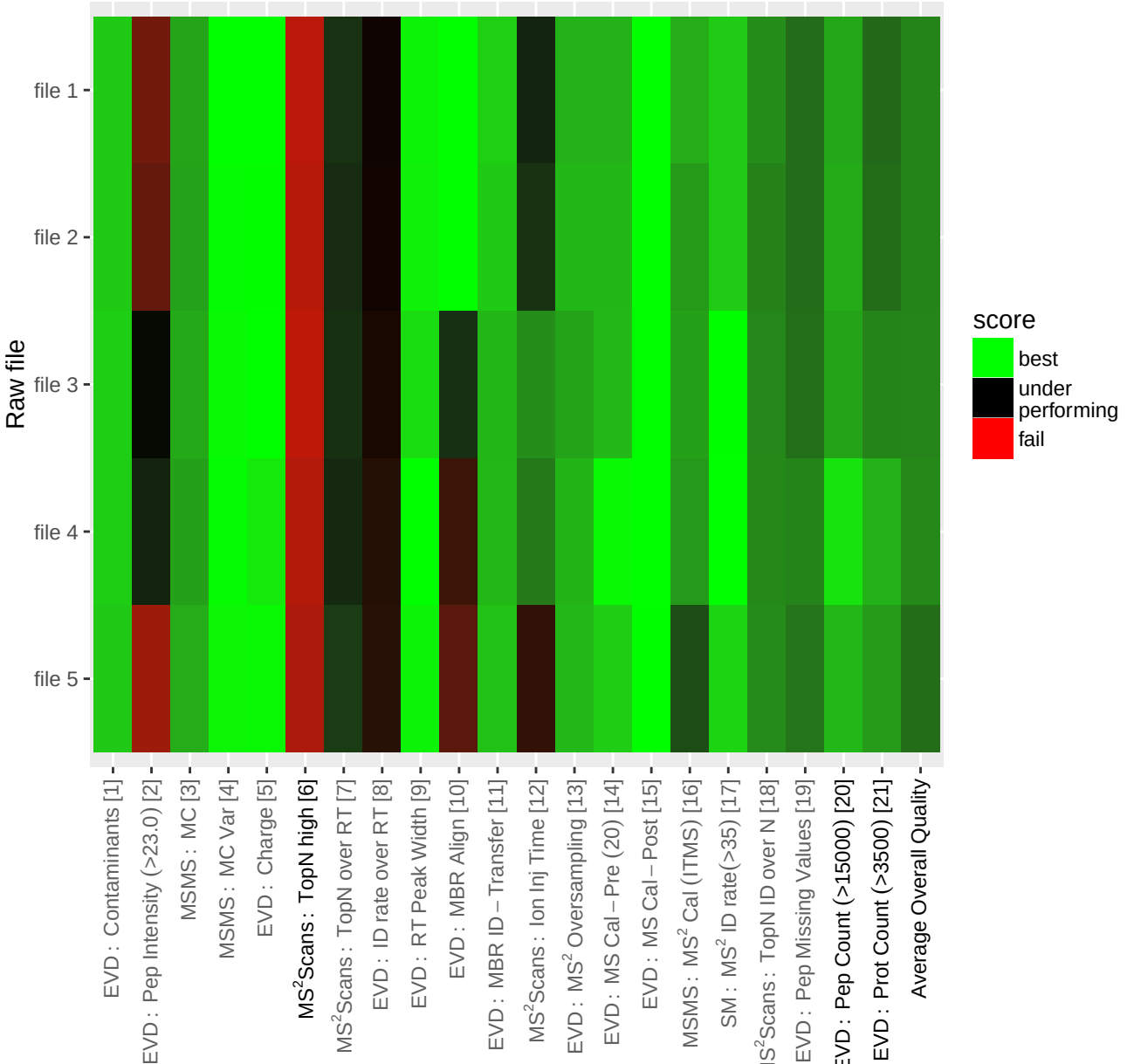
Performance overview



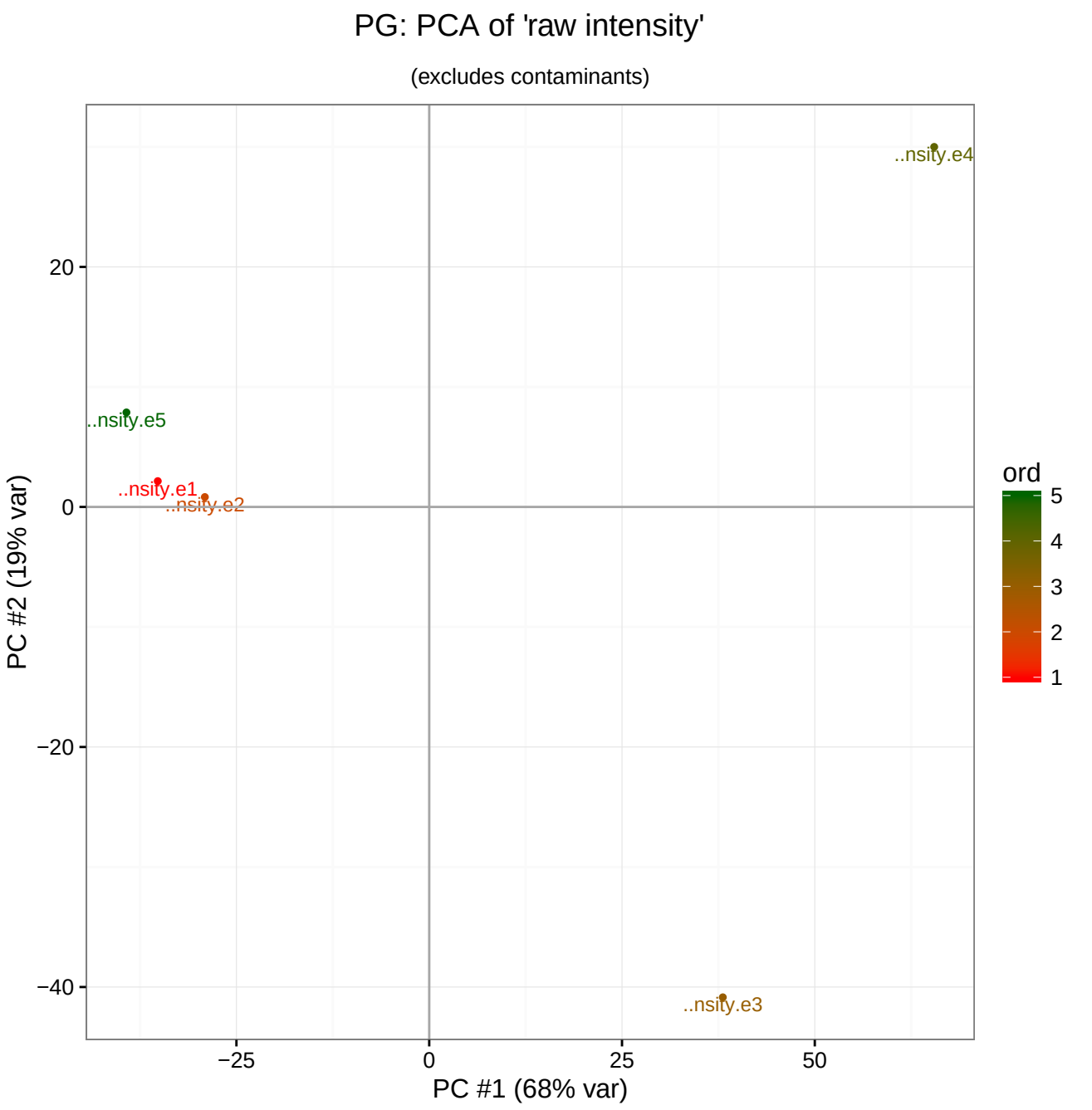
Mapping of Raw files to their short names
Mapping source: file (user−defined)
(automatic shortening of names was not sufficiently short − see 'best effort')

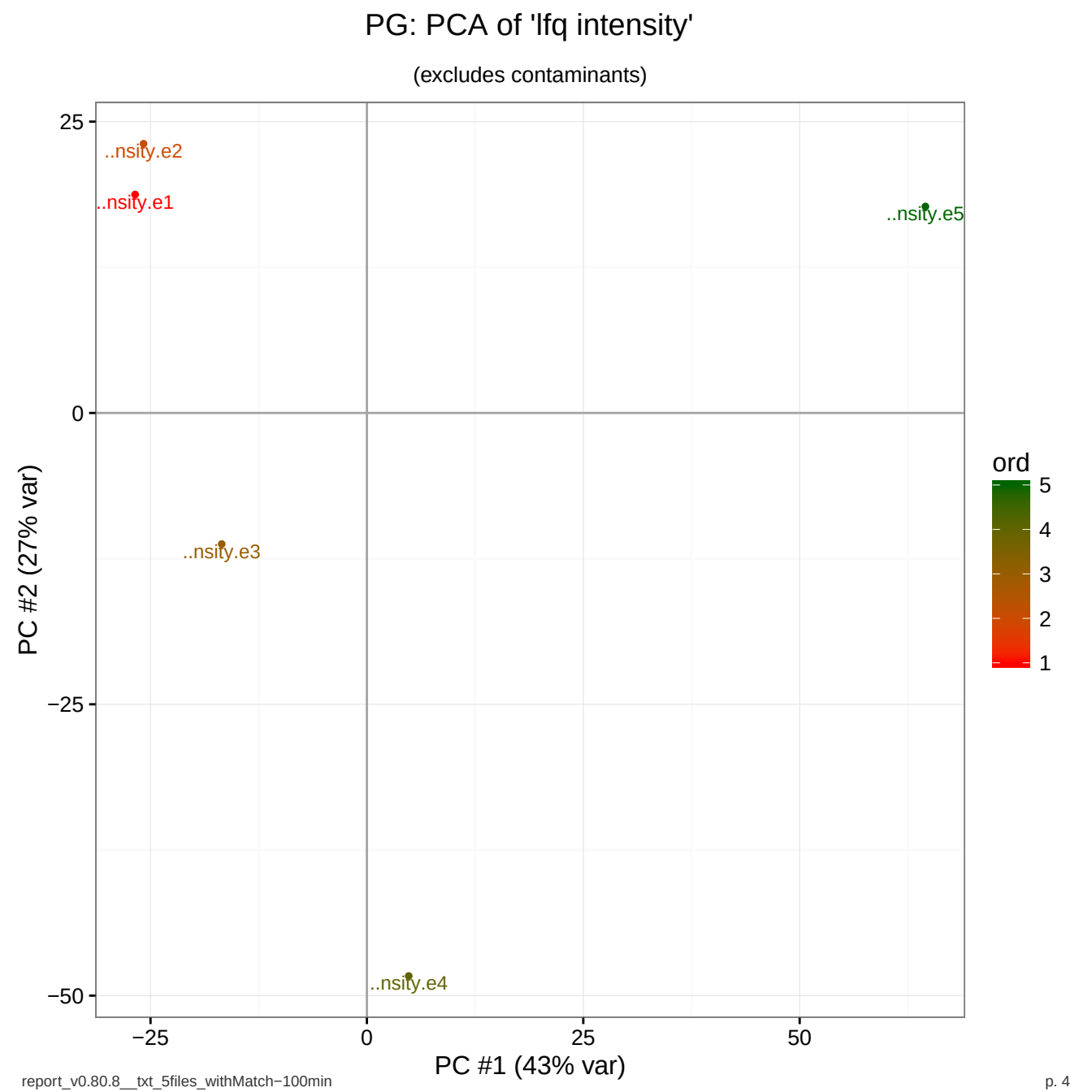
original	short name	best effort
Toni_20140521_GM_QC_01	file 1	..521_GM_QC_01
Toni_20140521_GM_QC_02	file 2	..521_GM_QC_02
Toni_20140522_GM_QC_01	file 3	..522_GM_QC_01
Toni_20140531_FB_QC_02	file 4	..531_FB_QC_02
Toni_20140608_FB_qc_01	file 5	..608_FB_qc_01

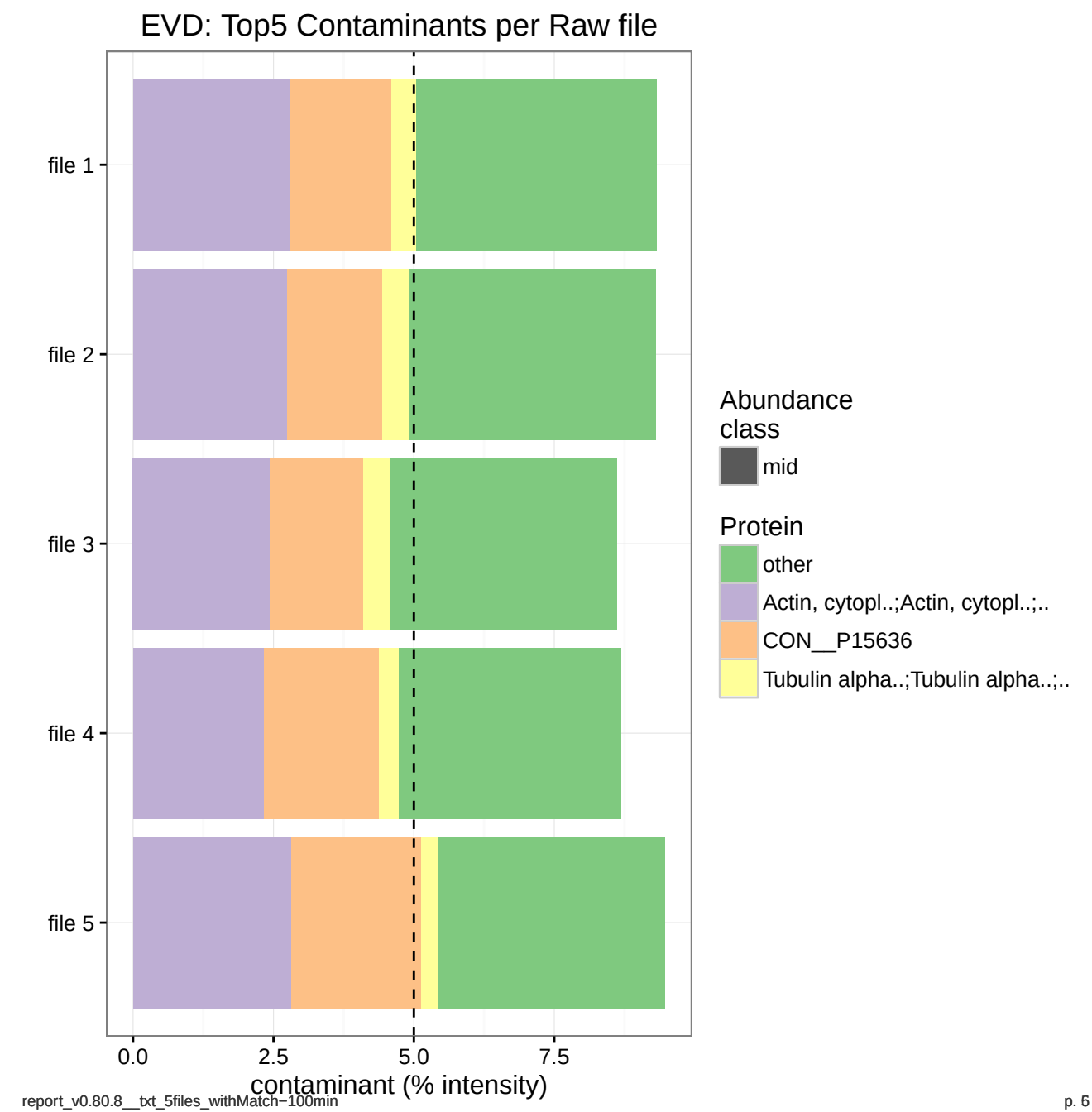
PAR: parameters

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)
25
0
−25
−50
PC #2 (27% var)
..nsity.e2
..nsity.e1
..nsity.e5
..nsity.e3
..nsity.e4
−25
0
25
50
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
contaminant (% intensity)
Abundance class
mid
Protein
other
Actin, cytopl..;Actin, cytopl..;..
CON__P15636
Tubulin alpha..;Tubulin alpha..;..

