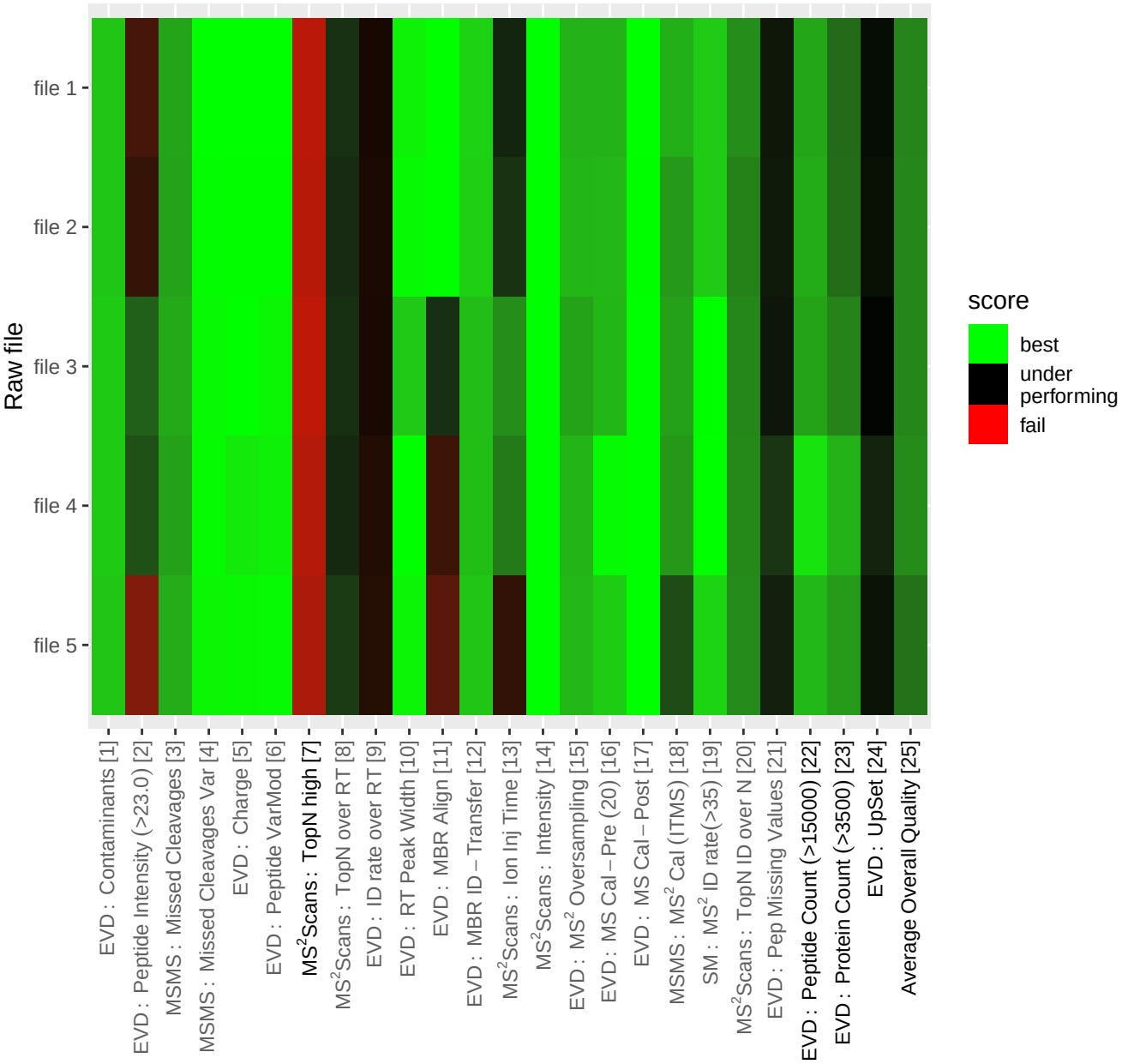
Performance overview



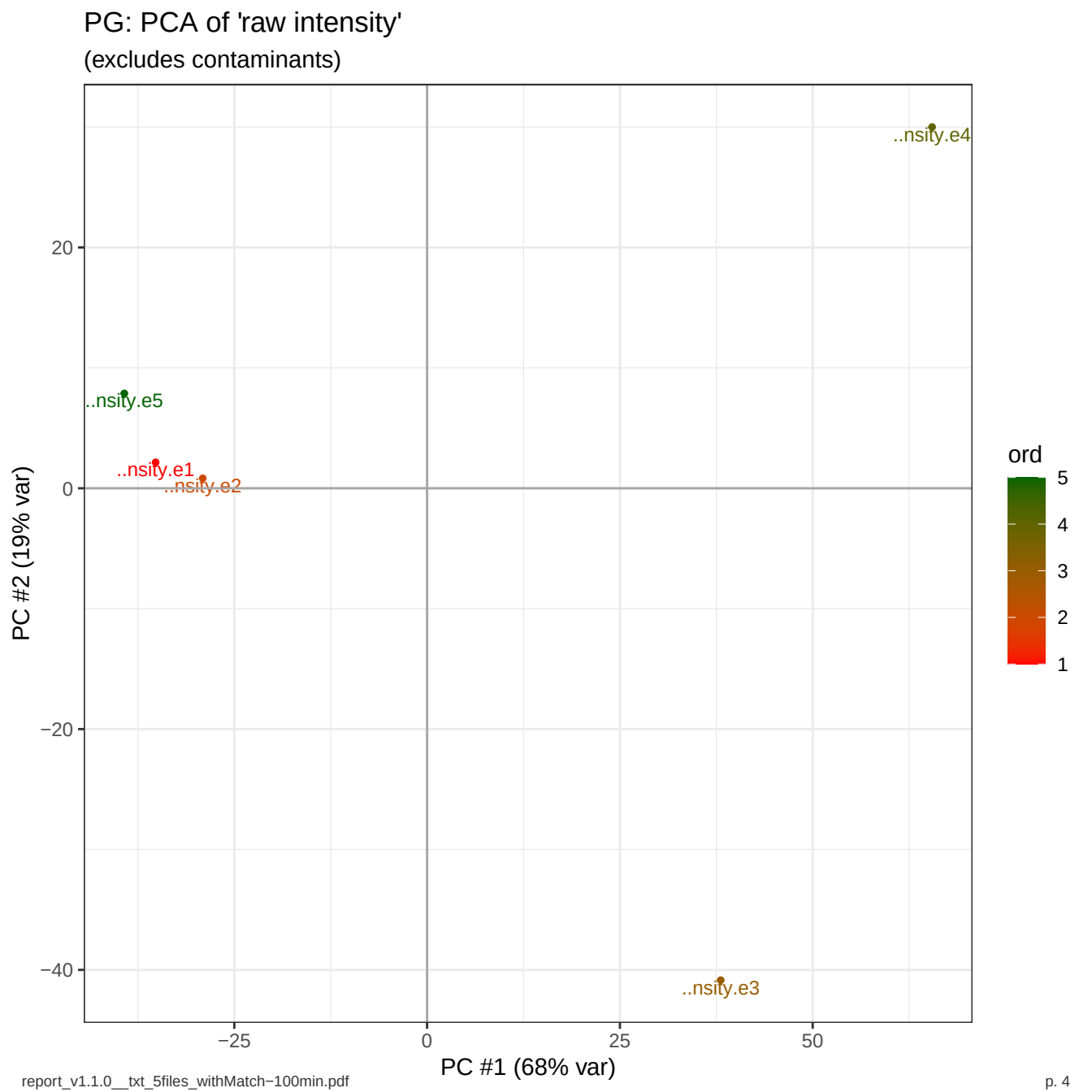
Mapping of Raw files to their short names
Mapping source: file (user−defined)
(automatic shortening of names was not sufficient − see 'best effort')

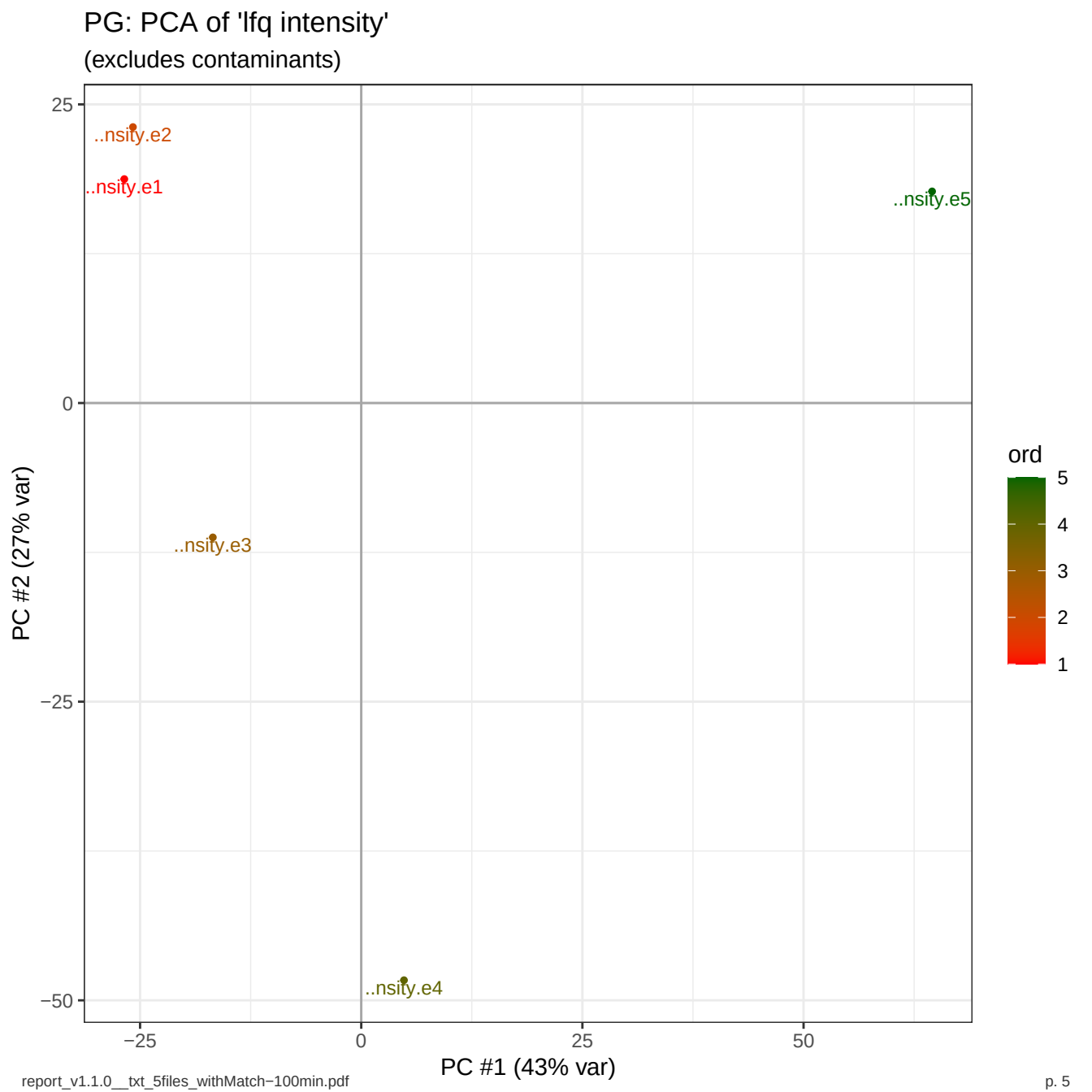
original	short name	best effort
Toni_20140521_GM_QC_01	file 1	..521_GM_QC_0.._01
Toni_20140521_GM_QC_02	file 2	..521_GM_QC_0.._02
Toni_20140522_GM_QC_01	file 3	..522_GM_QC_0.._01
Toni_20140531_FB_QC_02	file 4	..531_FB_QC_0.._02
Toni_20140608_FB_qc_01	file 5	..608_FB_qc_0.._01

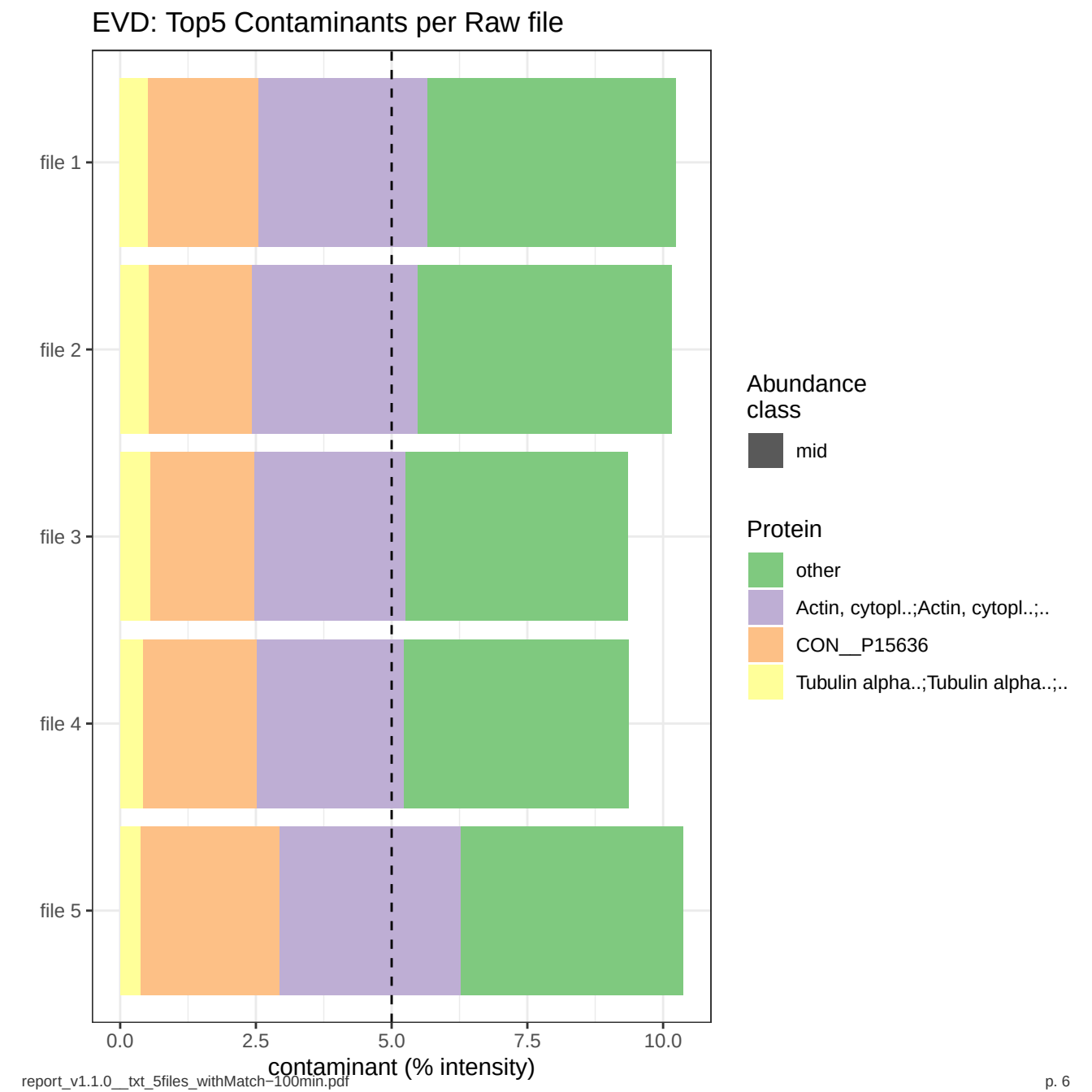
PAR: parameters

parameter	value	parameter	value
Advanced ratios	False	MS/MS deisotoping (ITMS)	False
Alignment time window [min]	100	MS/MS deisotoping (TOF)	False
Cut peaks	True	MS/MS deisotoping (Unknown)	False
Decoy mode	revert	MS/MS recalibration	False
Discard unmodified counterpa..	True	MS/MS tol. (FTMS)	20 ppm
Find dependent peptides	False	MS/MS tol. (ITMS)	0.5 Da
First pass AIF correlation	0.8	MS/MS tol. (TOF)	0.1 Da
Fixed modifications	Carbamidomethyl (C)	MS/MS tol. (Unknown)	0.5 Da
iBAQ	False	Peptides used for protein qu..	Razor
iBAQ log fit	False	Protein FDR	0.01
Include contaminants	True	PSM FDR	0.01
Labeled amino acid filtering	True	Re−quantify	True
Match between runs	True	RT shift	False
Matching time window [min]	1	Site FDR	0.01
Min. delta score for modifie..	17	Site quantification	Use least modified peptide
Min. delta score for unmodif..	0	Site tables	Oxidation (M)Sites.txt
Min. peptide Length	7	Special AAs	KR
Min. peptides	1	Top MS/MS peaks per 100 Da. ..	12
Min. ratio count	2	Top MS/MS peaks per 100 Da. ..	8
Min. razor peptides	1	Top MS/MS peaks per 100 Da. ..	10
Min. score for modified pept..	40	Top MS/MS peaks per 100 Da. ..	10
Min. score for unmodified pe..	0	Use delta score	False
Min. unique peptides	0	Use Normalized Ratios For Oc..	True
Modifications included in pr..	Acetyl (Protein N−term) Oxidation (M)	Use only unmodified peptides..	True
MS/MS deisotoping (FTMS)	True	Version	1.4.1.2

