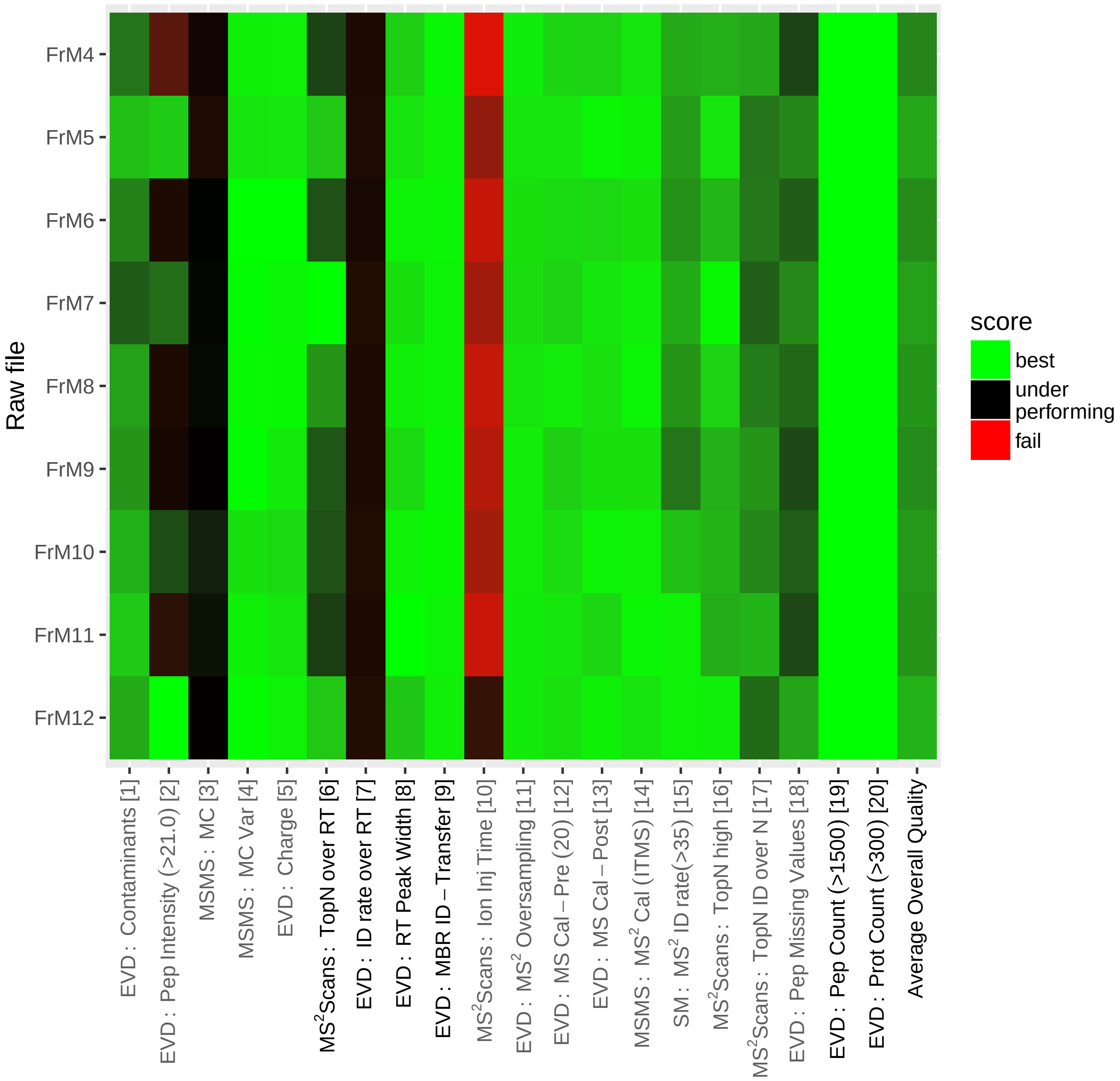
Performance overview



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
FrM4_Rep−GFP	FrM4	4_Rep−GFP
FrM5_Rep−GFP_PCNA_FLAG	FrM5	5_PCNA_FLAG
FrM6_PCNA_FLAG_control	FrM6	6_control
FrM7_Rep−GFP	FrM7	7_Rep−GFP
FrM8_Rep−GFP_PCNA_FLAG	FrM8	8_PCNA_FLAG
FrM9_PCNA_FLAG_control	FrM9	9_control
FrM10_Rep−GFP	FrM10	10_Rep−GFP
FrM11_Rep−GFP_PCNA_FLAG	FrM11	11_PCNA_FLAG
FrM12_PCNA_FLAG_control	FrM12	12_control

PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	Modifications included in pr..	Acetyl (Protein N−term) Deamidation (NQ) Oxidation (M)
Alignment time window [min]	20	MS/MS deisotoping (FTMS)	True
Date of writing	07/29/2016 11:53:45	MS/MS deisotoping (ITMS)	False
Decoy mode	revert	MS/MS deisotoping (TOF)	True
Dependent peptide FDR	0.01	MS/MS deisotoping (Unknown)	False
Discard unmodified counterpa..	True	MS/MS tol. (FTMS)	20 ppm
Find dependent peptides	True	MS/MS tol. (ITMS)	0.5 Da
First pass AIF correlation	0.8	MS/MS tol. (TOF)	40 ppm
Fixed modifications	Carbamidomethyl (C)	MS/MS tol. (Unknown)	0.5 Da
iBAQ	True	Peptides used for protein qu..	Razor
iBAQ log fit	True	Protein FDR	0.01
Include contaminants	True	PSM FDR	0.01
Labeled amino acid filtering	True	Re−quantify	False
Machine name	BICMAXQUANT2	RT shift	False
Mass bin size	0.0065	Site FDR	0.01
Match between runs	True	Site tables	Deamidation (NQ)Sites.txt Oxidation (M)Sites.txt
Matching time window [min]	0.7	Special AAs	KR
Min. delta score for modifie..	6	Top MS/MS peaks per 100 Da. ..	12
Min. delta score for unmodif..	0	Top MS/MS peaks per 100 Da. ..	8
Min. peptide Length	7	Top MS/MS peaks per 100 Da. ..	10
Min. peptides	1	Top MS/MS peaks per 100 Da. ..	8
Min. ratio count	2	Use delta score	False
Min. razor peptides	1	Use Normalized Ratios For Oc..	True
Min. score for modified pept..	40	Use only unmodified peptides..	True
Min. score for unmodified pe..	0	User name	LCMS
Min. unique peptides	0	Version	1.5.2.8

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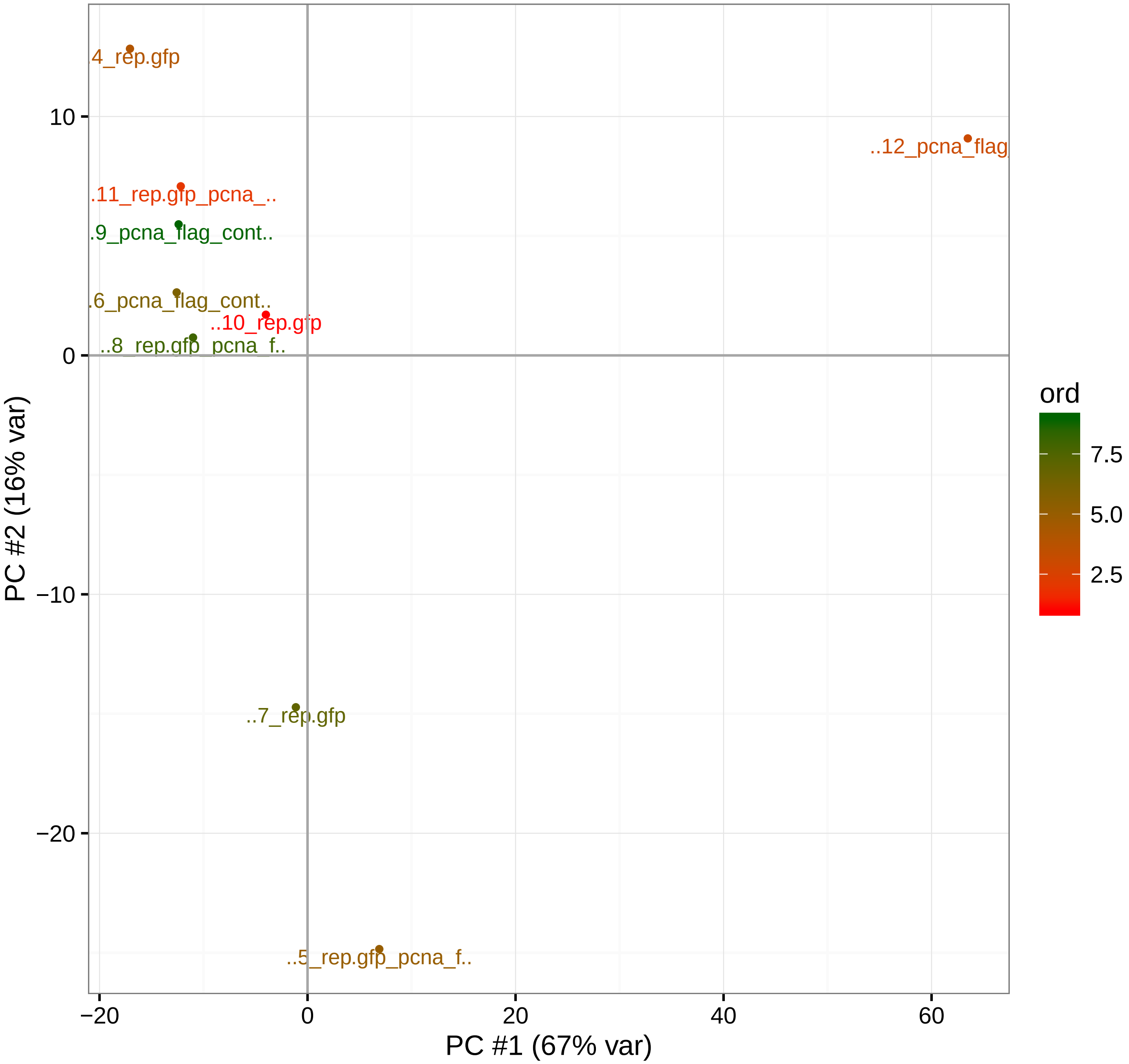
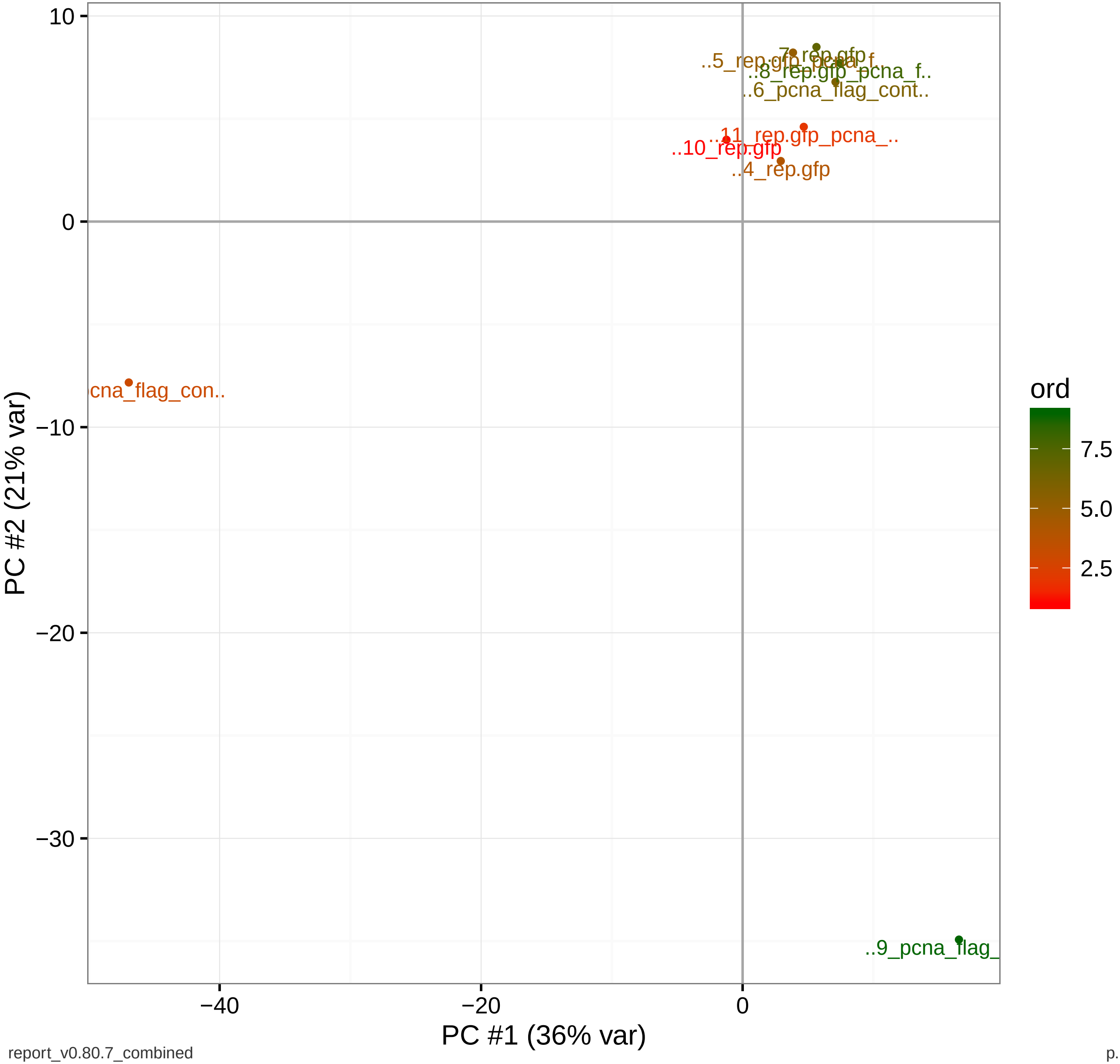
PG: PCA of 'raw intensity'

(excludes contaminants)

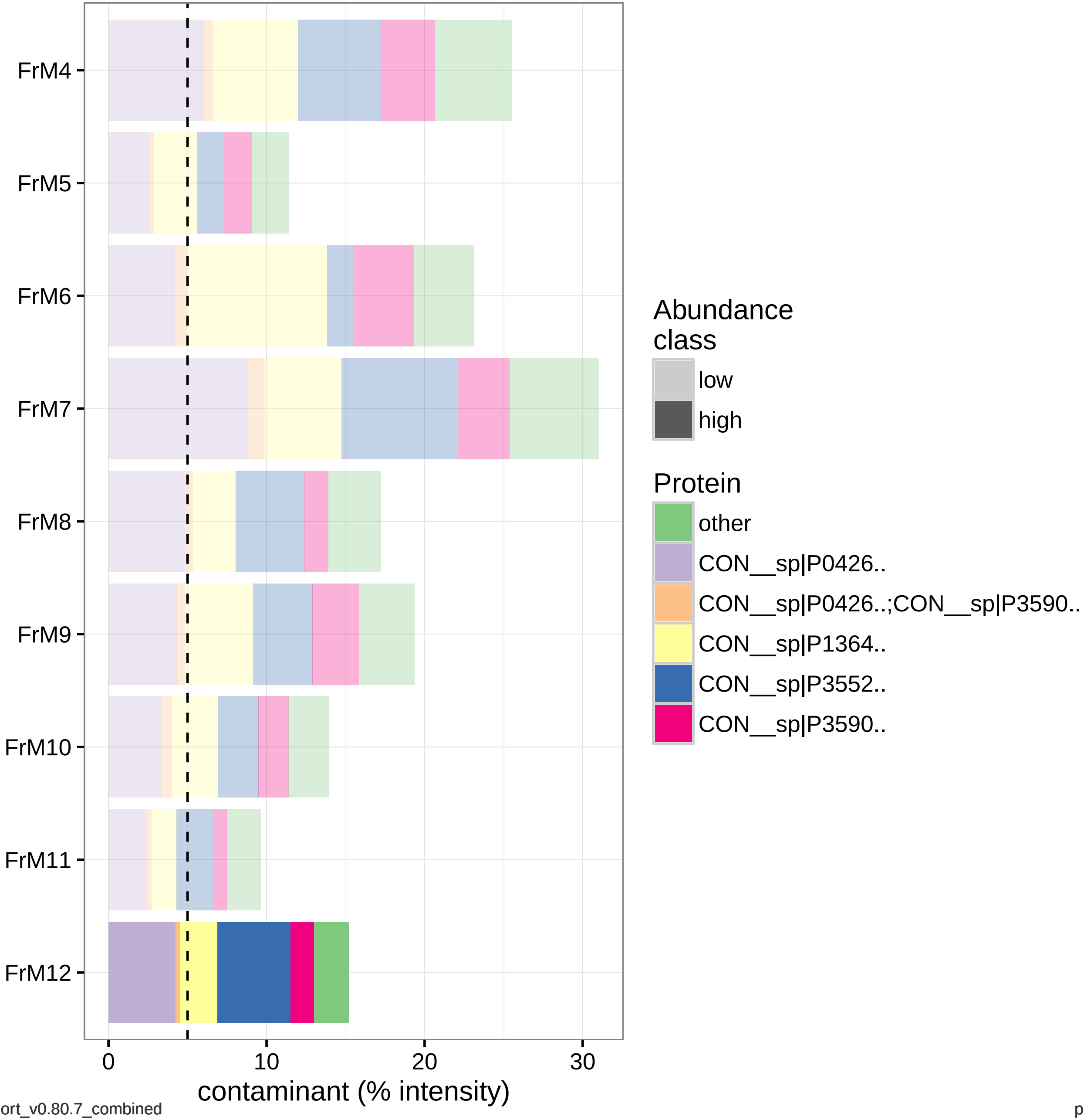


PG: PCA of 'lfq intensity'

