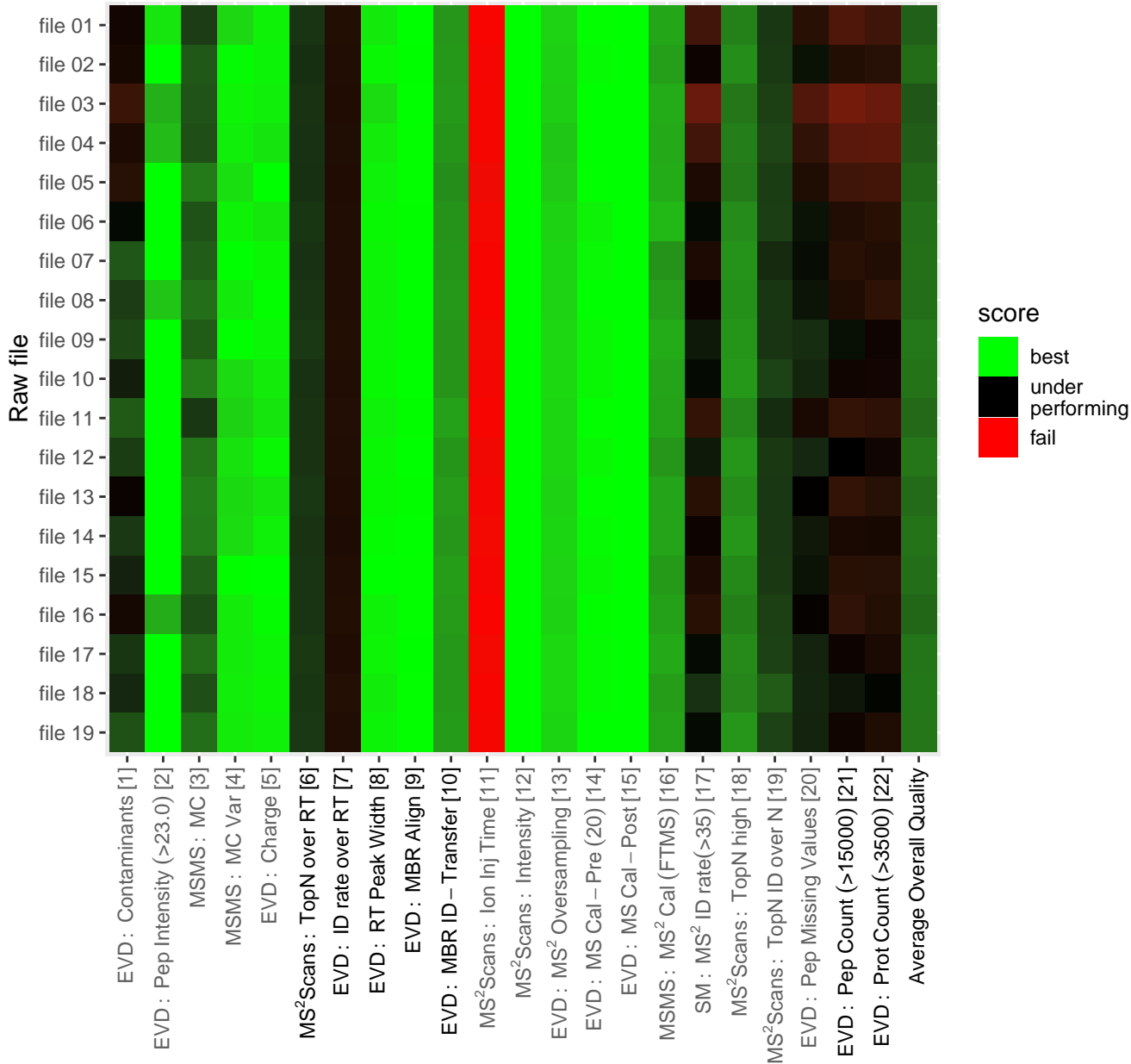


Performance overview



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 ..	0.01
Advanced site intensities	True	MS/MS deisotoping tolerance ..	Da
Alignment ion mobility windo..	1	MS/MS deisotoping tolerance ..	7
Alignment time window [min]	20	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	06/03/2021 00:23:50	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-c40mq-0648.n novalocal	MS/MS water loss (TOF)	True
Main search max. combination..	200	MS/MS water loss (Unknown)	True
Match between runs	True	Peptides used for protein qu..	Razor
Match ion mobility window [i..	0.05	Protein FDR	0.01
Match unidentified features	False	PSM FDR	0.01

/data/dnb03/galaxy_db/files/0/7/e/dataset_07e07cb6-d3eb-40b2-9040-eca7c86c7dd3.dat

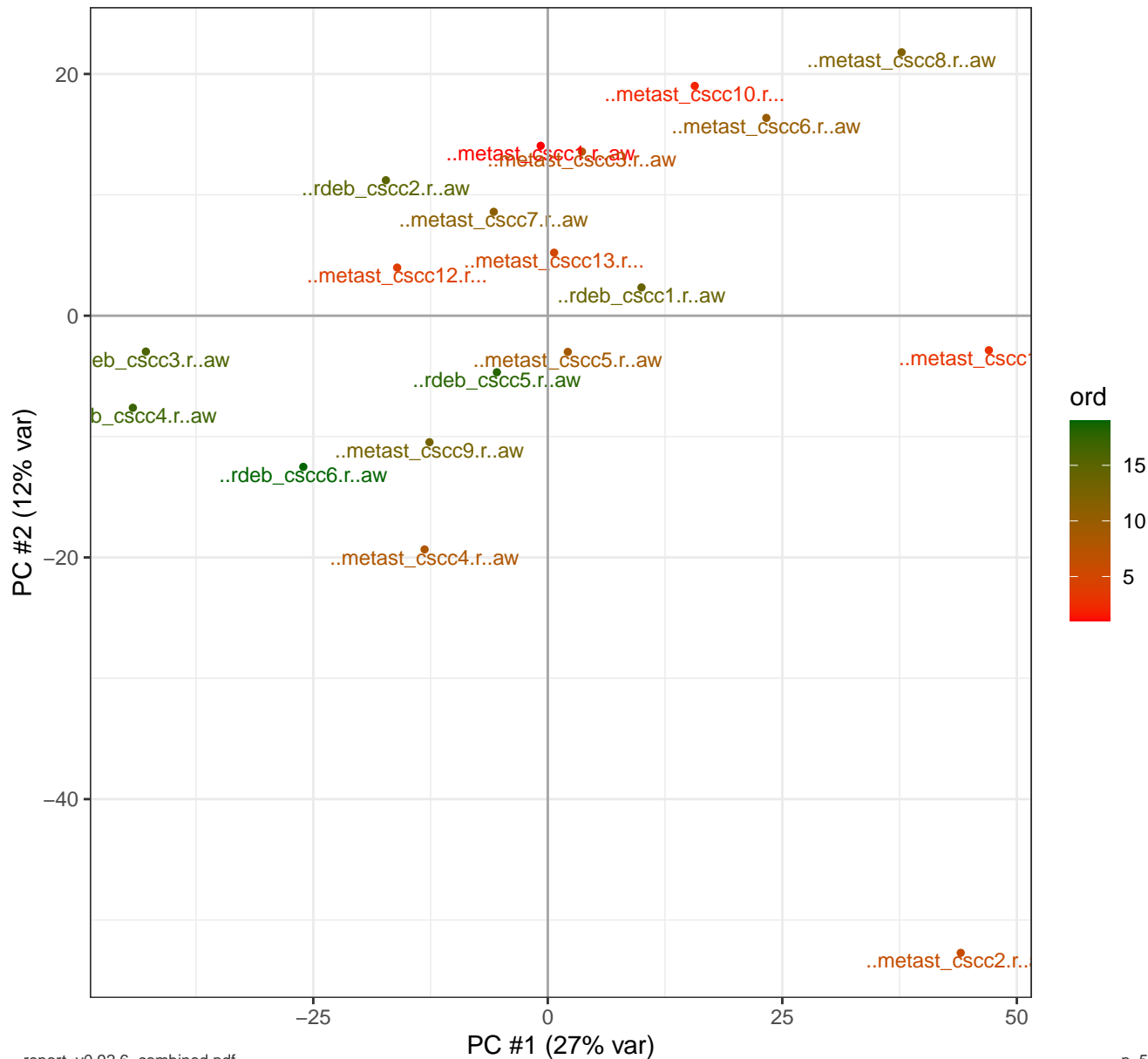
PAR: parameters

parameter	value	parameter	value
Matching time window [min]	0.7	PSM FDR Crosslink	0.01
Max mods in site table	3	Razor protein FDR	True
Max. peptide length for unsp..	25	Require MS/MS for LFQ compar..	True
Max. peptide mass [Da]	4600	Second peptides	True
Min. delta score for modifie..	6	Separate LFQ in parameter gr..	False
Min. delta score for unmodif..	0	Site FDR	0.01
Min. peptide Length	7	Site tables	Oxidation (M)Sites.txt
Min. peptide length for unsp..	8	Stabilize large LFQ ratios	True
Min. peptides	1	Temporary folder	
Min. razor peptides	1	Top MS/MS peaks per Da inter..	12
Min. score for modified pept..	40	Top MS/MS peaks per Da inter..	8
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	10
Min. unique peptides	1	Top MS/MS peaks per Da inter..	12
Modifications included in pr..	Acetyl (Protein N-term) Oxidation (M)	Use delta score	False
MS/MS ammonia loss (FTMS)	True	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (ITMS)	True	Use only unmodified peptides..	True
MS/MS ammonia loss (TOF)	True	User name	galaxy
MS/MS ammonia loss (Unknown)	True	Variation mode	None
MS/MS deisotoping (FTMS)	True	Version	1.6.10.43
MS/MS deisotoping (ITMS)	False	Write accumulatedPasefMsmsSc..	True
MS/MS deisotoping (TOF)	True	Write allPeptides table	True
MS/MS deisotoping (Unknown)	True	Write ms3Scans table	True
MS/MS deisotoping tolerance ..	7	Write msmsScans table	True
MS/MS deisotoping tolerance ..	ppm	Write msScans table	False
MS/MS deisotoping tolerance ..	0.15	Write mzRange table	True
MS/MS deisotoping tolerance ..	Da	Write pasefMsmsScans table	True

/data/dnb03/galaxy_db/files/0/7/e/dataset_07e07cb6-d3eb-40b2-9040-eca7c86c7dd3.dat

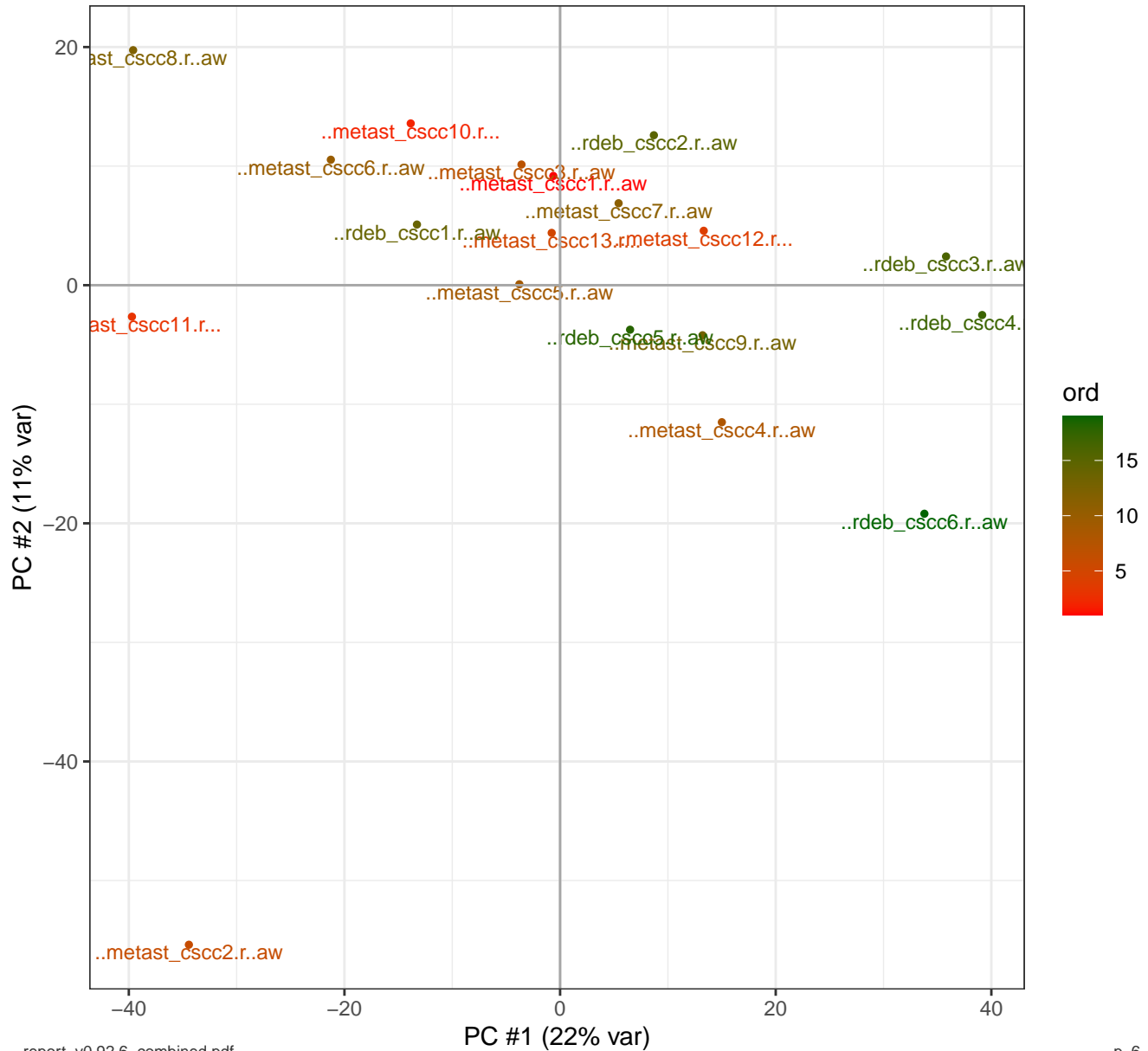
PG: PCA of 'raw intensity'

(excludes contaminants)

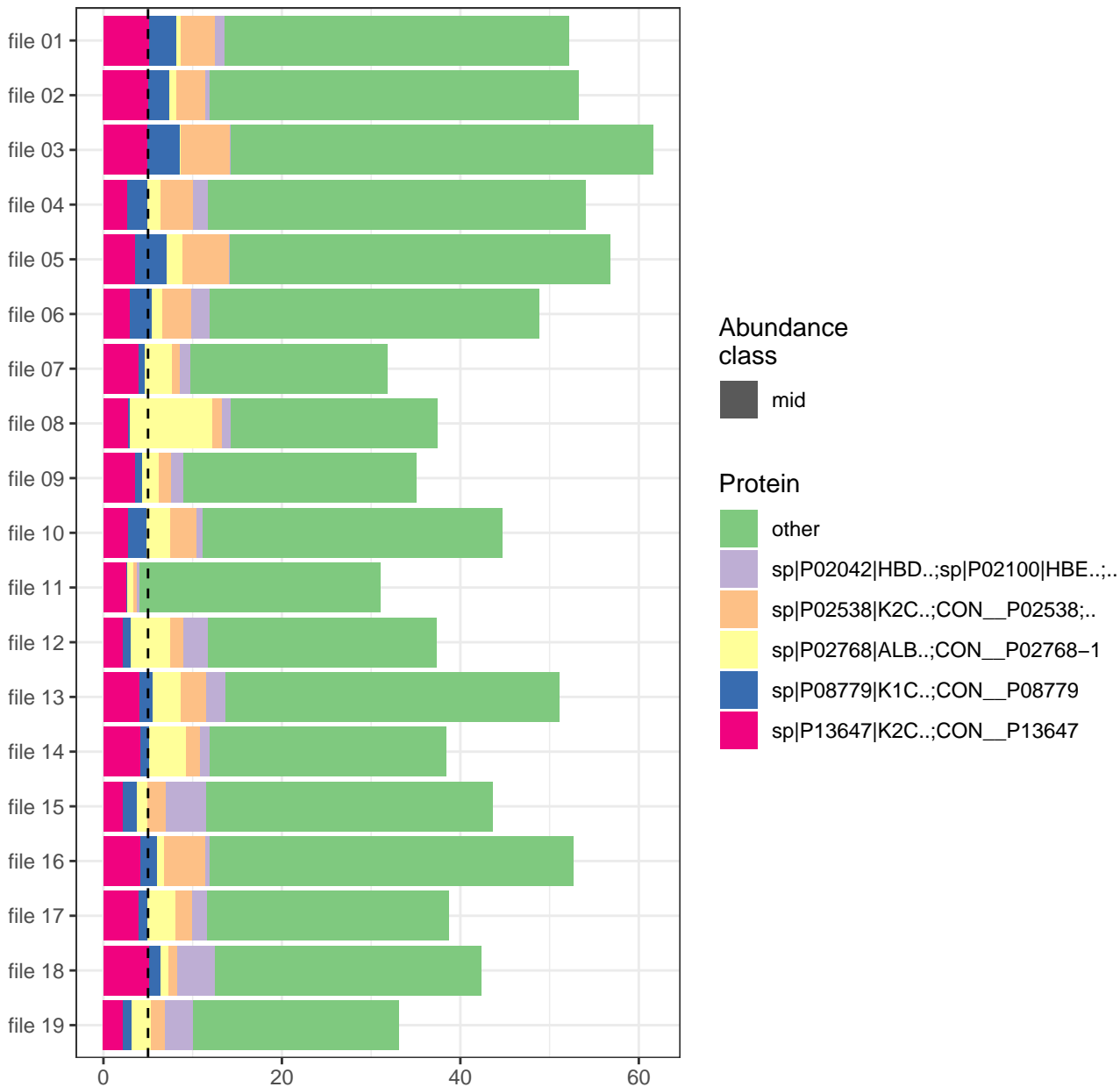


PG: PCA of 'lfq intensity'

(excludes contaminants)



EVD: Top5 Contaminants per Raw file



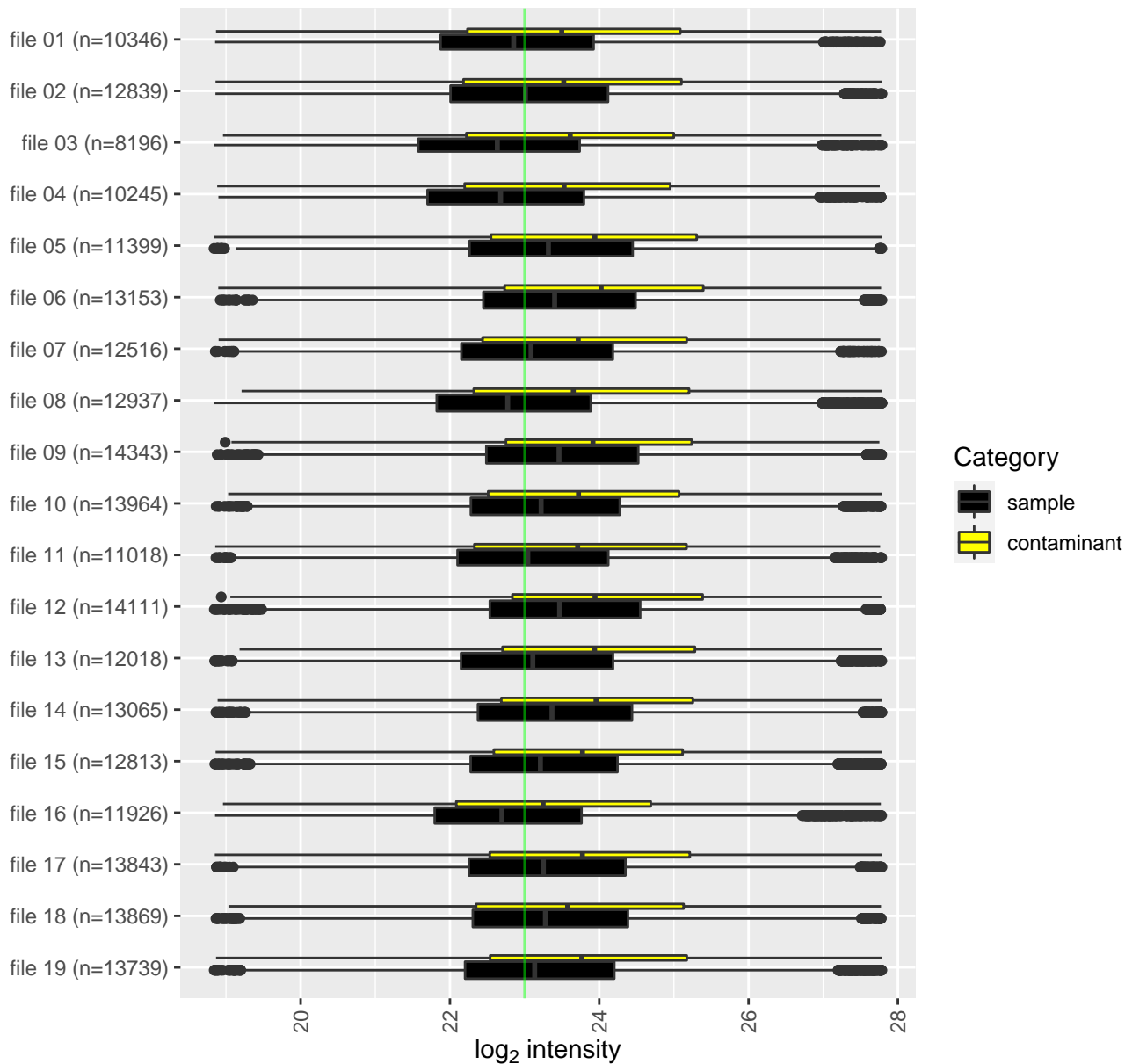
EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

Did you use the correct database?