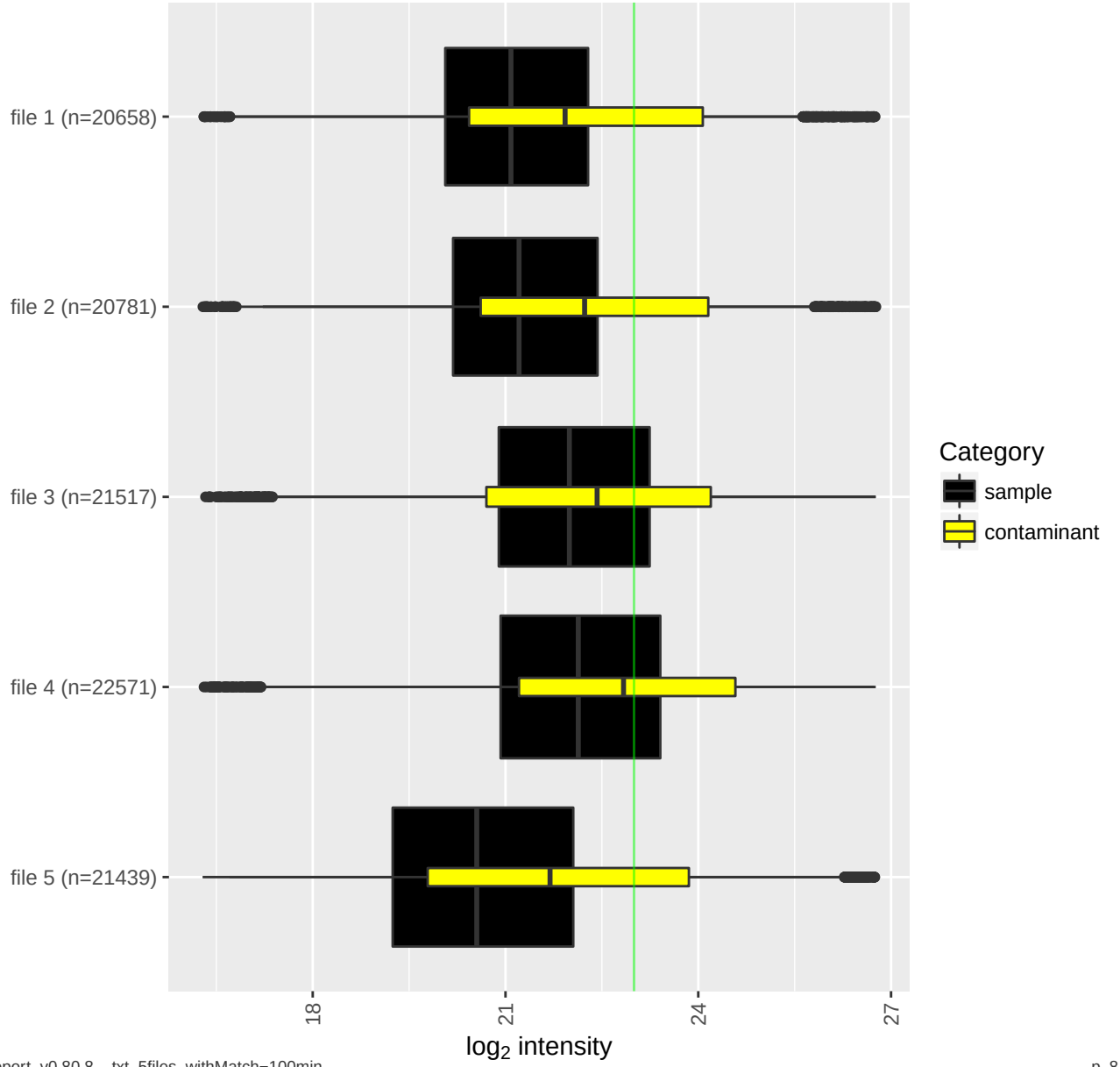
EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

Did you use the correct database?

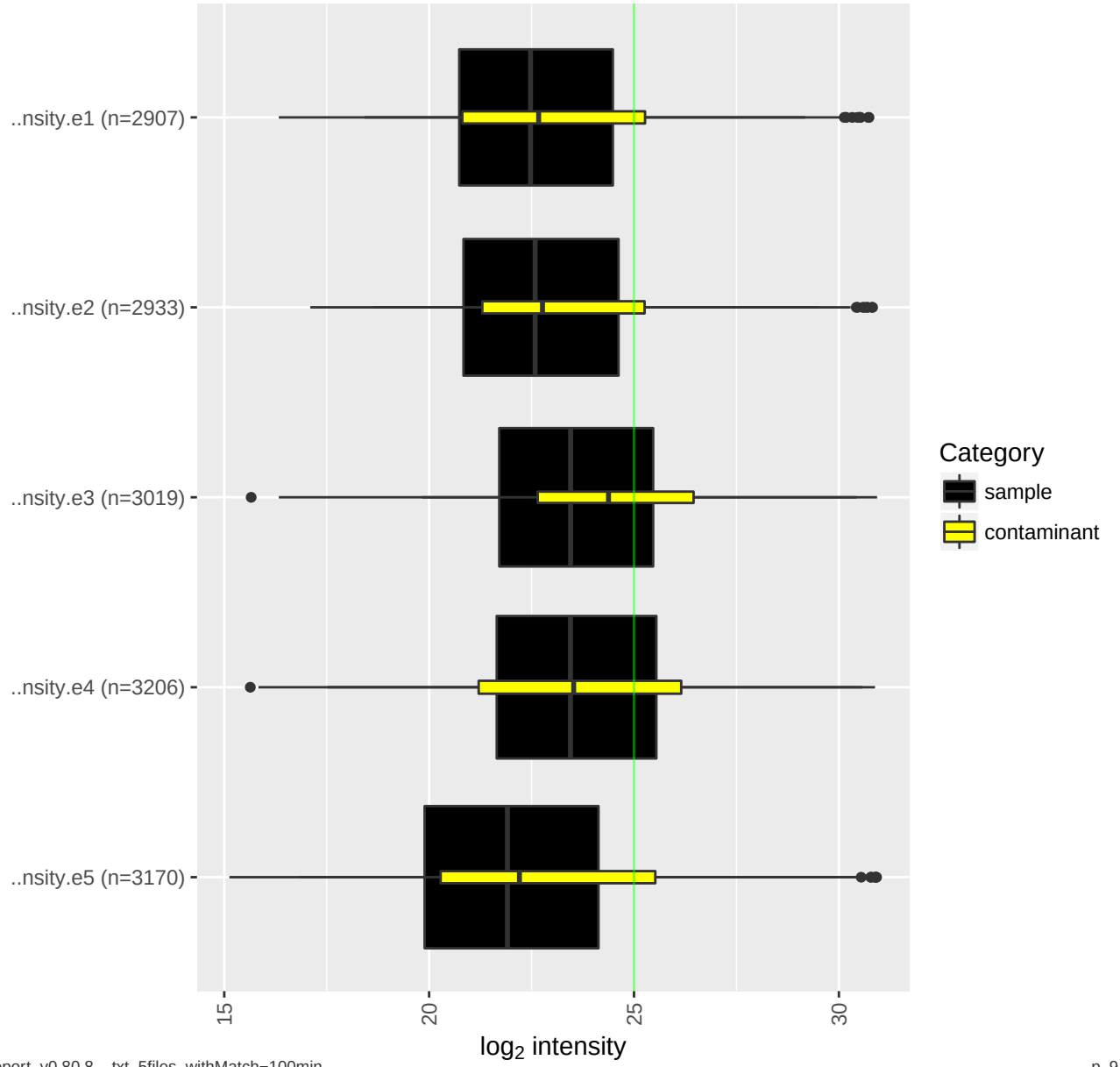
EVD: peptide intensity distribution

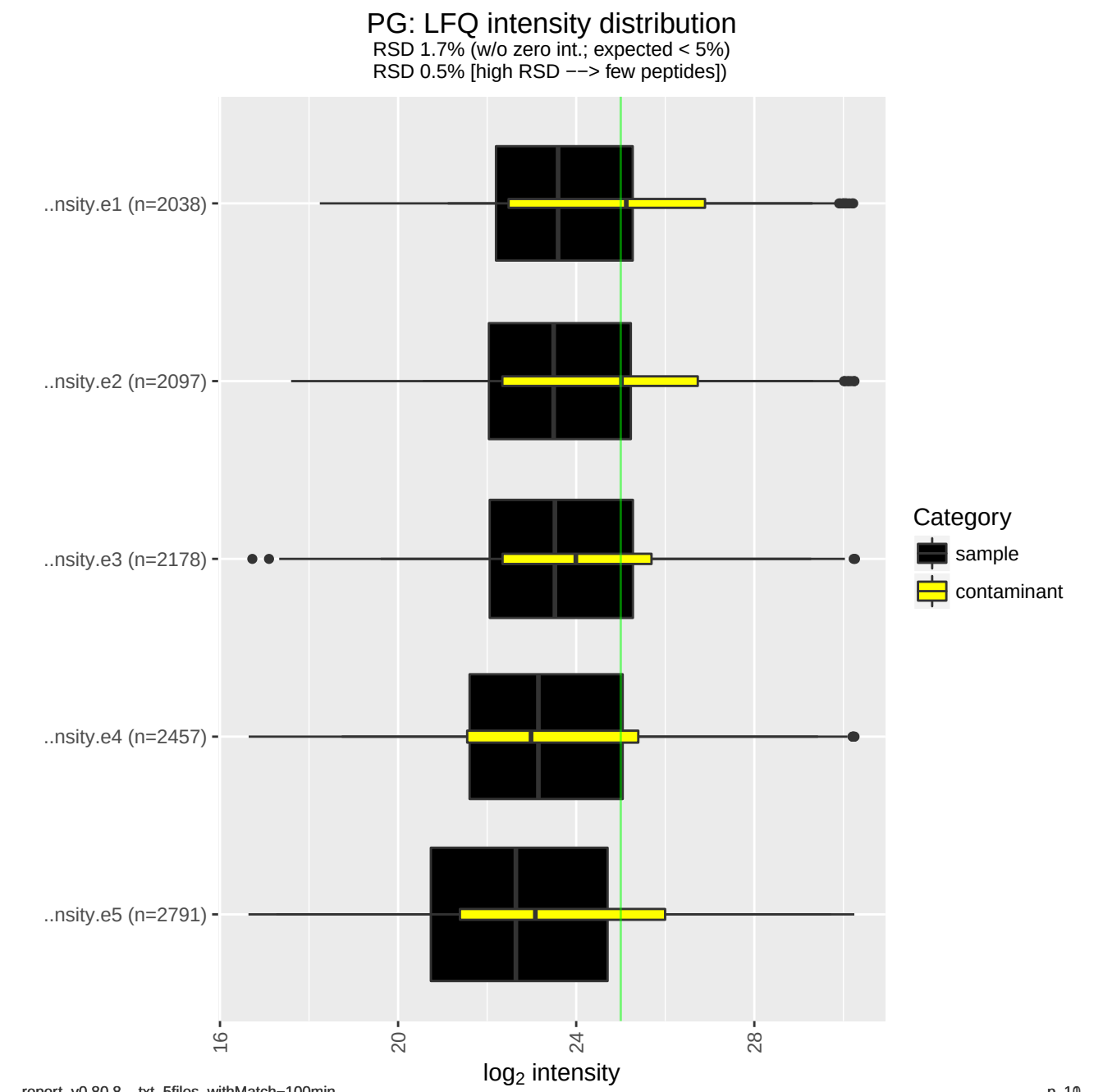
RSD 3.2% (expected < 5%)