(excludes contaminants)

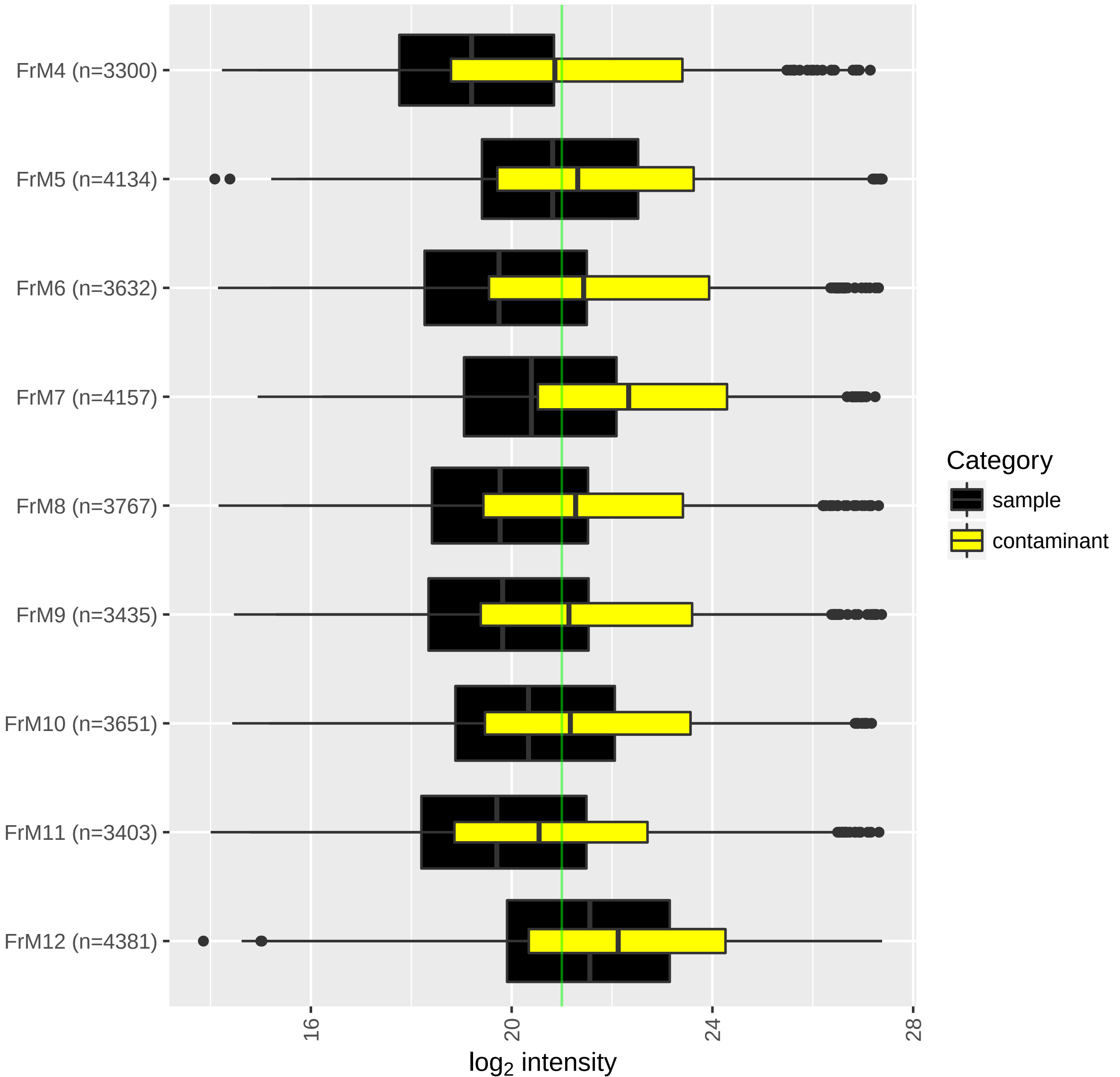


EVD: Top5 Contaminants per Raw file



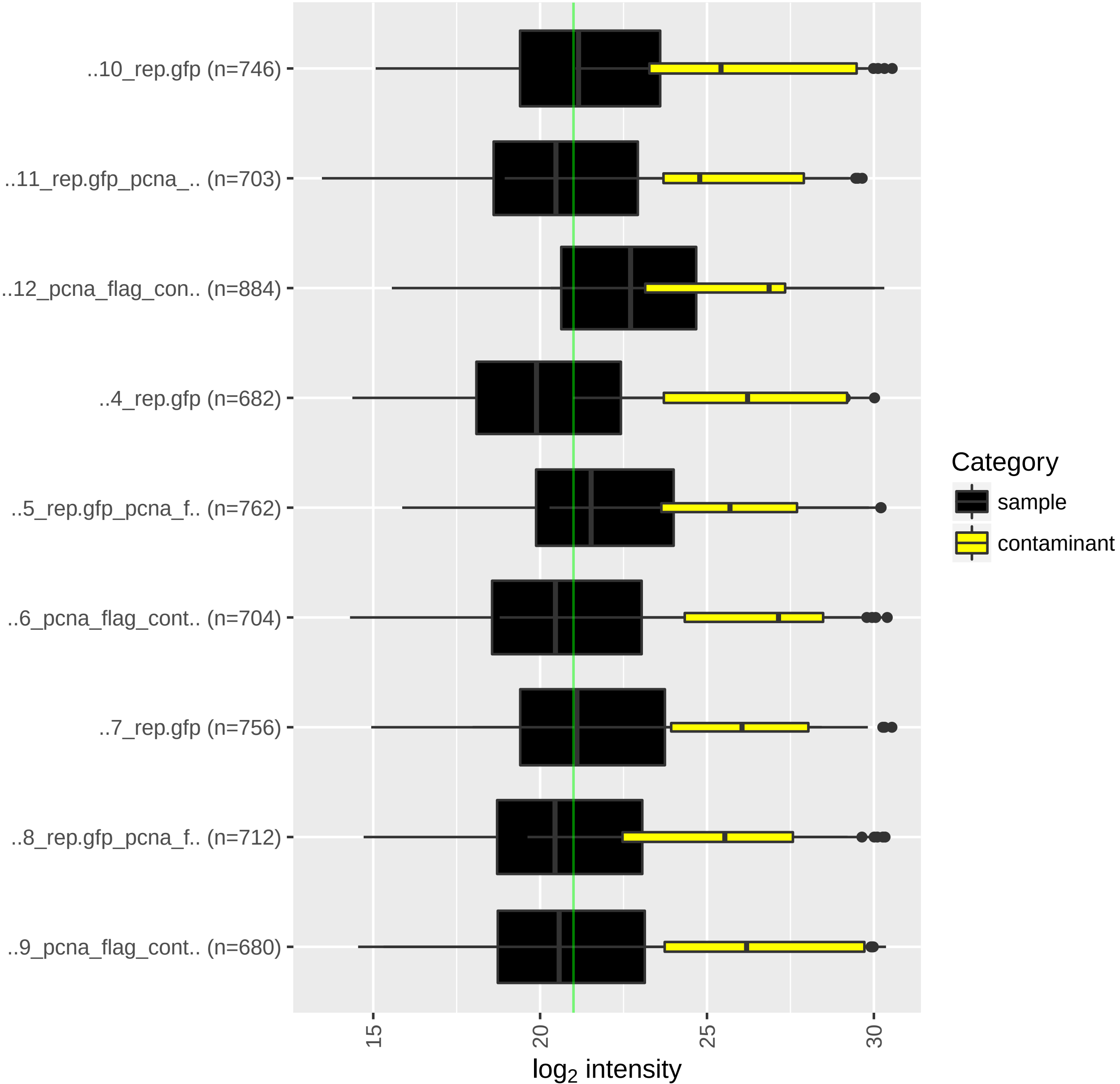
EVD: peptide intensity distribution

RSD 3.4% (expected < 5%)



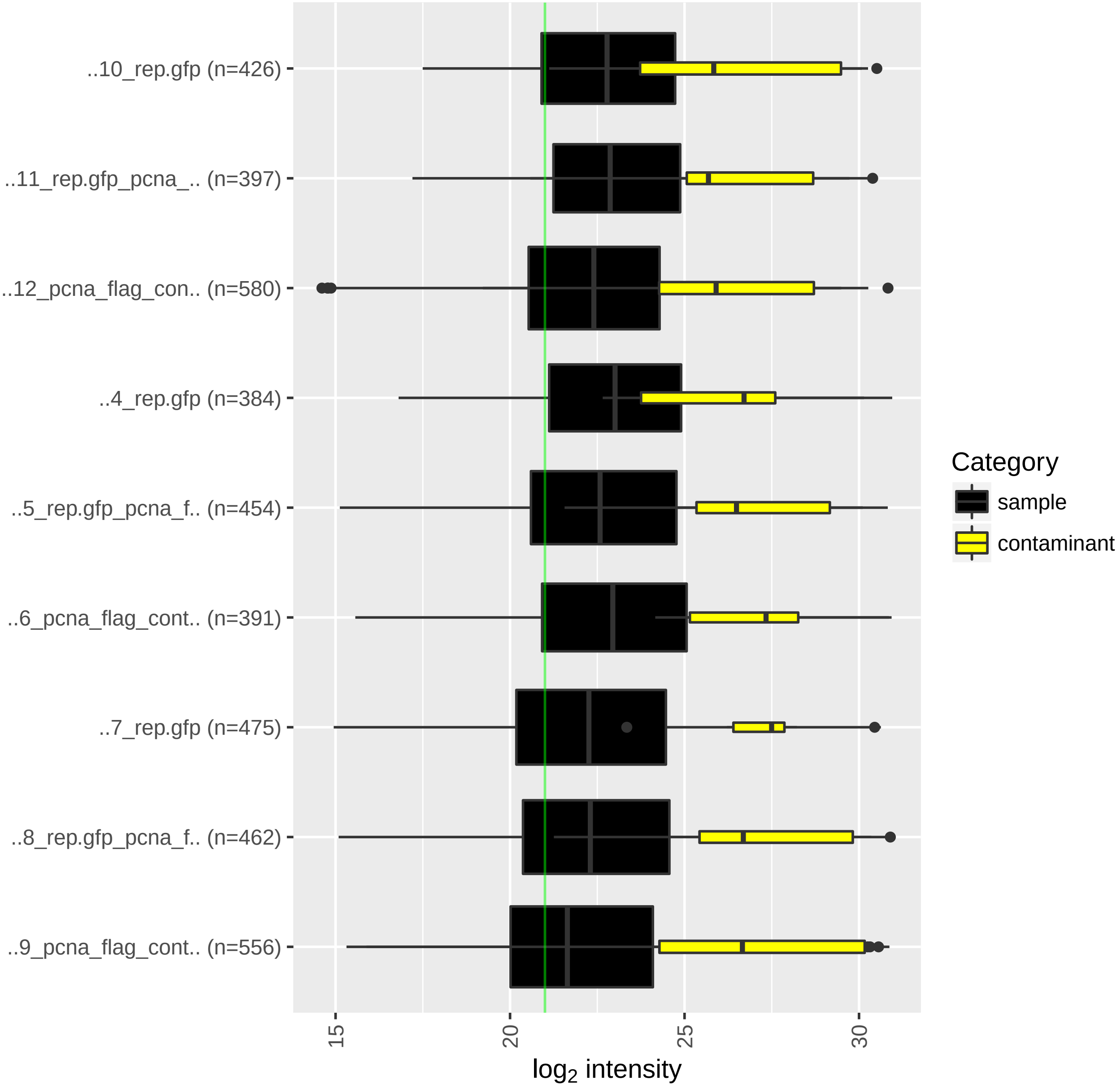
PG: intensity distribution

RSD 3.9% (w/o zero int.; expected < 5%)
RSD 6.1% [high RSD −−> few peptides])



