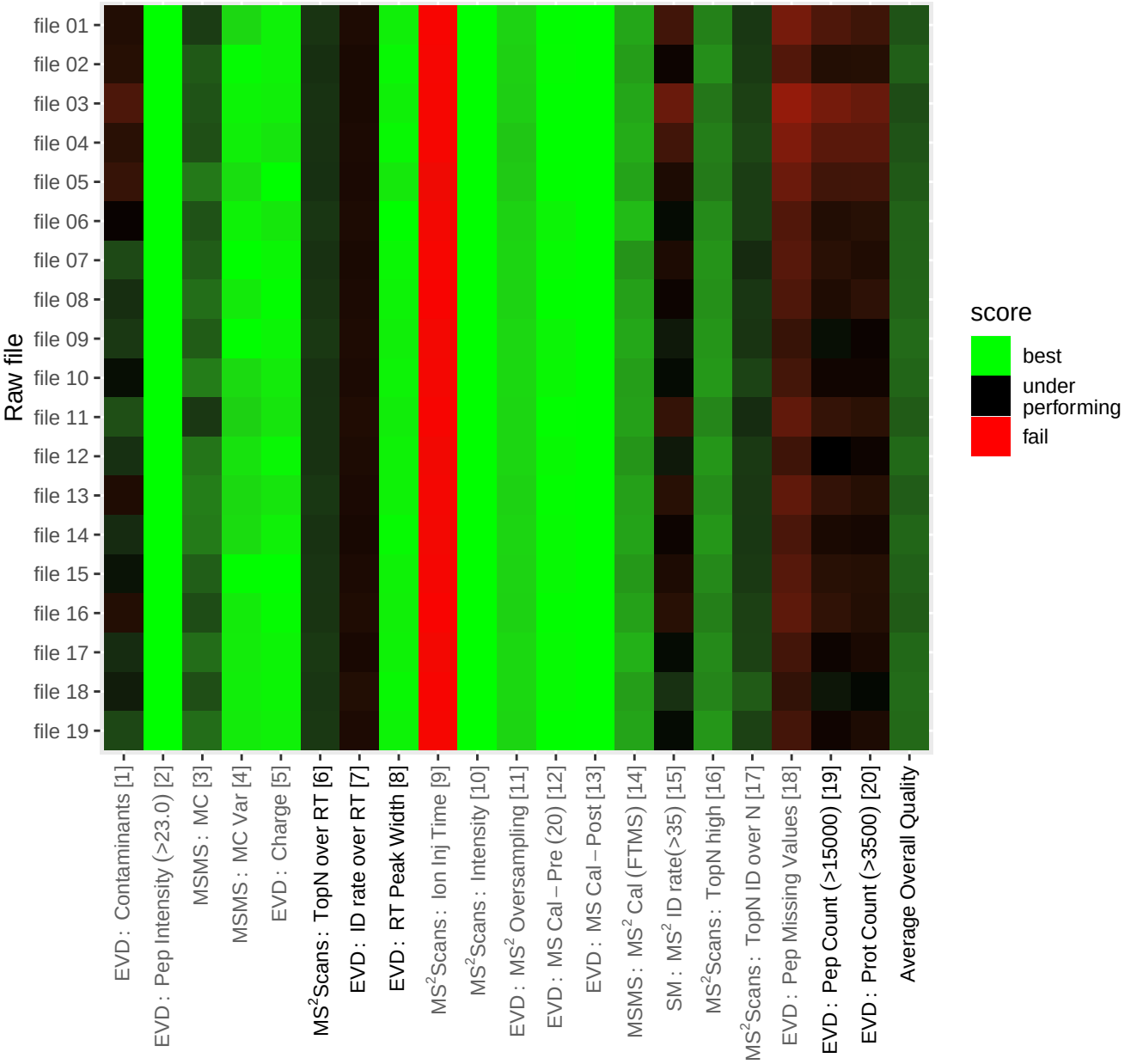
Performance overview



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

original	short name	best effort
RDEB_cSCC6.raw.thermo	file 01	..RDEB_cSCC6.r..mo
RDEB_cSCC5.raw.thermo	file 02	..RDEB_cSCC5.r..mo
RDEB_cSCC4.raw.thermo	file 03	..RDEB_cSCC4.r..mo
RDEB_cSCC3.raw.thermo	file 04	..RDEB_cSCC3.r..mo
RDEB_cSCC2.raw.thermo	file 05	..RDEB_cSCC2.r..mo
RDEB_cSCC1.raw.thermo	file 06	..RDEB_cSCC1.r..mo
metast_cSCC13.raw.thermo	file 07	..metast_cSCC13.r..mo
metast_cSCC12.raw.thermo	file 08	..metast_cSCC12.r..mo
metast_cSCC11.raw.thermo	file 09	..metast_cSCC11.r..mo
metast_cSCC10.raw.thermo	file 10	..metast_cSCC10.r..mo
metast_cSCC9.raw.thermo	file 11	..metast_cSCC9.r..mo
metast_cSCC8.raw.thermo	file 12	..metast_cSCC8.r..mo
metast_cSCC7.raw.thermo	file 13	..metast_cSCC7.r..mo
metast_cSCC6.raw.thermo	file 14	..metast_cSCC6.r..mo
metast_cSCC5.raw.thermo	file 15	..metast_cSCC5.r..mo
metast_cSCC4.raw.thermo	file 16	..metast_cSCC4.r..mo
metast_cSCC3.raw.thermo	file 17	..metast_cSCC3.r..mo
metast_cSCC2.raw.thermo	file 18	..metast_cSCC2.r..mo
metast_cSCC1.raw.thermo	file 19	..metast_cSCC1.r..mo

PAR: parameters

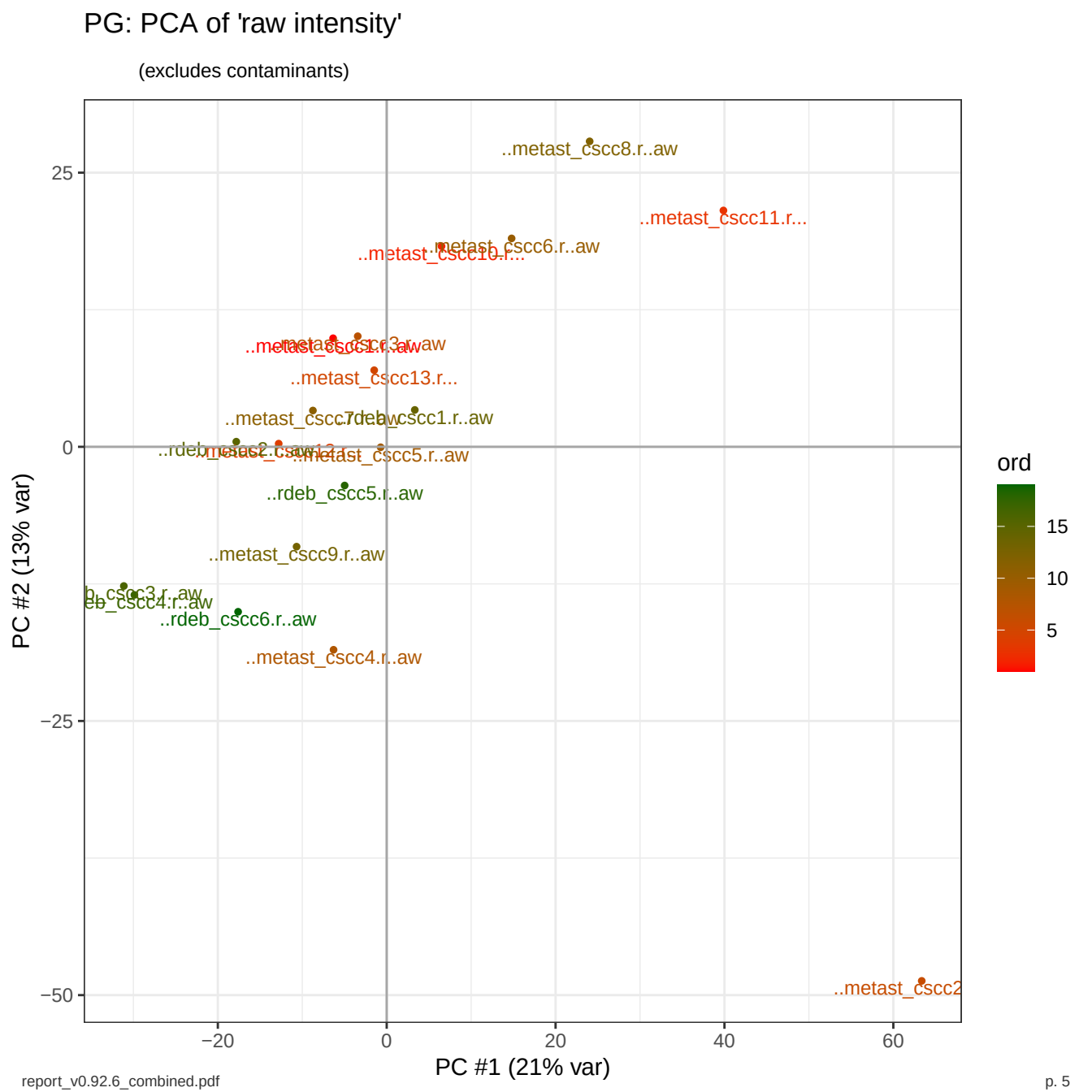
parameter	value	parameter	value
Advanced ratios	True	MS/MS deisotoping tolerance ..	7
Advanced site intensities	True	MS/MS deisotoping tolerance ..	ppm
Calculate peak properties	False	MS/MS dependent losses (FTMS..	True
Combined folder location		MS/MS dependent losses (ITMS..	True
Da interval. (FTMS)	100	MS/MS dependent losses (TOF)	True
Da interval. (ITMS)	100	MS/MS dependent losses (Unkn..	True
Da interval. (TOF)	100	MS/MS higher charges (FTMS)	True
Da interval. (Unknown)	100	MS/MS higher charges (ITMS)	True
Date of writing	02/17/2021 09:26:52	MS/MS higher charges (TOF)	True
Decoy mode	revert	MS/MS higher charges (Unknow..	True
Disable MD5	False	MS/MS recalibration (FTMS)	False
Discard unmodified counterpa..	False	MS/MS recalibration (ITMS)	False
Epsilon score for mutations		MS/MS recalibration (TOF)	False
Evaluate variant peptides se..	True	MS/MS recalibration (Unknown..	False
Find dependent peptides	False	MS/MS tol. (FTMS)	20 ppm
Fixed andromeda index folder		MS/MS tol. (ITMS)	0.5 Da
iBAQ	False	MS/MS tol. (TOF)	40 ppm
iBAQ log fit	False	MS/MS tol. (Unknown)	20 ppm
Include contaminants	True	MS/MS water loss (FTMS)	True
Label min. ratio count	2	MS/MS water loss (ITMS)	True
Machine name	vgcnbwc−worker−c20me−8620.novalocal	MS/MS water loss (TOF)	True
Main search max. combination..	200	MS/MS water loss (Unknown)	True
Match between runs	False	Peptides used for protein qu..	Razor
Match unidentified features	False	Protein FDR	0.01
Max mods in site table	3	PSM FDR	0.01
Max. peptide length for unsp..	25	PSM FDR Crosslink	0.01

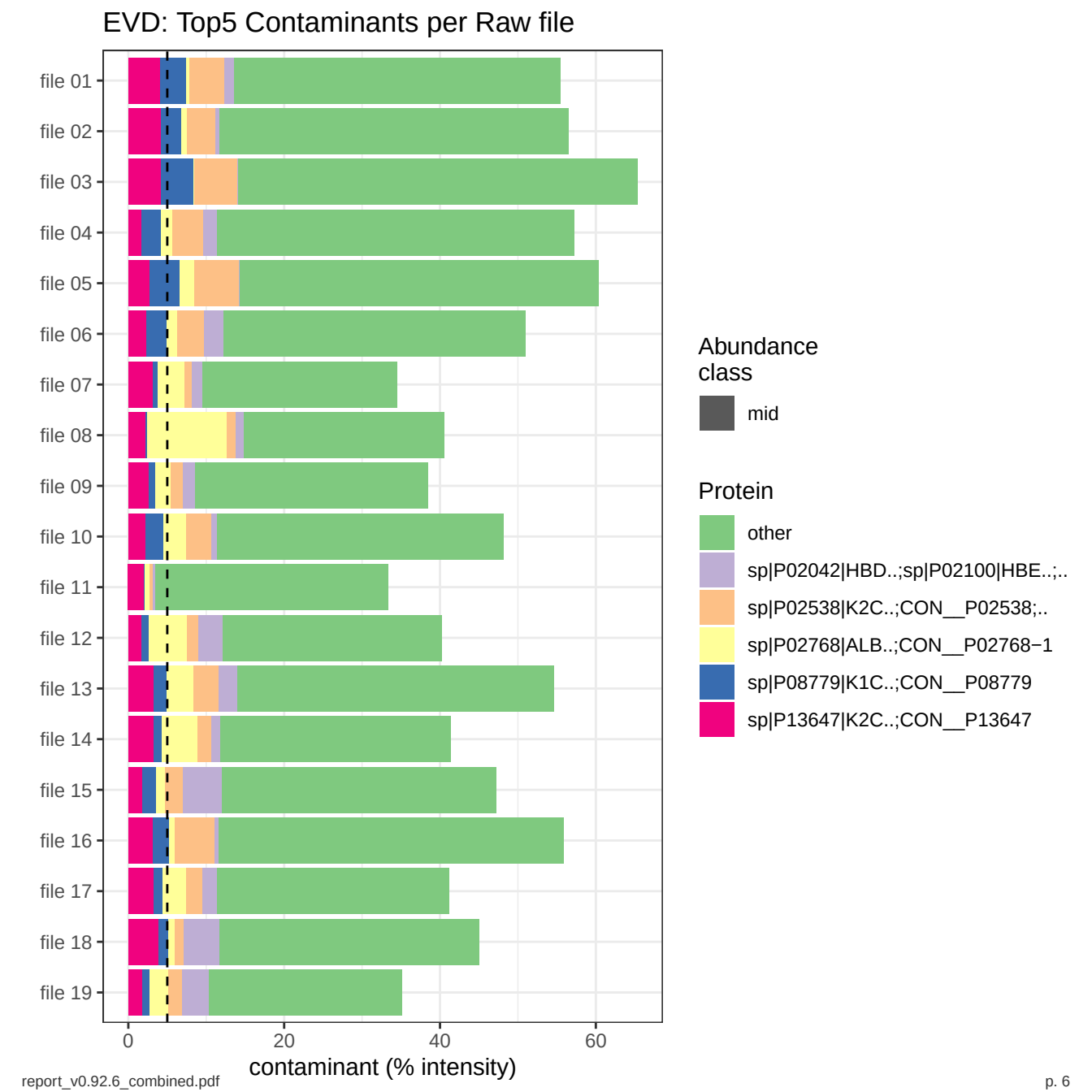
/data/dnb03/galaxy_db/files/8/0/c/dataset_80c72798−c781−4bfc−9256−55b3c2f2dca4.dat

PAR: parameters

parameter	value	parameter	value
Max. peptide mass [Da]	4600	Razor protein FDR	True
Min. delta score for modifie..	6	Require MS/MS for LFQ compar..	True
Min. delta score for unmodif..	0	Second peptides	True
Min. peptide Length	7	Separate LFQ in parameter gr..	False
Min. peptide length for unsp..	8	Site FDR	0.01
Min. peptides	1	Site tables	Oxidation (M)Sites.txt
Min. razor peptides	1	Stabilize large LFQ ratios	True
Min. score for modified pept..	40	Temporary folder	
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	12
Min. unique peptides	0	Top MS/MS peaks per Da inter..	8
Modifications included in pr..	Acetyl (Protein N−term) Oxidation (M)	Top MS/MS peaks per Da inter..	10
MS/MS ammonia loss (FTMS)	True	Top MS/MS peaks per Da inter..	12
MS/MS ammonia loss (ITMS)	True	Use delta score	False
MS/MS ammonia loss (TOF)	True	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (Unknown)	True	Use only unmodified peptides..	True
MS/MS deisotoping (FTMS)	True	User name	galaxy
MS/MS deisotoping (ITMS)	False	Variation mode	None
MS/MS deisotoping (TOF)	True	Version	1.6.10.43
MS/MS deisotoping (Unknown)	True	Write accumulatedPasefMsmsSc..	True
MS/MS deisotoping tolerance ..	7	Write allPeptides table	True
MS/MS deisotoping tolerance ..	ppm	Write ms3Scans table	True
MS/MS deisotoping tolerance ..	0.15	Write msmsScans table	True
MS/MS deisotoping tolerance ..	Da	Write msScans table	False
MS/MS deisotoping tolerance ..	0.01	Write mzRange table	True
MS/MS deisotoping tolerance ..	Da	Write pasefMsmsScans table	True

/data/dnb03/galaxy_db/files/8/0/c/dataset_80c72798−c781−4bfc−9256−55b3c2f2dca4.dat

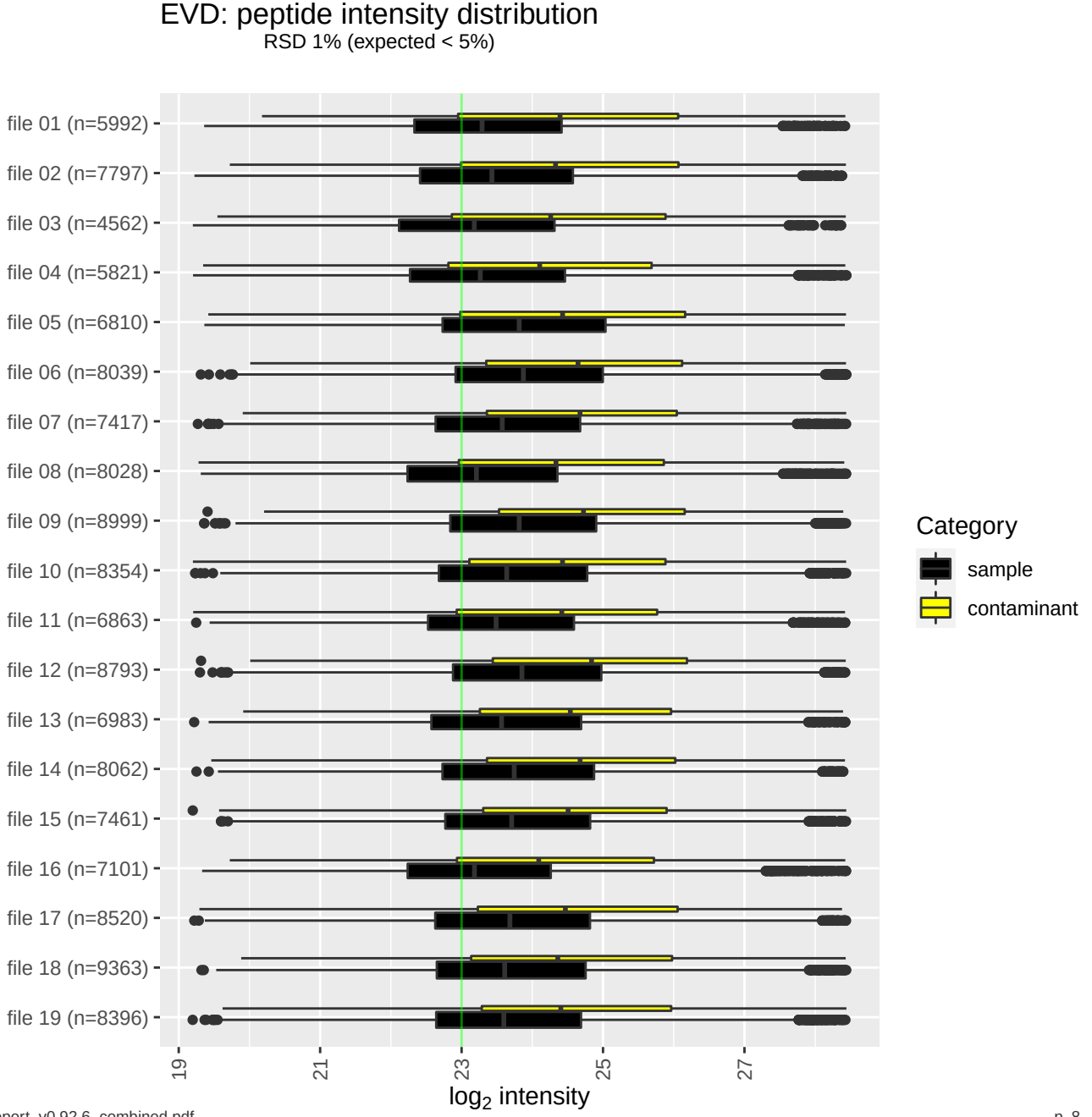

PG: PCA of 'raw intensity'
(excludes contaminants)
..metast_cscc8.r..aw
..metast_cscc11.r...
..metast_cscc6.r..aw
..metast_cscc10.r...
..metast_cscc1.r..aw
..metast_cscc3.r..aw
..metast_cscc13.r...
..metast_cscc7.r..aw
..rdeb_cscc1.r..aw
..metast_cscc5.r..aw
..rdeb_cscc5.r..aw
..metast_cscc9.r..aw
..rdeb_cscc6.r..aw
..metast_cscc4.r..aw
..metast_cscc2
ord
15
10
5
25
0
−25
−50
−20
0
20
40
60
PC #2 (13% var)
PC #1 (21% var)