EVD: peptide intensity distribution

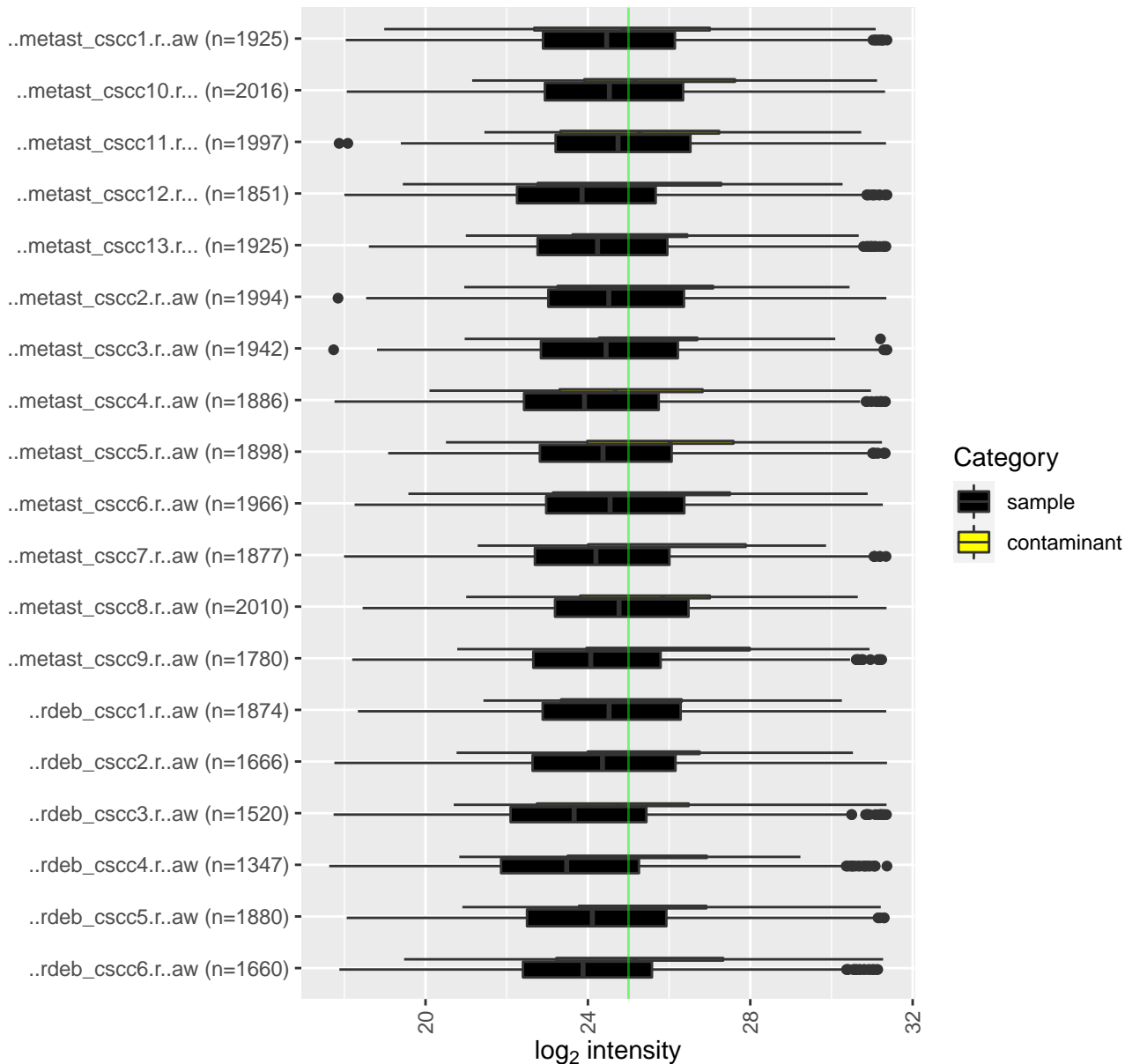
RSD 1.1% (expected < 5%)



PG: intensity distribution

RSD 1.5% (w/o zero int.; expected < 5%)

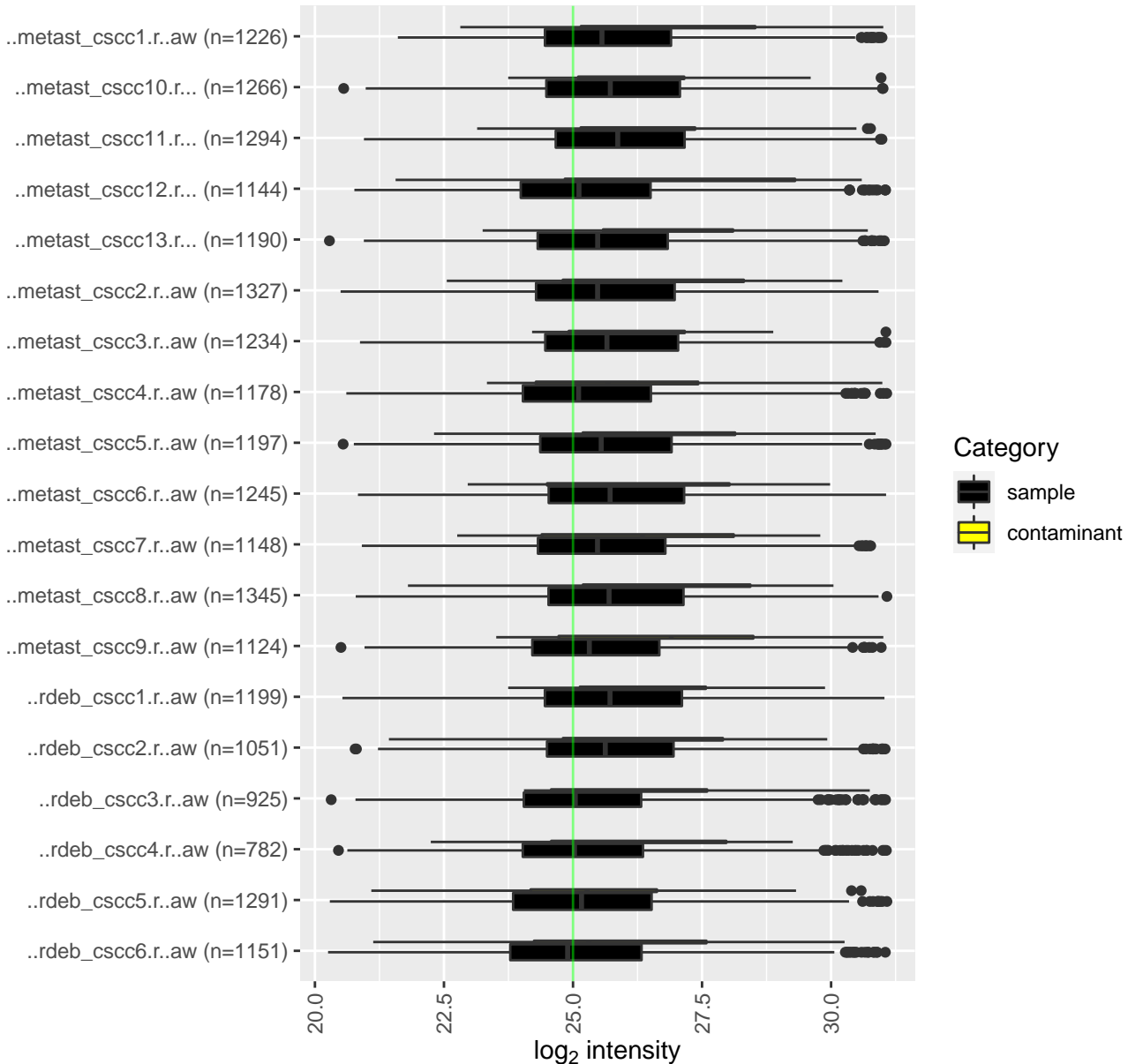
RSD 4.1% [high RSD --> few peptides]



PG: LFQ intensity distribution

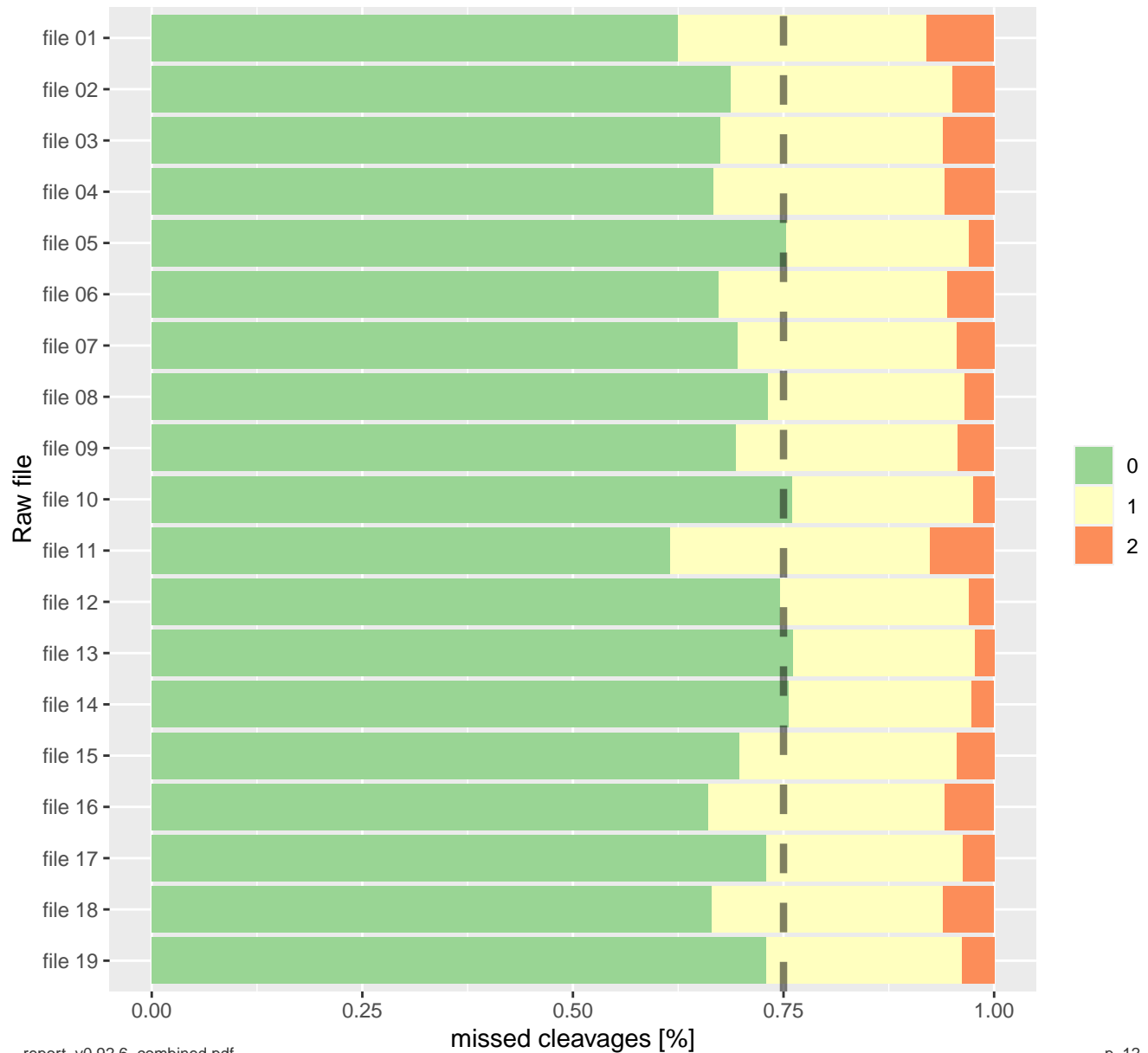
RSD 1.2% (w/o zero int.; expected < 5%)

RSD 299.6% [high RSD ---> few peptides]

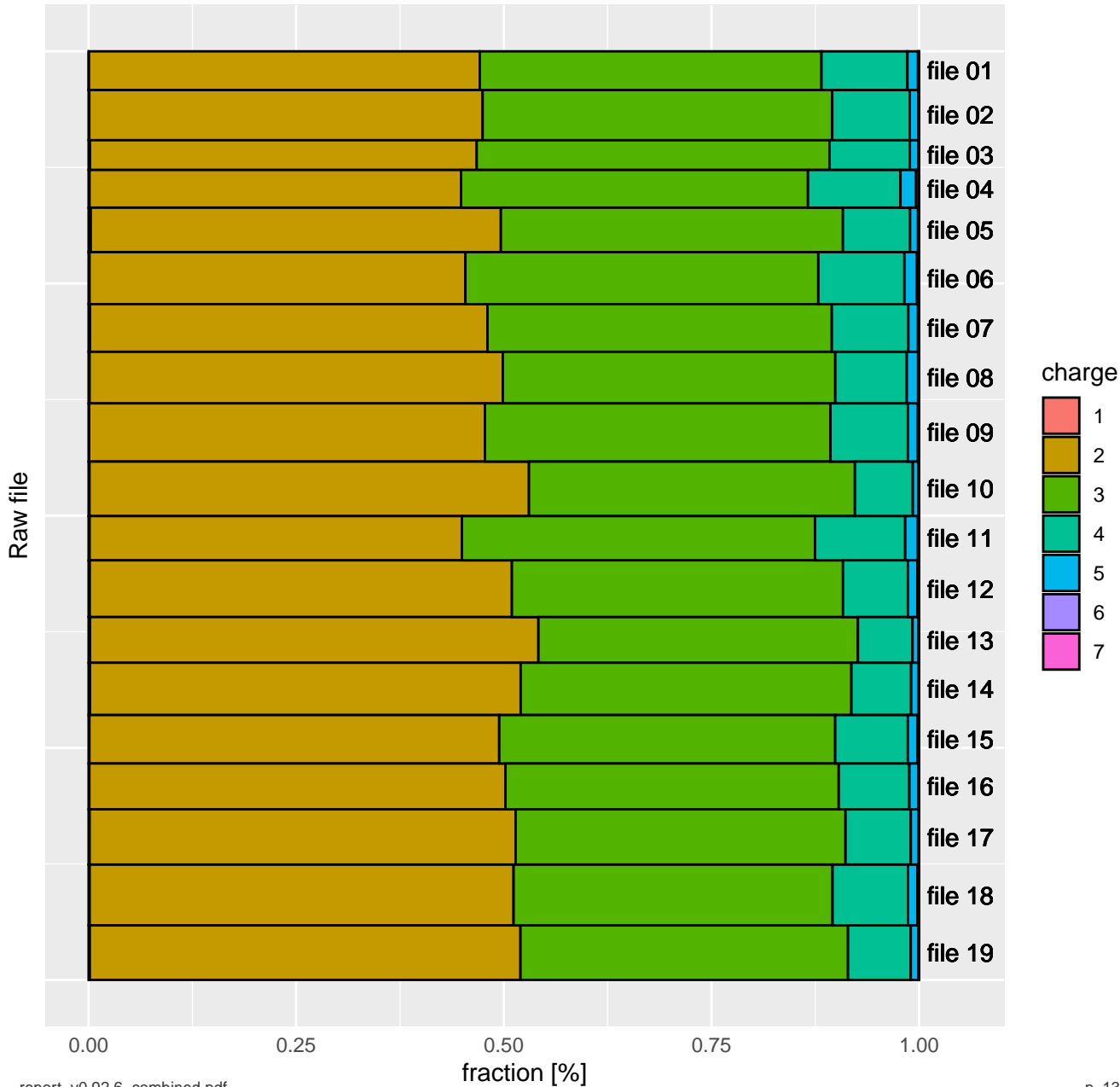


MSMS: Missed cleavages per Raw file

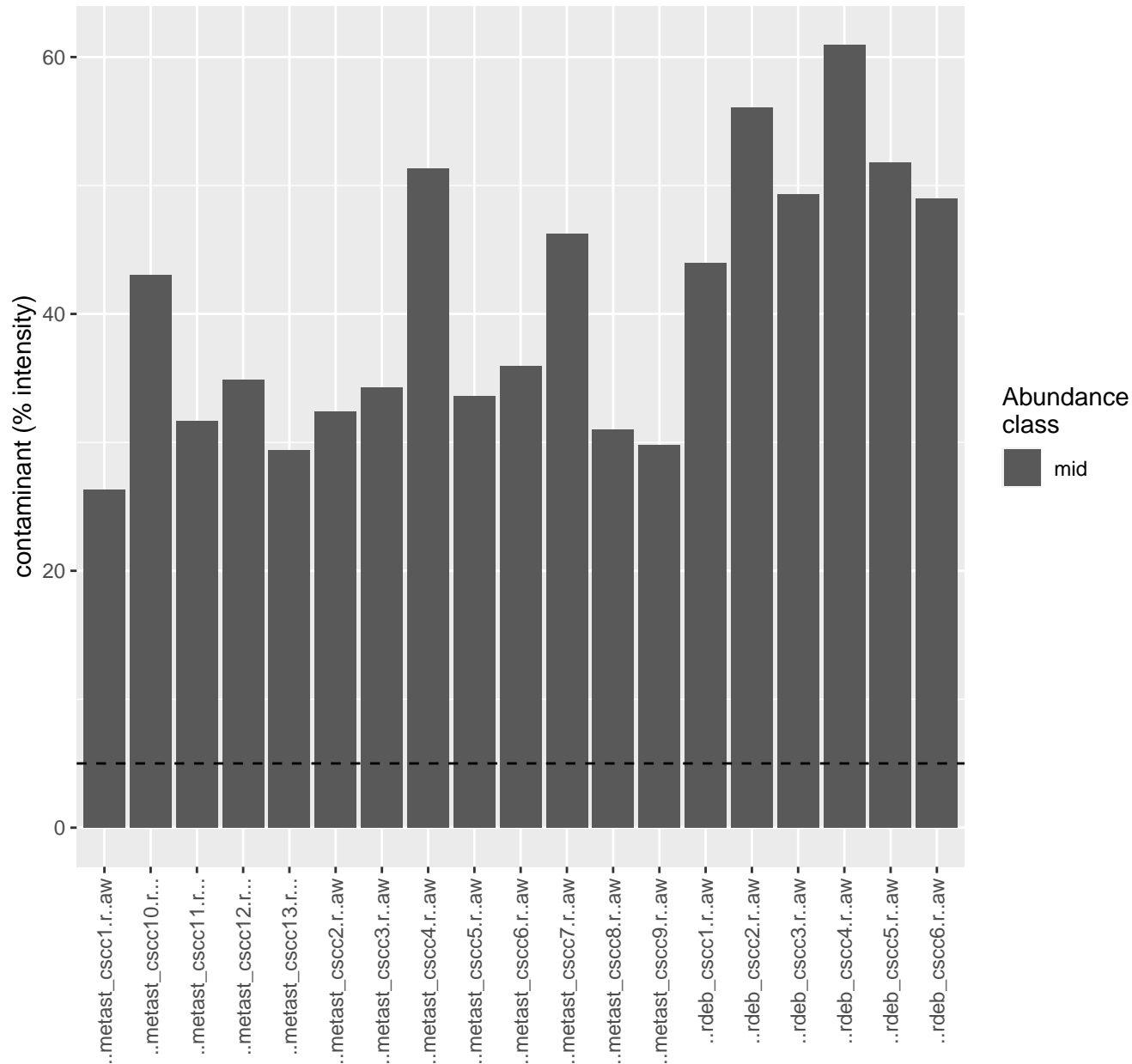
(excludes contaminants)



