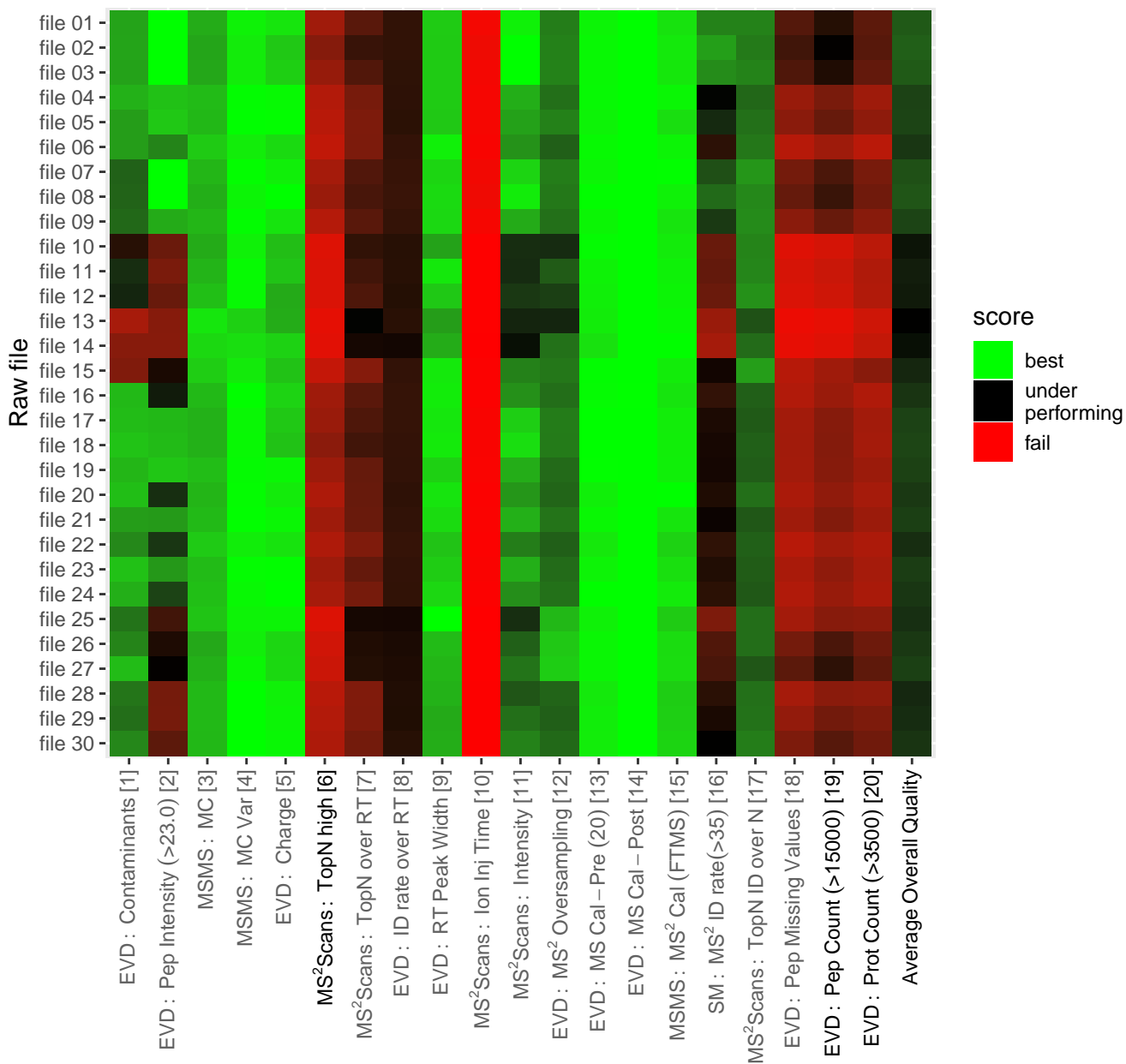


# Performance overview



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
20170427_144T_1a_170427152838	file 01	..20170427_144T_1a_170427152838
20170427_144T_1b	file 02	..20170427_144T_1b
20170427_144T_1c	file 03	..20170427_144T_1c
20170427_144T_2a	file 04	..20170427_144T_2a
20170427_144T_2b	file 05	..20170427_144T_2b
20170427_144T_2c	file 06	..20170427_144T_2c
20170427_159N_5a	file 07	..20170427_159N_5a
20170427_159N_5b	file 08	..20170427_159N_5b
20170427_159N_5c	file 09	..20170427_159N_5c
20170427_159T_3a	file 10	..20170427_159T_3a
20170427_159T_3b	file 11	..20170427_159T_3b
20170427_159T_3c	file 12	..20170427_159T_3c
20170427_159T_4a	file 13	..20170427_159T_4a
20170427_159T_4b	file 14	..20170427_159T_4b
20170427_159T_4c	file 15	..20170427_159T_4c

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
20170427_163N_8a	file 16	..20170427_163N_8a
20170427_163N_8b	file 17	..20170427_163N_8b
20170427_163N_8c	file 18	..20170427_163N_8c
20170427_163T_6a	file 19	..20170427_163T_6a
20170427_163T_6b	file 20	..20170427_163T_6b
20170427_163T_6c	file 21	..20170427_163T_6c
20170427_163T_7a	file 22	..20170427_163T_7a
20170427_163T_7b	file 23	..20170427_163T_7b
20170427_163T_7c	file 24	..20170427_163T_7c
144T_mlgG1	file 25	..144T_mlgG1
144T_mlgG2	file 26	..144T_mlgG2
144T_mlgG3	file 27	..144T_mlgG3
144T_Orf1_1	file 28	..144T_Orf1_1
144T_Orf1_2	file 29	..144T_Orf1_2
144T_Orf1_3	file 30	..144T_Orf1_3

## PAR: parameters

parameter	value	parameter	value
Advanced ratios	False	MS/MS deisotoping tolerance ..	0.01
Advanced site intensities	True	MS/MS deisotoping tolerance ..	Da
Alignment ion mobility windo..	0	MS/MS deisotoping tolerance ..	0.15
Alignment time window [min]	20	MS/MS deisotoping tolerance ..	Da
Calculate peak properties	False	MS/MS dependent losses (FTMS..	True
Combined folder location	G:\LaCava\CRC_v4	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	04/15/2019 08:59:48	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..	True	MS/MS recalibration (ITMS)	False
Epsilon score for mutations	G:\LaCava\CRC_v4	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	C:\Users\ProteHomics\Desкто op\MaxQuant\Andromeda_Index	MS/MS tol. (ITMS)	0.5 Da
iBAQ	True	MS/MS tol. (TOF)	40 ppm
iBAQ log fit	False	MS/MS tol. (Unknown)	0.5 Da
Include contaminants	True	MS/MS water loss (FTMS)	True
Label min. ratio count	2	MS/MS water loss (ITMS)	True
Machine name	DESKTOP-RHO63DE	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	Protein FDR	0.01
Match unidentified features	False	PSM FDR	0.01

ortho\_orf1.fasta

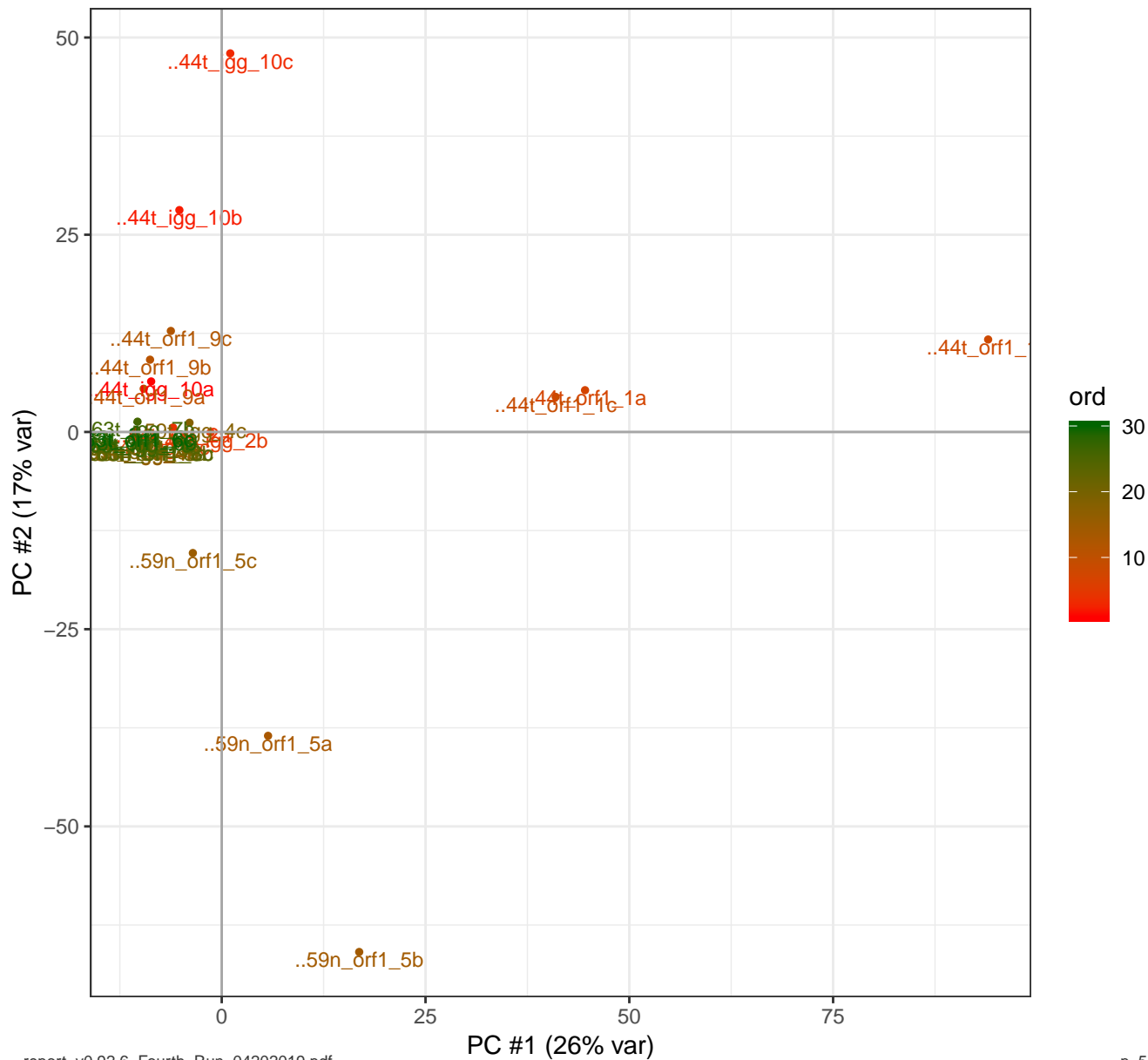
## PAR: parameters

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 Phospho (STY)Sites.txt
Min. peptide length for unsp..	8	Stabilize large LFQ ratios	True
Min. peptides	1	Temporary folder	E:\MQ_Temp
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	0	Top MS/MS peaks per Da inter..	8
Modifications included in pr..	Oxidation (M) Acetyl (Protein N-term) Carbamidomethyl (C)	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	ProteHomics
MS/MS ammonia loss (Unknown)	True	Variation mode	None
MS/MS deisotoping (FTMS)	True	Version	1.6.5.0
MS/MS deisotoping (ITMS)	False	Write accumulatedPasefMsmsSc..	True
MS/MS deisotoping (TOF)	True	Write allPeptides table	True
MS/MS deisotoping (Unknown)	False	Write ms3Scans table	True
MS/MS deisotoping tolerance ..	7	Write msmsScans table	True
MS/MS deisotoping tolerance ..	ppm	Write msScans table	True
MS/MS deisotoping tolerance ..	0.15	Write mzRange table	True
MS/MS deisotoping tolerance ..	Da	Write pasefMsmsScans table	True

ortho\_orf1.fasta

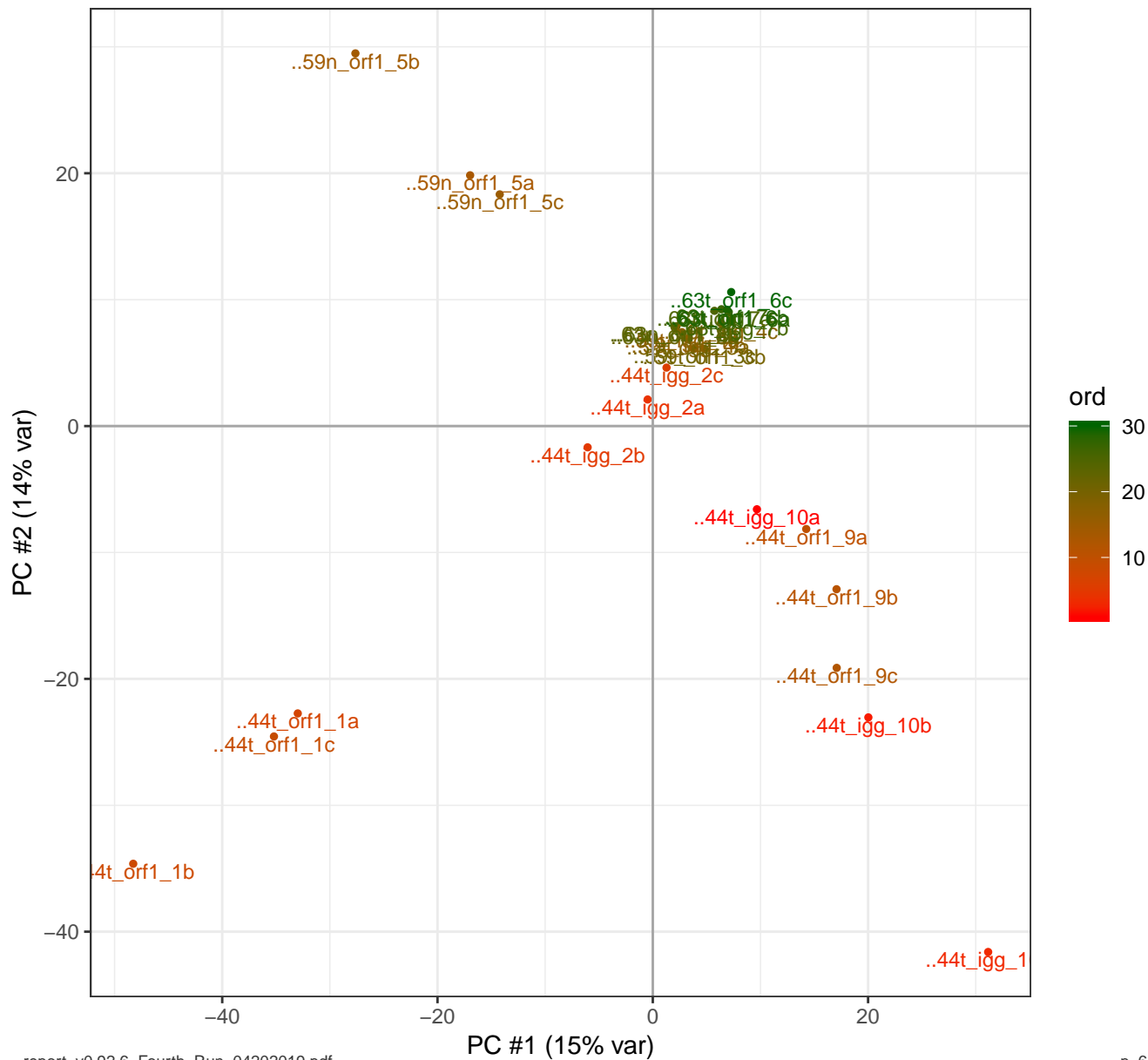
# PG: PCA of 'raw intensity'

(excludes contaminants)

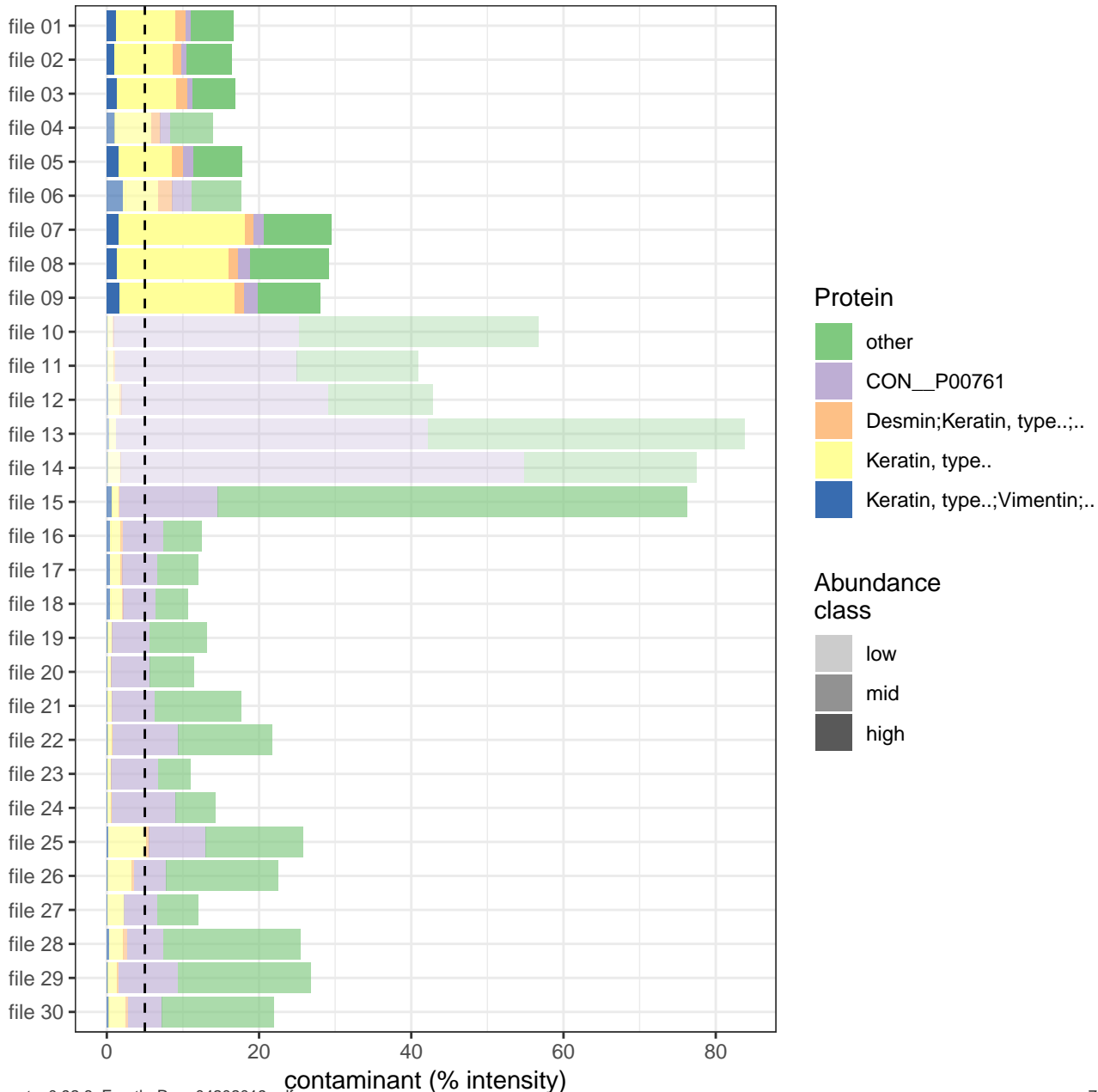


## PG: PCA of 'lfq intensity'

(excludes contaminants)



# EVD: Top5 Contaminants per Raw file





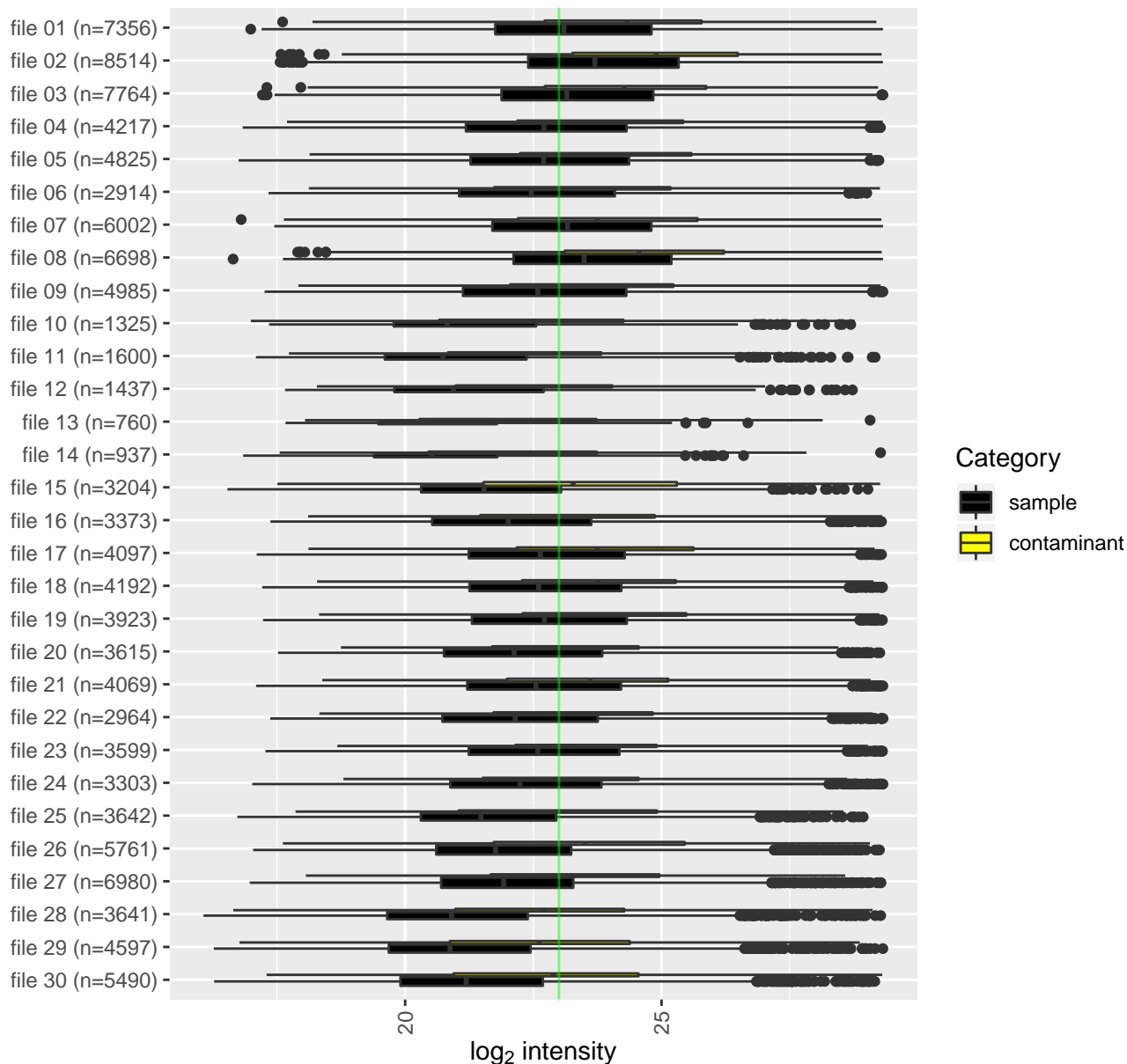
## EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

Did you use the correct database?

# EVD: peptide intensity distribution

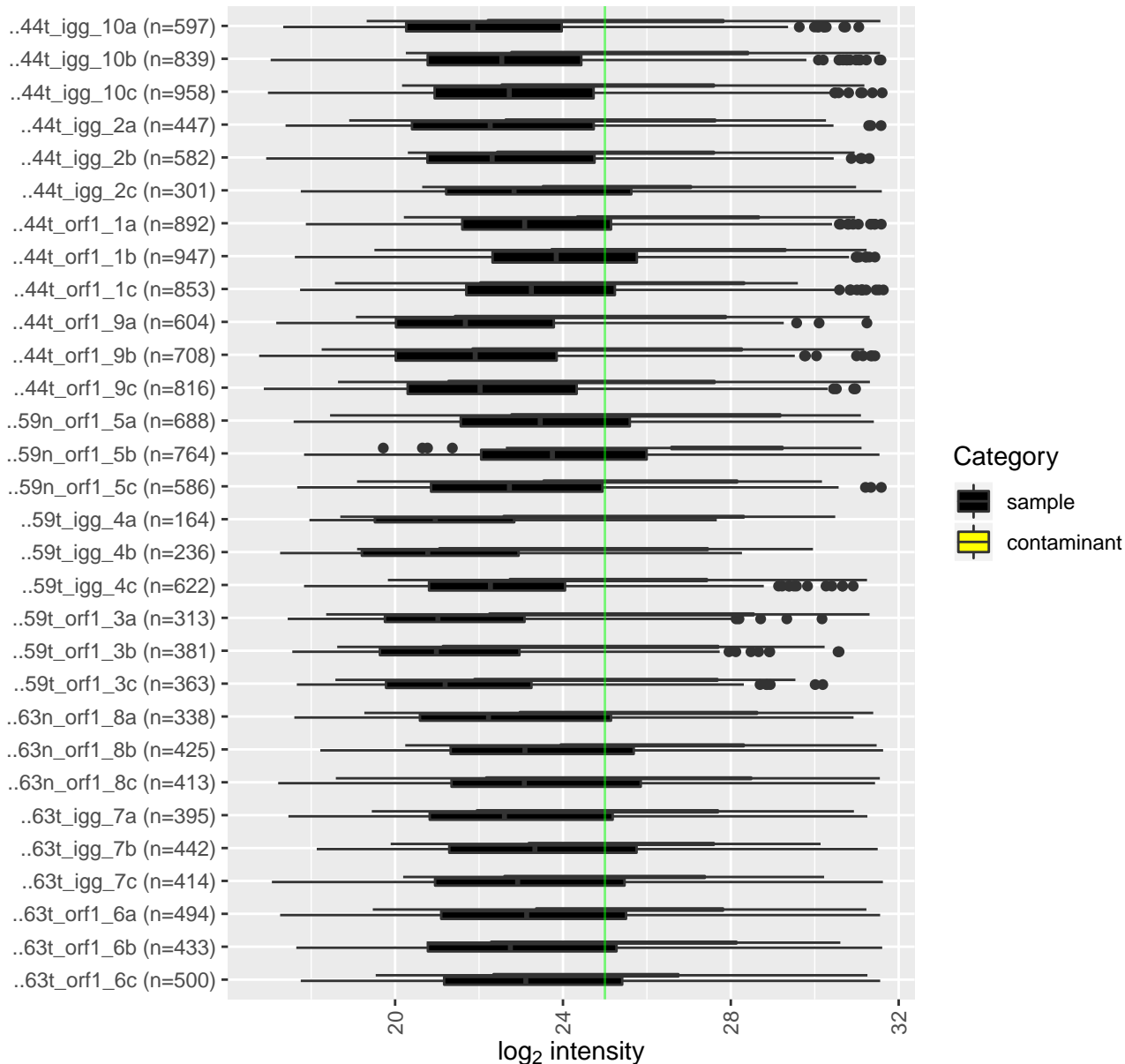
RSD 4% (expected < 5%)



# PG: intensity distribution

RSD 3.8% (w/o zero int.; expected < 5%)

