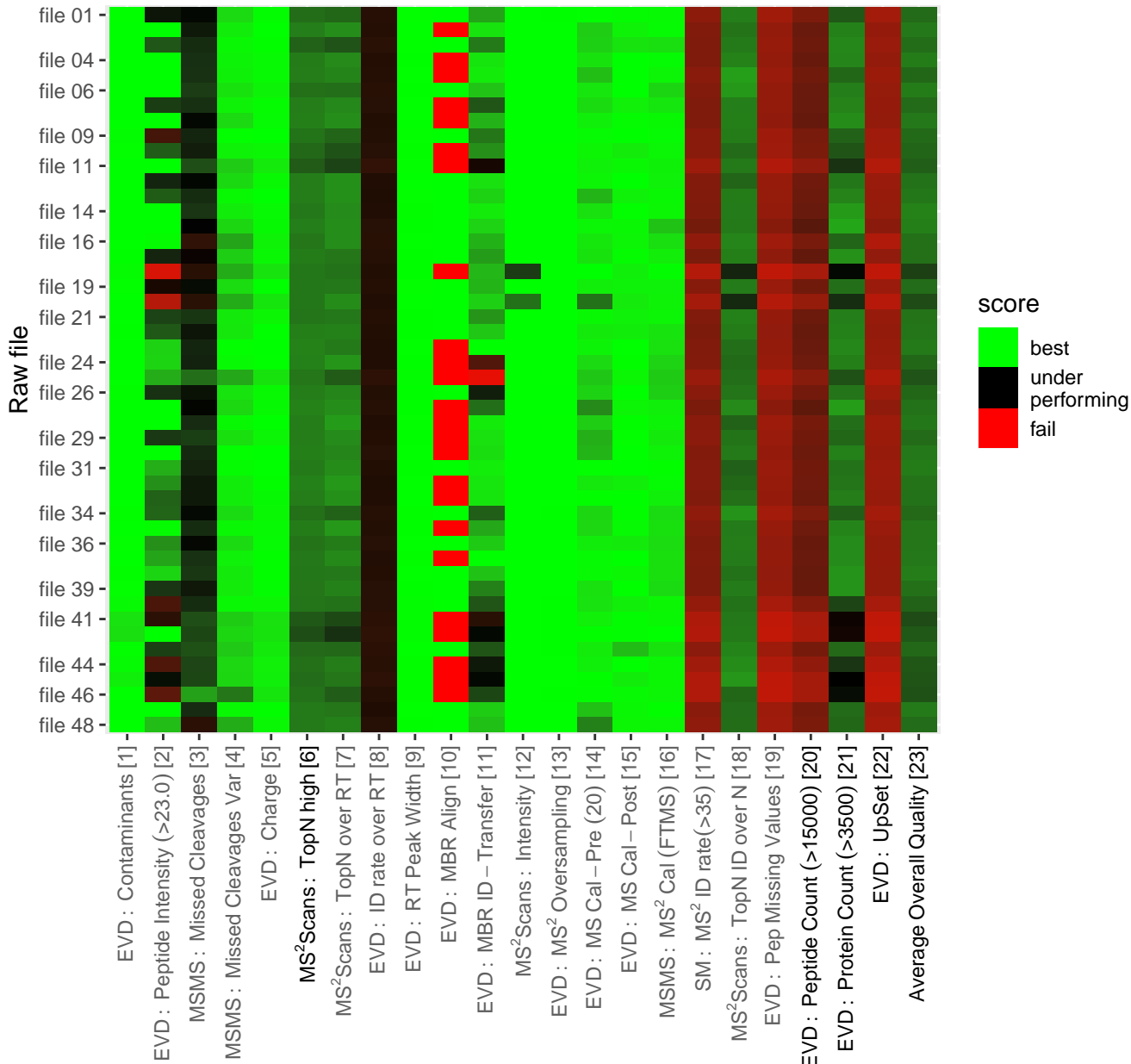


# Performance overview



# 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
drake_zsychev_18366_20211124_FAIMS_totalPr_26_s96_3408.raw.thermo	file 01	..26_s96_3408.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_25_s96_2583.raw.thermo	file 02	..25_s96_2583.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_24_s93_4571.raw.thermo	file 03	..24_s93_4571.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_21_s77CR_5496.raw.thermo	file 04	..21_s77CR_5496.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_20_s77CR_2042.raw.thermo	file 05	..20_s77CR_2042.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_19_s77CR_1018.raw.thermo	file 06	..19_s77CR_1018.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_18_s77_4327.raw.thermo	file 07	..18_s77_4327.r..mo
jdake_zsychev_18366_20211124_FAIMS_totalPr_16_s77_949.raw.thermo	file 08	..16_s77_949.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_15_s70CR_6134.raw.thermo	file 09	..15_s70CR_6134.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_14_s70CR_5206.raw.thermo	file 10	..14_s70CR_5206.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_13_s70CR_1015.raw.thermo	file 11	..13_s70CR_1015.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_11_s70_2099.raw.thermo	file 12	..11_s70_2099.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_10_s70_1205.raw.thermo	file 13	..10_s70_1205.r..mo
jdake_zsychev_18366_20211124_FAIMS_totalPr_9_s49_6052.raw.thermo	file 14	..9_s49_6052.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_08_s49_4385.raw.thermo	file 15	..08_s49_4385.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_07_s49_1261.raw.thermo	file 16	..07_s49_1261.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_06_s35CR_6378.raw.thermo	file 17	..06_s35CR_6378.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_05_s35CR_5490.raw.thermo	file 18	..05_s35CR_5490.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_04_s35CR_1339.raw.thermo	file 19	..04_s35CR_1339.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_03_s35_3853.raw.thermo	file 20	..03_s35_3853.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_02_s35_2564.raw.thermo	file 21	..02_s35_2564.r..mo
jdake_zsychev_18366_20211124_FAIMS_totalPr_01_s35_810.raw.thermo	file 22	..01_s35_810.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_54_s208_1_6719.raw.thermo	file 23	..54_s208_1_6719.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_53_s208_1_4865.raw.thermo	file 24	..53_s208_1_4865.r..mo