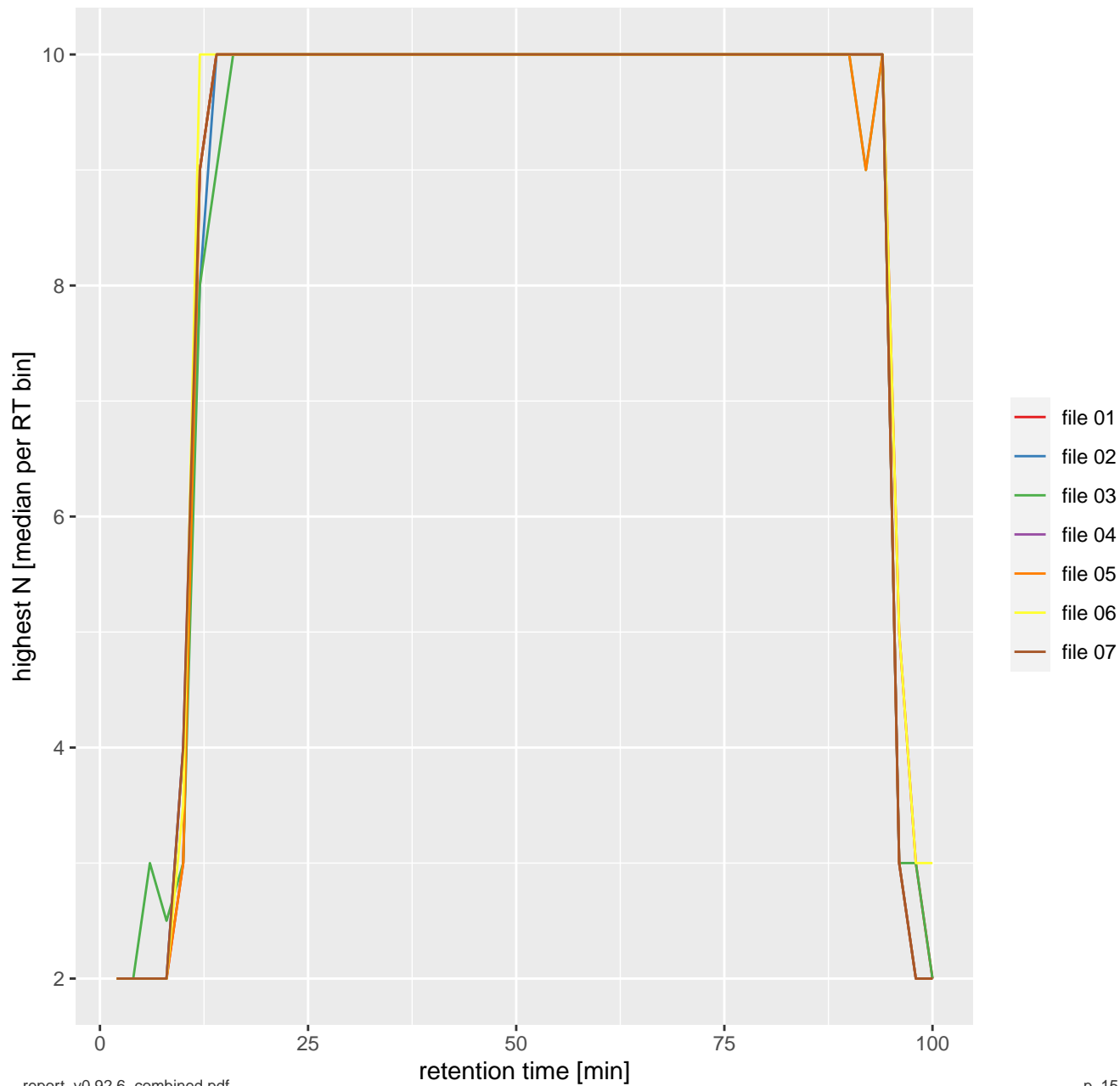
EVD: charge distribution



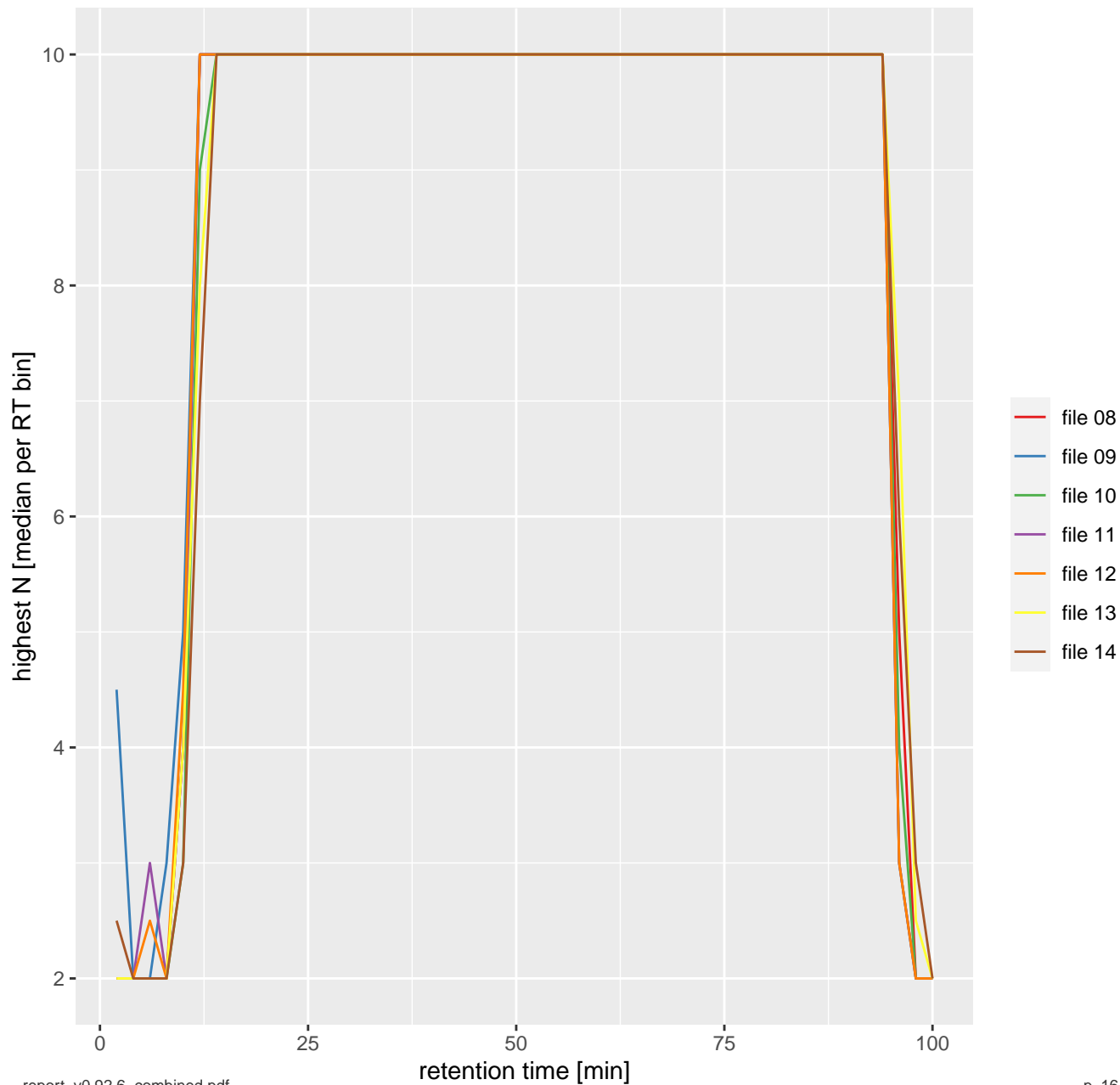
PG: Contaminant per condition



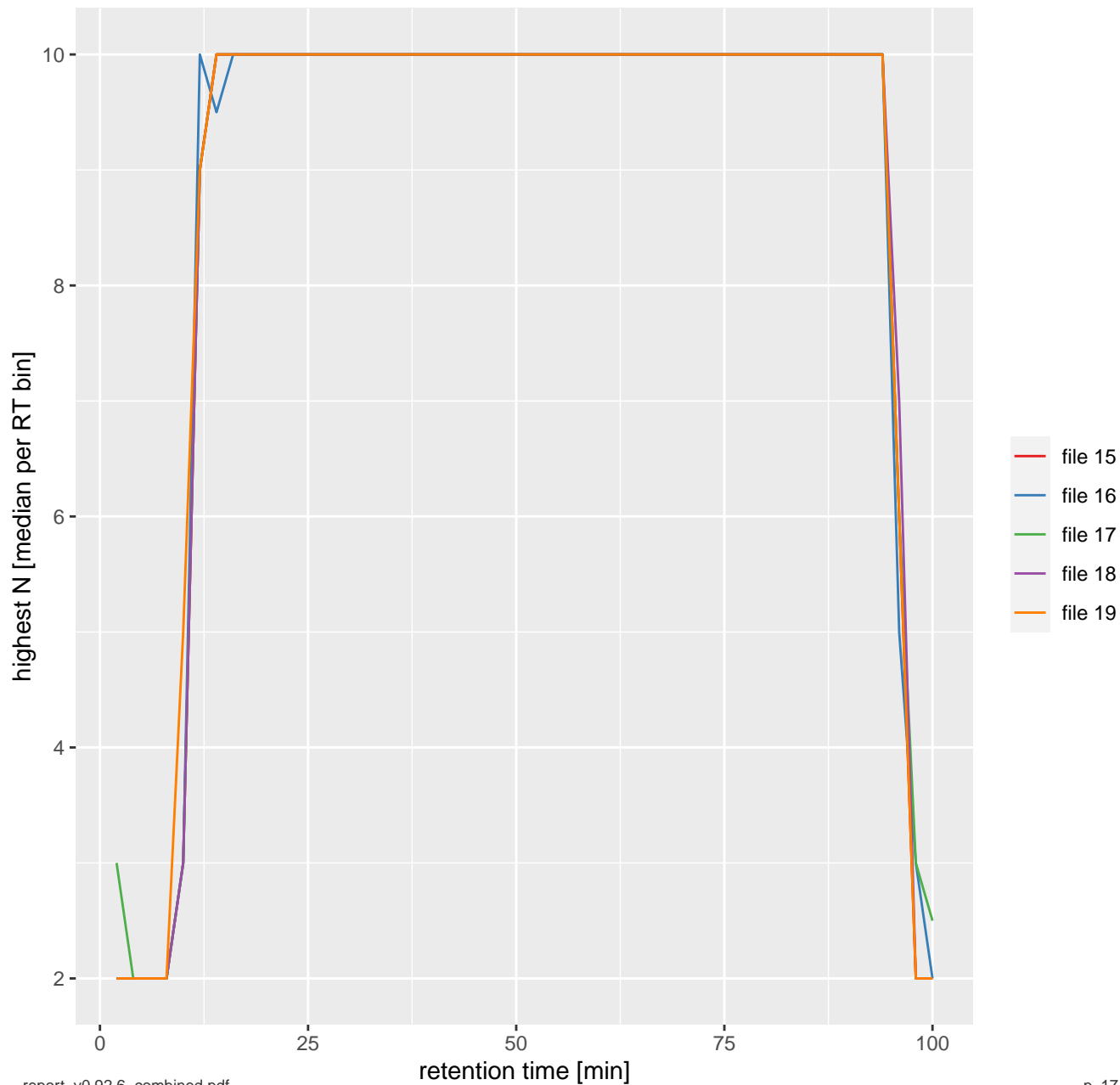
MSMSscans: TopN over RT



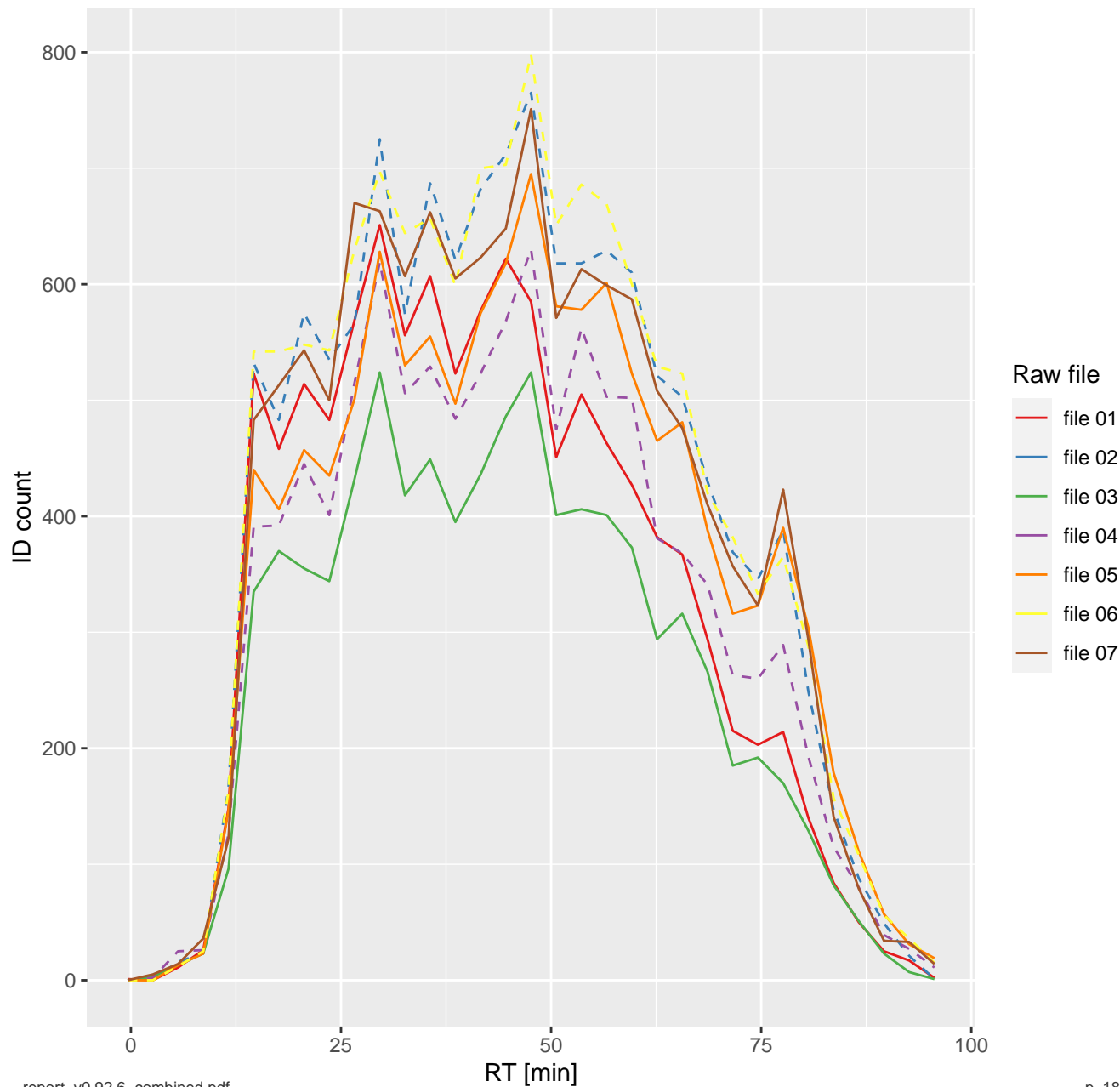
MSMSscans: TopN over RT



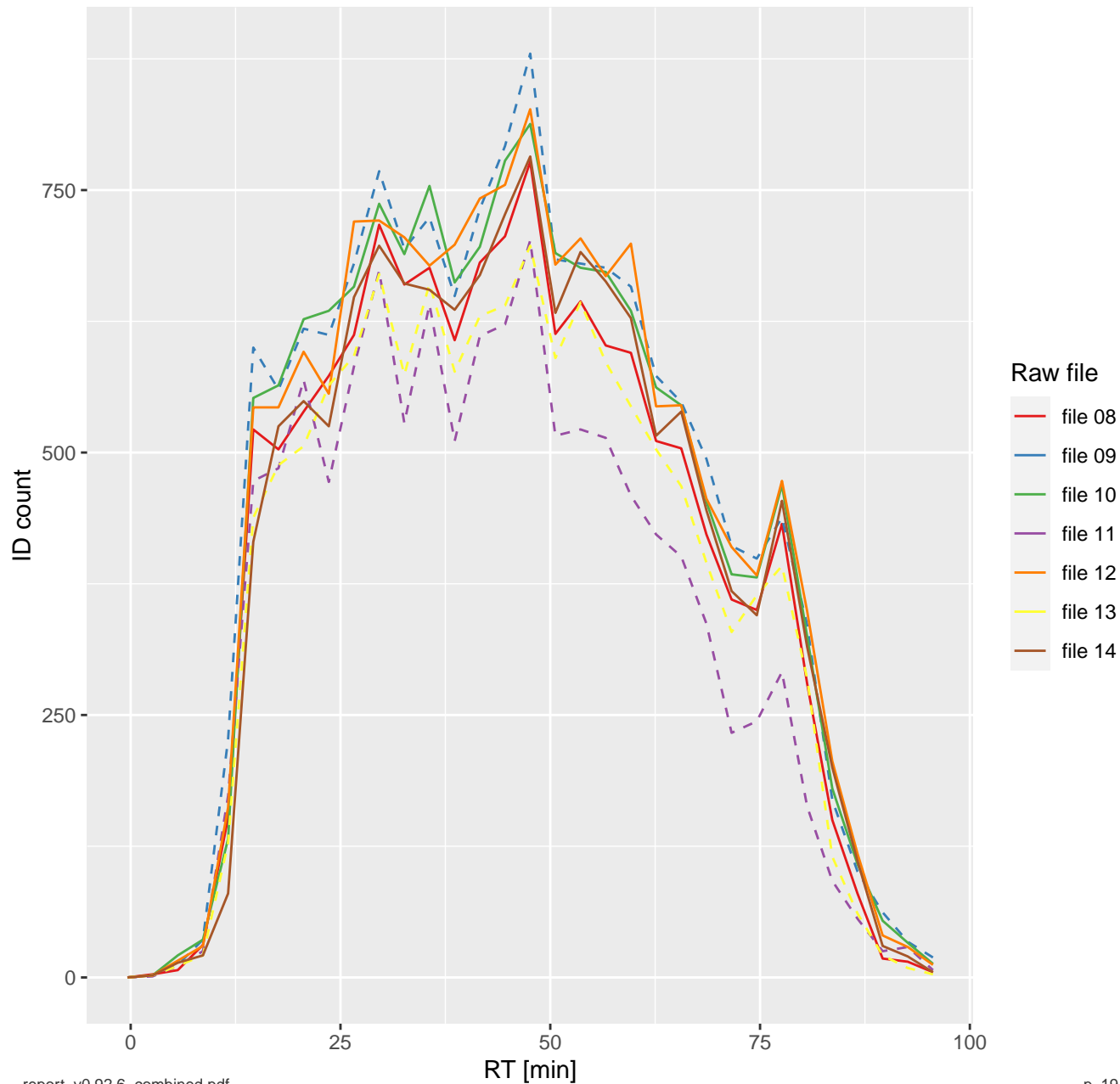
MSMSscans: TopN over RT



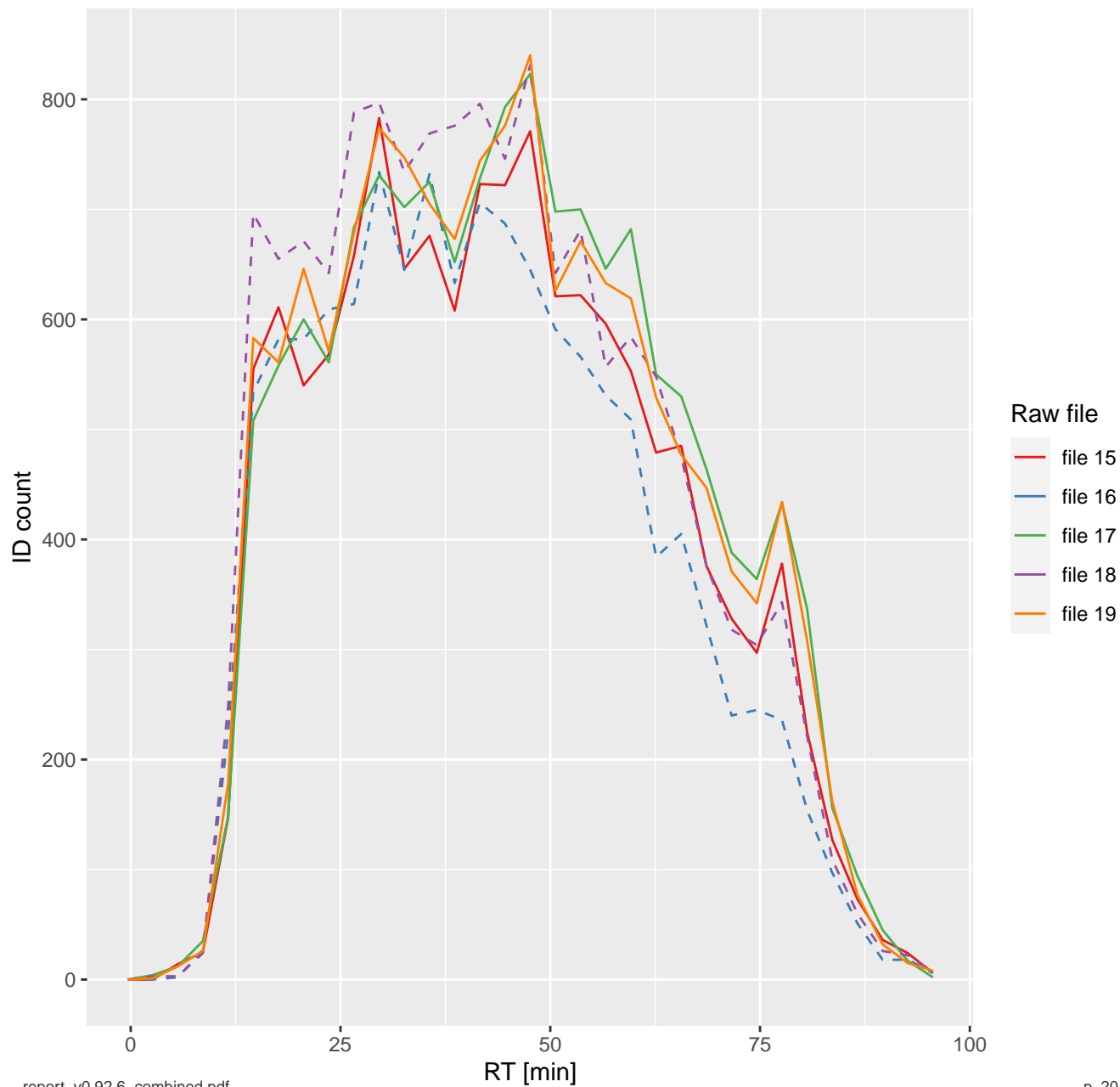
EVD: IDs over RT



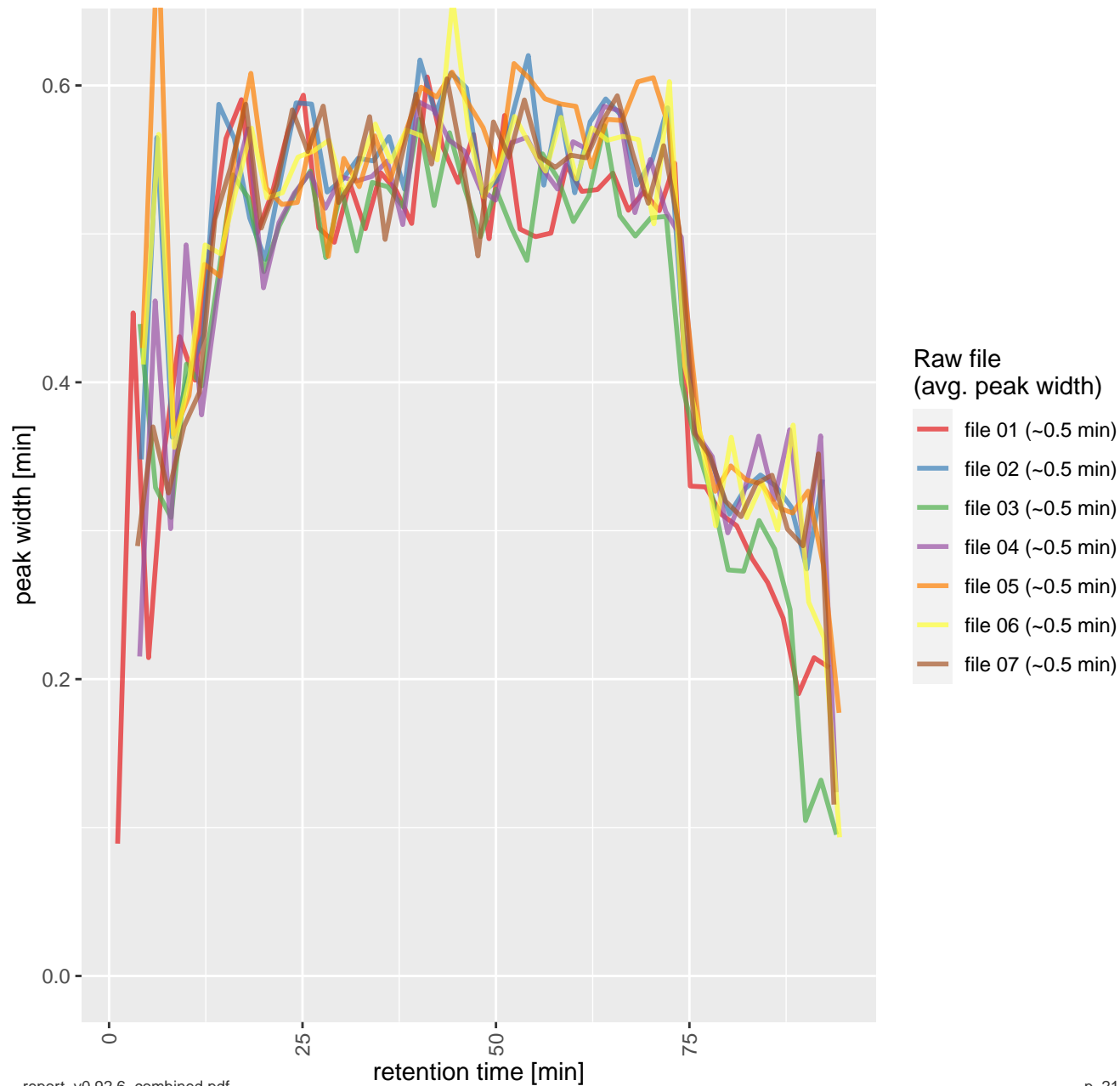
EVD: IDs over RT