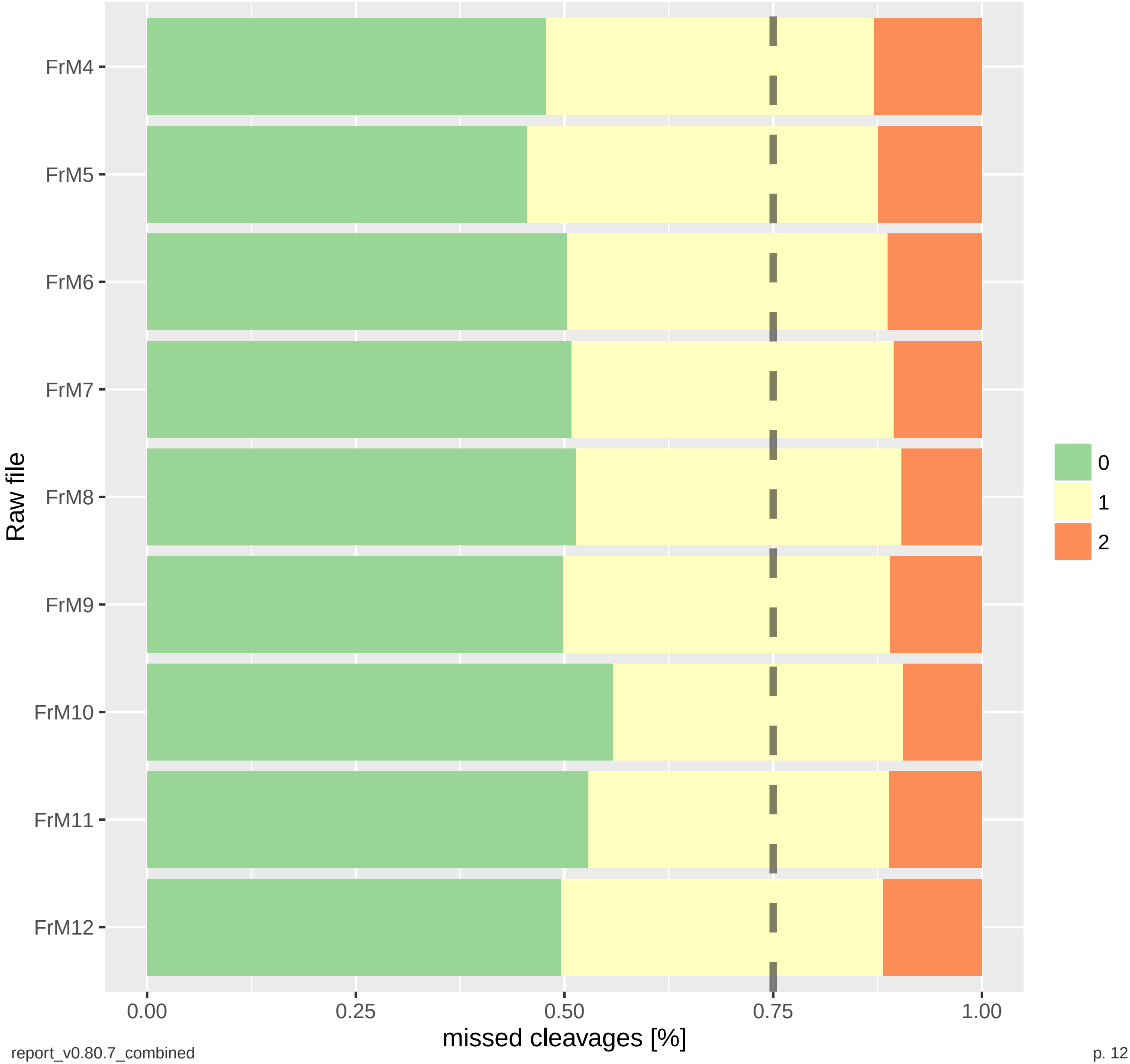
PG: LFQ intensity distribution

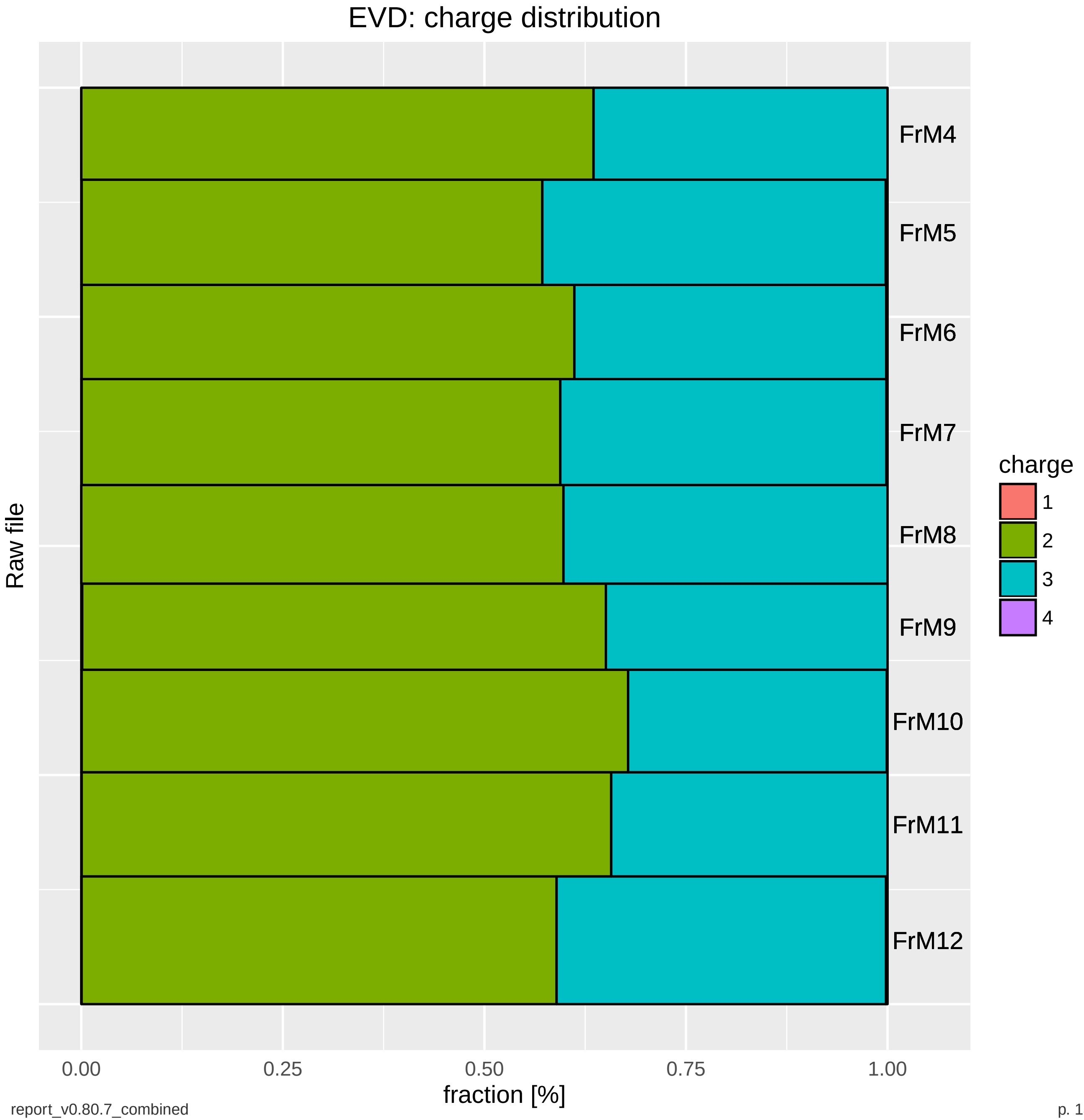
RSD 1.9% (w/o zero int.; expected < 5%)
RSD 198.5% [high RSD −−> few peptides])

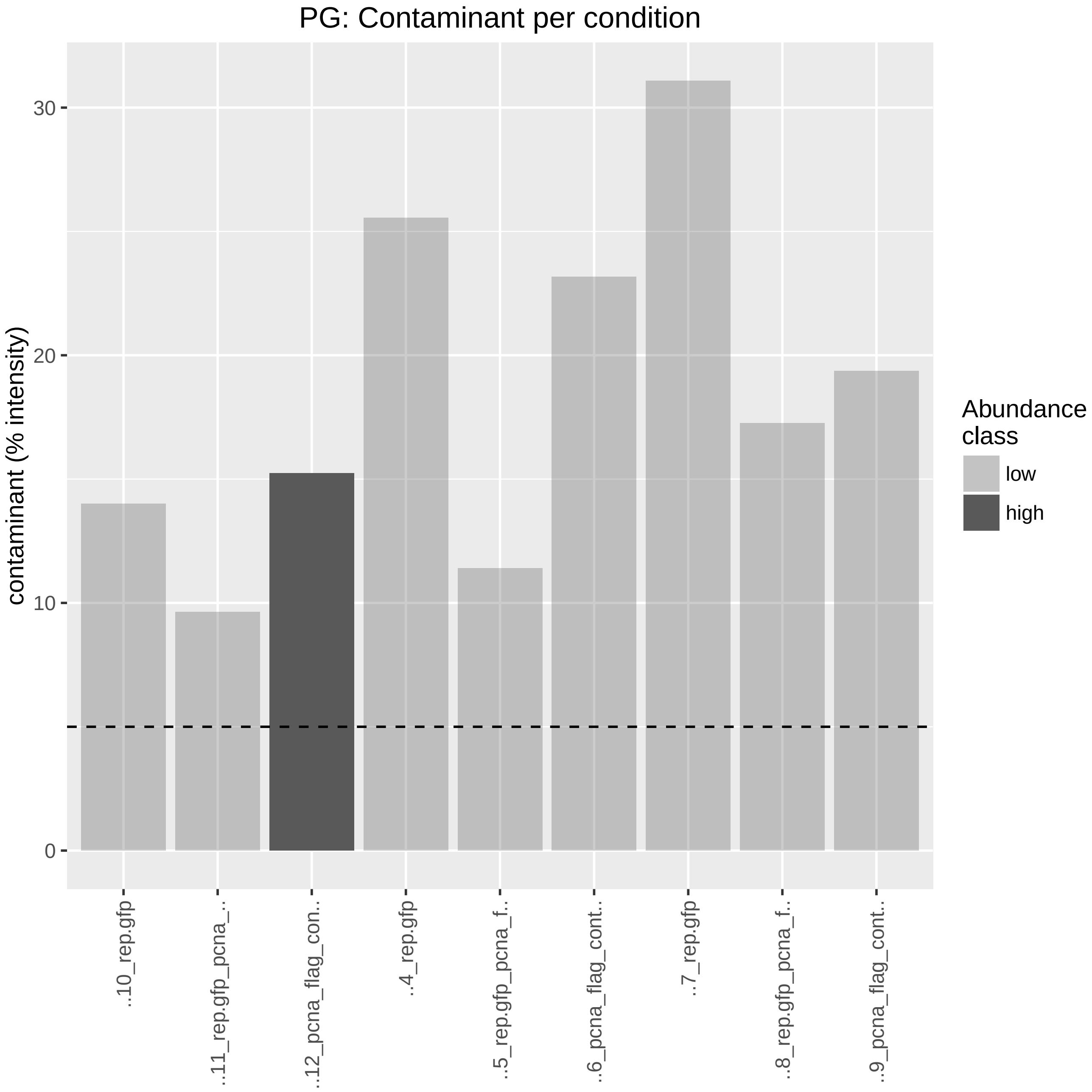


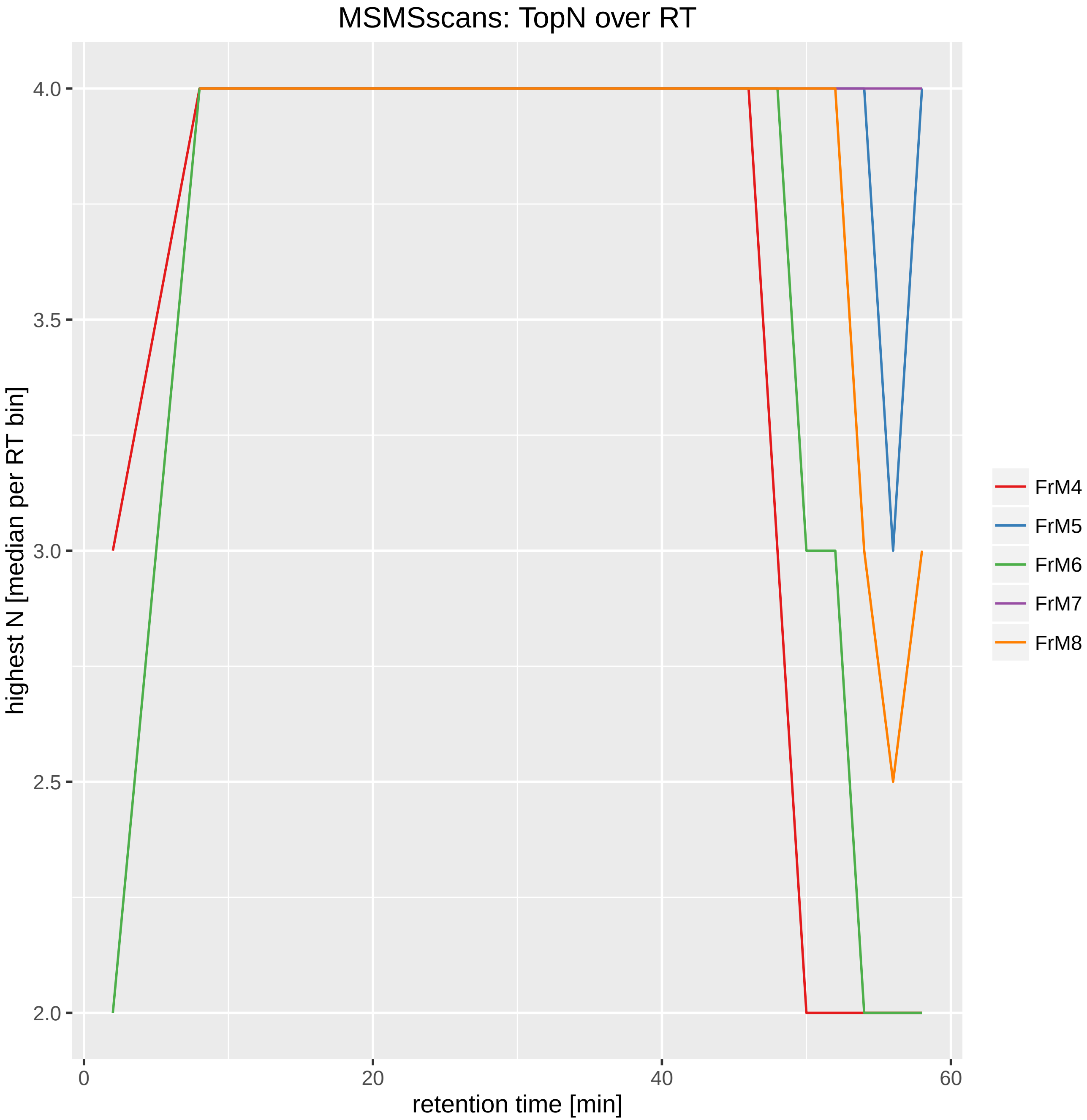
MSMS: Missed cleavages per Raw file

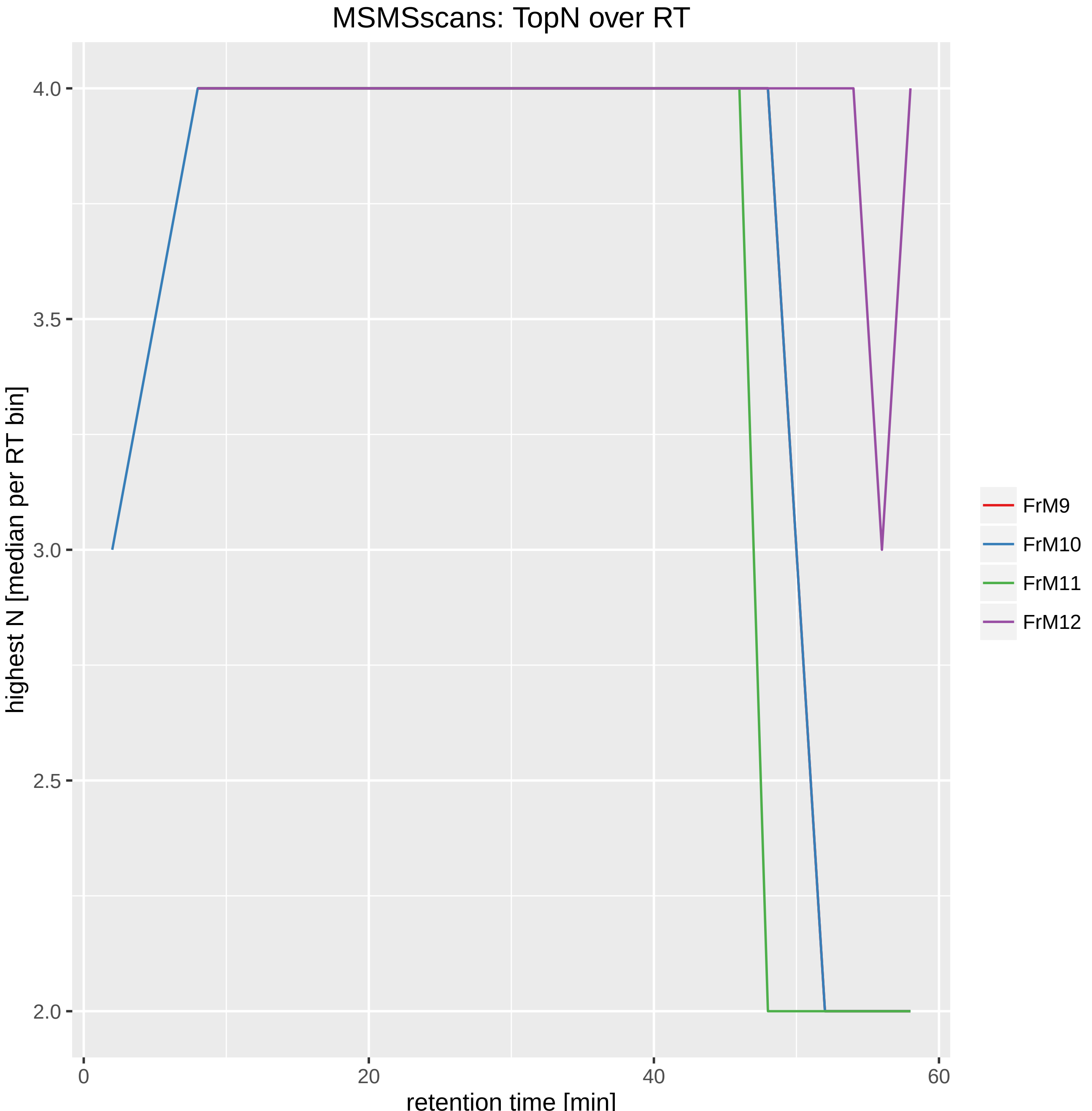
(excludes contaminants)