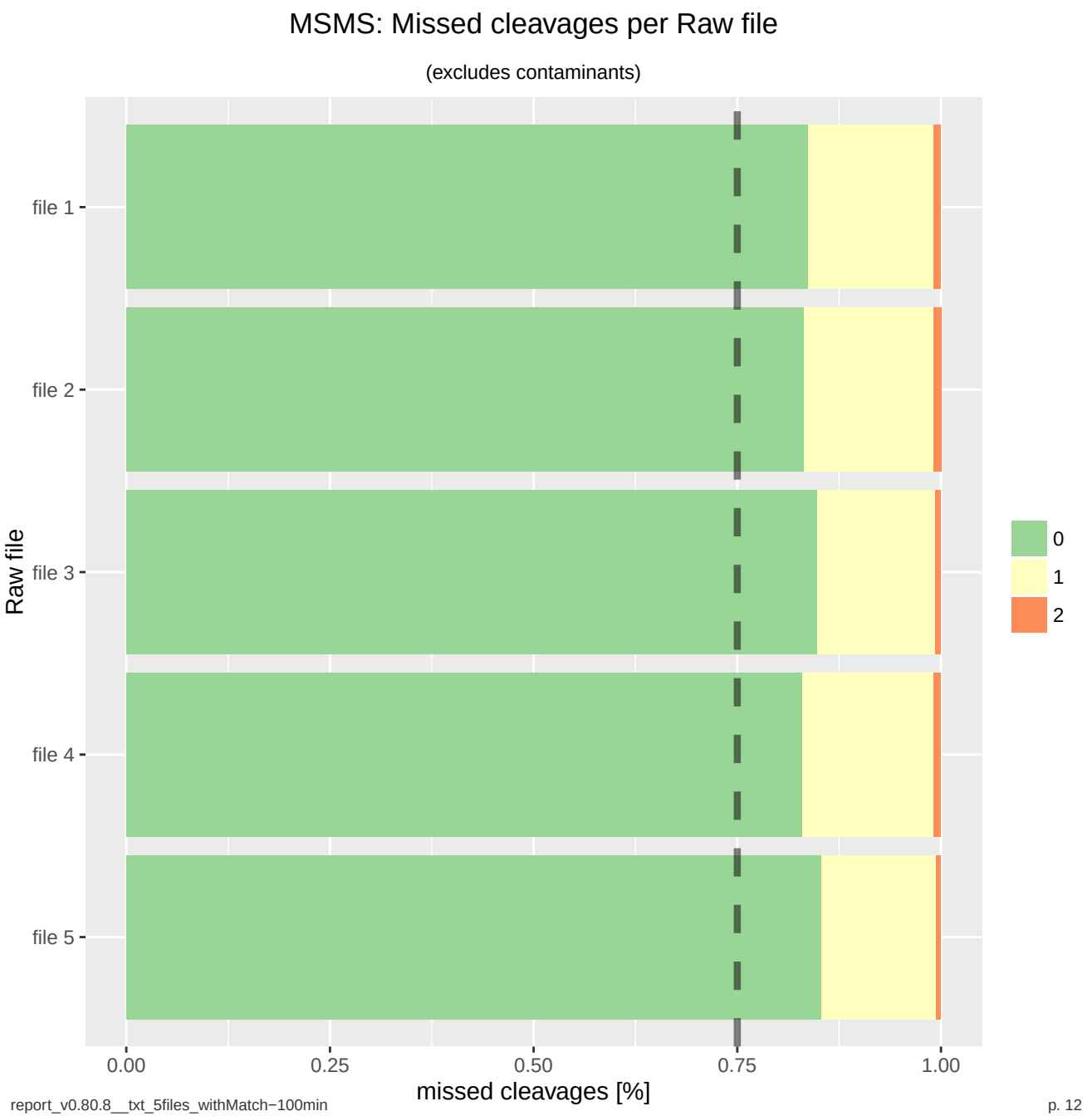


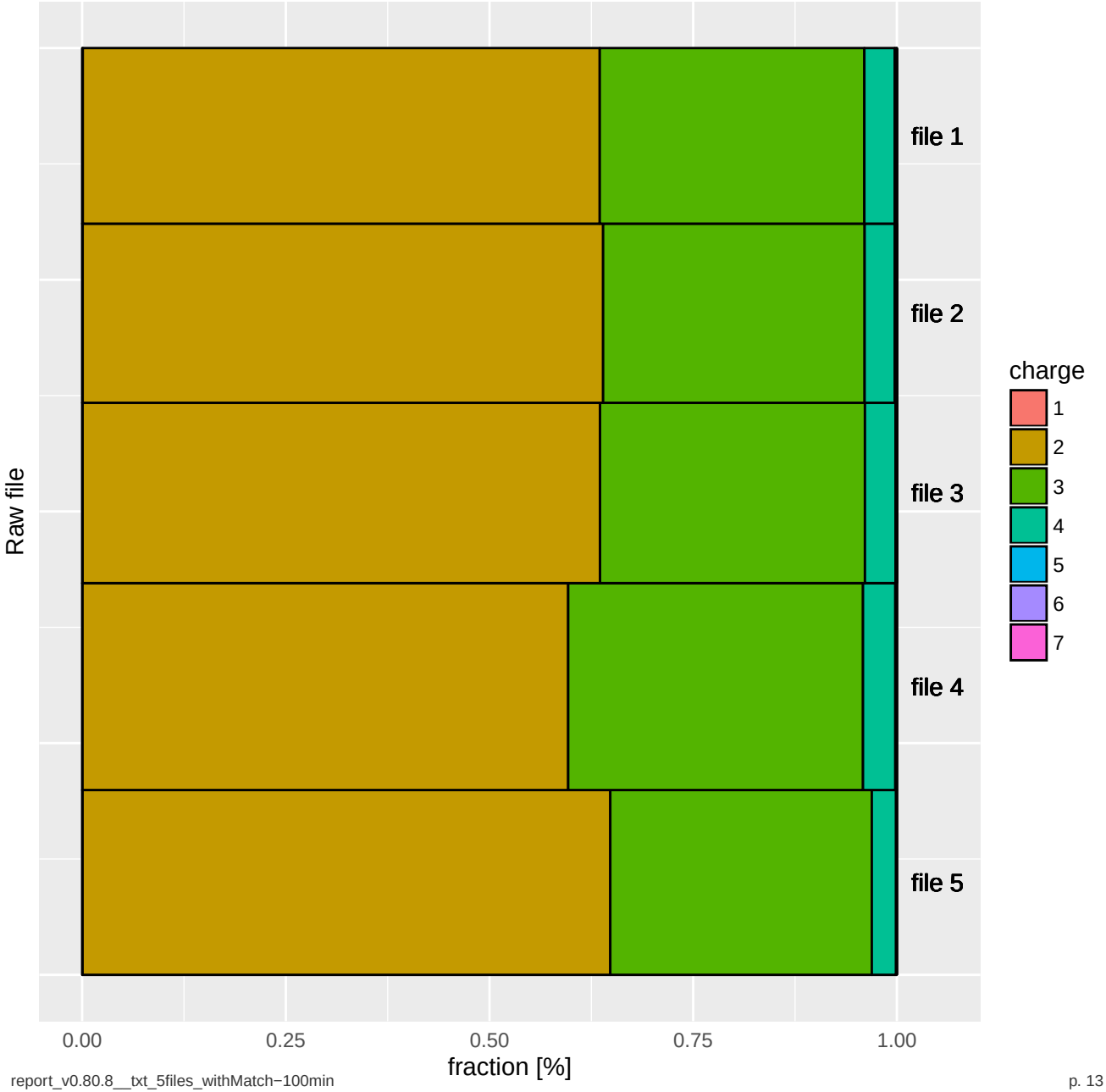
PG: intensity distribution

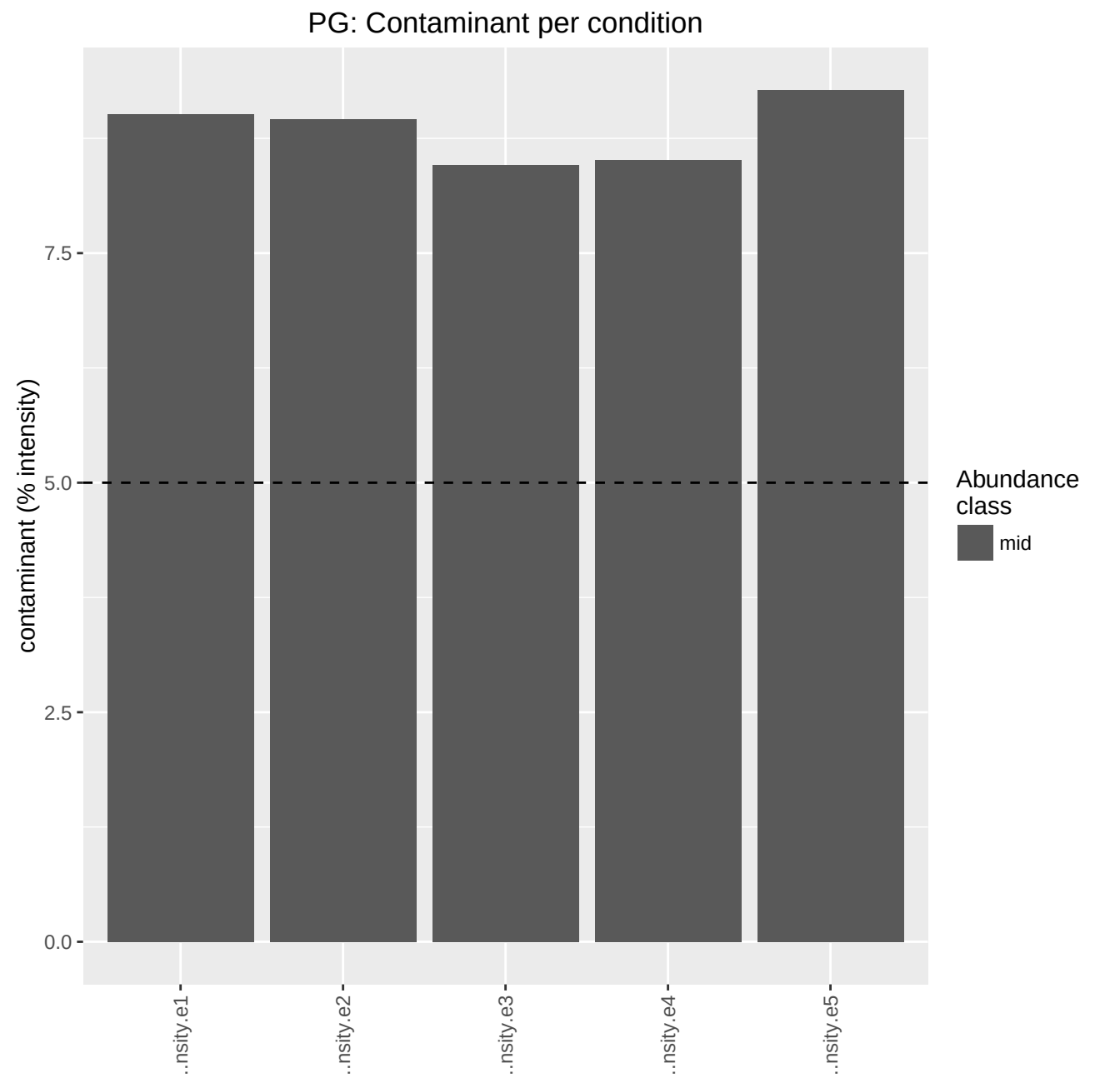
RSD 3% (w/o zero int.; expected < 5%)
RSD 3.2% [high RSD −−> few peptides])