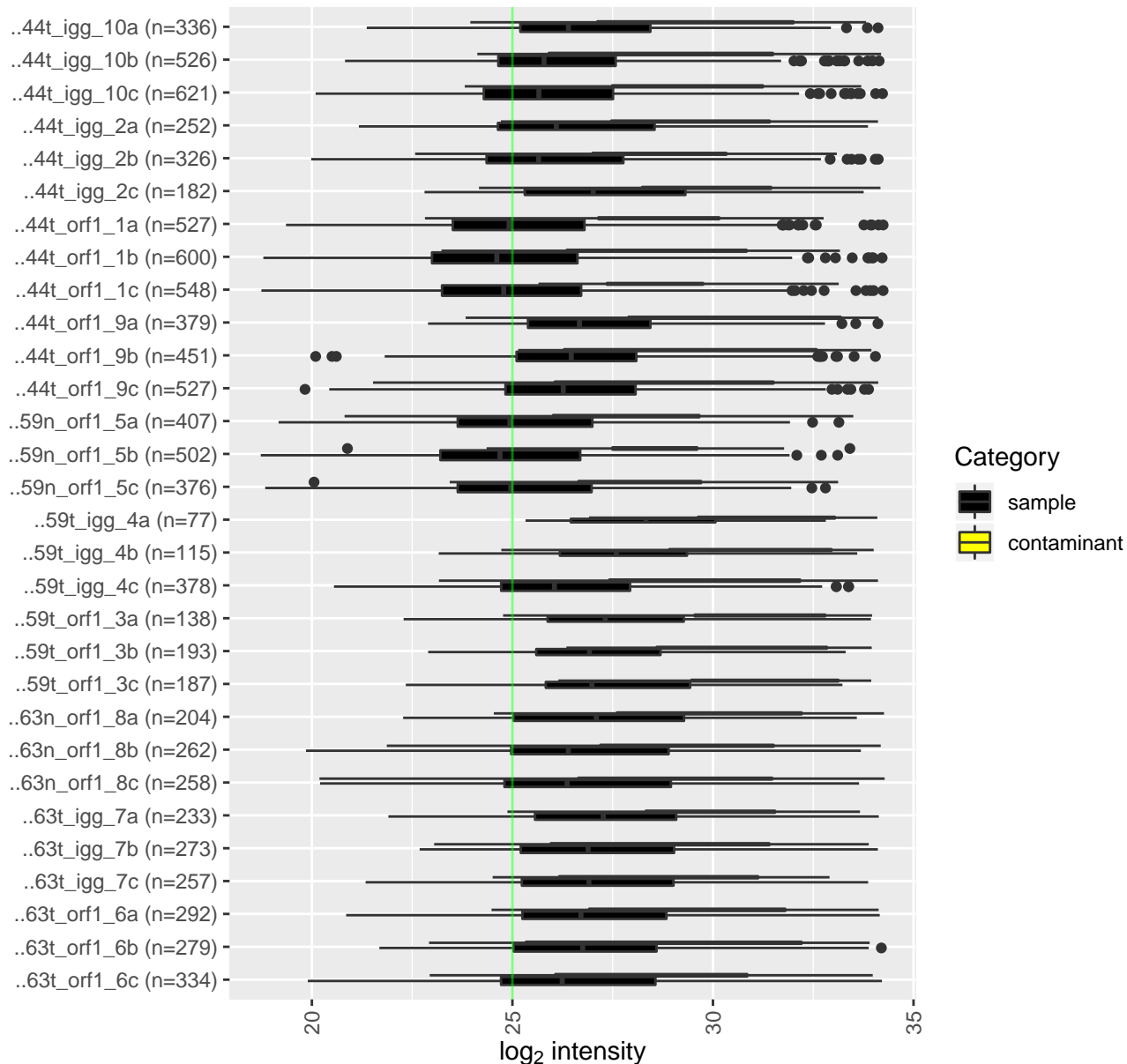
RSD NaN% [high RSD --> few peptides]



# PG: LFQ intensity distribution

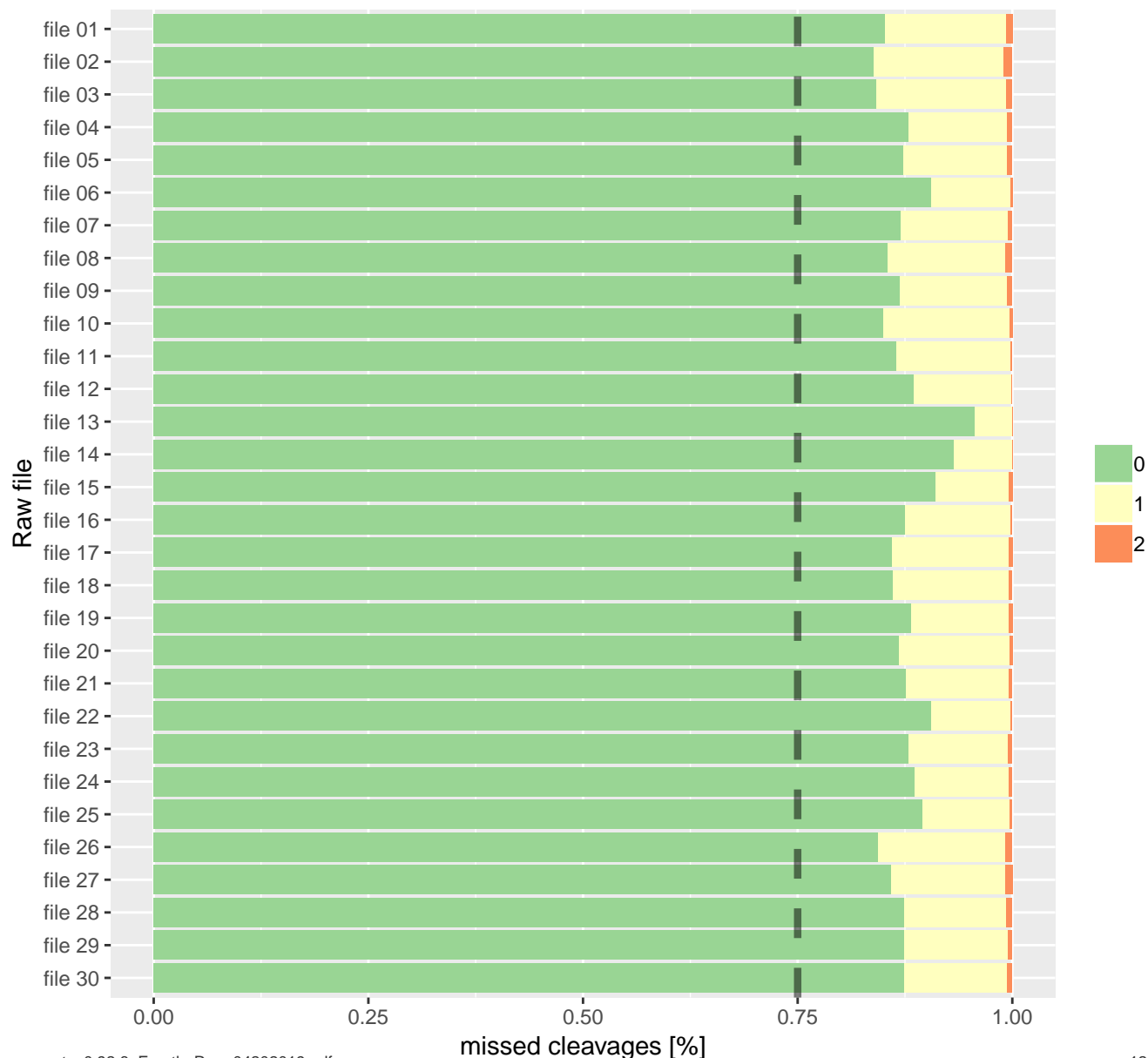
RSD 3.9% (w/o zero int.; expected < 5%)

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

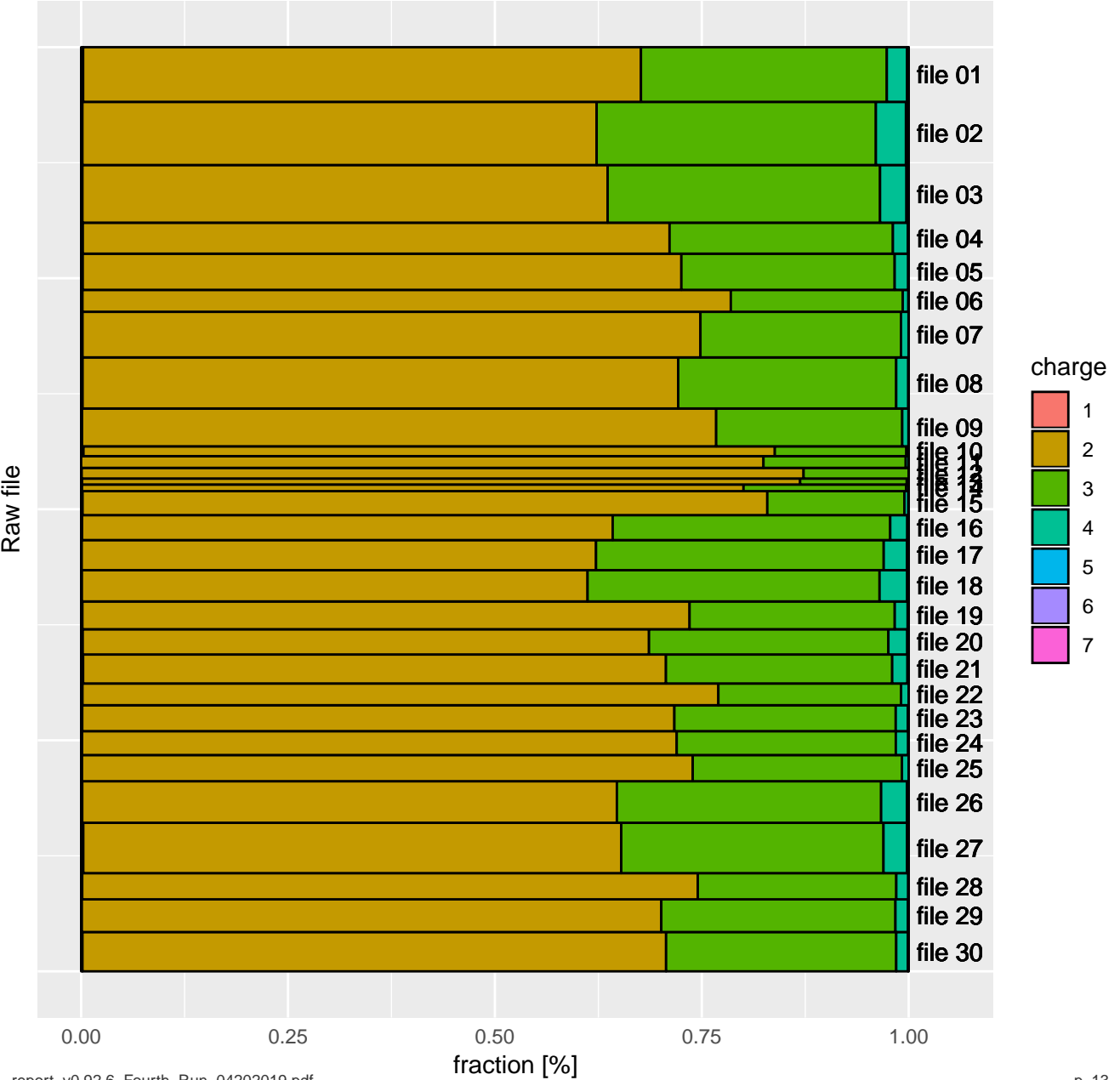


# MSMS: Missed cleavages per Raw file

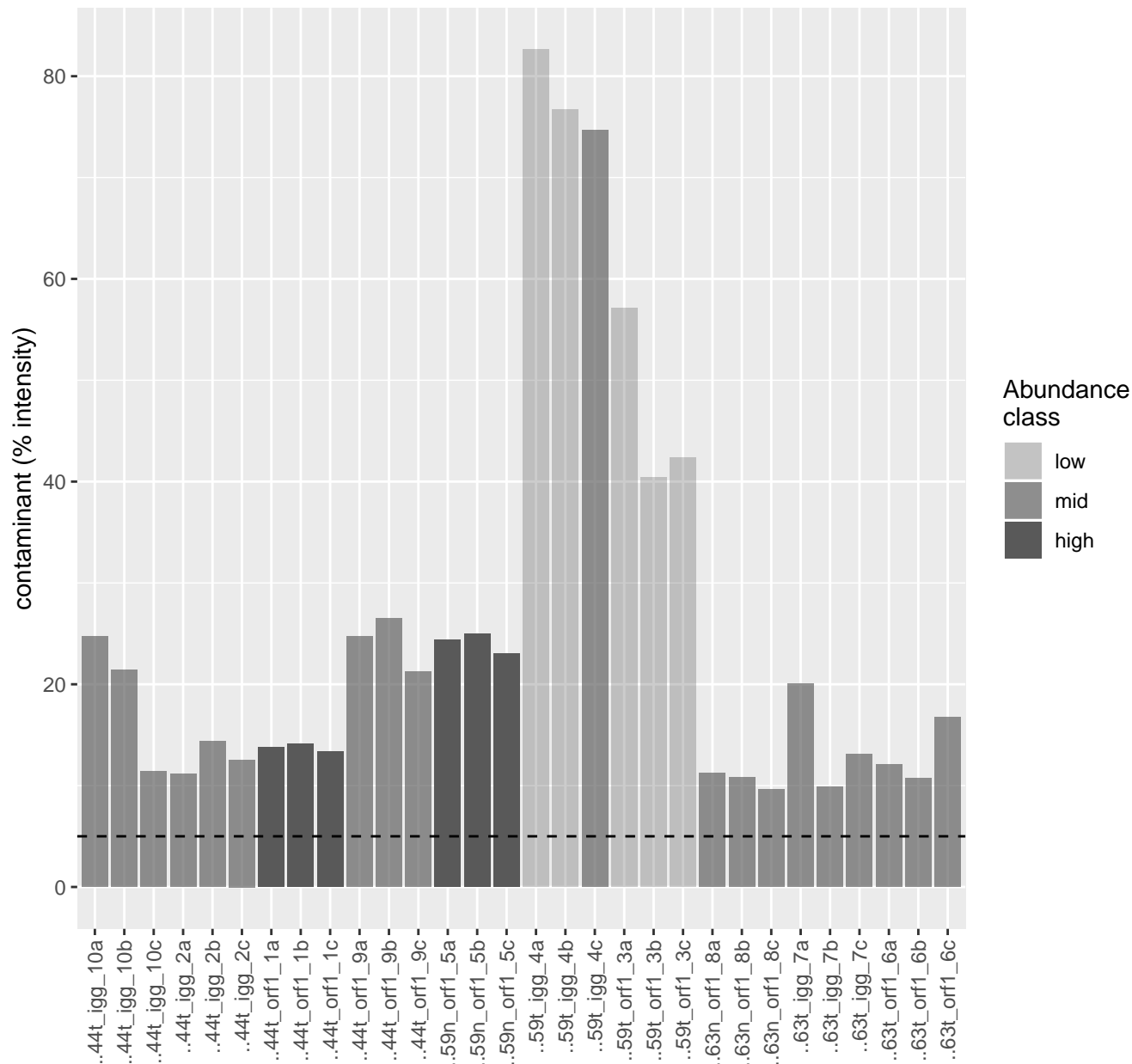
(excludes contaminants)



