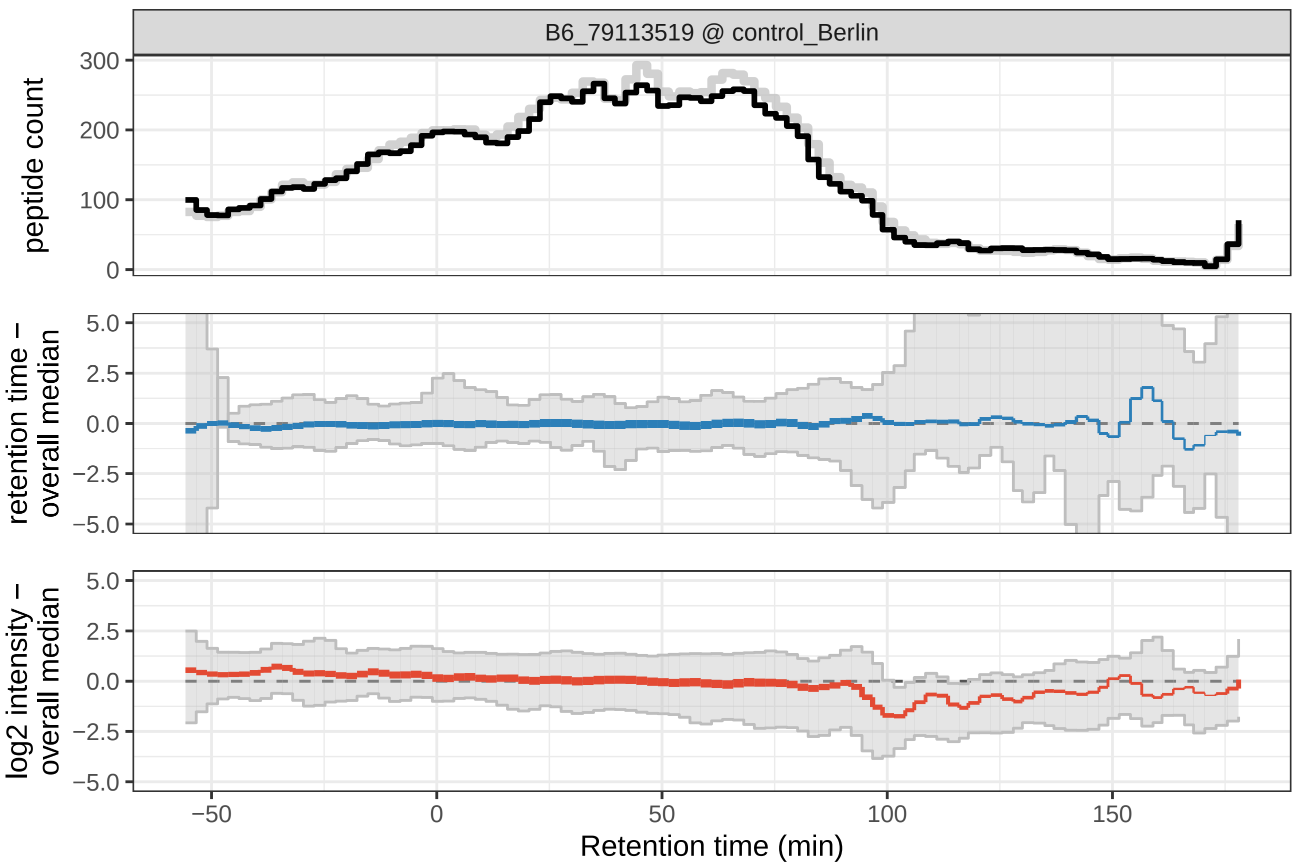
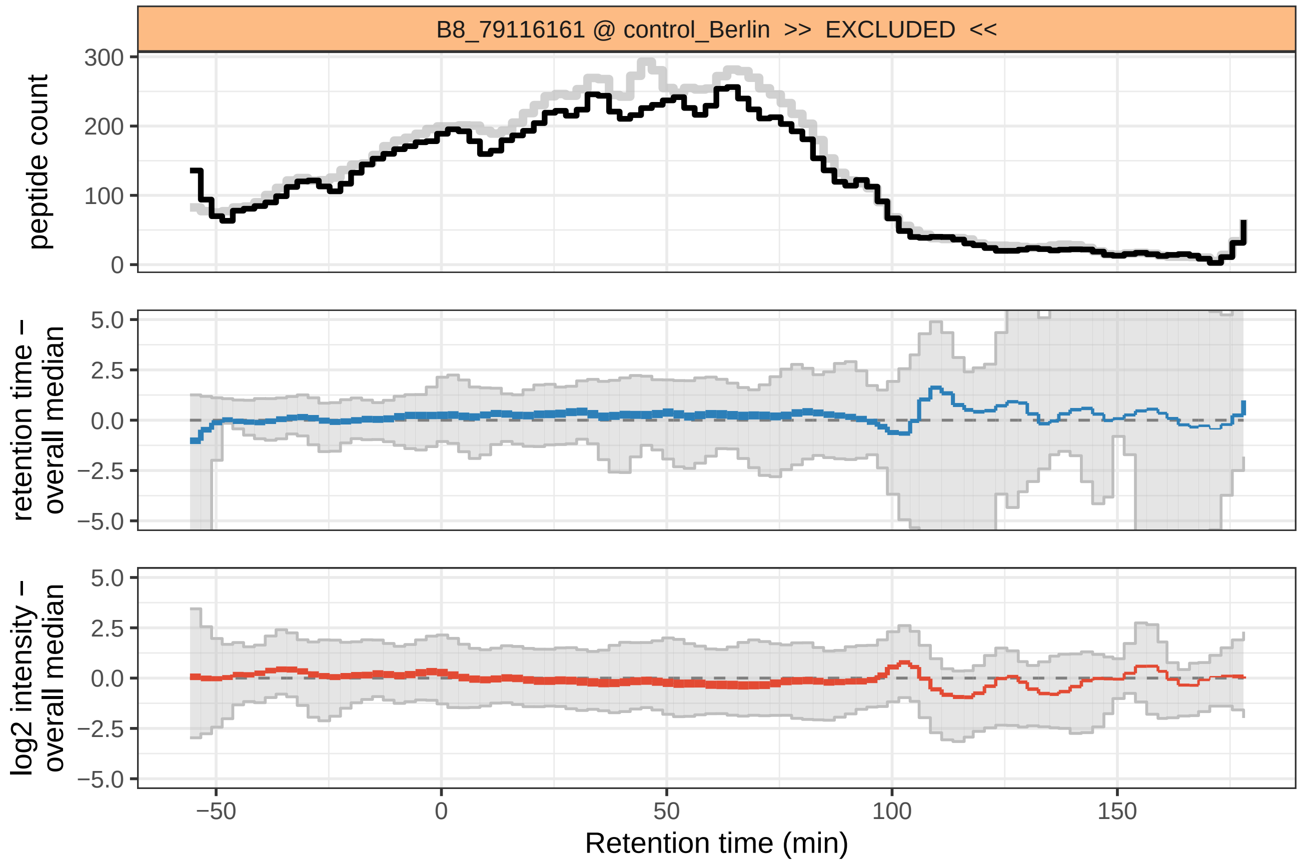
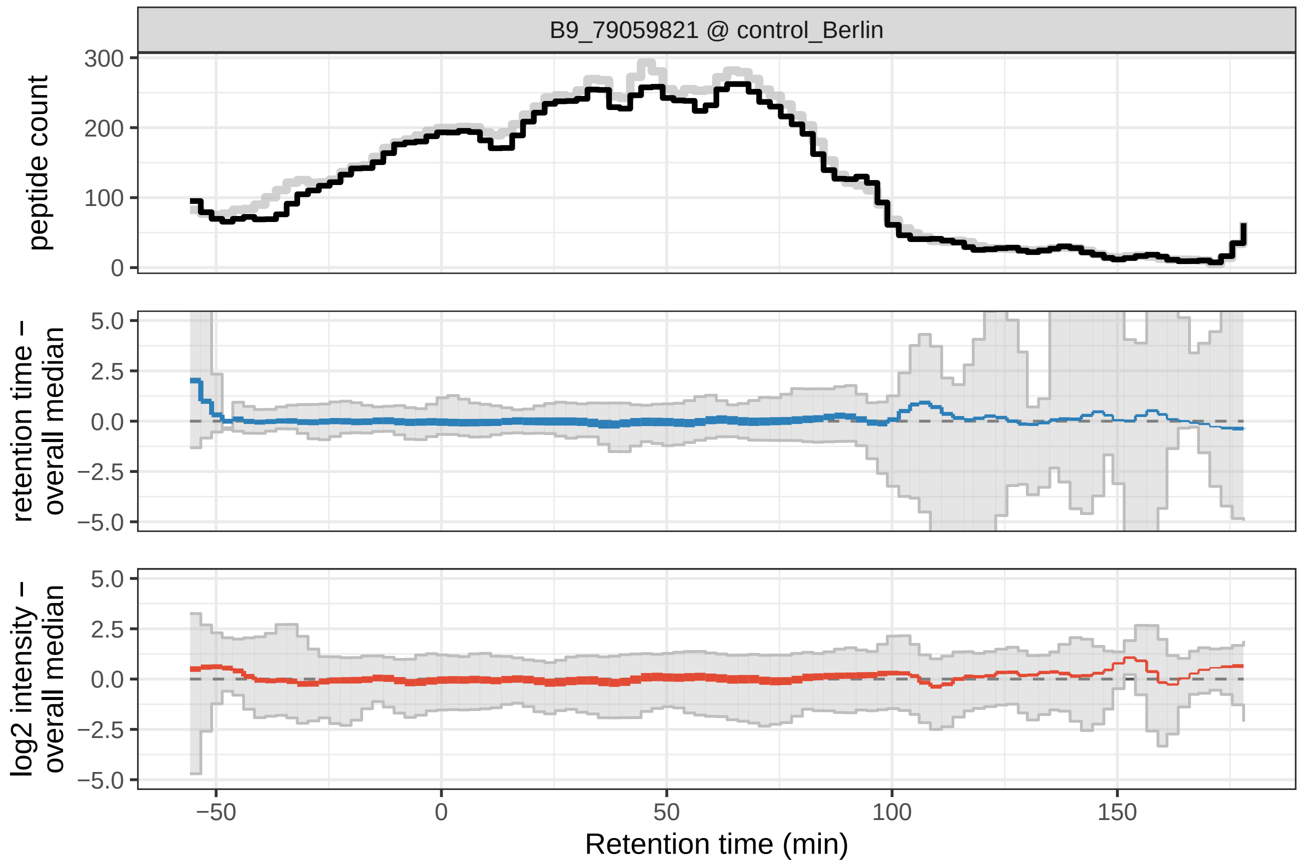
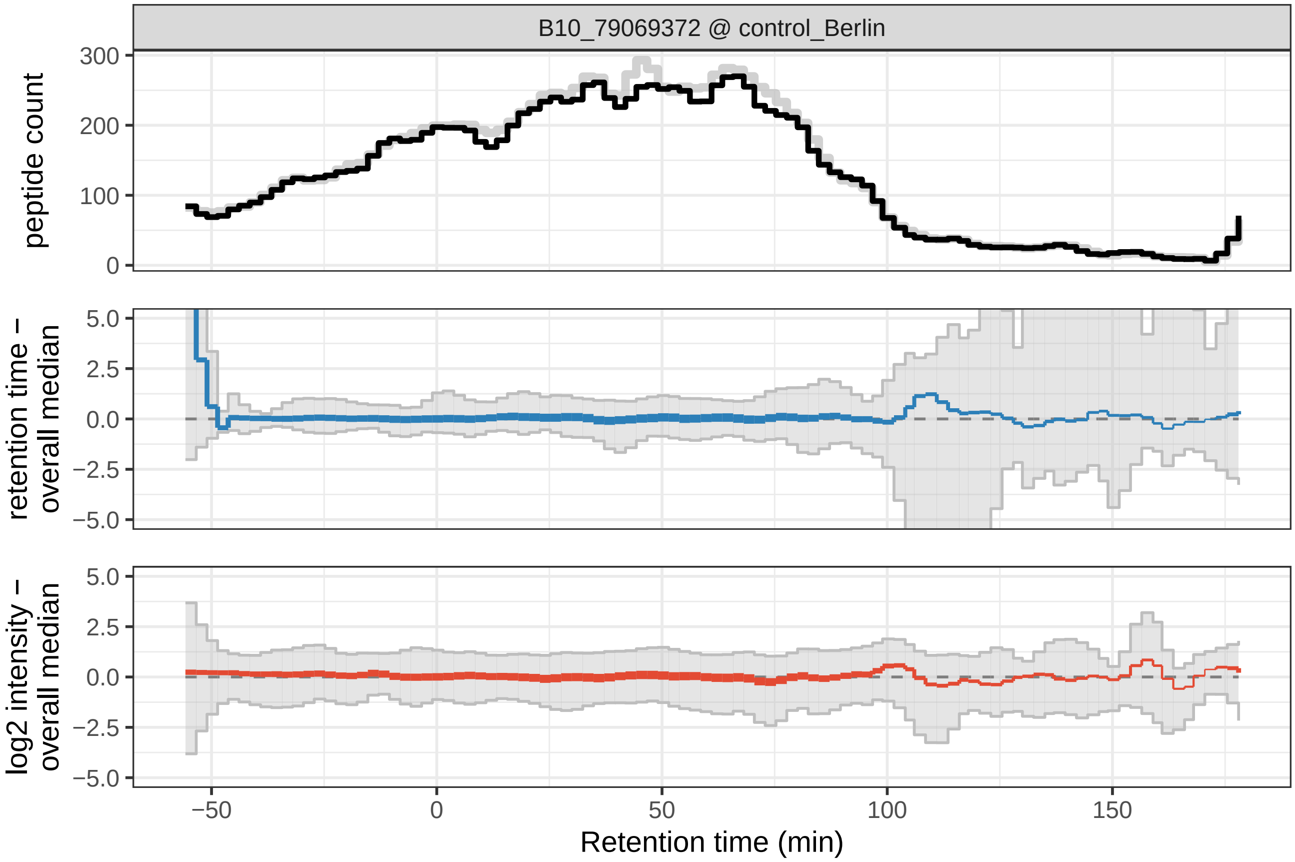
100
150
Retention time (min)


A12_190103450 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


B6_79113519 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


B8_79116161 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


B9_79059821 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


B10_79069372 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)
300
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0
5.0
2.5
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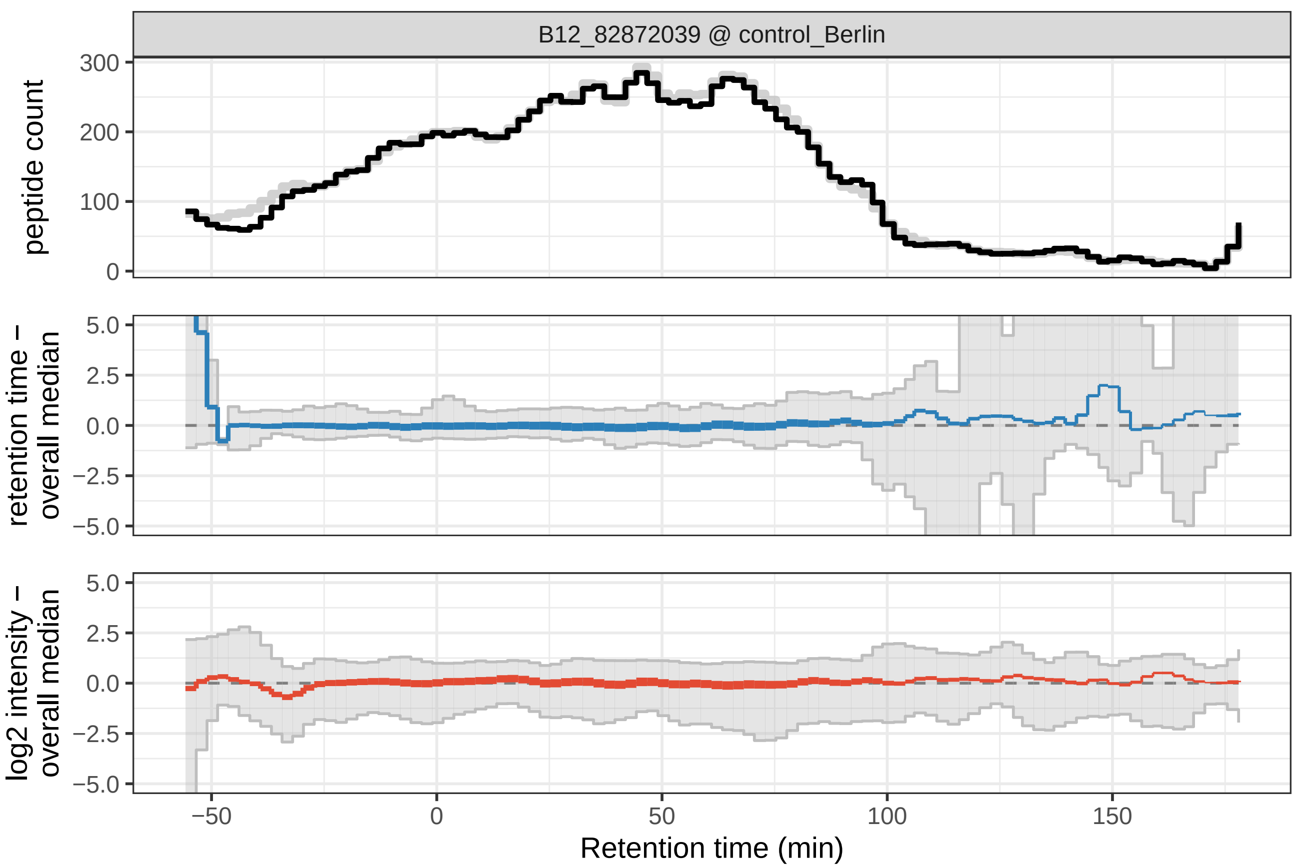
−2.5
−5.0
−50
0
50
100
150


B12_82872039 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)
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−5.0
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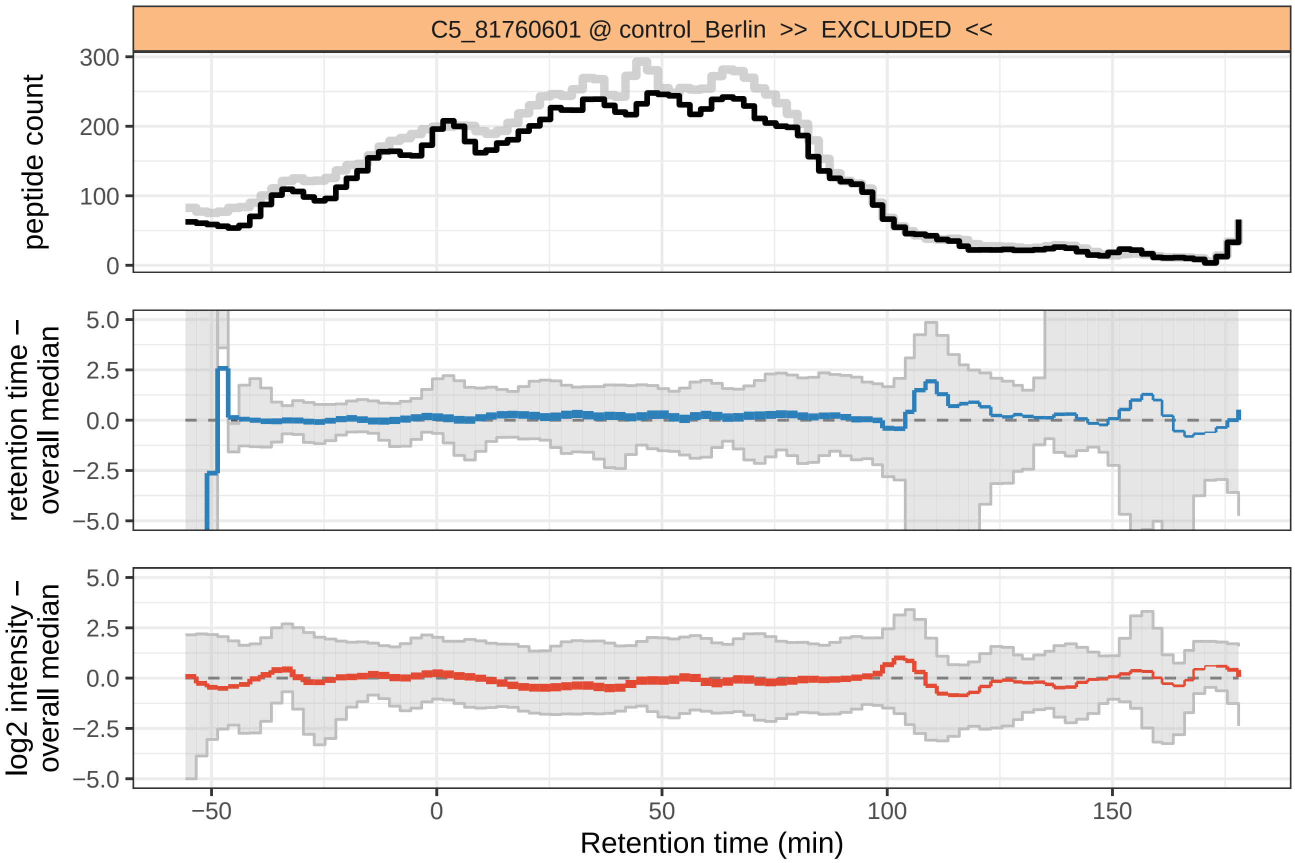
0
50
100
150


C5_81760601 @ control_Berlin >> EXCLUDED <<
peptide count
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100
0
retention time –
overall median
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
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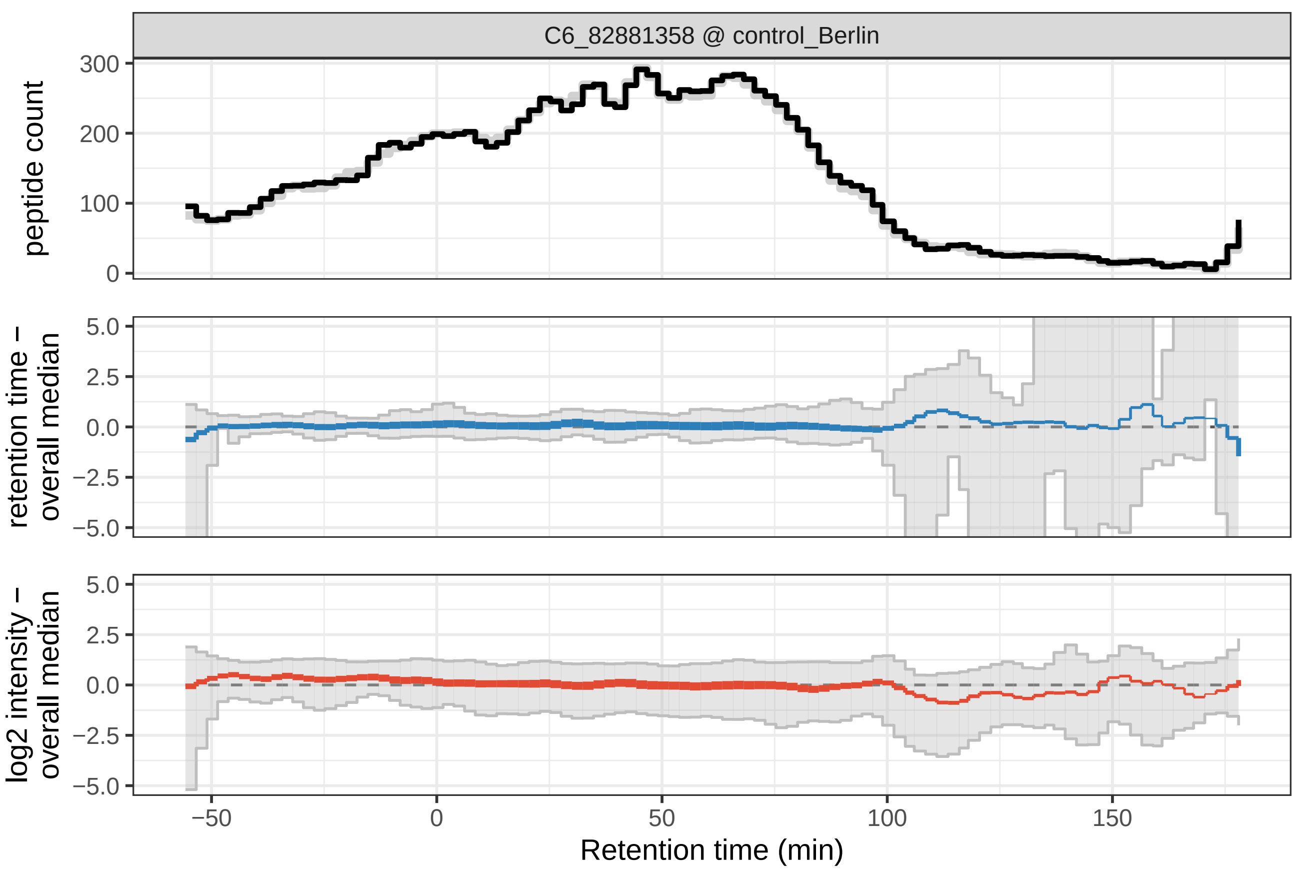
100
150
Retention time (min)


C6_82881358 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
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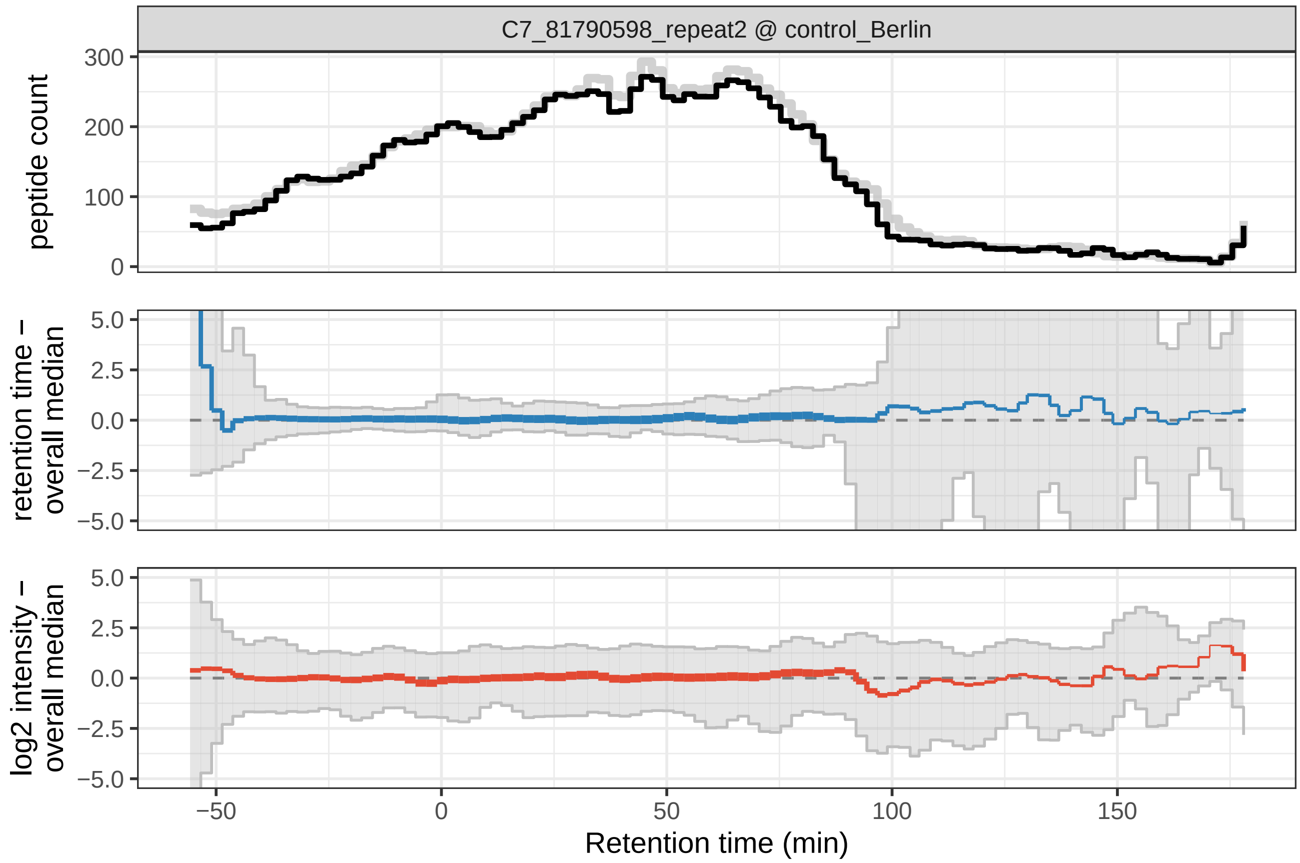
100
150
Retention time (min)


C7_81790598_repeat2 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
0
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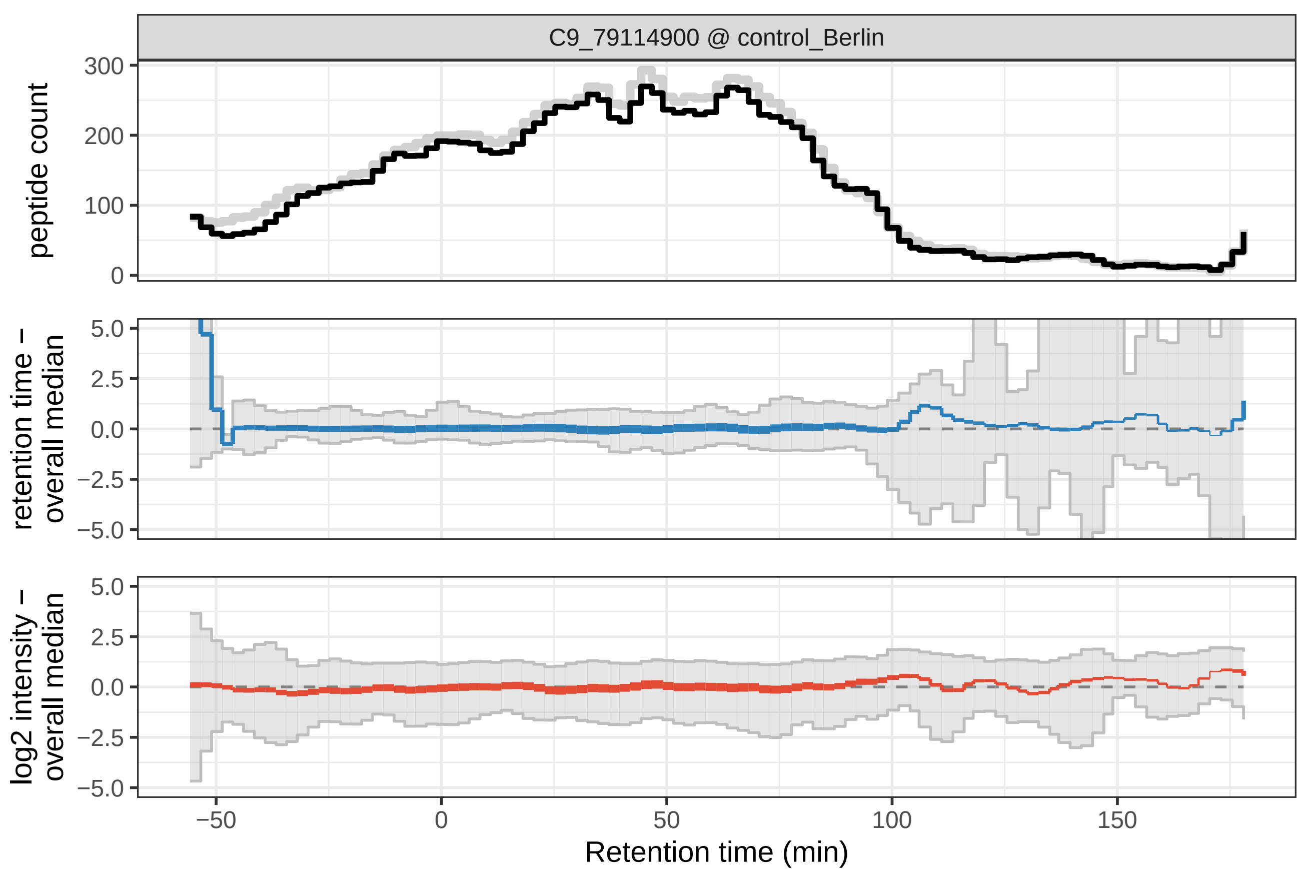
100
150
Retention time (min)


C9_79114900 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
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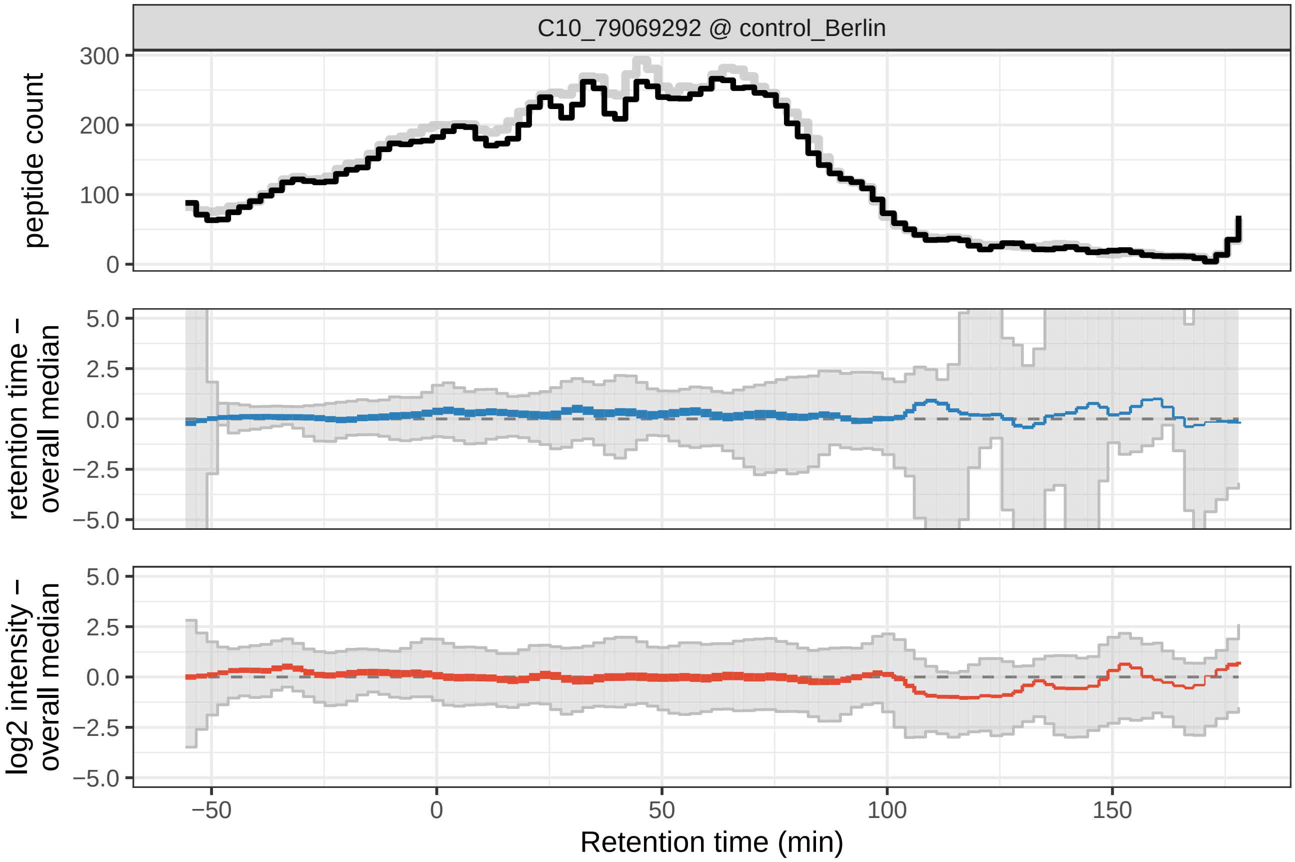
100
150
Retention time (min)


C10_79069292 @ control_Berlin
peptide count
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200
100
0
retention time –
overall median
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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2.5
0.0
−2.5
−5.0
−50
0
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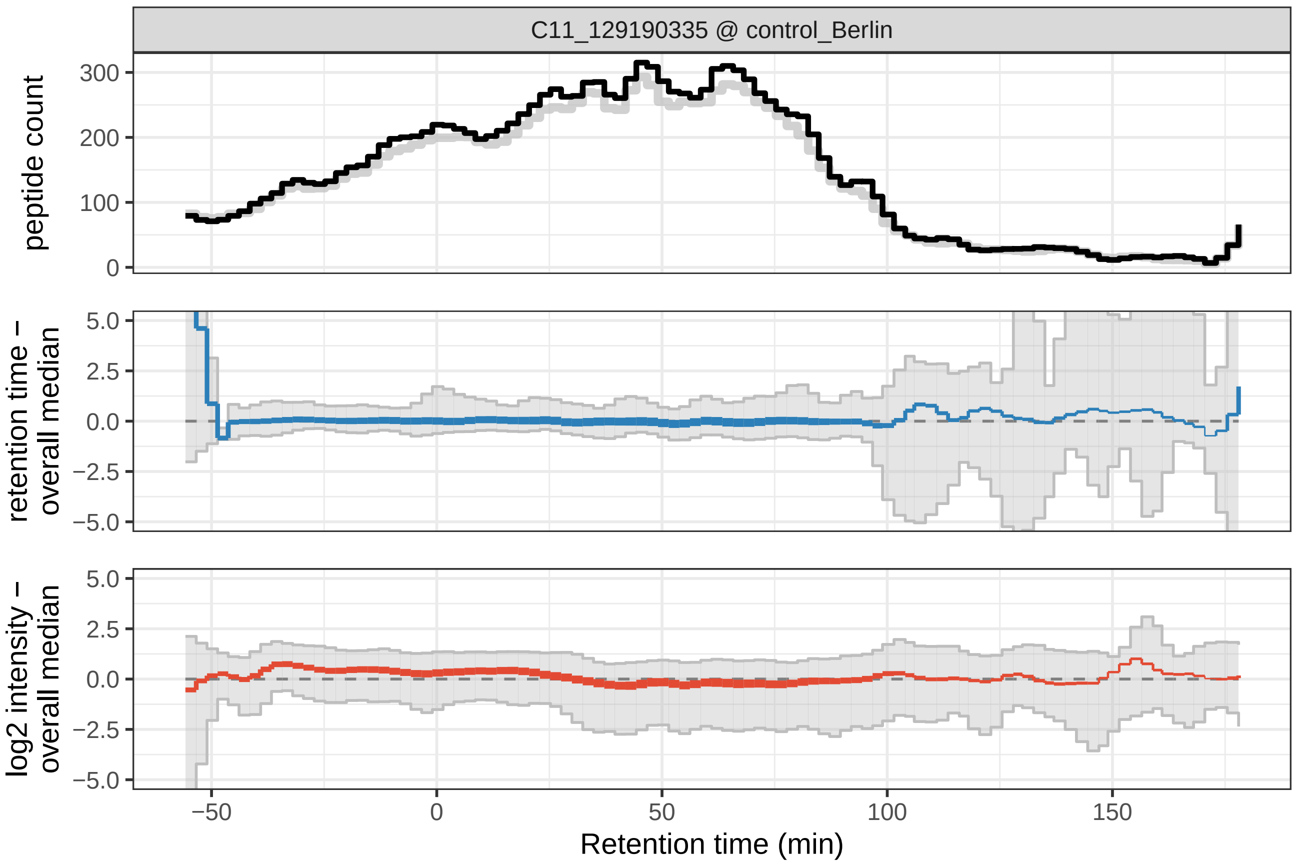
100
150
Retention time (min)


C11_129190335 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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2.5
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−5.0
log2 intensity –
overall median
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2.5
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−2.5
−5.0
−50
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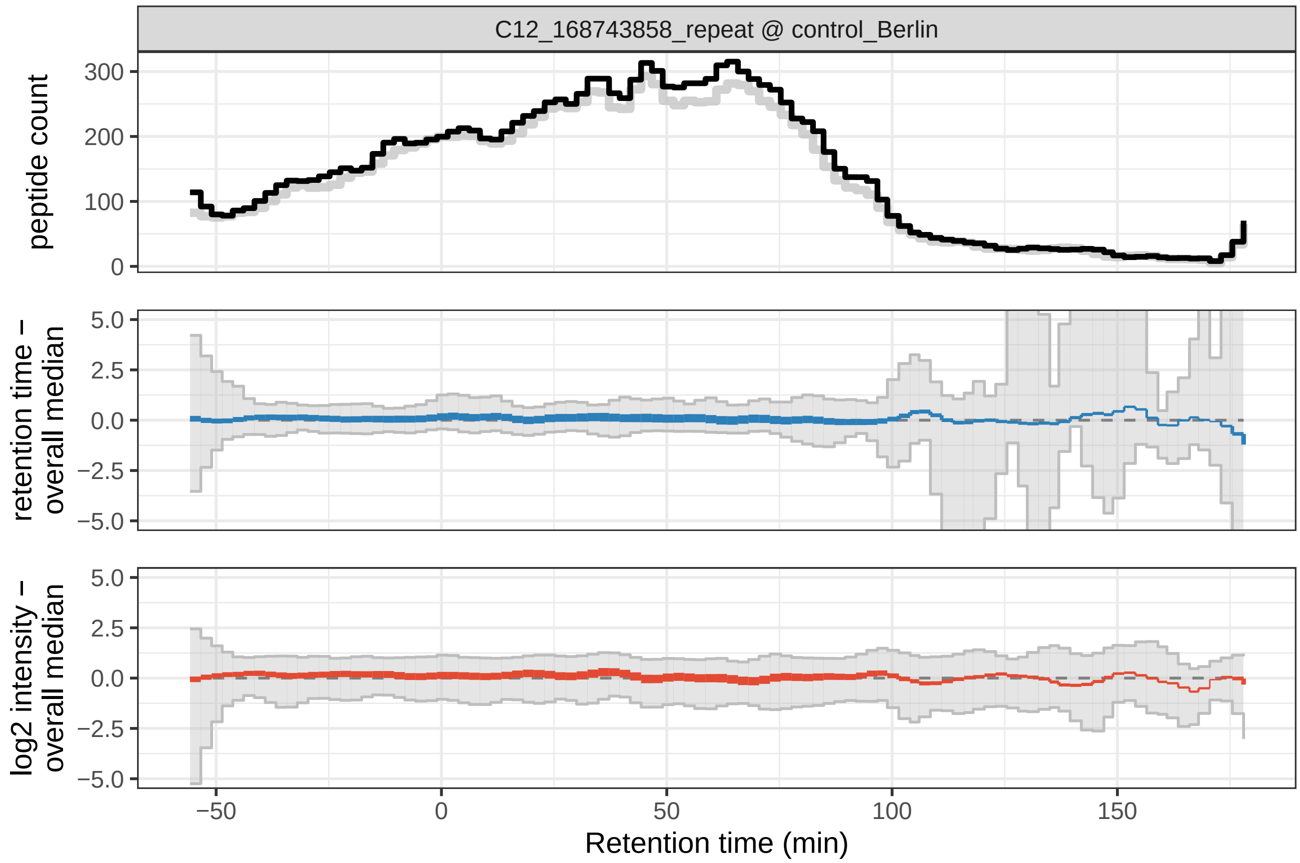
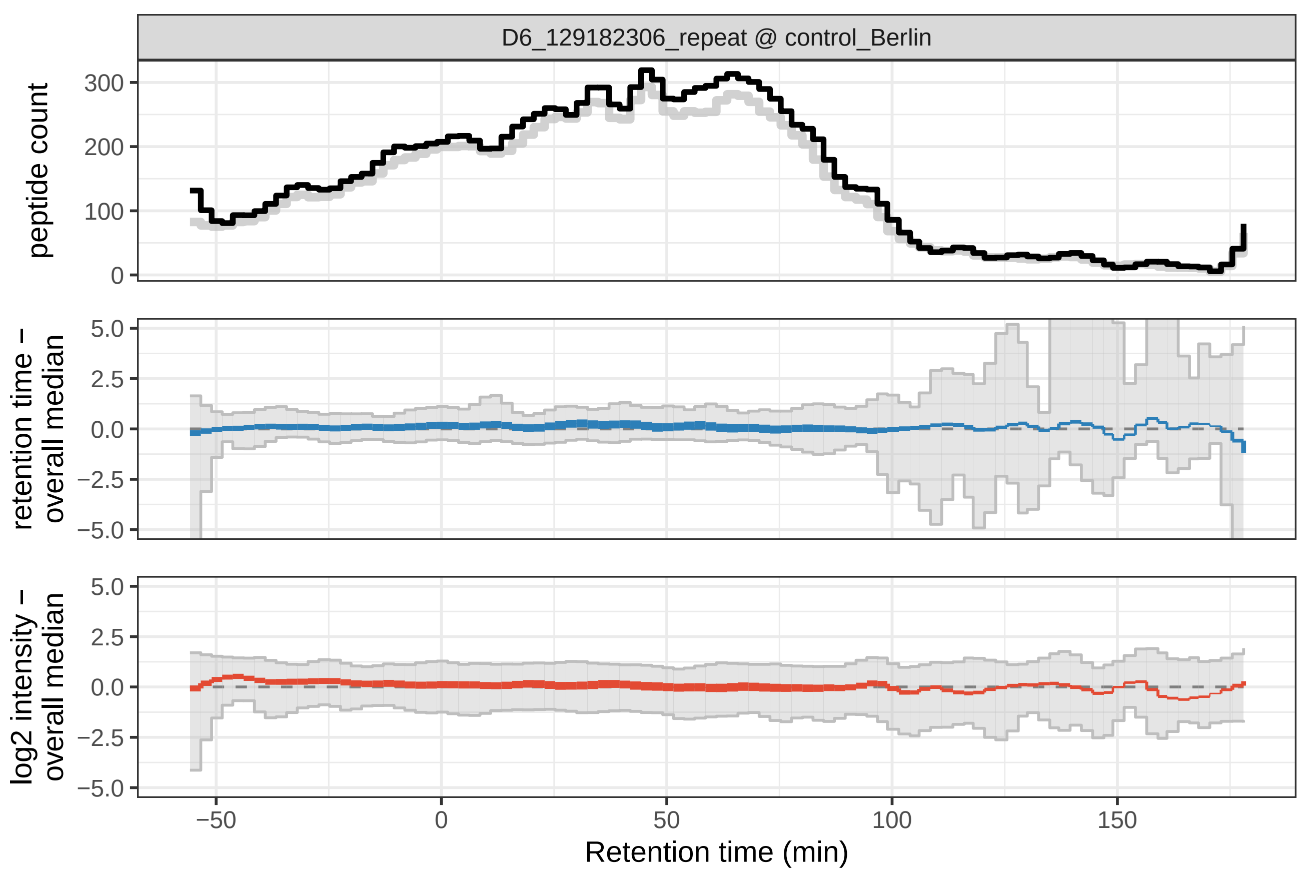
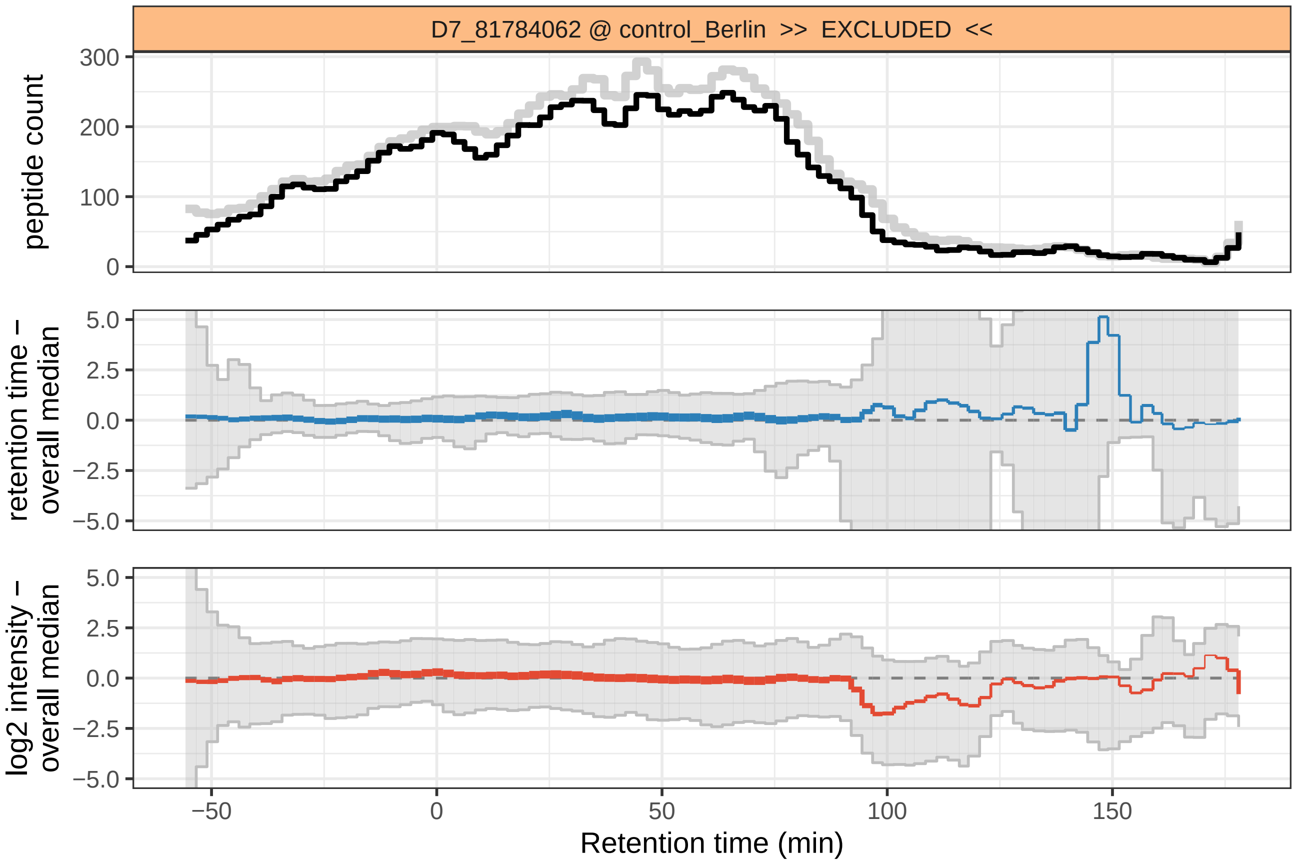
100
150
Retention time (min)


C12_168743858_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


D6_129182306_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)



D7_81784062 @ control_Berlin >> EXCLUDED <<
peptide count
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100
0
retention time –
overall median
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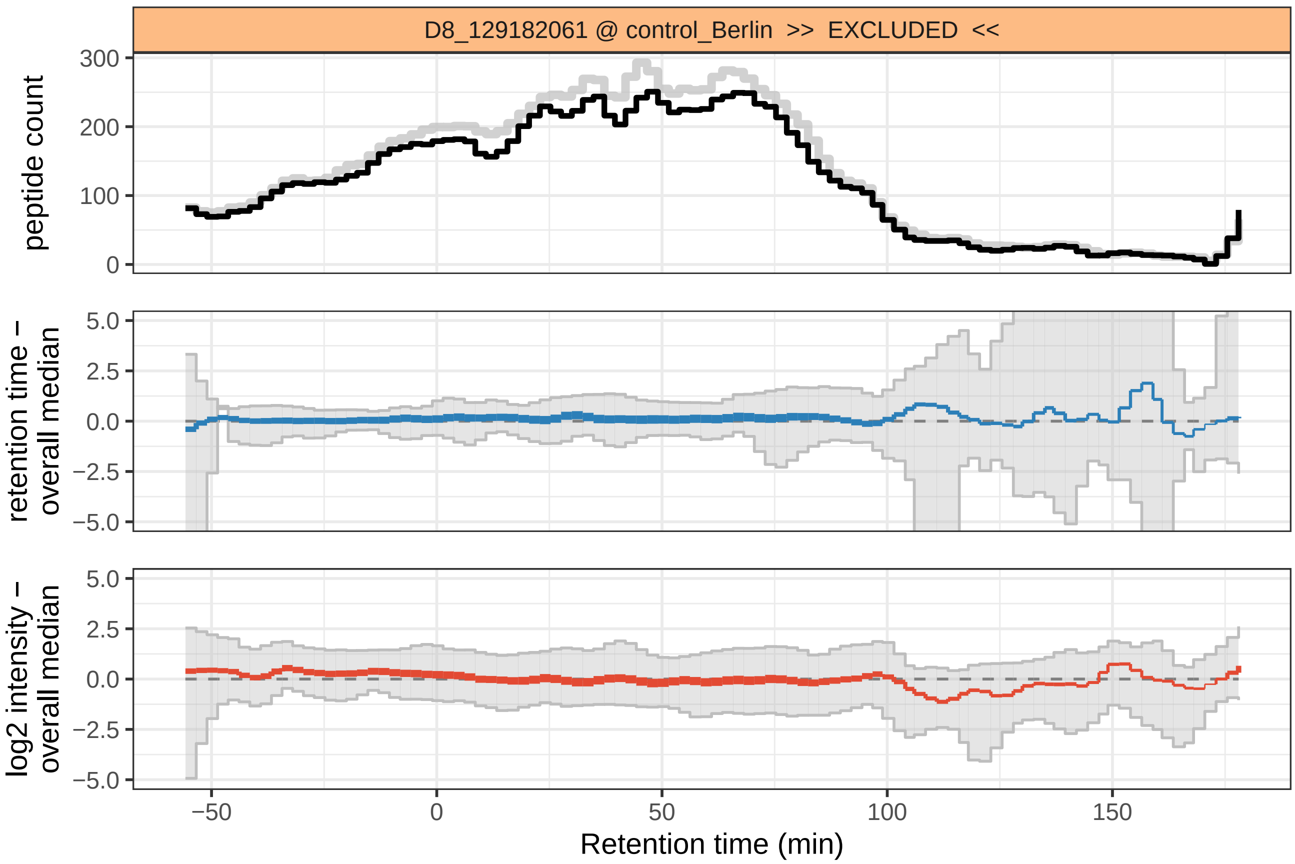
−2.5
−5.0
log2 intensity –
overall median
−50
0
50
100
150
Retention time (min)



D8_129182061 @ control_Berlin >> EXCLUDED <<
peptide count
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100
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retention time –
overall median
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−2.5
−5.0
log2 intensity –
overall median
−50
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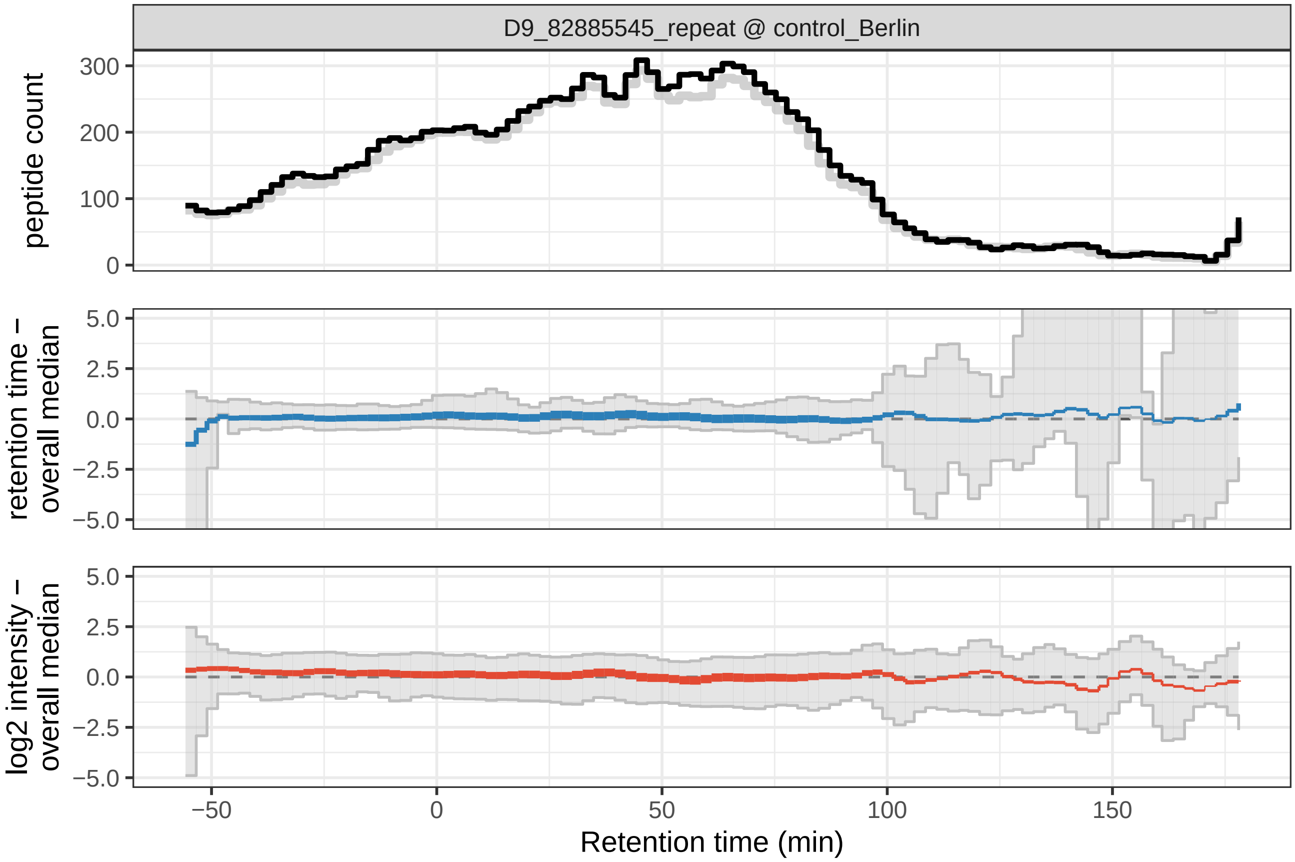
100
150
Retention time (min)


D9_82885545_repeat @ control_Berlin
peptide count
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100
0
retention time –
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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−2.5
−5.0
−50
0
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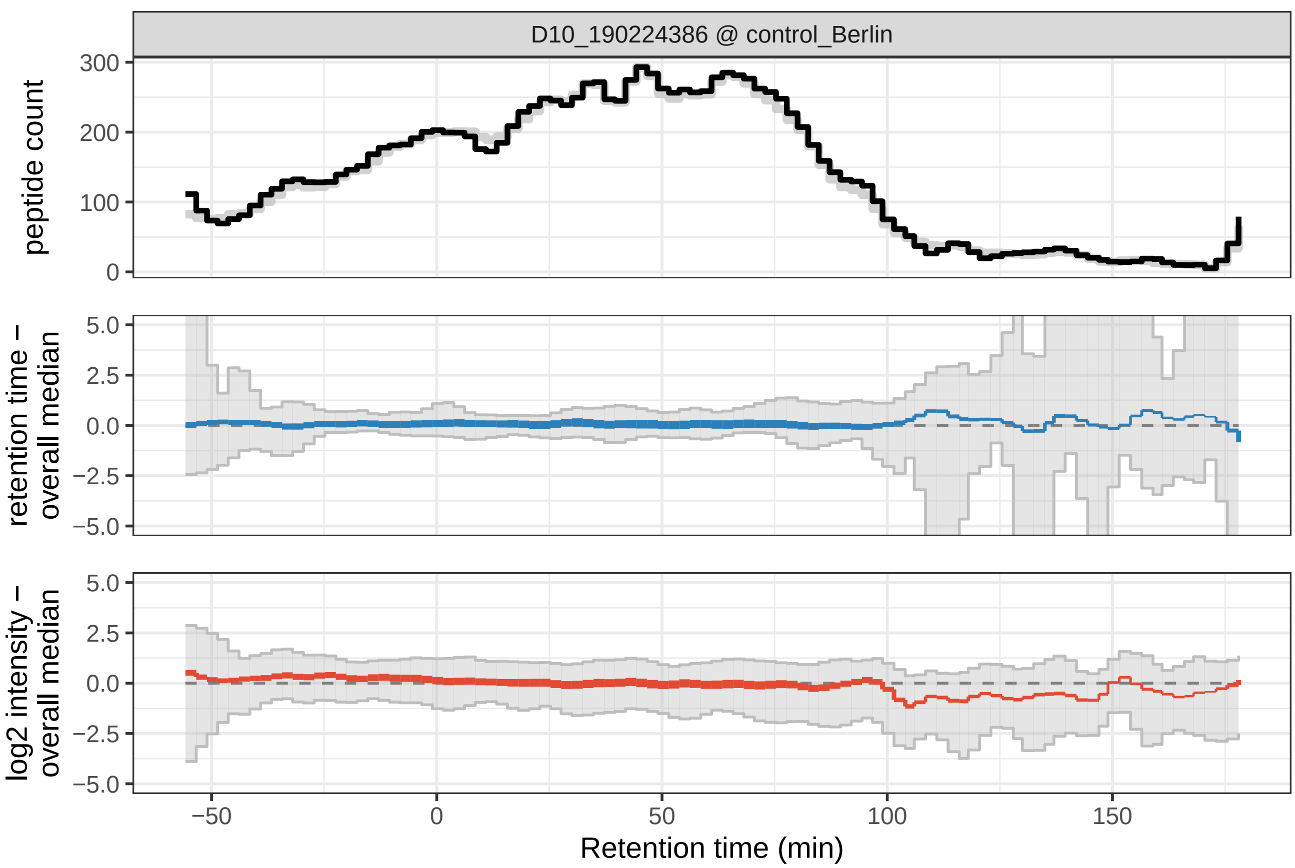
100
150
Retention time (min)


D10_190224386 @ control_Berlin
peptide count
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100
0
retention time –
overall median
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−5.0
log2 intensity –
overall median
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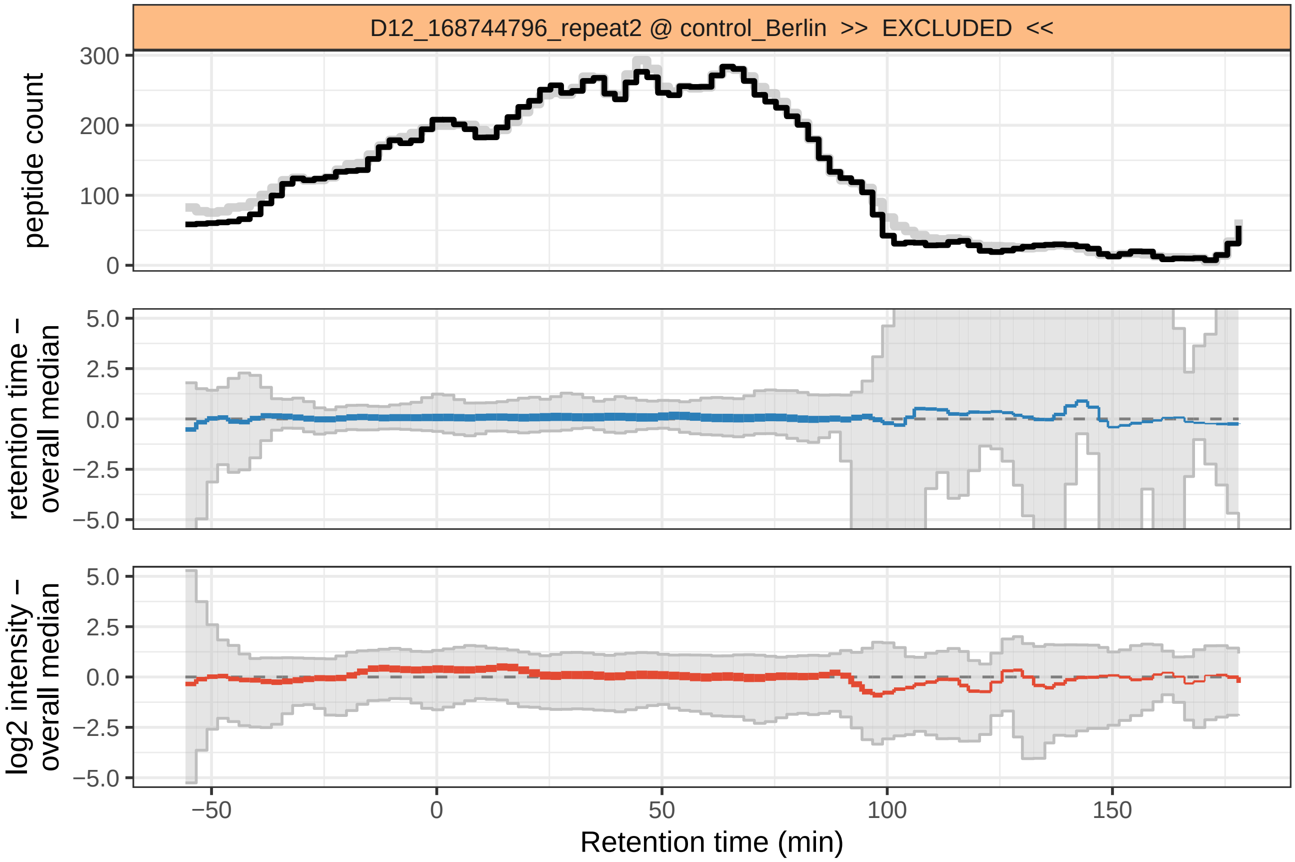
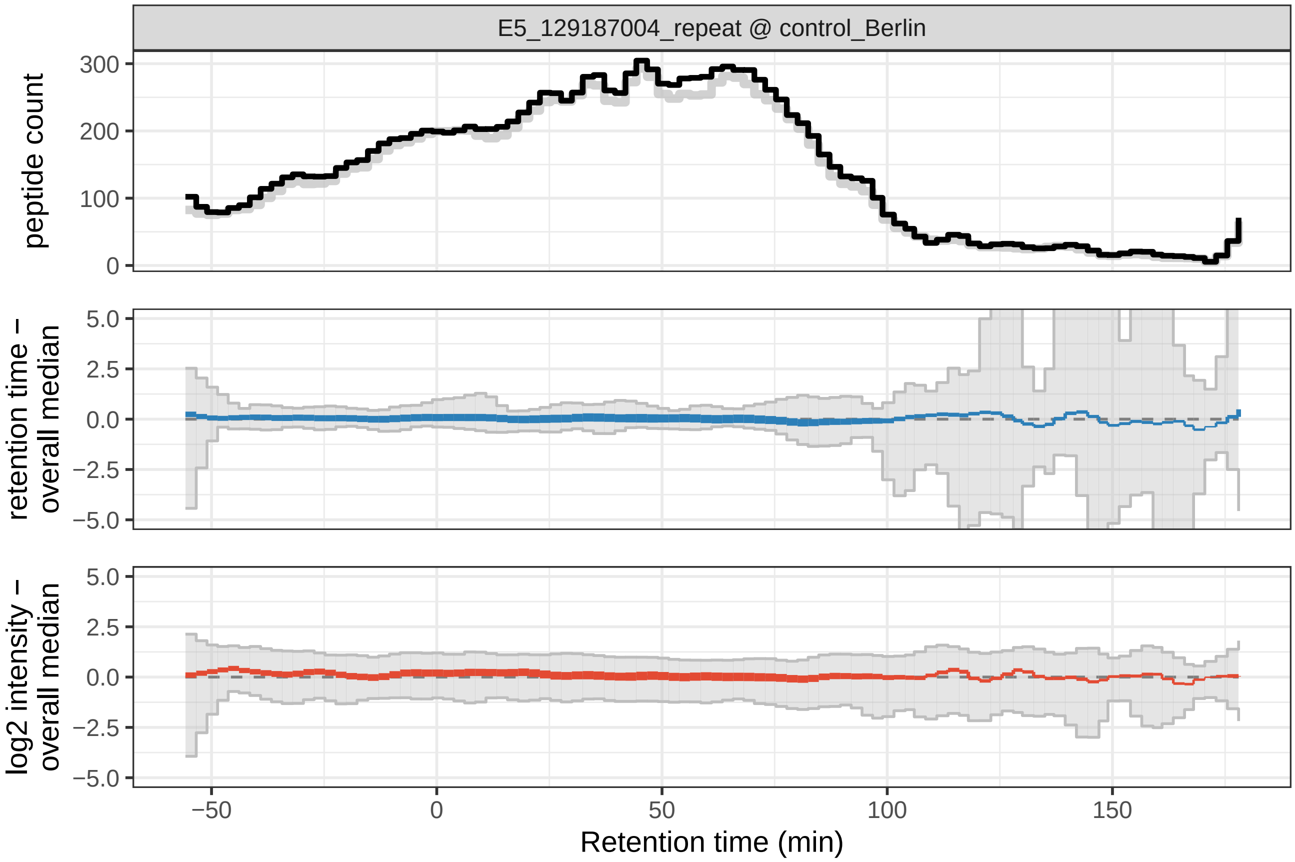
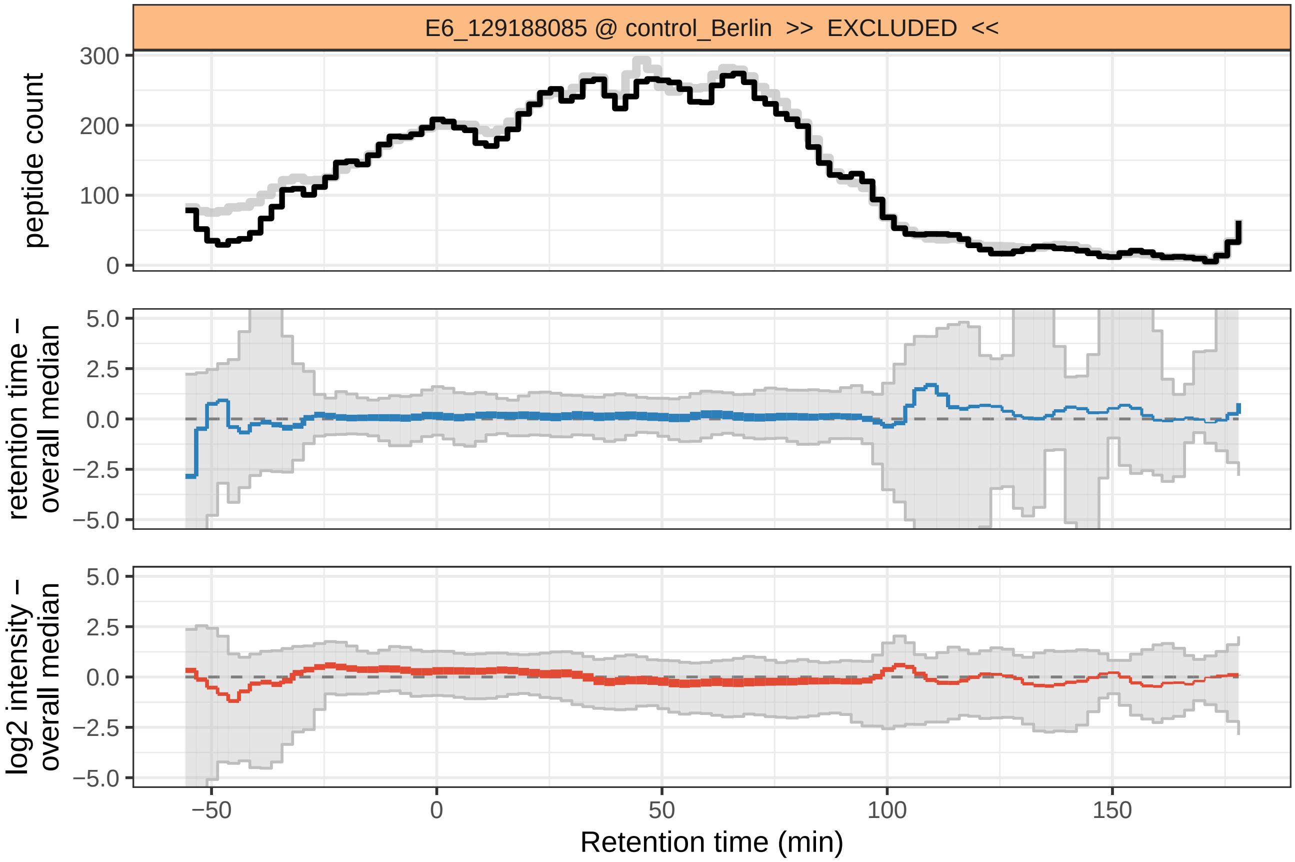
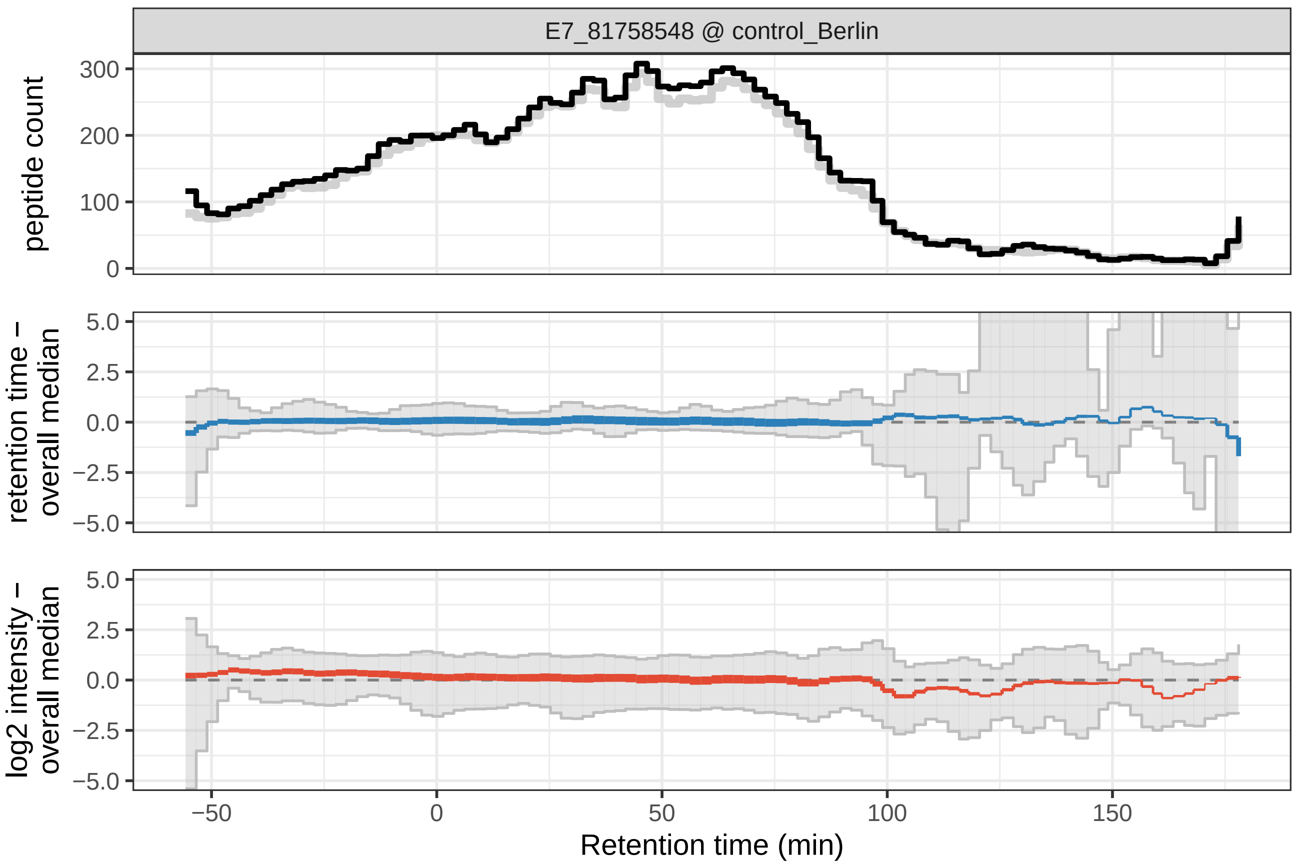
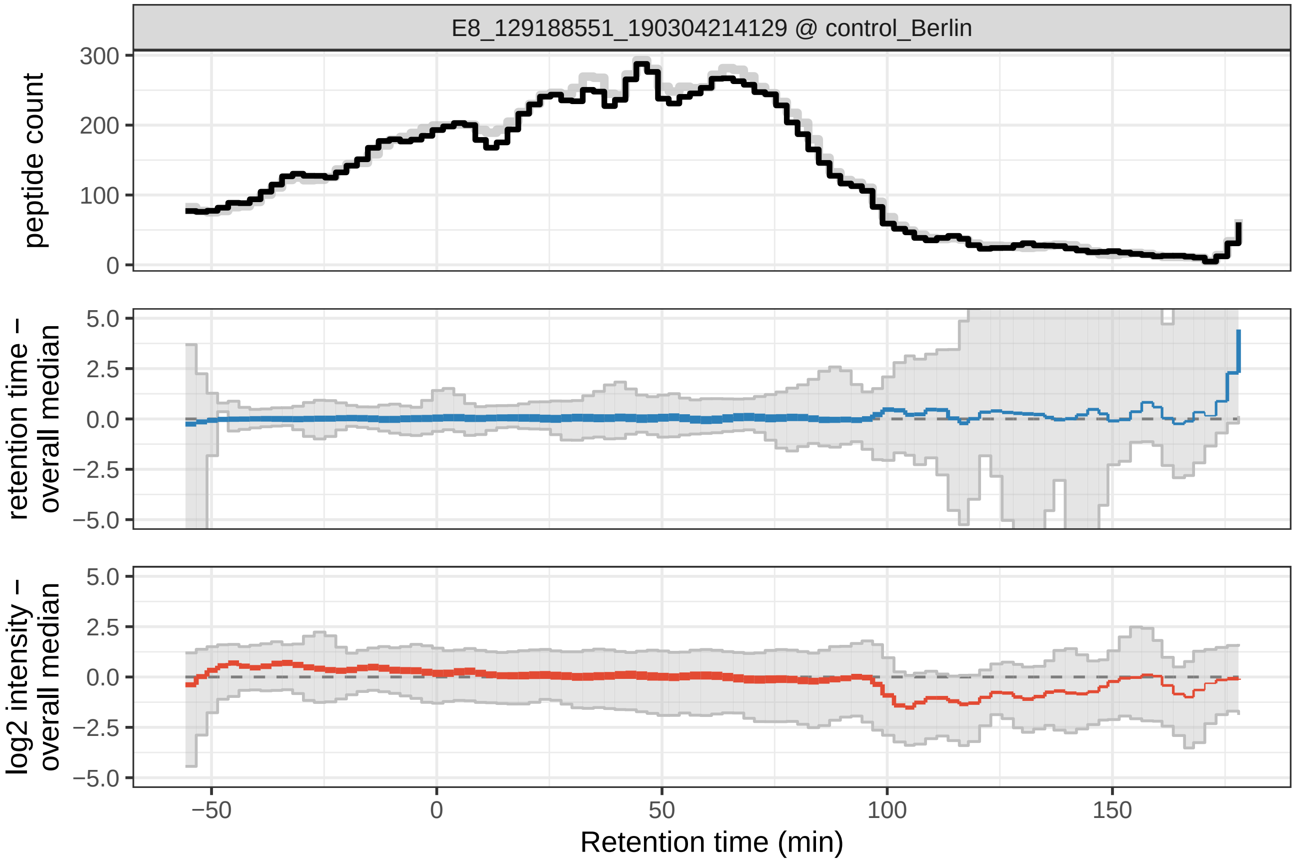
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


D12_168744796_repeat2 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


E5_129187004_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


E6_129188085 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


E7_81758548 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


E8_129188551_190304214129 @ control_Berlin
peptide count
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200
100
0
retention time – overall median
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2.5
0.0
−2.5
−5.0
log2 intensity – overall median
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2.5
0.0
−2.5
−5.0
−50
0
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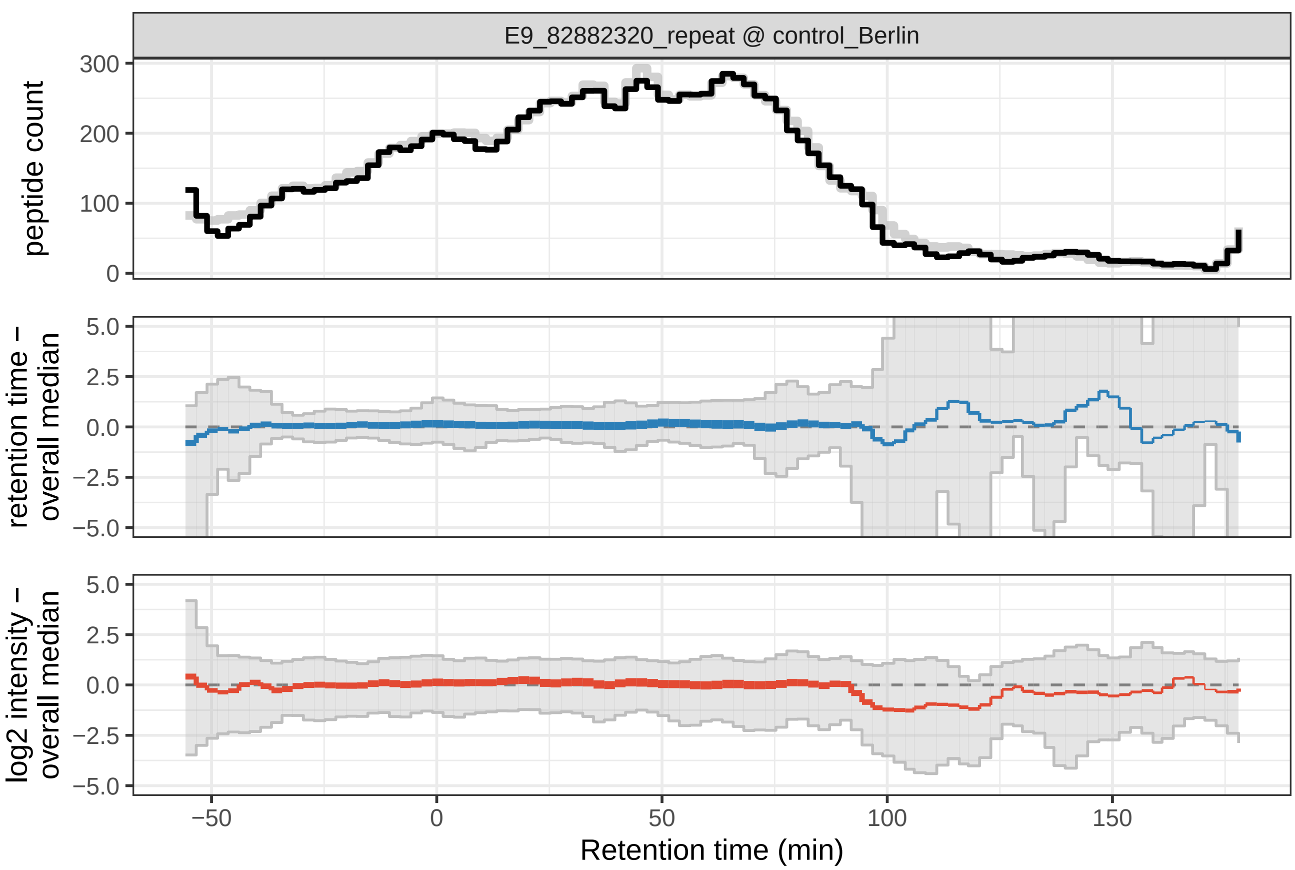
100
150
Retention time (min)