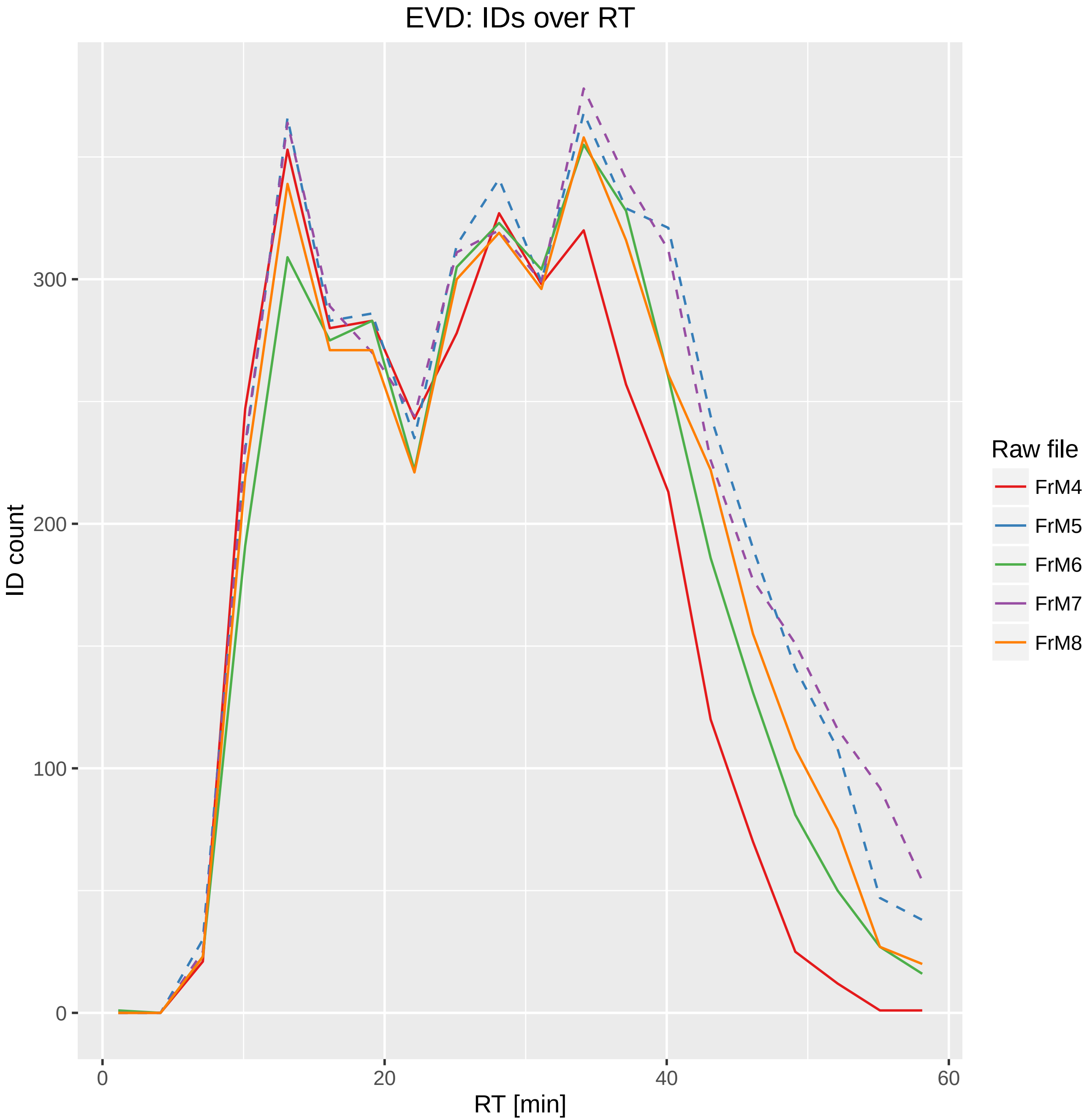


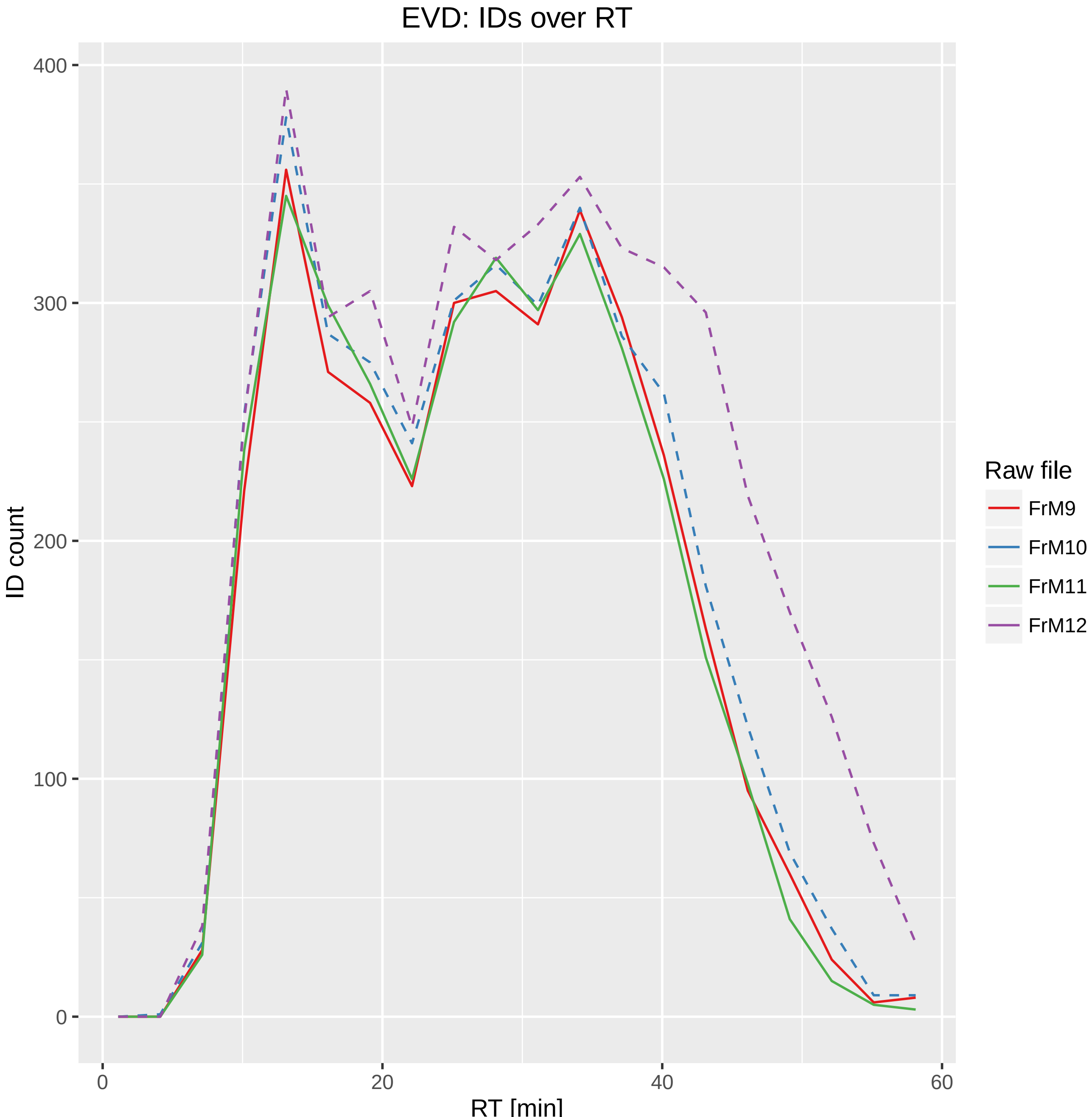

EVD: charge distribution
Raw file
fraction [%]
0.00
0.25
0.50
0.75
1.00
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
charge
1
2
3
4

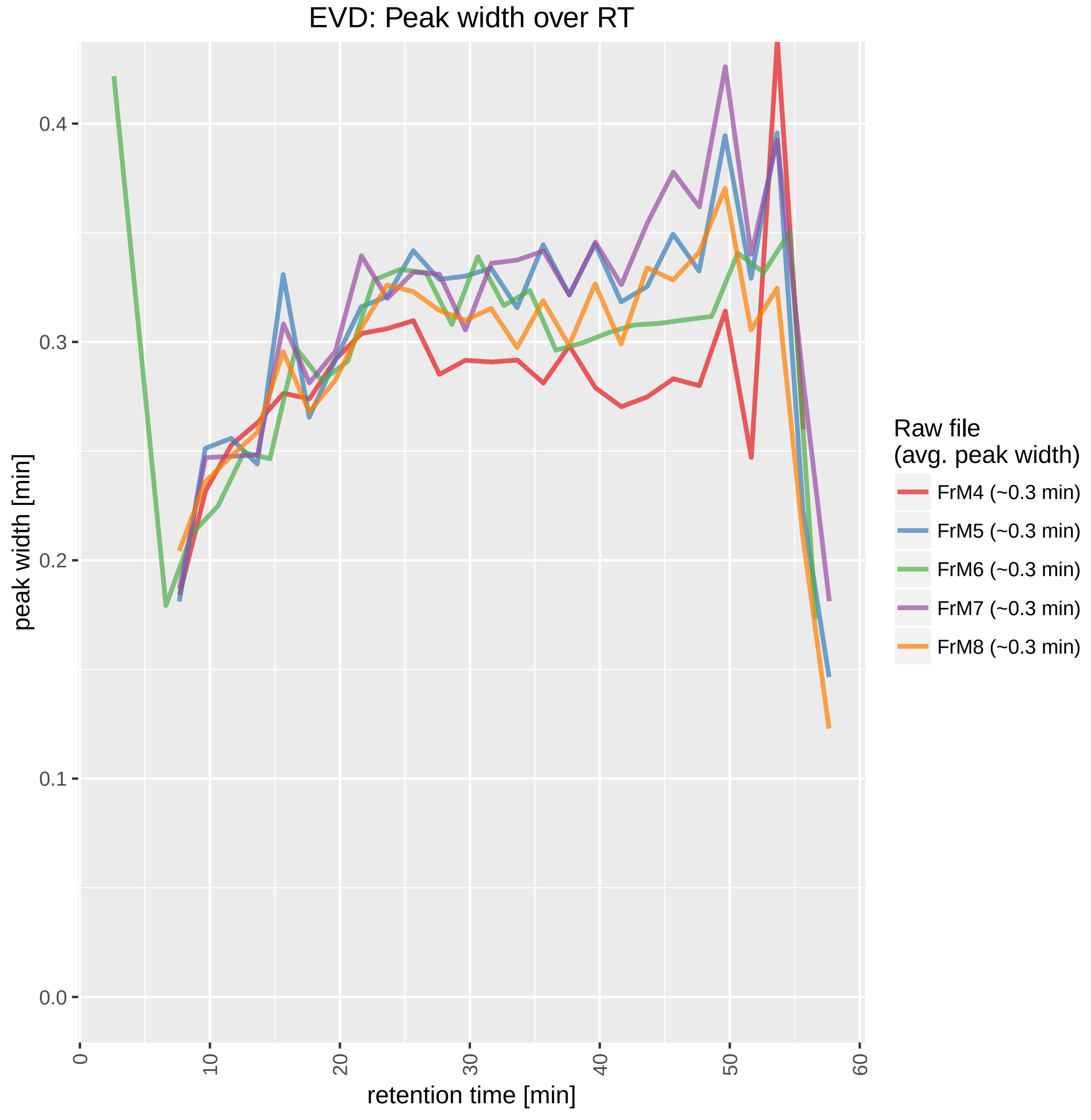

PG: Contaminant per condition
contaminant (% intensity)
0
10
20
30
..10_rep.gfp
..11_rep.gfp_pcna_..
..12_pcna_flag_con..
..4_rep.gfp
..5_rep.gfp_pcna_f..
..6_pcna_flag_cont..
..7_rep.gfp
..8_rep.gfp_pcna_f..
..9_pcna_flag_cont..
Abundance class
low
high

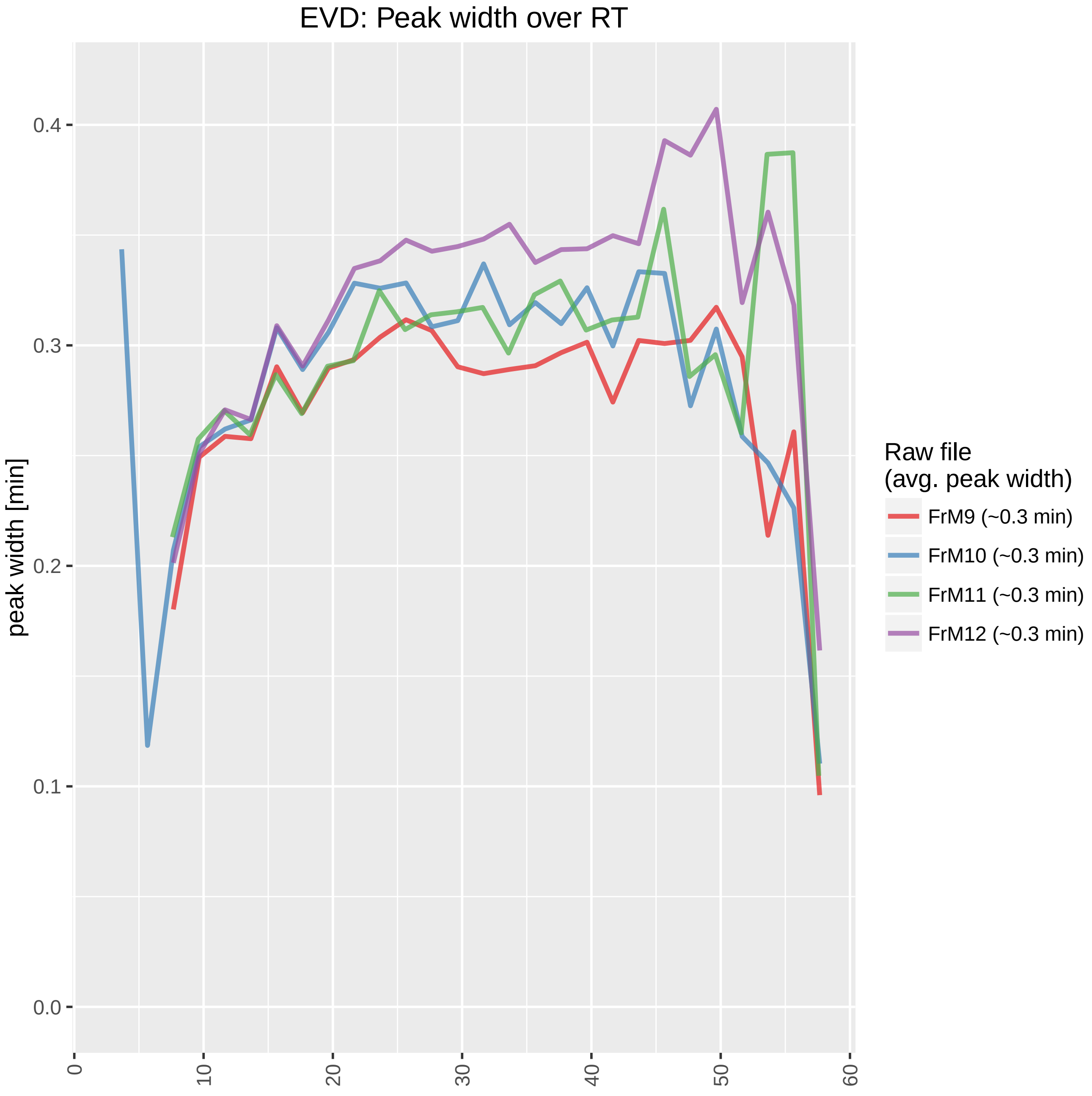

MSMSscans: TopN over RT
highest N [median per RT bin]
4.0
3.5
3.0
2.5
2.0
0
20
40
60
retention time [min]
FrM4
FrM5
FrM6
FrM7
FrM8


MSMSscans: TopN over RT
highest N [median per RT bin]
4.0
3.5
3.0
2.5
2.0
0
20
40
60
retention time [min]
FrM9
FrM10
FrM11
FrM12


EVD: IDs over RT
ID count
300
200
100
0
0
20
40
60
RT [min]
Raw file
FrM4
FrM5
FrM6
FrM7
FrM8