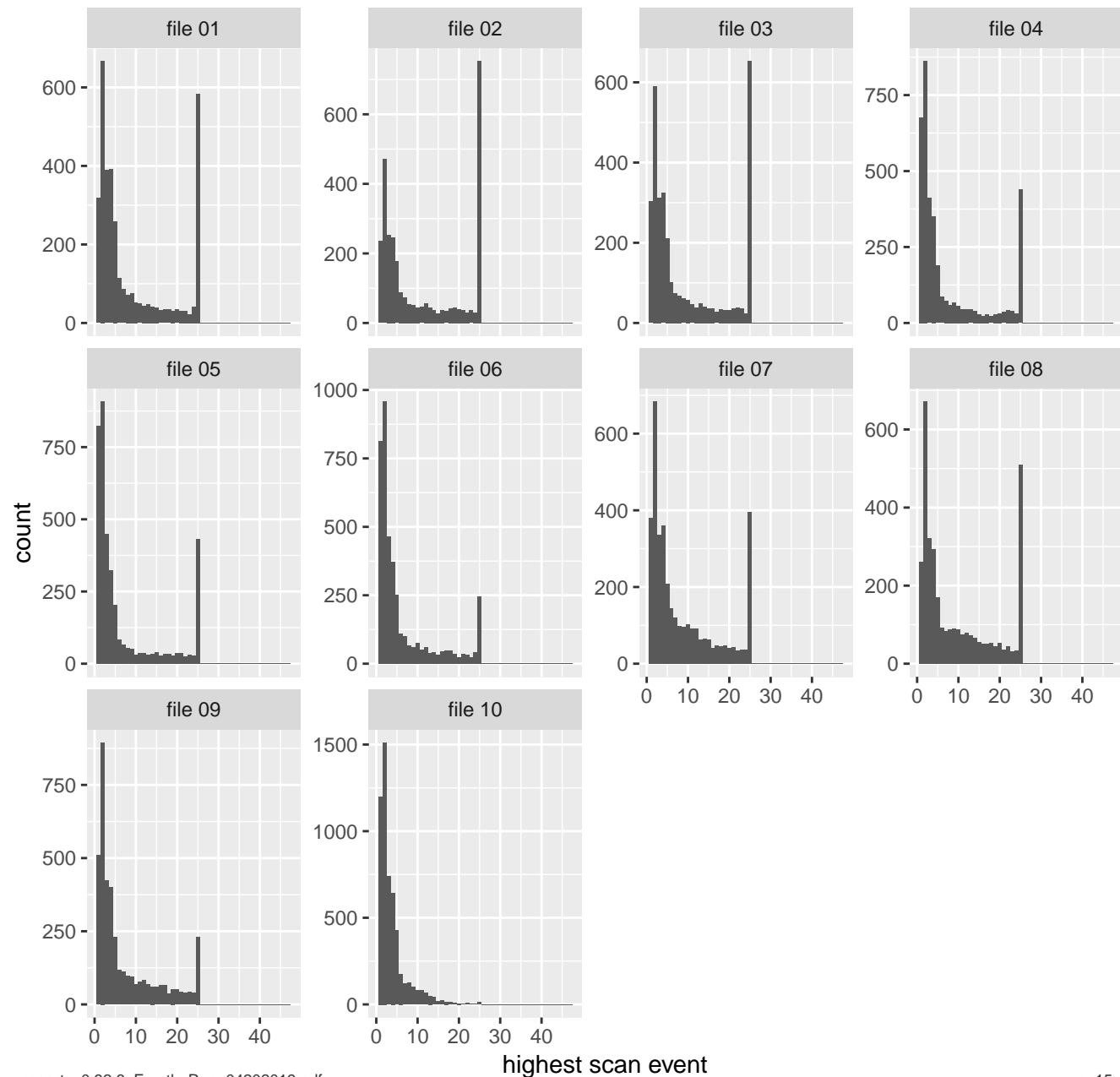
EVD: charge distribution



# PG: Contaminant per condition

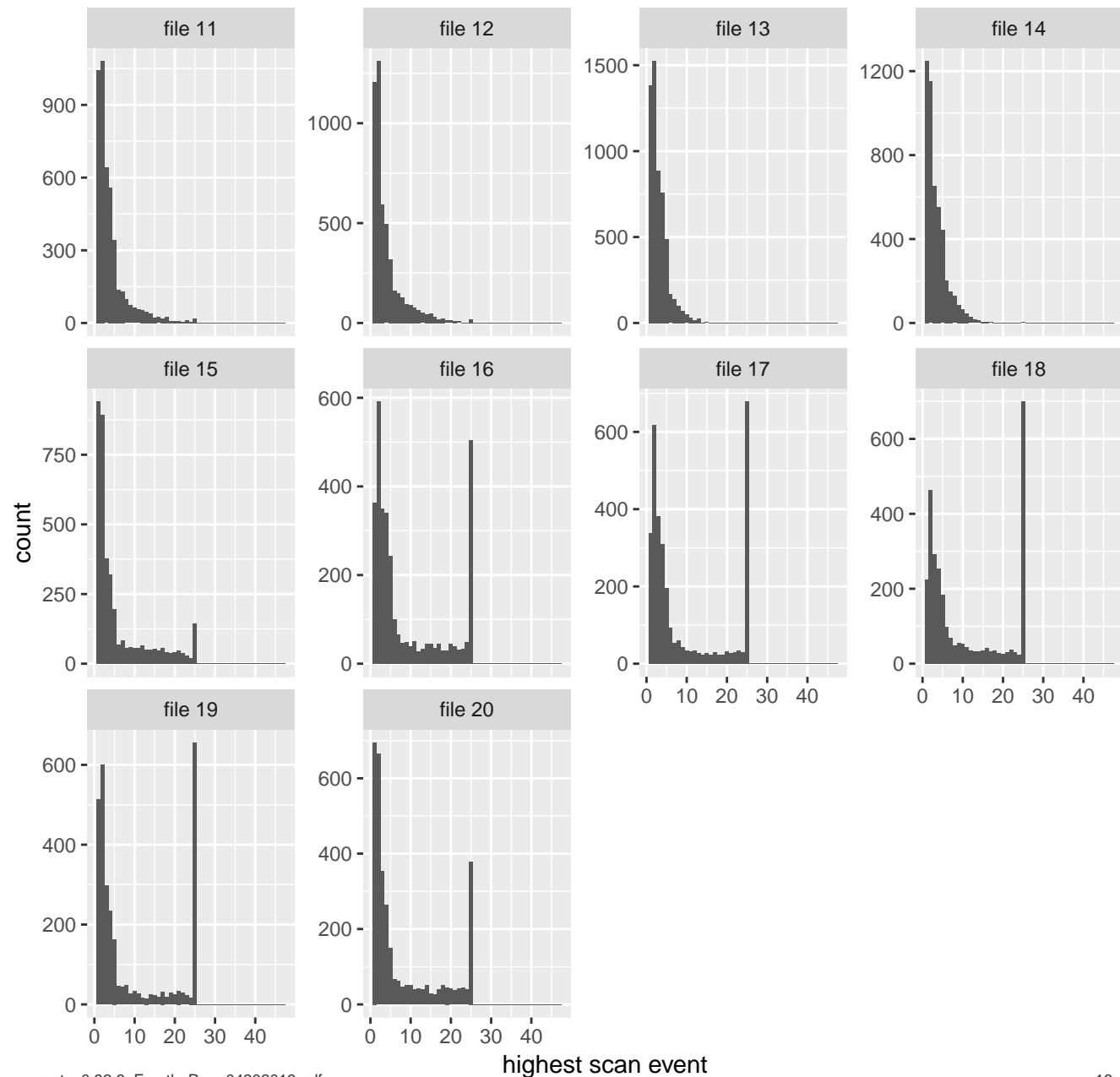


# MSMScans: TopN

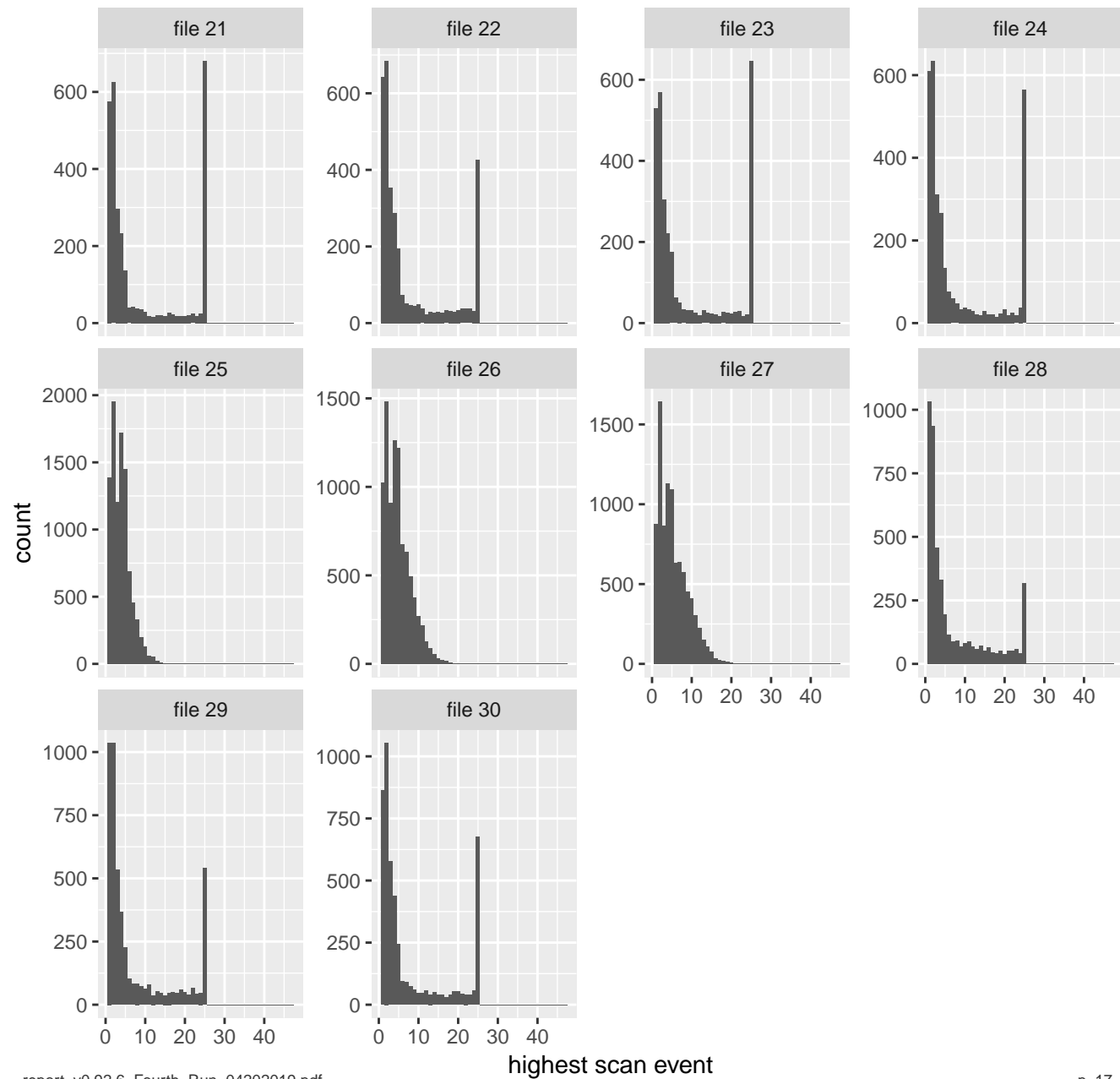




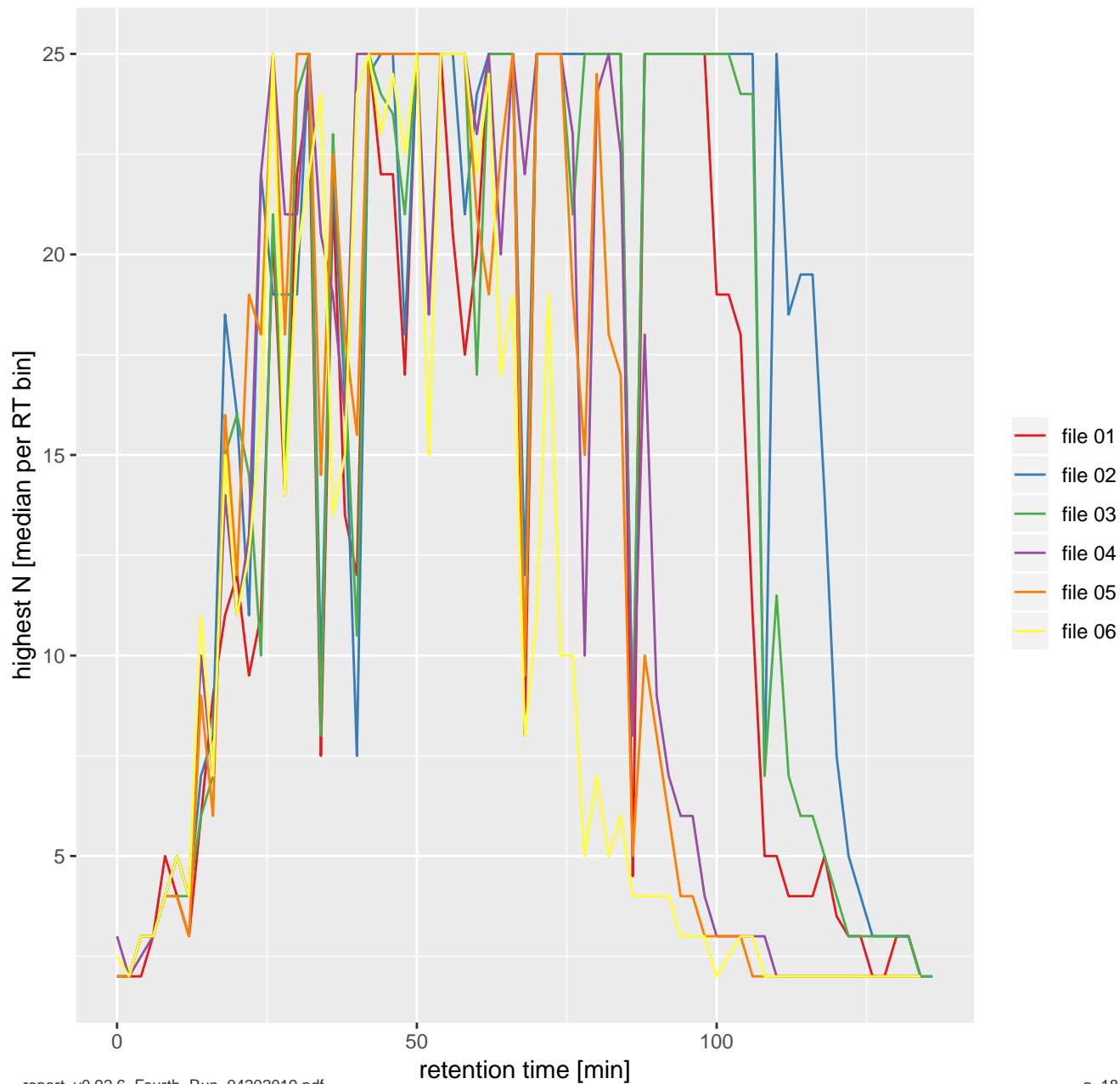
# MSMScans: TopN



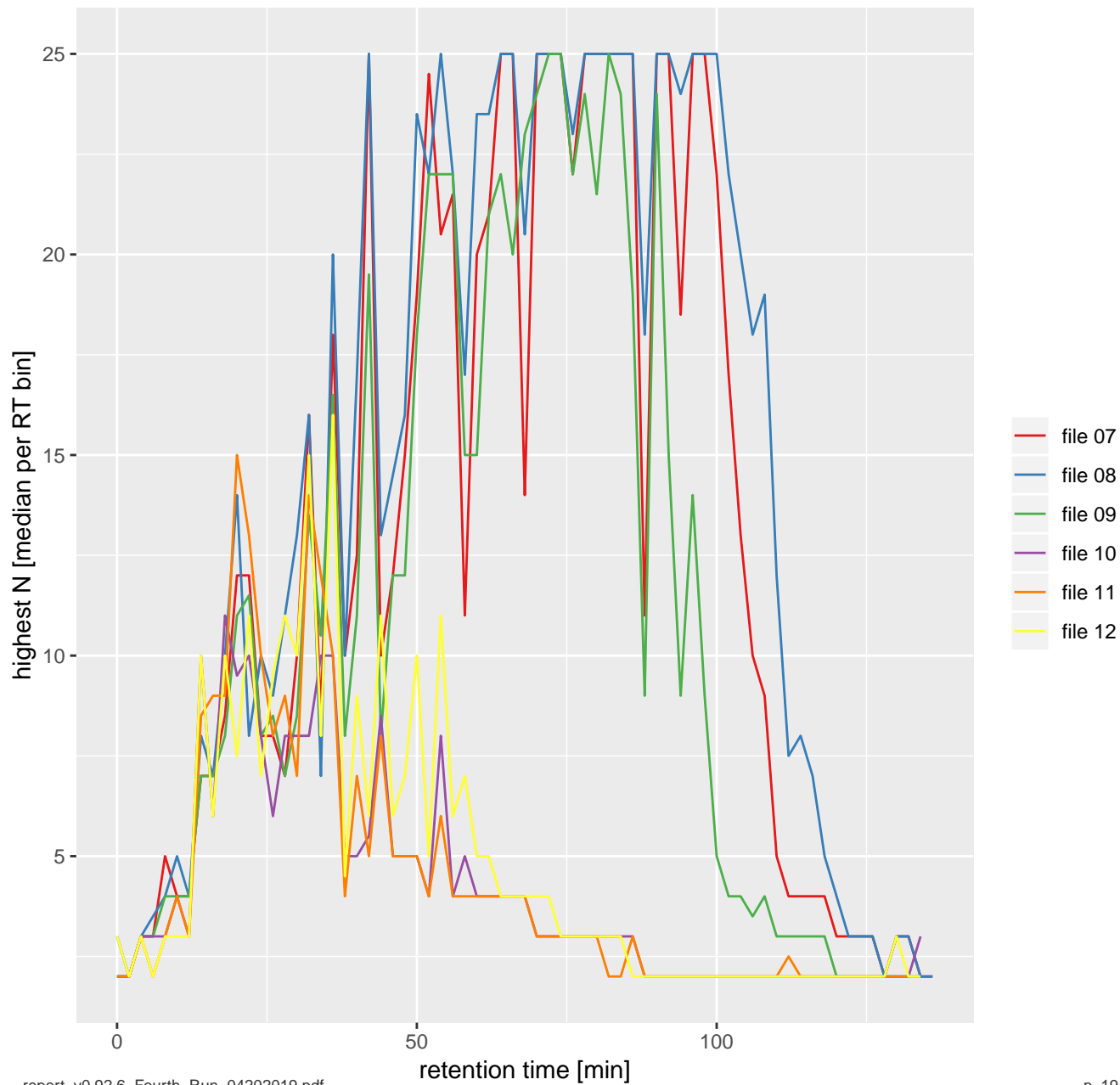
# MSMSScans: TopN



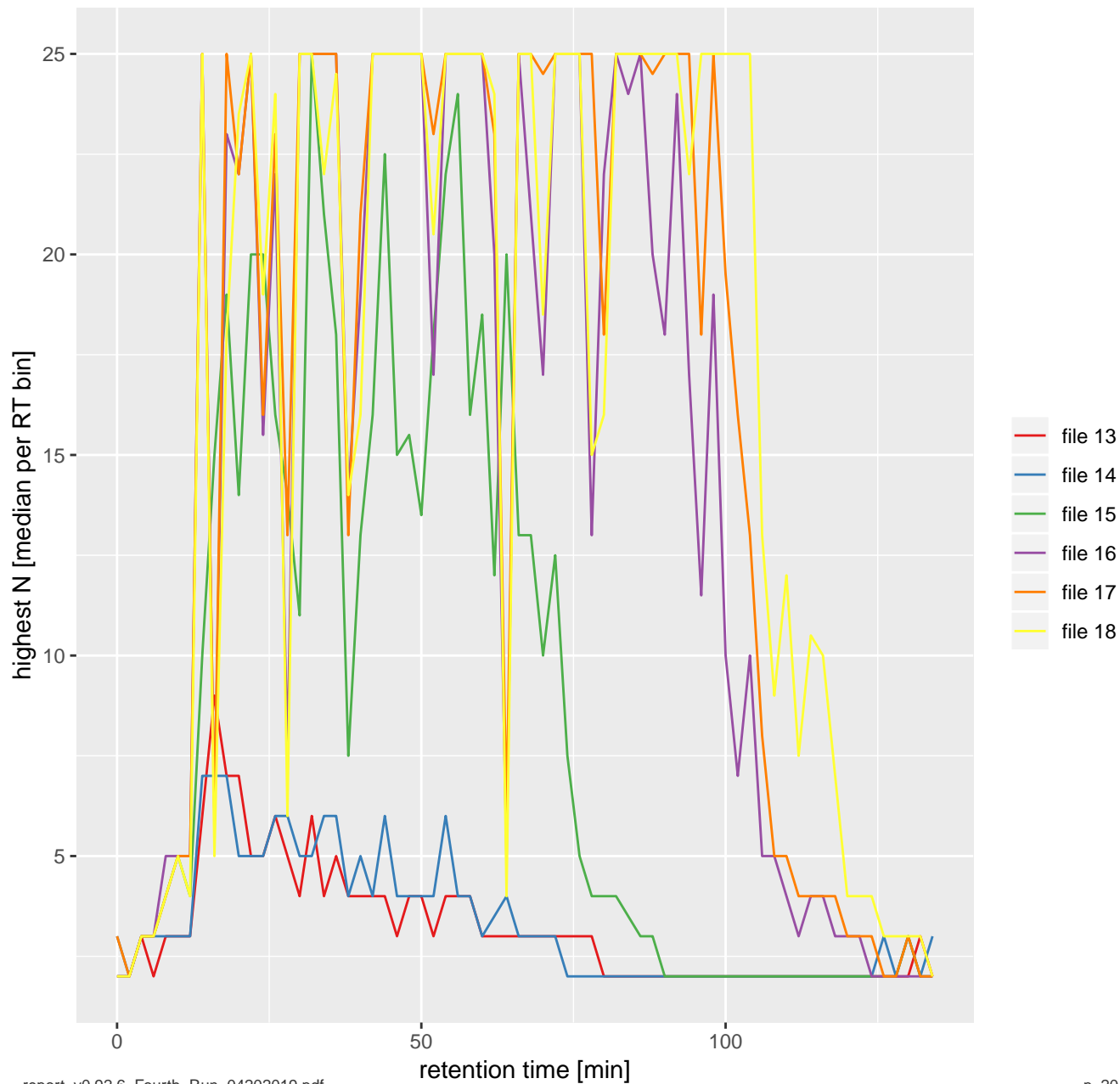
# MSMSscans: TopN over RT



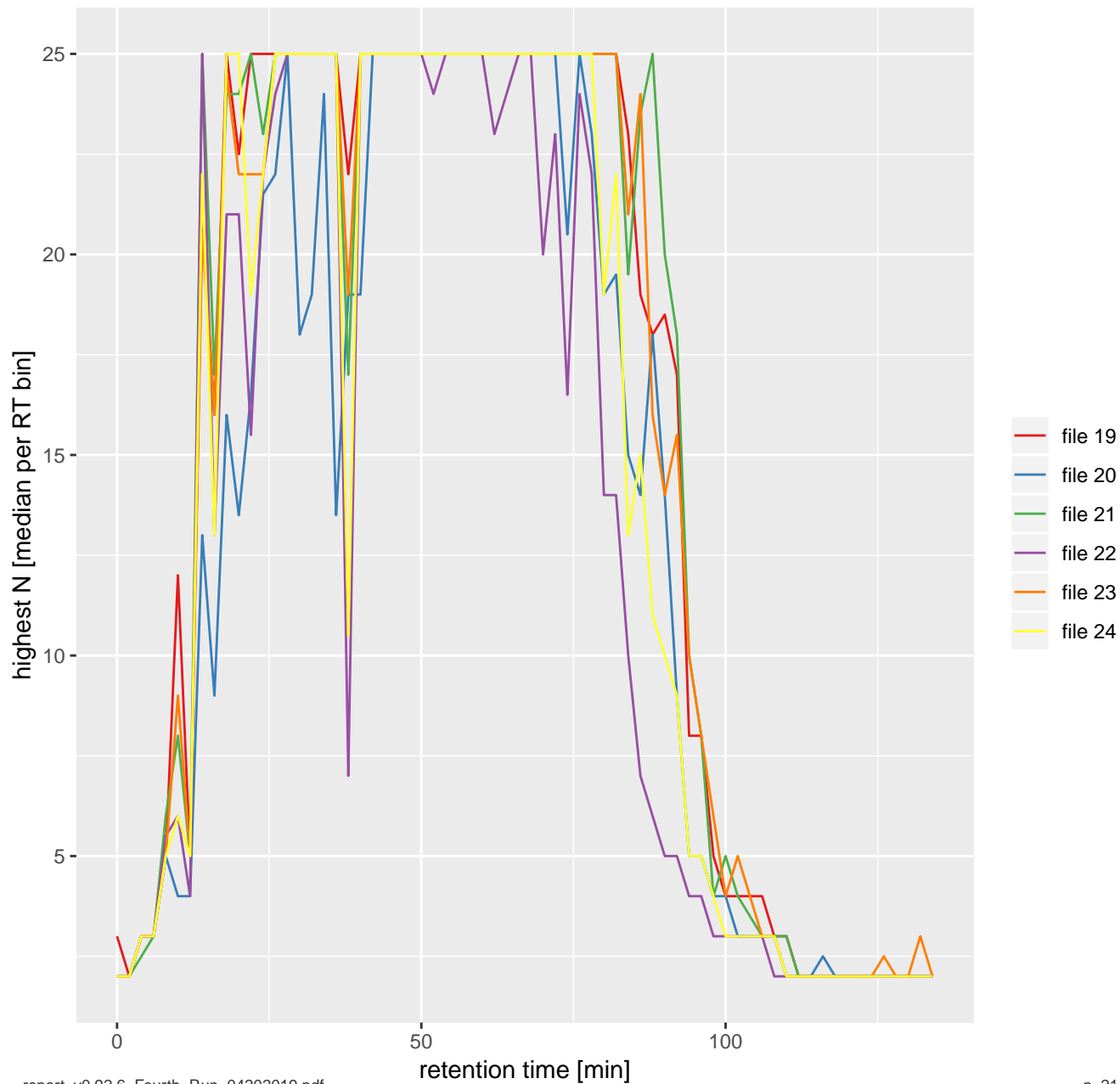
# MSMSscans: TopN over RT



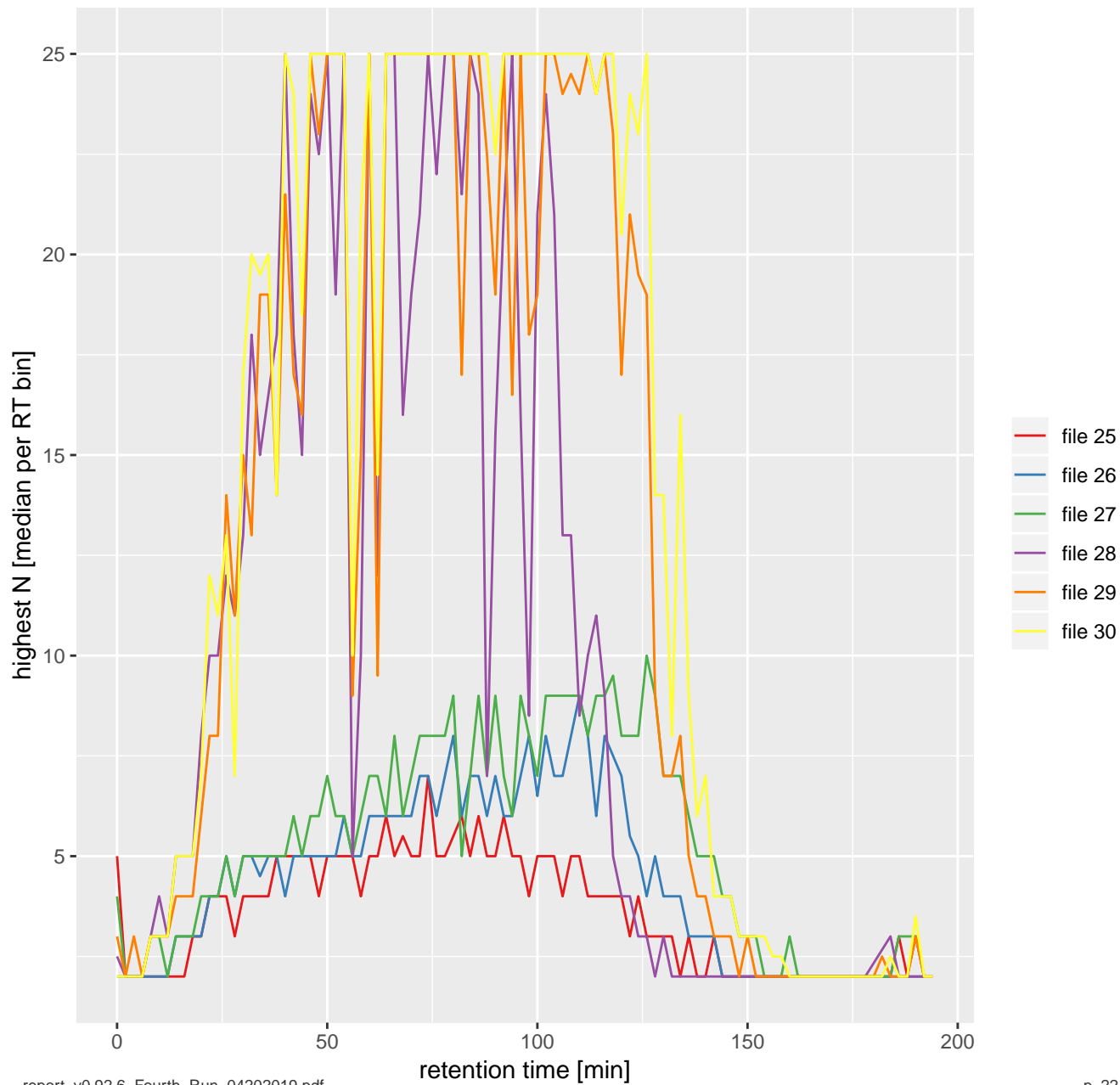
