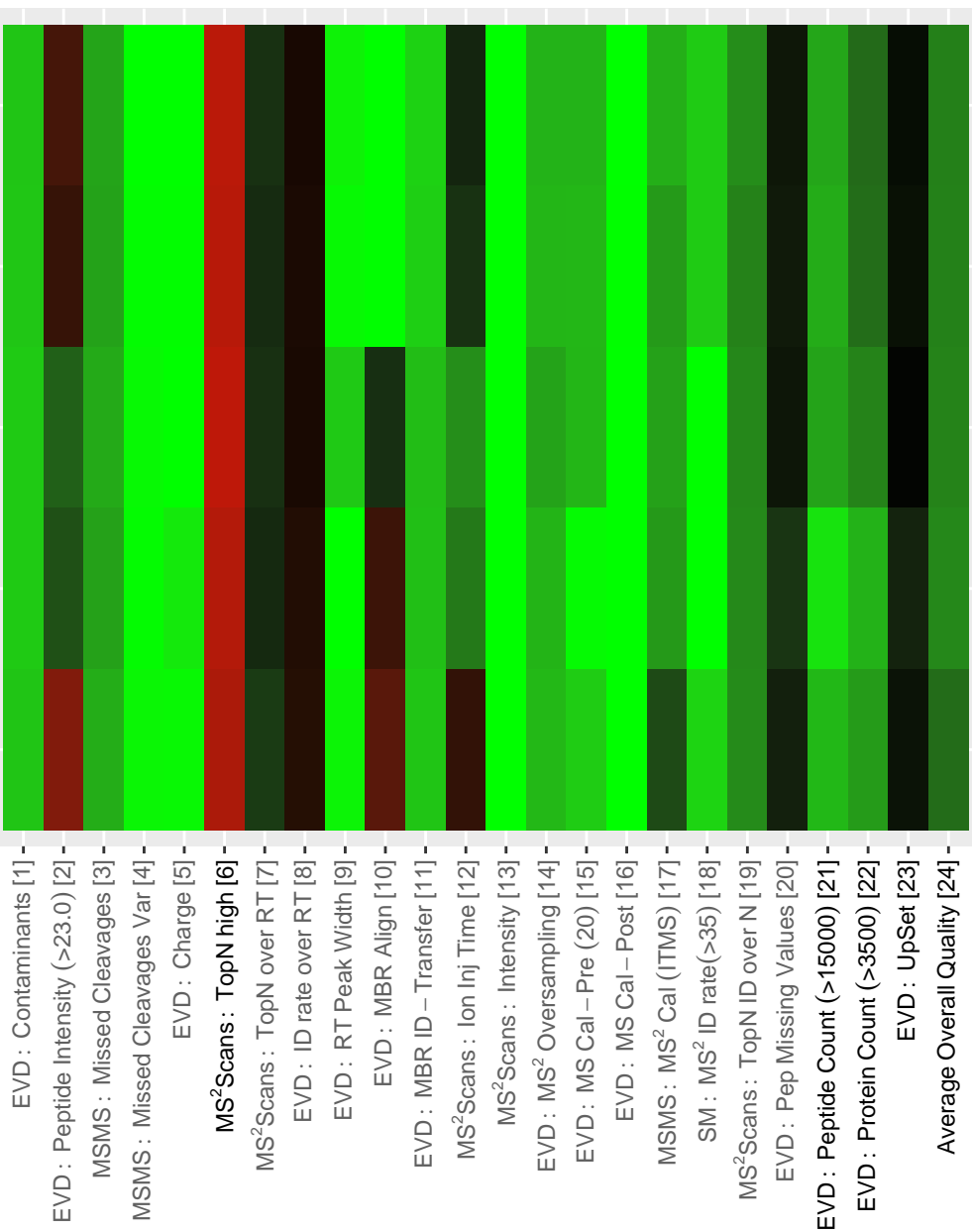


# Performance overview

Raw file

file 1  
file 2  
file 3  
file 4  
file 5



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

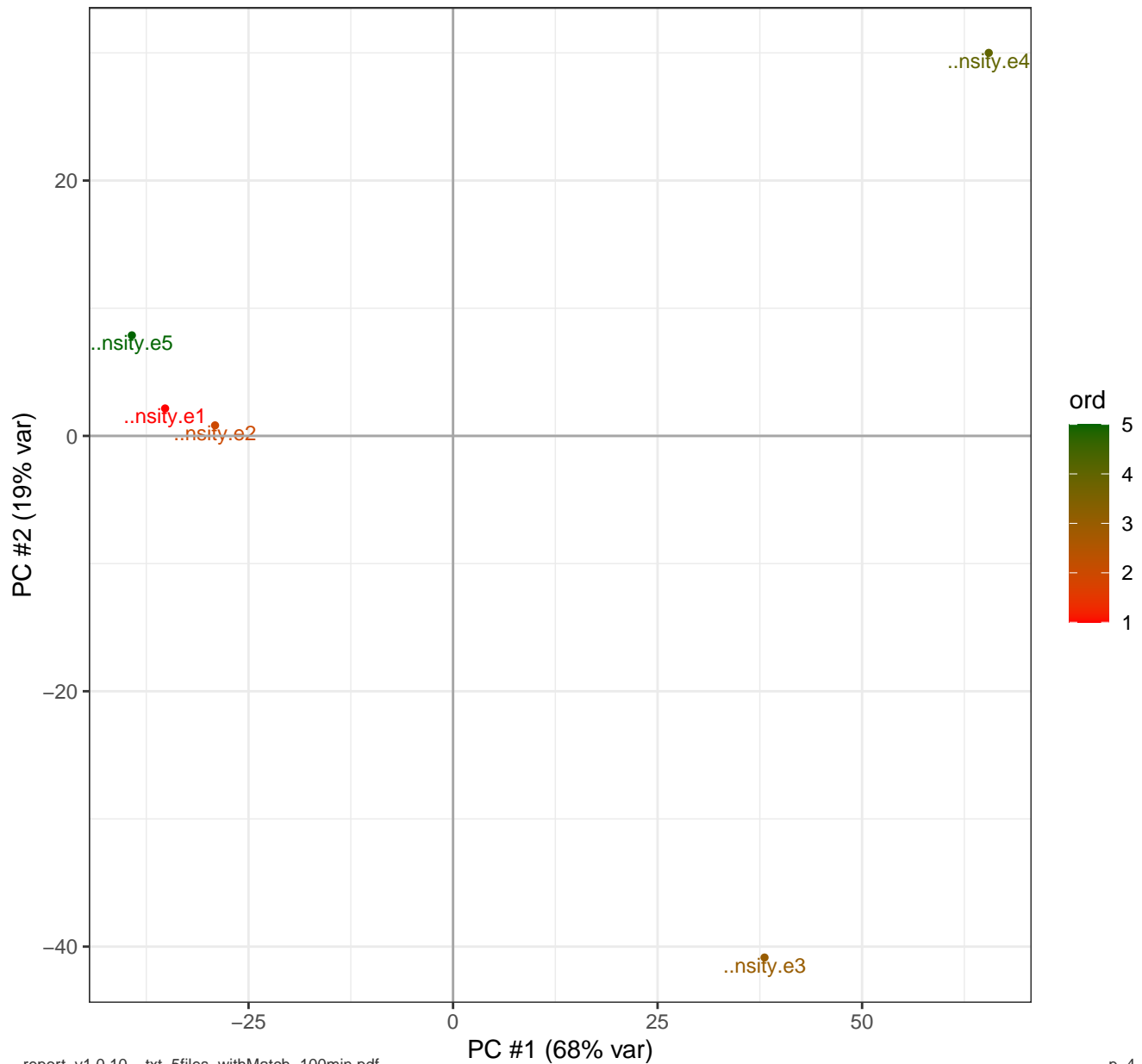
original	short name	best effort
Toni_20140521_GM_QC_01	file 1	..521_GM_QC_0.._01
Toni_20140521_GM_QC_02	file 2	..521_GM_QC_0.._02
Toni_20140522_GM_QC_01	file 3	..522_GM_QC_0.._01
Toni_20140531_FB_QC_02	file 4	..531_FB_QC_0.._02
Toni_20140608_FB_qc_01	file 5	..608_FB_qc_0.._01

## 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

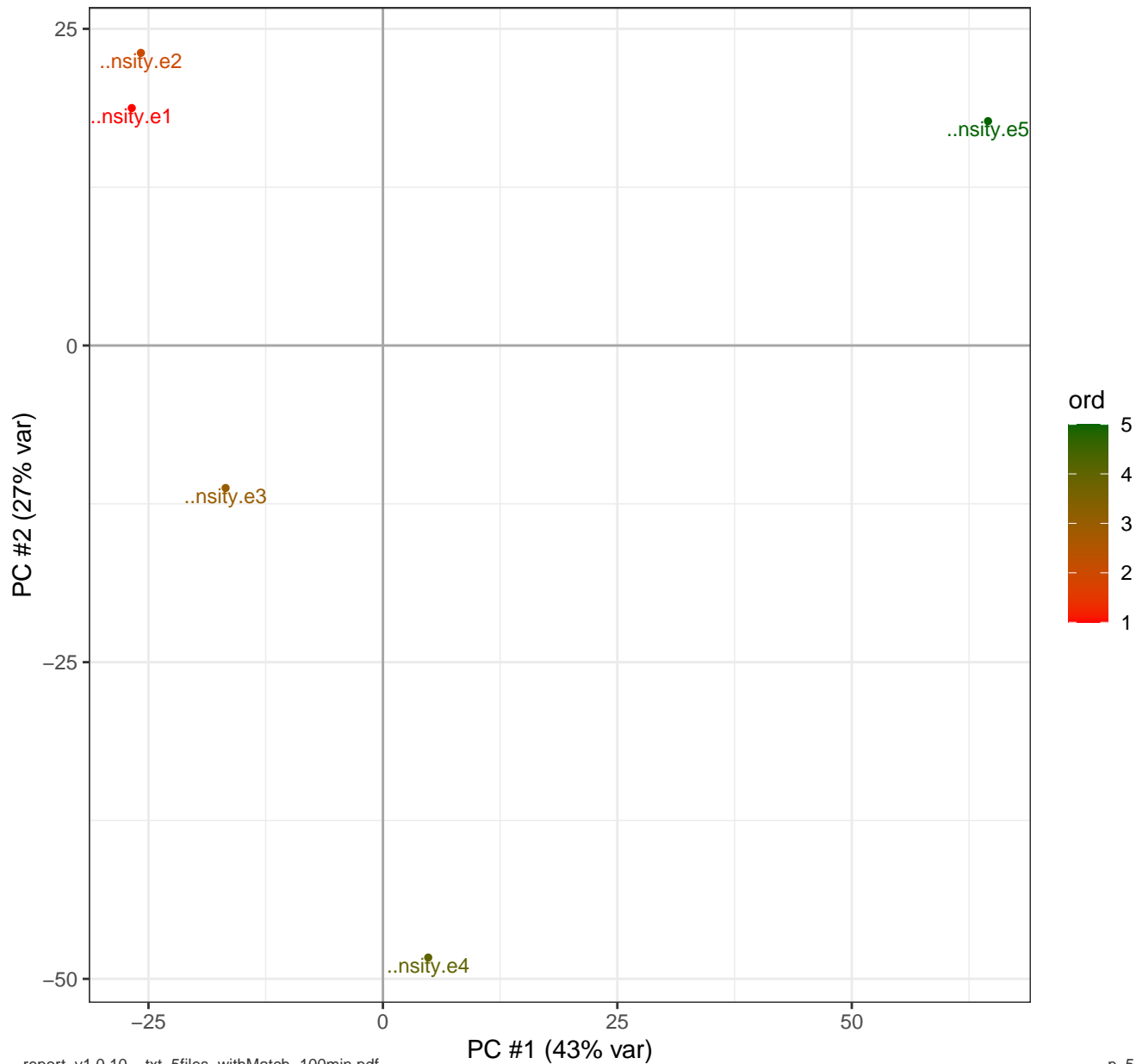
uniprot\_human\_canonical\_and\_isoforms\_20130513.fasta

PG: PCA of 'raw intensity'  
(excludes contaminants)

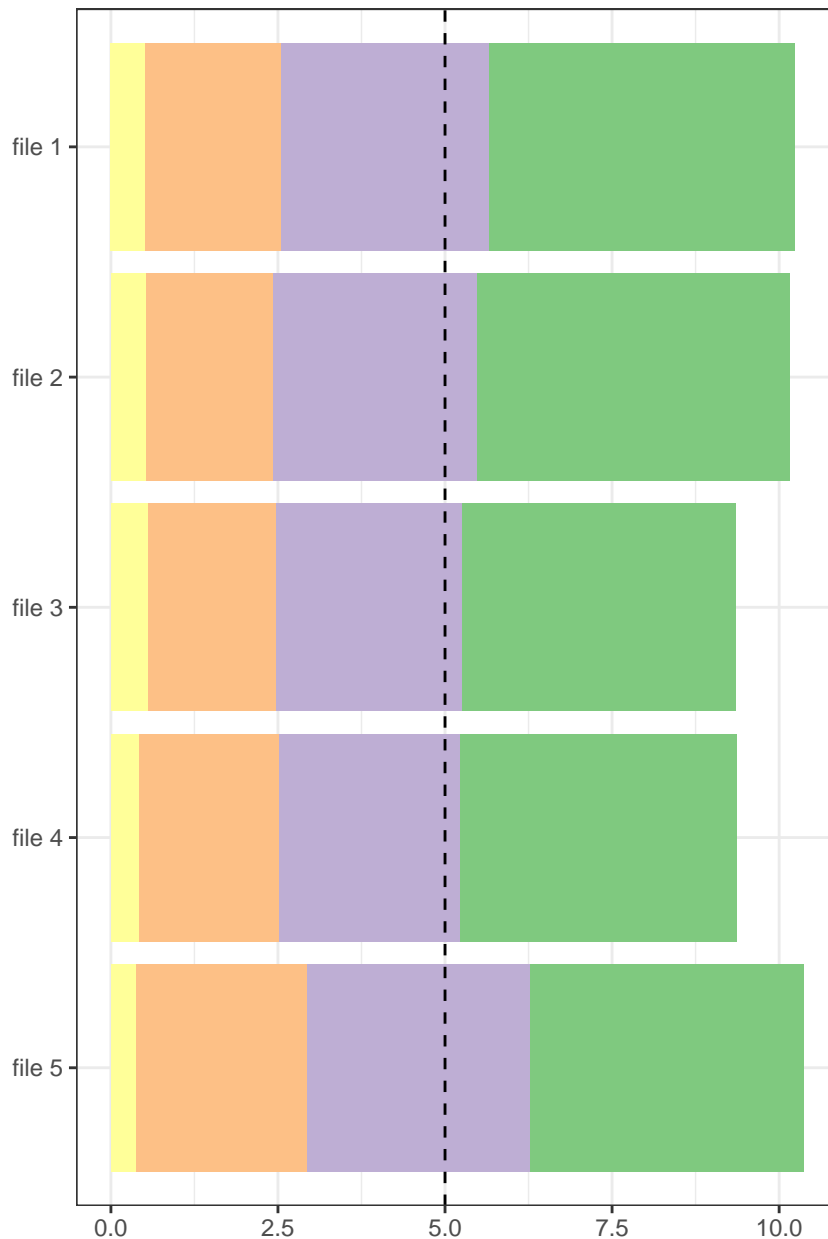


# PG: PCA of 'lfq intensity'

(excludes contaminants)



## EVD: Top5 Contaminants per Raw file



Abundance  
class



mid

Protein



other



Actin, cytopl.;Actin, cytopl.;...