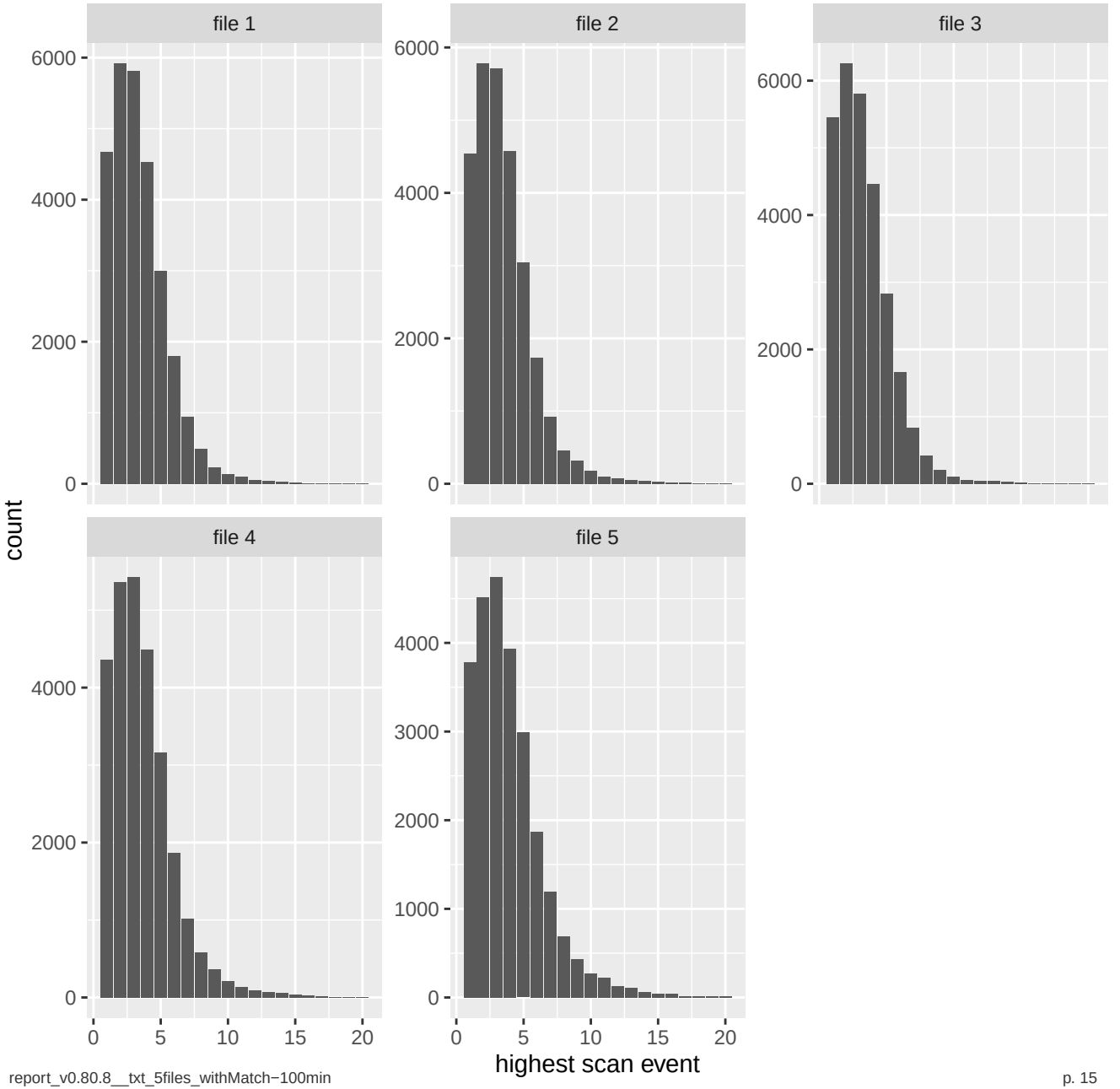


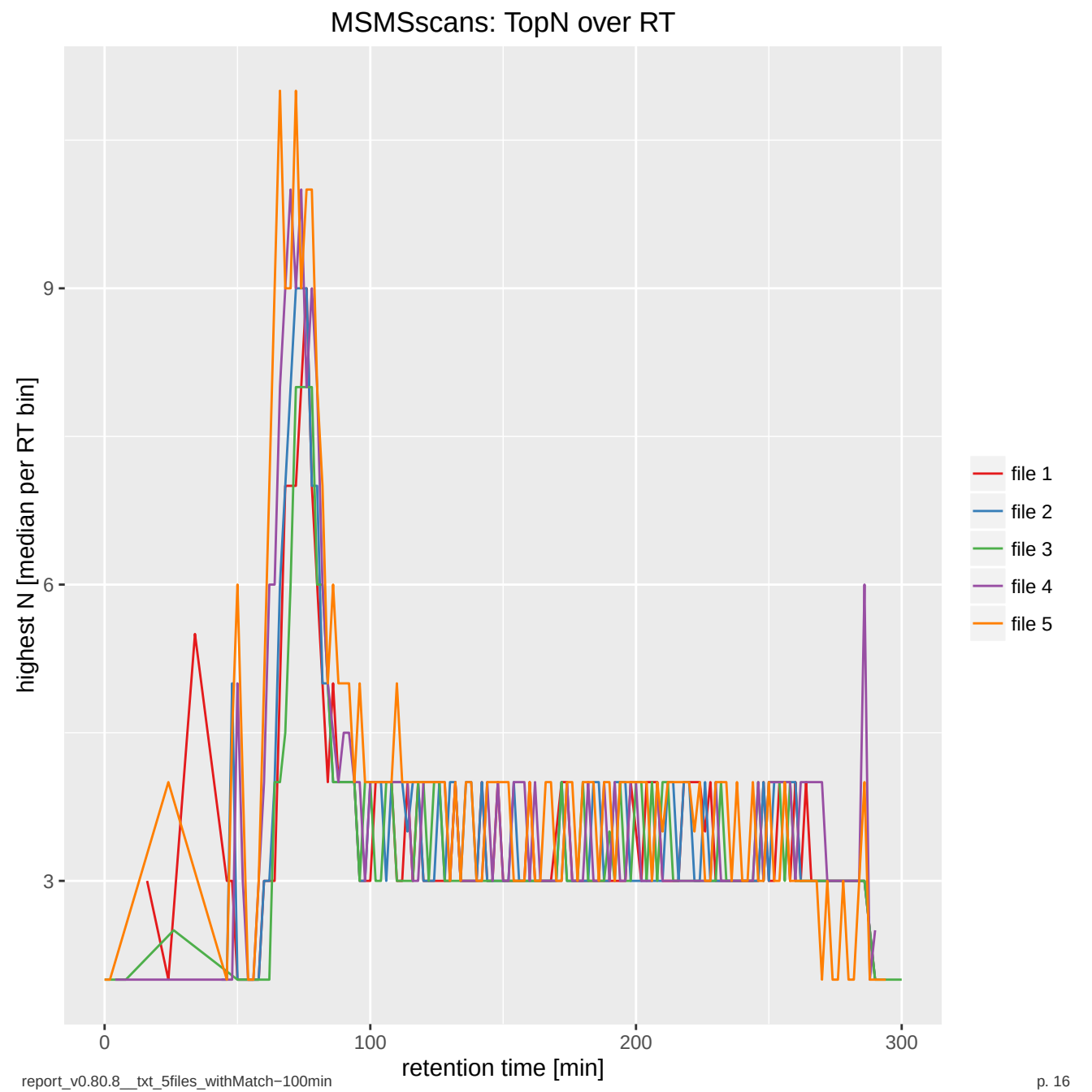

PG: LFQ intensity distribution
RSD 1.7% (w/o zero int.; expected < 5%)
RSD 0.5% [high RSD −−> few peptides])
..nsity.e1 (n=2038)
..nsity.e2 (n=2097)
..nsity.e3 (n=2178)
..nsity.e4 (n=2457)
..nsity.e5 (n=2791)
16
20
24
28
log2 intensity
Category
sample
contaminant


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

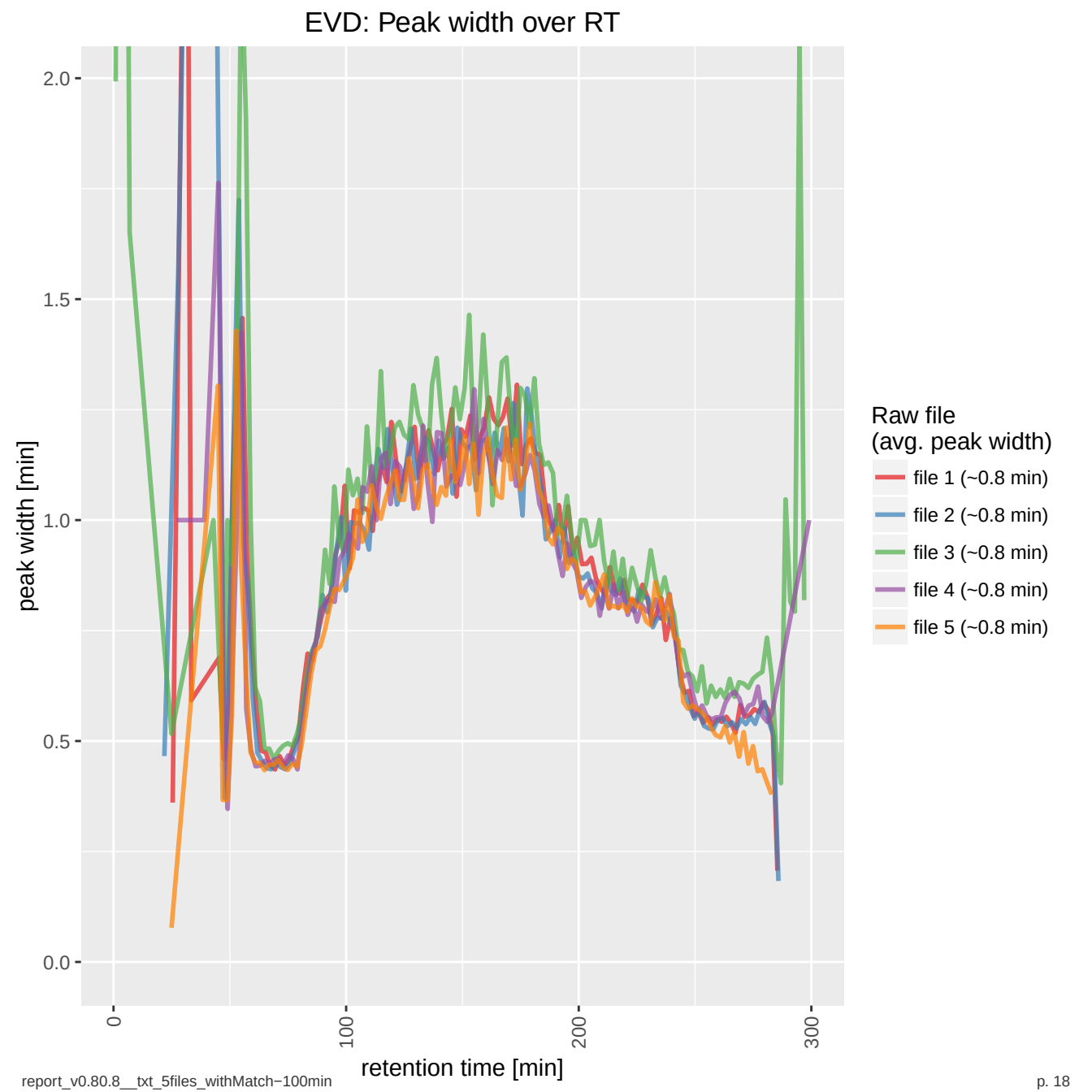

EVD: charge distribution
Raw file
file 1
file 2
file 3
file 4
file 5
charge
1
2
3
4
5
6
7
0.00
0.25
0.50
0.75
1.00
fraction [%]


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
file 1
file 2
file 3
file 4
file 5
count
highest scan event
0
2000
4000
6000
1000
3000
5
10
15
20

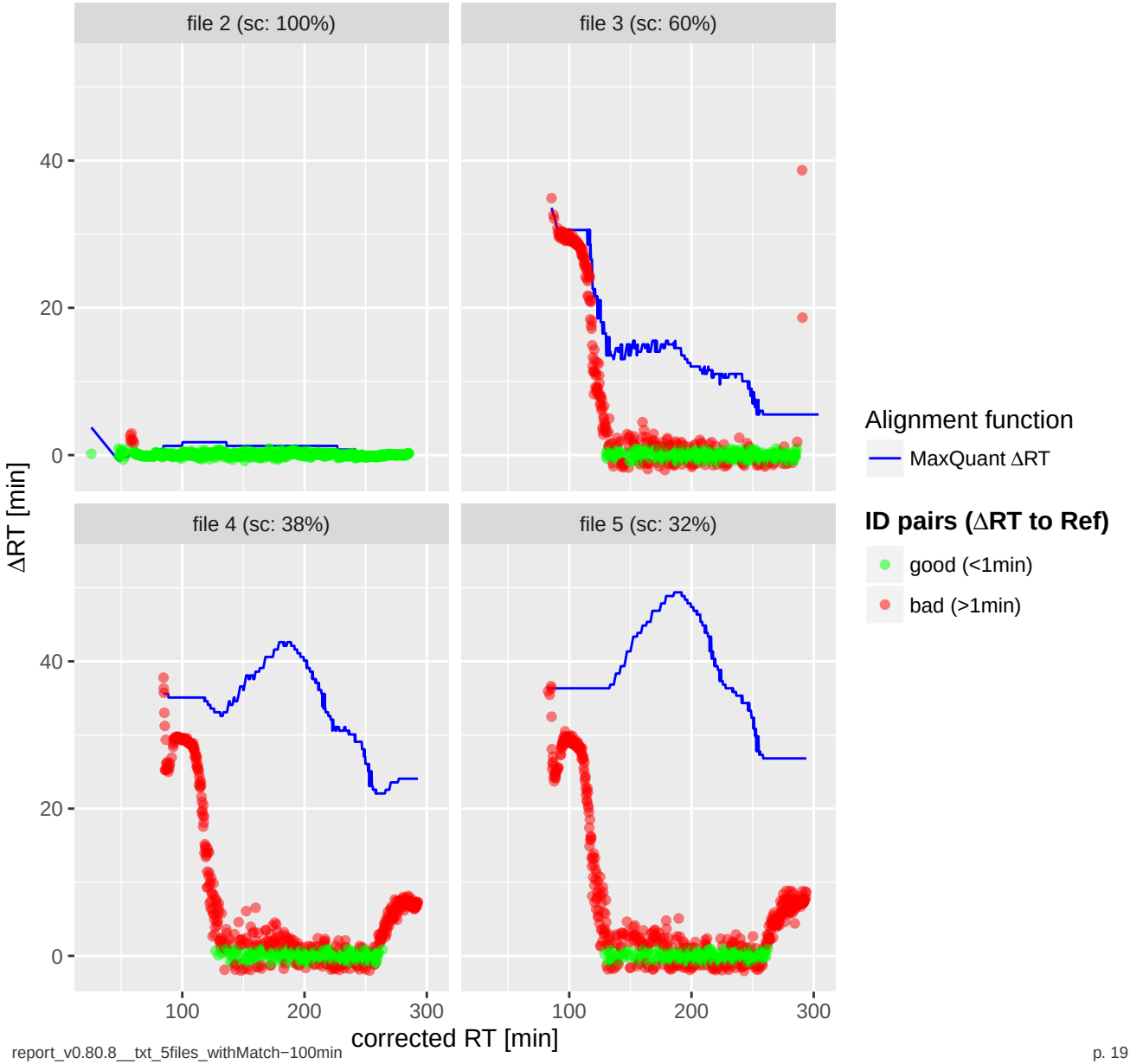

MSMSscans: TopN over RT
highest N [median per RT bin]
9
6
3
0
100
200
300
retention time [min]
file 1
file 2
file 3
file 4
file 5

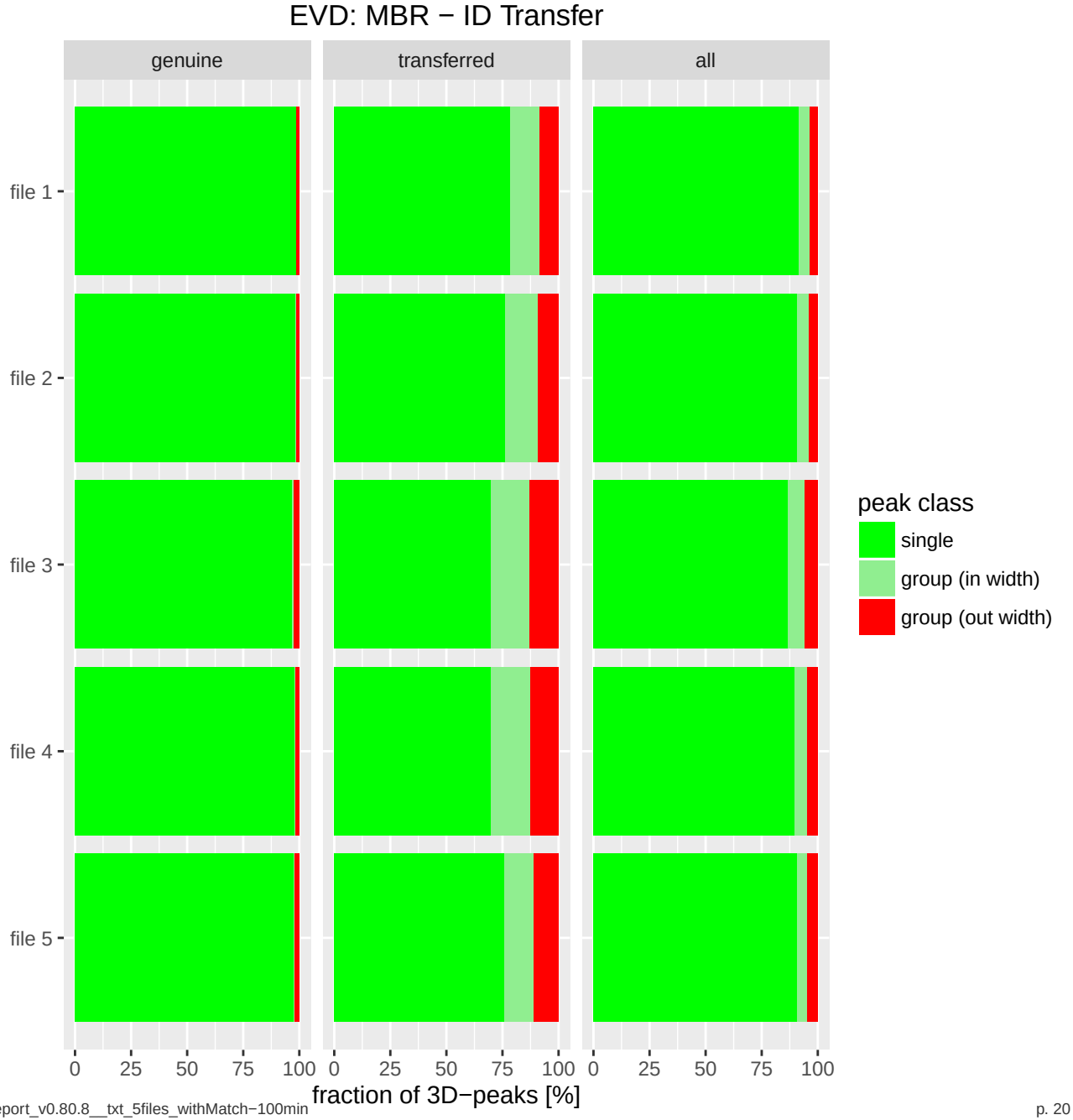

EVD: IDs over RT
ID count
400
200
0
0
100
200
300
RT [min]
Raw file
file 1
file 2
file 3
file 4
file 5