# MSMSscans: TopN over RT



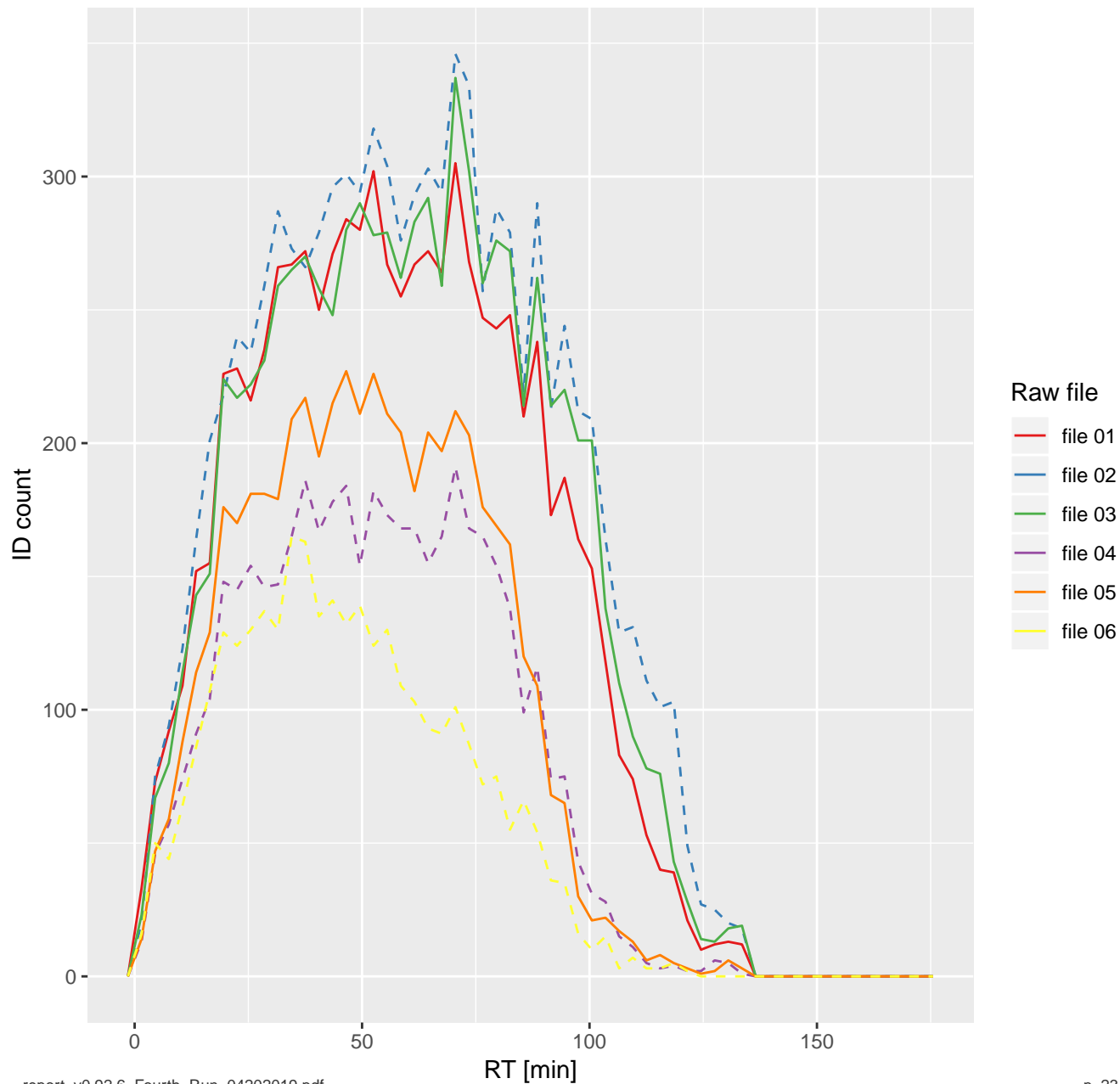
# MSMSscans: TopN over RT



# MSMSscans: TopN over RT

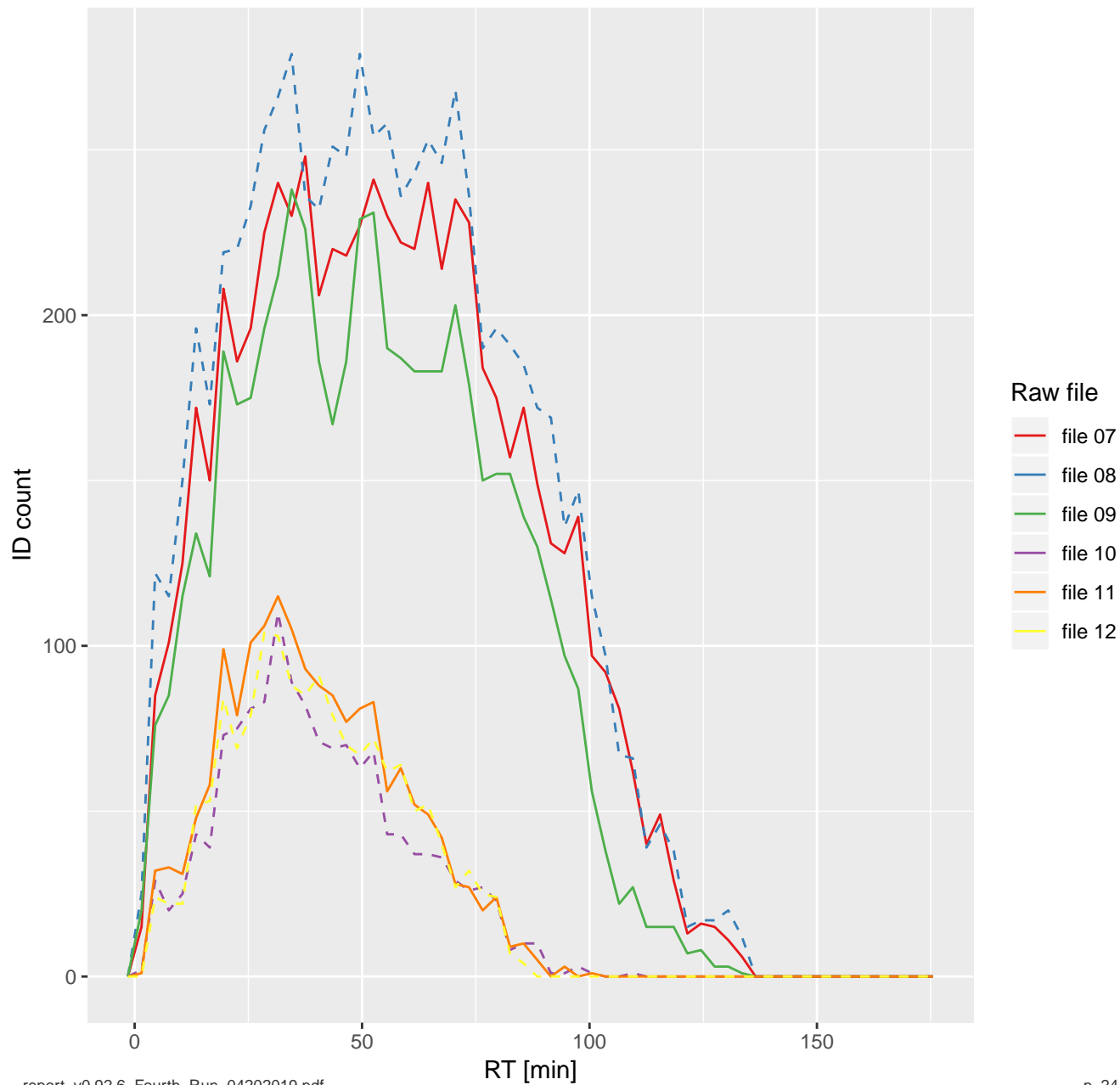


# EVD: IDs over RT

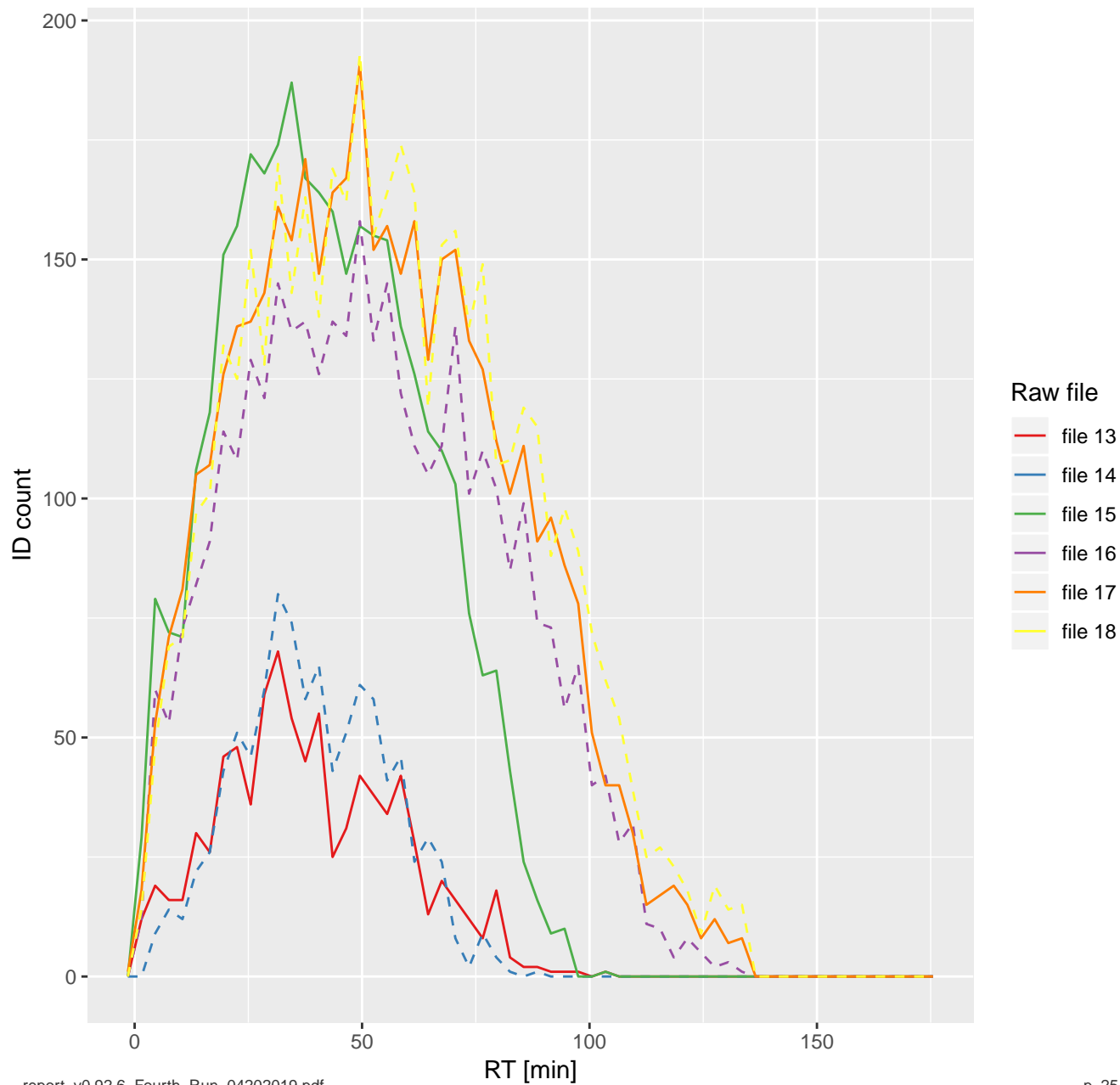




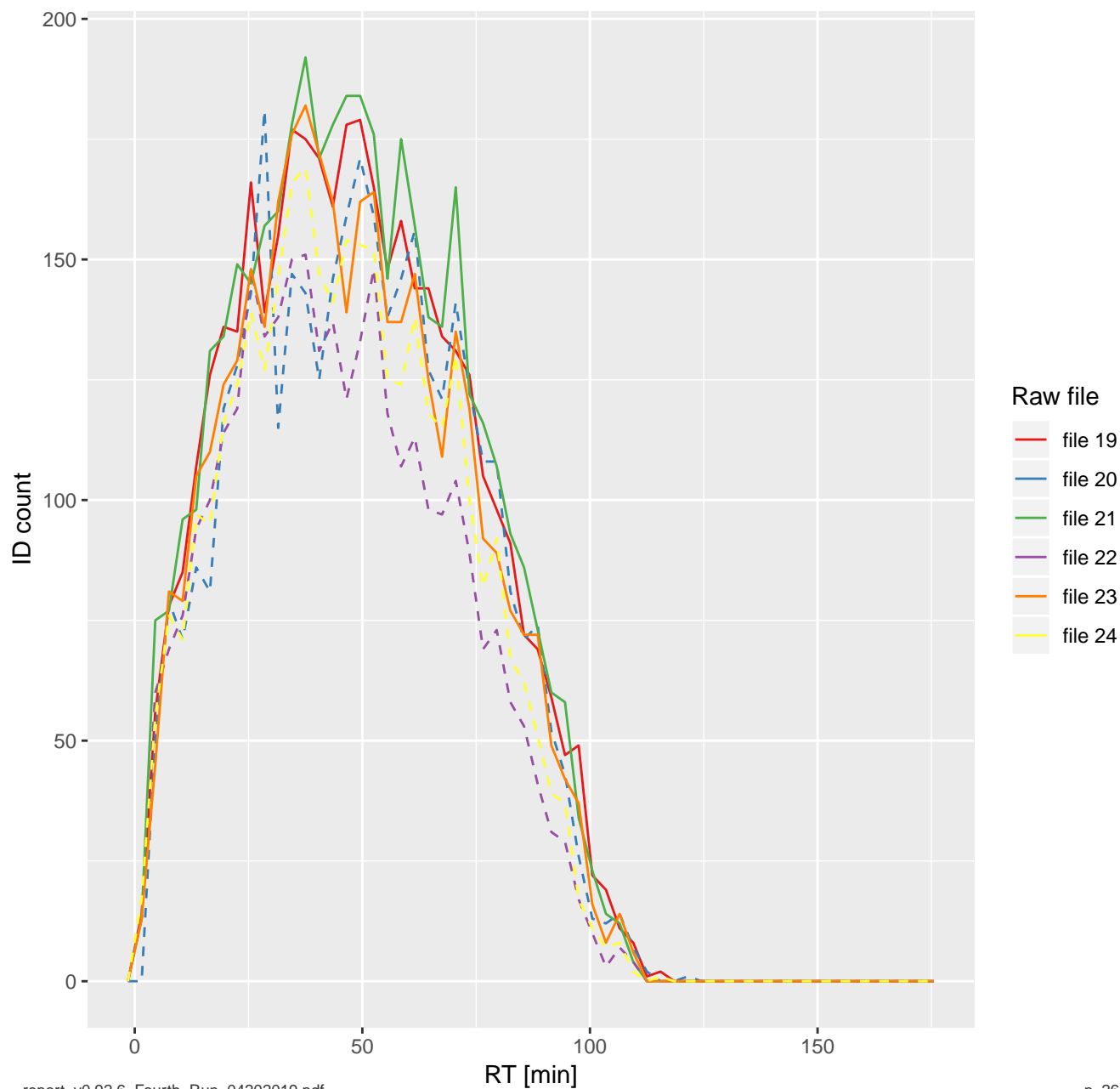
# EVD: IDs over RT



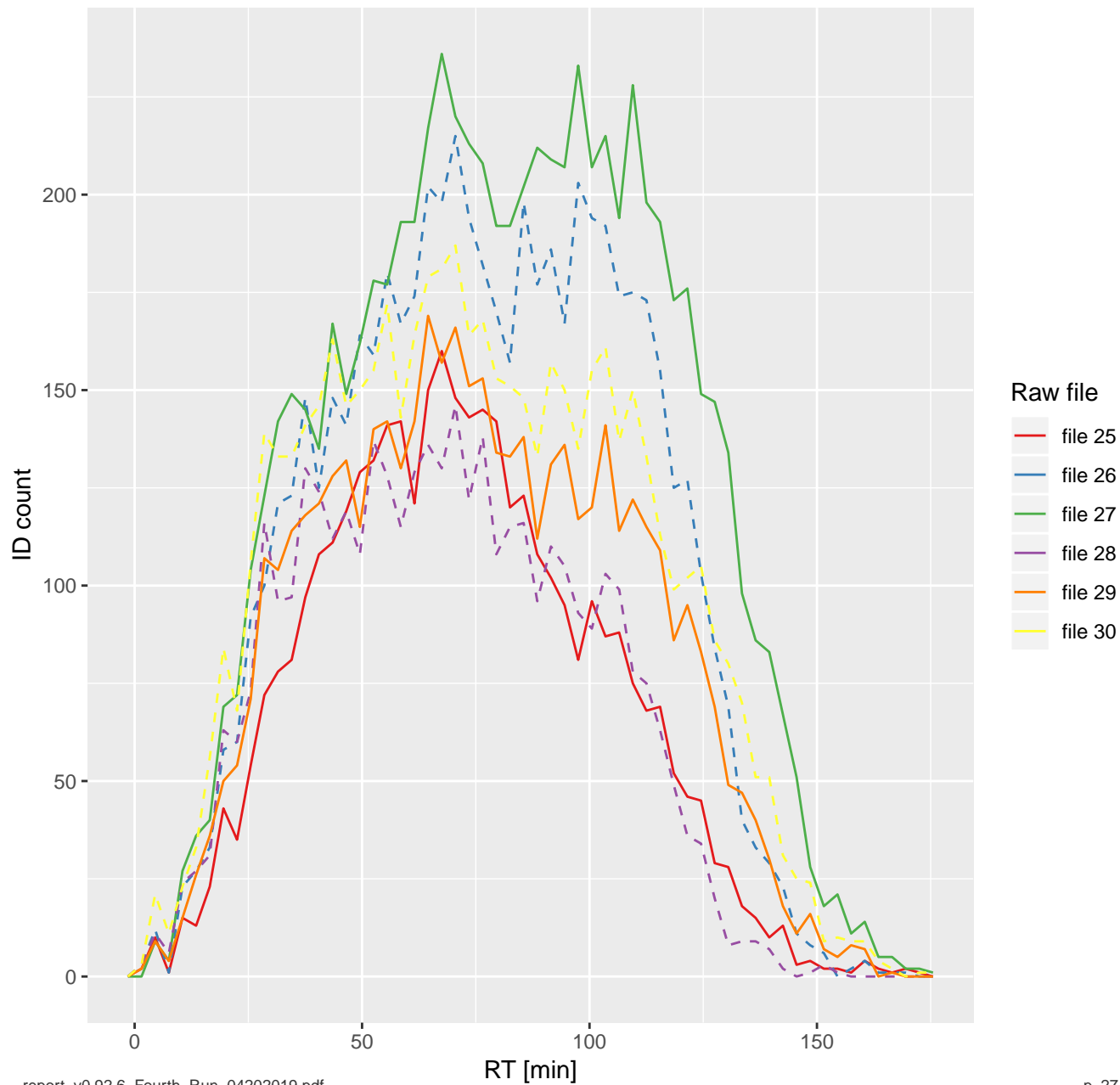
# EVD: IDs over RT



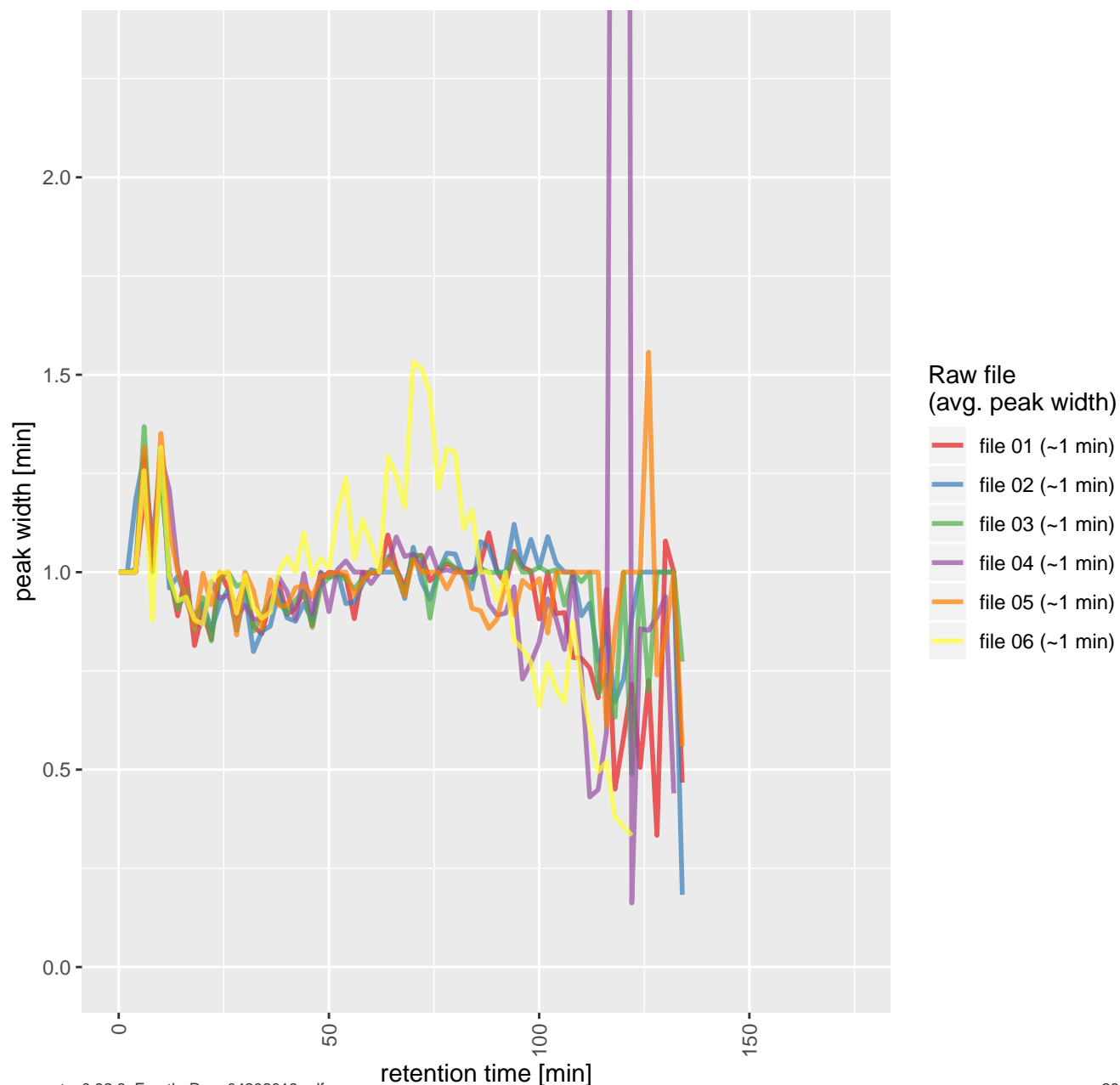
# EVD: IDs over RT



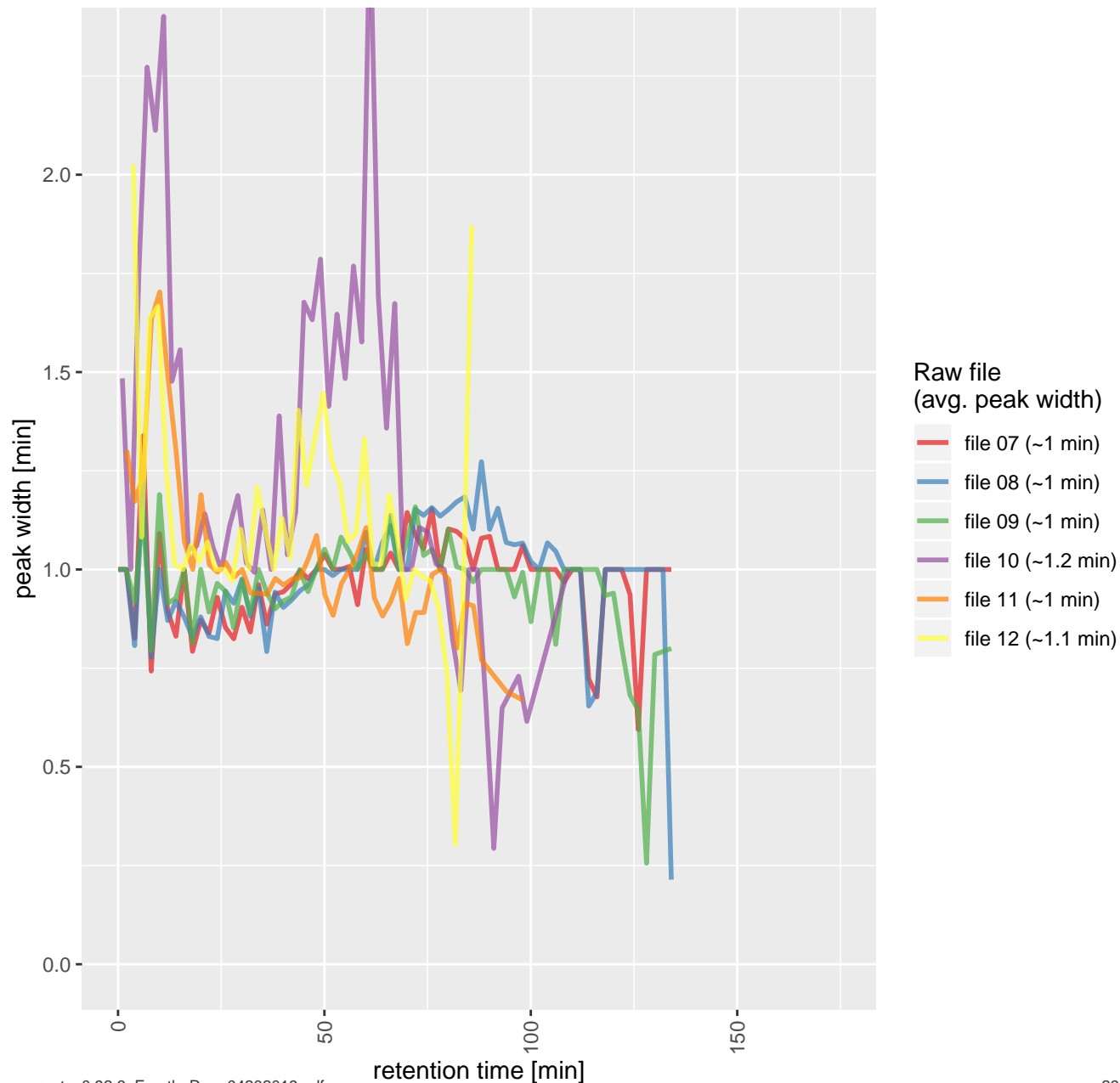
# EVD: IDs over RT



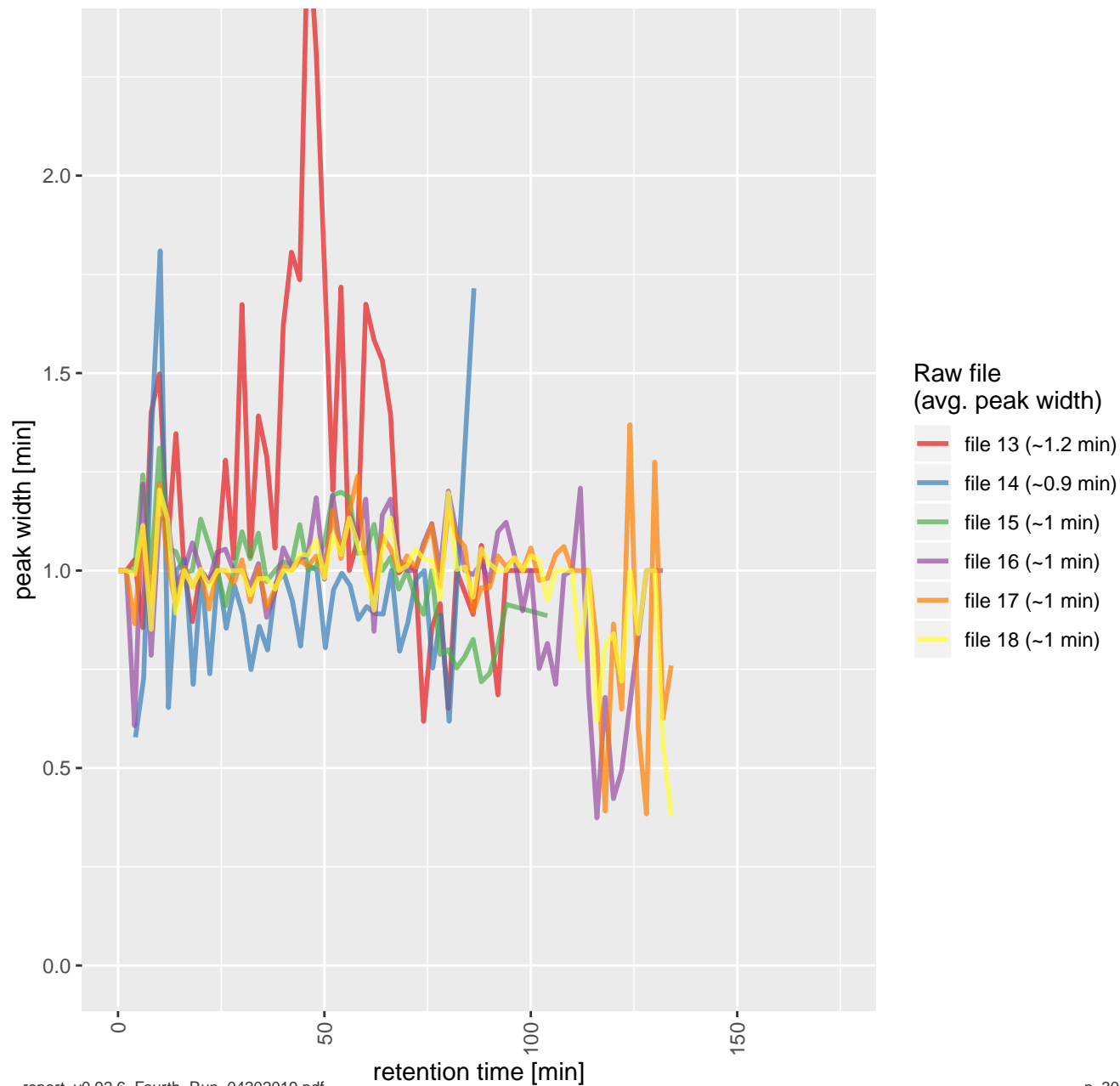