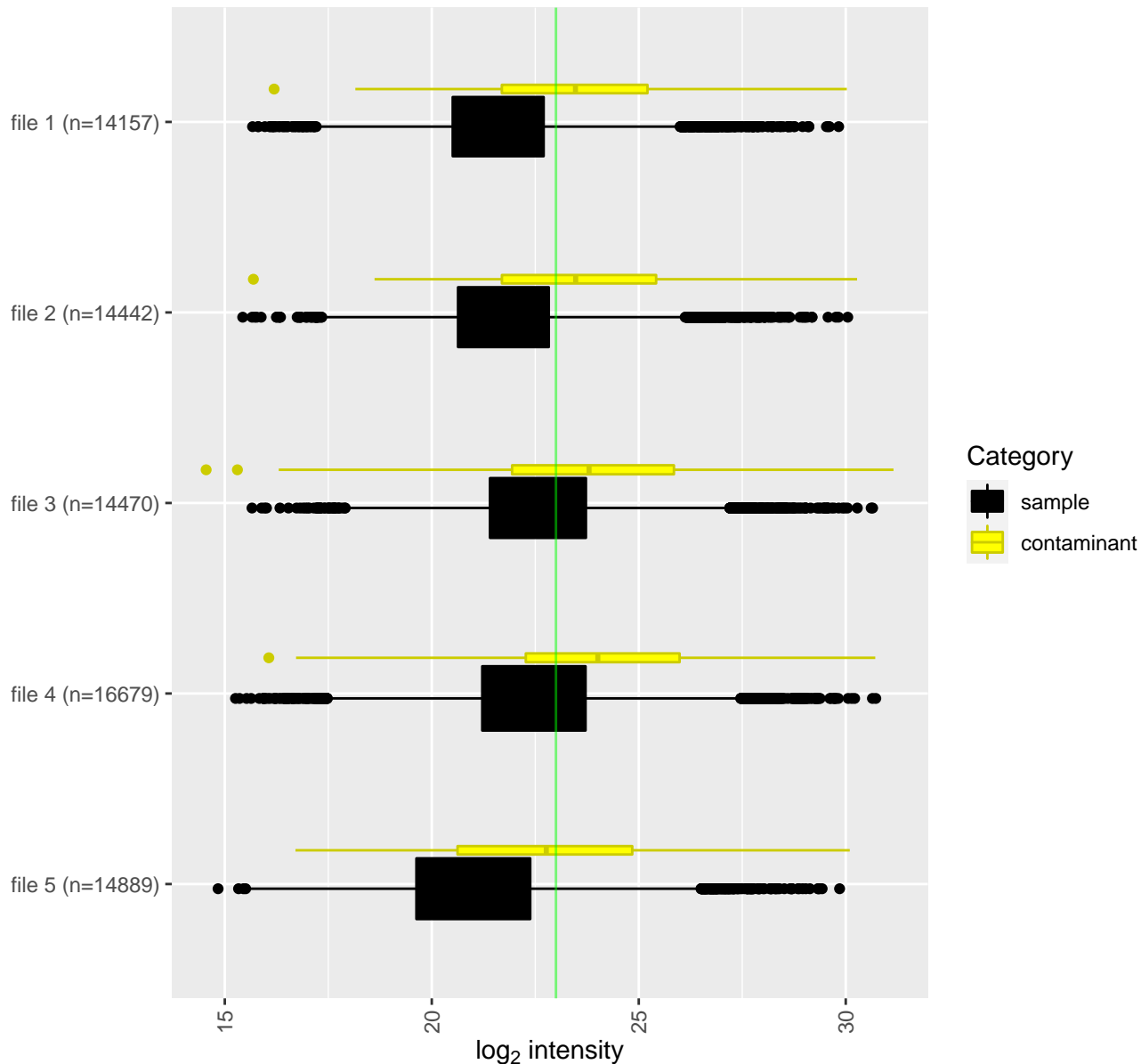
CON\_\_P15636



Tubulin alpha.;Tubulin alpha.;...

# EVD: peptide intensity distribution

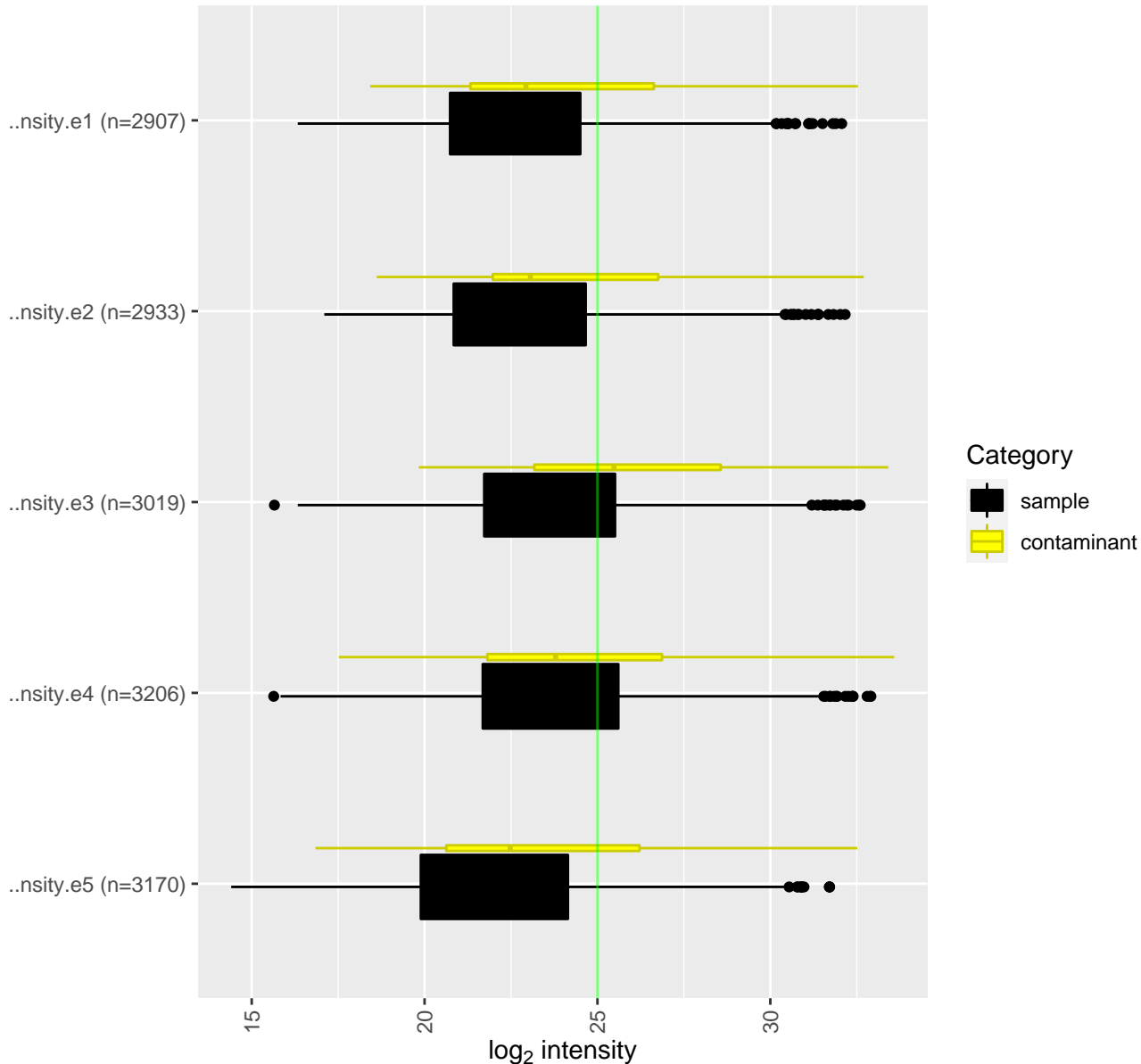
RSD 3% (expected < 5%)



## PG: intensity distribution

RSD 3% (w/o zero int.; expected < 5%)

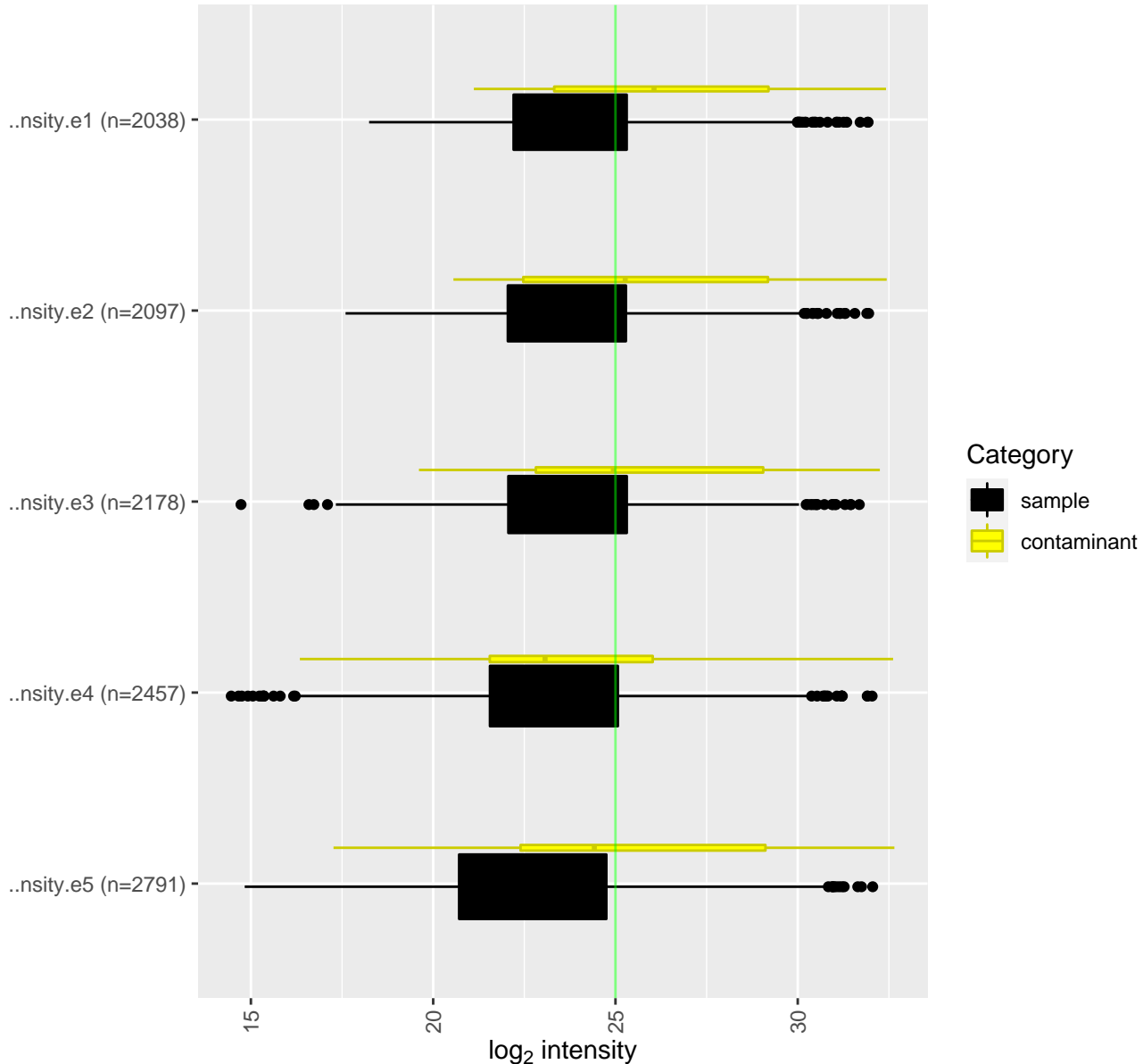
RSD 3.2% [high RSD --> few peptides]