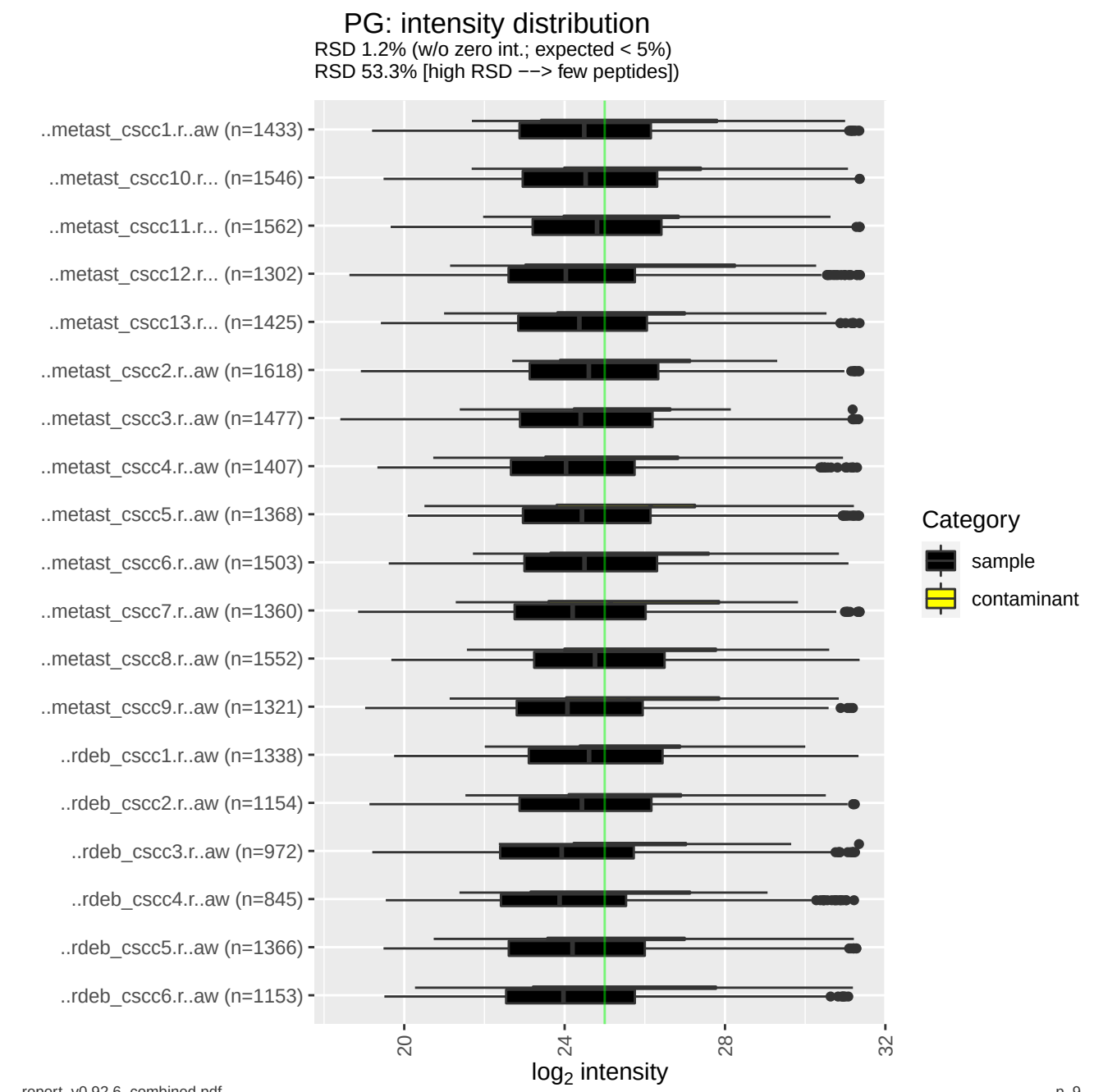

EVD: Top5 Contaminants per Raw file
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0
20
40
60
contaminant (% intensity)
Abundance class
mid
Protein
other
sp|P02042|HBD..;sp|P02100|HBE..;..
sp|P02538|K2C..;CON__P02538;..
sp|P02768|ALB..;CON__P02768−1
sp|P08779|K1C..;CON__P08779
sp|P13647|K2C..;CON__P13647

EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

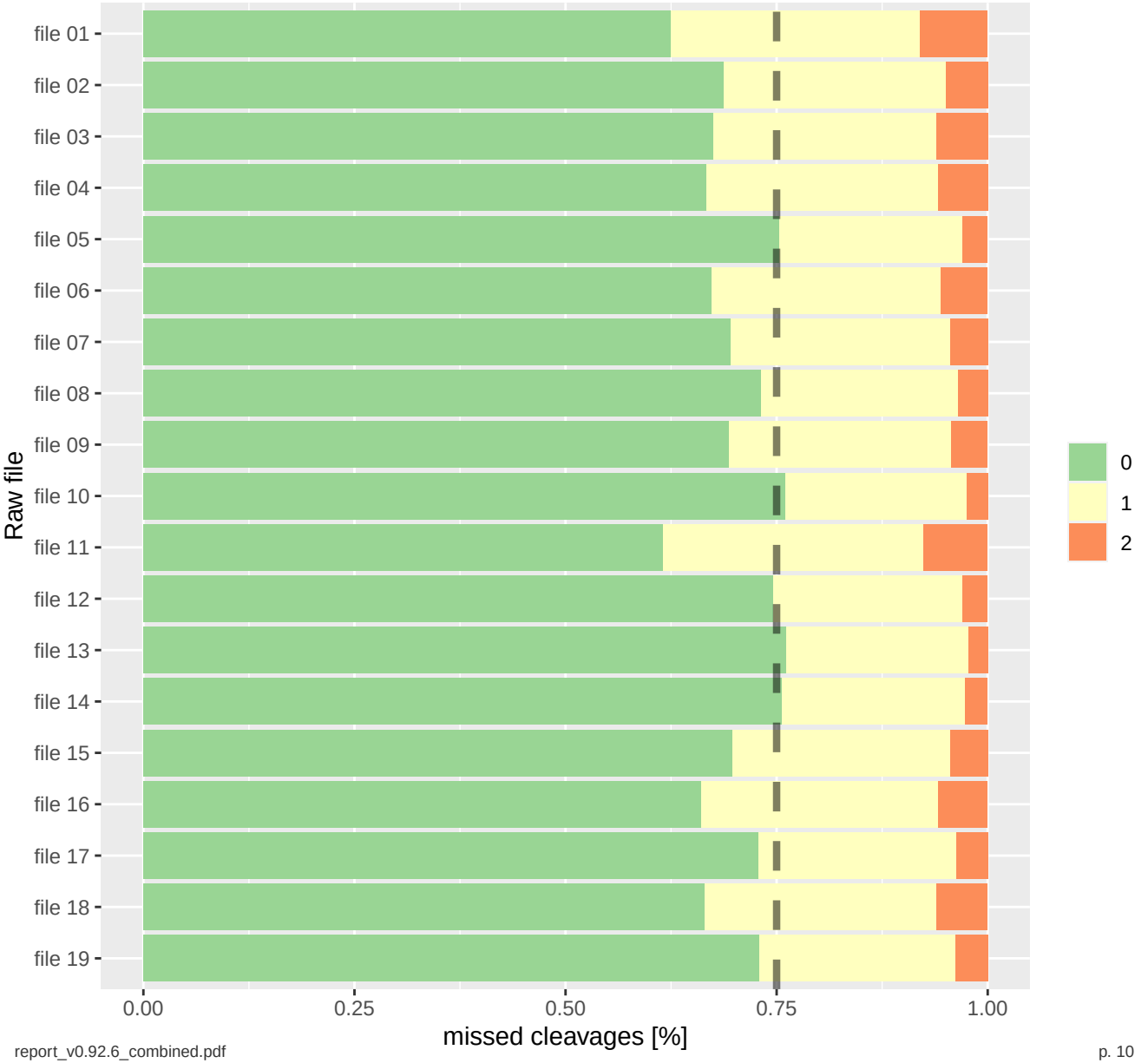
Did you use the correct database?

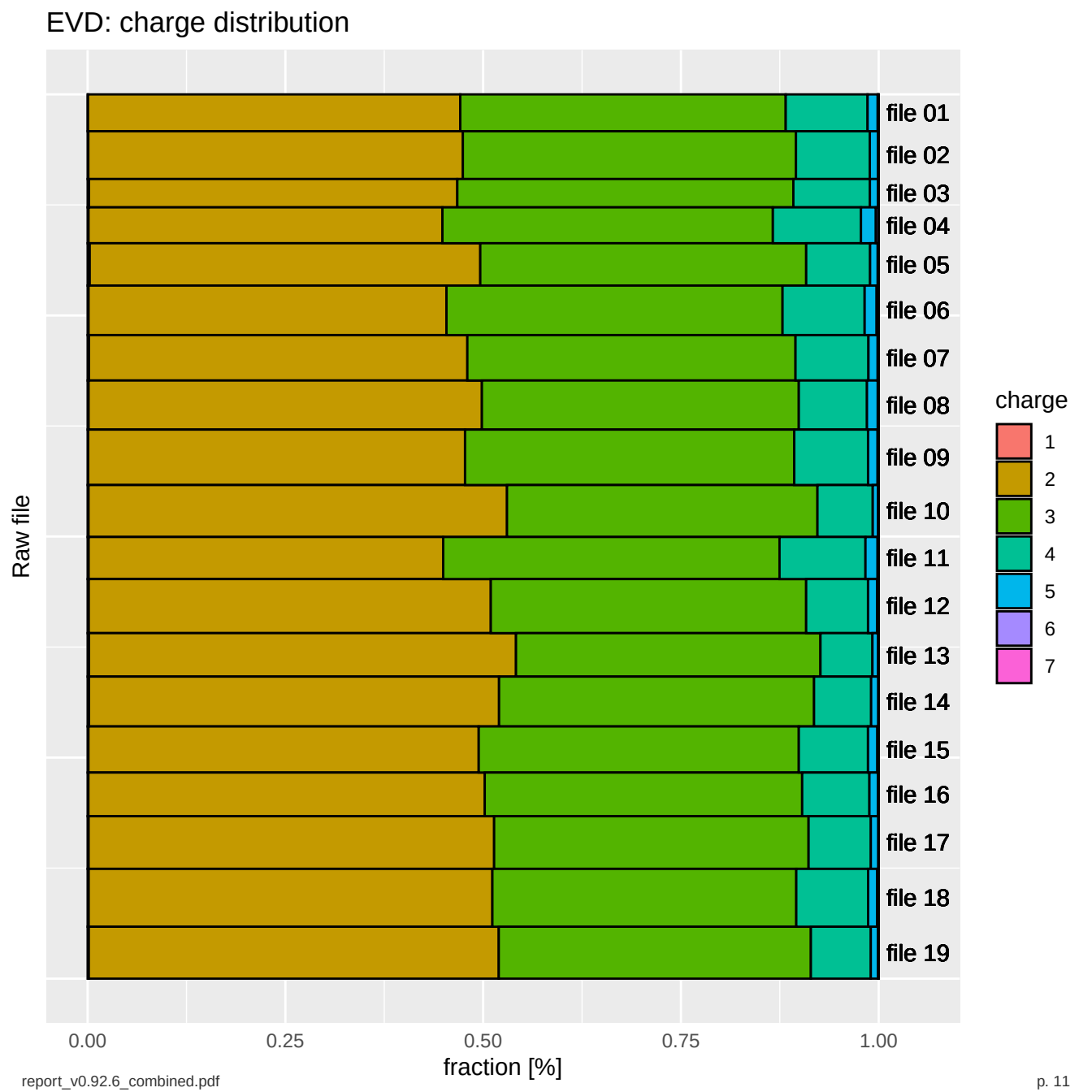

EVD: peptide intensity distribution
RSD 1% (expected < 5%)
file 01 (n=5992)
file 02 (n=7797)
file 03 (n=4562)
file 04 (n=5821)
file 05 (n=6810)
file 06 (n=8039)
file 07 (n=7417)
file 08 (n=8028)
file 09 (n=8999)
file 10 (n=8354)
file 11 (n=6863)
file 12 (n=8793)
file 13 (n=6983)
file 14 (n=8062)
file 15 (n=7461)
file 16 (n=7101)
file 17 (n=8520)
file 18 (n=9363)
file 19 (n=8396)
19
21
23
25
27
log2 intensity
Category
sample
contaminant

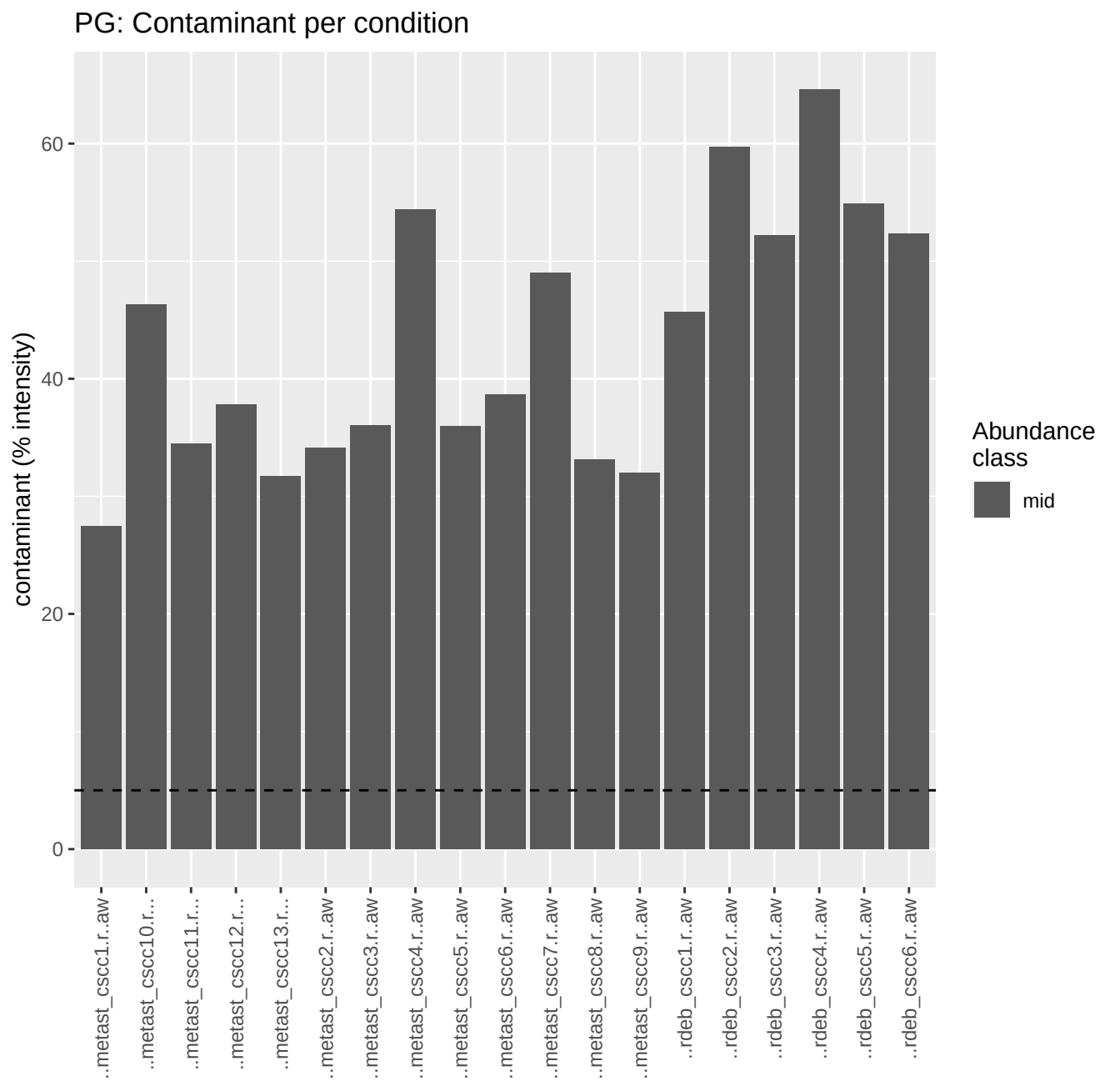

PG: intensity distribution
RSD 1.2% (w/o zero int.; expected < 5%)
RSD 53.3% [high RSD −−> few peptides])
..metast_cscc1.r..aw (n=1433)
..metast_cscc10.r... (n=1546)
..metast_cscc11.r... (n=1562)
..metast_cscc12.r... (n=1302)
..metast_cscc13.r... (n=1425)
..metast_cscc2.r..aw (n=1618)
..metast_cscc3.r..aw (n=1477)
..metast_cscc4.r..aw (n=1407)
..metast_cscc5.r..aw (n=1368)
..metast_cscc6.r..aw (n=1503)
..metast_cscc7.r..aw (n=1360)
..metast_cscc8.r..aw (n=1552)
..metast_cscc9.r..aw (n=1321)
..rdeb_cscc1.r..aw (n=1338)
..rdeb_cscc2.r..aw (n=1154)
..rdeb_cscc3.r..aw (n=972)
..rdeb_cscc4.r..aw (n=845)
..rdeb_cscc5.r..aw (n=1366)
..rdeb_cscc6.r..aw (n=1153)
20
24
28
32
log2 intensity
Category
sample
contaminant