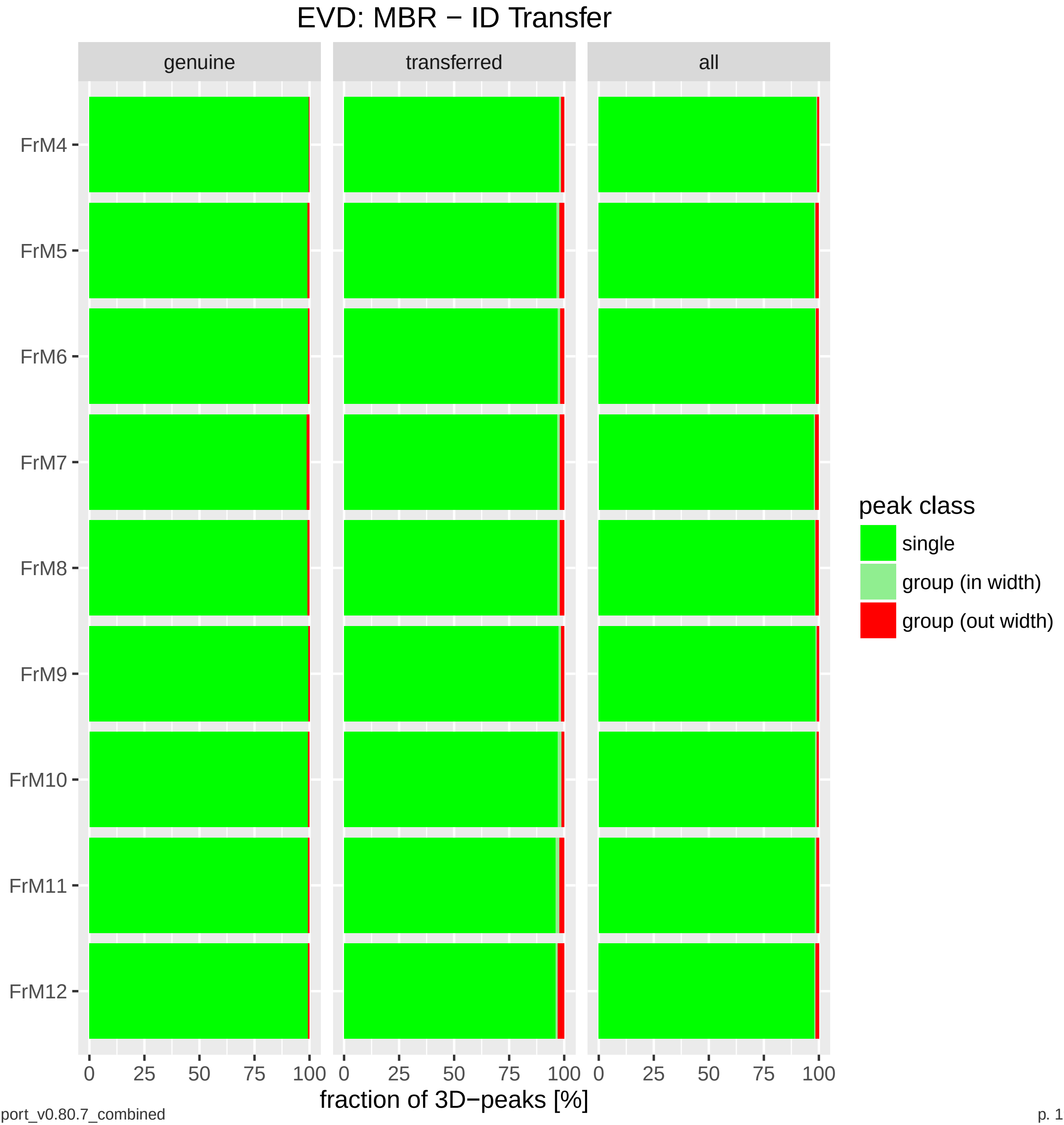

EVD: IDs over RT
ID count
400
300
200
100
0
0
20
40
60
RT [min]
Raw file
FrM9
FrM10
FrM11
FrM12


EVD: Peak width over RT
peak width [min]
0.0
0.1
0.2
0.3
0.4
retention time [min]
0
10
20
30
40
50
60
Raw file
(avg. peak width)
FrM4 (~0.3 min)
FrM5 (~0.3 min)
FrM6 (~0.3 min)
FrM7 (~0.3 min)
FrM8 (~0.3 min)


EVD: Peak width over RT
peak width [min]
0.0
0.1
0.2
0.3
0.4
retention time [min]
0
10
20
30
40
50
60
Raw file
(avg. peak width)
FrM9 (~0.3 min)
FrM10 (~0.3 min)
FrM11 (~0.3 min)
FrM12 (~0.3 min)

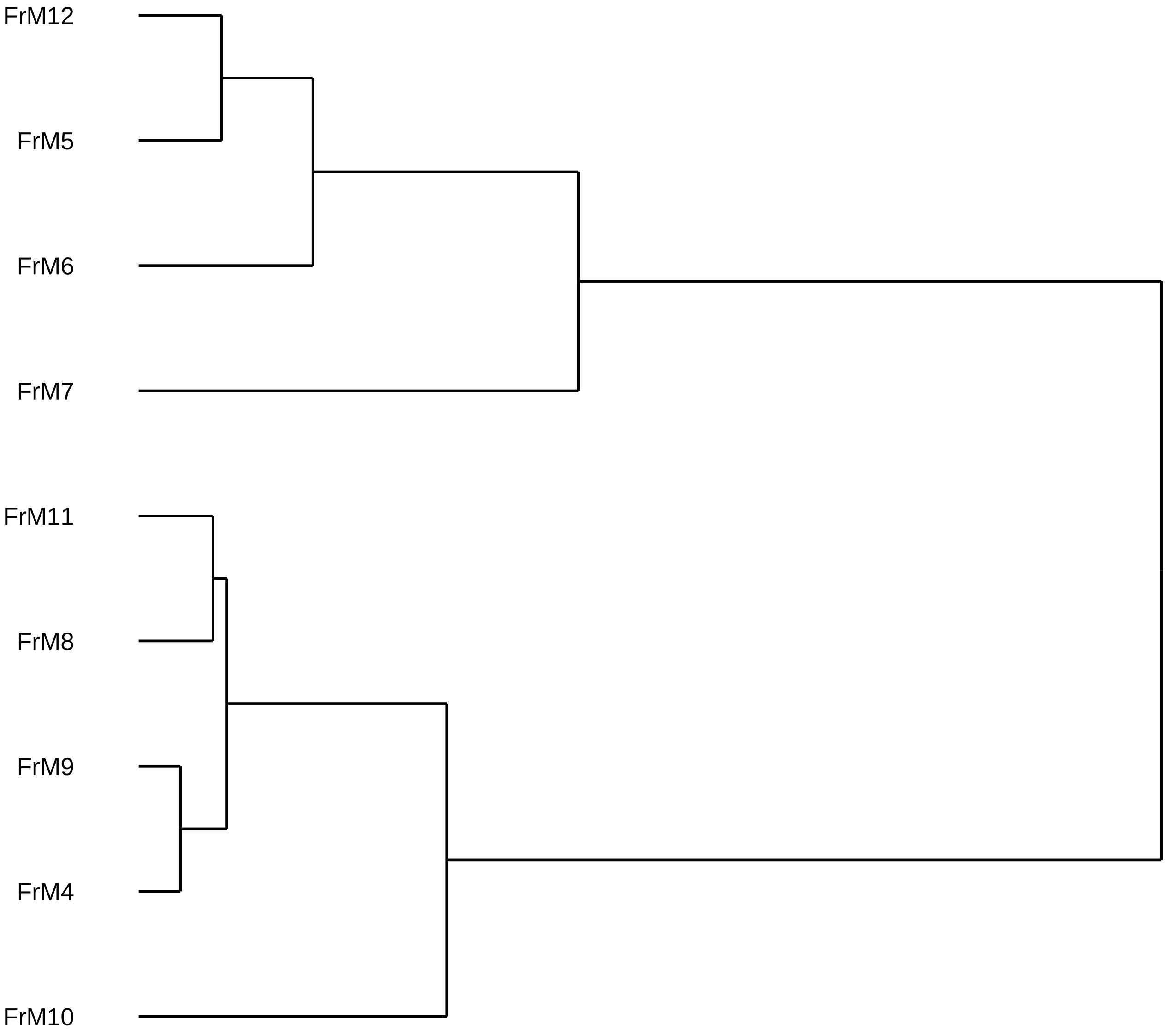
EVD: Alignment check

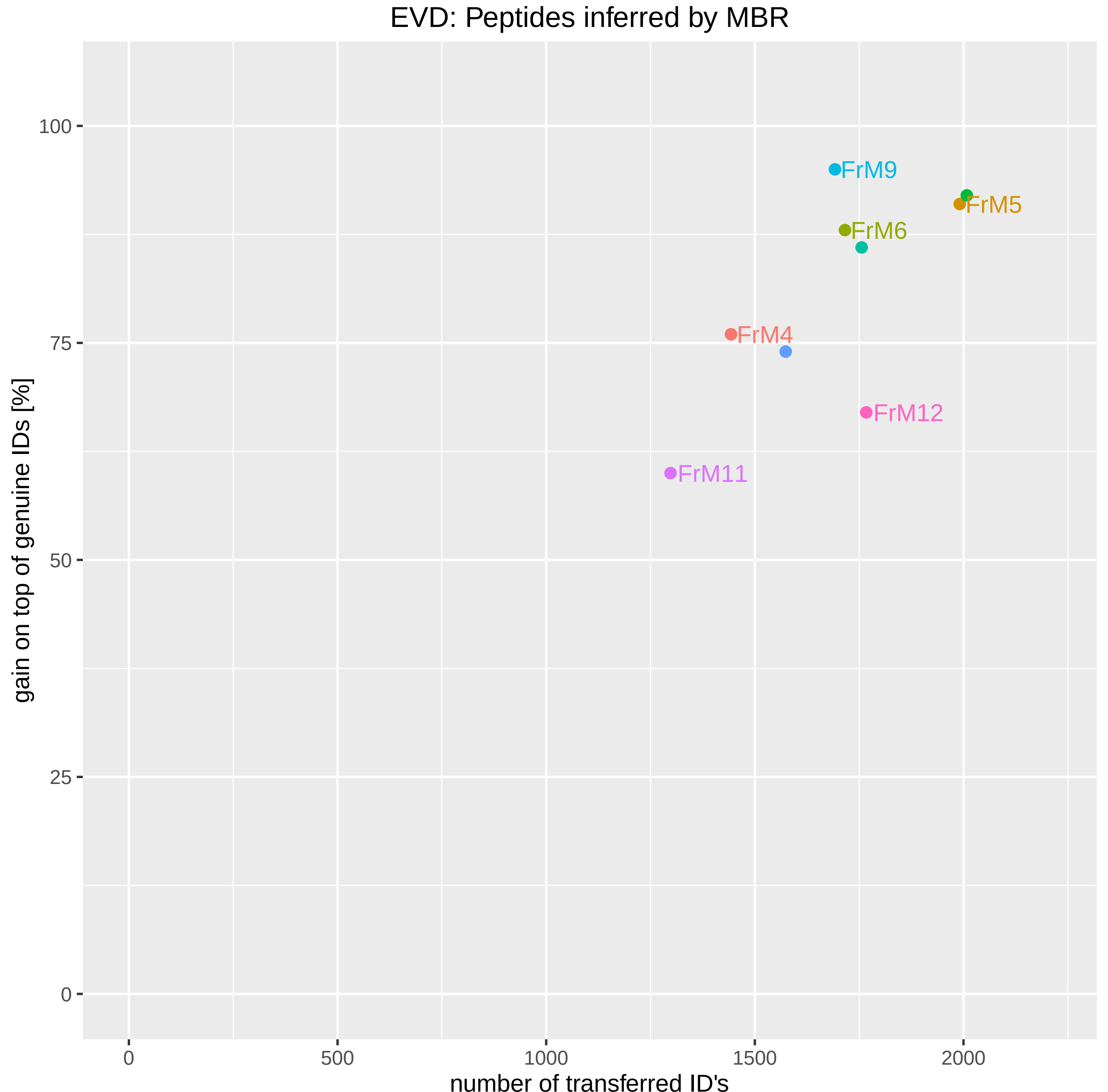
nd a unique reference Raw file (files: FrM10_Rep−GFP, FrM6_PCNA_FLAG

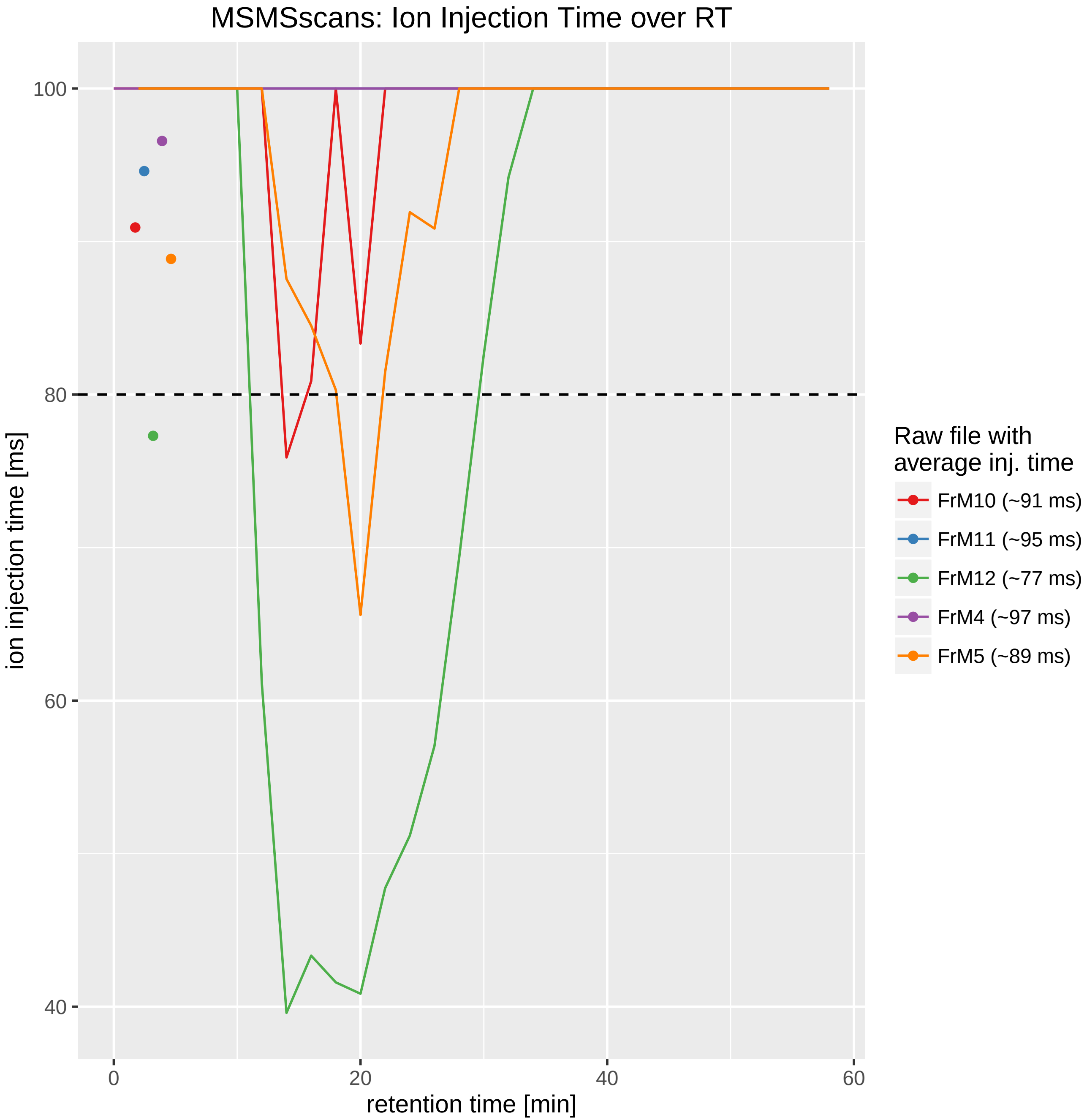

EVD: MBR − ID Transfer
genuine
transferred
all
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
0
25
50
75
100
fraction of 3D−peaks [%]
peak class
single
group (in width)
group (out width)