# PG: LFQ intensity distribution

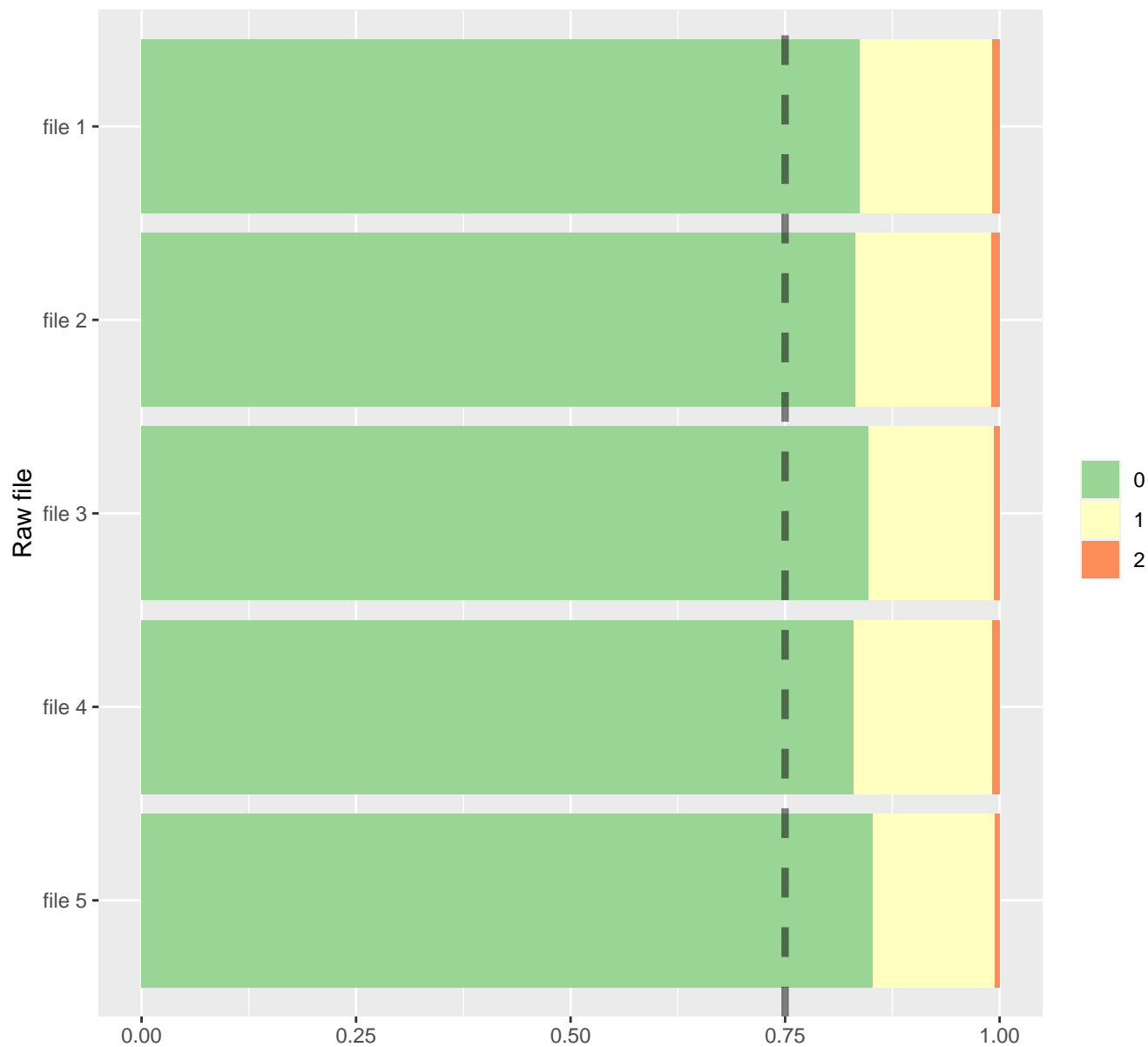
RSD 1.7% (w/o zero int.; expected < 5%)

RSD 0.5% [high RSD --> few peptides]

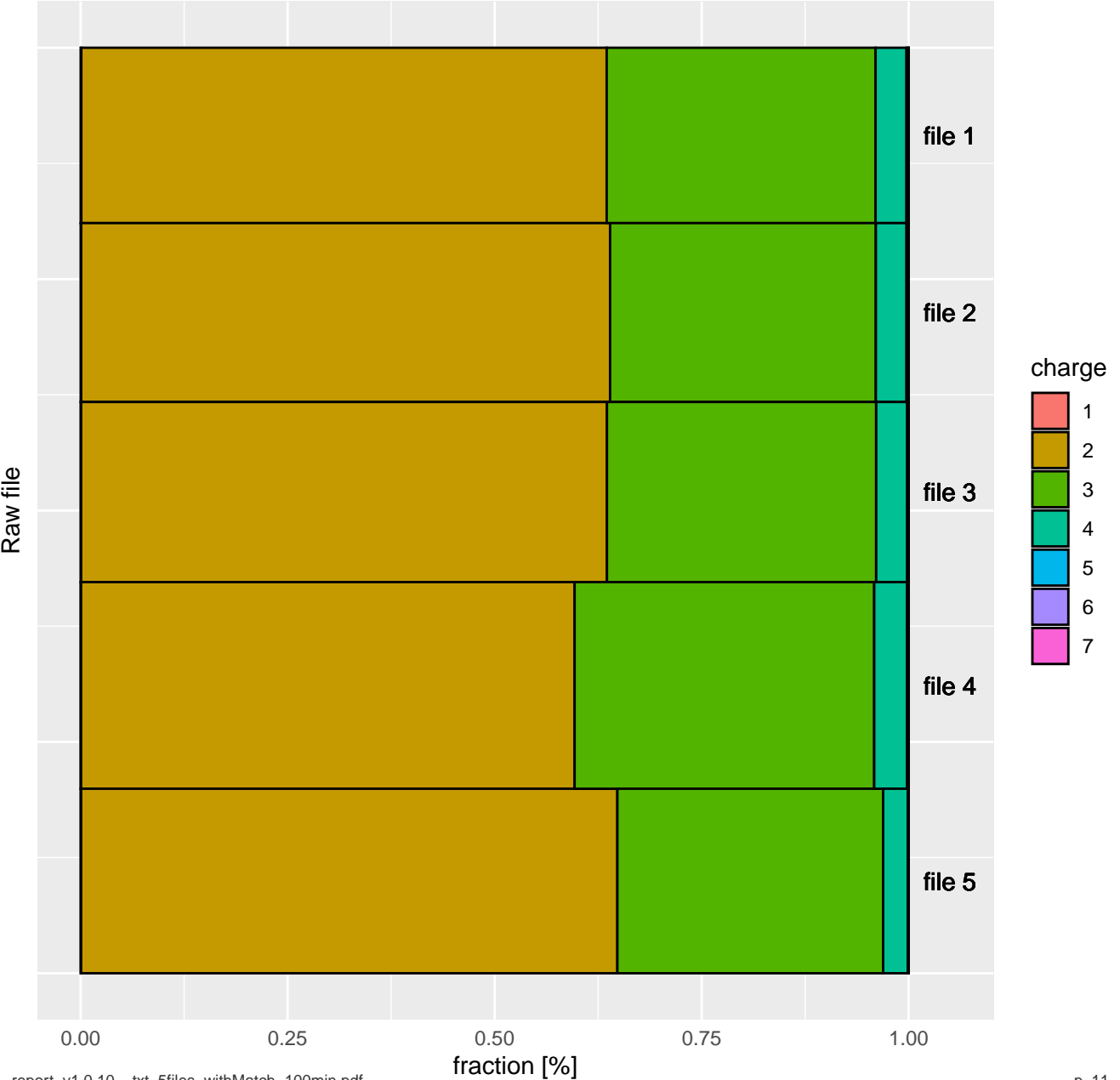


# MSMS: Missed cleavages per Raw file

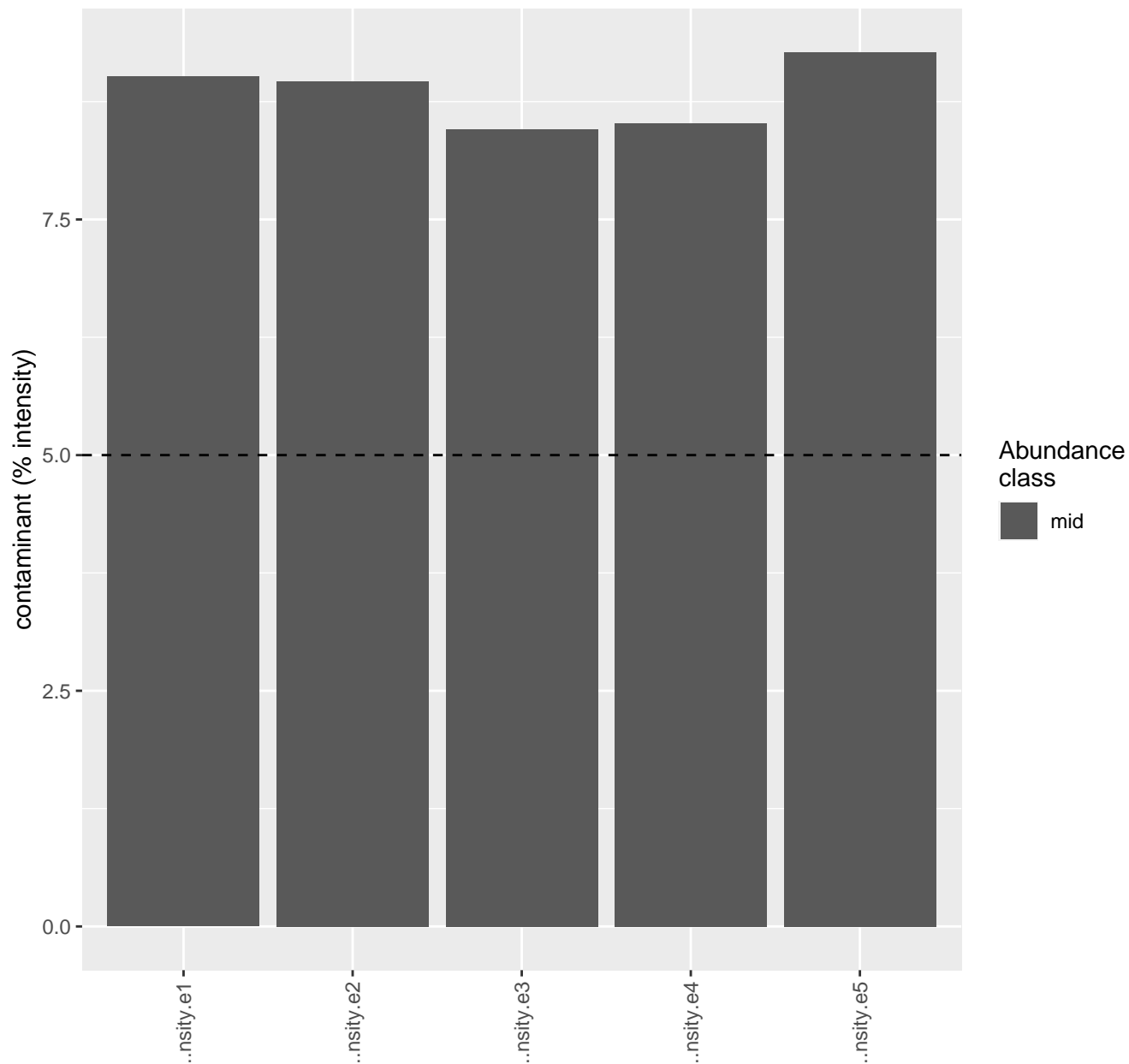
(excludes contaminants)