## EVD: Peak width over RT



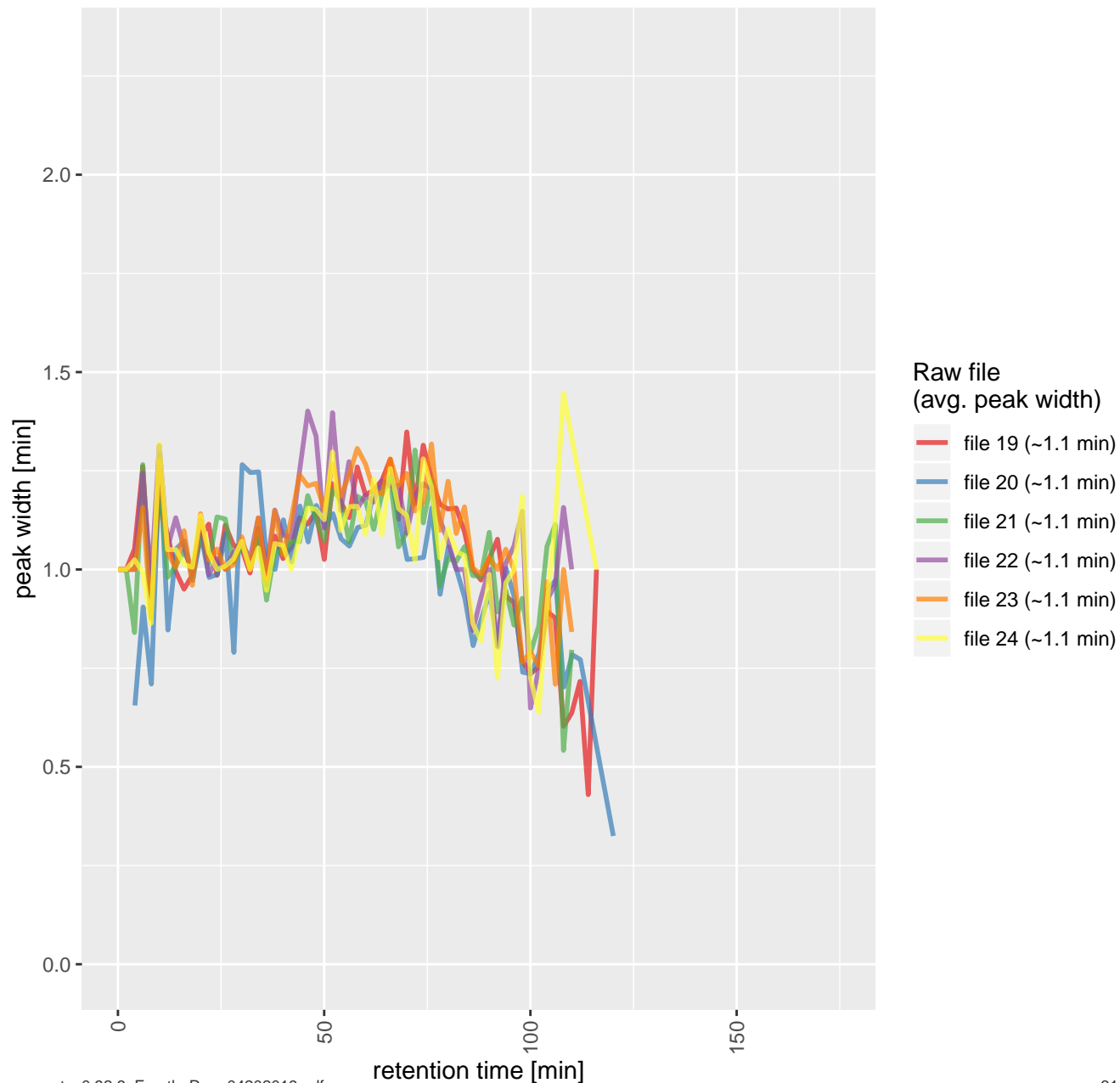
## EVD: Peak width over RT



## EVD: Peak width over RT

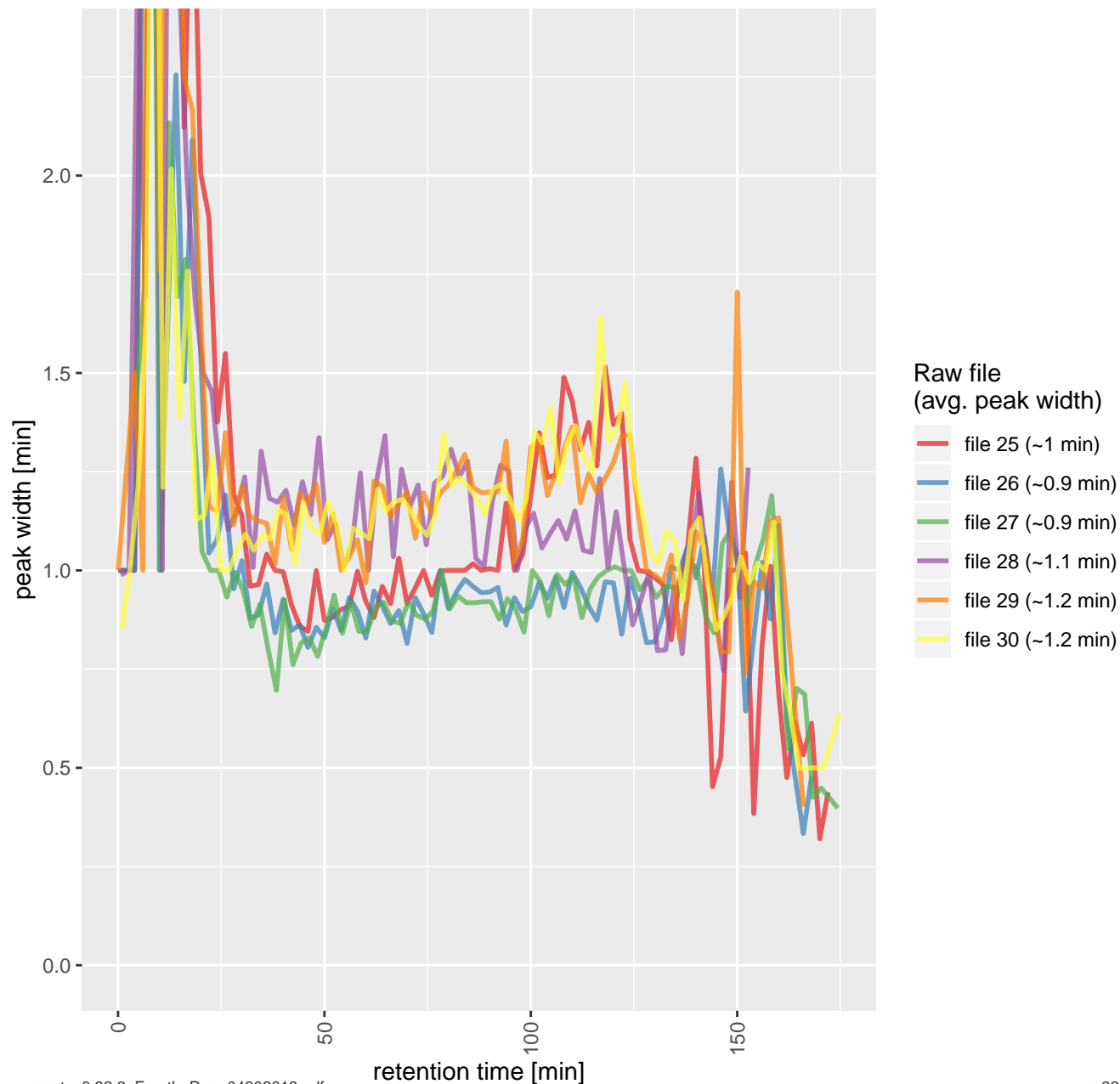


## EVD: Peak width over RT

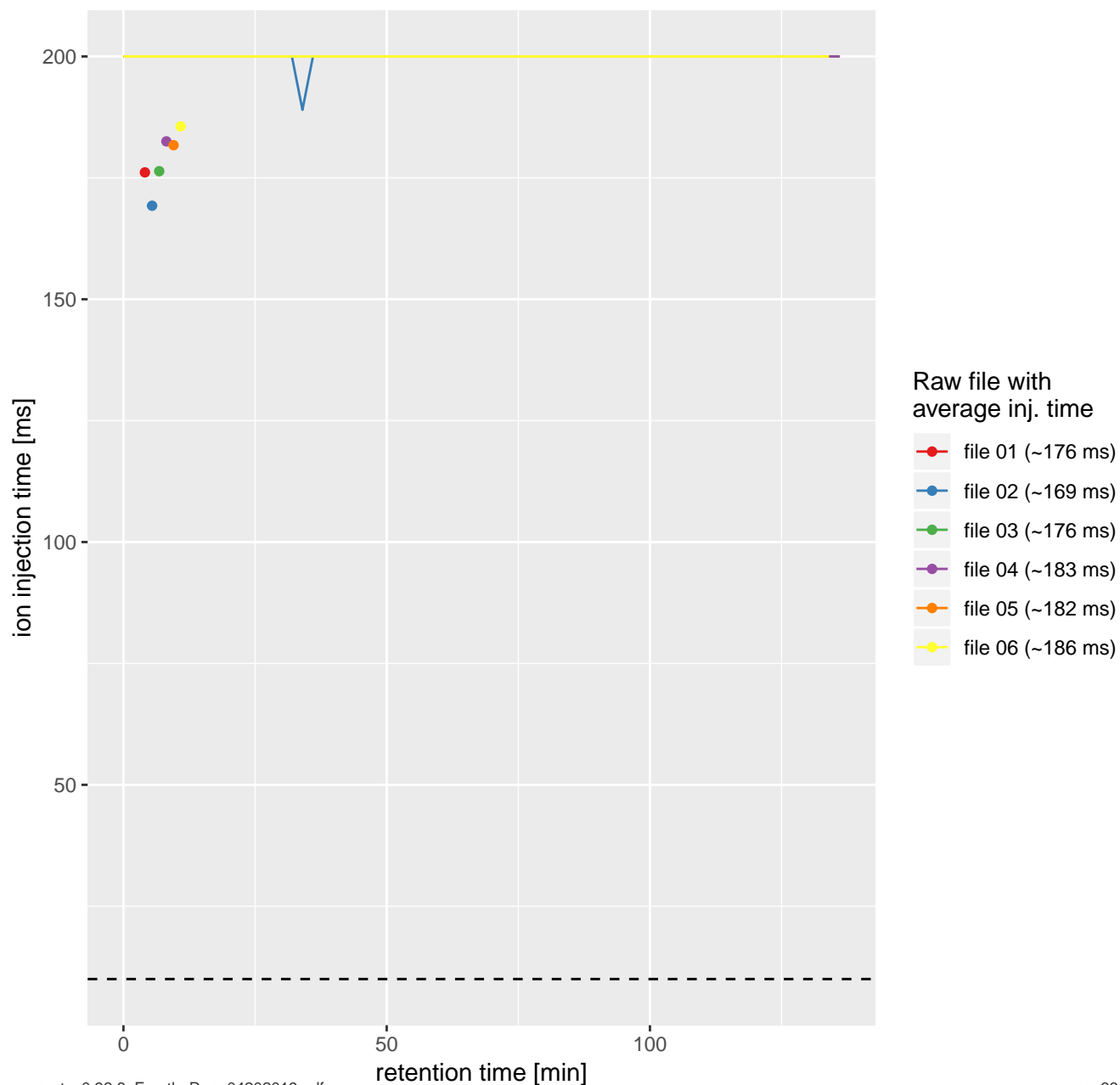




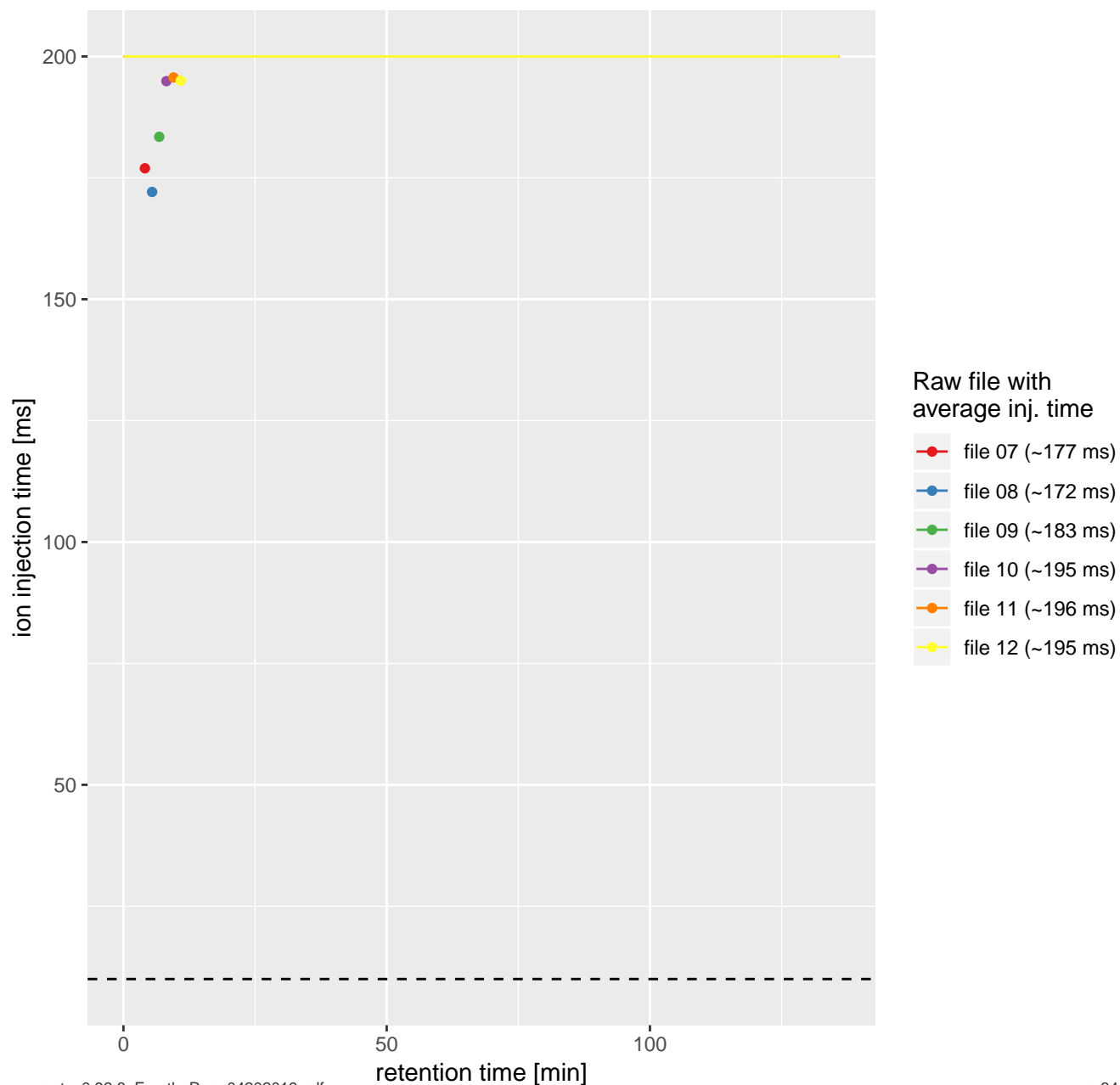
## EVD: Peak width over RT



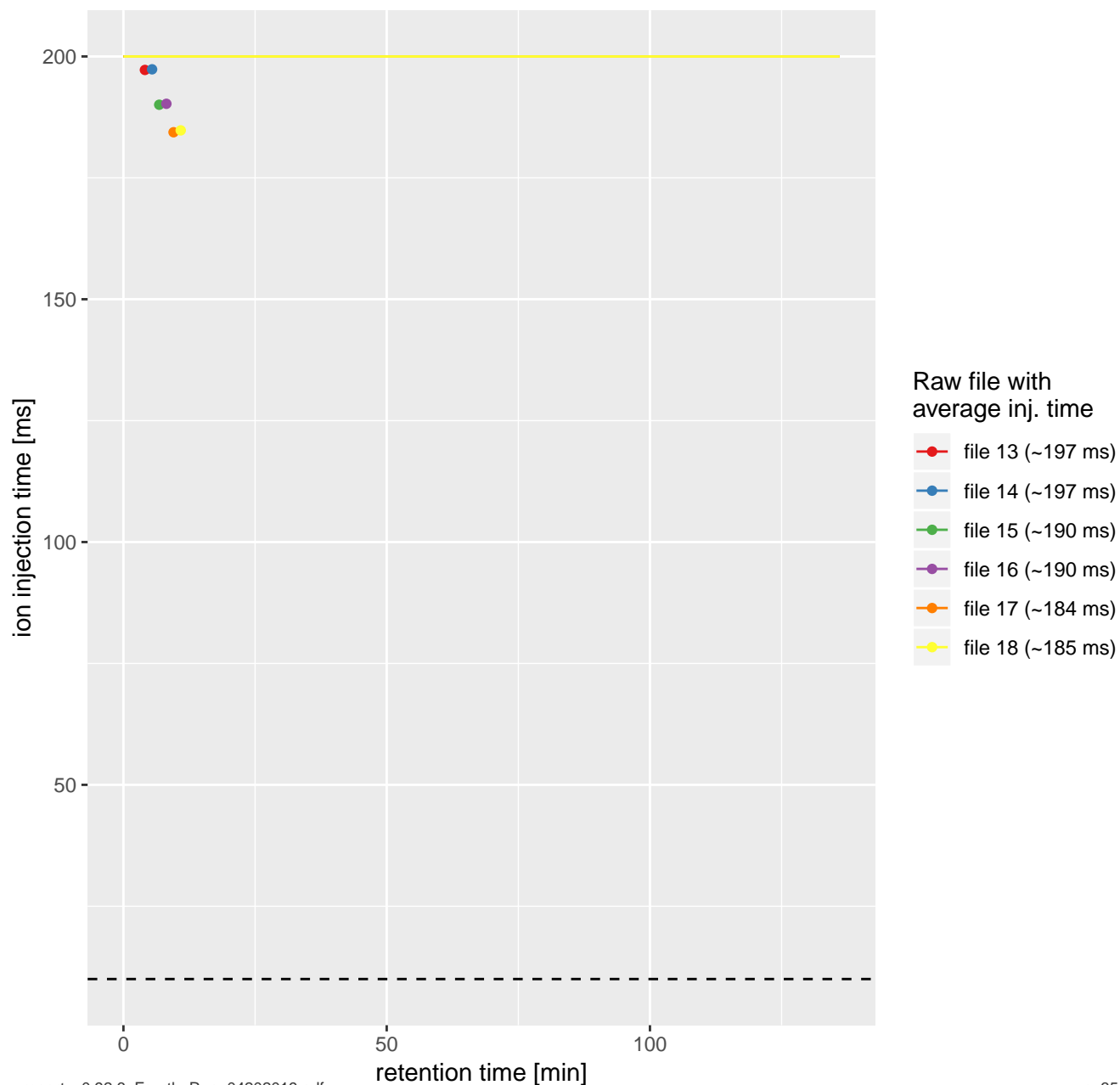
# MSMSscans: Ion Injection Time over RT



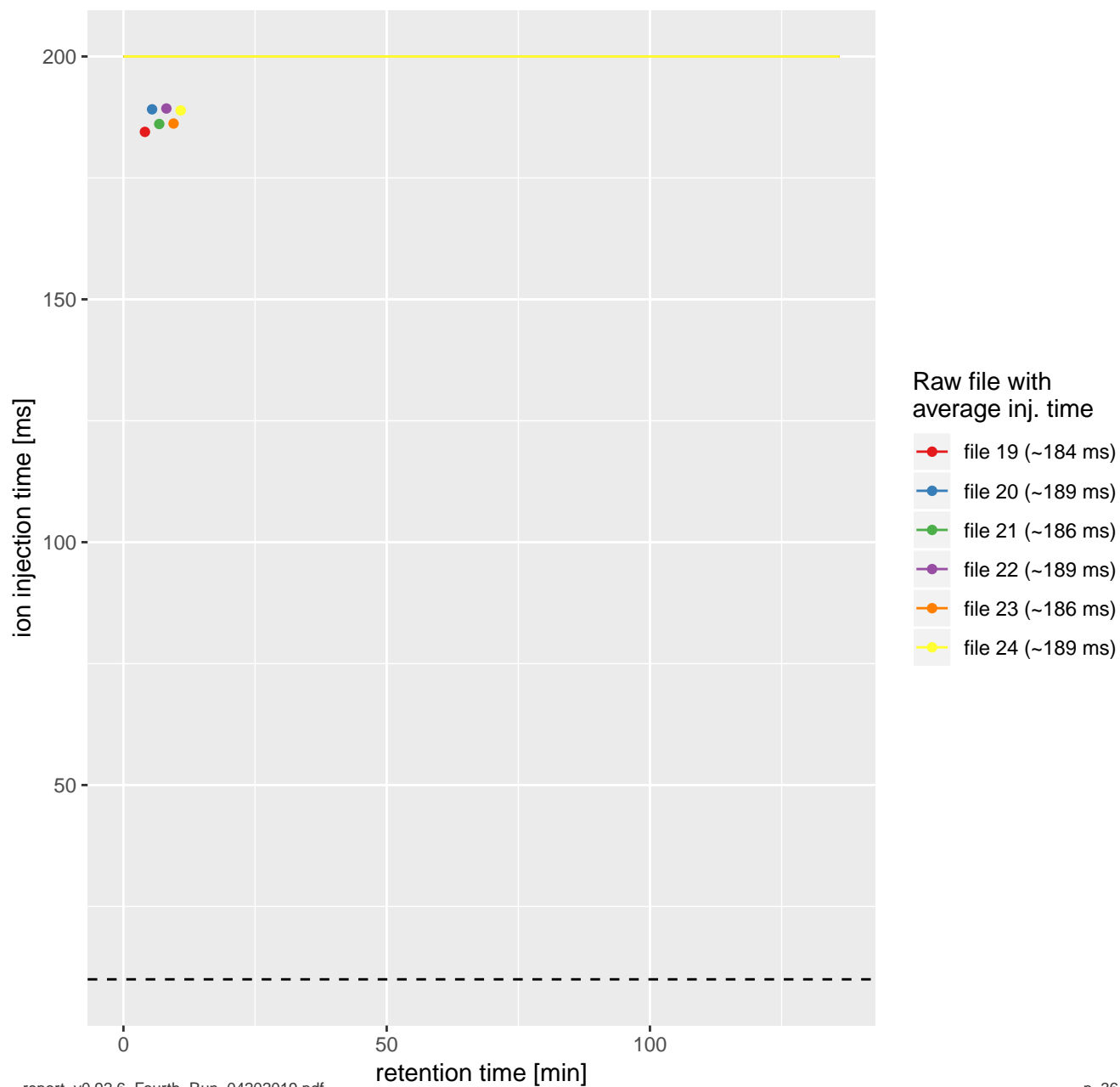
# MSMSscans: Ion Injection Time over RT



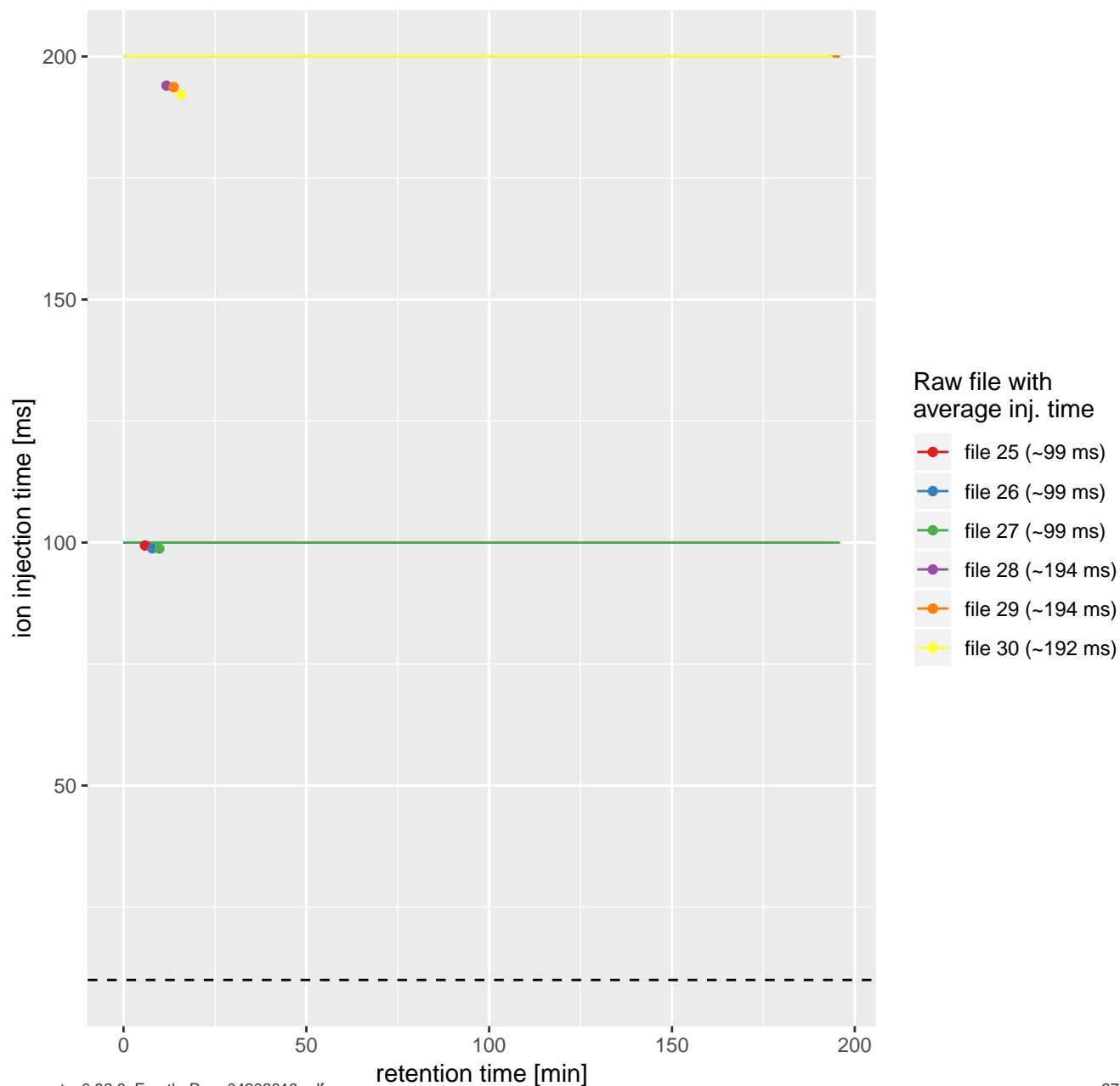