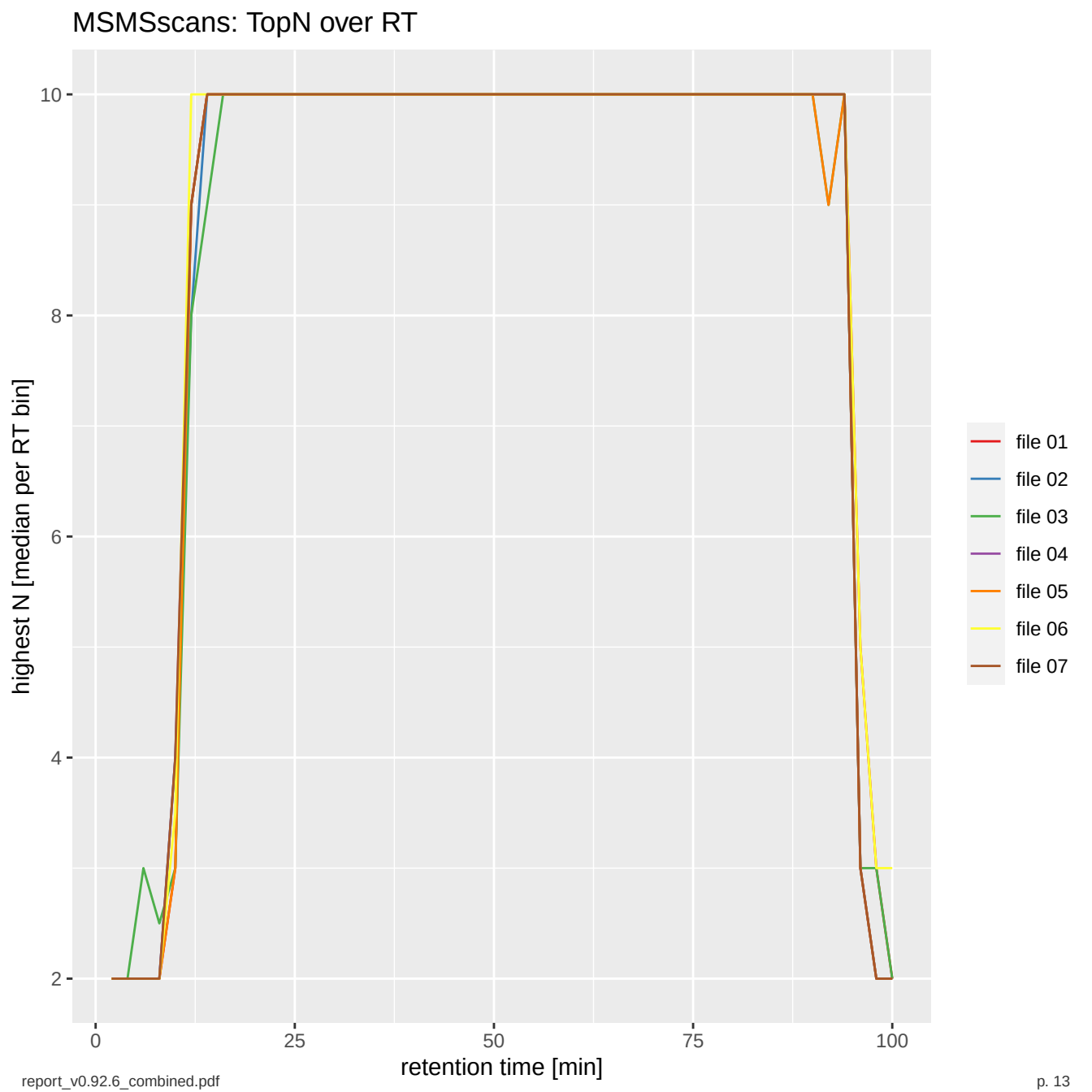
MSMS: Missed cleavages per Raw file

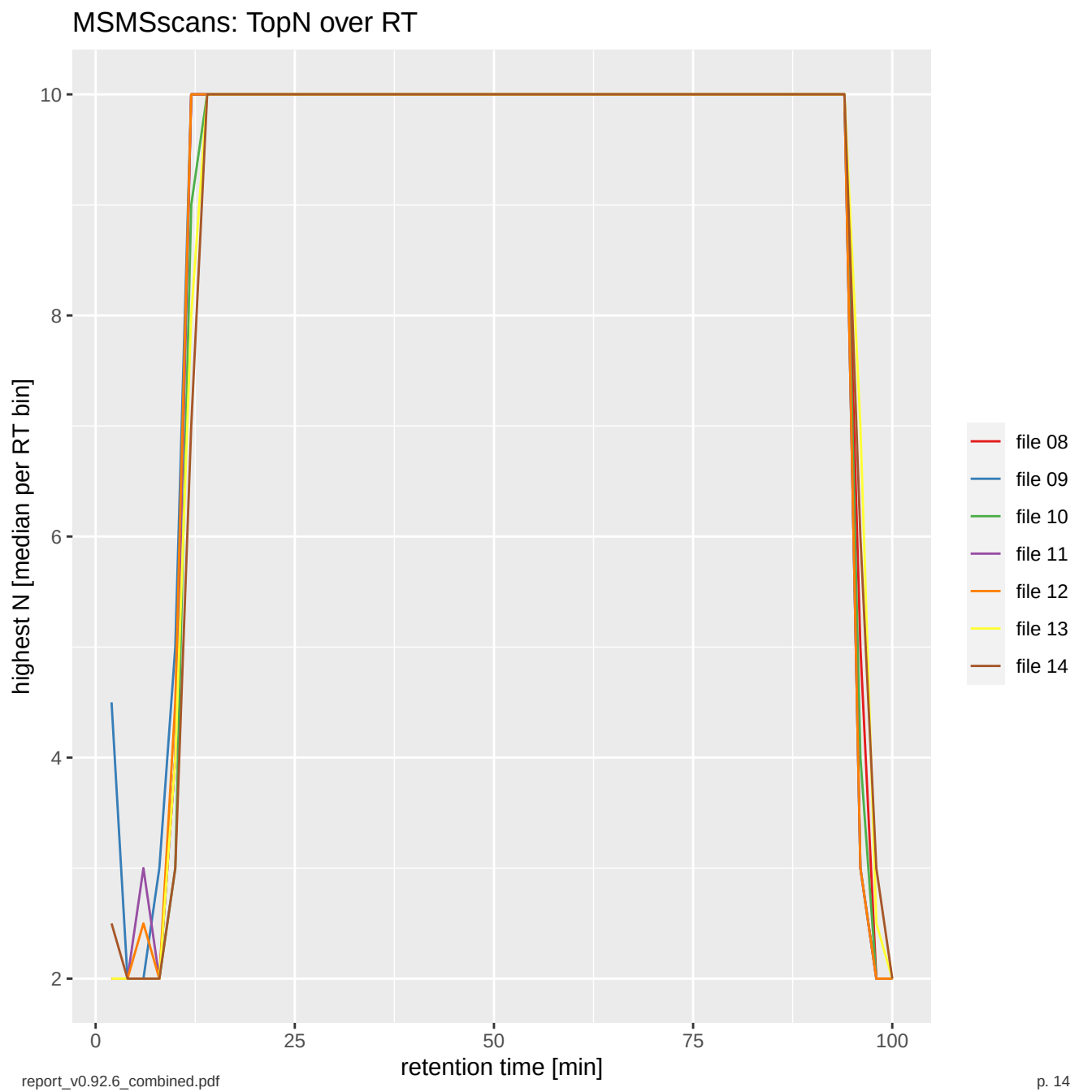
(excludes contaminants)

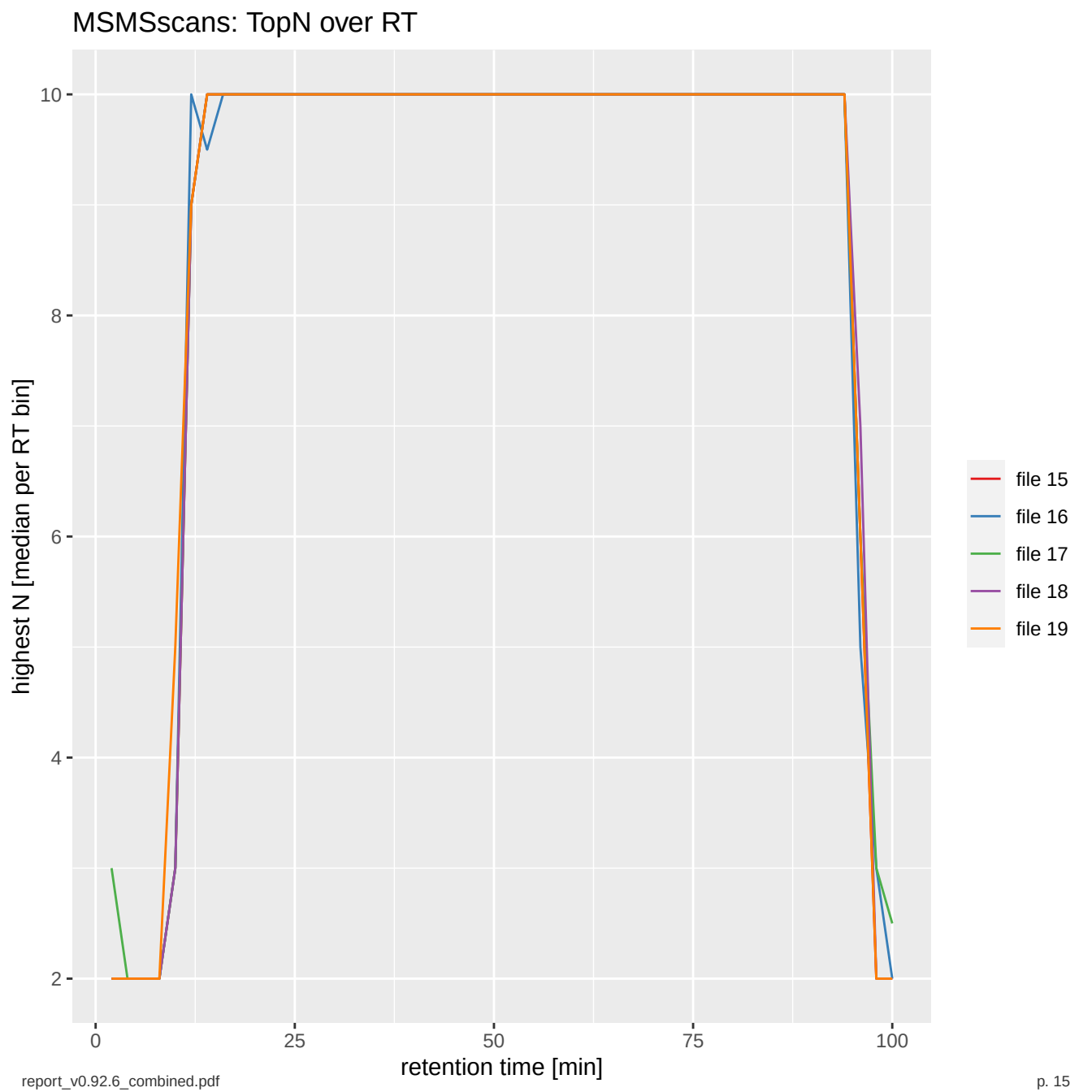


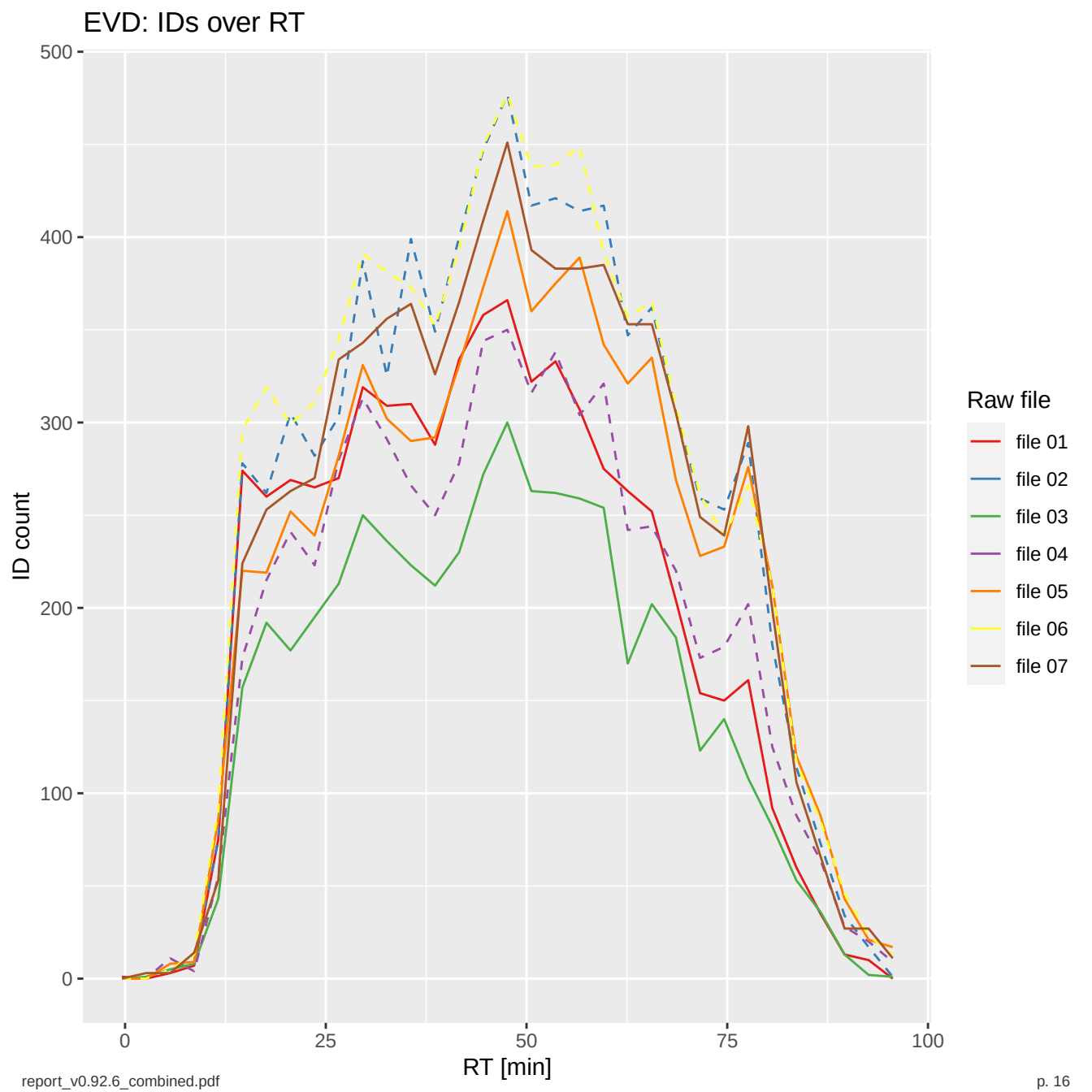

EVD: charge distribution
Raw file
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
charge
1
2
3
4
5
6
7
0.00
0.25
0.50
0.75
1.00
fraction [%]

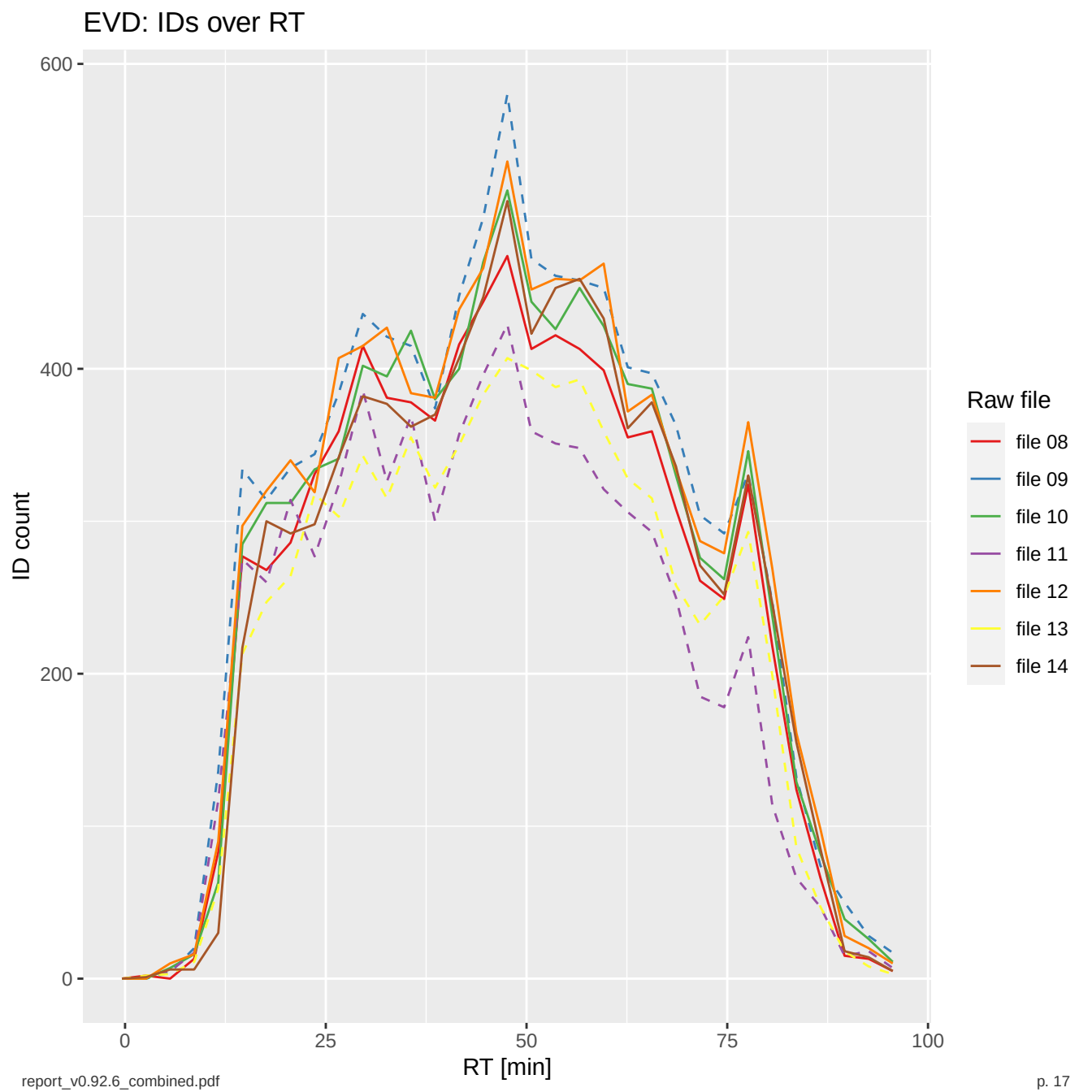

PG: Contaminant per condition
contaminant (% intensity)
0
20
40
60
..metast_cscc1.r..aw
..metast_cscc10.r...
..metast_cscc11.r...
..metast_cscc12.r...
..metast_cscc13.r...
..metast_cscc2.r..aw
..metast_cscc3.r..aw
..metast_cscc4.r..aw
..metast_cscc5.r..aw
..metast_cscc6.r..aw
..metast_cscc7.r..aw
..metast_cscc8.r..aw
..metast_cscc9.r..aw
..rdeb_cscc1.r..aw
..rdeb_cscc2.r..aw
..rdeb_cscc3.r..aw
..rdeb_cscc4.r..aw
..rdeb_cscc5.r..aw
..rdeb_cscc6.r..aw
Abundance class
mid

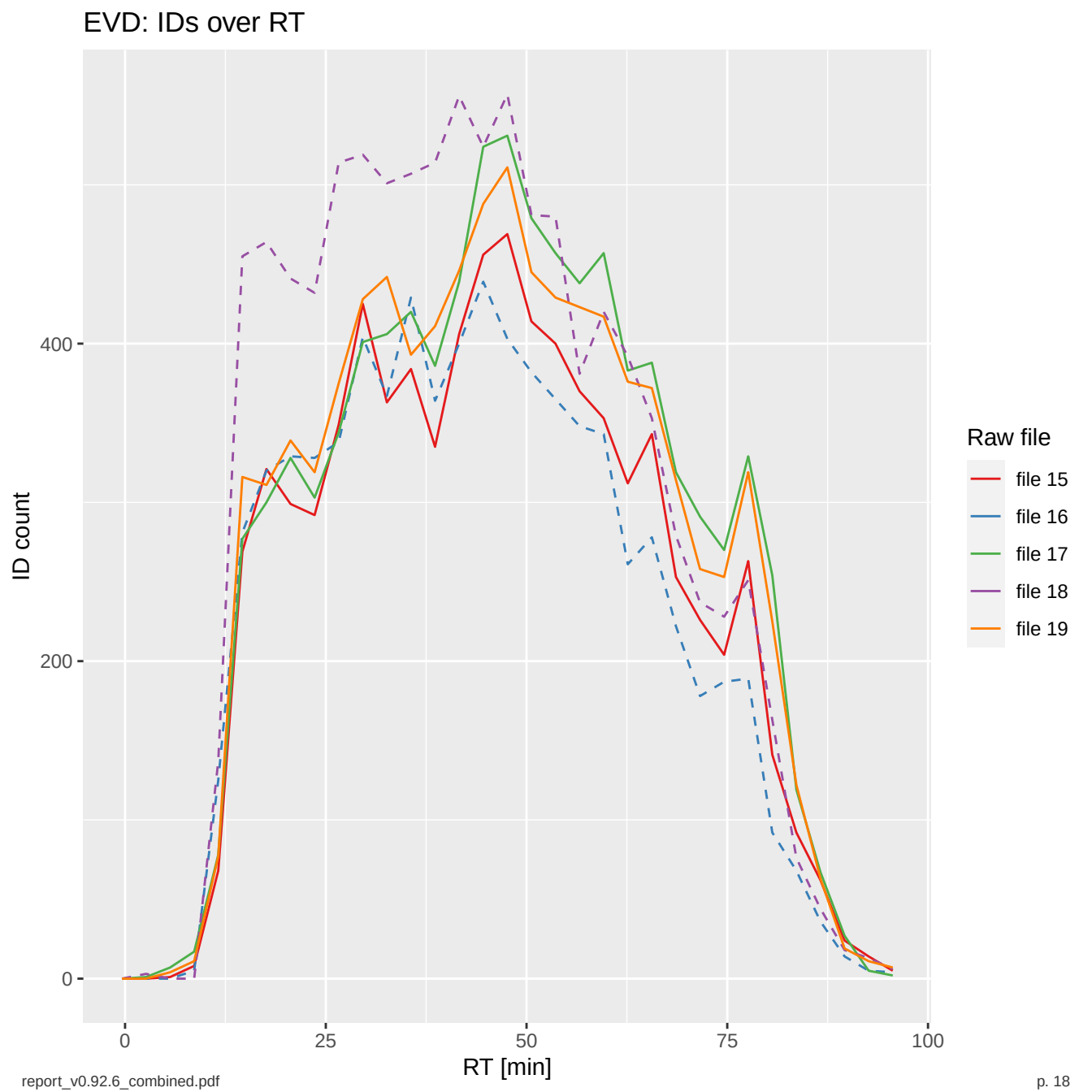

MSMSscans: TopN over RT
highest N [median per RT bin]
10
8
6
4
2
0
25
50
75
100
retention time [min]
file 01
file 02
file 03
file 04
file 05
file 06
file 07