E9_82882320_repeat @ control_Berlin
peptide count
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100
0
retention time – overall median
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−5.0
log2 intensity – overall median
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0.0
−2.5
−5.0
−50
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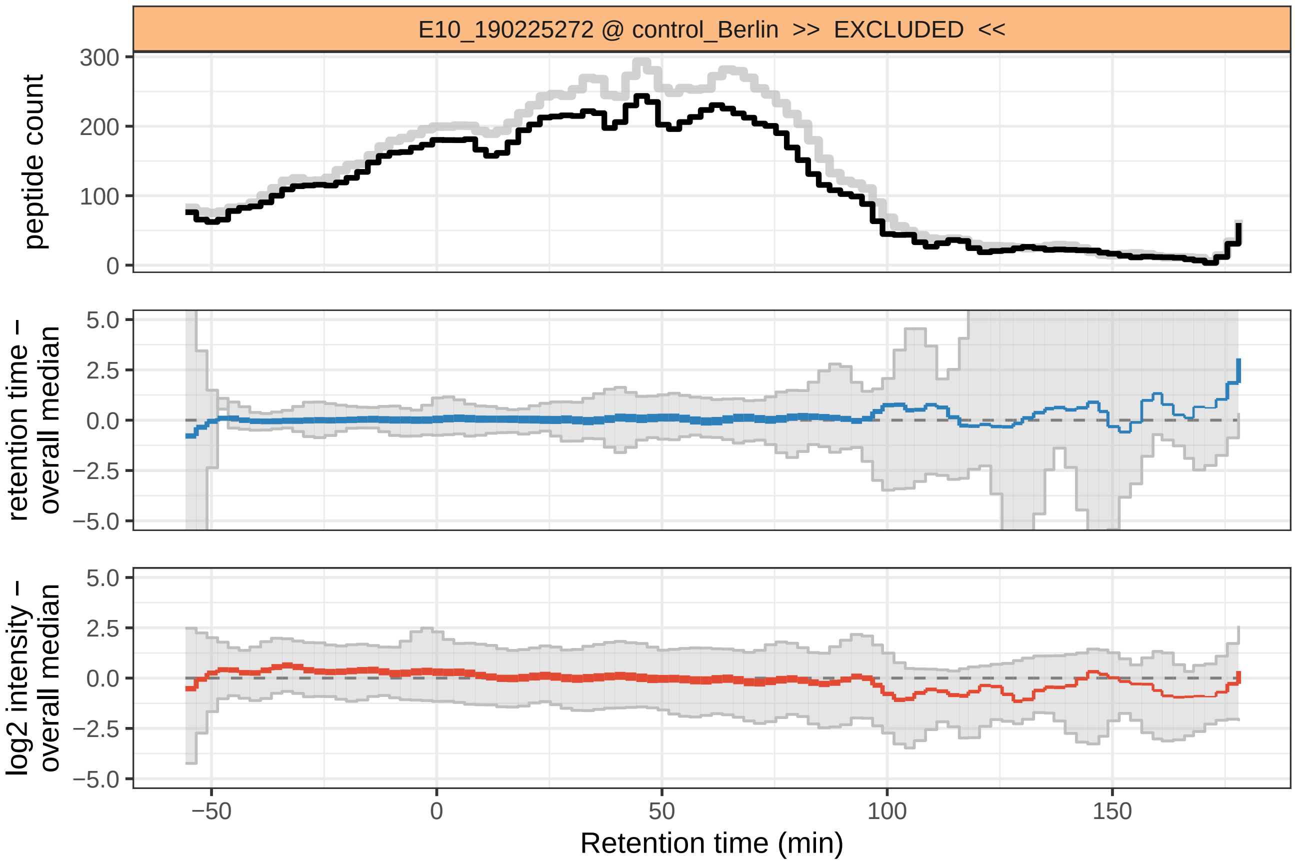
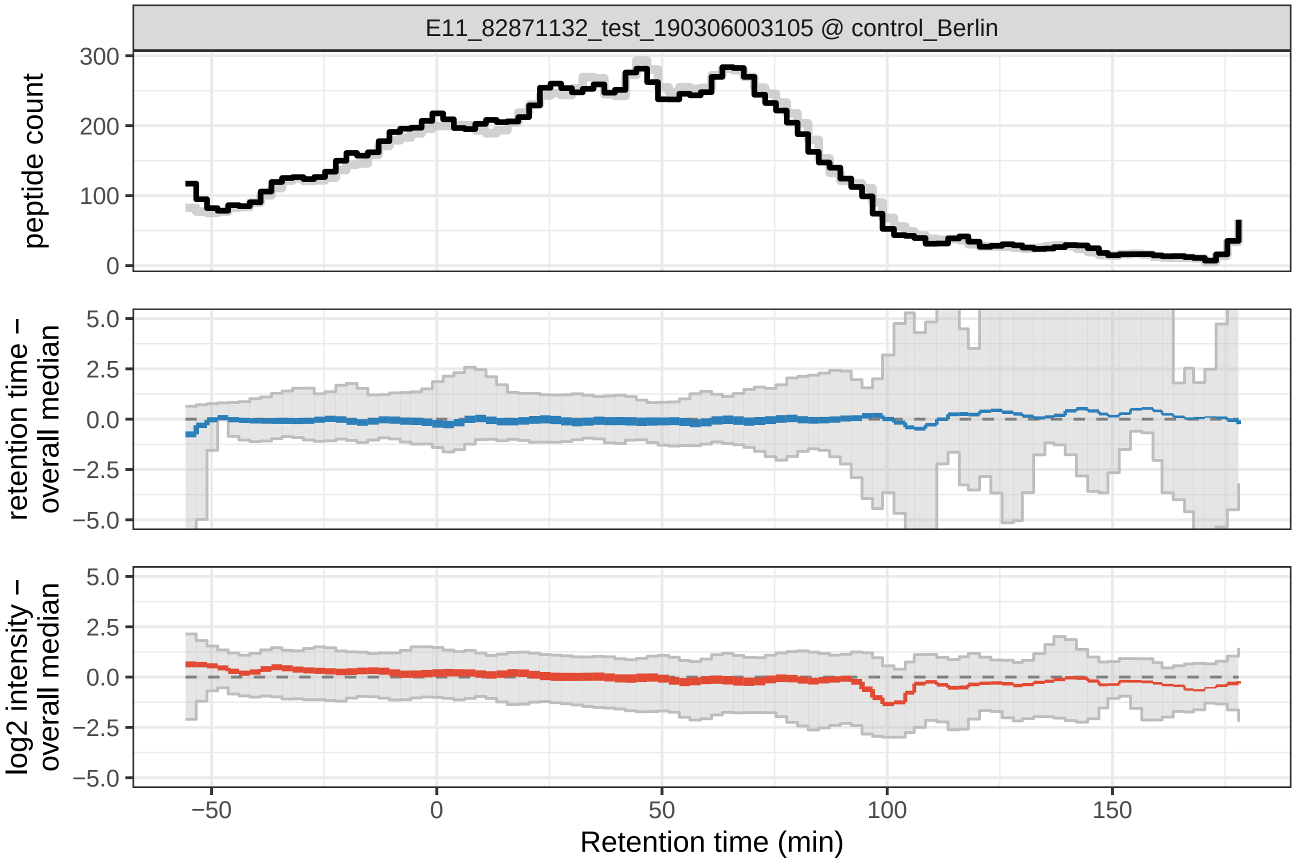
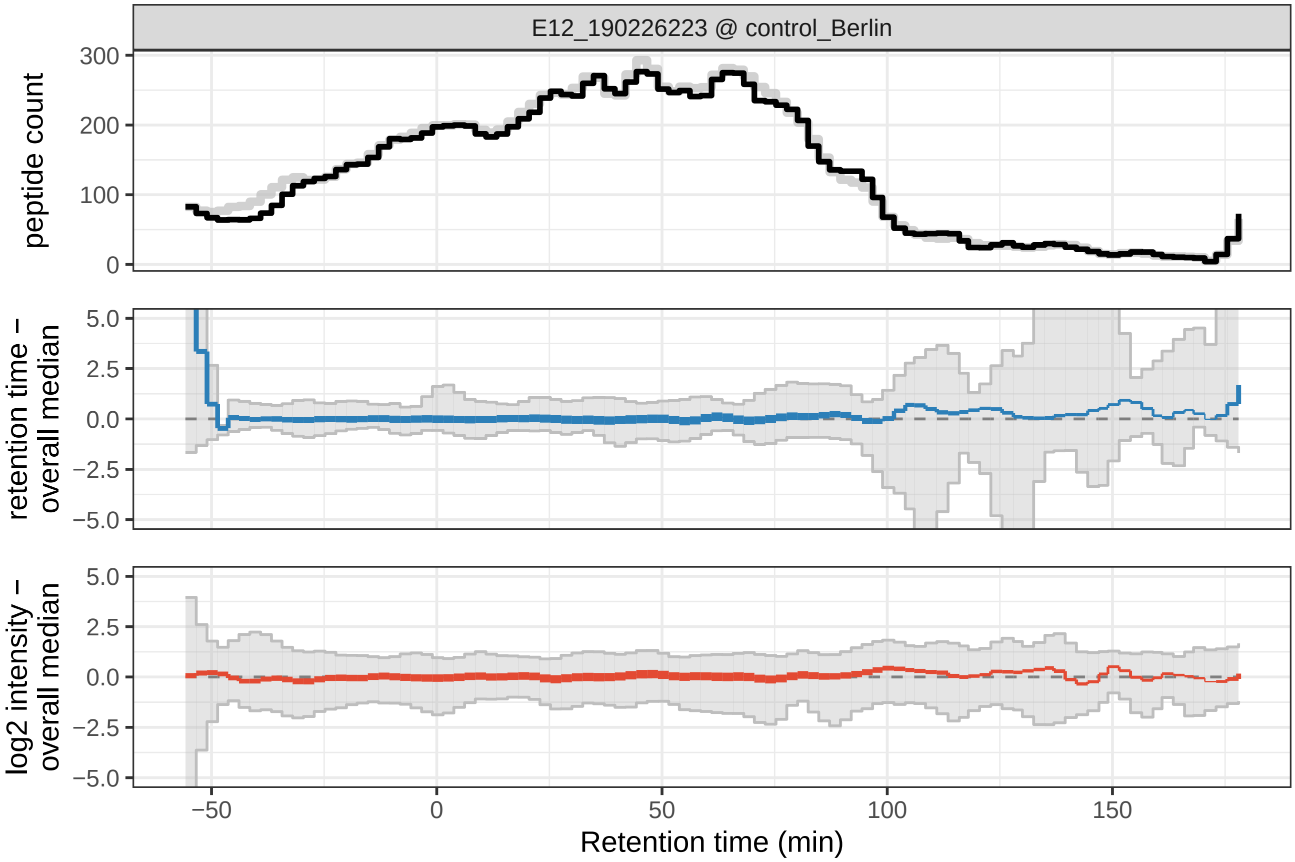
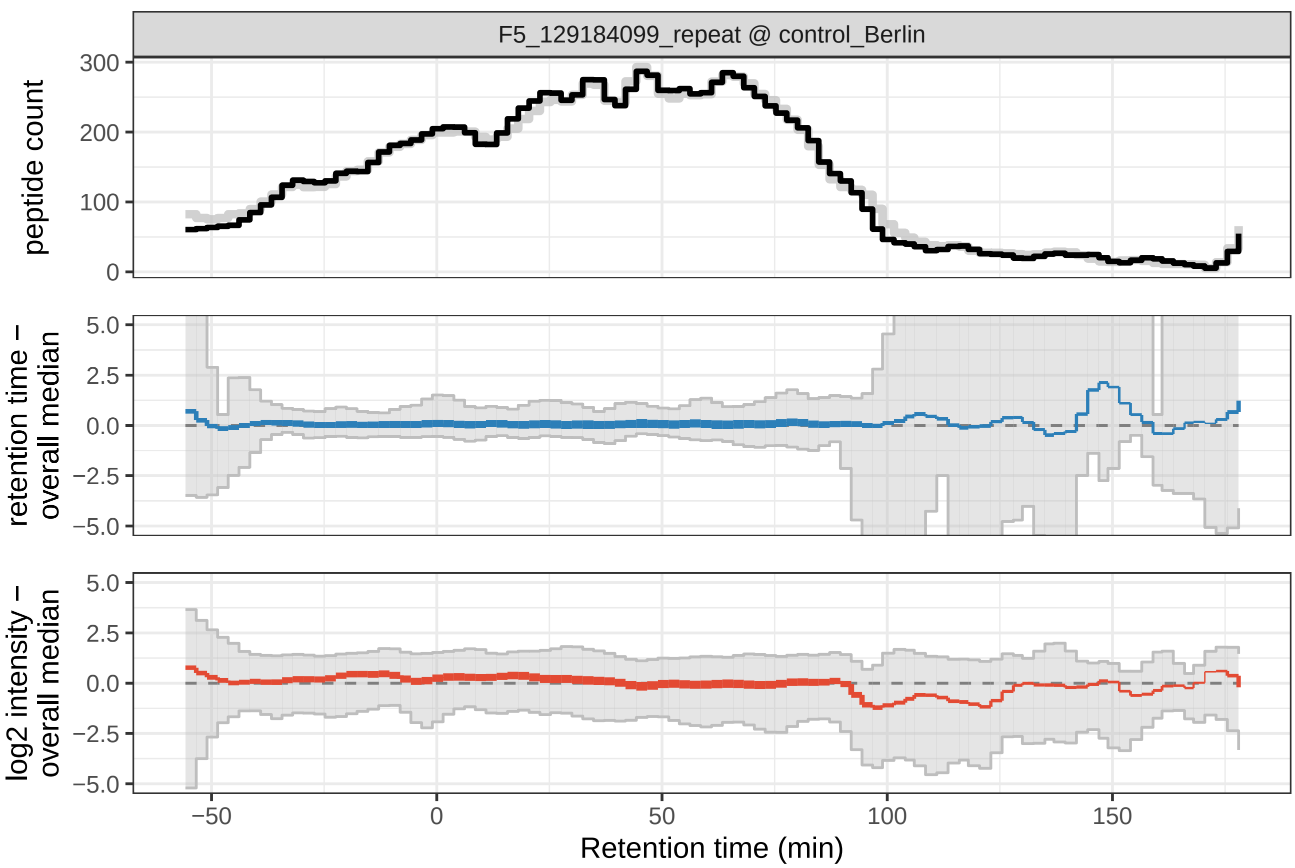
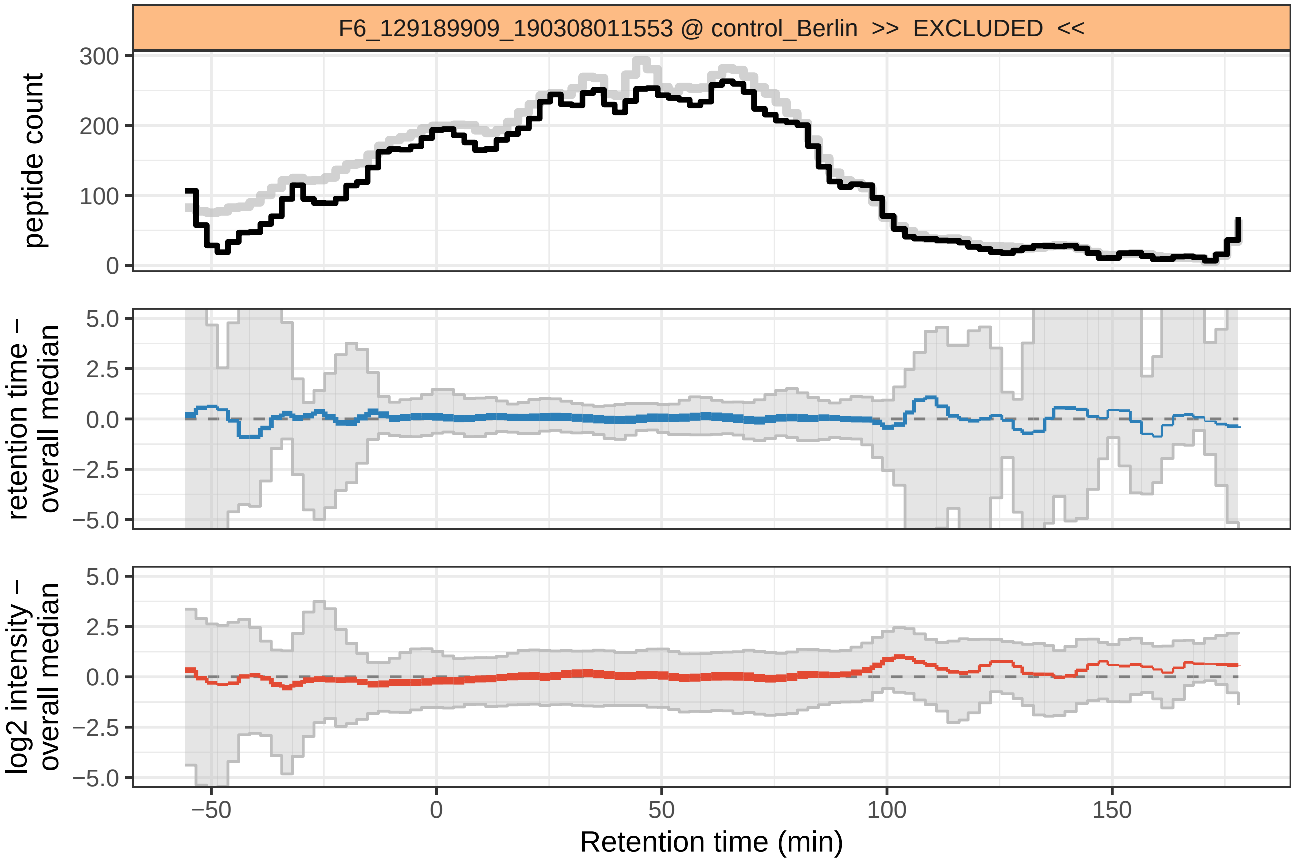
100
150
Retention time (min)

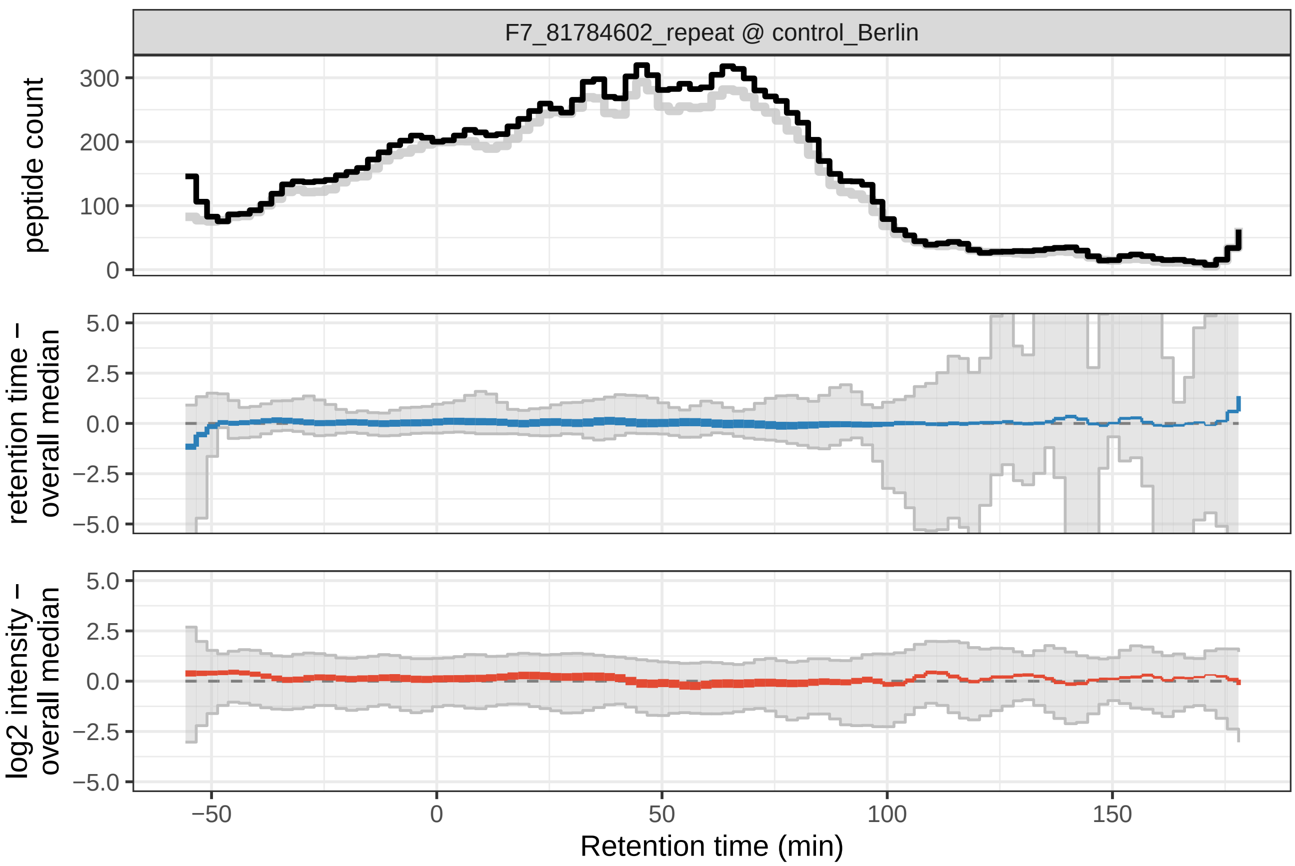

E10_190225272 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

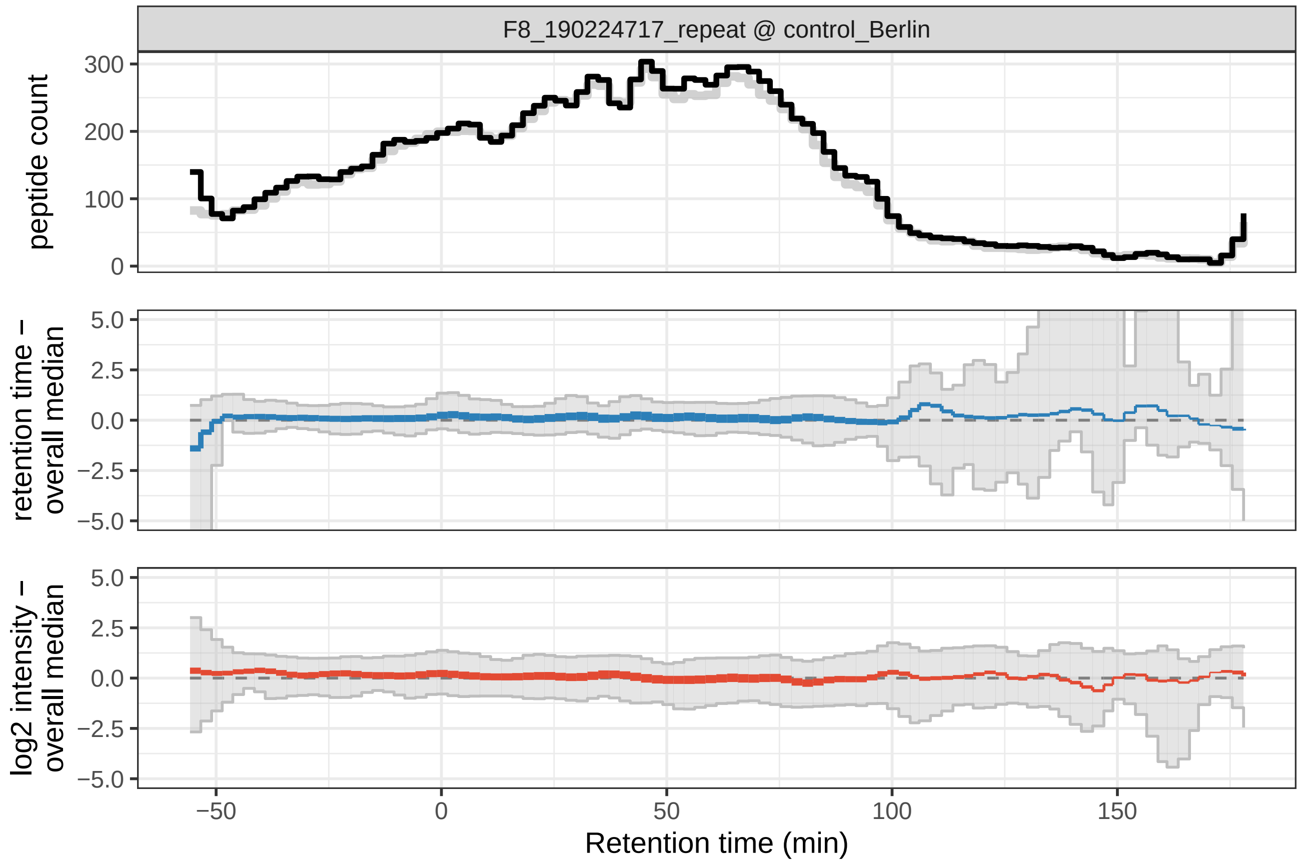

E11_82871132_test_190306003105 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

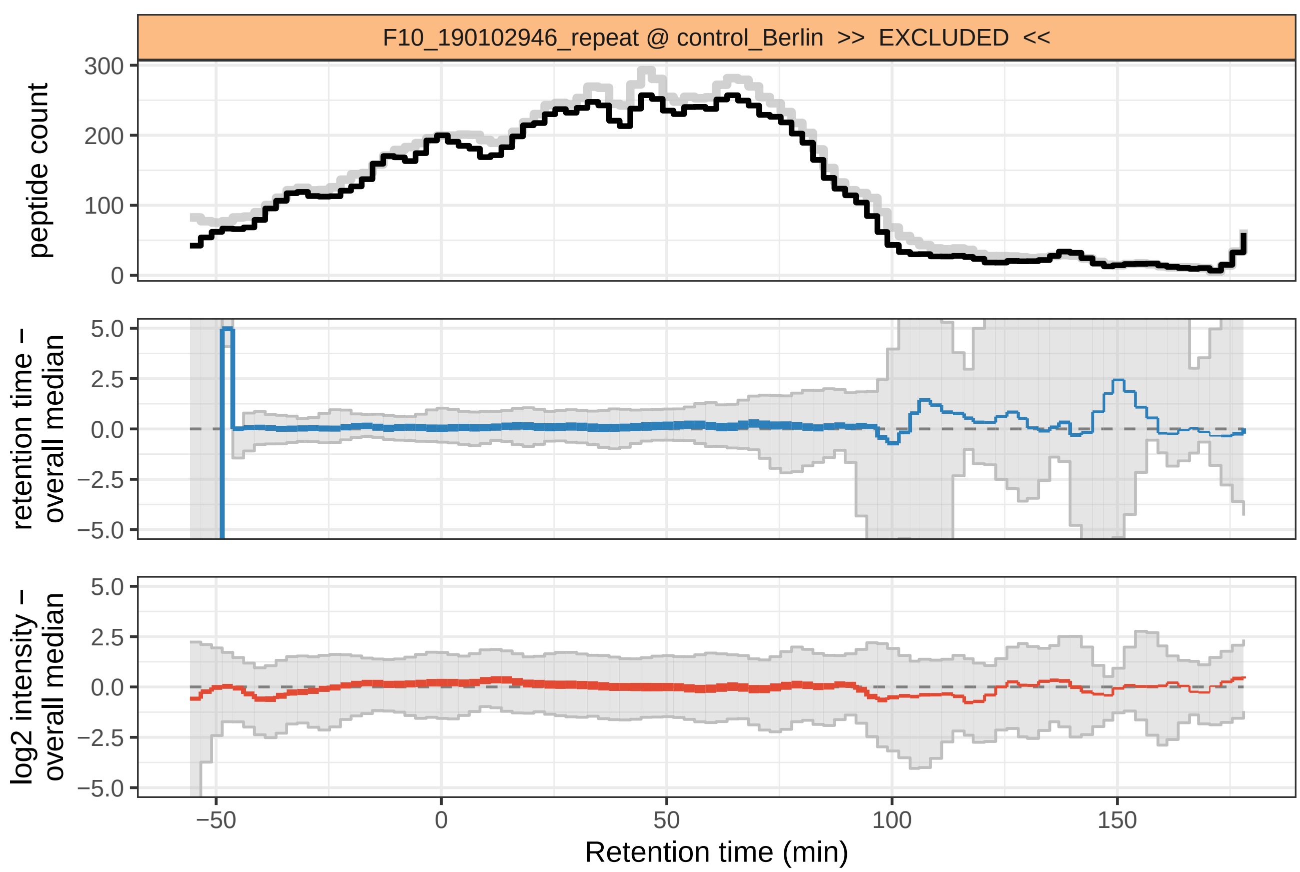

E12_190226223 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

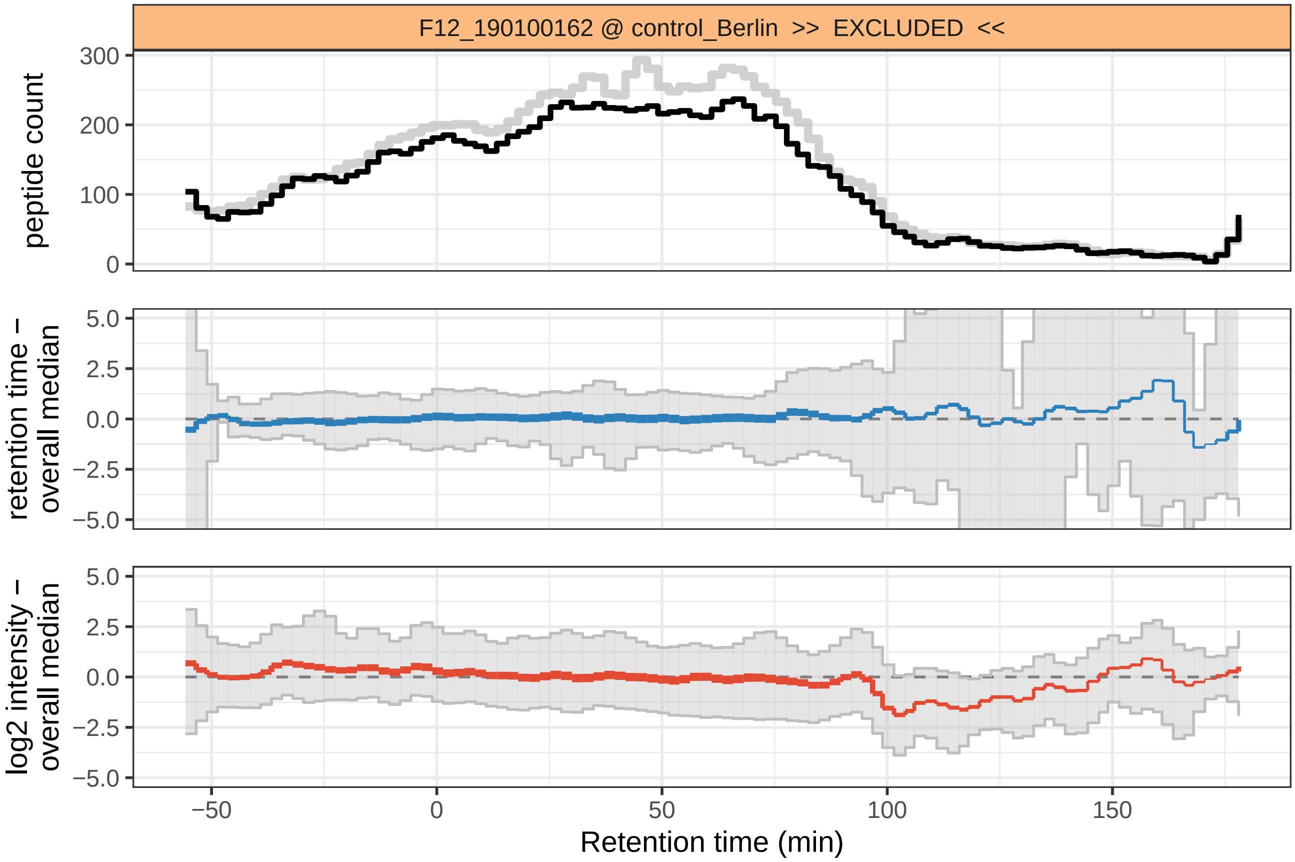

F5_129184099_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

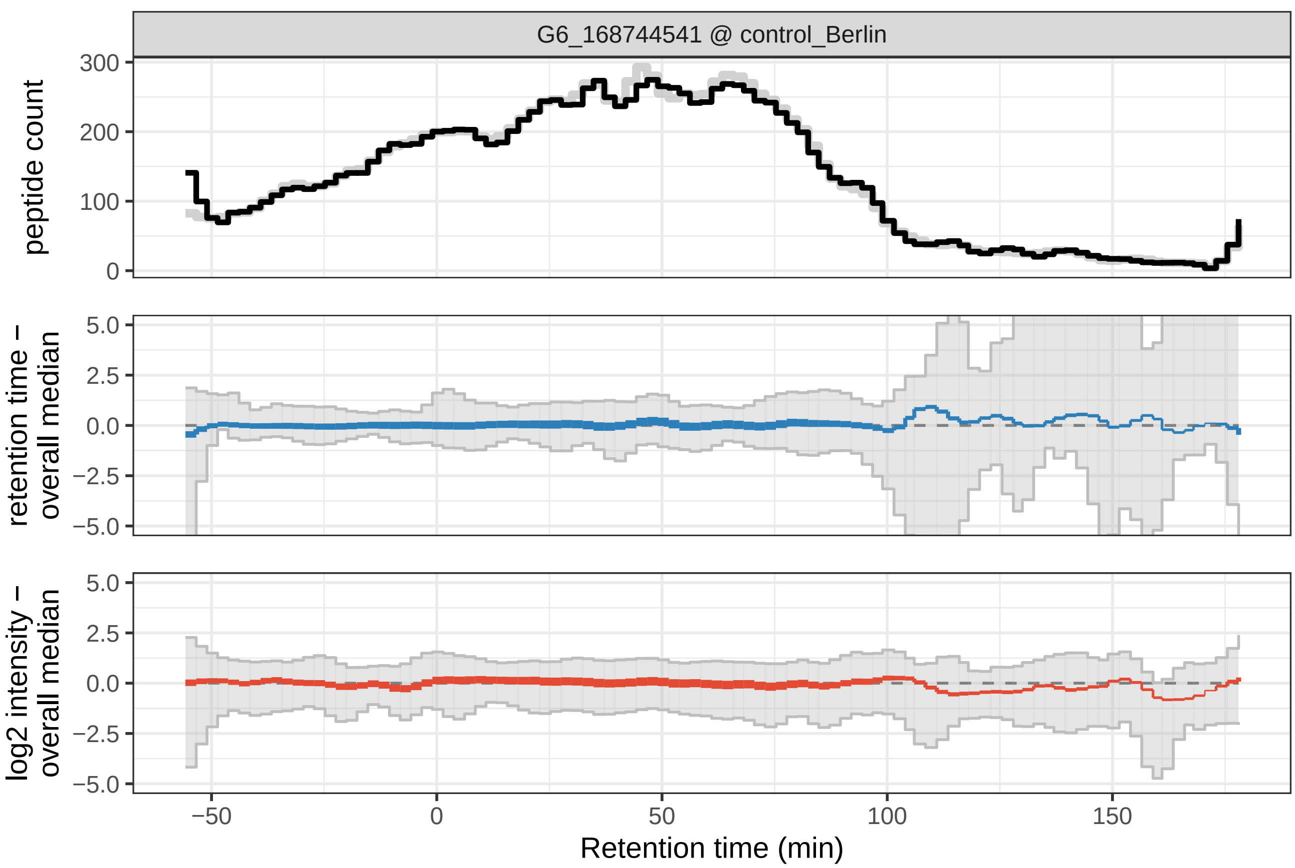

F6_129189909_190308011553 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

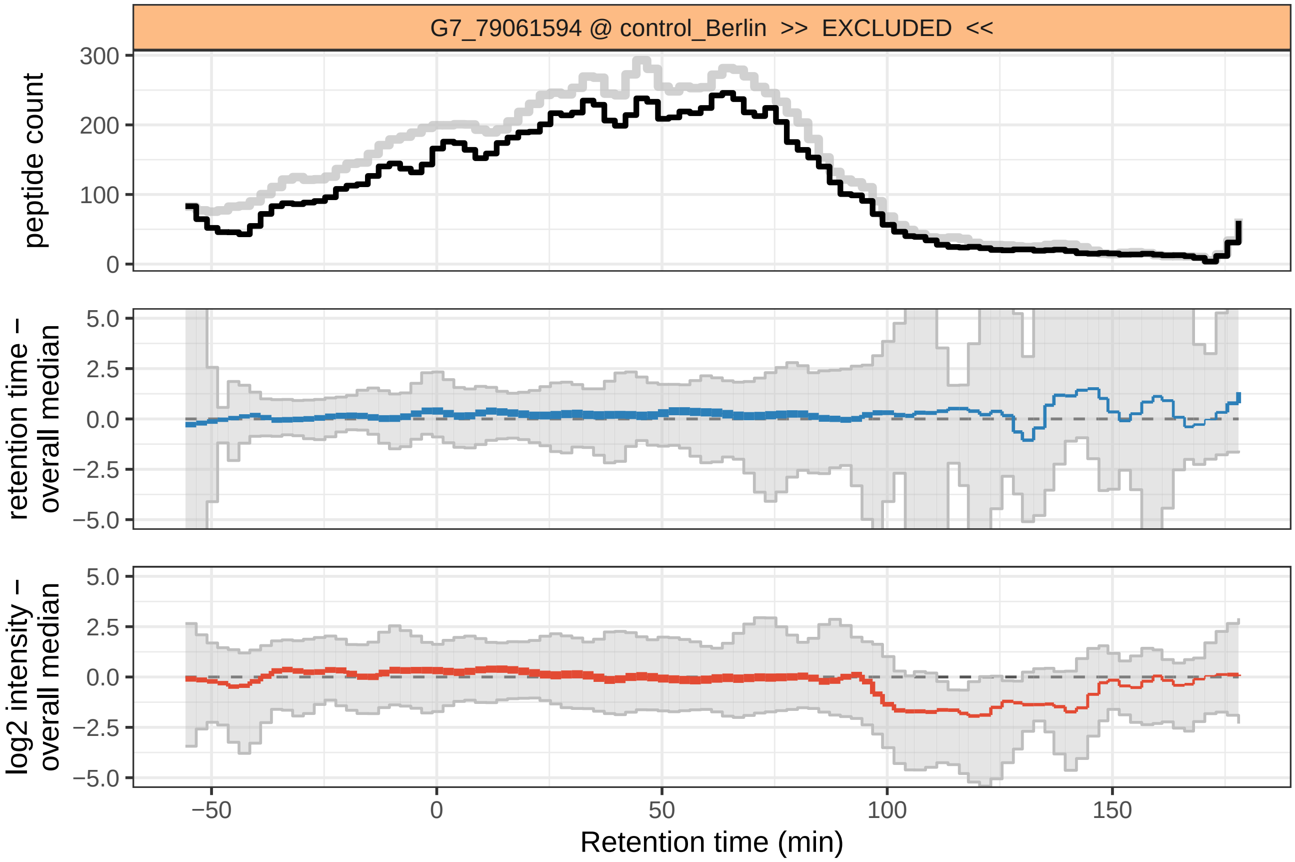

F7_81784602_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


F8_190224717_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


F10_190102946_repeat @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


F12_190100162 @ control_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


G6_168744541 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


G7_79061594 @ control_Berlin >> EXCLUDED <<
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retention time –
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2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
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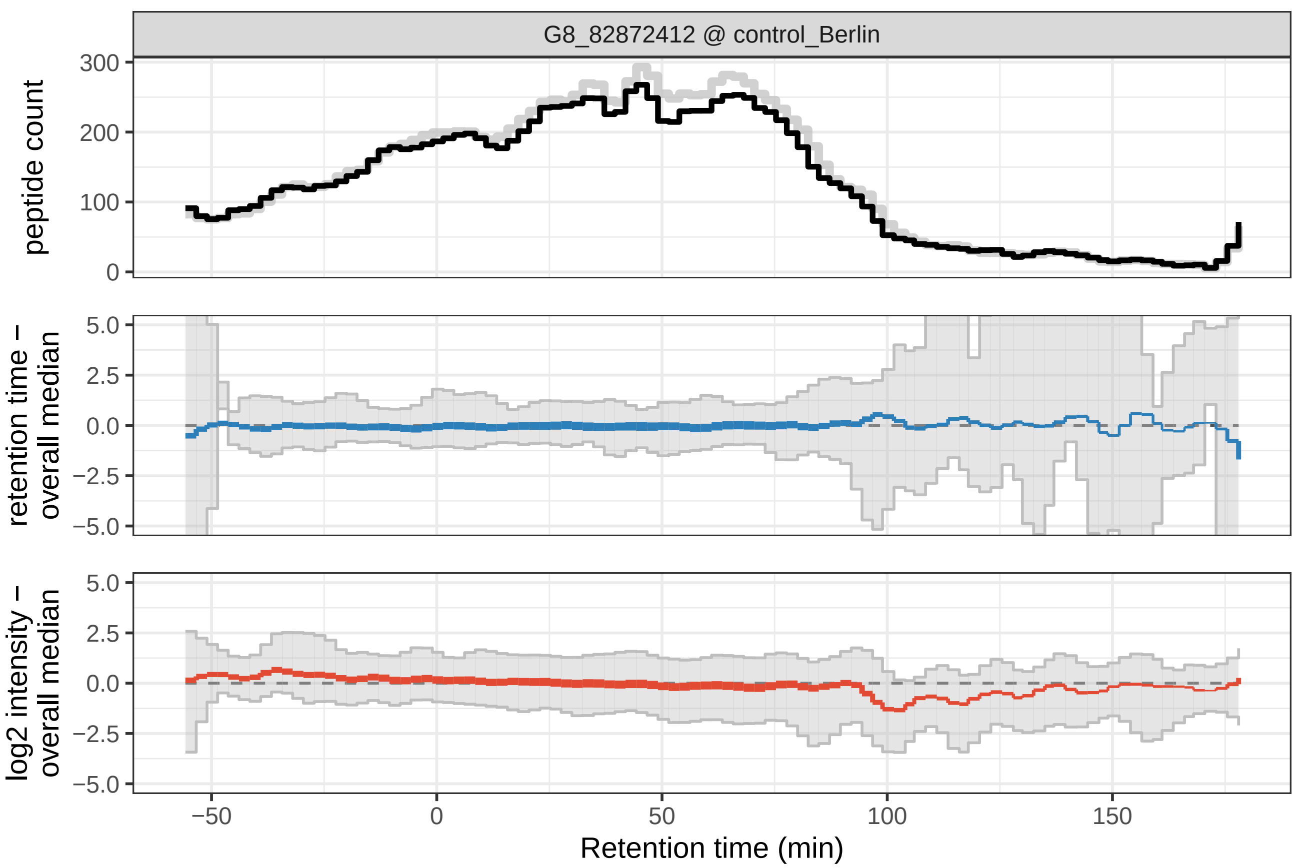
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


G8_82872412 @ control_Berlin
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log2 intensity –
overall median
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−50
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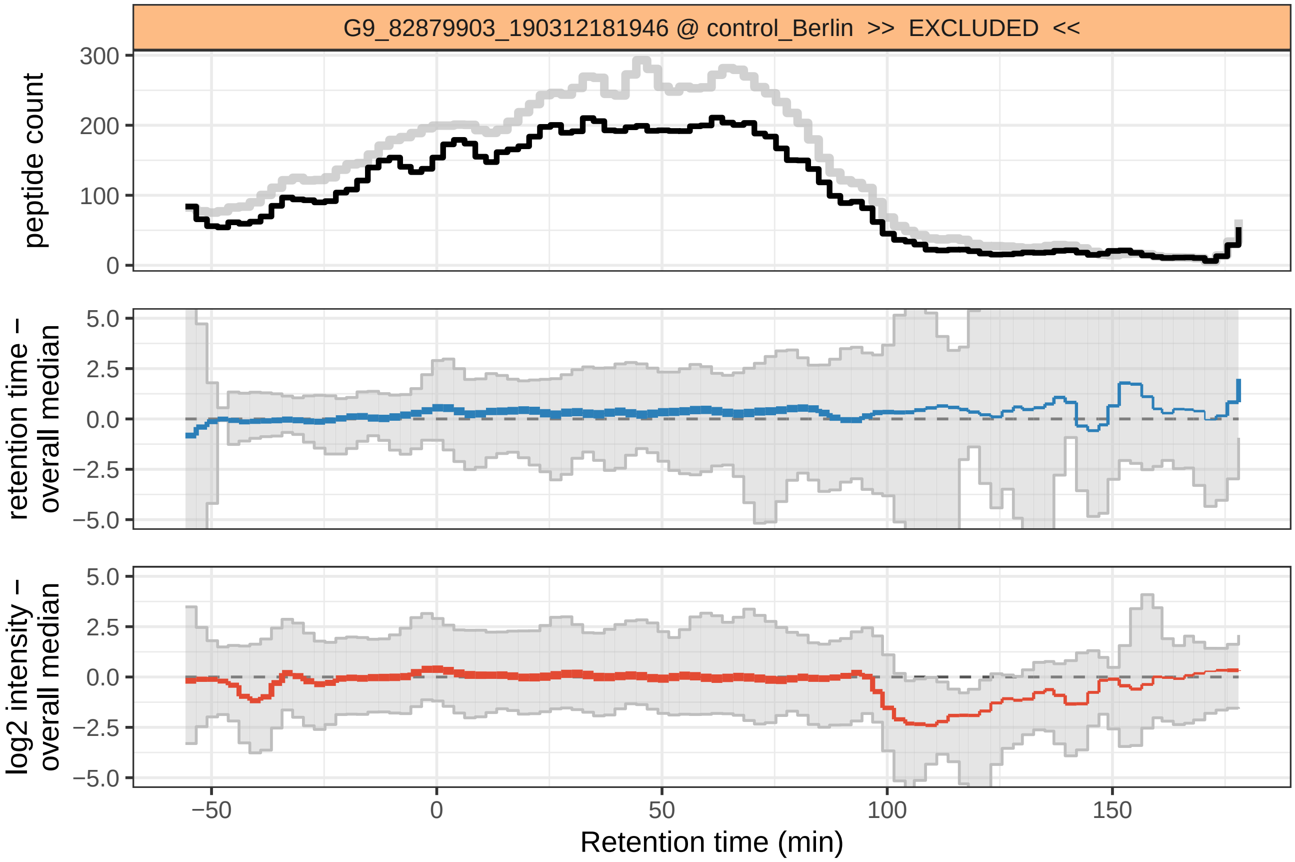
100
150
Retention time (min)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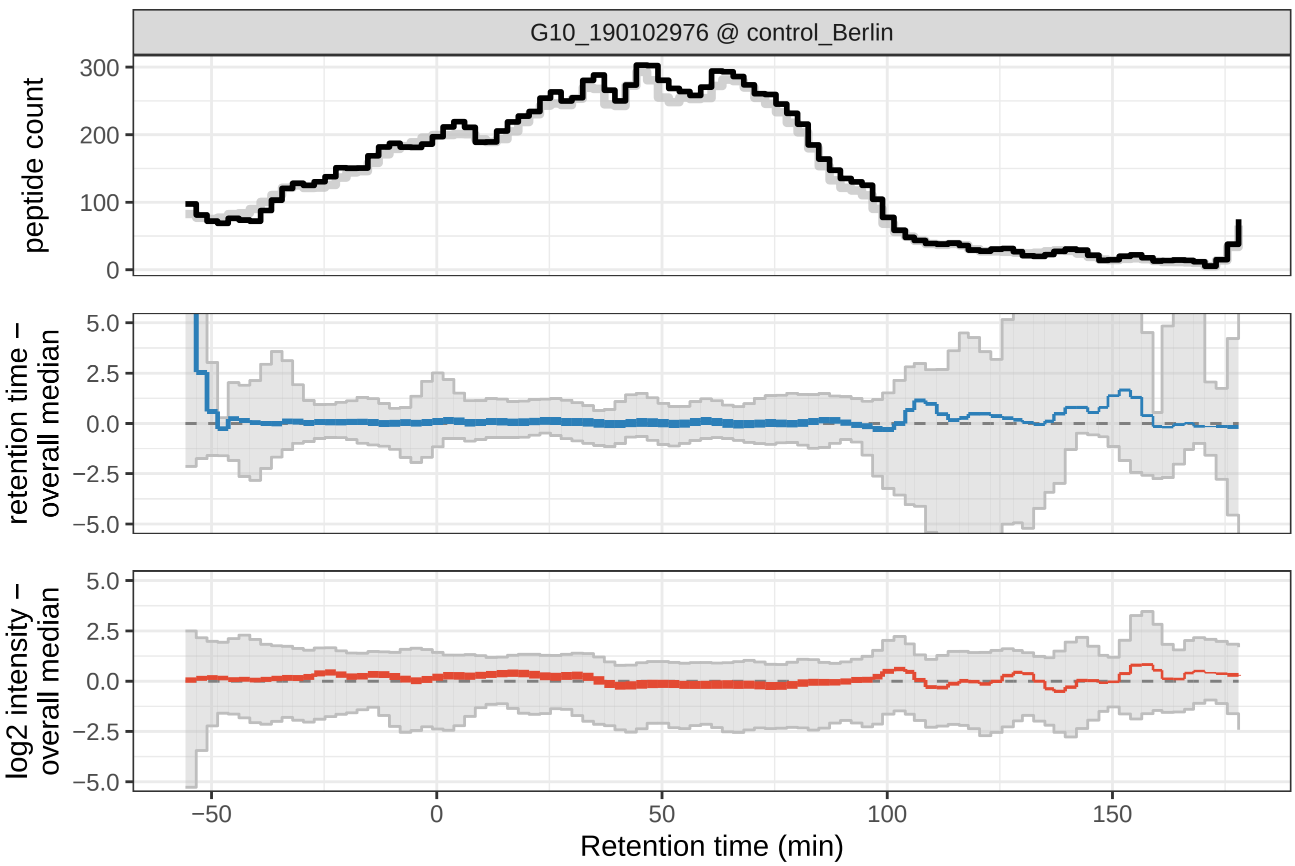
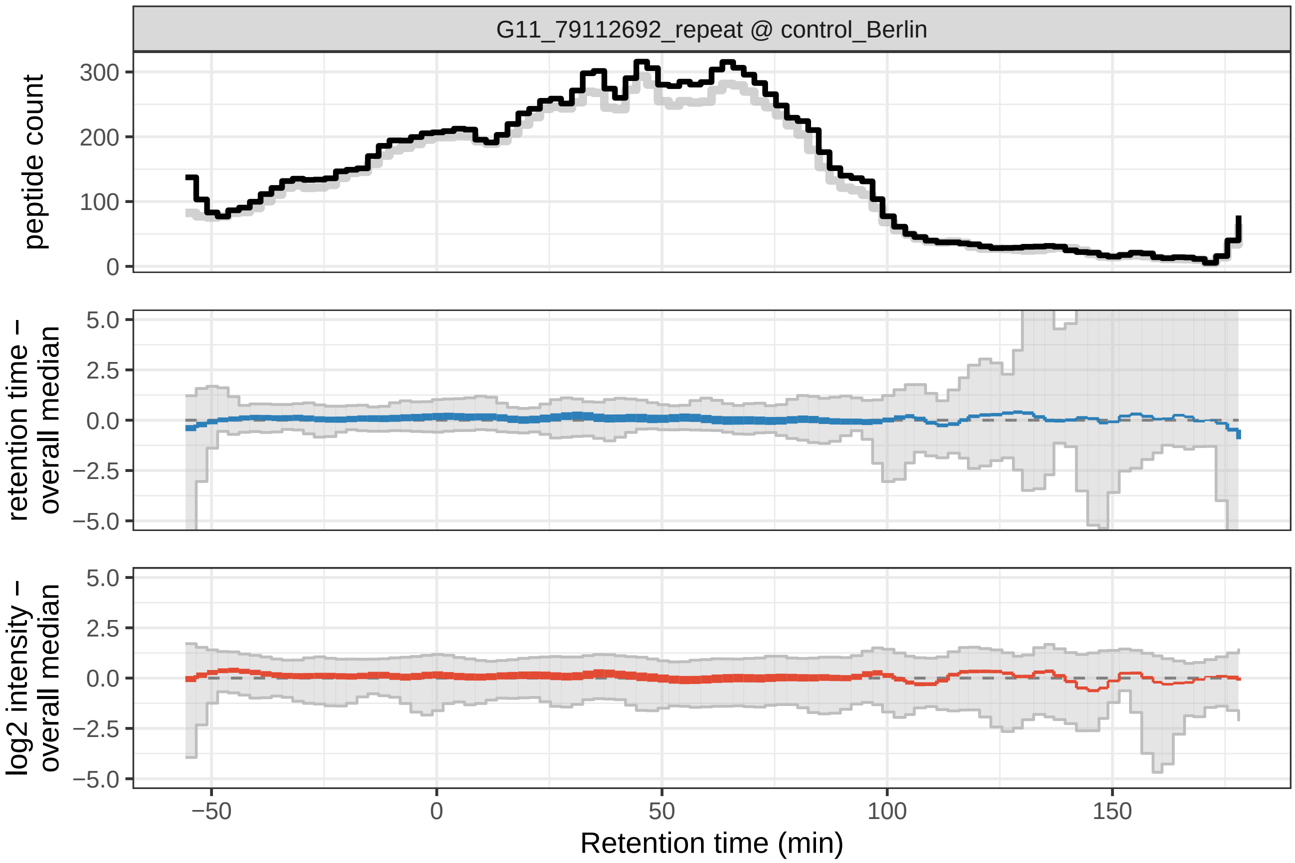
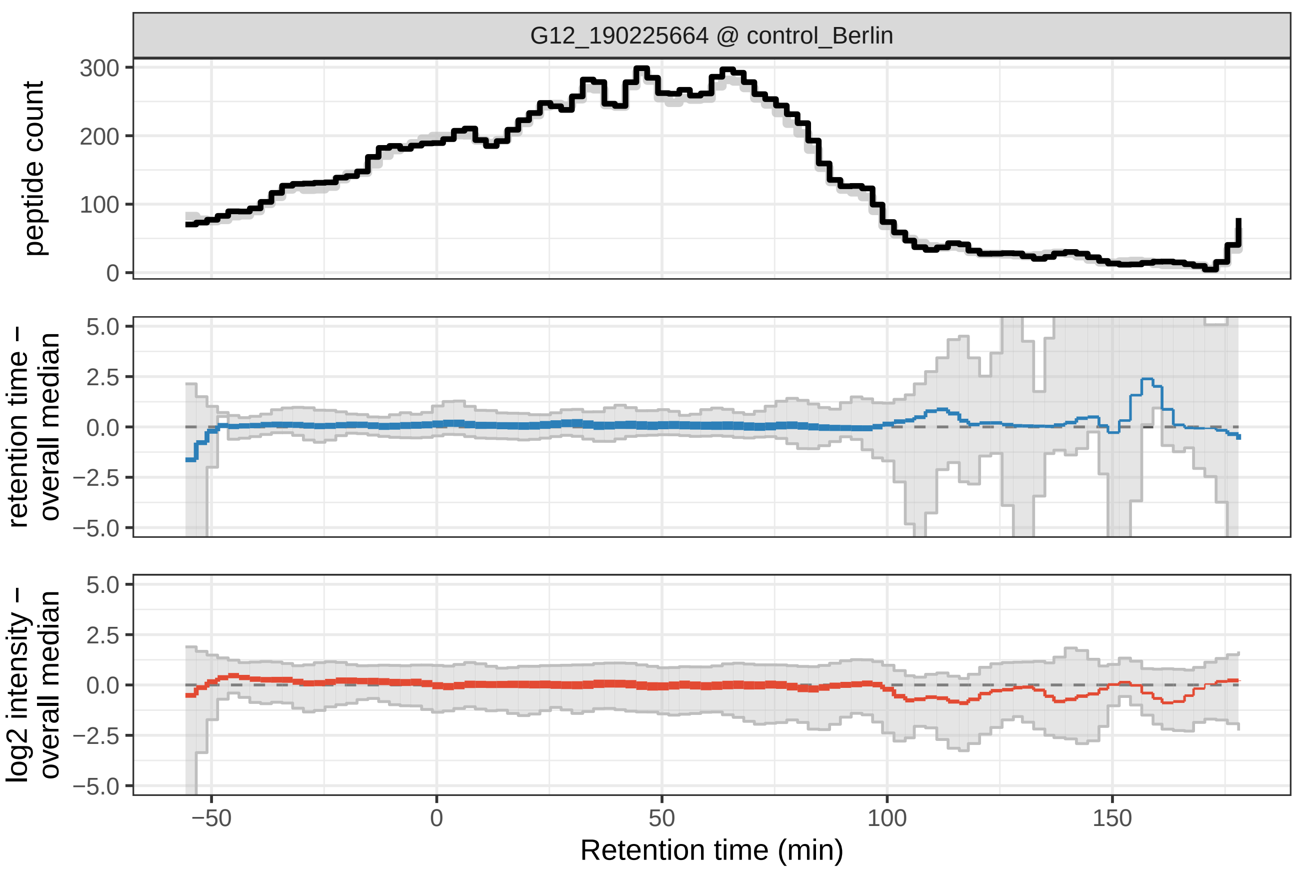
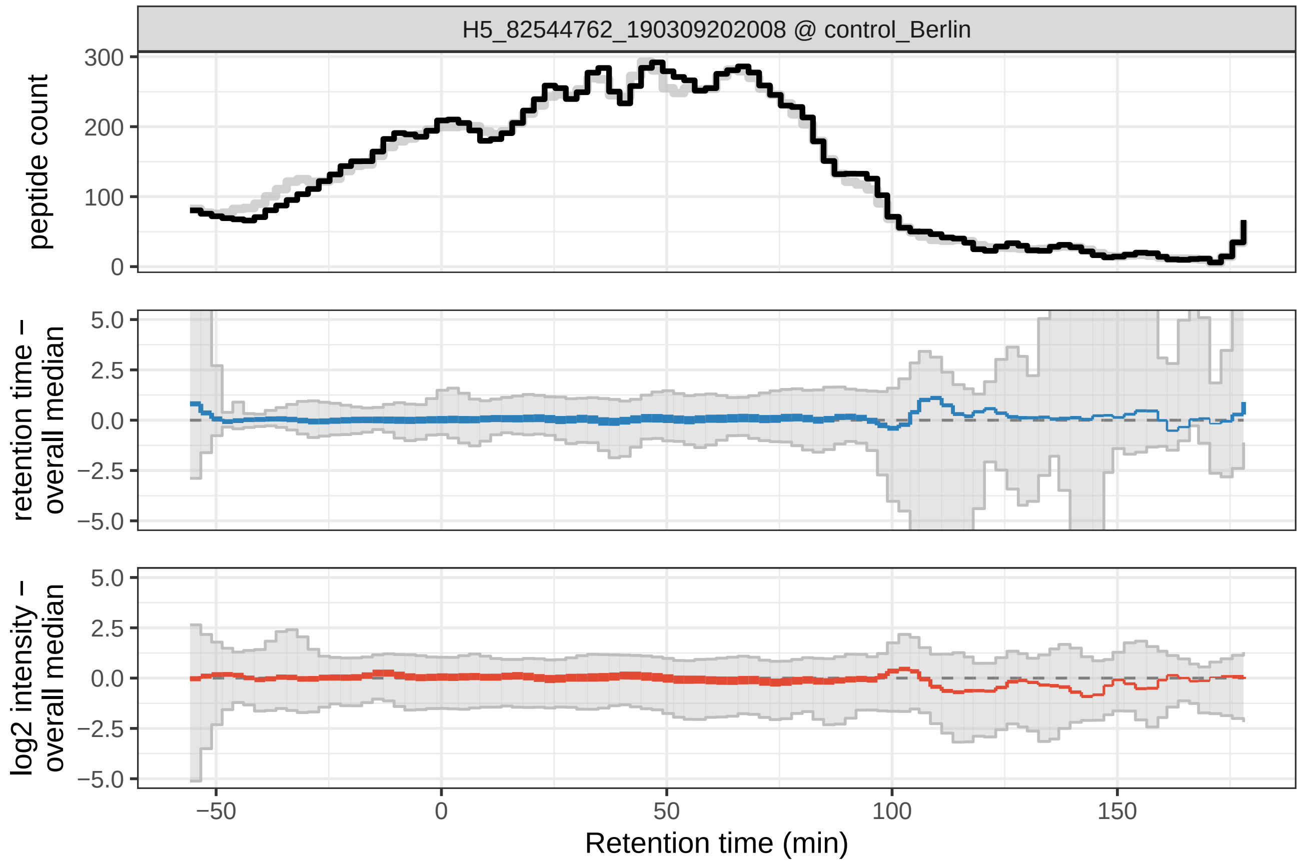
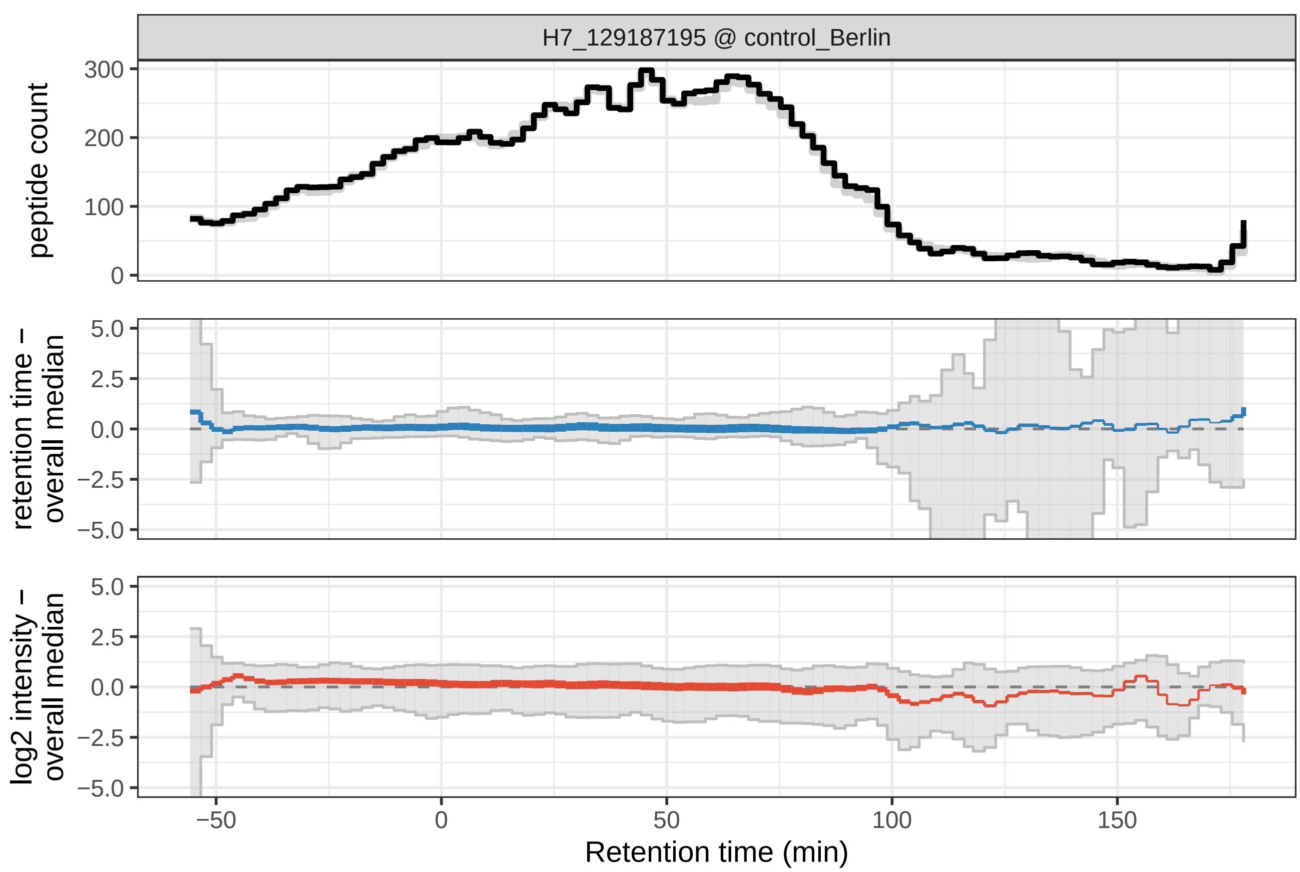
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

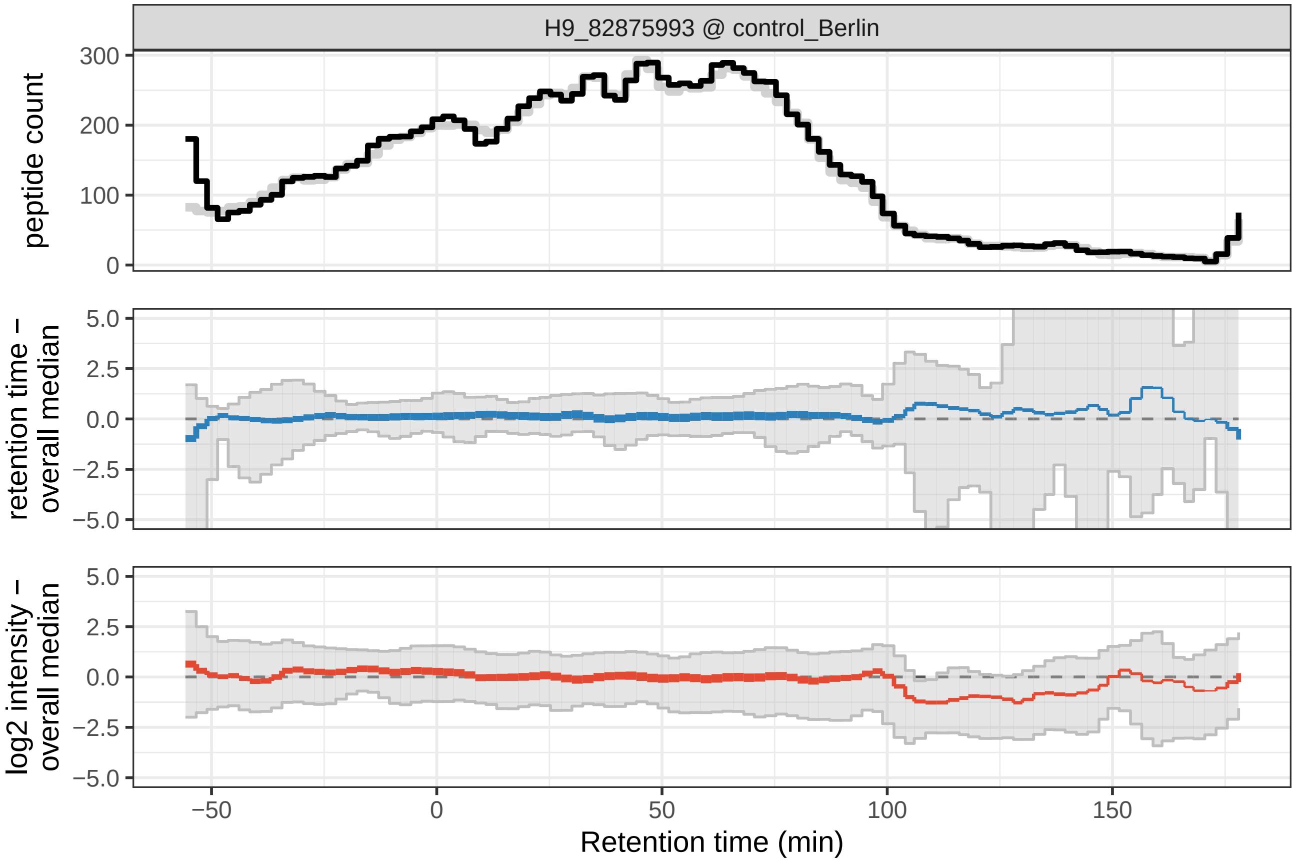

G10_190102976 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

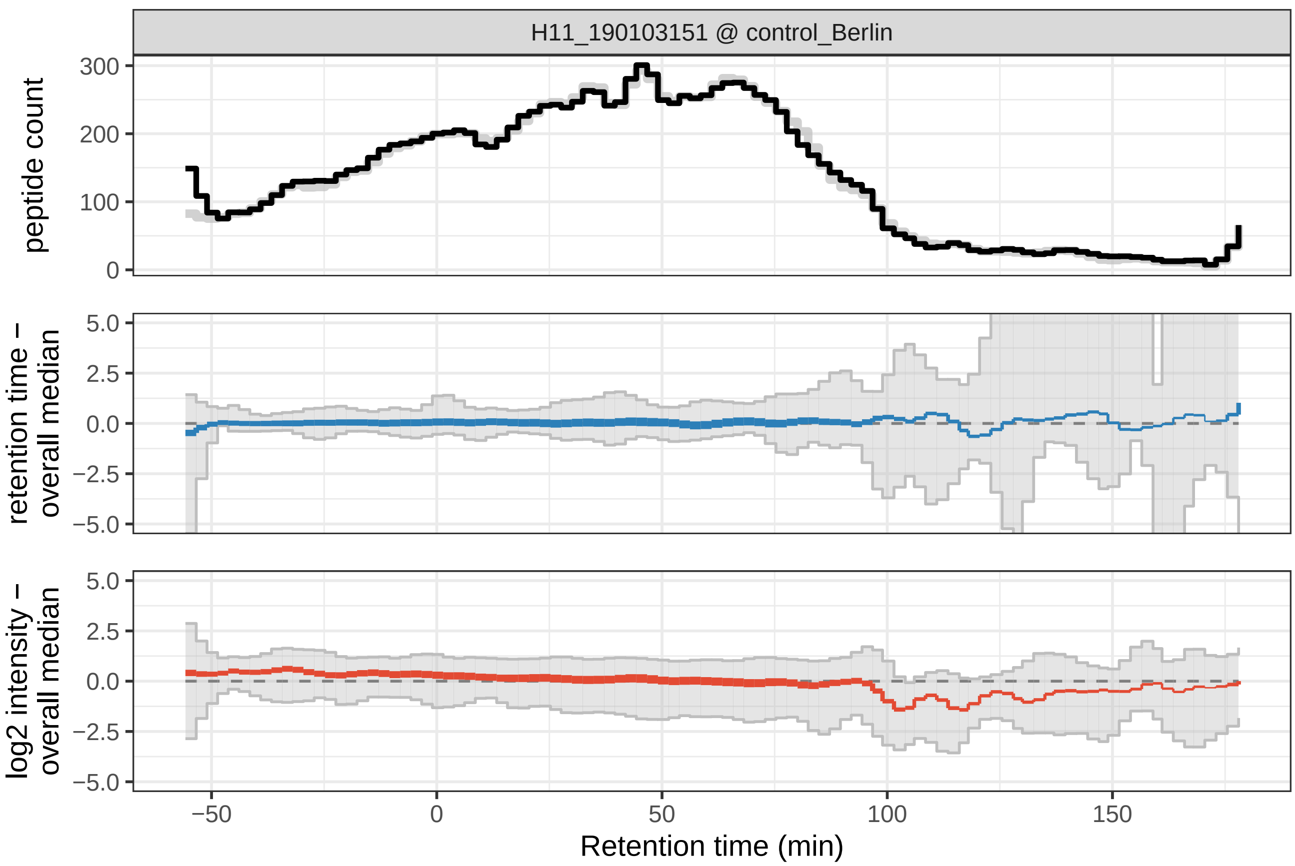

G11_79112692_repeat @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

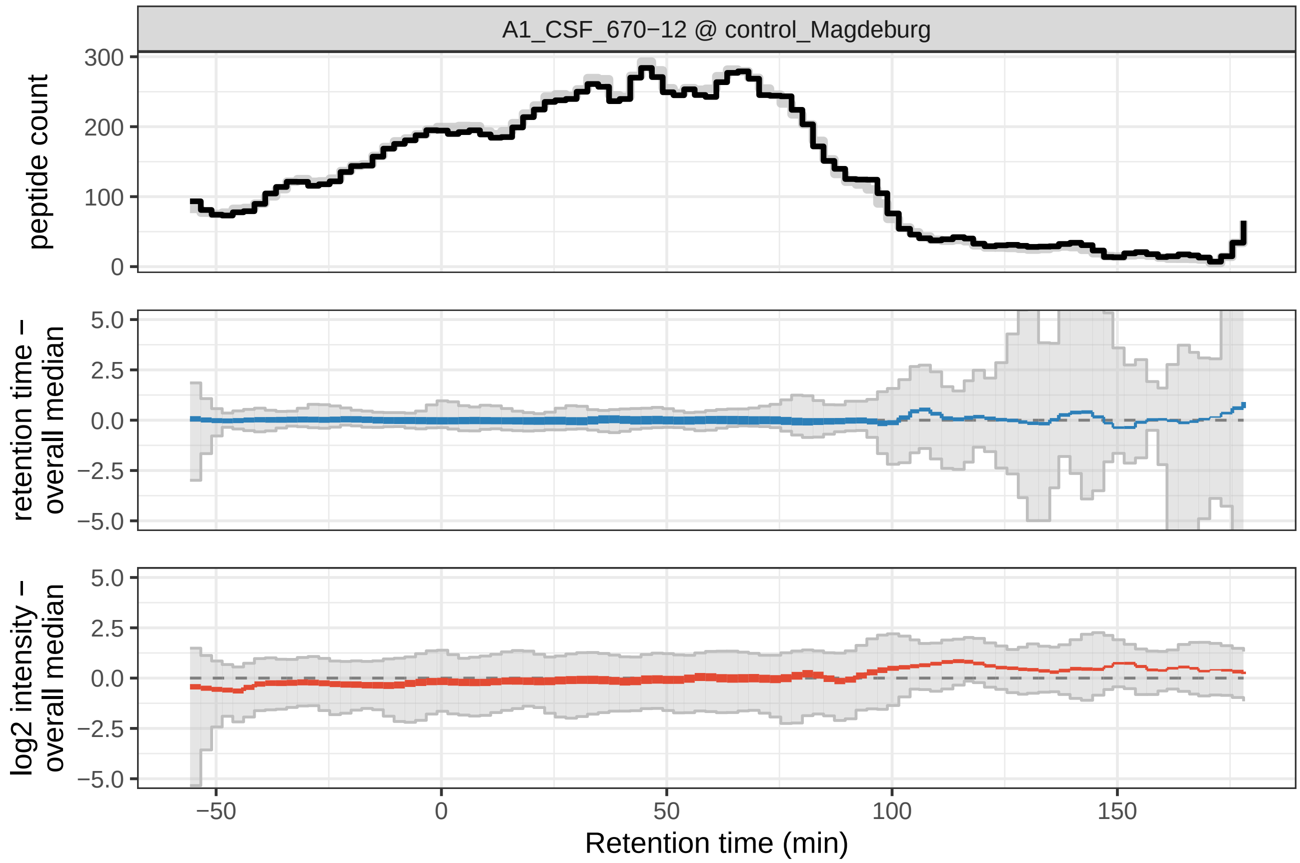

G12_190225664 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

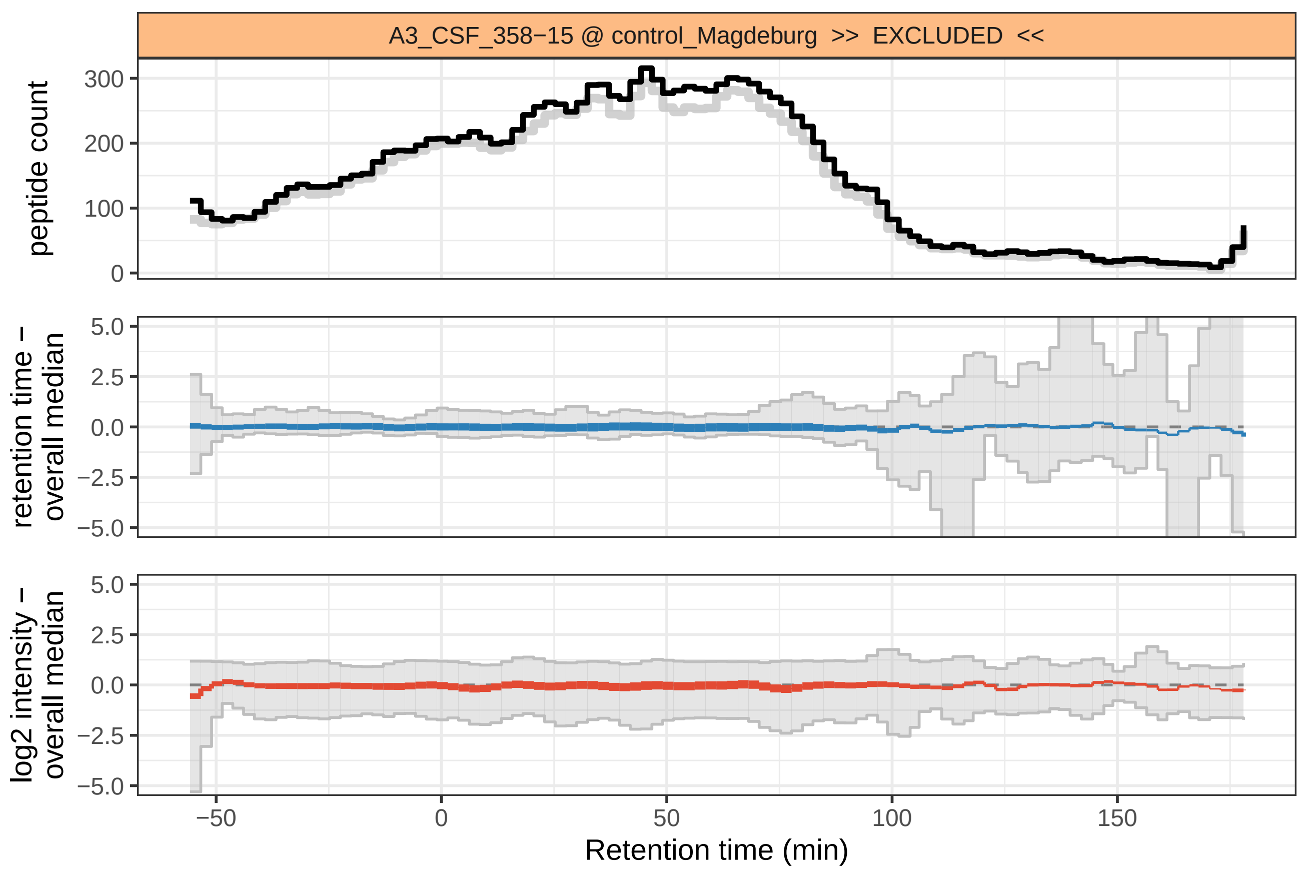

H5_82544762_190309202008 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

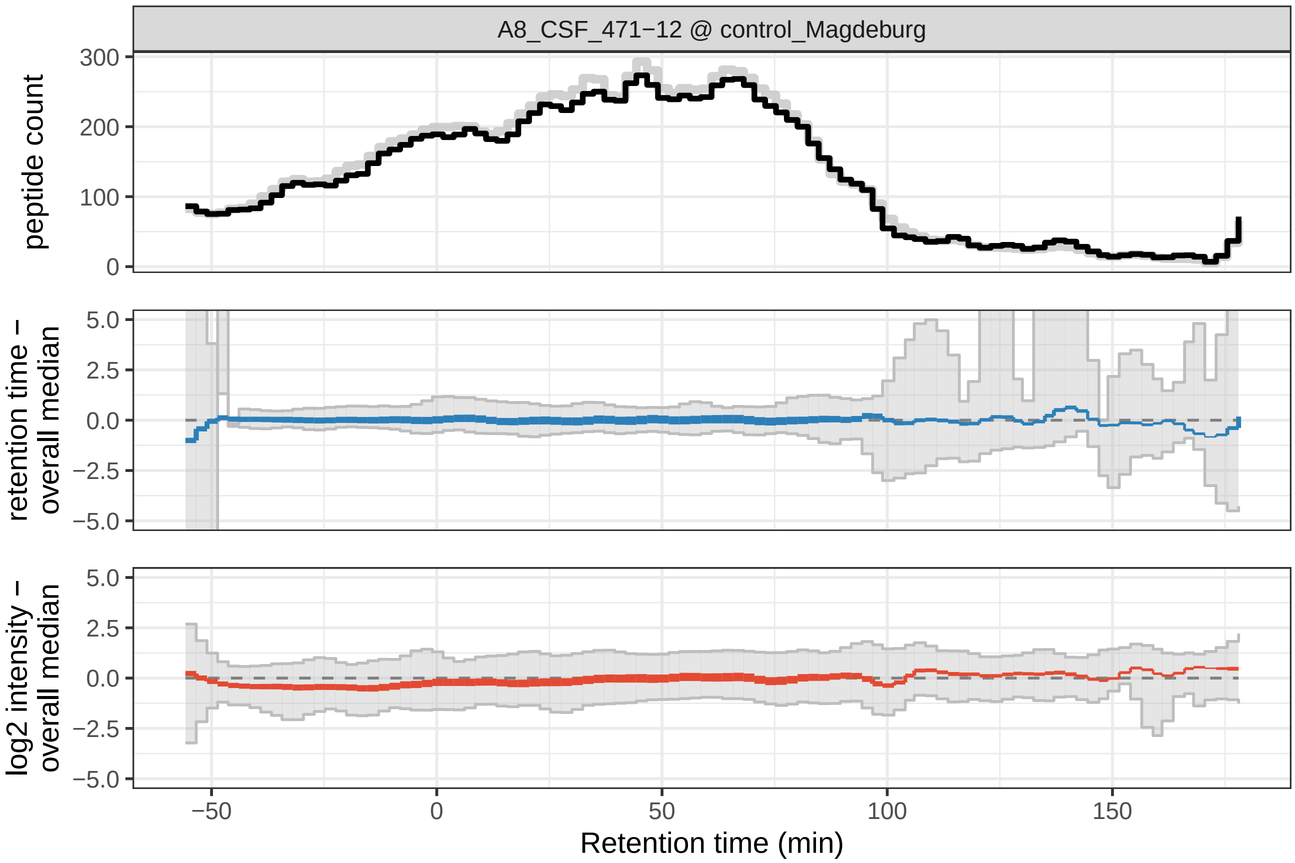

H7_129187195 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

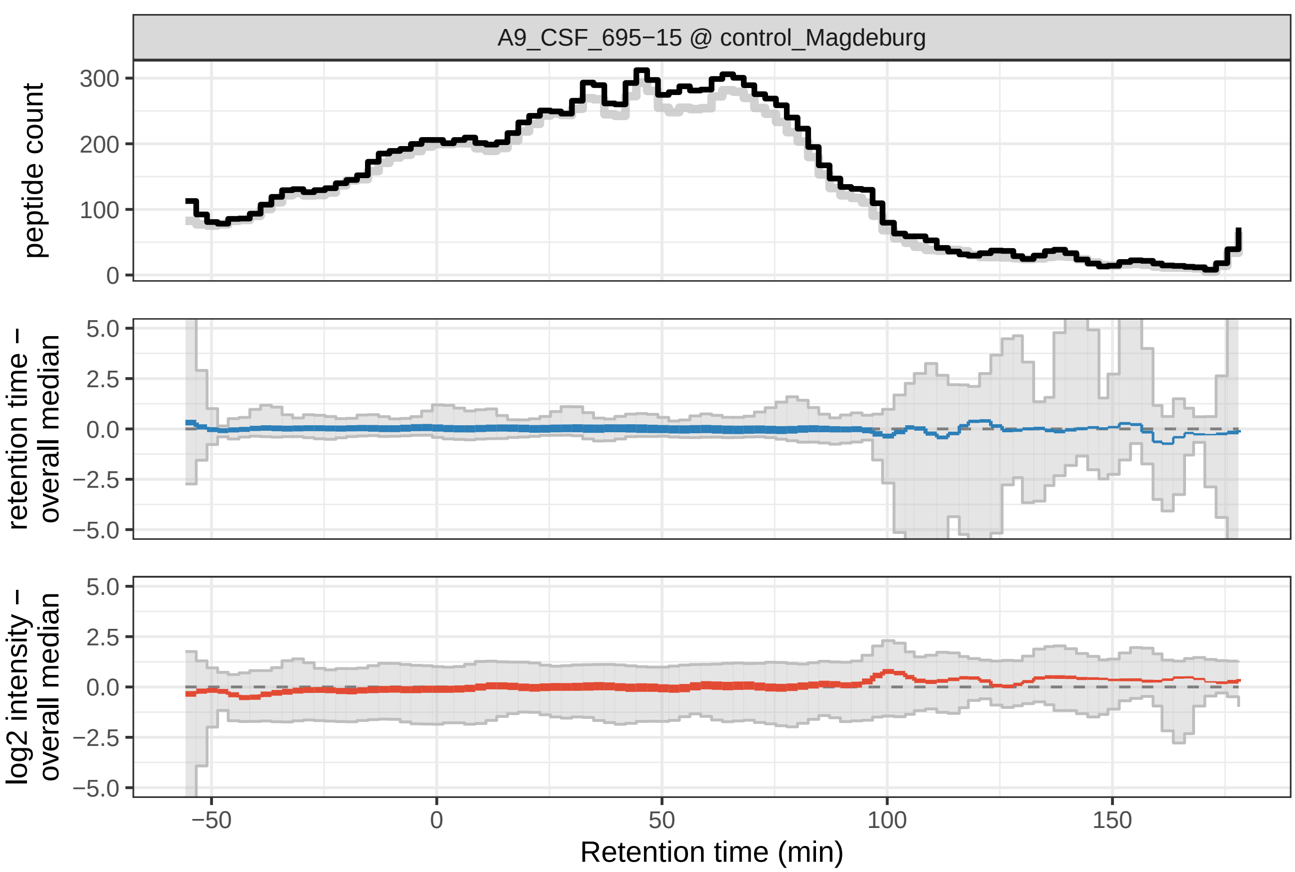

H9_82875993 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

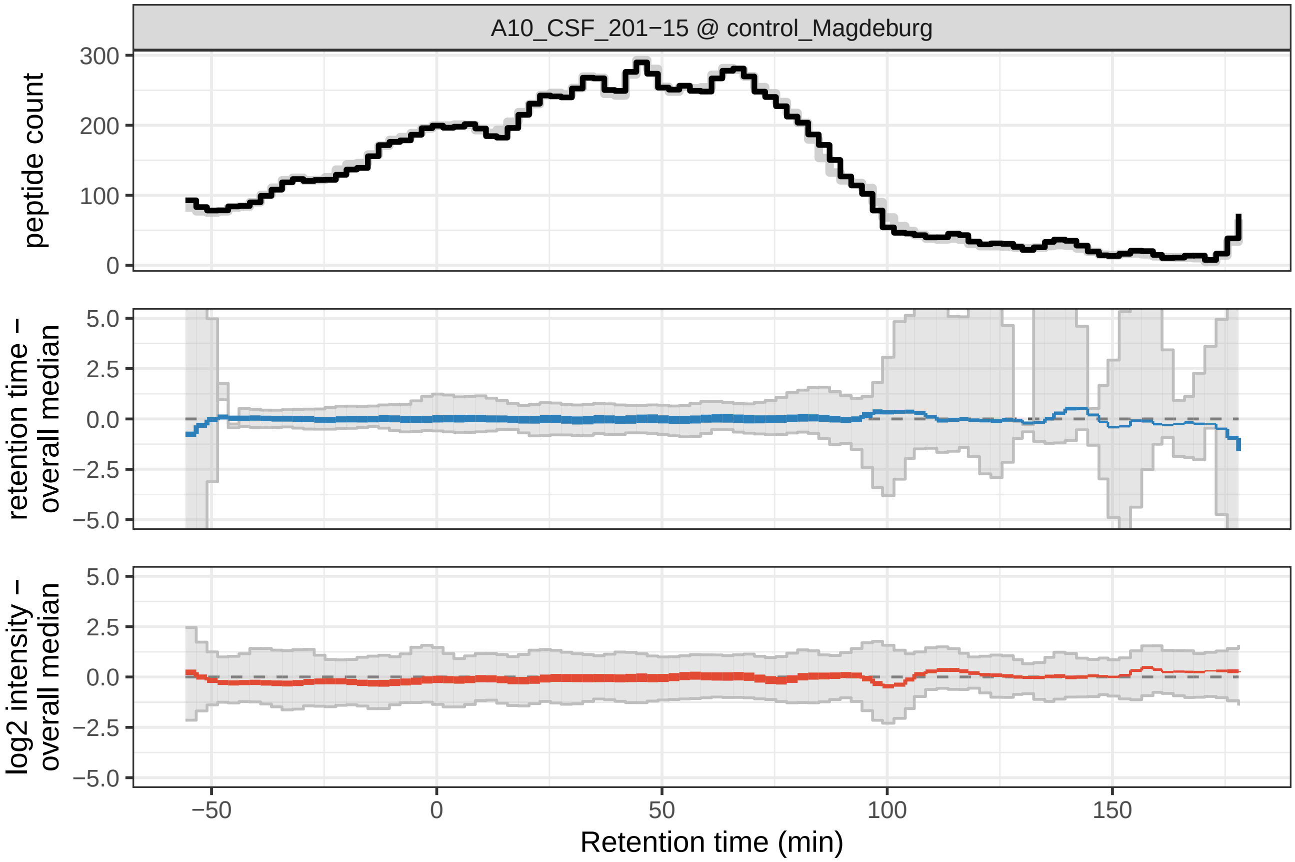

H11_190103151 @ control_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

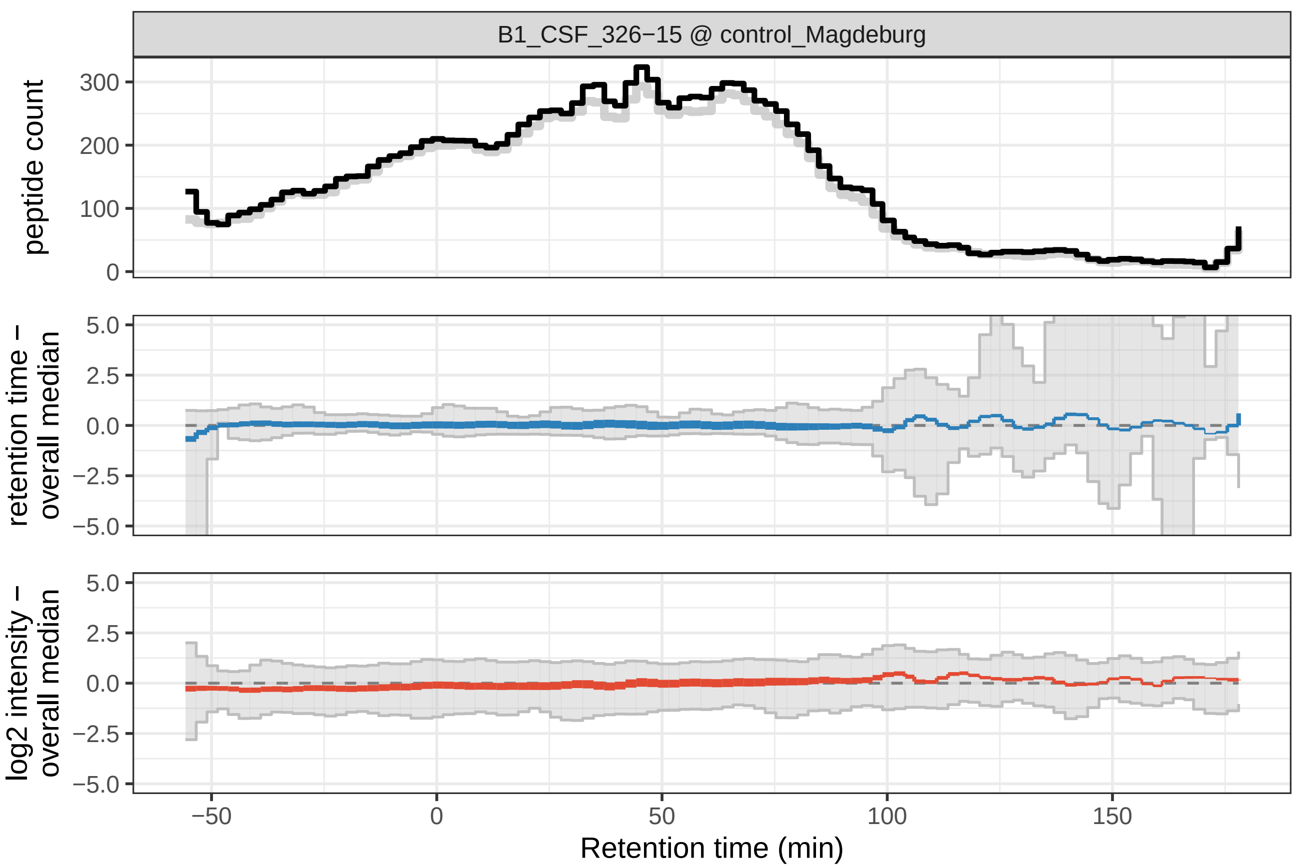

A1_CSF_670−12 @ control_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

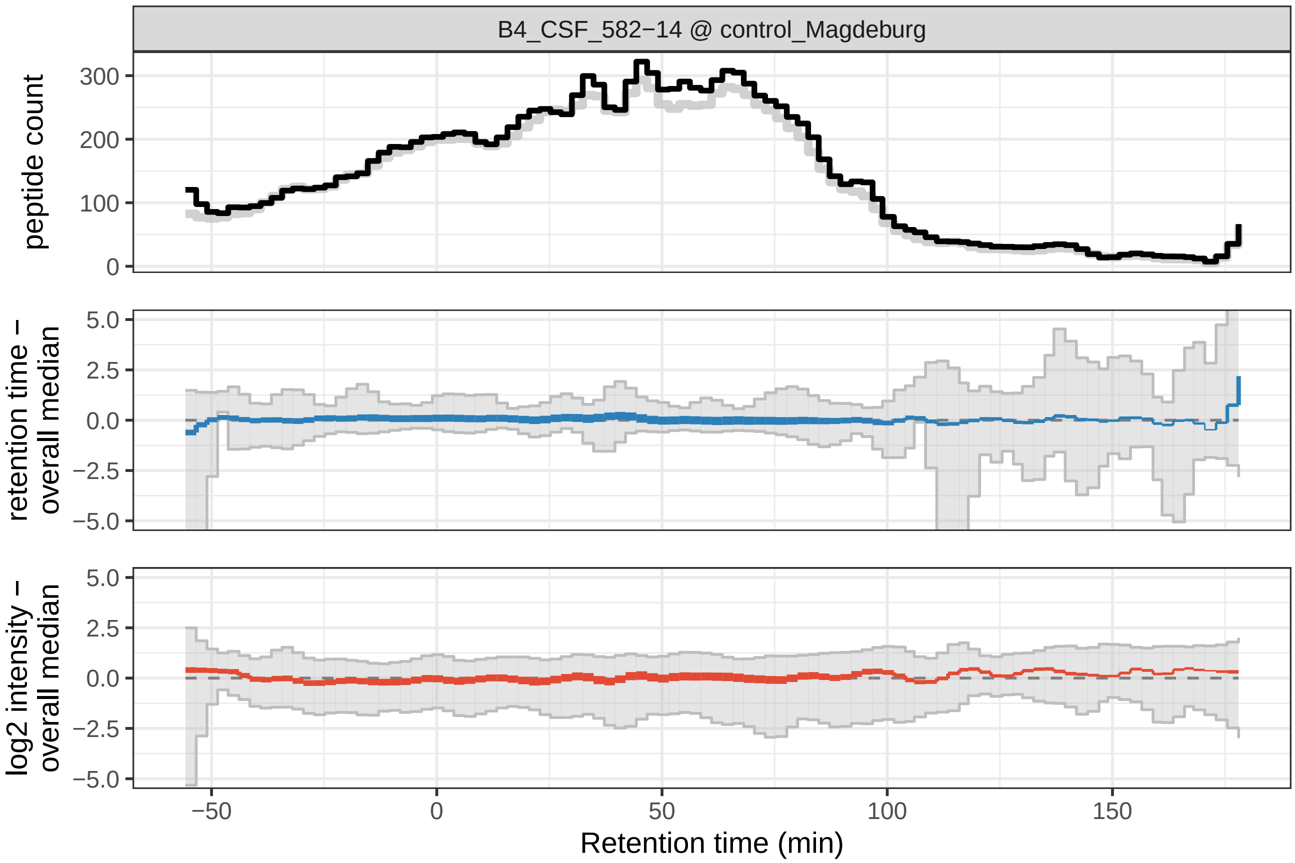

A3_CSF_358−15 @ control_Magdeburg >> EXCLUDED <<
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