uniprot_human_canonical_and_isoforms_20130513.fasta

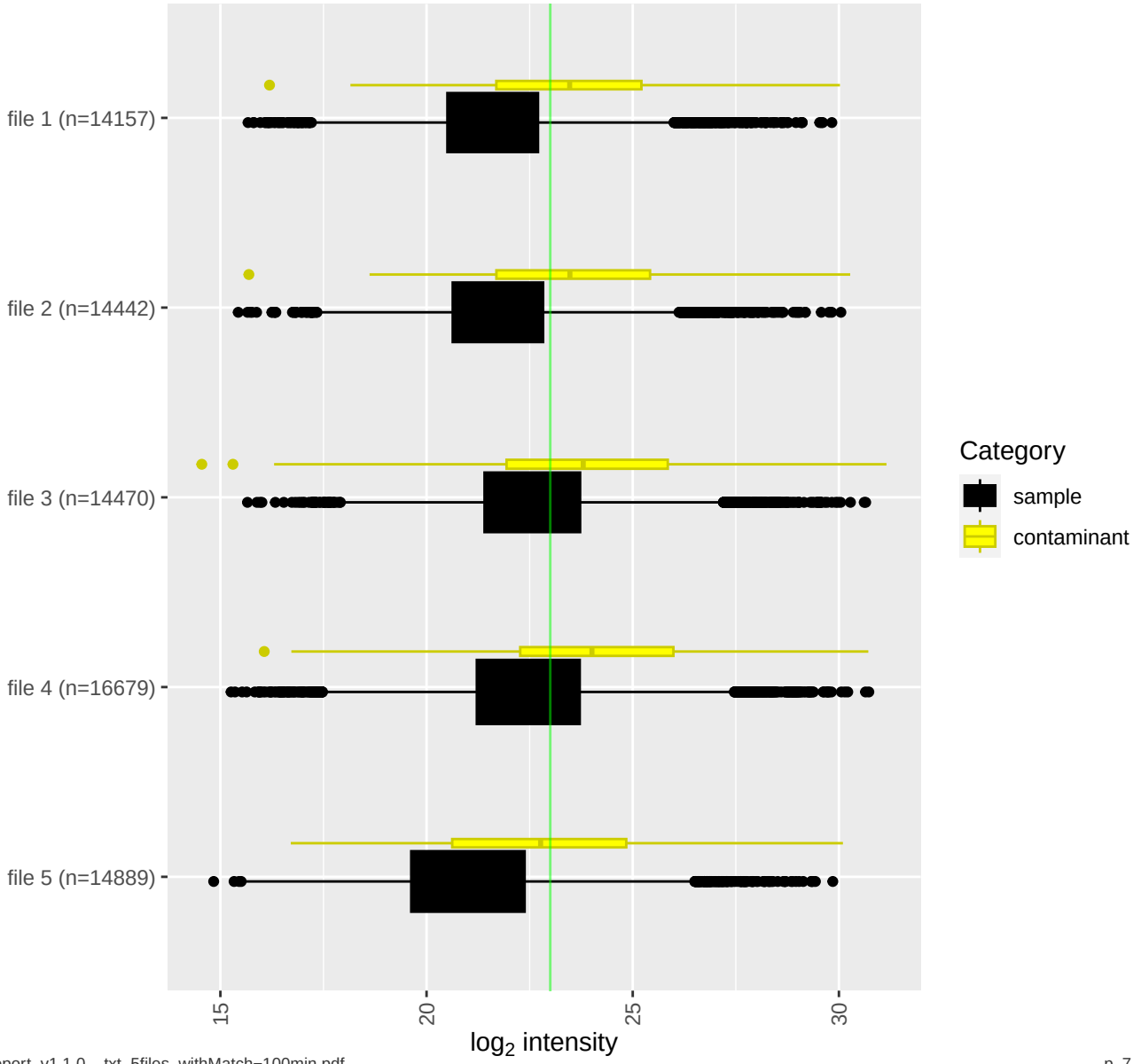

PG: PCA of 'raw intensity'
(excludes contaminants)
..nsity.e4
..nsity.e5
..nsity.e1
..nsity.e2
..nsity.e3
20
0
−20
−40
−25
0
25
50
PC #2 (19% var)
PC #1 (68% var)
ord
5
4
3
2
1


PG: PCA of 'lfq intensity'
(excludes contaminants)
..nsity.e2
..nsity.e1
..nsity.e5
..nsity.e3
..nsity.e4
25
0
−25
−50
−25
0
25
50
PC #2 (27% var)
PC #1 (43% var)
ord
5
4
3
2
1


EVD: Top5 Contaminants per Raw file
file 1
file 2
file 3
file 4
file 5
0.0
2.5
5.0
7.5
10.0
contaminant (% intensity)
Abundance class
mid
Protein
other
Actin, cytopl..;Actin, cytopl..;..
CON__P15636
Tubulin alpha..;Tubulin alpha..;..

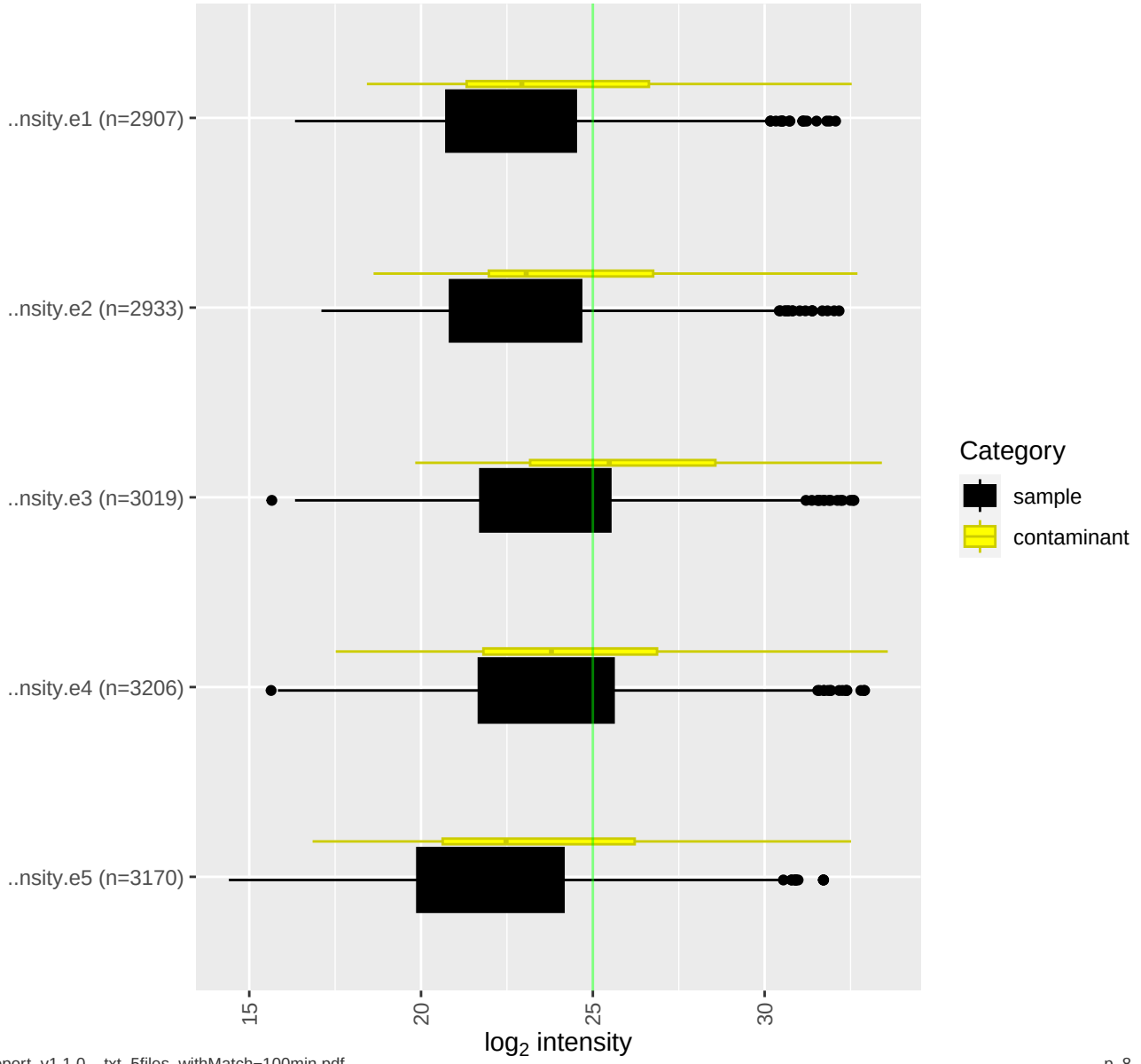
EVD: peptide intensity distribution

RSD 3% (expected < 5%)



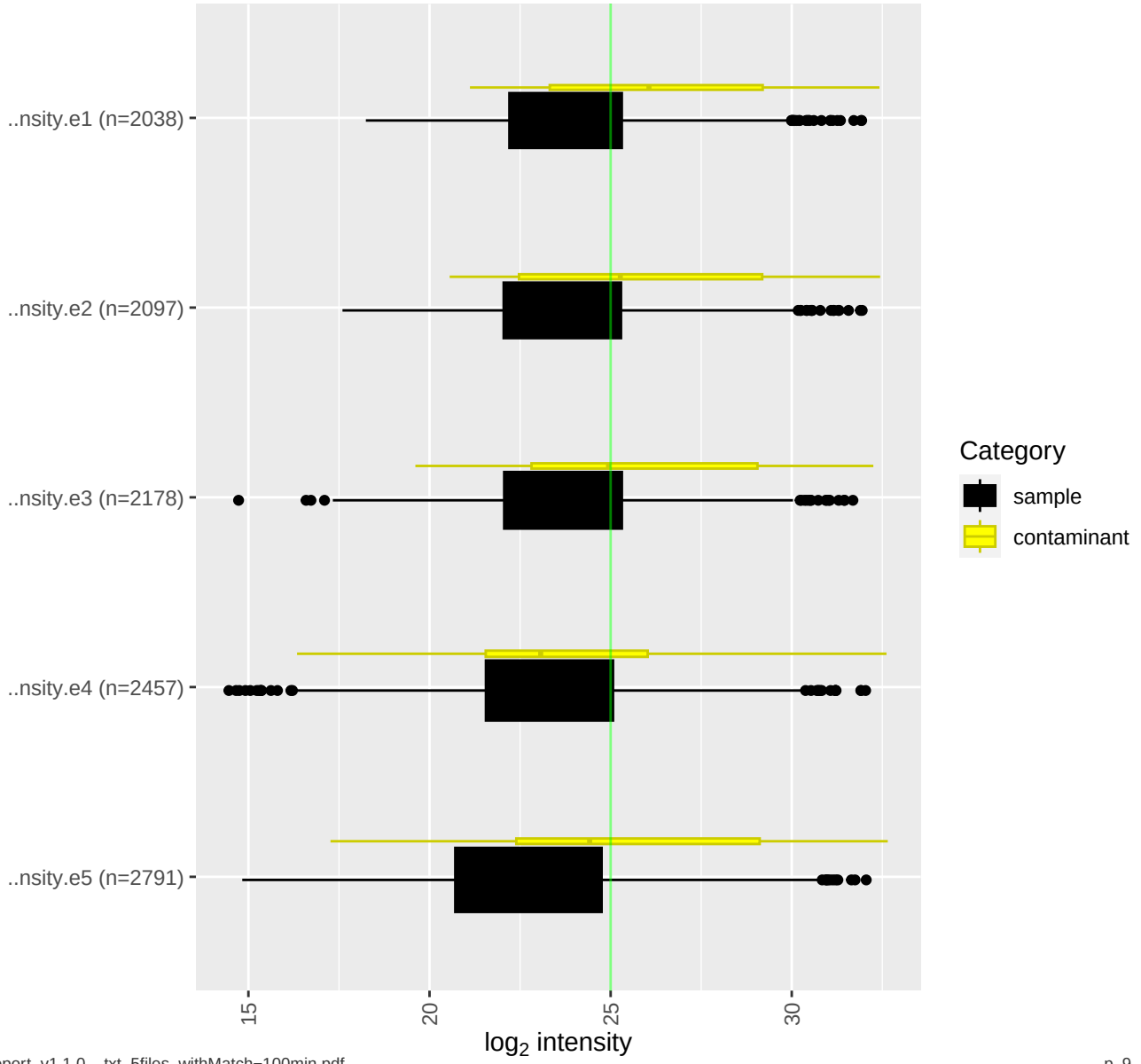
PG: intensity distribution

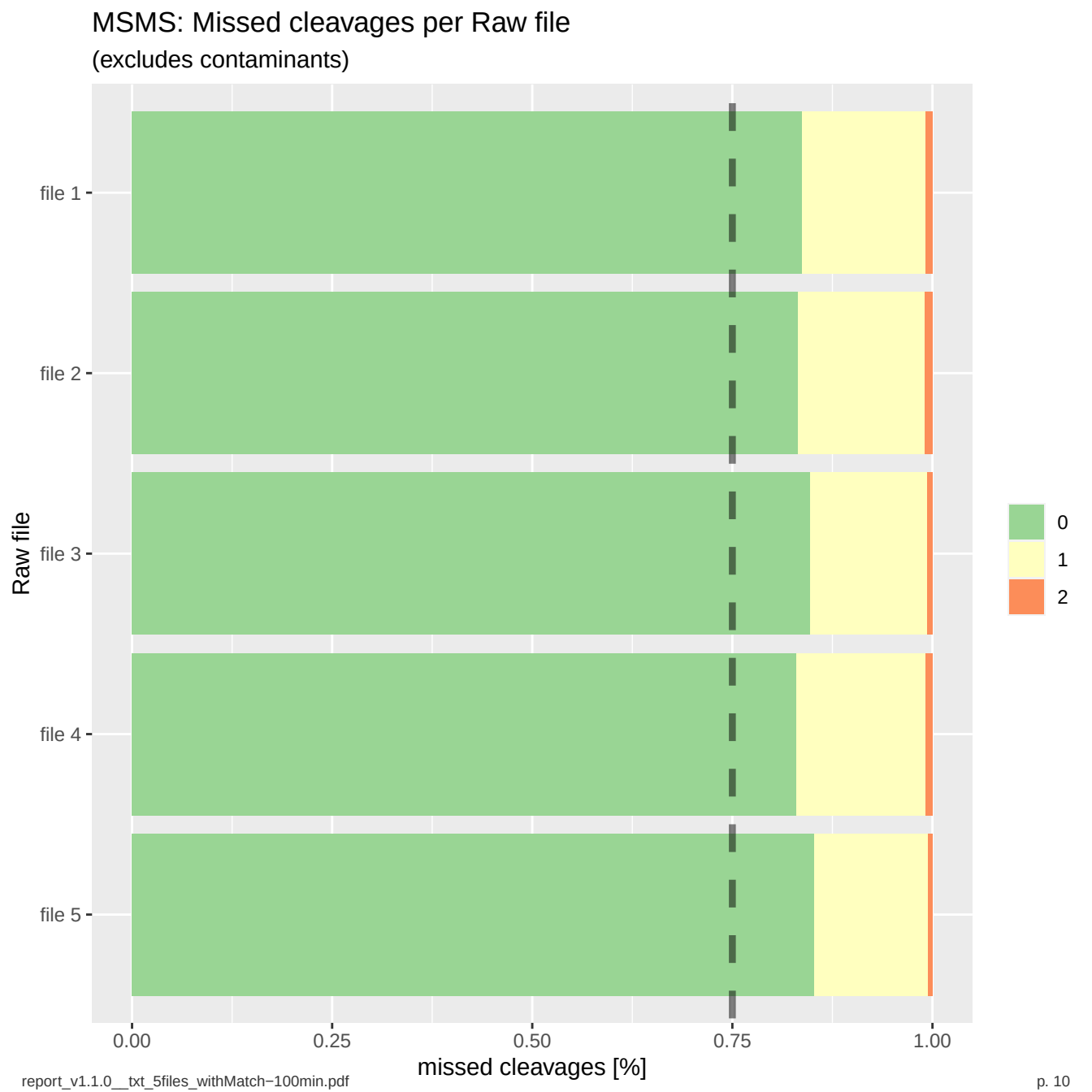
RSD 3% (w/o zero int.; expected < 5%)
RSD 3.2% [high RSD −−> few peptides])