[experimental] EVD: Clustering Tree of Raw files

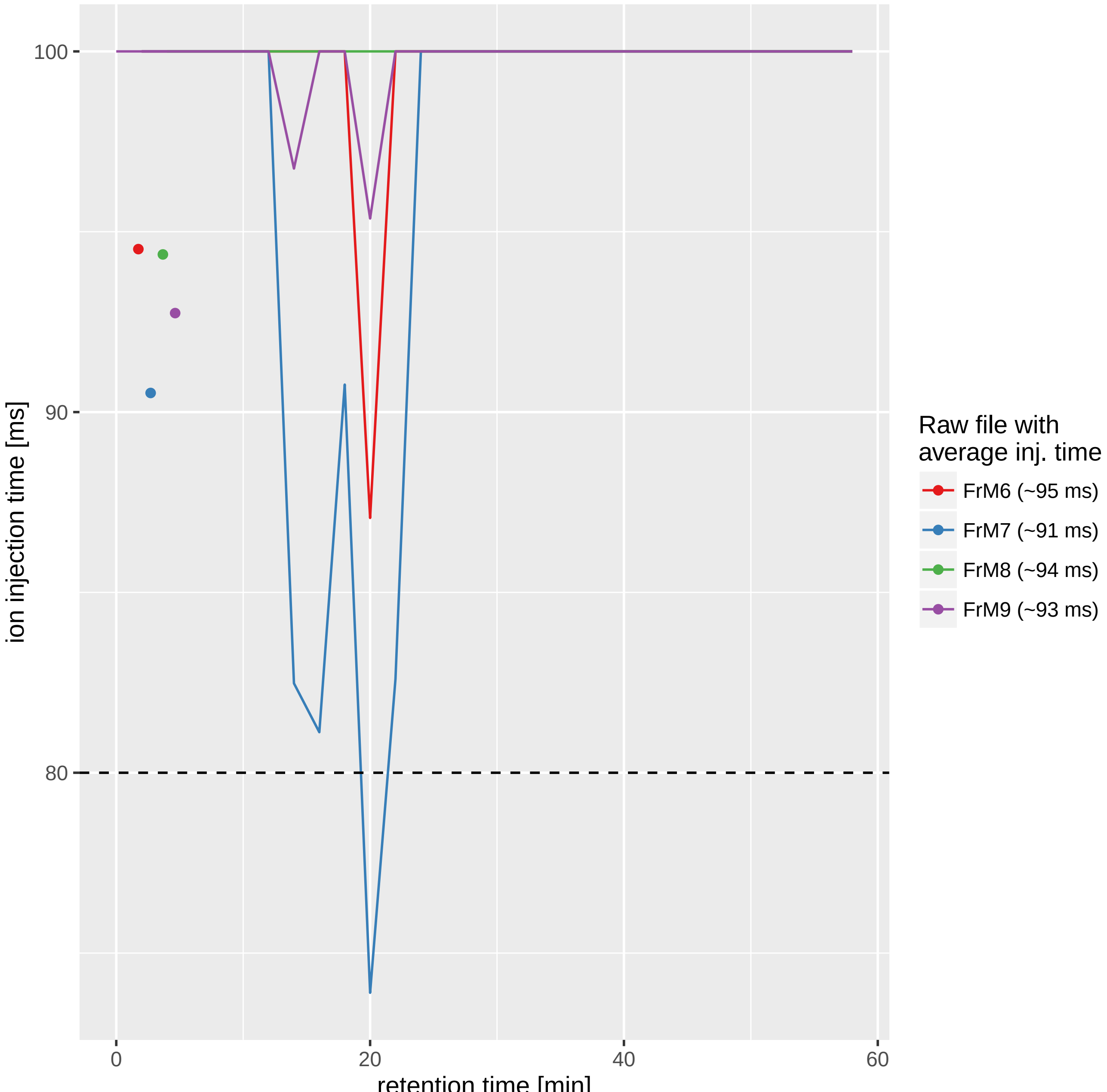
by Correlation of Corrected Retention Times

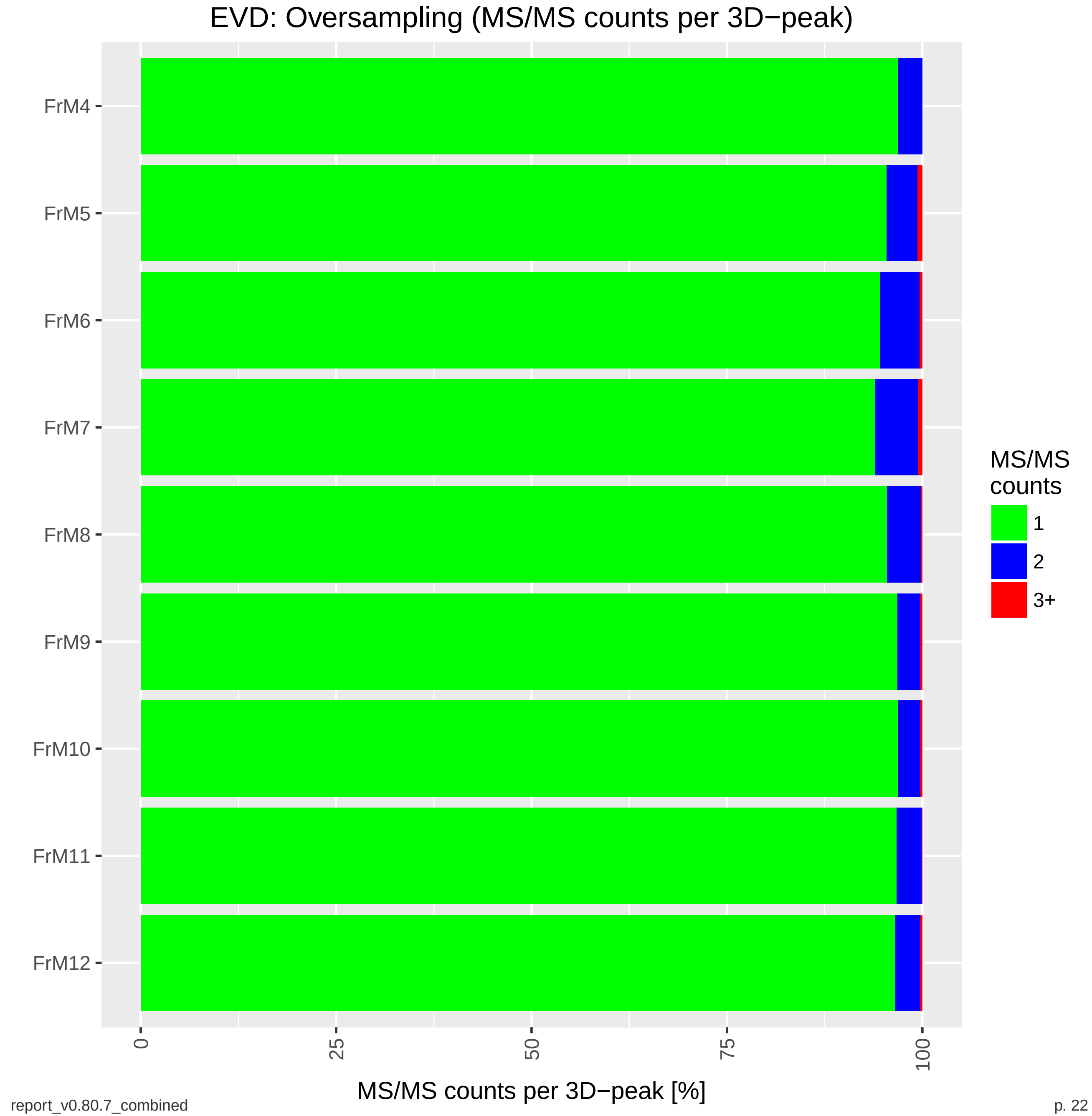



EVD: Peptides inferred by MBR
FrM9
FrM5
FrM6
FrM4
FrM12
FrM11
100
75
50
25
0
0
500
1000
1500
2000
gain on top of genuine IDs [%]
number of transferred ID's

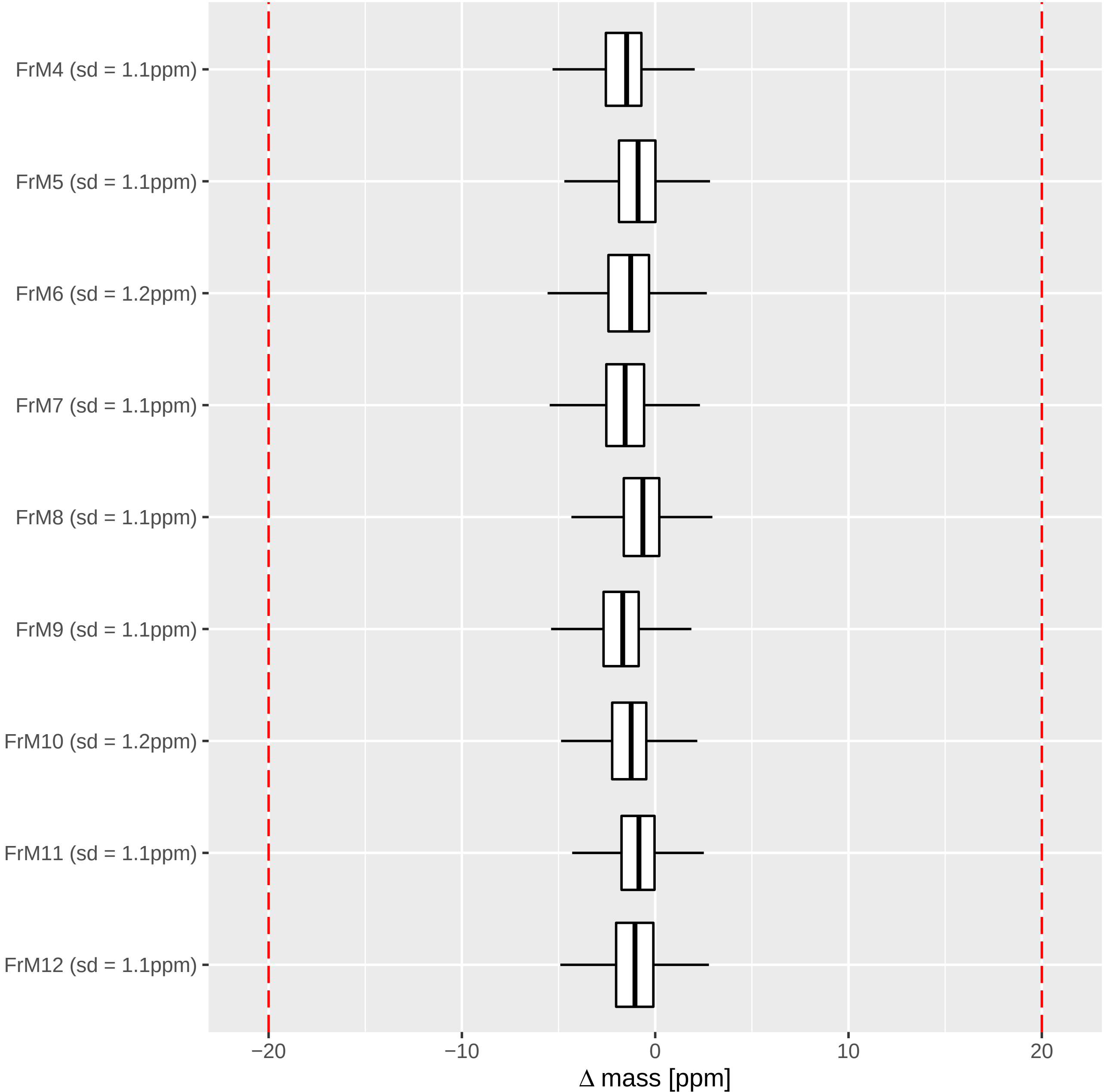

MSMSscans: Ion Injection Time over RT
100
80
60
40
0
20
40
60
ion injection time [ms]
retention time [min]
Raw file with
average inj. time
FrM10 (~91 ms)
FrM11 (~95 ms)
FrM12 (~77 ms)
FrM4 (~97 ms)
FrM5 (~89 ms)

MSMSscans: Ion Injection Time over RT

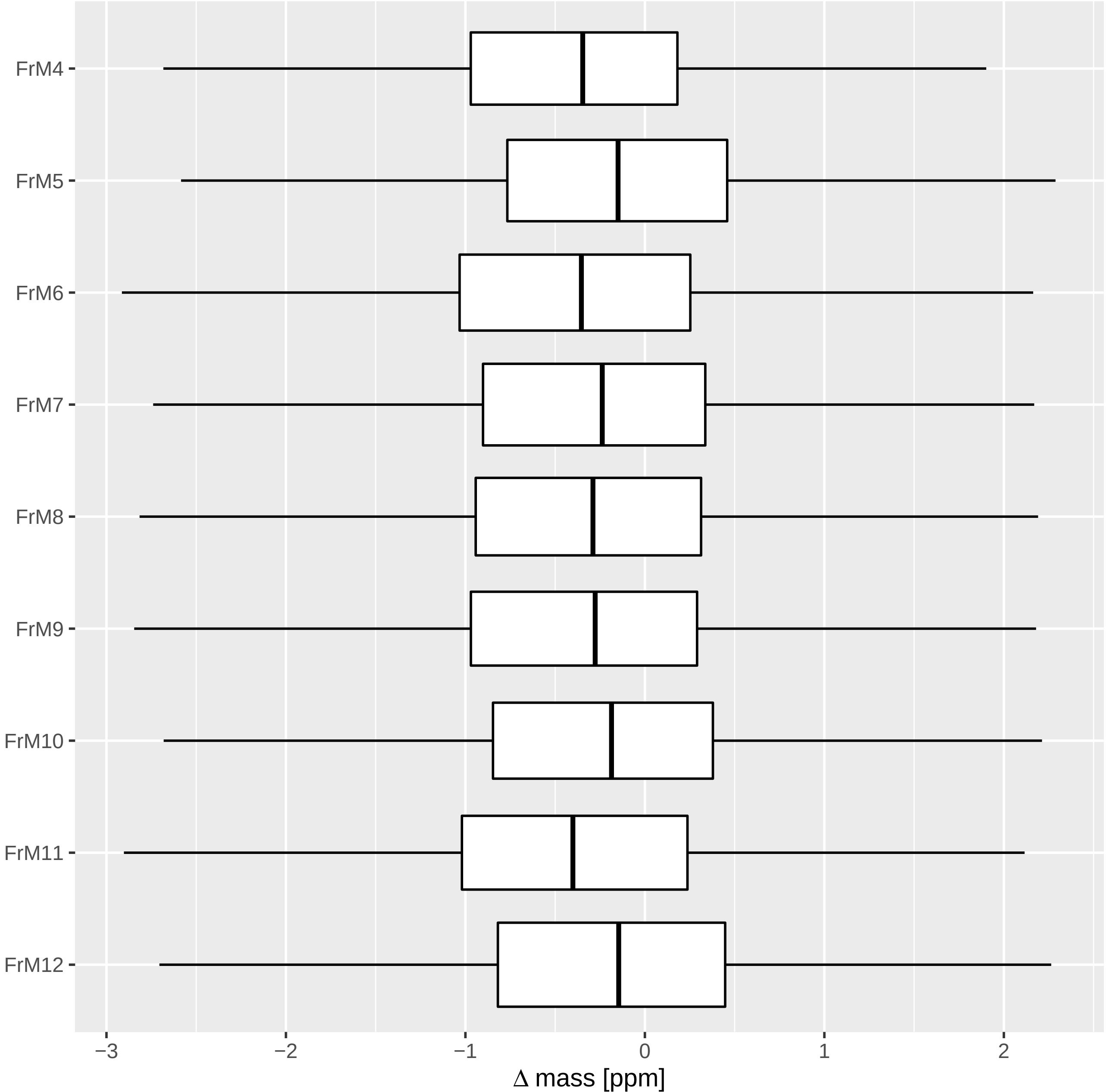



EVD: Oversampling (MS/MS counts per 3D−peak)
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
0
25
50
75
100
MS/MS counts per 3D−peak [%]
MS/MS counts
1
2
3+