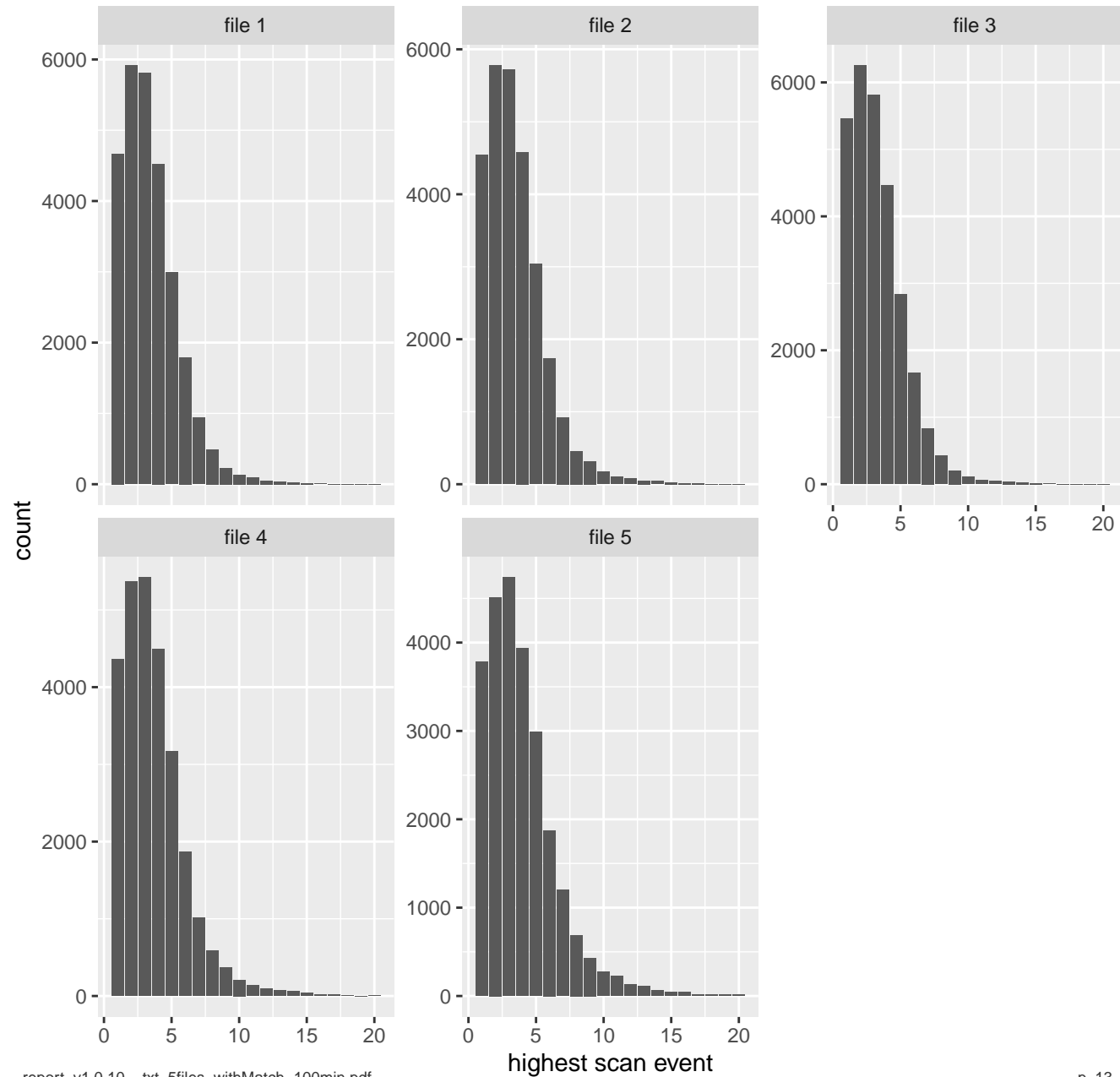
EVD: charge distribution



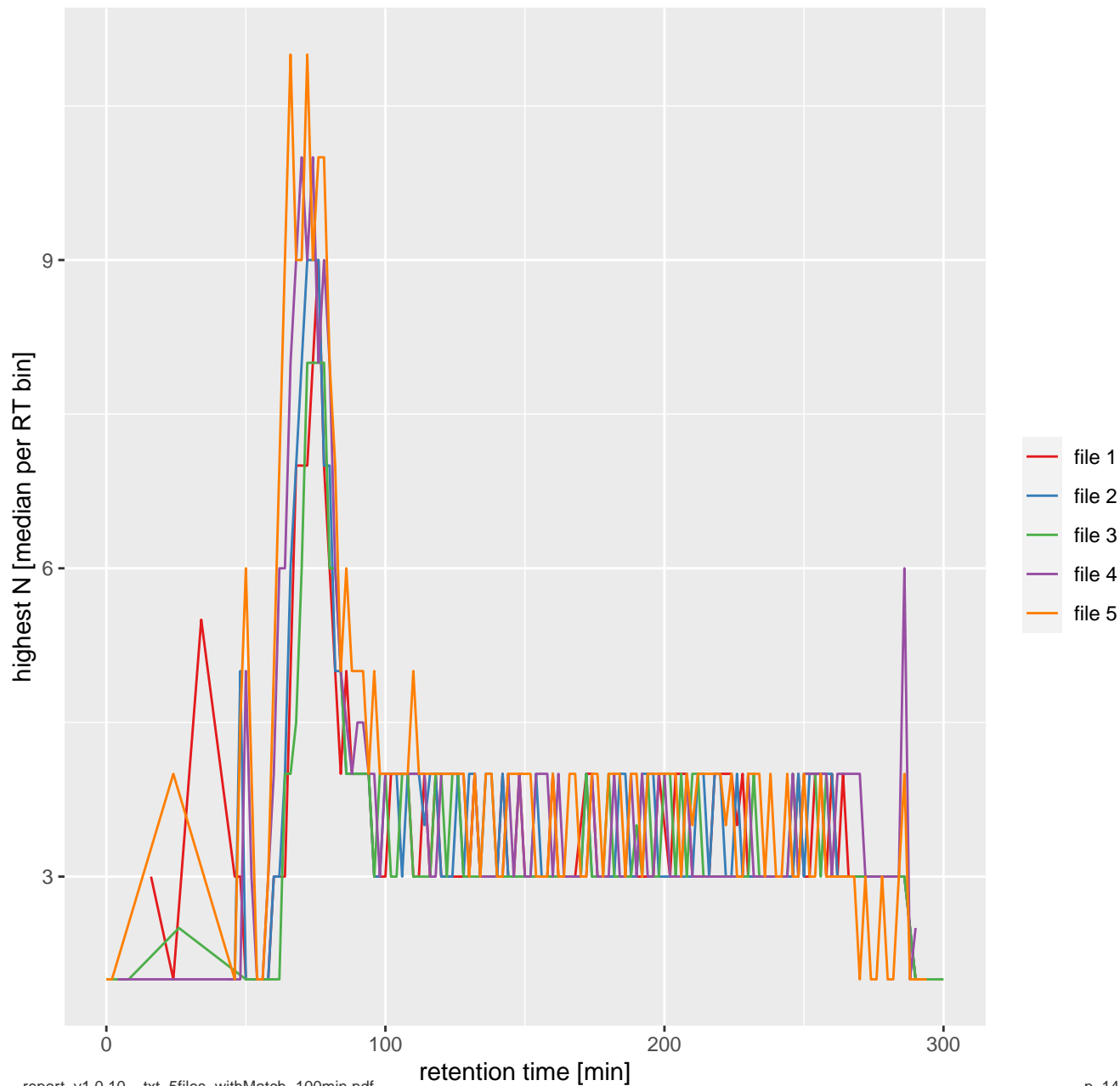
## PG: Contaminant per condition



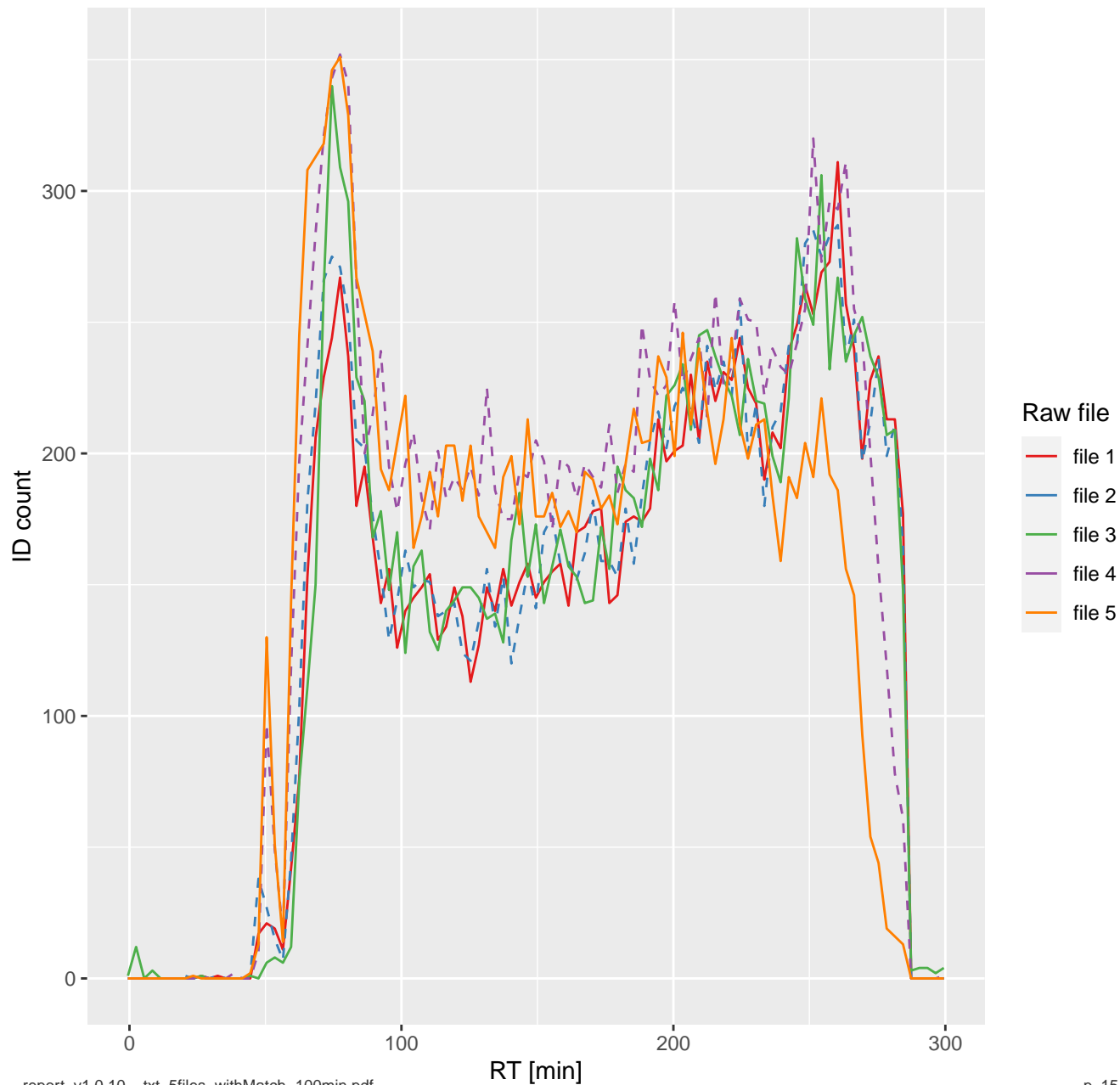
# MSMSscans: TopN



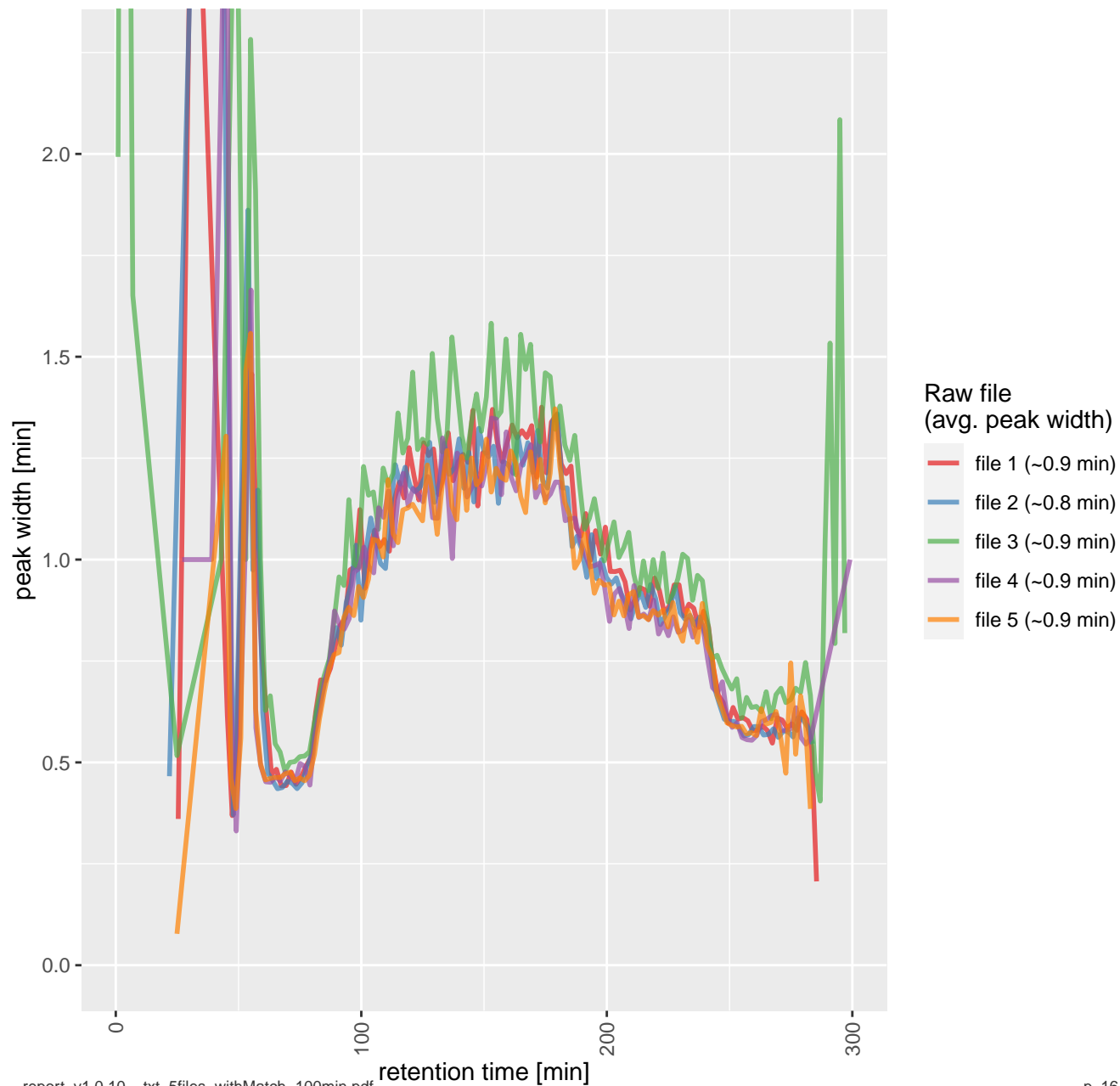
# MSMSscans: TopN over RT



# EVD: IDs over RT

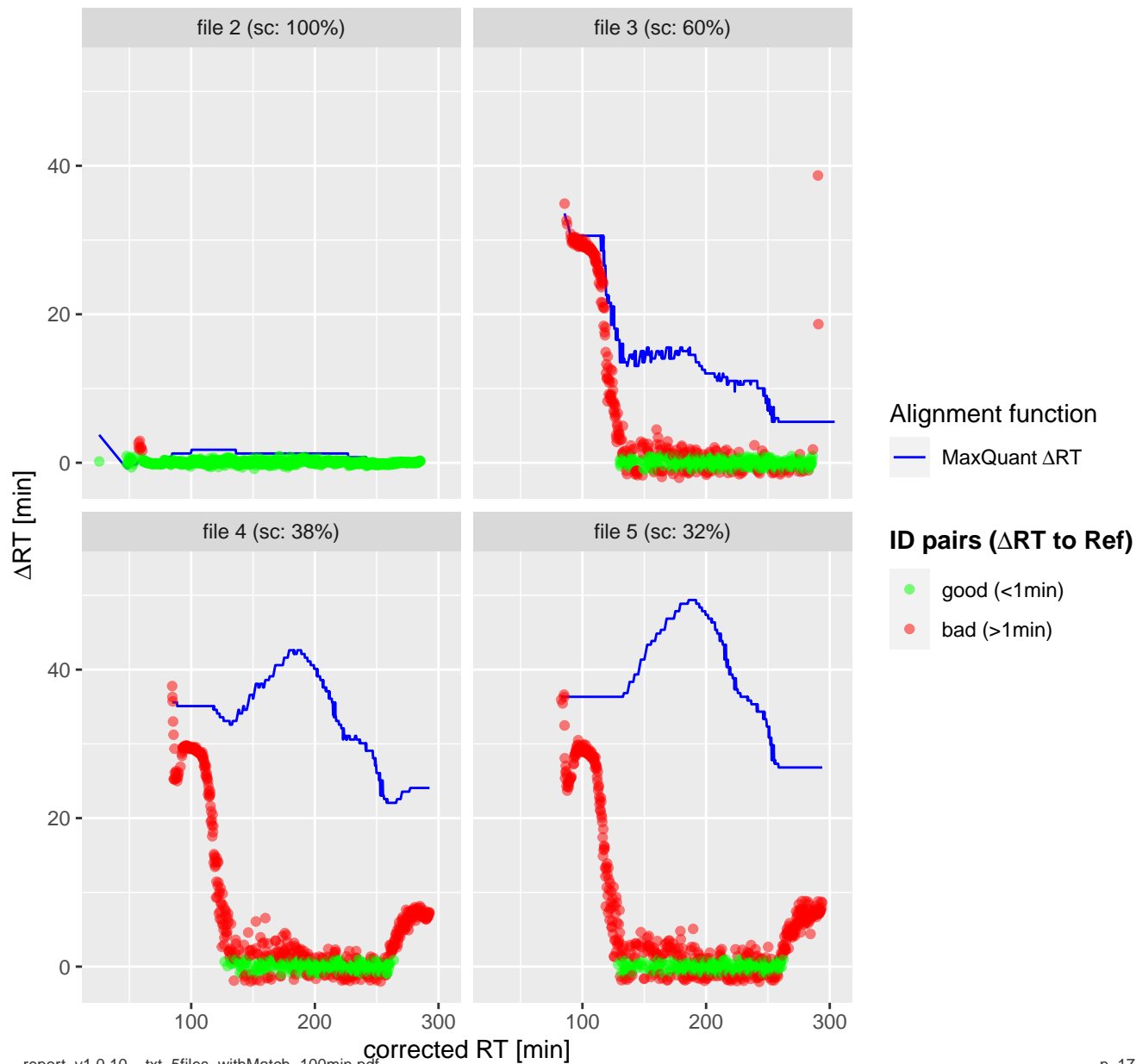