# 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
ie_zsychev_18366_20211124_FAIMS_totalPr_52_s208_1_4107.raw.thermo	file 25	..52_s208_1_4107.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_50_s173_1_2824.raw.thermo	file 26	..50_s173_1_2824.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_49_s173_1_2032.raw.thermo	file 27	..49_s173_1_2032.r..mo
ə_zsychev_18366_20211124_FAIMS_totalPr_48_s167CR_4675.raw.thermo	file 28	..48_s167CR_4675.r..mo
ə_zsychev_18366_20211124_FAIMS_totalPr_47_s167CR_1732.raw.thermo	file 29	..47_s167CR_1732.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_46_s167CR_964.raw.thermo	file 30	..46_s167CR_964.r..mo
rake_zsychev_18366_20211124_FAIMS_totalPr_45_s167_4895.raw.thermo	file 31	..45_s167_4895.r..mo
rake_zsychev_18366_20211124_FAIMS_totalPr_44_s167_2473.raw.thermo	file 32	..44_s167_2473.r..mo
rake_zsychev_18366_20211124_FAIMS_totalPr_43_s167_1532.raw.thermo	file 33	..43_s167_1532.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_42_s145_2_2467.raw.thermo	file 34	..42_s145_2_2467.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_41_s145_2_1396.raw.thermo	file 35	..41_s145_2_1396.r..mo
ike_zsychev_18366_20211124_FAIMS_totalPr_40_s145_2_829.raw.thermo	file 36	..40_s145_2_829.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_39_s145_1_2519.raw.thermo	file 37	..39_s145_1_2519.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_38_s145_1_1709.raw.thermo	file 38	..38_s145_1_1709.r..mo
ie_zsychev_18366_20211124_FAIMS_totalPr_37_s145_1_1003.raw.thermo	file 39	..37_s145_1_1003.r..mo
ə_zsychev_18366_20211124_FAIMS_totalPr_36_s105CR_4079.raw.thermo	file 40	..36_s105CR_4079.r..mo
ə_zsychev_18366_20211124_FAIMS_totalPr_35_s105CR_3738.raw.thermo	file 41	..35_s105CR_3738.r..mo
ə_zsychev_18366_20211124_FAIMS_totalPr_34_s105CR_2894.raw.thermo	file 42	..34_s105CR_2894.r..mo
rake_zsychev_18366_20211124_FAIMS_totalPr_33_s105_4539.raw.thermo	file 43	..33_s105_4539.r..mo
rake_zsychev_18366_20211124_FAIMS_totalPr_32_s105_4409.raw.thermo	file 44	..32_s105_4409.r..mo
drake_zsychev_18366_20211124_FAIMS_totalPr_31_s105_754.raw.thermo	file 45	..31_s105_754.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_30_s96CR_4465.raw.thermo	file 46	..30_s96CR_4465.r..mo
ke_zsychev_18366_20211124_FAIMS_totalPr_29_s96CR_4324.raw.thermo	file 47	..29_s96CR_4324.r..mo
ake_zsychev_18366_20211124_FAIMS_totalPr_28_s96CR_789.raw.thermo	file 48	..28_s96CR_789.r..mo

## PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	MS/MS deisotoping tolerance ..	Da
Advanced site intensities	True	MS/MS deisotoping tolerance ..	7
Alignment ion mobility windo..	1	MS/MS deisotoping tolerance ..	ppm
Alignment time window [min]	20	MS/MS dependent losses (FTMS..	True
Calculate peak properties	False	MS/MS dependent losses (ITMS..	True
Combined folder location		MS/MS dependent losses (TOF)	True
Da interval. (FTMS)	100	MS/MS dependent losses (Unkn..	True
Da interval. (ITMS)	100	MS/MS higher charges (FTMS)	True
Da interval. (TOF)	100	MS/MS higher charges (ITMS)	True
Da interval. (Unknown)	100	MS/MS higher charges (TOF)	True
Date of writing	03/22/2023 01:48:18	MS/MS higher charges (Unknow..	True
Decoy mode	revert	MS/MS recalibration (FTMS)	False
Disable MD5	False	MS/MS recalibration (ITMS)	False
Discard unmodified counterpa..	True	MS/MS recalibration (TOF)	False
Epsilon score for mutations		MS/MS recalibration (Unknown..	False
Evaluate variant peptides se..	True	MS/MS tol. (FTMS)	20 ppm
Find dependent peptides	False	MS/MS tol. (ITMS)	0.5 Da
Fixed andromeda index folder		MS/MS tol. (TOF)	40 ppm
iBAQ	False	MS/MS tol. (Unknown)	20 ppm
iBAQ log fit	False	MS/MS water loss (FTMS)	True
Include contaminants	True	MS/MS water loss (ITMS)	True
Label min. ratio count	2	MS/MS water loss (TOF)	True
Machine name	cn0272	MS/MS water loss (Unknown)	True
Main search max. combination..	200	Peptides used for protein qu..	Razor
Match between runs	True	Protein FDR	0.01
Match ion mobility window [i..	0.05	PSM FDR	0.01
Match unidentified features	True	PSM FDR Crosslink	0.01