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 (~0.8 min)
file 2 (~0.8 min)
file 3 (~0.8 min)
file 4 (~0.8 min)
file 5 (~0.8 min)

EVD: MBR − alignment

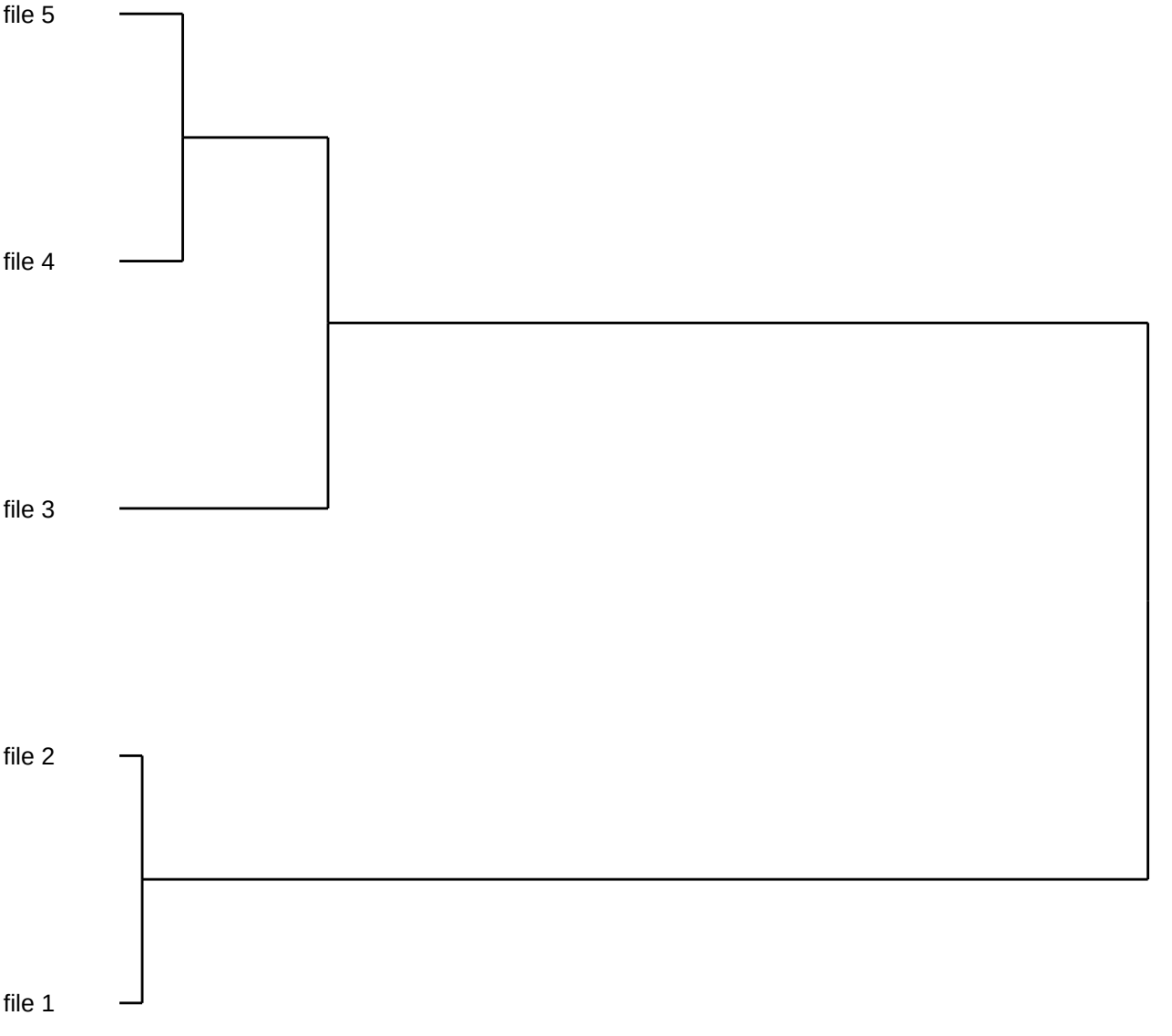
alignment reference: Toni_20140521_GM_QC_01

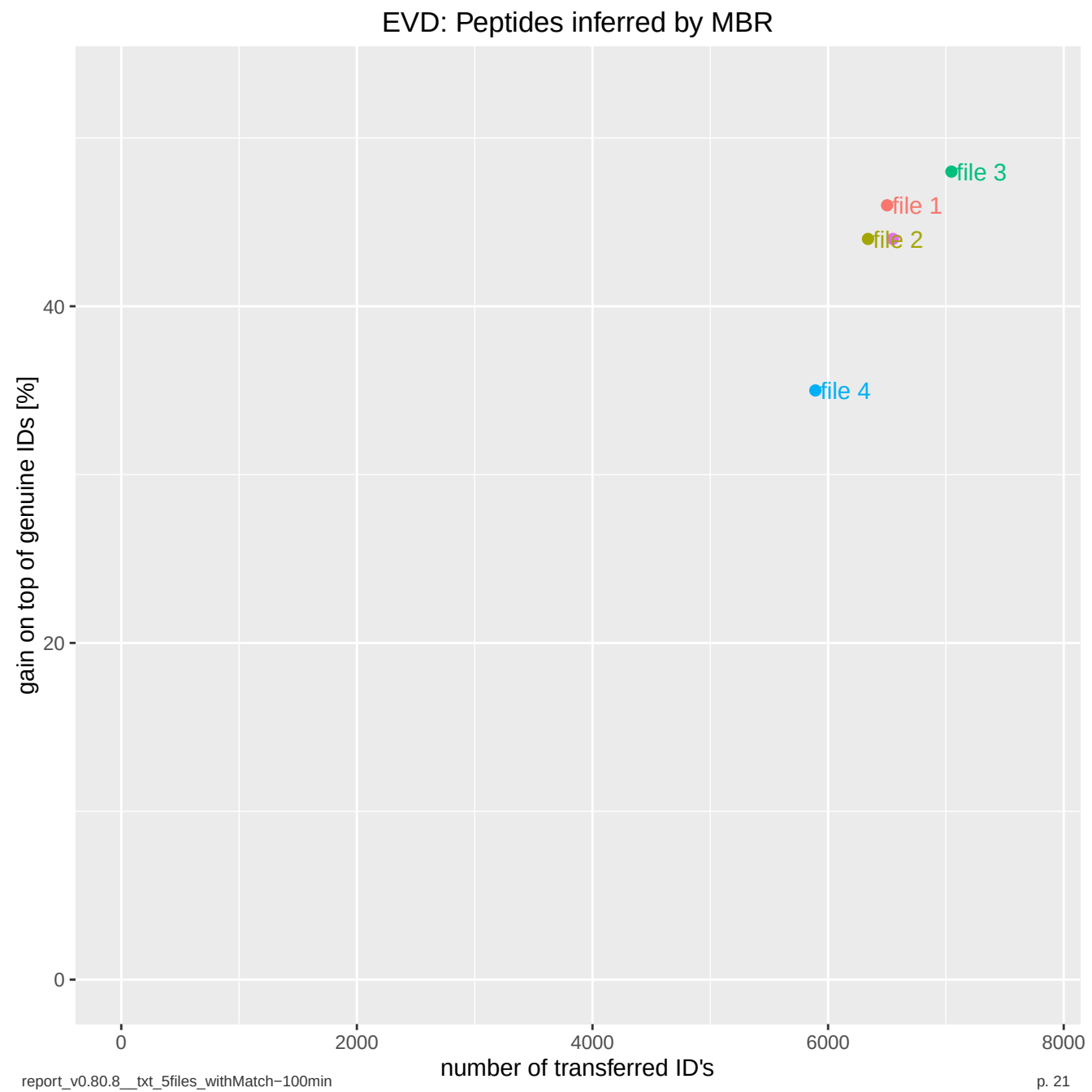


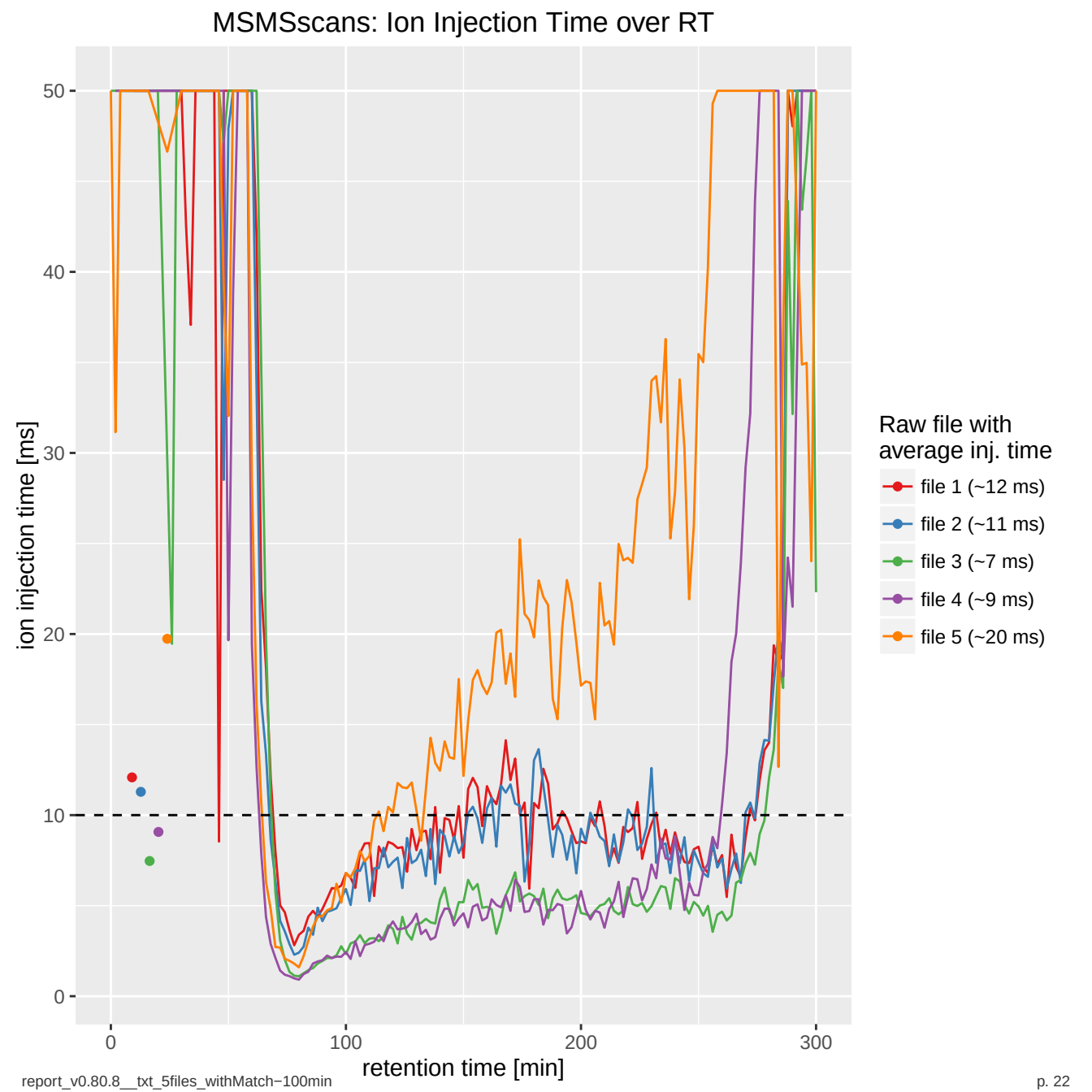

EVD: MBR − ID Transfer
genuine
transferred
all
file 1
file 2
file 3
file 4
file 5
0
25
50
75
100
fraction of 3D−peaks [%]
peak class
single
group (in width)
group (out width)