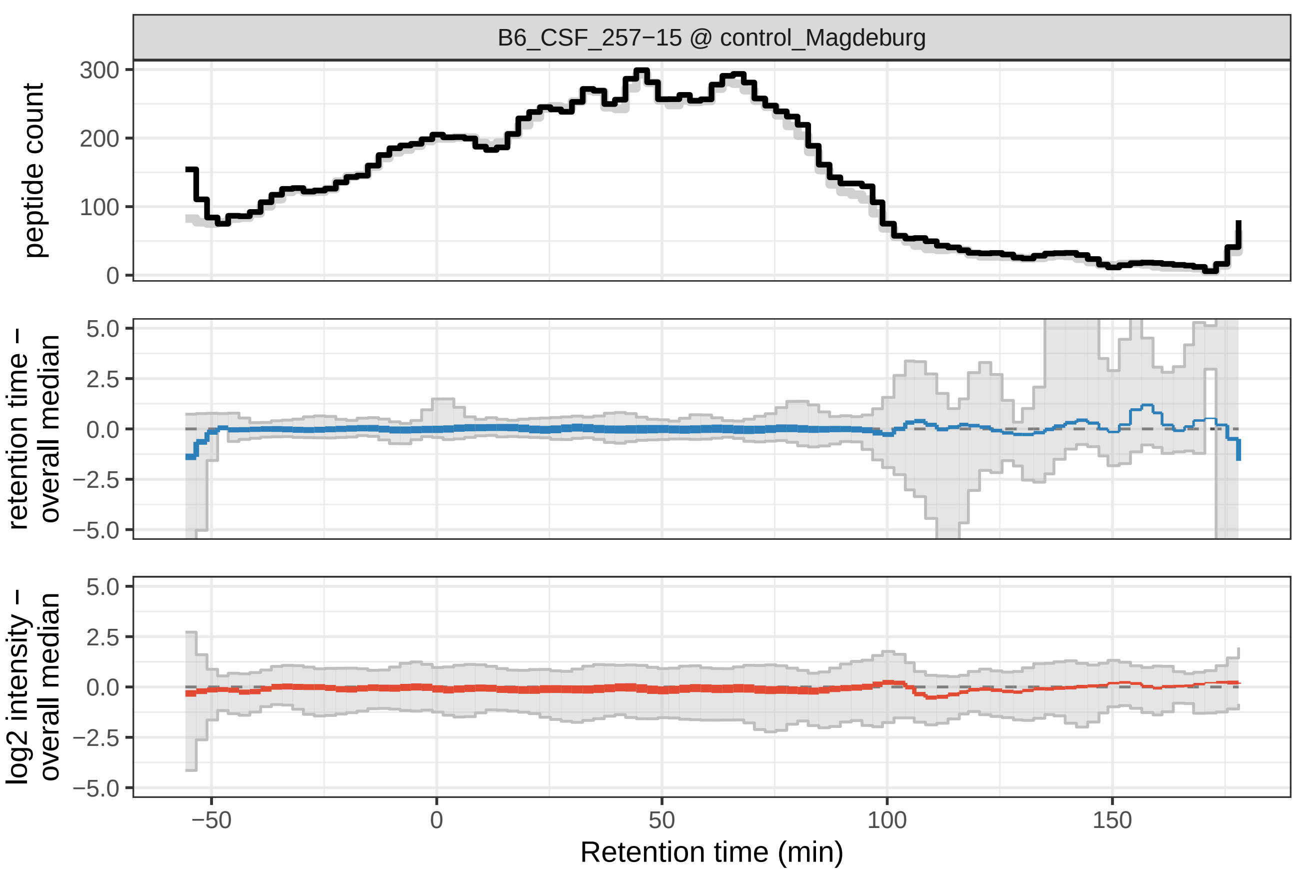

A8_CSF_471−12 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

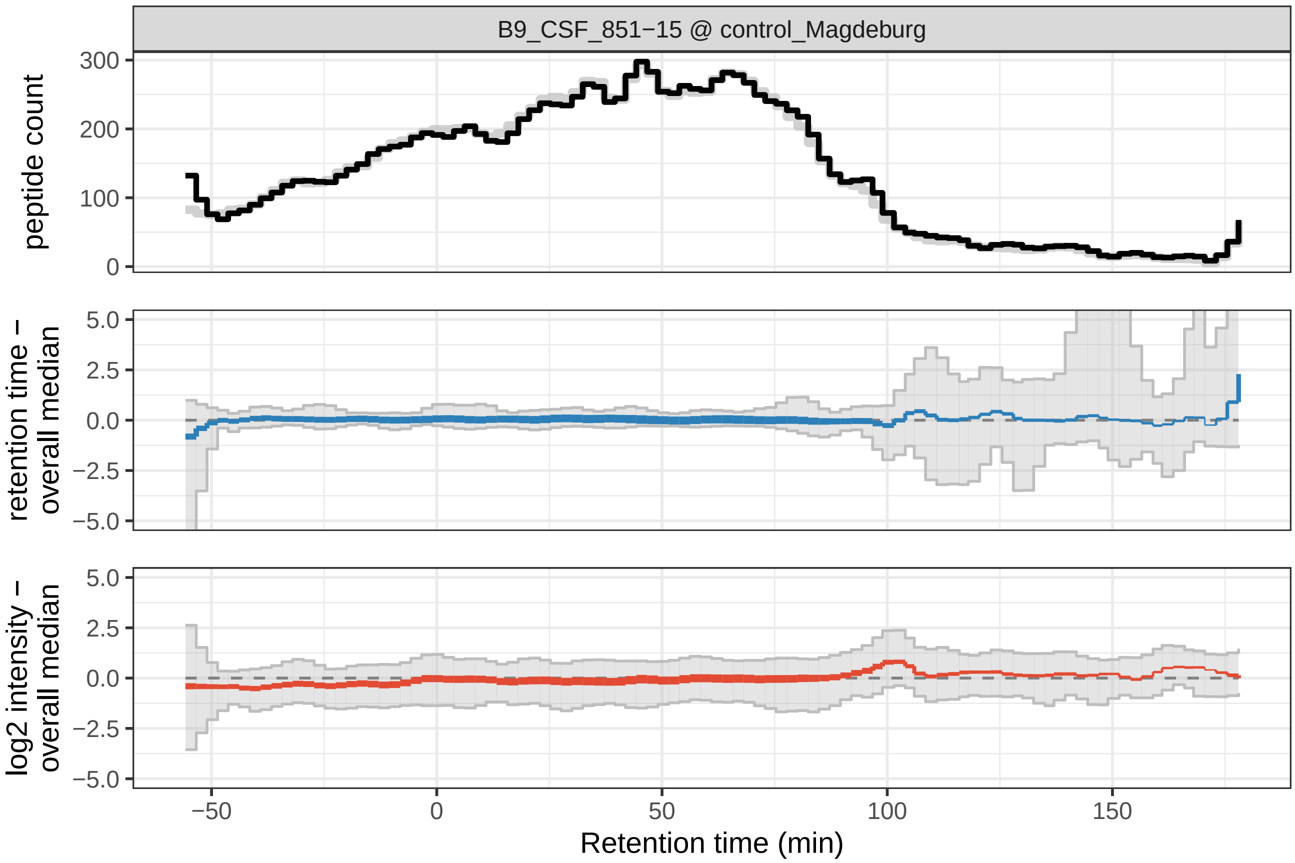

A9_CSF_695−15 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

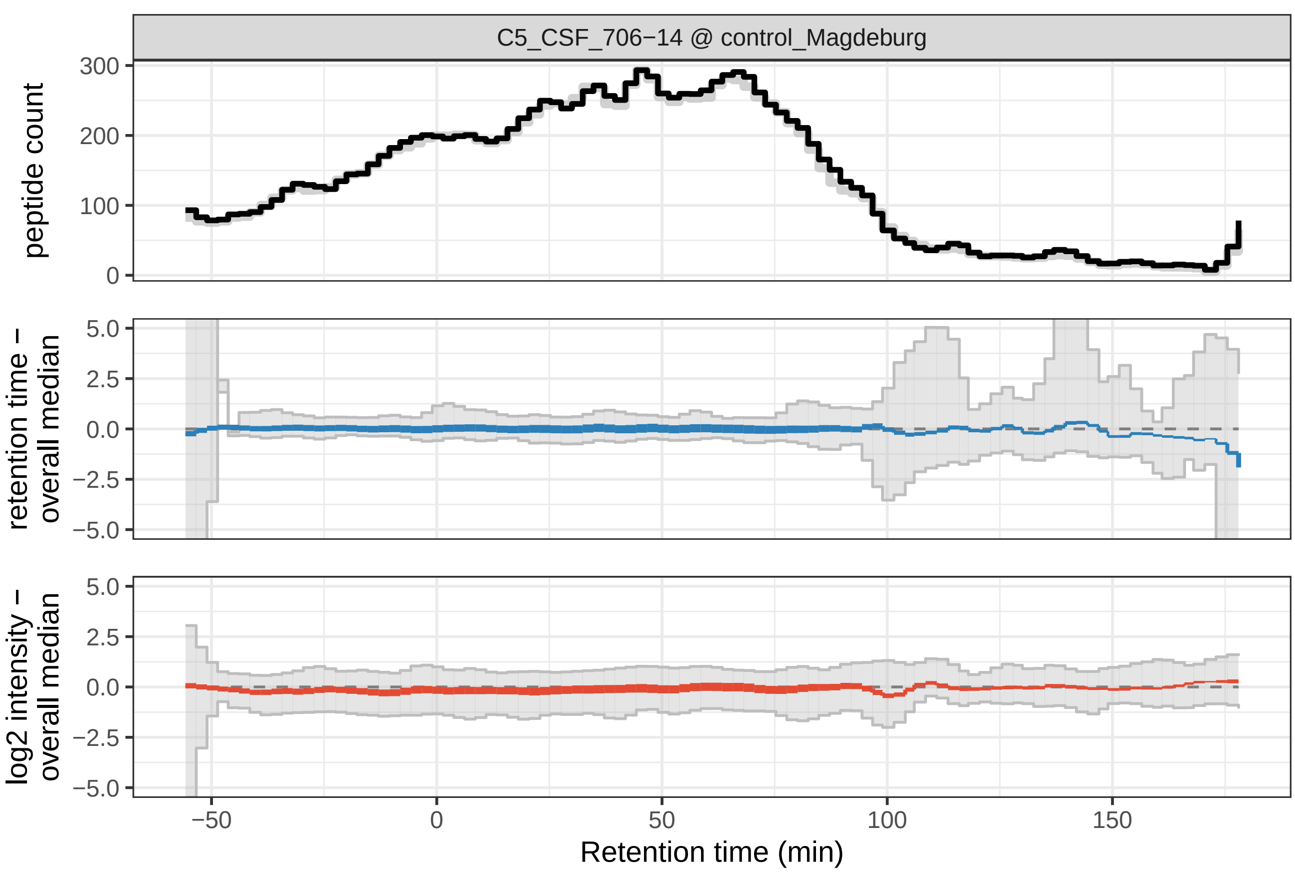

A10_CSF_201−15 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

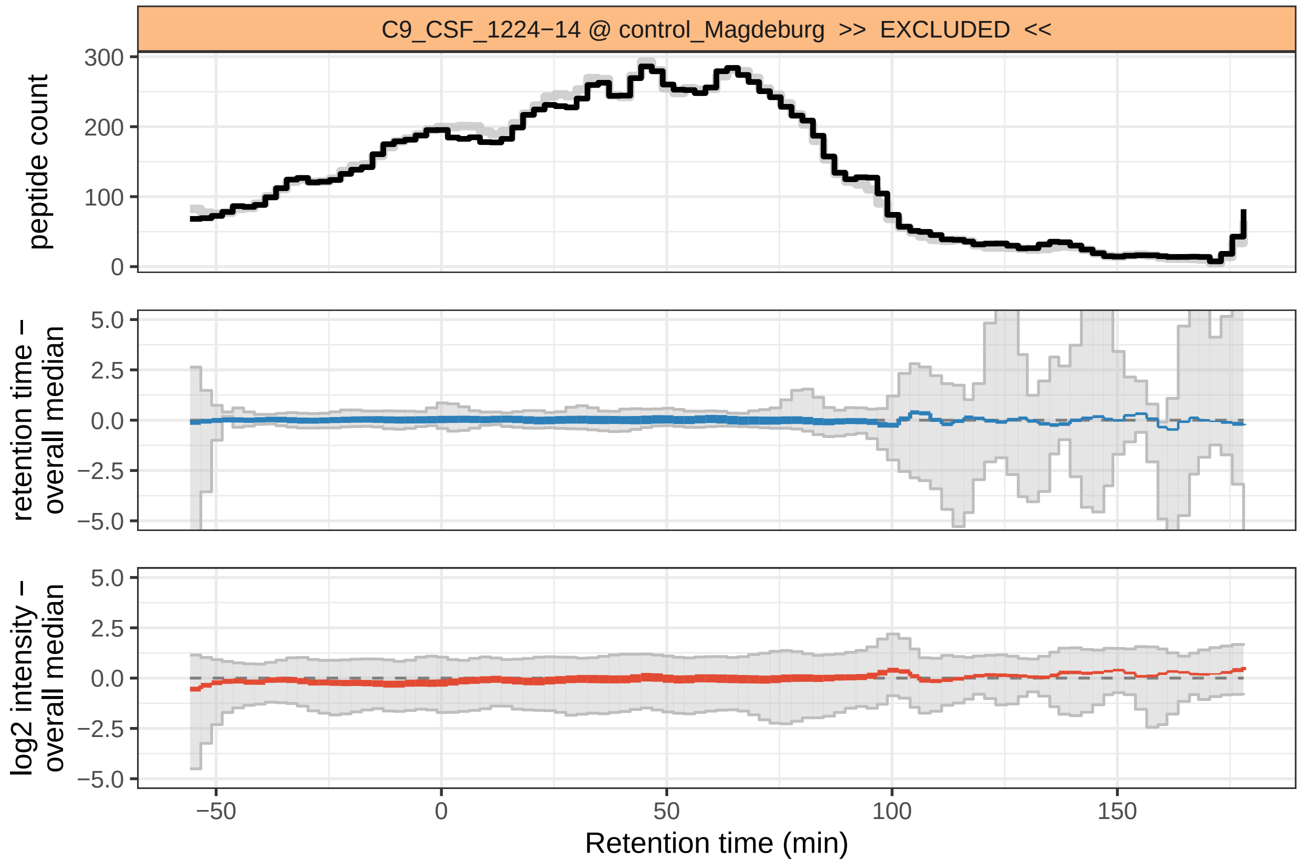

B1_CSF_326−15 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

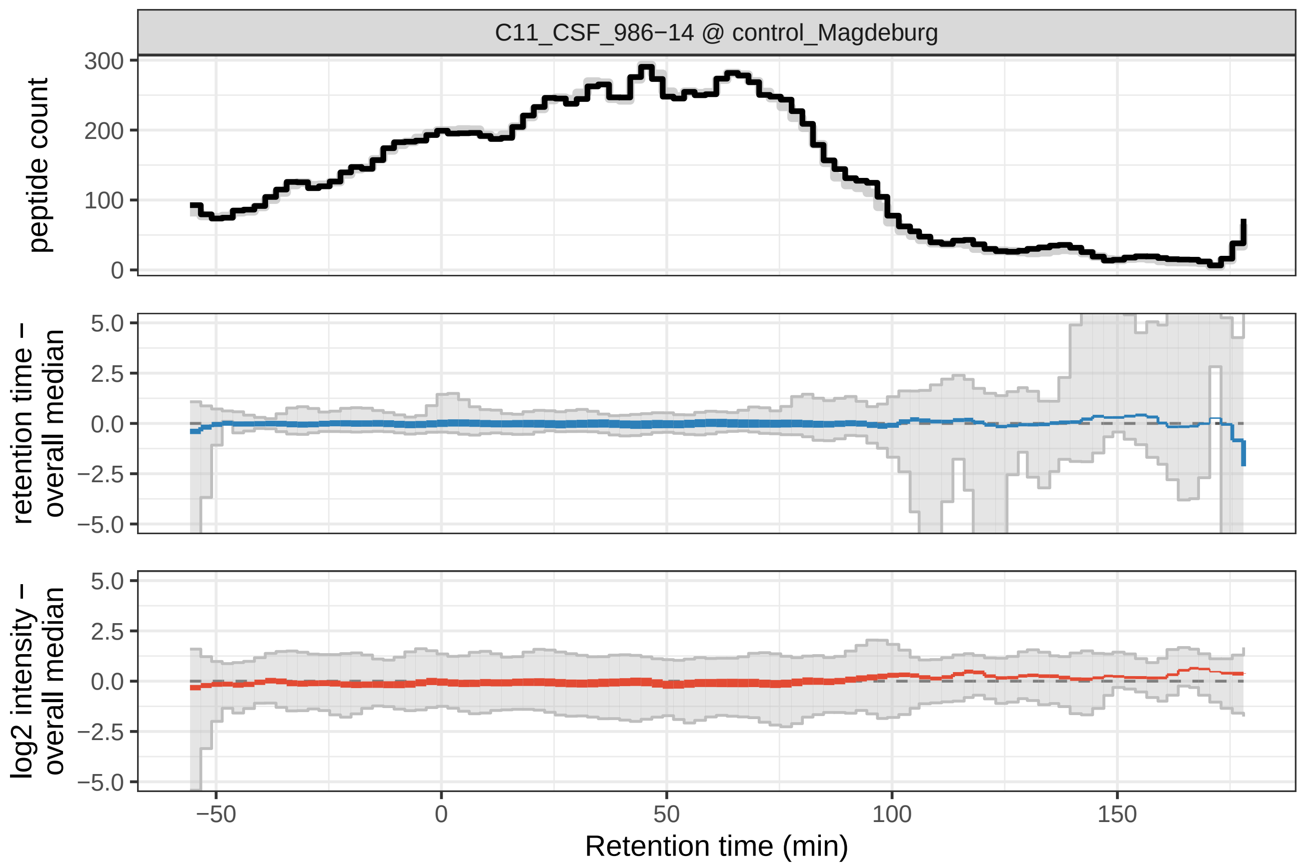

B4_CSF_582−14 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

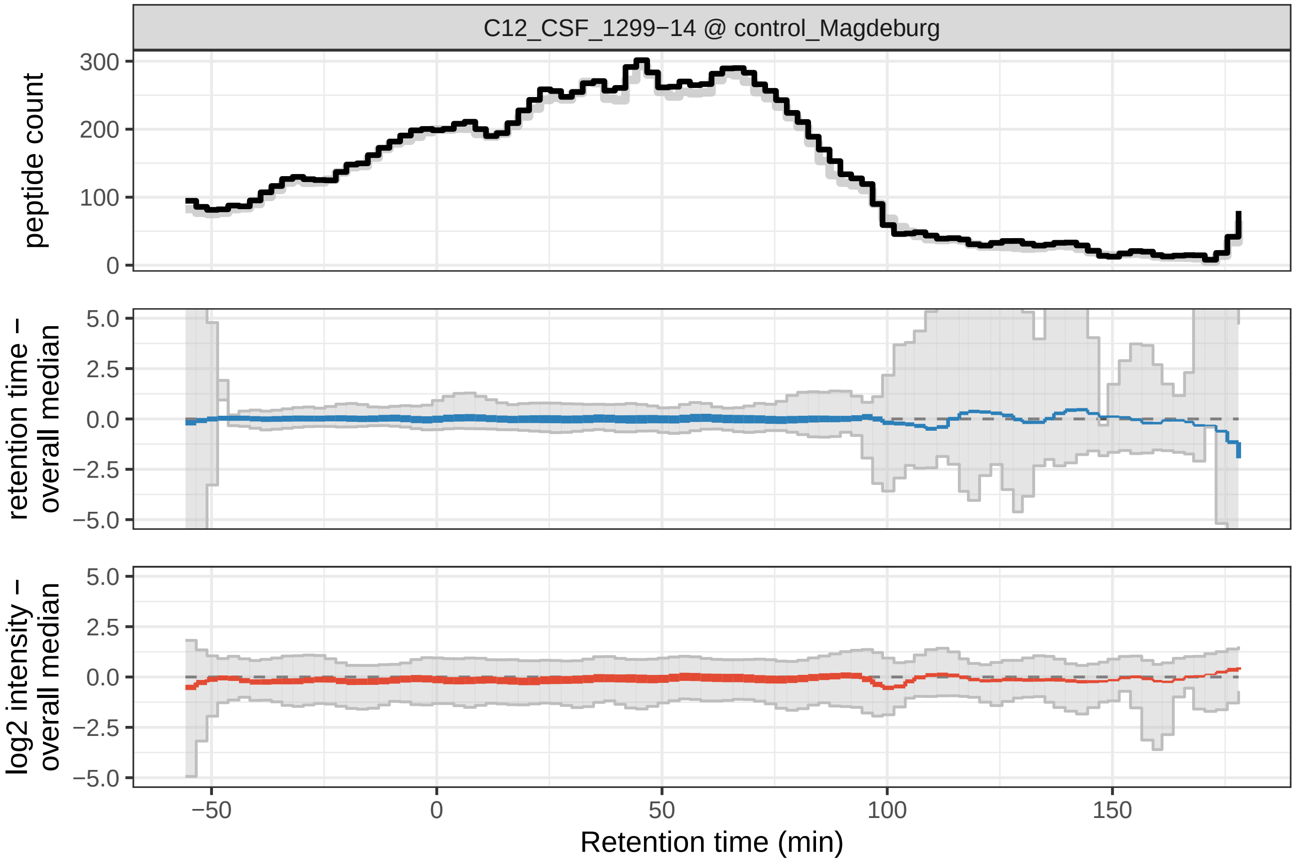

B6_CSF_257−15 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

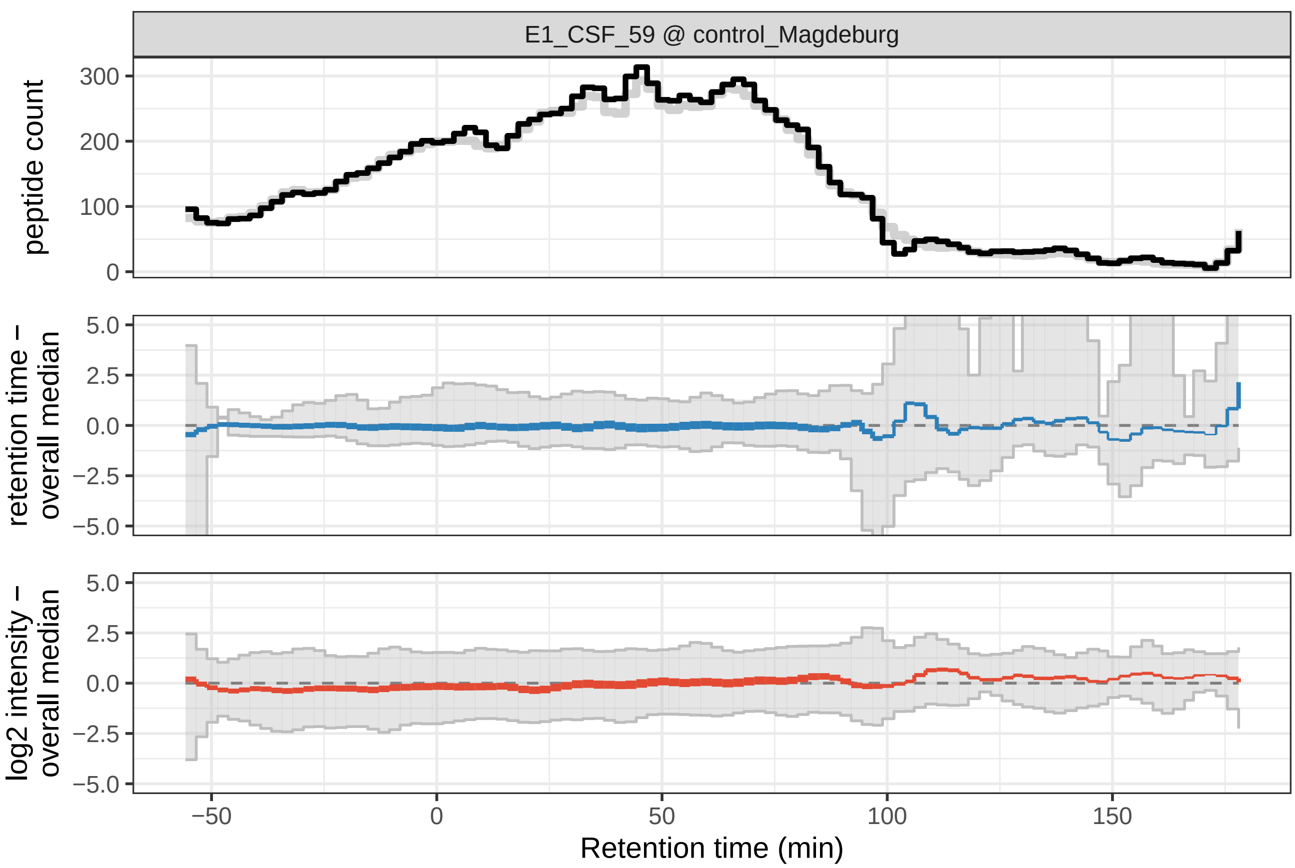

B9_CSF_851−15 @ control_Magdeburg
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

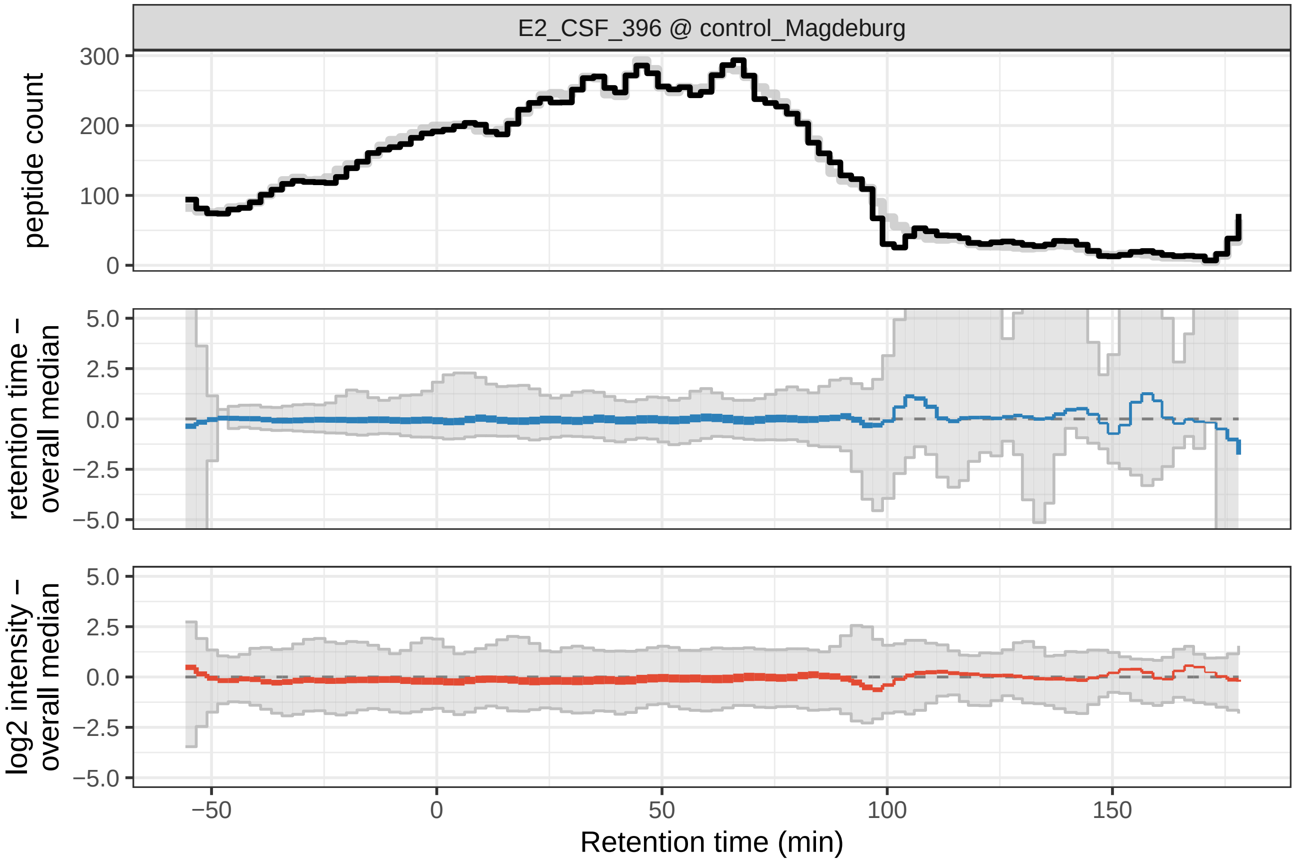

C5_CSF_706−14 @ control_Magdeburg
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

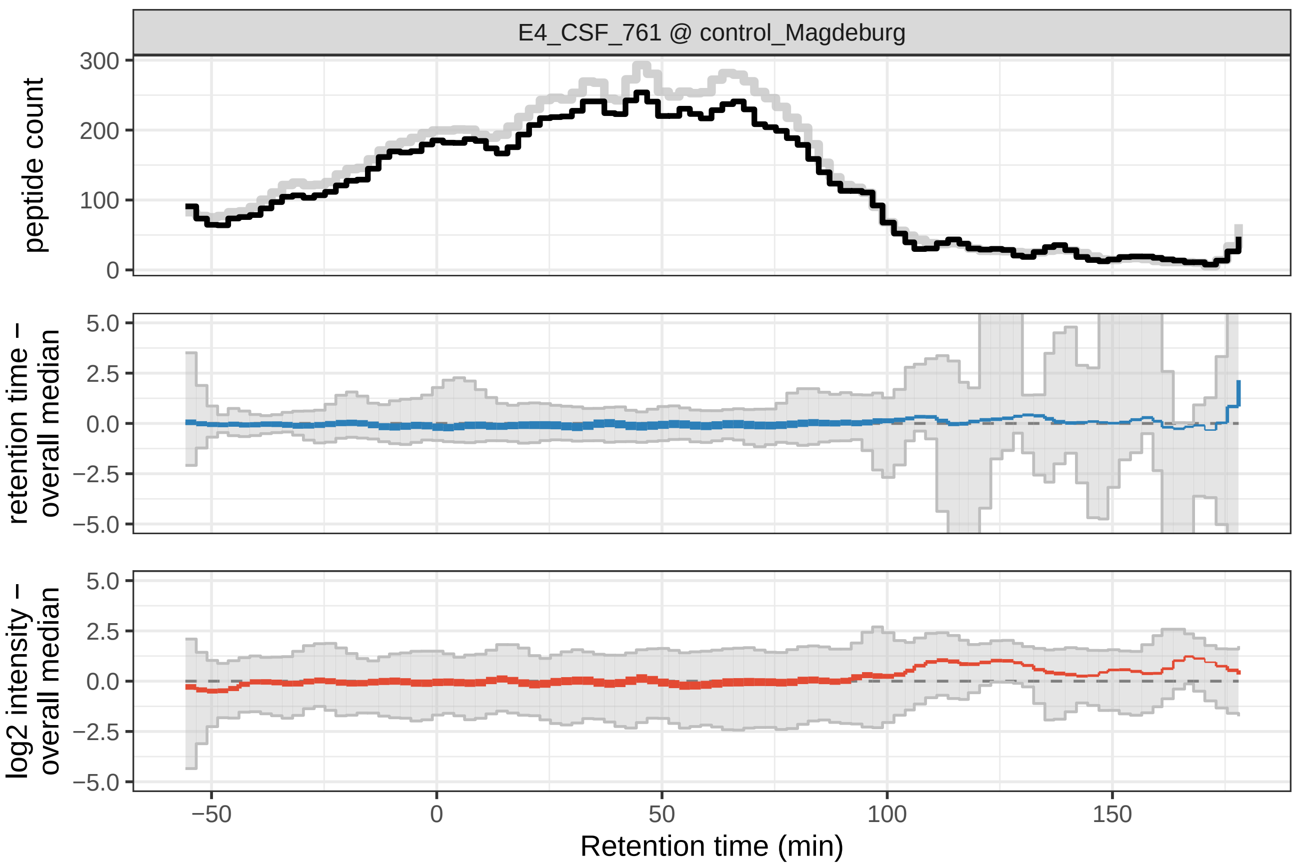

C9_CSF_1224−14 @ control_Magdeburg >> EXCLUDED <<
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

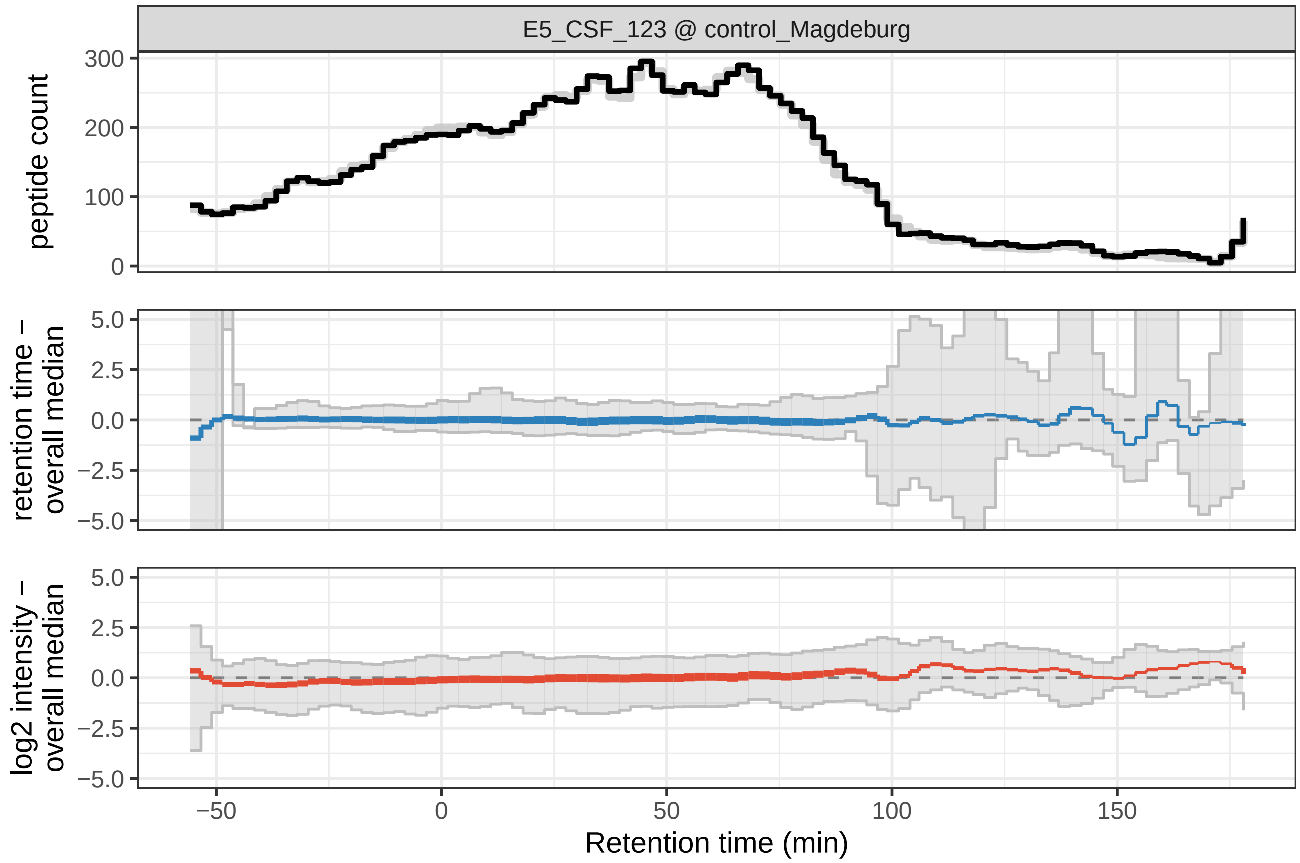

C11_CSF_986−14 @ control_Magdeburg
peptide count
retention time − overall median
log2 intensity − overall median
Retention time (min)

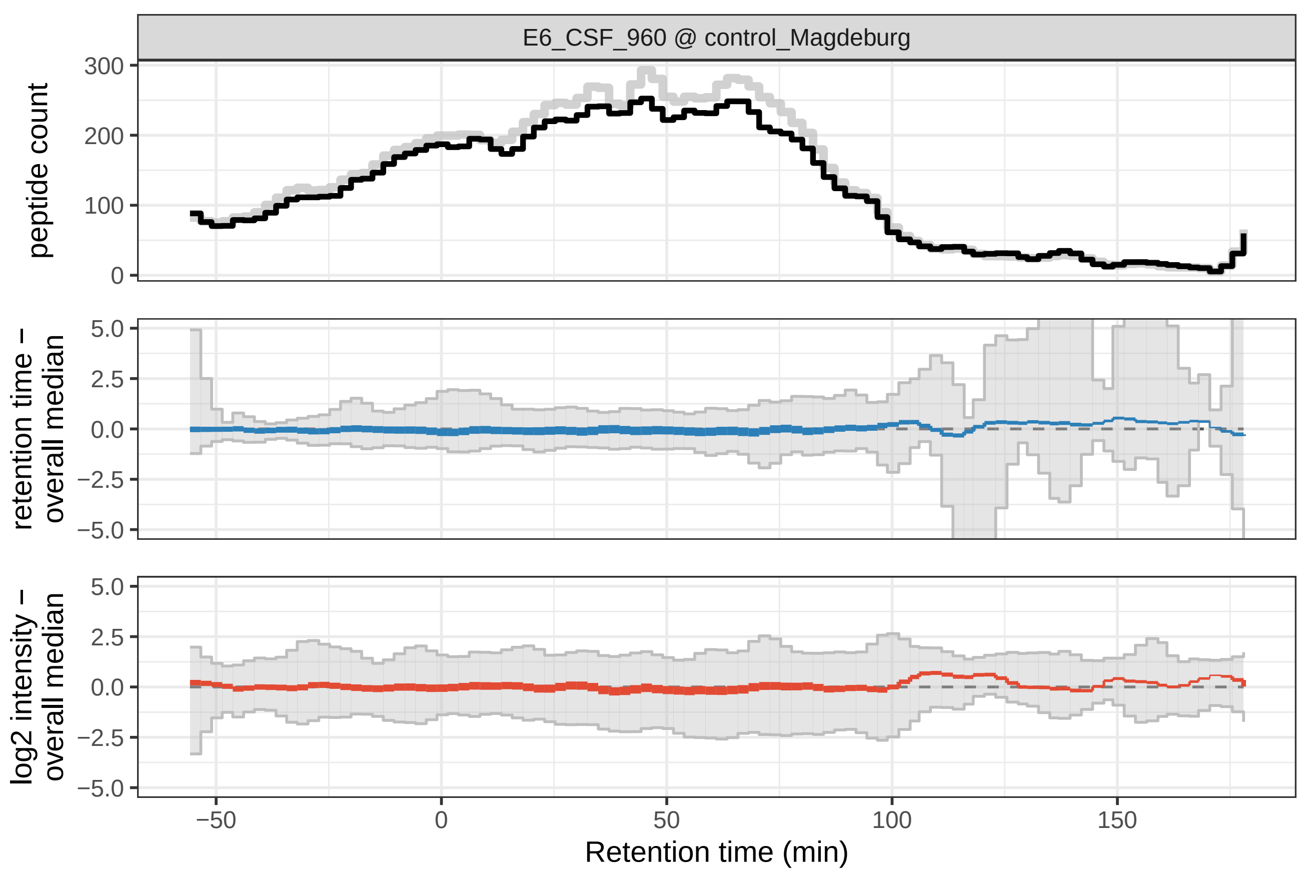

C12_CSF_1299−14 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

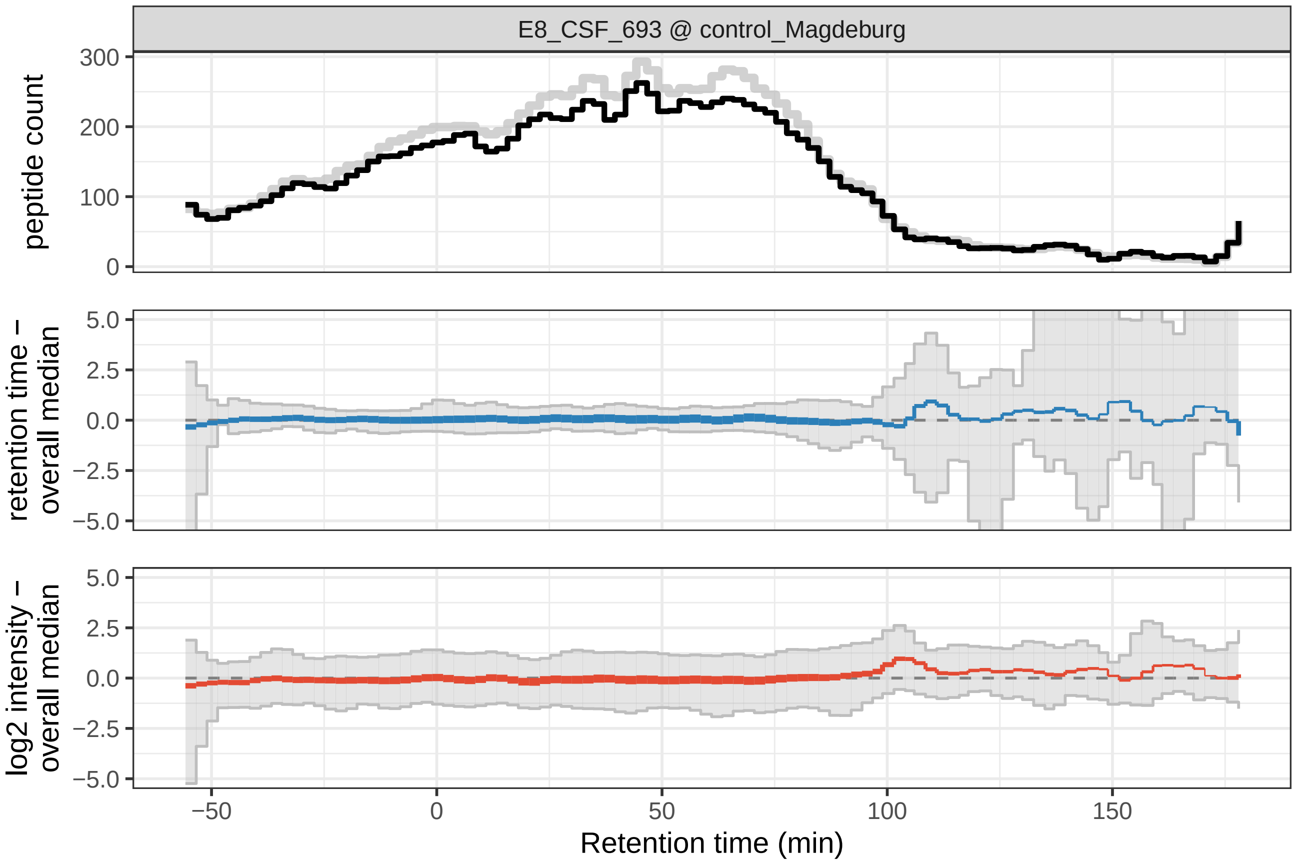

E1_CSF_59 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

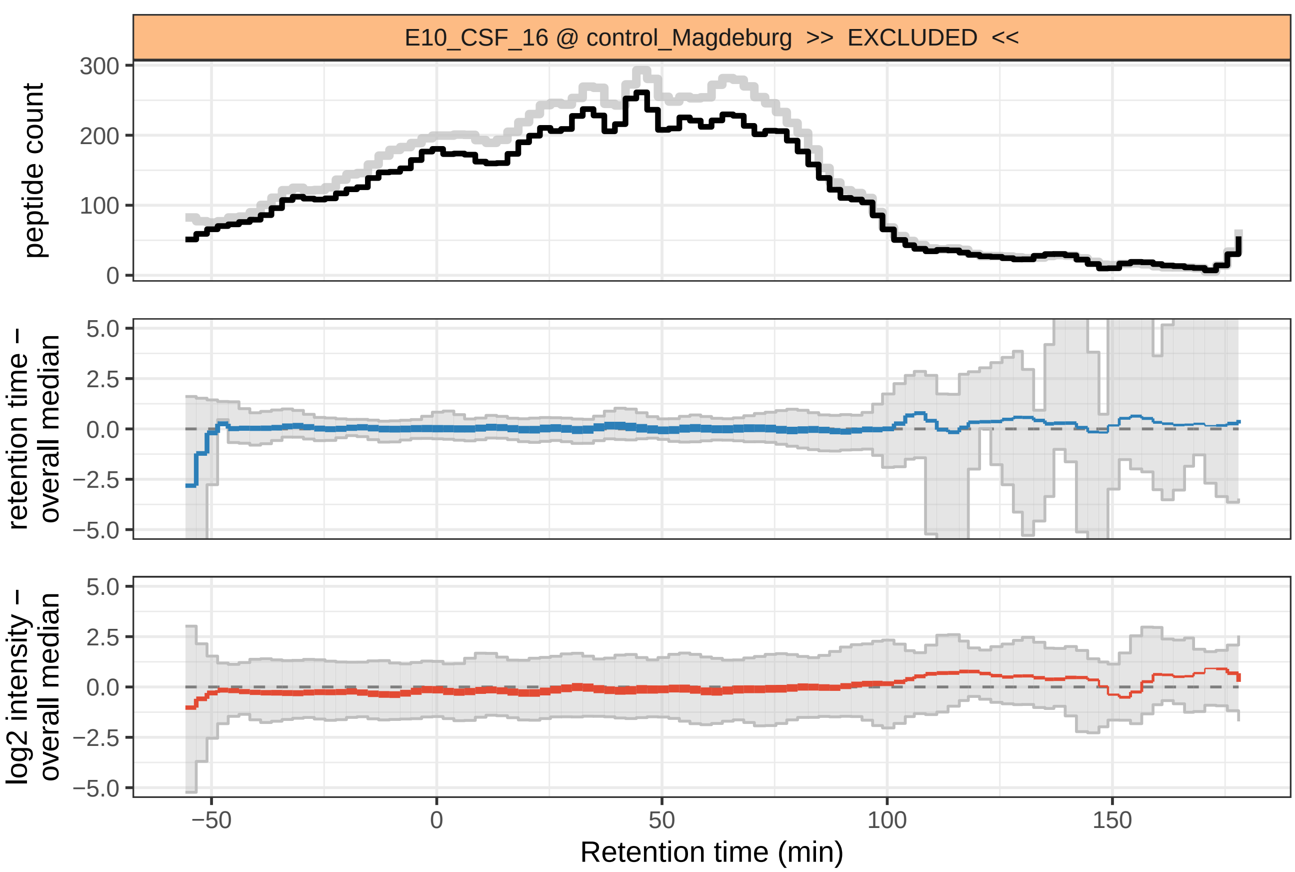

E2_CSF_396 @ control_Magdeburg
peptide count
retention time –
overall median
log2 intensity –
overall median
Retention time (min)

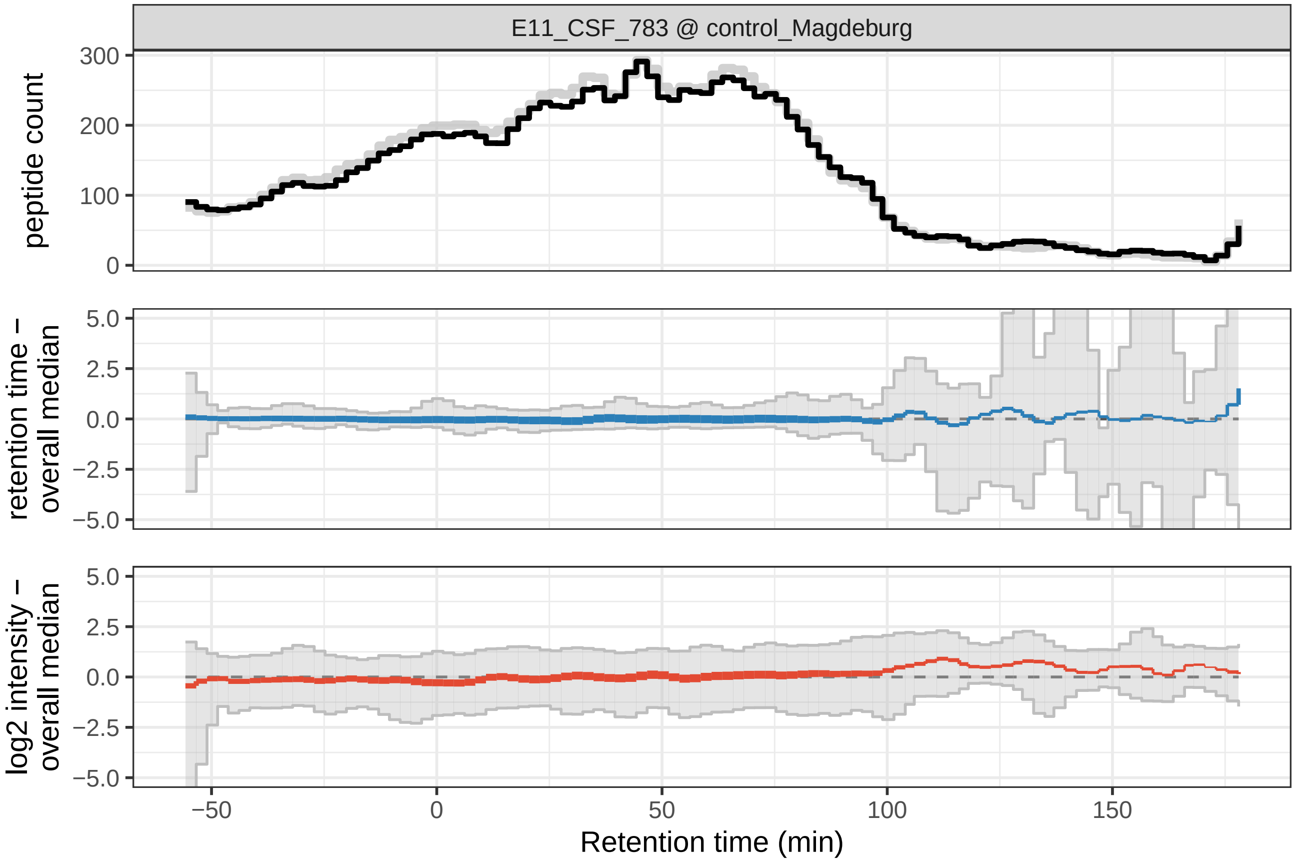

E4_CSF_761 @ control_Magdeburg
peptide count
retention time –
overall median
log2 intensity –
overall median
Retention time (min)

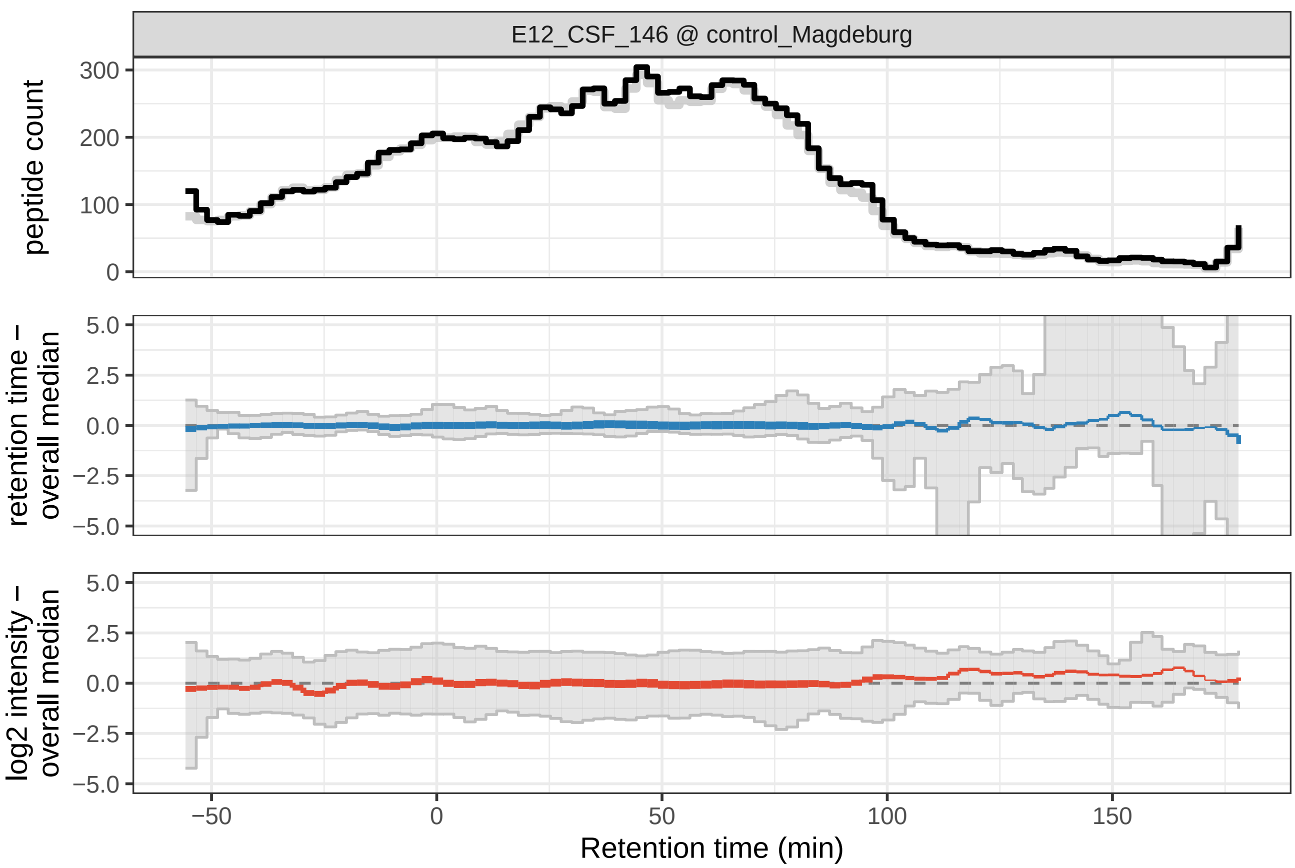

E5_CSF_123 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150

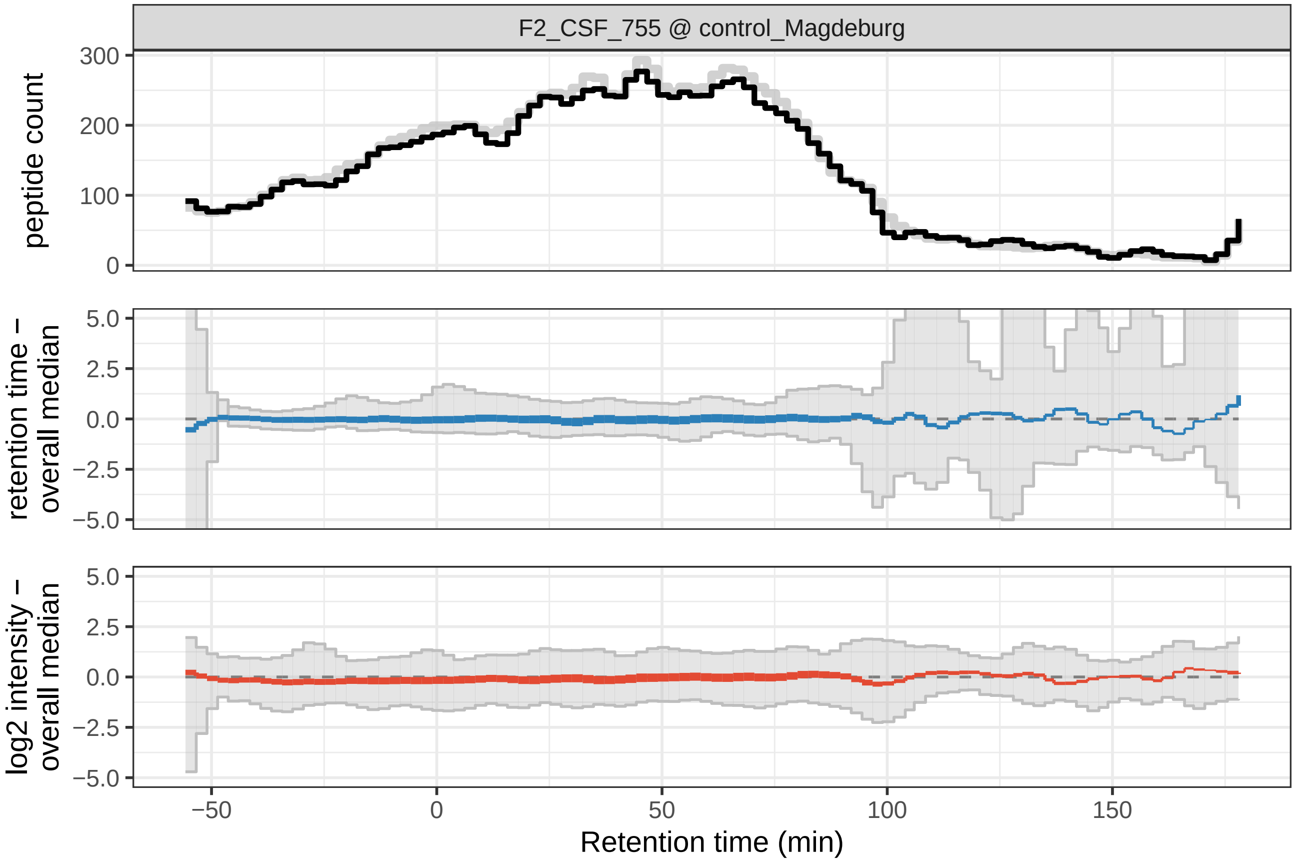

E6_CSF_960 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150

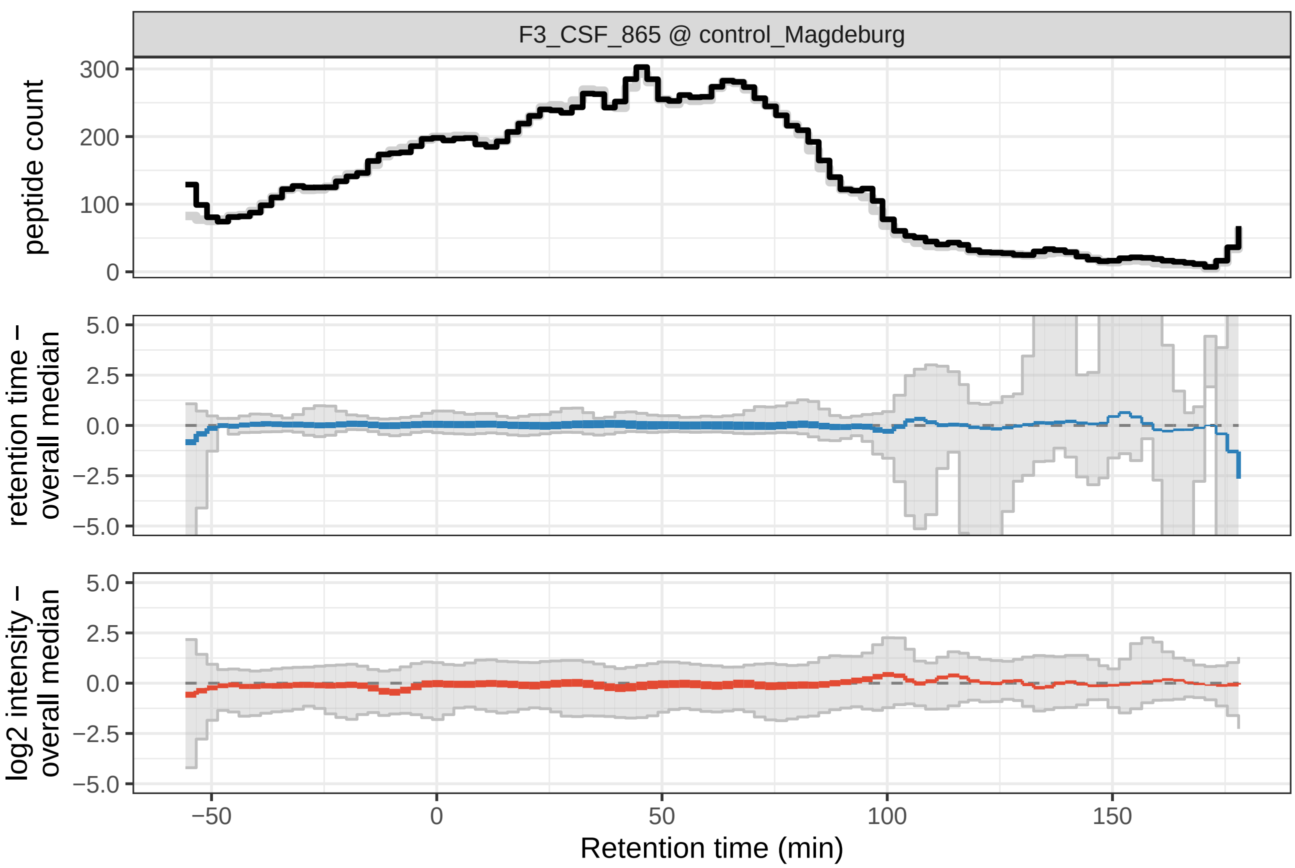

E8_CSF_693 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

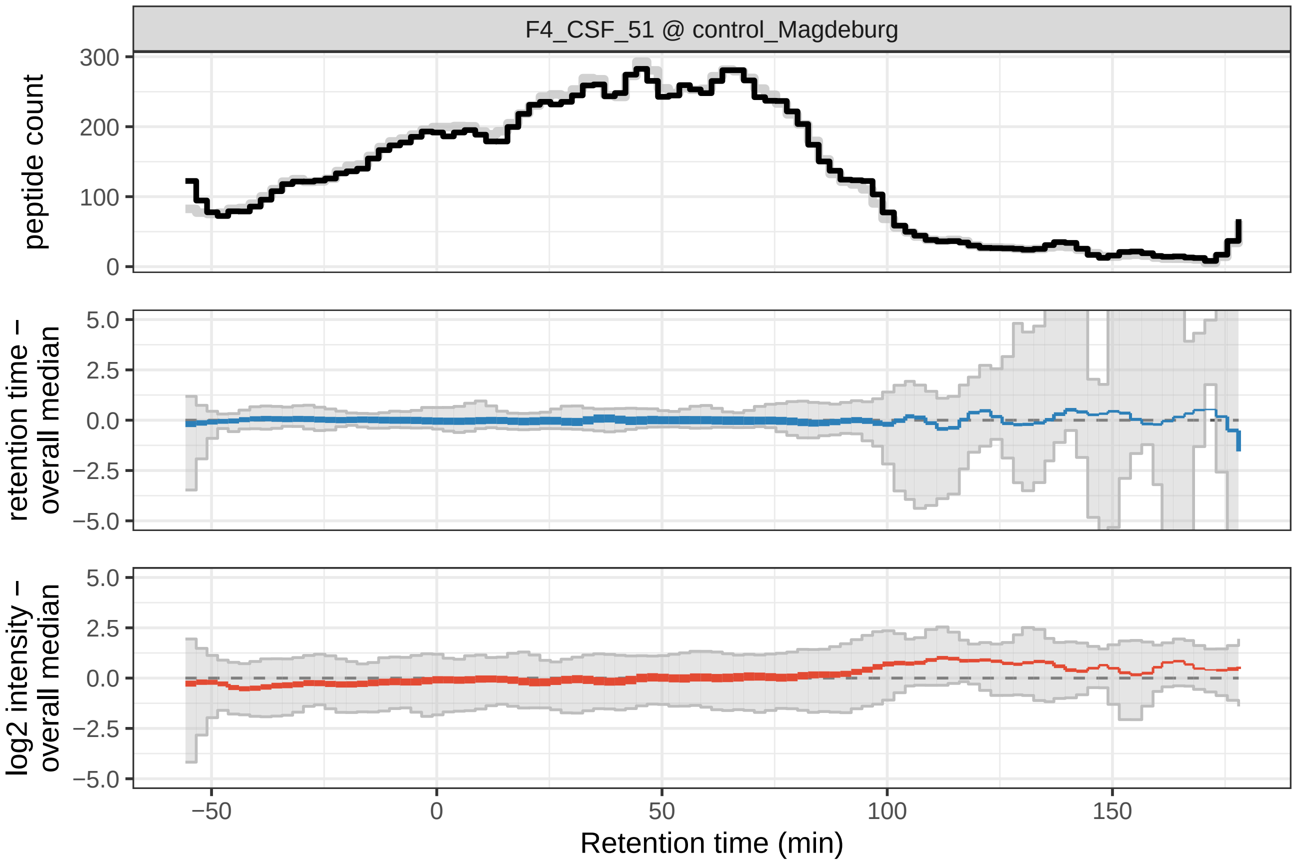

E10_CSF_16 @ control_Magdeburg >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

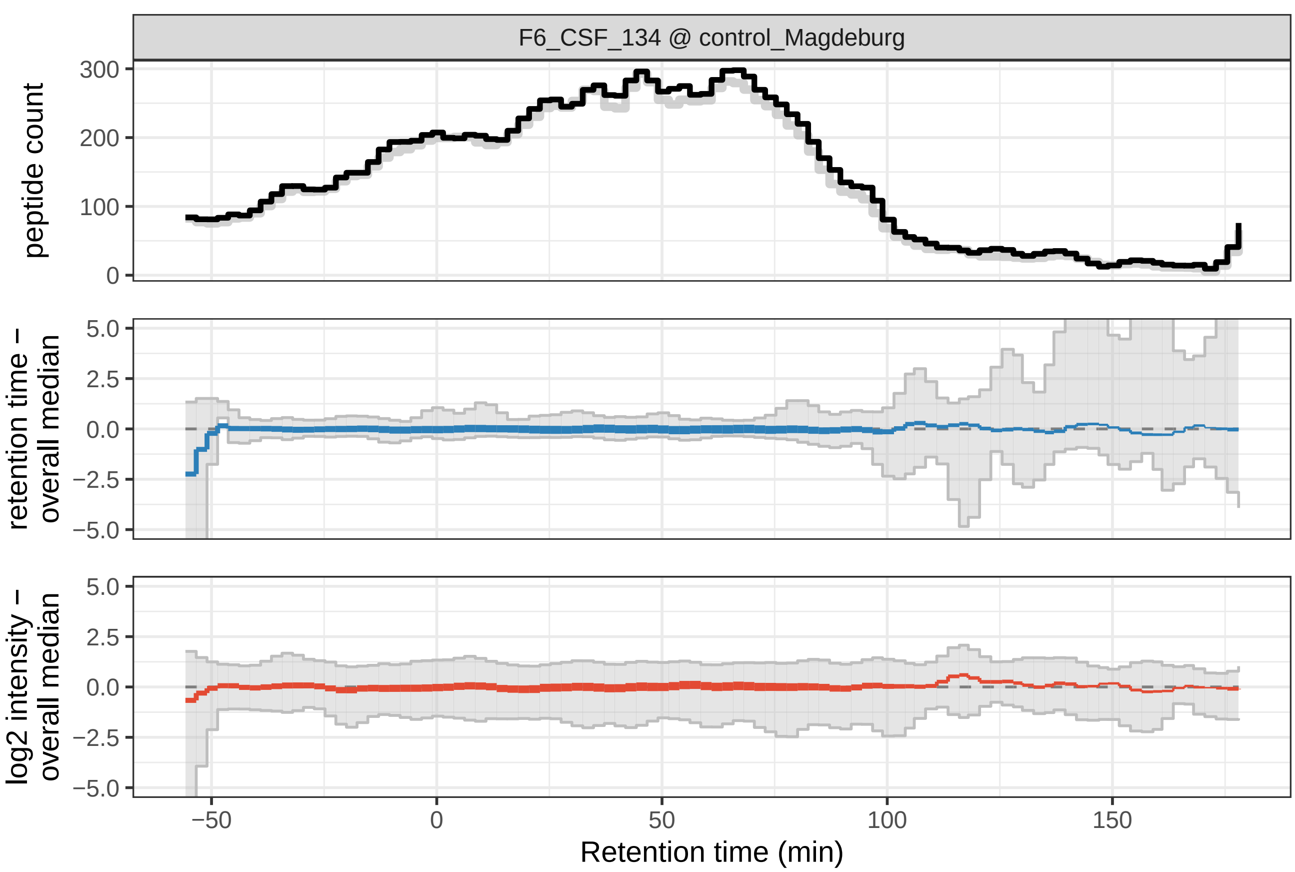

E11_CSF_783 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

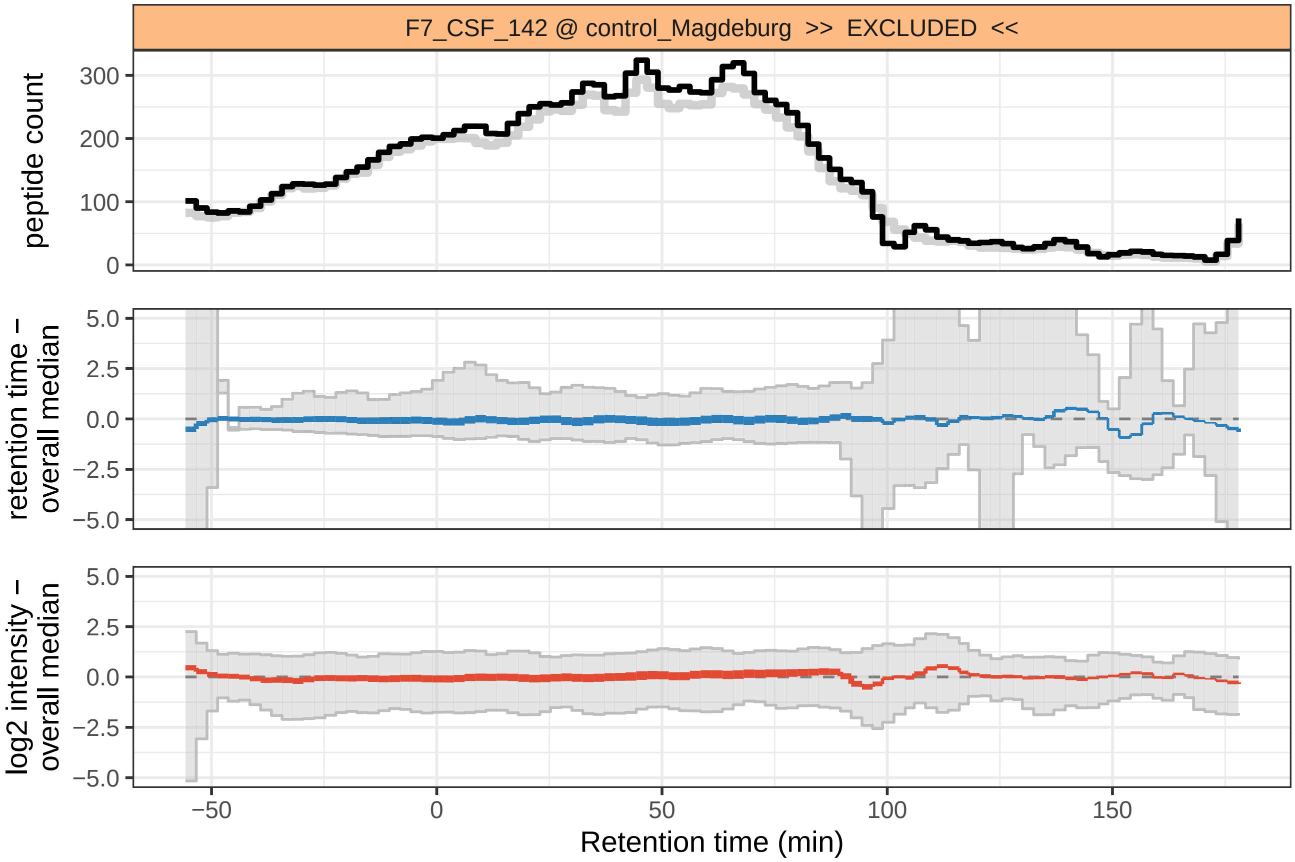

E12_CSF_146 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

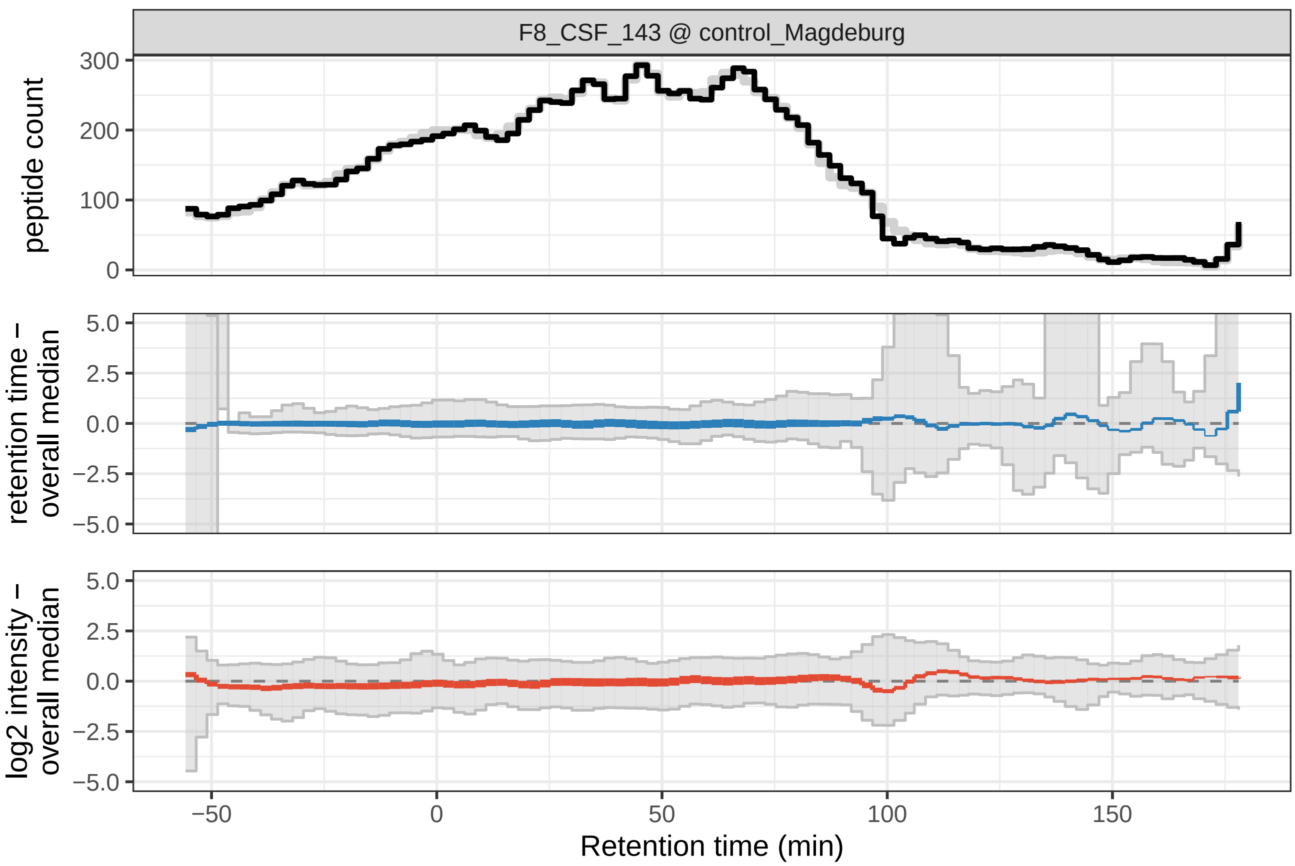

F2_CSF_755 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

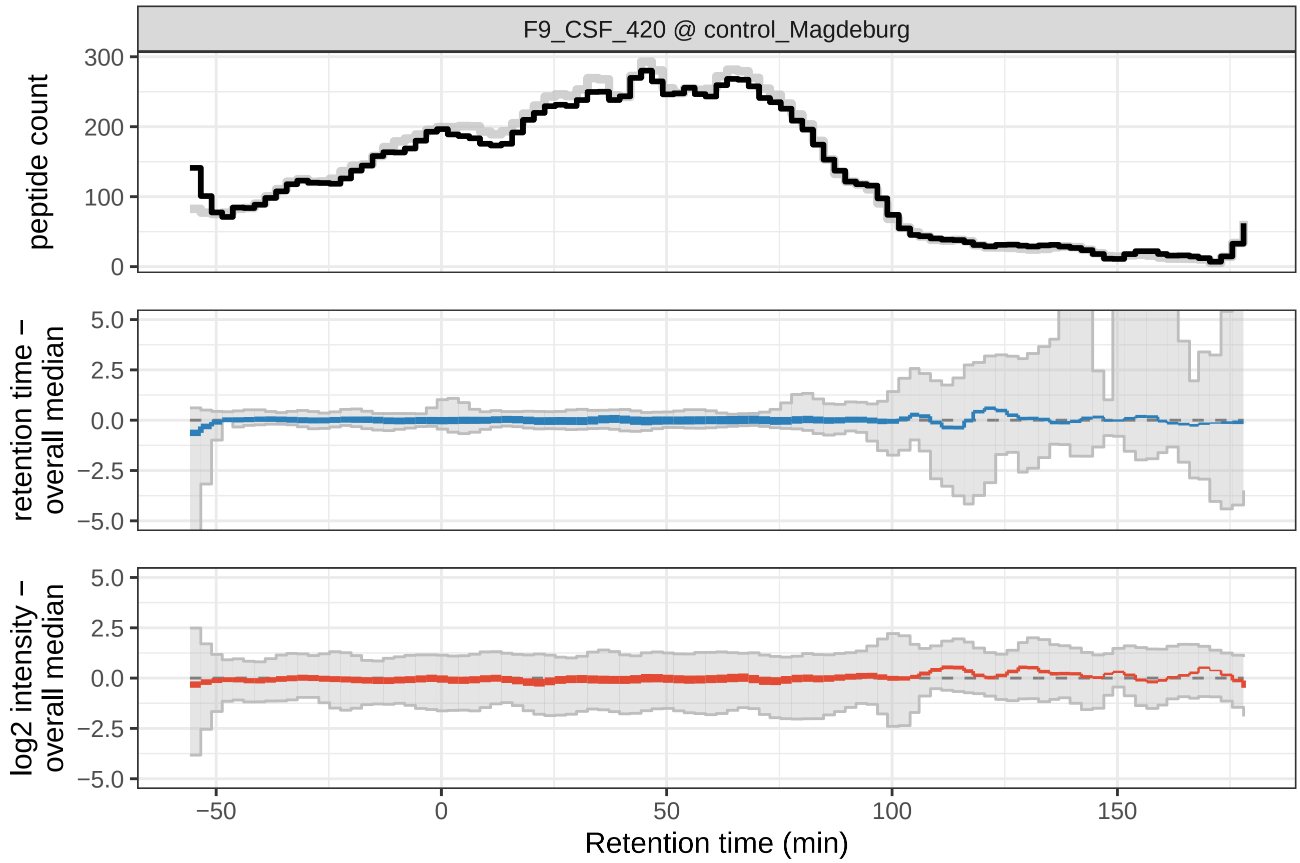

F3_CSF_865 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

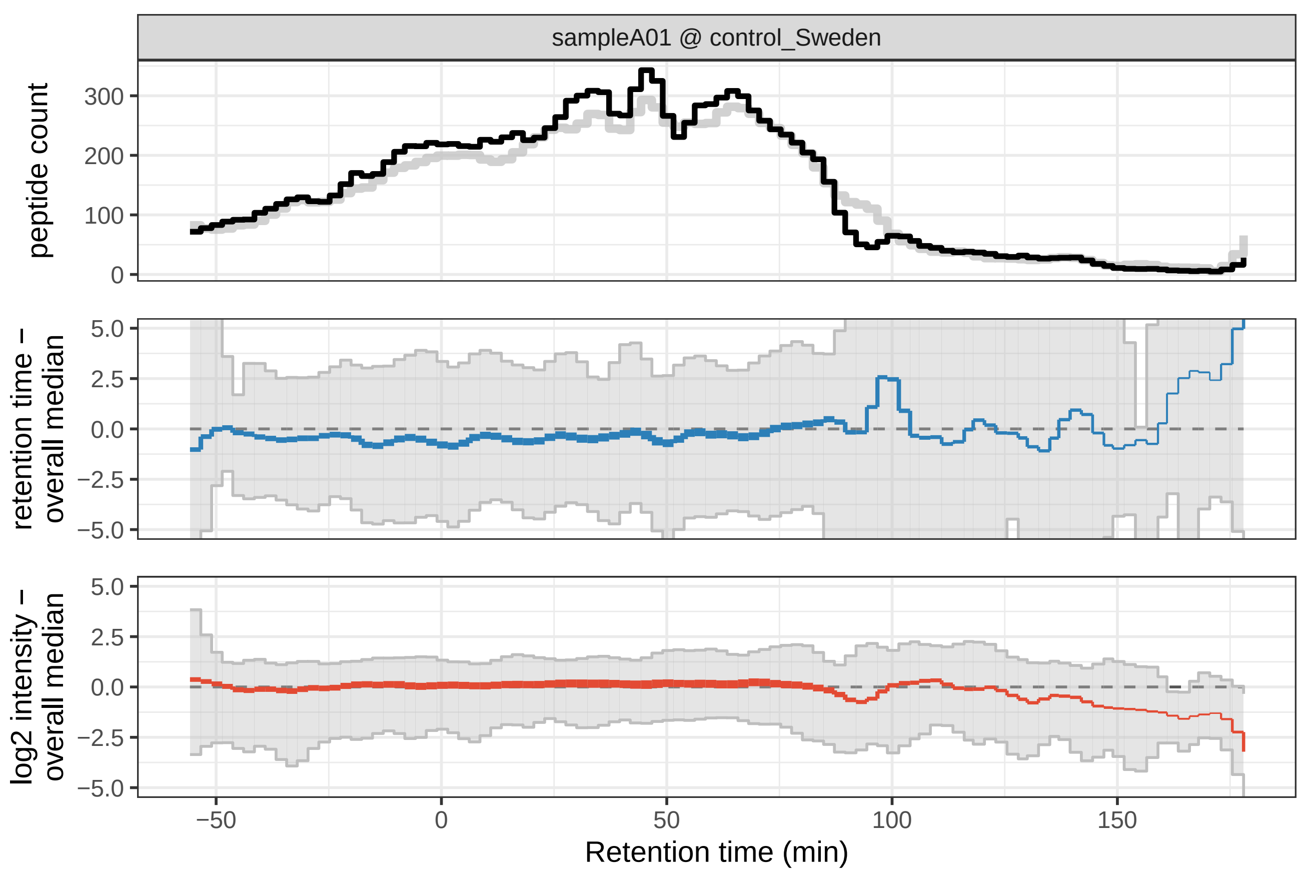

F4_CSF_51 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

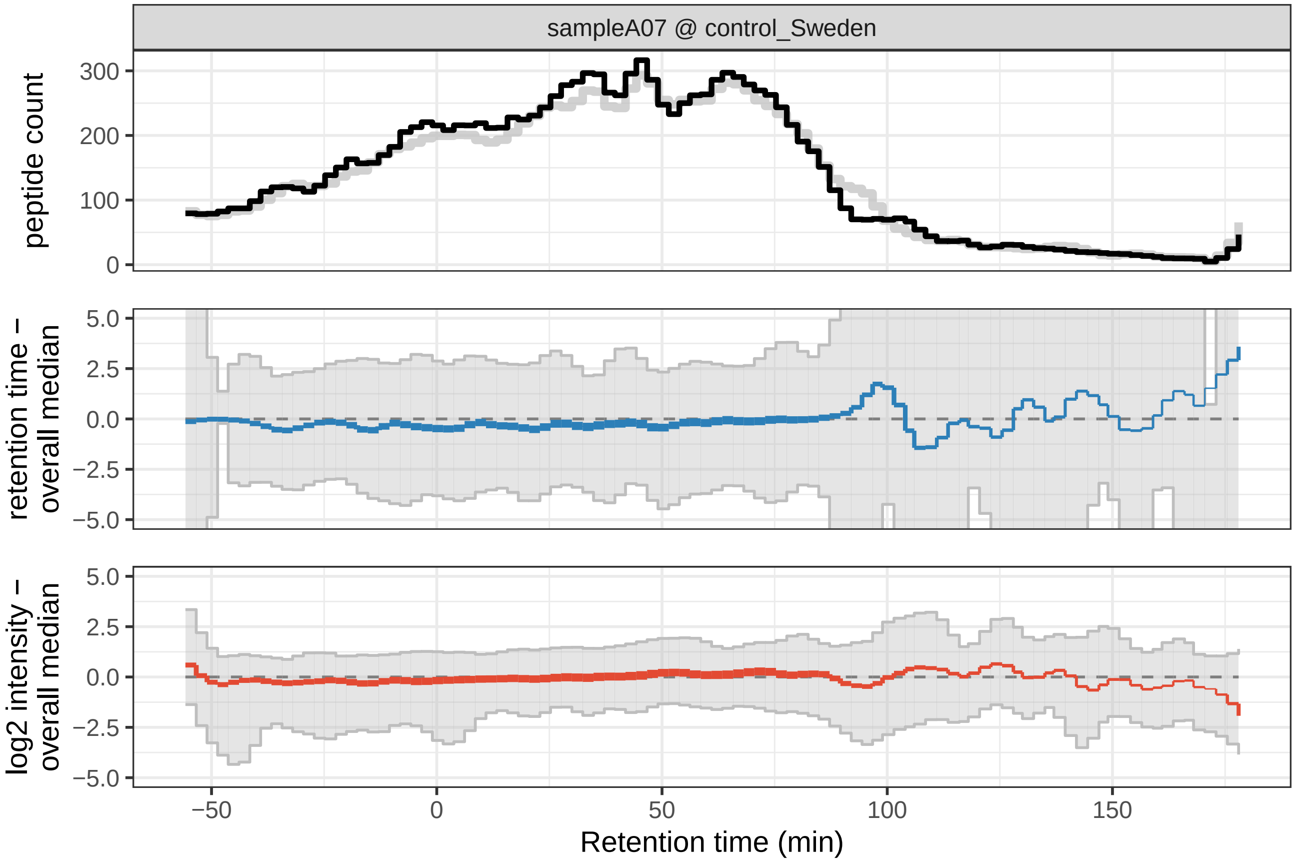

F6_CSF_134 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

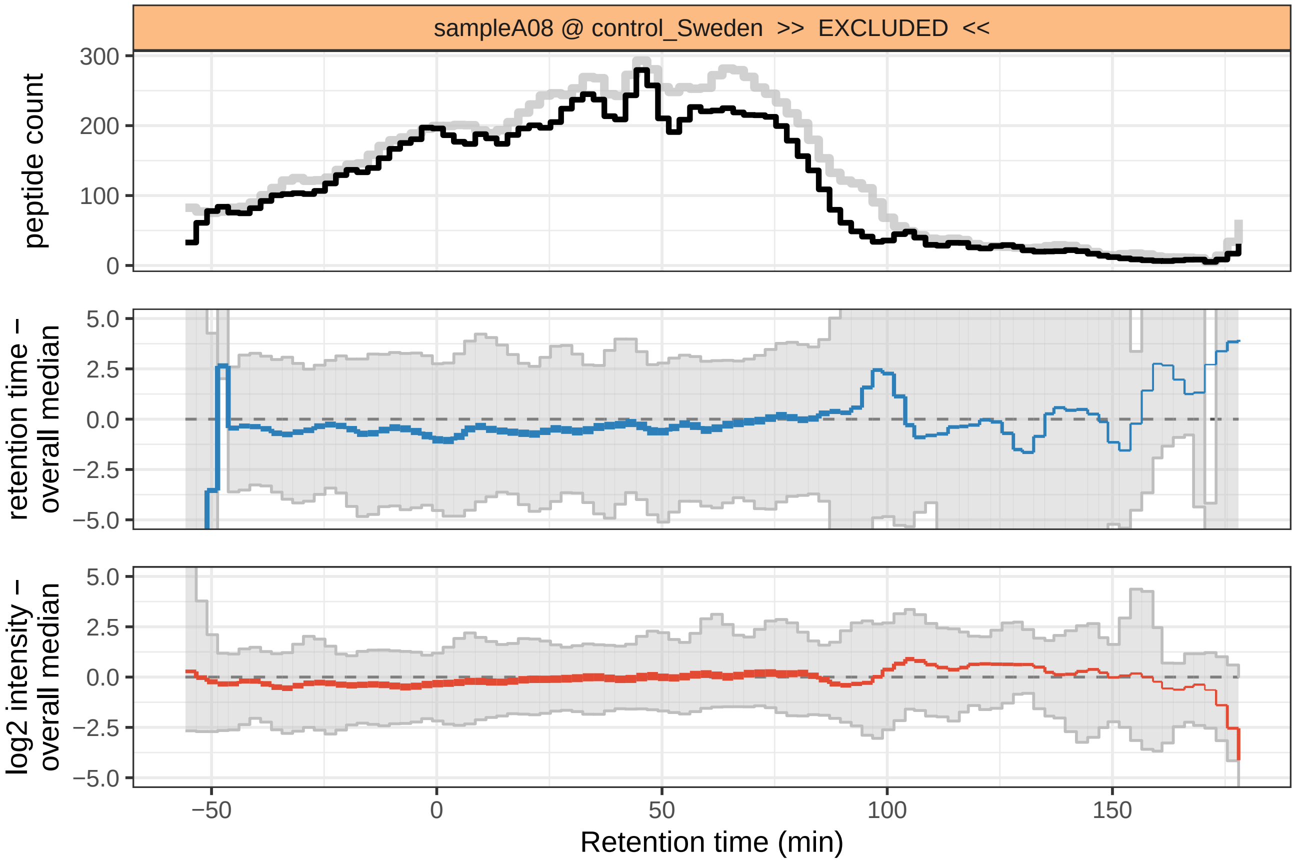

F7_CSF_142 @ control_Magdeburg >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