/panfs/roc/galaxy/PRODUCTION/database/files/001/498/dataset\_1498072.dat

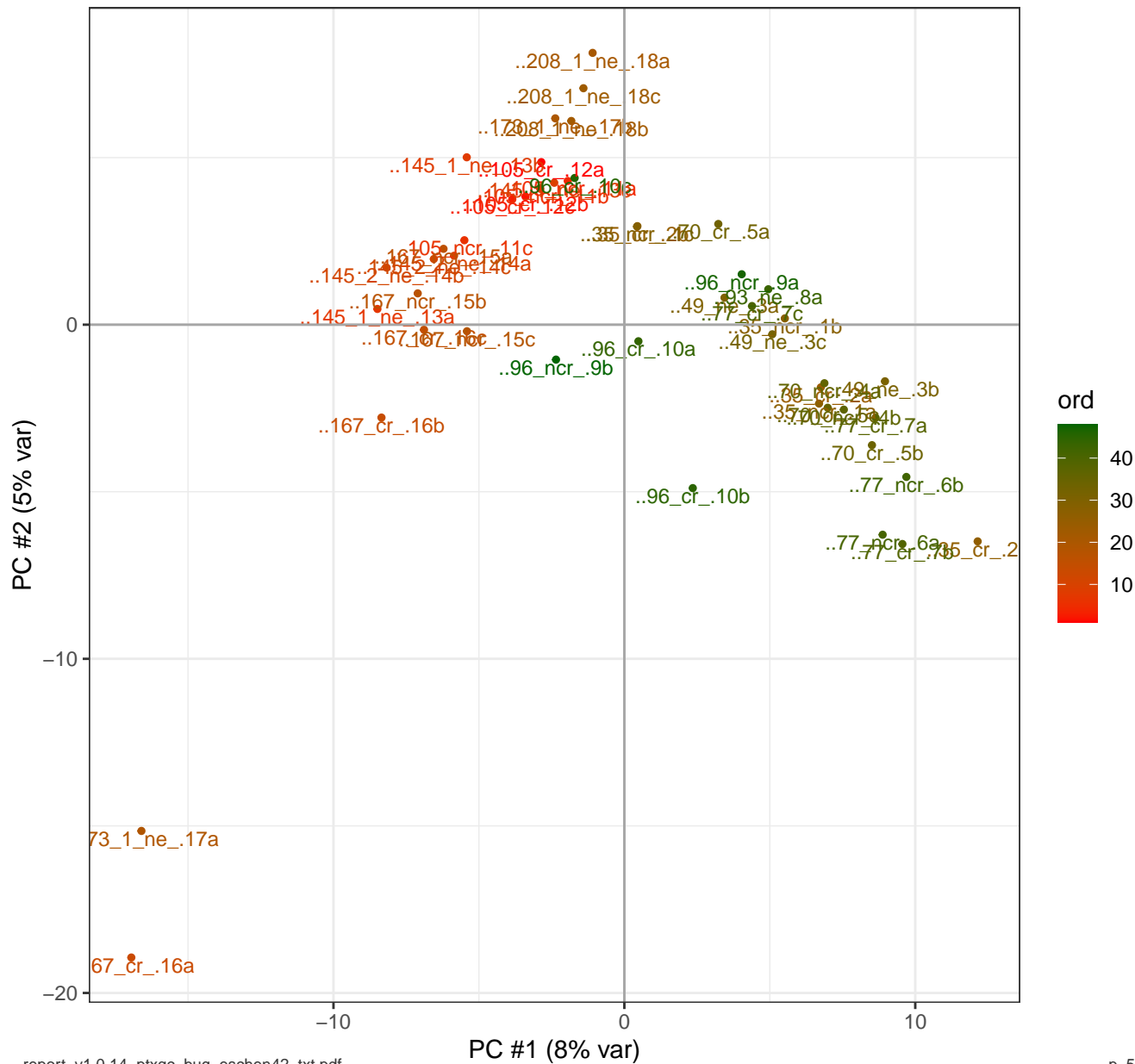
## PAR: parameters

parameter	value	parameter	value
Matching time window [min]	5	Razor protein FDR	True
Max mods in site table	3	Require MS/MS for LFQ compar..	True
Max. peptide length for unsp..	25	Second peptides	True
Max. peptide mass [Da]	4600	Separate LFQ in parameter gr..	False
Min. delta score for modifie..	6	Site FDR	0.01
Min. delta score for unmodif..	0	Site tables	Oxidation (M)Sites.txt Phospho (STY)Sites.txt
Min. peptide Length	9	Stabilize large LFQ ratios	True
Min. peptide length for unsp..	8	Top MS/MS peaks per Da inter..	12
Min. peptides	1	Top MS/MS peaks per Da inter..	8
Min. razor peptides	1	Top MS/MS peaks per Da inter..	10
Min. score for modified pept..	40	Top MS/MS peaks per Da inter..	12
Min. score for unmodified pe..	0	Use delta score	False
Min. unique peptides	0	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (FTMS)	True	Use only unmodified peptides..	False
MS/MS ammonia loss (ITMS)	True	User name	galaxy
MS/MS ammonia loss (TOF)	True	Variation mode	None
MS/MS ammonia loss (Unknown)	True	Version	1.6.17.0
MS/MS deisotoping (FTMS)	True	Write accumulatedPasefMsmsSc..	False
MS/MS deisotoping (ITMS)	False	Write allPeptides table	True
MS/MS deisotoping (TOF)	True	Write DIA fragments table	False
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
MS/MS deisotoping tolerance ..	0.01		