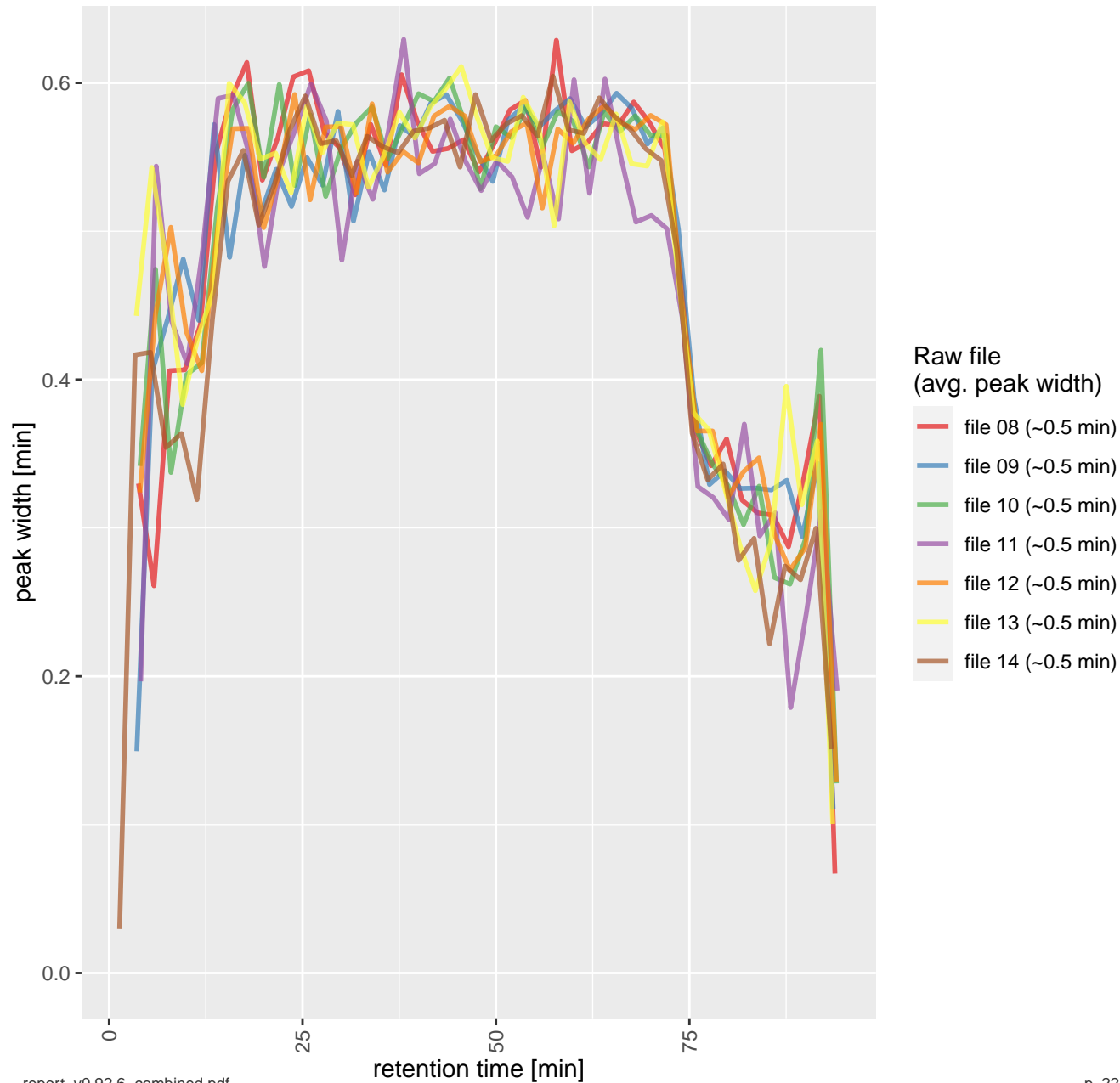
EVD: IDs over RT



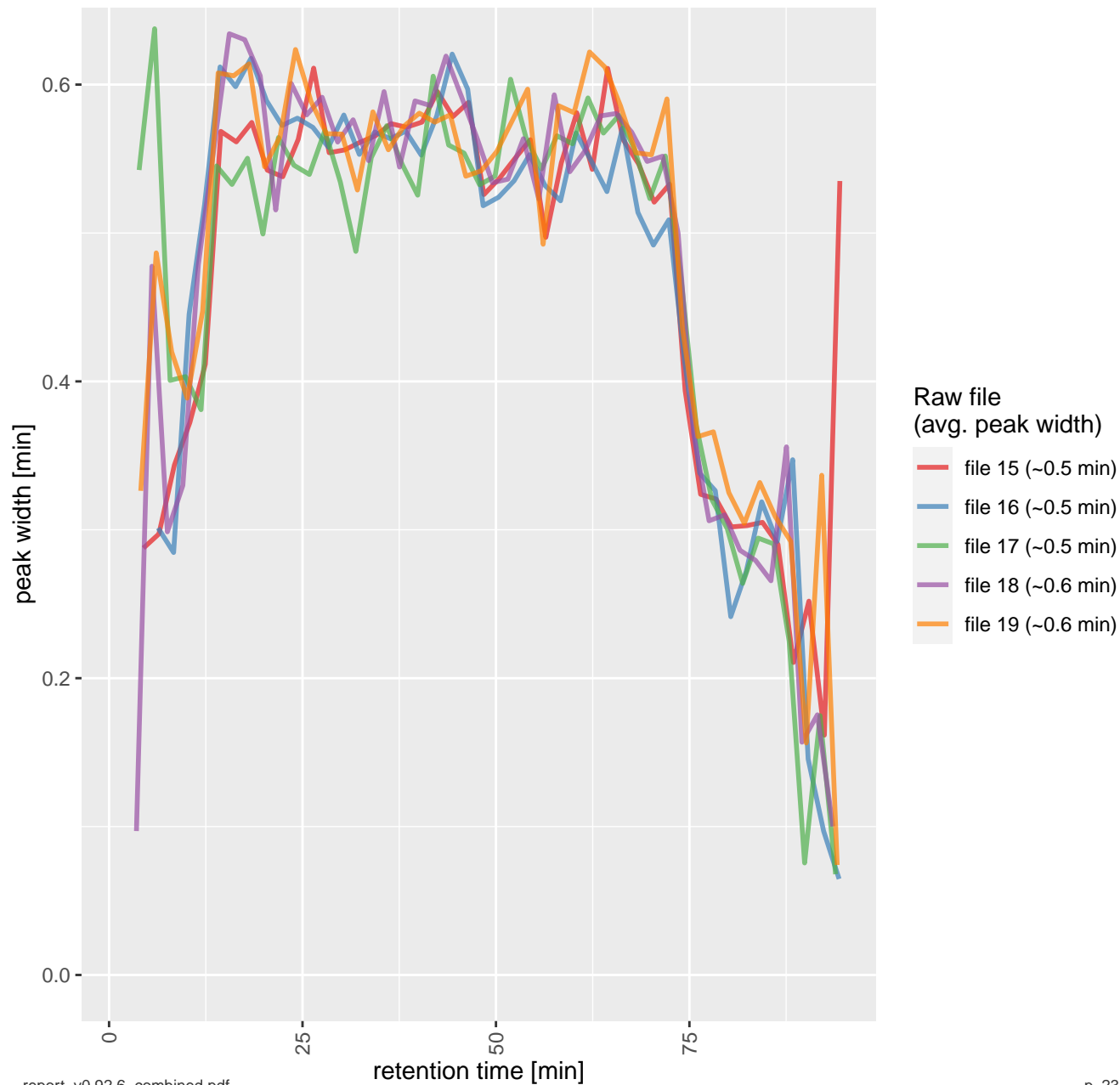
EVD: Peak width over RT



EVD: Peak width over RT

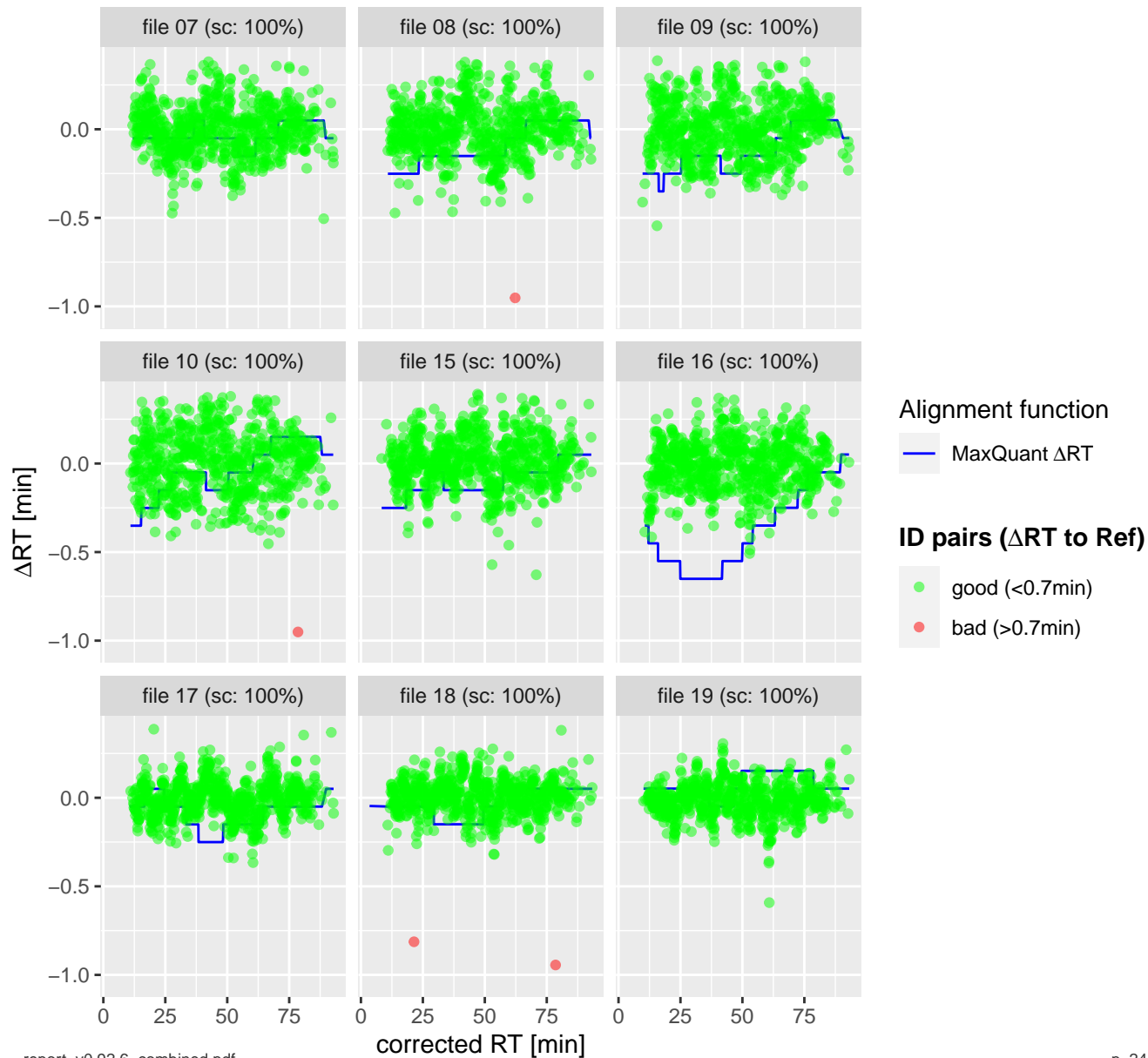


EVD: Peak width over RT



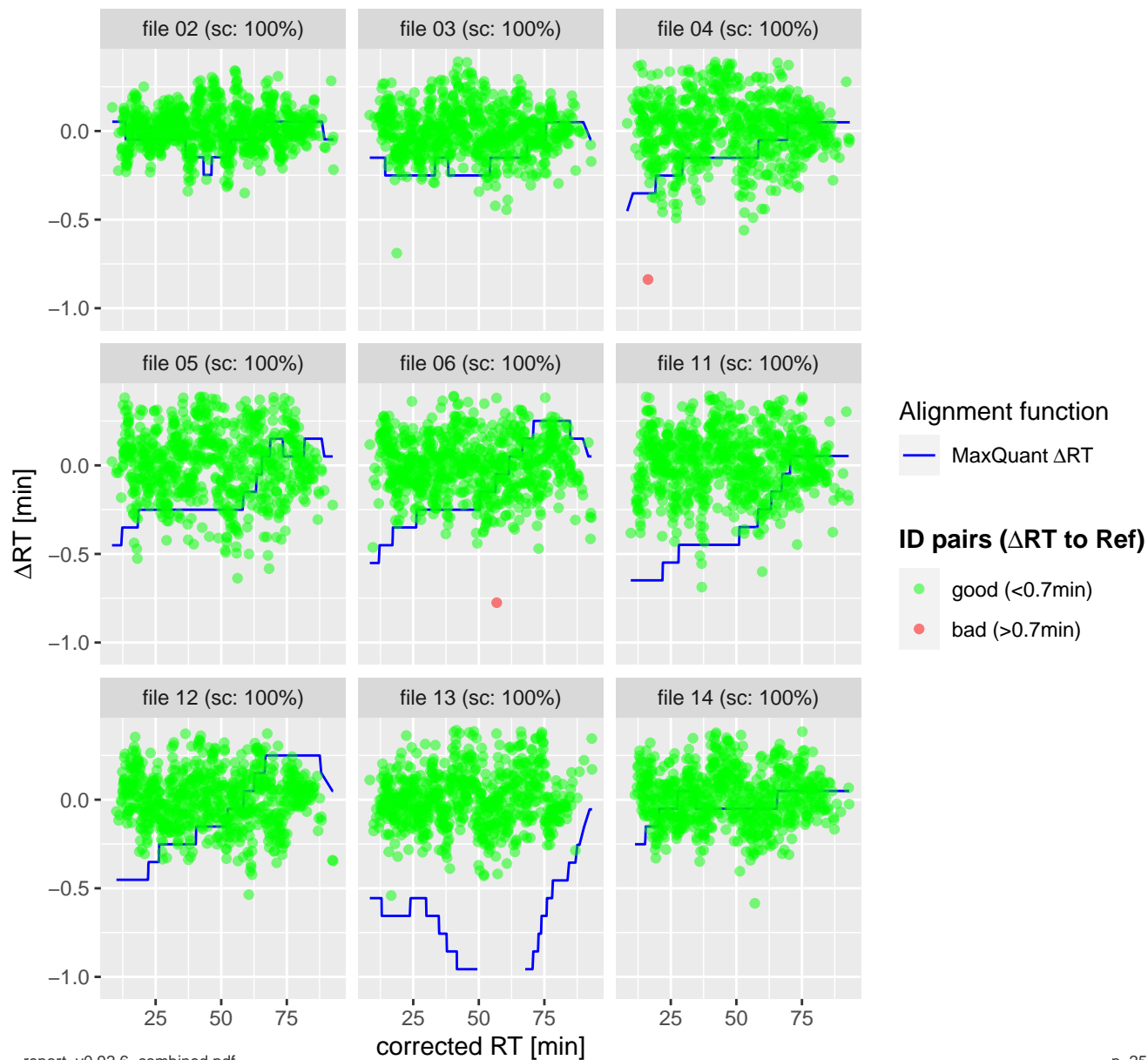
EVD: MBR – alignment

alignment reference: RDEB_cSCC6.raw.thermo

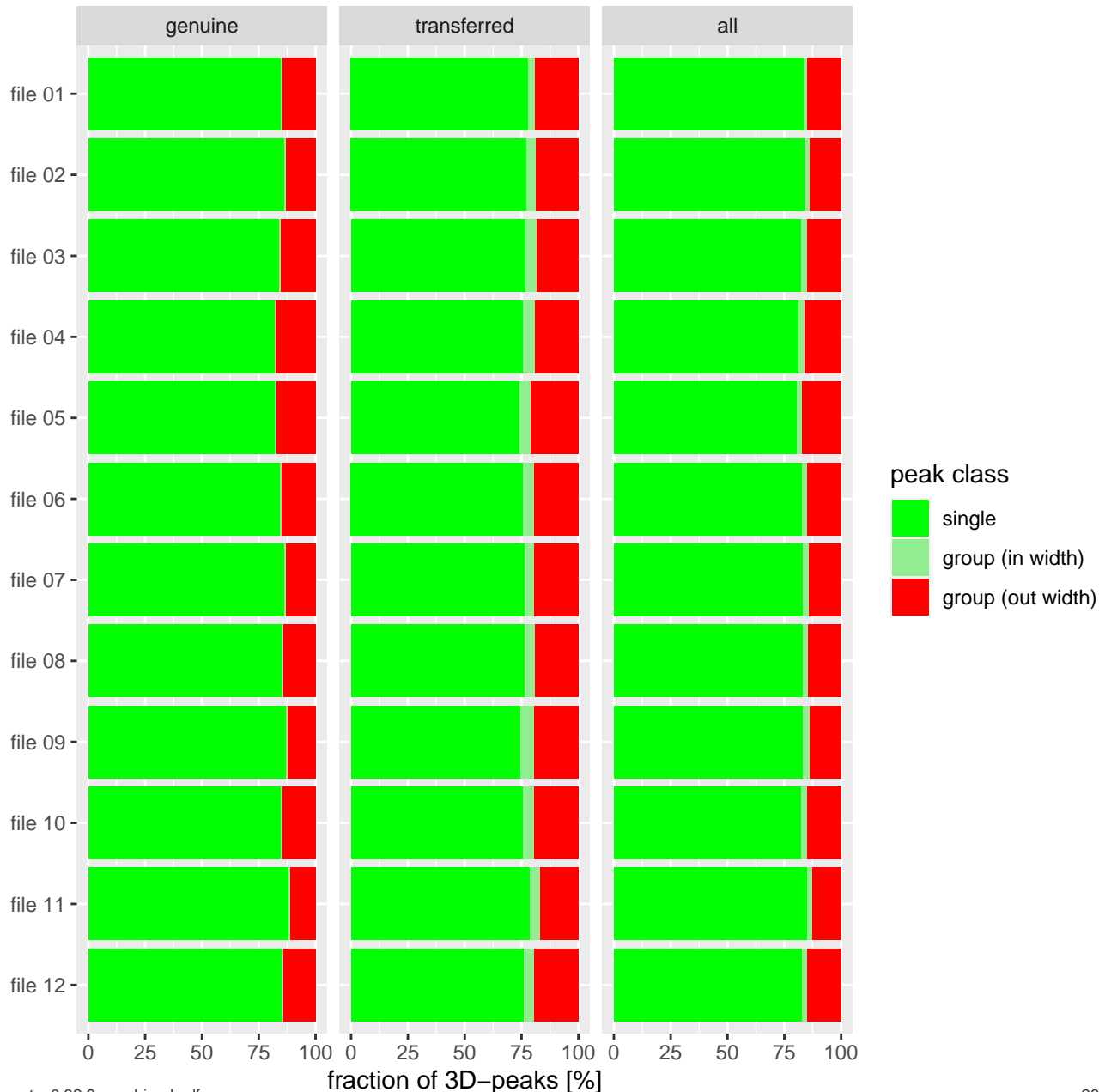


EVD: MBR – alignment

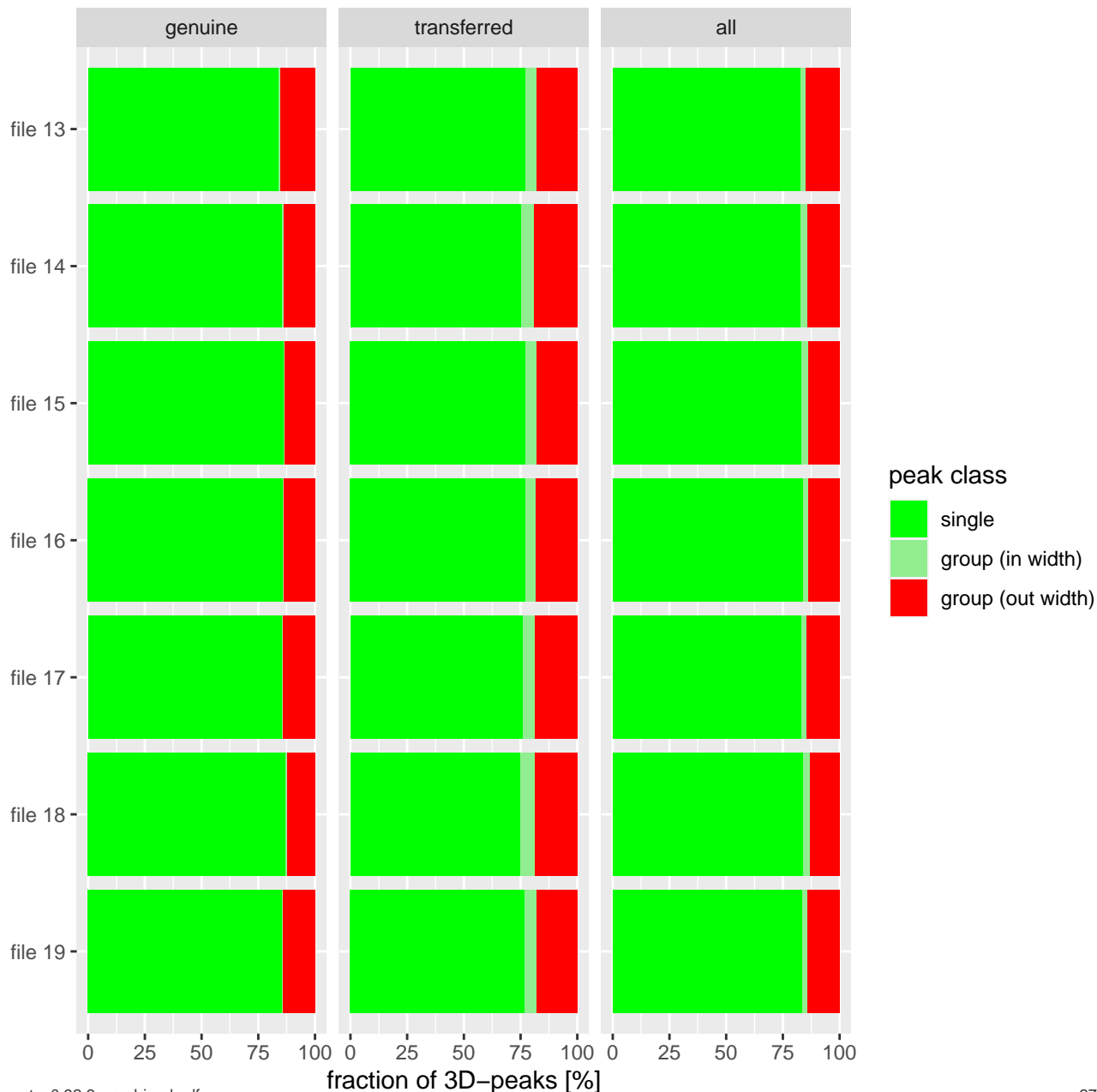
alignment reference: RDEB_cSCC6.raw.thermo