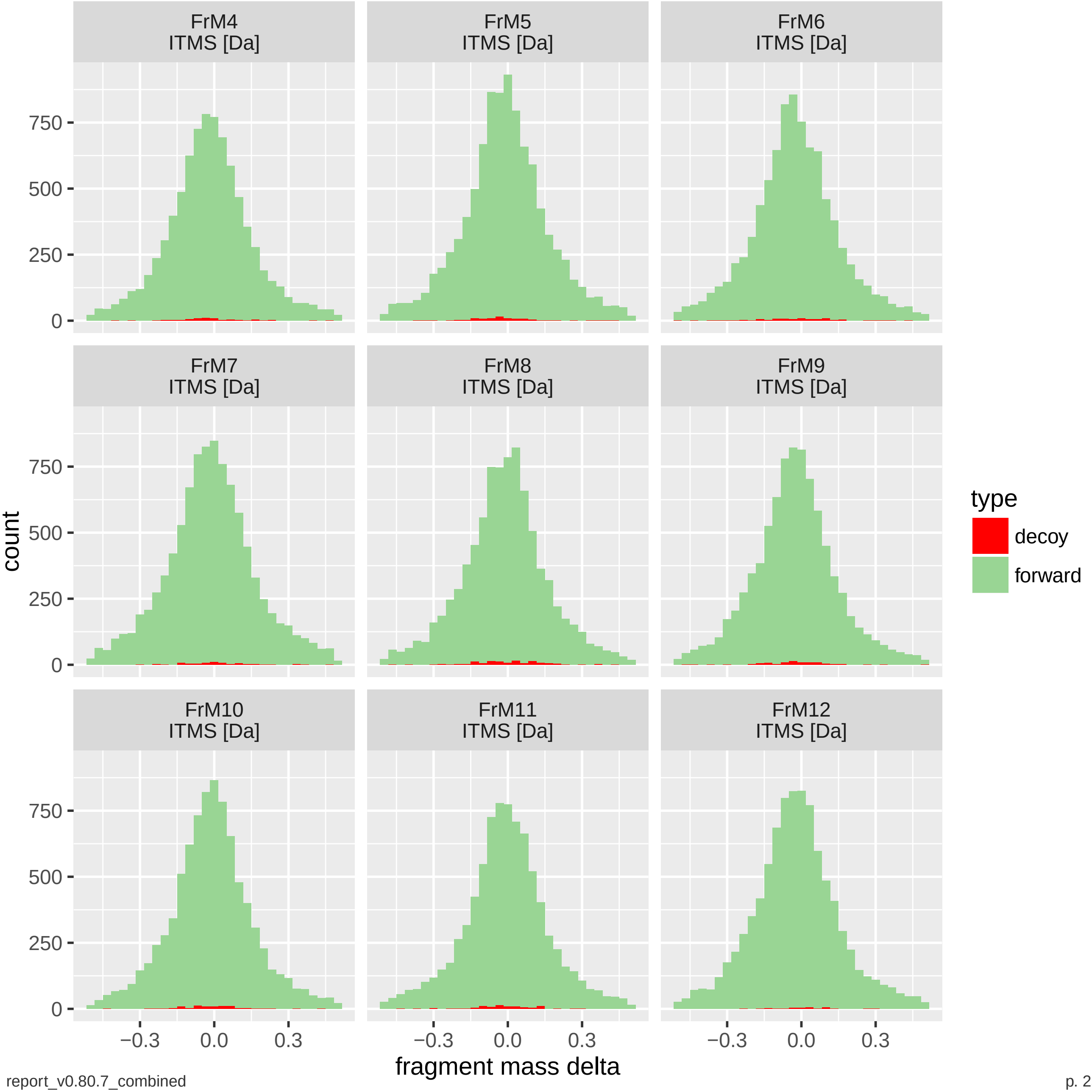
EVD: Uncalibrated mass error

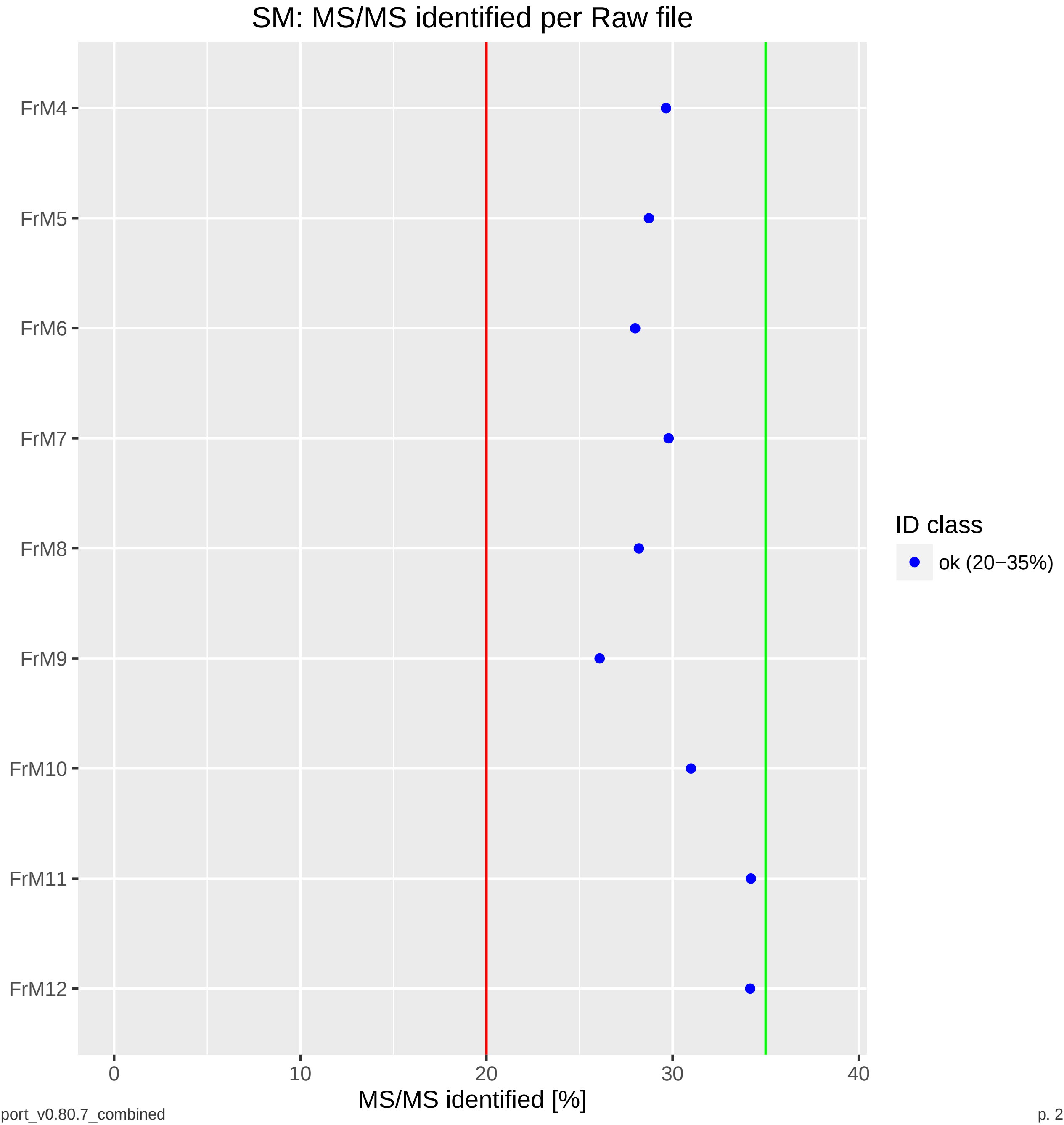


EVD: Calibrated mass error

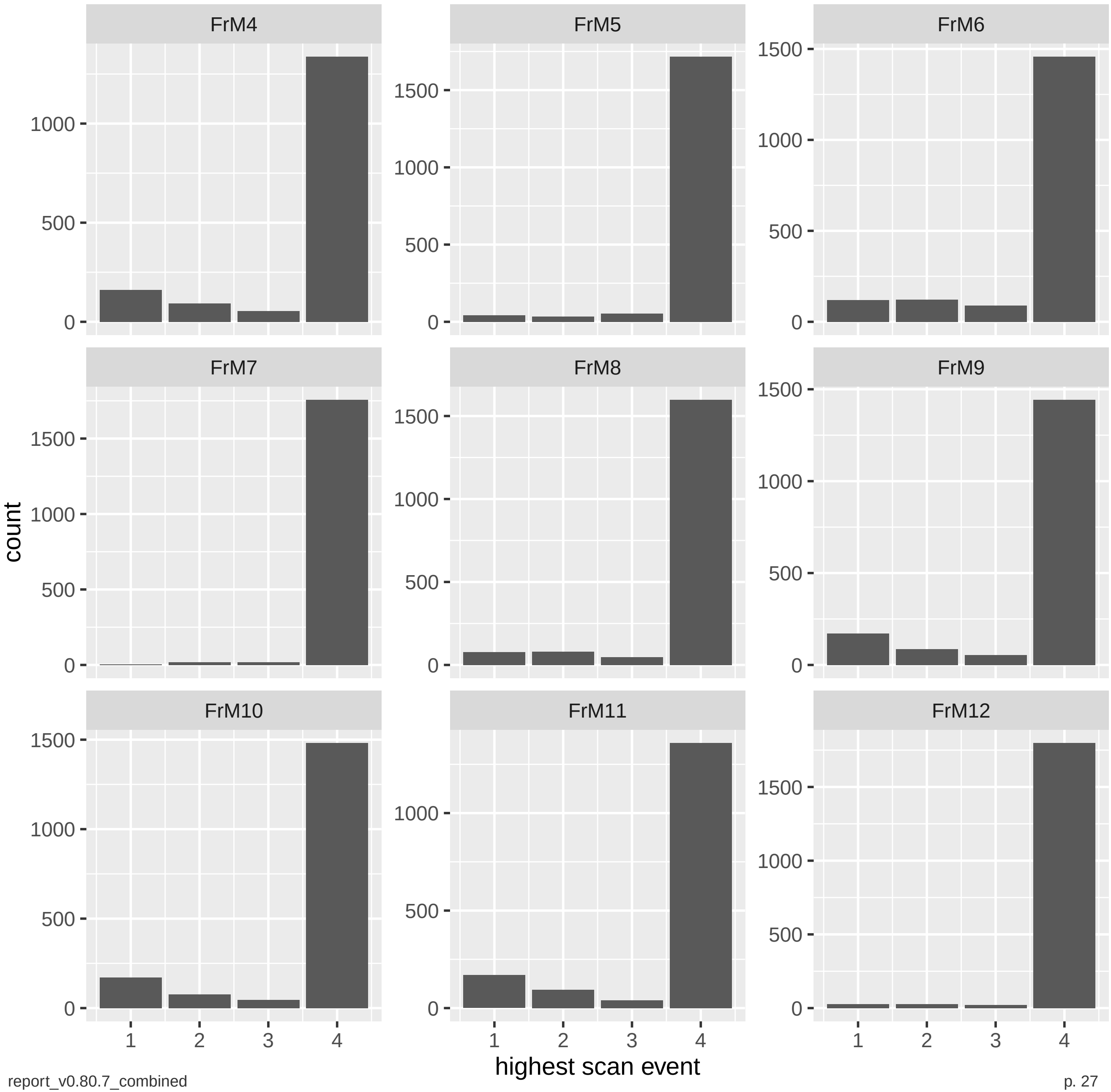


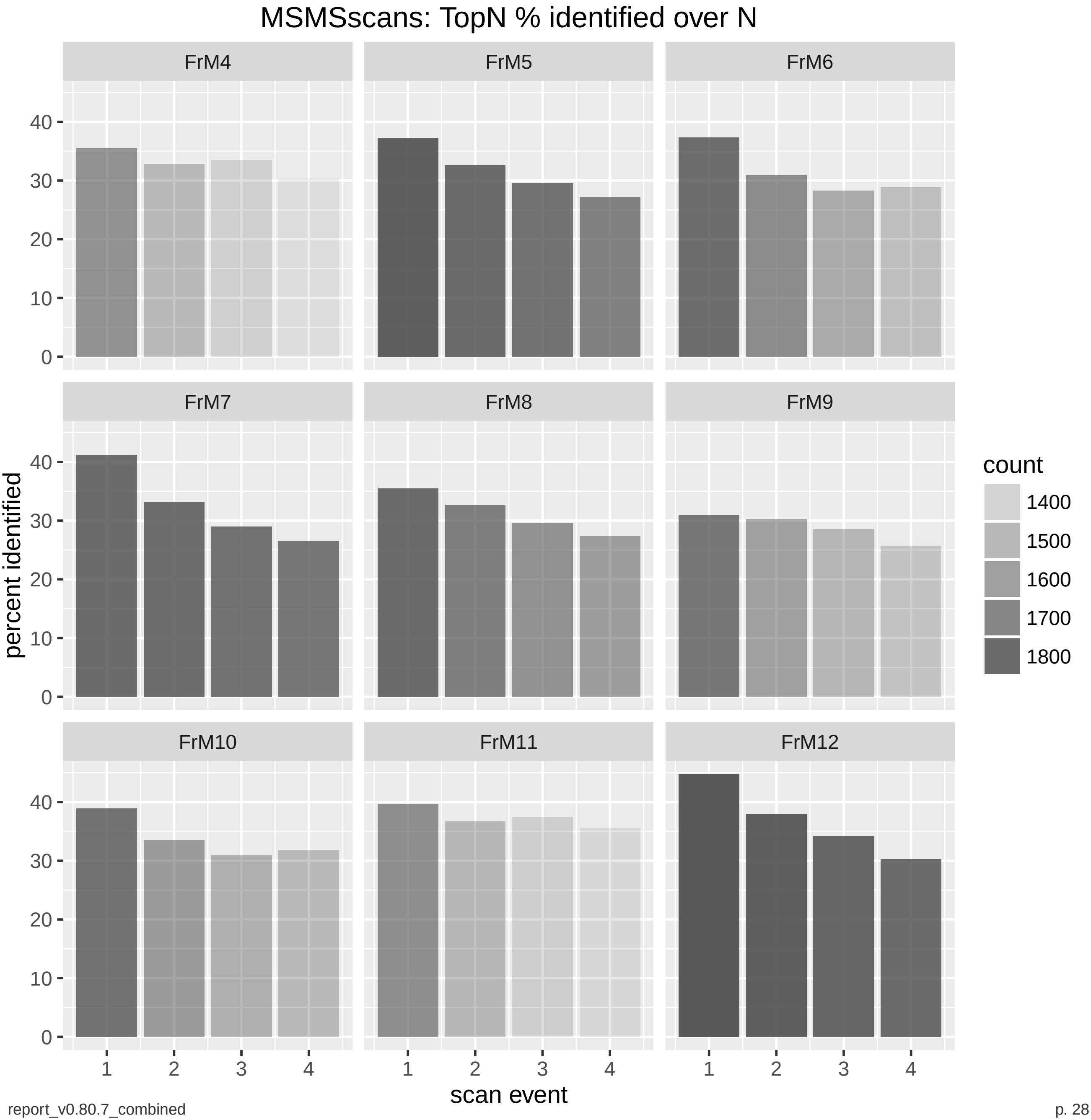
MSMS: Fragment mass errors per Raw file

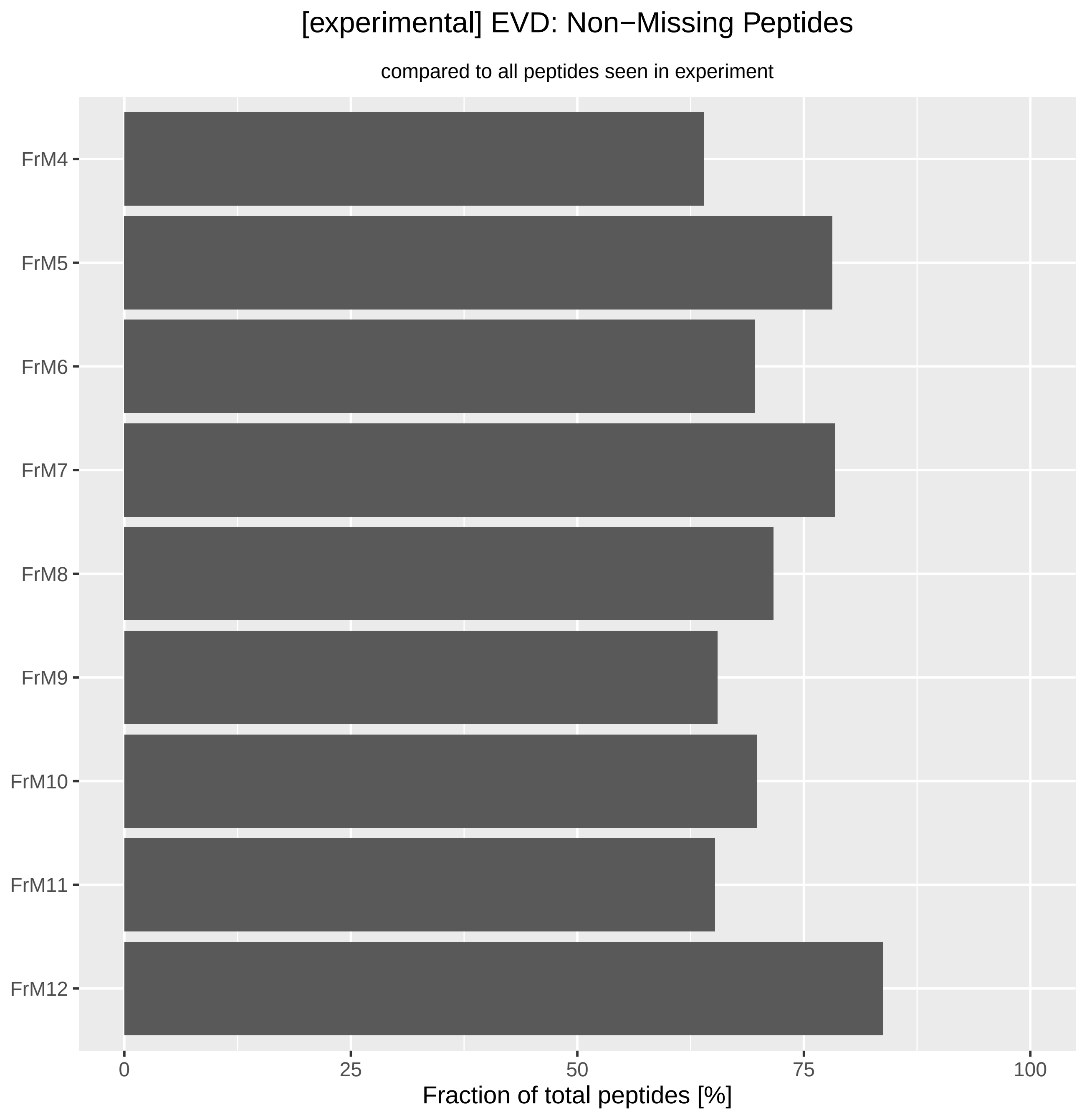


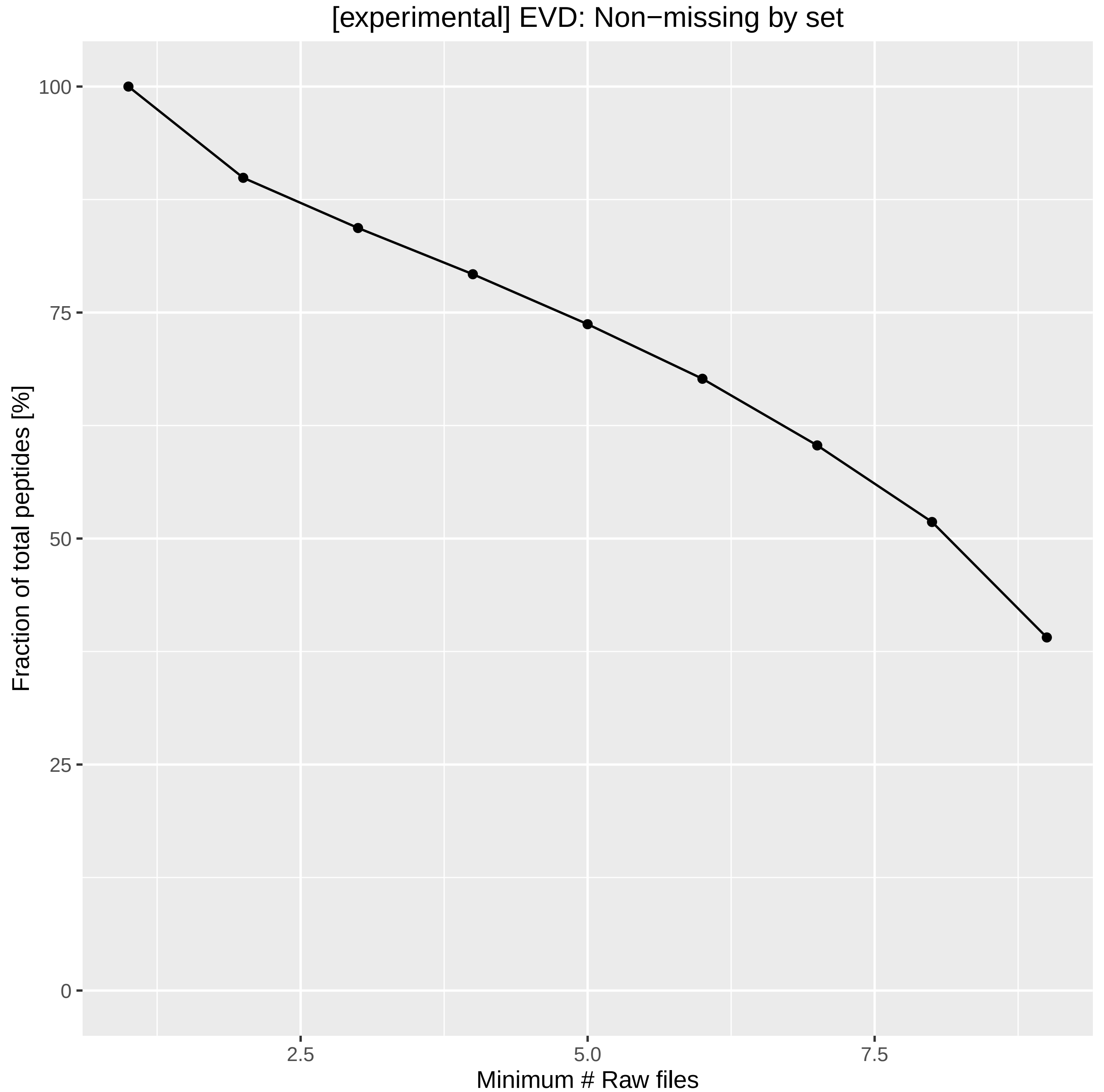

SM: MS/MS identified per Raw file
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
0
10
20
30
40
MS/MS identified [%]
ID class
● ok (20−35%)

MSMSscans: TopN

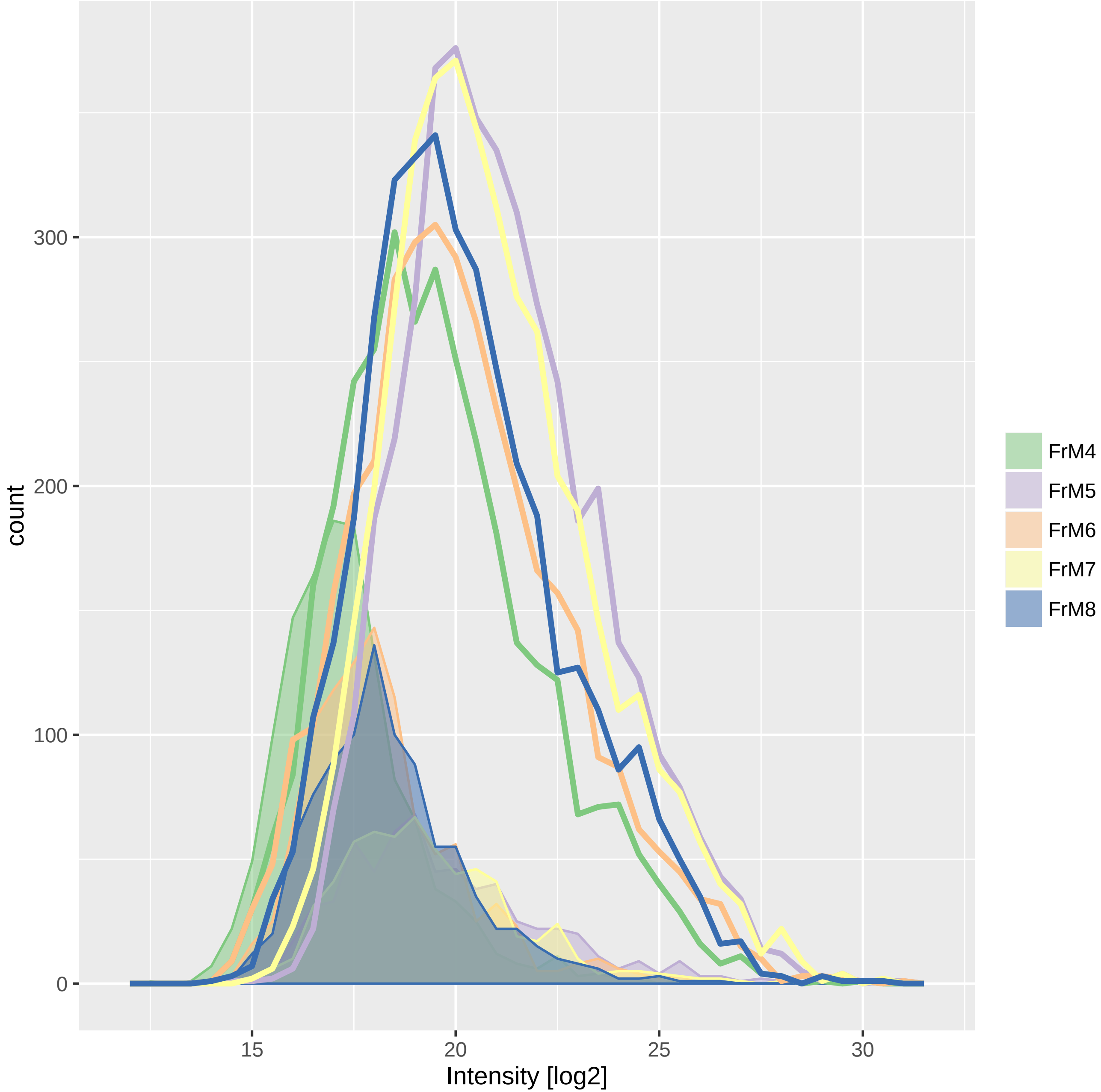



MSMSscans: TopN % identified over N
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
percent identified
0
10
20
30
40
scan event
1
2
3
4
count
1400
1500
1600
1700
1800