/panfs/roc/galaxy/PRODUCTION/database/files/001/498/dataset\_1498072.dat

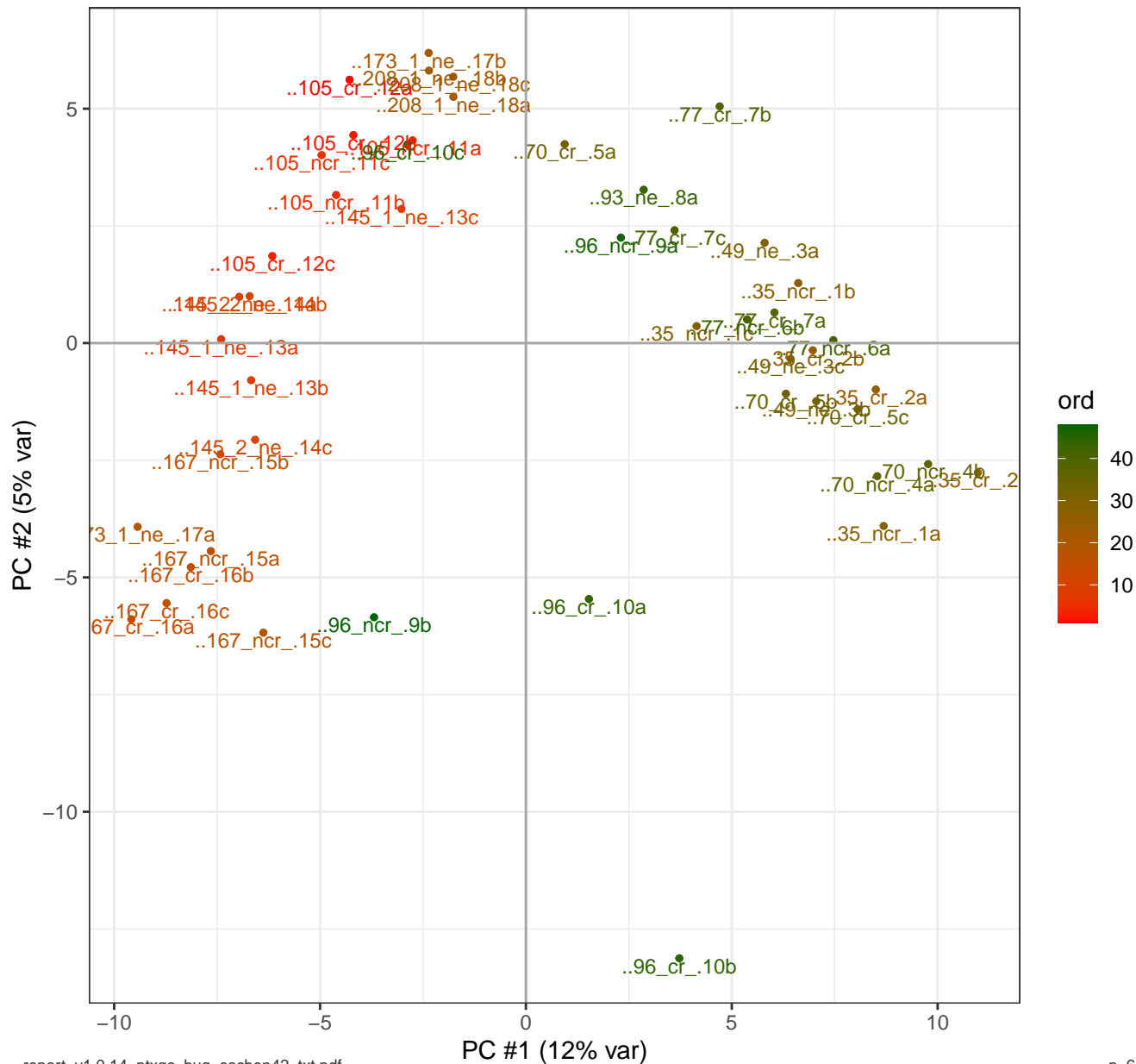
# PG: PCA of 'raw intensity'