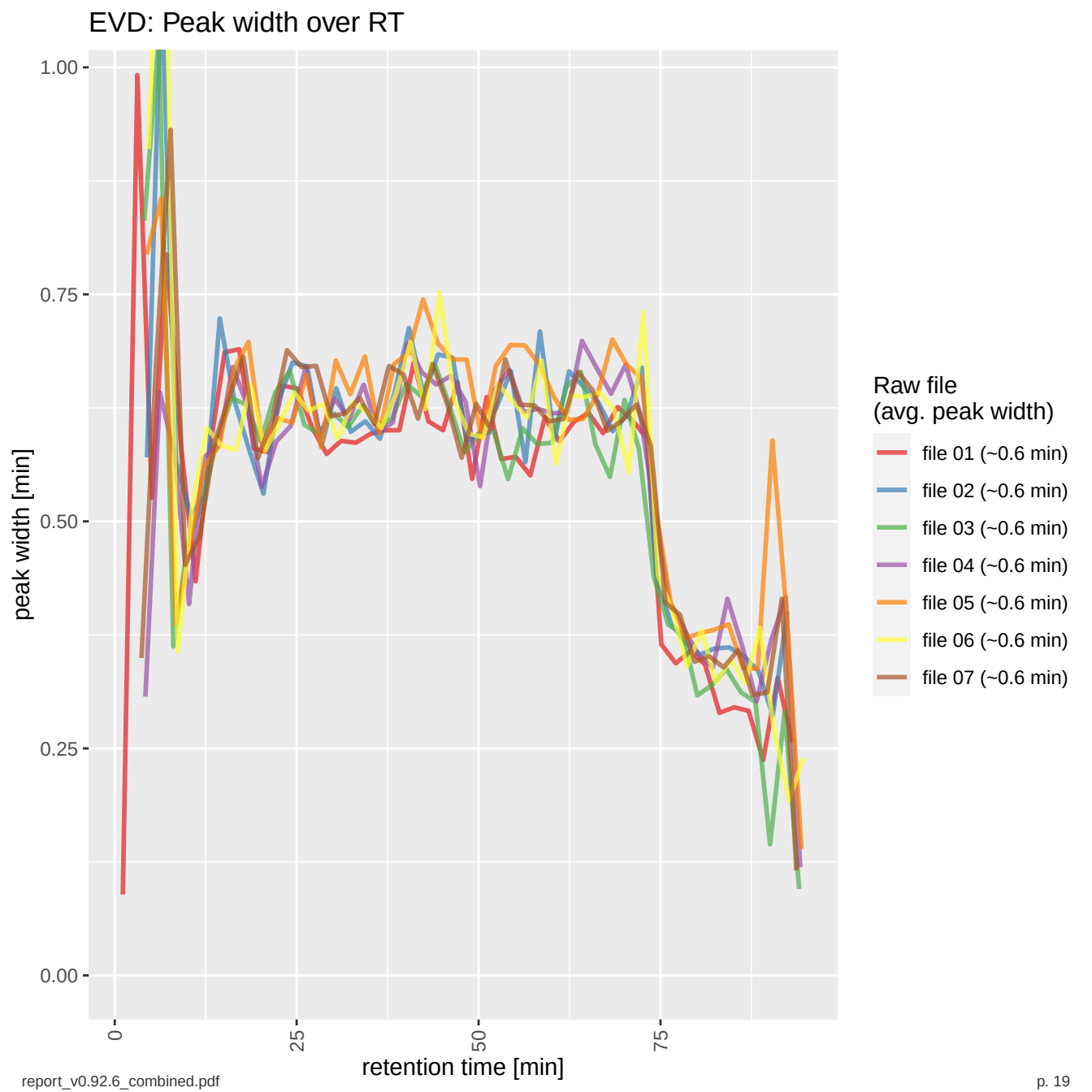

MSMSscans: TopN over RT
highest N [median per RT bin]
10
8
6
4
2
0
25
50
75
100
retention time [min]
file 08
file 09
file 10
file 11
file 12
file 13
file 14

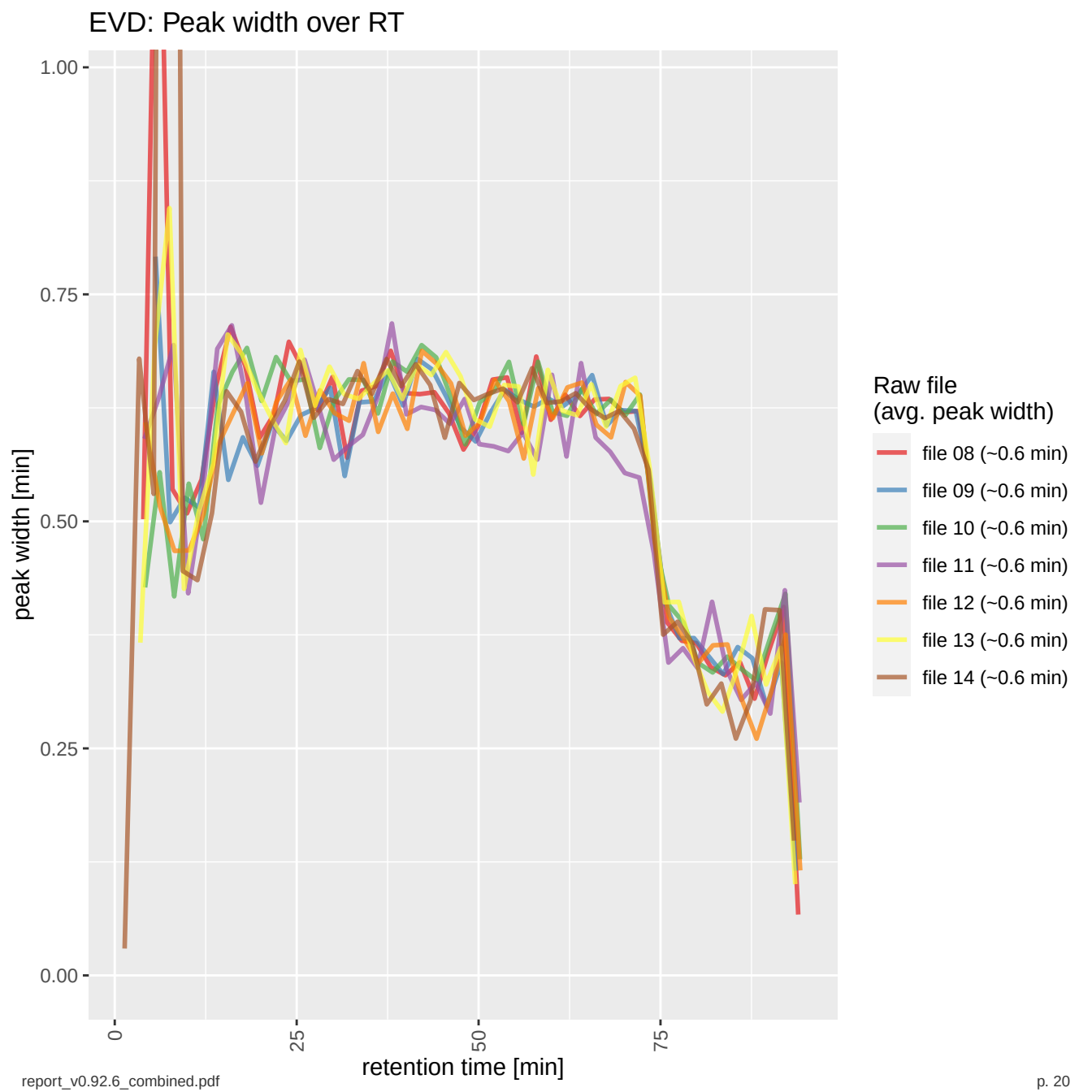

MSMSscans: TopN over RT
highest N [median per RT bin]
10
8
6
4
2
0
25
50
75
100
retention time [min]
file 15
file 16
file 17
file 18
file 19

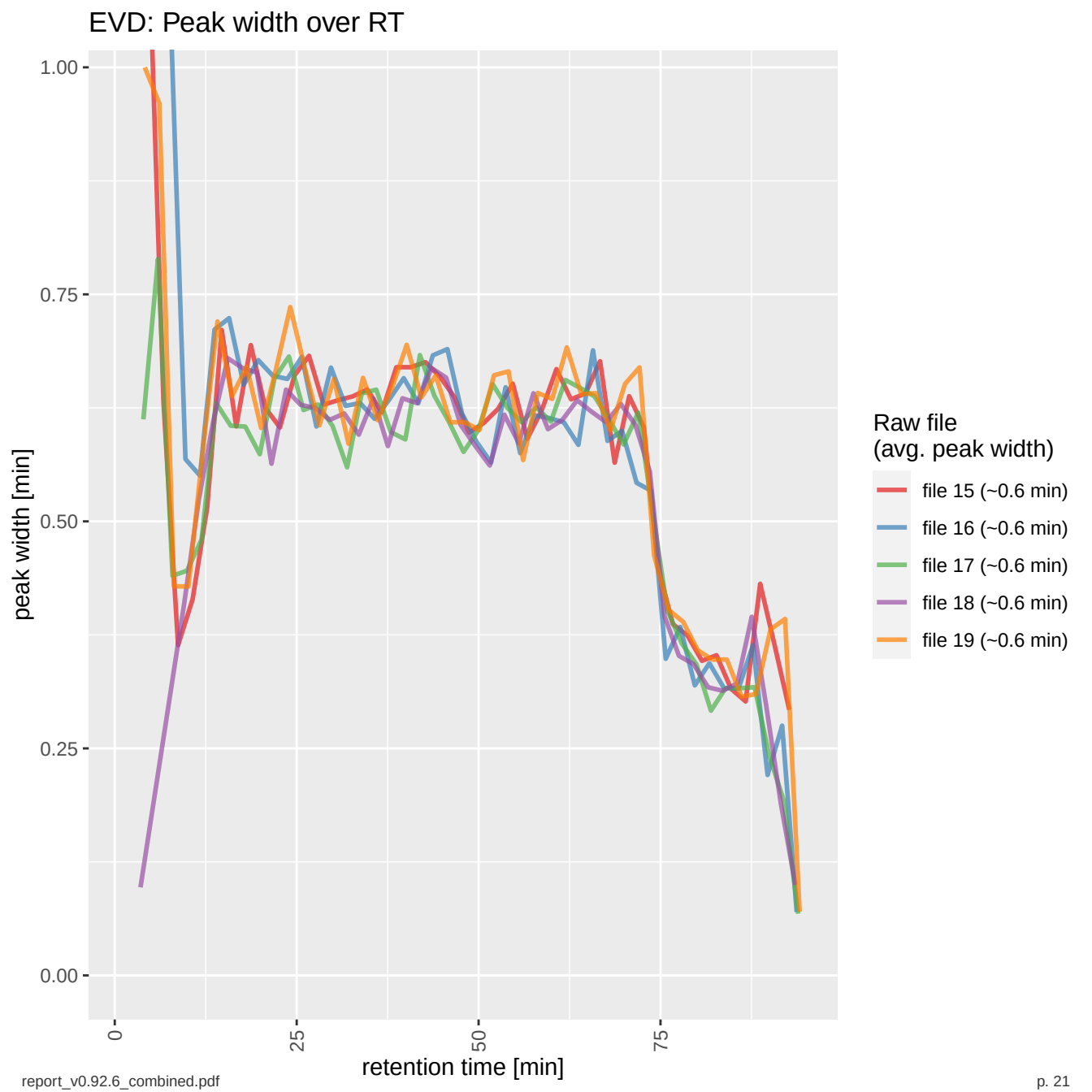

EVD: IDs over RT
ID count
RT [min]
Raw file
file 01
file 02
file 03
file 04
file 05
file 06
file 07
500
400
300
200
100
0
0
25
50
75
100

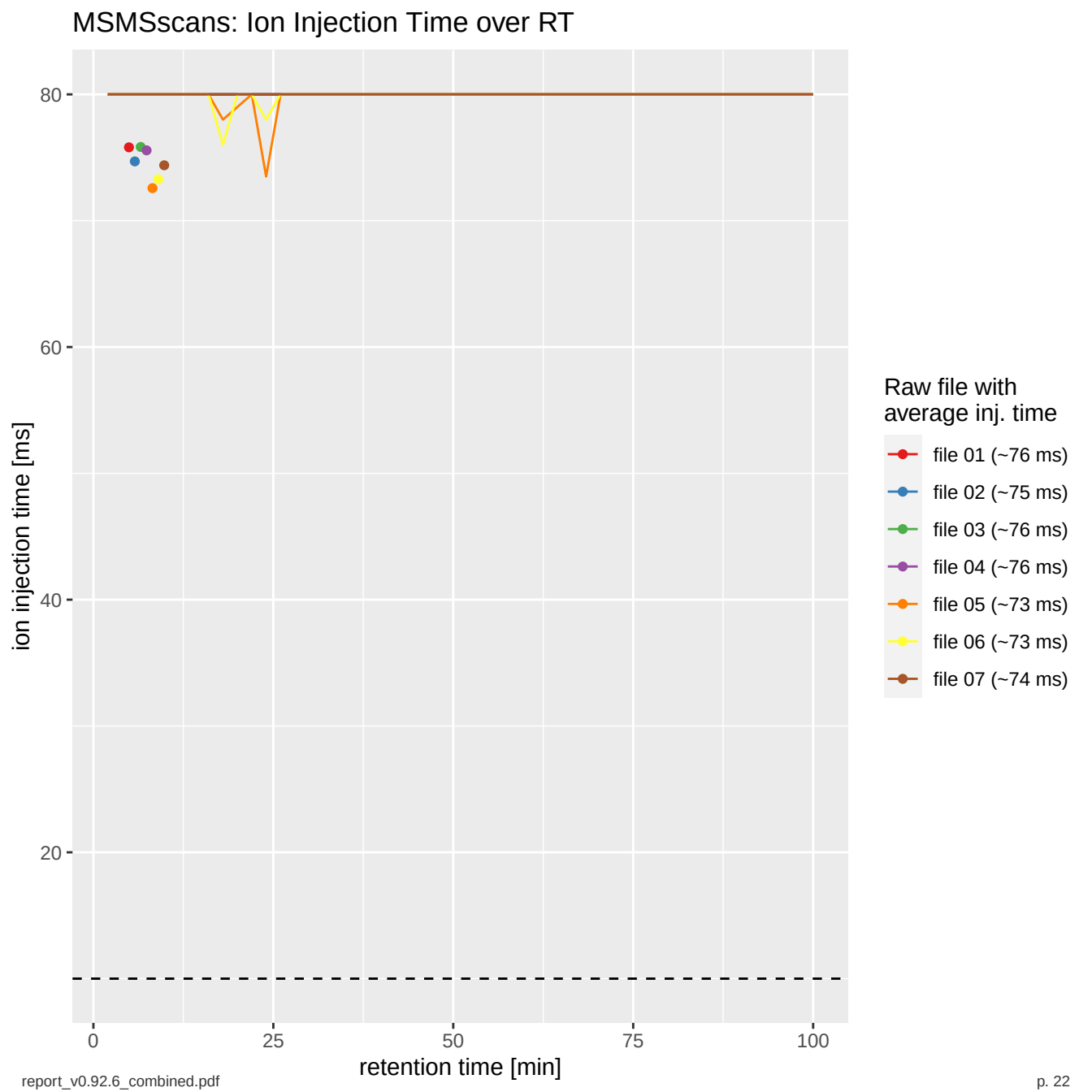

EVD: IDs over RT
600
400
200
0
ID count
0
25
50
75
100
RT [min]
Raw file
file 08
file 09
file 10
file 11
file 12
file 13
file 14

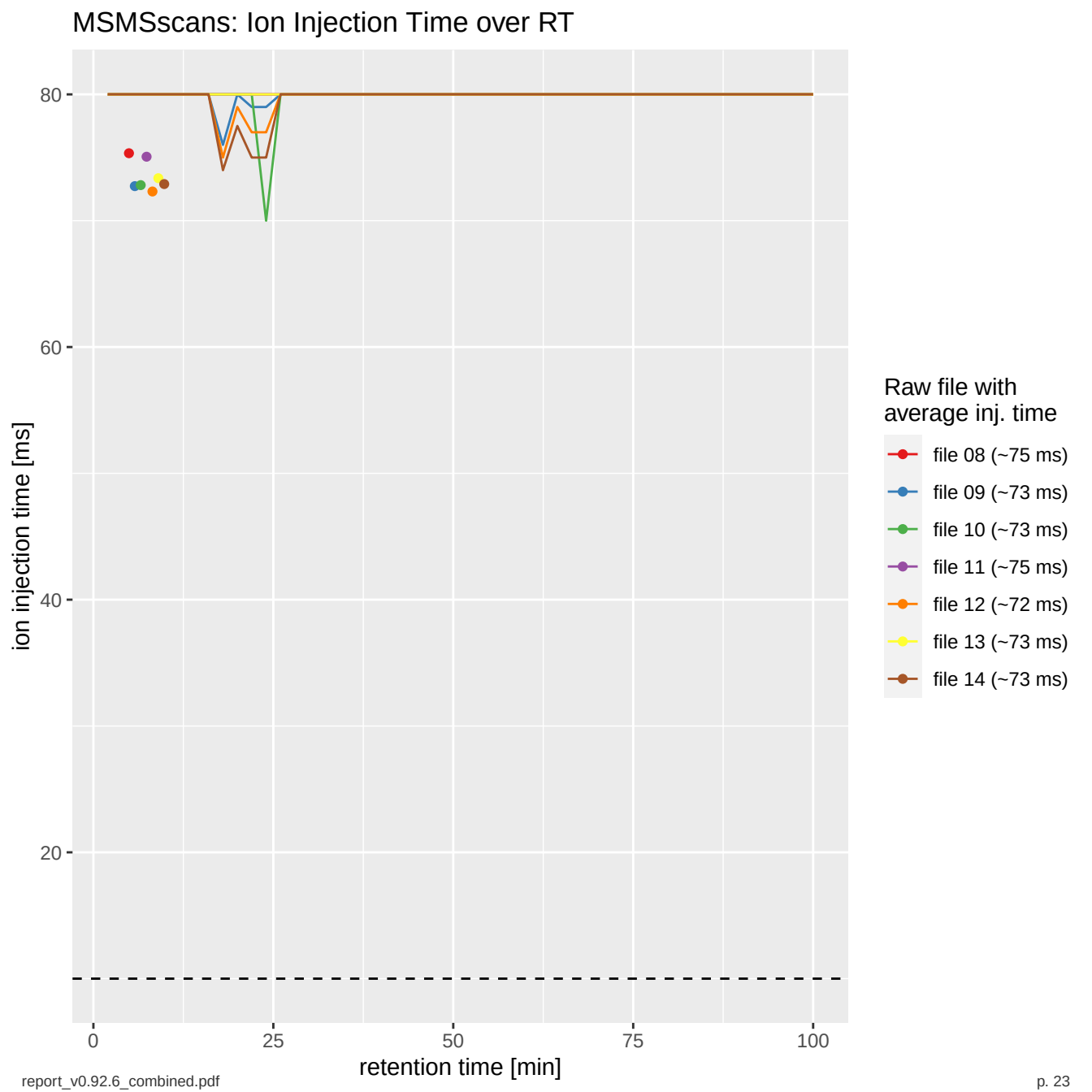

EVD: IDs over RT
ID count
400
200
0
0
25
50
75
100
RT [min]
Raw file
file 15
file 16
file 17
file 18
file 19

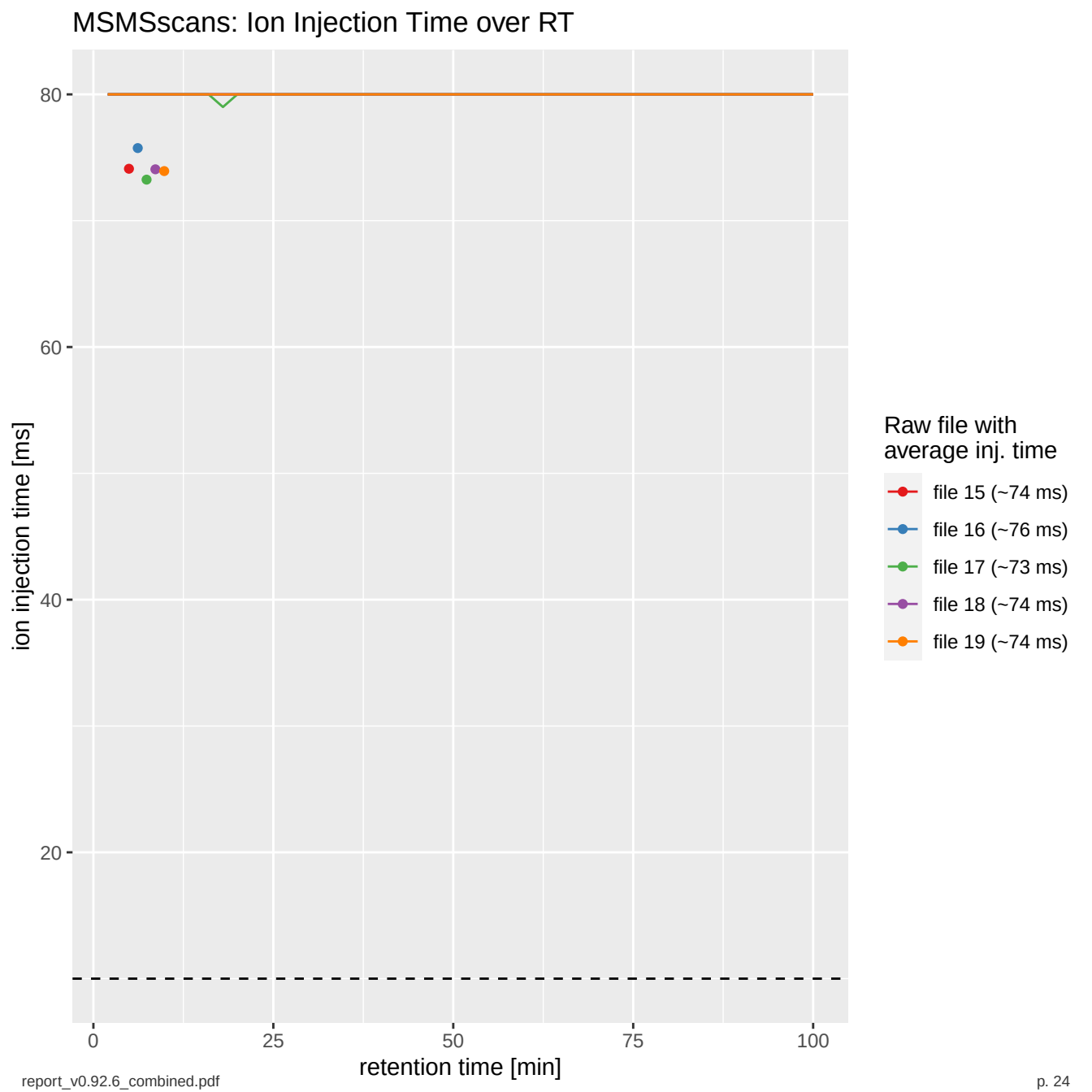

EVD: Peak width over RT
1.00
0.75
0.50
0.25
0.00
peak width [min]
0
25
50
75
retention time [min]
Raw file
(avg. peak width)
file 01 (~0.6 min)
file 02 (~0.6 min)
file 03 (~0.6 min)
file 04 (~0.6 min)
file 05 (~0.6 min)
file 06 (~0.6 min)
file 07 (~0.6 min)