## EVD: Peak width over RT

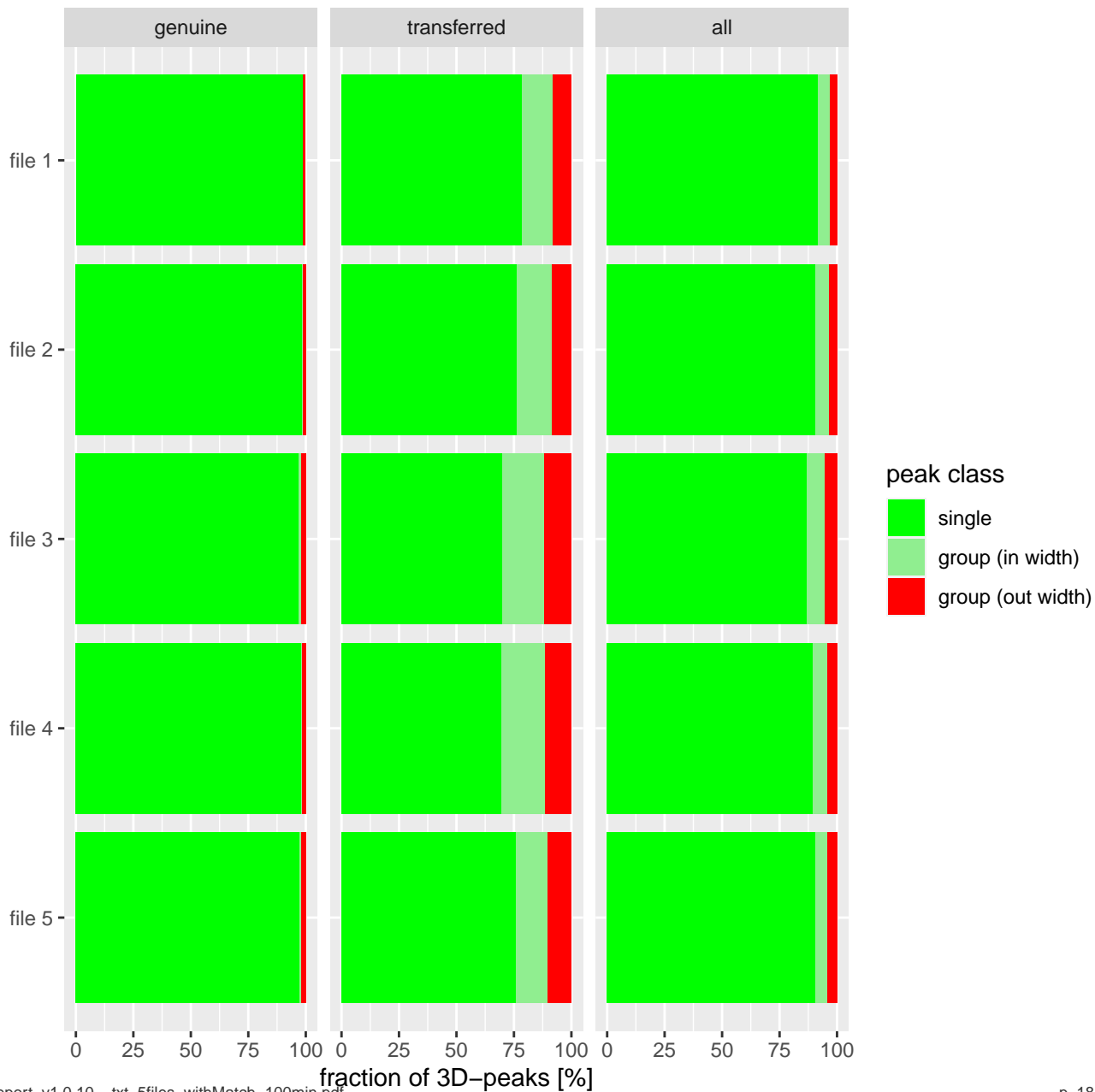


# EVD: MBR – alignment

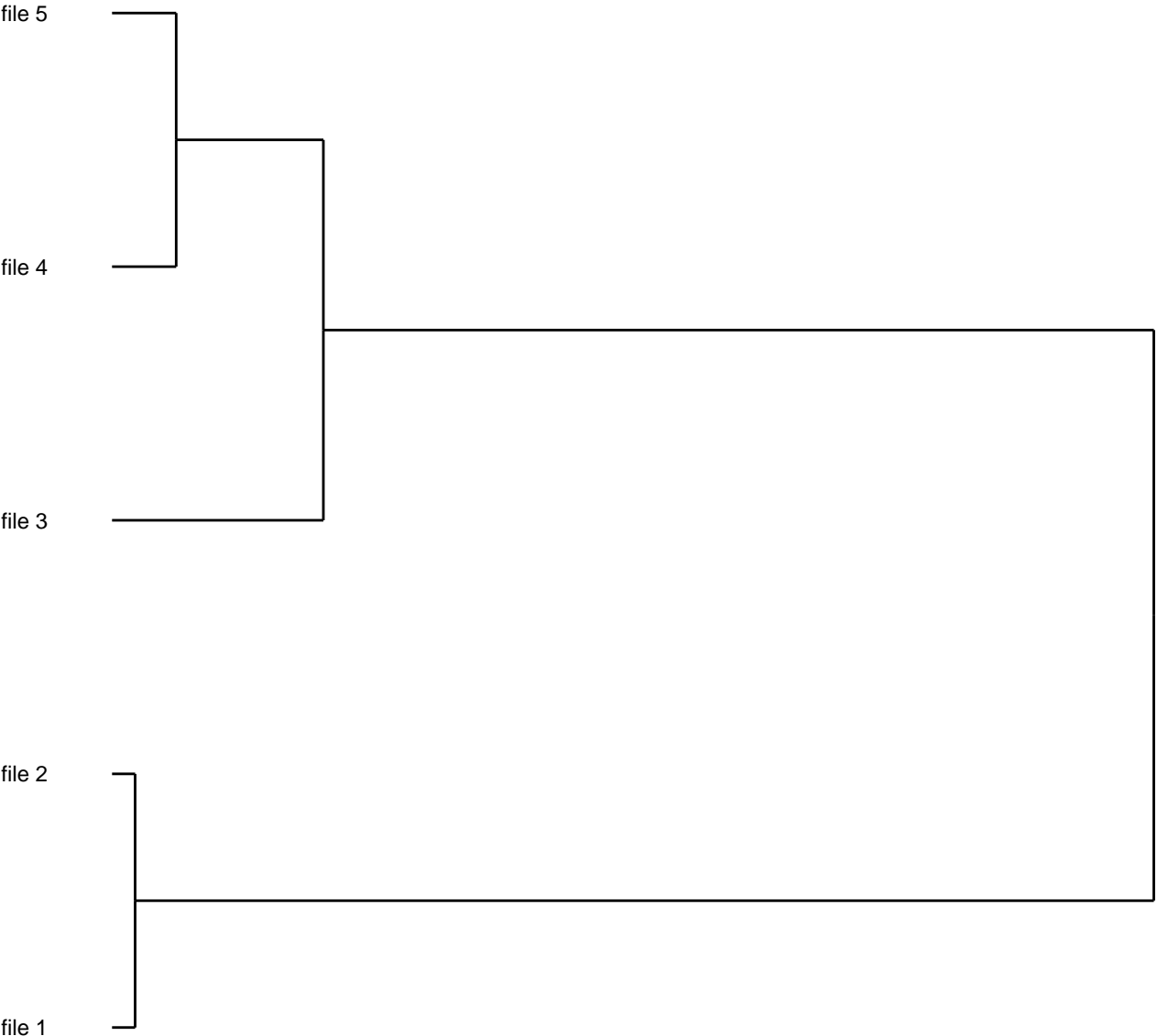
alignment reference: Toni\_20140521\_GM\_QC\_01



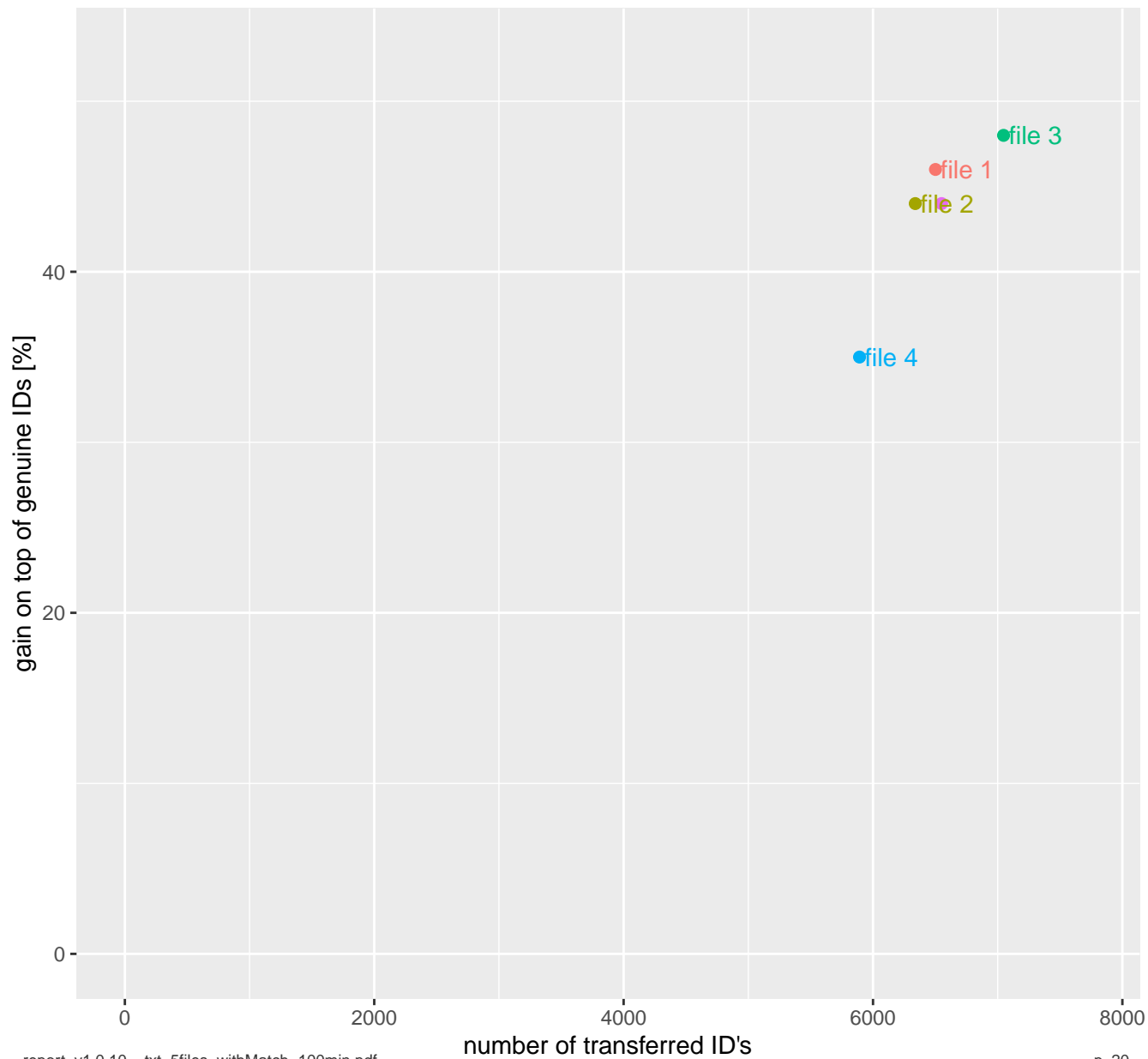
# EVD: MBR – ID Transfer



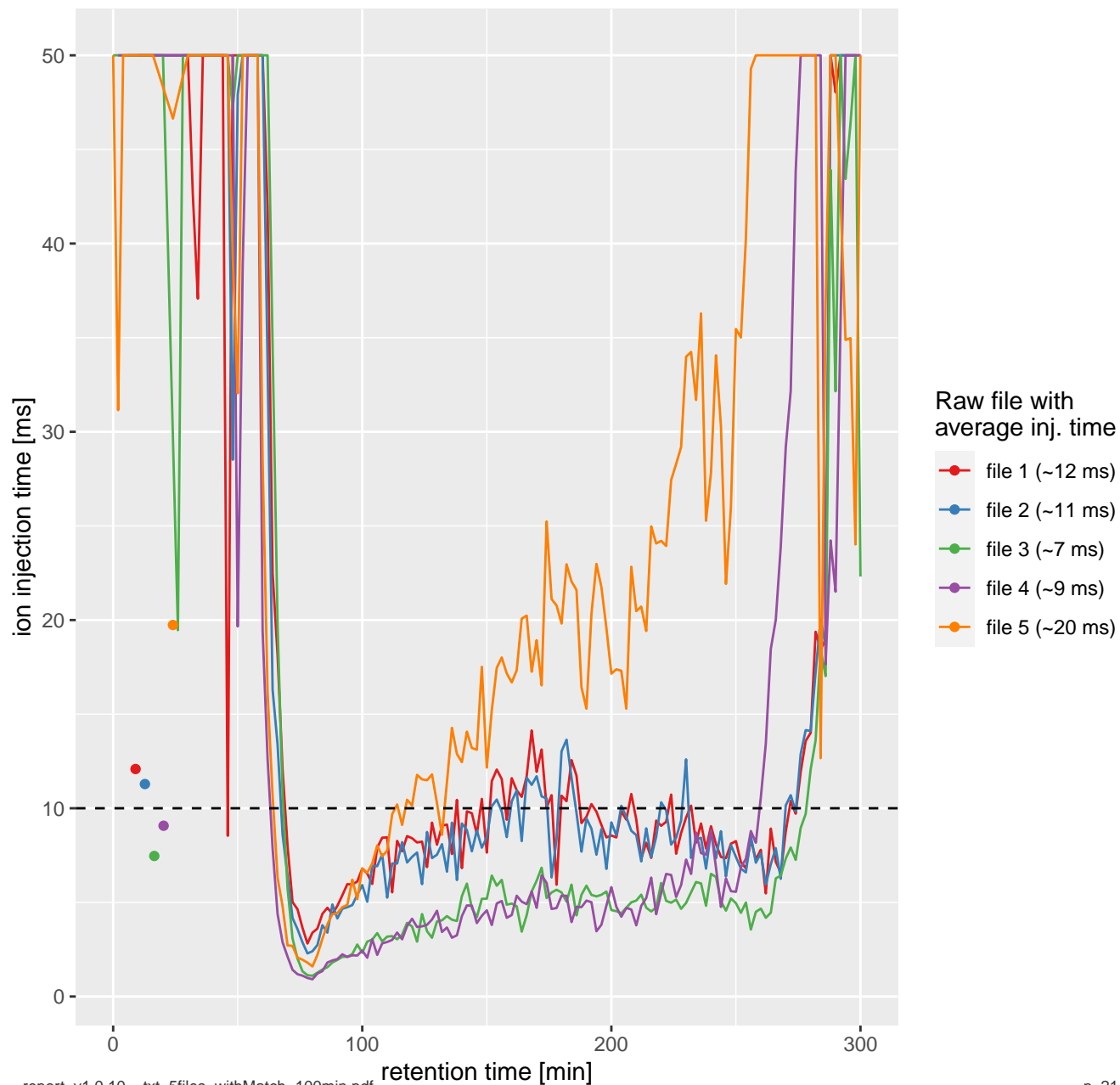
[experimental] EVD: Clustering Tree of Raw files  
by Correlation of Corrected Retention Times