(excludes contaminants)

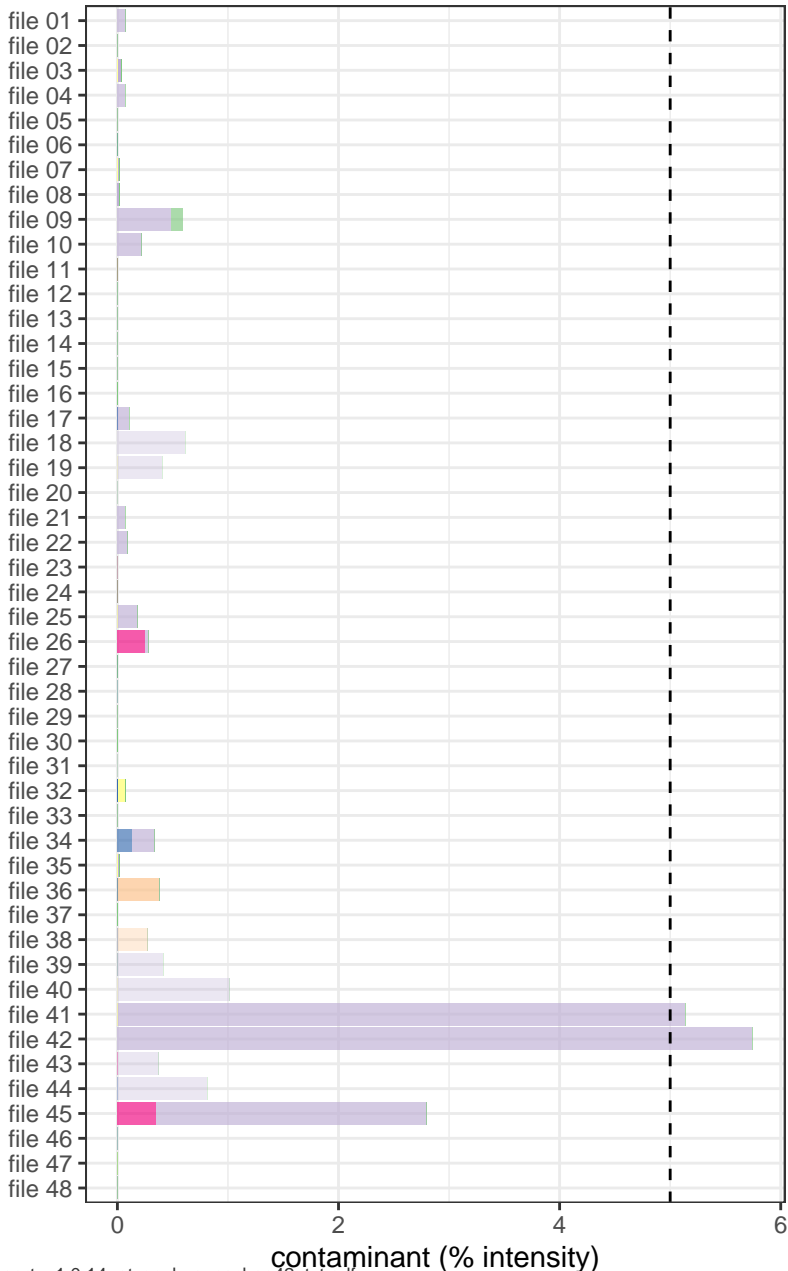


# PG: PCA of 'lfq intensity'

(excludes contaminants)



# EVD: Top5 Contaminants per Raw file



## Protein

- other
- CON\_\_P01966
- sp|P13647|K2C...;CON\_\_P13647;..
- sp|P97861|KRT...;tr|E9Q1Y9|E9Q...;
- sp|Q6IMF0|KRT...;tr|F5GYI5|F5G...;
- tr|C9JFR7|C9J...;generic|con\_C...;