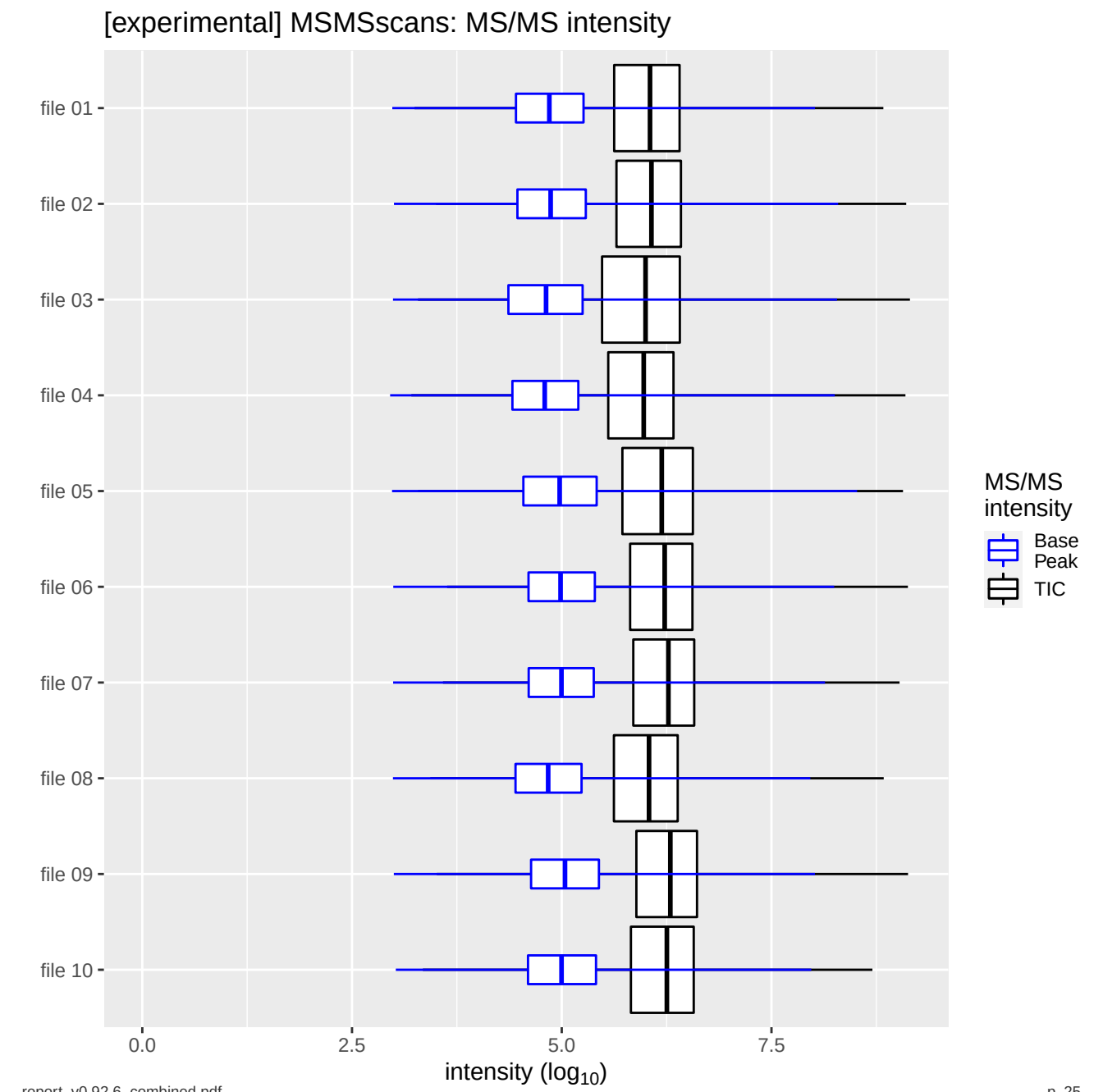

EVD: Peak width over RT
1.00
0.75
0.50
0.25
0.00
peak width [min]
0
25
50
75
retention time [min]
Raw file
(avg. peak width)
file 08 (~0.6 min)
file 09 (~0.6 min)
file 10 (~0.6 min)
file 11 (~0.6 min)
file 12 (~0.6 min)
file 13 (~0.6 min)
file 14 (~0.6 min)

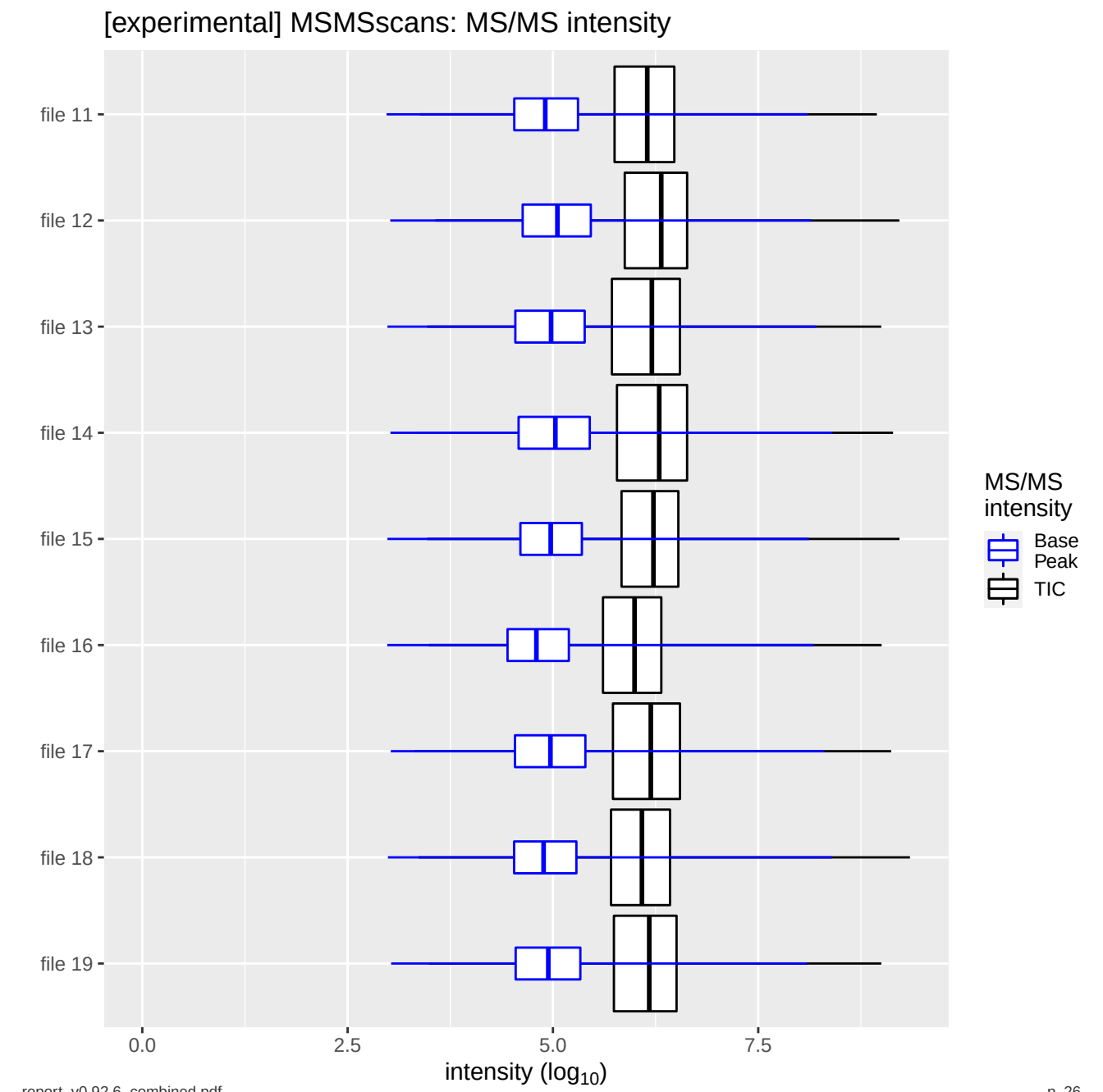

EVD: Peak width over RT
1.00
0.75
0.50
0.25
0.00
peak width [min]
0
25
50
75
retention time [min]
Raw file
(avg. peak width)
file 15 (~0.6 min)
file 16 (~0.6 min)
file 17 (~0.6 min)
file 18 (~0.6 min)
file 19 (~0.6 min)

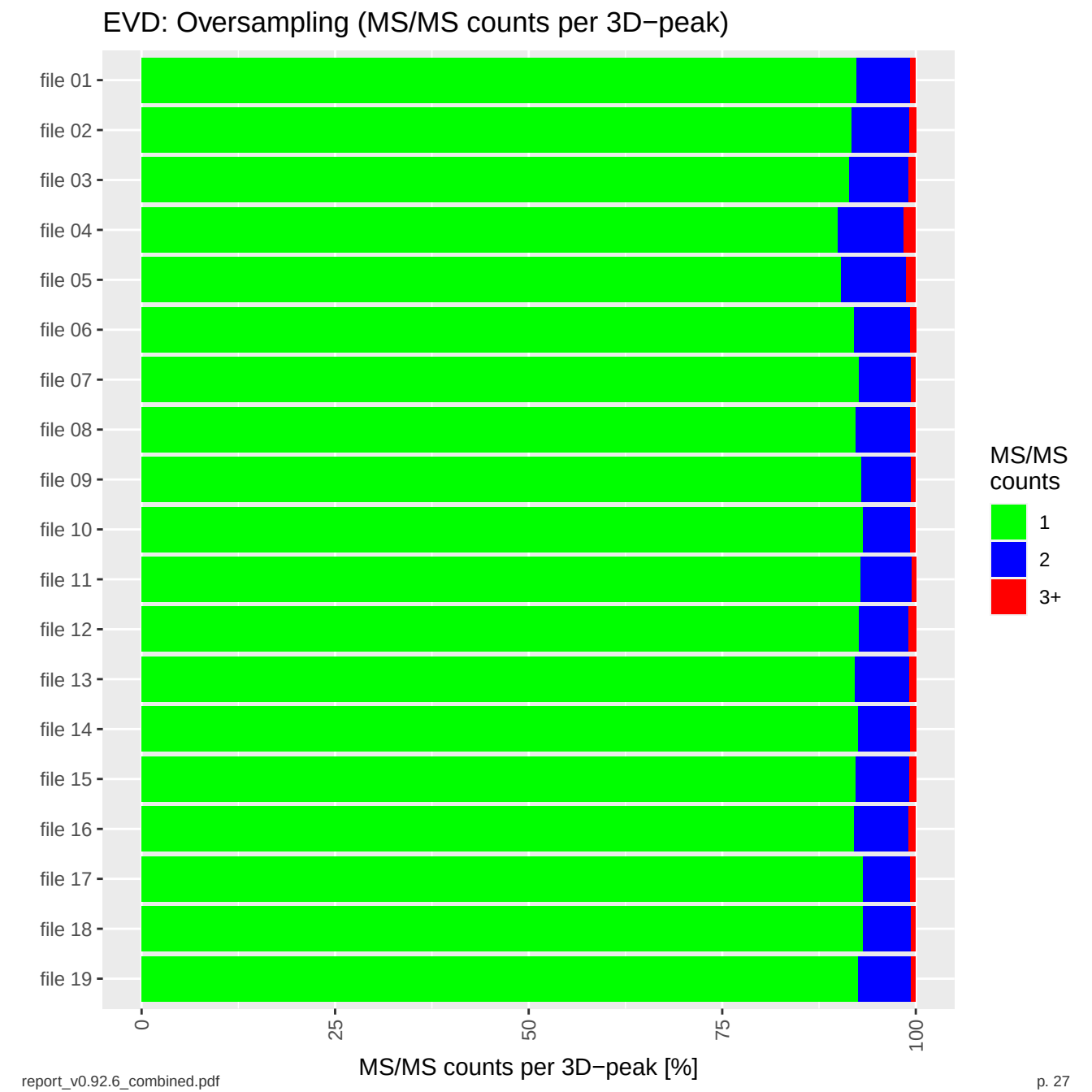

MSMSscans: Ion Injection Time over RT
ion injection time [ms]
80
60
40
20
0
25
50
75
100
retention time [min]
Raw file with average inj. time
file 01 (~76 ms)
file 02 (~75 ms)
file 03 (~76 ms)
file 04 (~76 ms)
file 05 (~73 ms)
file 06 (~73 ms)
file 07 (~74 ms)

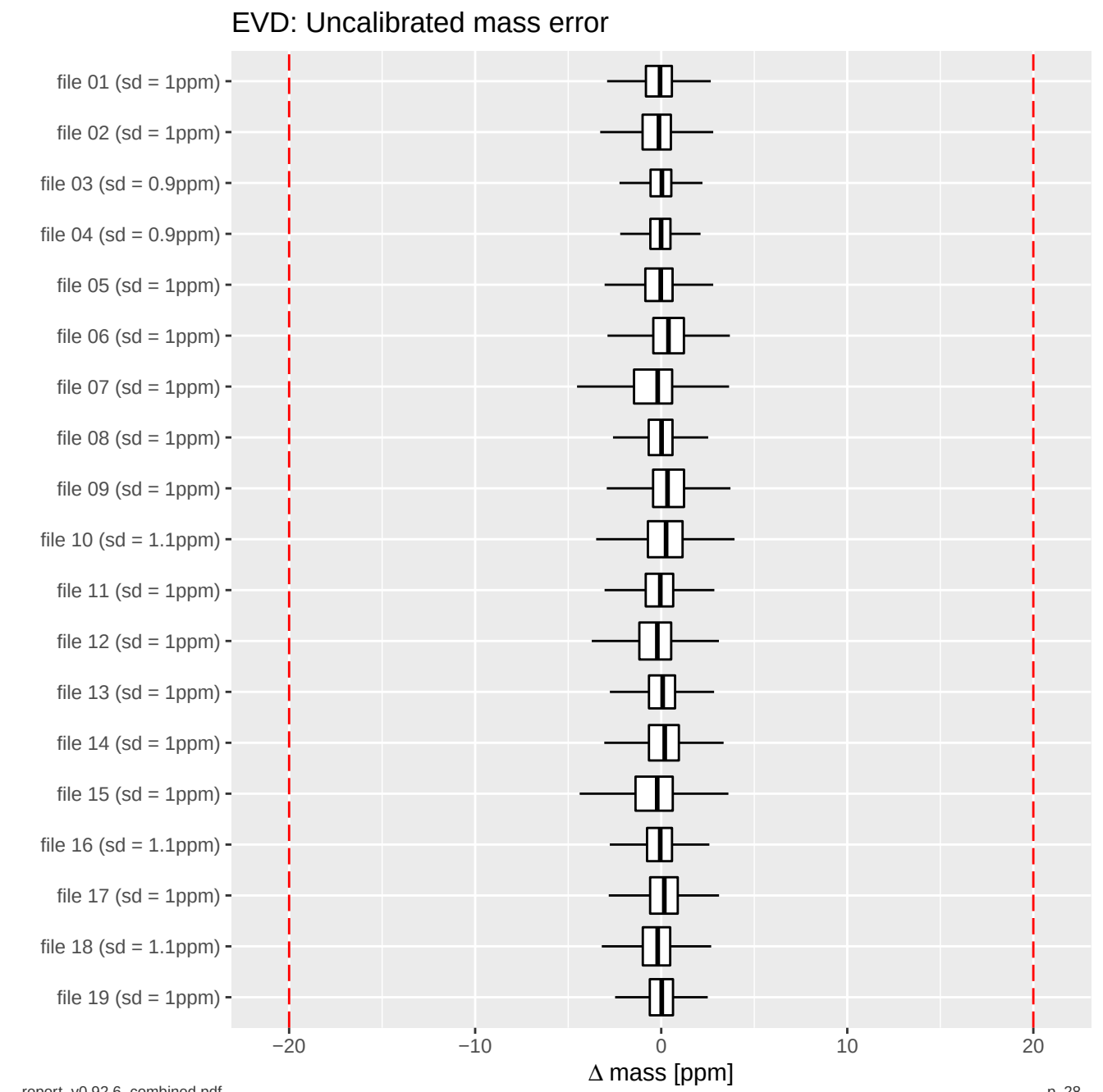

MSMSscans: Ion Injection Time over RT
ion injection time [ms]
80
60
40
20
0
25
50
75
100
retention time [min]
Raw file with average inj. time
file 08 (~75 ms)
file 09 (~73 ms)
file 10 (~73 ms)
file 11 (~75 ms)
file 12 (~72 ms)
file 13 (~73 ms)
file 14 (~73 ms)

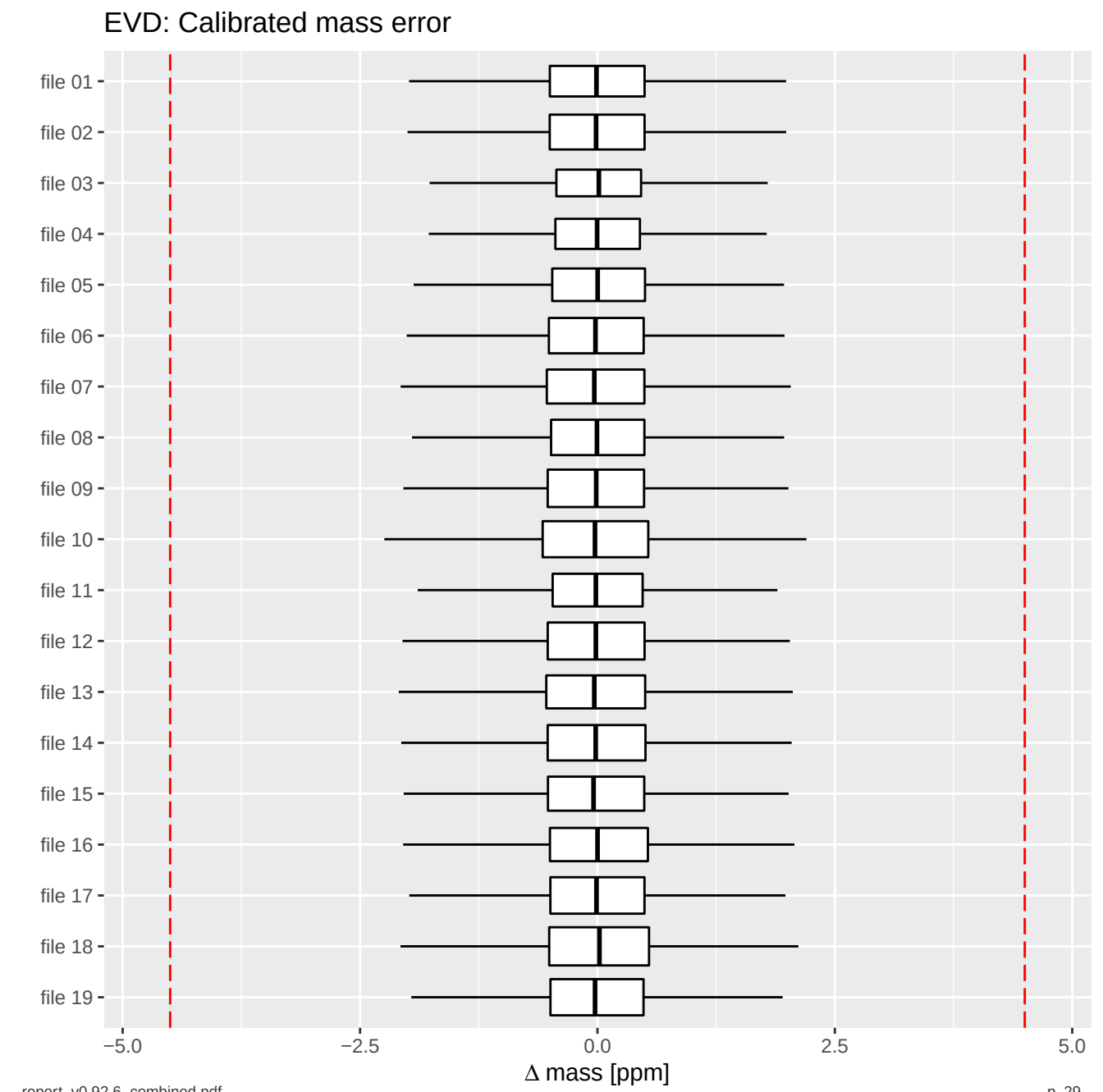

MSMSscans: Ion Injection Time over RT
ion injection time [ms]
80
60
40
20
0
25
50
75
100
retention time [min]
Raw file with average inj. time
file 15 (~74 ms)
file 16 (~76 ms)
file 17 (~73 ms)
file 18 (~74 ms)
file 19 (~74 ms)