EVD: MBR – ID Transfer

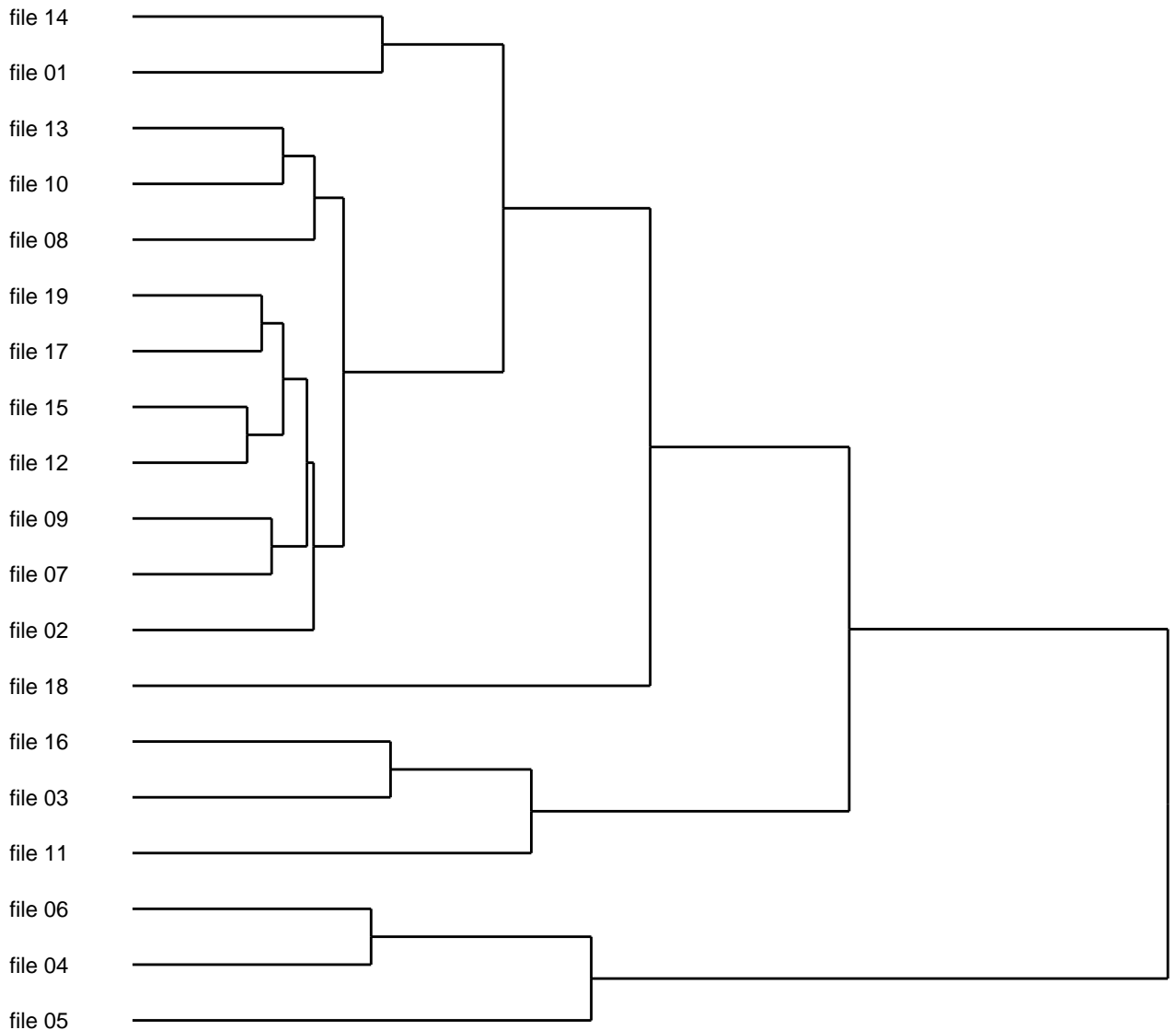


EVD: MBR – ID Transfer

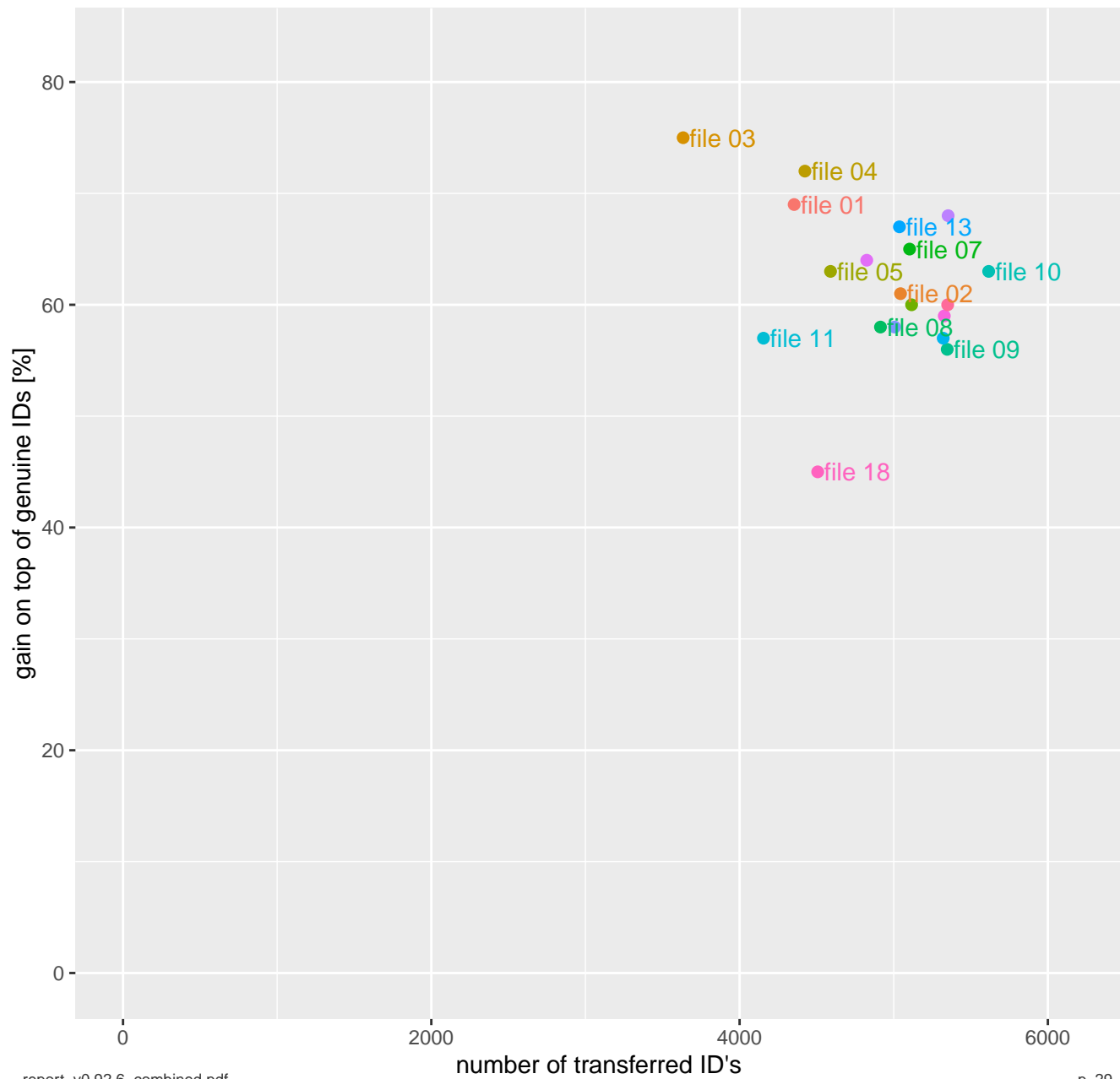


[experimental] EVD: Clustering Tree of Raw files

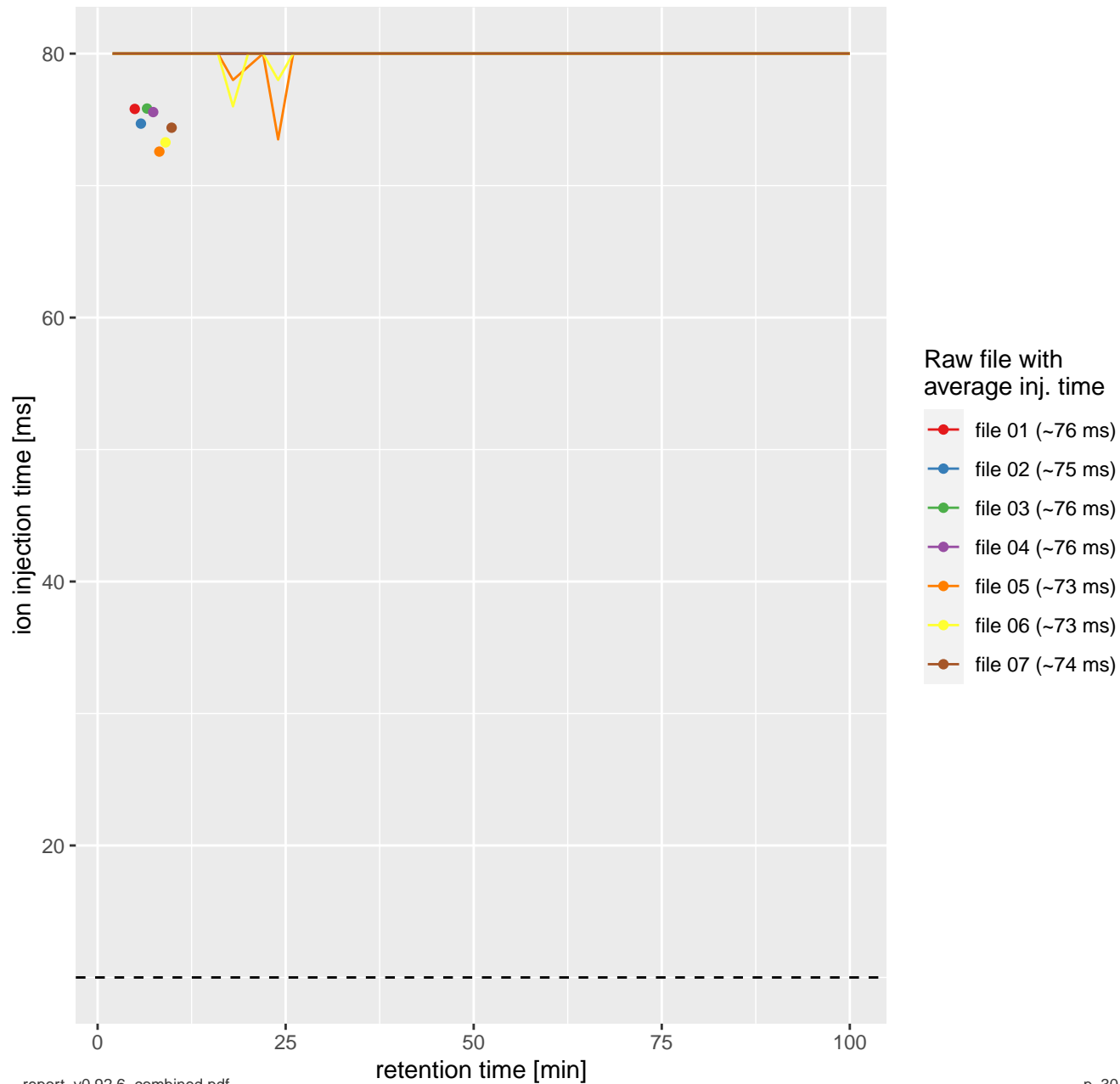
by Correlation of Corrected Retention Times