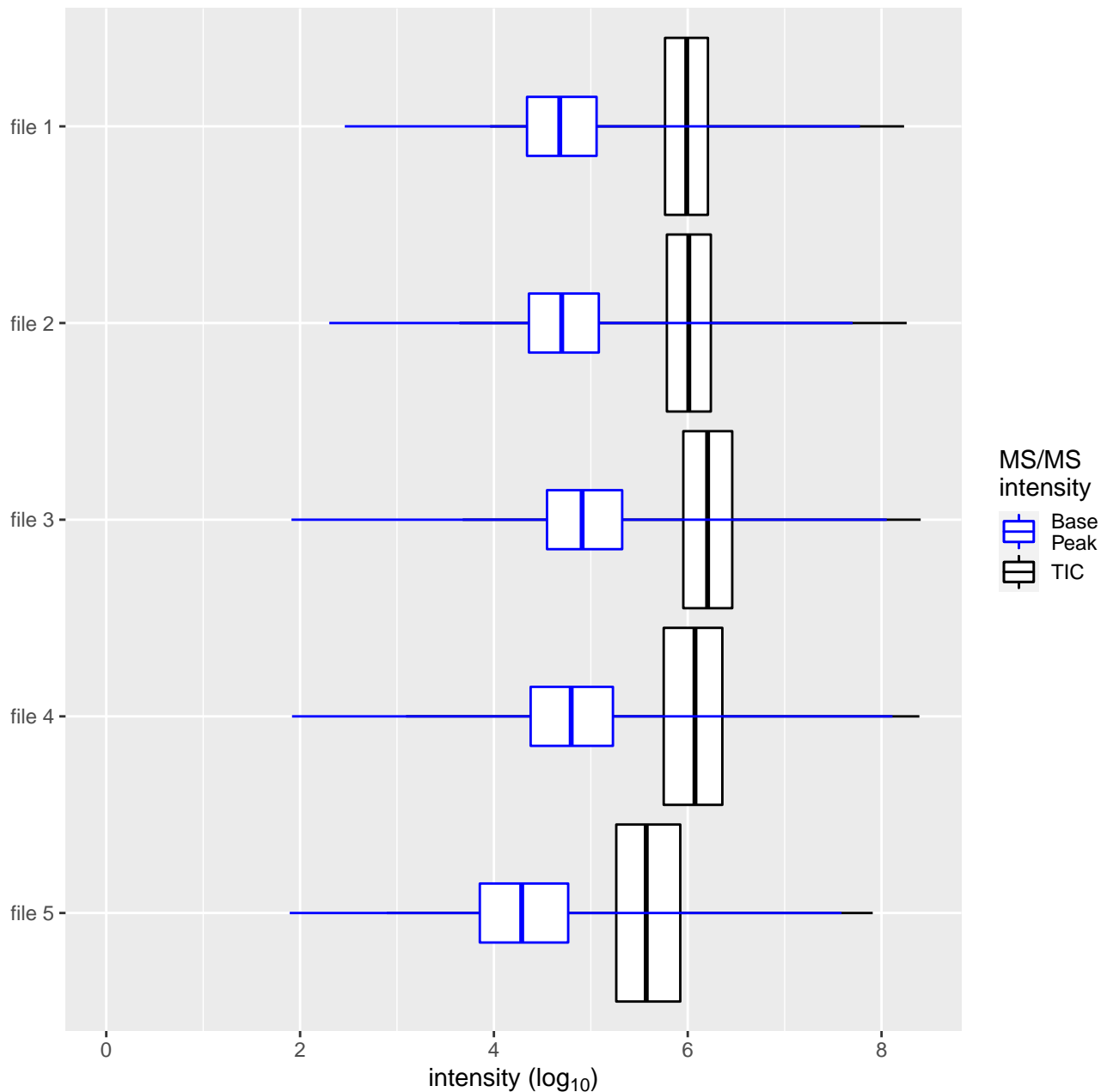
## EVD: Peptides inferred by MBR



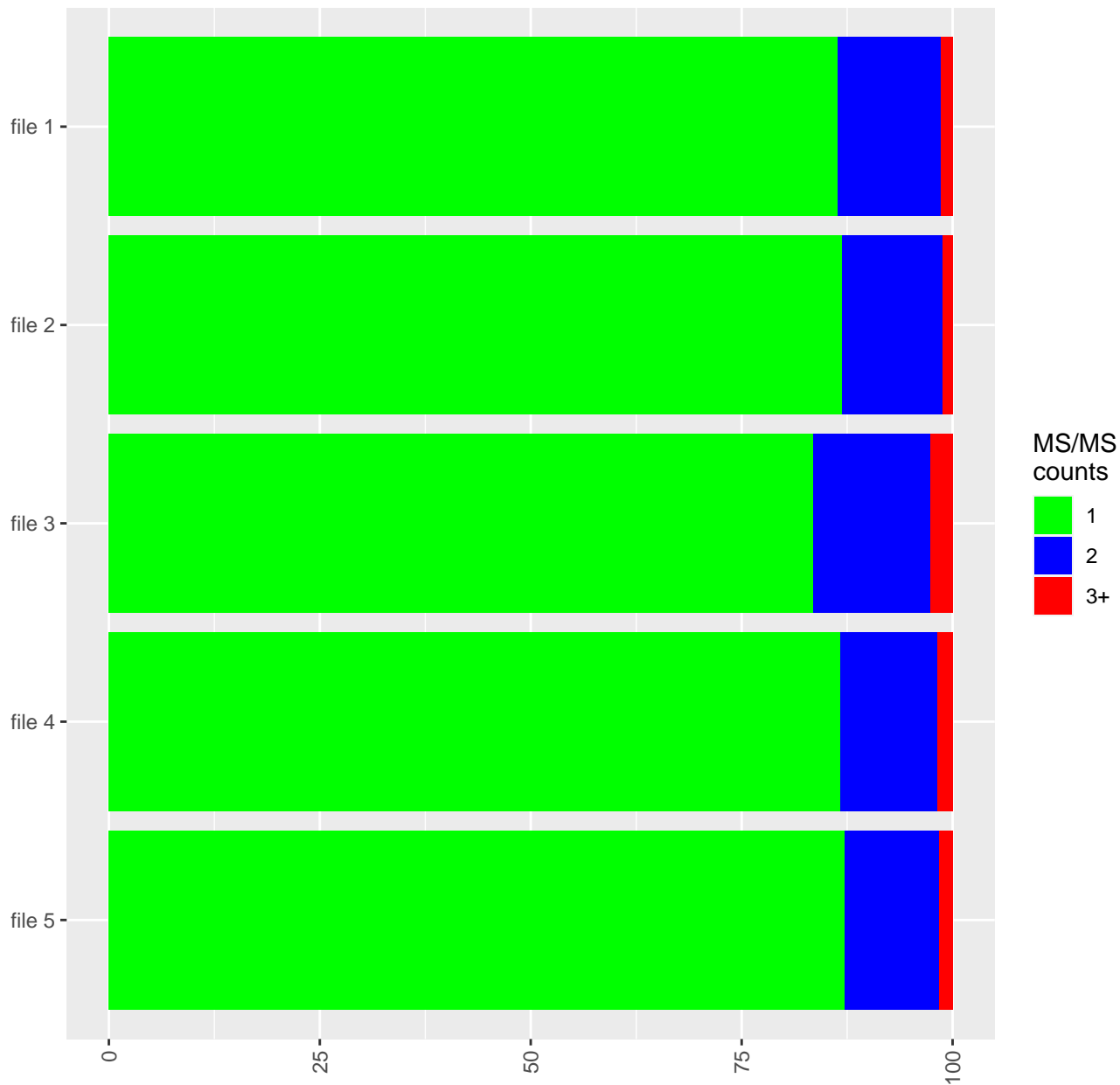
# MSMSscans: Ion Injection Time over RT



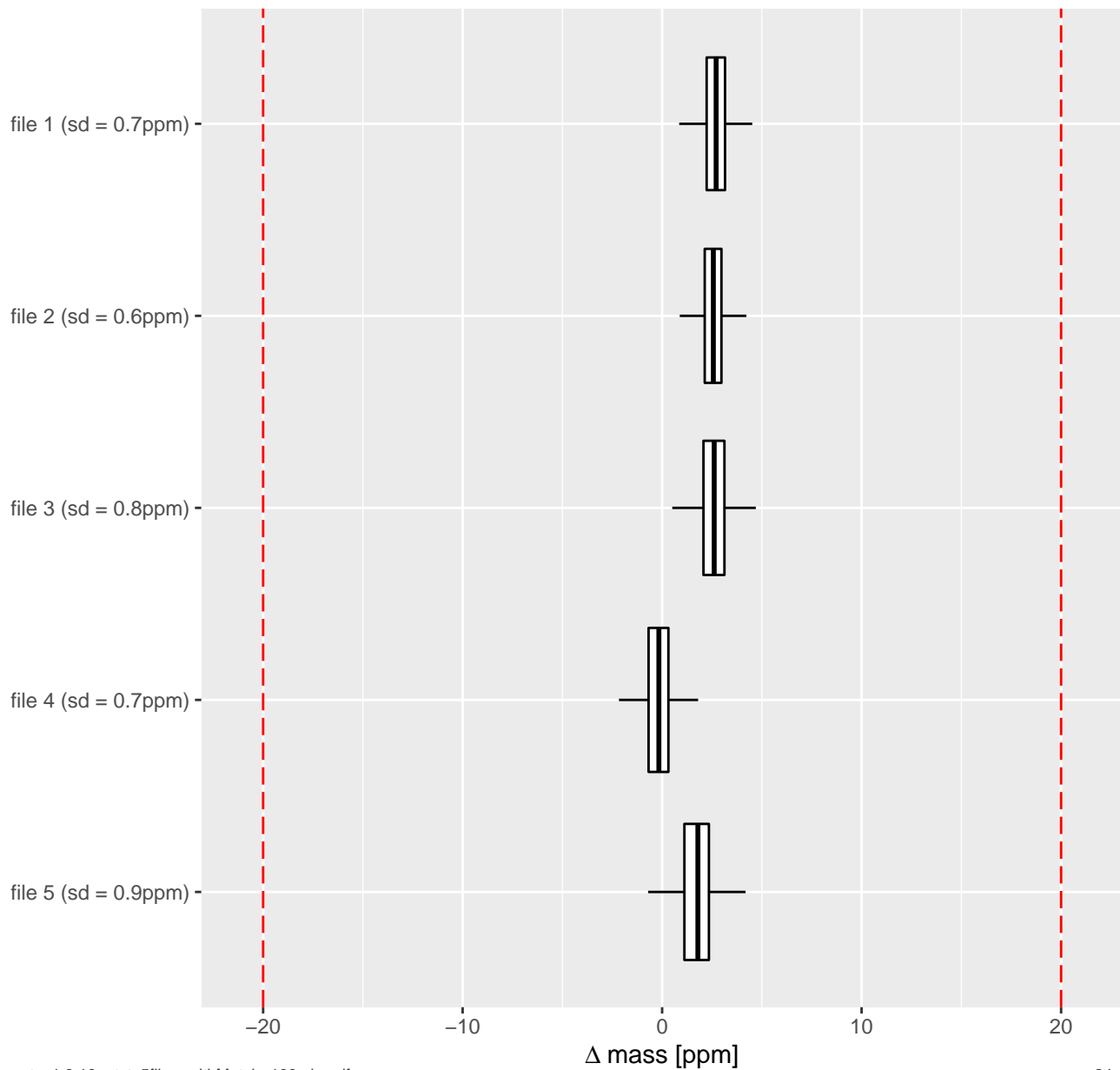
# [experimental] MSMSscans: MS/MS intensity