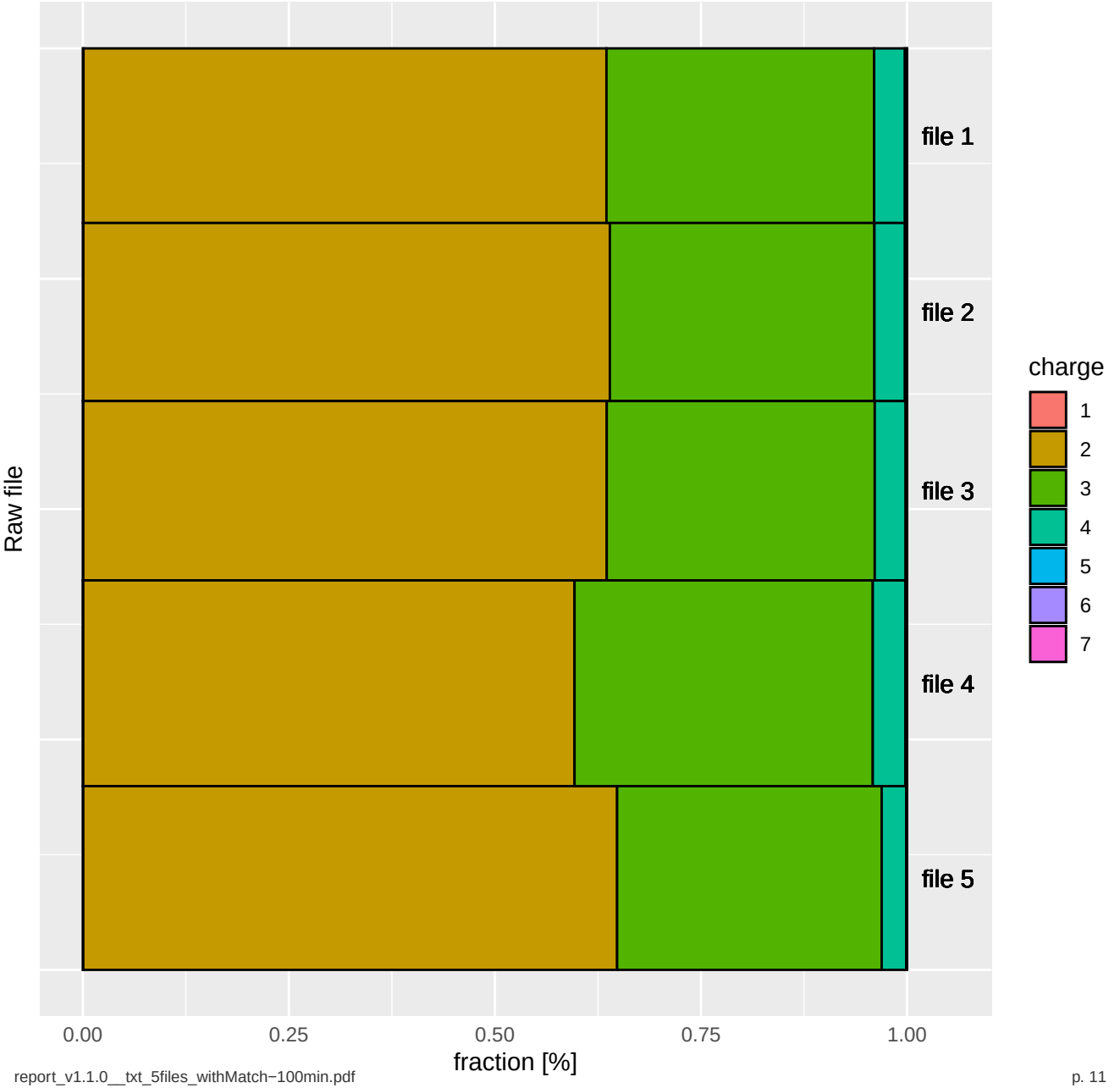
PG: LFQ intensity distribution

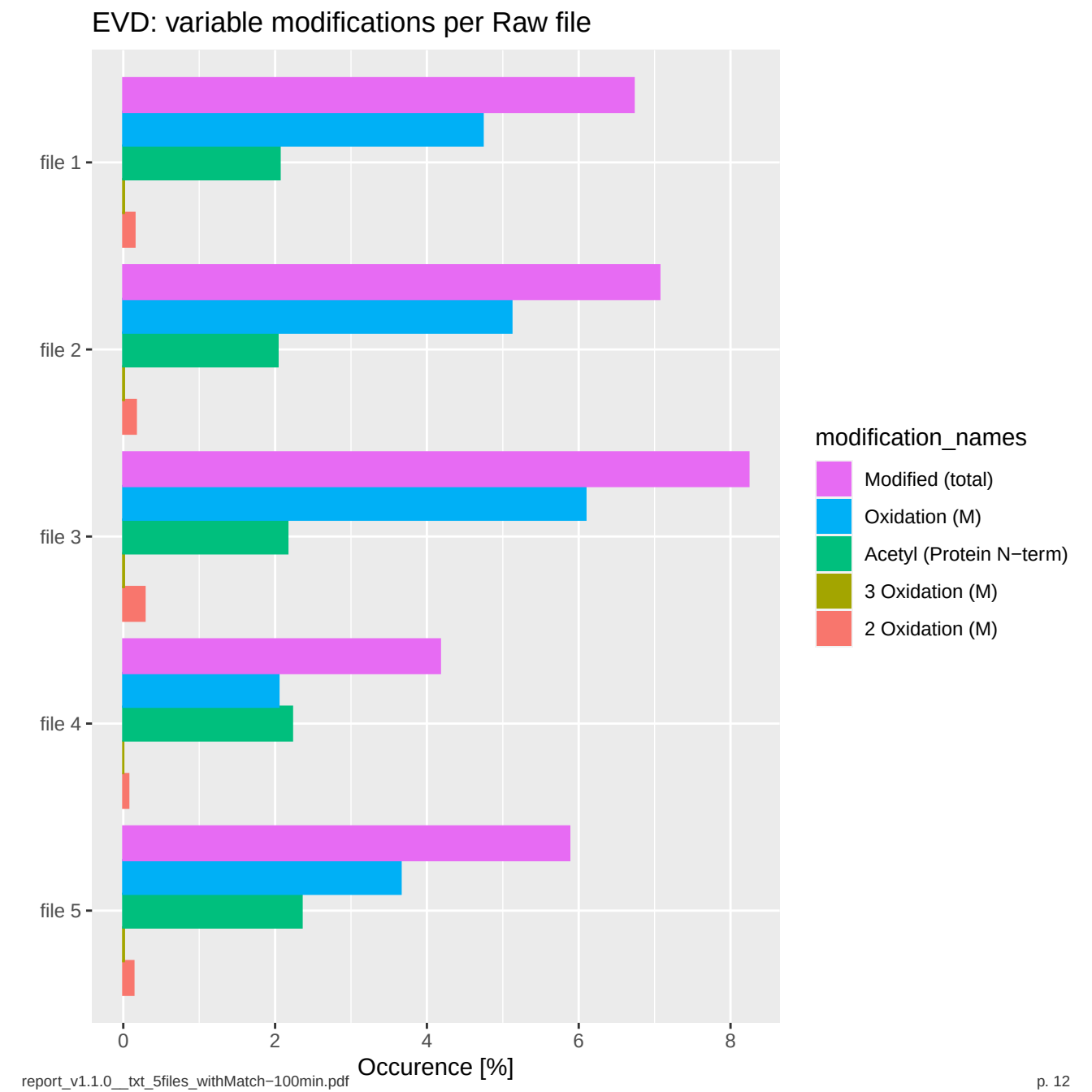
RSD 1.7% (w/o zero int.; expected < 5%)
RSD 0.5% [high RSD −−> few peptides])

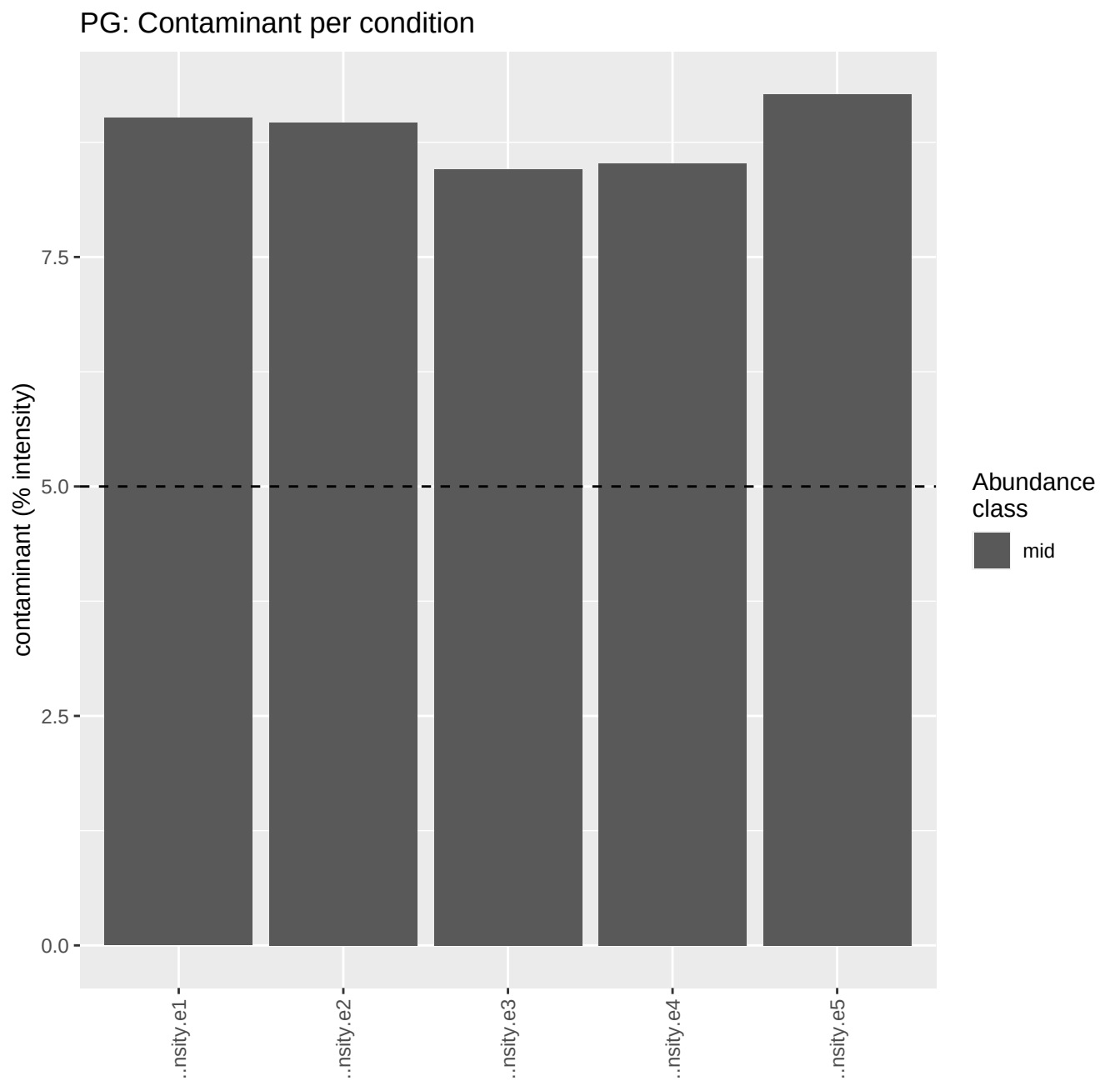



MSMS: Missed cleavages per Raw file
(excludes contaminants)
Raw file
file 1
file 2
file 3
file 4
file 5
0.00
0.25
0.50
0.75
1.00
missed cleavages [%]
0
1
2

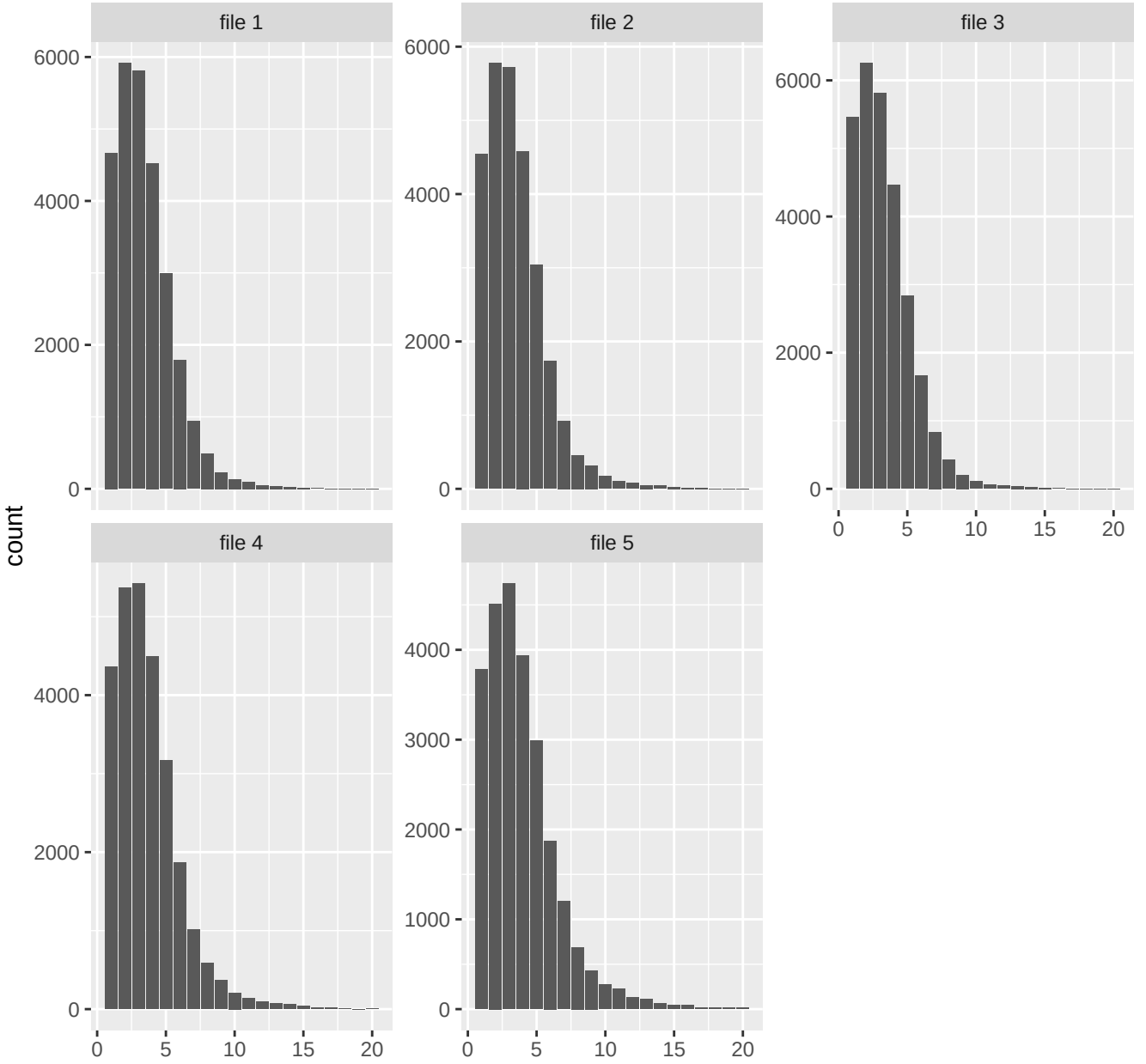
EVD: charge distribution



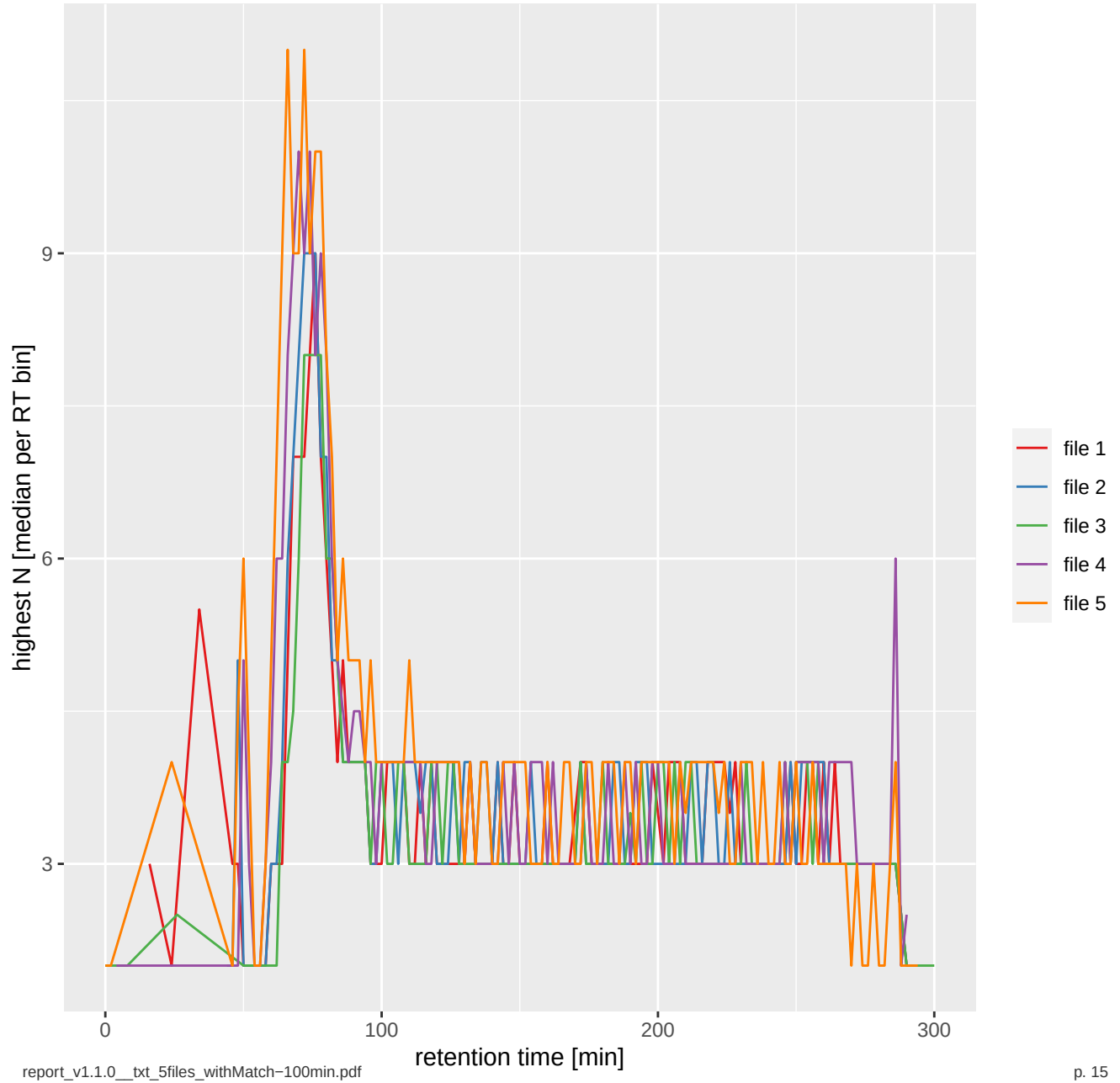

EVD: variable modifications per Raw file
file 1
file 2
file 3
file 4
file 5
0
2
4
6
8
Occurence [%]
modification_names
Modified (total)
Oxidation (M)
Acetyl (Protein N−term)
3 Oxidation (M)
2 Oxidation (M)