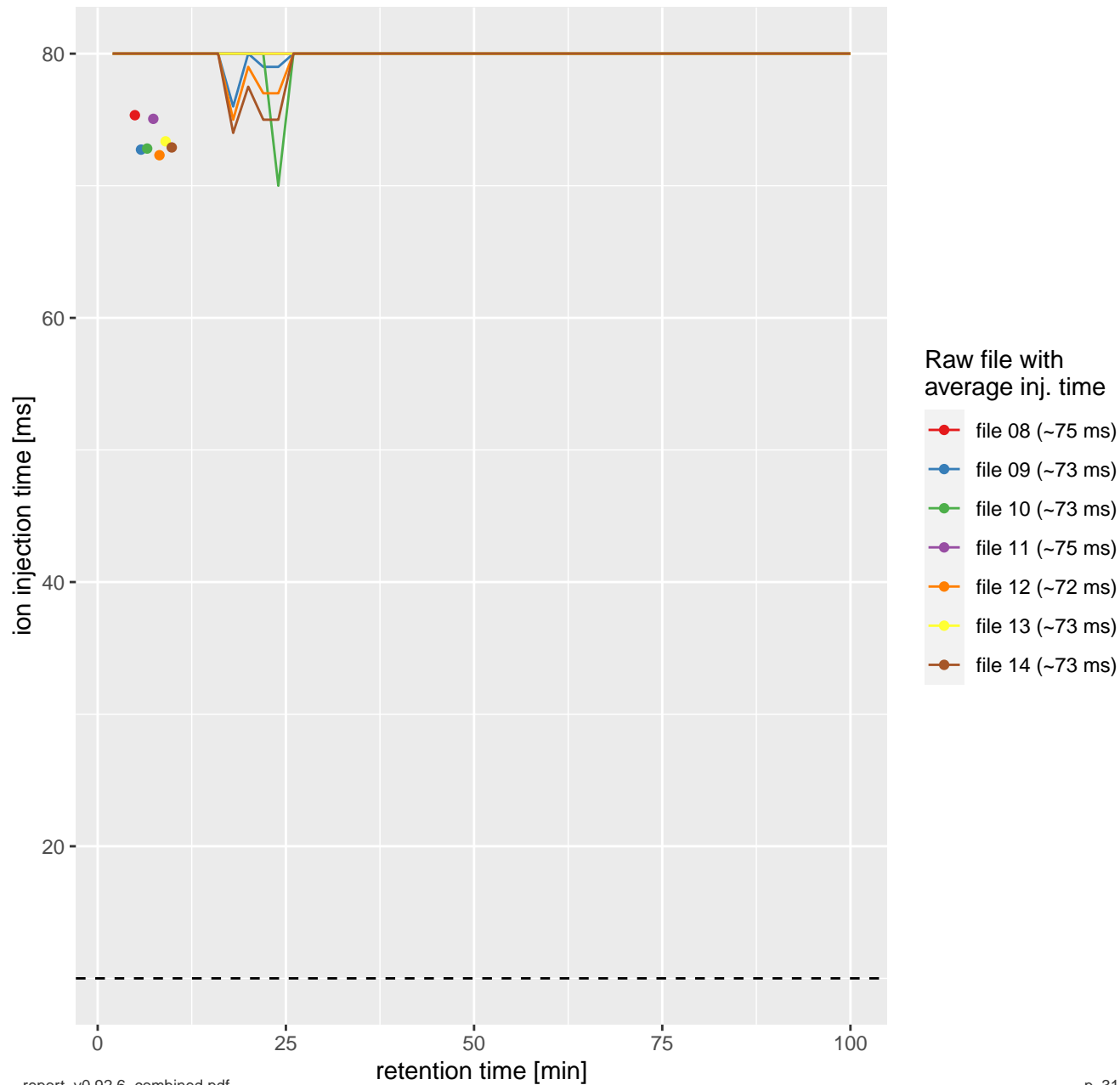
EVD: Peptides inferred by MBR



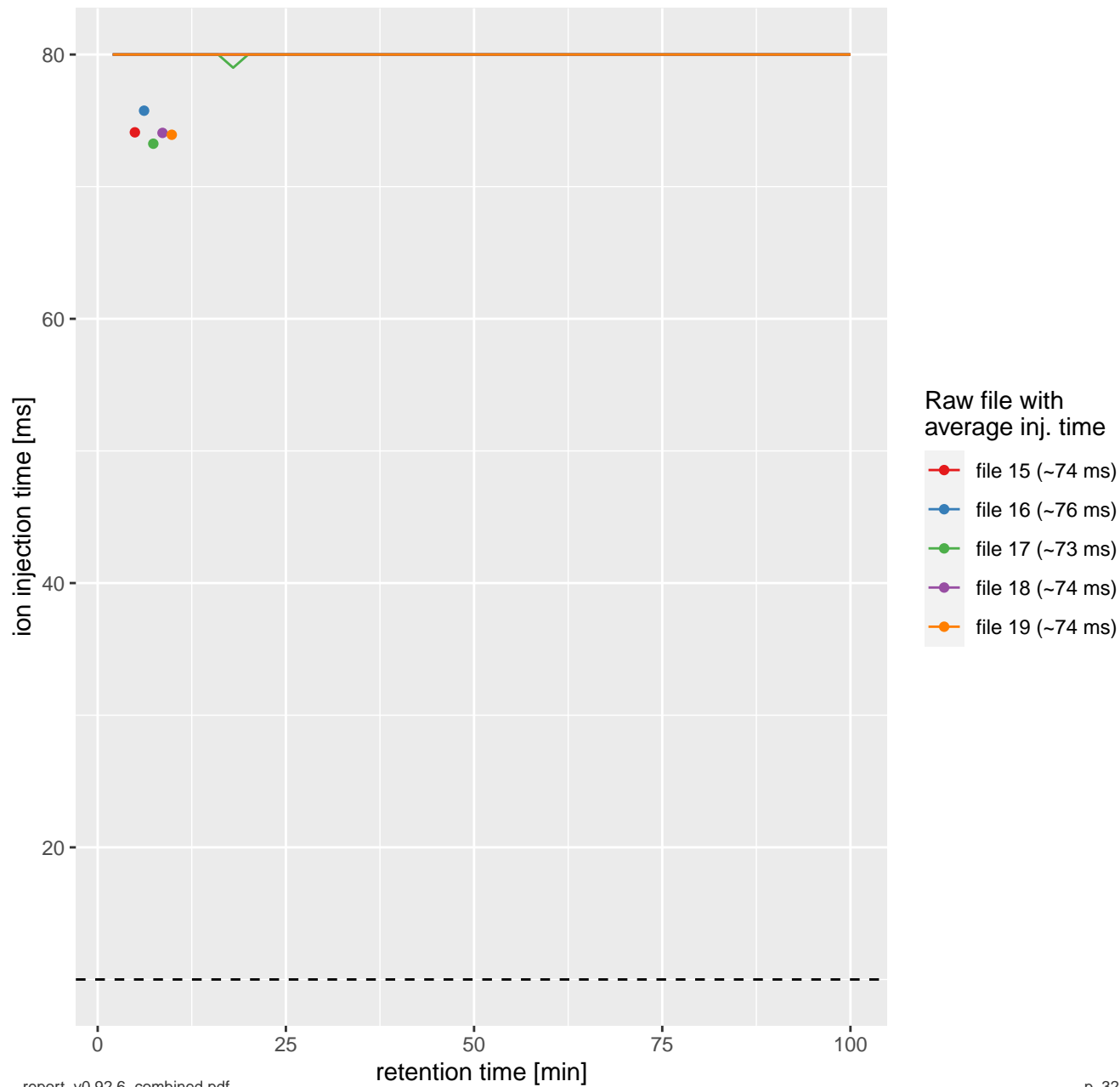
MSMSscans: Ion Injection Time over RT



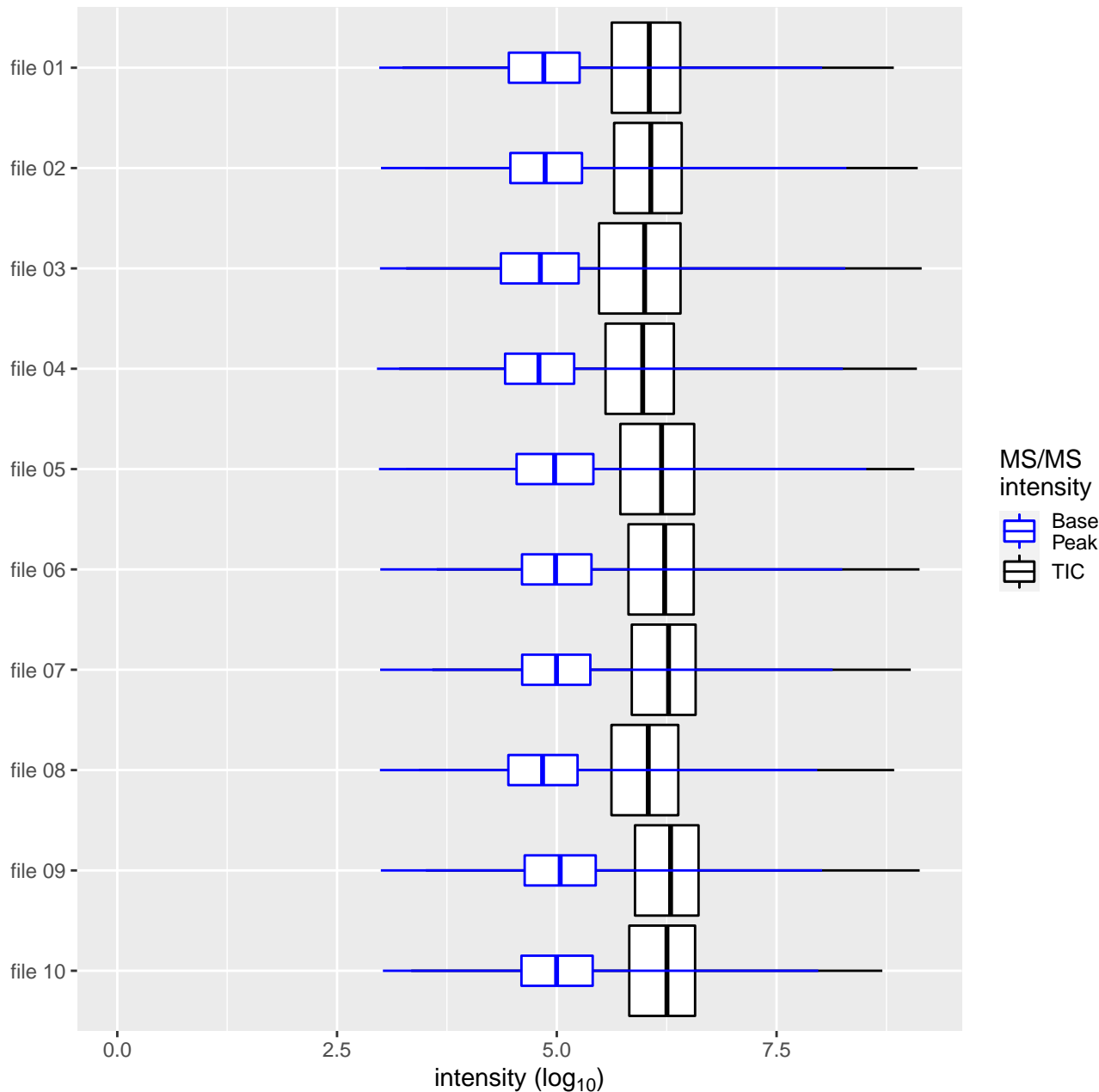
MSMSscans: Ion Injection Time over RT



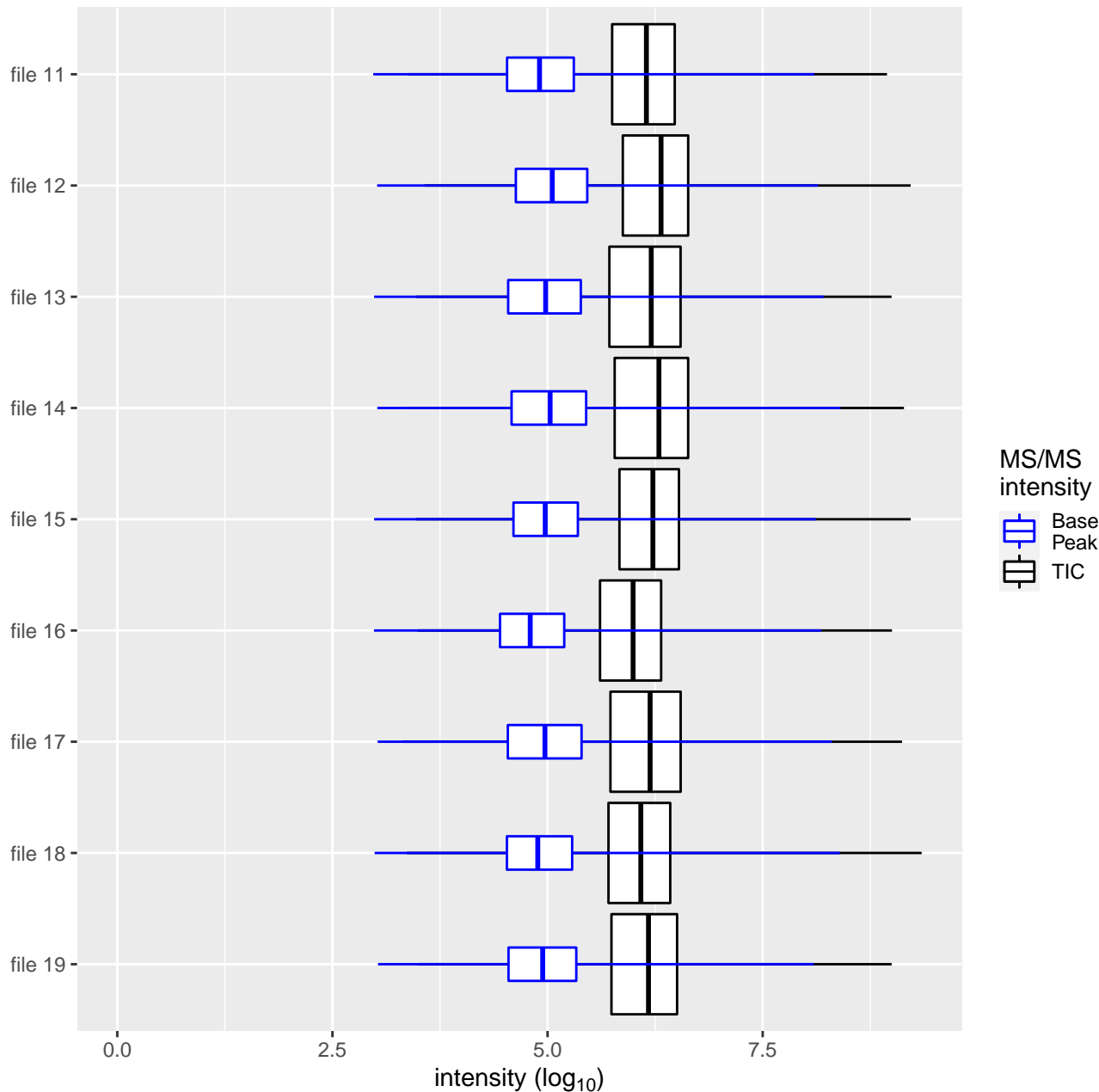
MSMSscans: Ion Injection Time over RT



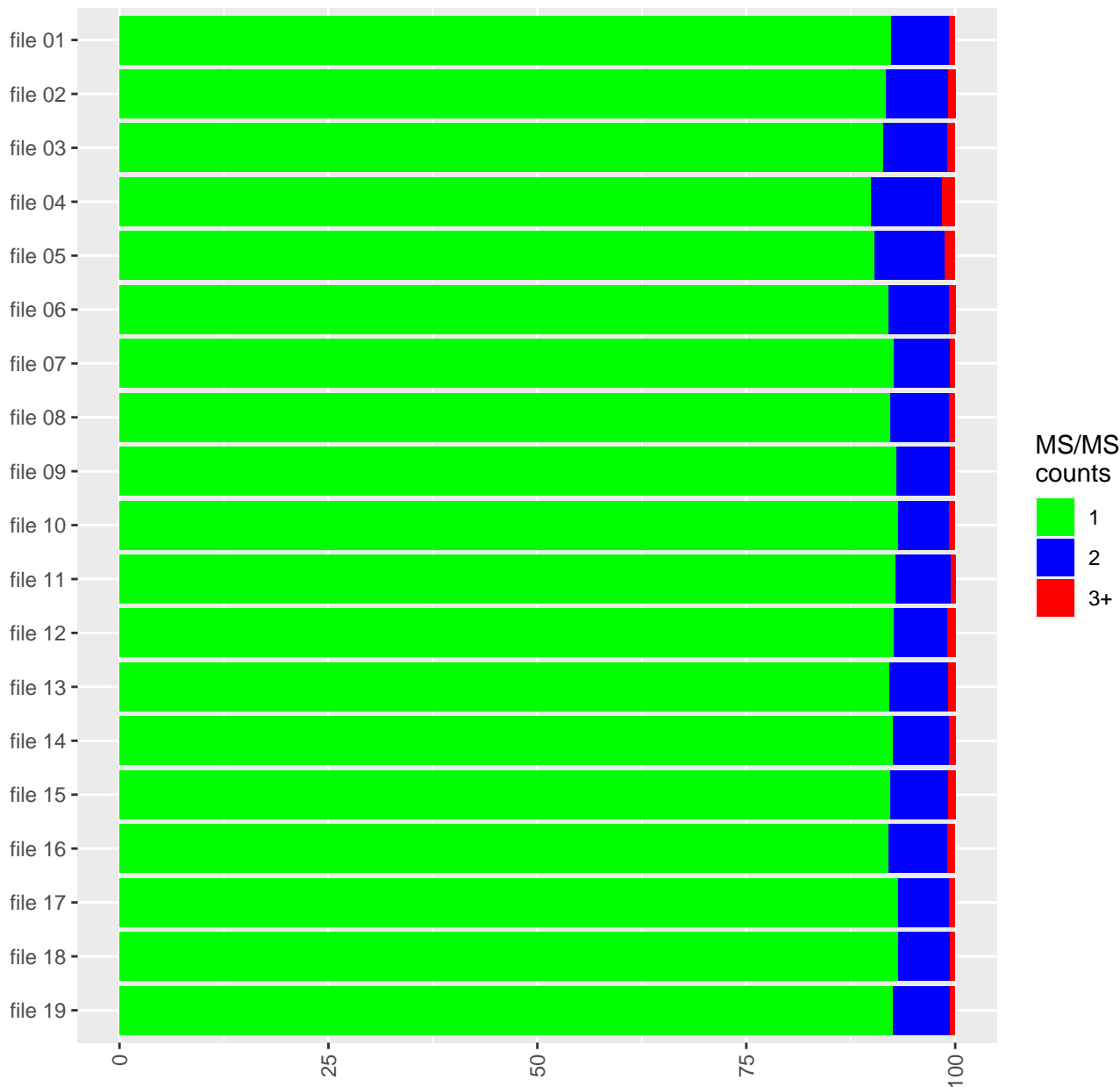
[experimental] MSMSscans: MS/MS intensity



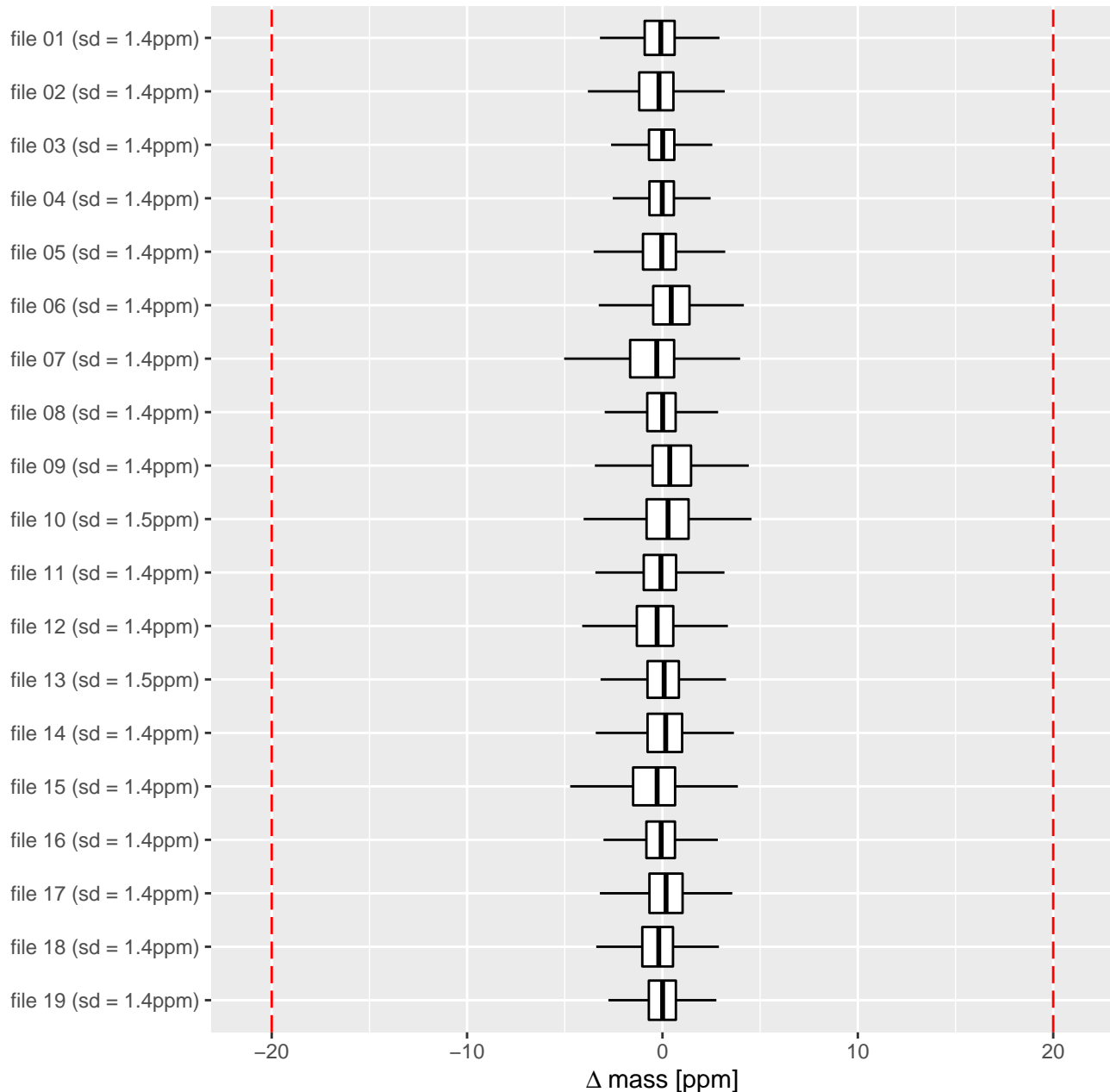
[experimental] MSMSscans: MS/MS intensity



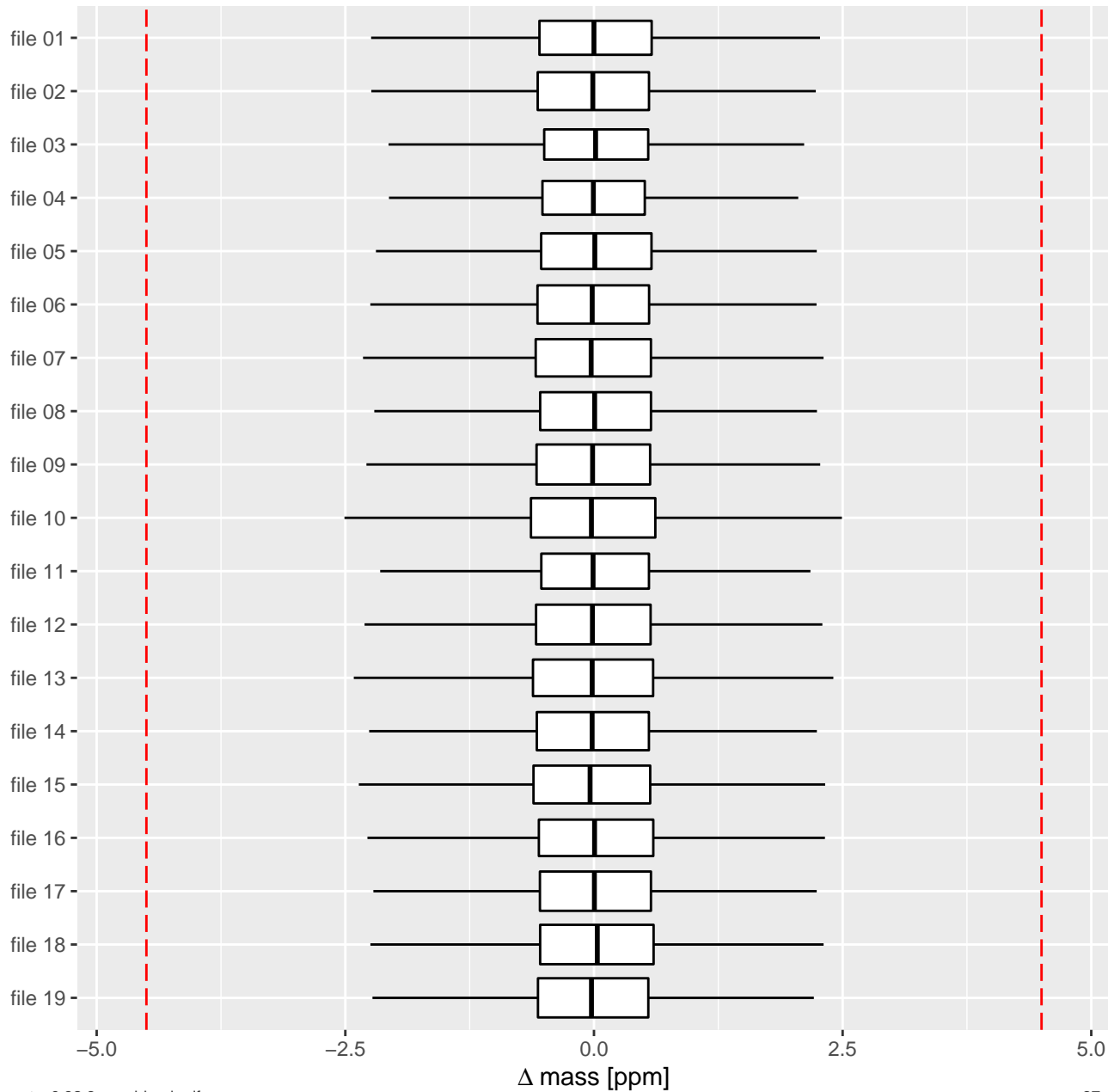
EVD: Oversampling (MS/MS counts per 3D-peak)