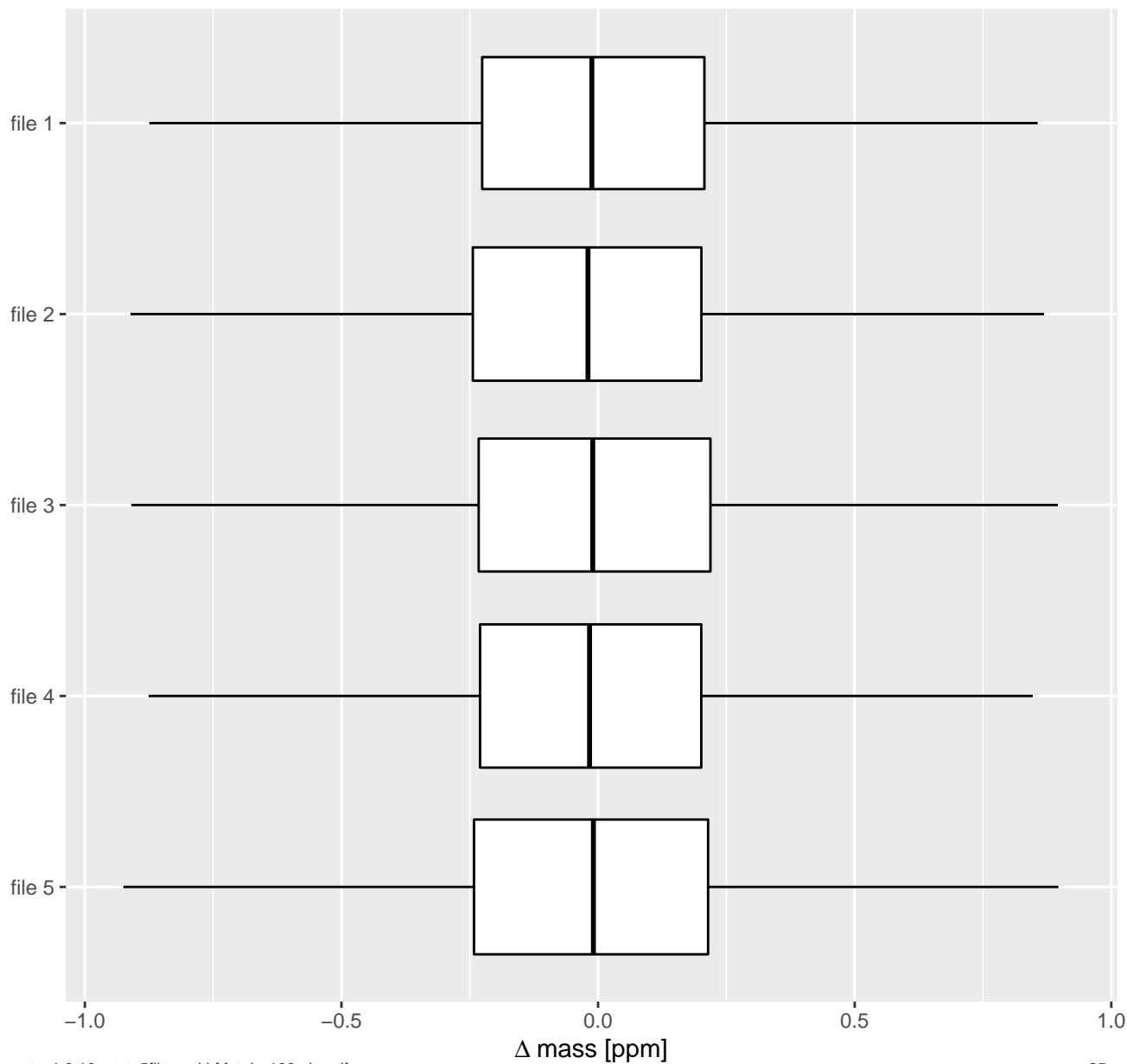
## EVD: Oversampling (MS/MS counts per 3D-peak)



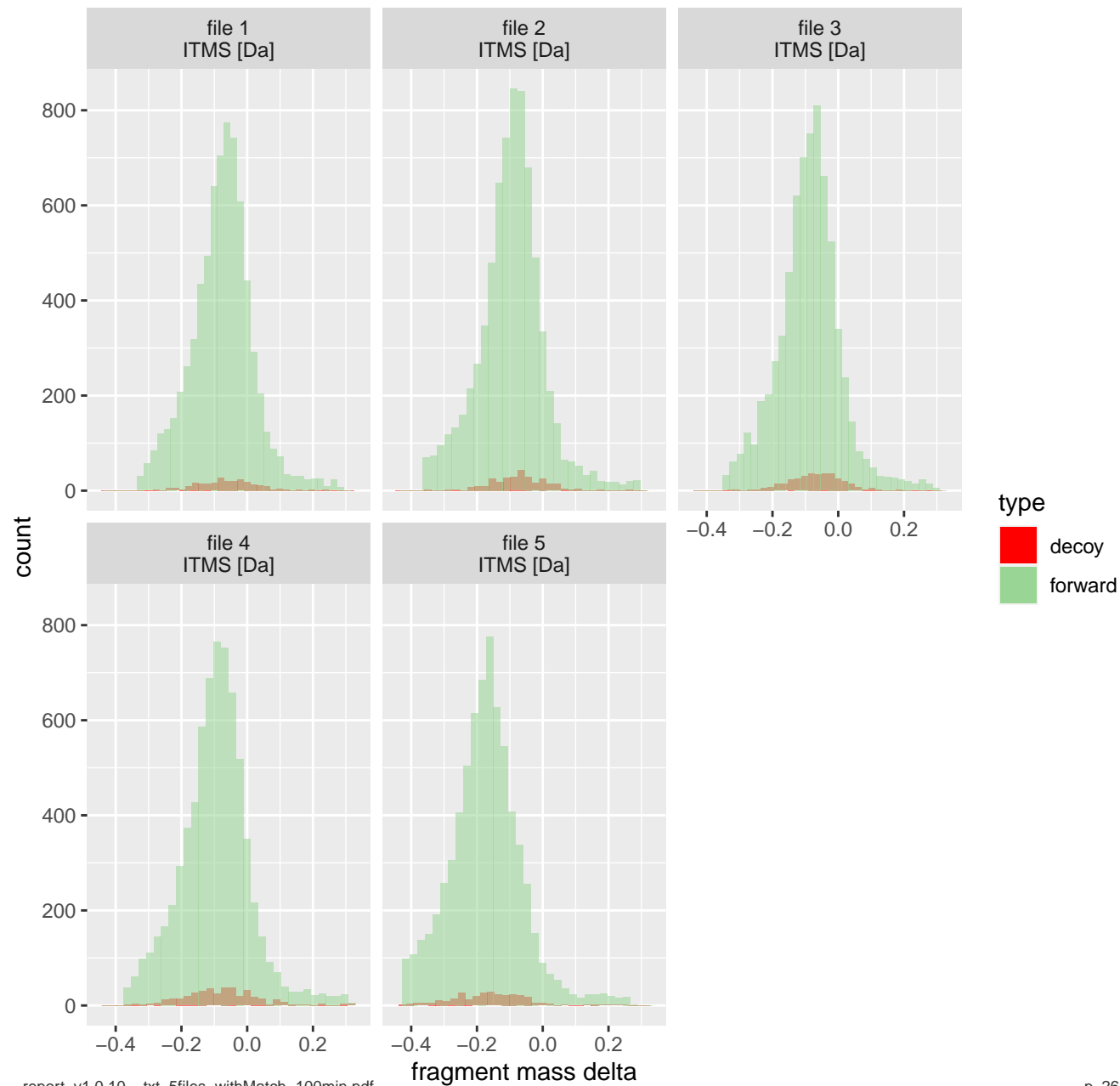
# EVD: Uncalibrated mass error



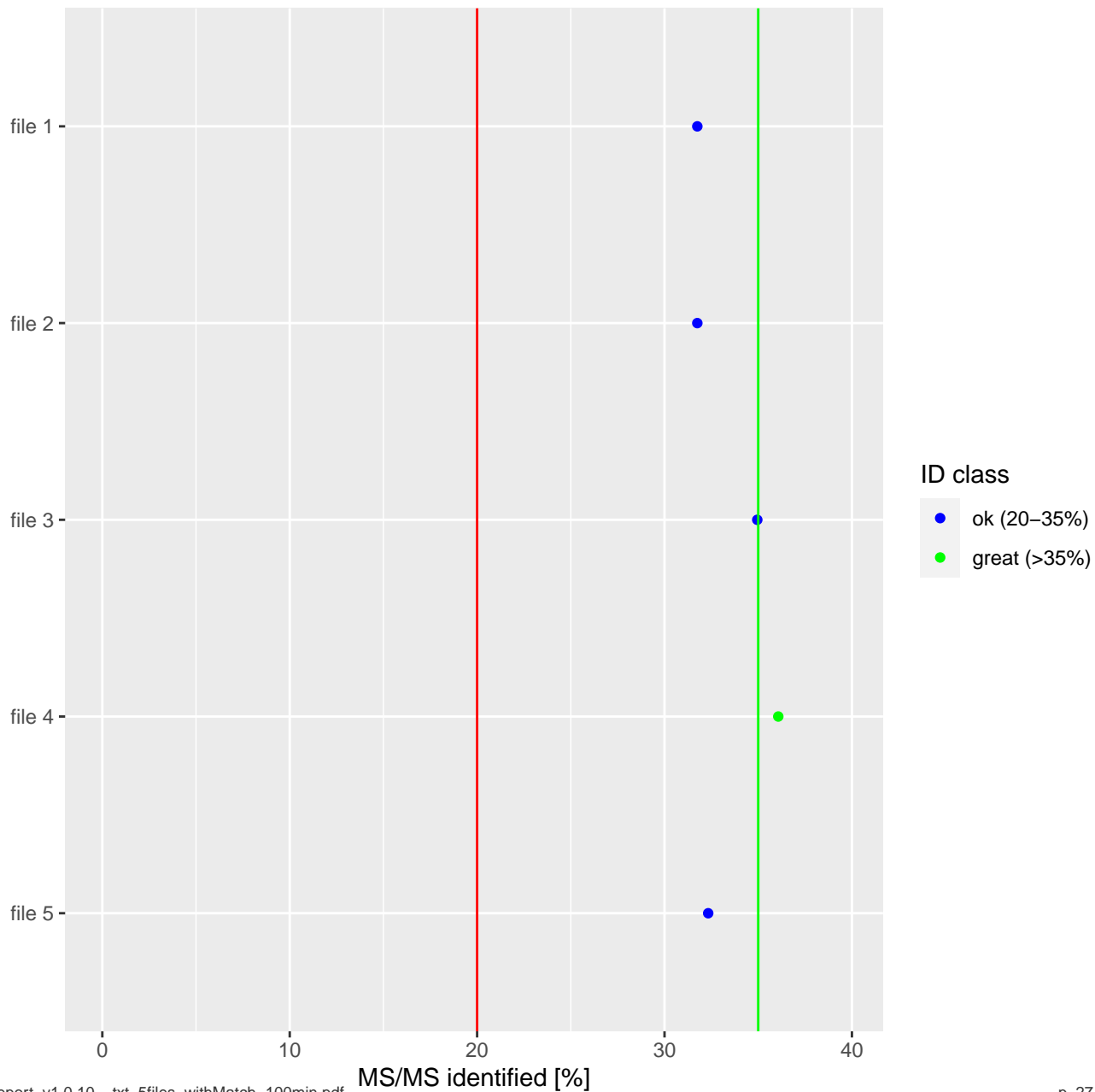
# EVD: Calibrated mass error



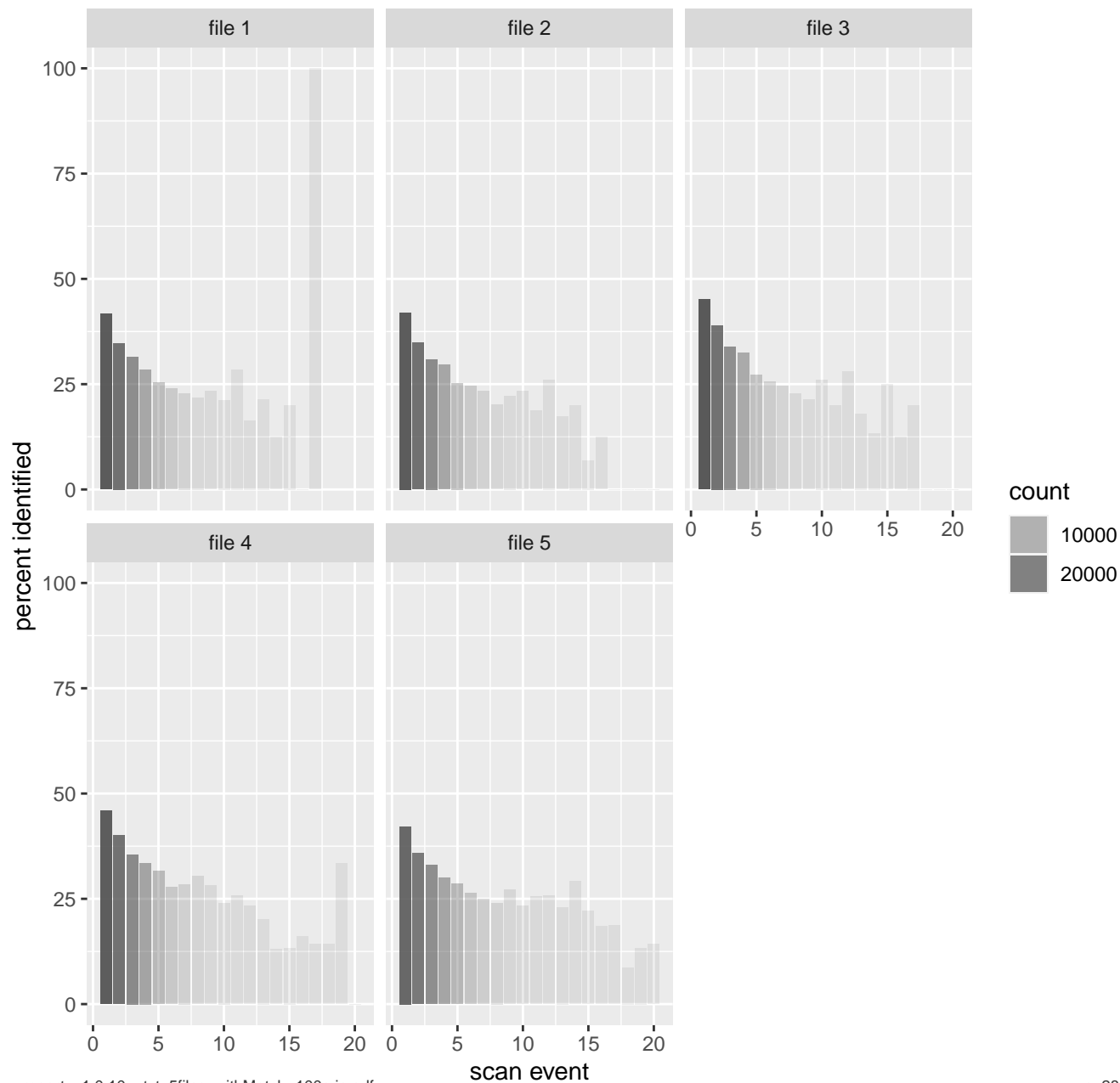
# MSMS: Fragment mass errors per Raw file