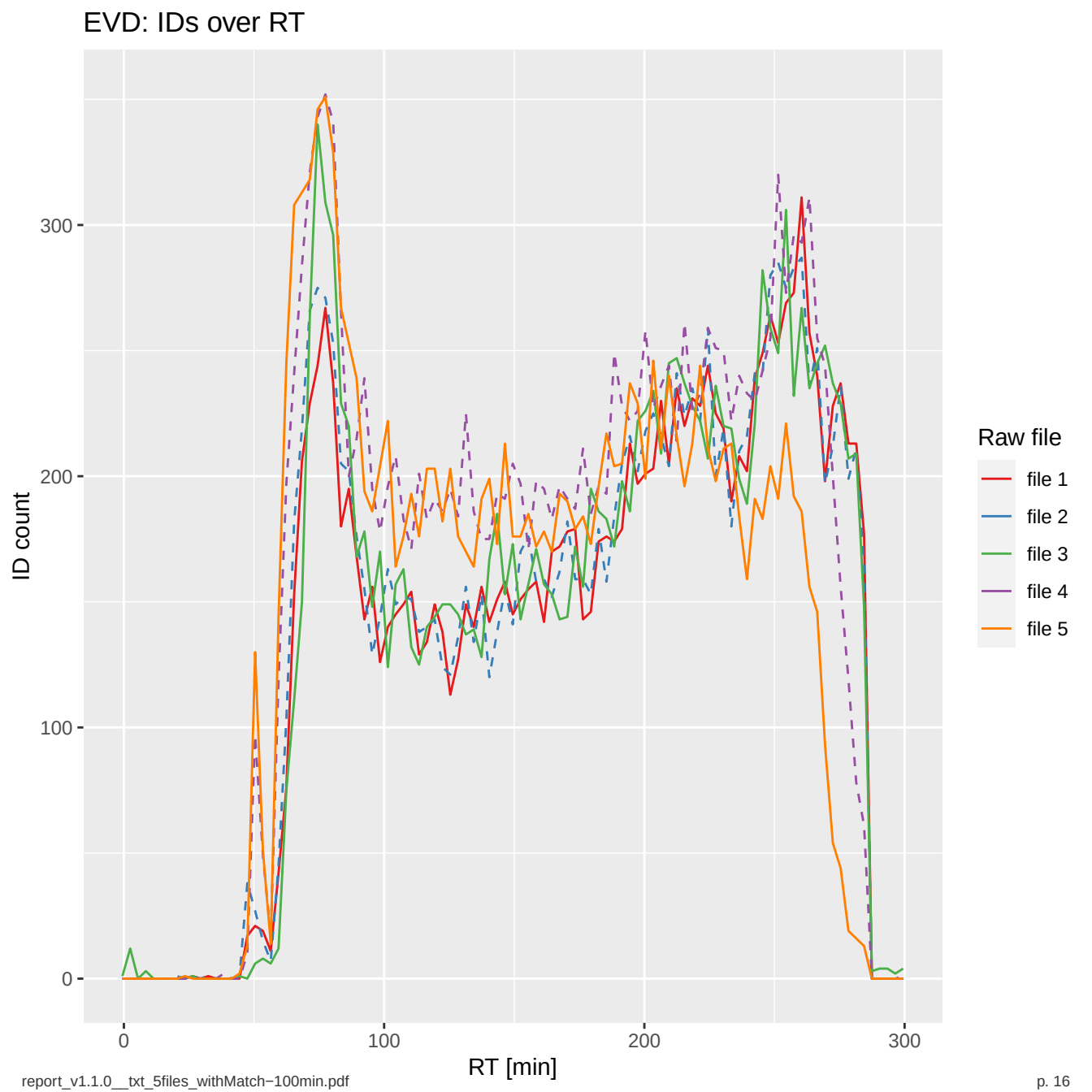

PG: Contaminant per condition
contaminant (% intensity)
7.5
5.0
2.5
0.0
..nsity.e1
..nsity.e2
..nsity.e3
..nsity.e4
..nsity.e5
Abundance class
mid

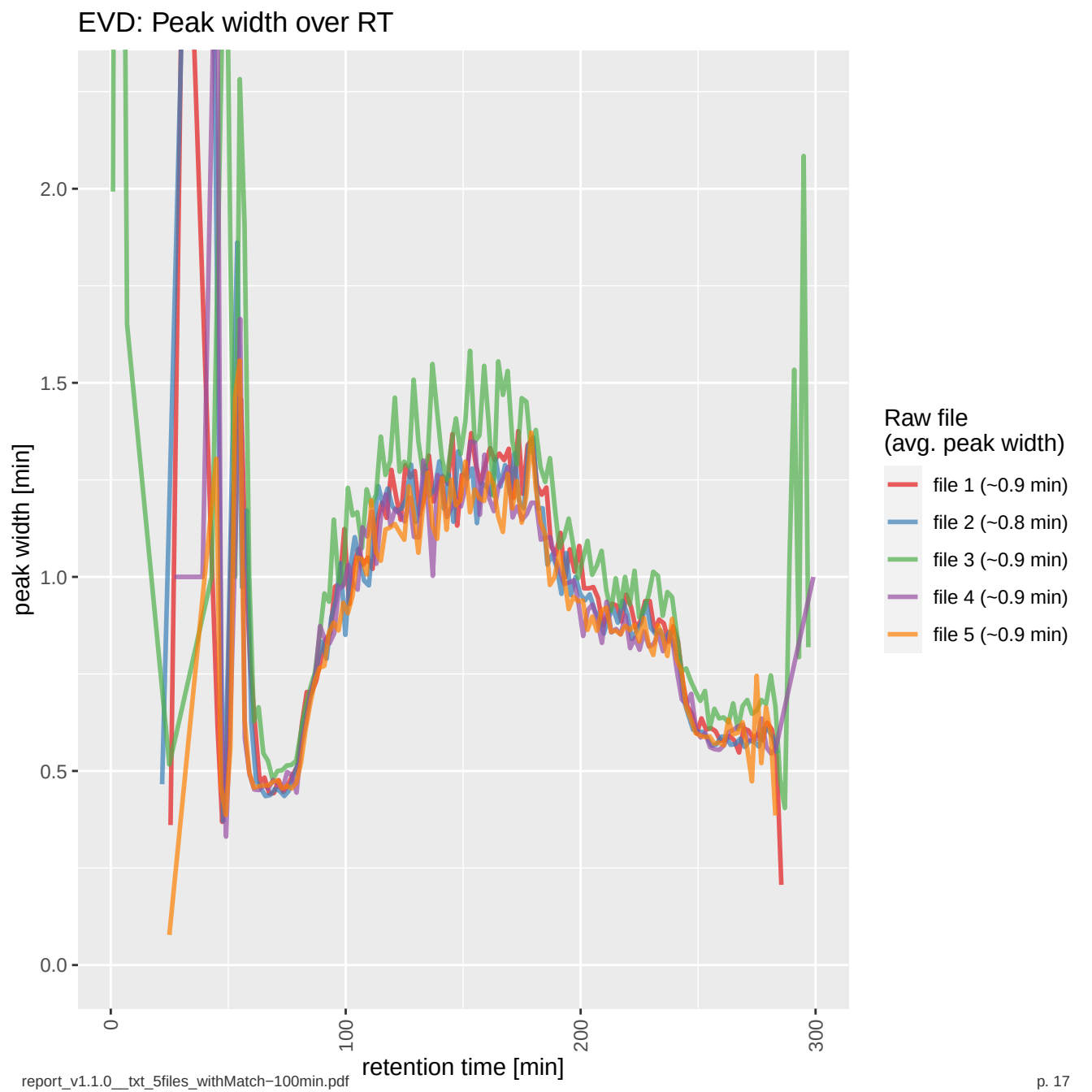
MSMSscans: TopN



MSMSscans: TopN over RT

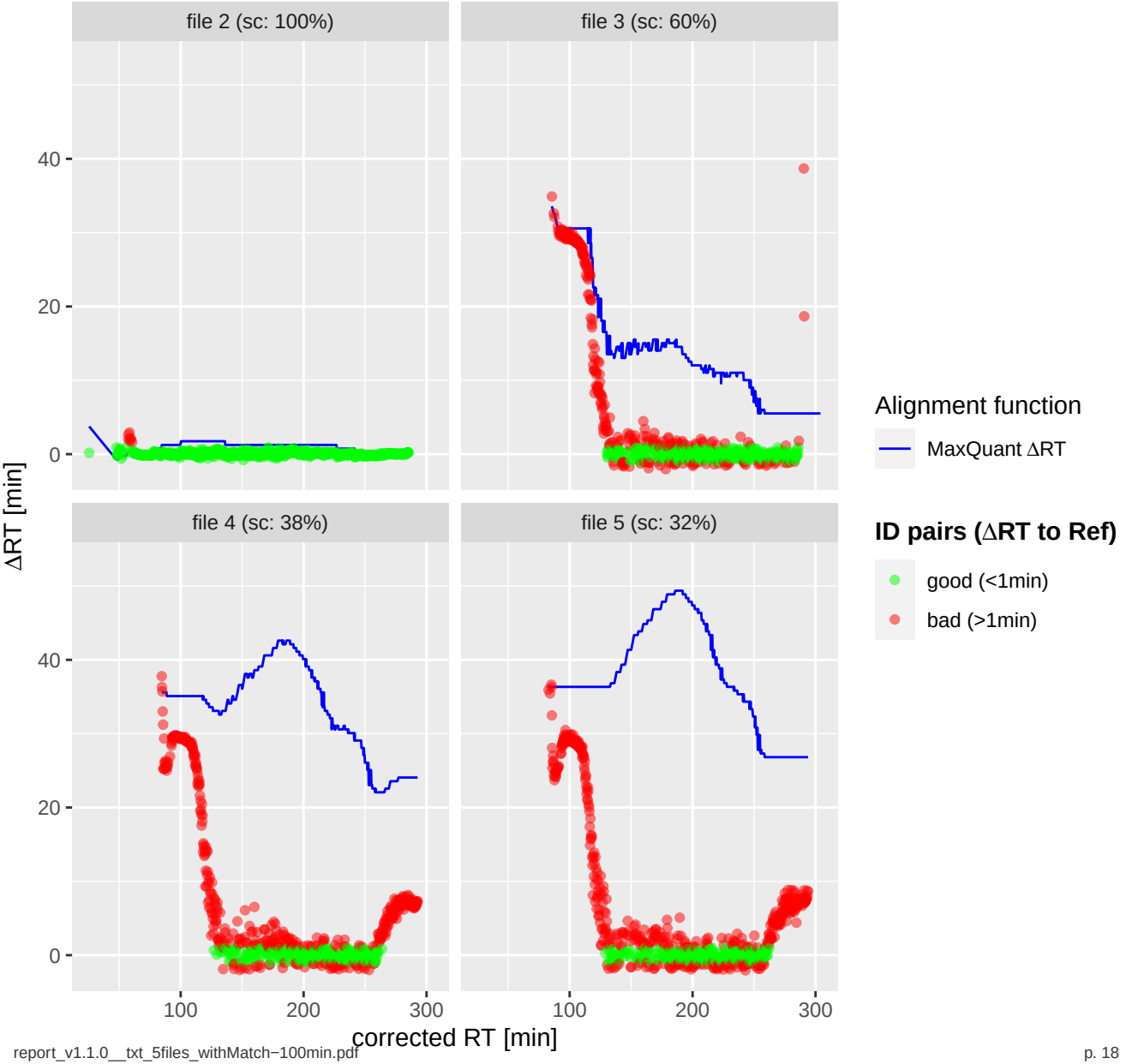


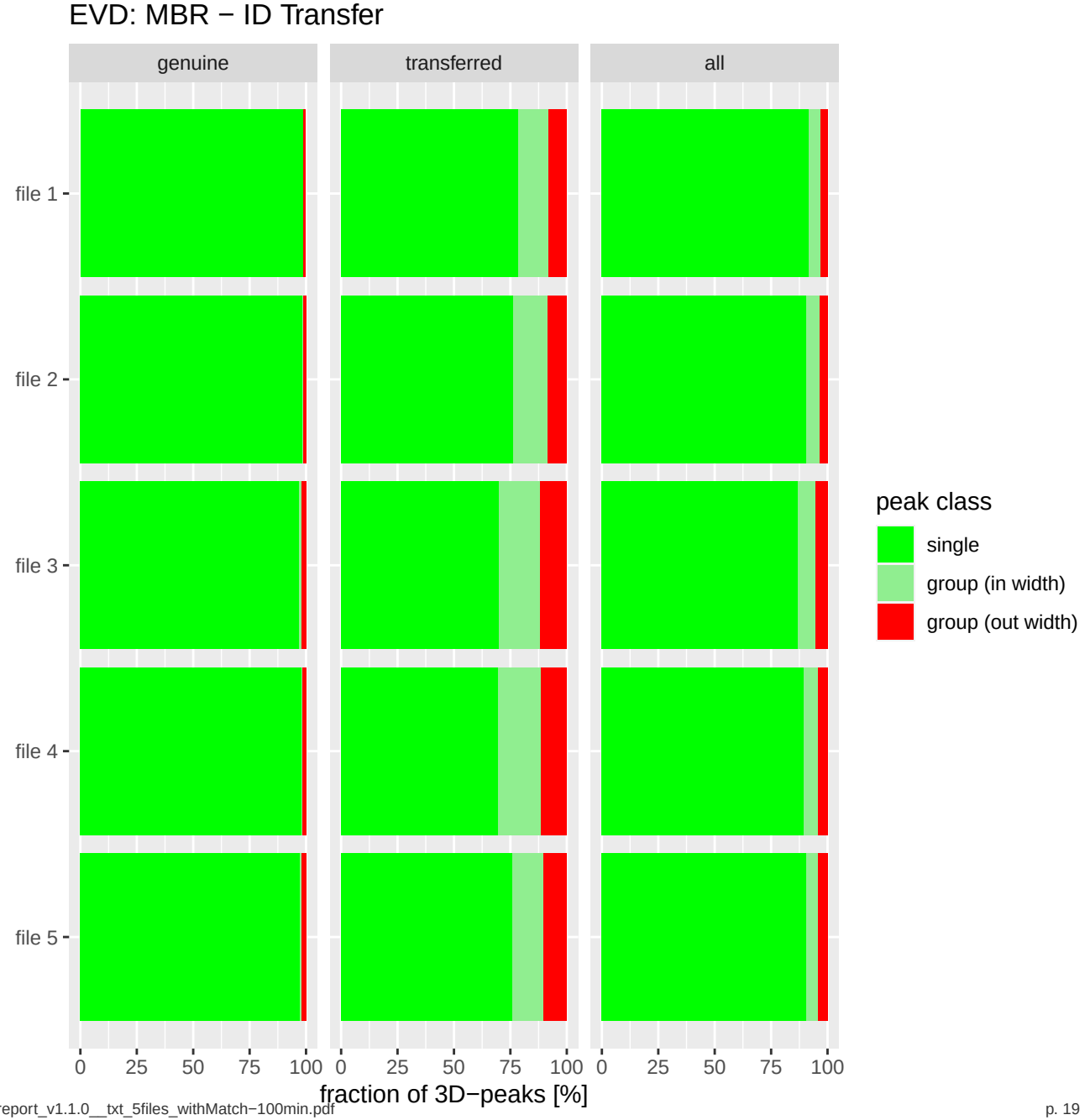

EVD: IDs over RT
ID count
300
200
100
0
0
100
200
300
RT [min]
Raw file
file 1
file 2
file 3
file 4
file 5


EVD: Peak width over RT
peak width [min]
2.0
1.5
1.0
0.5
0.0
0
100
200
300
retention time [min]
Raw file
(avg. peak width)
file 1 (~0.9 min)
file 2 (~0.8 min)
file 3 (~0.9 min)
file 4 (~0.9 min)
file 5 (~0.9 min)