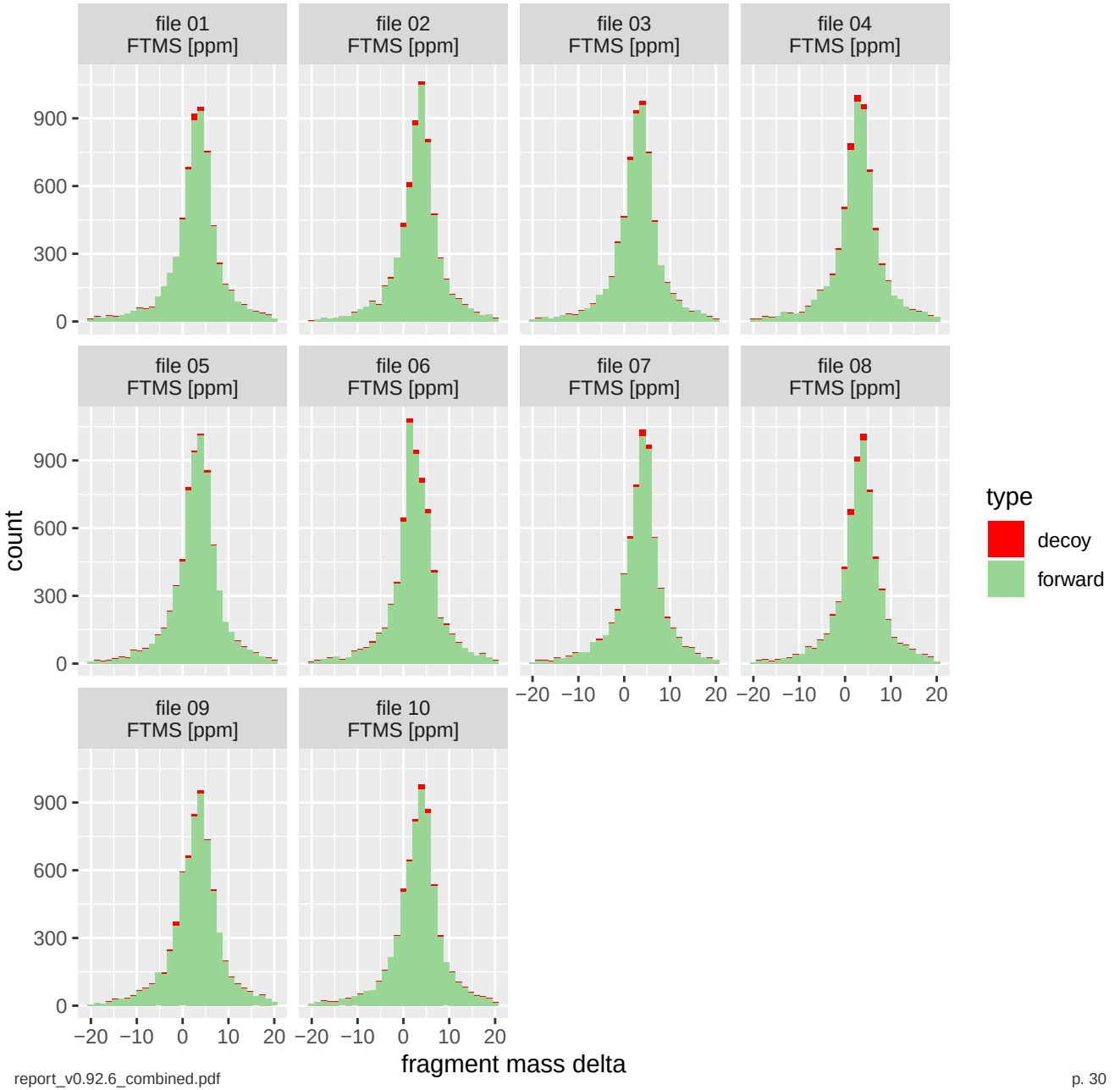

[experimental] MSMSscans: MS/MS intensity
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
0.0
2.5
5.0
7.5
intensity (log10)
MS/MS intensity
Base Peak
TIC

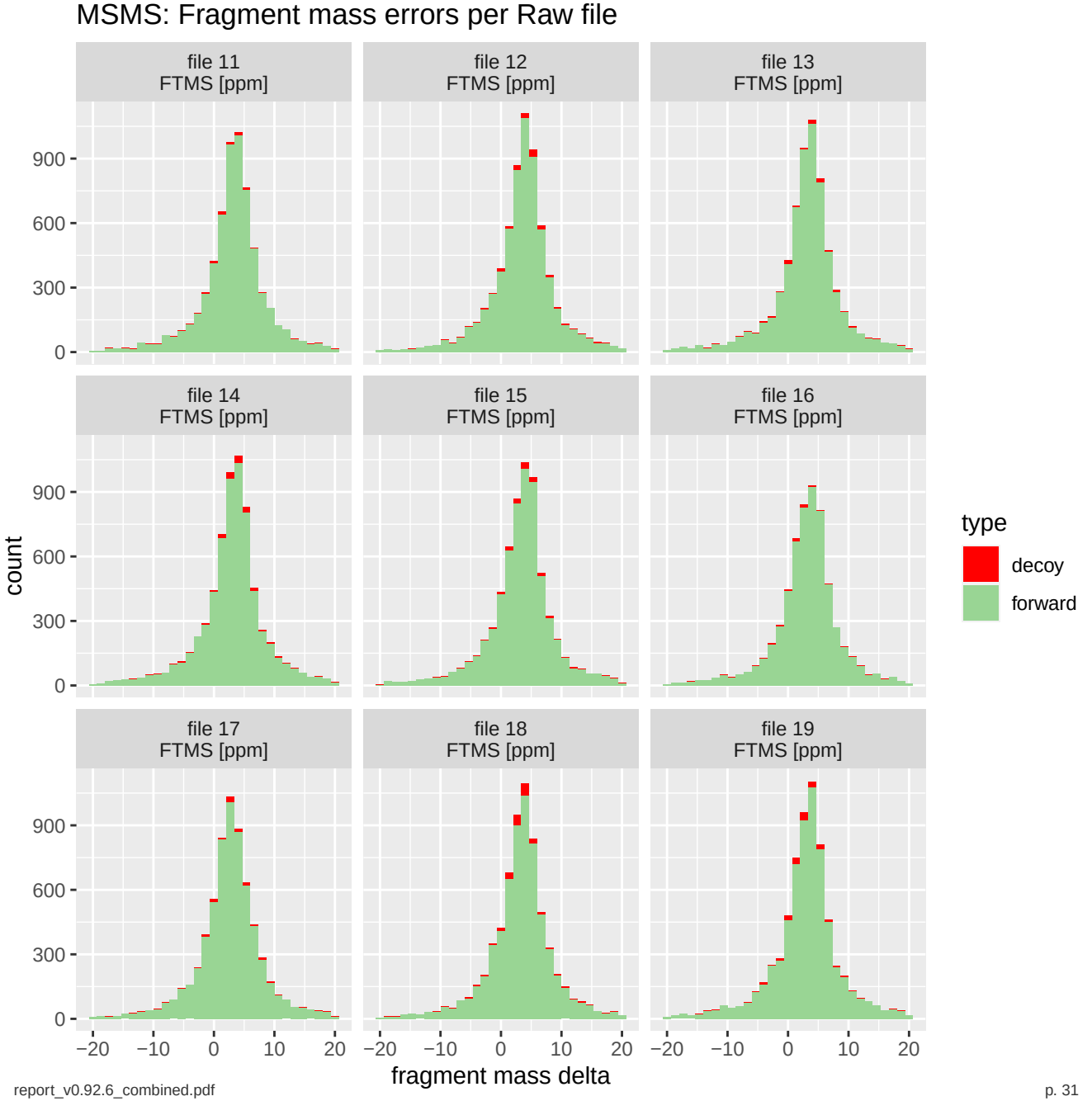

[experimental] MSMSscans: MS/MS intensity
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0.0
2.5
5.0
7.5
intensity (log10)
MS/MS intensity
Base Peak
TIC

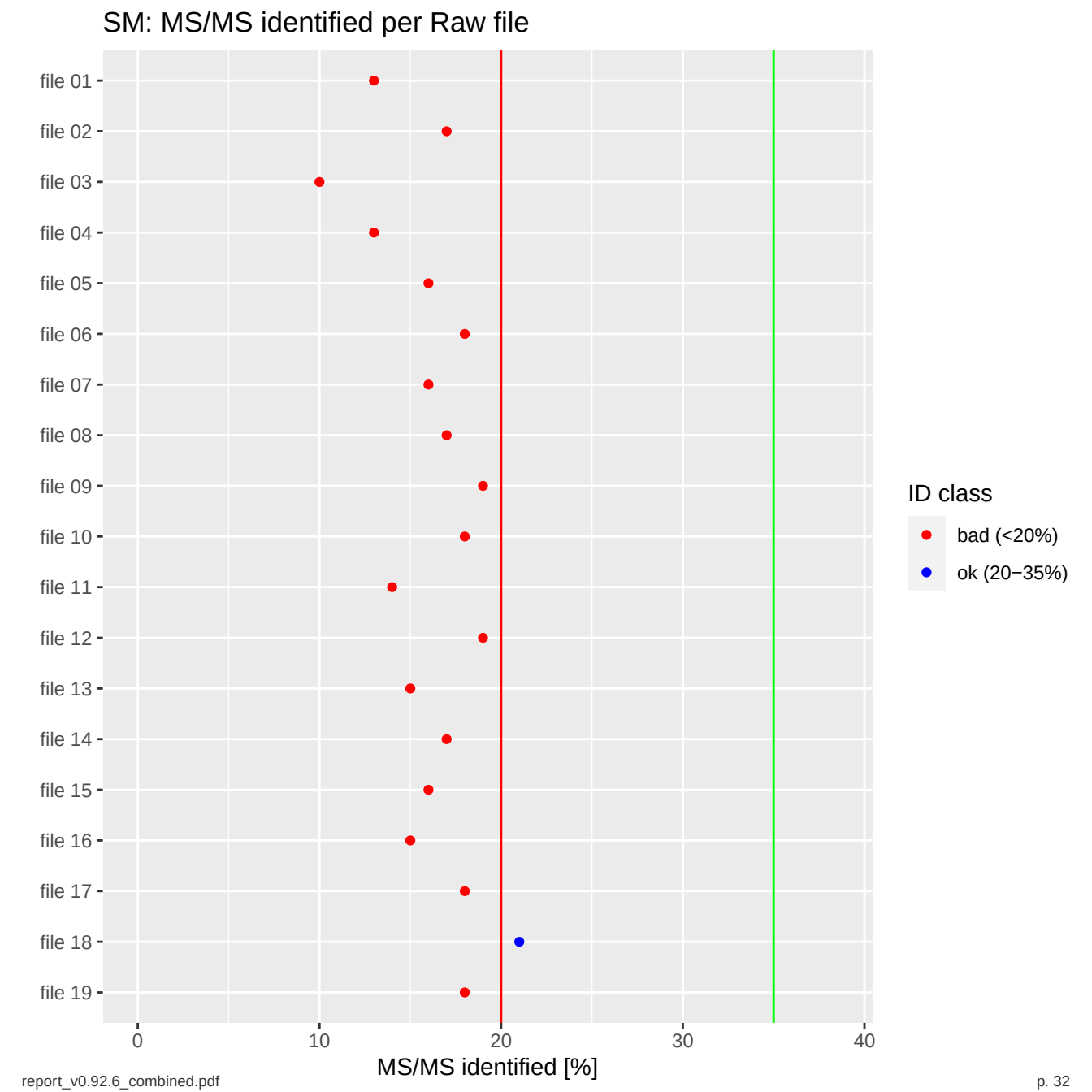

EVD: Oversampling (MS/MS counts per 3D−peak)
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0
25
50
75
100
MS/MS counts per 3D−peak [%]
MS/MS counts
1
2
3+


EVD: Uncalibrated mass error
file 01 (sd = 1ppm)
file 02 (sd = 1ppm)
file 03 (sd = 0.9ppm)
file 04 (sd = 0.9ppm)
file 05 (sd = 1ppm)
file 06 (sd = 1ppm)
file 07 (sd = 1ppm)
file 08 (sd = 1ppm)
file 09 (sd = 1ppm)
file 10 (sd = 1.1ppm)
file 11 (sd = 1ppm)
file 12 (sd = 1ppm)
file 13 (sd = 1ppm)
file 14 (sd = 1ppm)
file 15 (sd = 1ppm)
file 16 (sd = 1.1ppm)
file 17 (sd = 1ppm)
file 18 (sd = 1.1ppm)
file 19 (sd = 1ppm)
−20
−10
0
10
20
Δ mass [ppm]


EVD: Calibrated mass error
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
−5.0
−2.5
0.0
2.5
5.0
Δ mass [ppm]


MSMS: Fragment mass errors per Raw file
file 01
FTMS [ppm]
file 02
FTMS [ppm]
file 03
FTMS [ppm]
file 04
FTMS [ppm]
file 05
FTMS [ppm]
file 06
FTMS [ppm]
file 07
FTMS [ppm]
file 08
FTMS [ppm]
file 09
FTMS [ppm]
file 10
FTMS [ppm]
count
0
300
600
900
−20
−10
0
10
20
fragment mass delta
type
decoy
forward

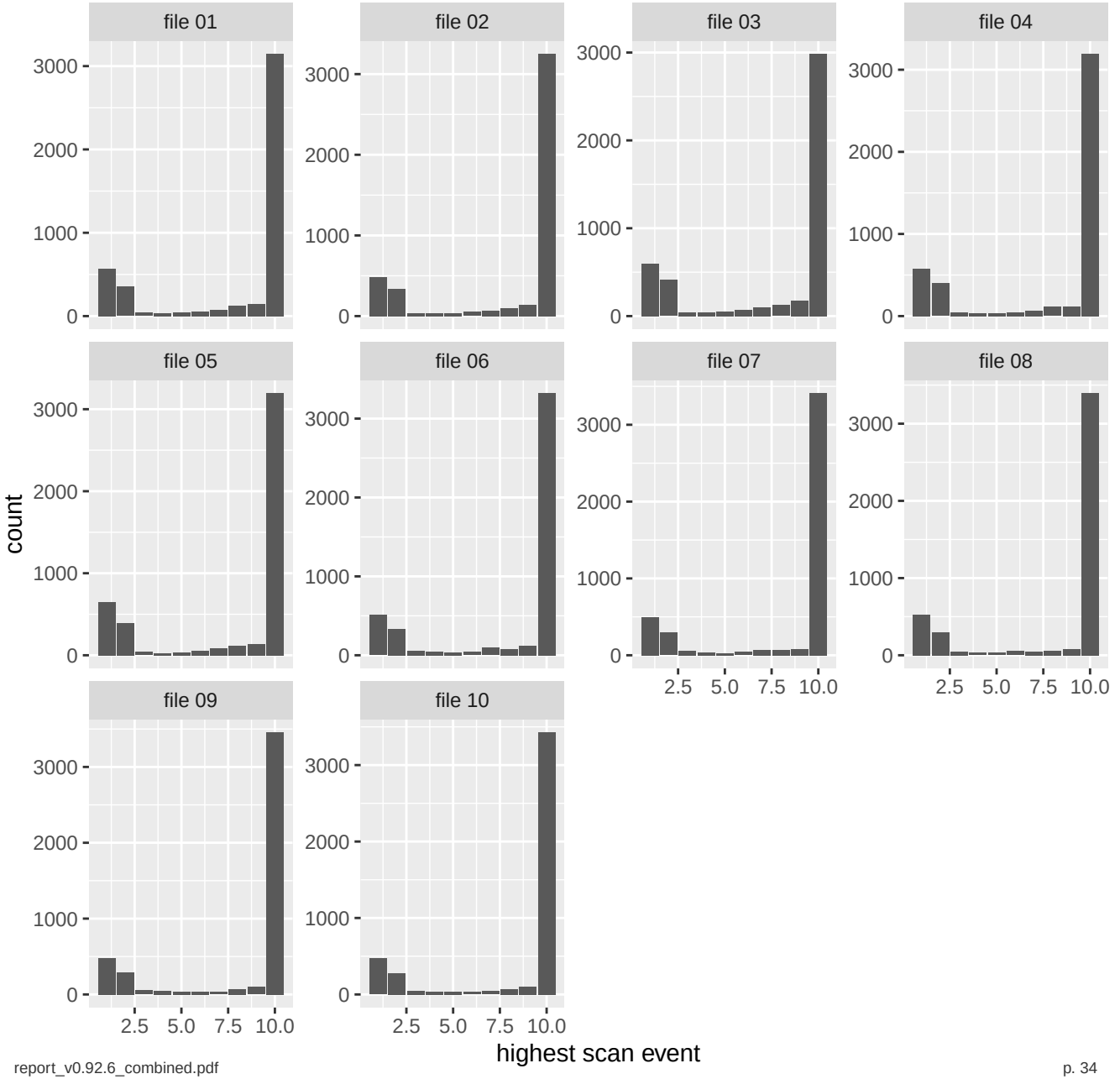

MSMS: Fragment mass errors per Raw file
file 11
FTMS [ppm]
file 12
FTMS [ppm]
file 13
FTMS [ppm]
file 14
FTMS [ppm]
file 15
FTMS [ppm]
file 16
FTMS [ppm]
file 17
FTMS [ppm]
file 18
FTMS [ppm]
file 19
FTMS [ppm]
count
0
300
600
900
−20
−10
0
10
20
fragment mass delta
type
decoy
forward