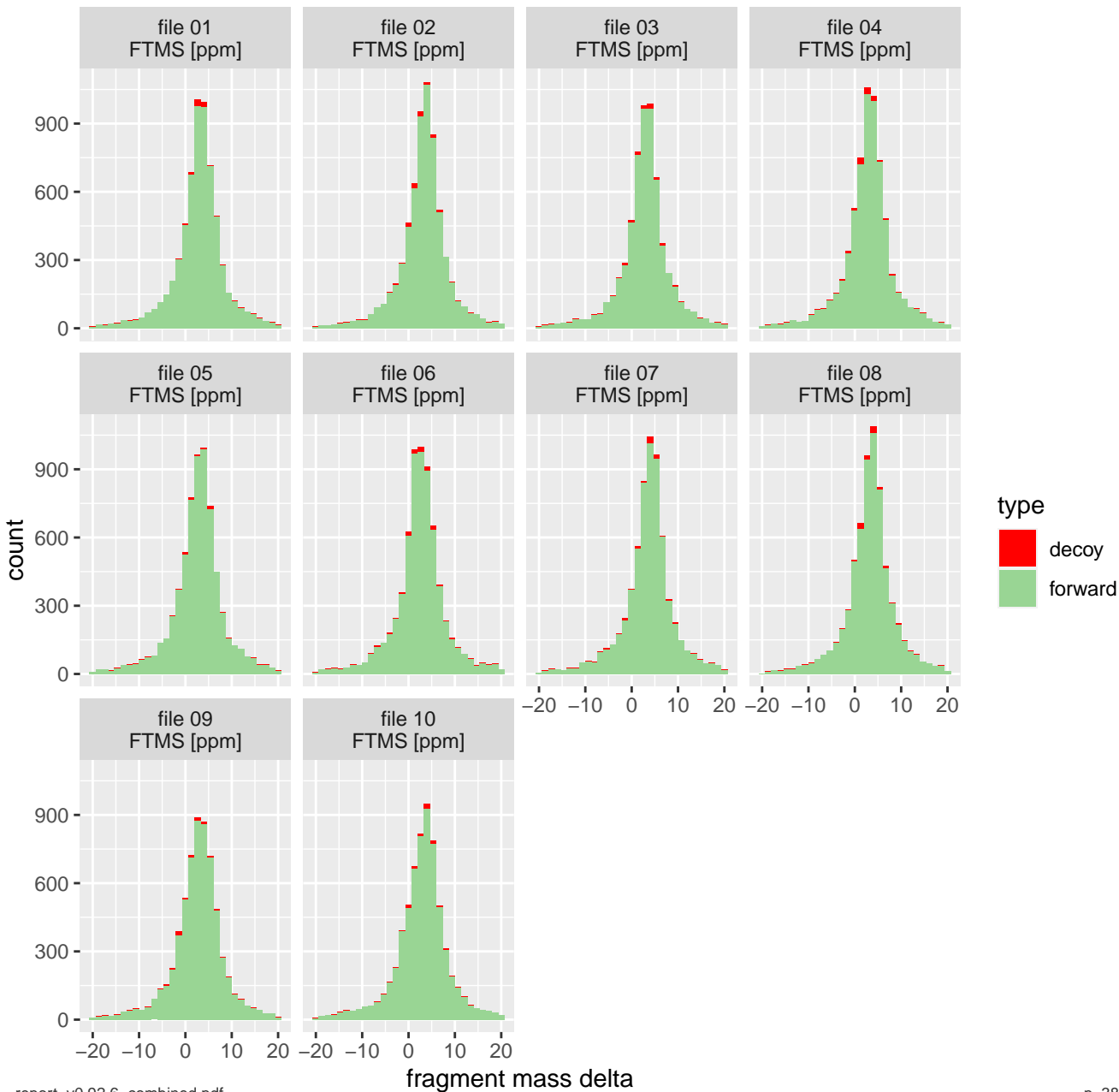
EVD: Uncalibrated mass error



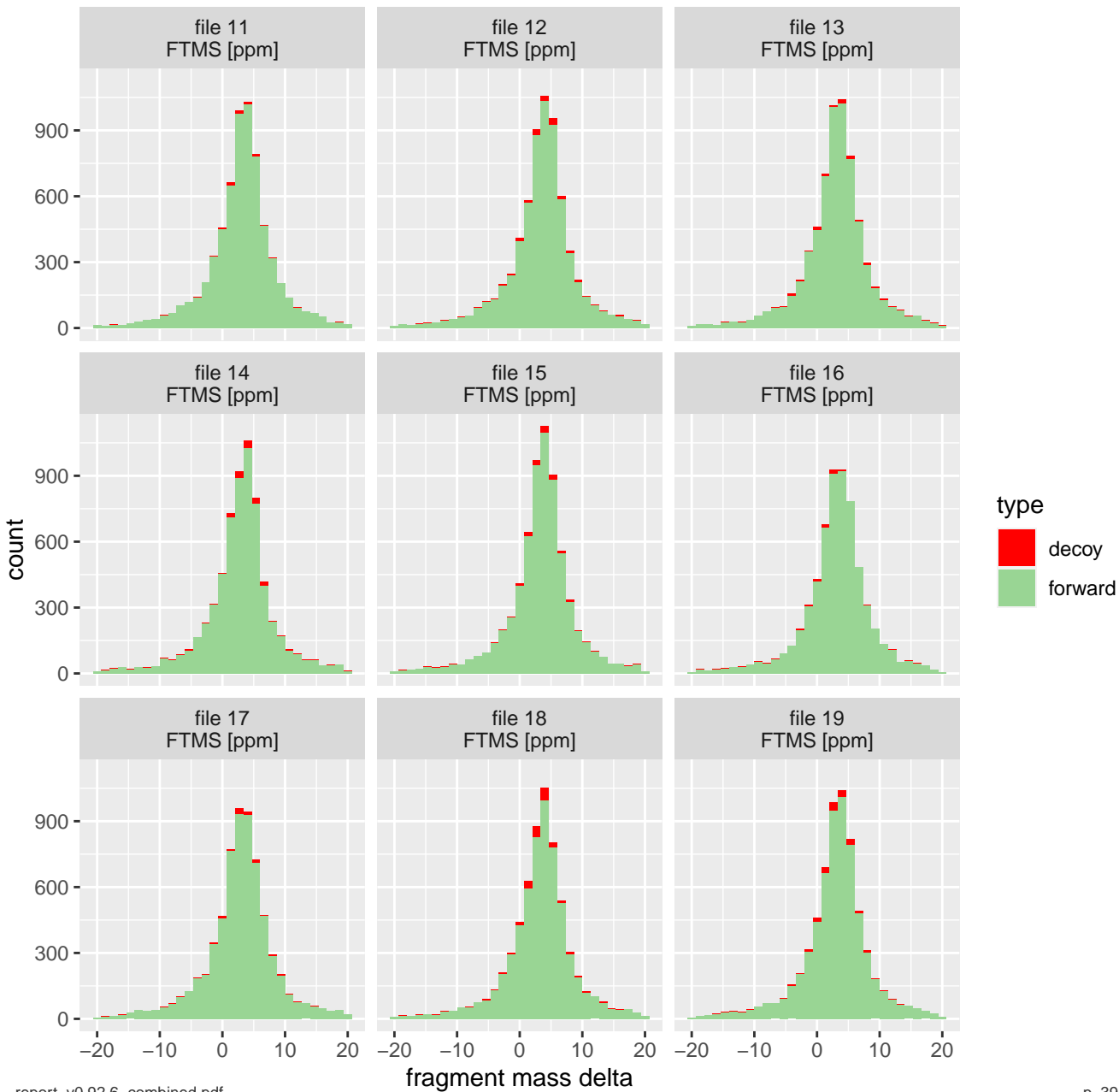
EVD: Calibrated mass error



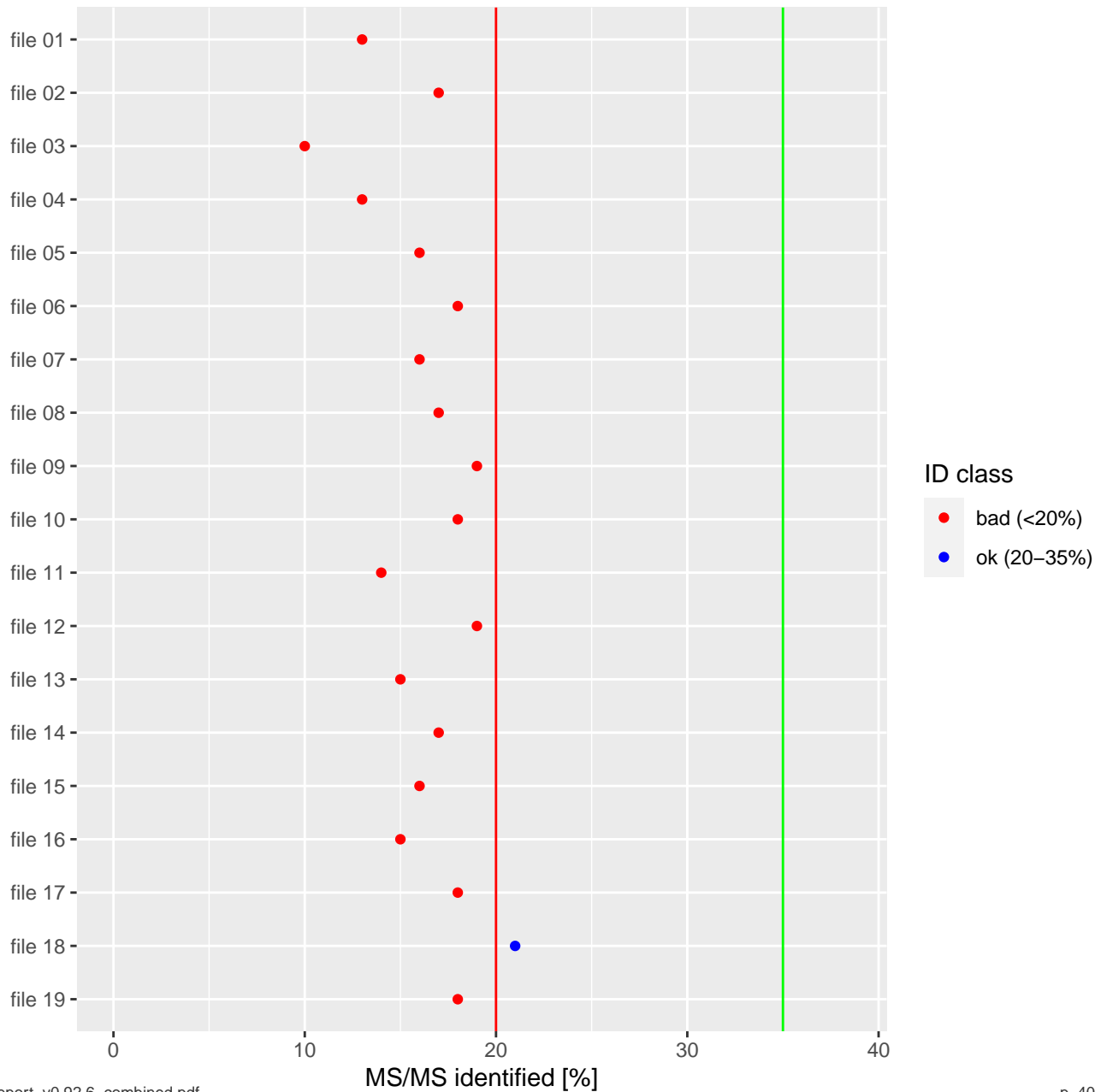
MSMS: Fragment mass errors per Raw file



MSMS: Fragment mass errors per Raw file



SM: MS/MS identified per Raw file

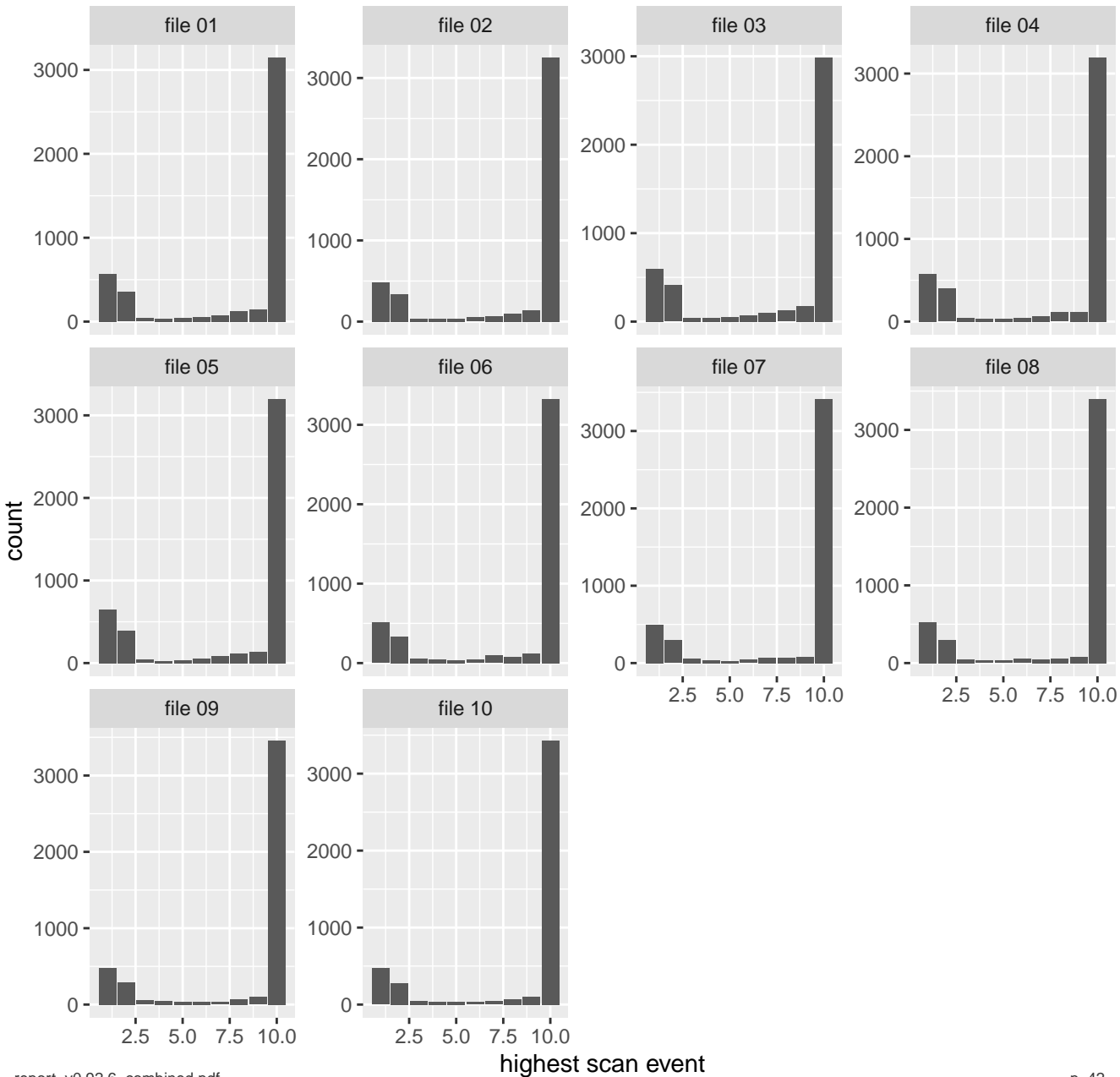


SM: Files with 'red' ID rate

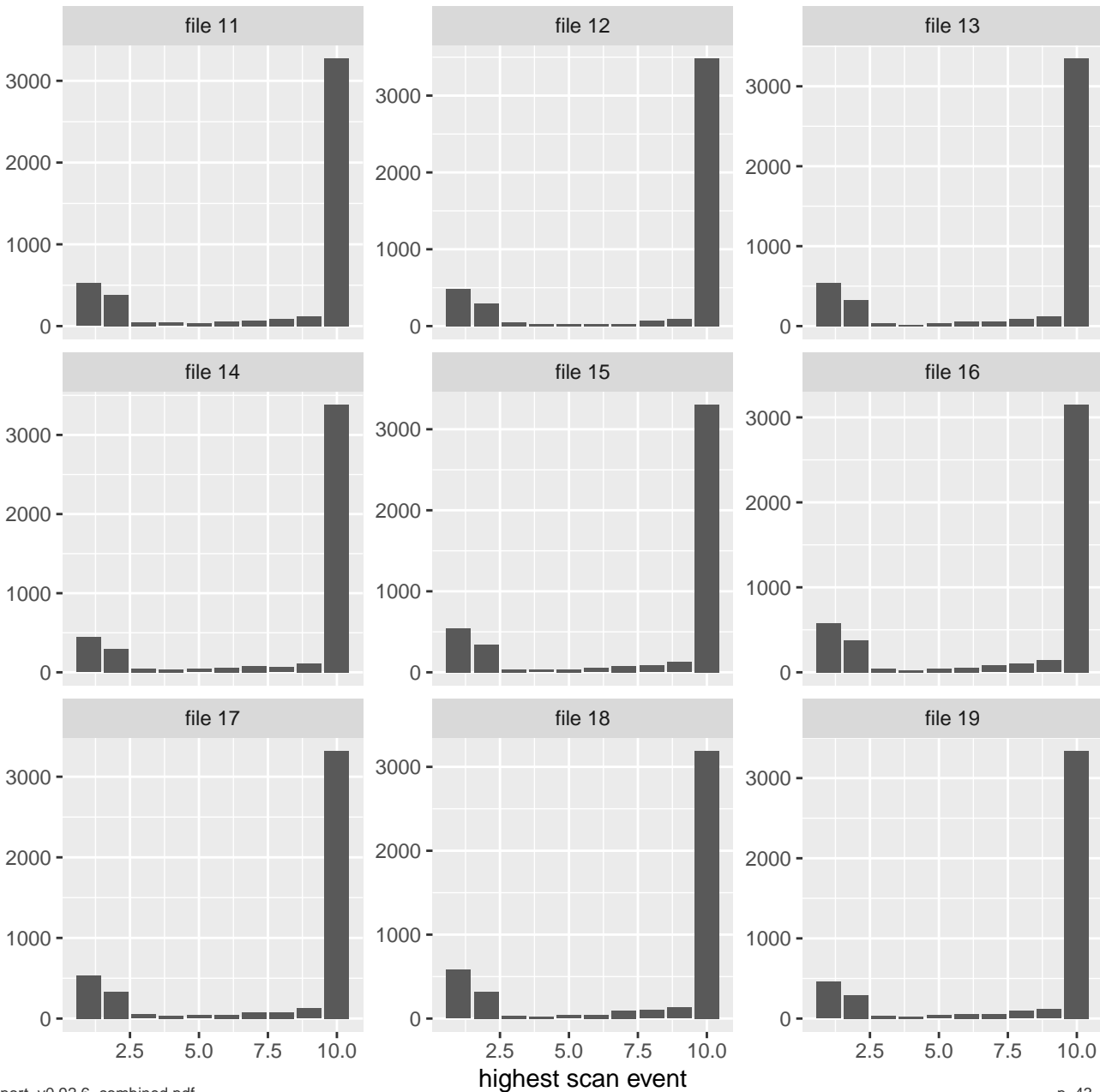
Raw file	% identified
RDEB_cSCC6.raw.thermo	13
RDEB_cSCC5.raw.thermo	17
RDEB_cSCC4.raw.thermo	10
RDEB_cSCC3.raw.thermo	13
RDEB_cSCC2.raw.thermo	16
RDEB_cSCC1.raw.thermo	18
metast_cSCC13.raw.thermo	16
metast_cSCC12.raw.thermo	17
metast_cSCC11.raw.thermo	19
metast_cSCC10.raw.thermo	18
metast_cSCC9.raw.thermo	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)