EVD: MBR − alignment

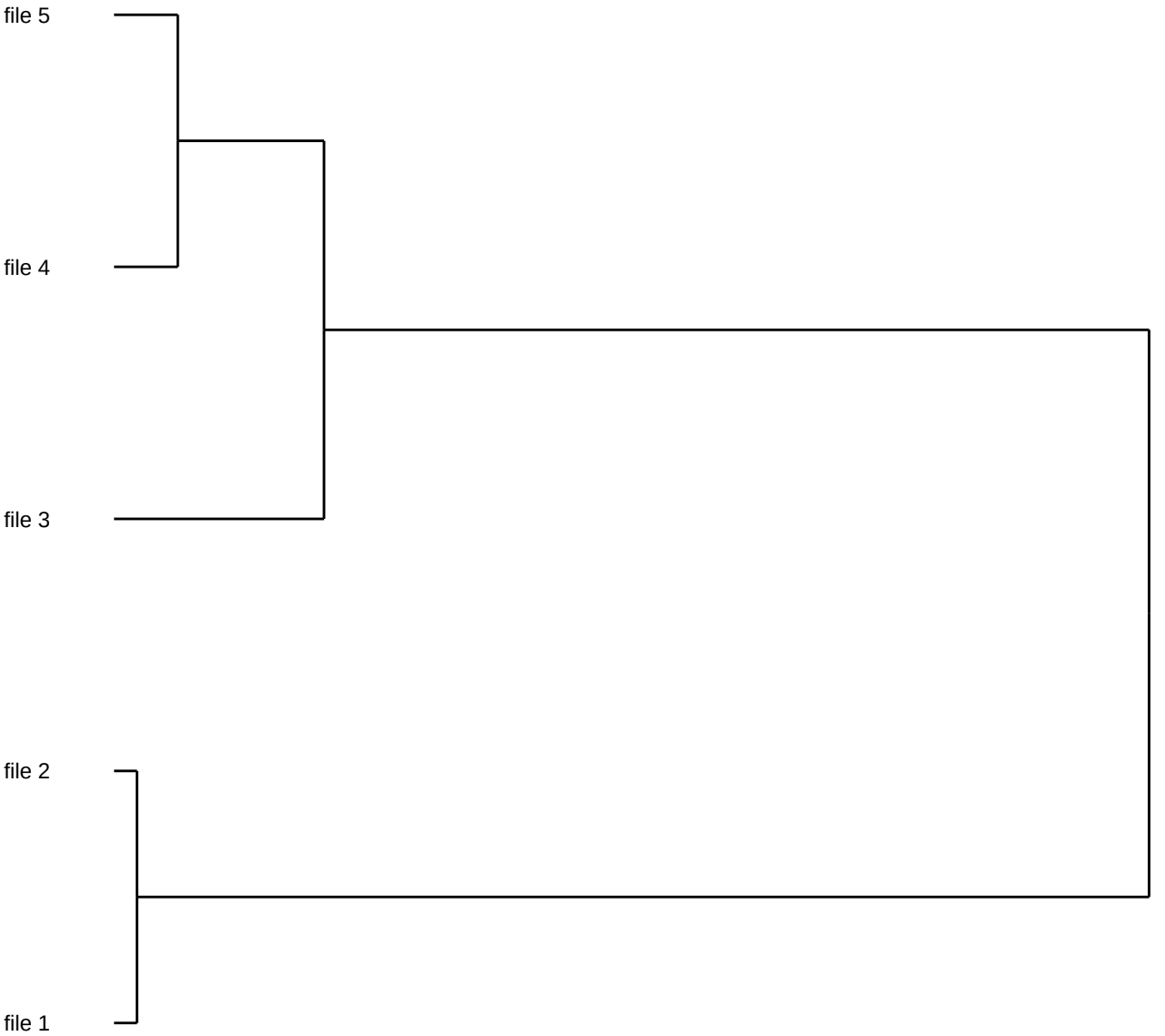
alignment reference: Toni_20140521_GM_QC_01

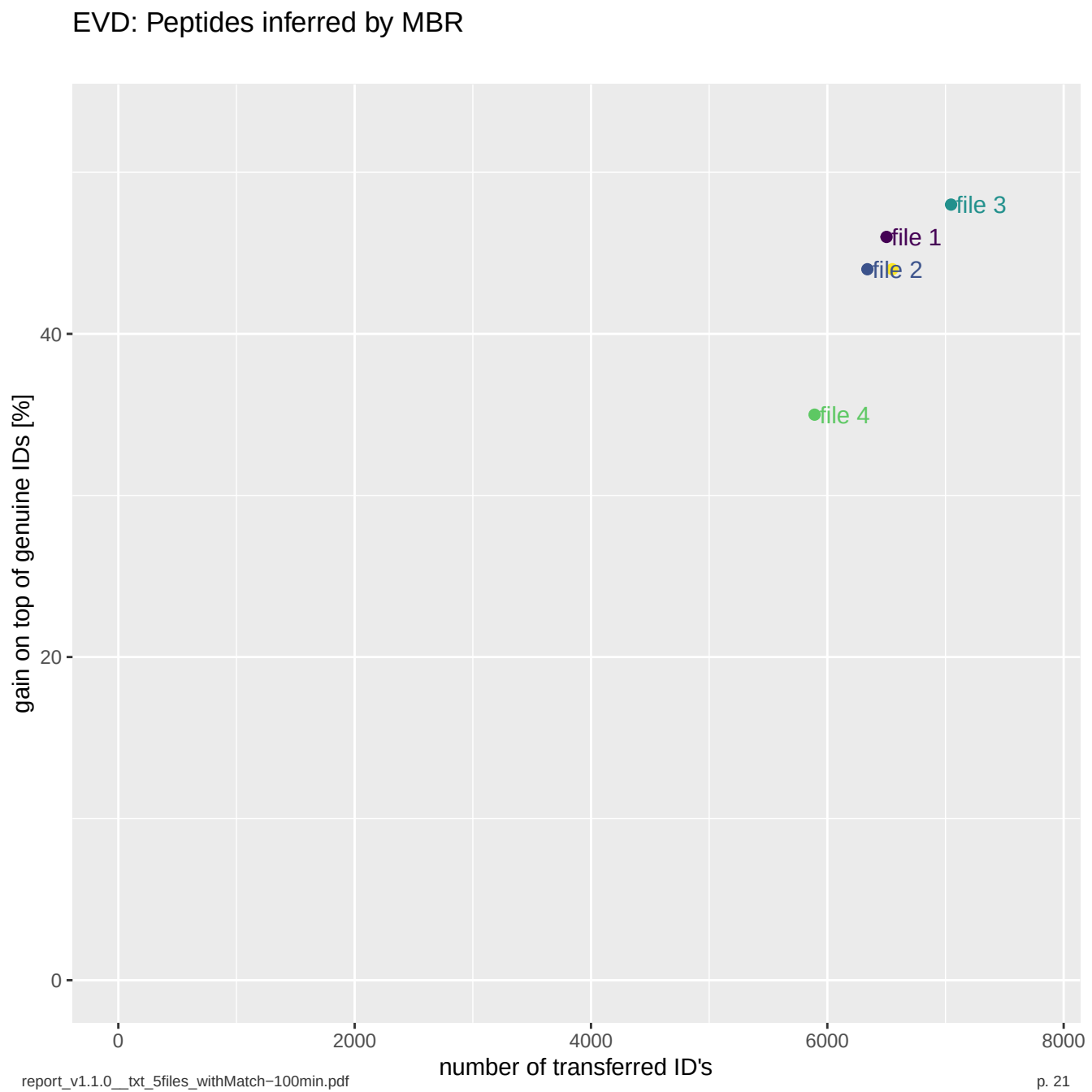


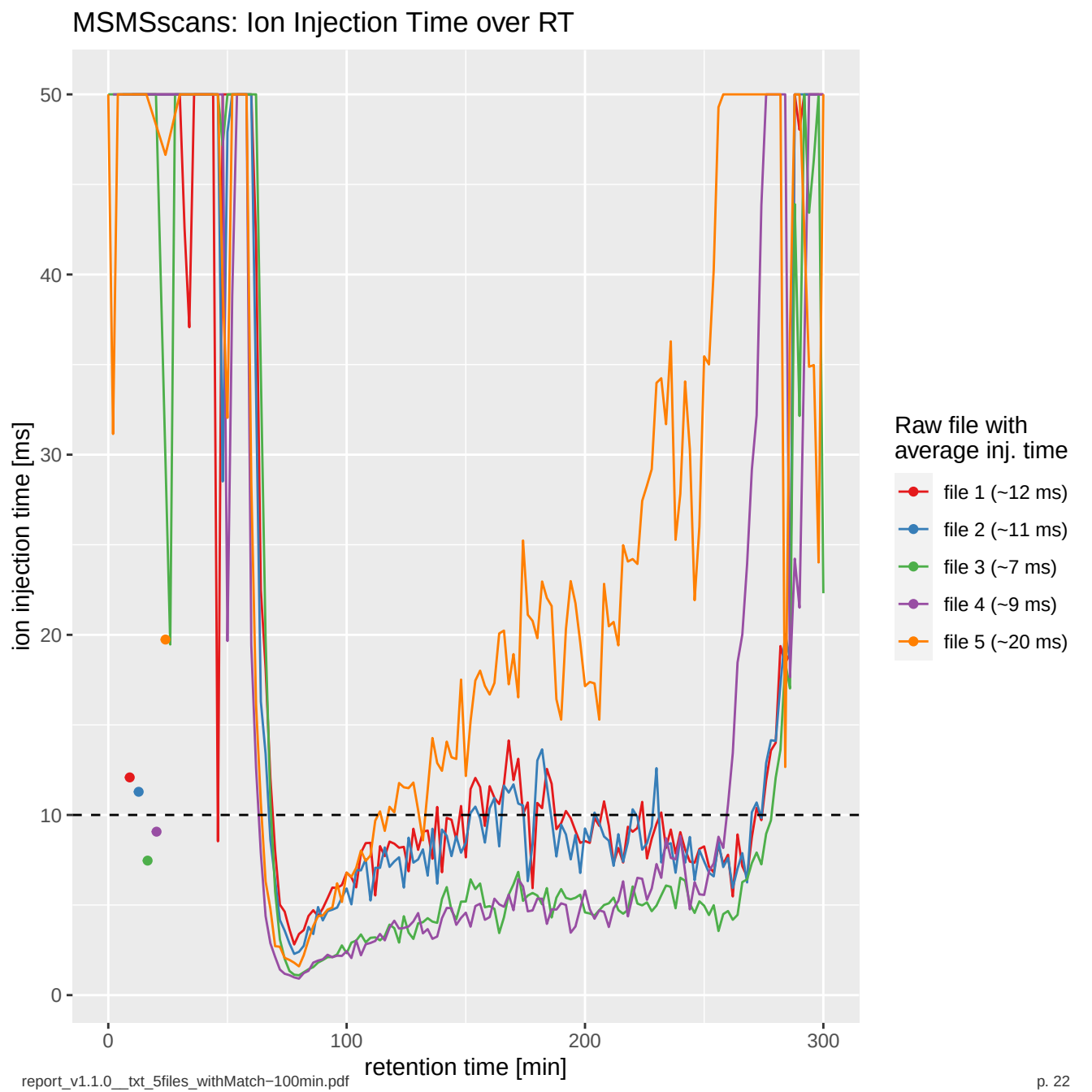

EVD: MBR − ID Transfer
genuine
transferred
all
file 1
file 2
file 3
file 4
file 5
0
25
50
75
100
fraction of 3D−peaks [%]
peak class
single
group (in width)
group (out width)

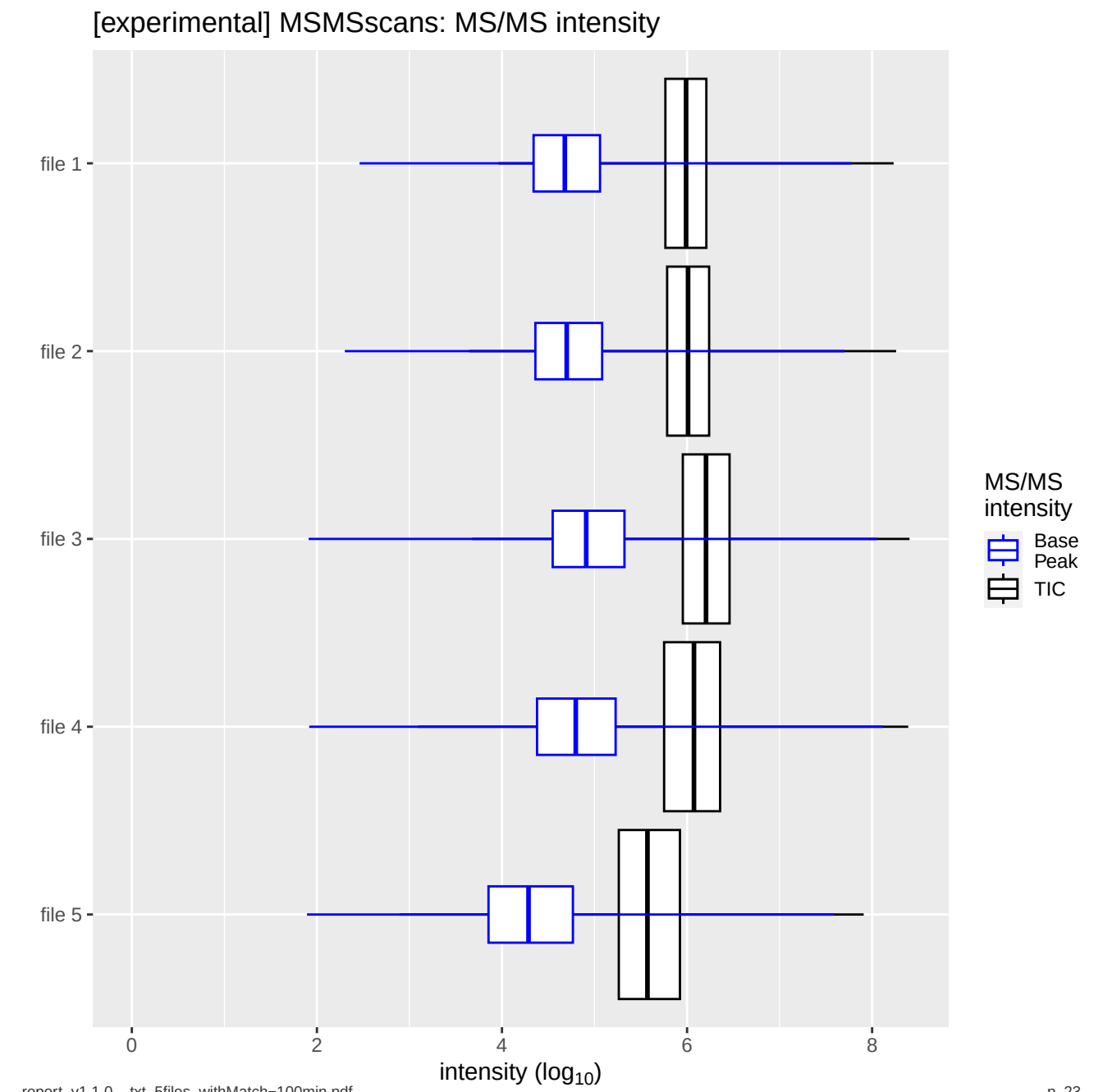
[experimental] EVD: Clustering Tree of Raw files

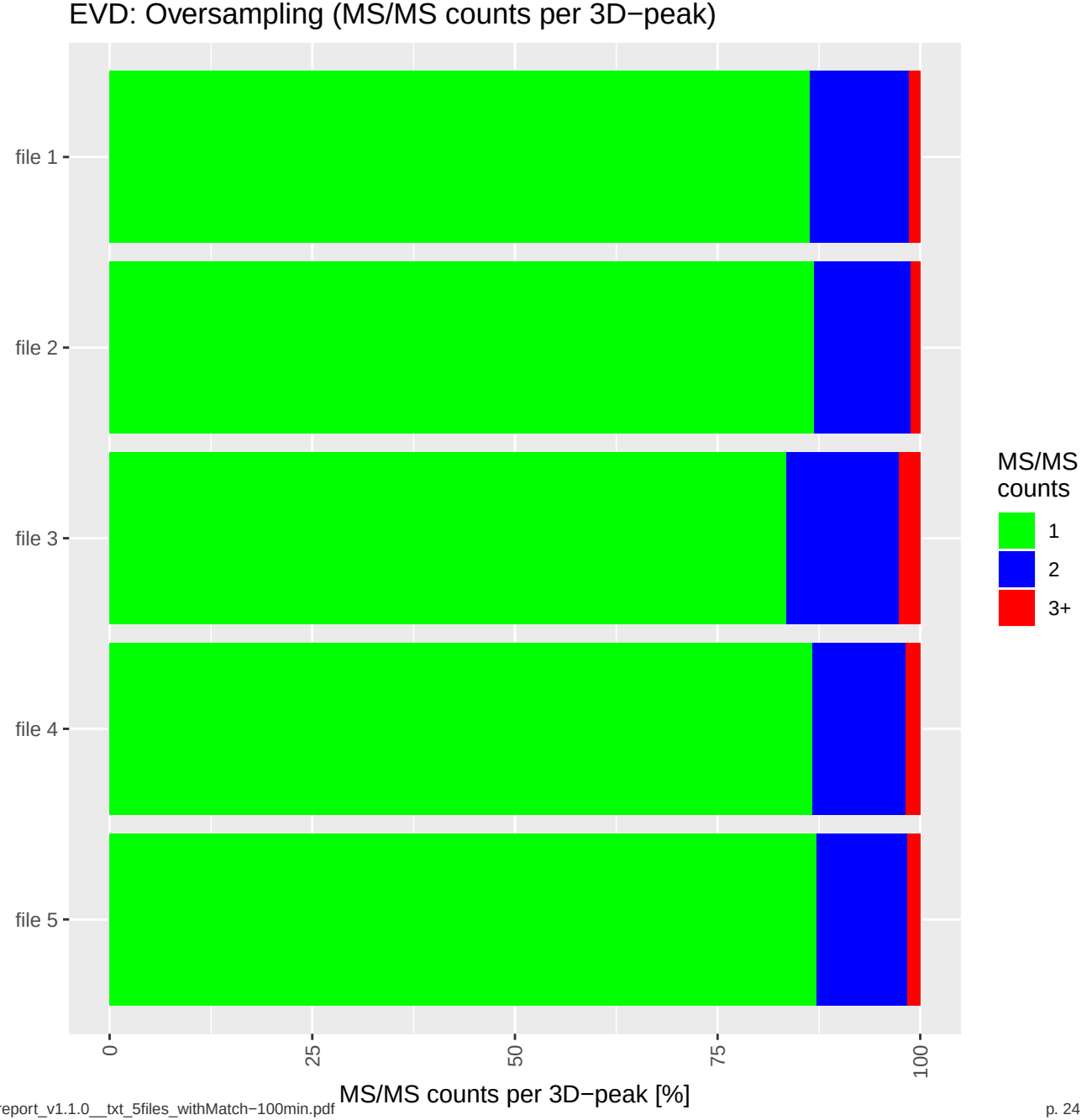
by Correlation of Corrected Retention Times