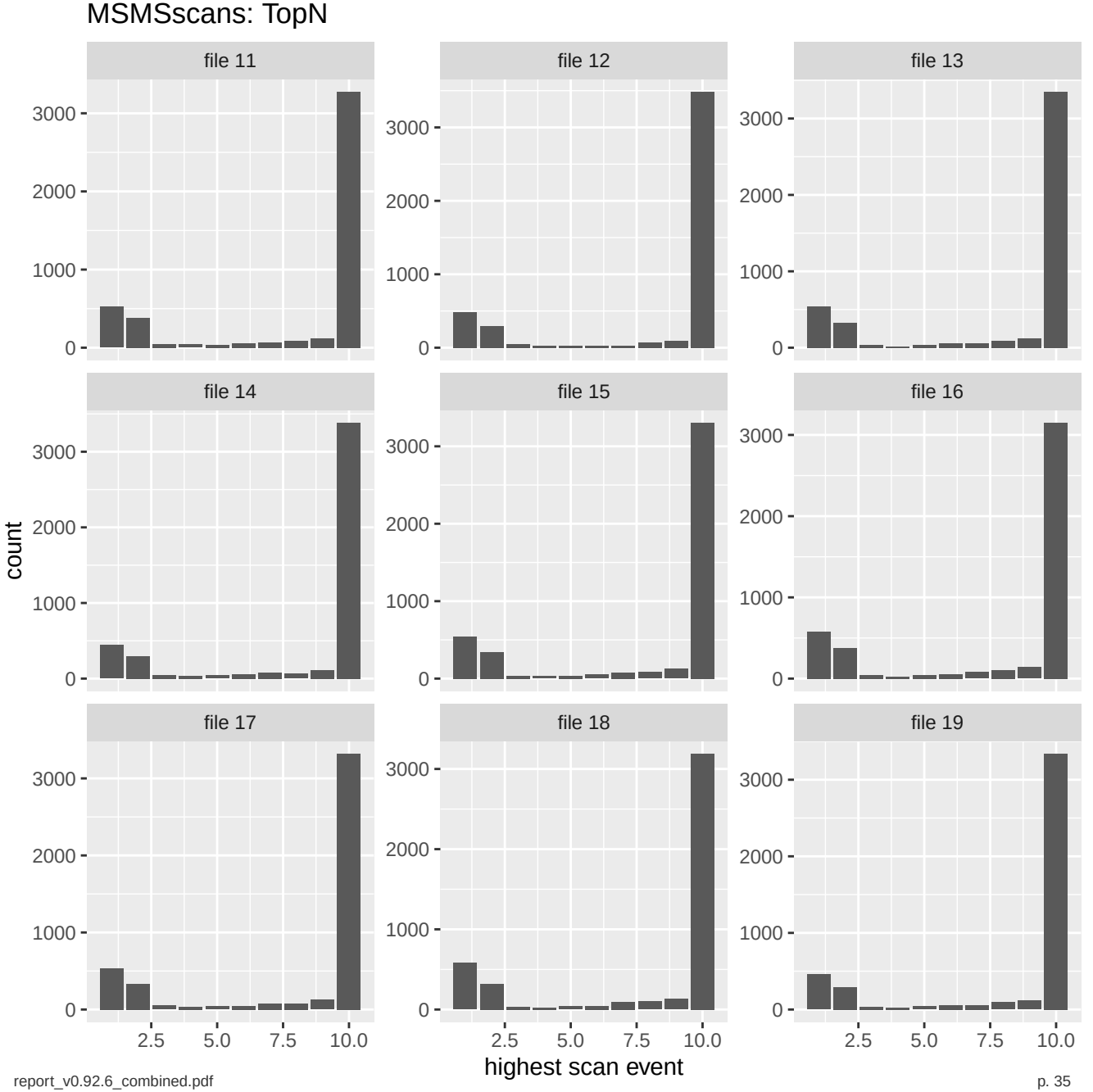

SM: MS/MS identified per Raw file
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0
10
20
30
40
MS/MS identified [%]
ID class
bad (<20%)
ok (20−35%)

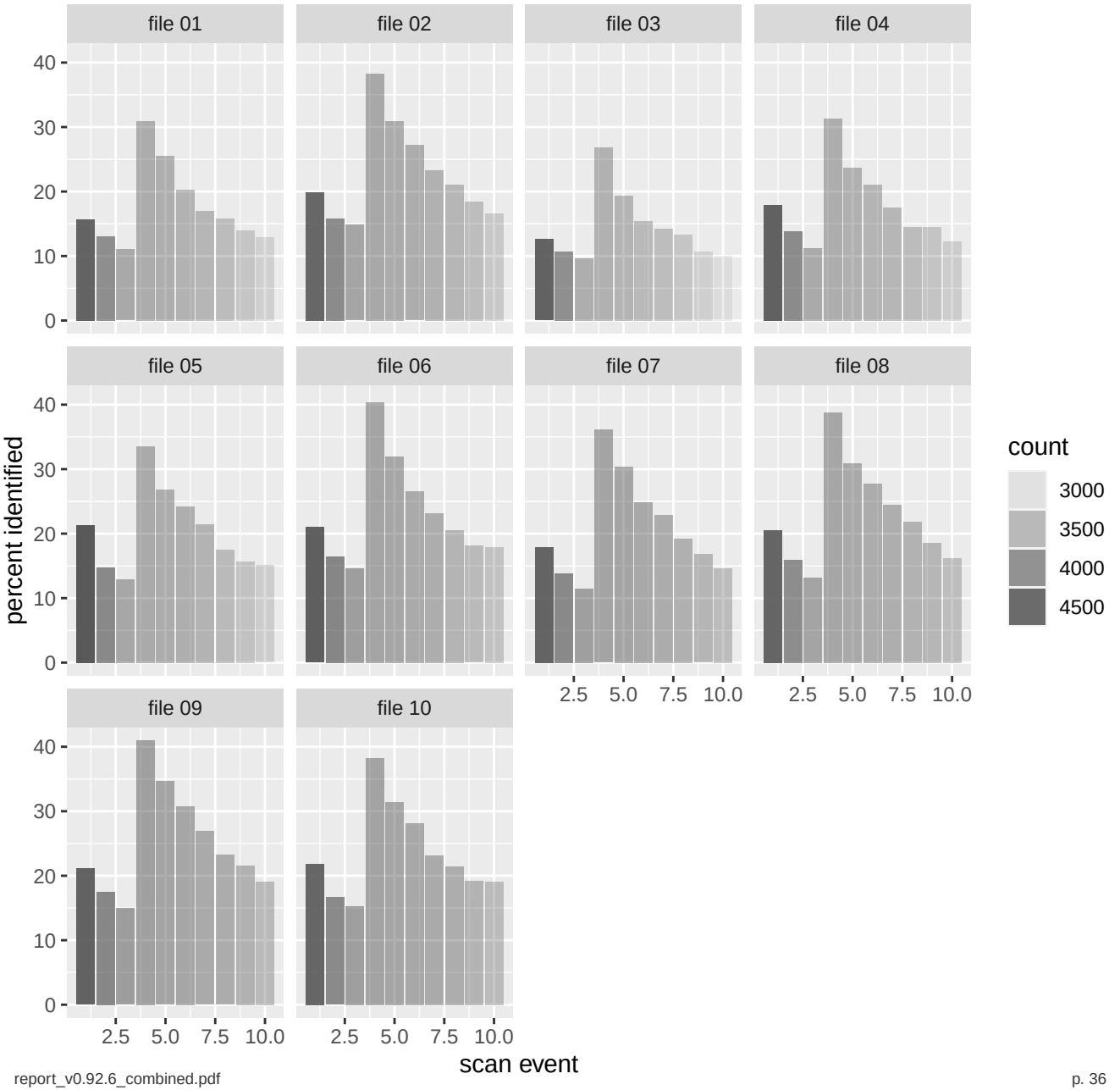
SM: Files with 'red' ID rate

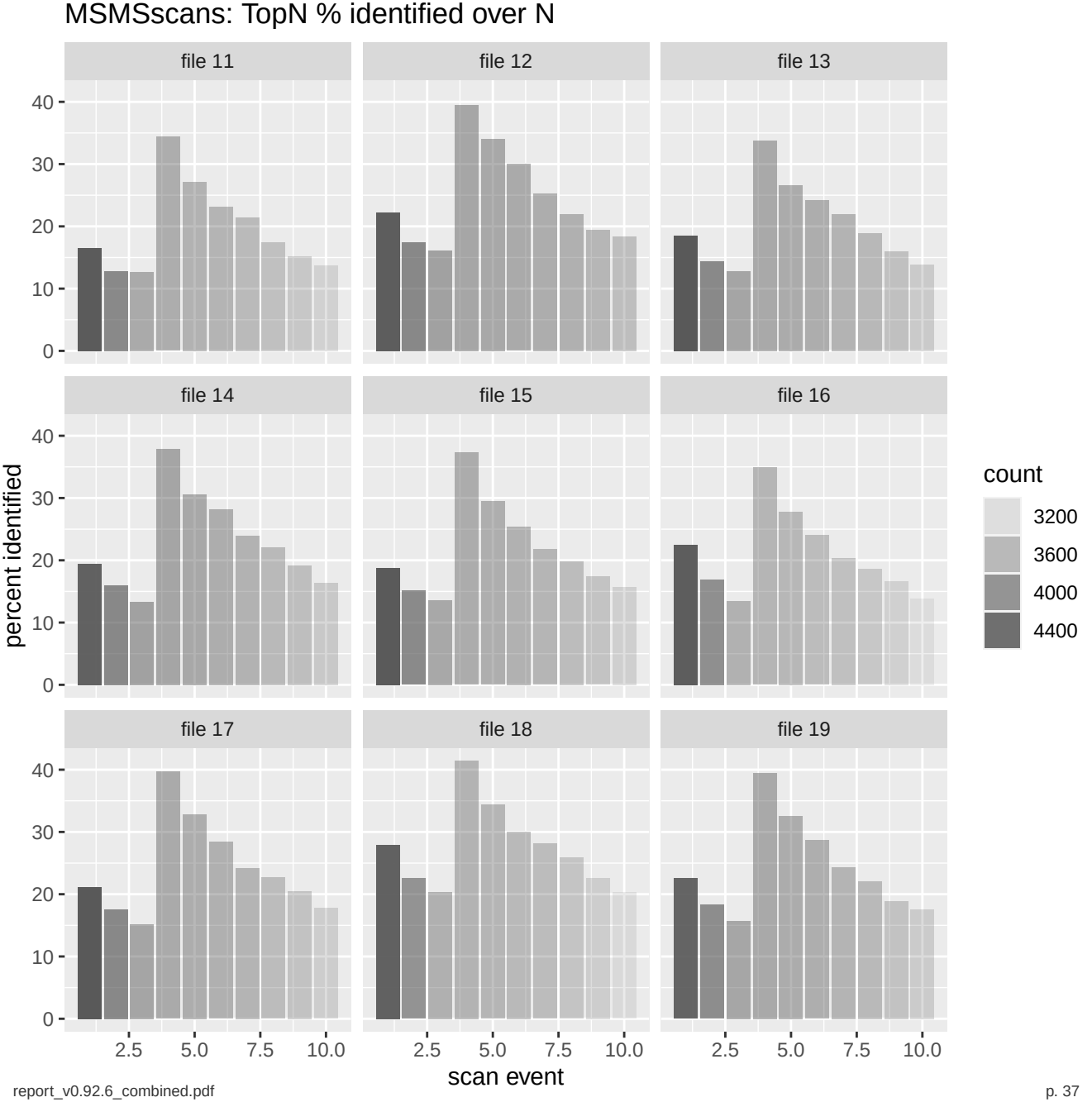
Raw file	% identified
RDEB_cSCC6.raw.thermo	13
RDEB_cSCC5.raw.thermo	17
RDEB_cSCC4.raw.thermo	10
RDEB_cSCC3.raw.thermo	13
RDEB_cSCC2.raw.thermo	16
RDEB_cSCC1.raw.thermo	18
metast_cSCC13.raw.thermo	16
metast_cSCC12.raw.thermo	17
metast_cSCC11.raw.thermo	19
metast_cSCC10.raw.thermo	18
metast_cSCC9.raw.thermo	14
metast_cSCC8.raw.thermo	19
metast_cSCC7.raw.thermo	15
metast_cSCC6.raw.thermo	17
metast_cSCC5.raw.thermo	16
metast_cSCC4.raw.thermo	15
metast_cSCC3.raw.thermo	18
metast_cSCC1.raw.thermo	18

95% of samples)


MSMSscans: TopN
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
count
highest scan event
0
1000
2000
3000
2.5
5.0
7.5
10.0

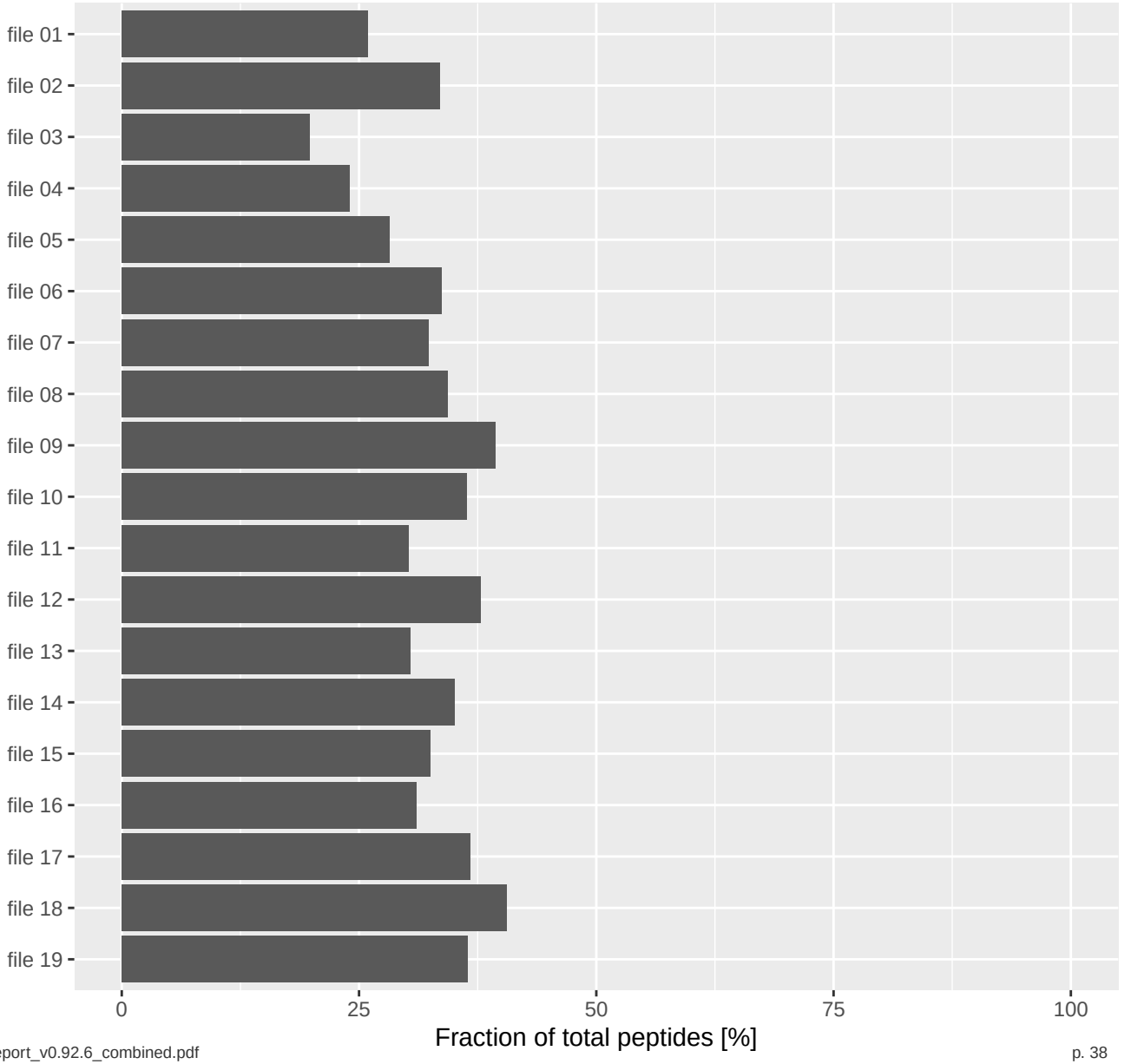

MSMSscans: TopN
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
count
highest scan event
0
1000
2000
3000
2.5
5.0
7.5
10.0

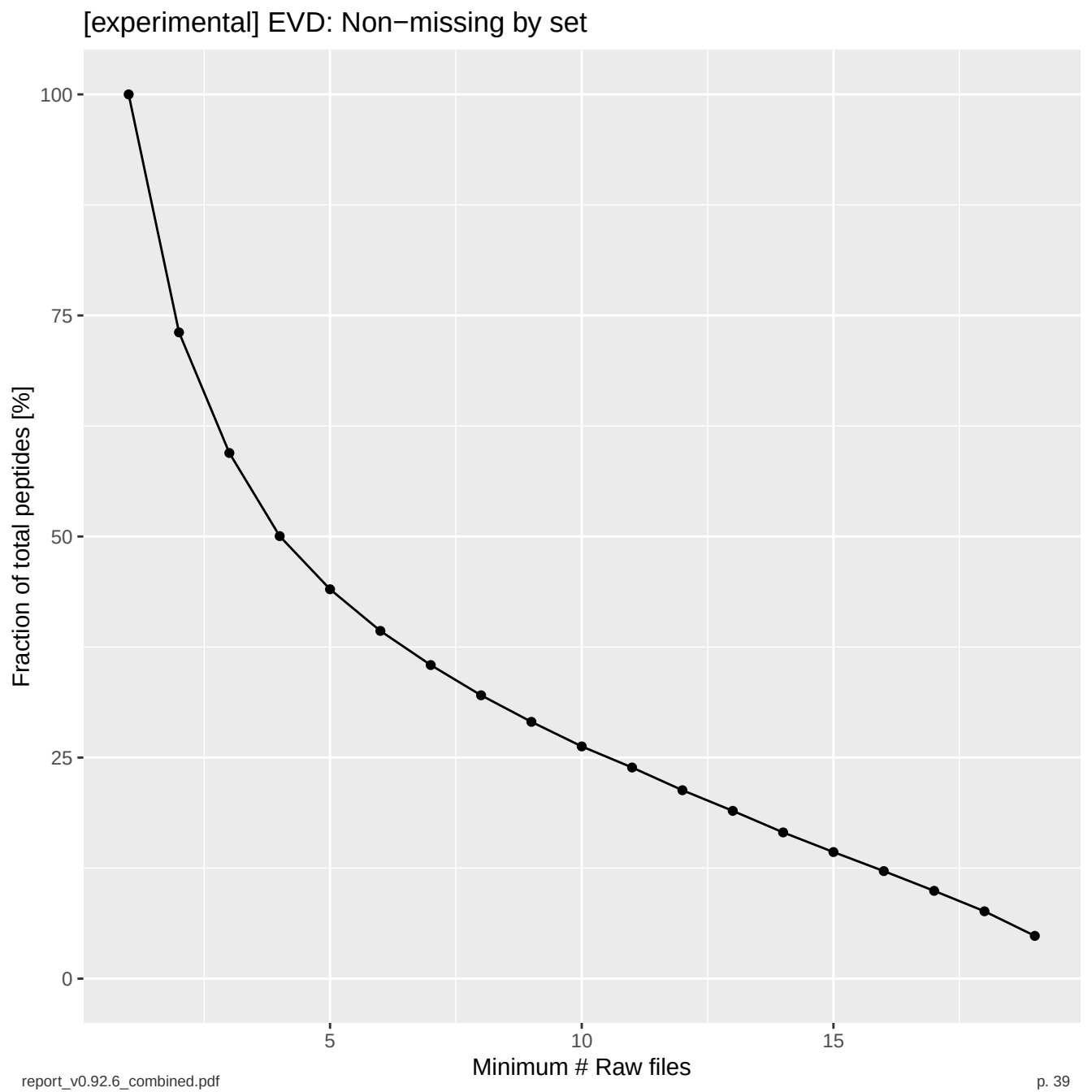

MSMSscans: TopN % identified over N
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
percent identified
0
10
20
30
40
2.5
5.0
7.5
10.0
scan event
count
3000
3500
4000
4500


MSMSscans: TopN % identified over N
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
percent identified
0
10
20
30
40
2.5
5.0
7.5
10.0
scan event
count
3200
3600
4000
4400

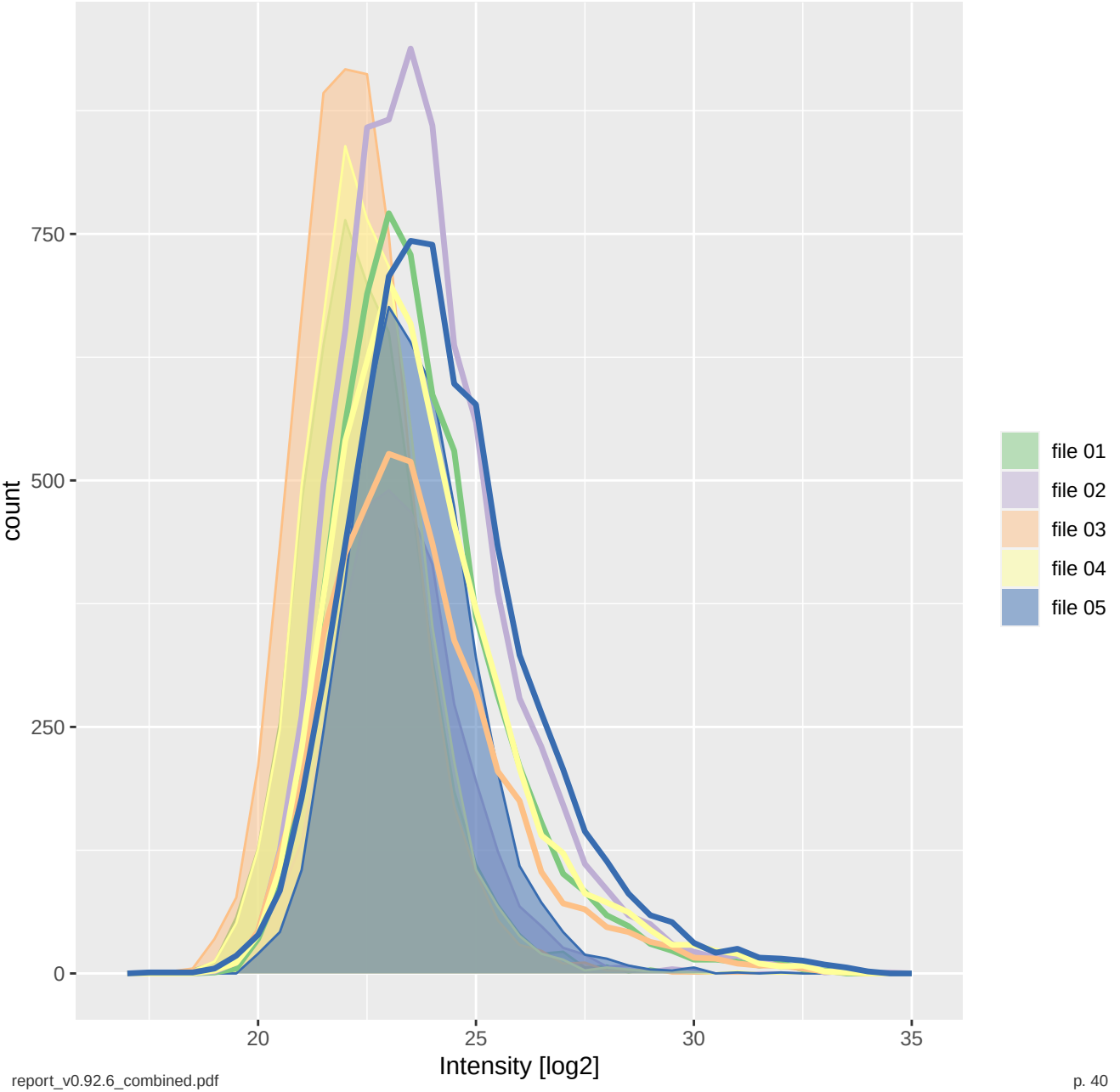
[experimental] EVD: Non−Missing Peptides