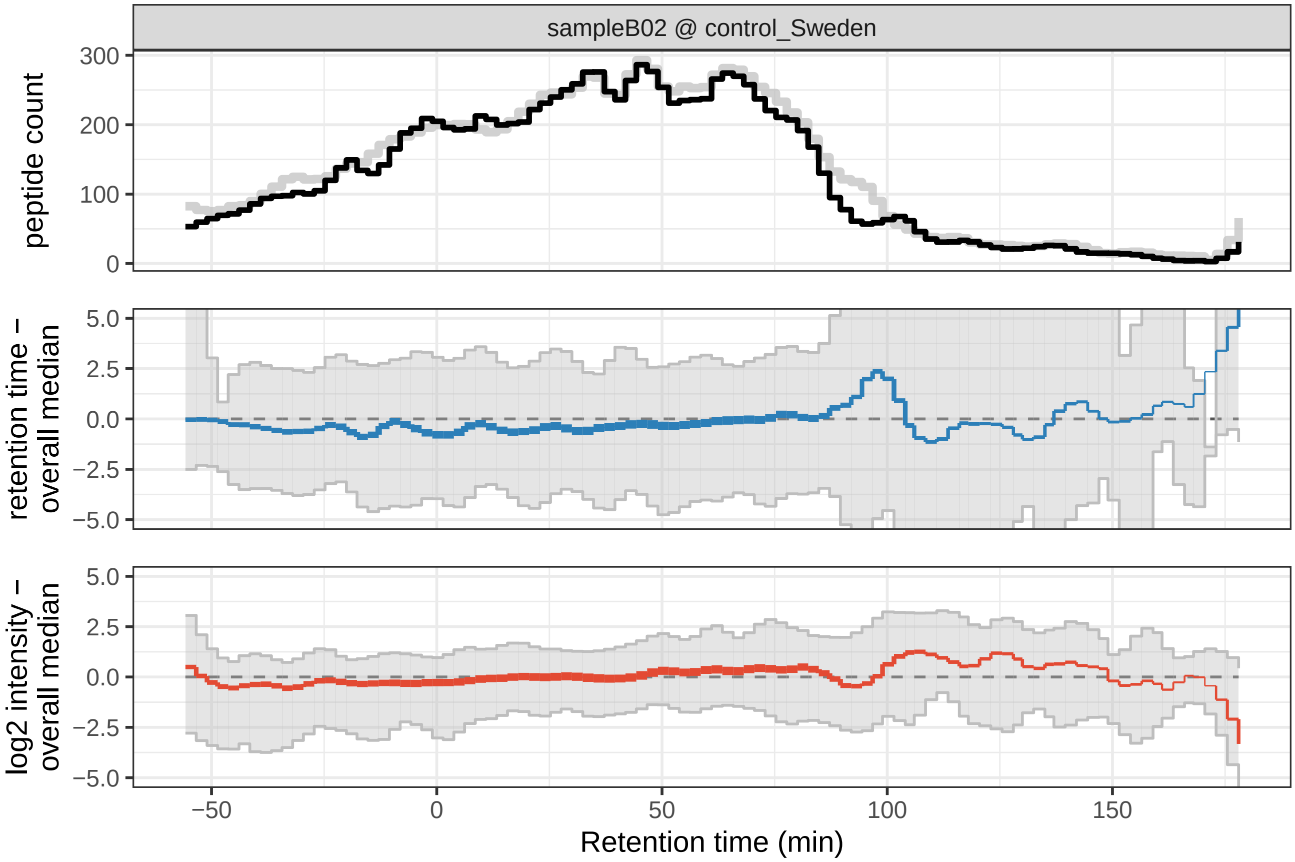

F8_CSF_143 @ control_Magdeburg
peptide count
retention time – overall median
log2 intensity – overall median
300
200
100
0
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

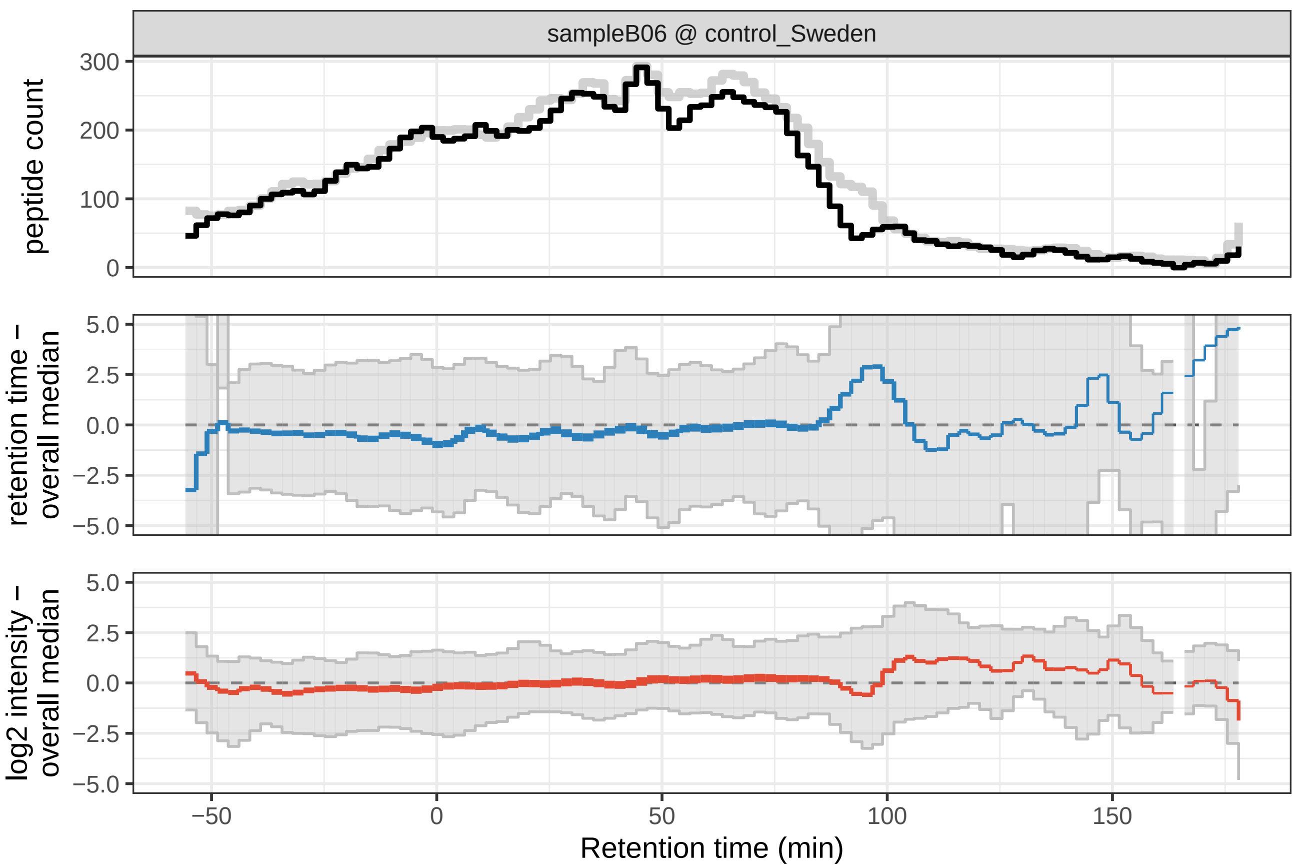

F9_CSF_420 @ control_Magdeburg
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

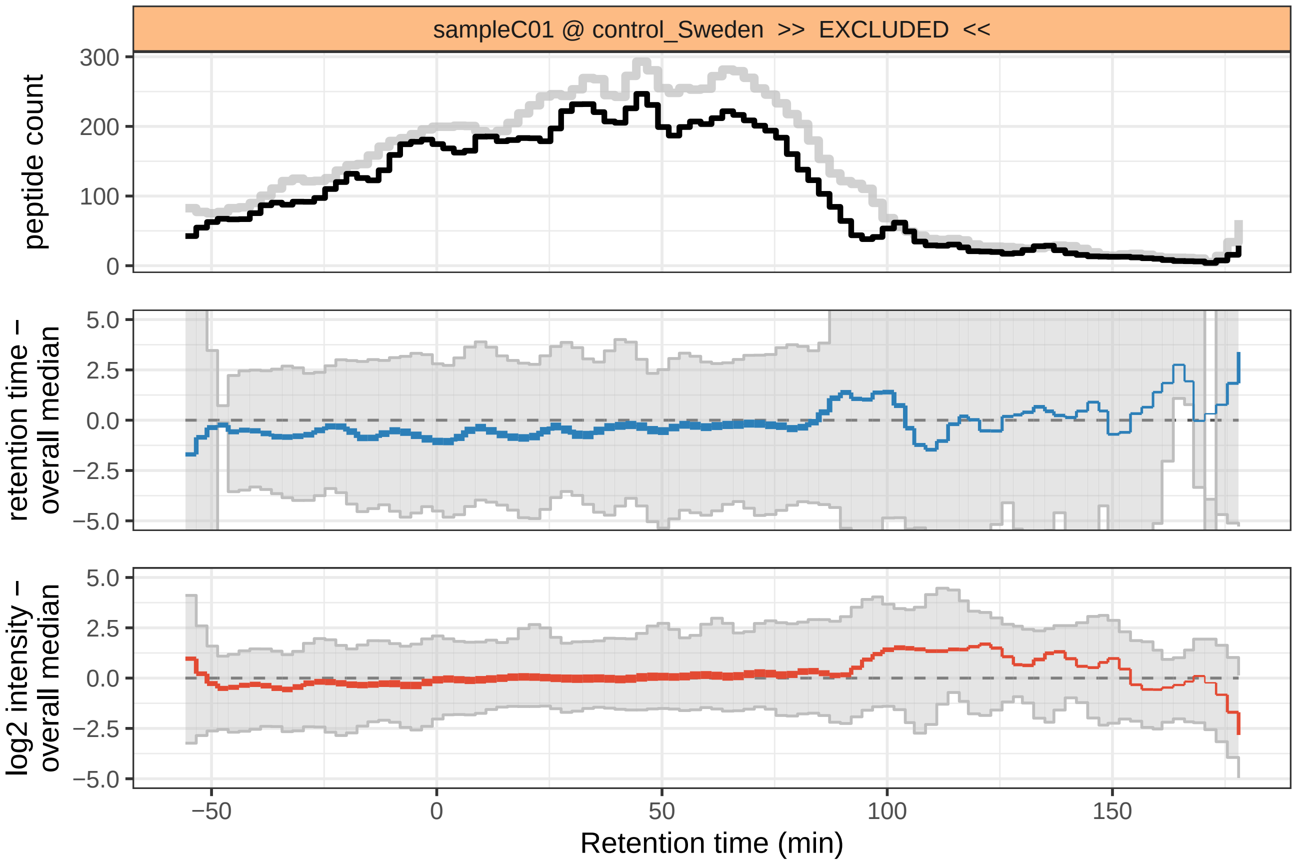

sampleA01 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleA07 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

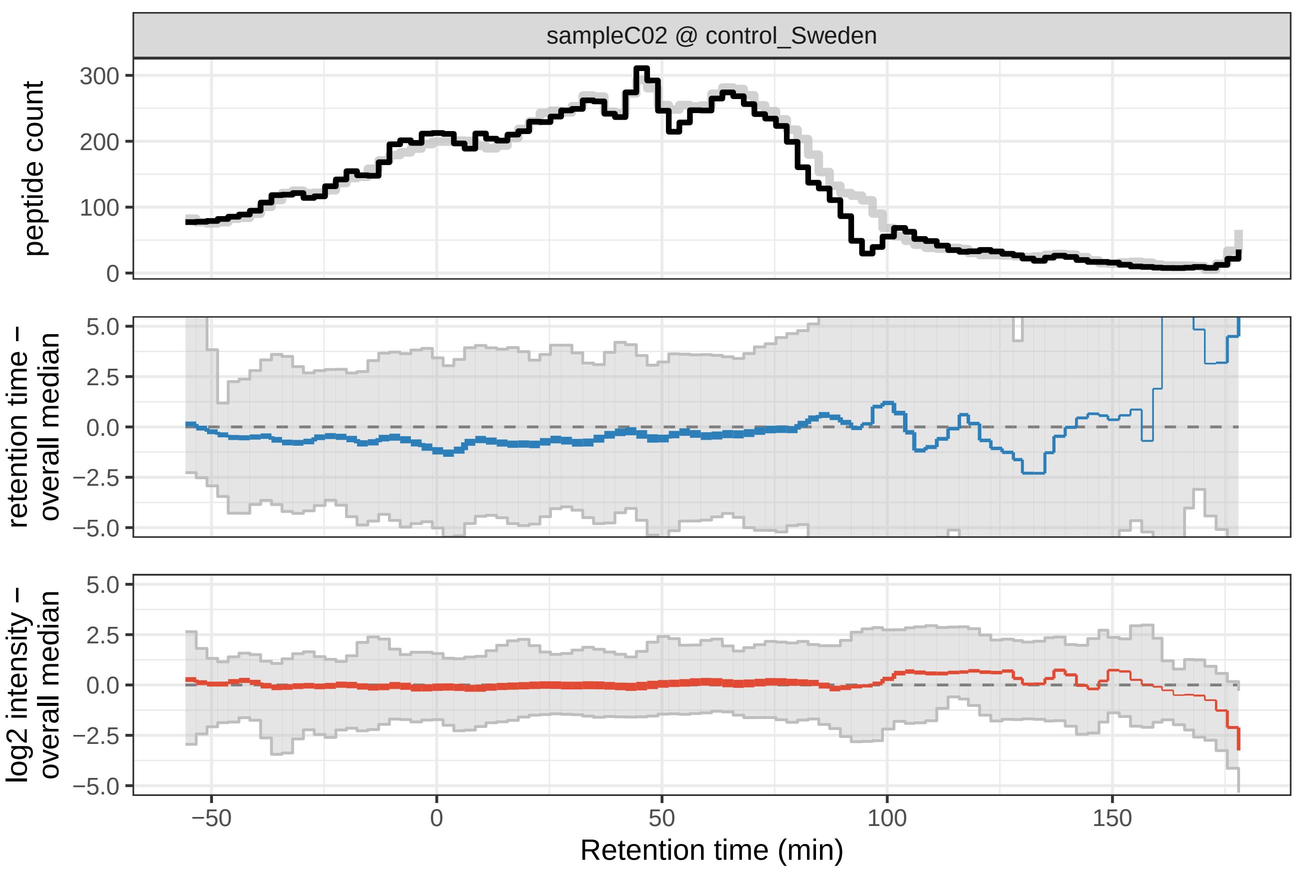

sampleA08 @ control_Sweden >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


sampleB02 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

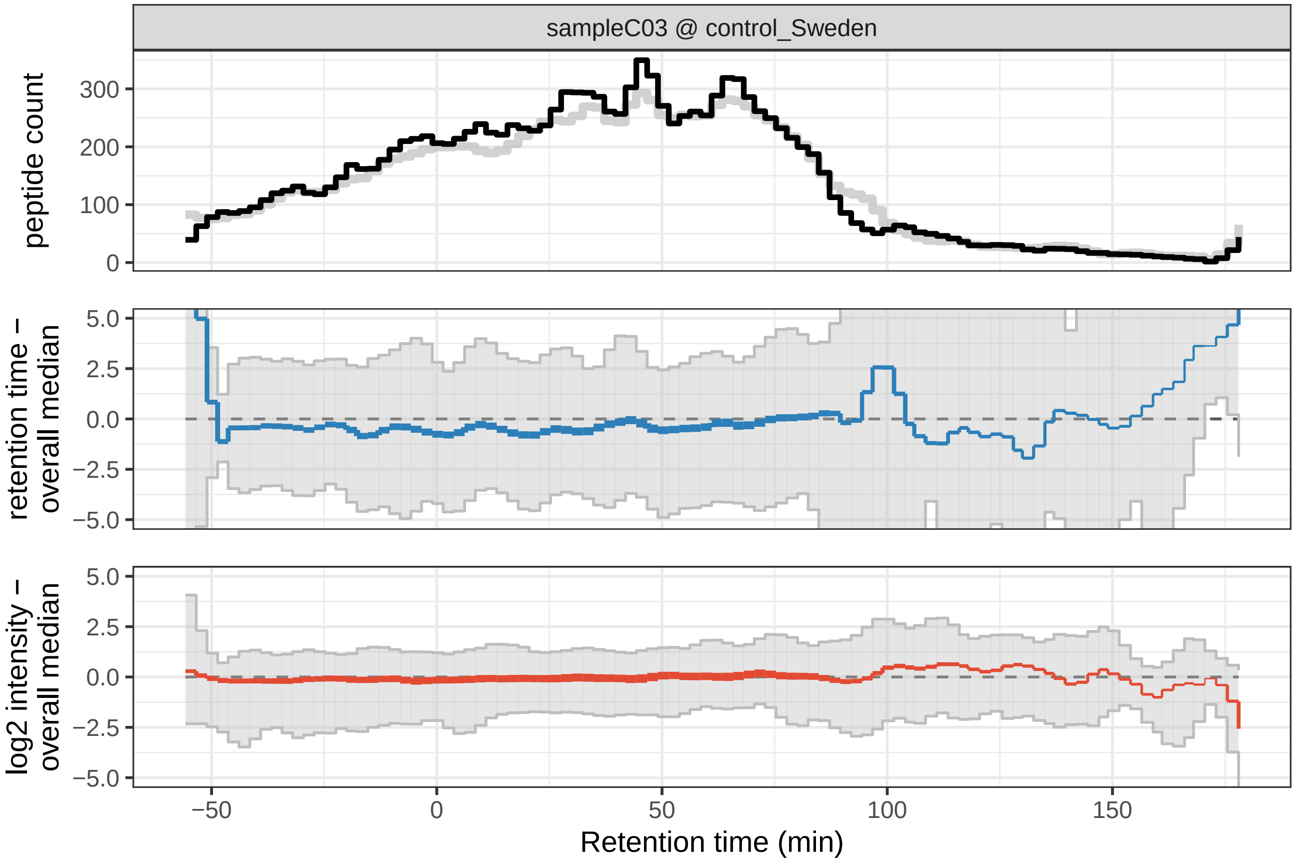

sampleB06 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

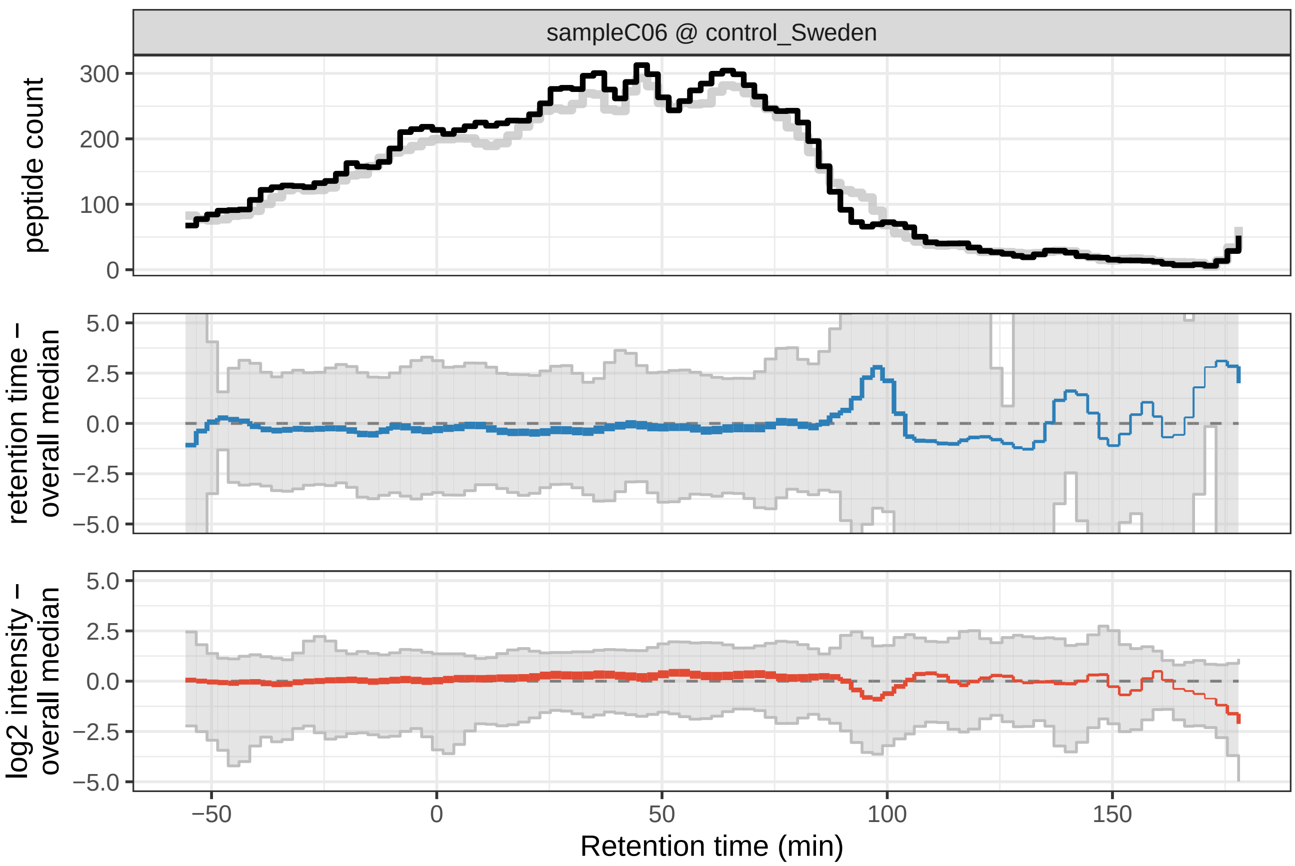


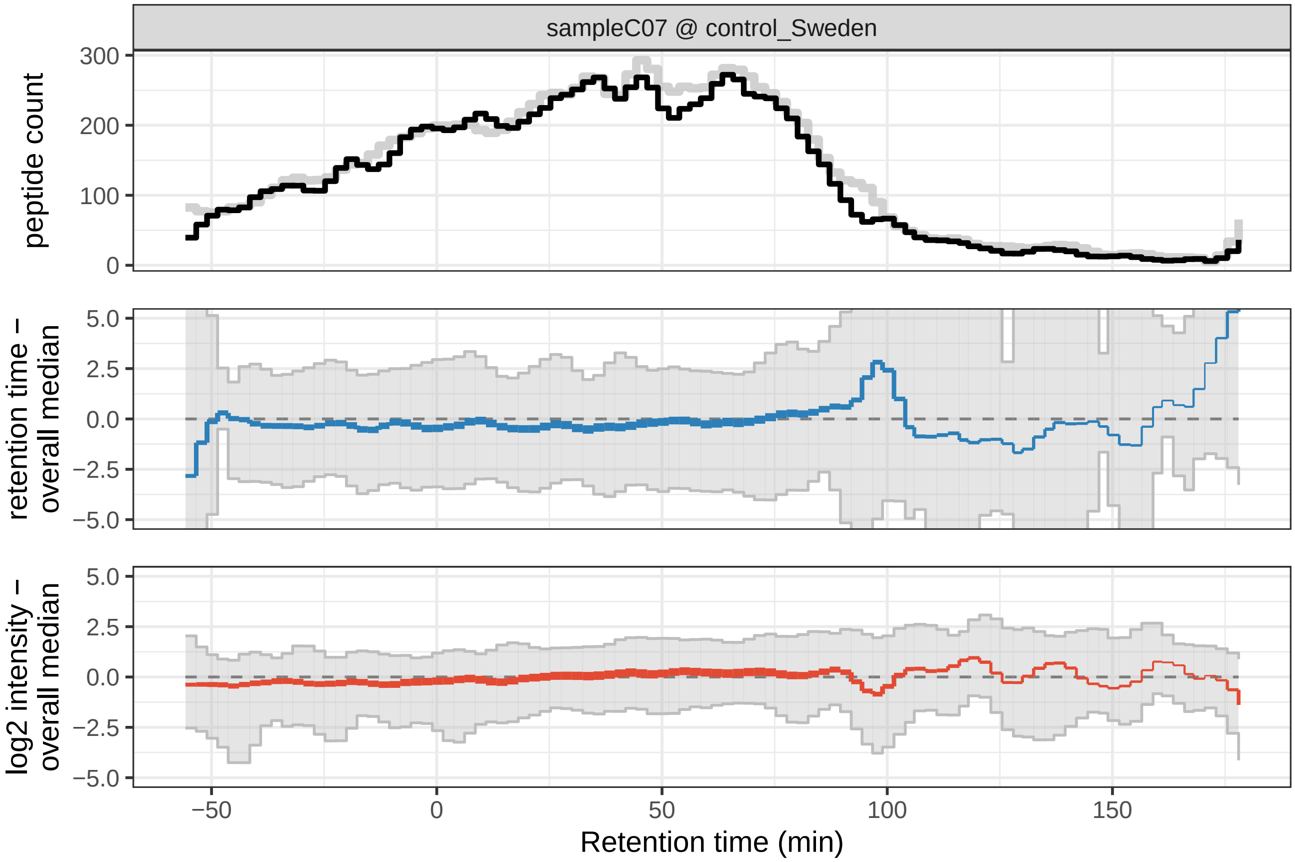
sampleC01 @ control_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

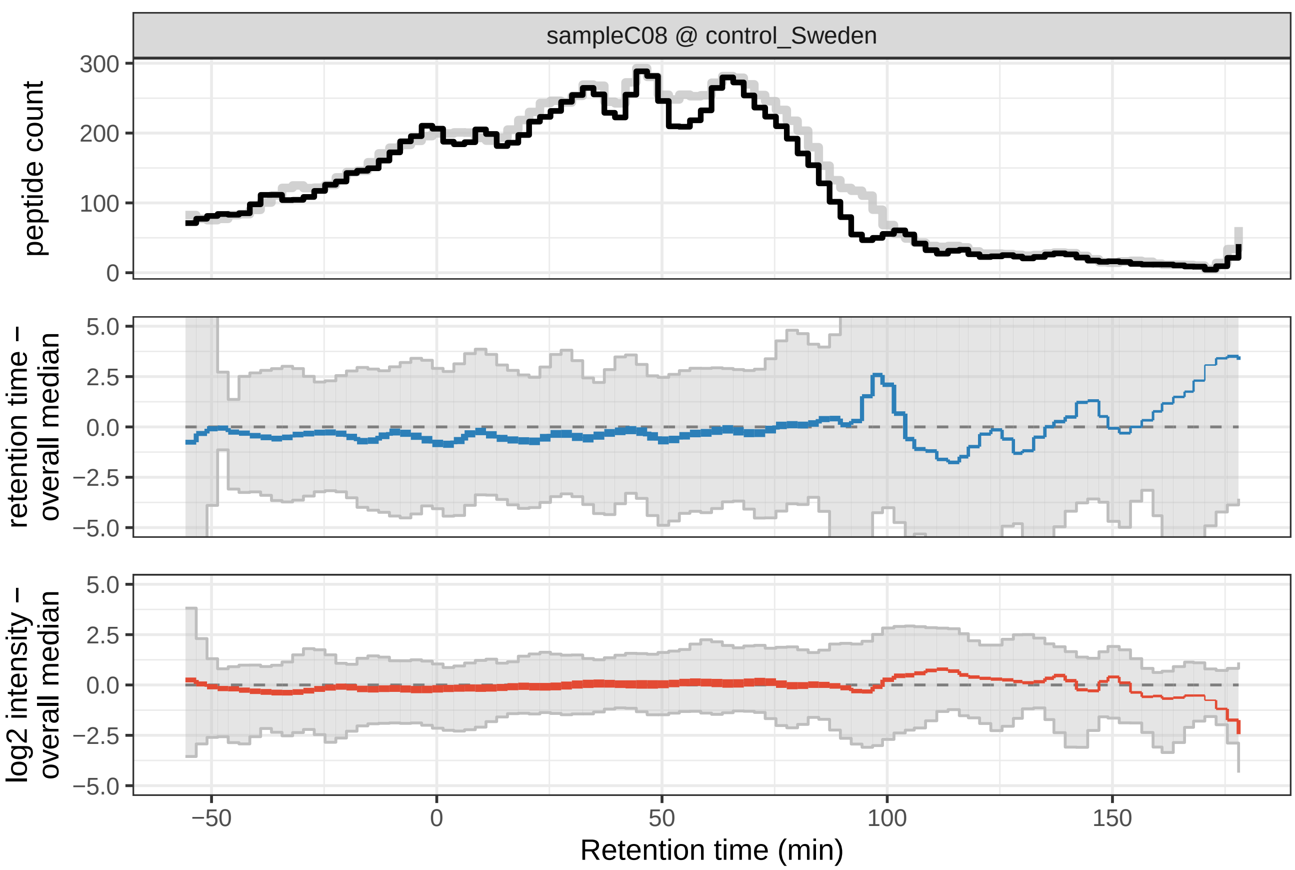


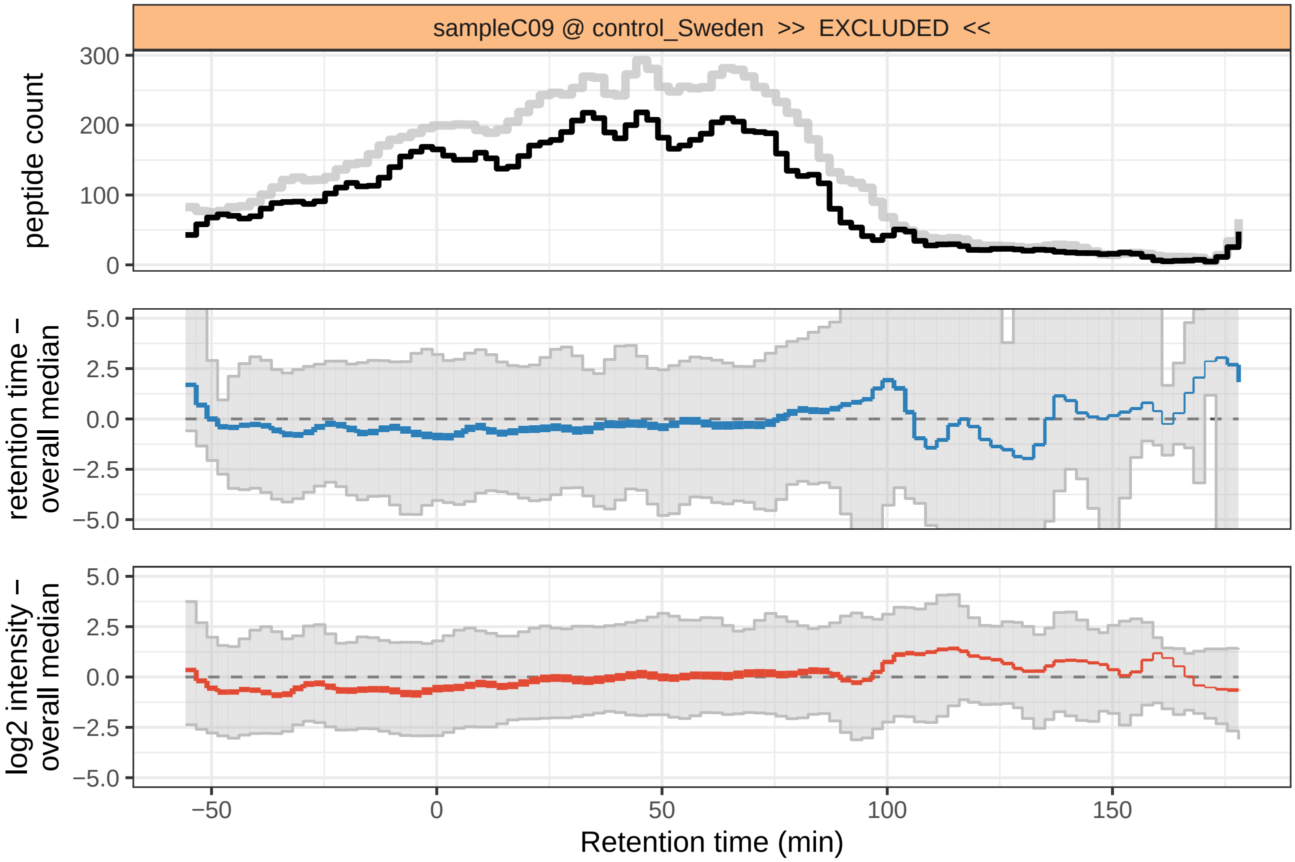
sampleC02 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

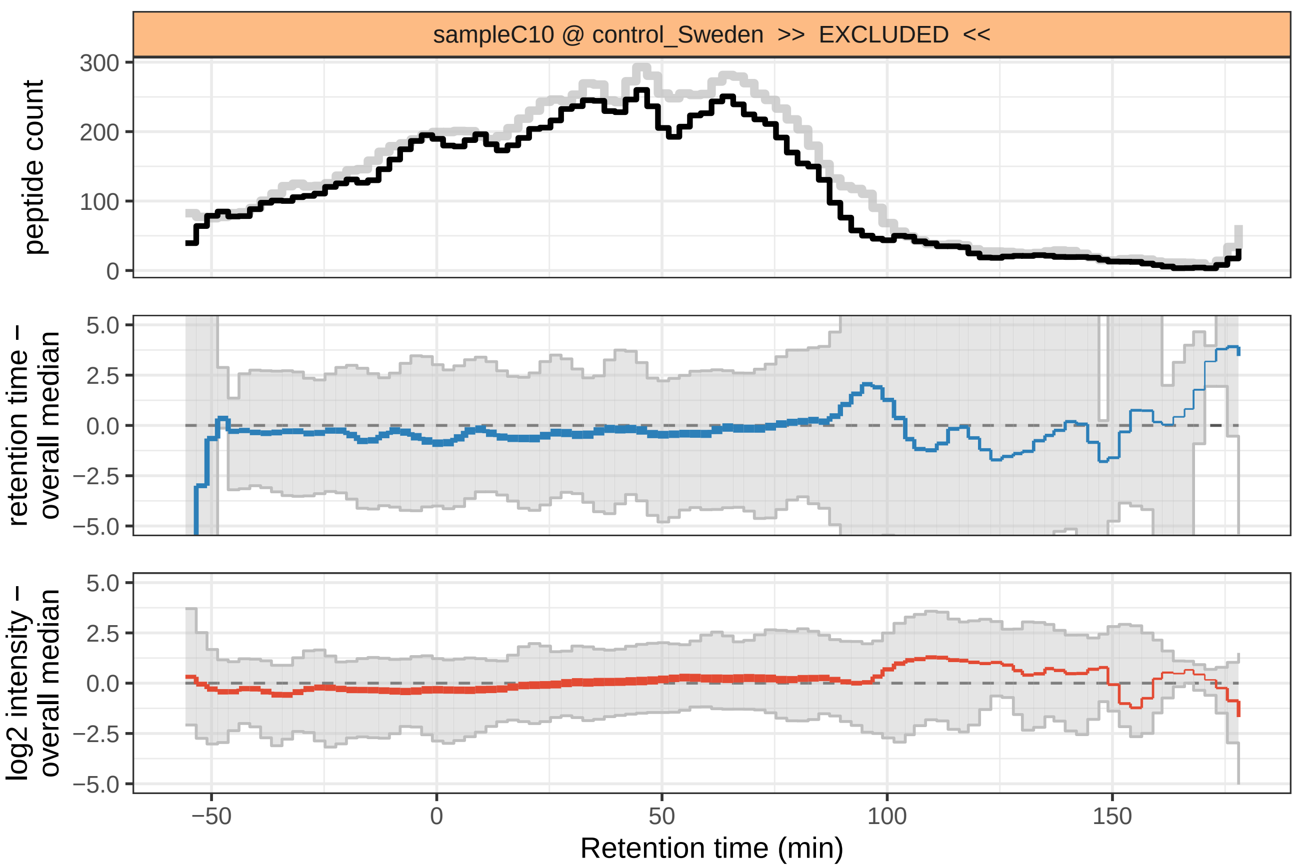

sampleC03 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

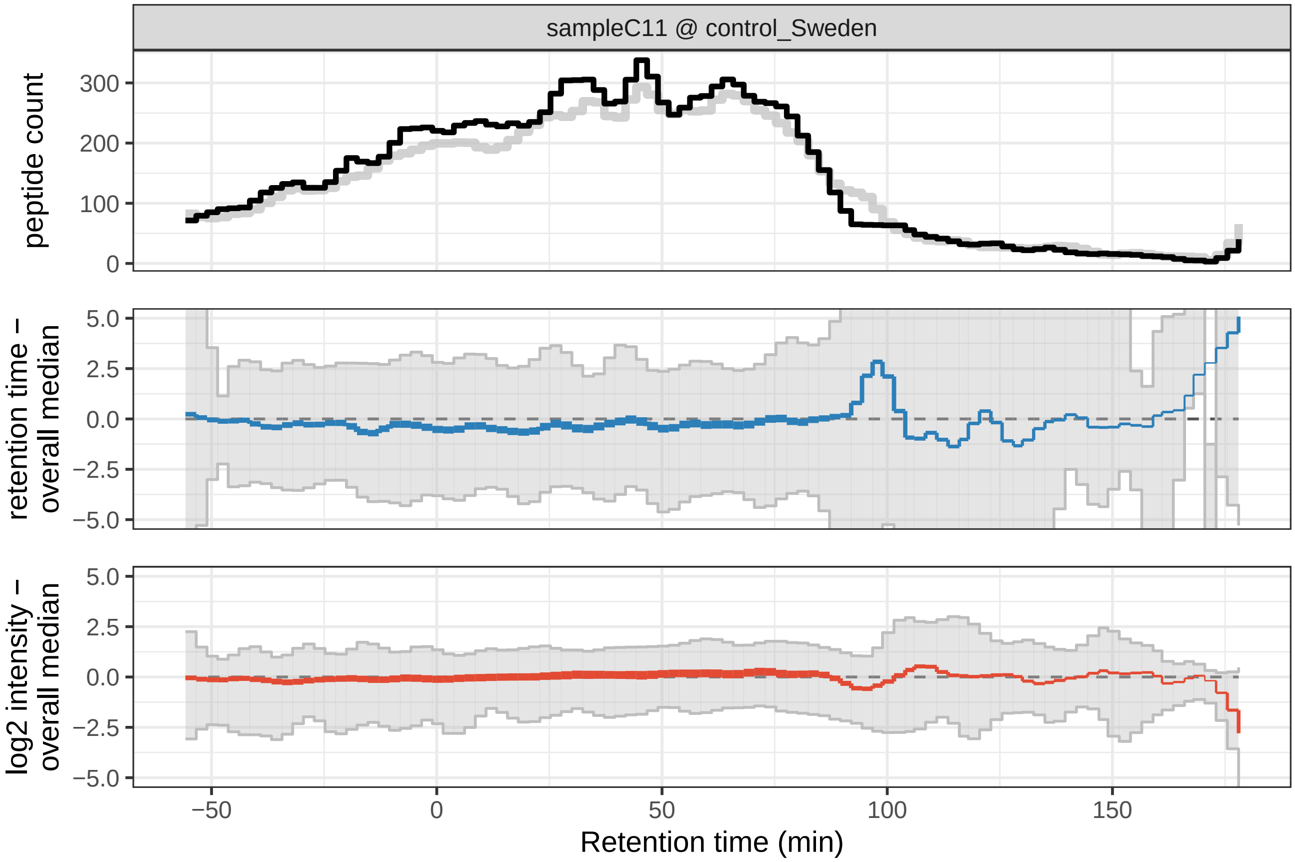

sampleC06 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

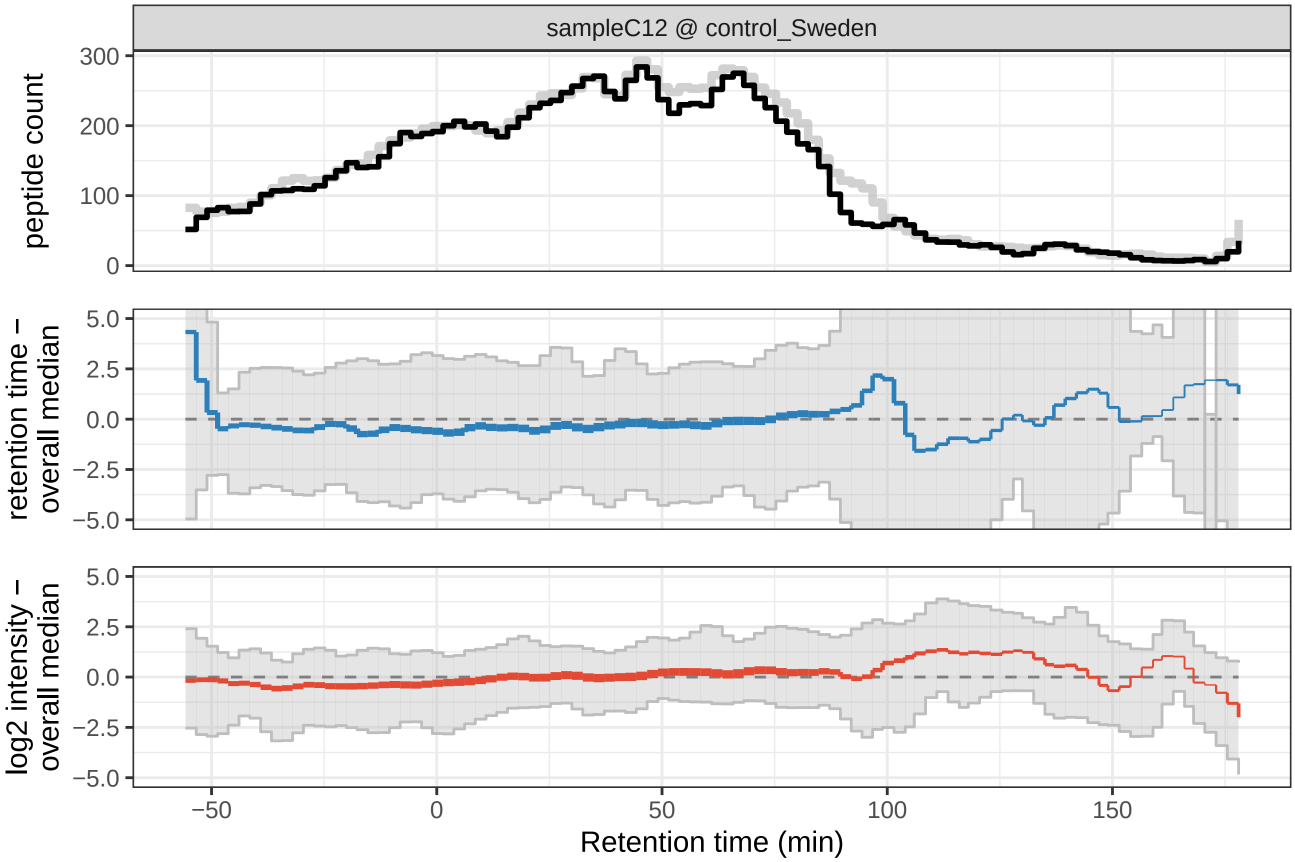

sampleC07 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

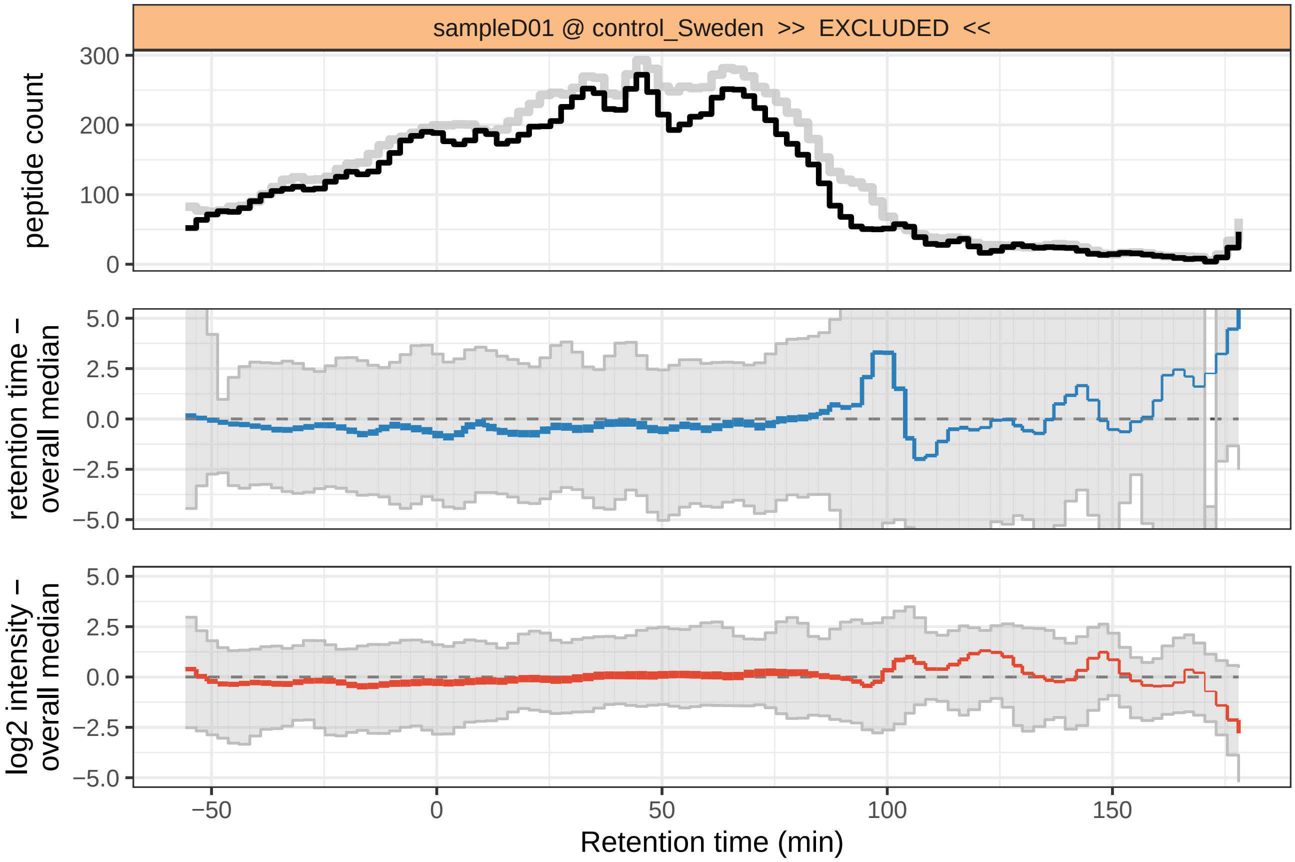

sampleC08 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

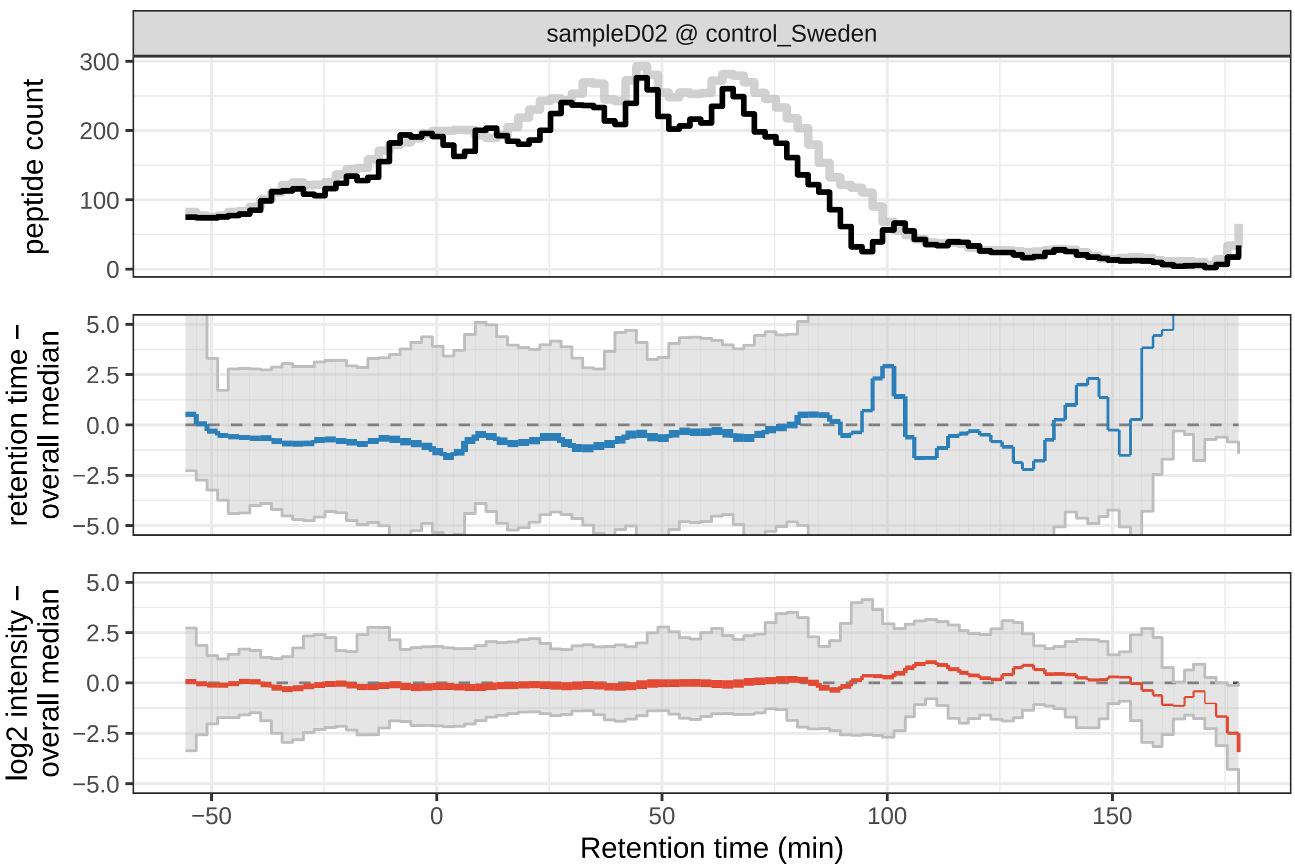

sampleC09 @ control_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

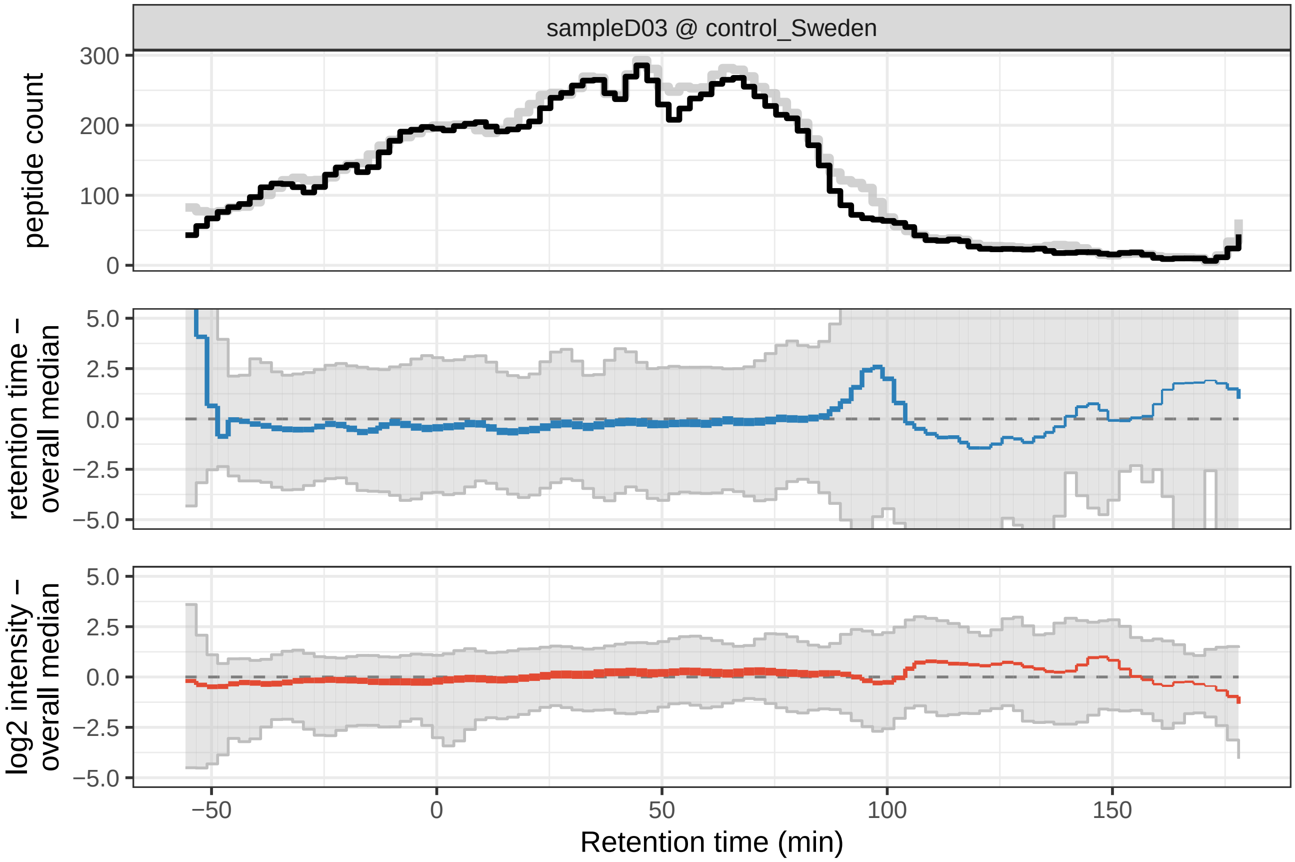

sampleC10 @ control_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

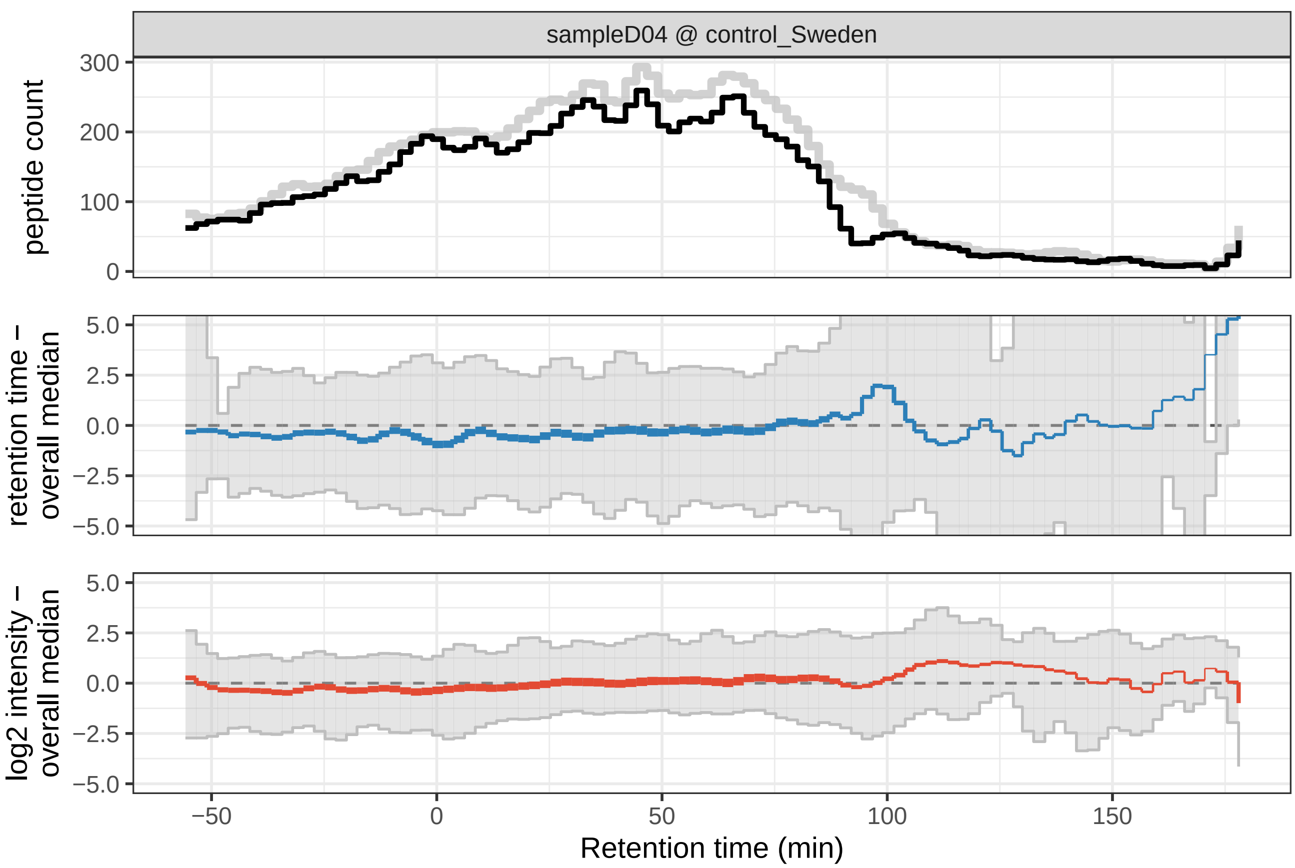

sampleC11 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

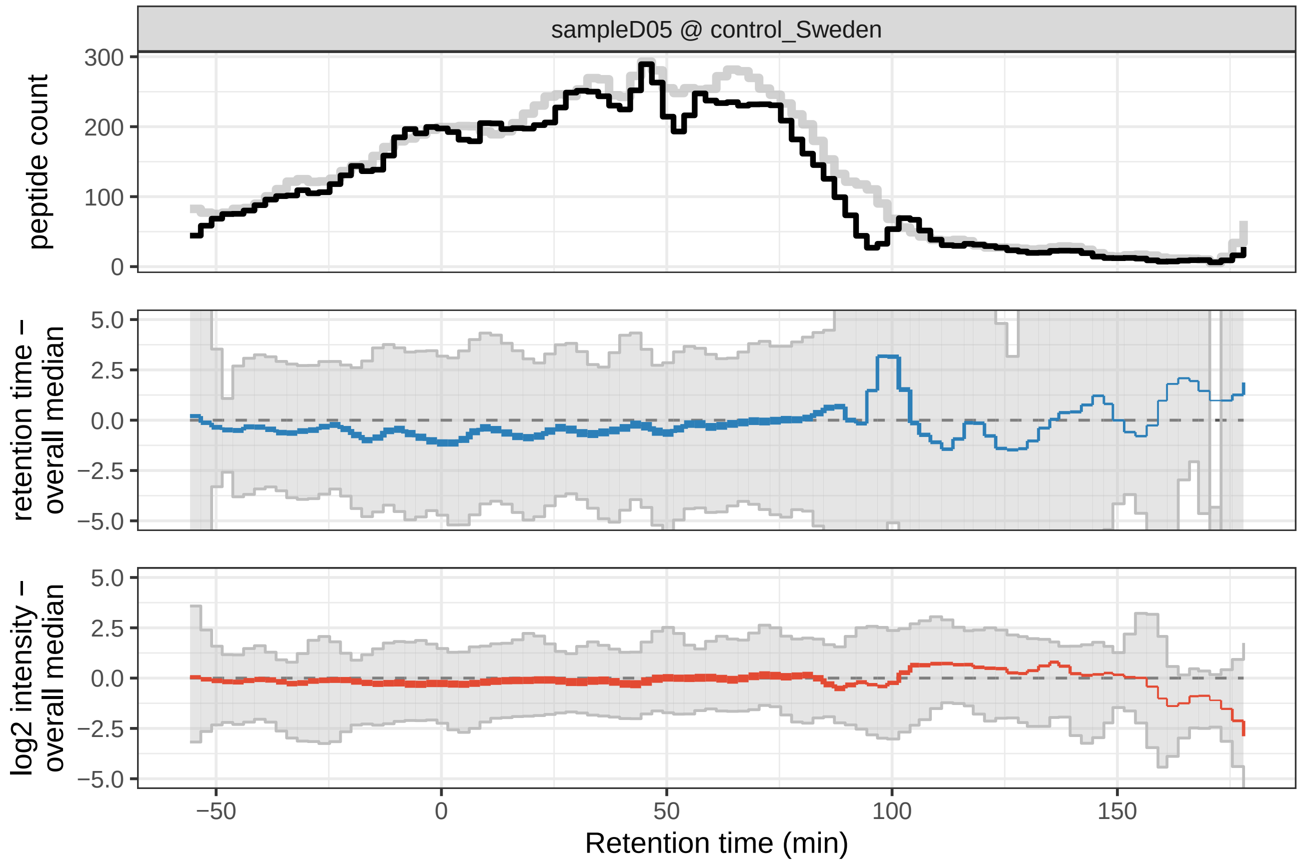

sampleC12 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

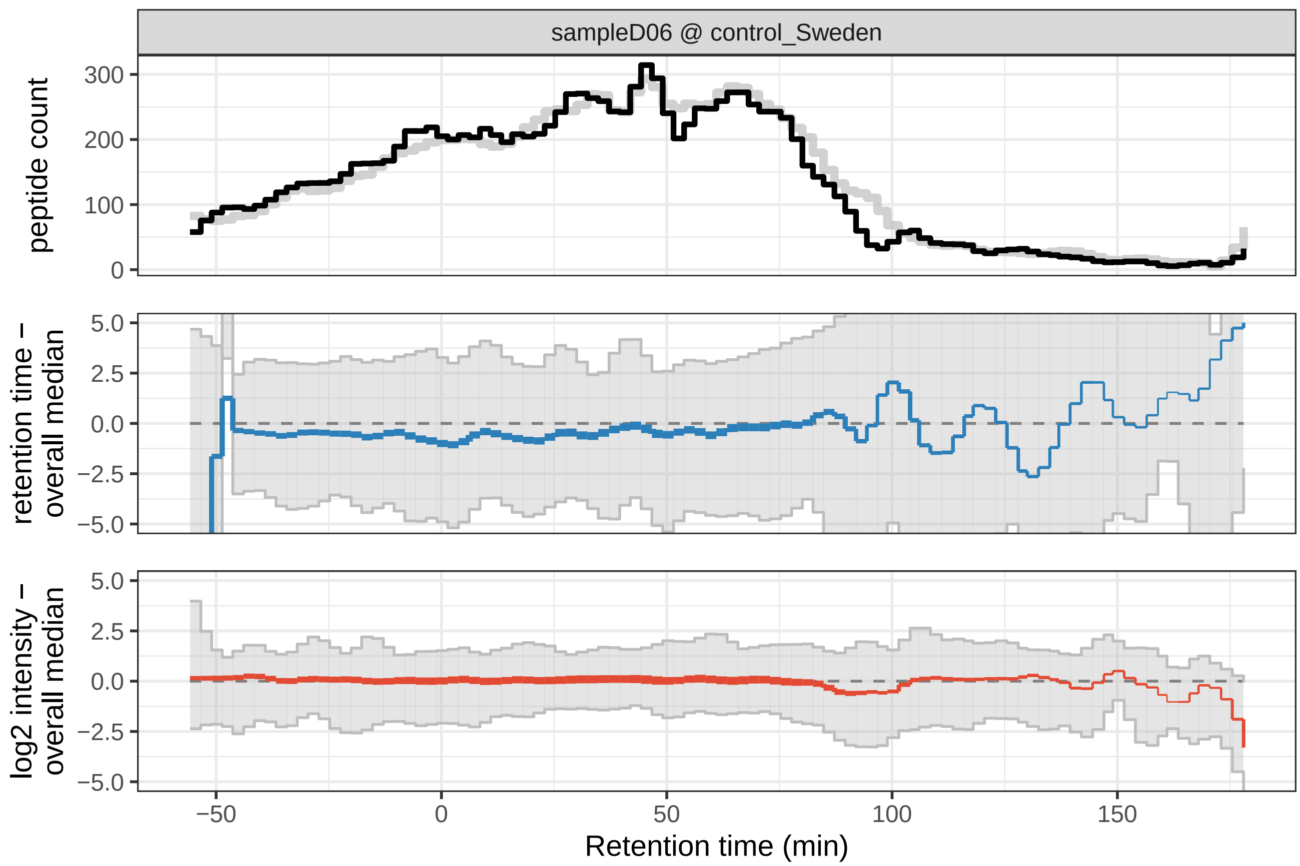

sampleD01 @ control_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

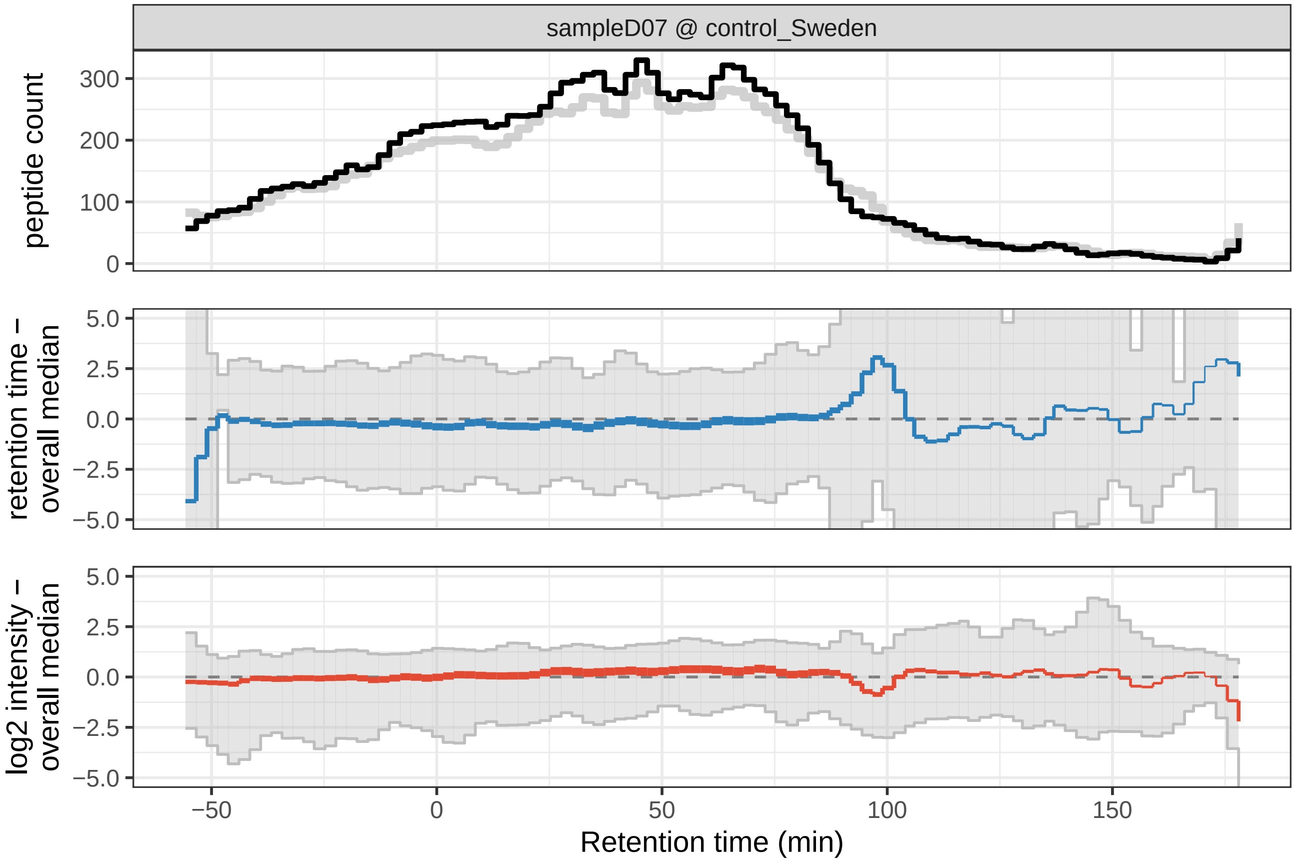

sampleD02 @ control_Sweden
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

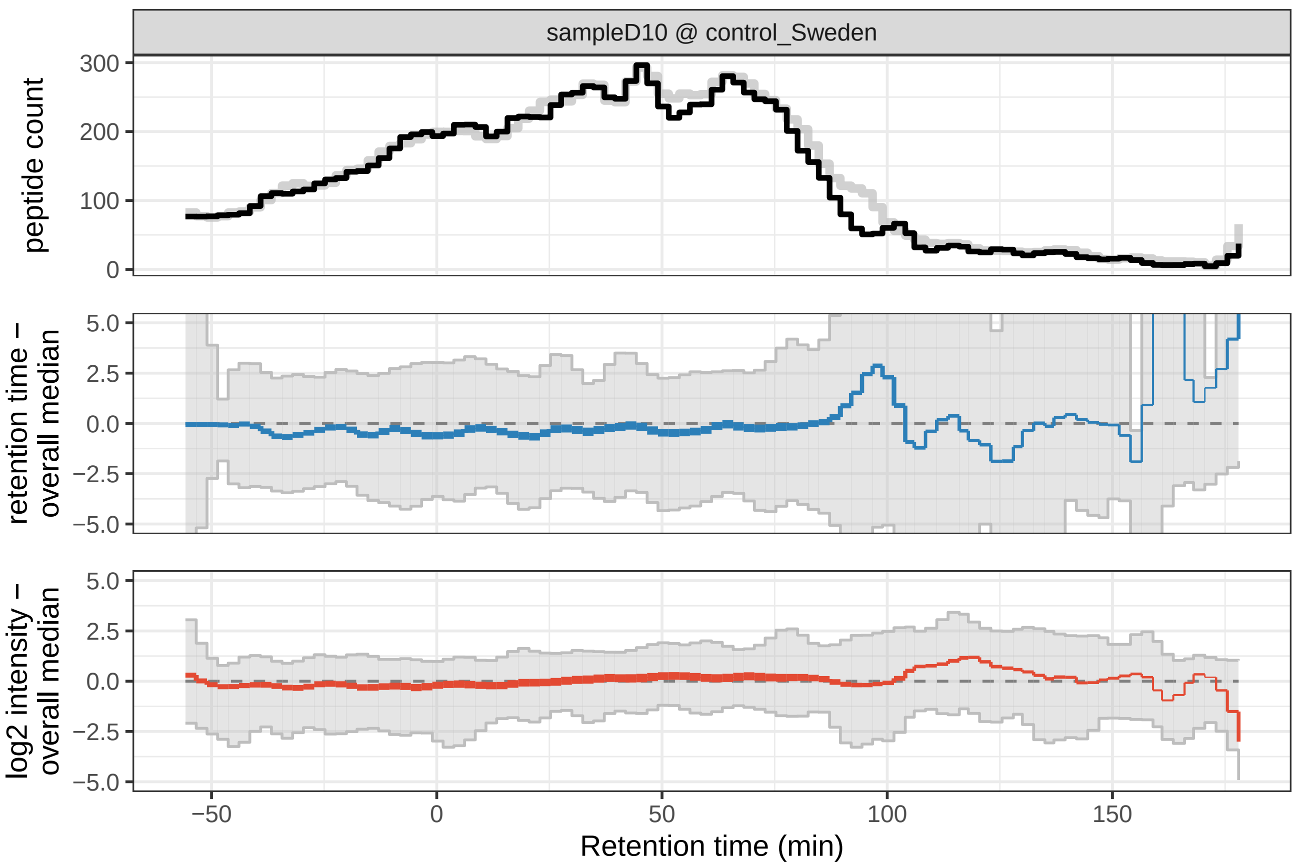

sampleD03 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

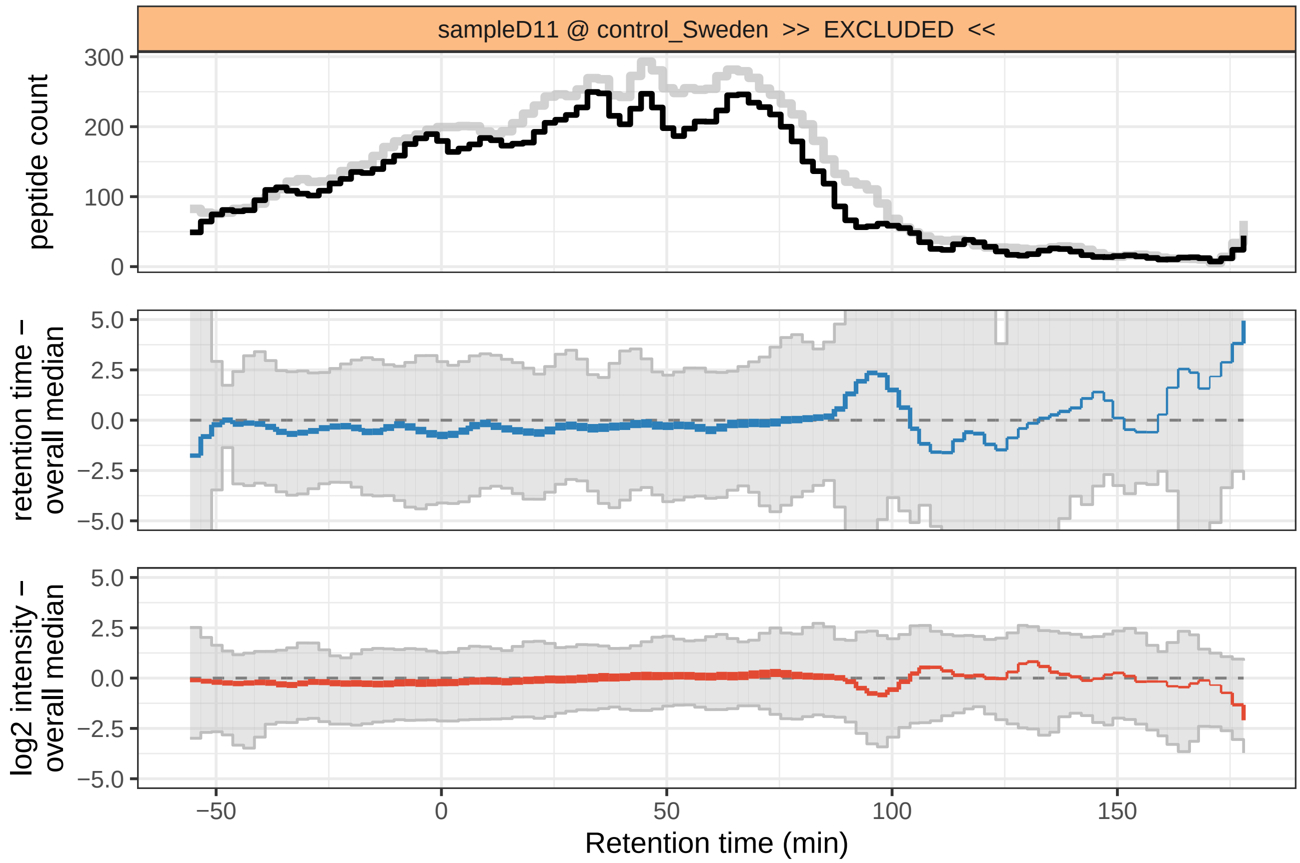

sampleD04 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

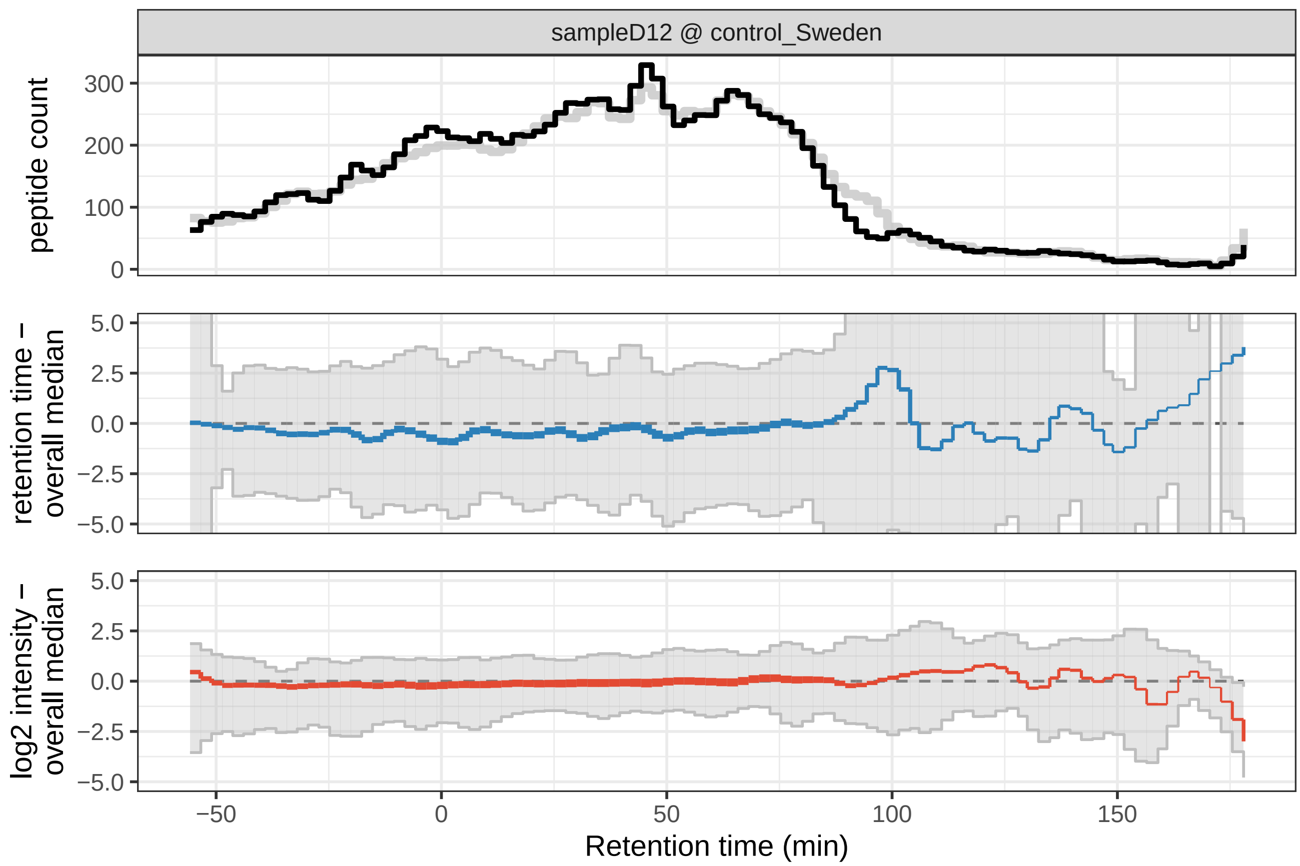

sampleD05 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

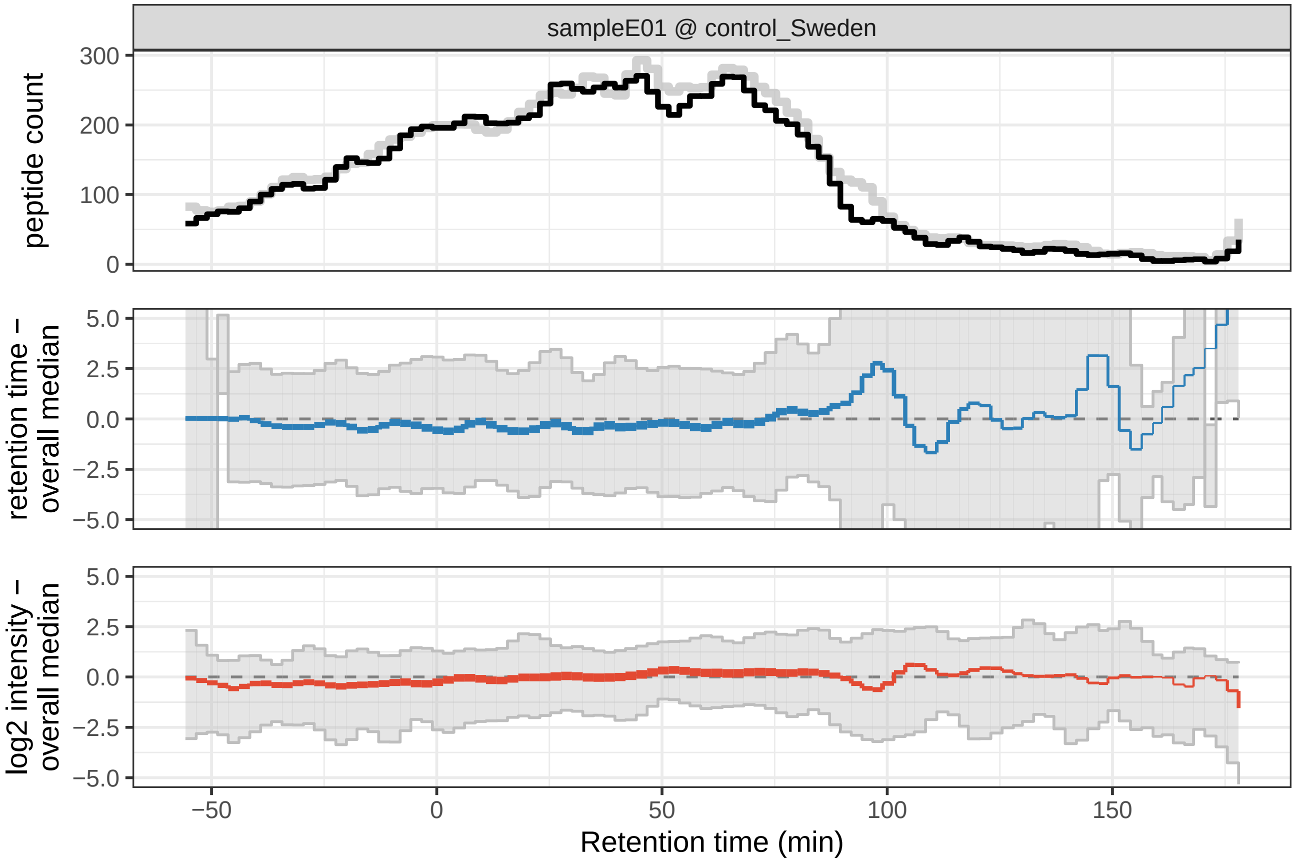

sampleD06 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

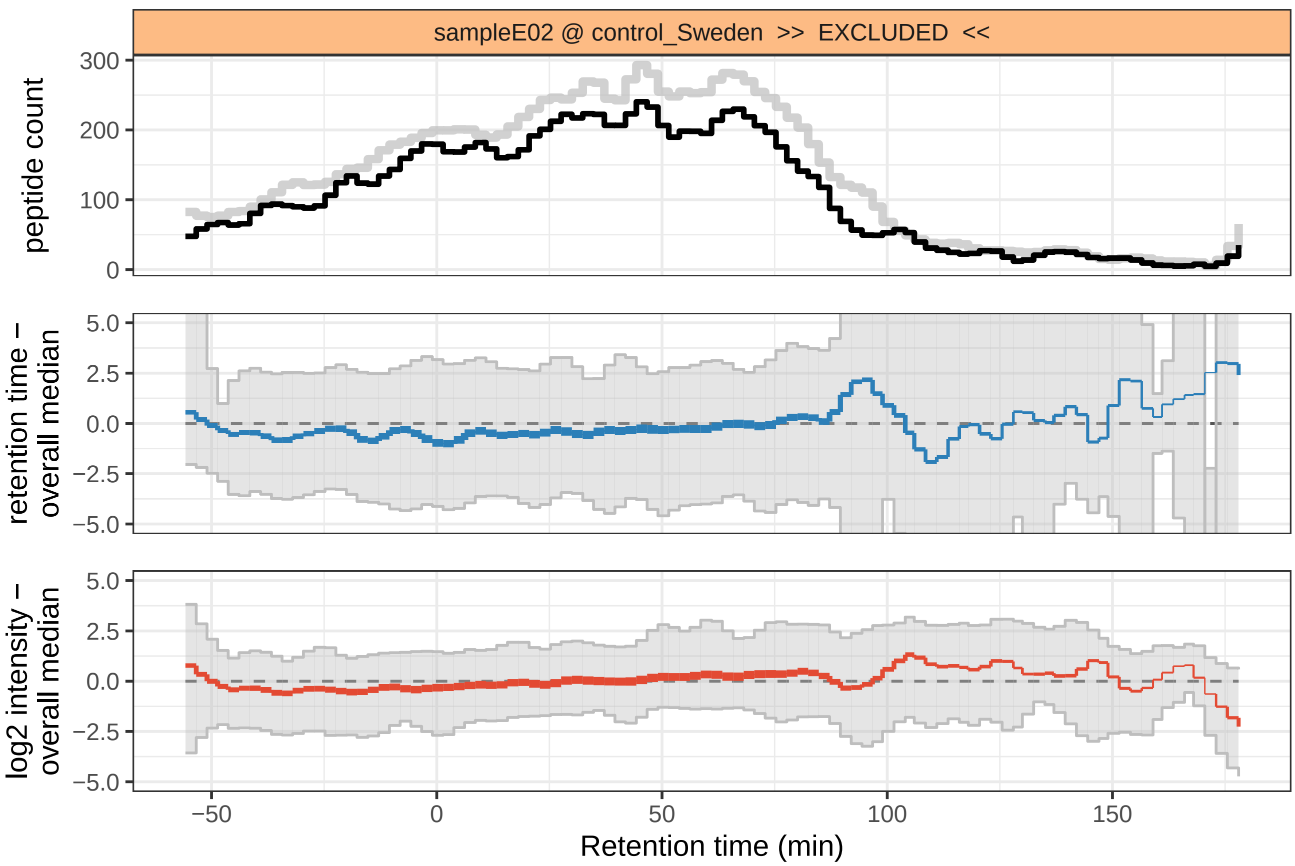

sampleD07 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

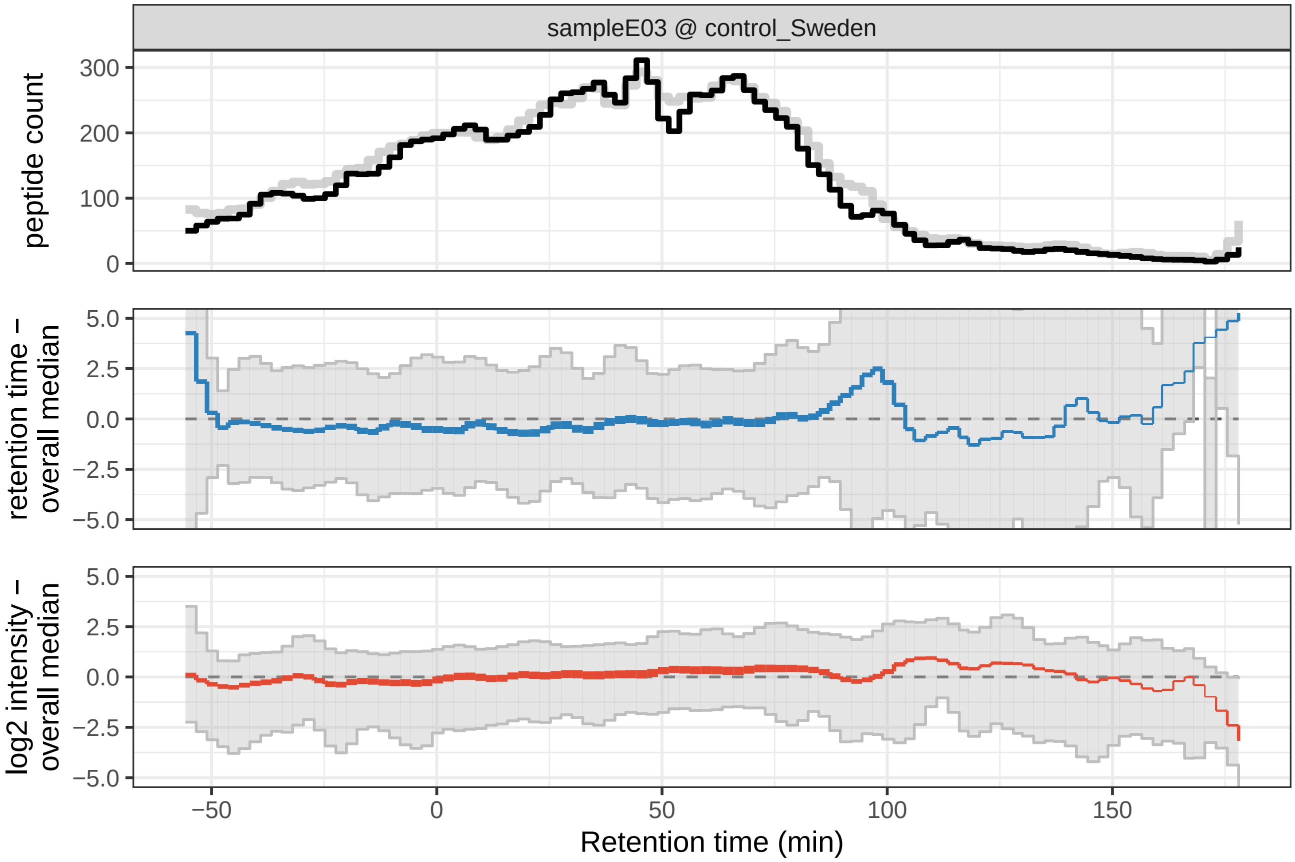

sampleD10 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleD11 @ control_Sweden >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