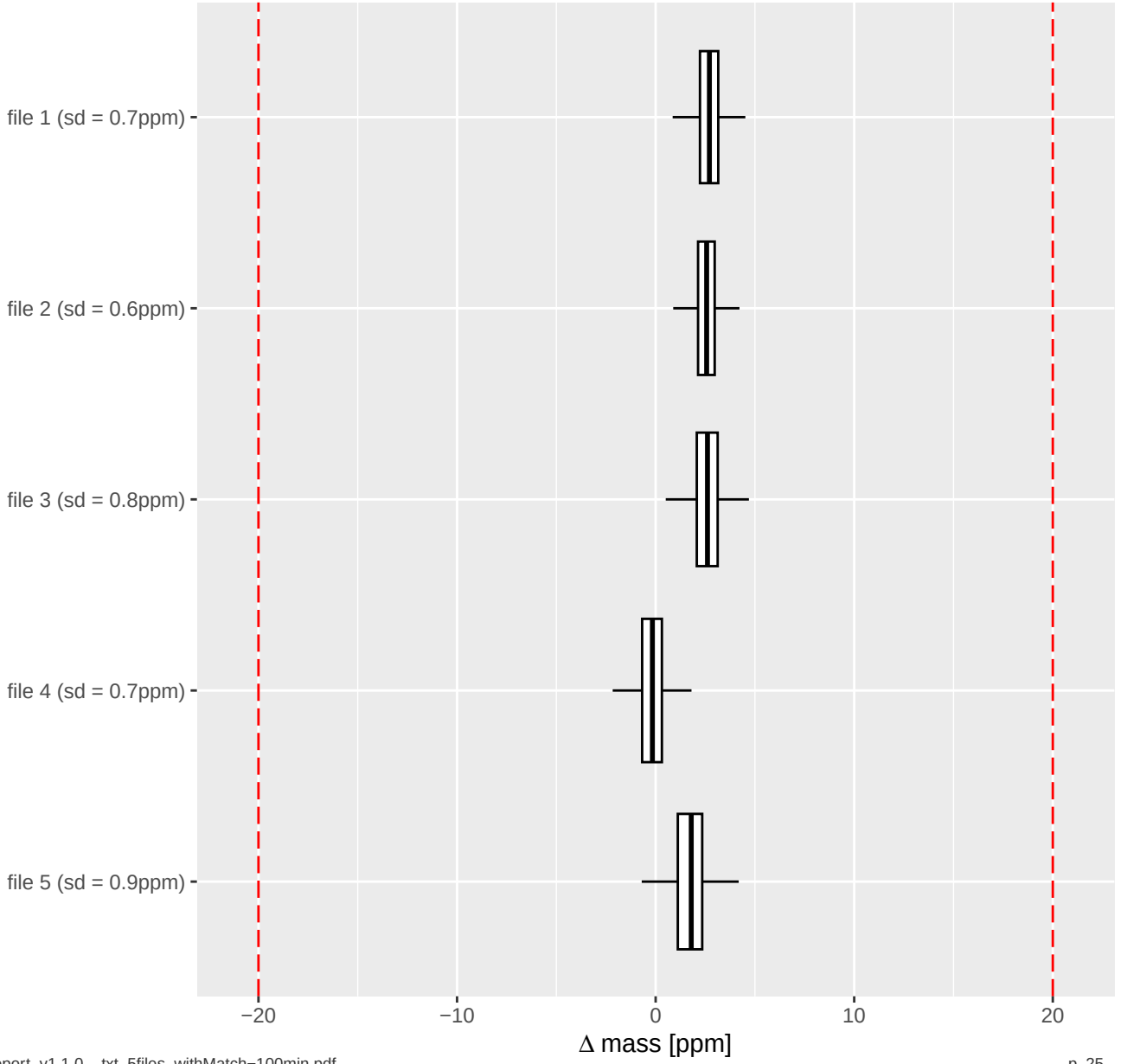

EVD: Peptides inferred by MBR
file 3
file 1
file 2
file 4
40
20
0
gain on top of genuine IDs [%]
0
2000
4000
6000
8000
number of transferred ID's


MSMSscans: Ion Injection Time over RT
ion injection time [ms]
50
40
30
20
10
0
0
100
200
300
retention time [min]
Raw file with average inj. time
file 1 (~12 ms)
file 2 (~11 ms)
file 3 (~7 ms)
file 4 (~9 ms)
file 5 (~20 ms)

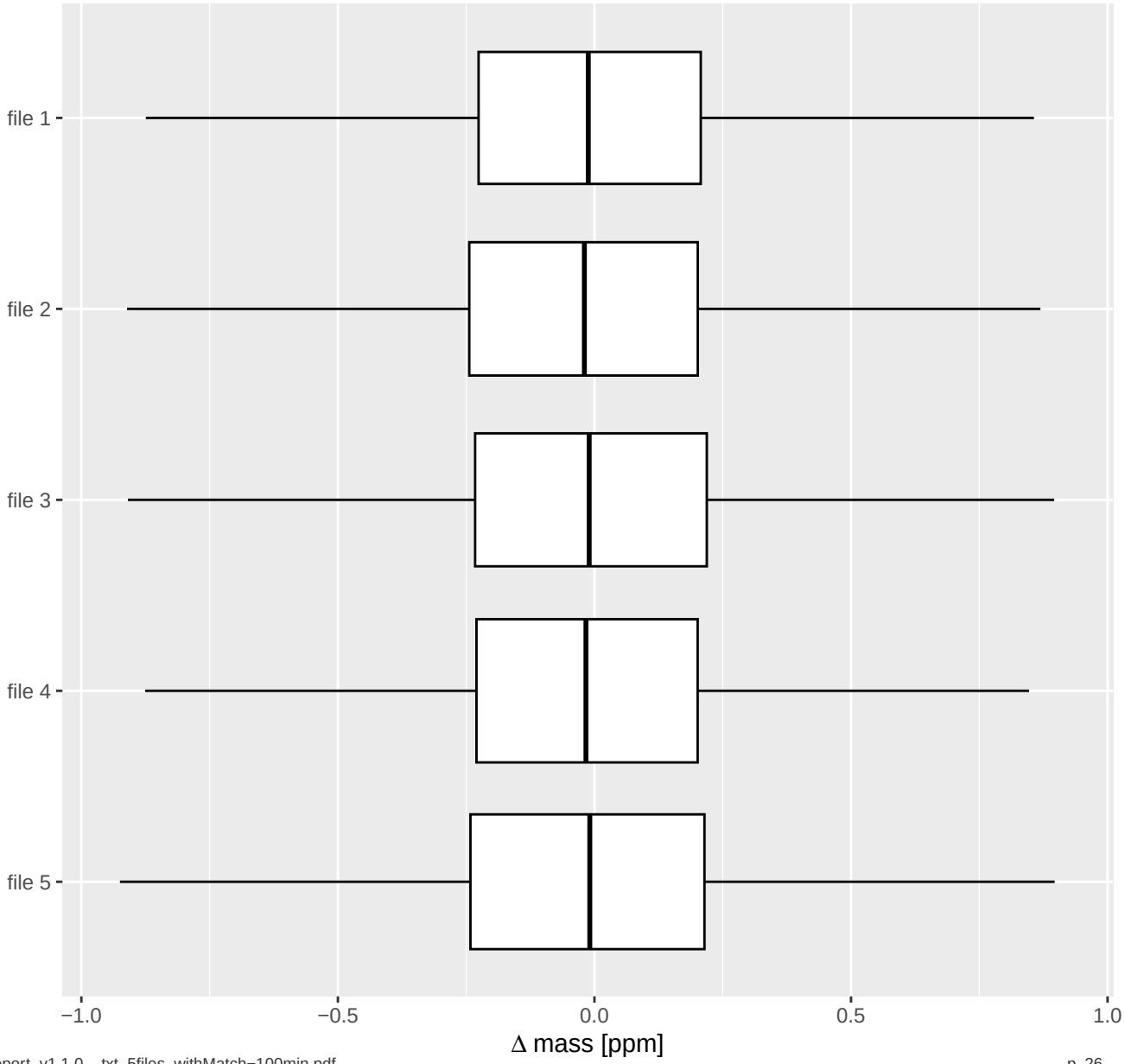

[experimental] MSMSscans: MS/MS intensity
file 1
file 2
file 3
file 4
file 5
0
2
4
6
8
intensity (log10)
MS/MS intensity
Base Peak
TIC


EVD: Oversampling (MS/MS counts per 3D−peak)
file 1
file 2
file 3
file 4
file 5
0
25
50
75
100
MS/MS counts per 3D−peak [%]
MS/MS counts
1
2
3+