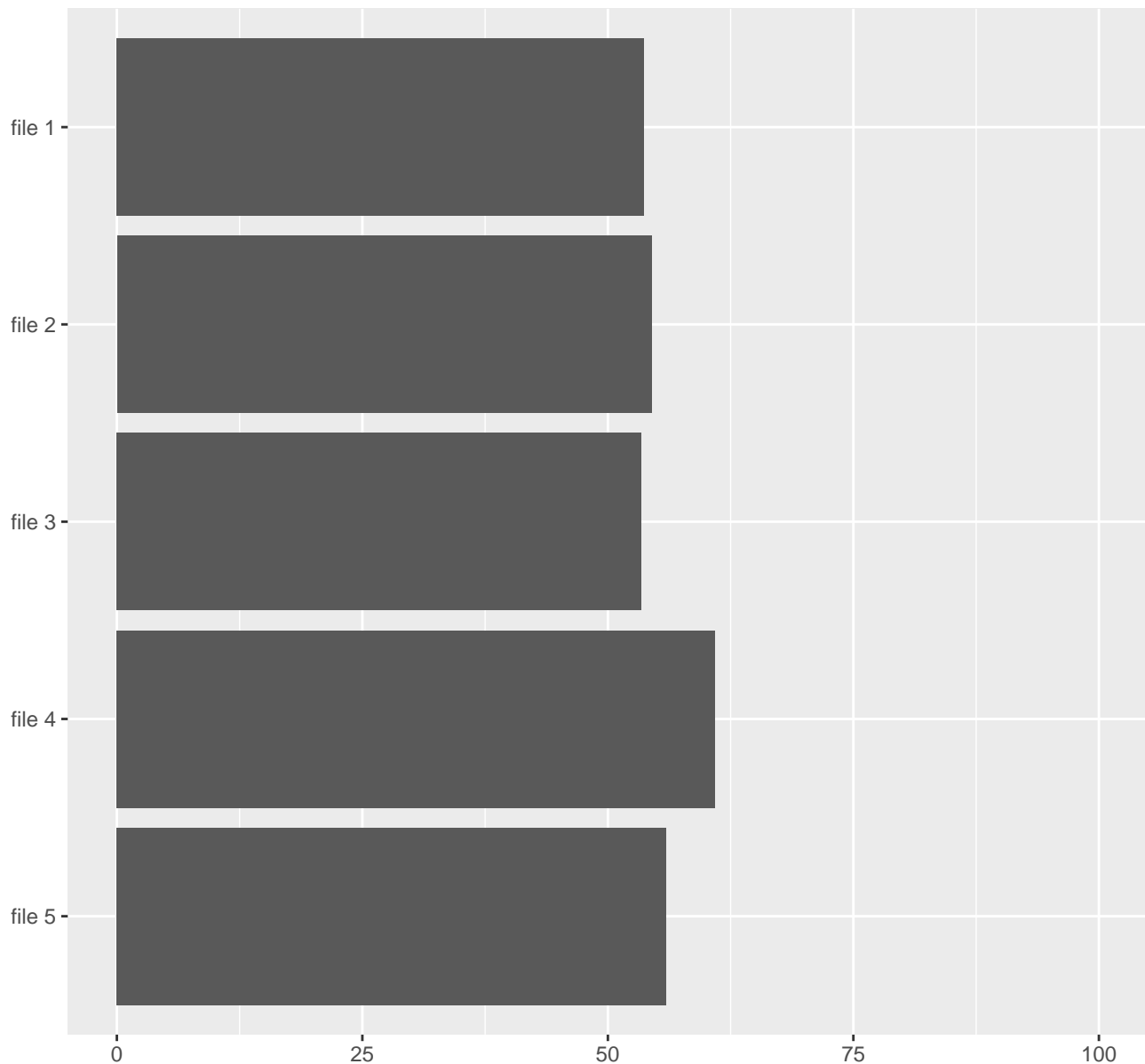
# SM: MS/MS identified per Raw file

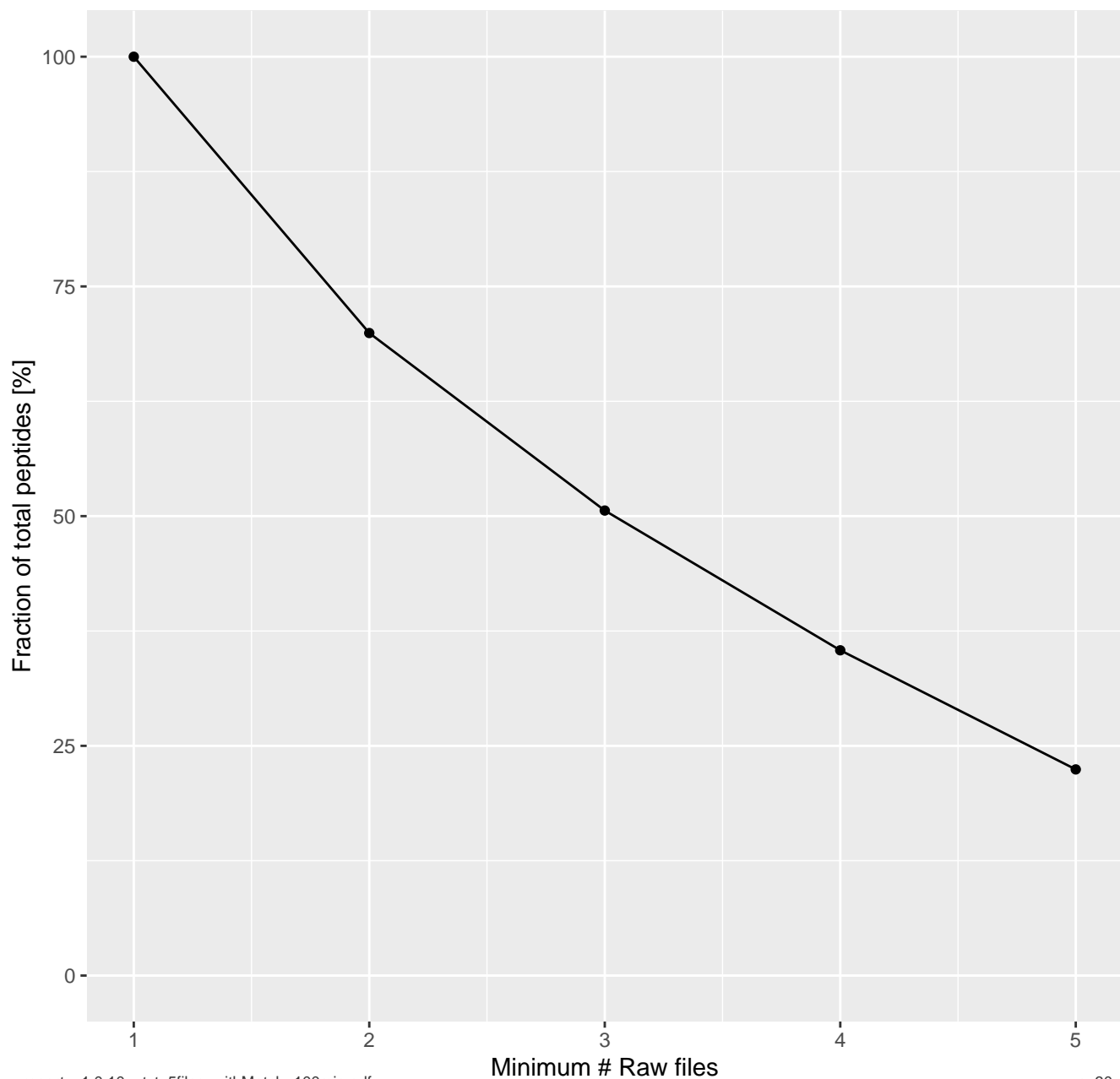


# MSMSScans: TopN % identified over N

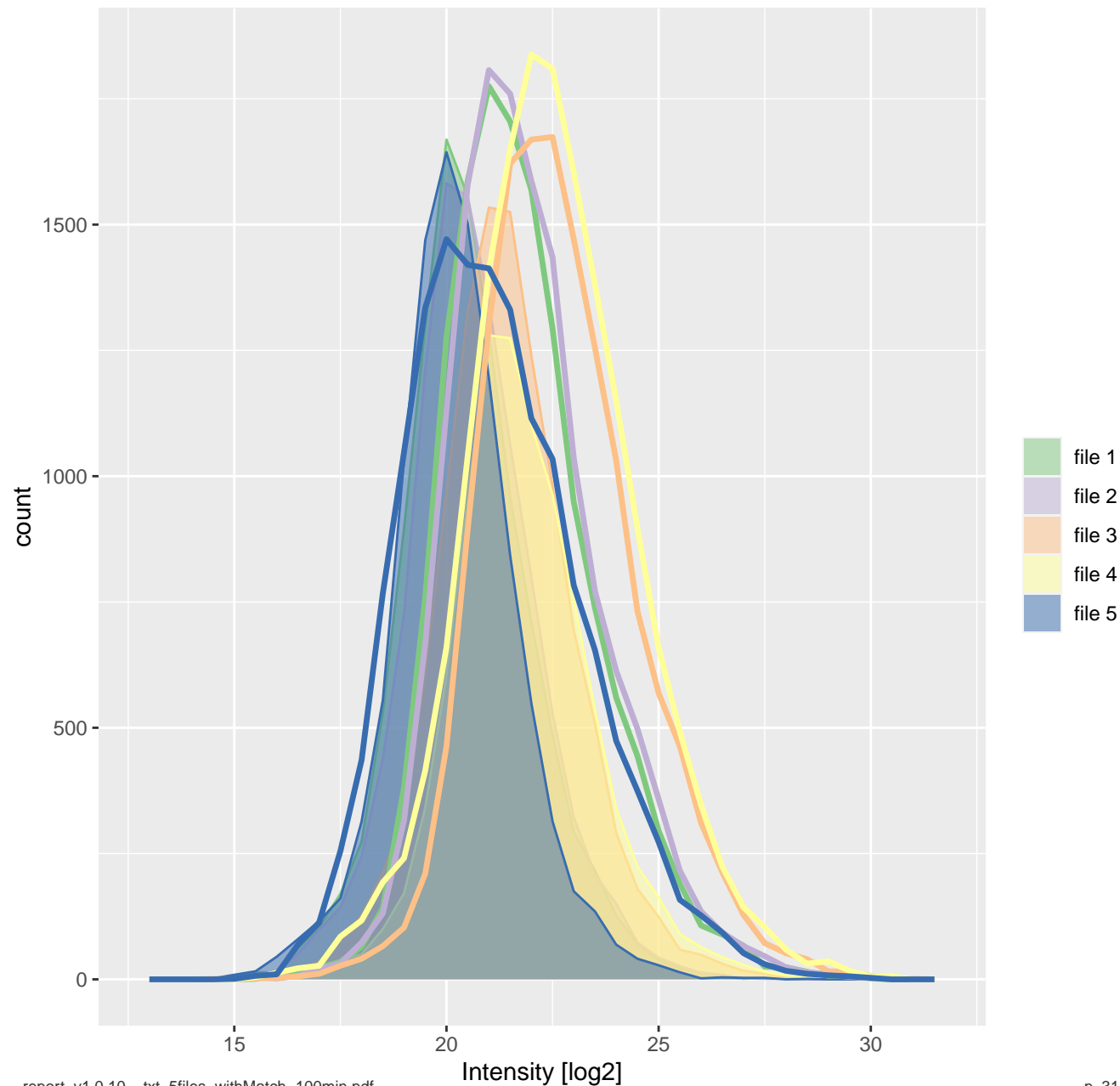


[experimental] EVD: Non-Missing Peptides  
compared to all peptides seen in experiment

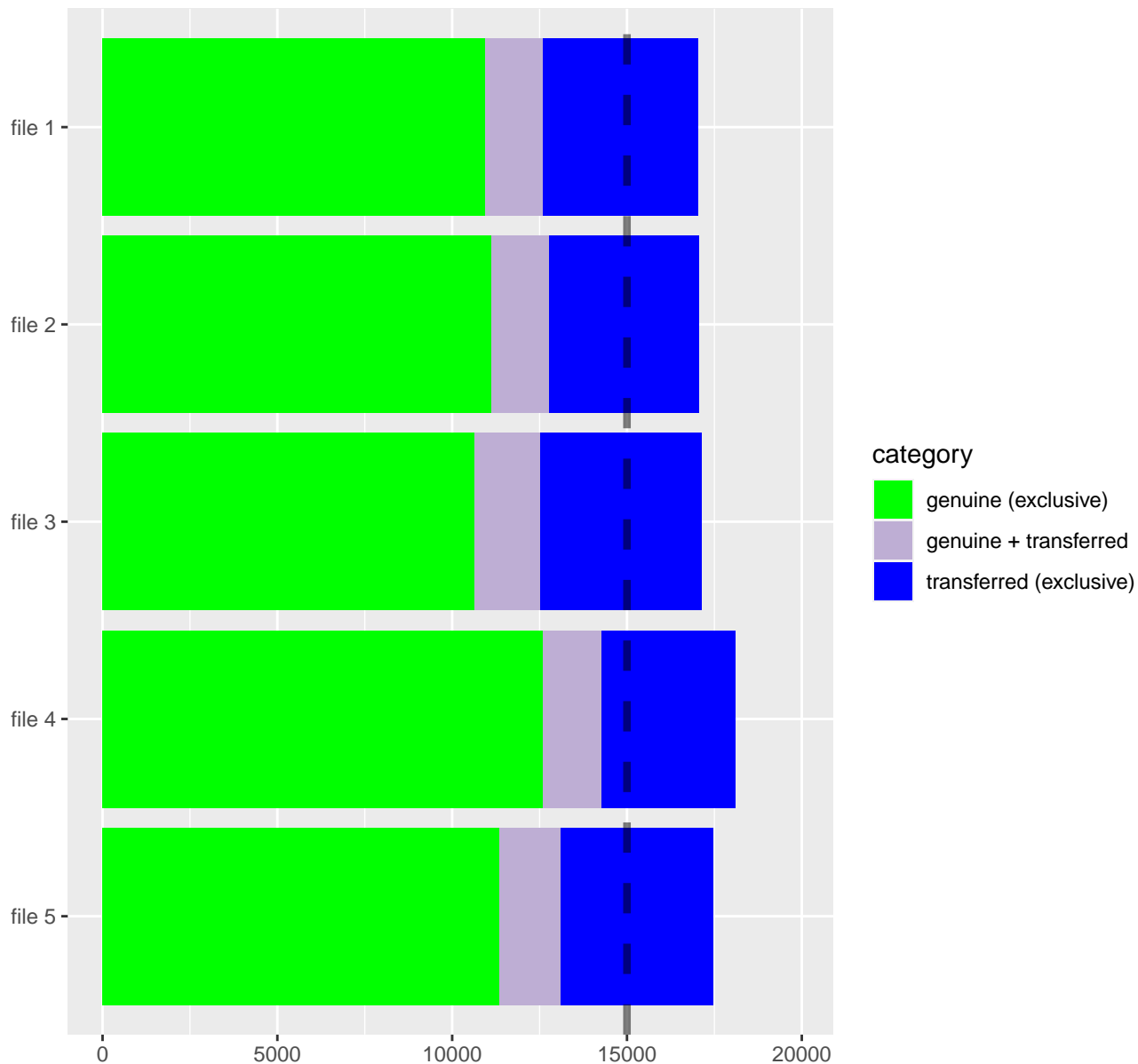




# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



## EVD: Peptide ID count



# EVD: ProteinGroups count

MBR gain: +14%