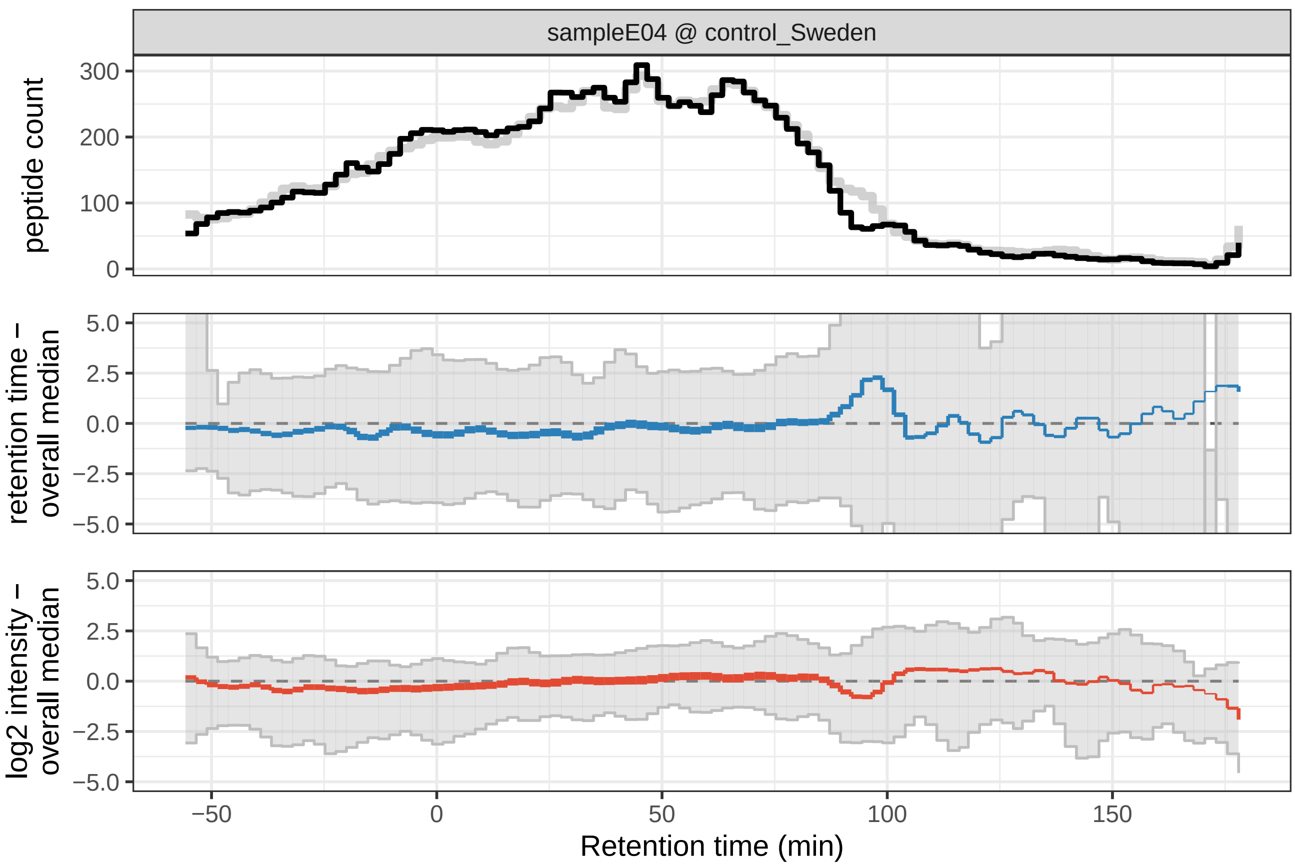

sampleD12 @ control_Sweden
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


sampleE01 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

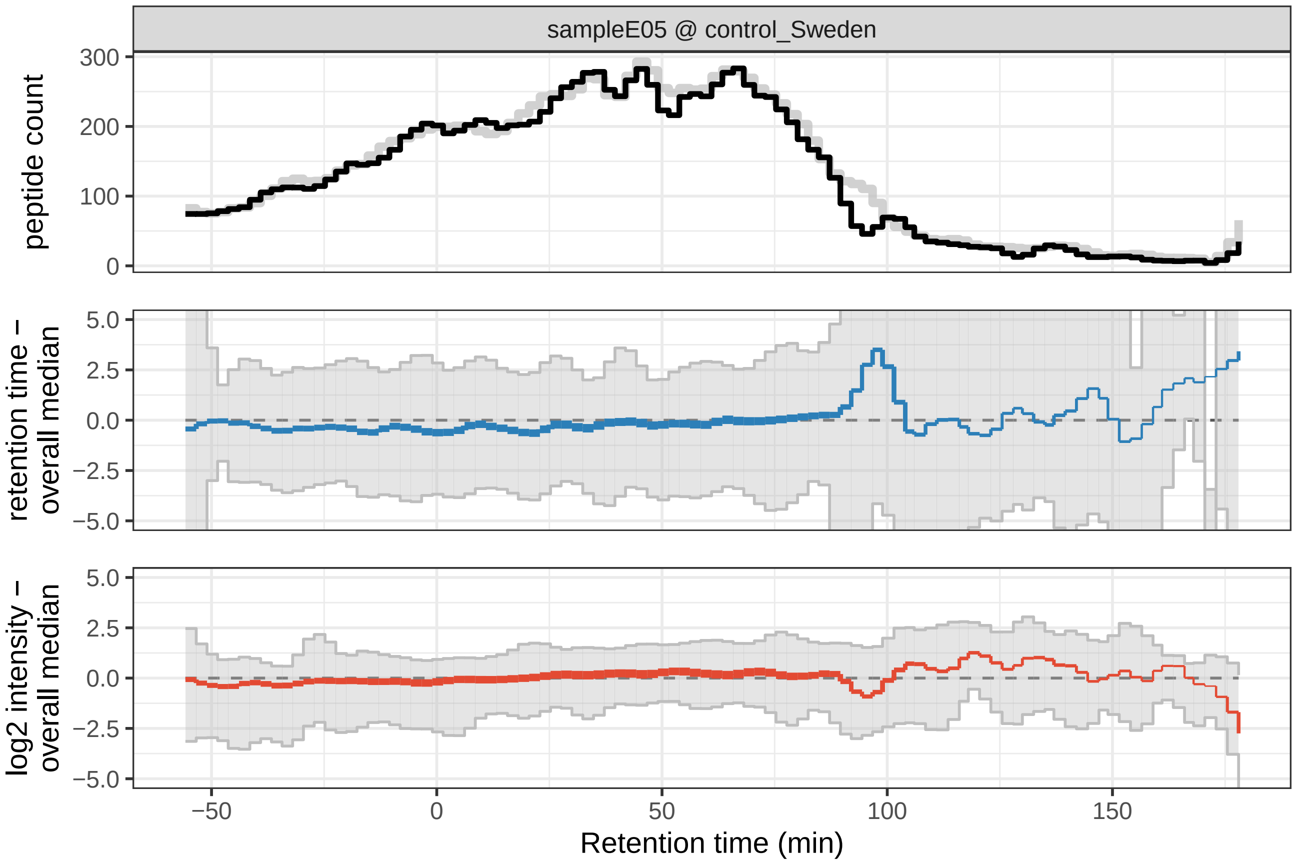

sampleE02 @ control_Sweden >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

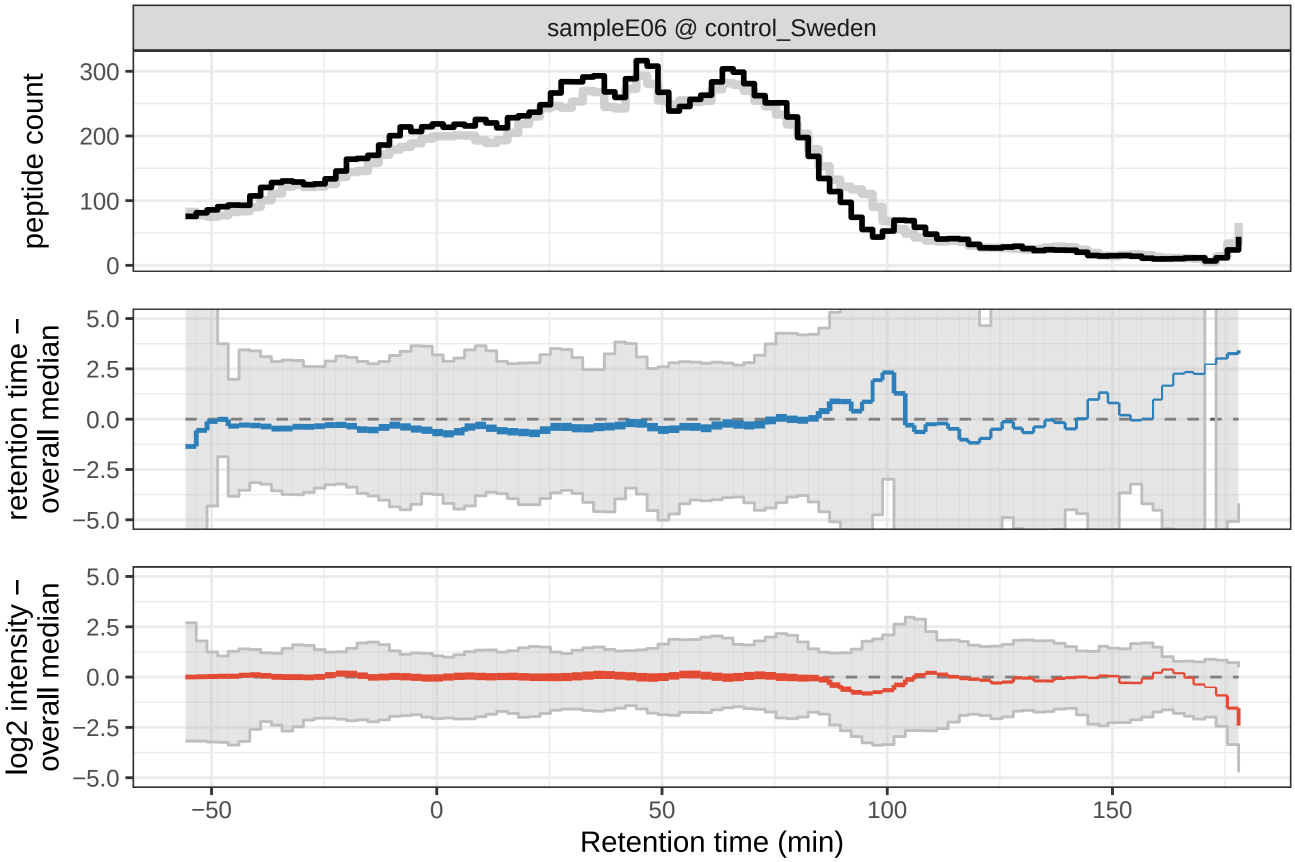


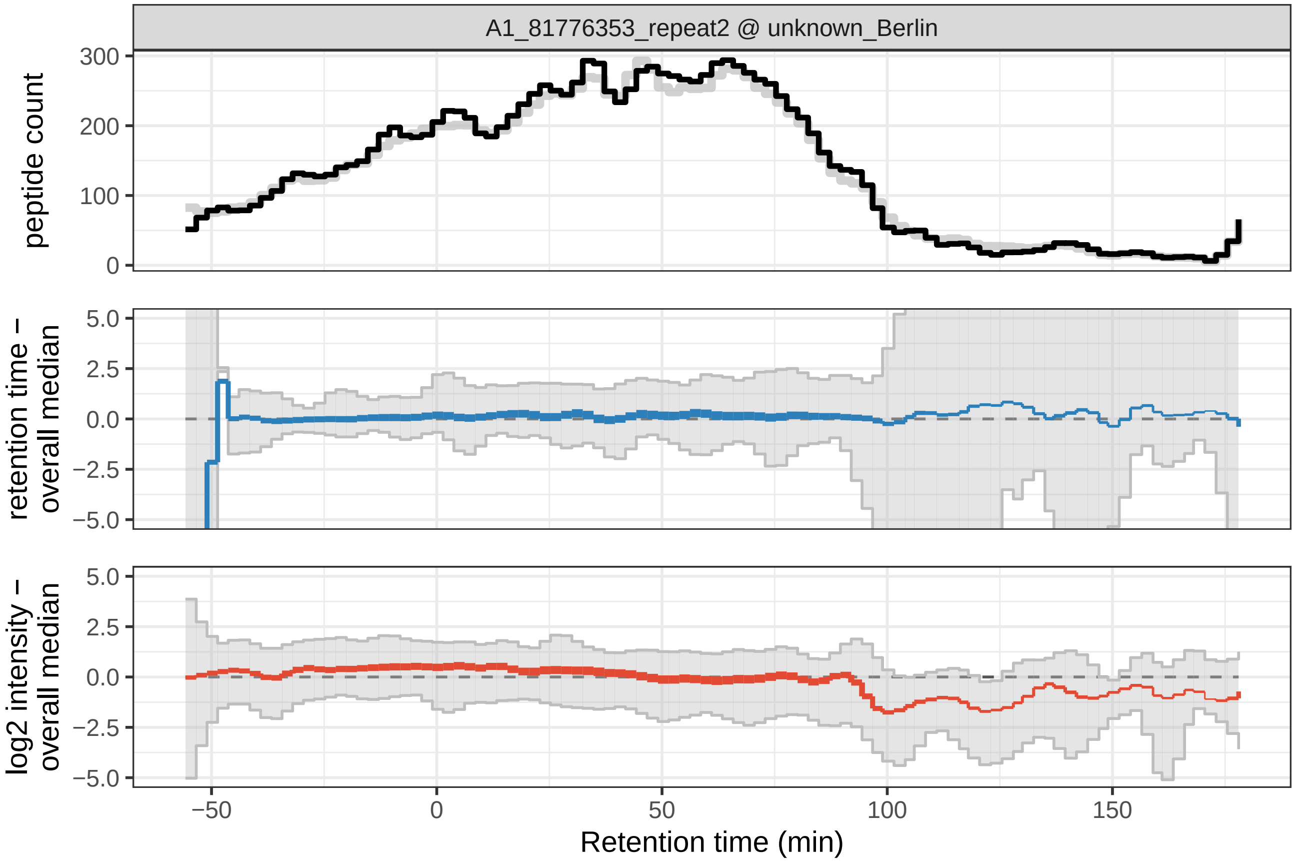
sampleE03 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

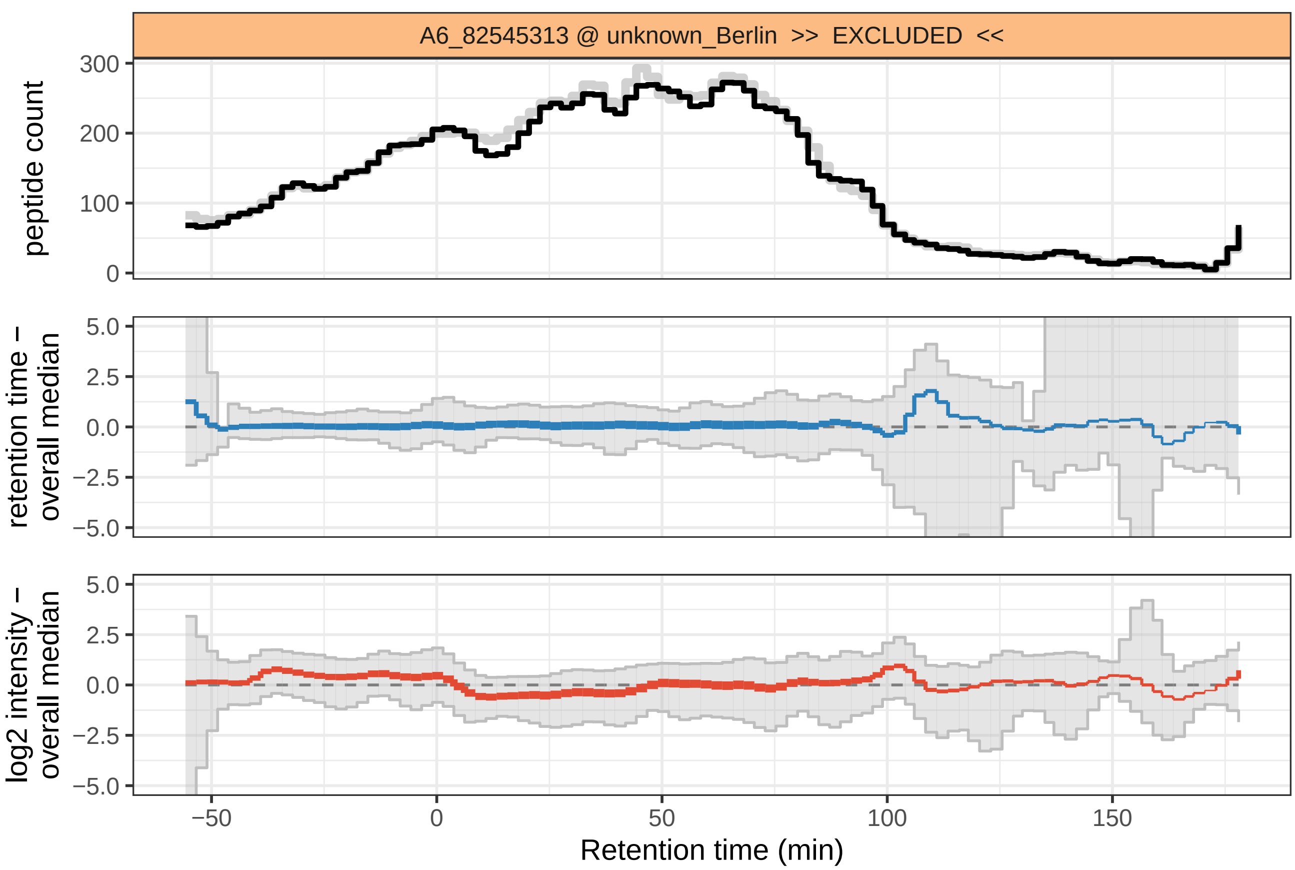


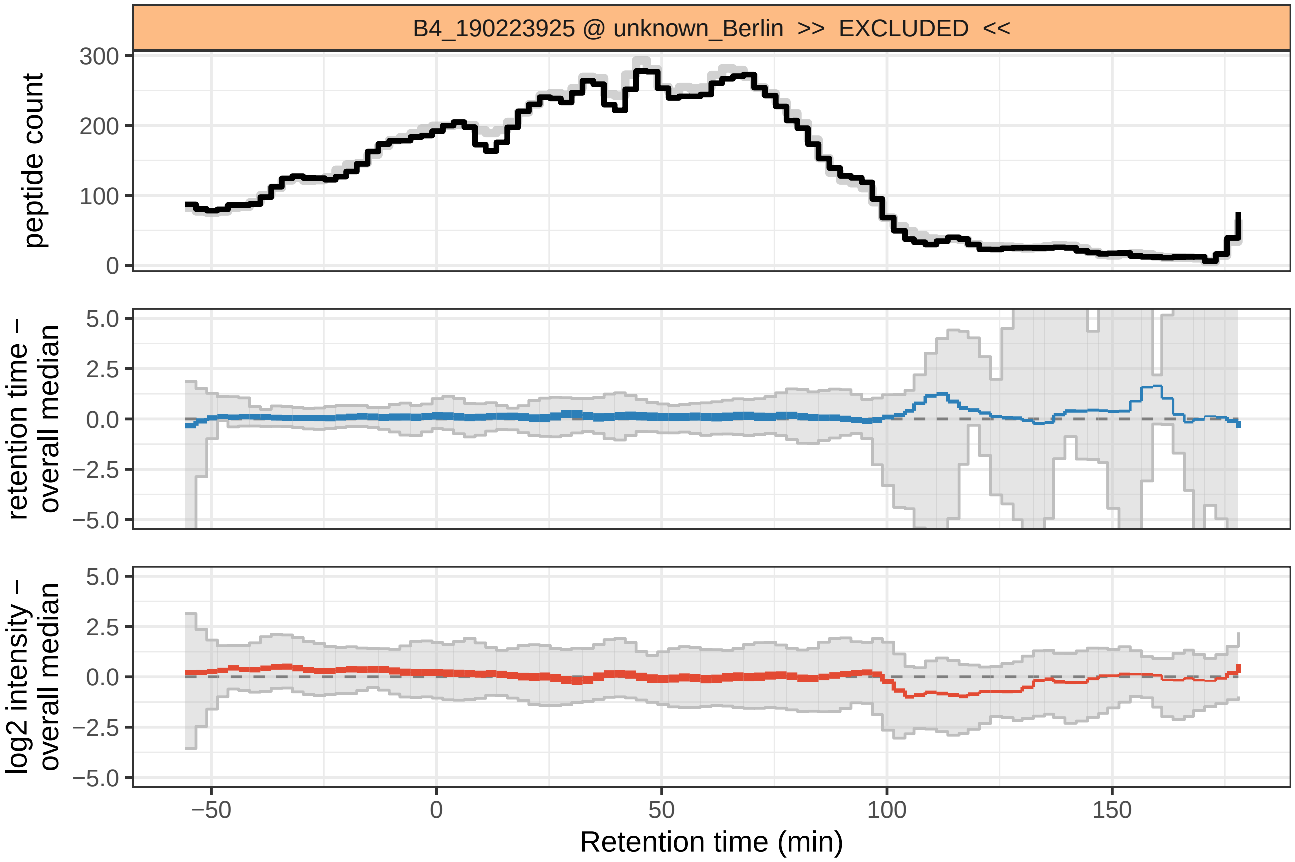
sampleE04 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

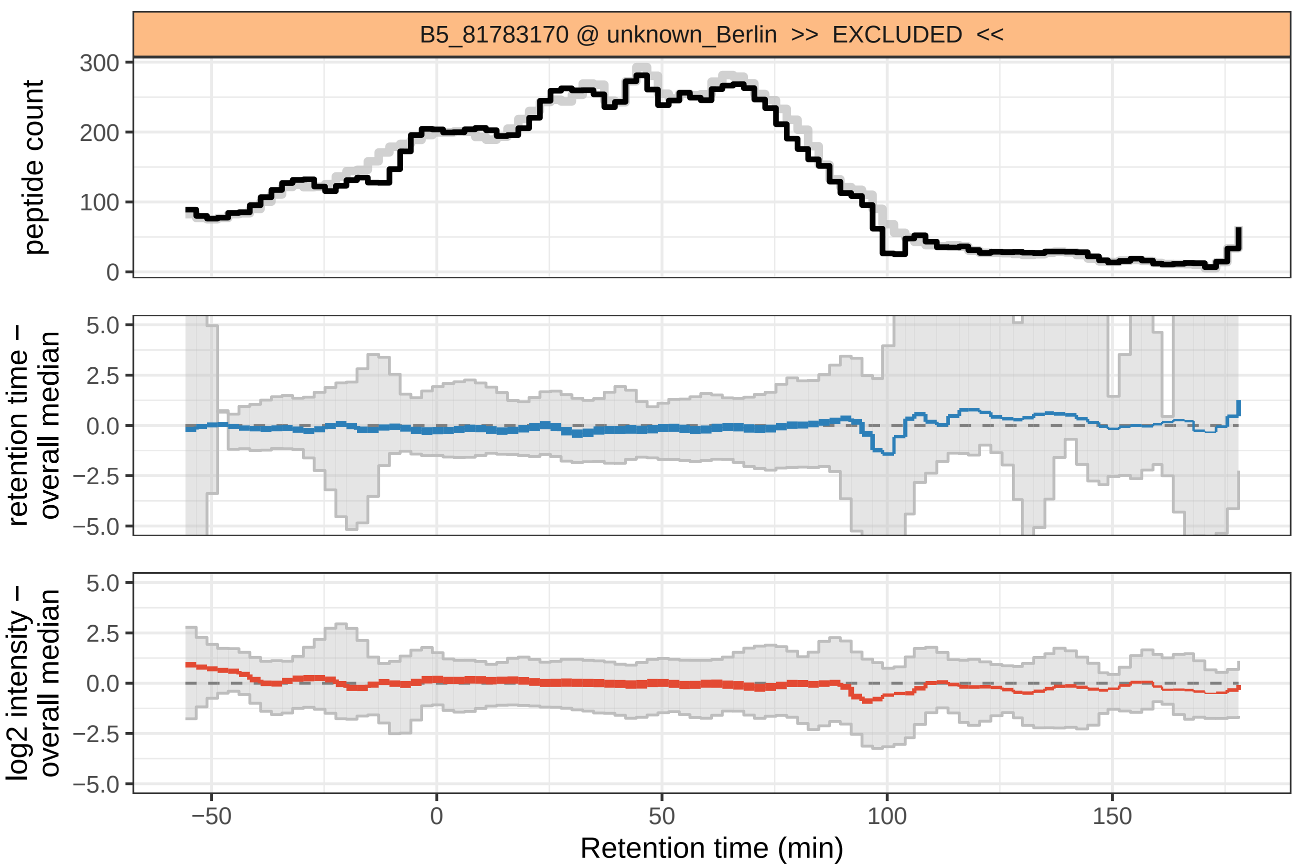

sampleE05 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

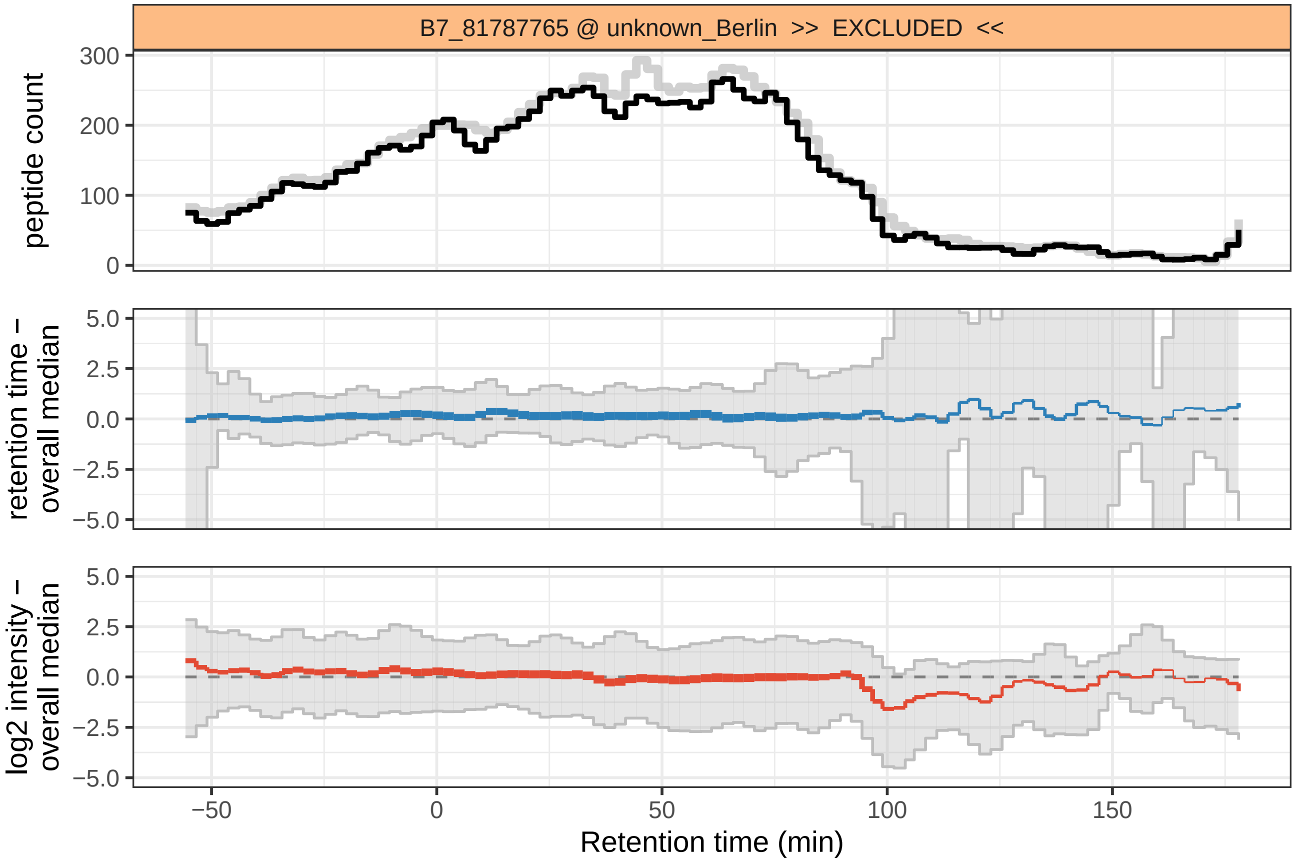

sampleE06 @ control_Sweden
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

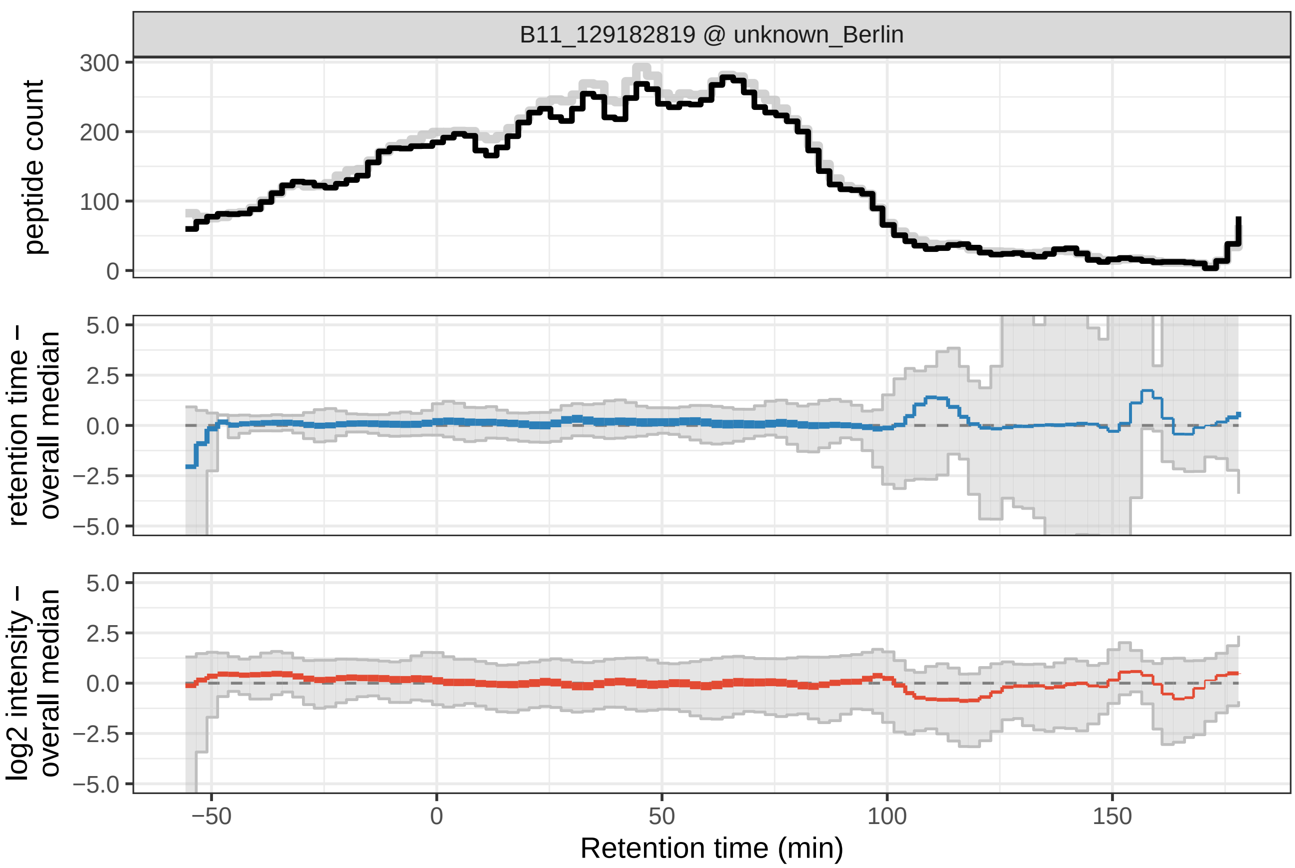

A1_81776353_repeat2 @ unknown_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

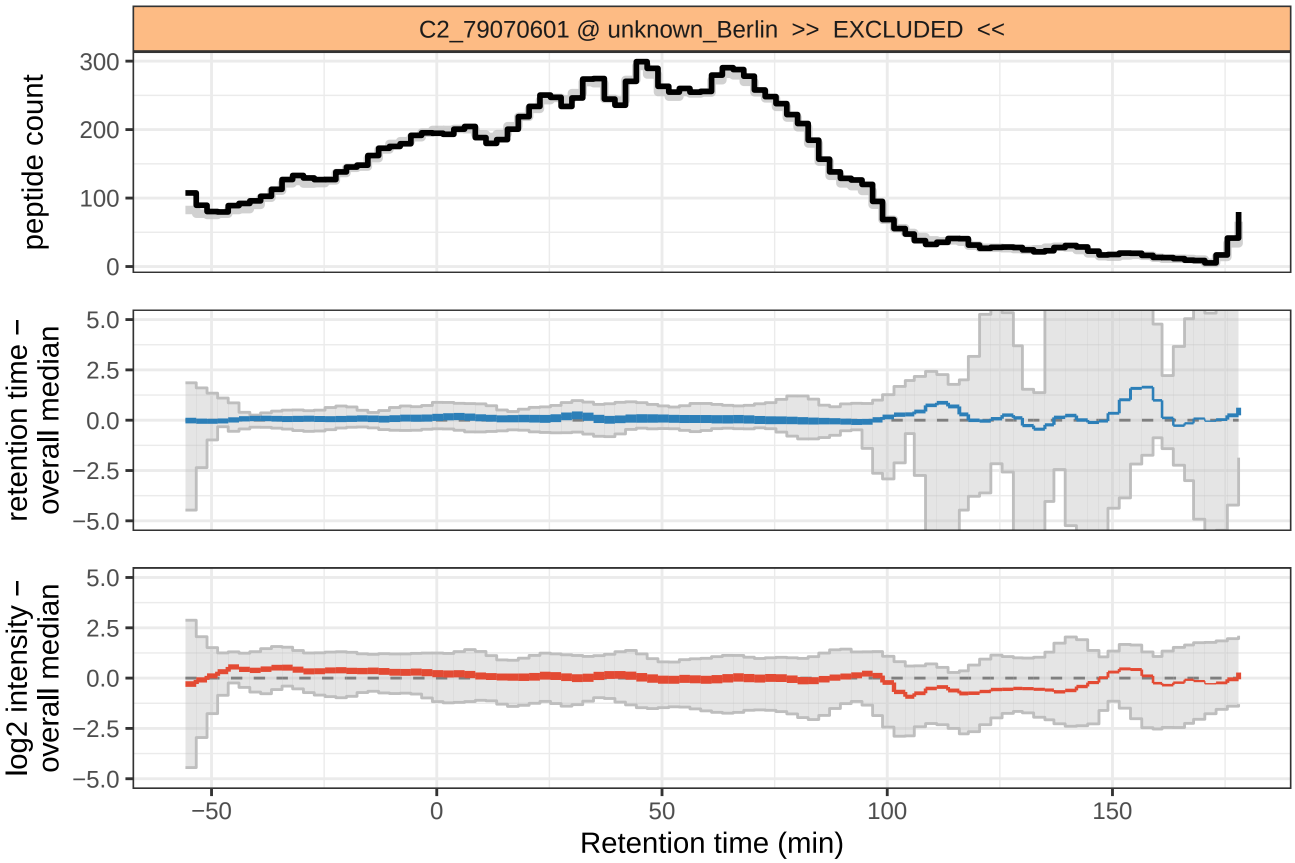

A6_82545313 @ unknown_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

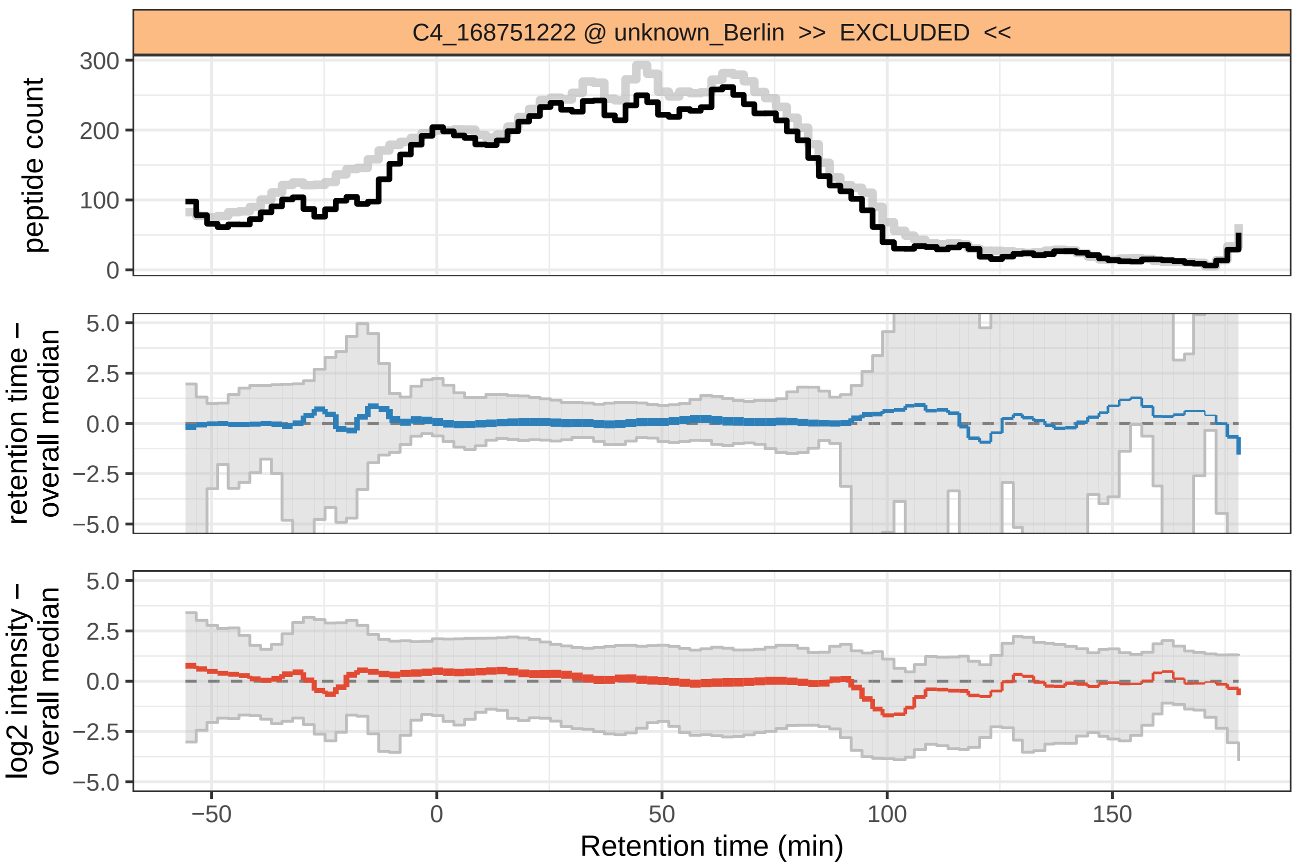

B4_190223925 @ unknown_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

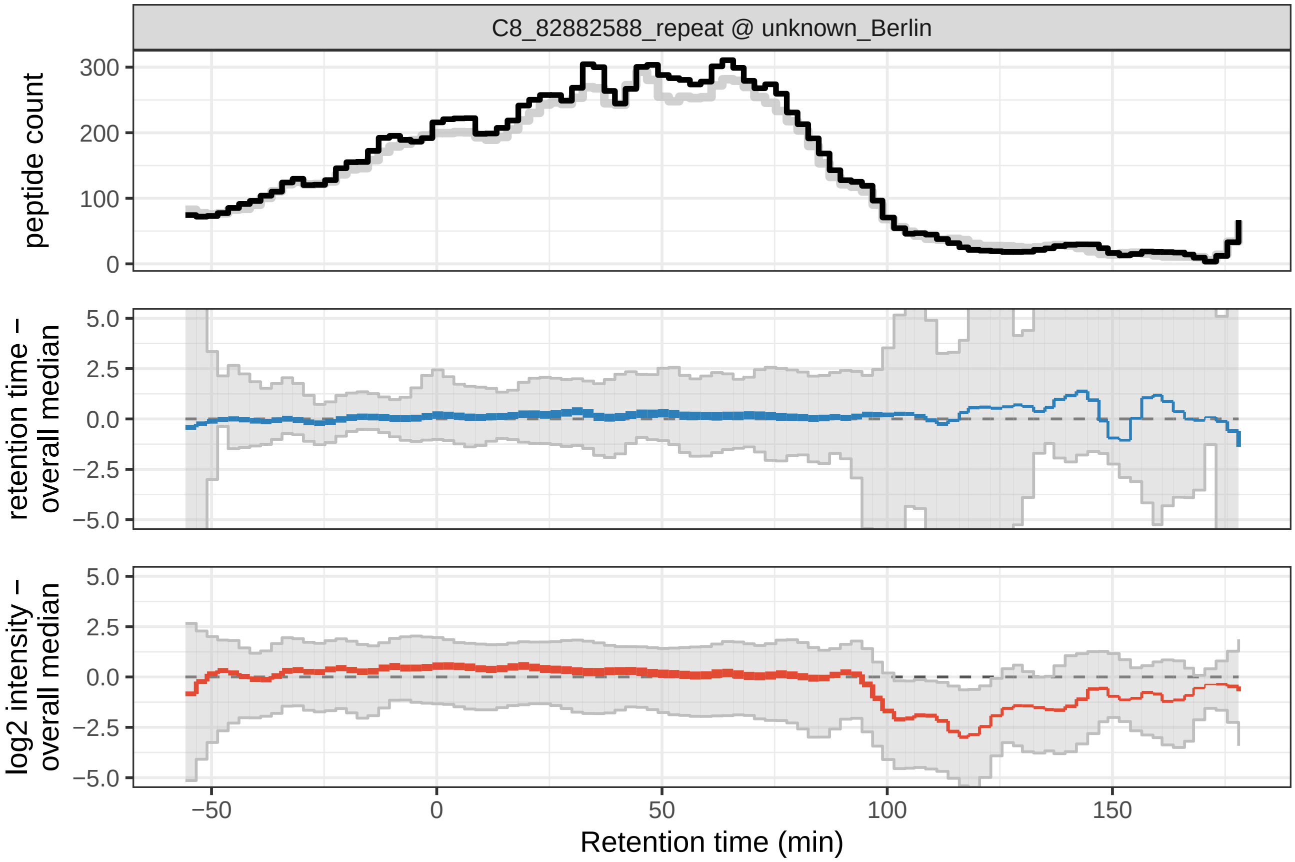

B5_81783170 @ unknown_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

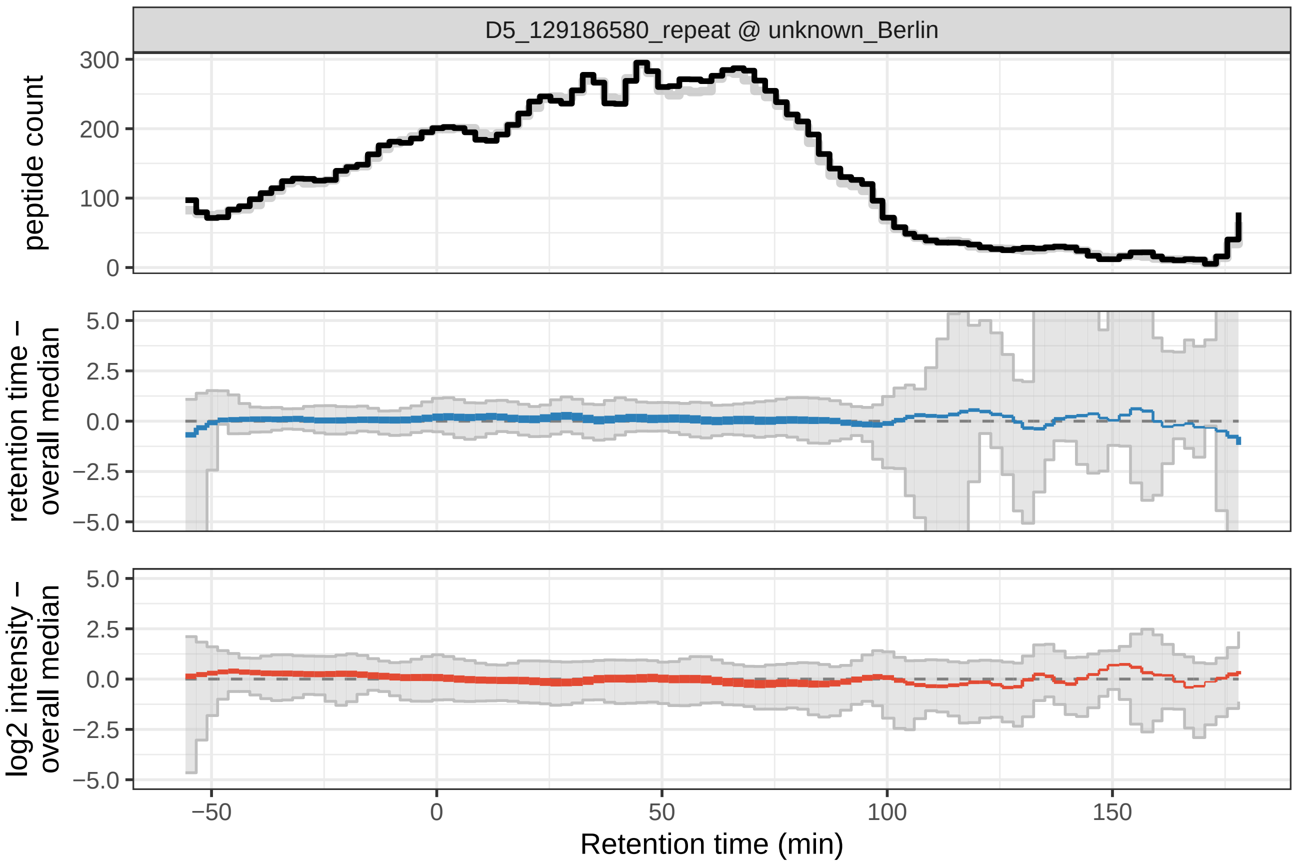

B7_81787765 @ unknown_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

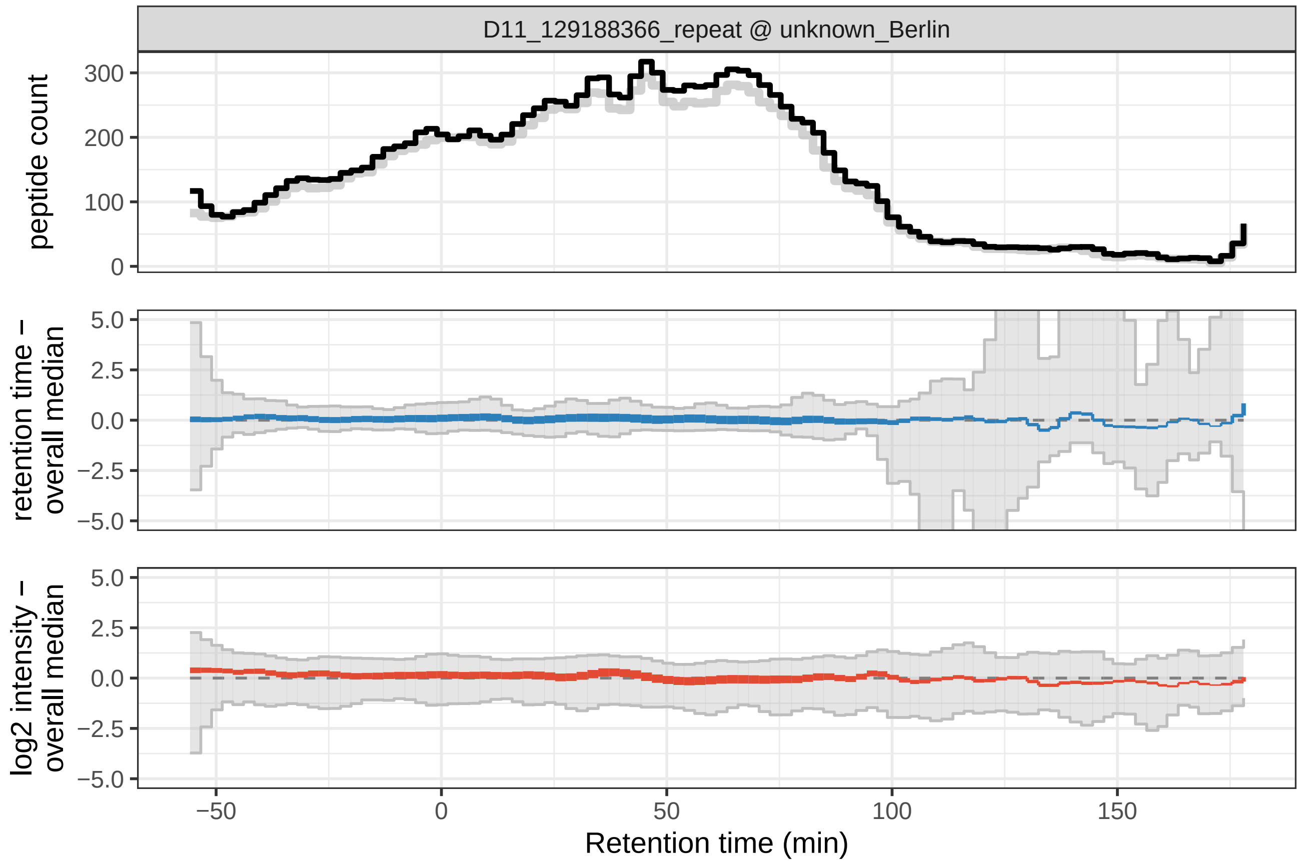

B11_129182819 @ unknown_Berlin
peptide count
300
200
100
0
retention time –
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity –
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

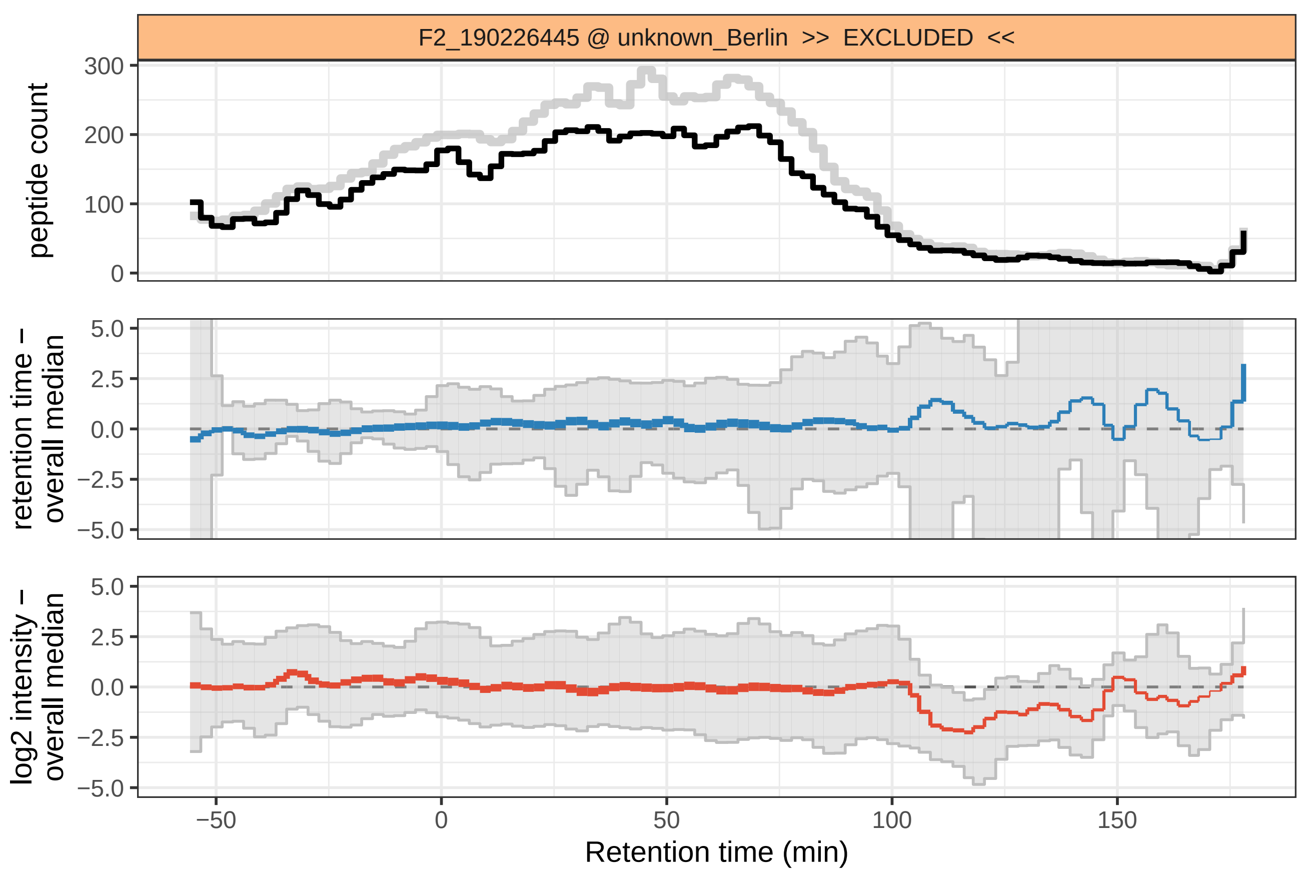

C2_79070601 @ unknown_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

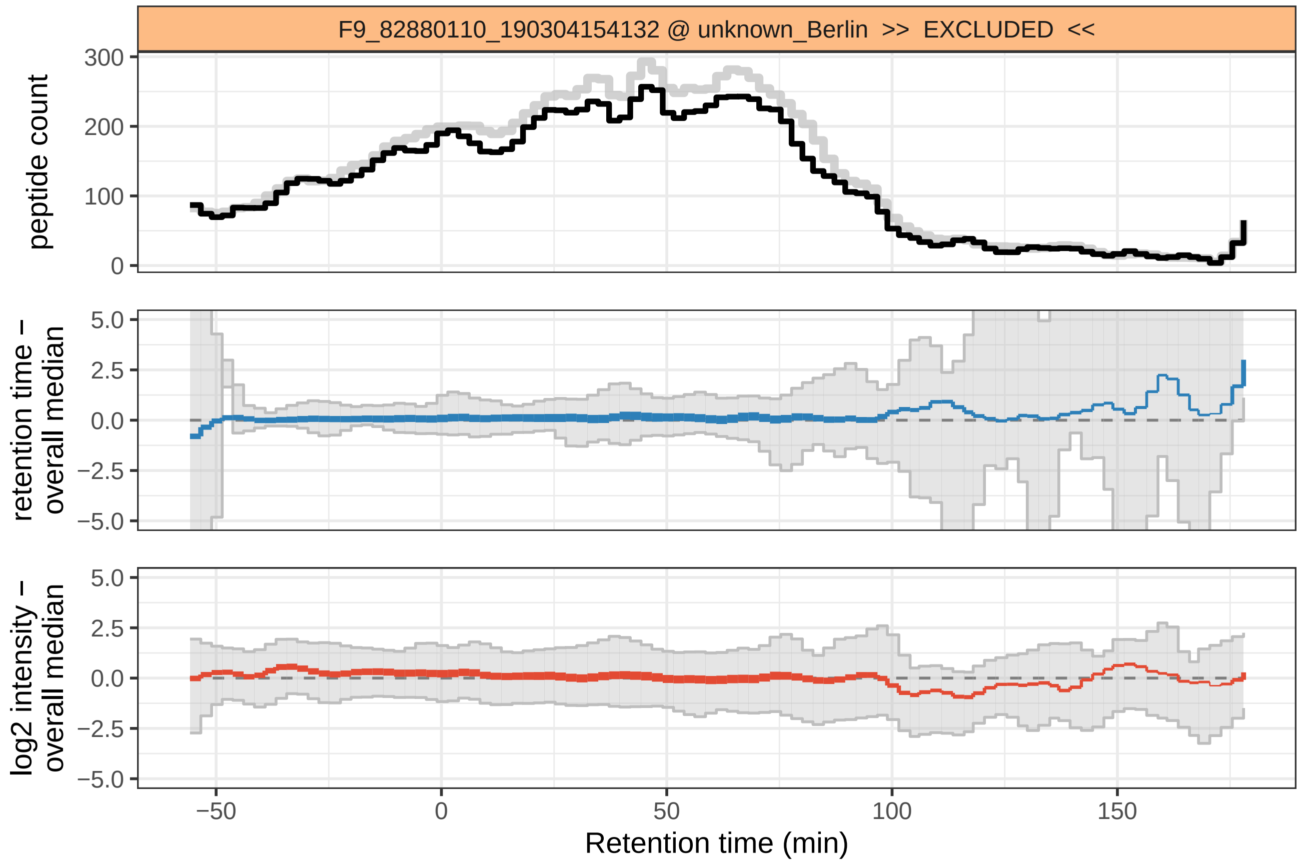

C4_168751222 @ unknown_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

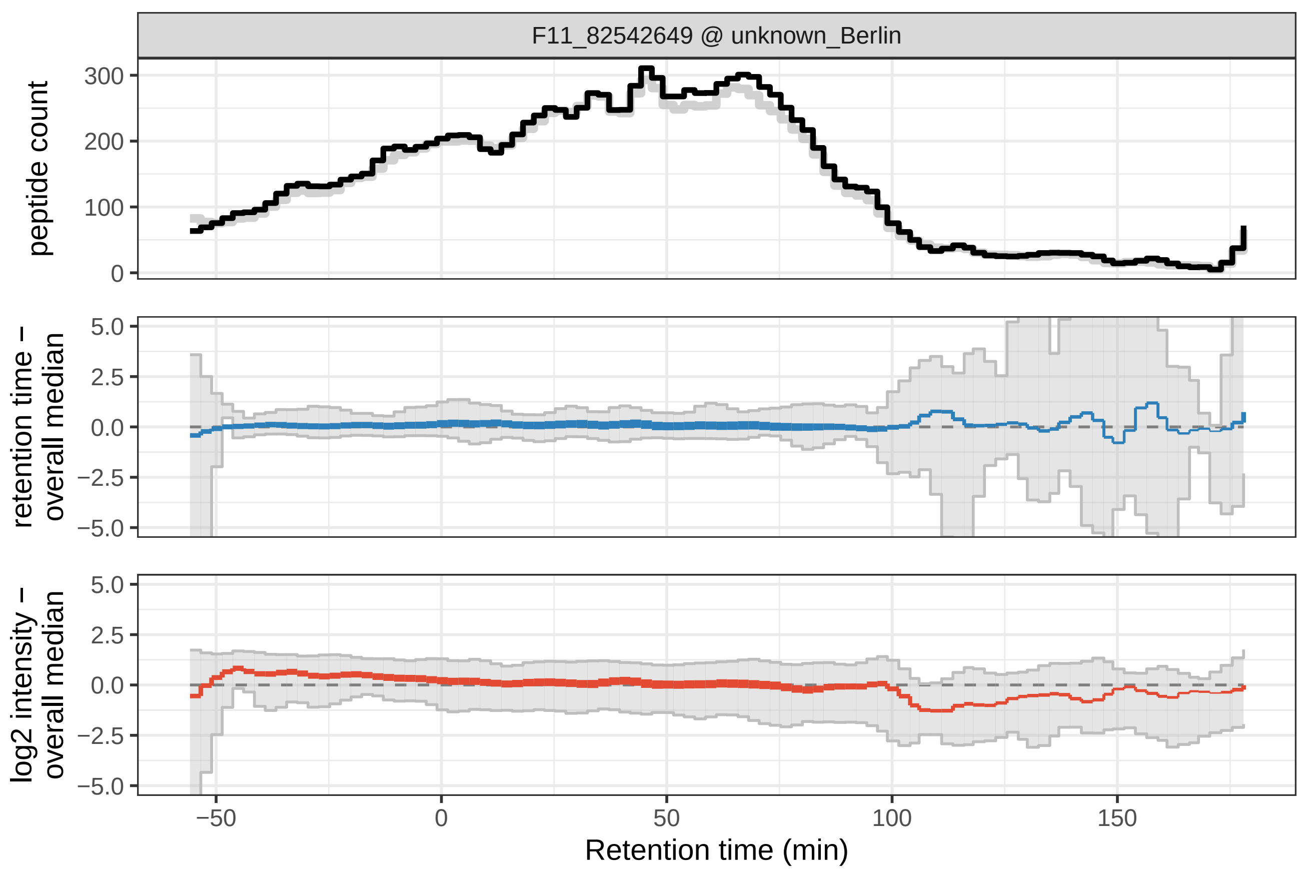

C8_82882588_repeat @ unknown_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

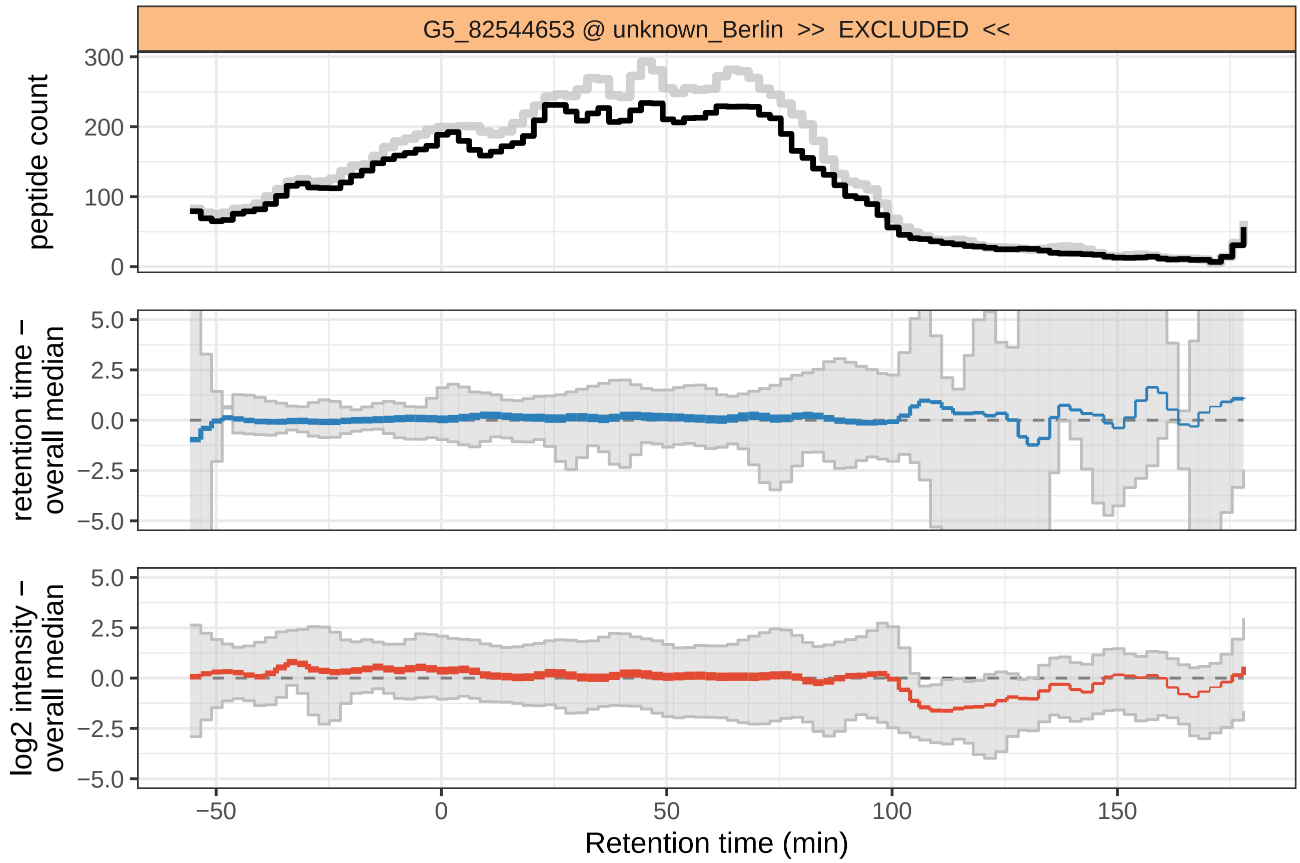

D5_129186580_repeat @ unknown_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

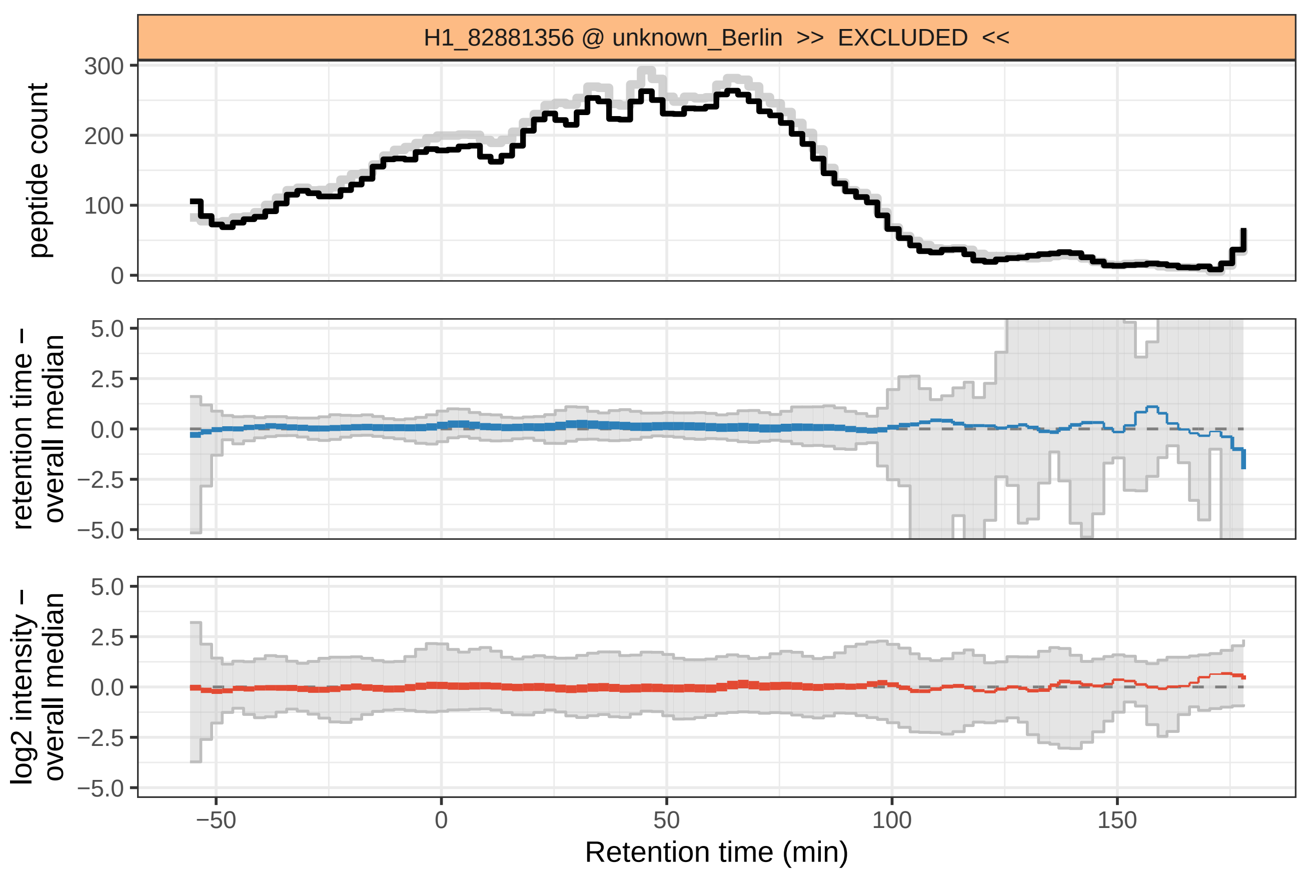

D11_129188366_repeat @ unknown_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

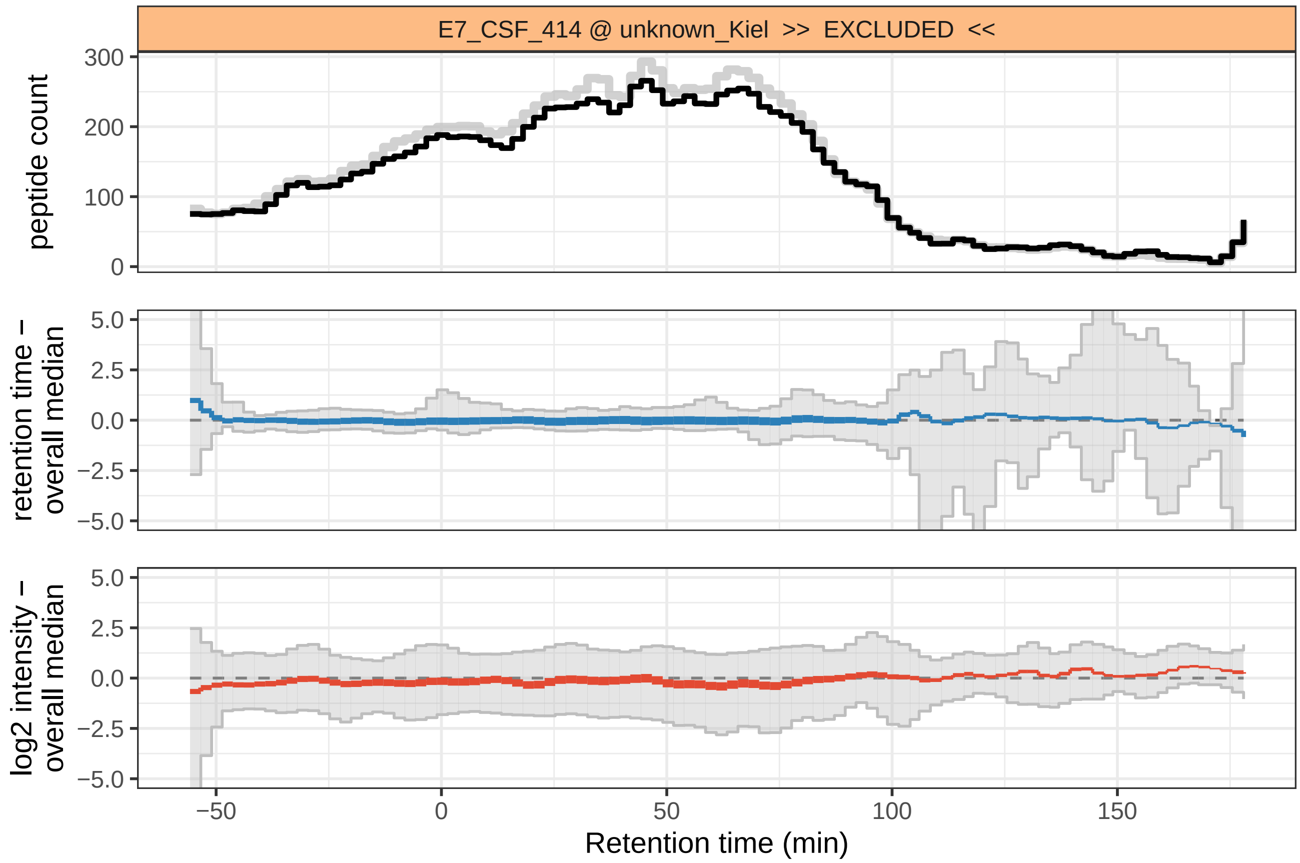

F2_190226445 @ unknown_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

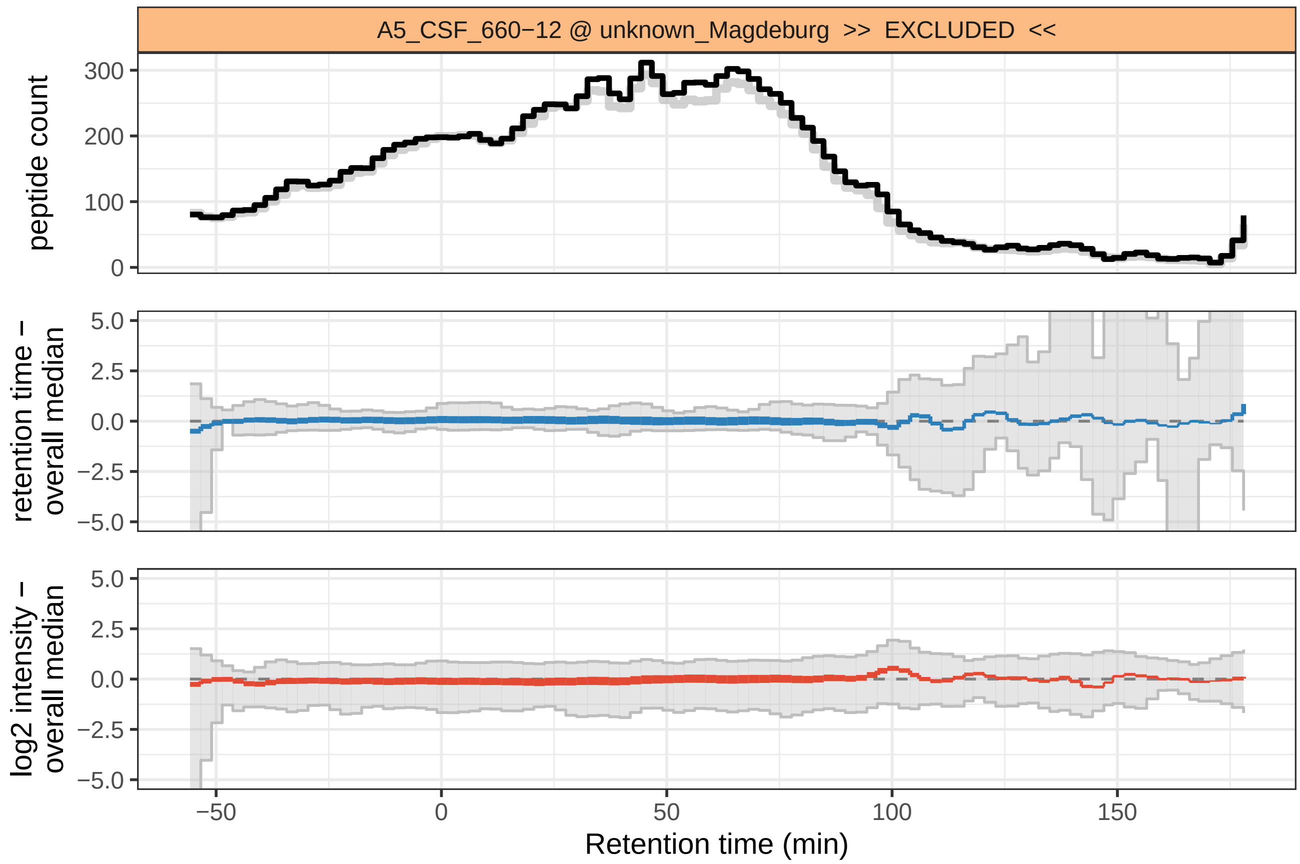

F9_82880110_190304154132 @ unknown_Berlin >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

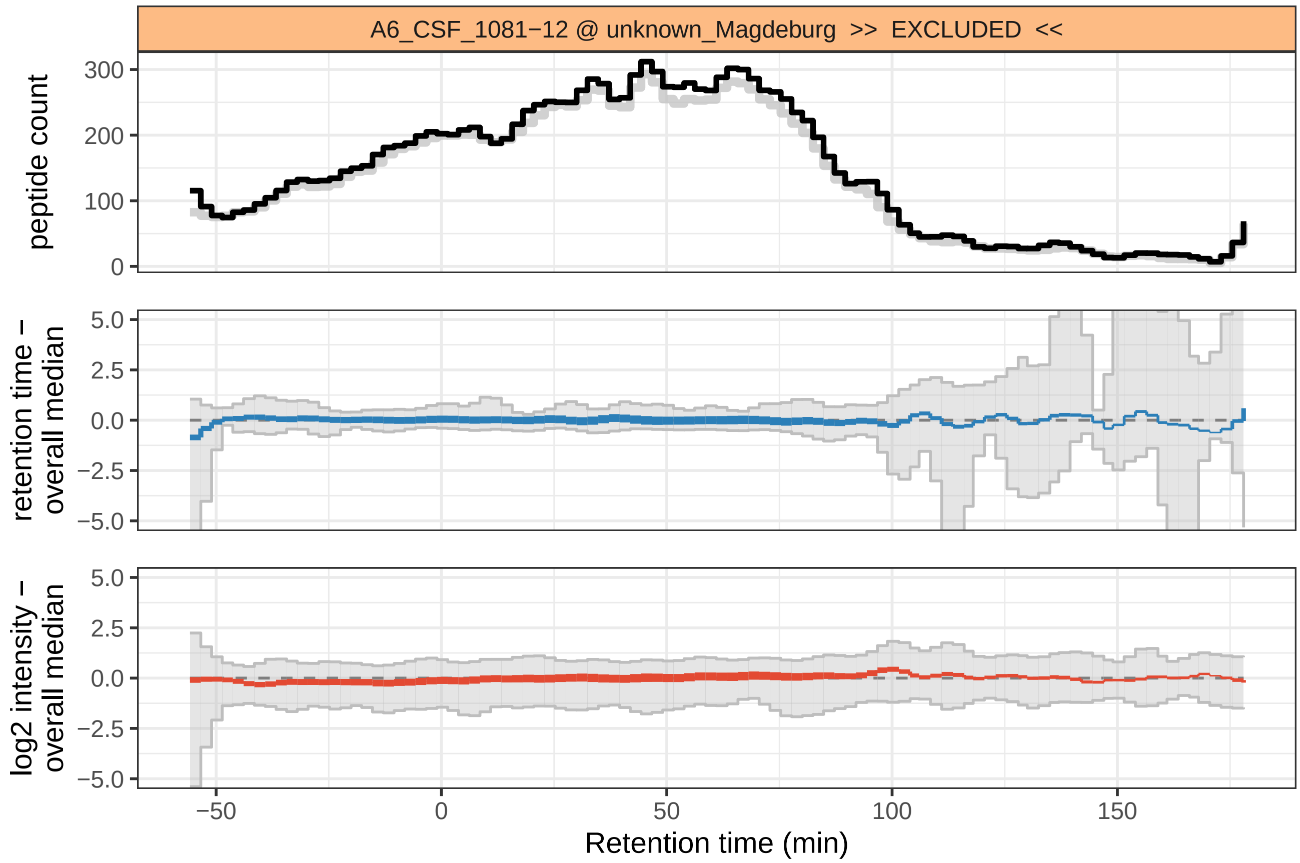

F11_82542649 @ unknown_Berlin
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

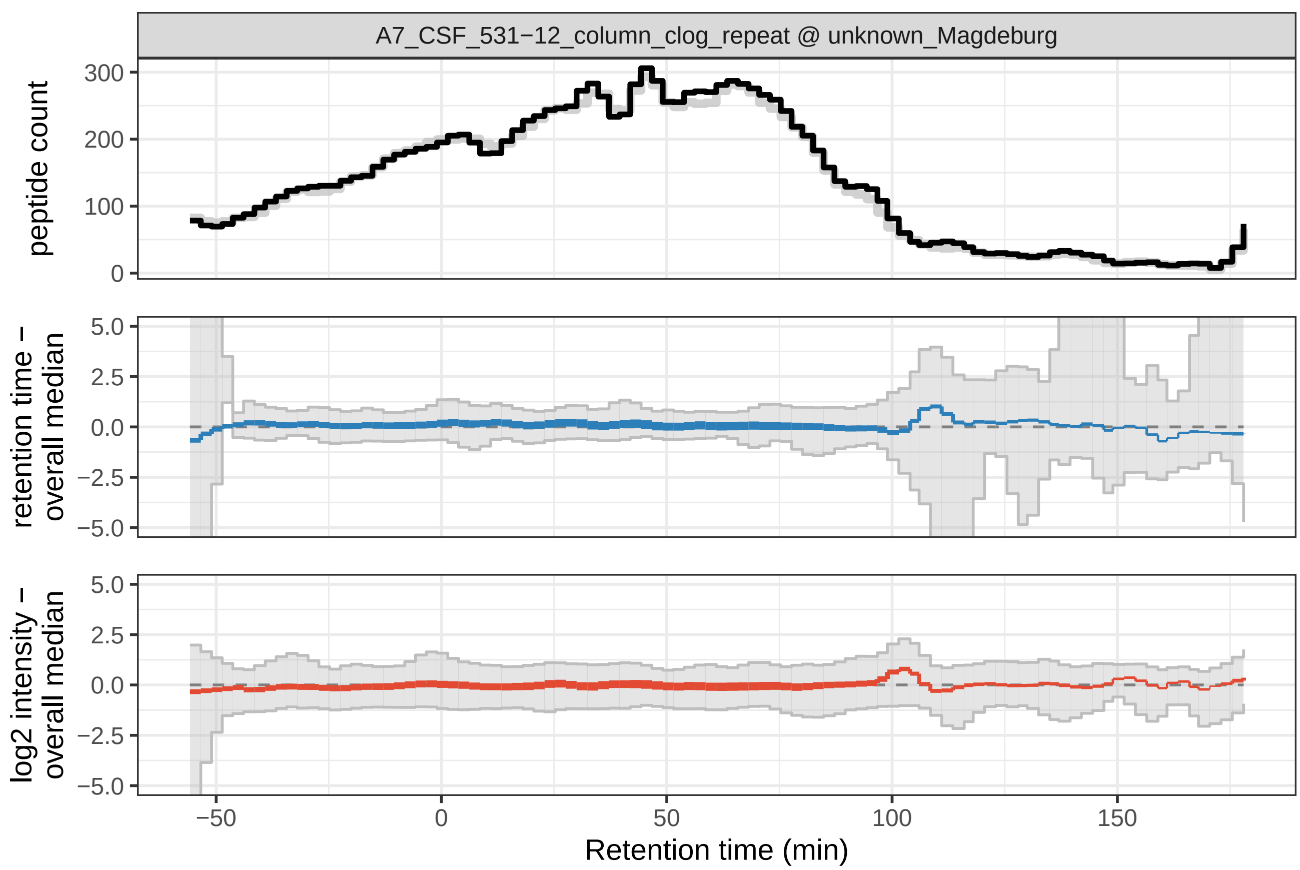

G5_82544653 @ unknown_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

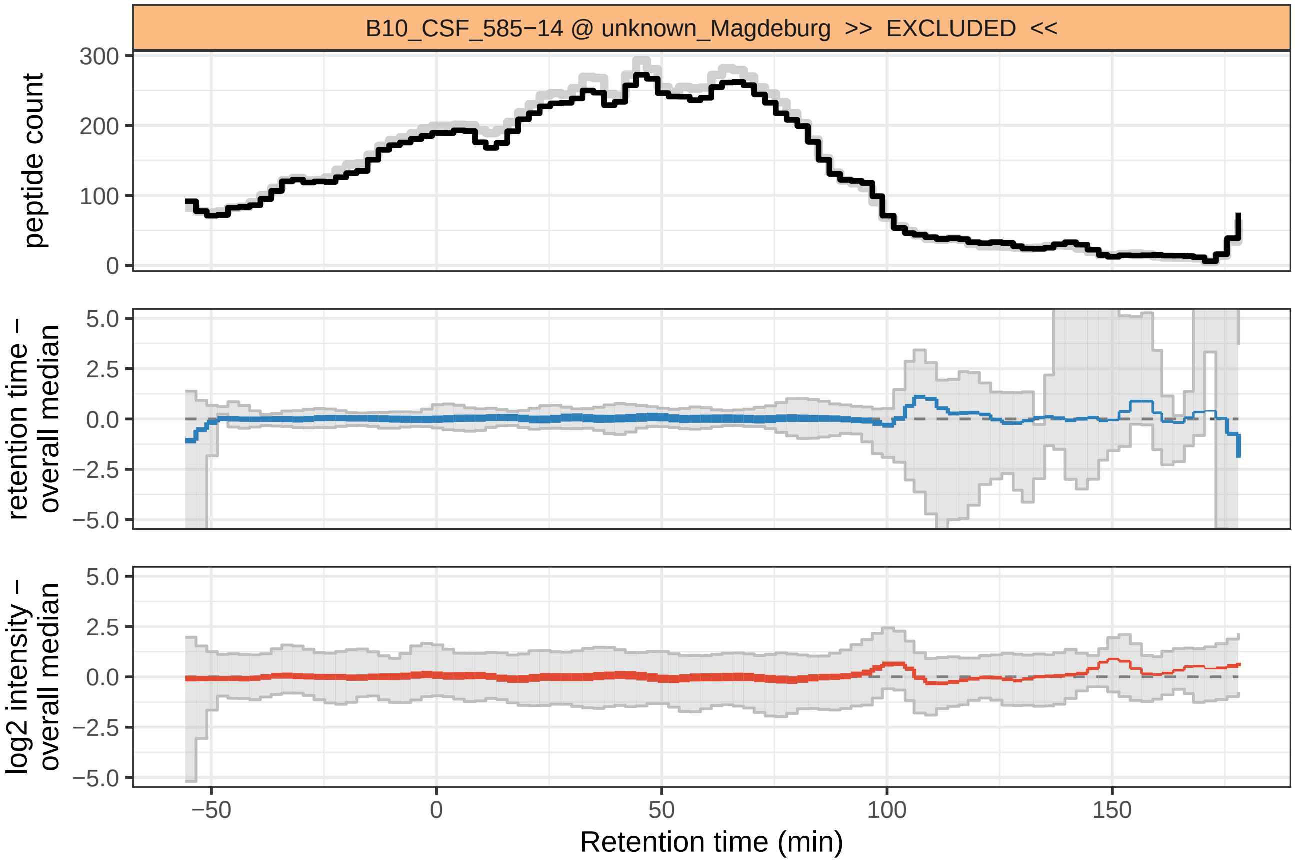

H1_82881356 @ unknown_Berlin >> EXCLUDED <<
peptide count
300
200
100
0
retention time – overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity – overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)