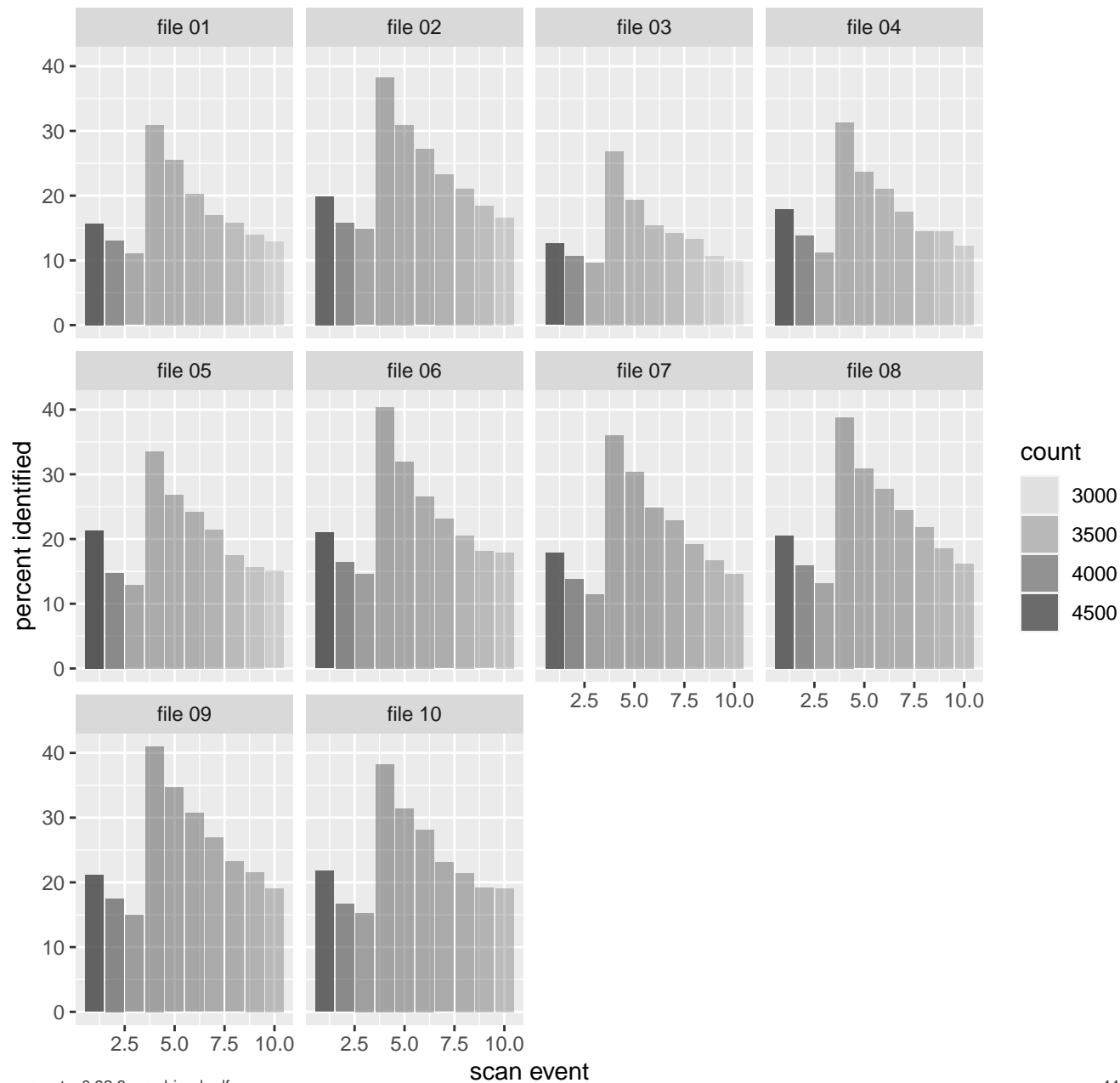
MSMScans: TopN



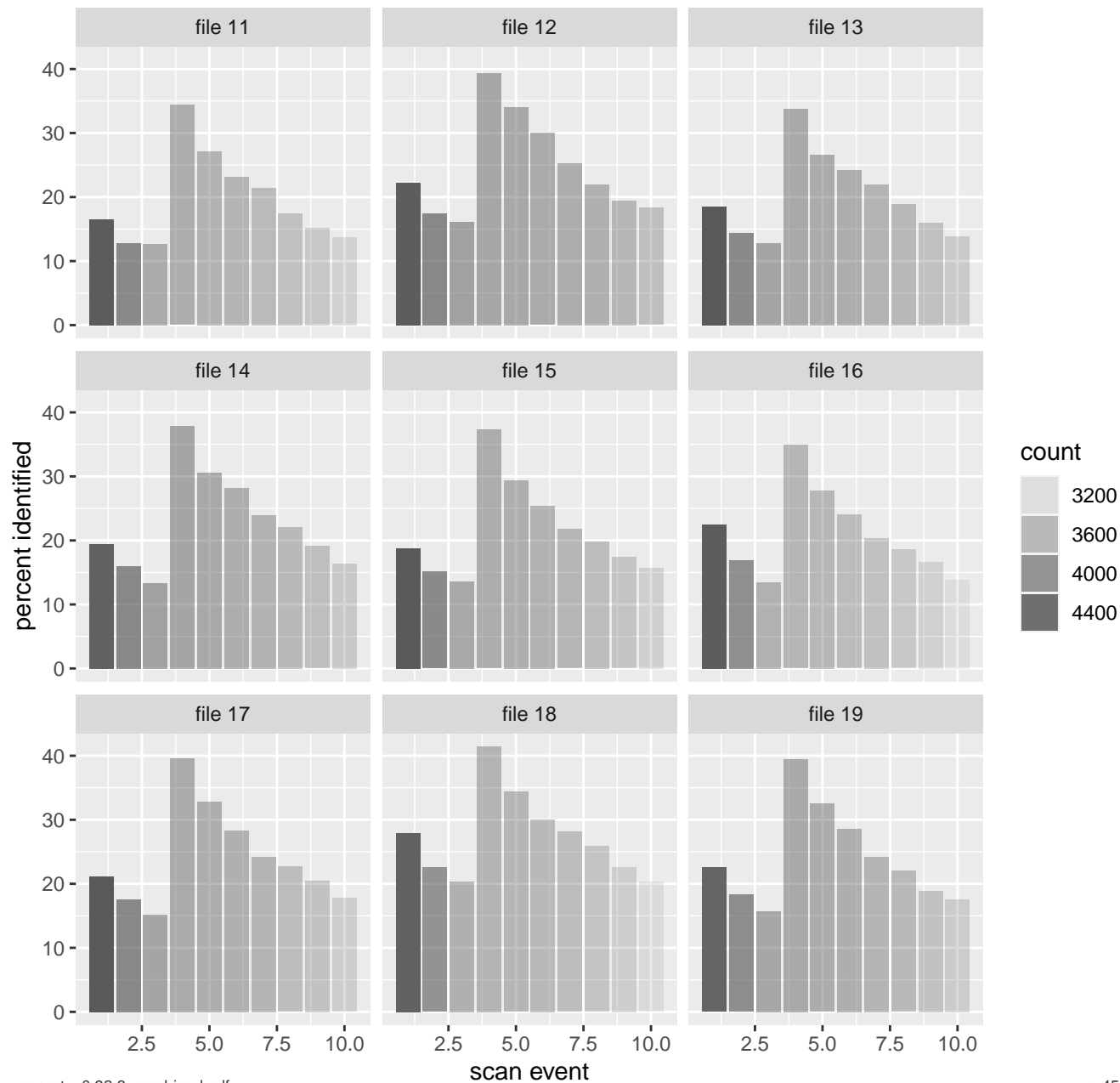
MSMSScans: TopN



MSMSscans: TopN % identified over N

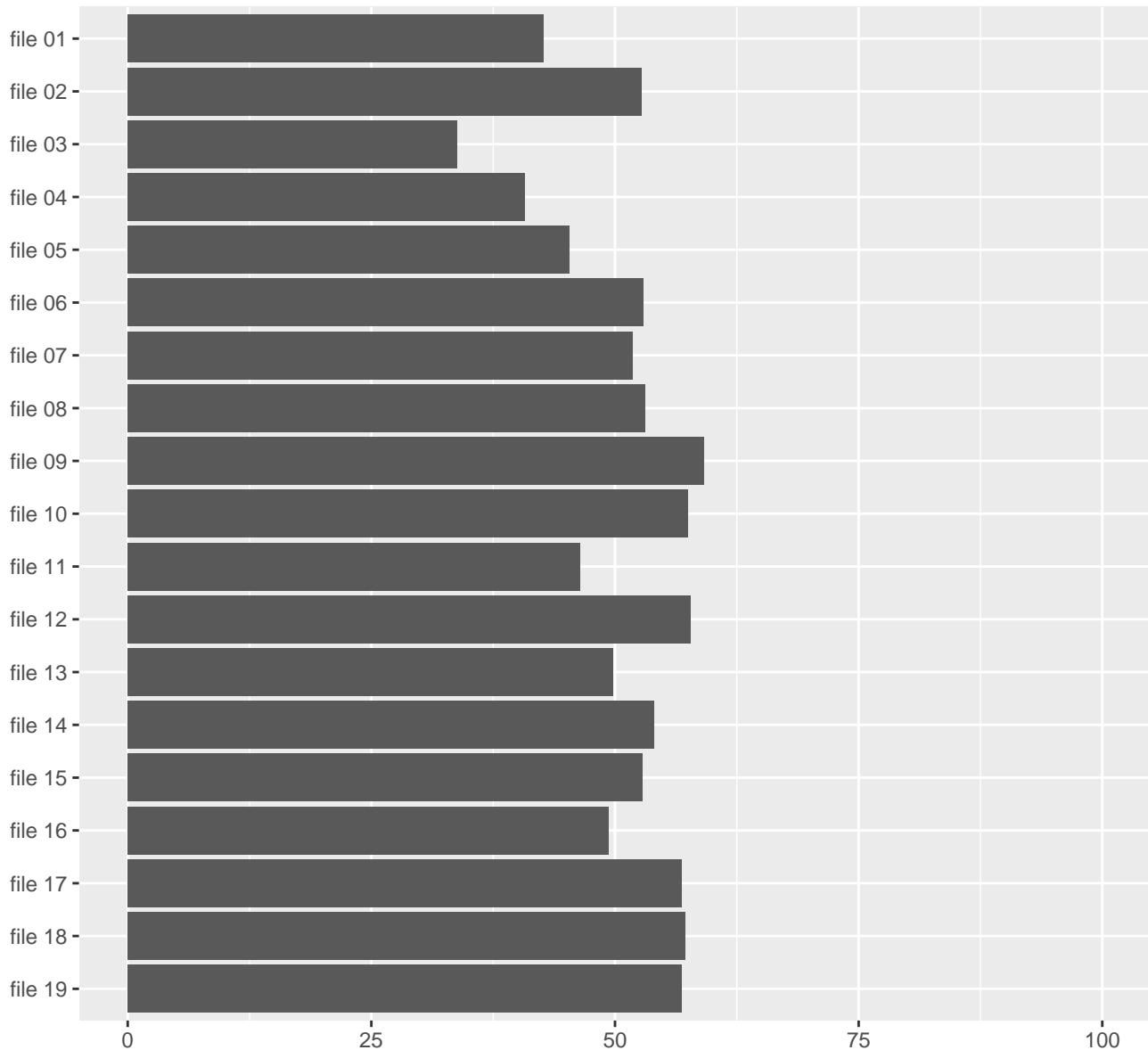


MSMSscans: TopN % identified over N

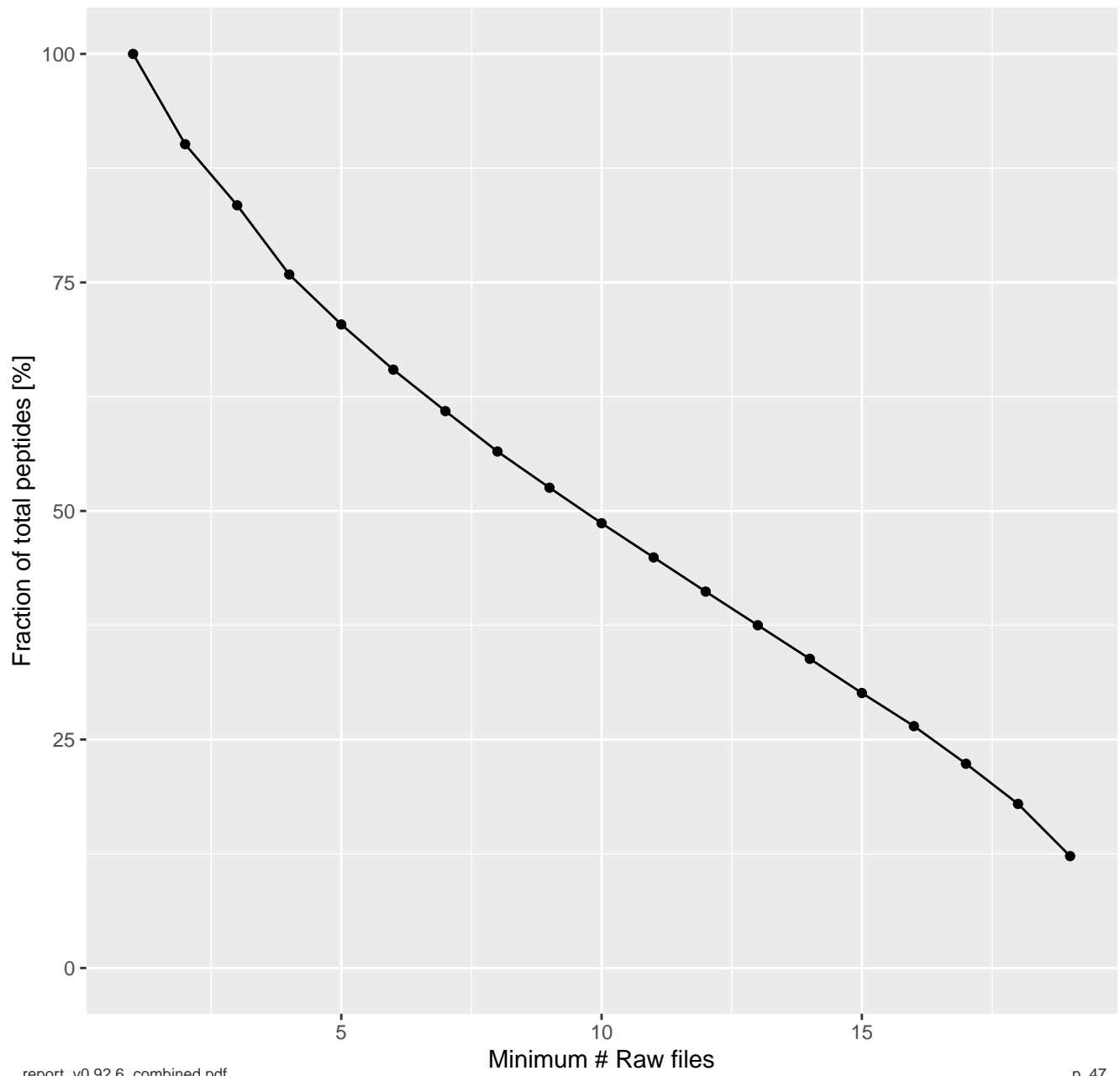


[experimental] EVD: Non-Missing Peptides

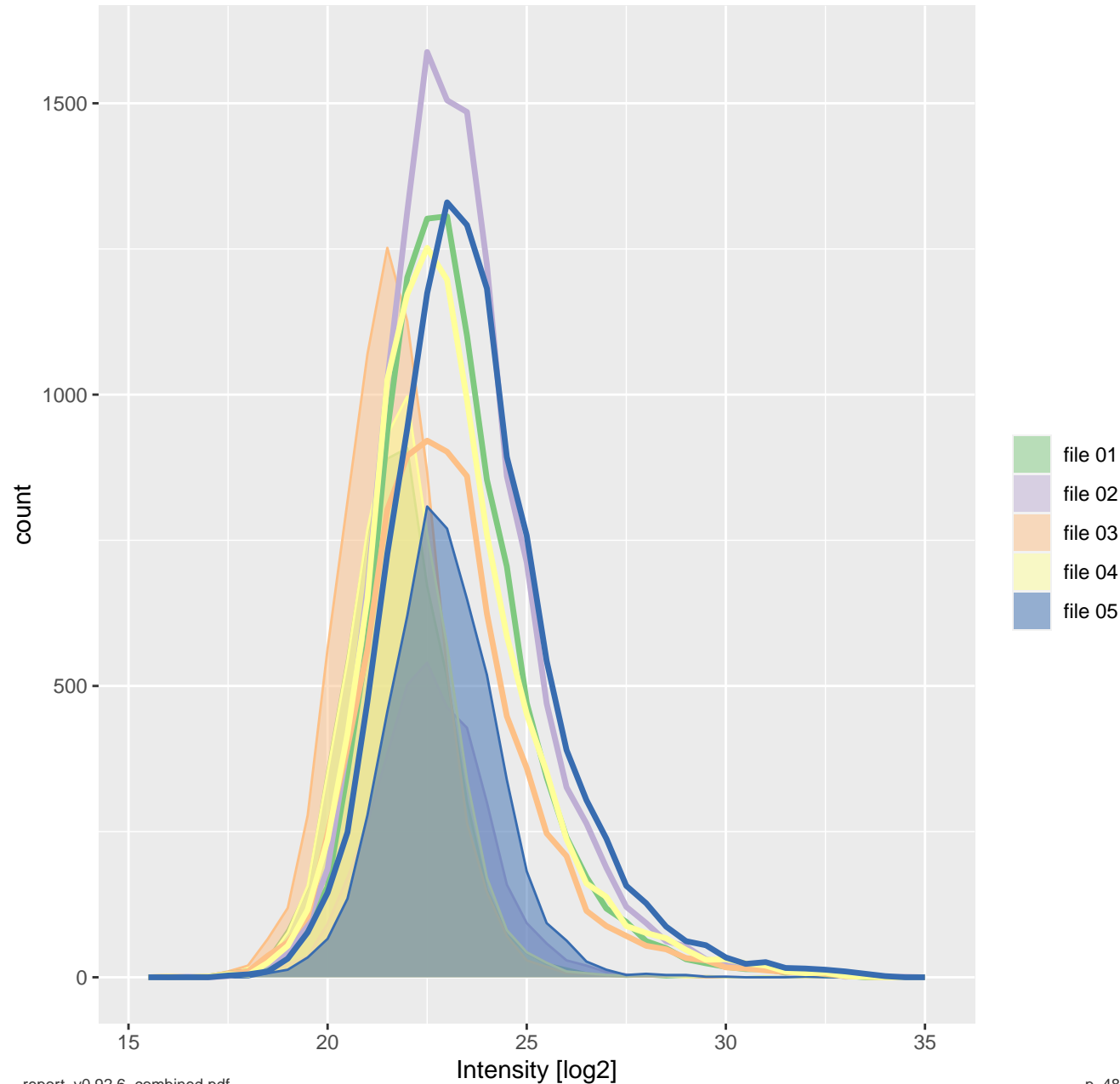
compared to all peptides seen in experiment



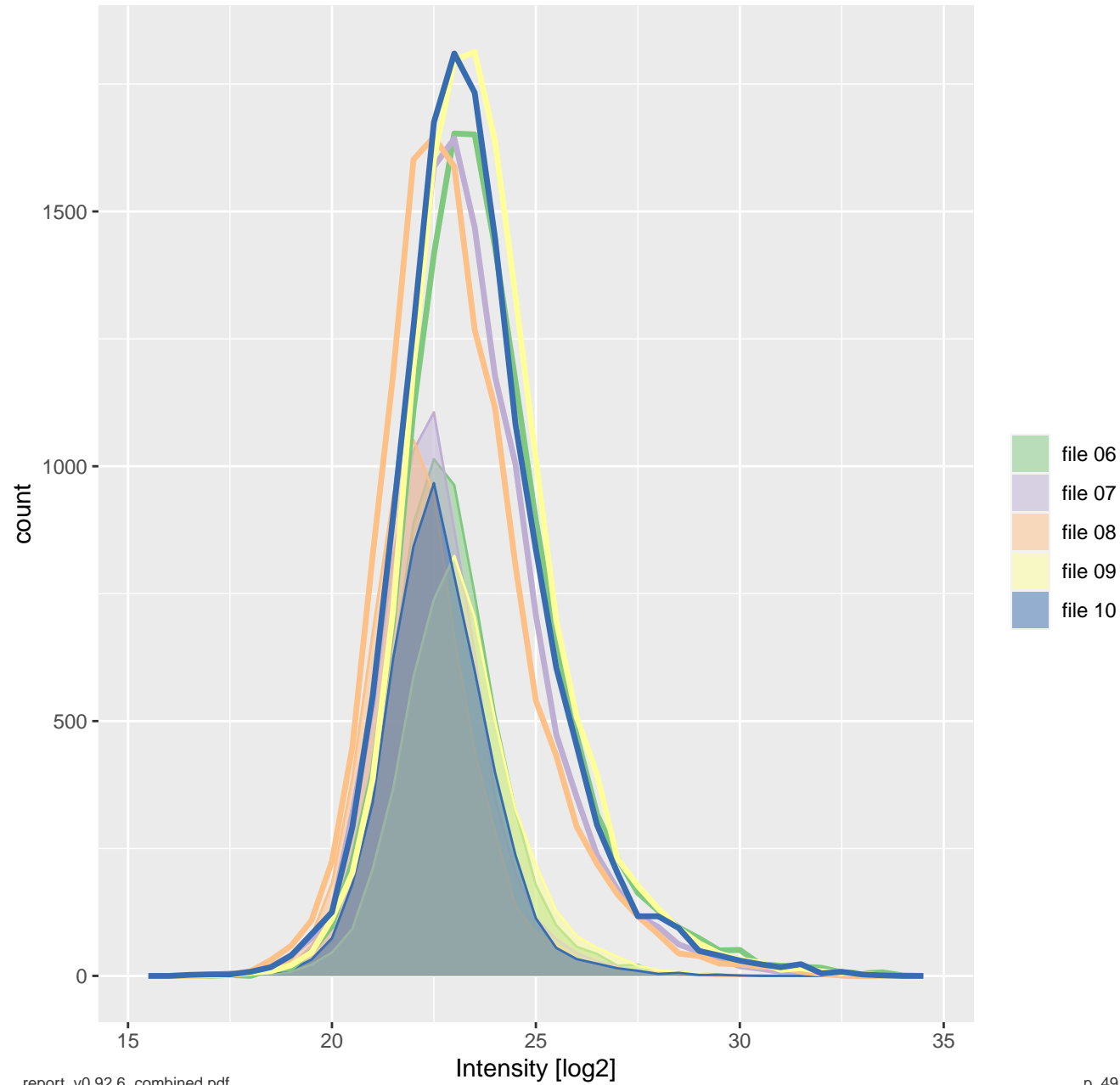
[experimental] EVD: Non-missing by set



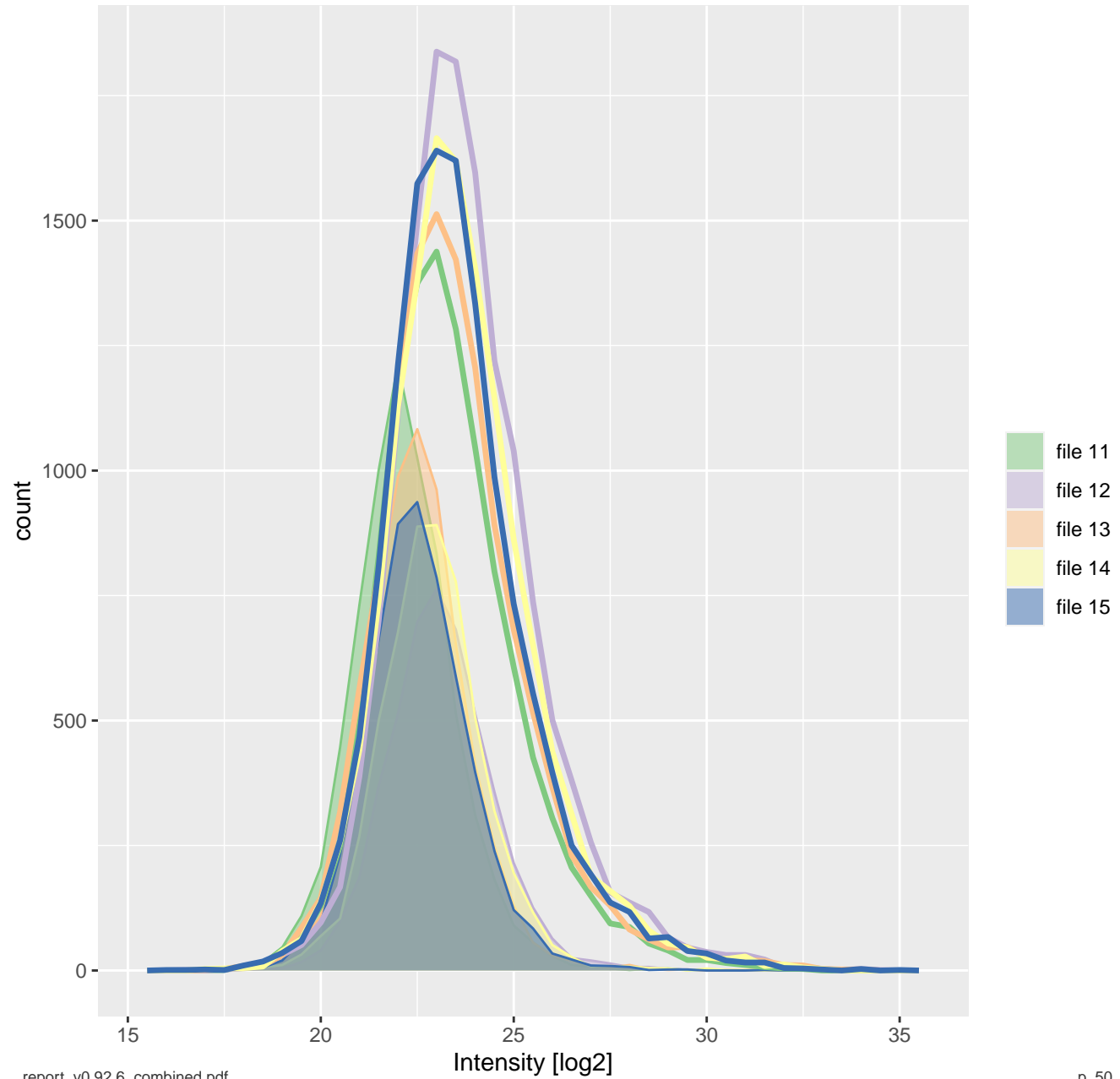
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



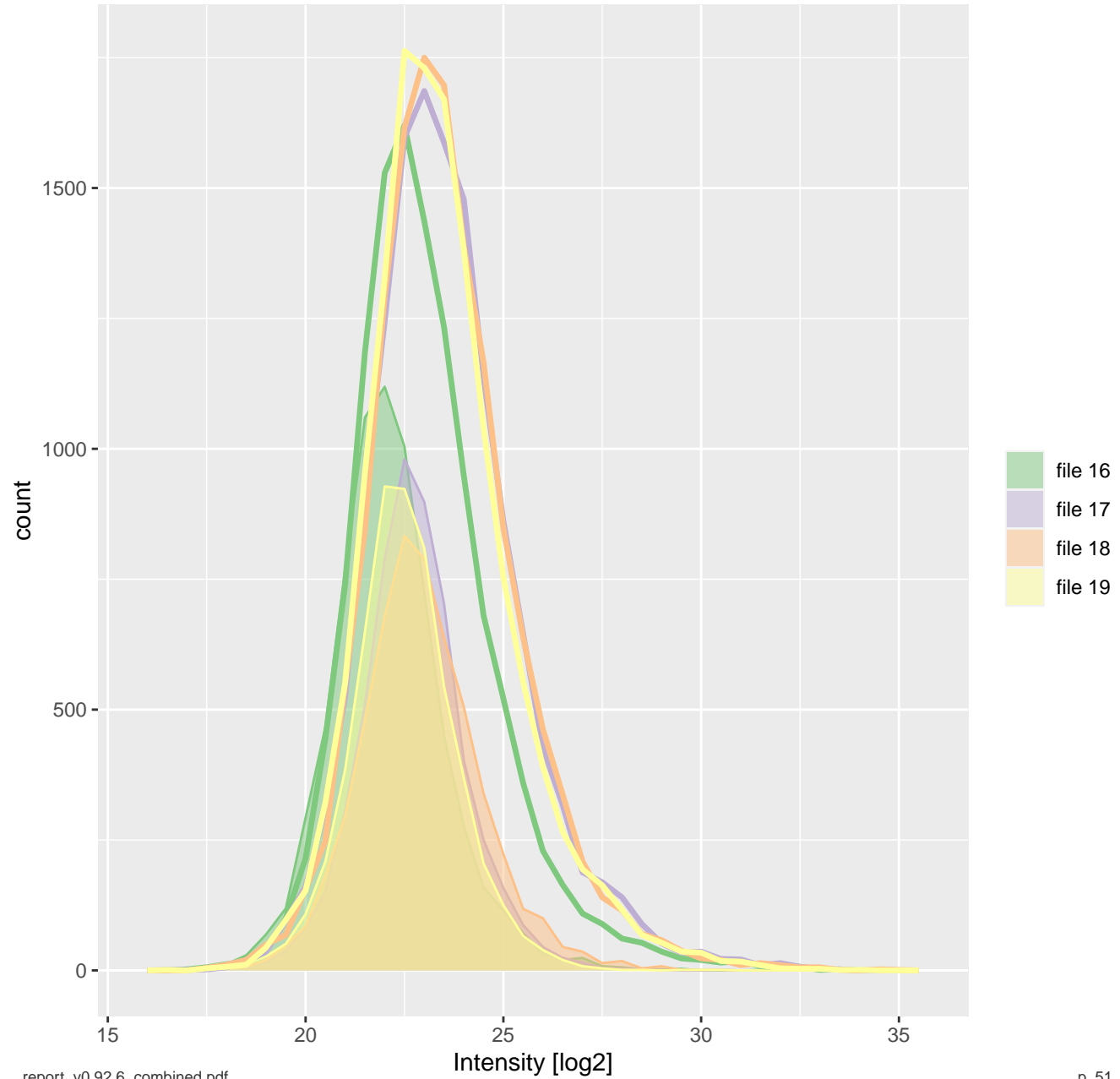
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



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

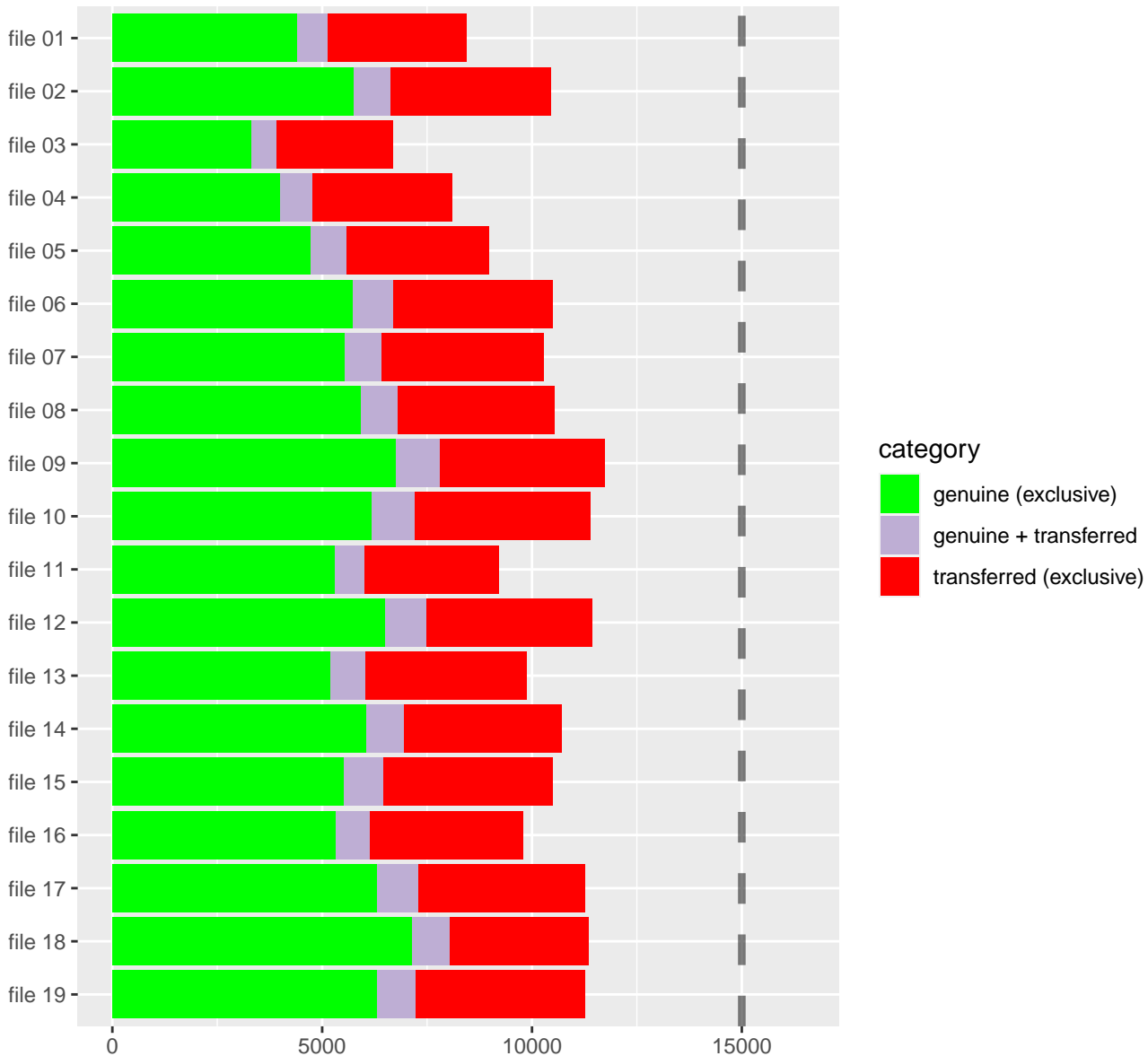


[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



EVD: Peptide ID count

MBR gain: +58%



EVD: ProteinGroups count

MBR gain: +32%