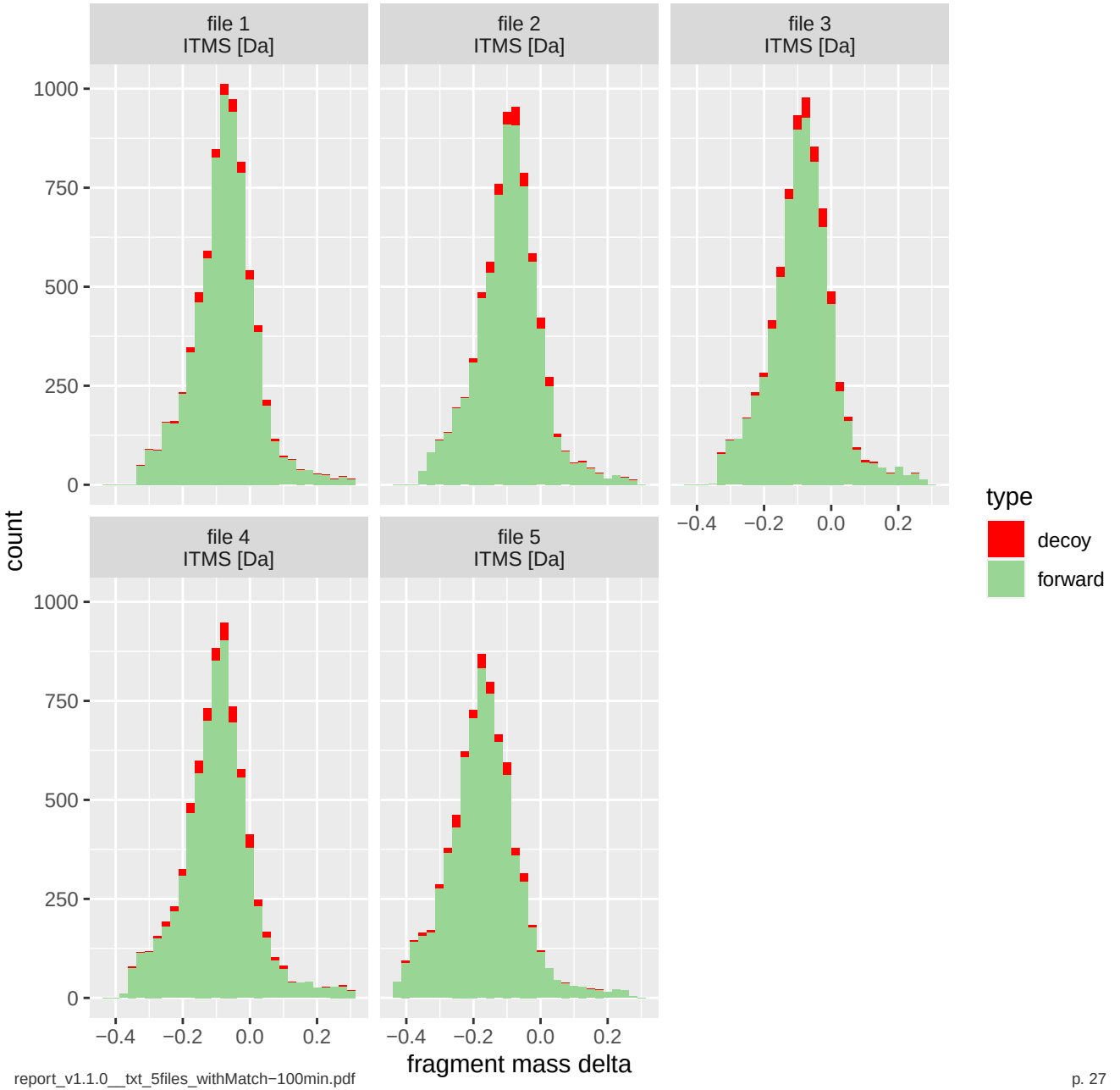
EVD: Uncalibrated mass error

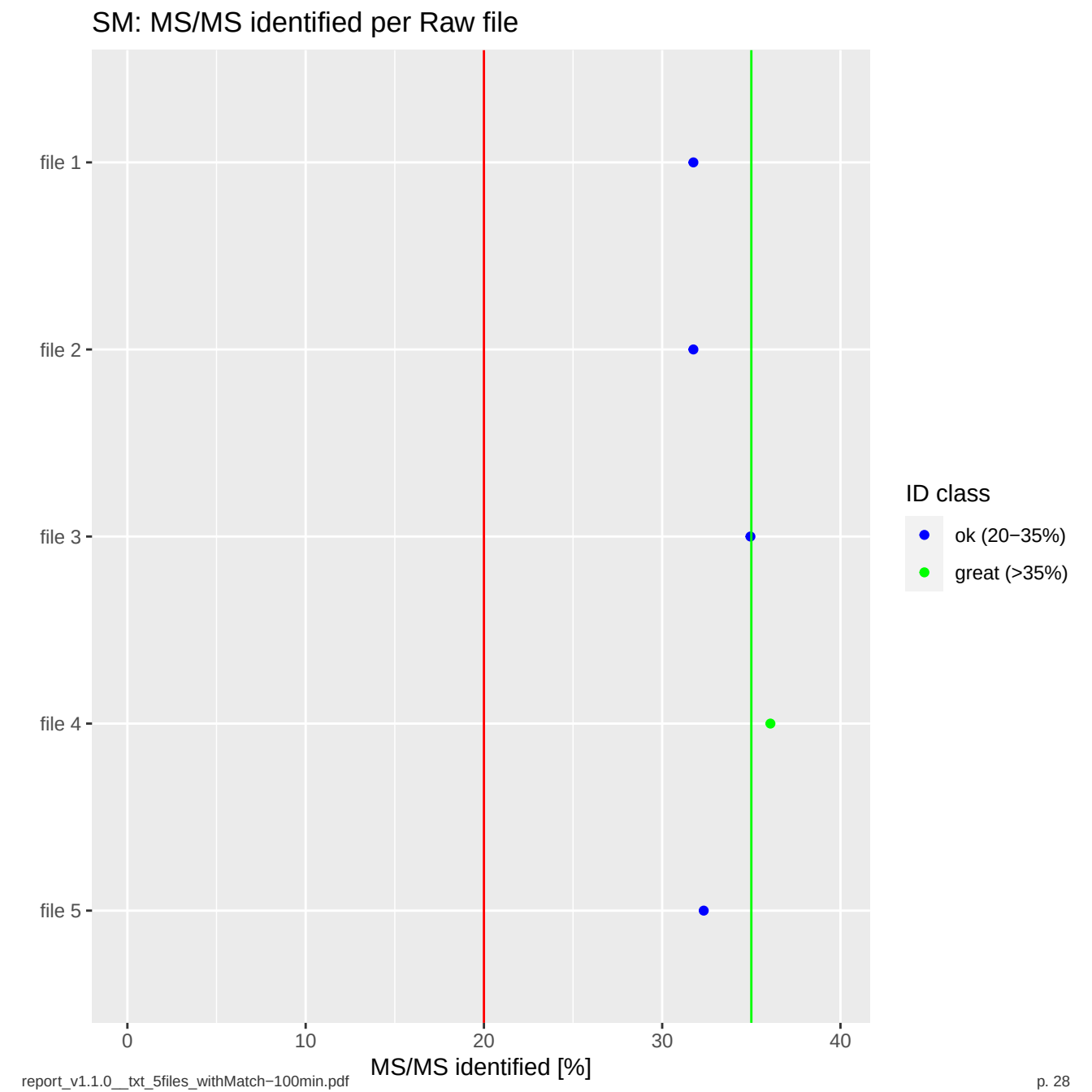


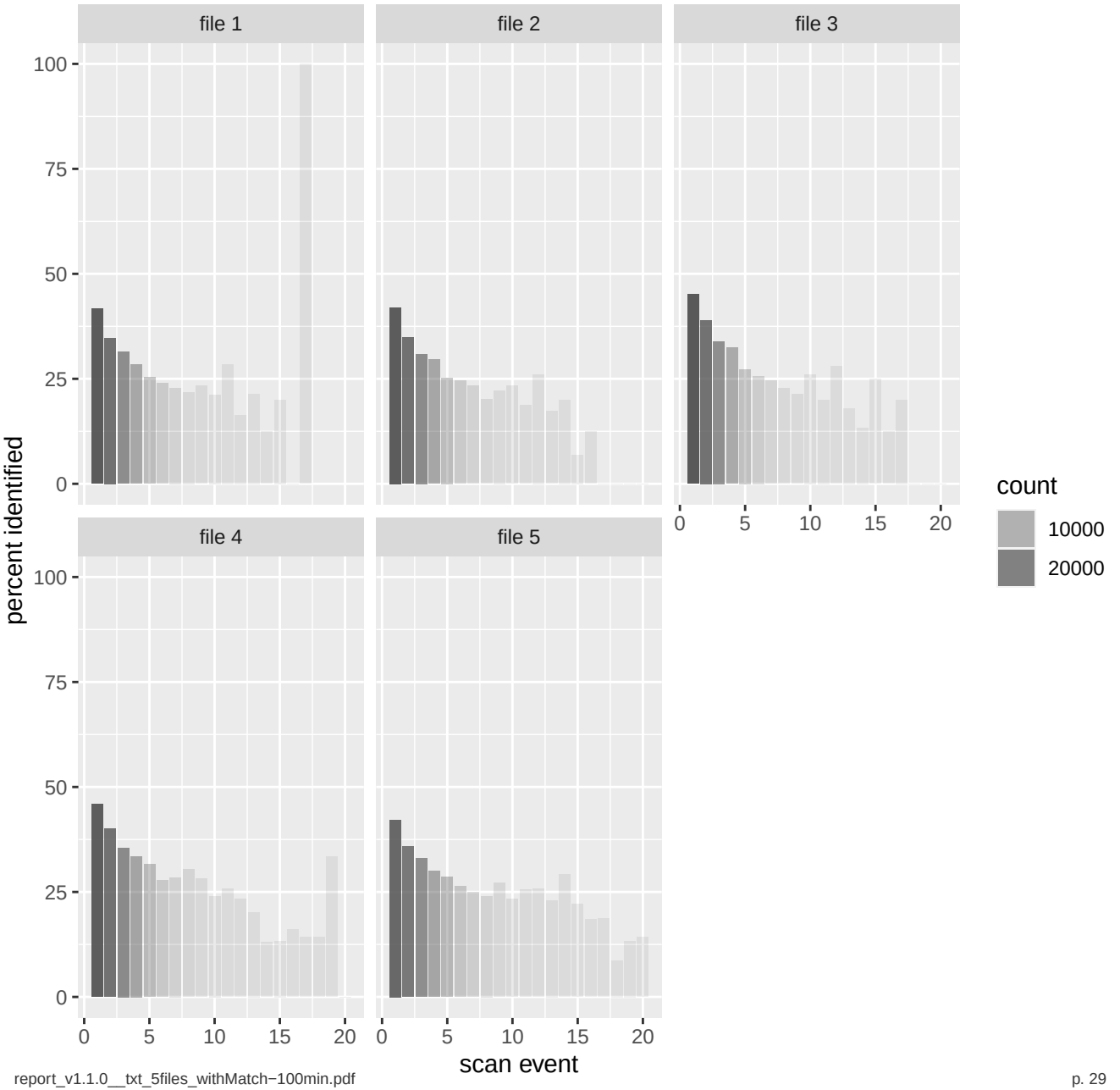
EVD: Calibrated mass error



MSMS: Fragment mass errors per Raw file

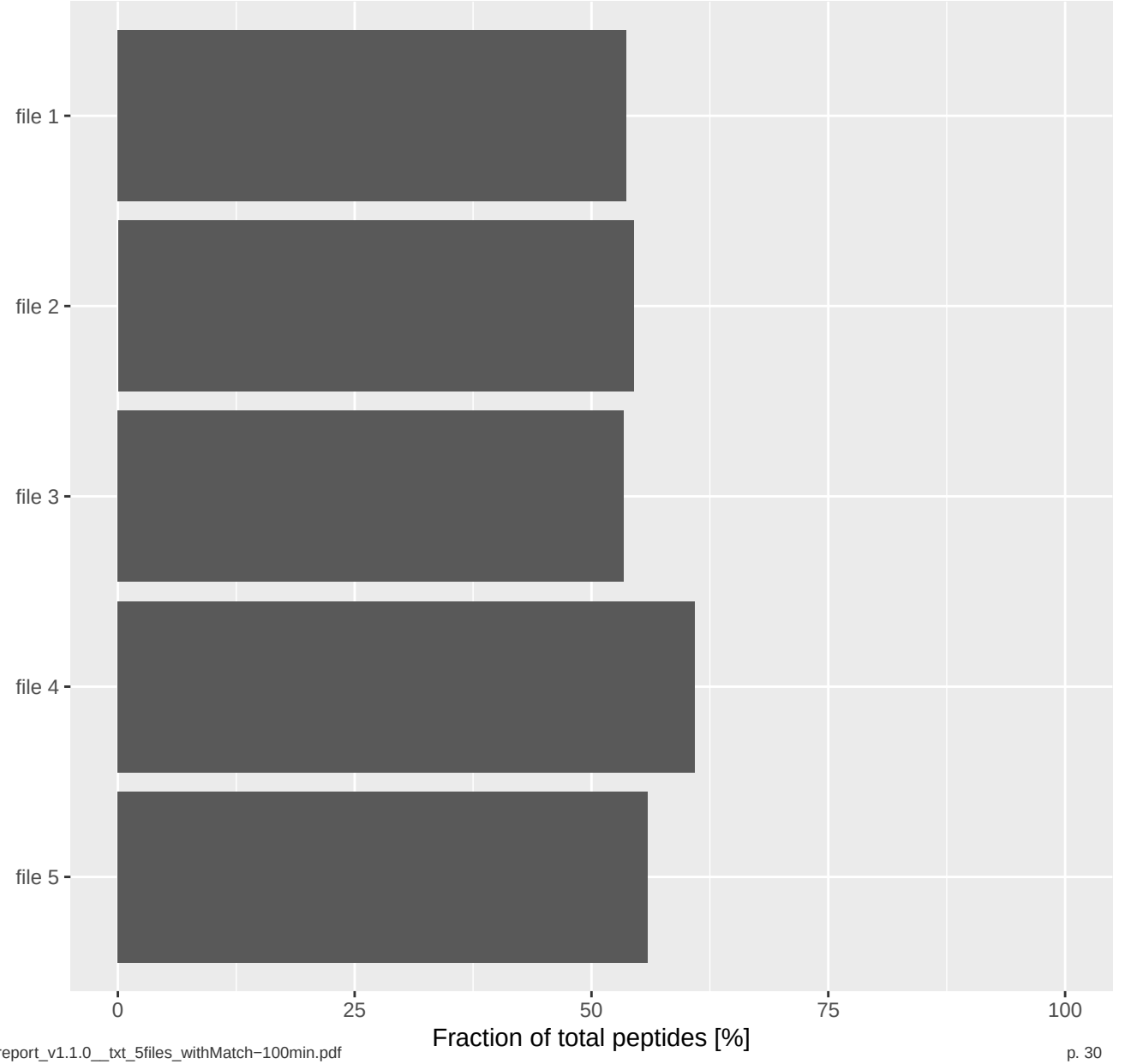


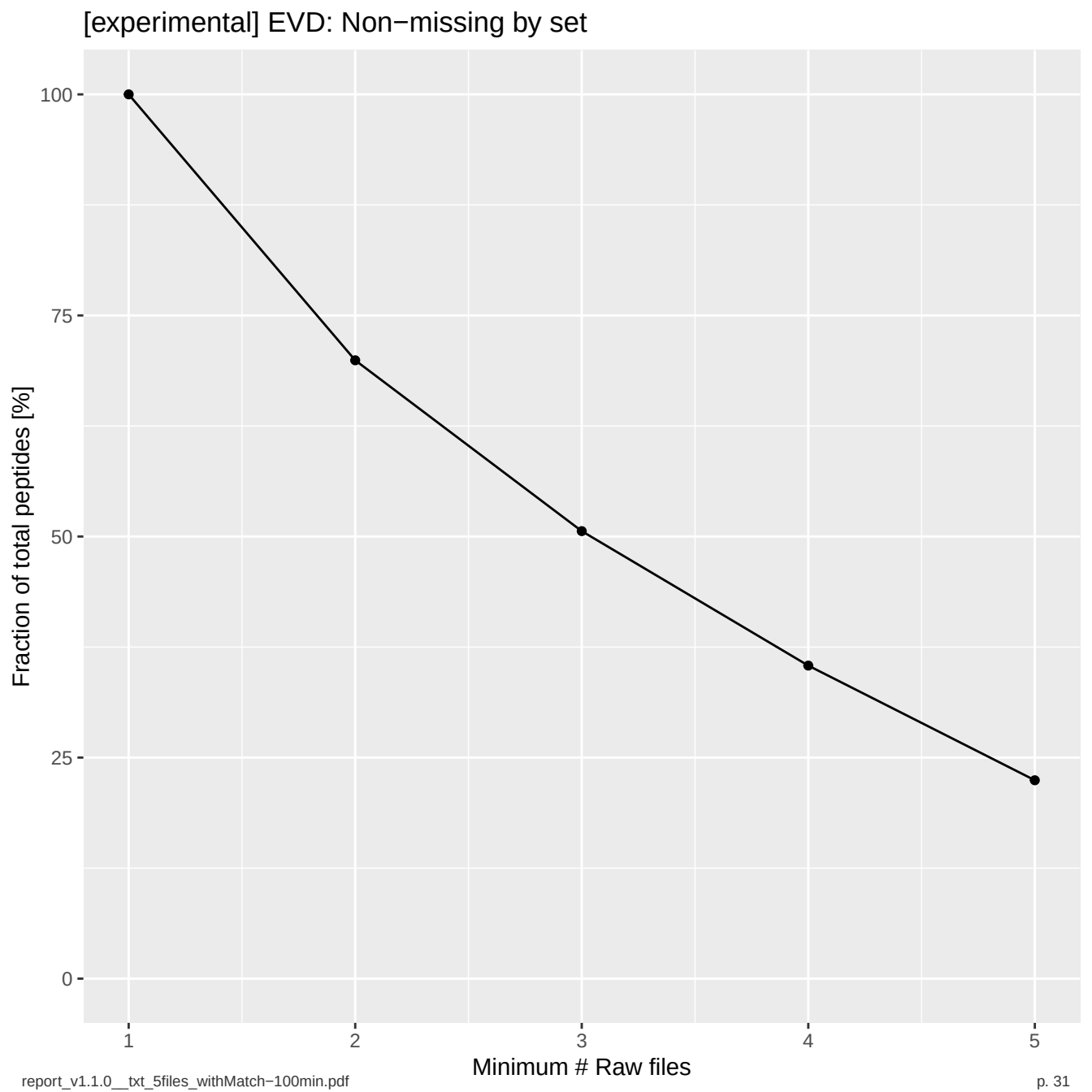

SM: MS/MS identified per Raw file
file 1
file 2
file 3
file 4
file 5
0
10
20
30
40
MS/MS identified [%]
ID class
ok (20−35%)
great (>35%)


MSMSscans: TopN % identified over N
file 1
file 2
file 3
file 4
file 5
percent identified
scan event
count
10000
20000

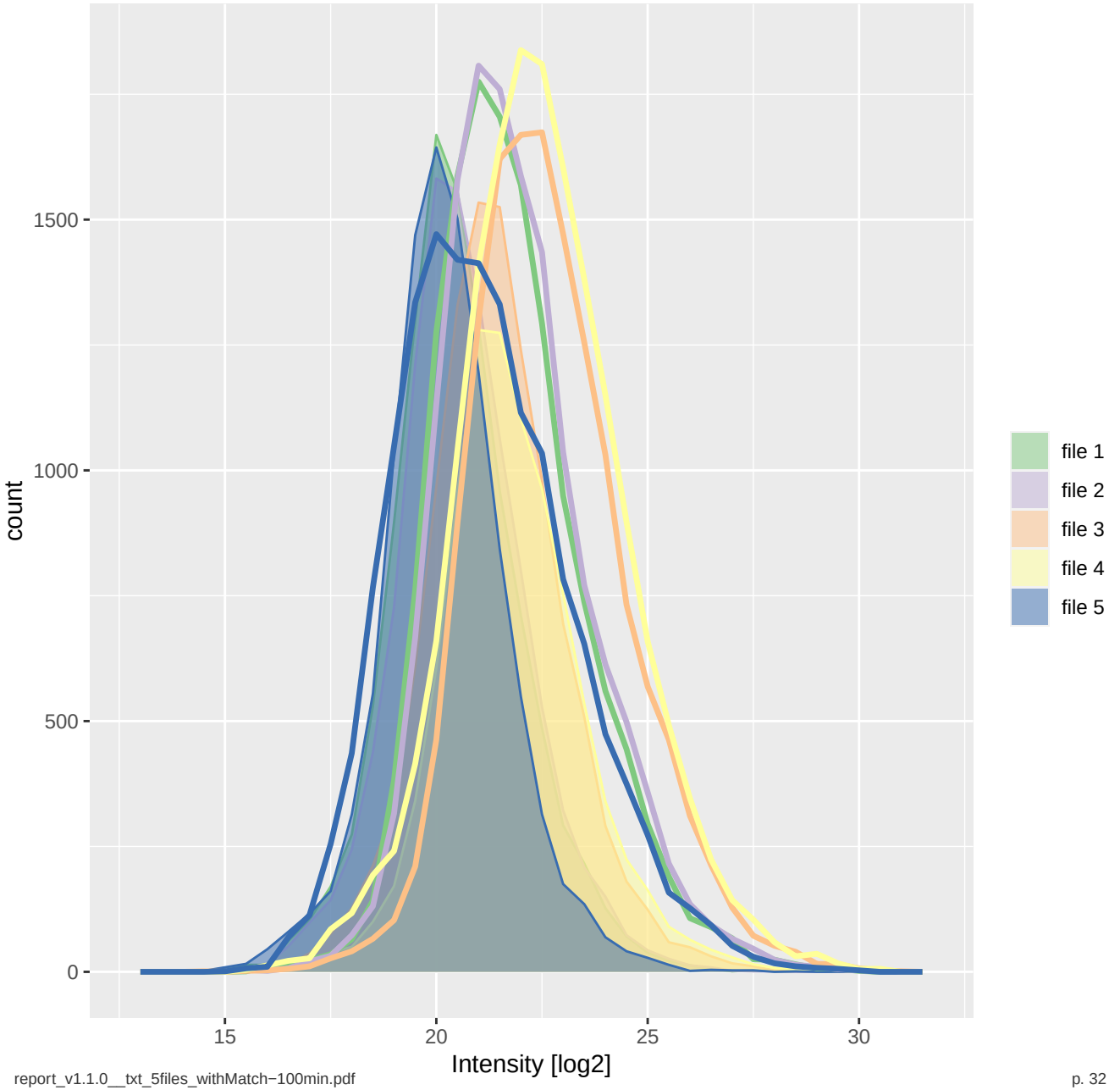
[experimental] EVD: Non−Missing Peptides

compared to all peptides seen in experiment

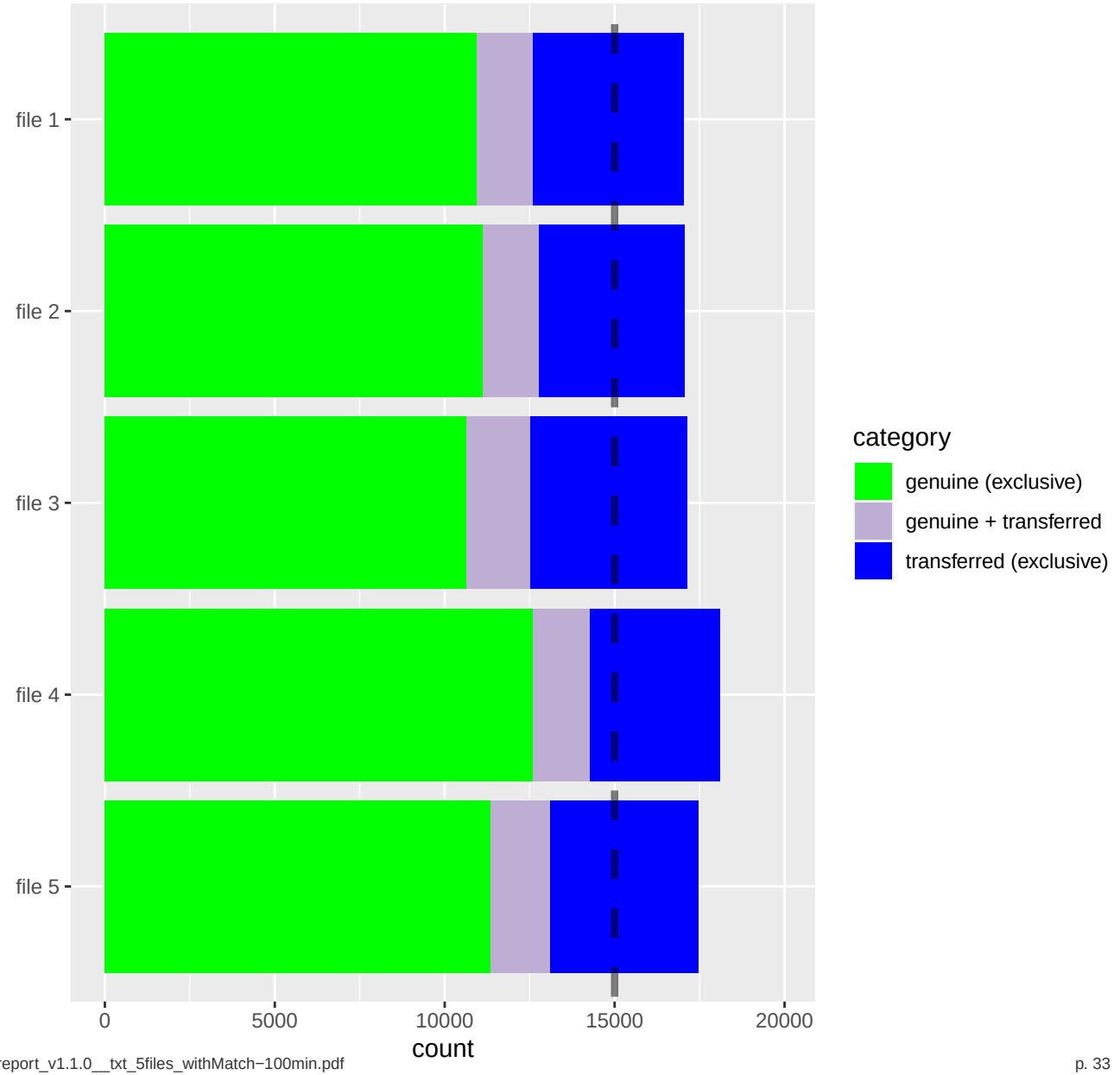



[experimental] EVD: Non−missing by set
Fraction of total peptides [%]
100
75
50
25
0
1
2
3
4
5
Minimum # Raw files