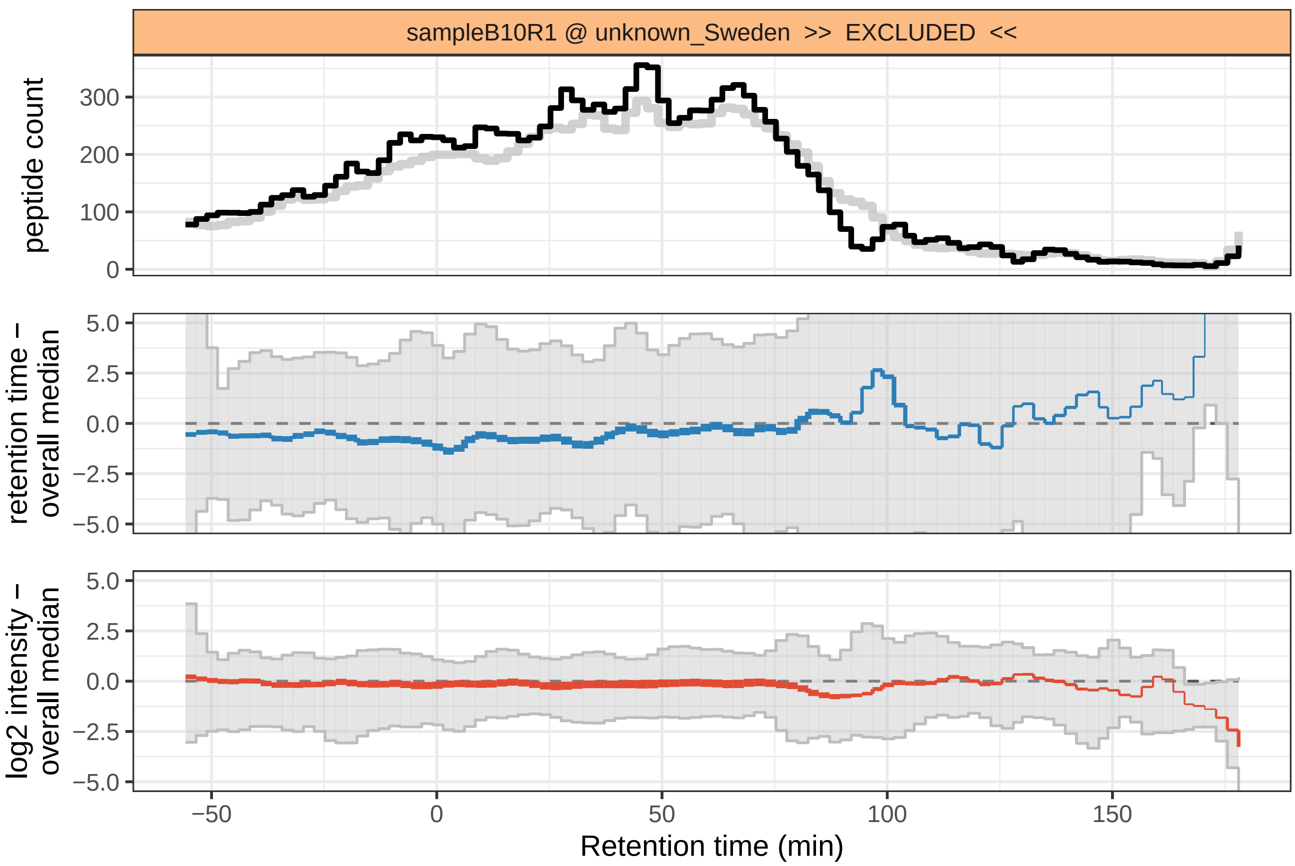

E7_CSF_414 @ unknown_Kiel >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


A5_CSF_660−12 @ unknown_Magdeburg >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)


A6_CSF_1081−12 @ unknown_Magdeburg >> EXCLUDED <<
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


A7_CSF_531−12_column_clog_repeat @ unknown_Magdeburg
peptide count
300
200
100
0
retention time −
overall median
5.0
2.5
0.0
−2.5
−5.0
log2 intensity −
overall median
5.0
2.5
0.0
−2.5
−5.0
−50
0
50
100
150
Retention time (min)


B10_CSF_585−14 @ unknown_Magdeburg >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

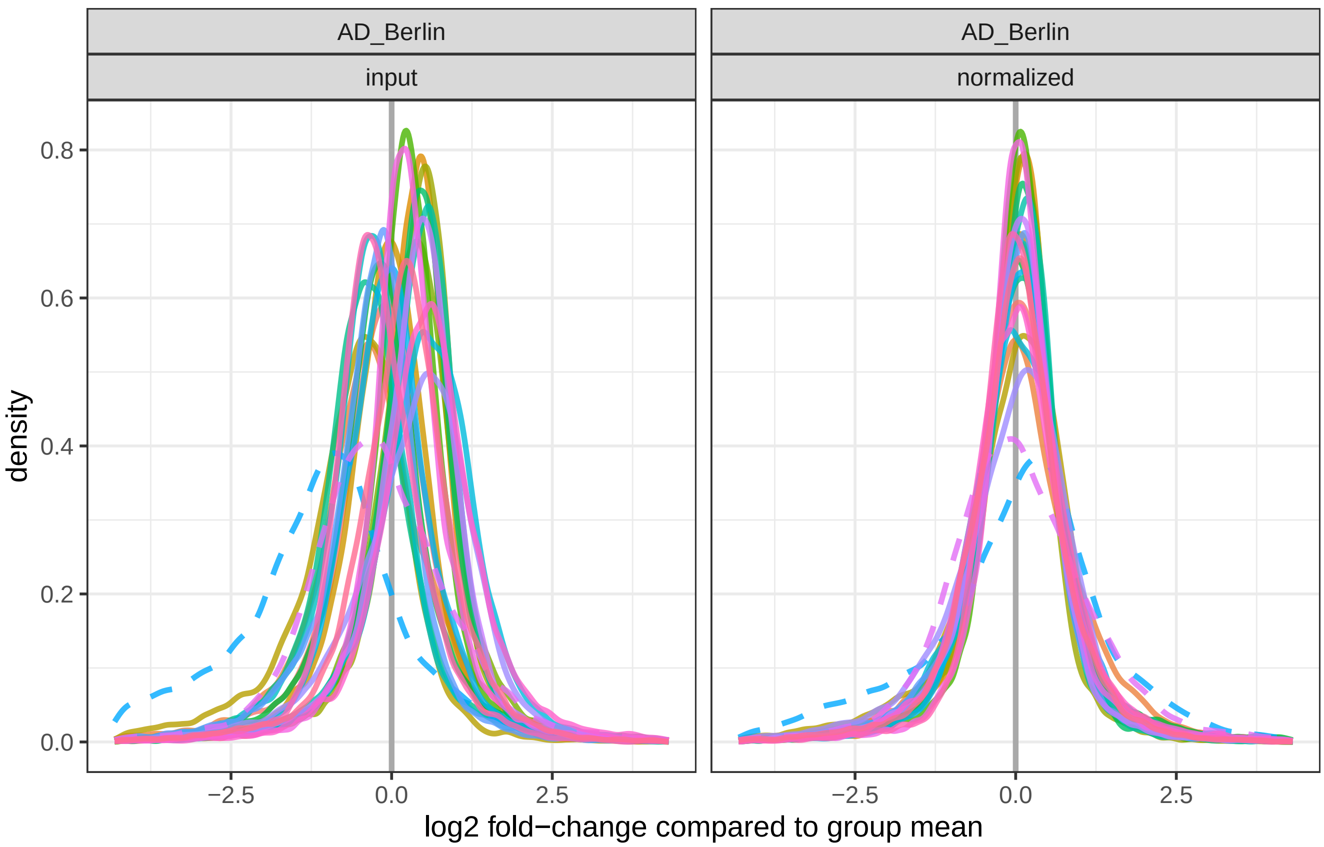

sampleB10R1 @ unknown_Sweden >> EXCLUDED <<
peptide count
retention time – overall median
log2 intensity – overall median
Retention time (min)

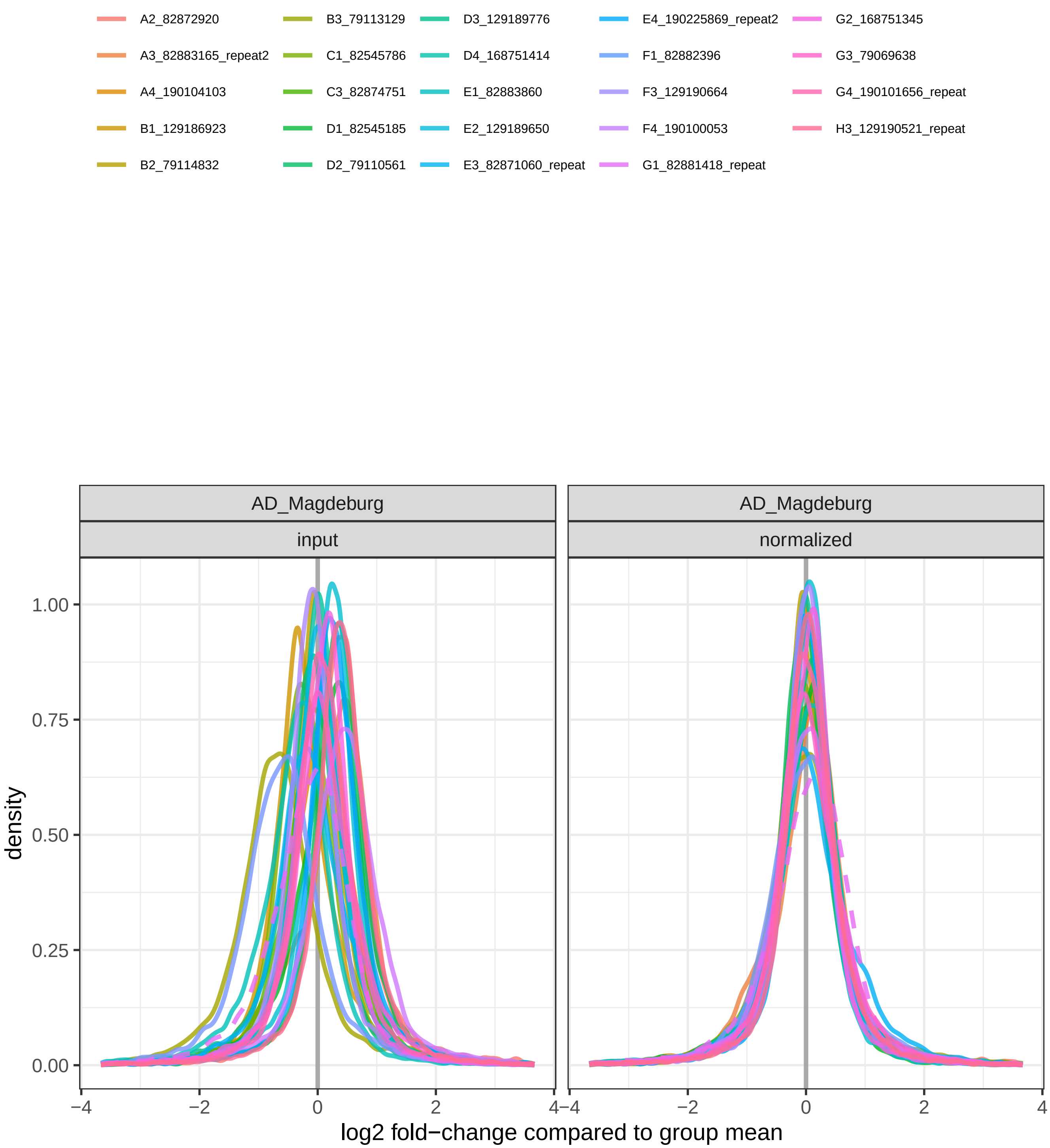
1.6 variation among replicates

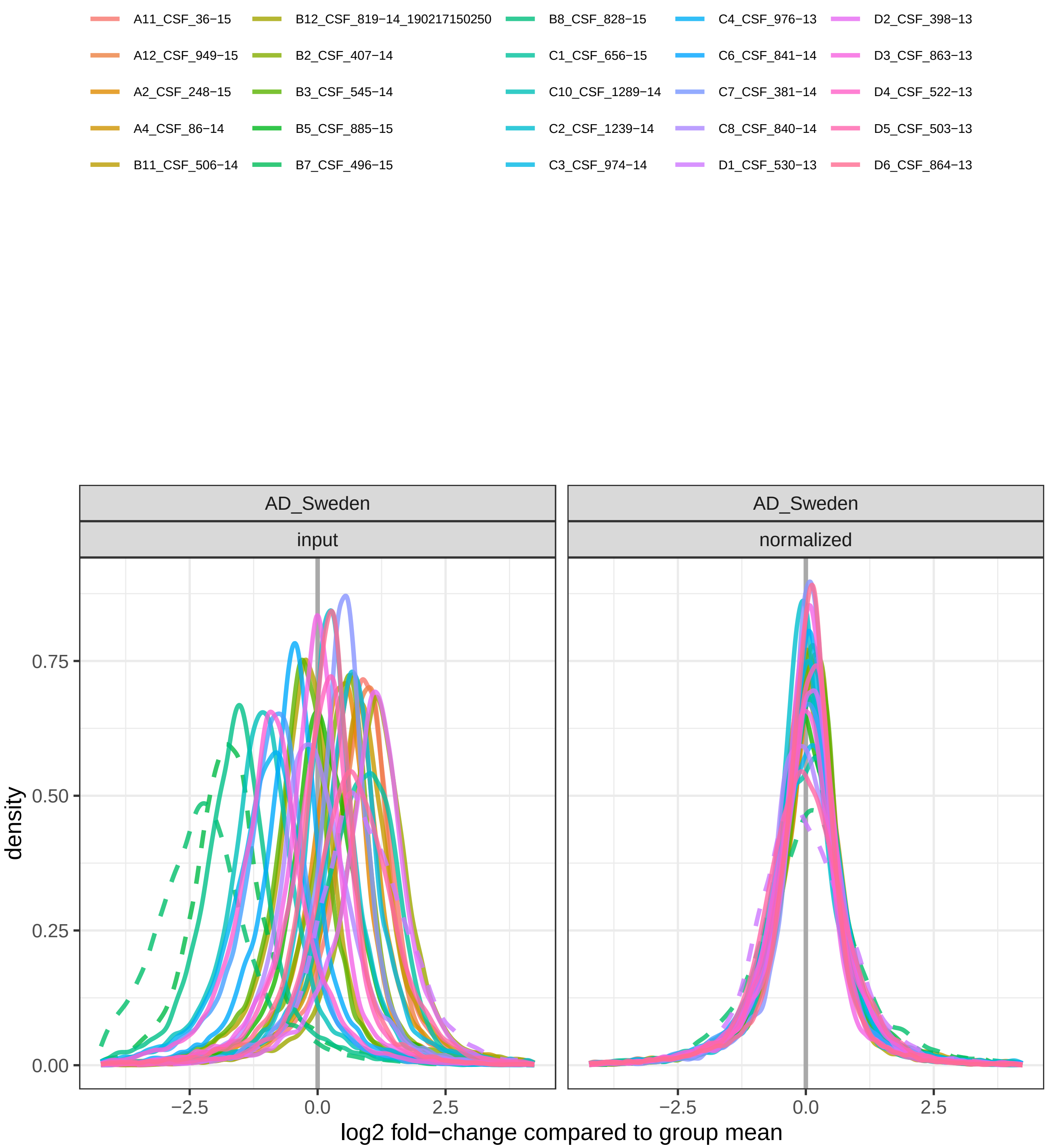
The reproducibility of replicate measurements is expressed in three different analyses. First, the difference between peptide intensities in each sample are compared to the mean value among all replicates (foldchange distributions). Next, the Coefficient of Variation (CoV) is used as a metric for reproducibility to explore how much the CoV within a sample group can be improved by removing a single sample (eg; if CoV strongly improved after removing sample s, it could be regarded as an outlier). Finally, the CoV within each sample group is visualized as a boxplot and a violin plot, figures commonly seen in proteomics literature and useful for comparing across experiments (of similar protocol).

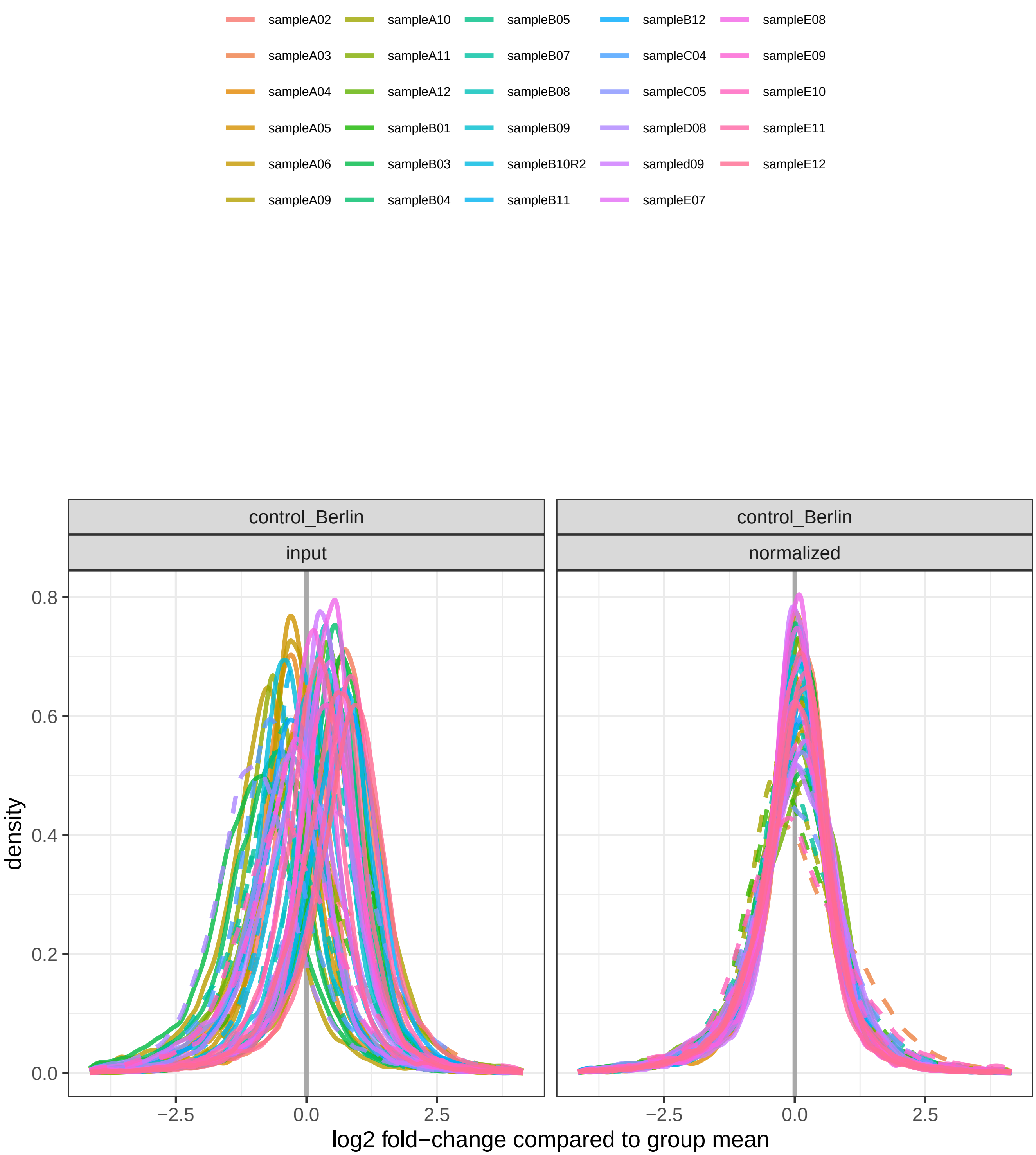
1.6.1 within-group foldchange distributions

The foldchange of all peptides in a sample is compared to their respective mean value over all samples in the group. This visualizes how strongly each sample deviates from other samples in the same group which helps identify outlier samples. The same data was used as detailed in the "retention time" section above. Samples marked as 'exclude' in the provided sample metadata table are visualized as dashed lines.

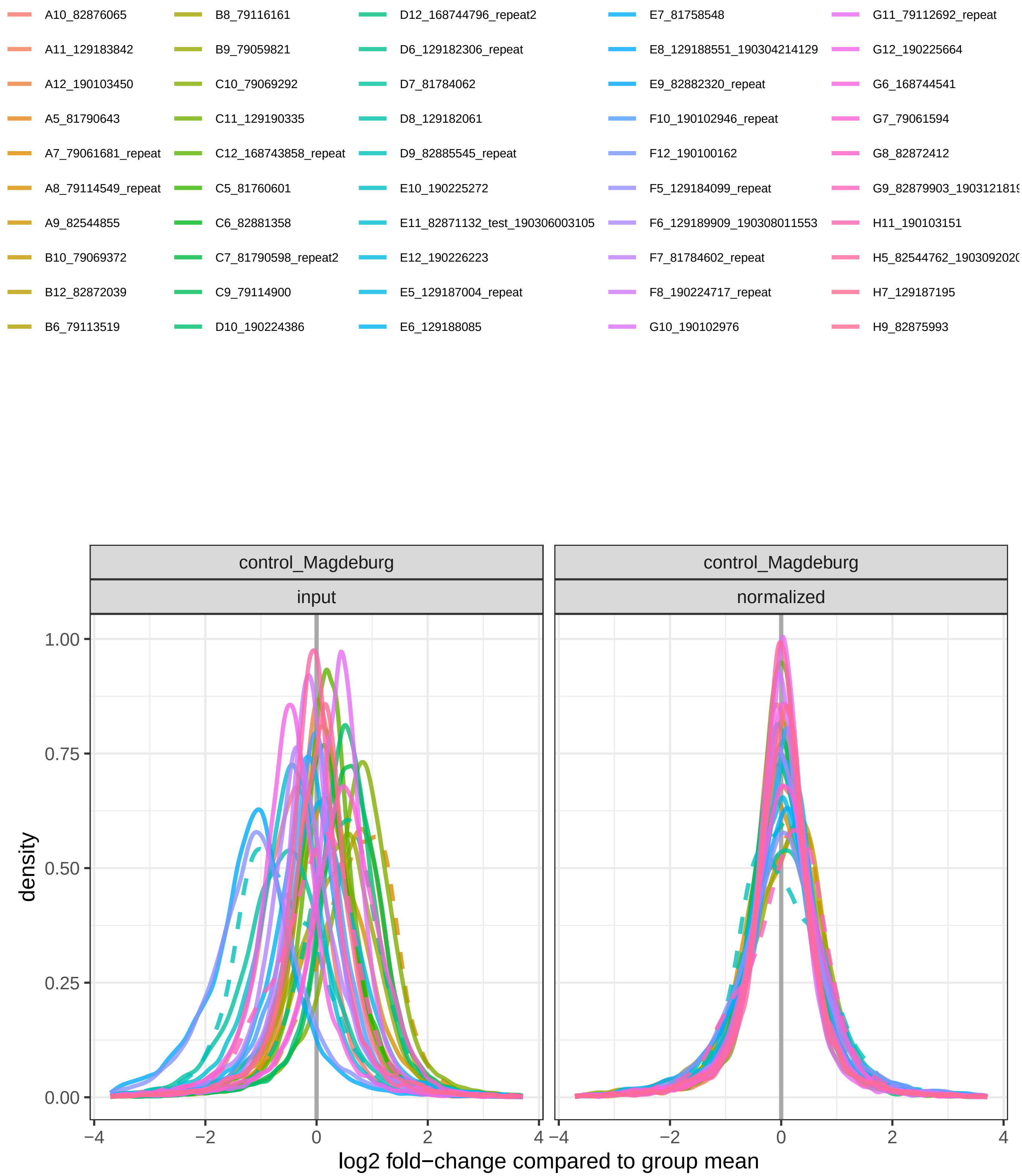


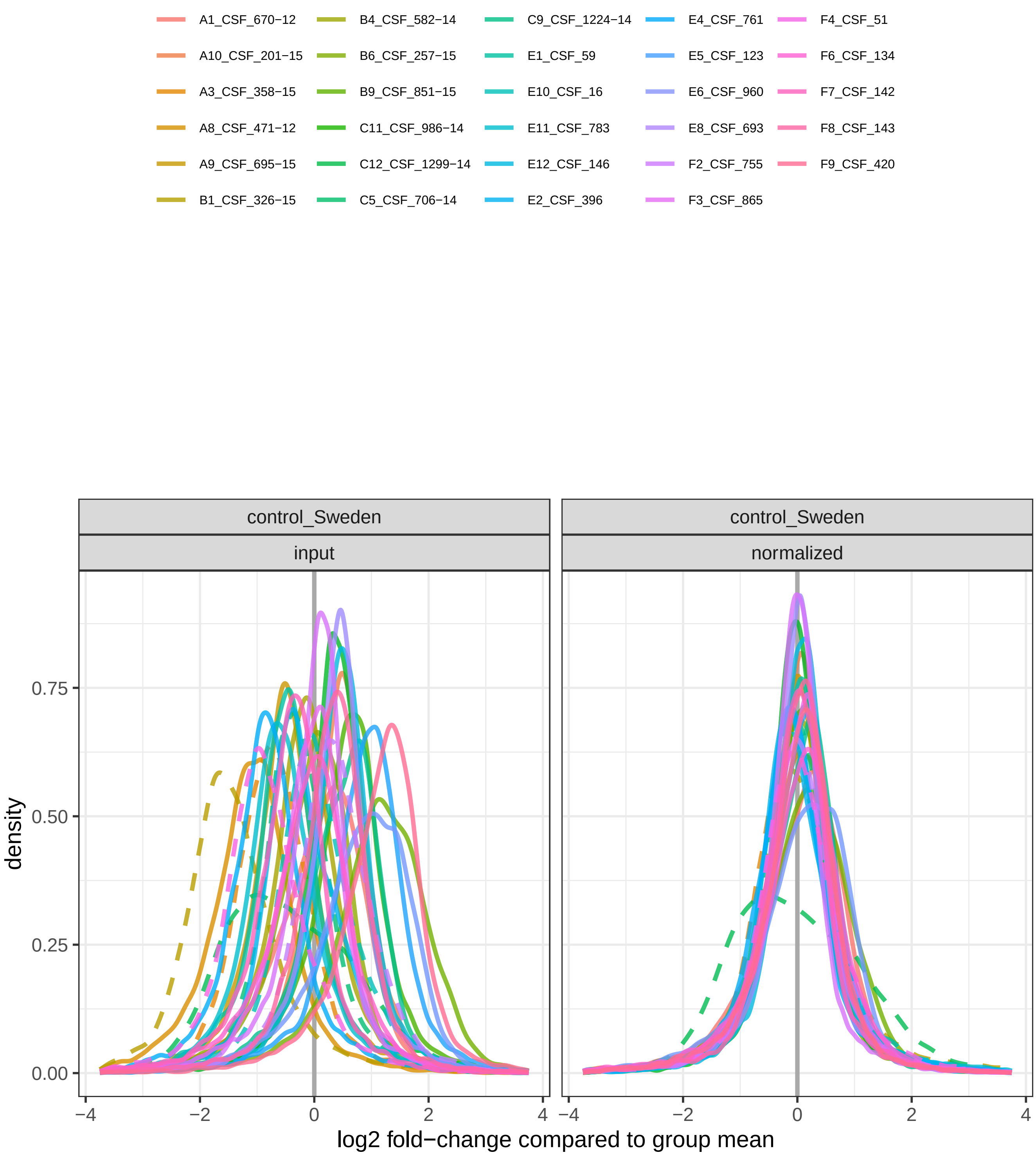

A2_82872920
A3_82883165_repeat2
A4_190104103
B1_129186923
B2_79114832
B3_79113129
C1_82545786
C3_82874751
D1_82545185
D2_79110561
D3_129189776
D4_168751414
E1_82883860
E2_129189650
E3_82871060_repeat
E4_190225869_repeat2
F1_82882396
F3_129190664
F4_190100053
G1_82881418_repeat
G2_168751345
G3_79069638
G4_190101656_repeat
H3_129190521_repeat
AD_Magdeburg
input
AD_Magdeburg
normalized
density
1.00
0.75
0.50
0.25
0.00
−4
−2
0
2
4
log2 fold−change compared to group mean

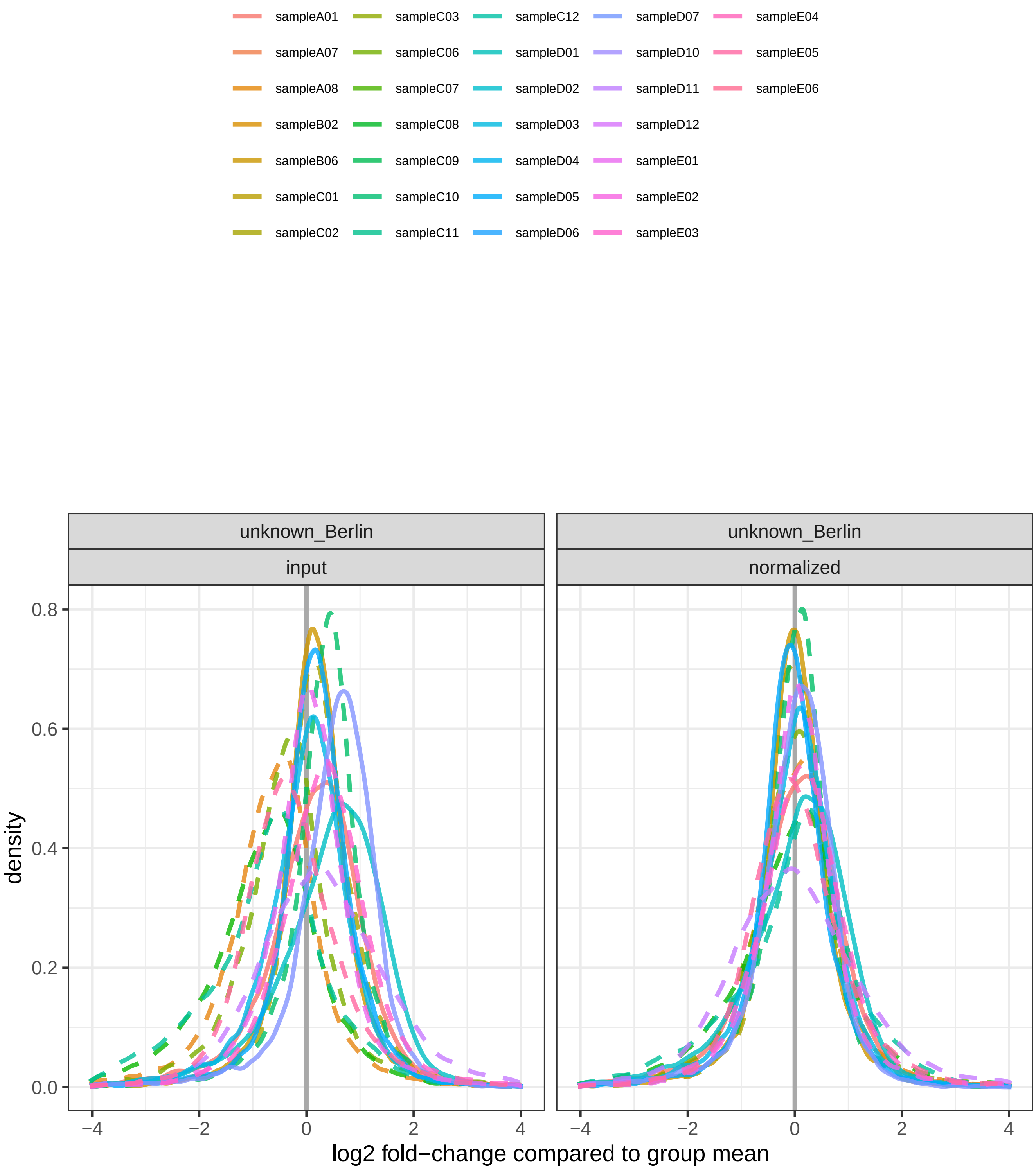

A11_CSF_36−15
A12_CSF_949−15
A2_CSF_248−15
A4_CSF_86−14
B11_CSF_506−14
B12_CSF_819−14_190217150250
B2_CSF_407−14
B3_CSF_545−14
B5_CSF_885−15
B7_CSF_496−15
B8_CSF_828−15
C1_CSF_656−15
C10_CSF_1289−14
C2_CSF_1239−14
C3_CSF_974−14
C4_CSF_976−13
C6_CSF_841−14
C7_CSF_381−14
C8_CSF_840−14
D1_CSF_530−13
D2_CSF_398−13
D3_CSF_863−13
D4_CSF_522−13
D5_CSF_503−13
D6_CSF_864−13
AD_Sweden
input
AD_Sweden
normalized
density
0.75
0.50
0.25
0.00
−2.5
0.0
2.5
log2 fold−change compared to group mean



sampleA02
sampleA03
sampleA04
sampleA05
sampleA06
sampleA09
sampleA10
sampleA11
sampleA12
sampleB01
sampleB03
sampleB04
sampleB05
sampleB07
sampleB08
sampleB09
sampleB10R2
sampleB11
sampleB12
sampleC04
sampleC05
sampleD08
sampled09
sampleE07
sampleE08
sampleE09
sampleE10
sampleE11
sampleE12
control_Berlin
input
control_Berlin
normalized
density
0.0
0.2
0.4
0.6
0.8
−2.5
0.0
2.5
log2 fold−change compared to group mean

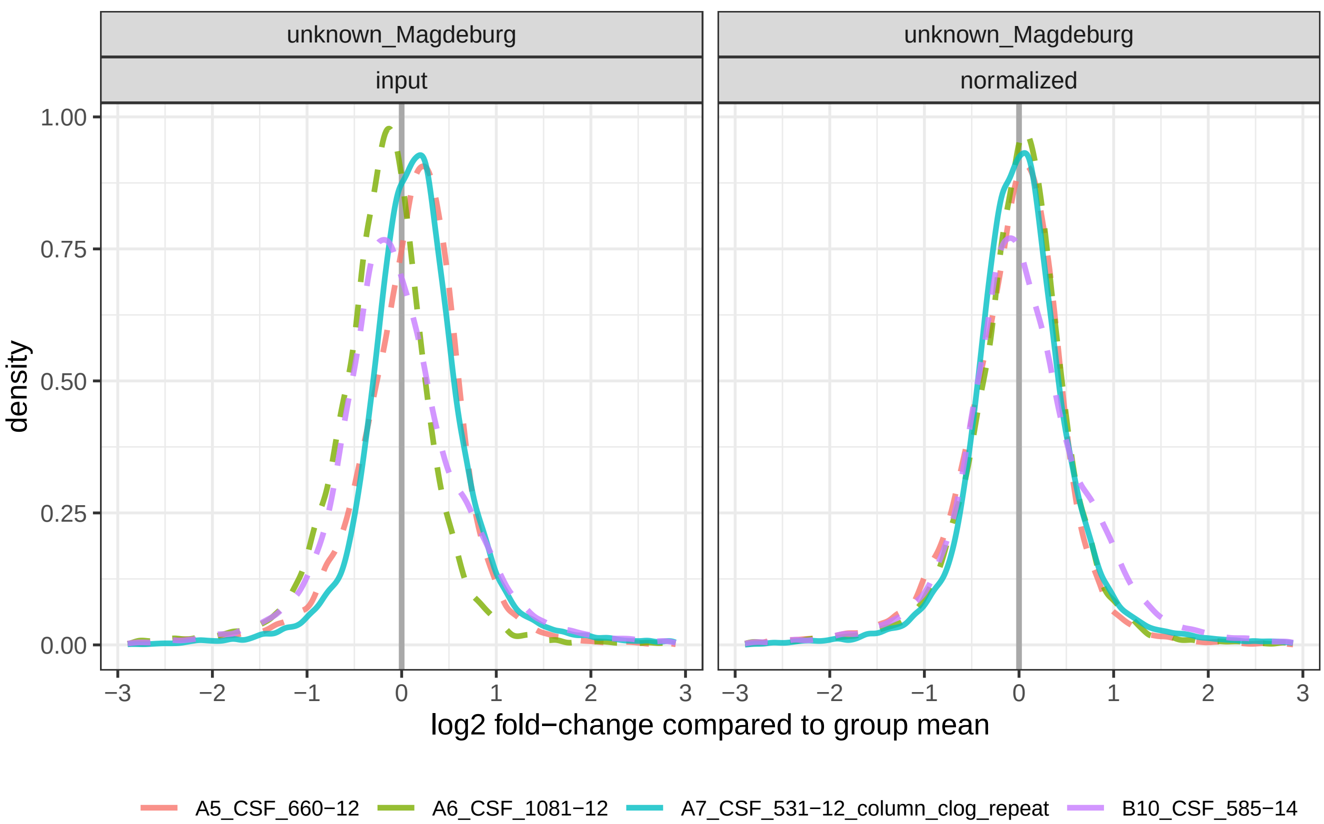

A10_82876065
A11_129183842
A12_190103450
A5_81790643
A7_79061681_repeat
A8_79114549_repeat
A9_82544855
B10_79069372
B12_82872039
B6_79113519
B8_79116161
B9_79059821
C10_79069292
C11_129190335
C12_168743858_repeat
C5_81760601
C6_82881358
C7_81790598_repeat2
C9_79114900
D10_190224386
D12_168744796_repeat2
D6_129182306_repeat
D7_81784062
D8_129182061
D9_82885545_repeat
E10_190225272
E11_82871132_test_190306003105
E12_190226223
E5_129187004_repeat
E6_129188085
E7_81758548
E8_129188551_190304214129
E9_82882320_repeat
F10_190102946_repeat
F12_190100162
F5_129184099_repeat
F6_129189909_190308011553
F7_81784602_repeat
F8_190224717_repeat
G10_190102976
G11_79112692_repeat
G12_190225664
G6_168744541
G7_79061594
G8_82872412
G9_82879903_190312181
H11_190103151
H5_82544762_190309202
H7_129187195
H9_82875993
control_Magdeburg
input
control_Magdeburg
normalized
density
1.00
0.75
0.50
0.25
0.00
−4
−2
0
2
4
log2 fold−change compared to group mean


A1_CSF_670−12
A10_CSF_201−15
A3_CSF_358−15
A8_CSF_471−12
A9_CSF_695−15
B1_CSF_326−15
B4_CSF_582−14
B6_CSF_257−15
B9_CSF_851−15
C11_CSF_986−14
C12_CSF_1299−14
C5_CSF_706−14
C9_CSF_1224−14
E1_CSF_59
E10_CSF_16
E11_CSF_783
E12_CSF_146
E2_CSF_396
E4_CSF_761
E5_CSF_123
E6_CSF_960
E8_CSF_693
F2_CSF_755
F3_CSF_865
F4_CSF_51
F6_CSF_134
F7_CSF_142
F8_CSF_143
F9_CSF_420
control_Sweden
input
control_Sweden
normalized
density
0.00
0.25
0.50
0.75
−4
−2
0
2
4
log2 fold−change compared to group mean



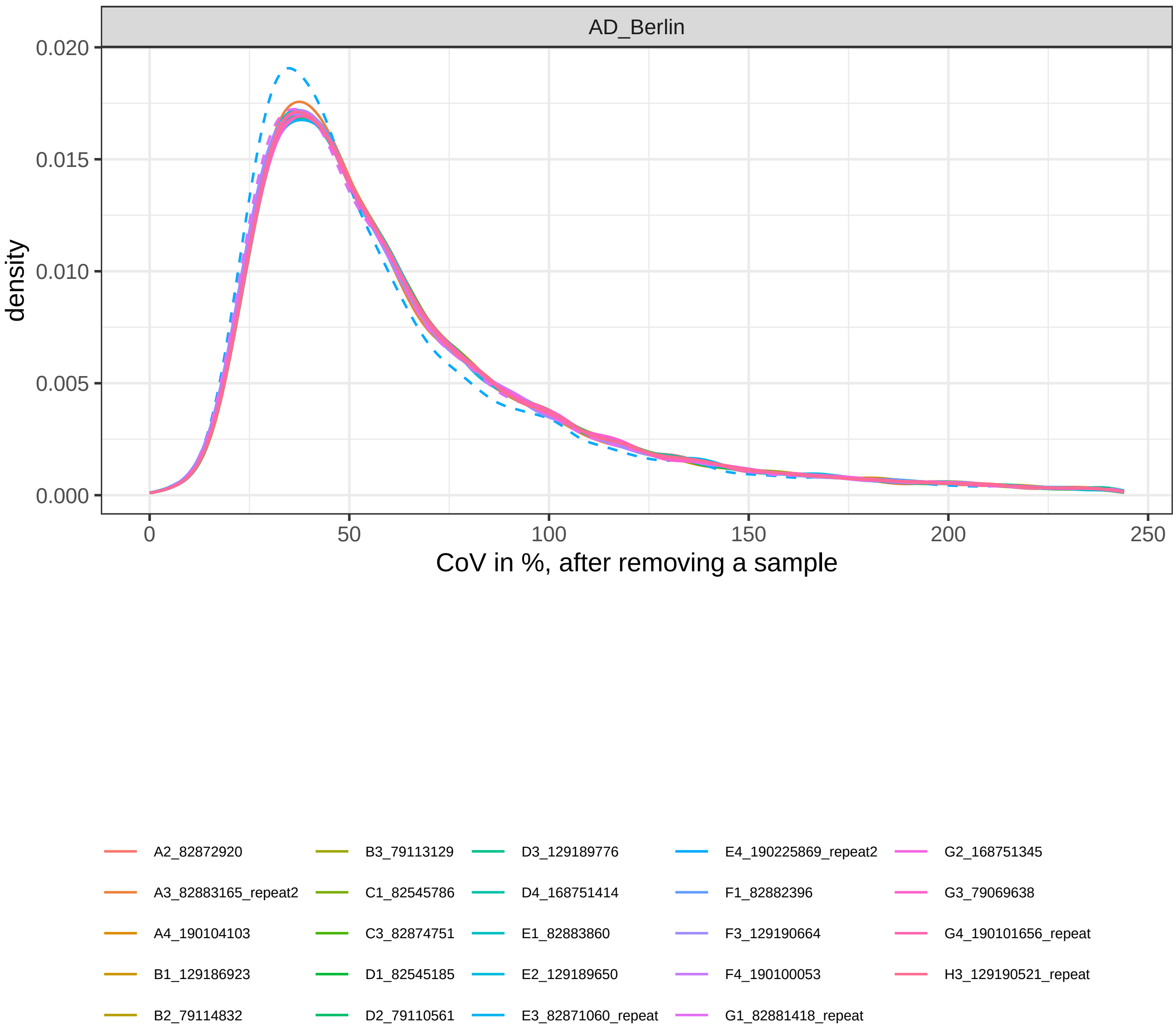
sampleA01
sampleA07
sampleA08
sampleB02
sampleB06
sampleC01
sampleC02
sampleC03
sampleC06
sampleC07
sampleC08
sampleC09
sampleC10
sampleC11
sampleC12
sampleD01
sampleD02
sampleD03
sampleD04
sampleD05
sampleD06
sampleD07
sampleD10
sampleD11
sampleD12
sampleE01
sampleE02
sampleE03
sampleE04
sampleE05
sampleE06
unknown_Berlin
input
unknown_Berlin
normalized
density
0.0
0.2
0.4
0.6
0.8
−4
−2
0
2
4
log2 fold−change compared to group mean

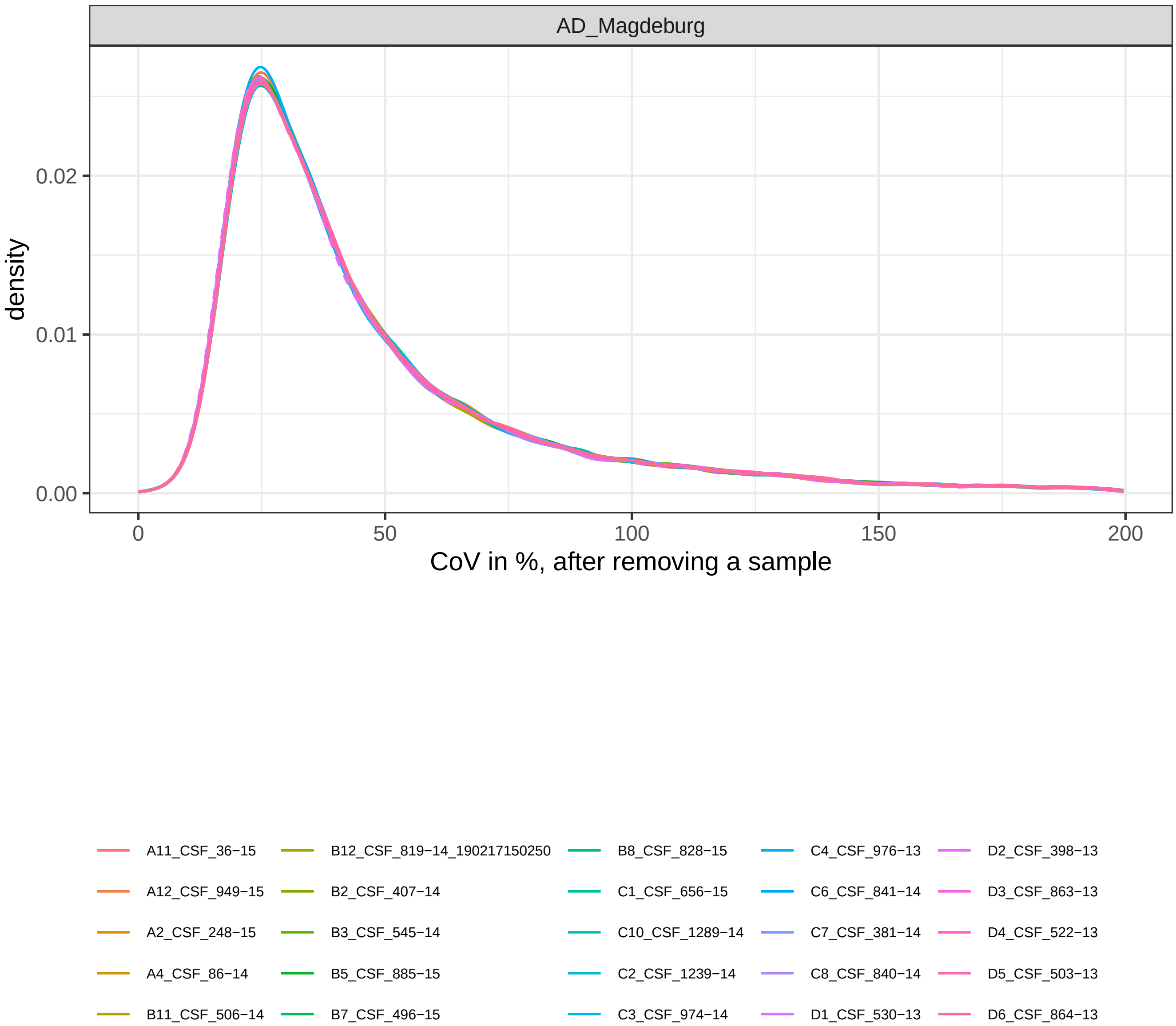

A1_81776353_repeat2
A6_82545313
B11_129182819
B4_190223925
B5_81783170
B7_81787765
C2_79070601
C4_168751222
C8_82882588_repeat
D11_129188366_repeat
D5_129186580_repeat
F11_82542649
F2_190226445
F9_82880110_190304154132
G5_82544653
H1_82881356

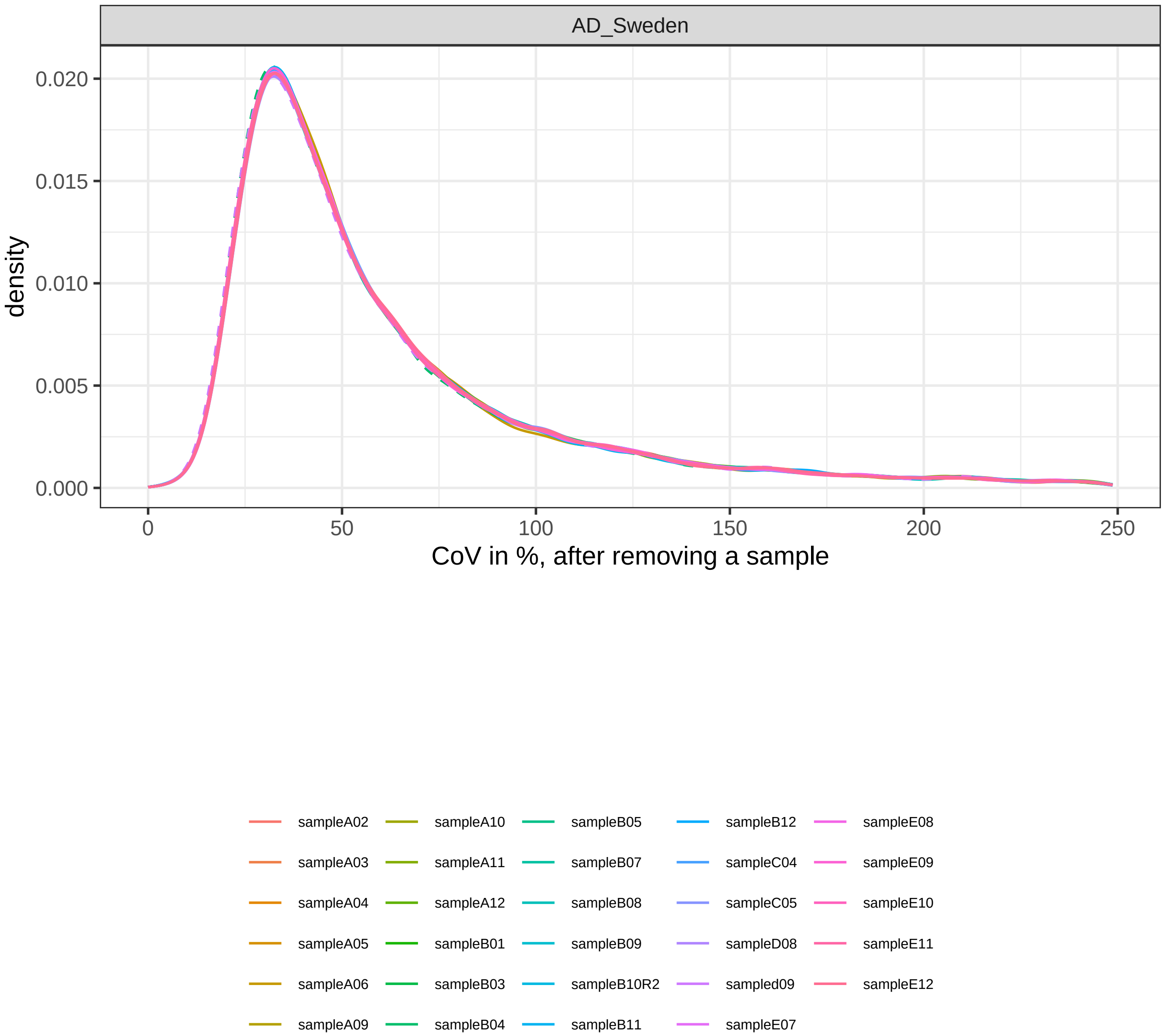

unknown_Magdeburg
input
unknown_Magdeburg
normalized
density
1.00
0.75
0.50
0.25
0.00
−3
−2
−1
0
1
2
3
log2 fold−change compared to group mean
A5_CSF_660−12
A6_CSF_1081−12
A7_CSF_531−12_column_clog_repeat
B10_CSF_585−14

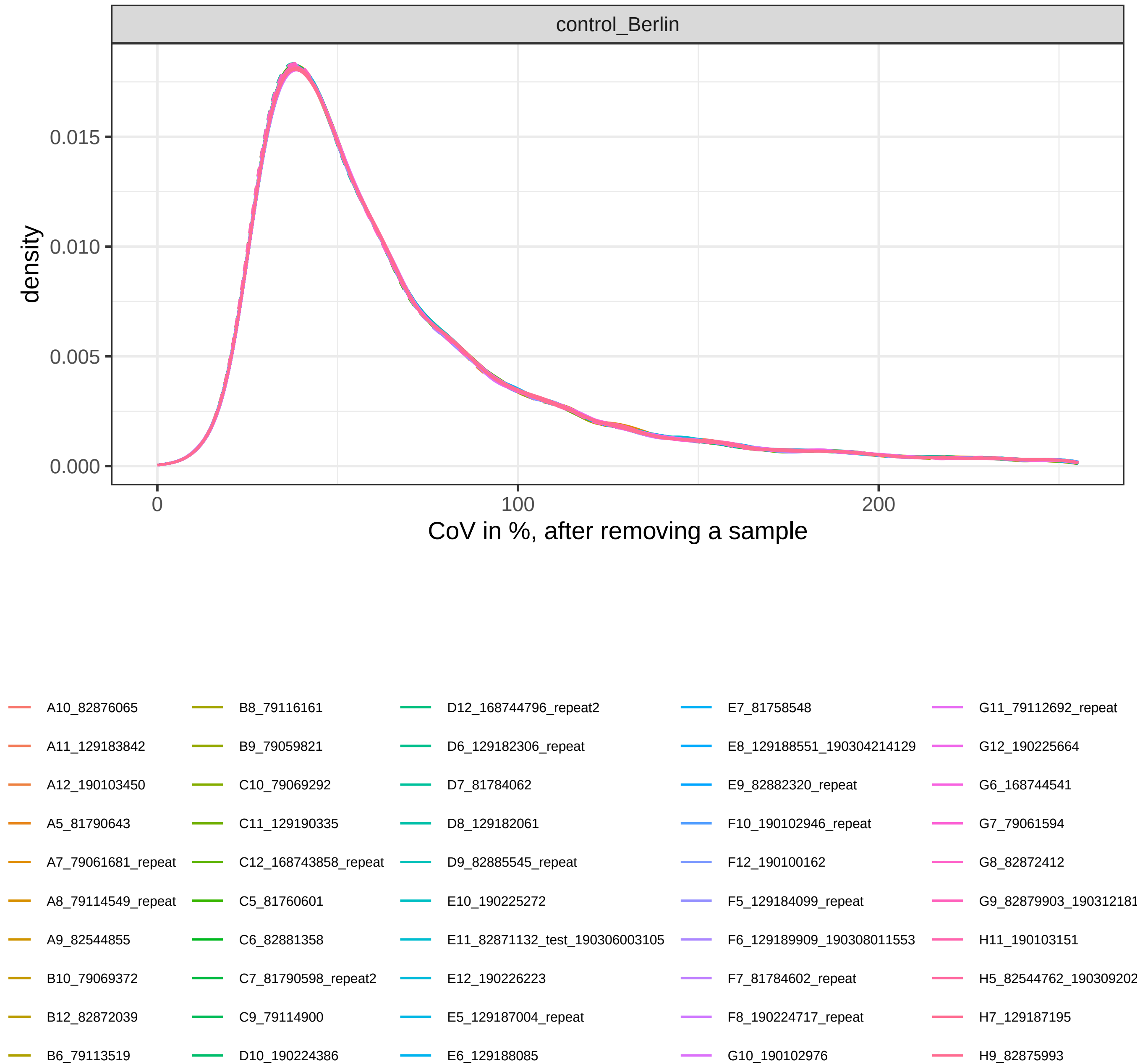
1.6.2 CoV, leave-one-out

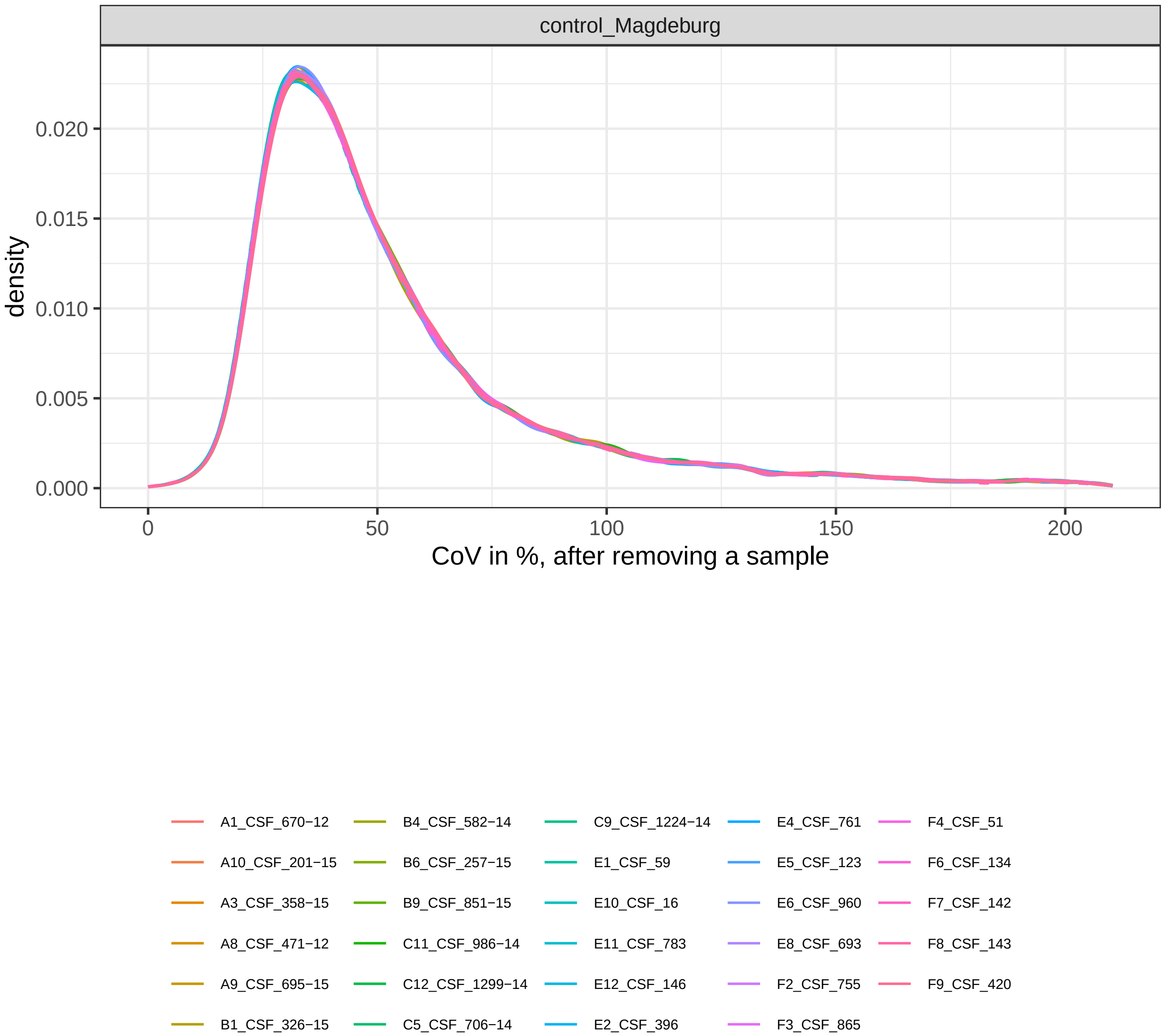
The figures below describe the effect of removing a particular sample prior to within-group Coefficient of Variation (CoV) computation. The lower the CoV distribution is for a sample, the better reproducibility we get by excluding it. Only sample groups with at least 4 replicates can be used for this analysis, so 3 samples remain after leaving one out. Samples marked as 'exclude' in the provided sample metadata are included in these analyses (shown as dashed lines), and only peptides with at least 3 data points across replicate samples (after leave-one-out) are used for each CoV computation.

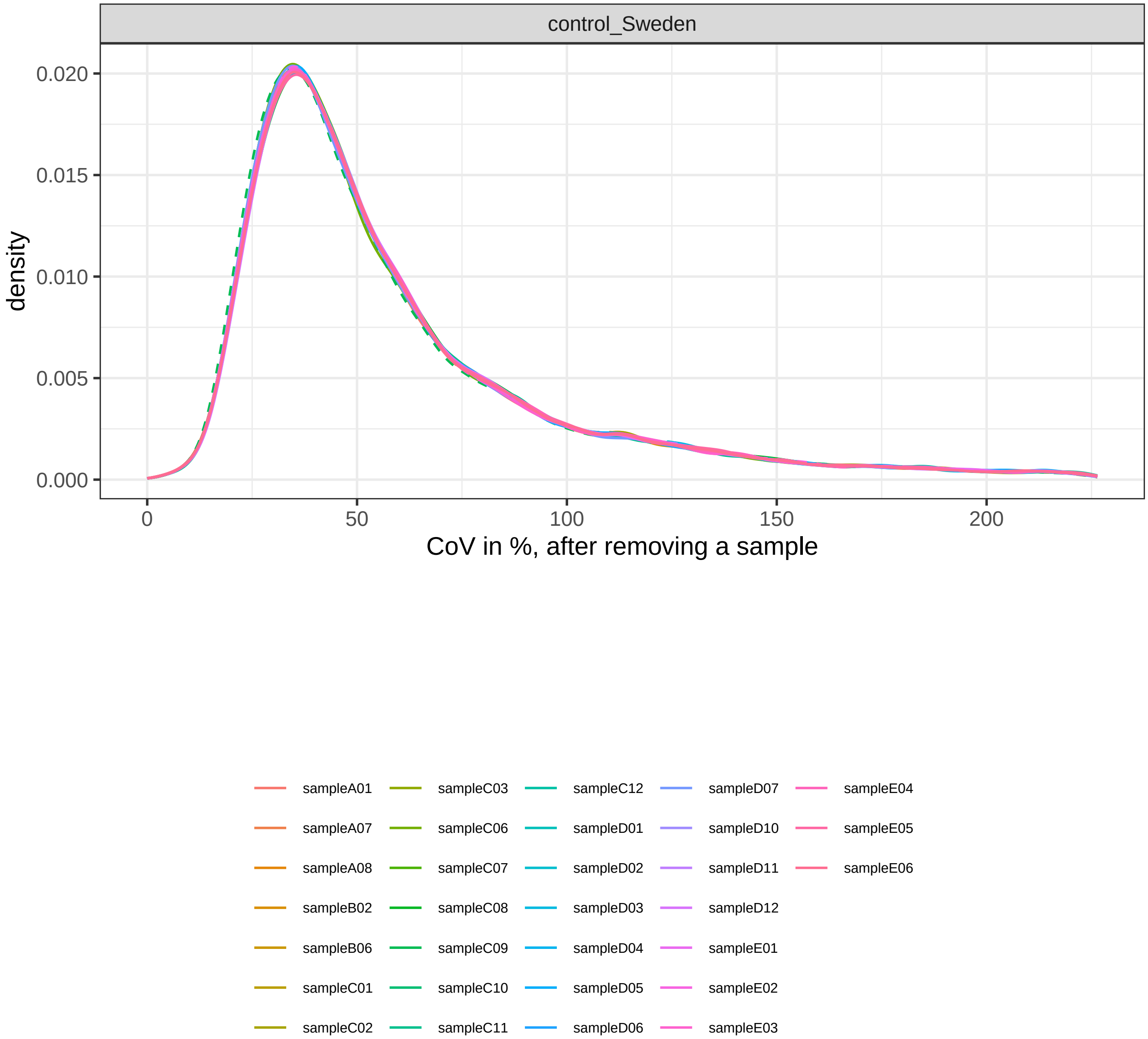


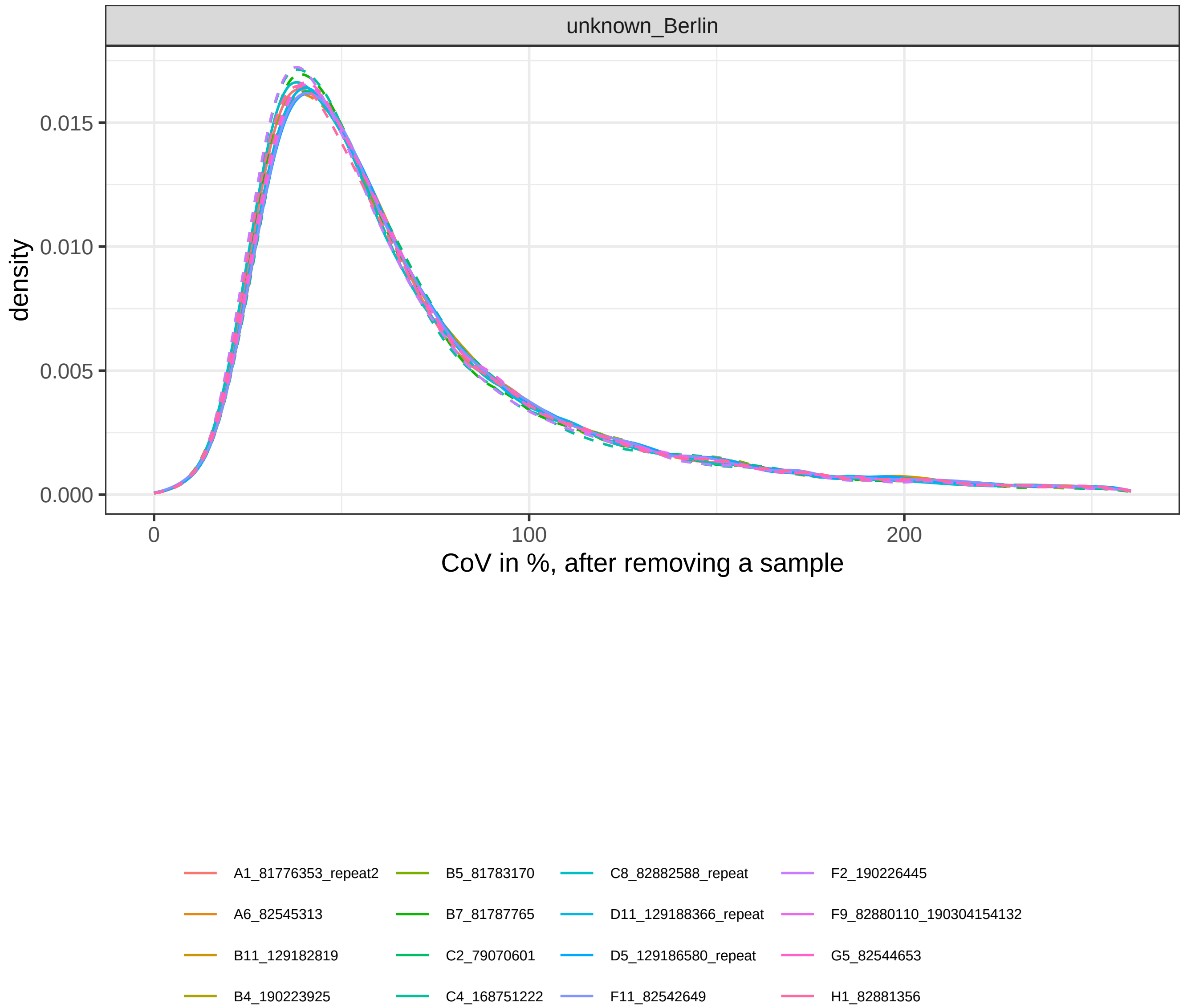

AD_Magdeburg
density
0.00
0.01
0.02
0
50
100
150
200
CoV in %, after removing a sample
A11_CSF_36−15
A12_CSF_949−15
A2_CSF_248−15
A4_CSF_86−14
B11_CSF_506−14
B12_CSF_819−14_190217150250
B2_CSF_407−14
B3_CSF_545−14
B5_CSF_885−15
B7_CSF_496−15
B8_CSF_828−15
C1_CSF_656−15
C10_CSF_1289−14
C2_CSF_1239−14
C3_CSF_974−14
C4_CSF_976−13
C6_CSF_841−14
C7_CSF_381−14
C8_CSF_840−14
D1_CSF_530−13
D2_CSF_398−13
D3_CSF_863−13
D4_CSF_522−13
D5_CSF_503−13
D6_CSF_864−13

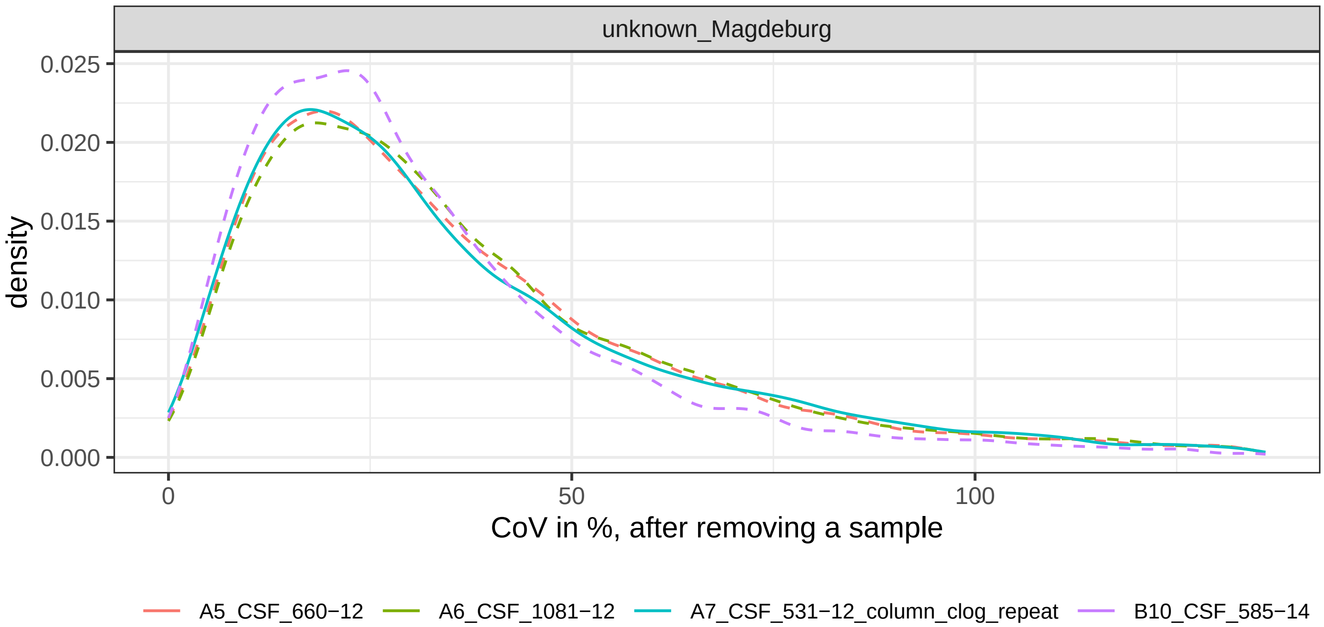

AD_Sweden
density
0.020
0.015
0.010
0.005
0.000
0
50
100
150
200
250
CoV in %, after removing a sample
sampleA02
sampleA03
sampleA04
sampleA05
sampleA06
sampleA09
sampleA10
sampleA11
sampleA12
sampleB01
sampleB03
sampleB04
sampleB05
sampleB07
sampleB08
sampleB09
sampleB10R2
sampleB11
sampleB12
sampleC04
sampleC05
sampleD08
sampled09
sampleE07
sampleE08
sampleE09
sampleE10
sampleE11
sampleE12

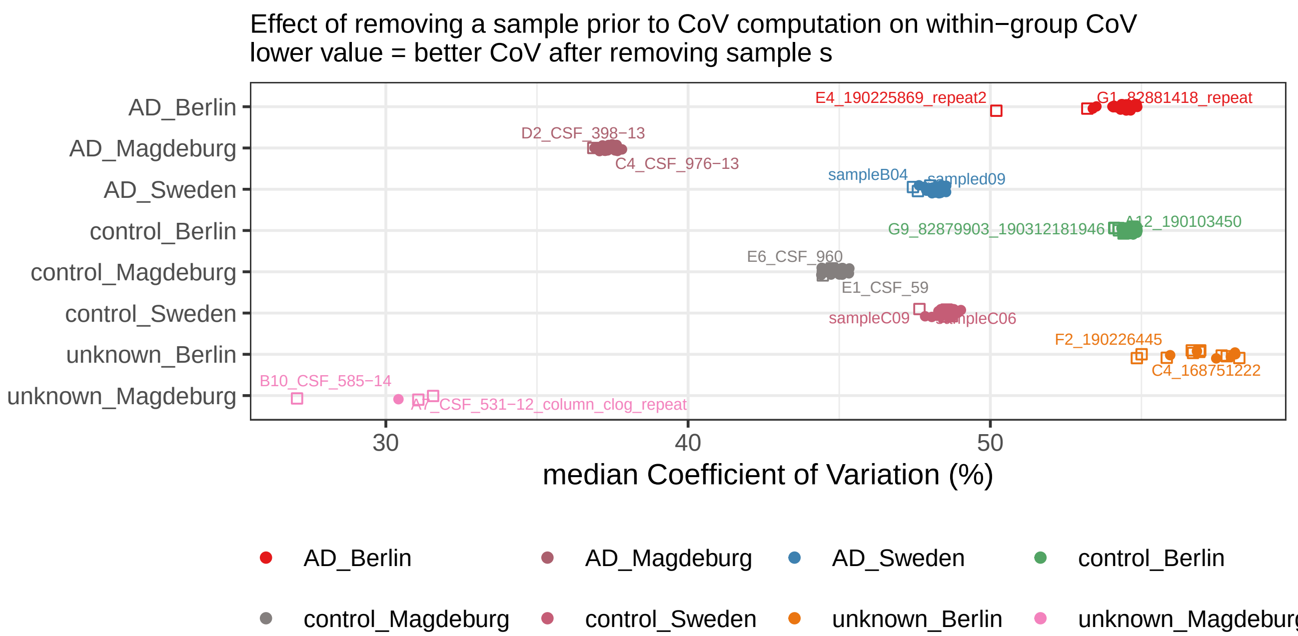

control_Berlin
density
0.015
0.010
0.005
0.000
0
100
200
CoV in %, after removing a sample
A10_82876065
A11_129183842
A12_190103450
A5_81790643
A7_79061681_repeat
A8_79114549_repeat
A9_82544855
B10_79069372
B12_82872039
B6_79113519
B8_79116161
B9_79059821
C10_79069292
C11_129190335
C12_168743858_repeat
C5_81760601
C6_82881358
C7_81790598_repeat2
C9_79114900
D10_190224386
D12_168744796_repeat2
D6_129182306_repeat
D7_81784062
D8_129182061
D9_82885545_repeat
E10_190225272
E11_82871132_test_190306003105
E12_190226223
E5_129187004_repeat
E6_129188085
E7_81758548
E8_129188551_190304214129
E9_82882320_repeat
F10_190102946_repeat
F12_190100162
F5_129184099_repeat
F6_129189909_190308011553
F7_81784602_repeat
F8_190224717_repeat
G10_190102976
G11_79112692_repeat
G12_190225664
G6_168744541
G7_79061594
G8_82872412
G9_82879903_190312181
H11_190103151
H5_82544762_190309202
H7_129187195
H9_82875993


control_Magdeburg
density
0.000
0.005
0.010
0.015
0.020
0
50
100
150
200
CoV in %, after removing a sample
A1_CSF_670−12
A10_CSF_201−15
A3_CSF_358−15
A8_CSF_471−12
A9_CSF_695−15
B1_CSF_326−15
B4_CSF_582−14
B6_CSF_257−15
B9_CSF_851−15
C11_CSF_986−14
C12_CSF_1299−14
C5_CSF_706−14
C9_CSF_1224−14
E1_CSF_59
E10_CSF_16
E11_CSF_783
E12_CSF_146
E2_CSF_396
E4_CSF_761
E5_CSF_123
E6_CSF_960
E8_CSF_693
F2_CSF_755
F3_CSF_865
F4_CSF_51
F6_CSF_134
F7_CSF_142
F8_CSF_143
F9_CSF_420


control_Sweden
density
0.020
0.015
0.010
0.005
0.000
0
50
100
150
200
CoV in %, after removing a sample
sampleA01
sampleA07
sampleA08
sampleB02
sampleB06
sampleC01
sampleC02
sampleC03
sampleC06
sampleC07
sampleC08
sampleC09
sampleC10
sampleC11
sampleC12
sampleD01
sampleD02
sampleD03
sampleD04
sampleD05
sampleD06
sampleD07
sampleD10
sampleD11
sampleD12
sampleE01
sampleE02
sampleE03
sampleE04
sampleE05
sampleE06


unknown_Berlin
density
0.015
0.010
0.005
0.000
0
100
200
CoV in %, after removing a sample
A1_81776353_repeat2
A6_82545313
B11_129182819
B4_190223925
B5_81783170
B7_81787765
C2_79070601
C4_168751222
C8_82882588_repeat
D11_129188366_repeat
D5_129186580_repeat
F11_82542649
F2_190226445
F9_82880110_190304154132
G5_82544653
H1_82881356


unknown_Magdeburg
density
0.025
0.020
0.015
0.010
0.005
0.000
0
50
100
CoV in %, after removing a sample
A5_CSF_660−12
A6_CSF_1081−12
A7_CSF_531−12_column_clog_repeat
B10_CSF_585−14


Effect of removing a sample prior to CoV computation on within−group CoV
lower value = better CoV after removing sample s
AD_Berlin
AD_Magdeburg
AD_Sweden
control_Berlin
control_Magdeburg
control_Sweden
unknown_Berlin
unknown_Magdeburg
E4_190225869_repeat2
G1_82881418_repeat
D2_CSF_398−13
C4_CSF_976−13
sampleB04
sampled09
G9_82879903_190312181946
A12_190103450
E6_CSF_960
E1_CSF_59
sampleC09
sampleC06
F2_190226445
C4_168751222
B10_CSF_585−14
A7_CSF_531−12_column_clog_repeat
30
40
50
median Coefficient of Variation (%)
AD_Berlin
AD_Magdeburg
AD_Sweden
control_Berlin
control_Magdeburg
control_Sweden
unknown_Berlin
unknown_Magdeburg

shortname	group	exclude	median CoV
E4_190225869_repeat2	AD_Berlin	TRUE	50.2
G1_82881418_repeat	AD_Berlin	TRUE	53.2
A3_82883165_repeat2	AD_Berlin	FALSE	53.4
F3_129190664	AD_Berlin	FALSE	53.5
E2_129189650	AD_Berlin	FALSE	54.0
B2_79114832	AD_Berlin	FALSE	54.1
D1_82545185	AD_Berlin	FALSE	54.1
A2_82872920	AD_Berlin	FALSE	54.2
G3_79069638	AD_Berlin	FALSE	54.3
D3_129189776	AD_Berlin	FALSE	54.3
H3_129190521_repeat	AD_Berlin	FALSE	54.3
E1_82883860	AD_Berlin	FALSE	54.4
F4_190100053	AD_Berlin	FALSE	54.5
F1_82882396	AD_Berlin	FALSE	54.5
C1_82545786	AD_Berlin	FALSE	54.5
E3_82871060_repeat	AD_Berlin	FALSE	54.6
G4_190101656_repeat	AD_Berlin	FALSE	54.6
B1_129186923	AD_Berlin	FALSE	54.6
D4_168751414	AD_Berlin	FALSE	54.6
G2_168751345	AD_Berlin	FALSE	54.8
D2_79110561	AD_Berlin	FALSE	54.8
A4_190104103	AD_Berlin	FALSE	54.8
C3_82874751	AD_Berlin	FALSE	54.8
B3_79113129	AD_Berlin	FALSE	54.9
D2_CSF_398-13	AD_Magdeburg	TRUE	36.9
C4_CSF_976-13	AD_Magdeburg	FALSE	36.9
B12_CSF_819-14_190217150250	AD_Magdeburg	FALSE	37.1
C7_CSF_381-14	AD_Magdeburg	FALSE	37.1
A12_CSF_949-15	AD_Magdeburg	FALSE	37.2
A2_CSF_248-15	AD_Magdeburg	FALSE	37.2
D1_CSF_530-13	AD_Magdeburg	FALSE	37.2
C10_CSF_1289-14	AD_Magdeburg	FALSE	37.3
D4_CSF_522-13	AD_Magdeburg	FALSE	37.3
B3_CSF_545-14	AD_Magdeburg	FALSE	37.3
A11_CSF_36-15	AD_Magdeburg	FALSE	37.4
B5_CSF_885-15	AD_Magdeburg	FALSE	37.4
B8_CSF_828-15	AD_Magdeburg	FALSE	37.5
B2_CSF_407-14	AD_Magdeburg	FALSE	37.5
A4_CSF_86-14	AD_Magdeburg	FALSE	37.5
B11_CSF_506-14	AD_Magdeburg	FALSE	37.6
D5_CSF_503-13	AD_Magdeburg	FALSE	37.6
C3_CSF_974-14	AD_Magdeburg	FALSE	37.6
B7_CSF_496-15	AD_Magdeburg	FALSE	37.6
C6_CSF_841-14	AD_Magdeburg	FALSE	37.6
C8_CSF_840-14	AD_Magdeburg	FALSE	37.7
D3_CSF_863-13	AD_Magdeburg	FALSE	37.7
C1_CSF_656-15	AD_Magdeburg	FALSE	37.7
C2_CSF_1239-14	AD_Magdeburg	FALSE	37.8
D6_CSF_864-13	AD_Magdeburg	FALSE	37.8
sampleB04	AD_Sweden	TRUE	47.4

shortname	group	exclude	median CoV
sampled09	AD_Sweden	TRUE	47.6
sampleA06	AD_Sweden	FALSE	47.6
sampleB11	AD_Sweden	FALSE	47.8
sampleE09	AD_Sweden	FALSE	47.9
sampleE11	AD_Sweden	FALSE	47.9
sampleB03	AD_Sweden	TRUE	48.0
sampleB01	AD_Sweden	FALSE	48.0
sampleB10R2	AD_Sweden	FALSE	48.1
sampleB07	AD_Sweden	FALSE	48.1
sampleD08	AD_Sweden	FALSE	48.1
sampleC04	AD_Sweden	FALSE	48.1
sampleA03	AD_Sweden	FALSE	48.2
sampleB08	AD_Sweden	FALSE	48.2
sampleA10	AD_Sweden	FALSE	48.2
sampleB05	AD_Sweden	FALSE	48.2
sampleE07	AD_Sweden	FALSE	48.2
sampleA12	AD_Sweden	FALSE	48.3
sampleA05	AD_Sweden	FALSE	48.3
sampleA11	AD_Sweden	FALSE	48.3
sampleB12	AD_Sweden	FALSE	48.3
sampleA04	AD_Sweden	FALSE	48.4
sampleE10	AD_Sweden	FALSE	48.4
sampleE08	AD_Sweden	FALSE	48.4
sampleA02	AD_Sweden	FALSE	48.4
sampleA09	AD_Sweden	FALSE	48.4
sampleE12	AD_Sweden	FALSE	48.5
sampleB09	AD_Sweden	FALSE	48.5
sampleC05	AD_Sweden	FALSE	48.5
G9_82879903_190312181946	control_Berlin	TRUE	54.1
A12_190103450	control_Berlin	TRUE	54.1
C5_81760601	control_Berlin	TRUE	54.2
D7_81784062	control_Berlin	TRUE	54.3
G7_79061594	control_Berlin	TRUE	54.3
C7_81790598_repeat2	control_Berlin	FALSE	54.3
A8_79114549_repeat	control_Berlin	FALSE	54.4
F7_81784602_repeat	control_Berlin	FALSE	54.4
F12_190100162	control_Berlin	TRUE	54.4
B8_79116161	control_Berlin	TRUE	54.5
G10_190102976	control_Berlin	FALSE	54.5
C11_129190335	control_Berlin	FALSE	54.5
F10_190102946_repeat	control_Berlin	TRUE	54.5
F6_129189909_190308011553	control_Berlin	TRUE	54.5
F5_129184099_repeat	control_Berlin	FALSE	54.6
C9_79114900	control_Berlin	FALSE	54.6
E10_190225272	control_Berlin	TRUE	54.6
B6_79113519	control_Berlin	FALSE	54.6
G8_82872412	control_Berlin	FALSE	54.6
E8_129188551_190304214129	control_Berlin	FALSE	54.6
H11_190103151	control_Berlin	FALSE	54.6
D12_168744796_repeat2	control_Berlin	TRUE	54.6

shortname	group	exclude	median CoV
H9_82875993	control_Berlin	FALSE	54.6
B12_82872039	control_Berlin	FALSE	54.6
A9_82544855	control_Berlin	FALSE	54.6
E7_81758548	control_Berlin	FALSE	54.6
C10_79069292	control_Berlin	FALSE	54.7
B9_79059821	control_Berlin	FALSE	54.7
E11_82871132_test_190306003105	control_Berlin	FALSE	54.7
A10_82876065	control_Berlin	FALSE	54.7
E6_129188085	control_Berlin	TRUE	54.7
D8_129182061	control_Berlin	TRUE	54.7
A5_81790643	control_Berlin	FALSE	54.7
E5_129187004_repeat	control_Berlin	FALSE	54.7
E12_190226223	control_Berlin	FALSE	54.7
E9_82882320_repeat	control_Berlin	FALSE	54.7
C6_82881358	control_Berlin	FALSE	54.7
H7_129187195	control_Berlin	FALSE	54.7
D6_129182306_repeat	control_Berlin	FALSE	54.7
D10_190224386	control_Berlin	FALSE	54.8
B10_79069372	control_Berlin	FALSE	54.8
G6_168744541	control_Berlin	FALSE	54.8
G12_190225664	control_Berlin	FALSE	54.8
A11_129183842	control_Berlin	FALSE	54.8
H5_82544762_190309202008	control_Berlin	FALSE	54.8
C12_168743858_repeat	control_Berlin	FALSE	54.8
A7_79061681_repeat	control_Berlin	FALSE	54.8
D9_82885545_repeat	control_Berlin	FALSE	54.9
G11_79112692_repeat	control_Berlin	FALSE	54.9
F8_190224717_repeat	control_Berlin	FALSE	54.9
E6_CSF_960	control_Magdeburg	FALSE	44.4
E1_CSF_59	control_Magdeburg	FALSE	44.4
E10_CSF_16	control_Magdeburg	TRUE	44.5
B4_CSF_582-14	control_Magdeburg	FALSE	44.5
F7_CSF_142	control_Magdeburg	TRUE	44.5
E4_CSF_761	control_Magdeburg	FALSE	44.5
C9_CSF_1224-14	control_Magdeburg	TRUE	44.7
A9_CSF_695-15	control_Magdeburg	FALSE	44.7
E8_CSF_693	control_Magdeburg	FALSE	44.7
A3_CSF_358-15	control_Magdeburg	TRUE	44.8
E12_CSF_146	control_Magdeburg	FALSE	44.8
B6_CSF_257-15	control_Magdeburg	FALSE	44.9
E2_CSF_396	control_Magdeburg	FALSE	44.9
F6_CSF_134	control_Magdeburg	FALSE	45.0
A1_CSF_670-12	control_Magdeburg	FALSE	45.0
A8_CSF_471-12	control_Magdeburg	FALSE	45.0
C11_CSF_986-14	control_Magdeburg	FALSE	45.0
E5_CSF_123	control_Magdeburg	FALSE	45.0
E11_CSF_783	control_Magdeburg	FALSE	45.1
C12_CSF_1299-14	control_Magdeburg	FALSE	45.1
F9_CSF_420	control_Magdeburg	FALSE	45.1
A10_CSF_201-15	control_Magdeburg	FALSE	45.1

shortname	group	exclude	median CoV
F2_CSF_755	control_Magdeburg	FALSE	45.1
B1_CSF_326-15	control_Magdeburg	FALSE	45.1
F4_CSF_51	control_Magdeburg	FALSE	45.1
C5_CSF_706-14	control_Magdeburg	FALSE	45.2
F8_CSF_143	control_Magdeburg	FALSE	45.3
F3_CSF_865	control_Magdeburg	FALSE	45.3
B9_CSF_851-15	control_Magdeburg	FALSE	45.3
sampleC09	control_Sweden	TRUE	47.7
sampleC06	control_Sweden	FALSE	47.8
sampleD07	control_Sweden	FALSE	48.1
sampleA01	control_Sweden	FALSE	48.2
sampleB02	control_Sweden	FALSE	48.3
sampleE03	control_Sweden	FALSE	48.4
sampleD02	control_Sweden	FALSE	48.4
sampleD05	control_Sweden	FALSE	48.5
sampleE02	control_Sweden	TRUE	48.5
sampleC01	control_Sweden	TRUE	48.6
sampleE01	control_Sweden	FALSE	48.6
sampleC02	control_Sweden	FALSE	48.6
sampleD04	control_Sweden	FALSE	48.6
sampleD01	control_Sweden	TRUE	48.6
sampleC07	control_Sweden	FALSE	48.6
sampleC11	control_Sweden	FALSE	48.6
sampleC03	control_Sweden	FALSE	48.6
sampleB06	control_Sweden	FALSE	48.7
sampleD06	control_Sweden	FALSE	48.7
sampleA08	control_Sweden	TRUE	48.7
sampleE06	control_Sweden	FALSE	48.7
sampleD11	control_Sweden	TRUE	48.7
sampleC10	control_Sweden	TRUE	48.7
sampleA07	control_Sweden	FALSE	48.7
sampleC12	control_Sweden	FALSE	48.7
sampleE04	control_Sweden	FALSE	48.8
sampleE05	control_Sweden	FALSE	48.8
sampleD10	control_Sweden	FALSE	48.8
sampleD03	control_Sweden	FALSE	48.8
sampleC08	control_Sweden	FALSE	48.9
sampleD12	control_Sweden	FALSE	49.0
F2_190226445	unknown_Berlin	TRUE	54.8
C4_168751222	unknown_Berlin	TRUE	55.0
B7_81787765	unknown_Berlin	TRUE	55.8
C8_82882588_repeat	unknown_Berlin	FALSE	55.9
B5_81783170	unknown_Berlin	TRUE	56.7
H1_82881356	unknown_Berlin	TRUE	56.7
A1_81776353_repeat2	unknown_Berlin	FALSE	56.8
G5_82544653	unknown_Berlin	TRUE	56.9
A6_82545313	unknown_Berlin	TRUE	56.9
D11_129188366_repeat	unknown_Berlin	FALSE	57.5
F9_82880110_190304154132	unknown_Berlin	TRUE	57.7
B4_190223925	unknown_Berlin	TRUE	57.8

shortname	group	exclude	median CoV
F11_82542649	unknown_Berlin	FALSE	58.0
D5_129186580_repeat	unknown_Berlin	FALSE	58.1
B11_129182819	unknown_Berlin	FALSE	58.1
C2_79070601	unknown_Berlin	TRUE	58.2
B10_CSF_585-14	unknown_Magdeburg	TRUE	27.1
A7_CSF_531-12_column_clog_repeat	unknown_Magdeburg	FALSE	30.4
A5_CSF_660-12	unknown_Magdeburg	TRUE	31.1
A6_CSF_1081-12	unknown_Magdeburg	TRUE	31.6

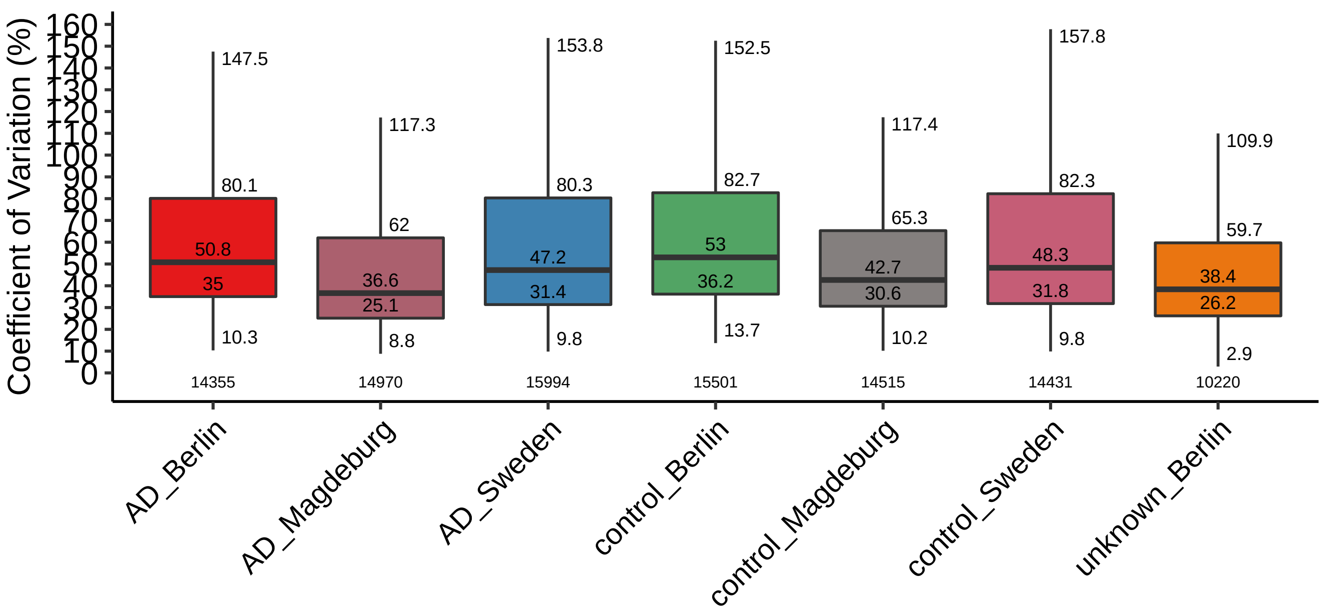
Leave-one-out impact on within-group CoV (%)

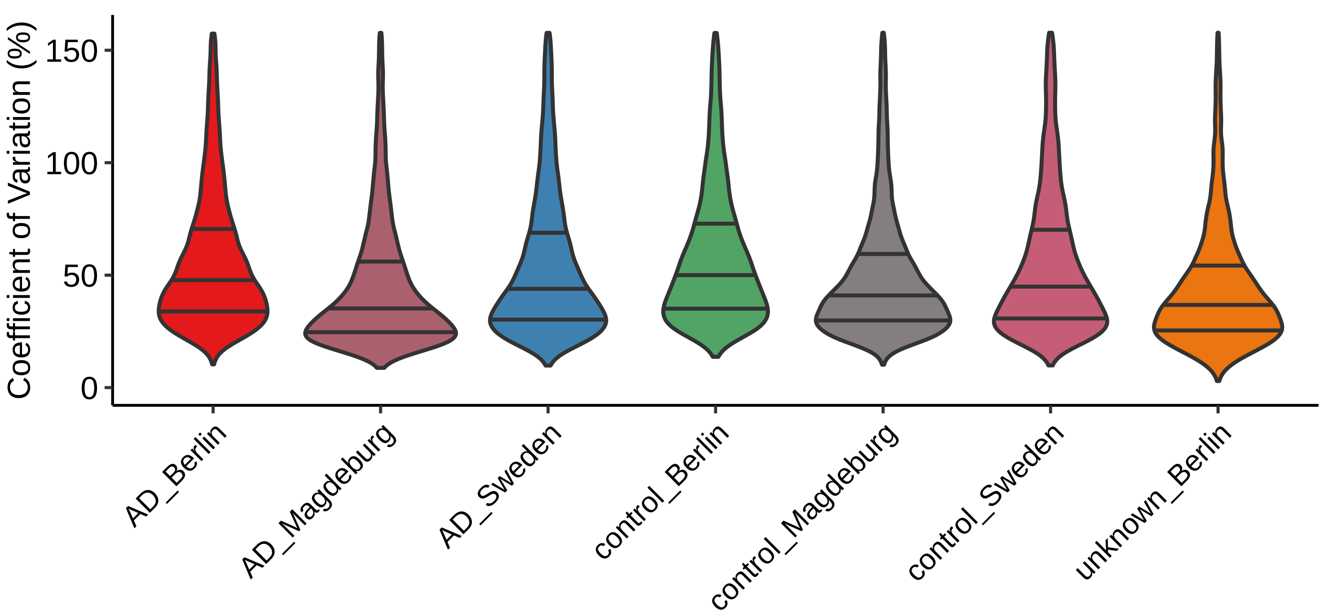
1.6.3 Coefficient of Variation

The Coefficient of Variation (CoV) is a quality metric for the reproducibility of replicate measurements, here visualized using box- and violin-plots.