# MSMSscans: Ion Injection Time over RT



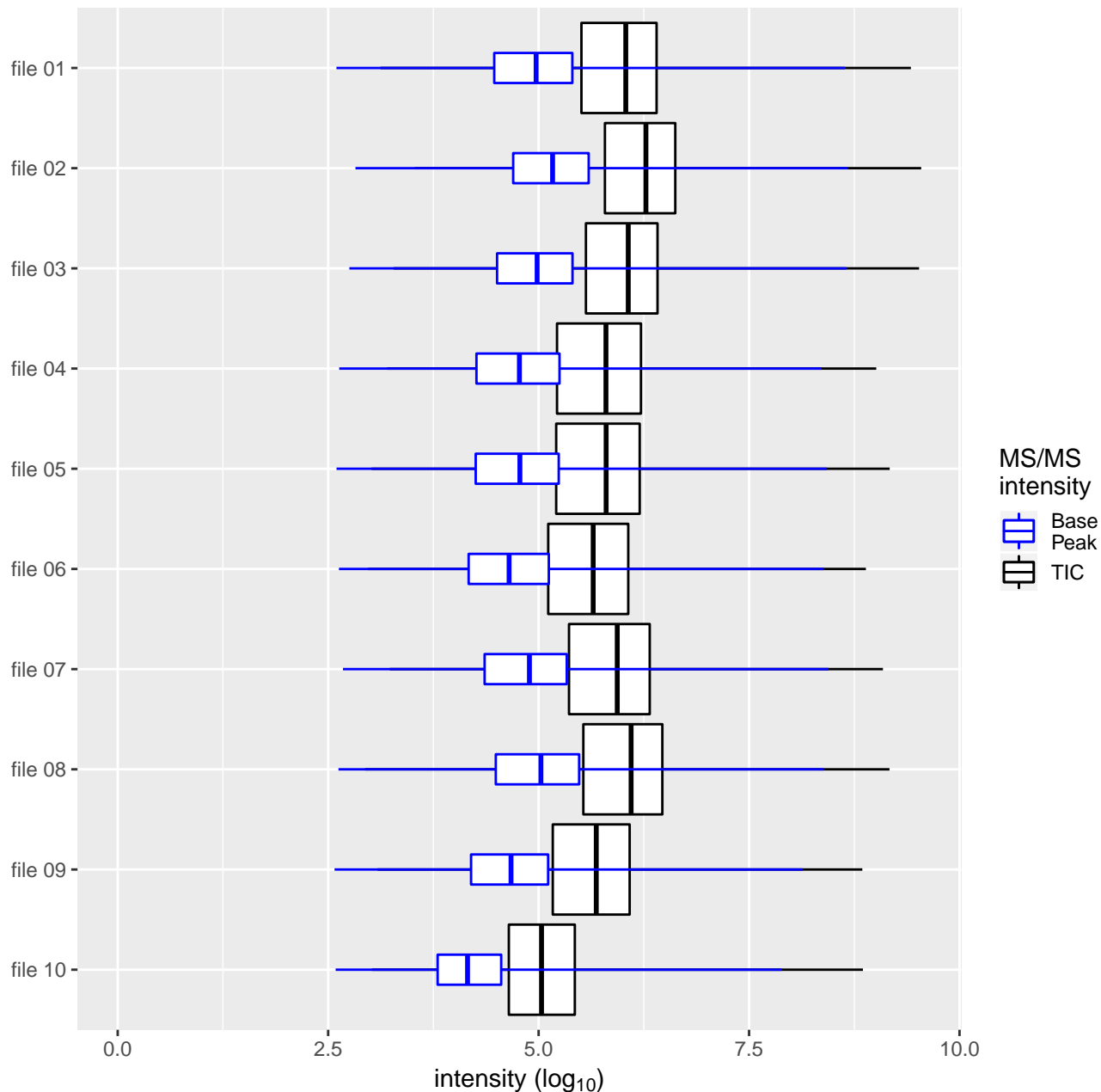
# MSMSscans: Ion Injection Time over RT



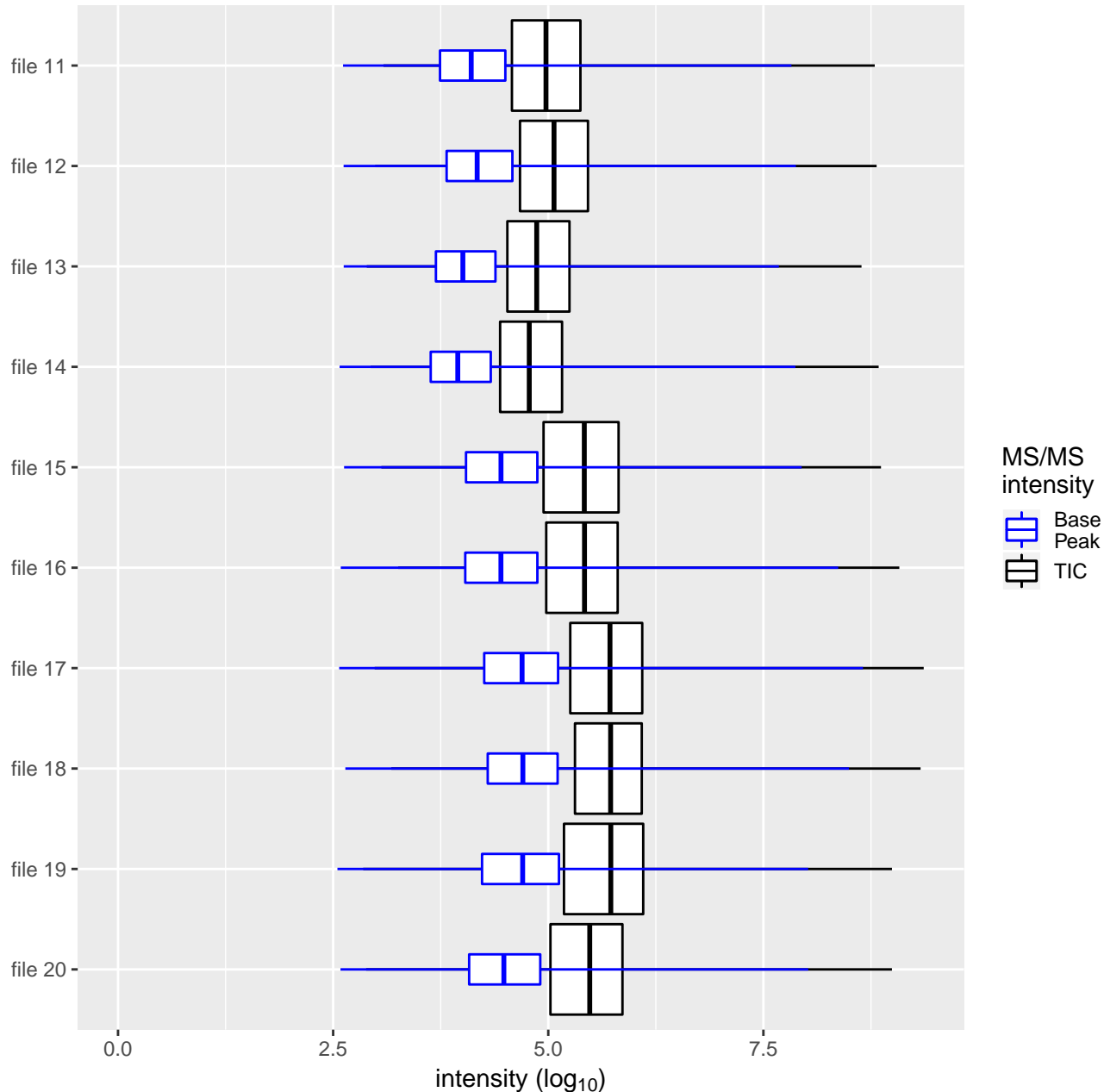
# MSMSscans: Ion Injection Time over RT



# [experimental] MSMSscans: MS/MS intensity

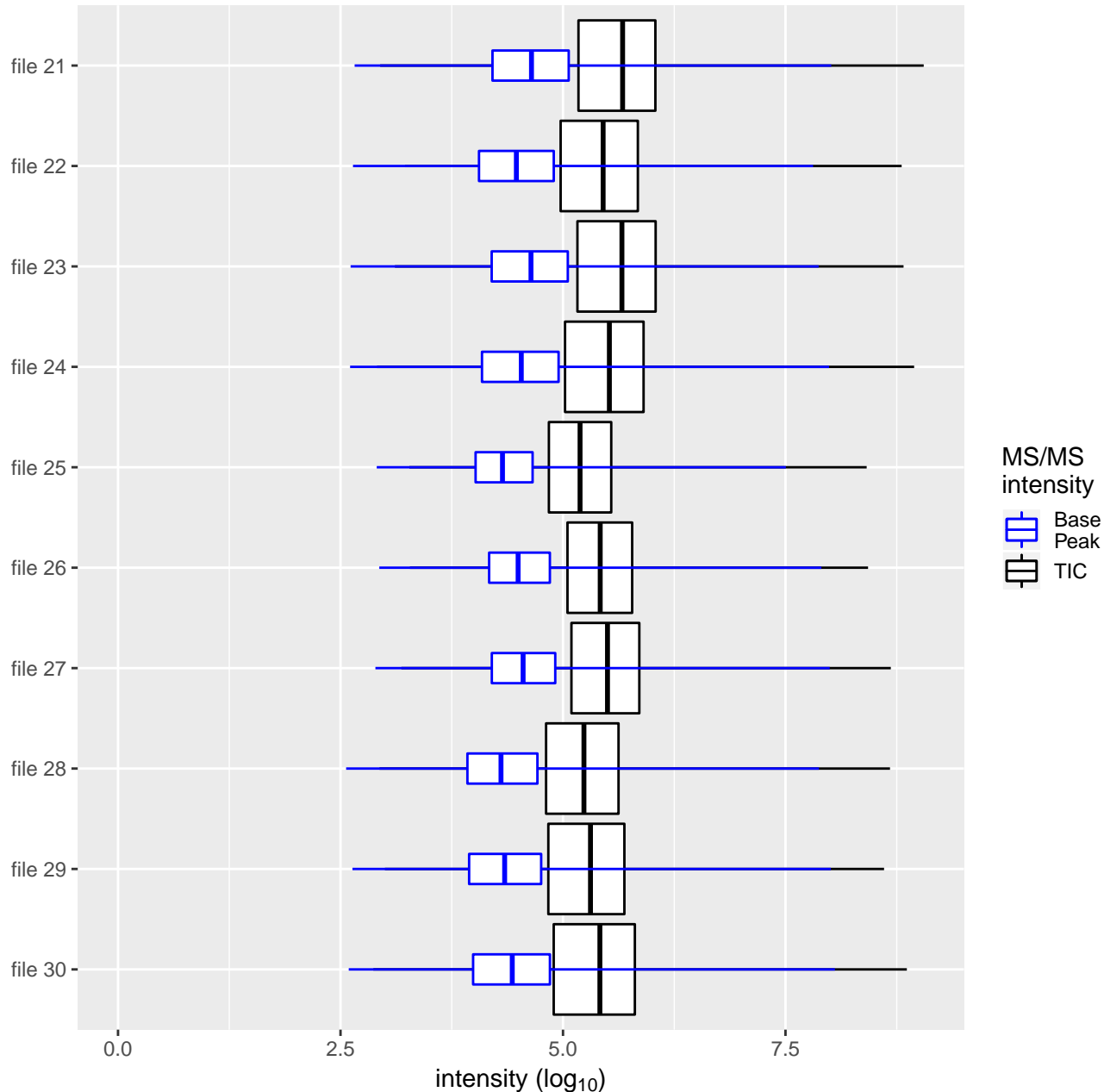


# [experimental] MSMSscans: MS/MS intensity

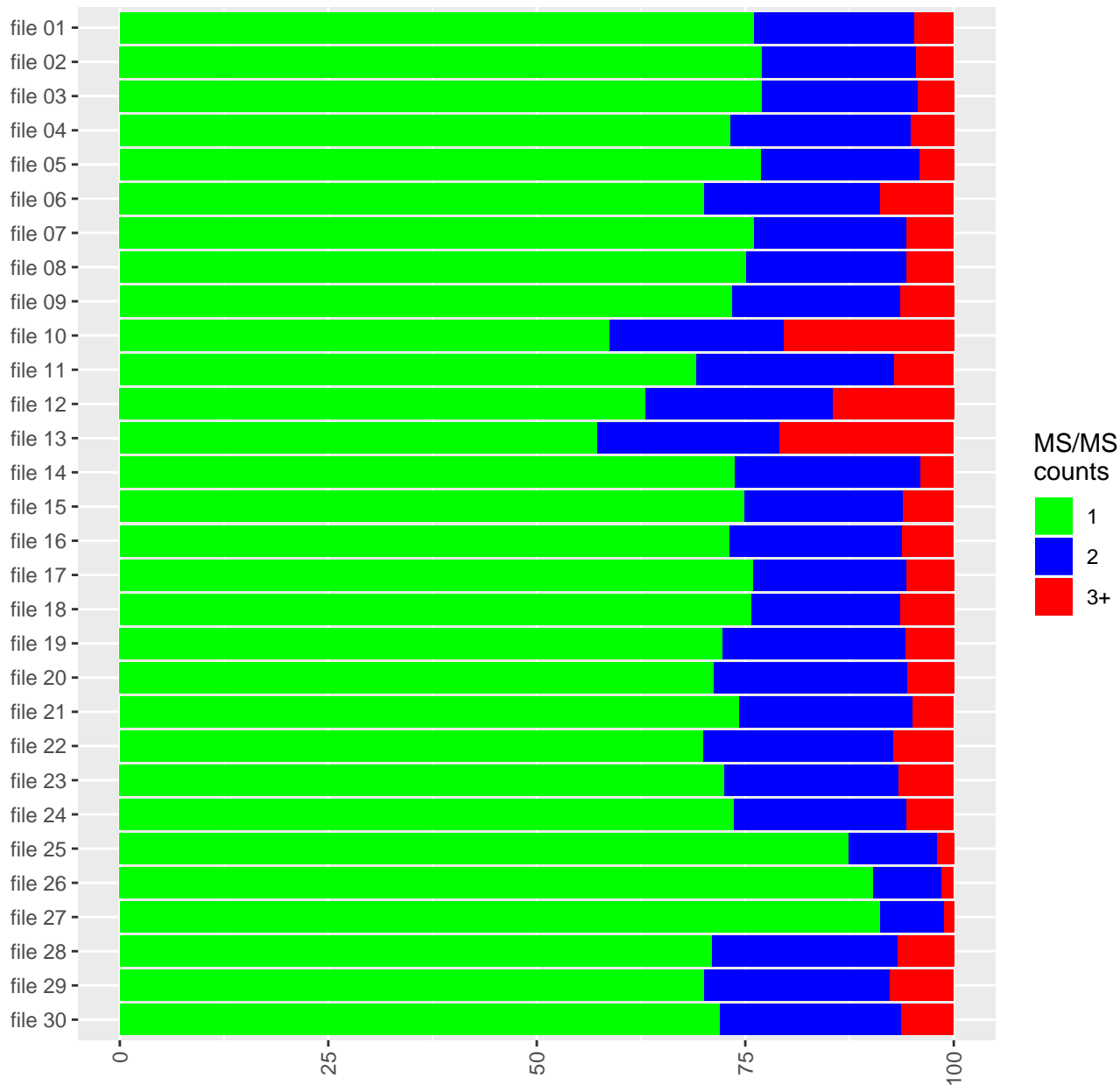




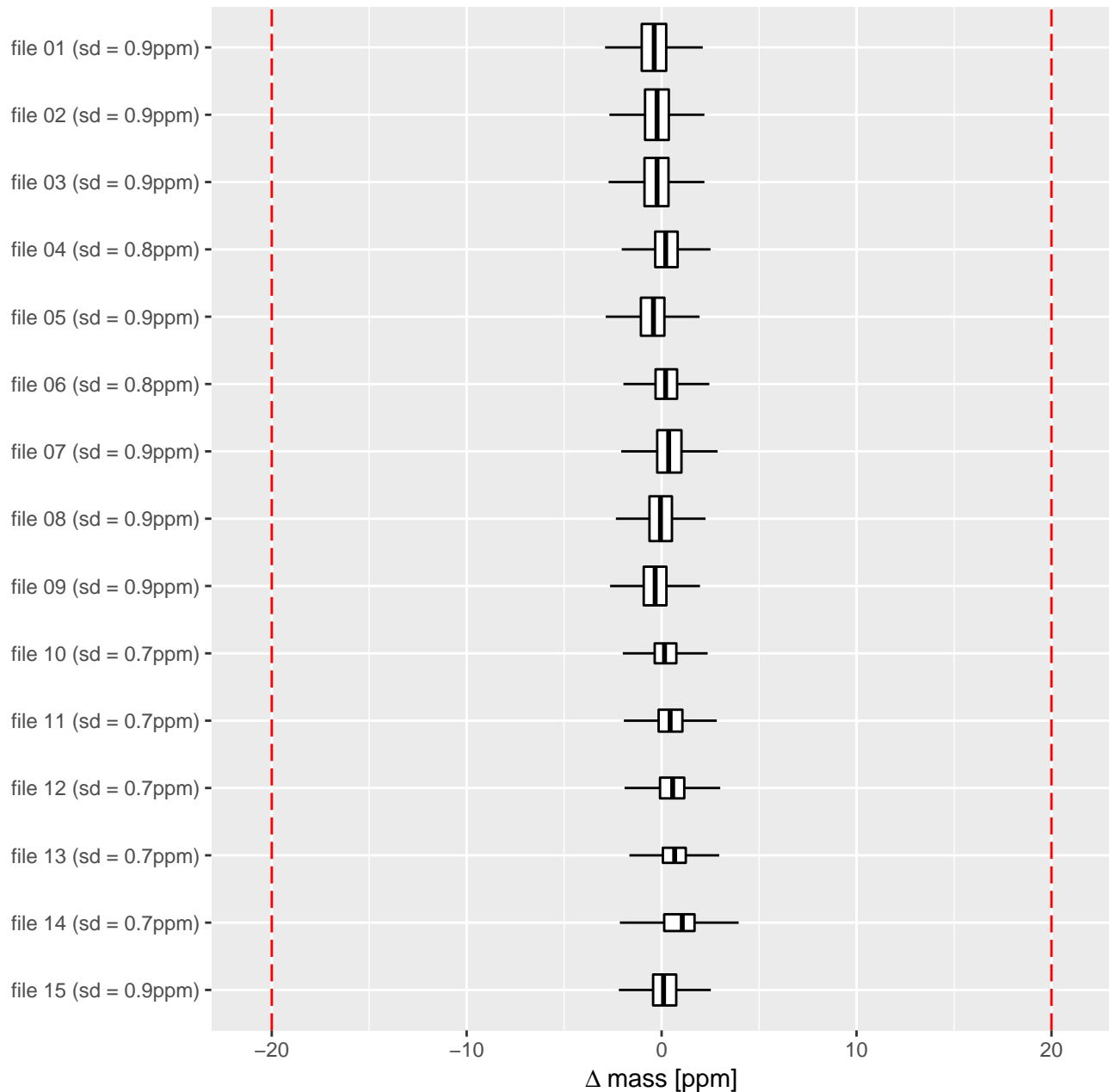
# [experimental] MSMSscans: MS/MS intensity



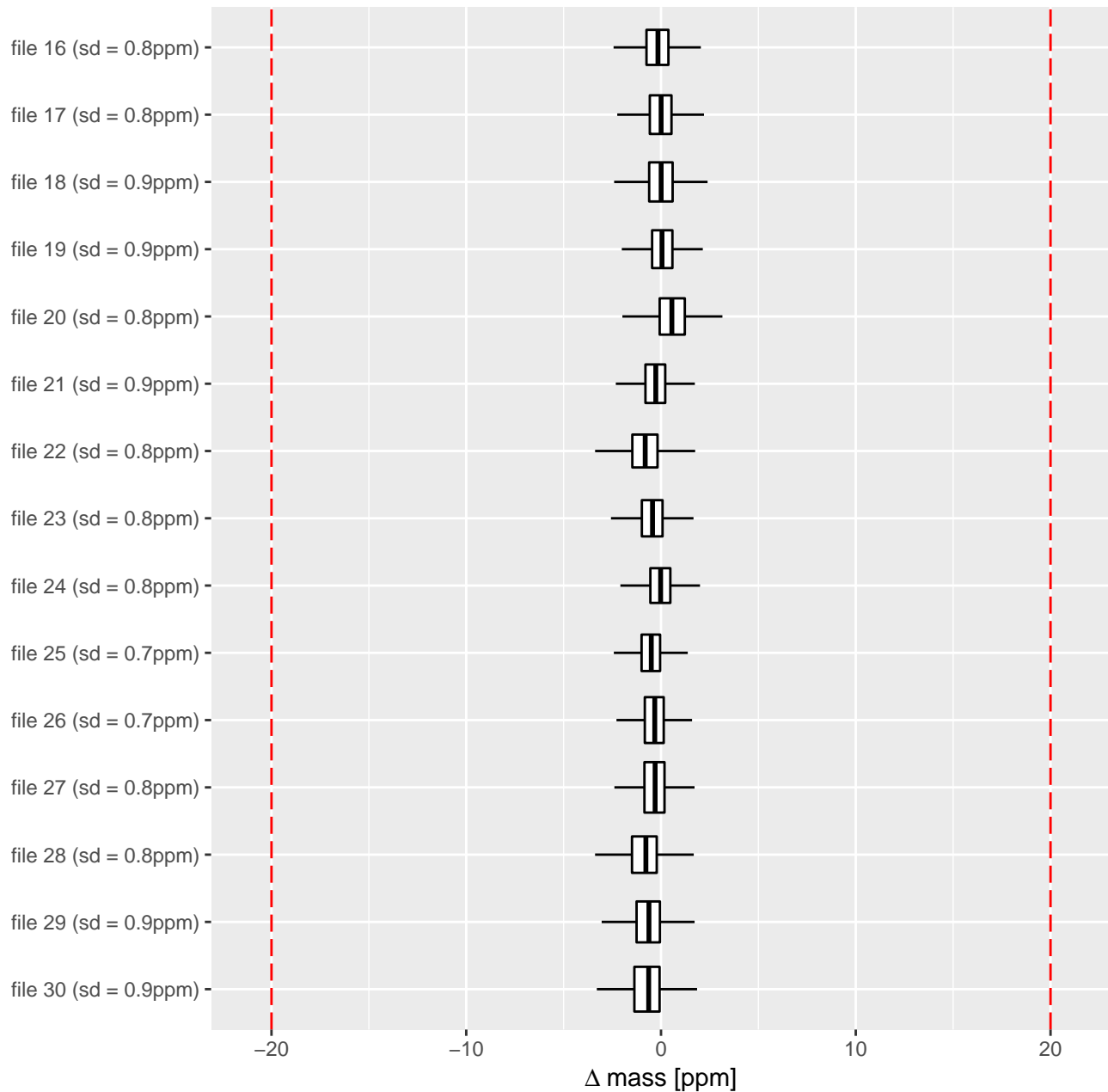
# EVD: Oversampling (MS/MS counts per 3D-peak)