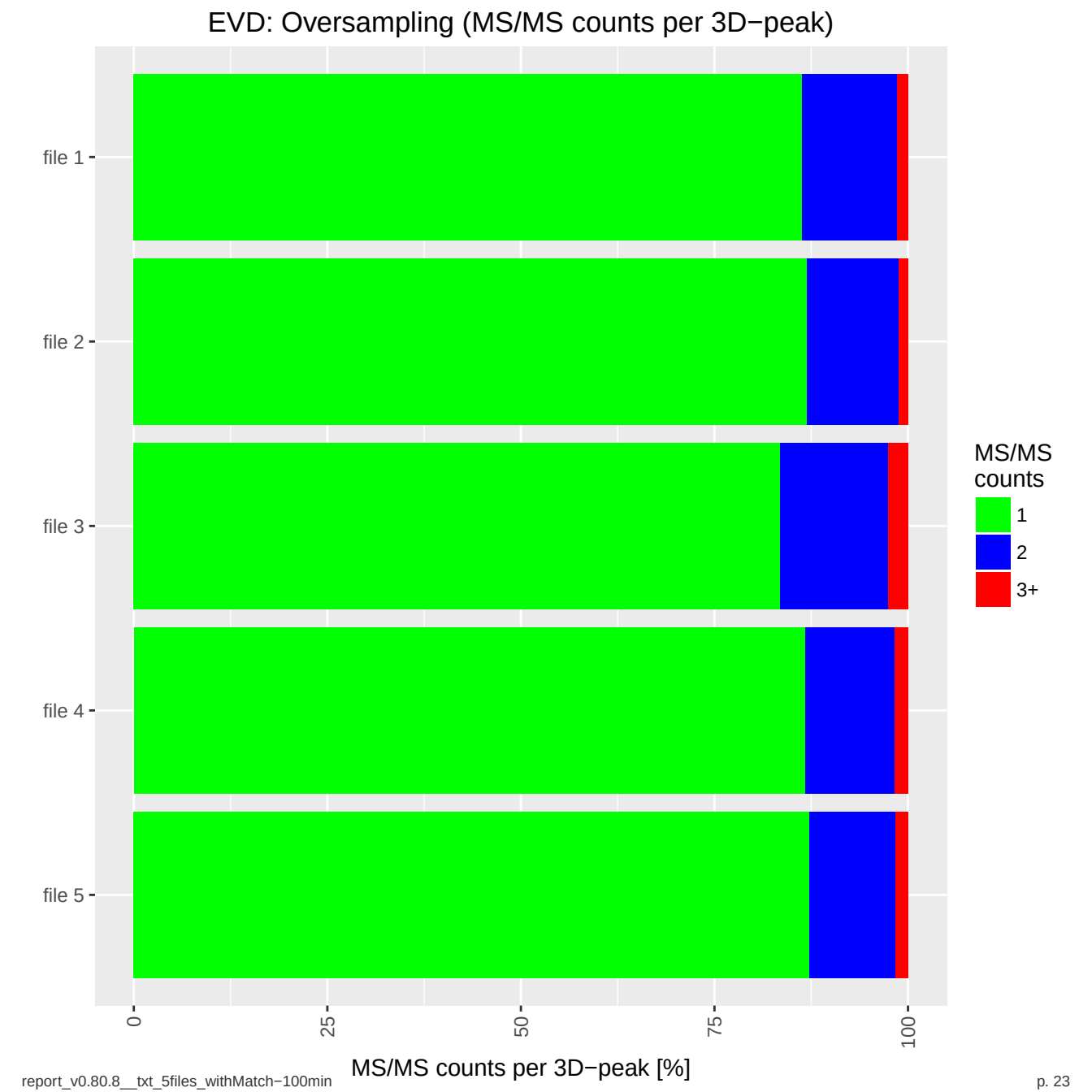
[experimental] EVD: Clustering Tree of Raw files

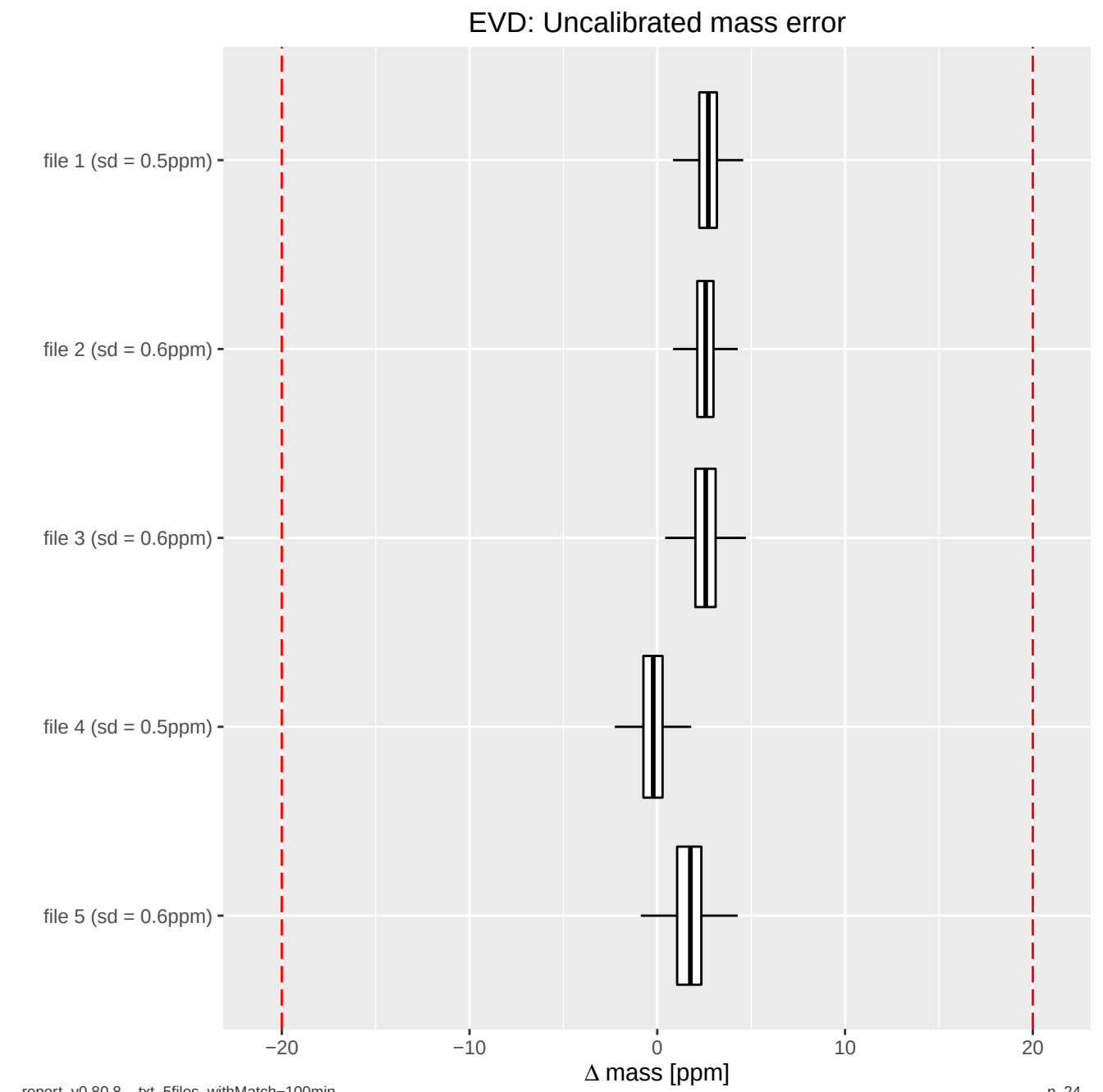
by Correlation of Corrected Retention Times

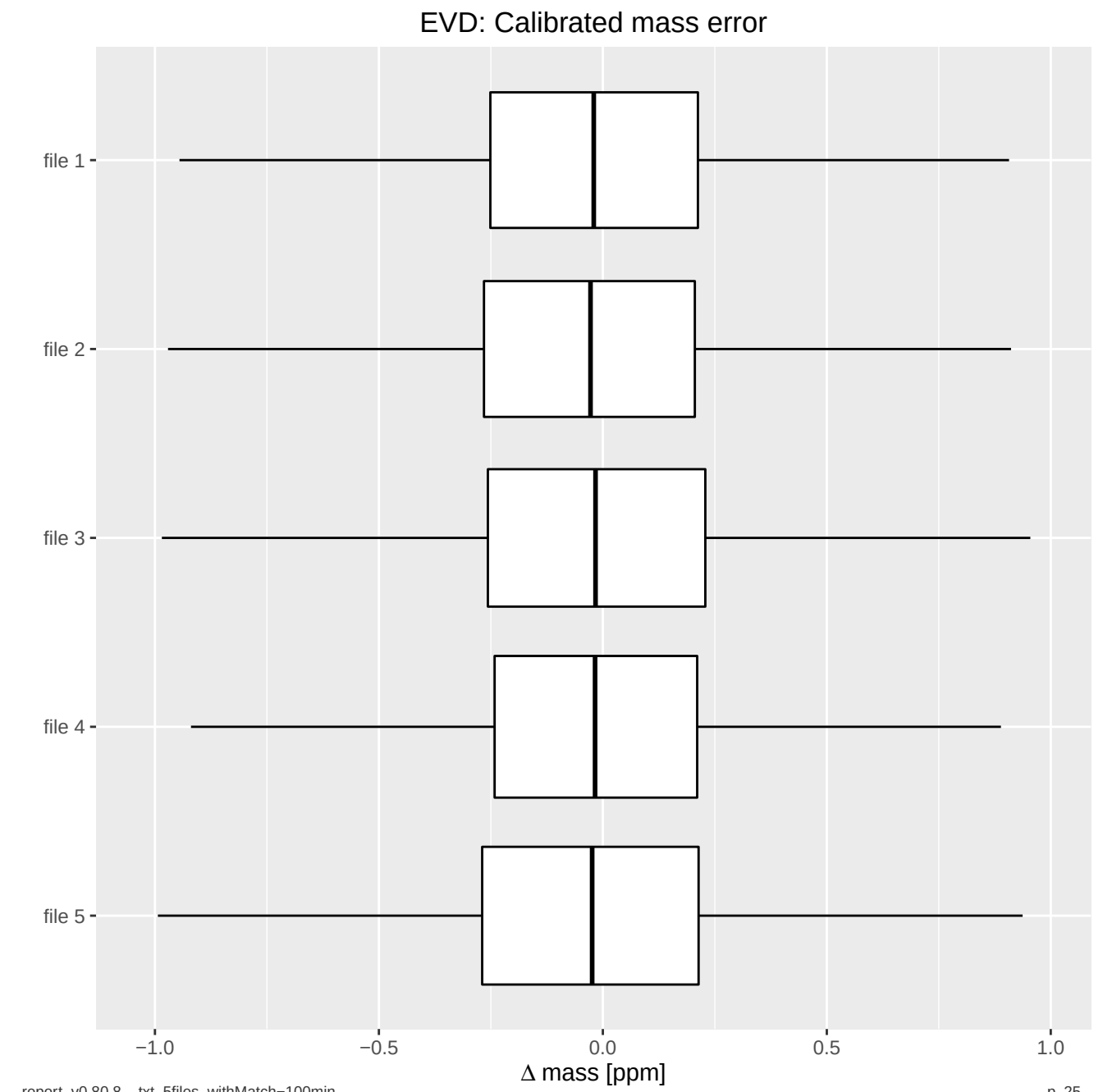



EVD: Peptides inferred by MBR
file 3
file 1
file 2
file 4
40
20
0
gain on top of genuine IDs [%]
0
2000
4000
6000
8000
number of transferred ID's

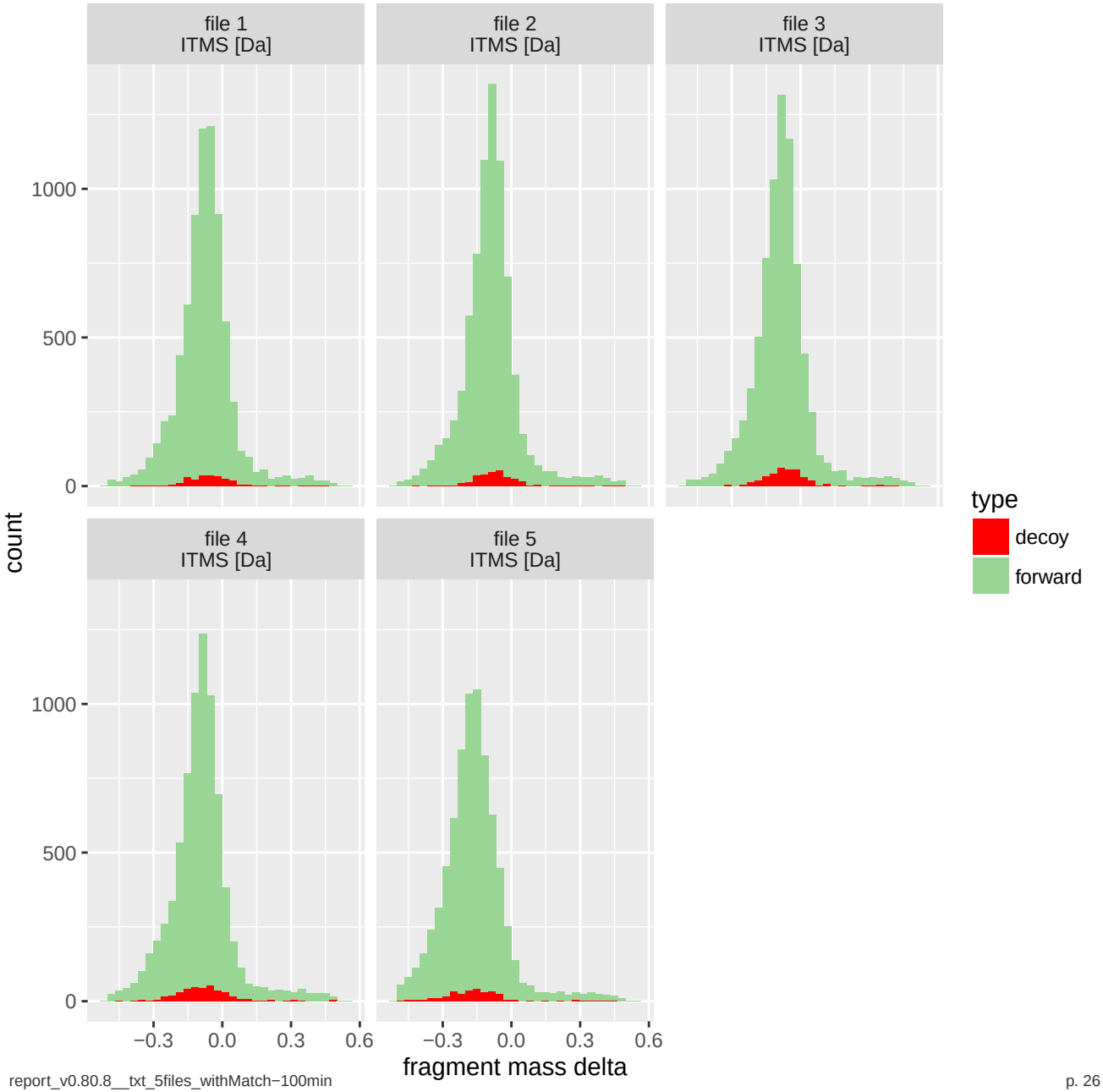

MSMSscans: Ion Injection Time over RT
ion injection time [ms]
retention time [min]
0
10
20
30
40
50
0
100
200
300
Raw file with average inj. time
file 1 (~12 ms)
file 2 (~11 ms)
file 3 (~7 ms)
file 4 (~9 ms)
file 5 (~20 ms)