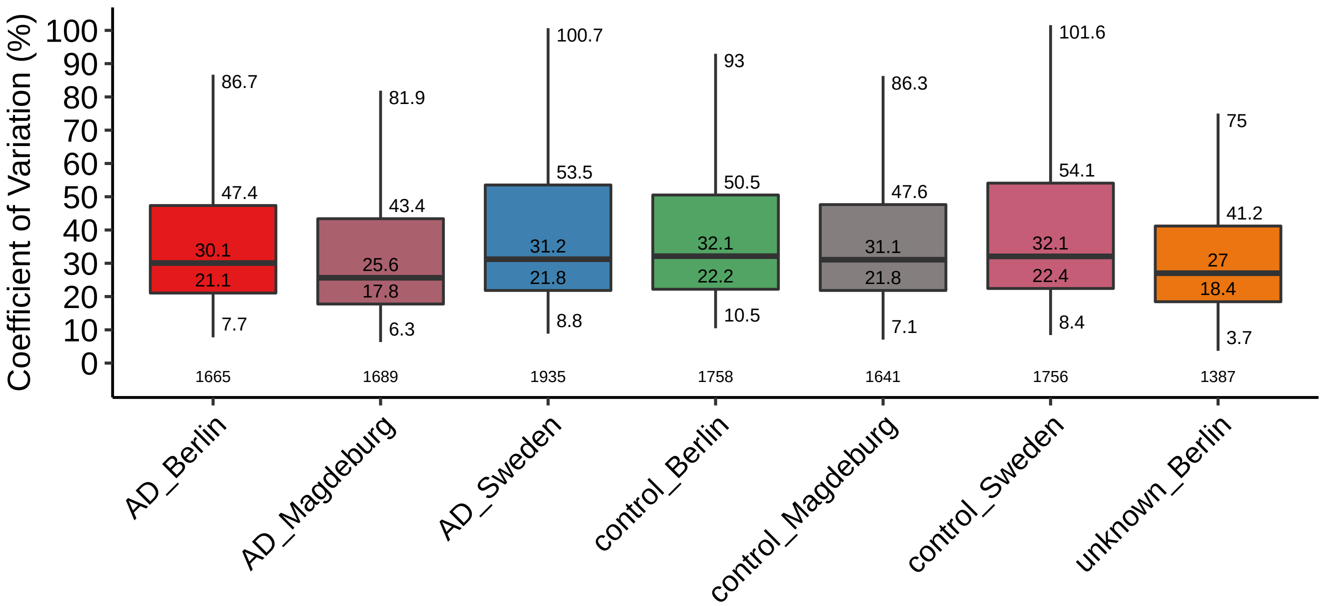
Only samples that are NOT marked 'exclude' in the provided sample metadata and are in a sample group among at least 3 replicates are used for these figures. The user-specified filtering rules (eg; filter_min_detect, filter_min_peptide_per_prot, etc.) were applied within each sample group independently and remaining peptides were subsequently normalized. Only peptides with at least 3 data points across replicate samples are used for each CoV computation.

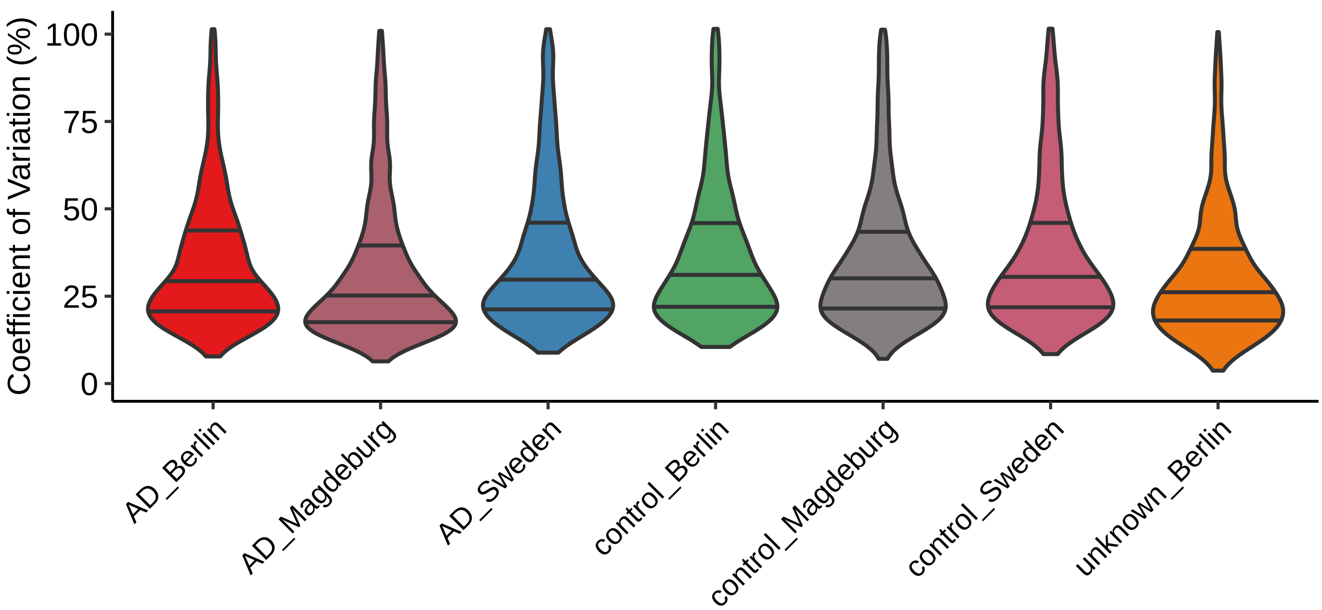
Peptide-level CoV:





Protein-level CoV: (analogous to peptide CoV's, but with additional MaxLFQ rollup to protein abundances)





1.7 PCA

A visualization of the first three PCA dimensions illustrates sample clustering. The goal of these figures is to detect global effects from a quality control perspective, such as samples from the same experiment batch clustering together, not to be sensitive to a minor subset of differentially abundant proteins (for which specialized statistical models can be applied downstream).

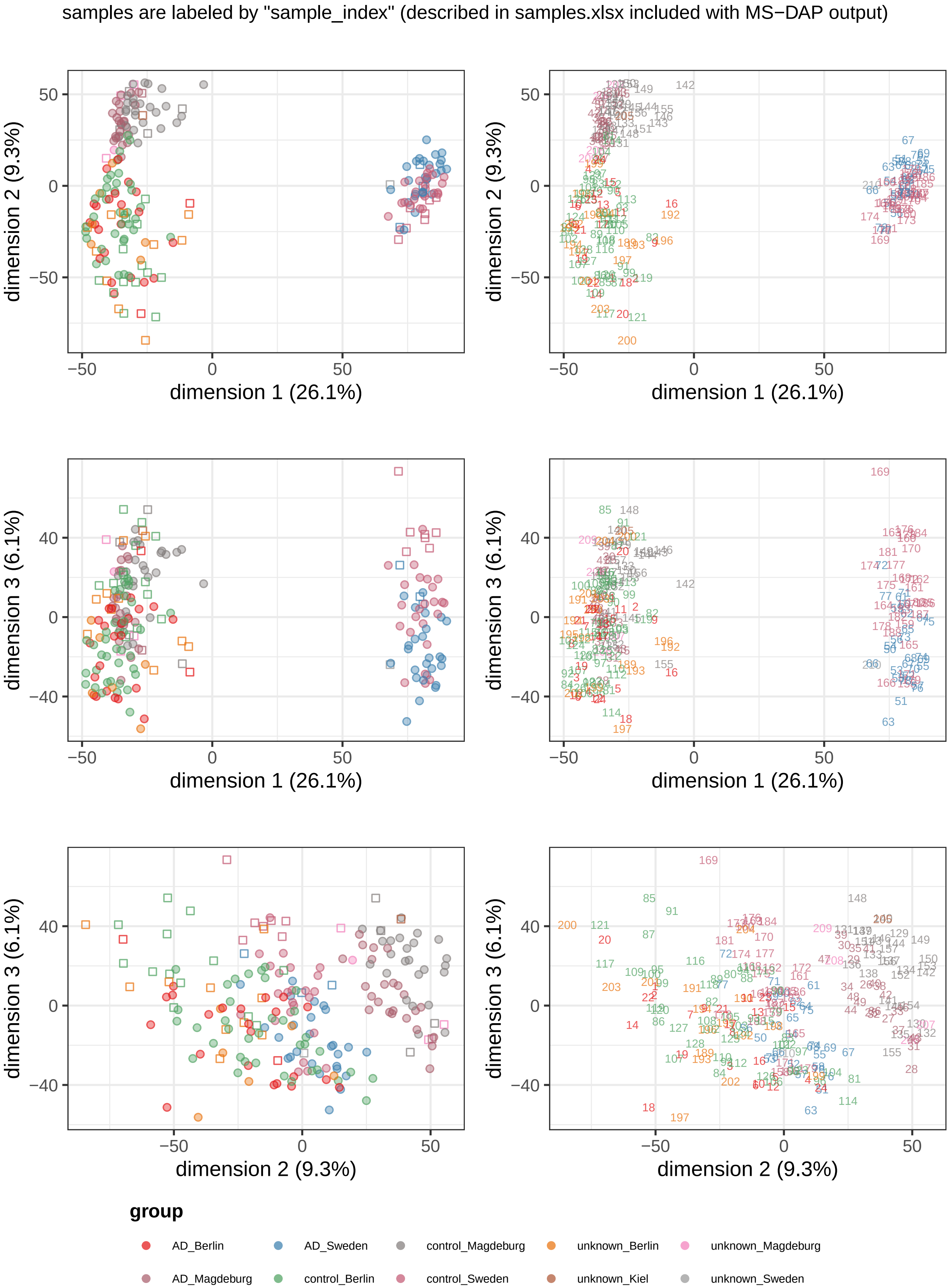
If additional sample metadata was provided, such as experiment batch, sample-prep dates, gel, etc., multiple PCA figures will be generated with respective color-codings. Users are encouraged to provide relevant experiment information as sample metadata and use these figures to search for unexpected batch effects.

The pcaMethods R package is used here to perform the Probabilistic PCA (PPCA). The set of peptides used for this analysis consists of those peptides that pass your filter criteria in every sample group. If any samples are marked as 'exclude' in the provided sample metadata, an additional PCA plot is generated with these samples included (depicting the 'exclude' samples as square symbols).

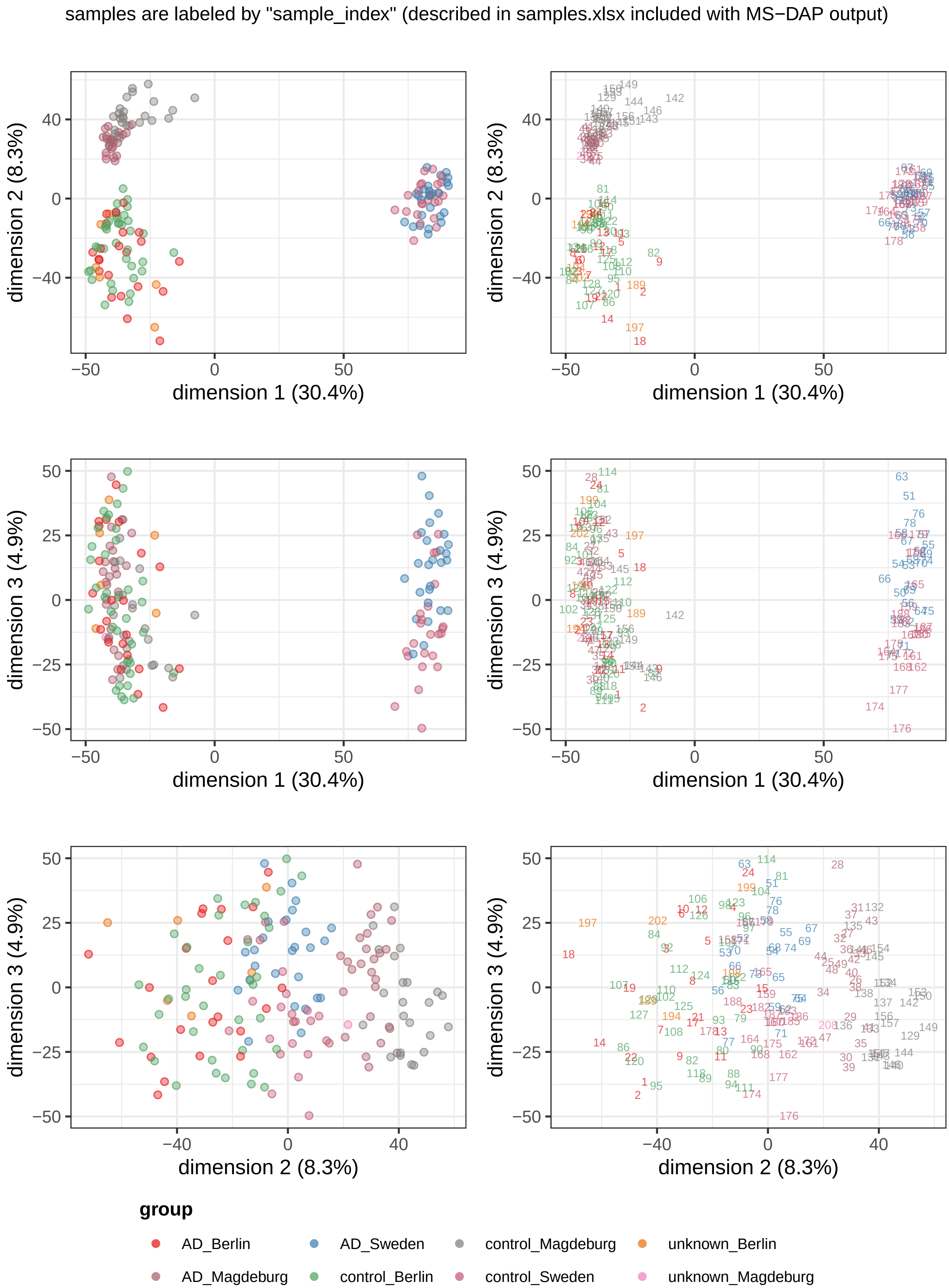
Rationale behind data filter
As mentioned above, the aim of the PCA figures is to identify global effects. To achieve this, we compute sample distances on the subset of peptides identified in each group which prevents rarely detected peptides/proteins from having a disproportionate effect on sample clustering. This pertains not only to 'randomly detected contaminant proteins' but also to proteins with abundance levels near the detection limit, which may be detected in only a subset of samples (eg; some measurements will be more successful/sensitive than others).

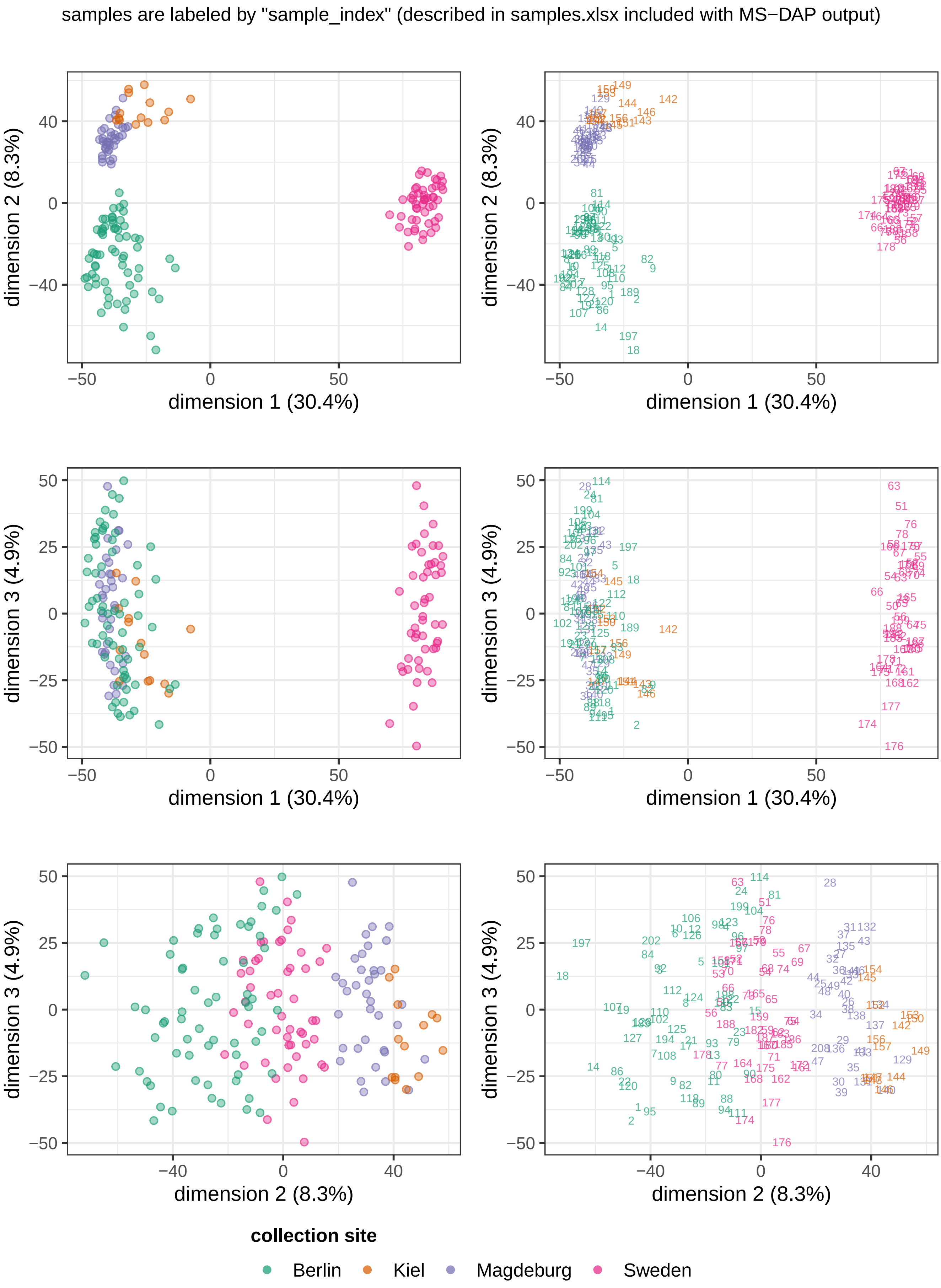
Figure legends
The first 3 principle components compared visually (1 *vs* 2, 1 *vs* 3, 2 *vs* 3) on the rows. Left- and right-side panels on each row represent the same figure without and with sample labels. The principle components are shown on the axis labels together with their respective percentage of variance explained. Samples marked as 'exclude' in the provided sample metadata, if any, are visualized as square shapes.

PCA of all samples, including those flagged as 'exclude', using 8892 peptides

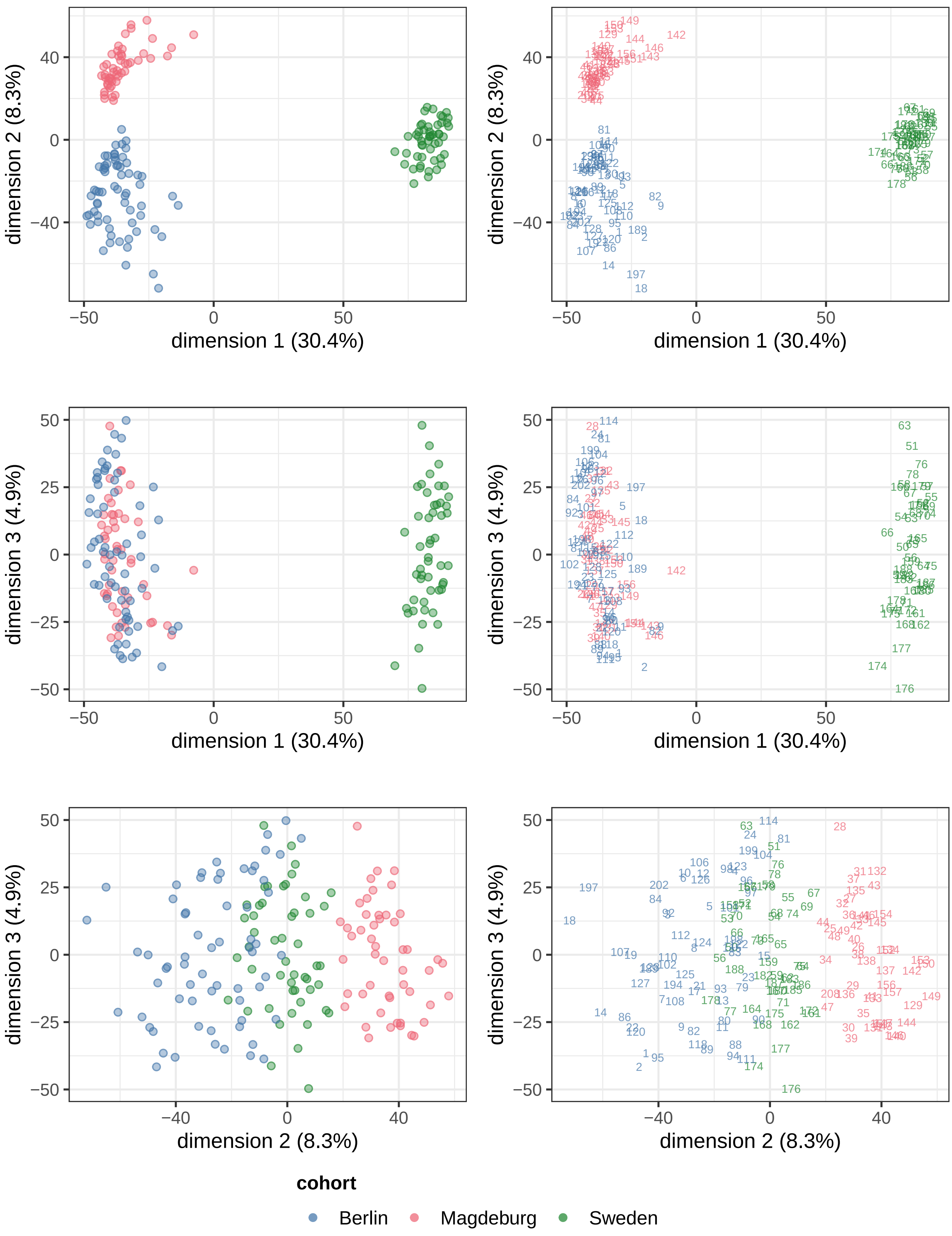


PCA only on samples not flagged as 'exclude', using 9164 peptides

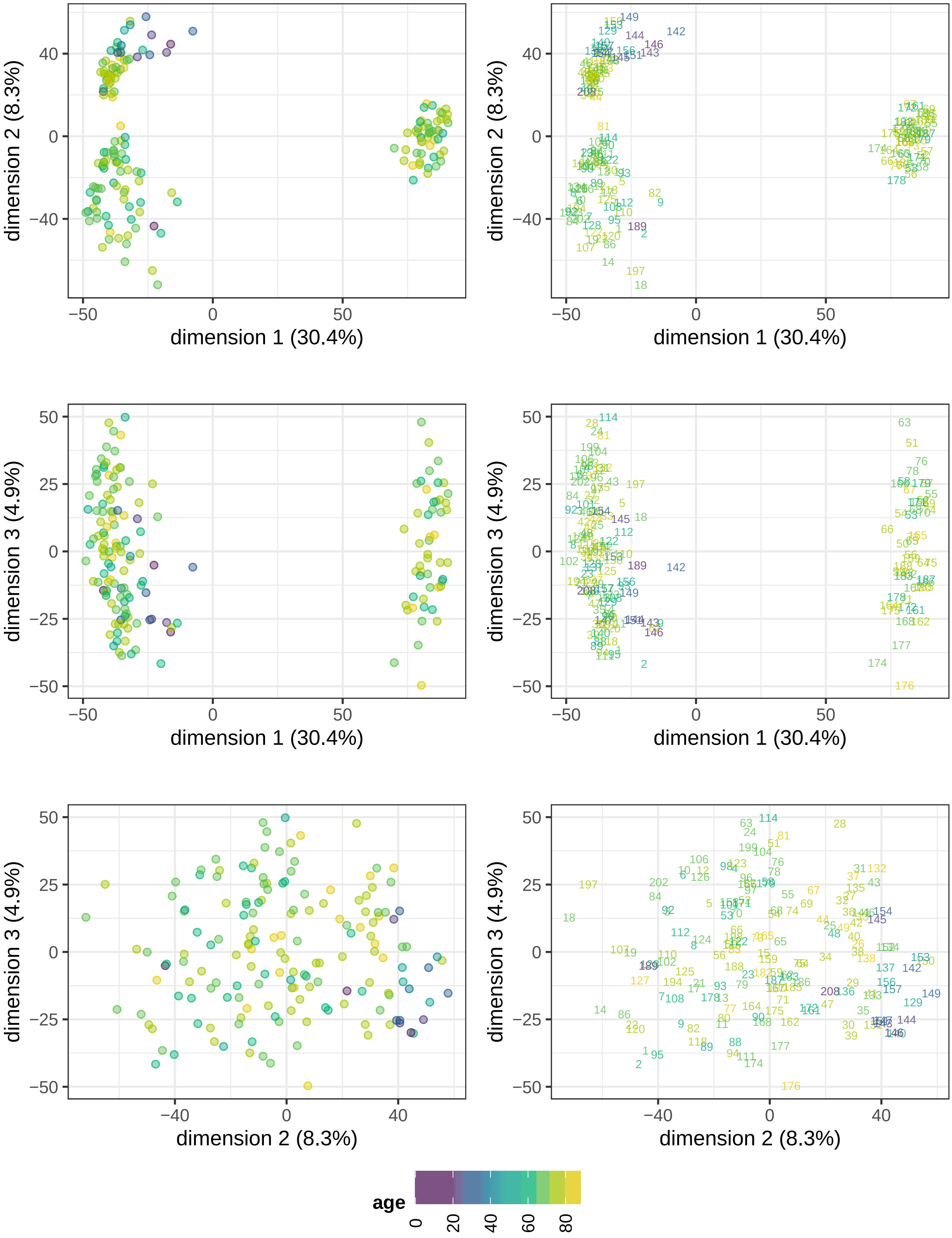


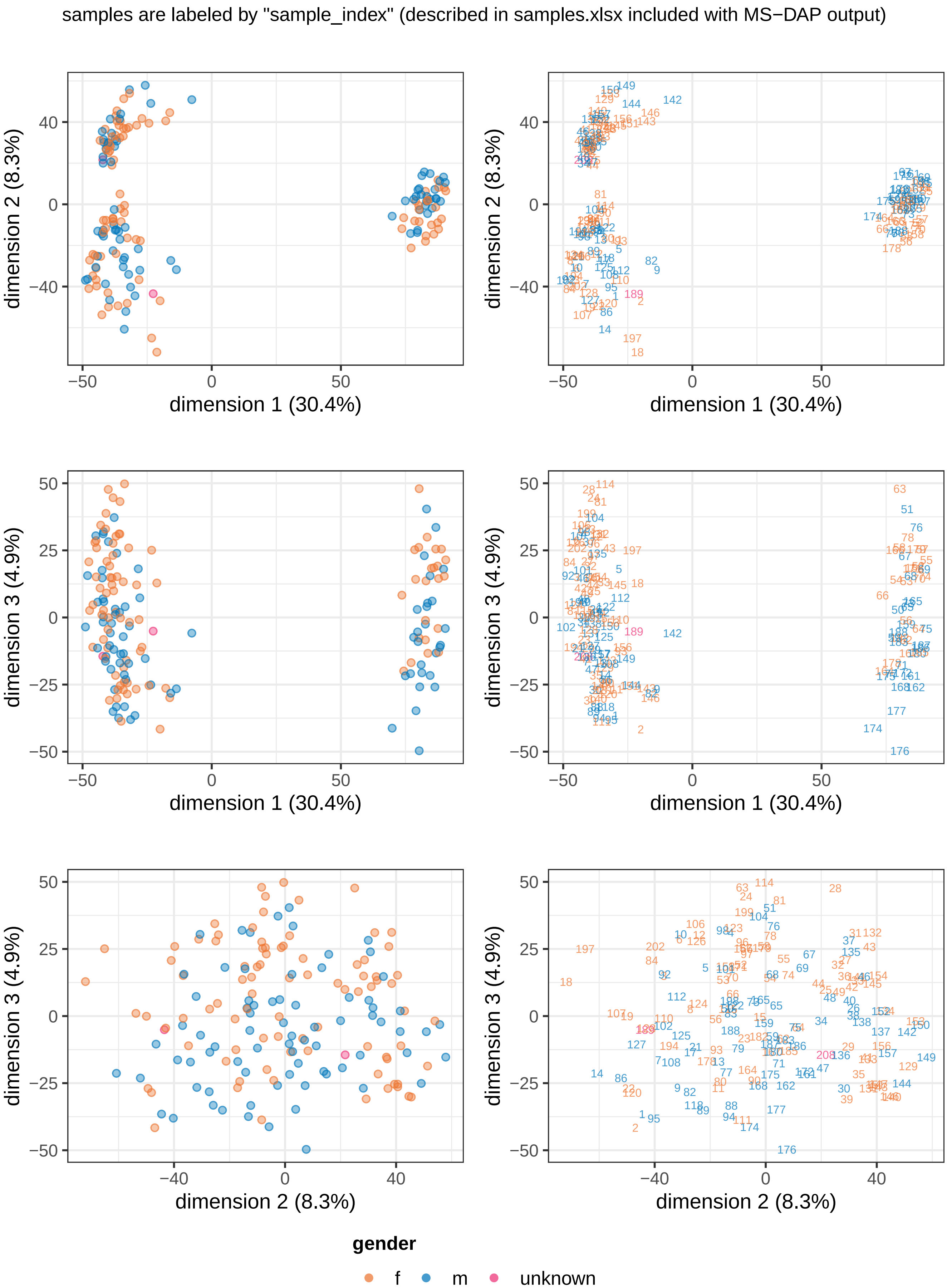

samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)
dimension 1 (30.4%)
dimension 2 (8.3%)
dimension 3 (4.9%)
collection site
Berlin
Kiel
Magdeburg
Sweden

samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)

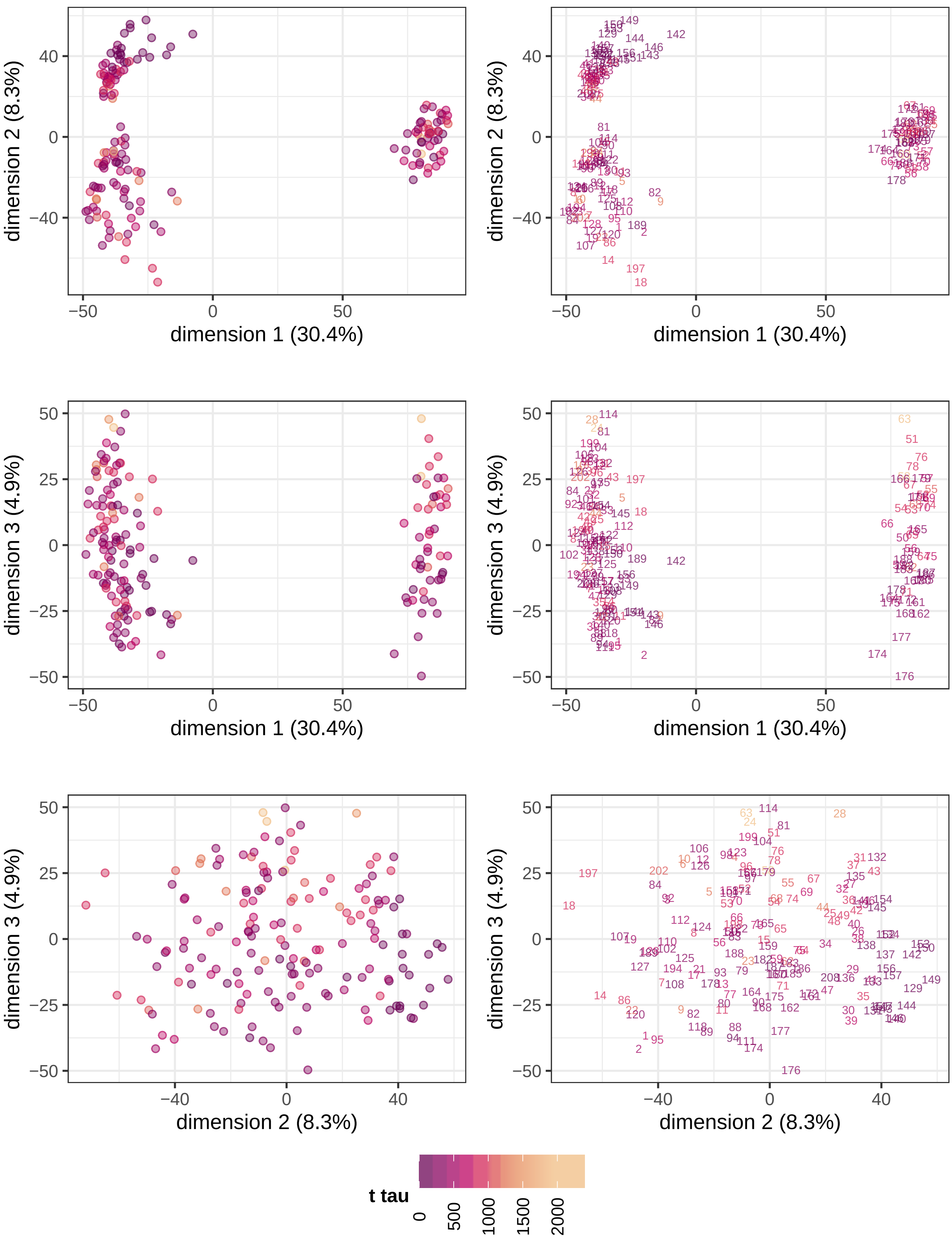


samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)

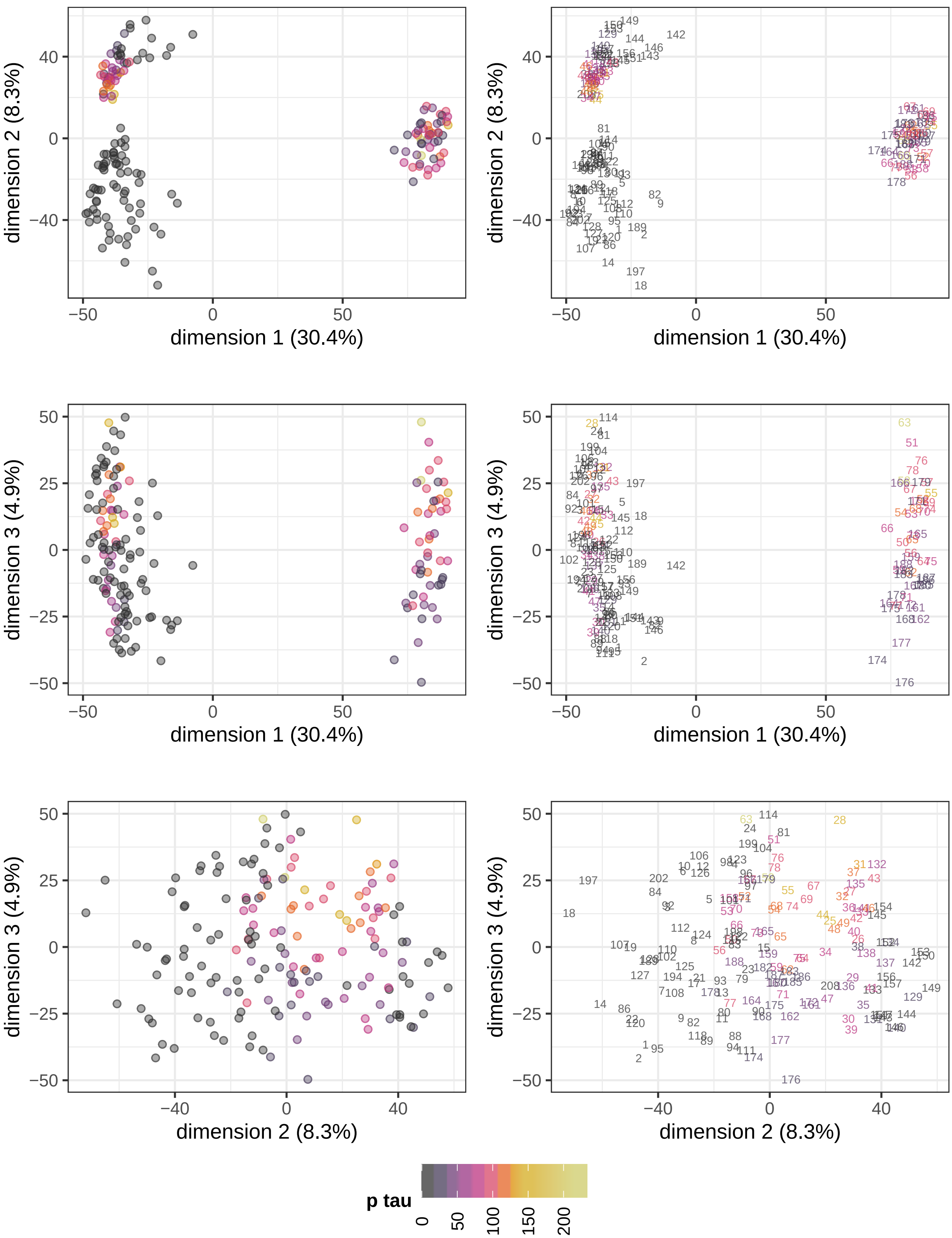



samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)
dimension 1 (30.4%)
dimension 2 (8.3%)
dimension 3 (4.9%)
gender
f
m
unknown

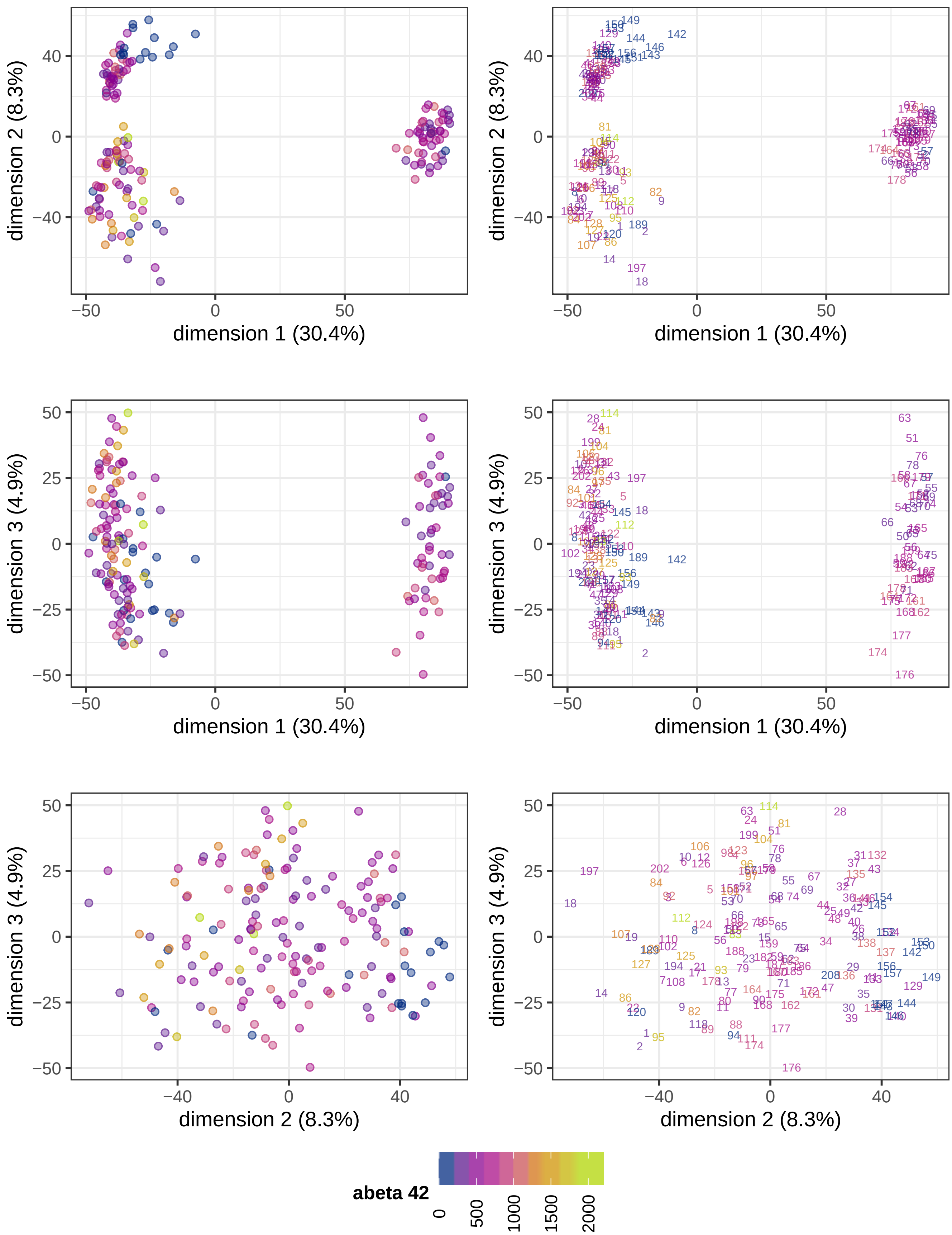
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



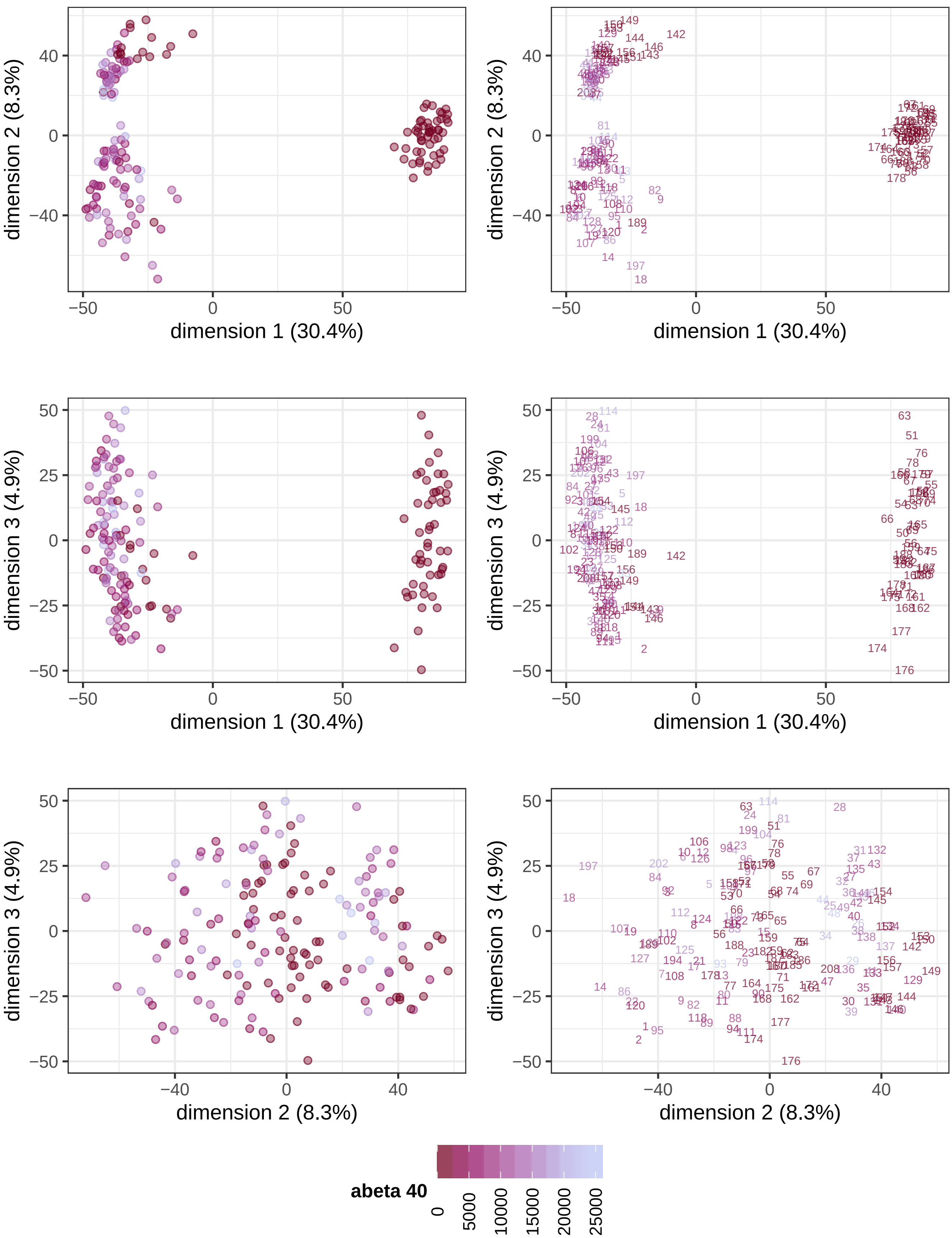
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



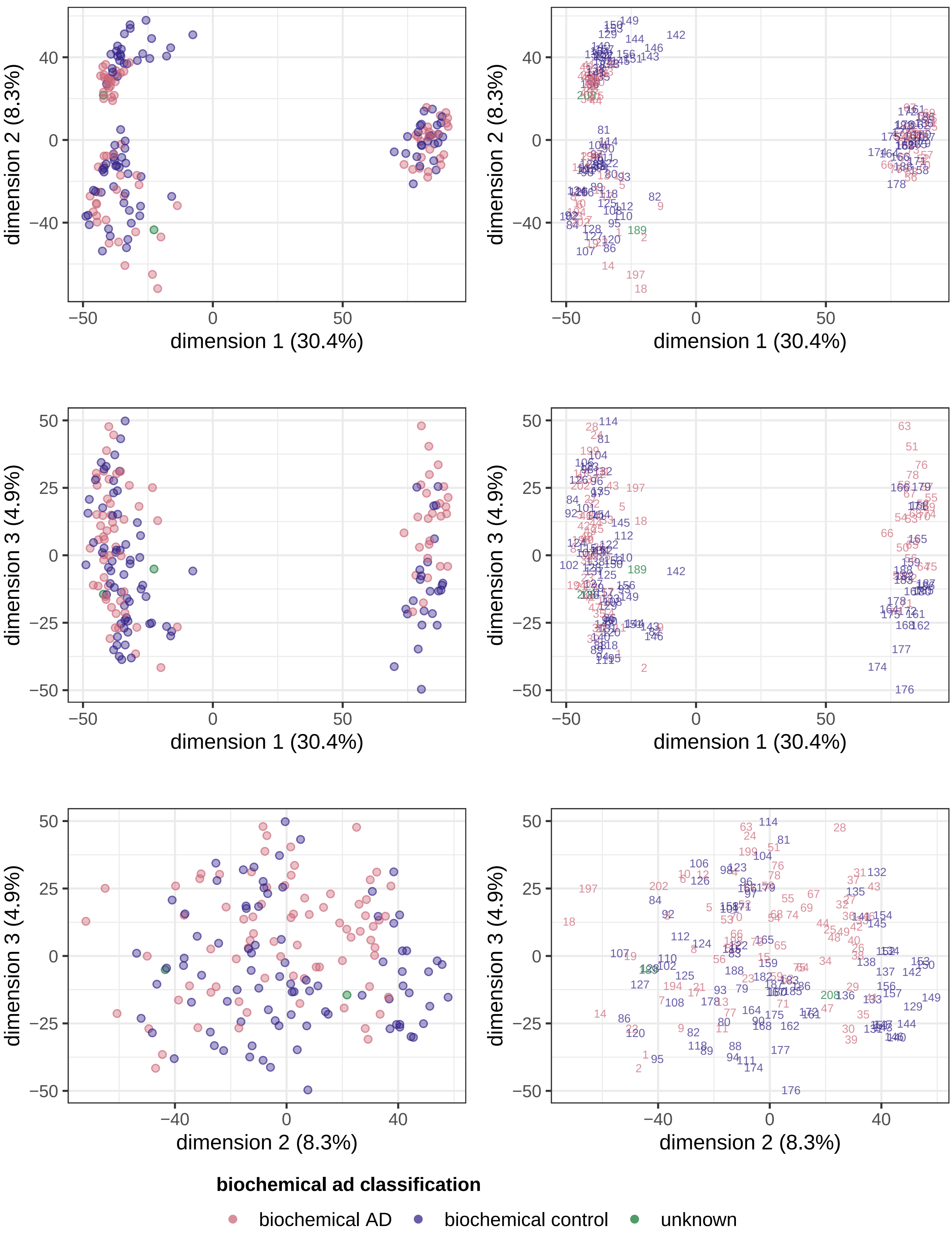
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



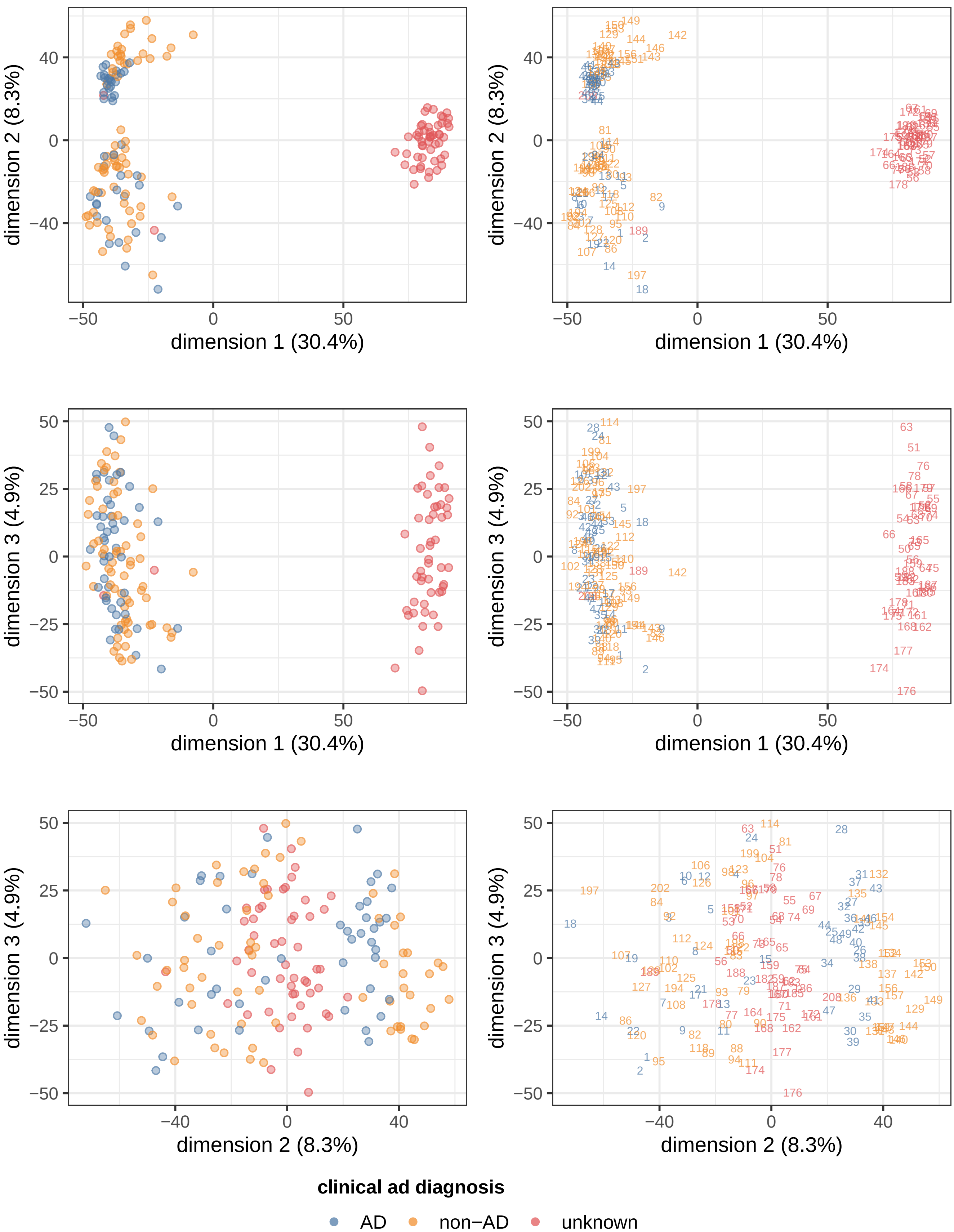
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



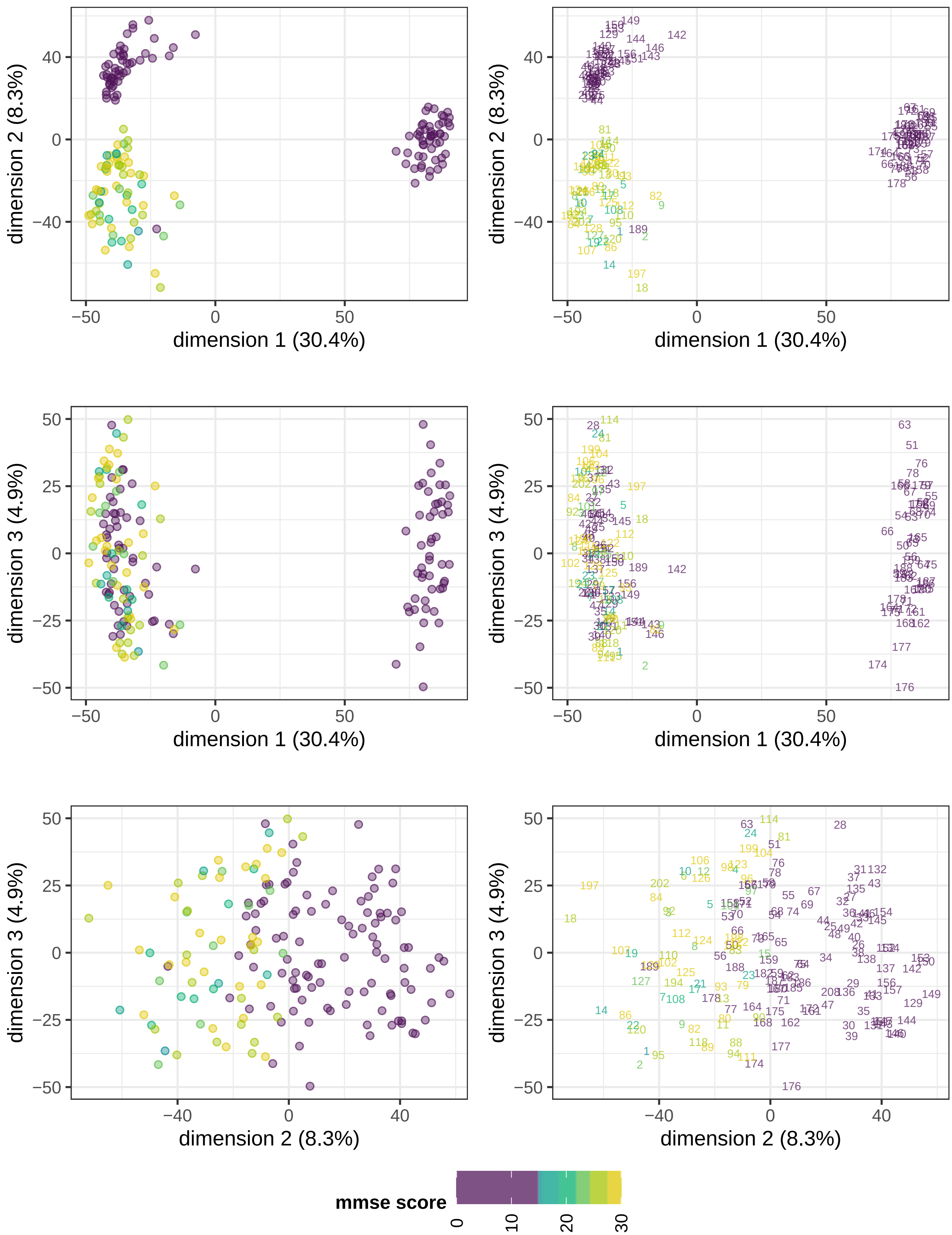
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



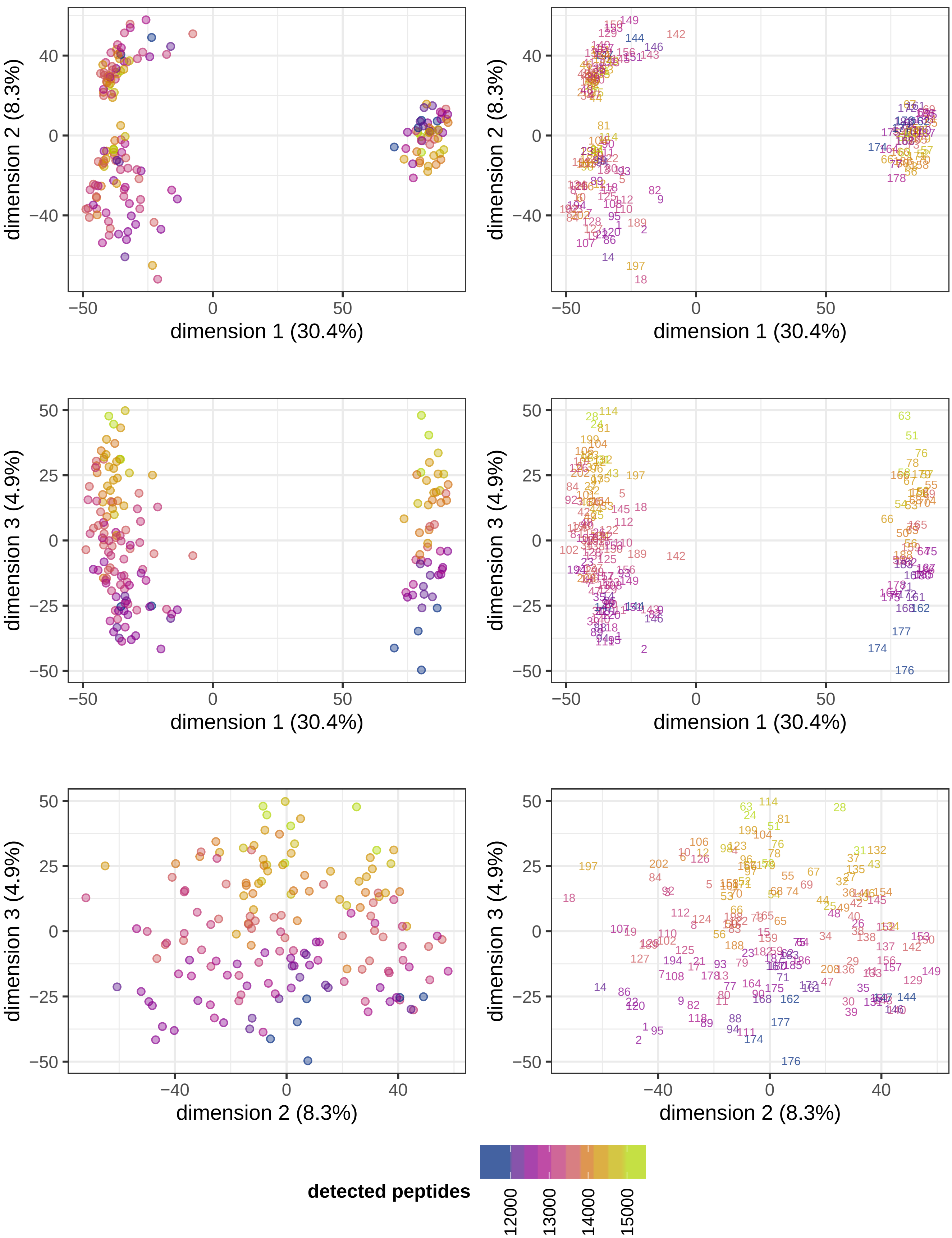
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



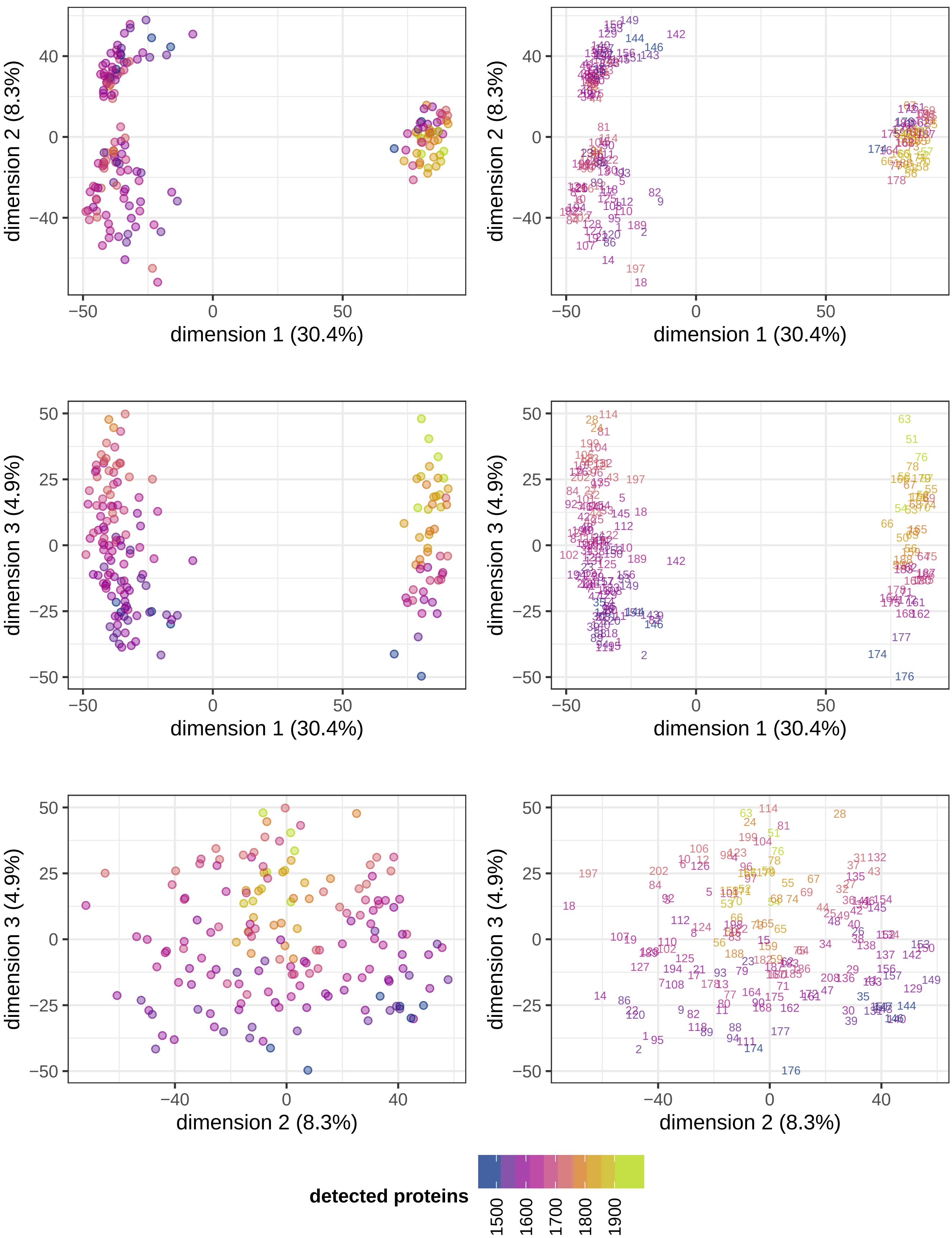
samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



samples are labeled by "sample_index" (described in samples.xlsx included with MS−DAP output)



2 Differential abundance analysis

goal: maximize reliable features for quantification

In a pairwise analysis of two groups of samples, only peptides with N data-points in both groups are used for quantitative analysis (where N = defined by user settings). For example; if peptide *p* is consistently quantified in sample groups A and B but not in C/D/E, it can be used when comparing group A *versus* group B but should not be used in any other group comparisons. This approach is particularly suited to maximize the number of peptides used for statistical analysis in experimental designs with many sample groups.

A common alternative strategy is a global filtering approach where peptides are selected based on their properties in the overall dataset (eg; present in x% of samples or x% of replicates in all groups) and subsequentially the resulting data matrix is used for all downstream statistical analyses. In the example above where peptide *p* is present in a subset of sample groups, *p* would either be left out (not present in majority of samples in entire dataset) or erronously used when applying t-statistics to groups B and C (since *p* is not present in group C, it may differentially detected but there are no features available for quantitative analysis)

2.1 control_Berlin vs AD_Berlin

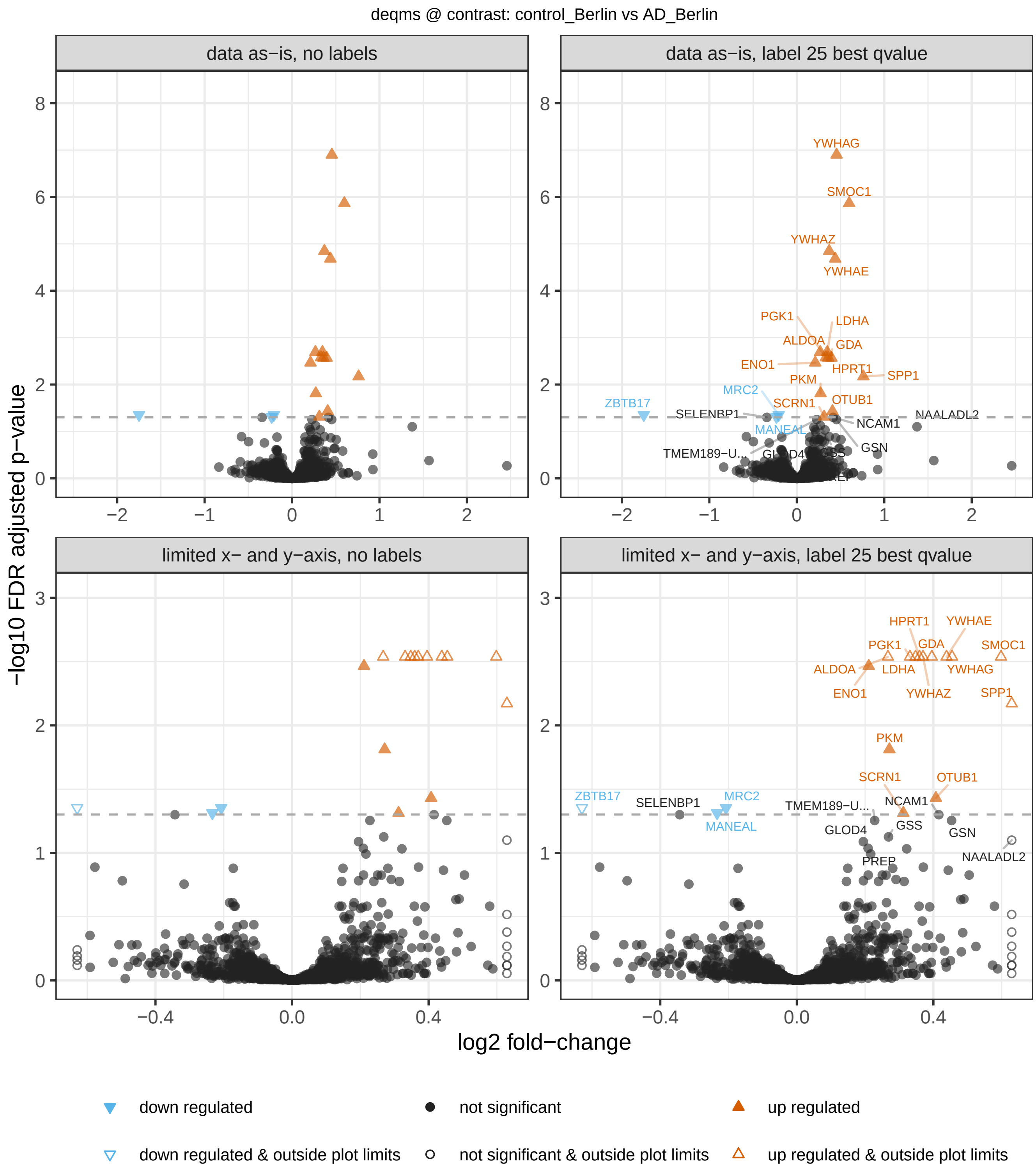
- **user setting:** using 'filter by contrast' peptide filtering approach
- 14318 peptides in 1662 proteins remain in the current contrast after peptide filters and are used for the statistical analysis in this section
- qvalue threshold: 0.05
- log2 foldchange threshold: 0

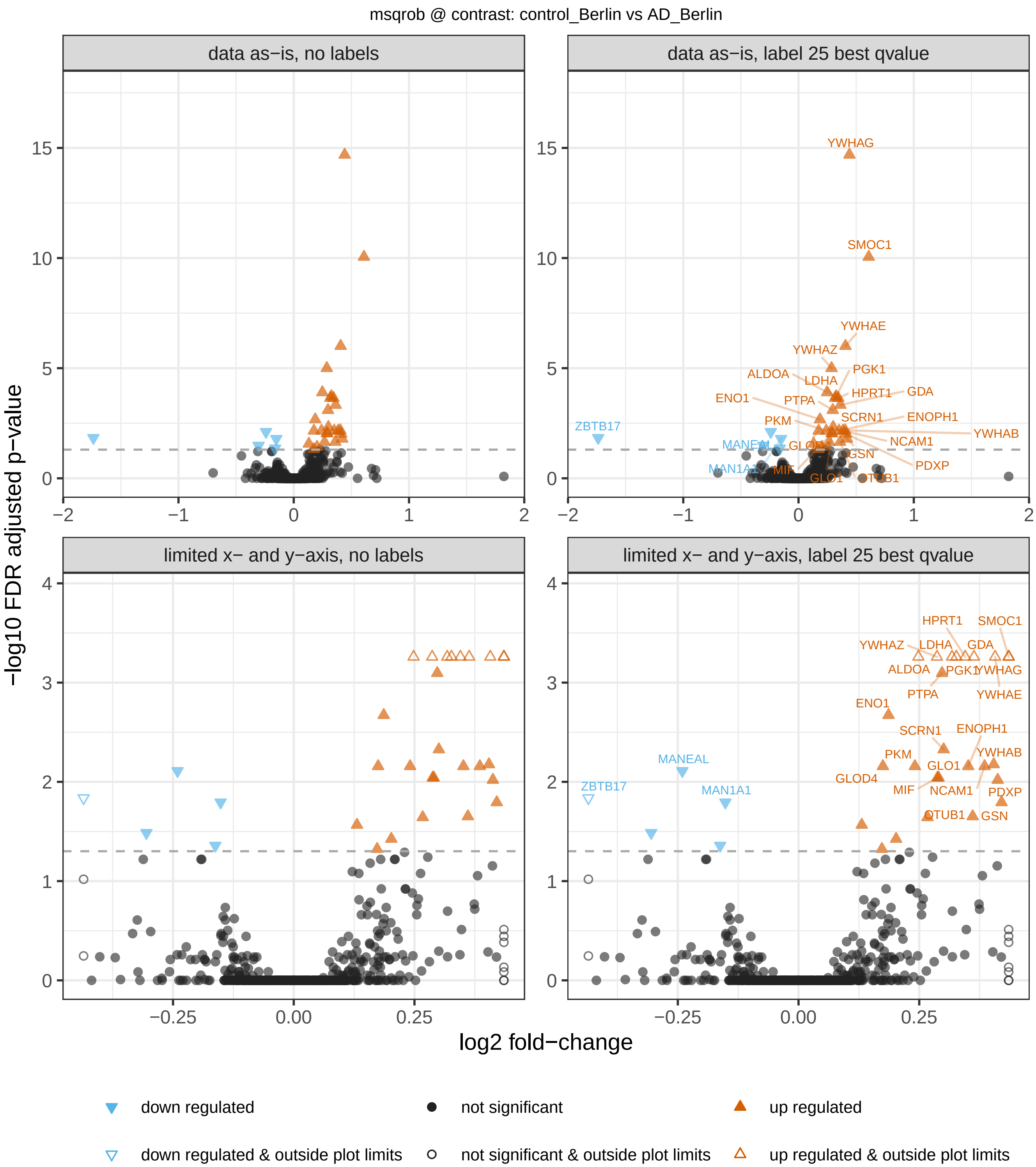
2.1.1 volcano

The plot title shows the statistical model and contrast (sample groups in the comparison). Left- and right-side figure panels on each row represent the same figure without and with labels for the 25 proteins with lowest p-value.

Bottom figure panels have limited x- and y-axis. For datasets with a small number of strong outliers in p-value or fold-change, which may have a profound effect on the plot scales, this allows inspection of the remainder of the volcano plot without disproportionate influence by 'extreme' values.