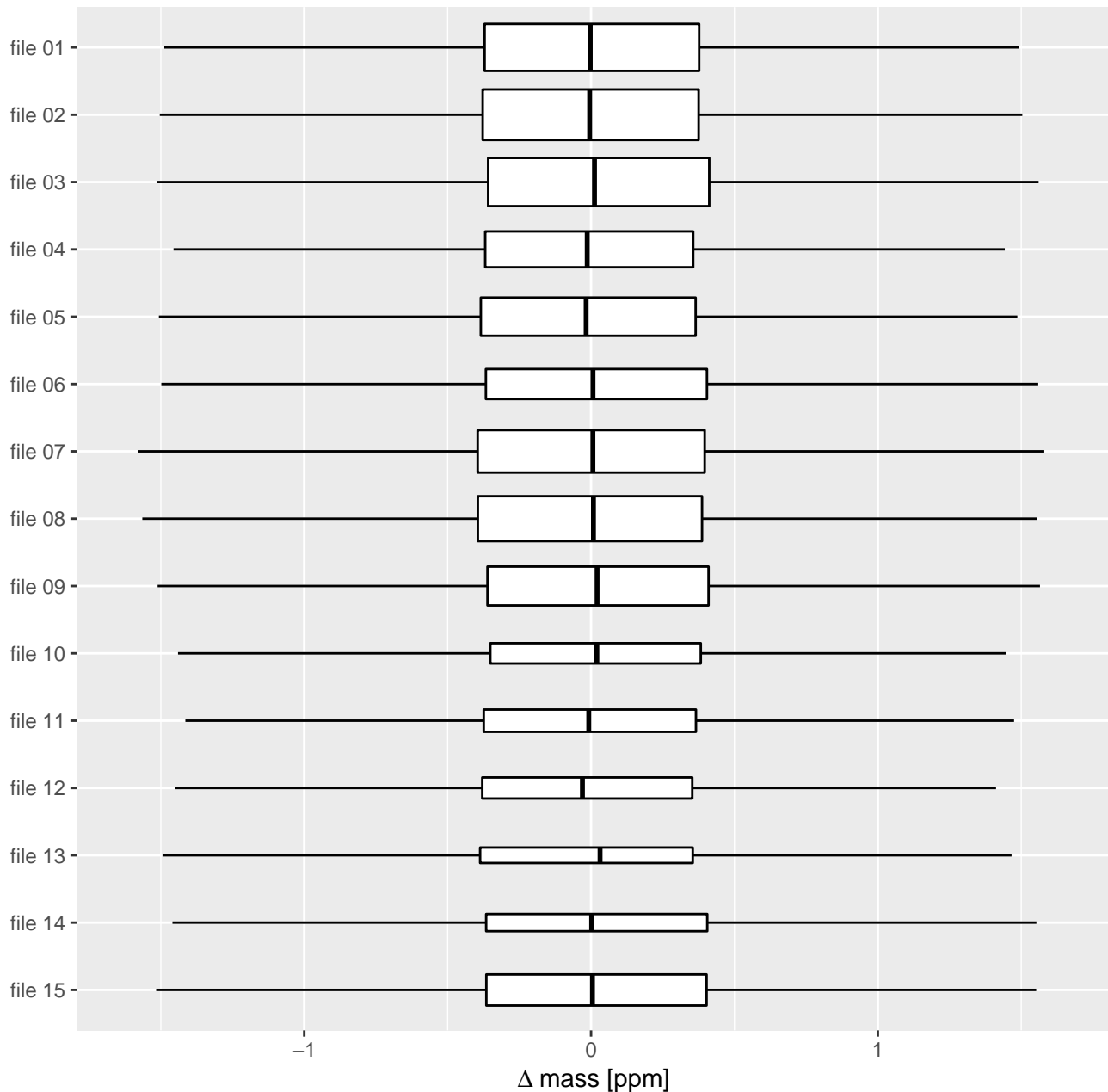
## EVD: Uncalibrated mass error



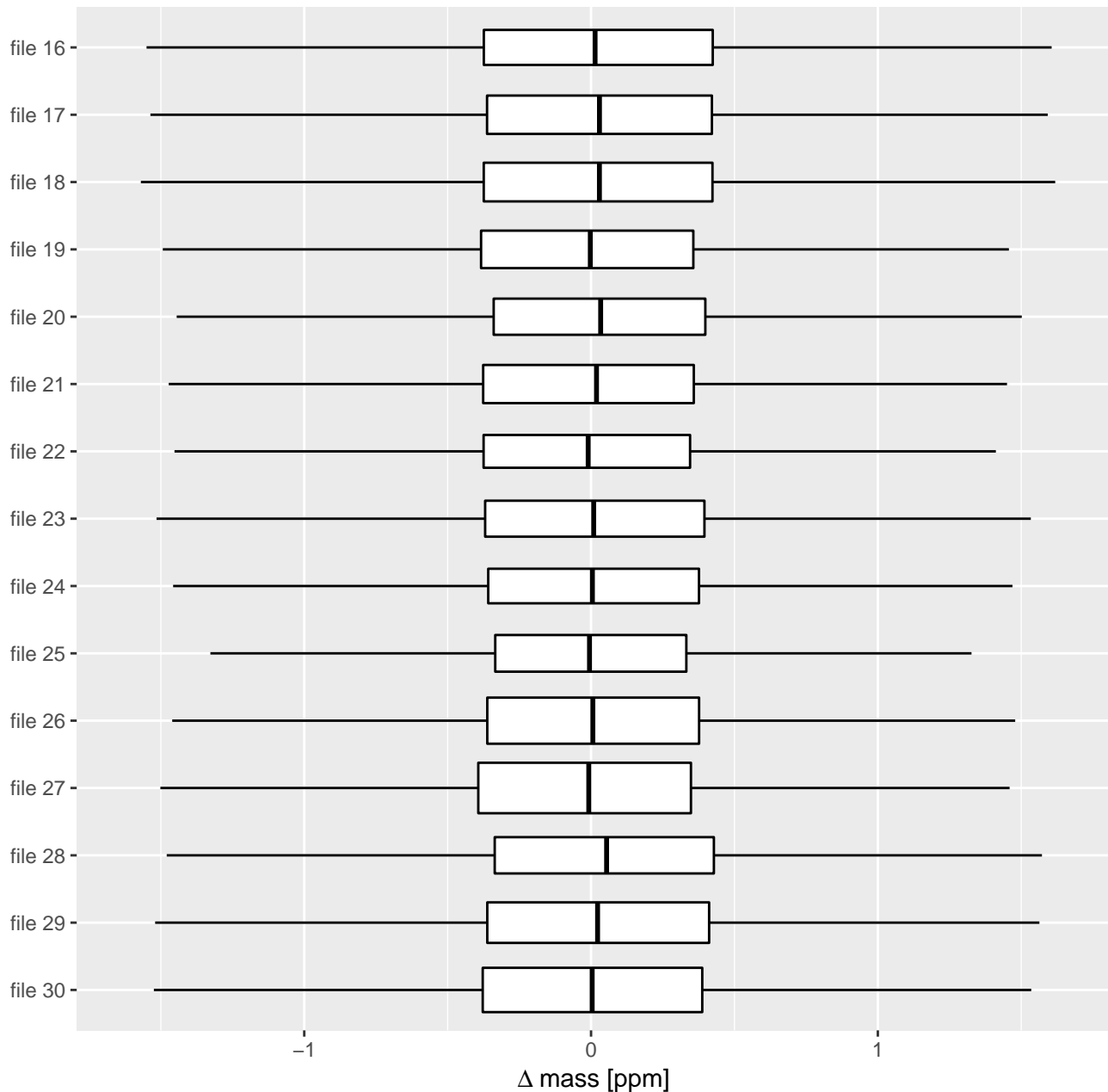
## EVD: Uncalibrated mass error



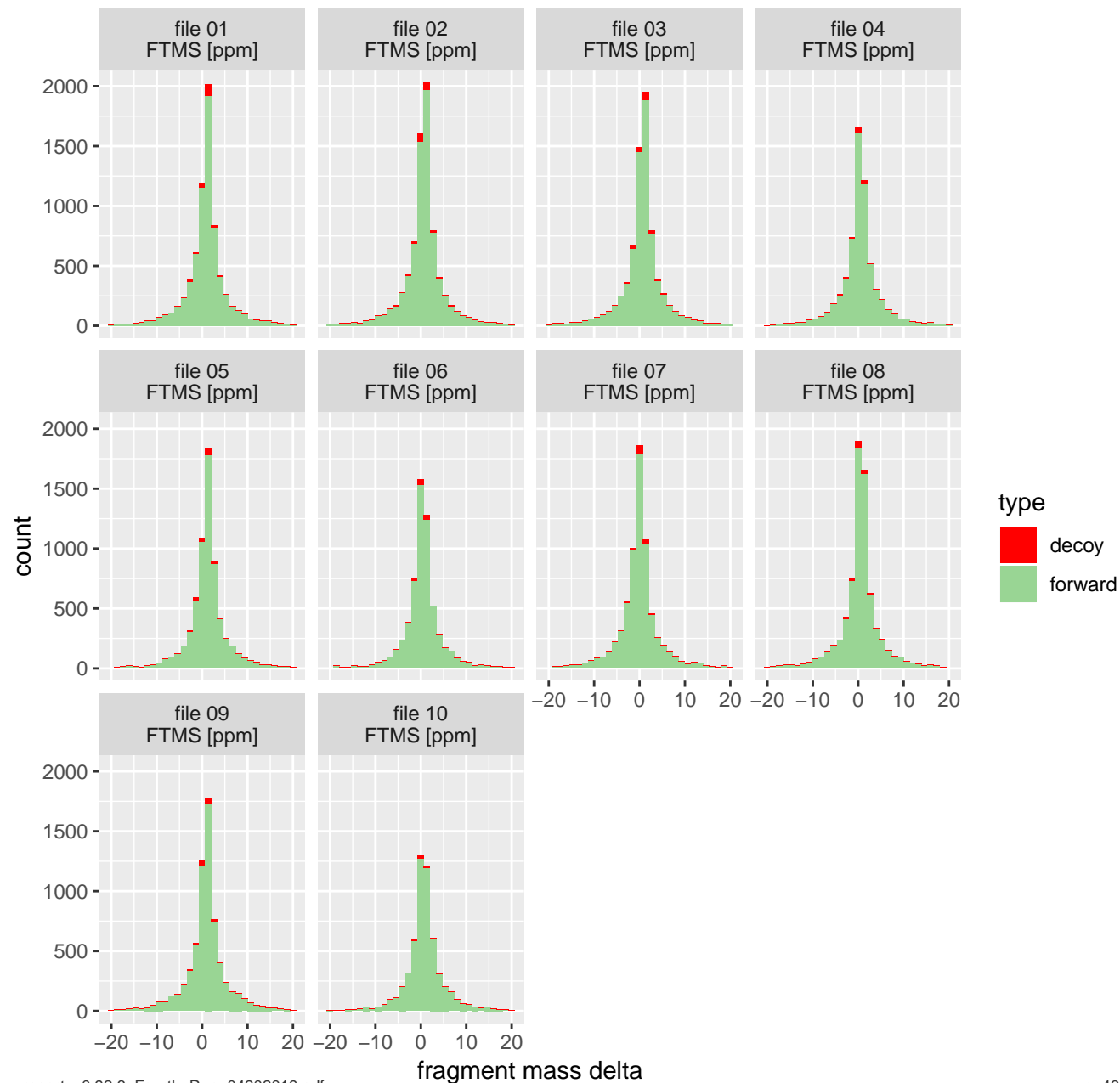
# EVD: Calibrated mass error



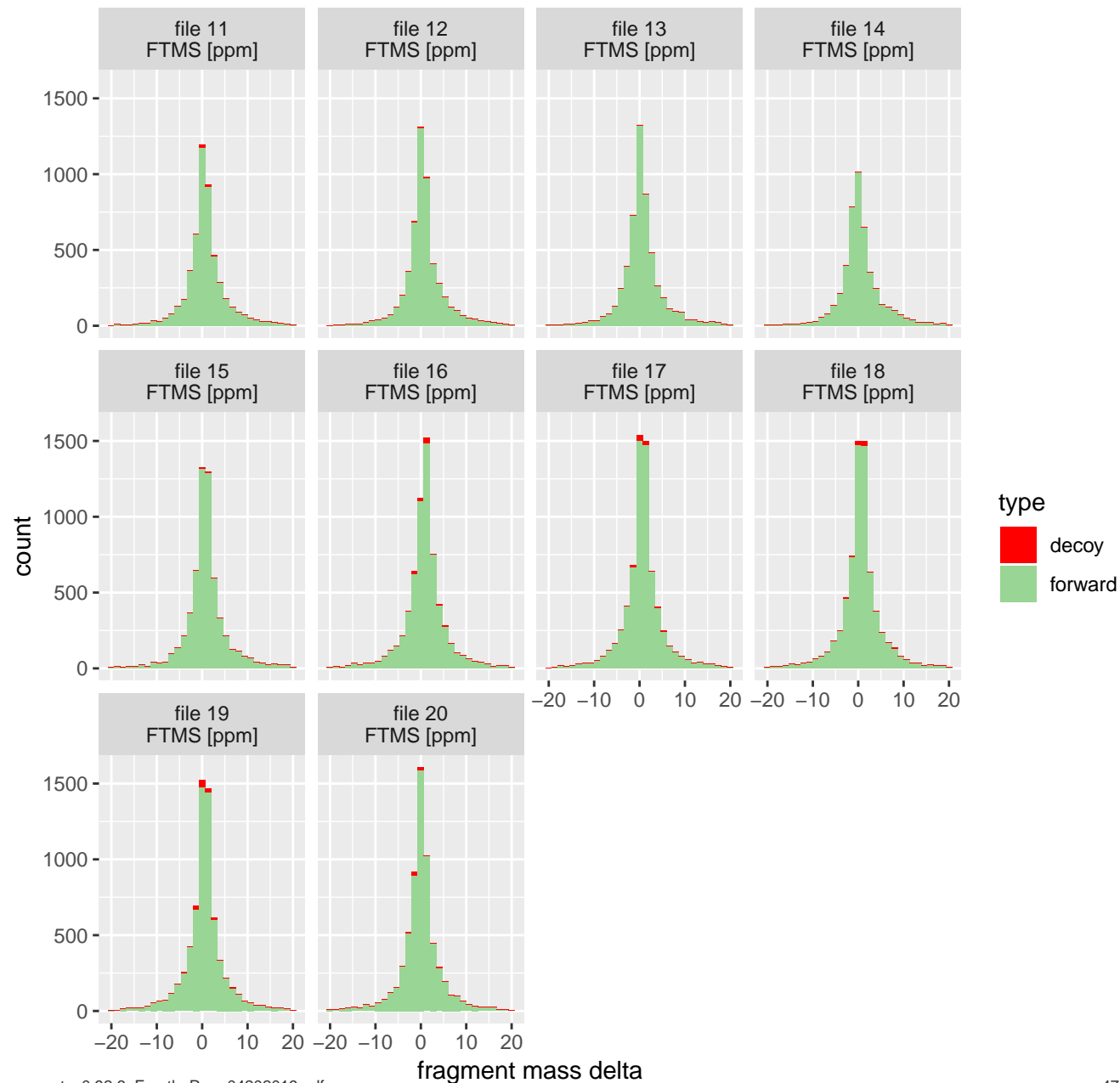
# EVD: Calibrated mass error



# MSMS: Fragment mass errors per Raw file

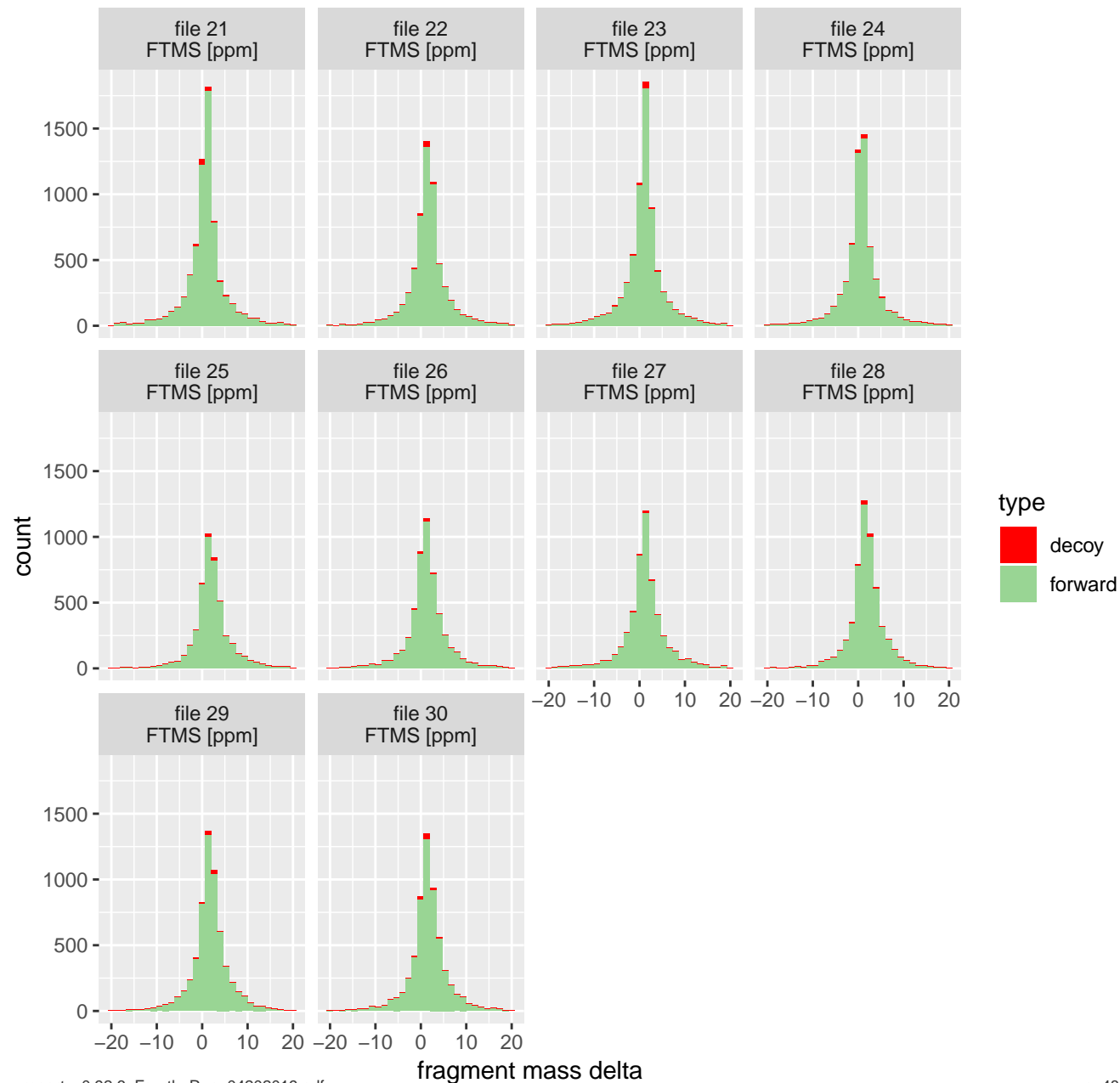


# MSMS: Fragment mass errors per Raw file

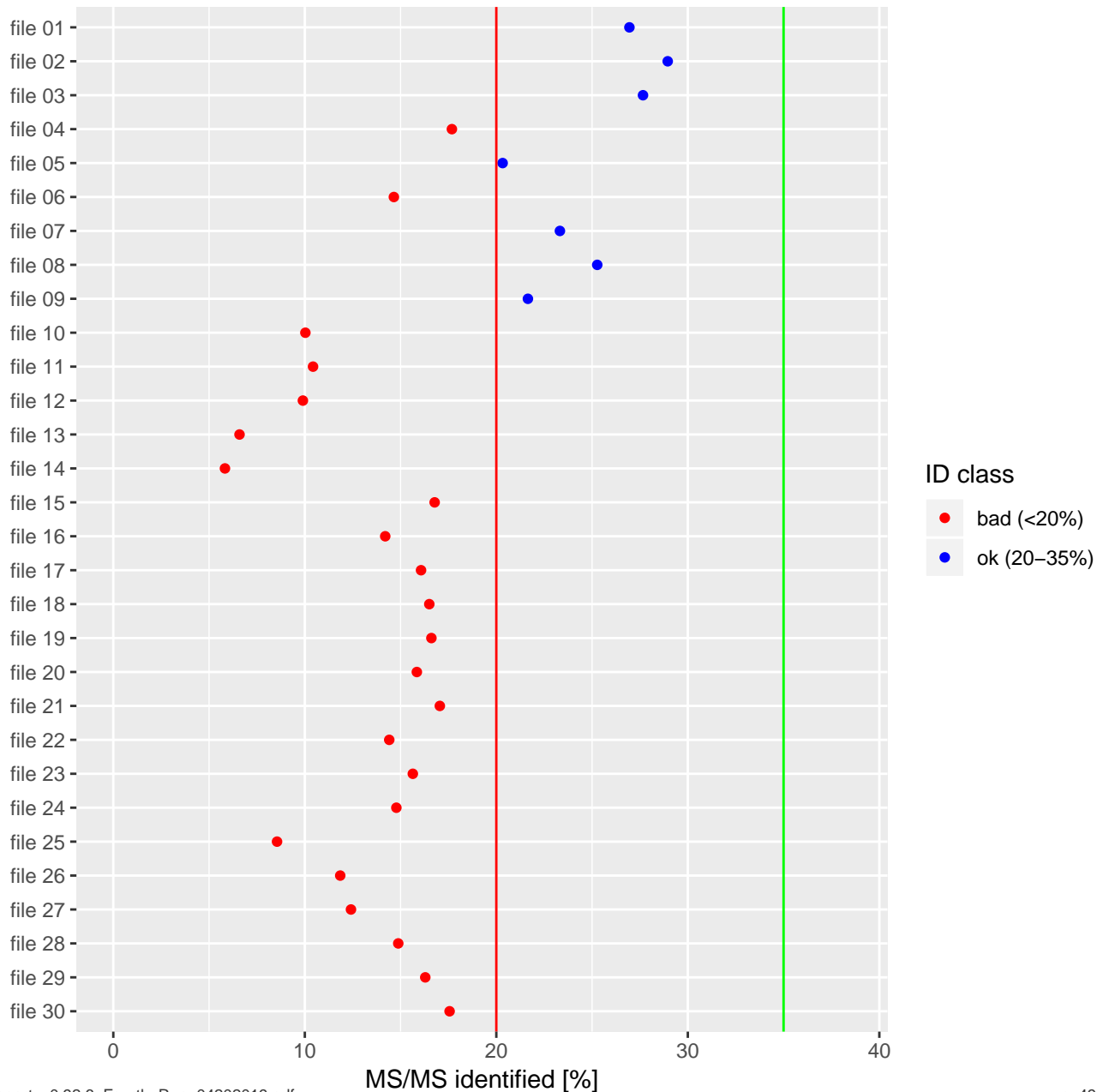




# MSMS: Fragment mass errors per Raw file



# SM: MS/MS identified per Raw file

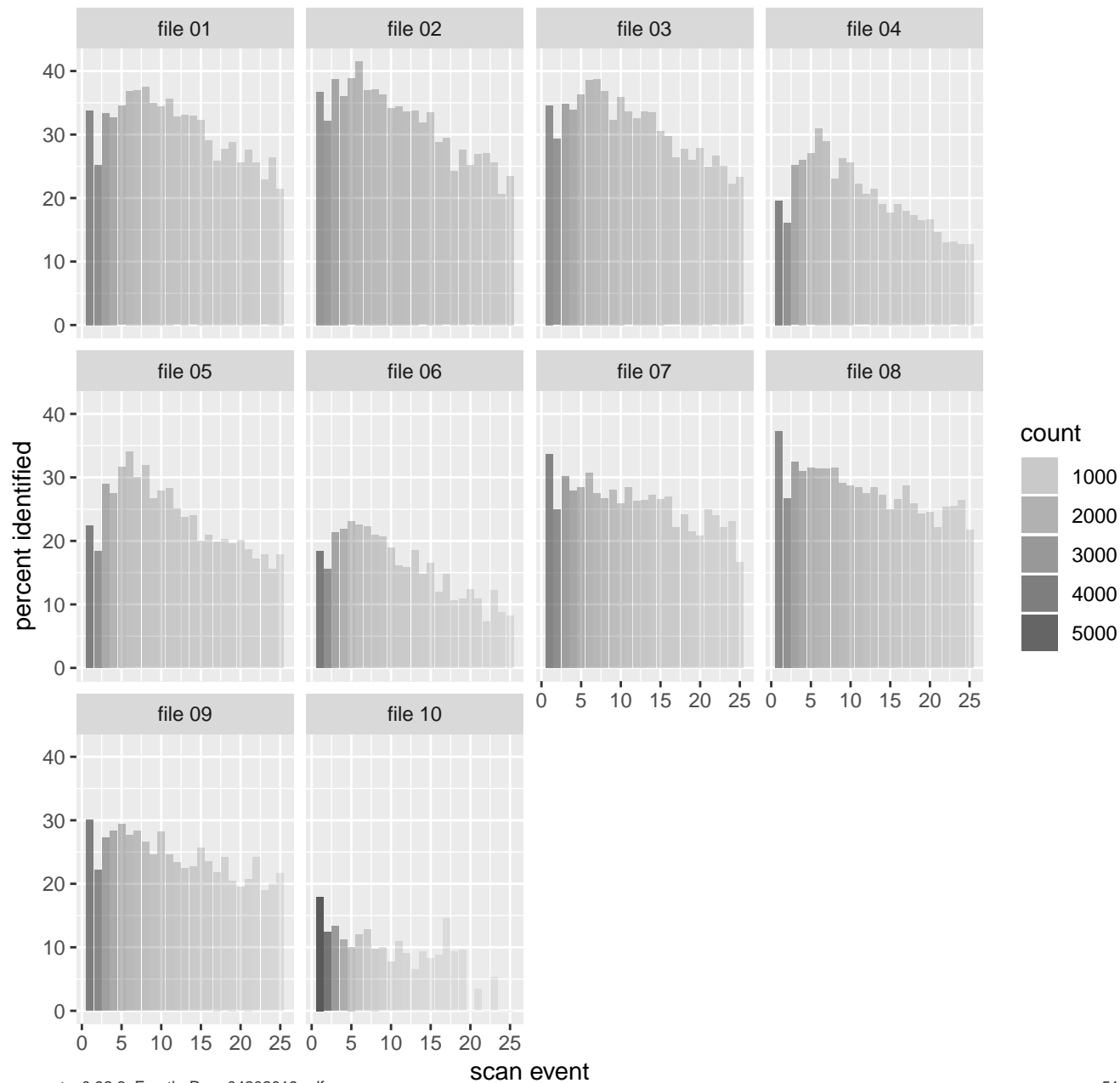


SM: Files with 'red' ID rate

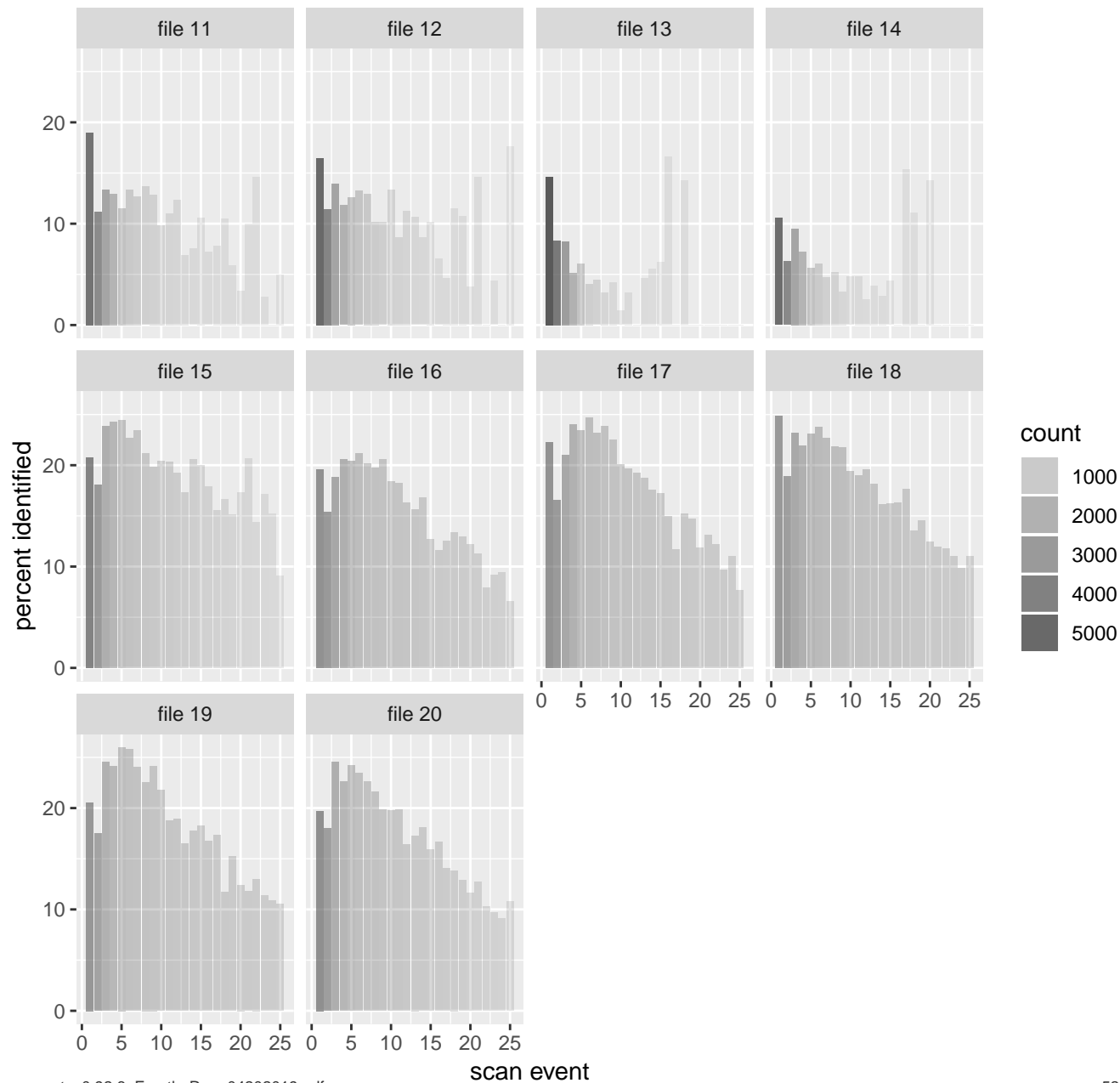
Raw file	% identified
20170427_144T_2a	17.68
20170427_144T_2c	14.65
20170427_159T_3a	10.03
20170427_159T_3b	10.43
20170427_159T_3c	9.90
20170427_159T_4a	6.59
20170427_159T_4b	5.83
20170427_159T_4c	16.78
20170427_163N_8a	14.20
20170427_163N_8b	16.07
20170427_163N_8c	16.50
20170427_163T_6a	16.61
20170427_163T_6b	15.85
20170427_163T_6c	17.05
20170427_163T_7a	14.41
20170427_163T_7b	15.64
20170427_163T_7c	14.78
144T_mlgG1	8.55
144T_mlgG2	11.85
144T_mlgG3	12.41
144T_Orf1_1	14.88
144T_Orf1_2	16.29
144T_Orf1_3	17.56

77% of samples)