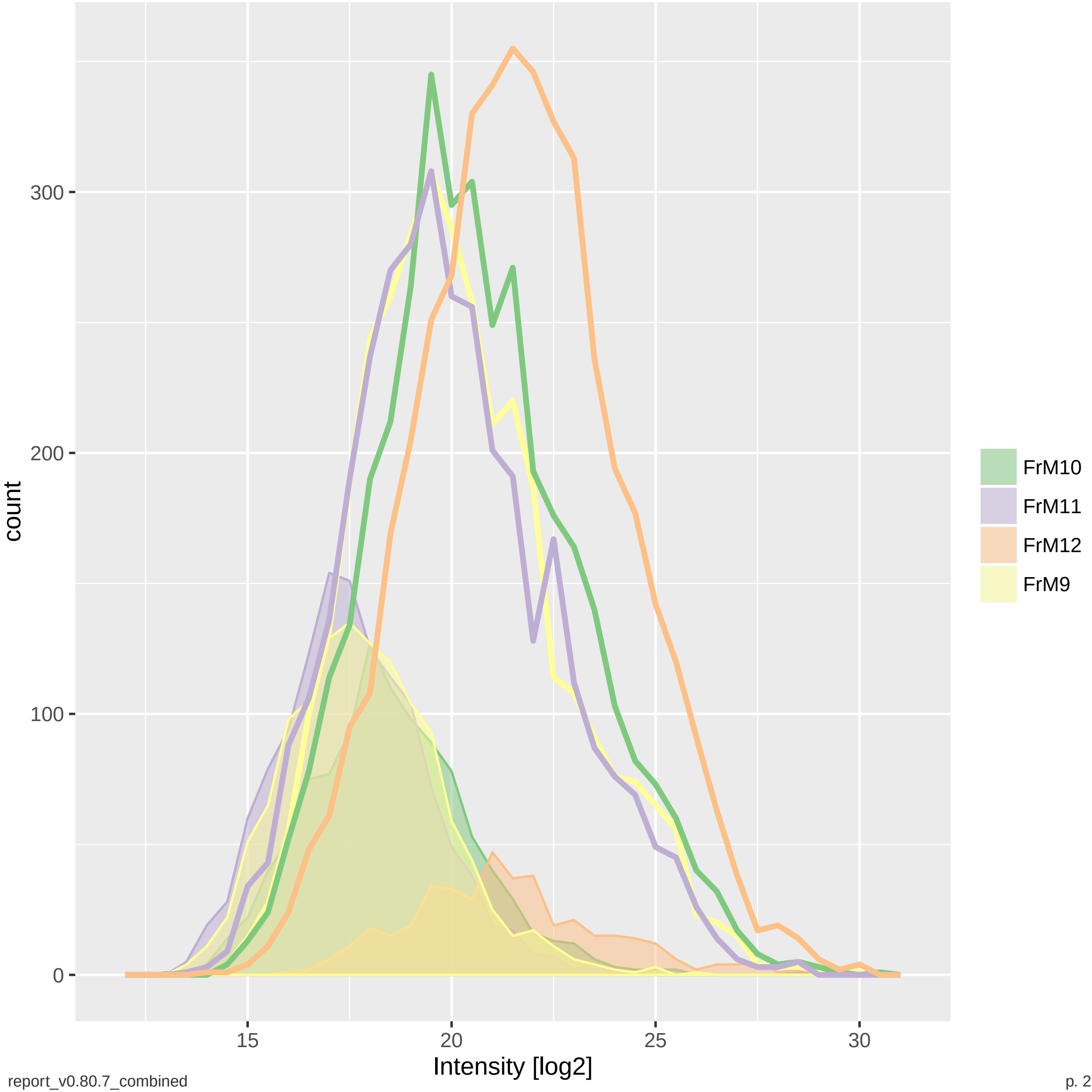

[experimental] EVD: Non−Missing Peptides
compared to all peptides seen in experiment
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
0
25
50
75
100
Fraction of total peptides [%]

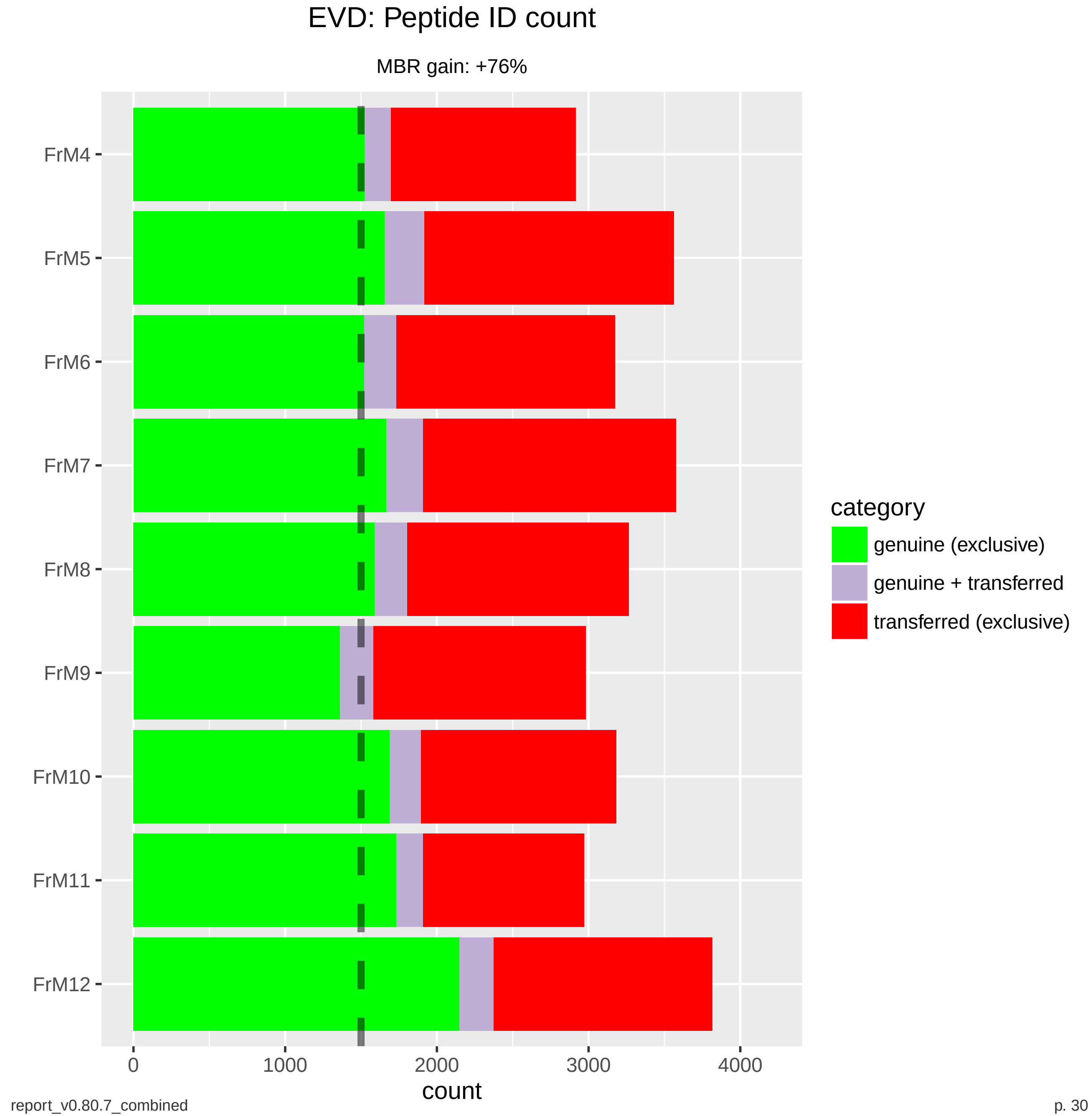

[experimental] EVD: Non−missing by set
Fraction of total peptides [%]
100
75
50
25
0
2.5
5.0
7.5
Minimum # Raw files

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



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




EVD: Peptide ID count
MBR gain: +76%
FrM4
FrM5
FrM6
FrM7
FrM8
FrM9
FrM10
FrM11
FrM12
0
1000
2000
3000
4000
count
category
genuine (exclusive)
genuine + transferred
transferred (exclusive)

EVD: ProteinGroups count

MBR gain: +46%