Labels for proteins that are more than 12 characters long are truncated for visual clarity (indicated by trailing …). For protein identifiers that are ambiguous, e.g. a protein-group with assigned genes "gene1a;gene1b", only the first label/ID is shown for visual clarity (indicated by trailing *).


deqms @ contrast: control_Berlin vs AD_Berlin
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
YWHAG
SMOC1
YWHAZ
YWHAE
PGK1
LDHA
ALDOA
GDA
ENO1
HPRT1
SPP1
PKM
MRC2
ZBTB17
SCRN1
OTUB1
SELENBP1
NAALADL2
NCAM1
MANEAL
GSN
TMEM189−U...
GLOD4
GSS
PREP
−log10 FDR adjusted p−value
log2 fold−change
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

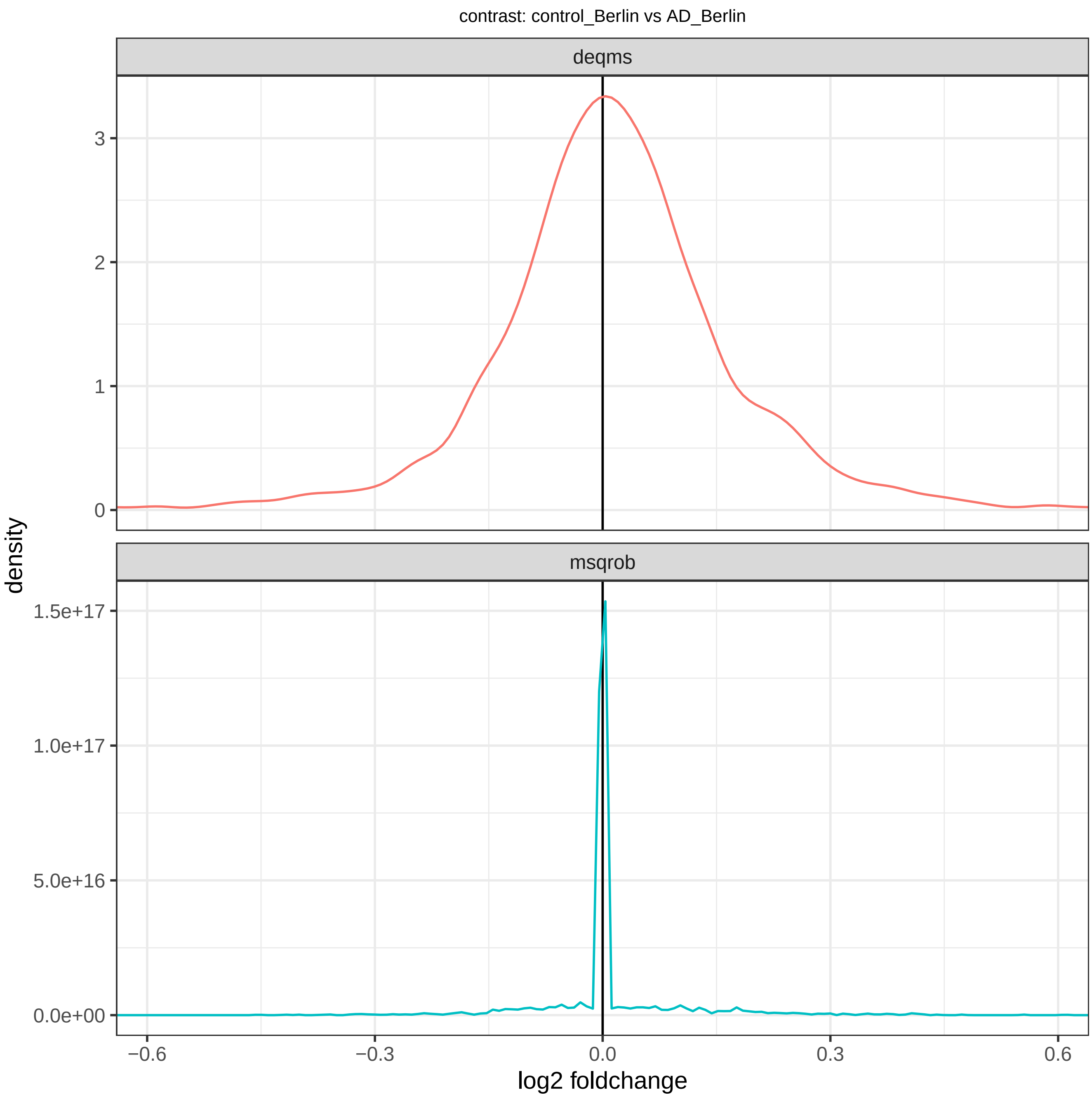


msqrob @ contrast: control_Berlin vs AD_Berlin
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

2.1.2 foldchange distribution

Distributions of estimated foldchanges produced by the statistical models. If the mode is far from 0, consider alternative normalization strategies. Do note the scale on the x-axis, for some experiments the foldchanges are very low which in turn may exaggerate this figure.

note; the MSqRob model tends to assign zero (log)foldchange for proteins with minor difference between conditions where the model is very sure the null hypothesis cannot be rejected (shrinkage by the ridge regression model). As a result, many foldchanges will be zero and the density plot for MSqRob may look like a spike instead of the expected Gaussian shape observed in other models



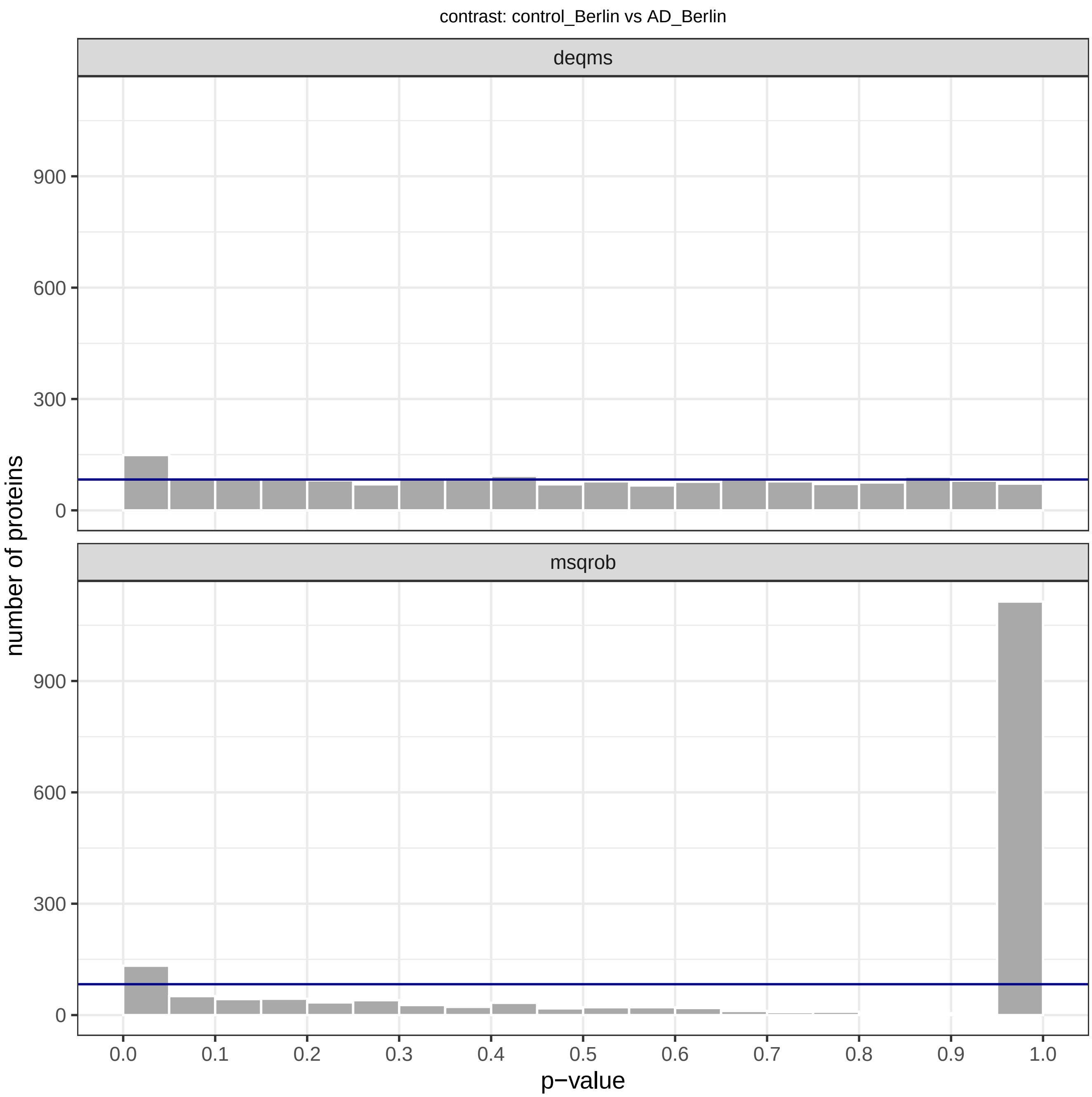
2.1.3 p-value distribution

Histogram of p-values computed by differential expression analysis algorithms, as-is, for quality-control inspection. The horizontal line indicates the expected counts assuming a uniform distribution (total number of p-values divided by number of histogram bins)

See further: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6164648/

See further: http://varianceexplained.org/statistics/interpreting-pvalue-histogram/

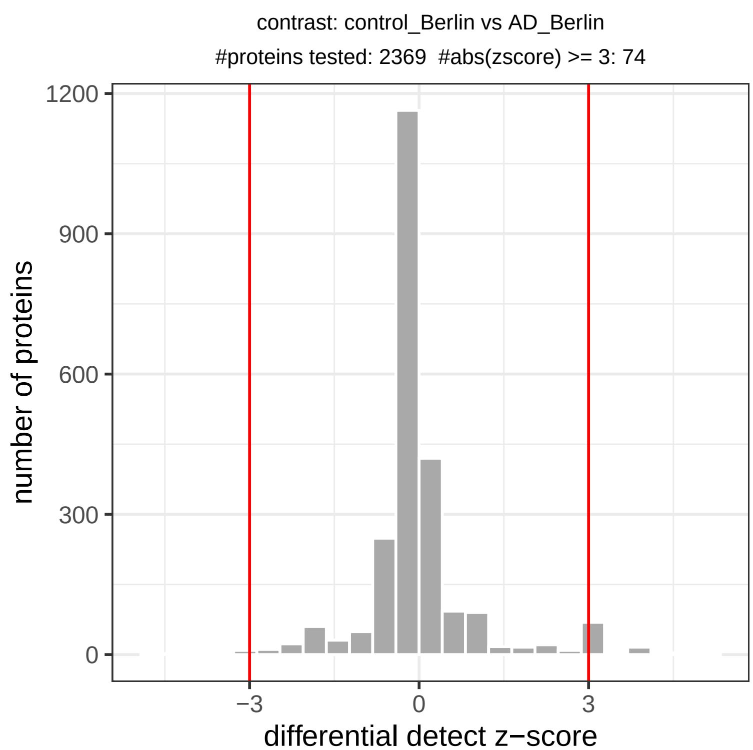
note; the MSqRob and MS-EmpiRe models often yield p-value distributions that show a large peak at p-value 1, these are typically proteins with estimated log foldchanges at/near zero where these models are very sure the null hypothesis cannot be rejected



2.1.4 differential detect

Some proteins may not have peptides with sufficient data points over samples to be used for differential expression analysis (depending on the user-defined filtering criteria in how many replicates peptides should be observed), but do show a strong difference in the number of detected peptides between sample groups. In some proteomics experimental designs, for example a wildtype-knockout APMS study, those are interesting proteins. The DEA based on peptide abundance values (volcano plots above) are the main result for differential testing in MS-DAP but as a situationally useful tool MS-DAP also includes a 'protein detection' z-score, based on the number of times a peptide for each protein was detected per sample group (/experimental condition), as an alternative means of differential testing.

Below figure shows the distribution of these scores with thresholds at 3 std. Both the z-scores and the counts these are based upon are available in the statistical result Excel table.



2.2 control_Magdeburg vs AD_Magdeburg

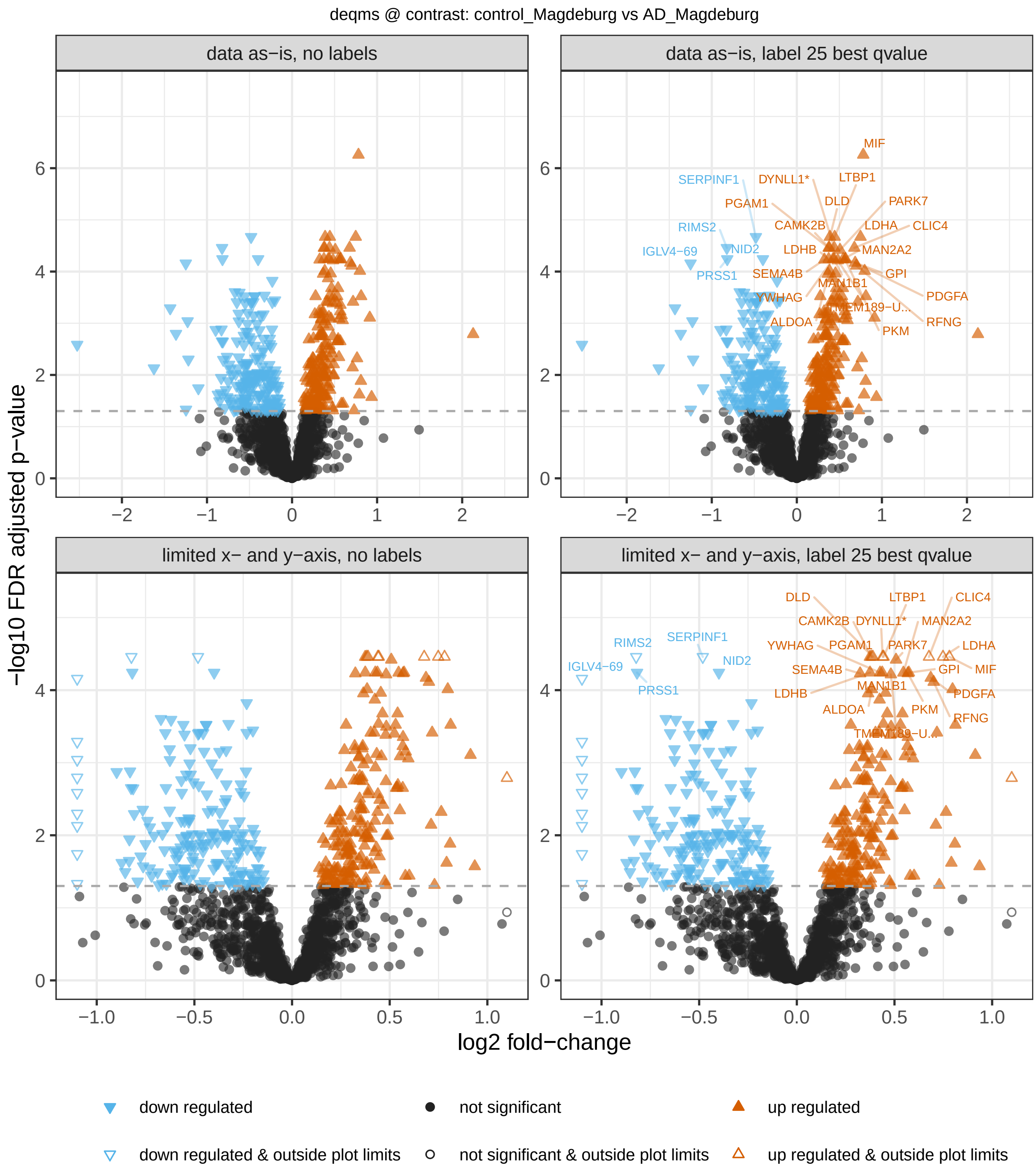
- **user setting:** using 'filter by contrast' peptide filtering approach
- 14255 peptides in 1617 proteins remain in the current contrast after peptide filters and are used for the statistical analysis in this section
- qvalue threshold: 0.05
- log2 foldchange threshold: 0

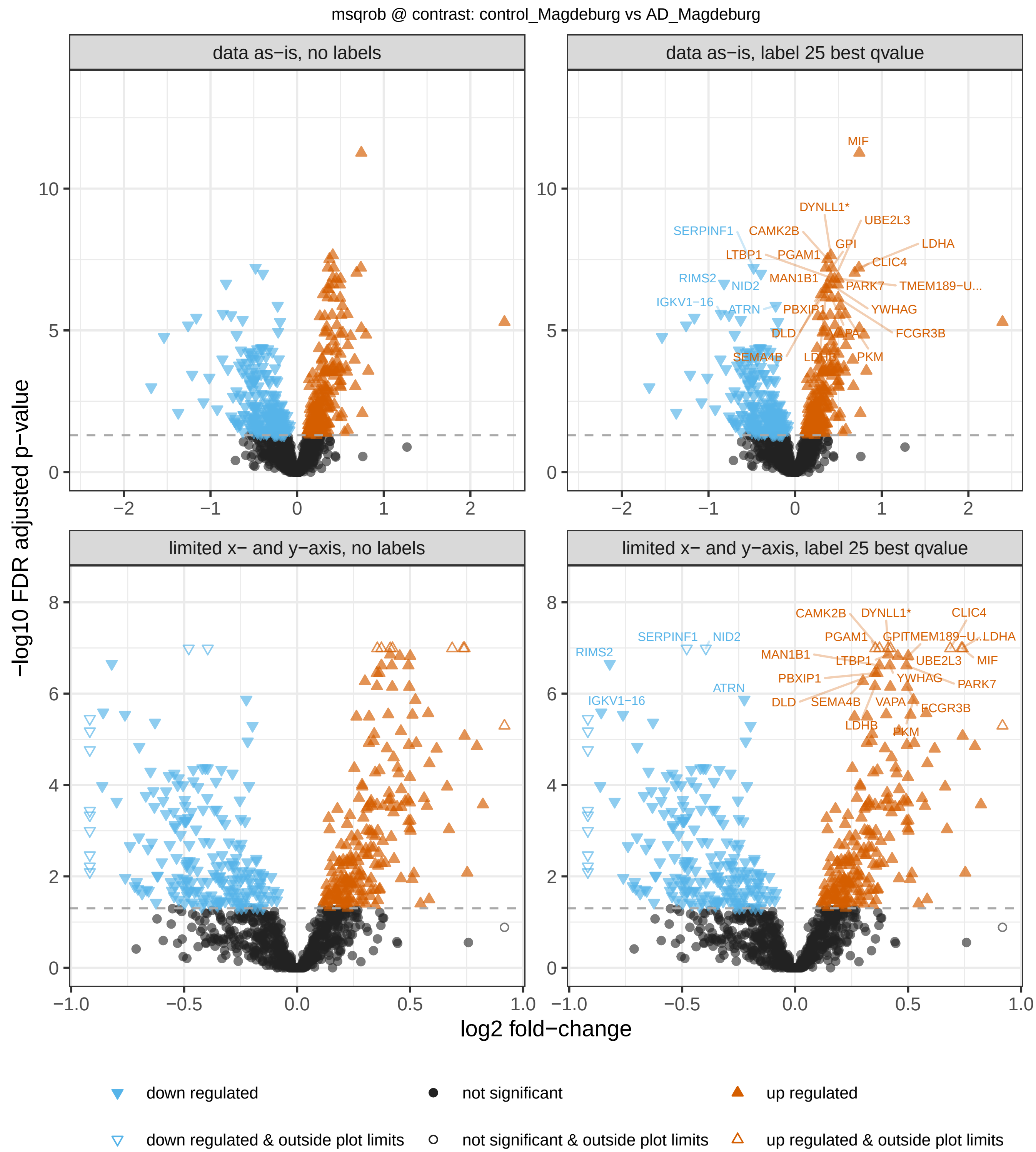
2.2.1 volcano

The plot title shows the statistical model and contrast (sample groups in the comparison). Left- and right-side figure panels on each row represent the same figure without and with labels for the 25 proteins with lowest p-value.

Bottom figure panels have limited x- and y-axis. For datasets with a small number of strong outliers in p-value or fold-change, which may have a profound effect on the plot scales, this allows inspection of the remainder of the volcano plot without disproportionate influence by 'extreme' values.

Labels for proteins that are more than 12 characters long are truncated for visual clarity (indicated by trailing …). For protein identifiers that are ambiguous, e.g. a protein-group with assigned genes "gene1a;gene1b", only the first label/ID is shown for visual clarity (indicated by trailing *).

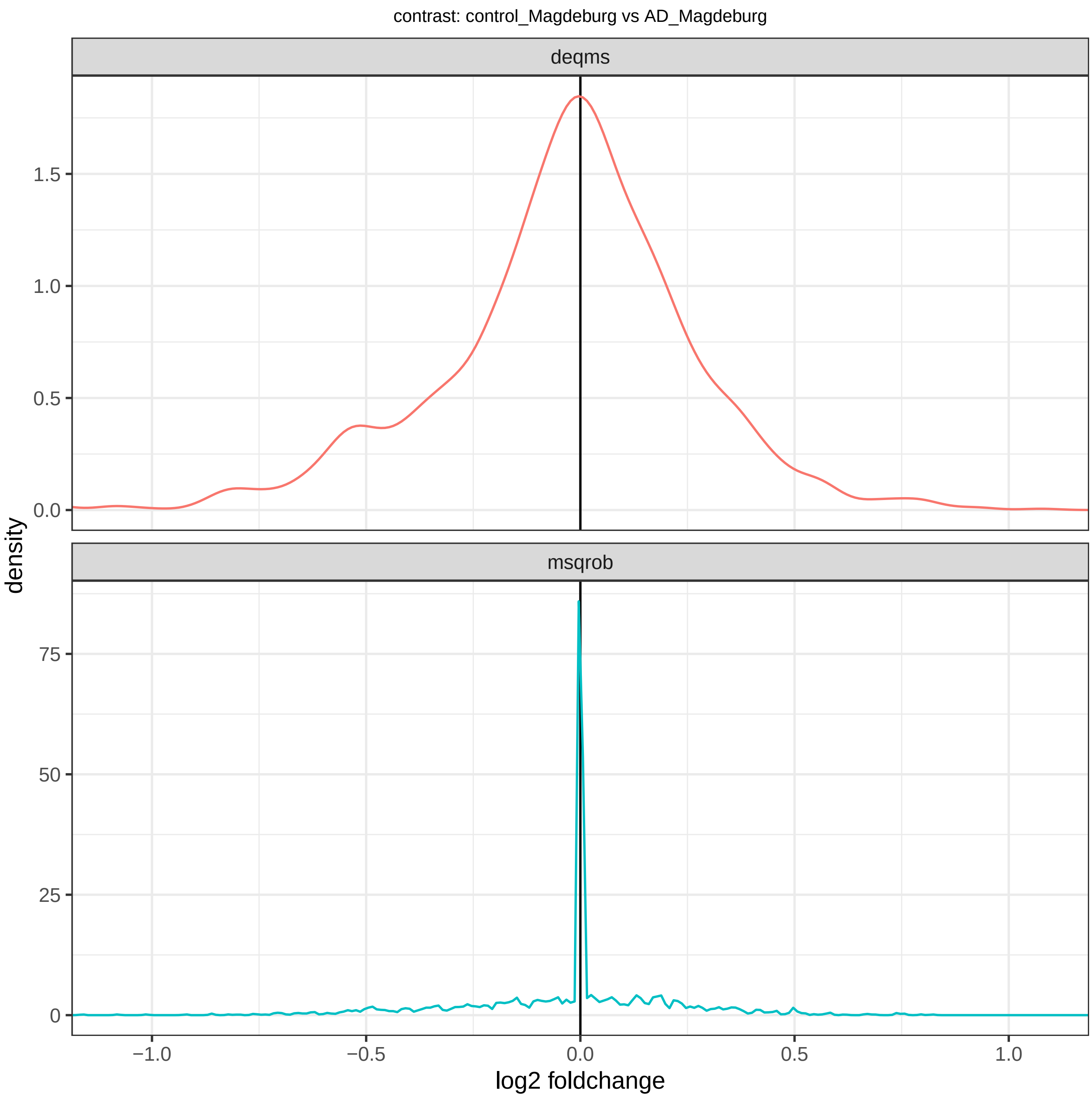

deqms @ contrast: control_Magdeburg vs AD_Magdeburg
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
MIF
SERPINF1
DYNLL1*
LTBP1
PGAM1
DLD
PARK7
RIMS2
CAMK2B
LDHA
CLIC4
IGLV4−69
NID2
LDHB
MAN2A2
PRSS1
SEMA4B
GPI
MAN1B1
YWHAG
PDGFA
TMEM189−U...
ALDOA
RFNG
PKM
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits


msqrob @ contrast: control_Magdeburg vs AD_Magdeburg
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
MIF
DYNLL1*
UBE2L3
SERPINF1
CAMK2B
GPI
LDHA
LTBP1
PGAM1
CLIC4
RIMS2
NID2
MAN1B1
PARK7
TMEM189−U...
IGKV1−16
ATRN
PBXIP1
YWHAG
DLD
FCGR3B
SEMA4B
PKM
VAPA
LDHB
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

2.2.2 foldchange distribution

Distributions of estimated foldchanges produced by the statistical models. If the mode is far from 0, consider alternative normalization strategies. Do note the scale on the x-axis, for some experiments the foldchanges are very low which in turn may exaggerate this figure.

note; the MSqRob model tends to assign zero (log)foldchange for proteins with minor difference between conditions where the model is very sure the null hypothesis cannot be rejected (shrinkage by the ridge regression model). As a result, many foldchanges will be zero and the density plot for MSqRob may look like a spike instead of the expected Gaussian shape observed in other models



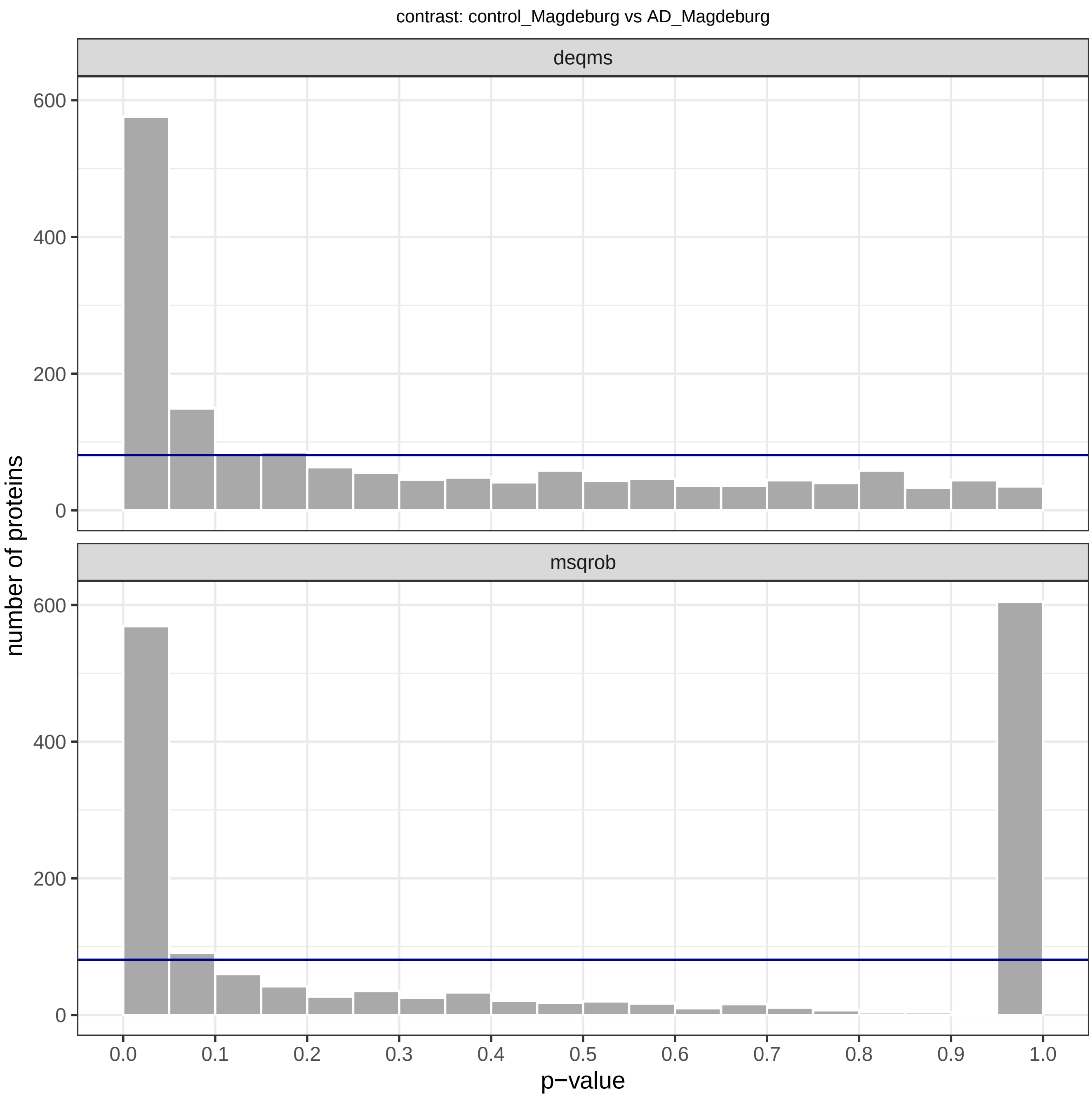
2.2.3 p-value distribution

Histogram of p-values computed by differential expression analysis algorithms, as-is, for quality-control inspection. The horizontal line indicates the expected counts assuming a uniform distribution (total number of p-values divided by number of histogram bins)

See further: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6164648/

See further: http://varianceexplained.org/statistics/interpreting-pvalue-histogram/

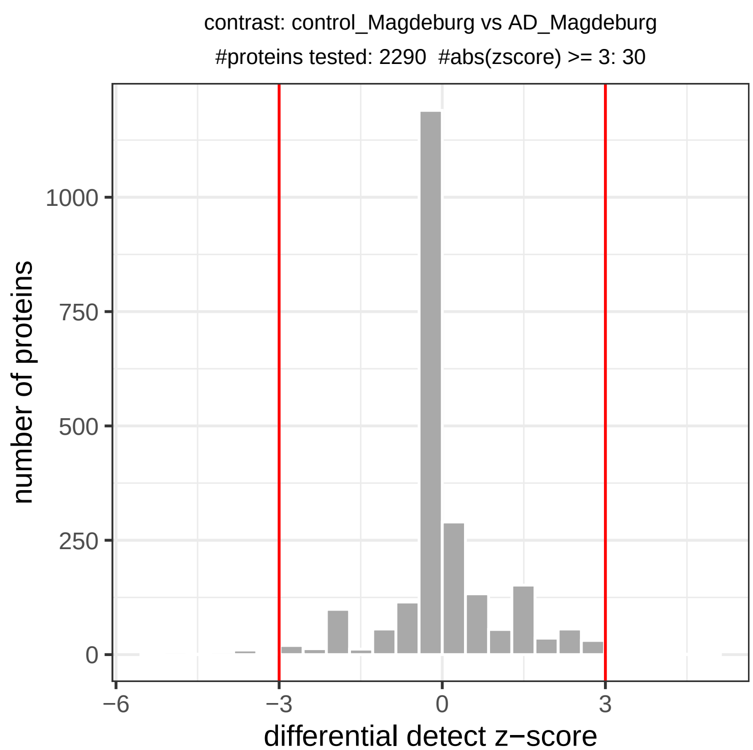
note; the MSqRob and MS-EmpiRe models often yield p-value distributions that show a large peak at p-value 1, these are typically proteins with estimated log foldchanges at/near zero where these models are very sure the null hypothesis cannot be rejected



2.2.4 differential detect

Some proteins may not have peptides with sufficient data points over samples to be used for differential expression analysis (depending on the user-defined filtering criteria in how many replicates peptides should be observed), but do show a strong difference in the number of detected peptides between sample groups. In some proteomics experimental designs, for example a wildtype-knockout APMS study, those are interesting proteins. The DEA based on peptide abundance values (volcano plots above) are the main result for differential testing in MS-DAP but as a situationally useful tool MS-DAP also includes a 'protein detection' z-score, based on the number of times a peptide for each protein was detected per sample group (/experimental condition), as an alternative means of differential testing.

Below figure shows the distribution of these scores with thresholds at 3 std. Both the z-scores and the counts these are based upon are available in the statistical result Excel table.



2.3 control_Sweden vs AD_Sweden

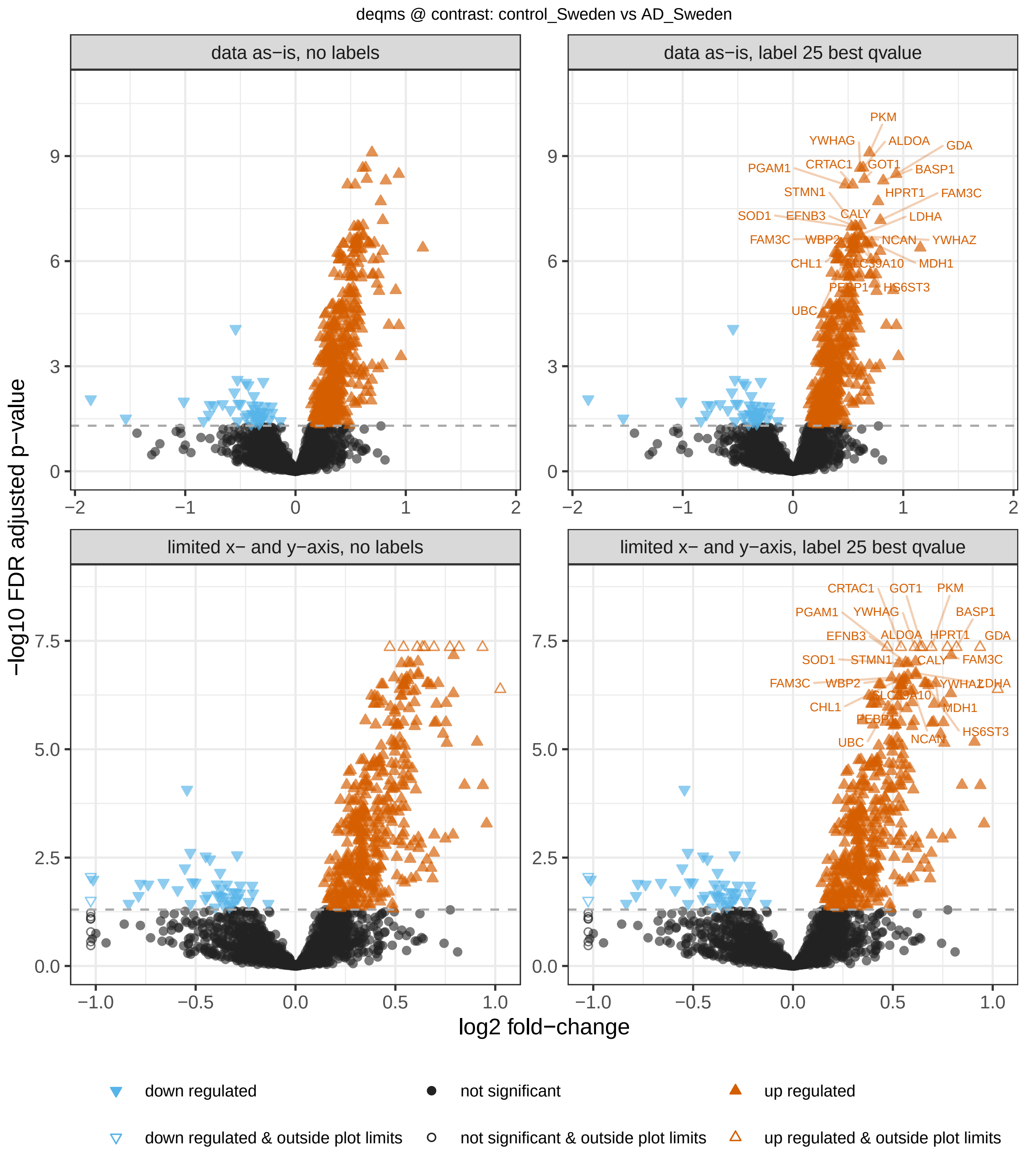
- **user setting:** using 'filter by contrast' peptide filtering approach
- 14272 peptides in 1732 proteins remain in the current contrast after peptide filters and are used for the statistical analysis in this section
- qvalue threshold: 0.05
- log2 foldchange threshold: 0

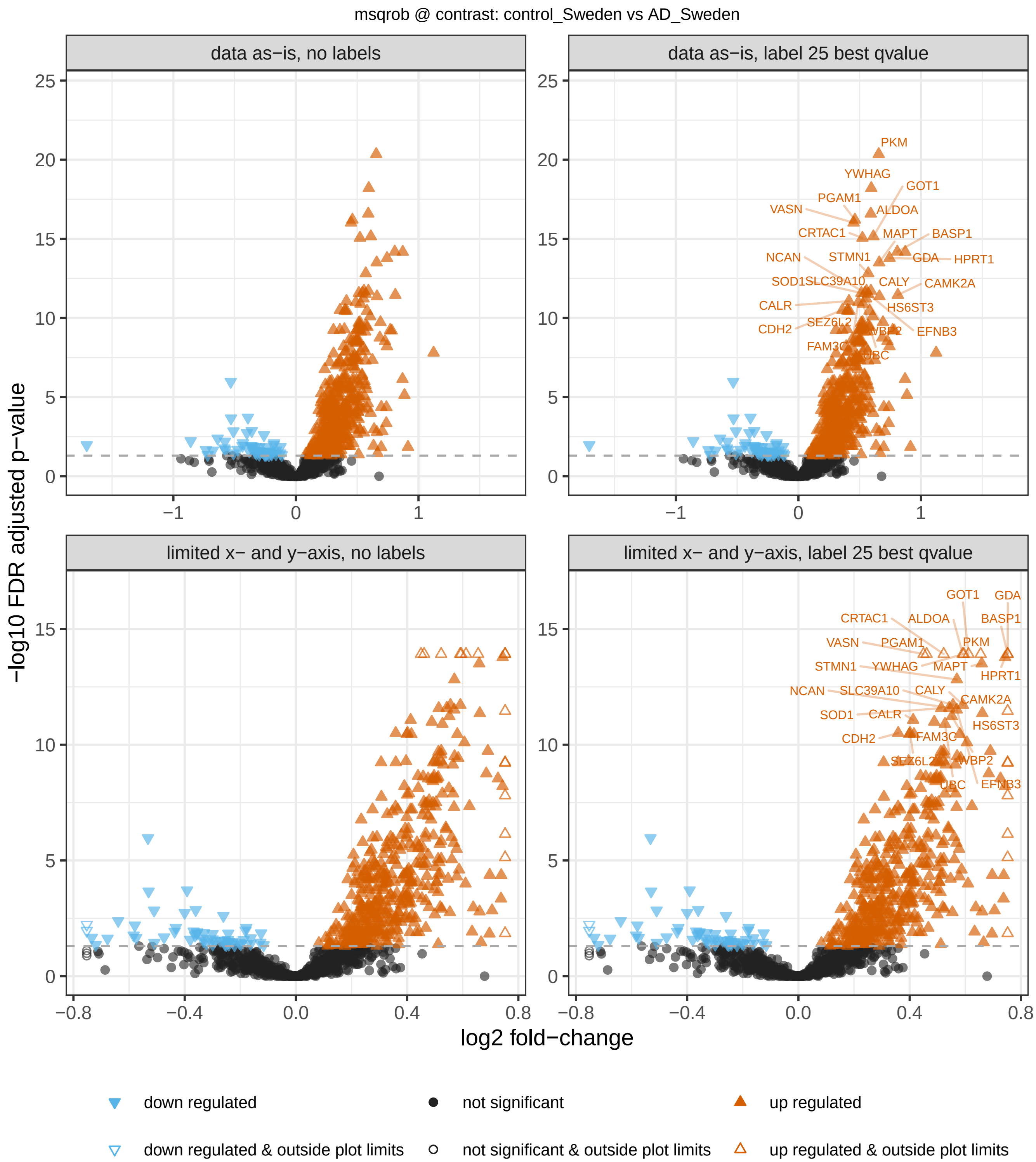
2.3.1 volcano

The plot title shows the statistical model and contrast (sample groups in the comparison). Left- and right-side figure panels on each row represent the same figure without and with labels for the 25 proteins with lowest p-value.

Bottom figure panels have limited x- and y-axis. For datasets with a small number of strong outliers in p-value or fold-change, which may have a profound effect on the plot scales, this allows inspection of the remainder of the volcano plot without disproportionate influence by 'extreme' values.

Labels for proteins that are more than 12 characters long are truncated for visual clarity (indicated by trailing …). For protein identifiers that are ambiguous, e.g. a protein-group with assigned genes "gene1a;gene1b", only the first label/ID is shown for visual clarity (indicated by trailing *).


deqms @ contrast: control_Sweden vs AD_Sweden
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
PKM
YWHAG
ALDOA
GDA
PGAM1
CRTAC1
GOT1
BASP1
STMN1
HPRT1
FAM3C
SOD1
EFNB3
CALY
LDHA
WBP2
NCAN
YWHAZ
CHL1
MDH1
HS6ST3
UBC
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

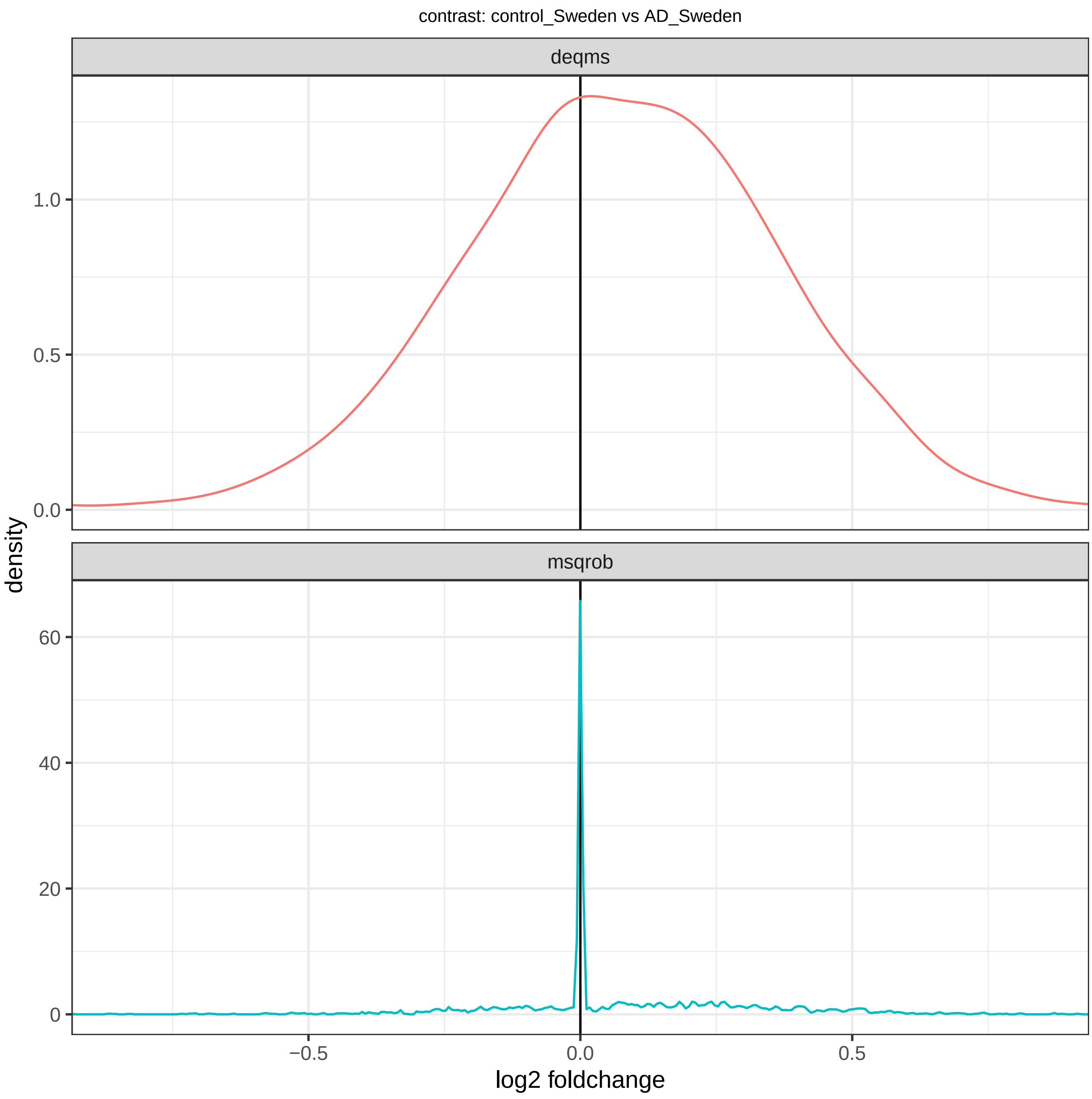


msqrob @ contrast: control_Sweden vs AD_Sweden
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

2.3.2 foldchange distribution

Distributions of estimated foldchanges produced by the statistical models. If the mode is far from 0, consider alternative normalization strategies. Do note the scale on the x-axis, for some experiments the foldchanges are very low which in turn may exaggerate this figure.

note; the MSqRob model tends to assign zero (log)foldchange for proteins with minor difference between conditions where the model is very sure the null hypothesis cannot be rejected (shrinkage by the ridge regression model). As a result, many foldchanges will be zero and the density plot for MSqRob may look like a spike instead of the expected Gaussian shape observed in other models



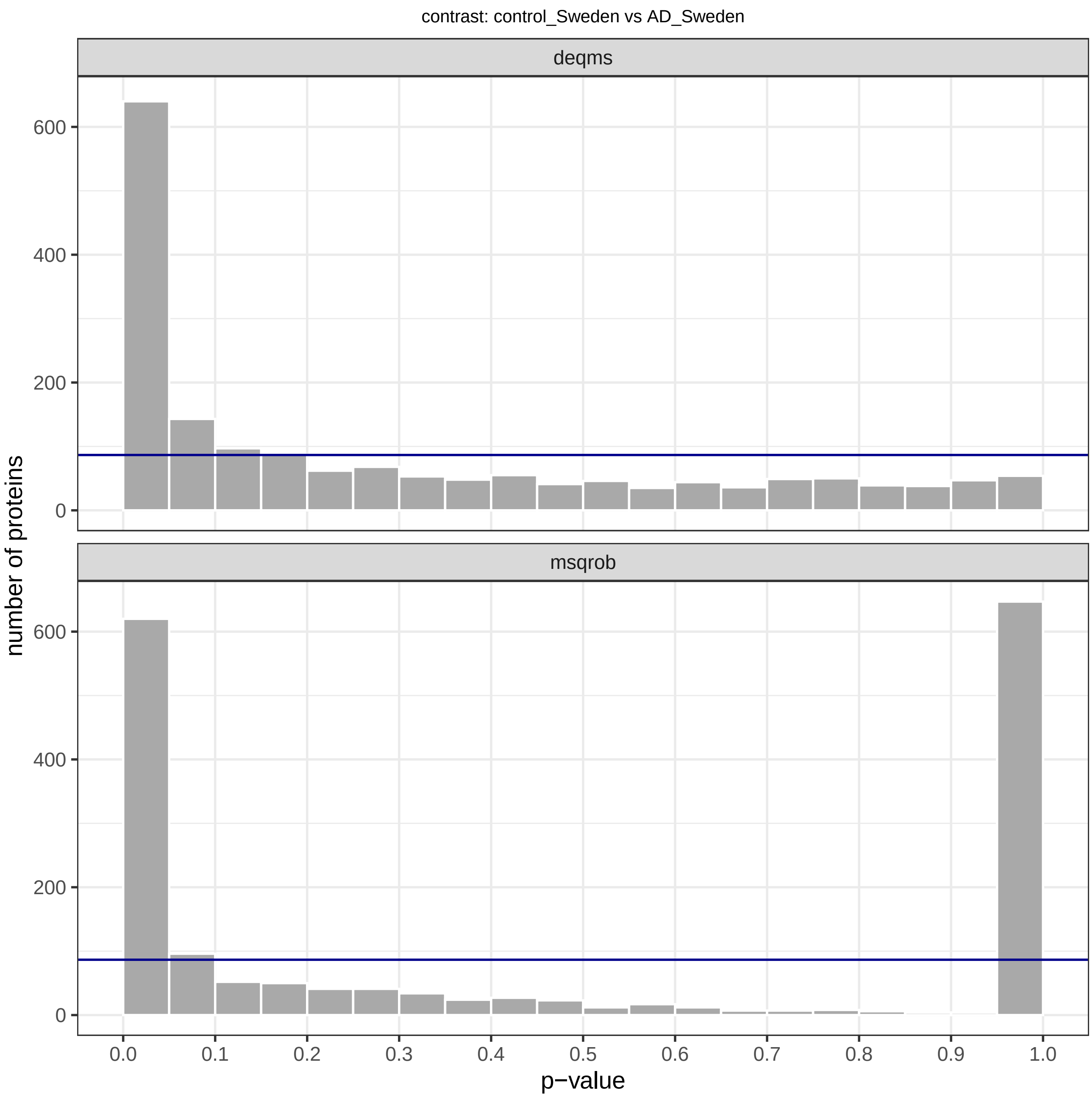
2.3.3 p-value distribution

Histogram of p-values computed by differential expression analysis algorithms, as-is, for quality-control inspection. The horizontal line indicates the expected counts assuming a uniform distribution (total number of p-values divided by number of histogram bins)

See further: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6164648/

See further: http://varianceexplained.org/statistics/interpreting-pvalue-histogram/

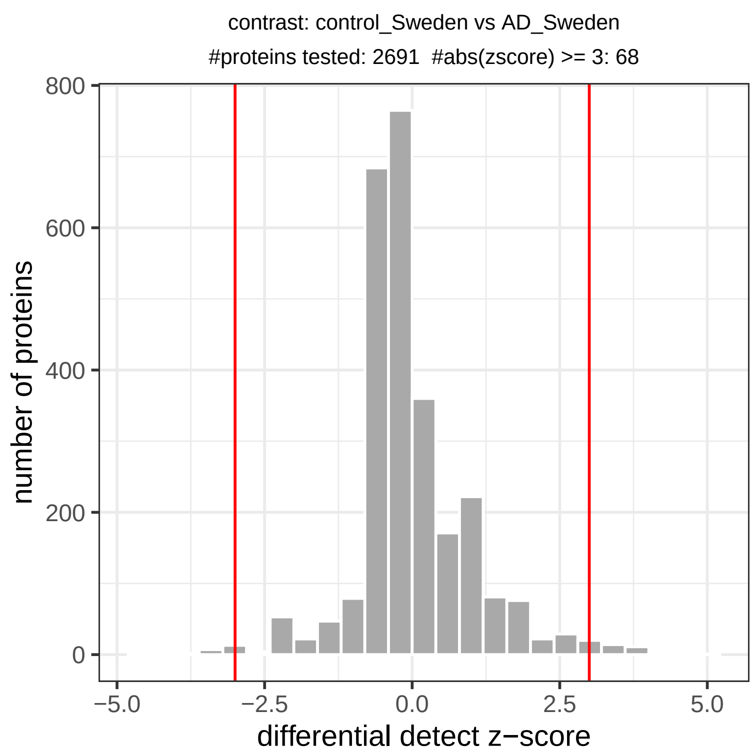
note; the MSqRob and MS-EmpiRe models often yield p-value distributions that show a large peak at p-value 1, these are typically proteins with estimated log foldchanges at/near zero where these models are very sure the null hypothesis cannot be rejected



2.3.4 differential detect

Some proteins may not have peptides with sufficient data points over samples to be used for differential expression analysis (depending on the user-defined filtering criteria in how many replicates peptides should be observed), but do show a strong difference in the number of detected peptides between sample groups. In some proteomics experimental designs, for example a wildtype-knockout APMS study, those are interesting proteins. The DEA based on peptide abundance values (volcano plots above) are the main result for differential testing in MS-DAP but as a situationally useful tool MS-DAP also includes a 'protein detection' z-score, based on the number of times a peptide for each protein was detected per sample group (/experimental condition), as an alternative means of differential testing.

Below figure shows the distribution of these scores with thresholds at 3 std. Both the z-scores and the counts these are based upon are available in the statistical result Excel table.



2.4 control__Berlin,control__Magdeburg... vs AD__Berlin,AD__Magdeburg,AD__Sweden

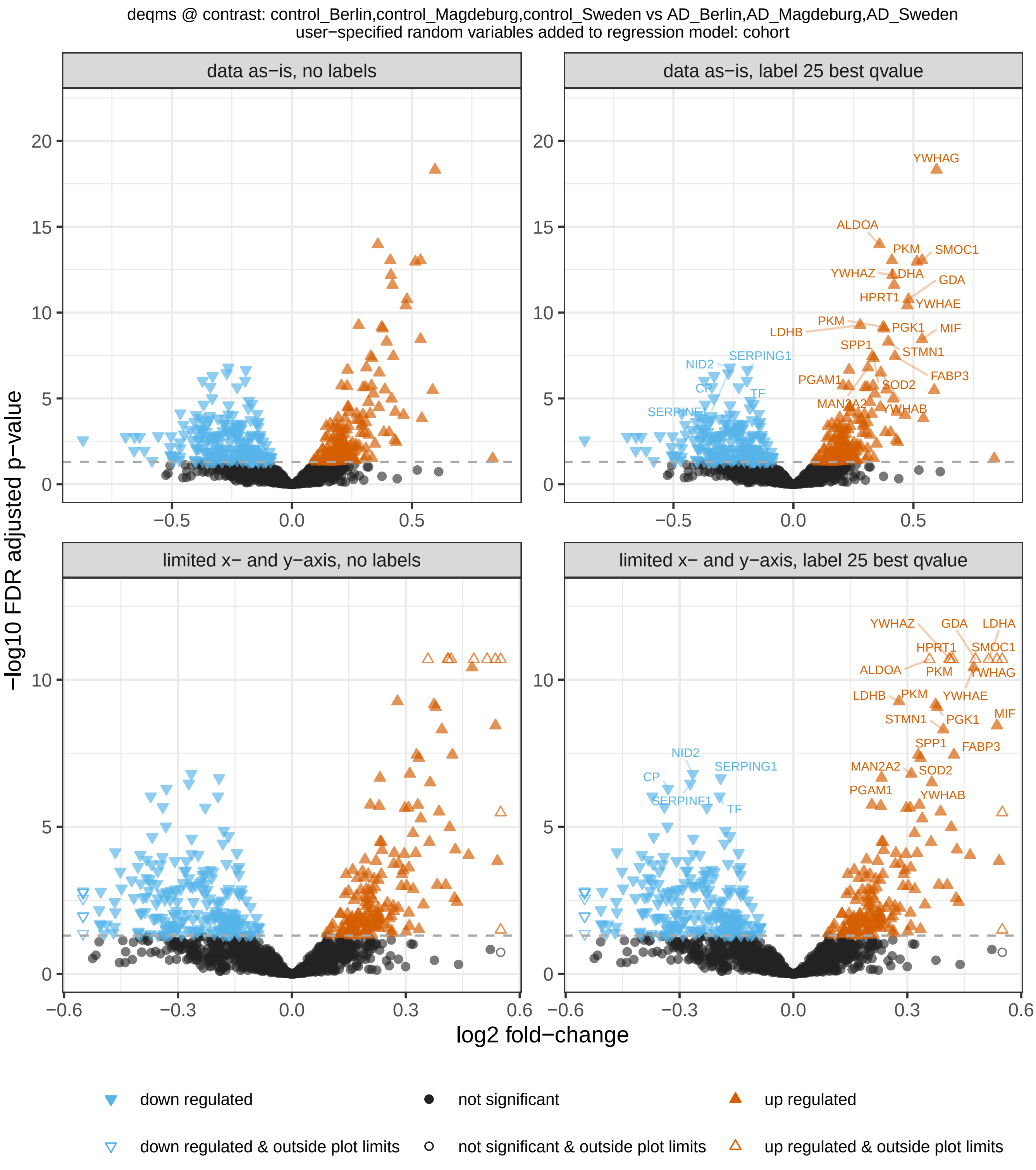
- **user setting:** using 'filter by contrast' peptide filtering approach
- 11824 peptides in 1445 proteins remain in the current contrast after peptide filters and are used for the statistical analysis in this section
- qvalue threshold: 0.05
- log2 foldchange threshold: 0

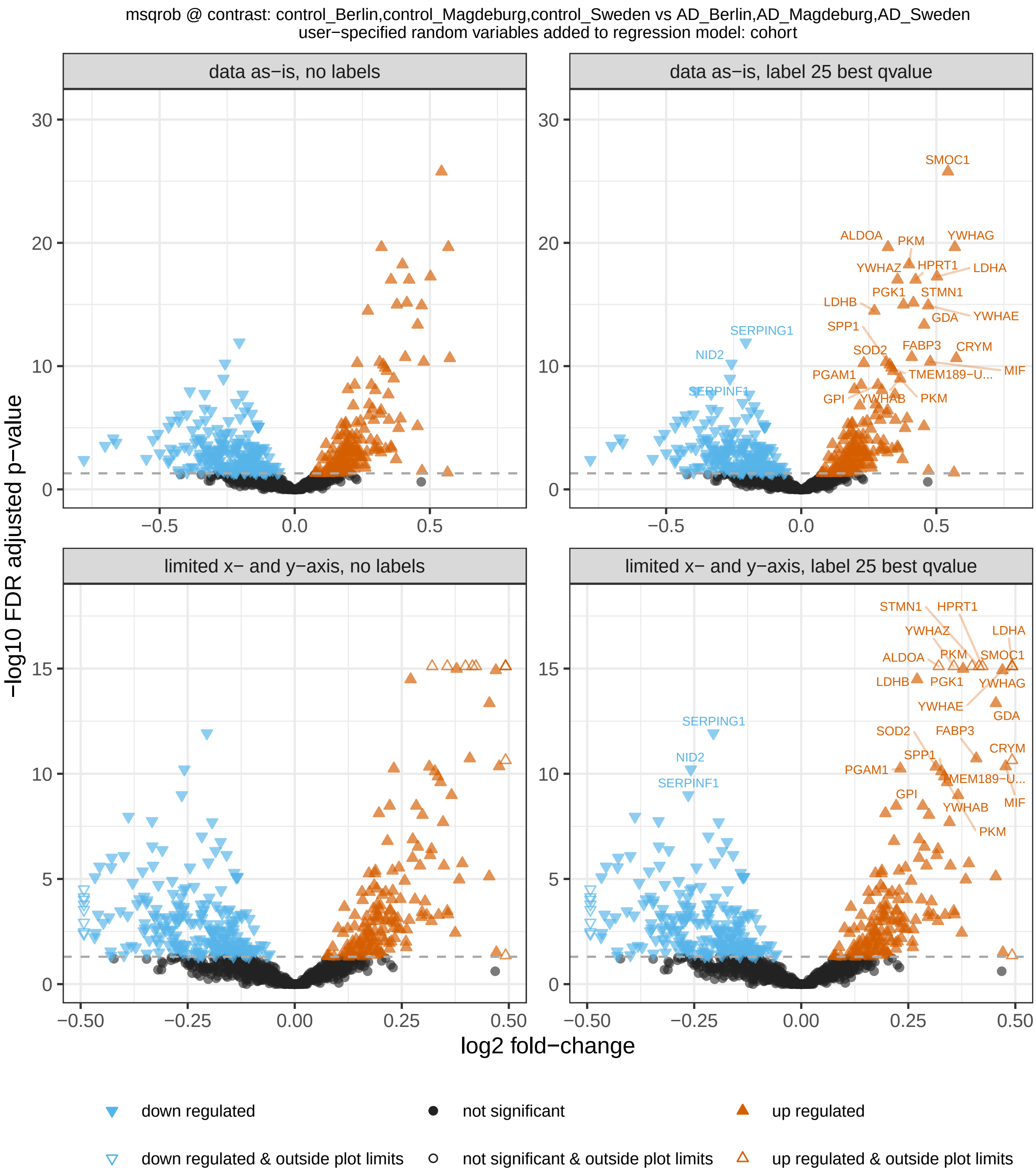
2.4.1 volcano

The plot title shows the statistical model and contrast (sample groups in the comparison). Left- and right-side figure panels on each row represent the same figure without and with labels for the 25 proteins with lowest p-value.

Bottom figure panels have limited x- and y-axis. For datasets with a small number of strong outliers in p-value or fold-change, which may have a profound effect on the plot scales, this allows inspection of the remainder of the volcano plot without disproportionate influence by 'extreme' values.

Labels for proteins that are more than 12 characters long are truncated for visual clarity (indicated by trailing …). For protein identifiers that are ambiguous, e.g. a protein-group with assigned genes "gene1a;gene1b", only the first label/ID is shown for visual clarity (indicated by trailing *).


deqms @ contrast: control_Berlin,control_Magdeburg,control_Sweden vs AD_Berlin,AD_Magdeburg,AD_Sweden
user−specified random variables added to regression model: cohort
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
YWHAG
ALDOA
PKM
SMOC1
YWHAZ
LDHA
GDA
HPRT1
YWHAE
LDHB
PGK1
MIF
SPP1
STMN1
NID2
SERPING1
FABP3
PGAM1
SOD2
CP
TF
SERPINF1
MAN2A2
YWHAB
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

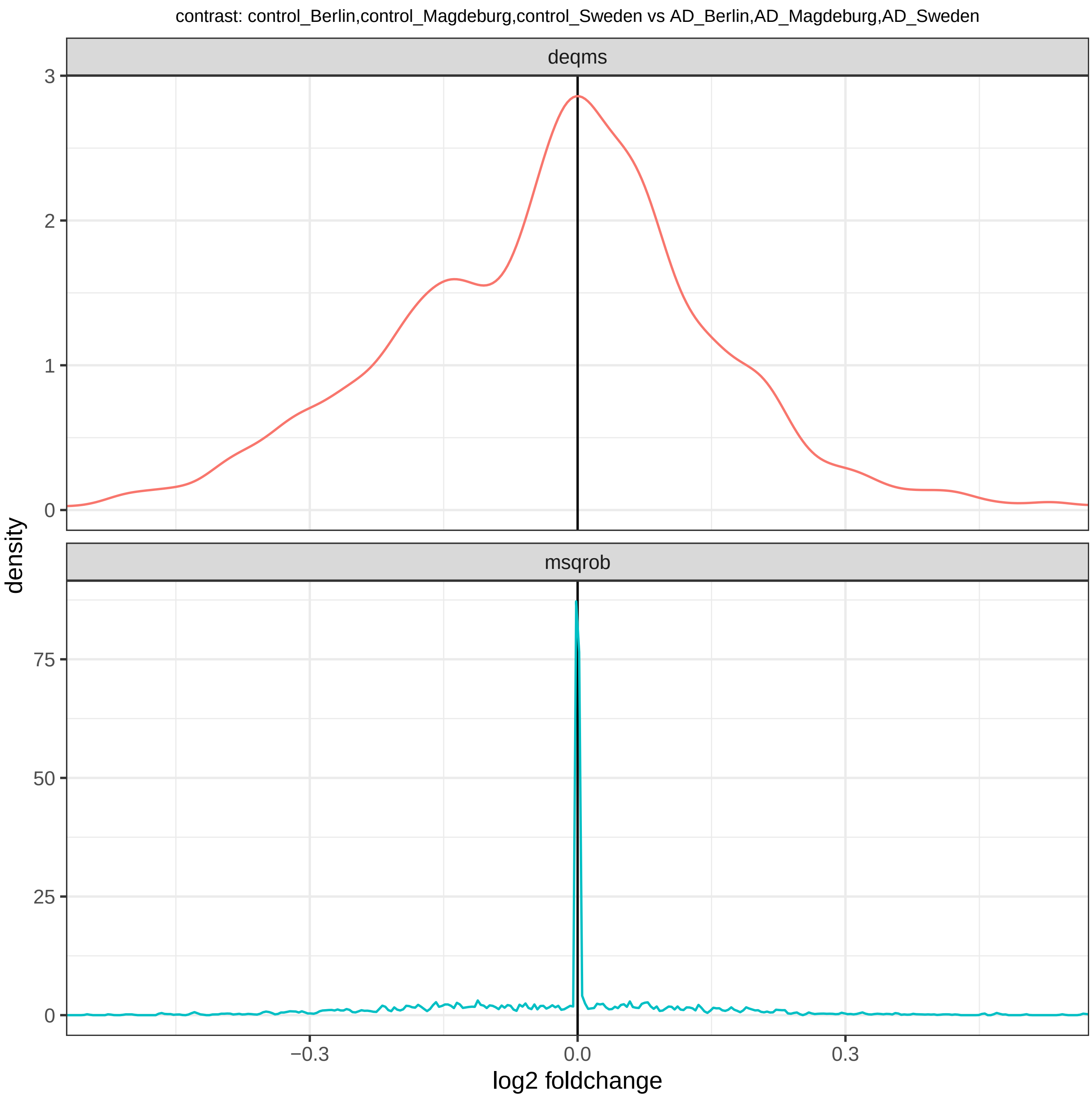


msqrob @ contrast: control_Berlin,control_Magdeburg,control_Sweden vs AD_Berlin,AD_Magdeburg,AD_Sweden
user−specified random variables added to regression model: cohort
data as−is, no labels
data as−is, label 25 best qvalue
limited x− and y−axis, no labels
limited x− and y−axis, label 25 best qvalue
−log10 FDR adjusted p−value
log2 fold−change
SMOC1
ALDOA
PKM
YWHAG
YWHAZ
HPRT1
LDHA
PGK1
STMN1
LDHB
GDA
YWHAE
SPP1
SERPING1
SOD2
FABP3
CRYM
NID2
PGAM1
TMEM189−U...
MIF
SERPINF1
GPI
YWHAB
down regulated
not significant
up regulated
down regulated & outside plot limits
not significant & outside plot limits
up regulated & outside plot limits

2.4.2 foldchange distribution

Distributions of estimated foldchanges produced by the statistical models. If the mode is far from 0, consider alternative normalization strategies. Do note the scale on the x-axis, for some experiments the foldchanges are very low which in turn may exaggerate this figure.

note; the MSqRob model tends to assign zero (log)foldchange for proteins with minor difference between conditions where the model is very sure the null hypothesis cannot be rejected (shrinkage by the ridge regression model). As a result, many foldchanges will be zero and the density plot for MSqRob may look like a spike instead of the expected Gaussian shape observed in other models



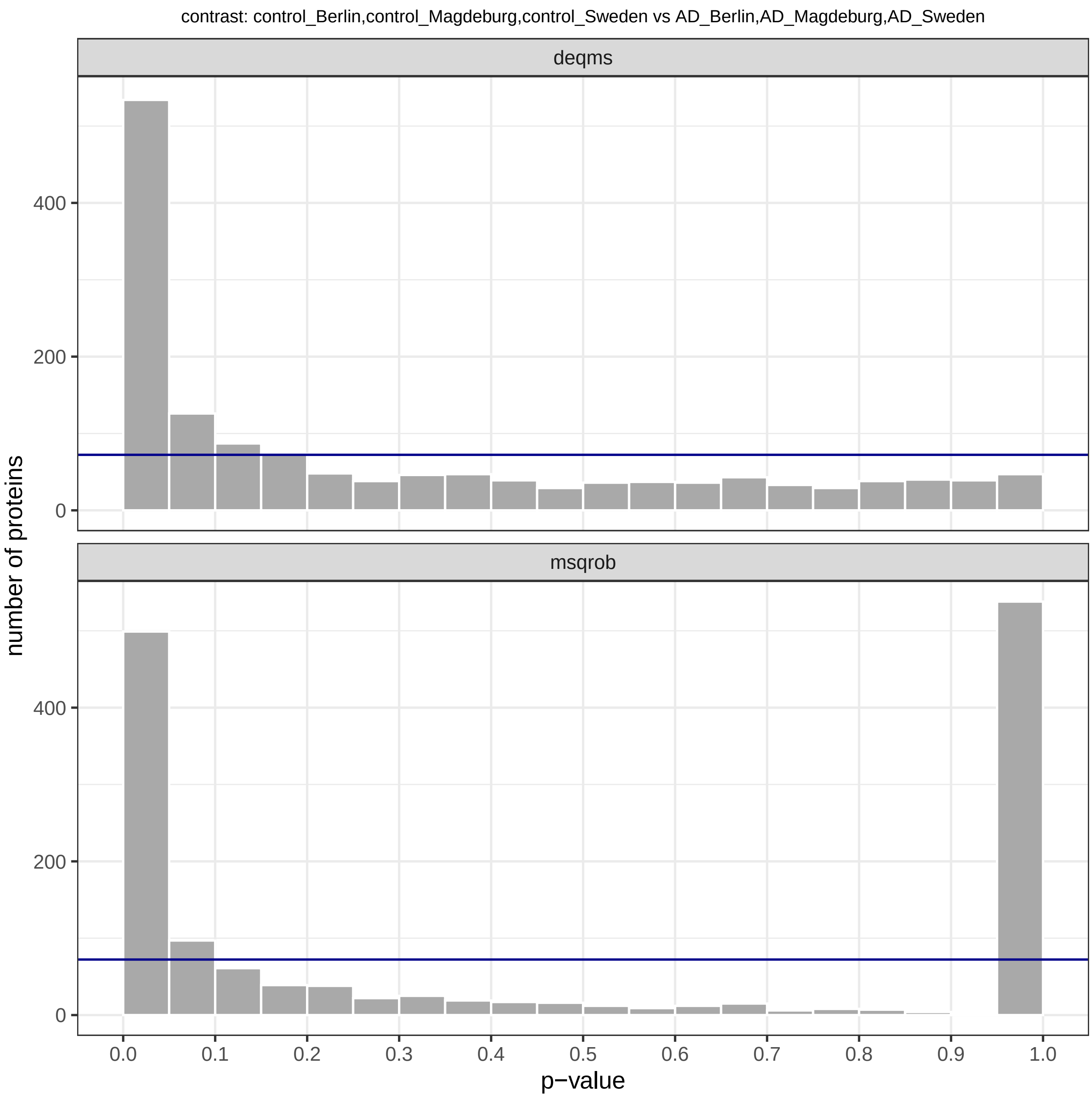
2.4.3 p-value distribution

Histogram of p-values computed by differential expression analysis algorithms, as-is, for quality-control inspection. The horizontal line indicates the expected counts assuming a uniform distribution (total number of p-values divided by number of histogram bins)

See further: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6164648/

See further: http://varianceexplained.org/statistics/interpreting-pvalue-histogram/

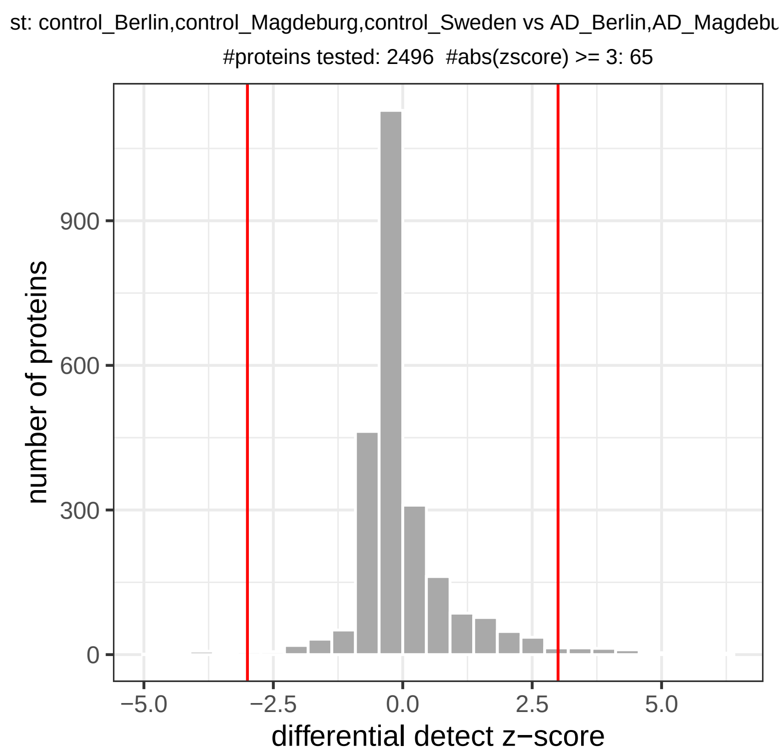
note; the MSqRob and MS-EmpiRe models often yield p-value distributions that show a large peak at p-value 1, these are typically proteins with estimated log foldchanges at/near zero where these models are very sure the null hypothesis cannot be rejected



2.4.4 differential detect

Some proteins may not have peptides with sufficient data points over samples to be used for differential expression analysis (depending on the user-defined filtering criteria in how many replicates peptides should be observed), but do show a strong difference in the number of detected peptides between sample groups. In some proteomics experimental designs, for example a wildtype-knockout APMS study, those are interesting proteins. The DEA based on peptide abundance values (volcano plots above) are the main result for differential testing in MS-DAP but as a situationally useful tool MS-DAP also includes a 'protein detection' z-score, based on the number of times a peptide for each protein was detected per sample group (/experimental condition), as an alternative means of differential testing.

Below figure shows the distribution of these scores with thresholds at 3 std. Both the z-scores and the counts these are based upon are available in the statistical result Excel table.



3 Summary of differential testing

Differential Expression Analysis: number of proteins found statistically significant.

contrast	algorithm	#test	#hits	top10 significant
control_Berlin vs AD_Berlin	deqms	1662	17	ywhag, smoc1, ywhaz, ywhae, aldoa, ldha, pgk1, gda, hprt1, eno1
control_Berlin vs AD_Berlin	msqrob	1662	31	ywhag, smoc1, ywhae, ywhaz, aldoa, pgk1, ldha, hprt1, gda, ptpa
control_Magdeburg vs AD_Magdeburg	deqms	1617	384	mif, ldha, dld, serpinf1, ltbp1, camk2b, rims2, dynll1;..., clic4, pgam1
control_Magdeburg vs AD_Magdeburg	msqrob	1617	411	mif, dynll1;..., camk2b, gpi, ldha, serpinf1, pgam1, clic4, nid2, ltbp1
control_Sweden vs AD_Sweden	deqms	1732	453	pkm, aldoa, ywhag, gda, got1, basp1, pgam1, crtac1, hprt1, fam3c
control_Sweden vs AD_Sweden	msqrob	1732	492	pkm, ywhag, aldoa, pgam1, vasn, got1, crtac1, basp1, gda, hprt1
control_Berlin,... vs AD_Berlin,AD_Ma...	deqms	1445	380	ywhag, aldoa, smoc1, pkm, ldha, ywhaz, hprt1, gda, ywhae, ldhb
control_Berlin,... vs AD_Berlin,AD_Ma...	msqrob	1445	379	smoc1, ywhag, aldoa, pkm, ldha, hprt1, ywhaz, stmn1, pgk1, ywhae

Differential Detection: prioritize proteins with more peptide detections in some group. A simple metric to complement results from DEA, which is the main result (eg; consider proteins with too few data points for DEA).

contrast	#proteins tested	#abs(zscore) >= 3	top10
control_Berlin vs AD_Berlin	2369	74	park7, grm4, acly, arl3, sdk2, ptprc, sema5a, mgat4a, cct2, psmd1
control_Magdeburg vs AD_Magdeburg	2290	30	crhbp, ppp3ca, wars, btf3, stx1b, mydgf, hspa4, brinp1, pcyox1, slitrk6
control_Sweden vs AD_Sweden	2691	68	hnrnpk, ddx6, rps10-n..., tomm22, rab14, ssrp1, glul, dlat, hist1h2..., ccsmst1
control_Berlin,... vs AD_Berlin,AD_Ma...	2496	65	tubb, park7, plppr4, smarce1, cdon, glce, dlat, gsta4, rbmxl1;..., sqstm1

4 log

[info] reading Spectronaut report...

[info] 22557/31469 precursors remain after selecting the 'best' precursor for each modified sequence

[info] 6882/6882 protein accessions and 2771/2771 protein groups were mapped to provided fasta file(s)

[info] contrast: control__Berlin vs AD__Berlin

[info] contrast: control__Magdeburg vs AD__Magdeburg

[info] contrast: control__Sweden vs AD__Sweden

[info] contrast: control__Berlin,control__Magdeburg,control__Sweden vs AD__Berlin,AD__Magdeburg,AD__Sweden

[info] using 23 threads for multiprocessing

[progress] caching filter data took 2.5 minutes

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 2 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 2 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 2 seconds

[progress] peptide filtering and normalization took 4.1 minutes

[info] peptide to protein rollup strategy: maxlfq

[info] differential expression analysis for contrast: control__Berlin vs AD__Berlin

[info] using data from peptide filter: filter by contrast

[info] random variables that are *not* applicable for current contrast due to lack of unique values (compared to sample groups/condition): cohort

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] DEqMS took 1 seconds

[info] msqrob linear regression formulas (these are prioritized. eg; if a model fit fails due to lack of data, the next formula is used); expression ~ (1 | condition) + (1 | sample_id) + (1 | peptide_id) , expression ~ (1 | condition)

[progress] msqrob took 6.5 minutes

[info] differential expression analysis for contrast: control__Magdeburg vs AD__Magdeburg

[info] using data from peptide filter: filter by contrast

[info] random variables that are *not* applicable for current contrast due to lack of unique values (compared to sample groups/condition): cohort

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] DEqMS took 1 seconds

[info] msqrob linear regression formulas (these are prioritized. eg; if a model fit fails due to lack of data, the next formula is used); expression ~ (1 | condition) + (1 | sample_id) + (1 | peptide_id) , expression ~ (1 | condition)

[progress] msqrob took 5.7 minutes

[info] differential expression analysis for contrast: control__Sweden vs AD__Sweden

[info] using data from peptide filter: filter by contrast

[info] random variables that are *not* applicable for current contrast due to lack of unique values (compared to sample groups/condition): cohort

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] DEqMS took 1 seconds

[info] msqrob linear regression formulas (these are prioritized. eg; if a model fit fails due to lack of data, the next formula is used); expression ~ (1 | condition) + (1 | sample_id) + (1 | peptide_id) , expression ~ (1 | condition)

[progress] msqrob took 5.6 minutes

[info] differential expression analysis for contrast: control__Berlin,control__Magdeburg,control__Sweden vs AD__Berlin,AD__Magdeburg,AD__Sweden

[info] using data from peptide filter: filter by contrast

[info] random variables used in current contrast: cohort

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds [progress] DEqMS took 1 seconds

[info] msqrob linear regression formulas (these are prioritized. eg; if a model fit fails due to lack of data, the next formula is used); expression ~ (1 | condition) + (1 | sample_id) + (1 | peptide_id) + (1 | cohort) , expression ~ (1 | condition) + (1 | cohort) , expression ~ (1 | condition)

[progress] msqrob took 10.3 minutes

[info] differential detection analysis: min_samples_observed=3

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] creating PDF report…

[progress] report: constructing plots specific for each contrast

[progress] report: rendering report (this may take a while depending on dataset size)

[progress] RT plots: preparing data took 20 seconds

[progress] RT plots: creating plots took 7 seconds

[info] skipping within-group foldchange plots for sample group 'unknown_Kiel', require at least 2 replicates

[info] skipping within-group foldchange plots for sample group 'unknown_Sweden', require at least 2 replicates

[info] No data available for CoV leave-one-out computation in sample group 'unknown_Kiel', skipping plots

[info] No data available for CoV leave-one-out computation in sample group 'unknown_Sweden', skipping plots

[progress] leave-one-out CoV plot computations took 8 seconds

[info] no CoV computation for sample group 'unknown_Kiel', require at least 3 replicates

[info] no CoV computation for sample group 'unknown_Magdeburg', require at least 3 replicates

[info] no CoV computation for sample group 'unknown_Sweden', require at least 3 replicates

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[info] no CoV computation for sample group 'unknown_Kiel', require at least 3 replicates

[info] no CoV computation for sample group 'unknown_Magdeburg', require at least 3 replicates

[info] no CoV computation for sample group 'unknown_Sweden', require at least 3 replicates

5 R command history

This shows the history commands from your R script that starts this pipeline, thereby automatically documenting the parameters/settings used. All lines of executed code since (last) importing data using this R package are shown.

Using this feature

Do not use RStudio's `source` option to execute our pipeline since it will only write `source(...yourscript.R)` to the session history, and consequentially that is all you see in this 'code log'. Instead, select all lines in your script (`control + A`) and then "run" the selected code (either click the run button in RStudio, or use `control + enter`). All lines shown in this section are the same as shown in the RStudio 'History' pane (a tab on the top-right of its UI).

```
dataset = import_dataset_spectronaut(
  filename = "C:/DATA/PMID32485097/20200914_185722_SNA-fSN1.1_CLib1.1 with deamidation_SNA-SER1.1 BGS default_all final raw files Zet Ma
  confidence_threshold = 0.05,
  use_normalized_intensities = FALSE,
  use_irt = TRUE, do_plot = TRUE
)
dataset = import_fasta(dataset,
  files = c(
    "C:/fasta/UniProt_2018-05/UP000005640_9606.fasta",
    "C:/fasta/UniProt_2018-05/UP000005640_9606_additional.fasta",
    "C:/fasta/UniProt_2017-06/UP000005640_9606.fasta",
    "C:/fasta/UniProt_2017-06/UP000005640_9606_additional.fasta"
  )
)
dataset = import_sample_metadata(dataset,
  filename = "C:/DATA/PMID32485097/sample_metadata.xlsx"
)
dataset = setup_contrasts(dataset,
  contrast_list = list(
    c(
      "control_Berlin",
      "AD_Berlin"
    ),
    c(
      "control_Magdeburg",
      "AD_Magdeburg"
    ),
    c(
      "control_Sweden",
      "AD_Sweden"
    ),
    list(
      c(
        "control_Berlin",
        "control_Magdeburg",
        "control_Sweden"
      ),
      c(
        "AD_Berlin",
        "AD_Magdeburg",
        "AD_Sweden"
      )
    )
  ),
  random_variables = "cohort"
)
dataset = analysis_quickstart(dataset,
  filter_min_detect = 8,
  filter_by_contrast = TRUE,
  filter_topn_peptides = 0,
  filter_min_peptide_per_prot = 1,
  norm_algorithm = c(
    "vsn",
    "modebetween_protein"
  ),
  dea_algorithm = c(
    "deqms",
```

```
    "msqrob"
  ), dea_qvalue_threshold = 0.05,
  output_qc_report = TRUE,
  output_dir = "C:/DATA/PMID32485097/",
  dump_all_data = TRUE,
  output_within_timestamped_subdirectory = TRUE
)
```

6 R session info

The computer system and versioning of all R packages used to run this analysis are shown below to facilitate, in combination with the previous section, reproducibility.

setting	value
version	R version 3.6.3 (2020-02-29)
os	Windows 10 x64
system	x86_64, mingw32
ui	RStudio
language	(EN)
collate	English_United States.1252
ctype	English_United States.1252
tz	Europe/Berlin
date	2021-05-23

System

package	loadedversion	source
dplyr	1.0.0	CRAN (R 3.6.3)
ggplot2	3.3.2	CRAN (R 3.6.3)
msdap	0.2.8.1	local
rlang	0.4.6	CRAN (R 3.6.3)
testthat	2.3.2	CRAN (R 3.6.3)
tibble	3.0.1	CRAN (R 3.6.3)
tidyr	1.1.0	CRAN (R 3.6.3)

Attached packages

package	loadedversion	source
abind	1.4-5	CRAN (R 3.6.0)
affy	1.64.0	Bioconductor
affyio	1.56.0	Bioconductor
AnnotationDbi	1.48.0	Bioconductor
arrangements	1.1.8	CRAN (R 3.6.3)
askpass	1.1	CRAN (R 3.6.3)
assertthat	0.2.1	CRAN (R 3.6.3)
backports	1.1.7	CRAN (R 3.6.3)
bigassertr	0.1.4	CRAN (R 3.6.3)
bigparallelr	0.3.1	CRAN (R 3.6.3)
bigstatsr	1.5.1	CRAN (R 3.6.3)
Biobase	2.46.0	Bioconductor
BiocFileCache	1.10.2	Bioconductor
BiocGenerics	0.32.0	Bioconductor
BiocManager	1.30.10	CRAN (R 3.6.3)
BiocParallel	1.20.1	Bioconductor
biomaRt	2.45.8	Github (grimbough/biomaRt@61c3ee0)
bit	1.1-15.2	CRAN (R 3.6.2)
bit64	0.9-7	CRAN (R 3.6.2)
bitops	1.0-6	CRAN (R 3.6.0)
blob	1.2.1	CRAN (R 3.6.3)
boot	1.3-24	CRAN (R 3.6.3)
broom	0.5.6	CRAN (R 3.6.3)
callr	3.4.3	CRAN (R 3.6.3)
car	3.0-8	CRAN (R 3.6.3)
carData	3.0-4	CRAN (R 3.6.3)
caTools	1.18.0	CRAN (R 3.6.3)
cellranger	1.1.0	CRAN (R 3.6.3)
cli	2.0.2	CRAN (R 3.6.3)
codetools	0.2-16	CRAN (R 3.6.3)
colorRamps	2.3	CRAN (R 3.6.0)
colorspace	1.4-1	CRAN (R 3.6.3)
cowplot	1.0.0	CRAN (R 3.6.3)
crayon	1.3.4	CRAN (R 3.6.3)
curl	4.3	CRAN (R 3.6.3)
data.table	1.12.8	CRAN (R 3.6.3)
DBI	1.1.0	CRAN (R 3.6.3)
dbplyr	1.4.4	CRAN (R 3.6.3)
DEqMS	1.4.0	Bioconductor
desc	1.2.0	CRAN (R 3.6.3)
devtools	2.3.0	CRAN (R 3.6.3)
diann	1.0.1	Github (vdemichev/diann-rpackage@af538f6)
digest	0.6.25	CRAN (R 3.6.3)
doParallel	1.0.15	CRAN (R 3.6.3)
ellipsis	0.3.1	CRAN (R 3.6.3)
eulerr	6.1.0	CRAN (R 3.6.3)
evaluate	0.14	CRAN (R 3.6.3)
fansi	0.4.1	CRAN (R 3.6.3)
farver	2.0.3	CRAN (R 3.6.3)
flock	0.7	CRAN (R 3.6.3)

package	loadedversion	source
forcats	0.5.0	CRAN (R 3.6.3)
foreach	1.5.0	CRAN (R 3.6.3)
foreign	0.8-75	CRAN (R 3.6.3)
formatR	1.7	CRAN (R 3.6.3)
fs	1.4.1	CRAN (R 3.6.3)
gdata	2.18.0	CRAN (R 3.6.3)
generics	0.1.0	CRAN (R 3.6.3)
ggpubr	0.4.0	CRAN (R 3.6.3)
ggrepel	0.8.2	CRAN (R 3.6.3)
ggsignif	0.6.0	CRAN (R 3.6.3)
glue	1.4.1	CRAN (R 3.6.3)
gmp	0.6-0	CRAN (R 3.6.3)
gplots	3.0.4	CRAN (R 3.6.3)
gridExtra	2.3	CRAN (R 3.6.3)
gtable	0.3.0	CRAN (R 3.6.3)
gtools	3.8.2	CRAN (R 3.6.3)
haven	2.3.1	CRAN (R 3.6.3)
hms	0.5.3	CRAN (R 3.6.3)
htmltools	0.5.0	CRAN (R 3.6.3)
httr	1.4.1	CRAN (R 3.6.3)
impute	1.60.0	Bioconductor
iq	1.9	CRAN (R 3.6.3)
IRanges	2.20.2	Bioconductor
iterators	1.0.12	CRAN (R 3.6.3)
KernSmooth	2.23-16	CRAN (R 3.6.3)
knitr	1.29	CRAN (R 3.6.3)
labeling	0.3	CRAN (R 3.6.0)
lattice	0.20-38	CRAN (R 3.6.3)
lifecycle	0.2.0	CRAN (R 3.6.3)
limma	3.42.2	Bioconductor
lme4	1.1-23	CRAN (R 3.6.3)
magrittr	1.5	CRAN (R 3.6.3)
MALDIquant	1.19.3	CRAN (R 3.6.3)
MASS	7.3-51.5	CRAN (R 3.6.3)
Matrix	1.2-18	CRAN (R 3.6.3)
matrixStats	0.56.0	CRAN (R 3.6.3)
memoise	1.1.0	CRAN (R 3.6.3)
mgcv	1.8-31	CRAN (R 3.6.3)
minqa	1.2.4	CRAN (R 3.6.3)
msEmpiRe	0.1.0	Github (zimmerlab/MS-EmpiRe@8a85757)
MSnbase	2.12.0	Bioconductor
munsell	0.5.0	CRAN (R 3.6.3)
mzID	1.24.0	Bioconductor
mzR	2.20.0	Bioconductor
ncdf4	1.17	CRAN (R 3.6.1)
nlme	3.1-144	CRAN (R 3.6.3)
nloptr	1.2.2.1	CRAN (R 3.6.3)
openssl	1.4.2	CRAN (R 3.6.3)
openxlsx	4.1.5	CRAN (R 3.6.3)
packrat	0.5.0	CRAN (R 3.6.3)

package	loadedversion	source
patchwork	1.0.1	CRAN (R 3.6.3)
pbkrtest	0.4-8.6	CRAN (R 3.6.3)
pcaMethods	1.78.0	Bioconductor
pdftools	2.3.1	CRAN (R 3.6.3)
pillar	1.4.4	CRAN (R 3.6.3)
pkgbuild	1.0.8	CRAN (R 3.6.3)
pkgconfig	2.0.3	CRAN (R 3.6.3)
pkgload	1.1.0	CRAN (R 3.6.3)
plyr	1.8.6	CRAN (R 3.6.3)
preprocessCore	1.48.0	Bioconductor
prettyunits	1.1.1	CRAN (R 3.6.3)
pROC	1.16.2	CRAN (R 3.6.3)
processx	3.4.2	CRAN (R 3.6.3)
progress	1.2.2	CRAN (R 3.6.3)
ProtGenerics	1.18.0	Bioconductor
ps	1.3.3	CRAN (R 3.6.3)
purrr	0.3.4	CRAN (R 3.6.3)
qpdf	1.1	CRAN (R 3.6.3)
R.methodsS3	1.8.0	CRAN (R 3.6.2)
R.oo	1.23.0	CRAN (R 3.6.2)
R.utils	2.9.2	CRAN (R 3.6.3)
R6	2.4.1	CRAN (R 3.6.3)
rappdirs	0.3.1	CRAN (R 3.6.3)
RColorBrewer	1.1-2	CRAN (R 3.6.0)
Rcpp	1.0.4.6	CRAN (R 3.6.3)
RcppEigen	0.3.3.7.0	CRAN (R 3.6.3)
readr	1.3.1	CRAN (R 3.6.3)
readxl	1.3.1	CRAN (R 3.6.3)
remotes	2.1.1	CRAN (R 3.6.3)
reshape2	1.4.4	CRAN (R 3.6.3)
rio	0.5.16	CRAN (R 3.6.3)
rmarkdown	2.3	CRAN (R 3.6.3)
rprojroot	1.3-2	CRAN (R 3.6.3)
rsconnect	0.8.16	CRAN (R 3.6.3)
RSQLite	2.2.0	CRAN (R 3.6.3)
rstatix	0.6.0	CRAN (R 3.6.3)
rstudioapi	0.11	CRAN (R 3.6.3)
S4Vectors	0.24.4	Bioconductor
scales	1.1.1	CRAN (R 3.6.3)
sessioninfo	1.1.1	CRAN (R 3.6.3)
statmod	1.4.34	CRAN (R 3.6.3)
stringi	1.4.6	CRAN (R 3.6.2)
stringr	1.4.0	CRAN (R 3.6.3)
styler	1.3.2	CRAN (R 3.6.3)
tidyselect	1.1.0	CRAN (R 3.6.3)
tinytex	0.24	CRAN (R 3.6.3)
usethis	1.6.1	CRAN (R 3.6.3)
variancePartition	1.16.1	Bioconductor
vctrs	0.3.1	CRAN (R 3.6.3)
viridis	0.5.1	CRAN (R 3.6.3)

package	loadedversion	source
viridisLite	0.3.0	CRAN (R 3.6.3)
vsn	3.54.0	Bioconductor
withr	2.2.0	CRAN (R 3.6.3)
xfun	0.15	CRAN (R 3.6.3)
XML	3.99-0.3	CRAN (R 3.6.3)
xml2	1.3.2	CRAN (R 3.6.3)
xtable	1.8-4	CRAN (R 3.6.3)
yaml	2.2.1	CRAN (R 3.6.3)
zip	2.0.4	CRAN (R 3.6.3)
zlibbioc	1.32.0	Bioconductor

Packages that are not attached