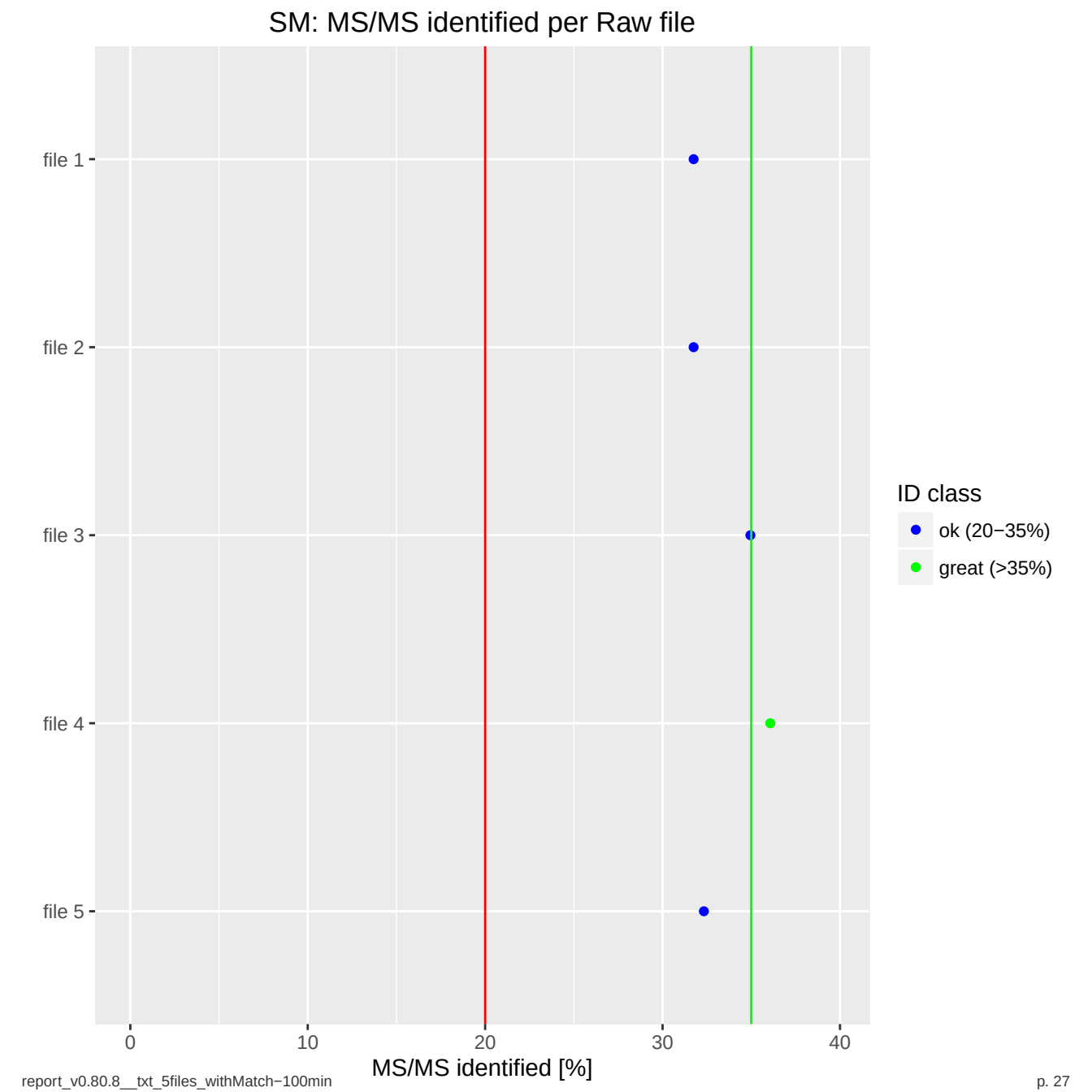

EVD: Oversampling (MS/MS counts per 3D−peak)
file 1
file 2
file 3
file 4
file 5
0
25
50
75
100
MS/MS counts per 3D−peak [%]
MS/MS counts
1
2
3+

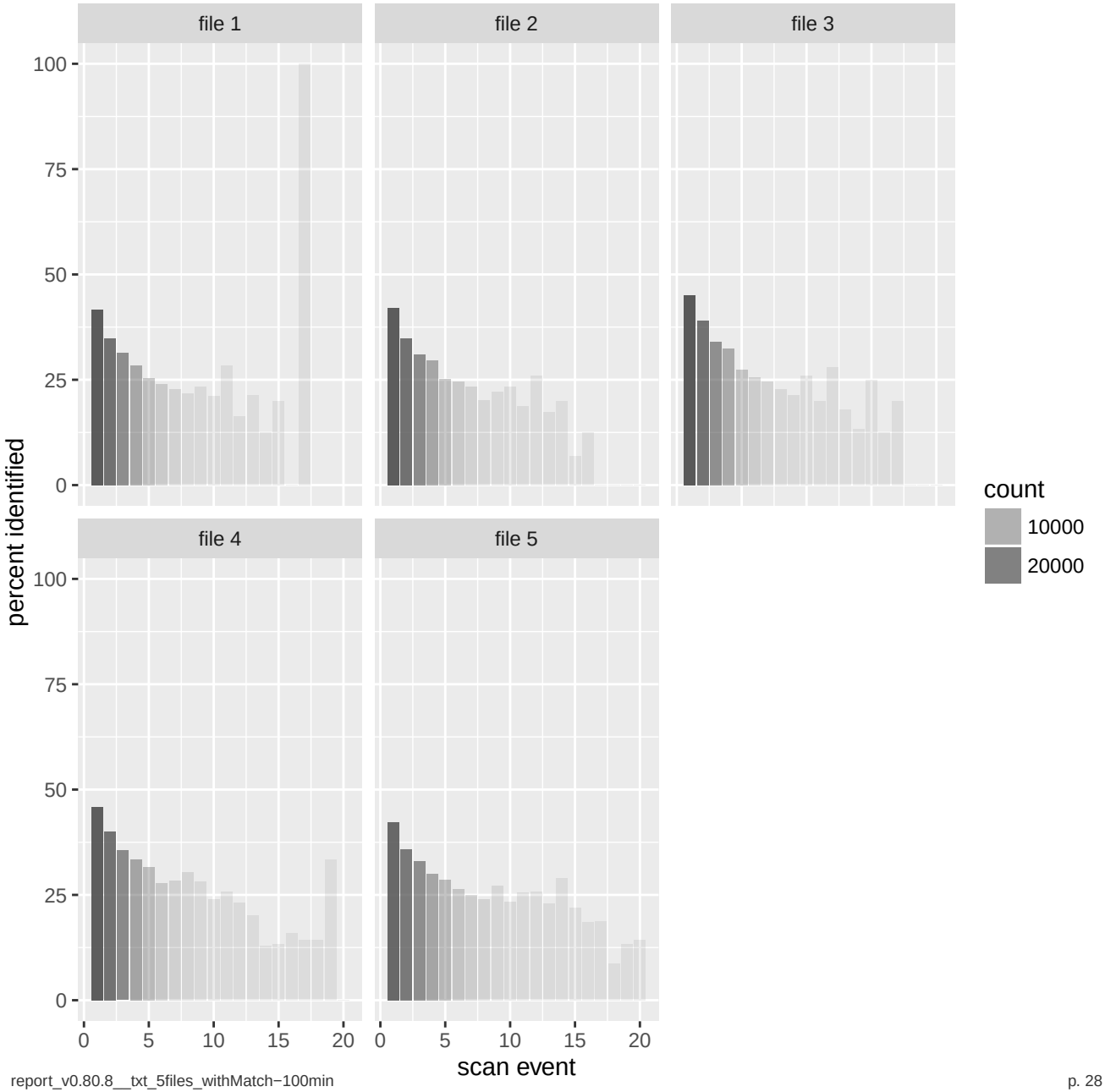

EVD: Uncalibrated mass error
file 1 (sd = 0.5ppm)
file 2 (sd = 0.6ppm)
file 3 (sd = 0.6ppm)
file 4 (sd = 0.5ppm)
file 5 (sd = 0.6ppm)
−20
−10
0
10
20
Δ mass [ppm]

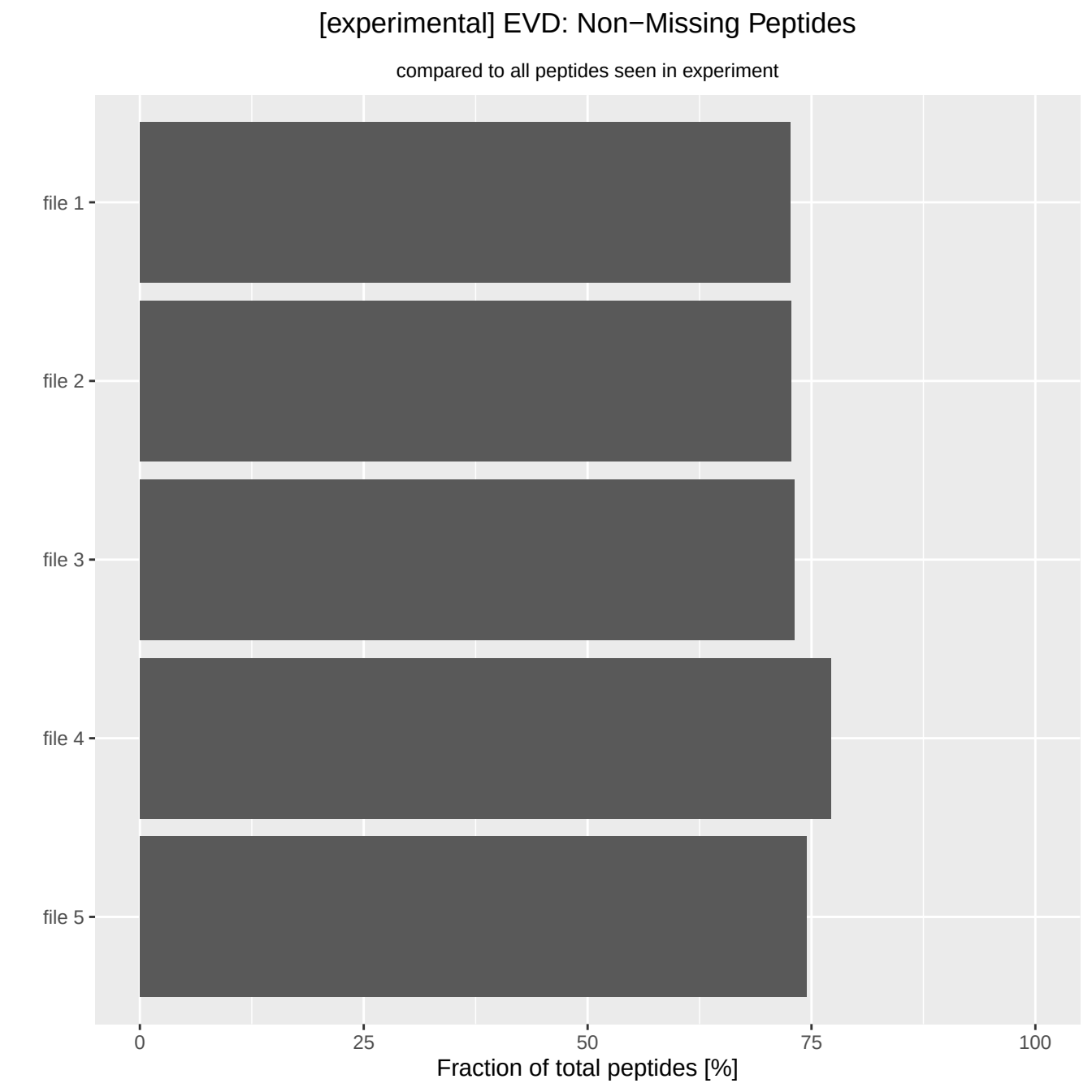

EVD: Calibrated mass error
file 1
file 2
file 3
file 4
file 5
−1.0
−0.5
0.0
0.5
1.0
Δ mass [ppm]