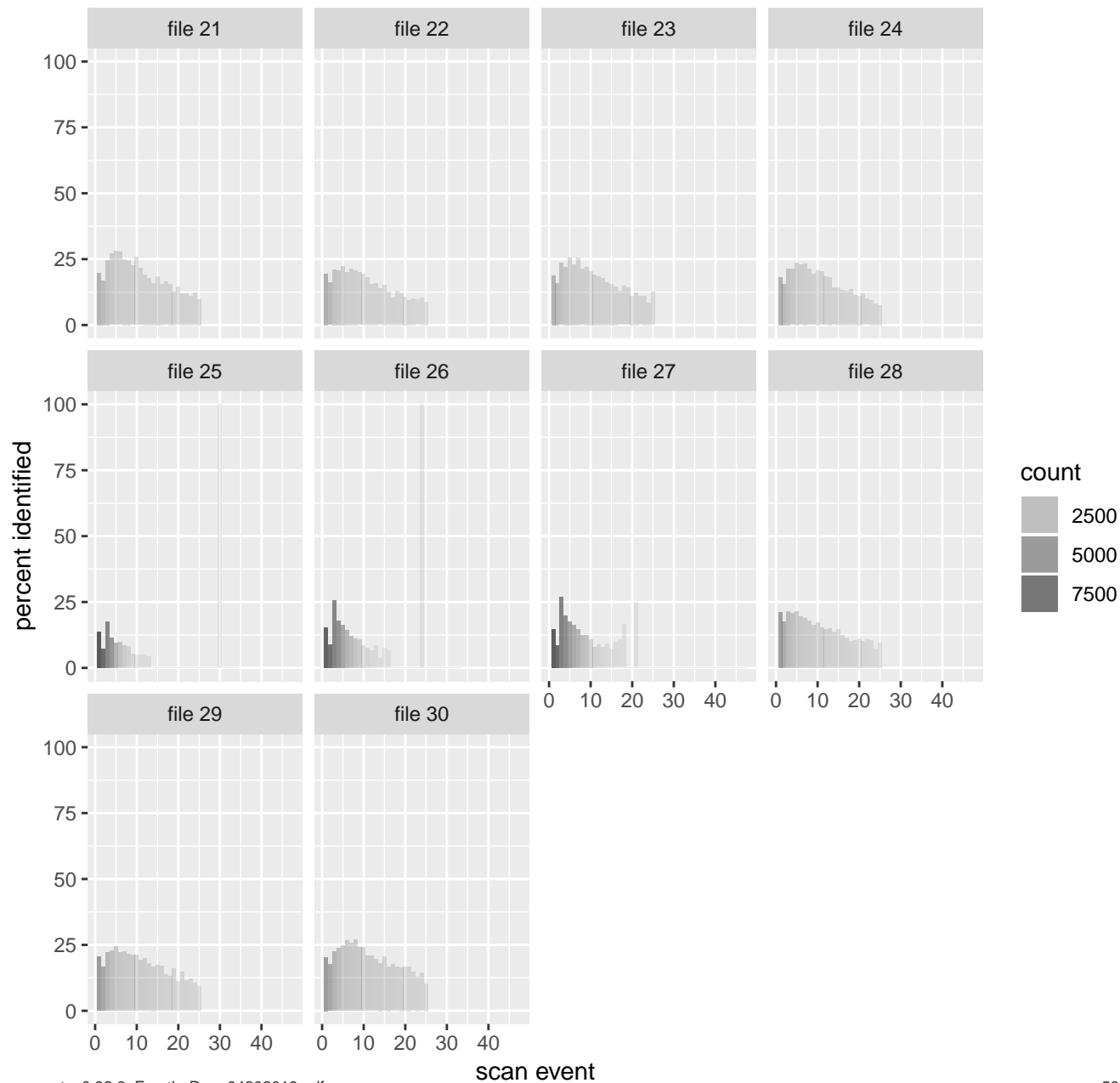
# MSMSscans: TopN % identified over N



# MSMSscans: TopN % identified over N

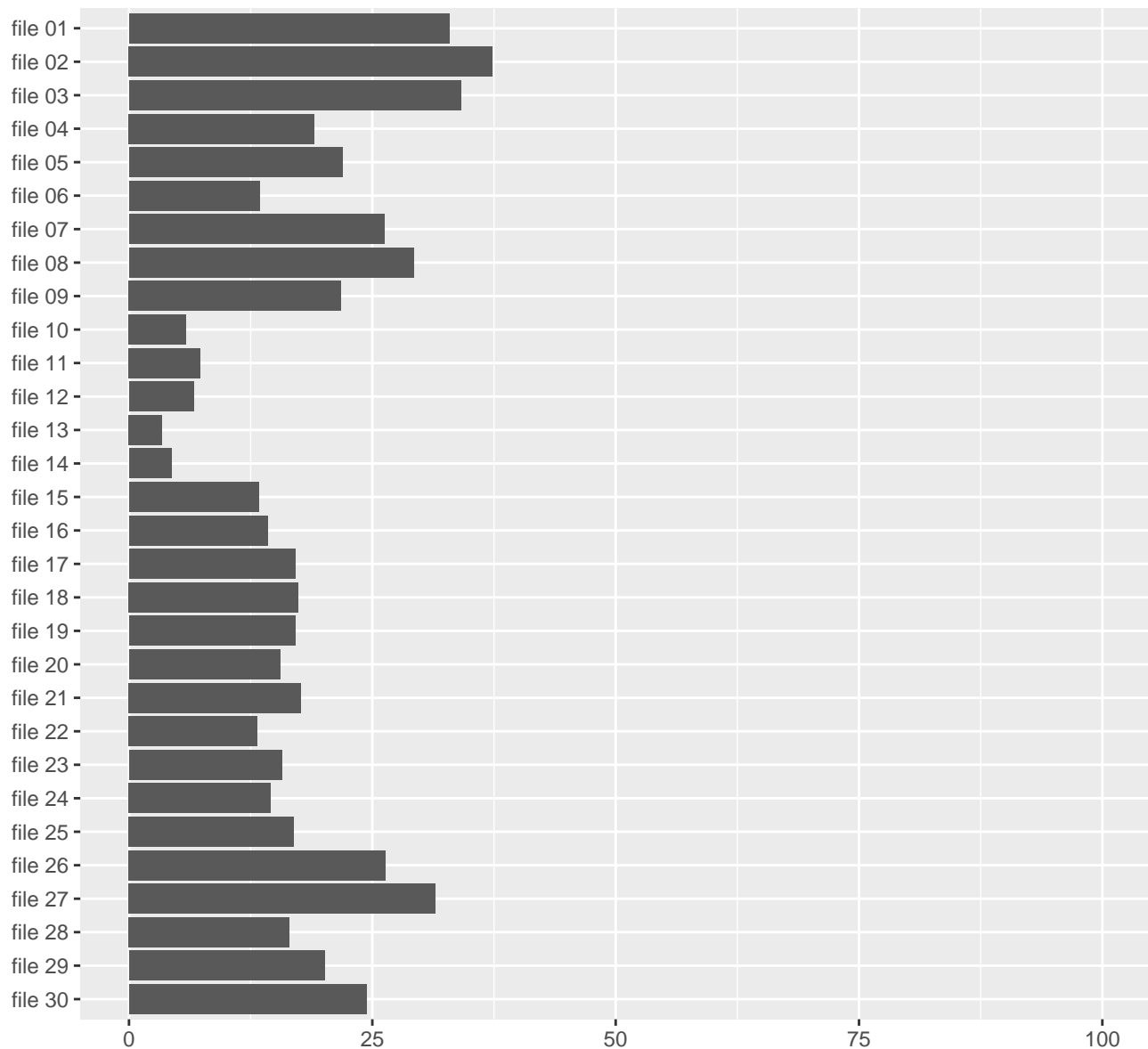


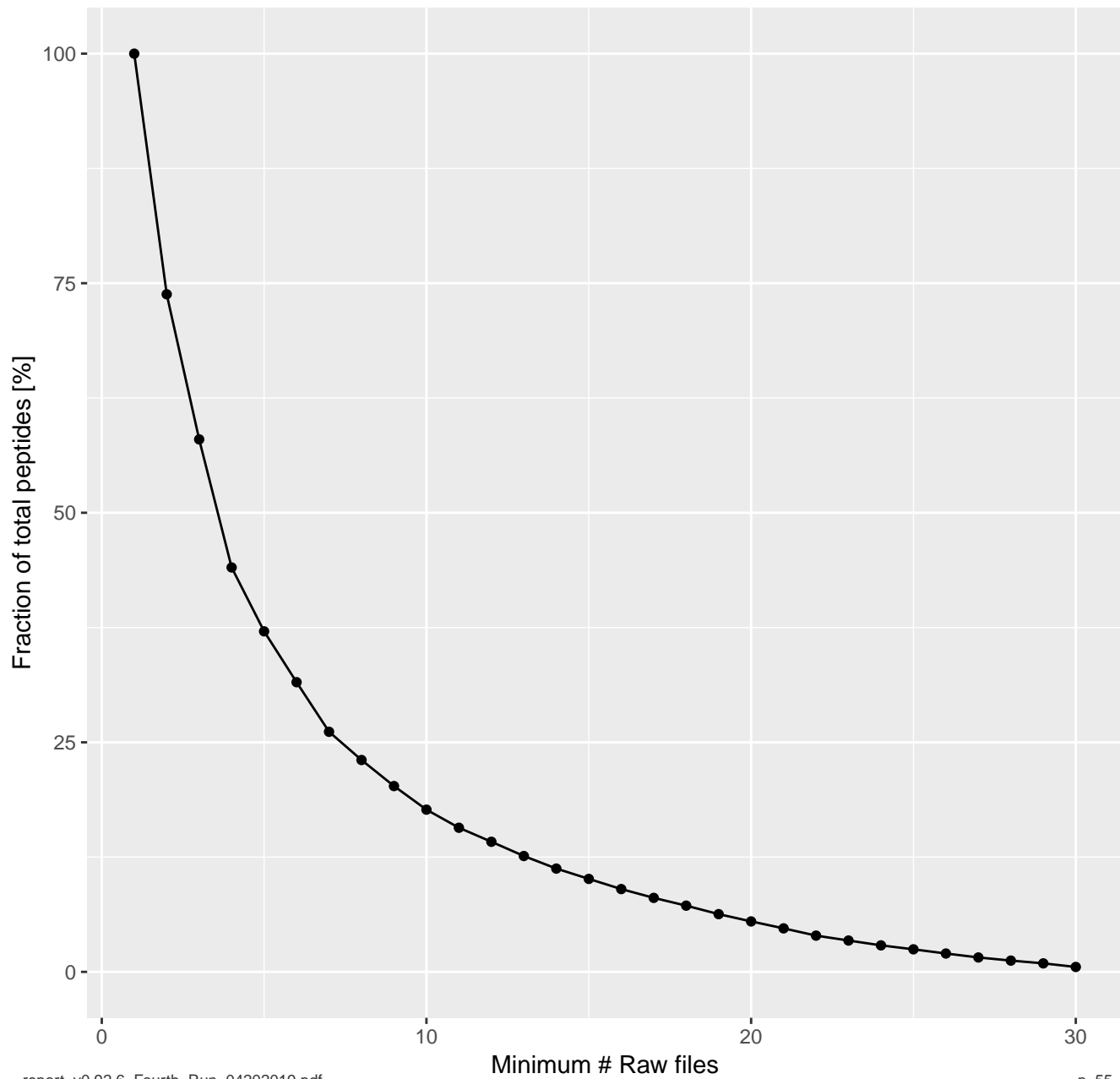
# MSMScans: TopN % identified over N



# [experimental] EVD: Non-Missing Peptides

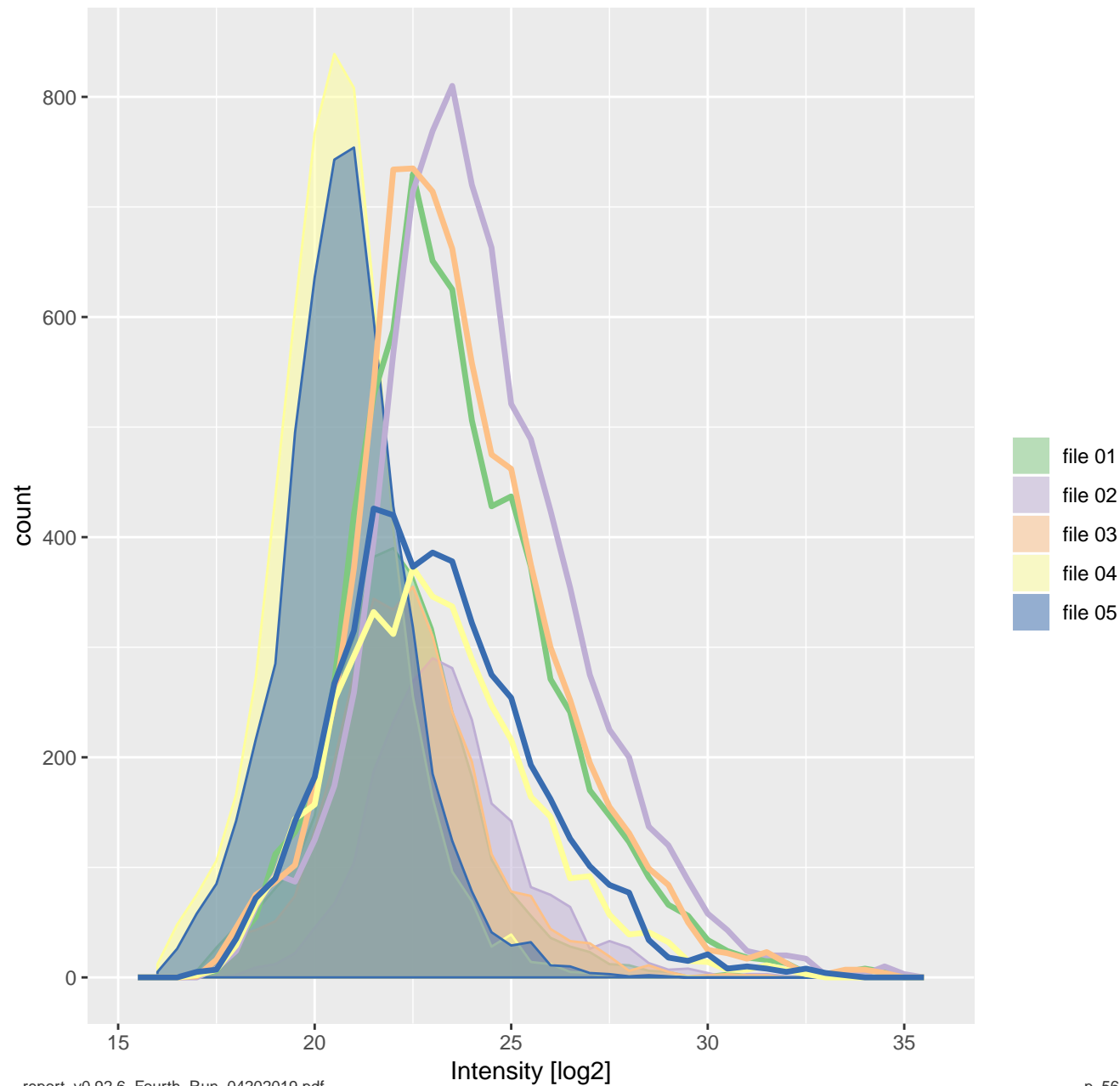
compared to all peptides seen in experiment



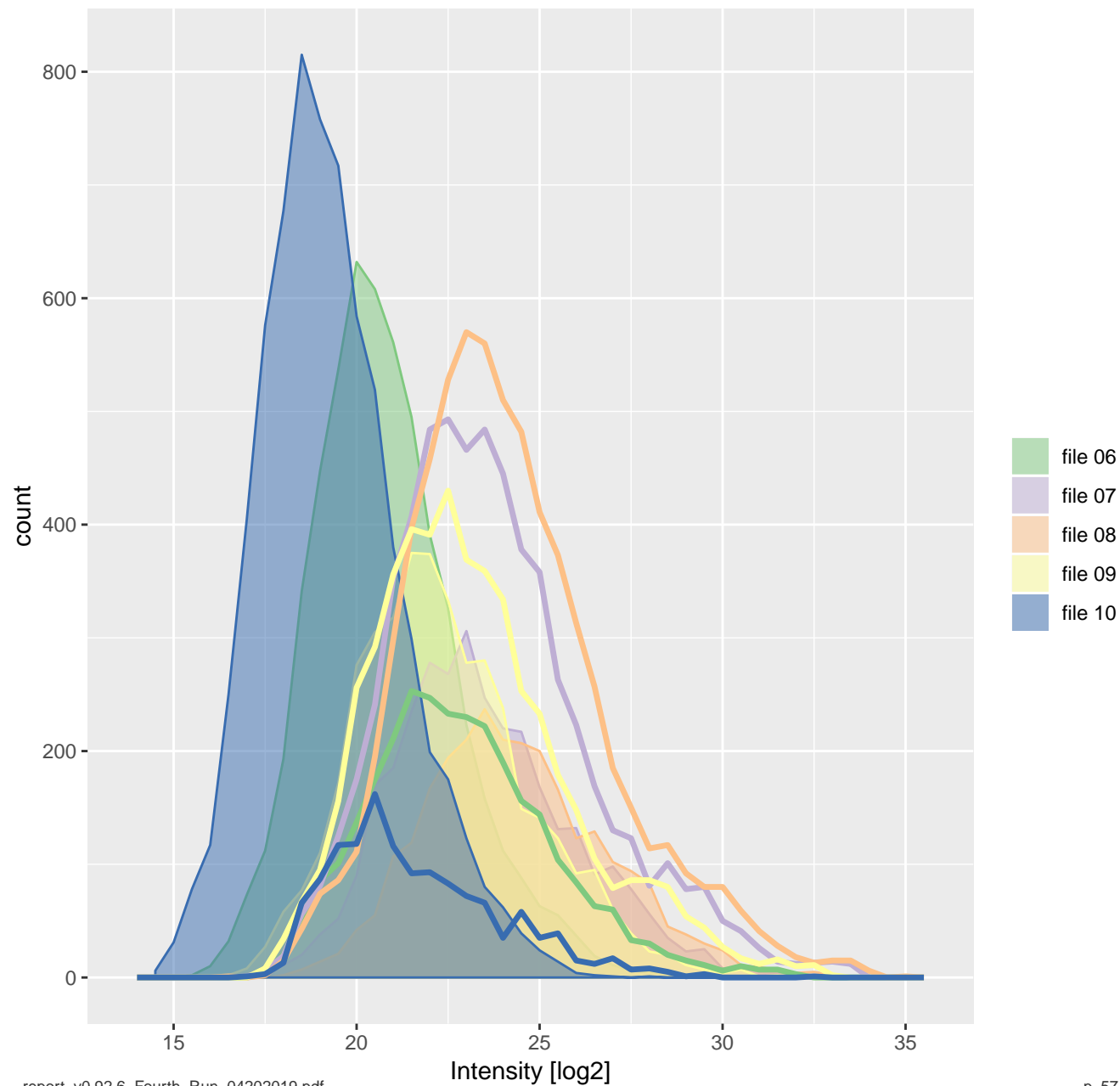




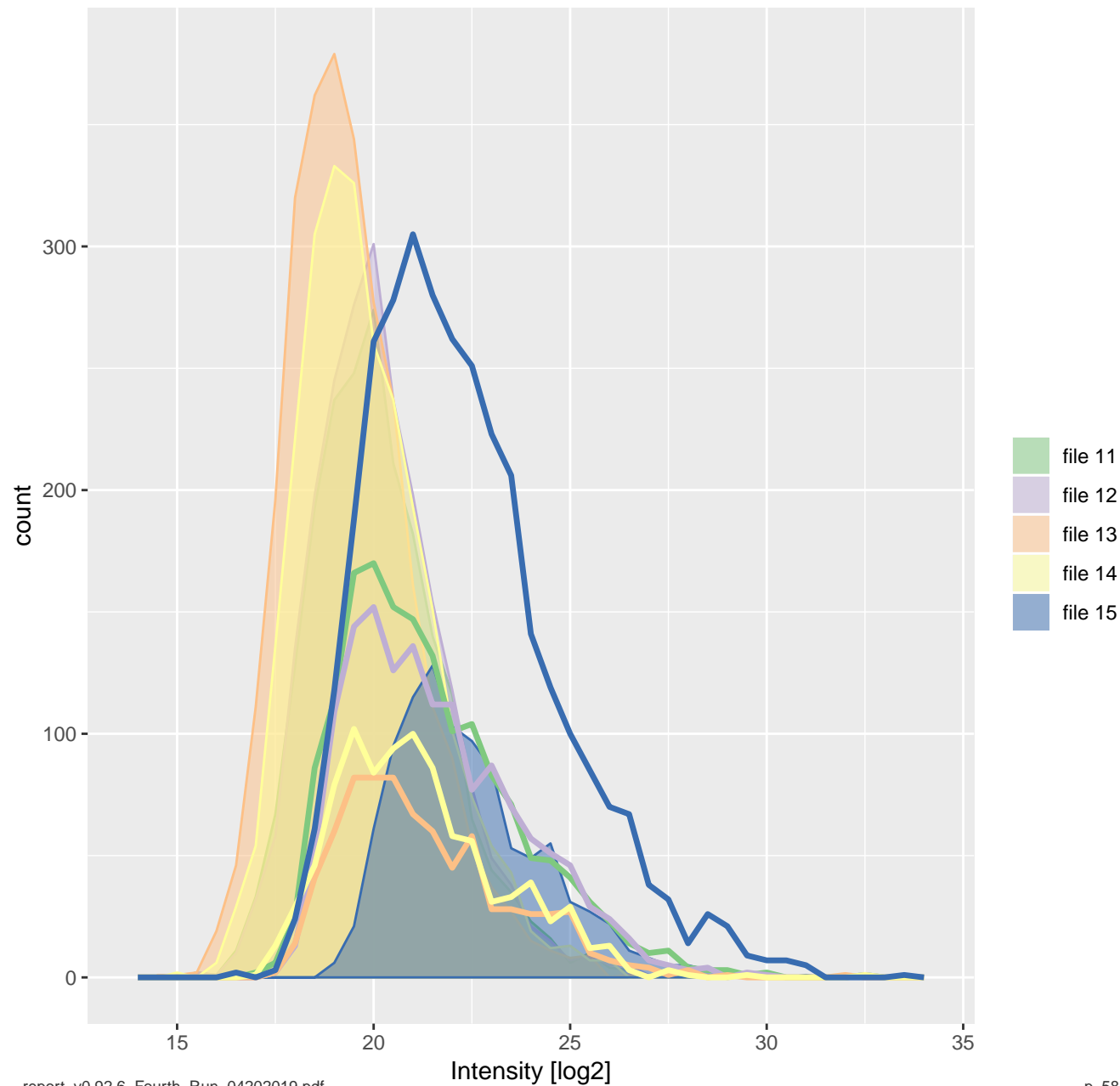
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



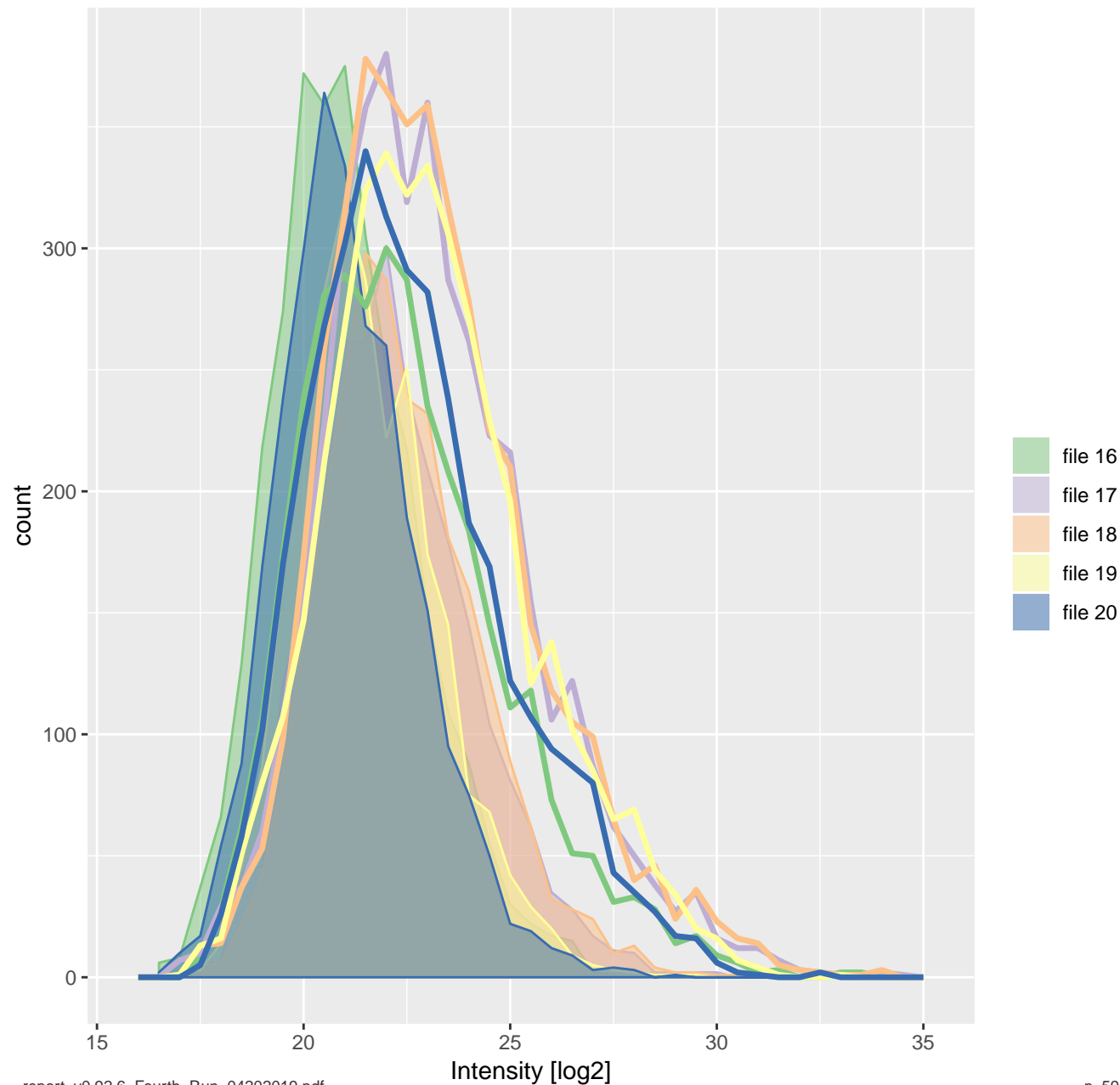
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



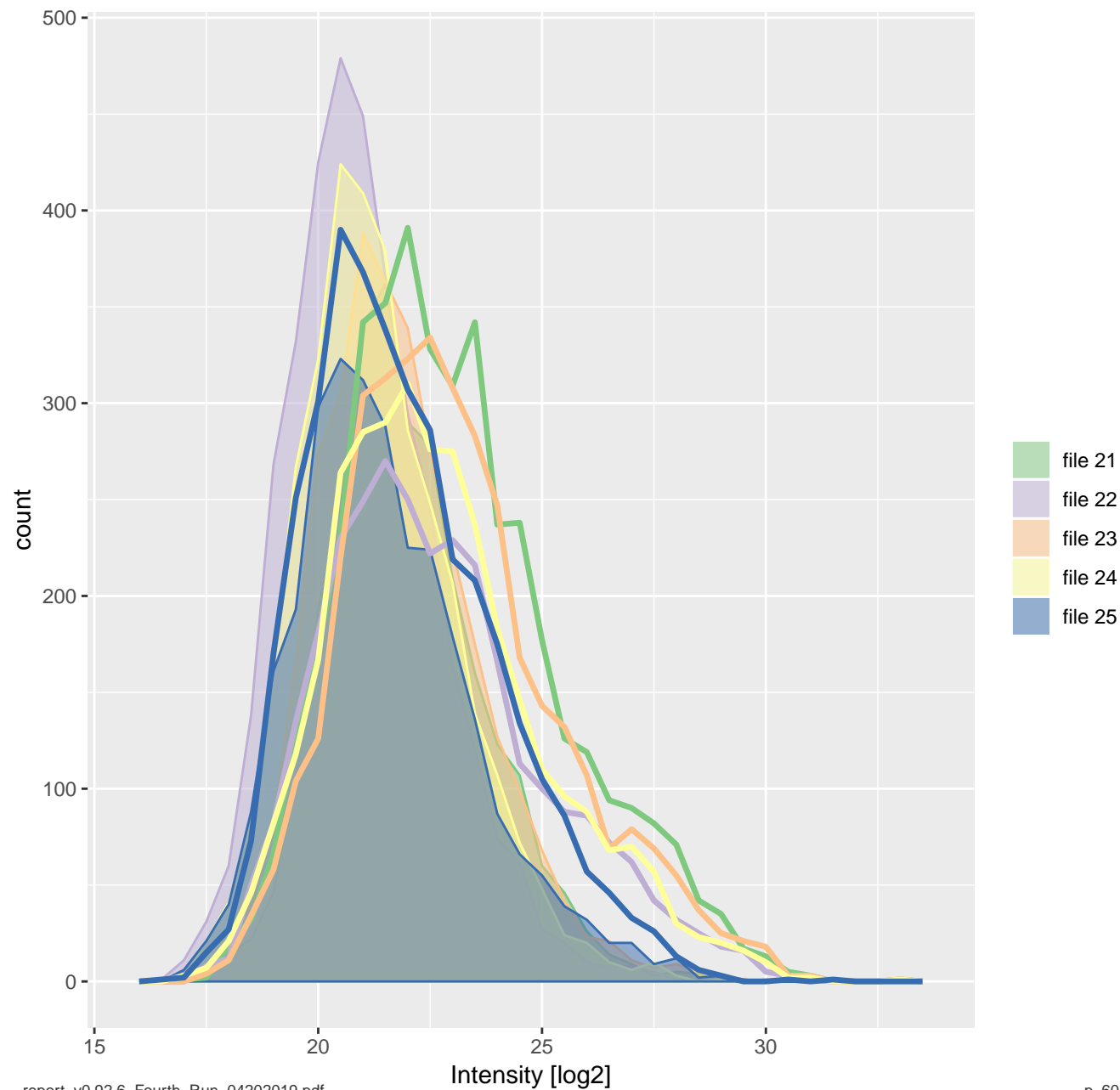
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



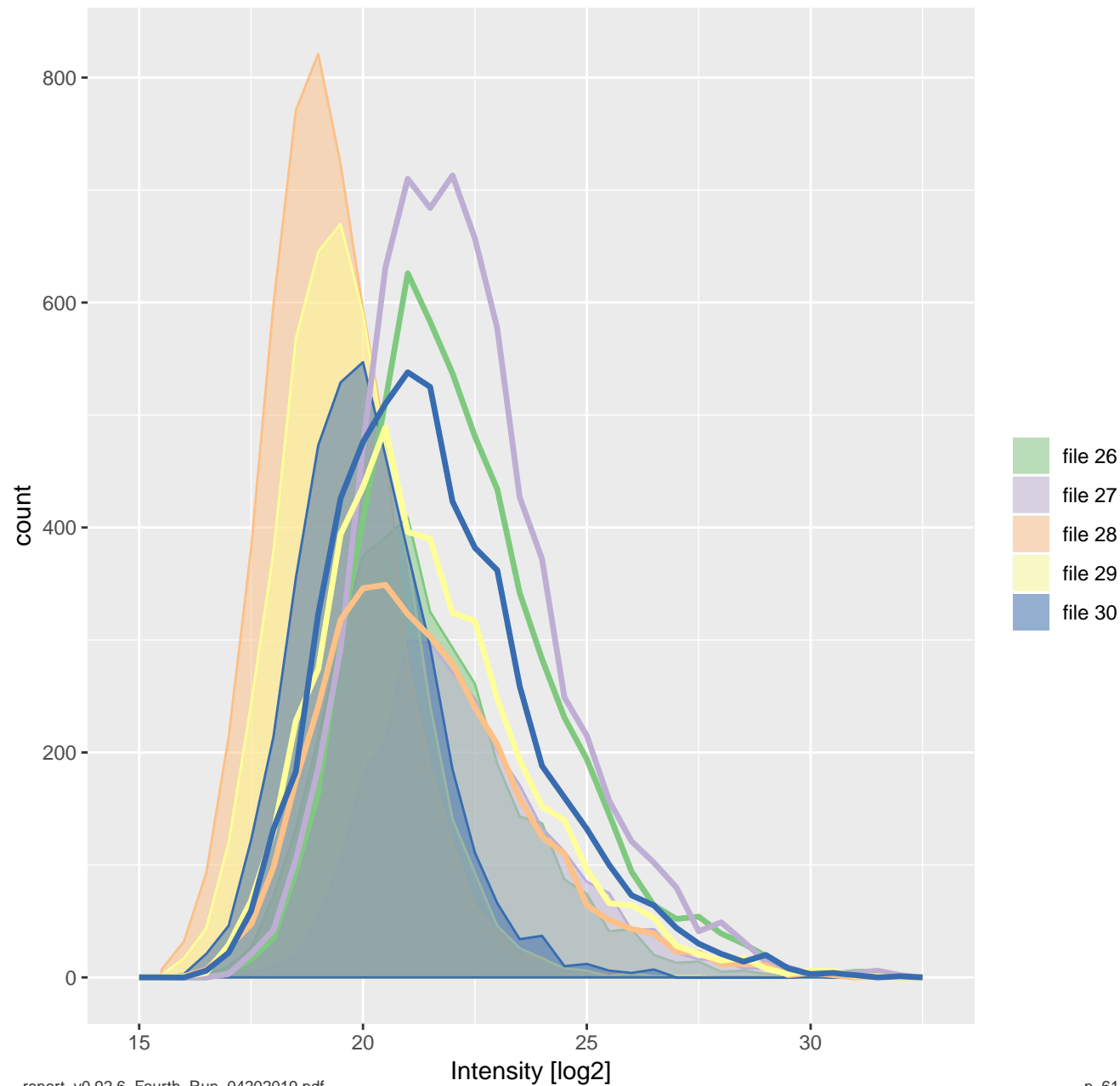
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



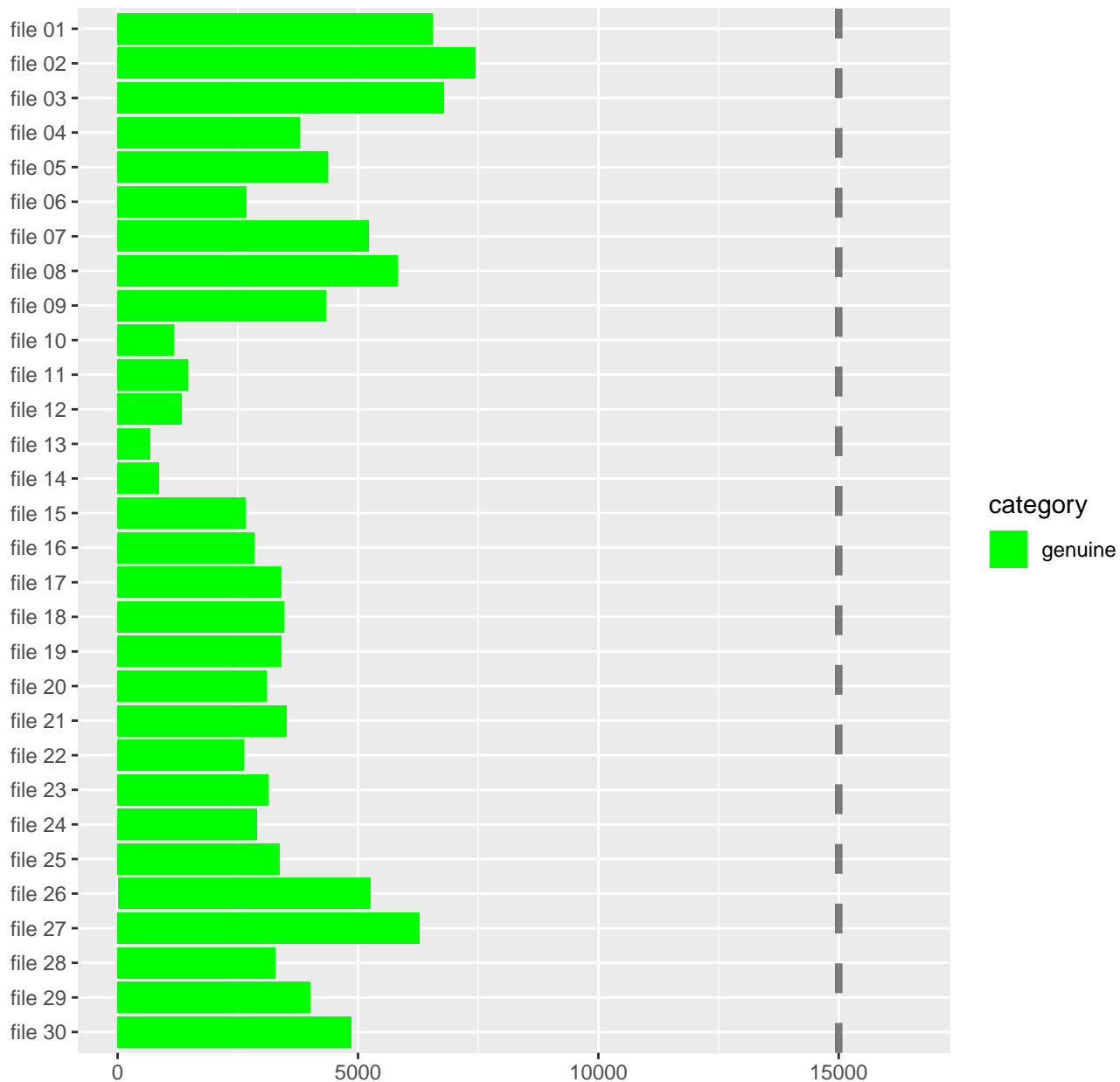
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



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



## EVD: Peptide ID count



## EVD: ProteinGroups count