[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values

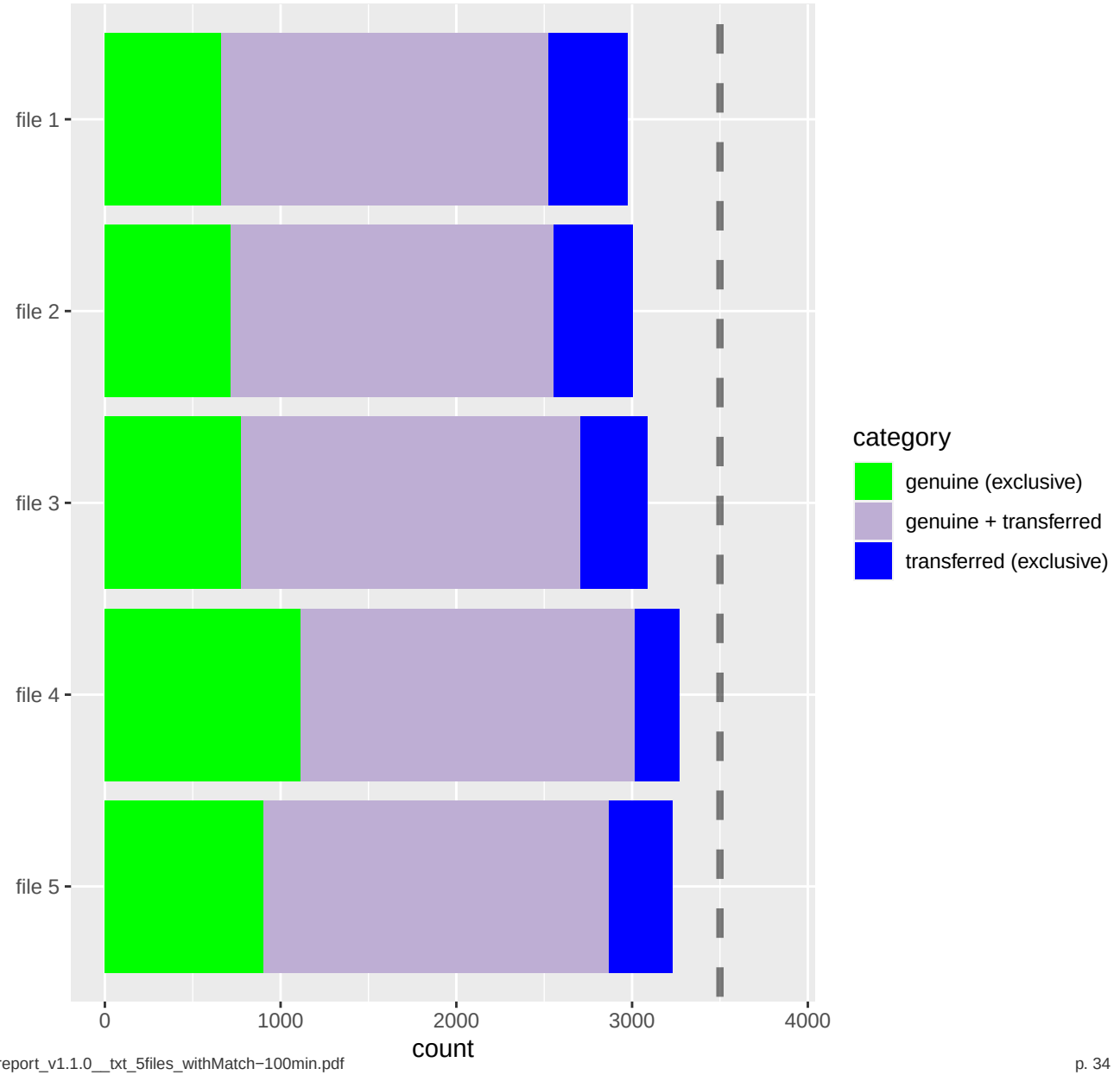


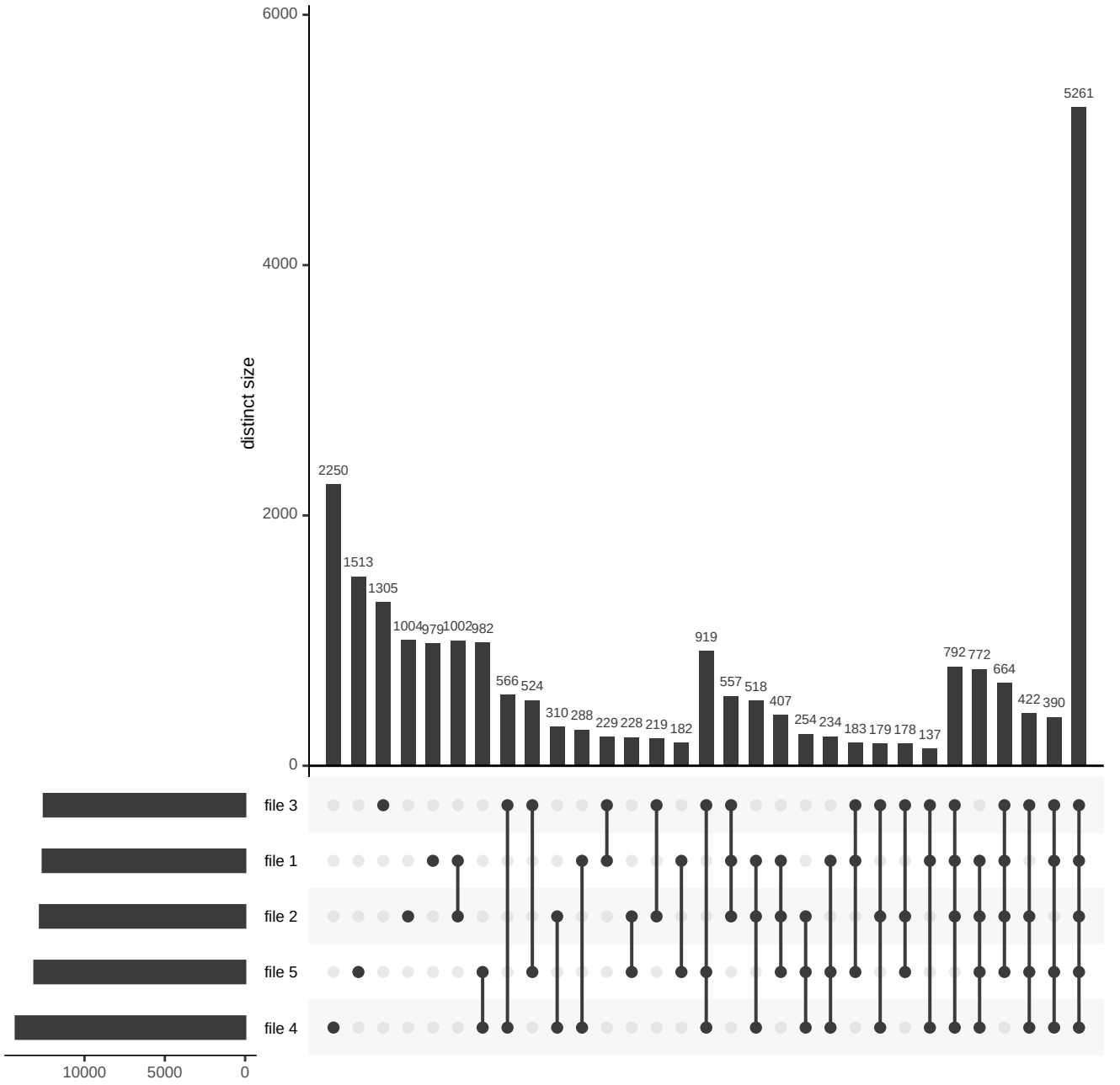
EVD: Peptide ID count

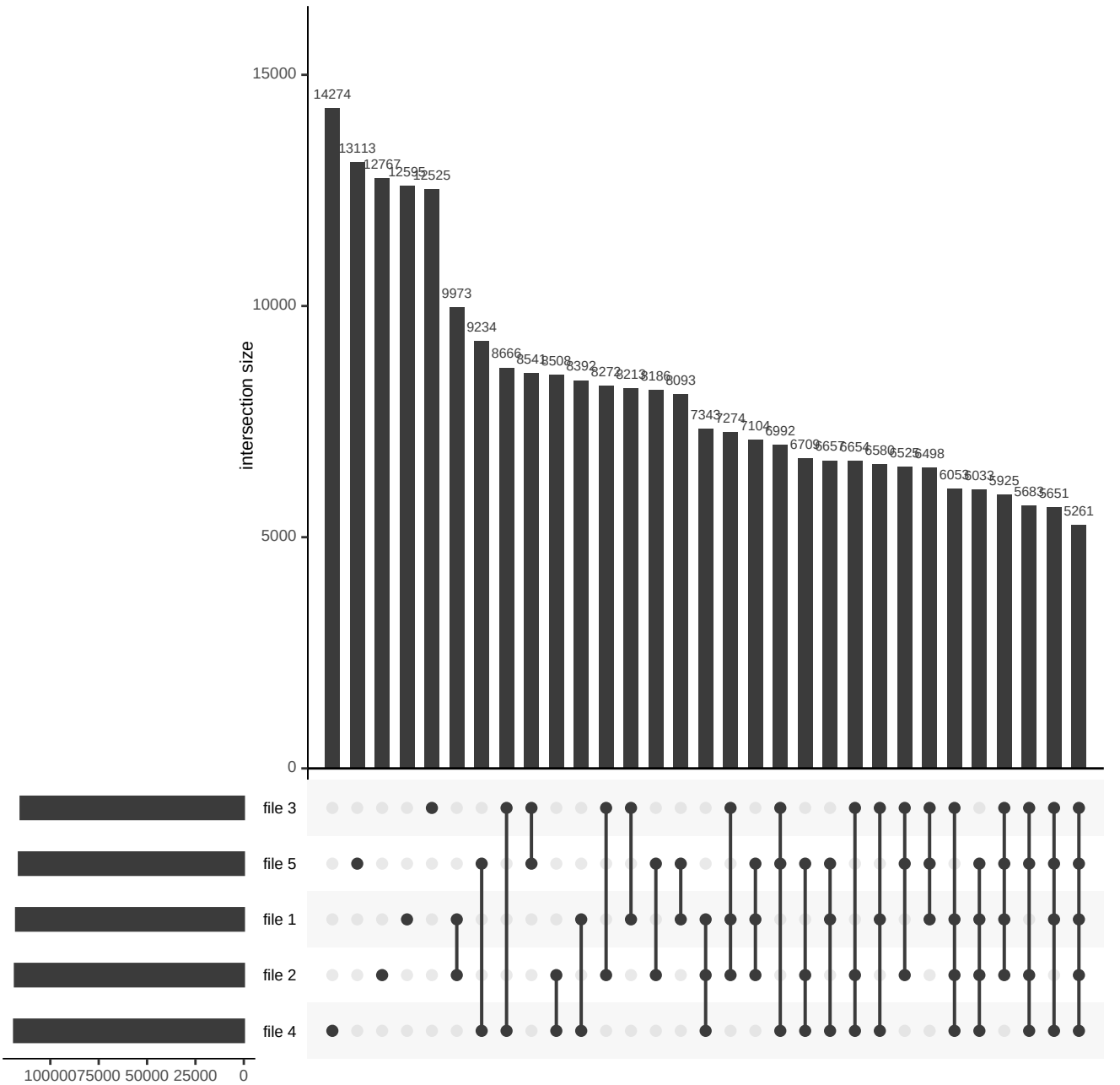


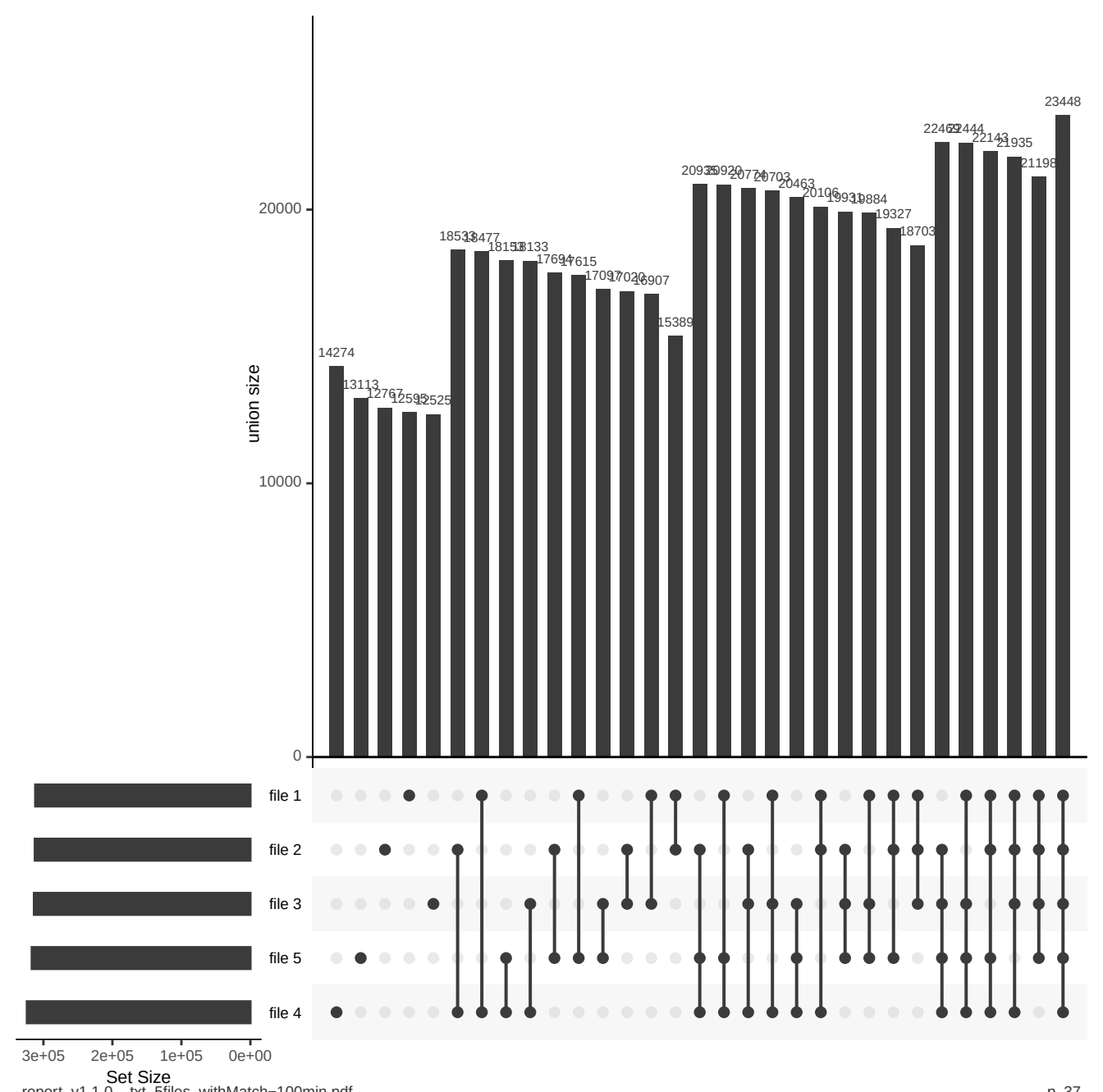
EVD: ProteinGroups count

MBR gain: +14%




6000
4000
2000
0
distinct size
2250
1513
1305
1004
979
1002
982
566
524
310
288
229
228
219
182
919
557
518
407
254
234
183
179
178
137
792
772
664
422
390
5261
file 3
file 1
file 2
file 5
file 4
10000
5000
0
Set Size


intersection size
15000
10000
5000
0
14274
13113
12767
12595
12525
9973
9234
8666
8541
8508
8392
8272
8213
8186
8093
7343
7274
7104
6992
6709
6657
6654
6580
6525
6498
6053
6033
5925
5683
5651
5261
file 3
file 5
file 1
file 2
file 4
10000075000 50000 25000 0
Set Size


union size
20000
10000
0
14274
13113
12767
12595
12525
18533
18477
18153
18133
17694
17615
17097
17020
16907
15389
20935
20920
20774
20703
20463
20106
19931
19884
19327
18703
22462
22444
22143
21935
21198
23448
file 1
file 2
file 3
file 5
file 4
3e+05
2e+05
1e+05
0e+00
Set Size