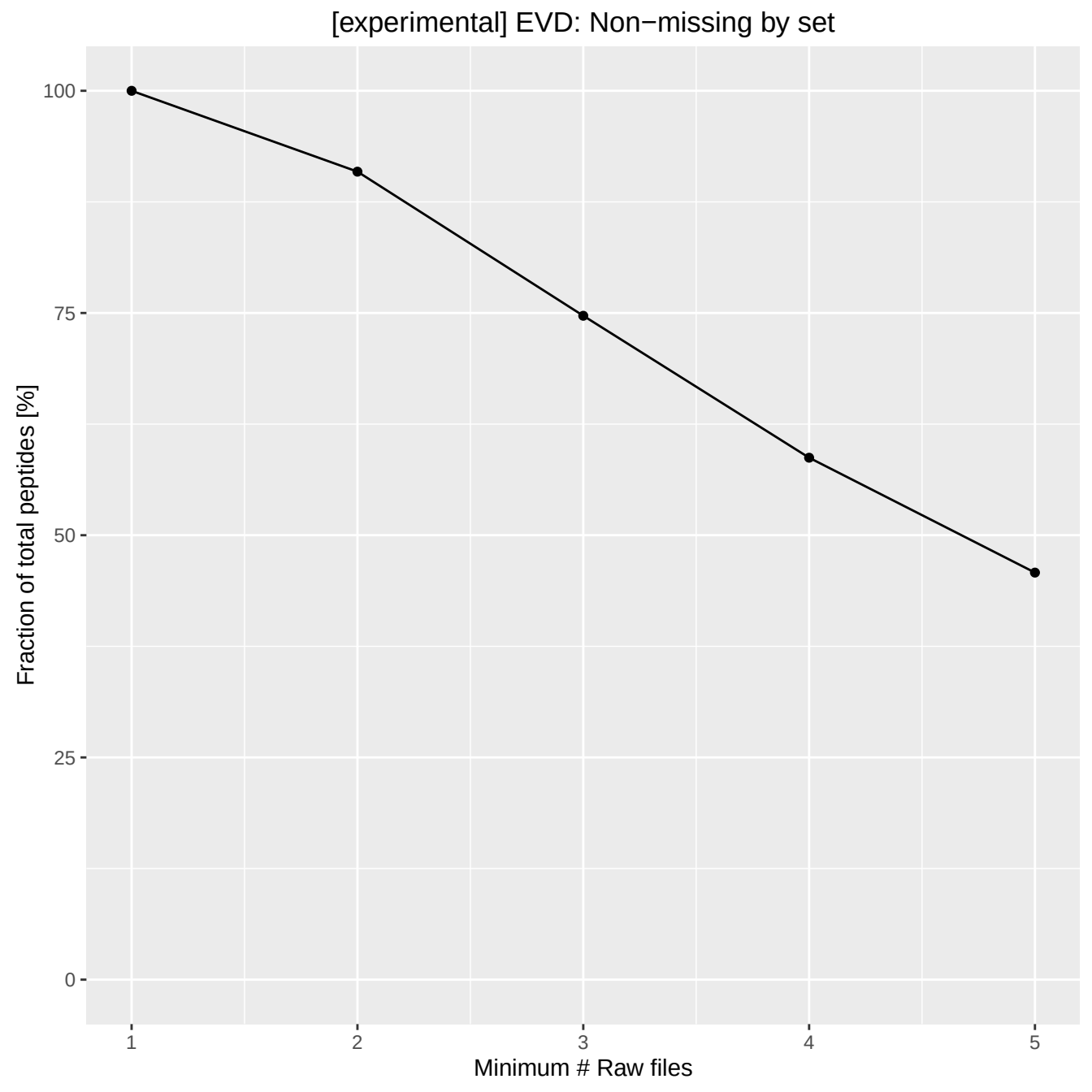
MSMS: Fragment mass errors per Raw file



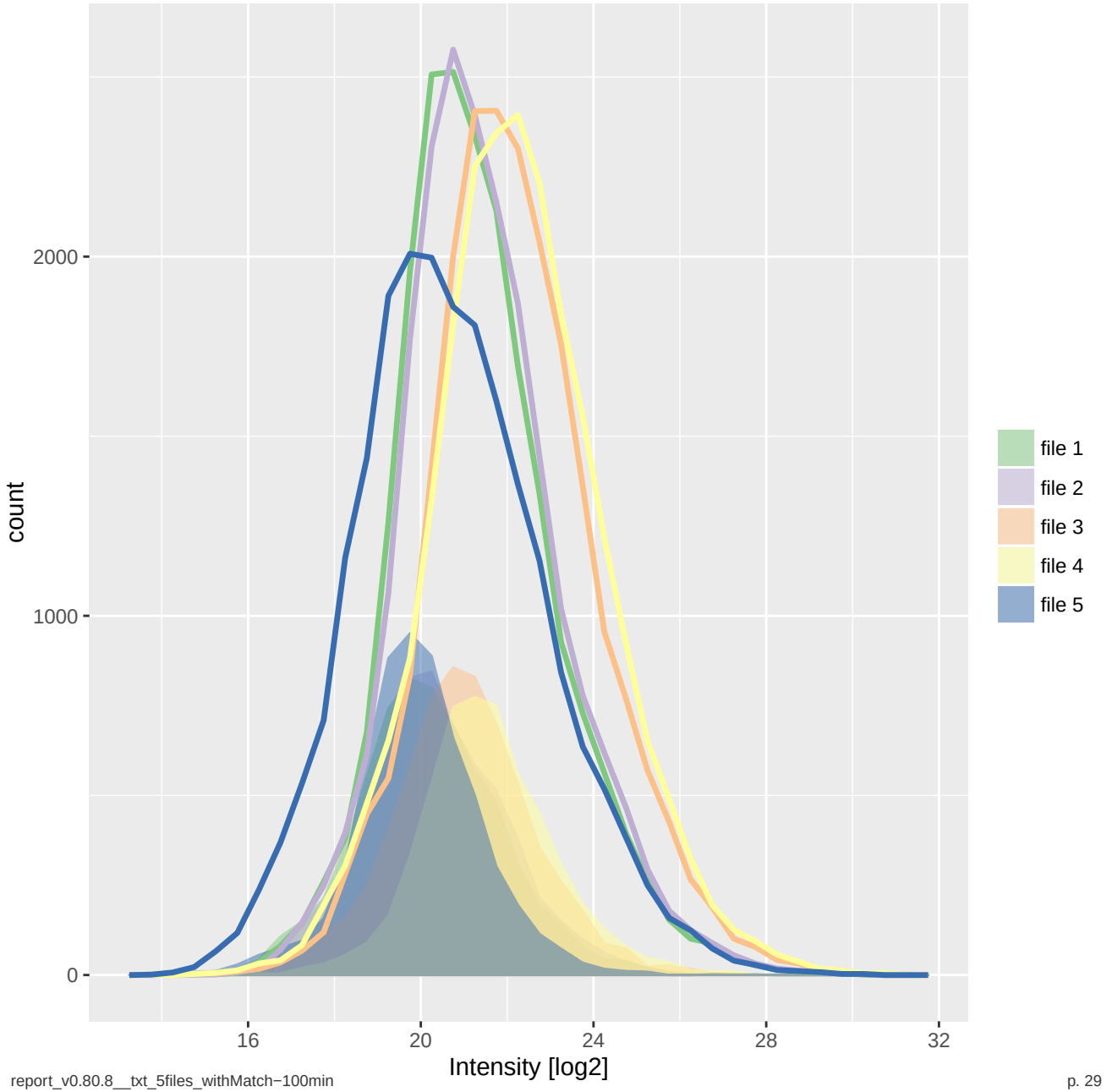

SM: MS/MS identified per Raw file
file 1
file 2
file 3
file 4
file 5
0
10
20
30
40
MS/MS identified [%]
ID class
ok (20−35%)
great (>35%)

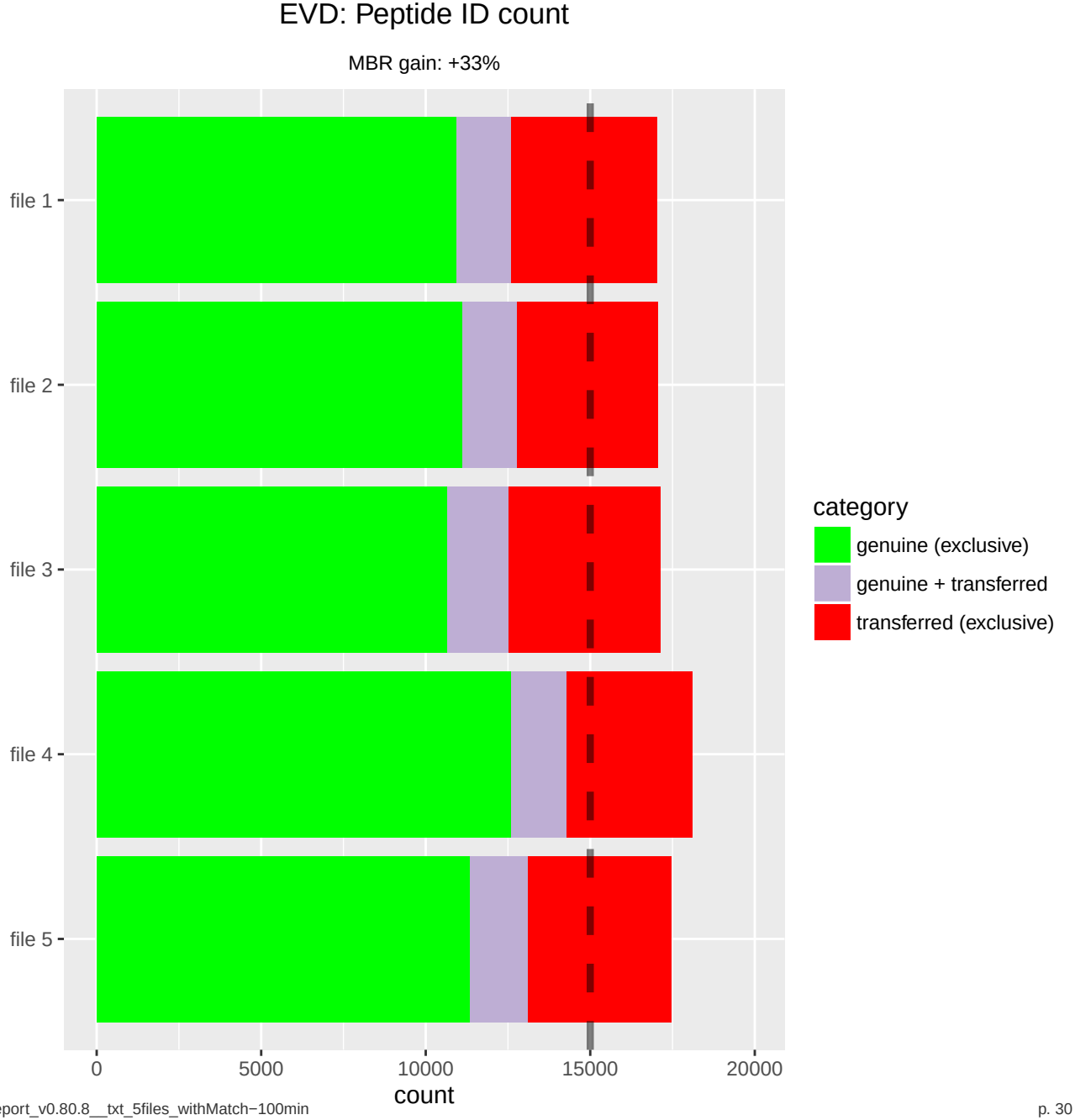

MSMSscans: TopN % identified over N
file 1
file 2
file 3
file 4
file 5
percent identified
100
75
50
25
0
0
5
10
15
20
scan event
count
10000
20000

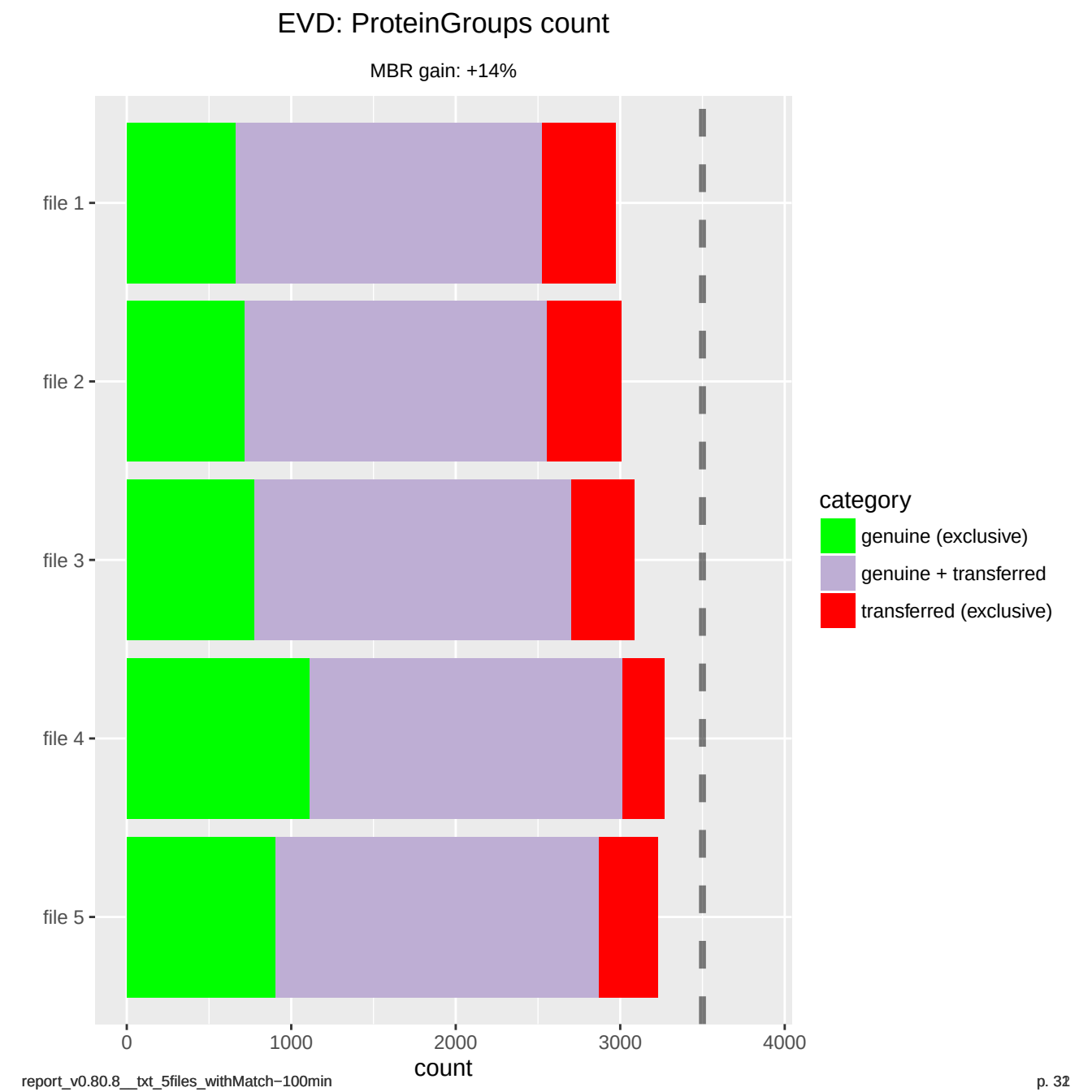

[experimental] EVD: Non−Missing Peptides
compared to all peptides seen in experiment
file 1
file 2
file 3
file 4
file 5
0
25
50
75
100
Fraction of total peptides [%]


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

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




EVD: Peptide ID count
MBR gain: +33%
file 1
file 2
file 3
file 4
file 5
0
5000
10000
15000
20000
count
category
genuine (exclusive)
genuine + transferred
transferred (exclusive)


EVD: ProteinGroups count
MBR gain: +14%
file 1
file 2
file 3
file 4
file 5
0
1000
2000
3000
4000
count
category
genuine (exclusive)
genuine + transferred
transferred (exclusive)