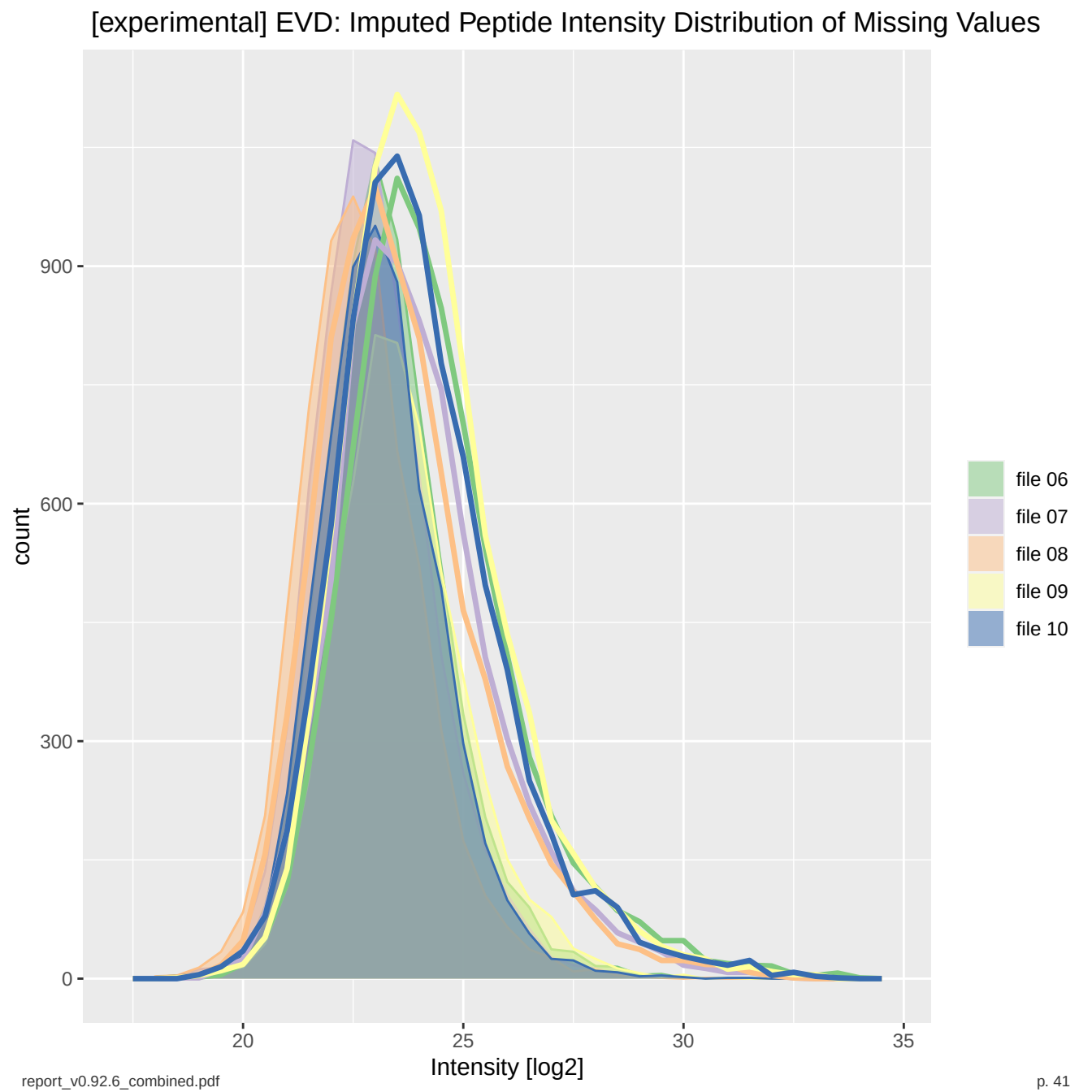
compared to all peptides seen in experiment

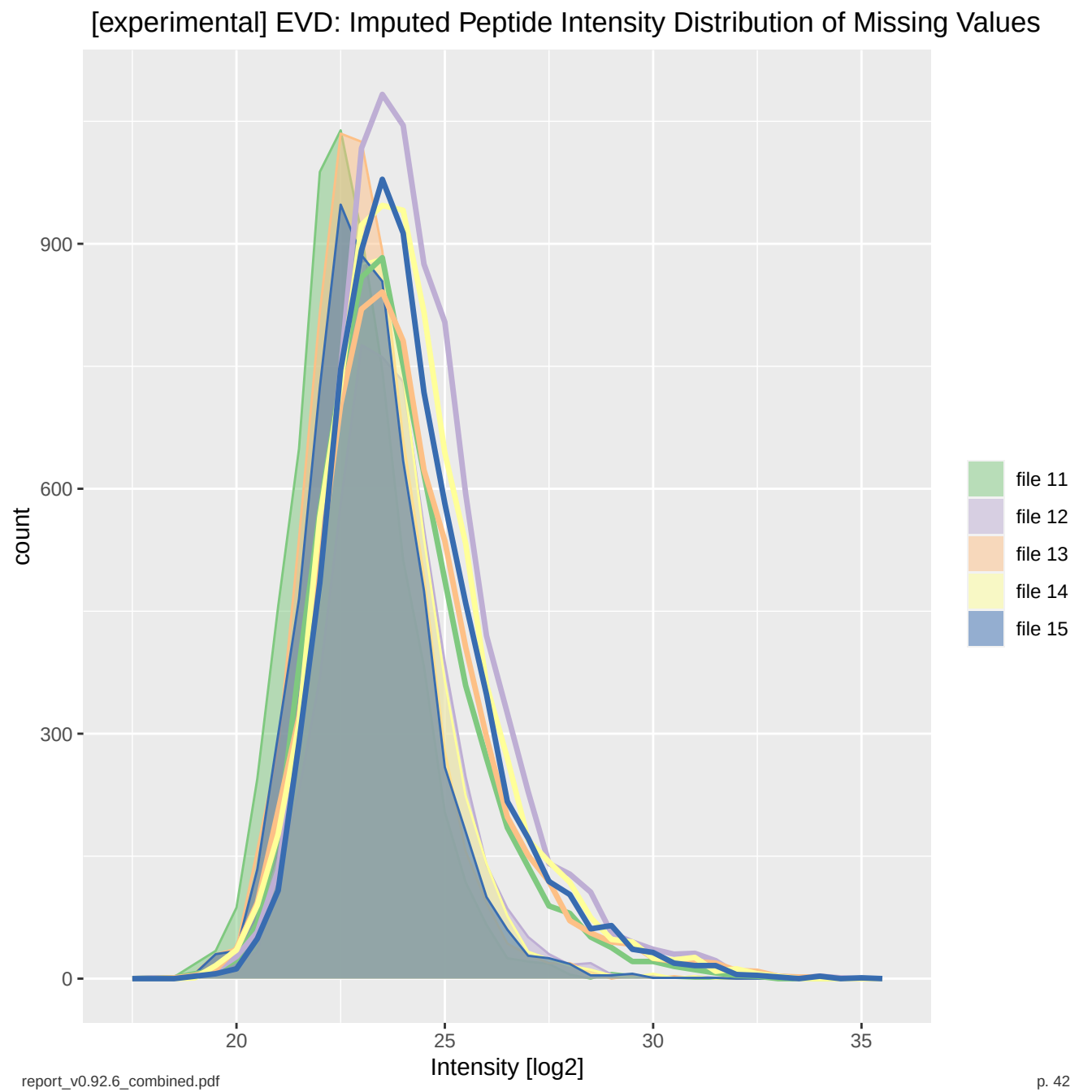


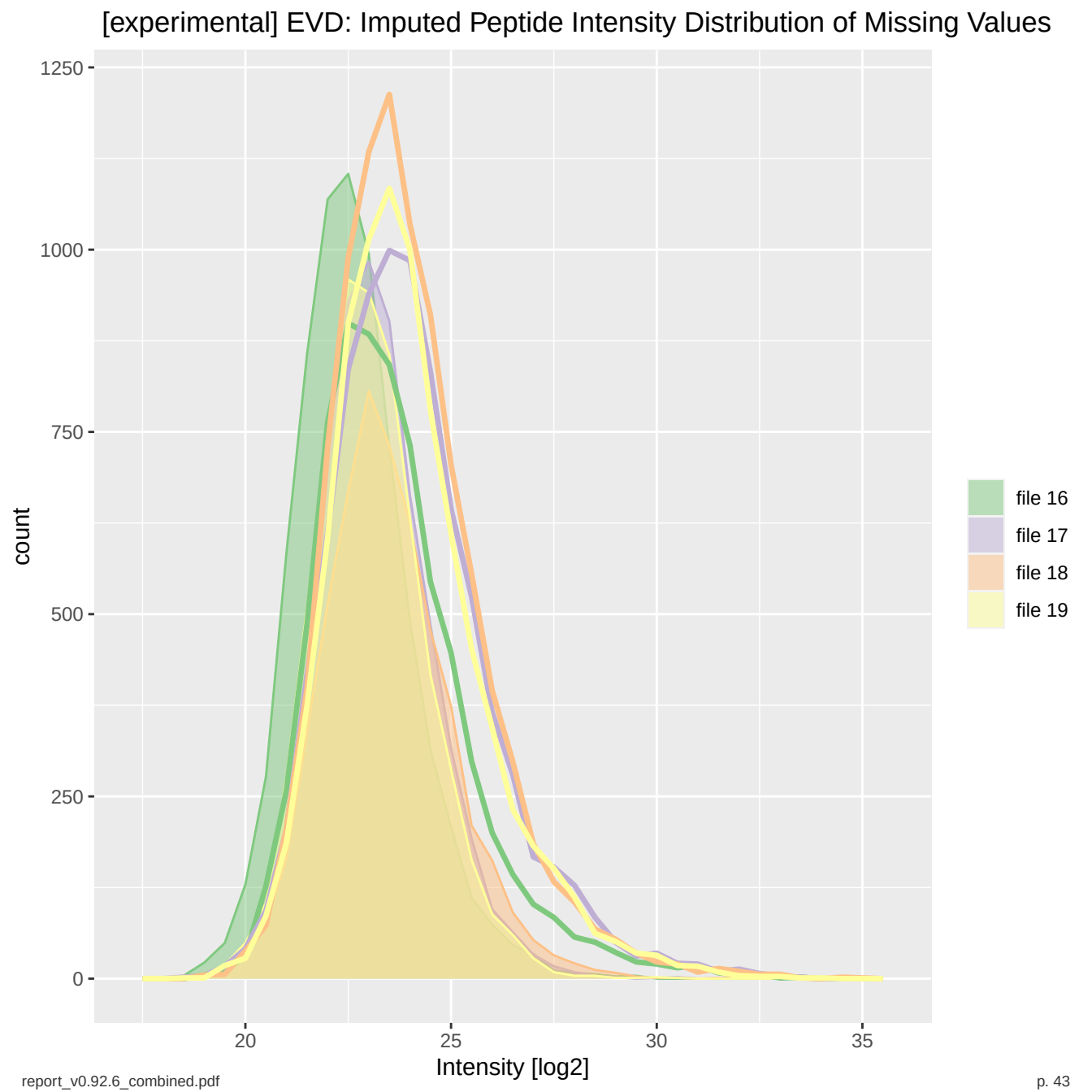

[experimental] EVD: Non−missing by set
100
75
50
25
0
Fraction of total peptides [%]
5
10
15
Minimum # Raw files

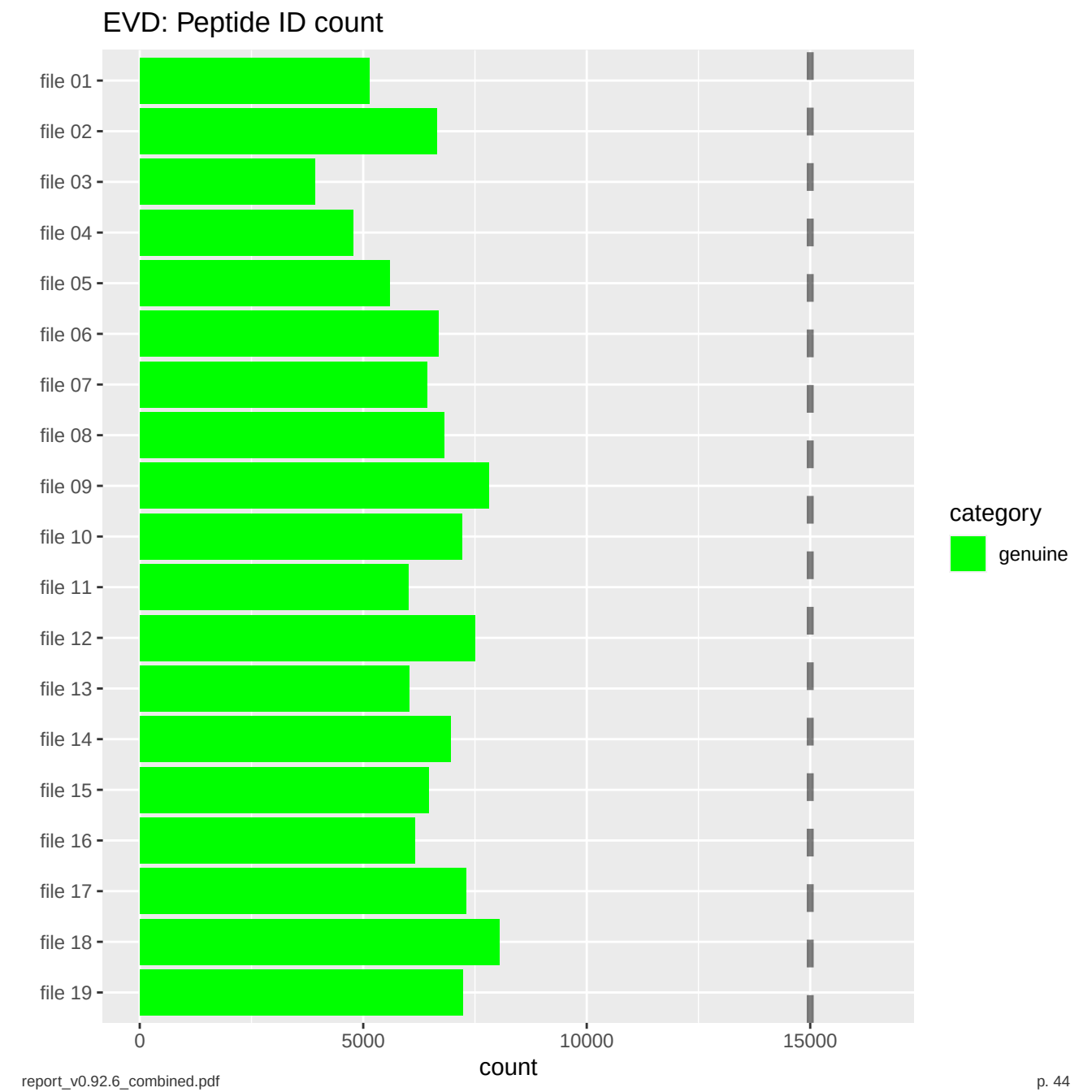
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values

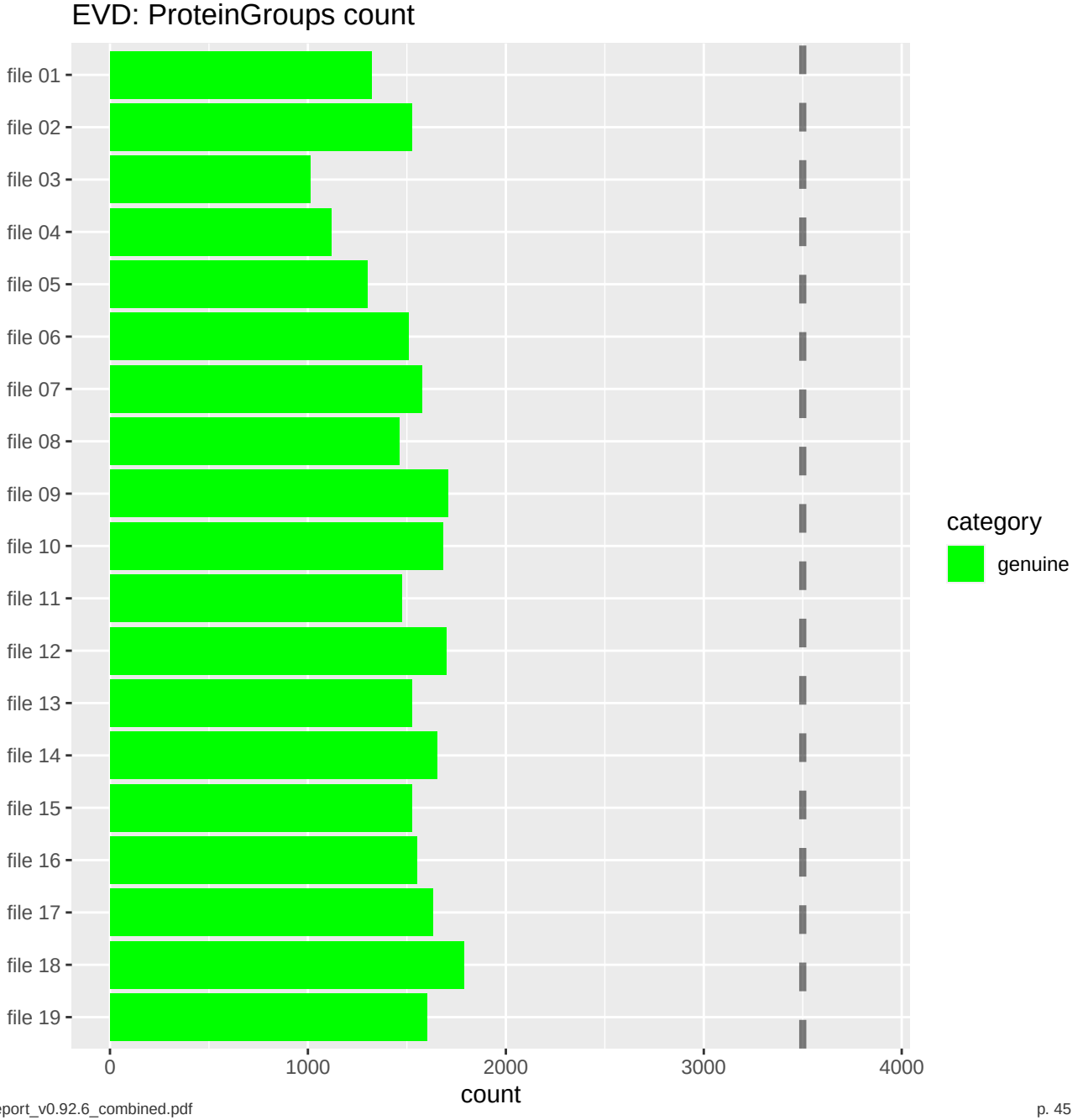



[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values
count
900
600
300
0
20
25
30
35
Intensity [log2]
file 06
file 07
file 08
file 09
file 10


[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values
count
900
600
300
0
20
25
30
35
Intensity [log2]
file 11
file 12
file 13
file 14
file 15


[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values
count
1250
1000
750
500
250
0
20
25
30
35
Intensity [log2]
file 16
file 17
file 18
file 19


EVD: Peptide ID count
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0
5000
10000
15000
count
category
genuine


EVD: ProteinGroups count
file 01
file 02
file 03
file 04
file 05
file 06
file 07
file 08
file 09
file 10
file 11
file 12
file 13
file 14
file 15
file 16
file 17
file 18
file 19
0
1000
2000
3000
4000
count
category
genuine