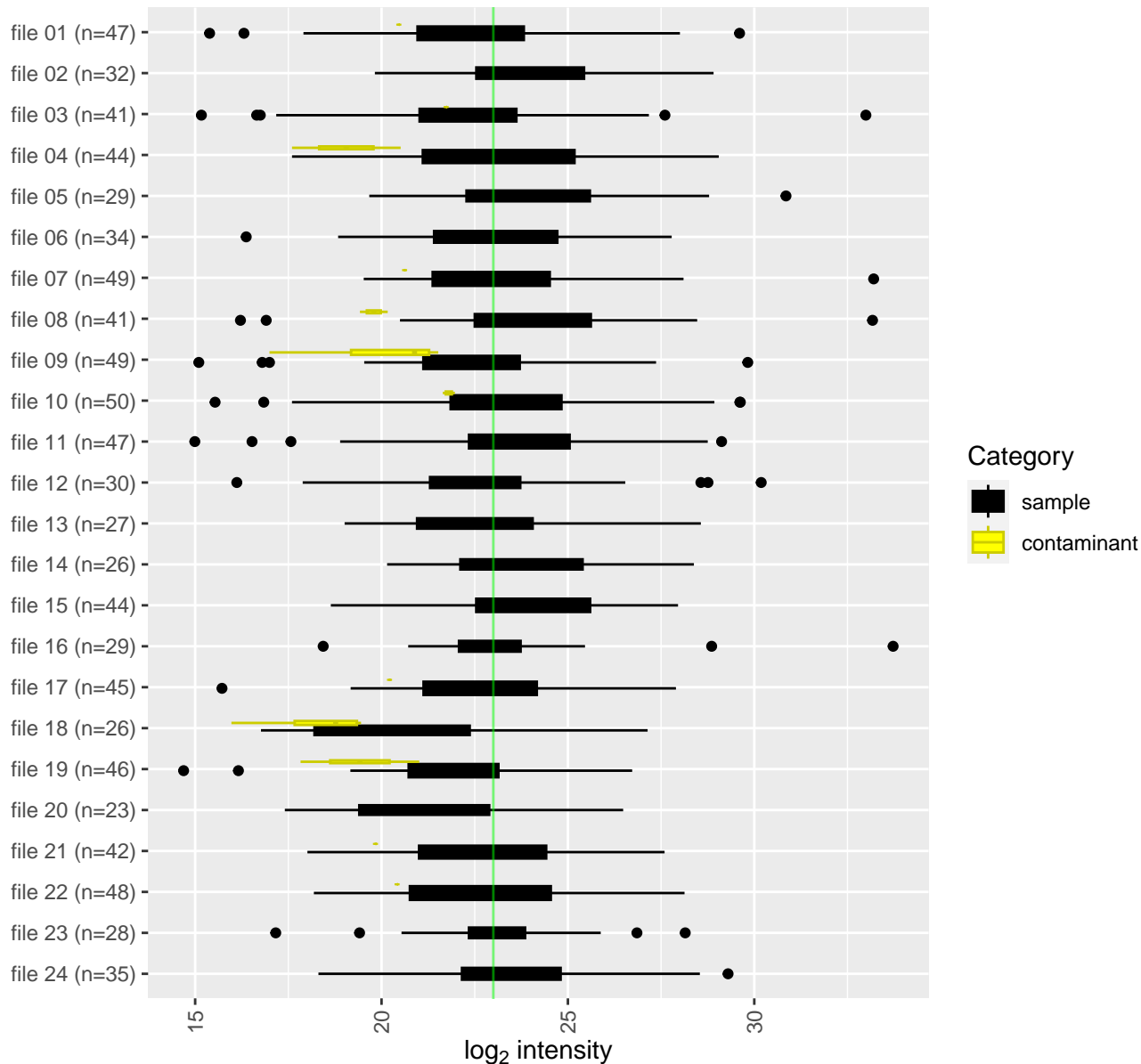
## Abundance class

- low
- mid
- high



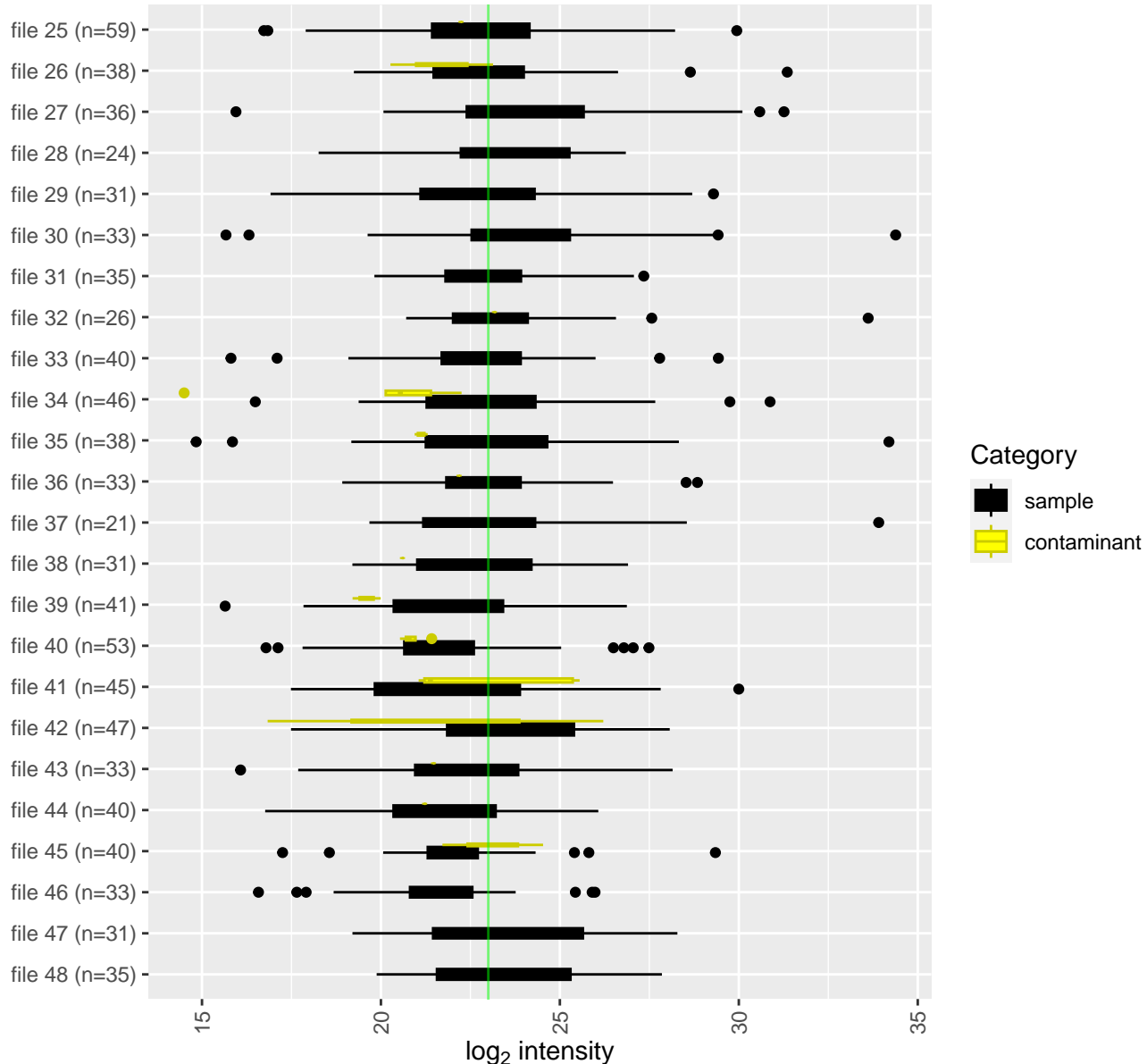
# EVD: peptide intensity distribution

RSD 3.9% (expected < 5%)



# EVD: peptide intensity distribution

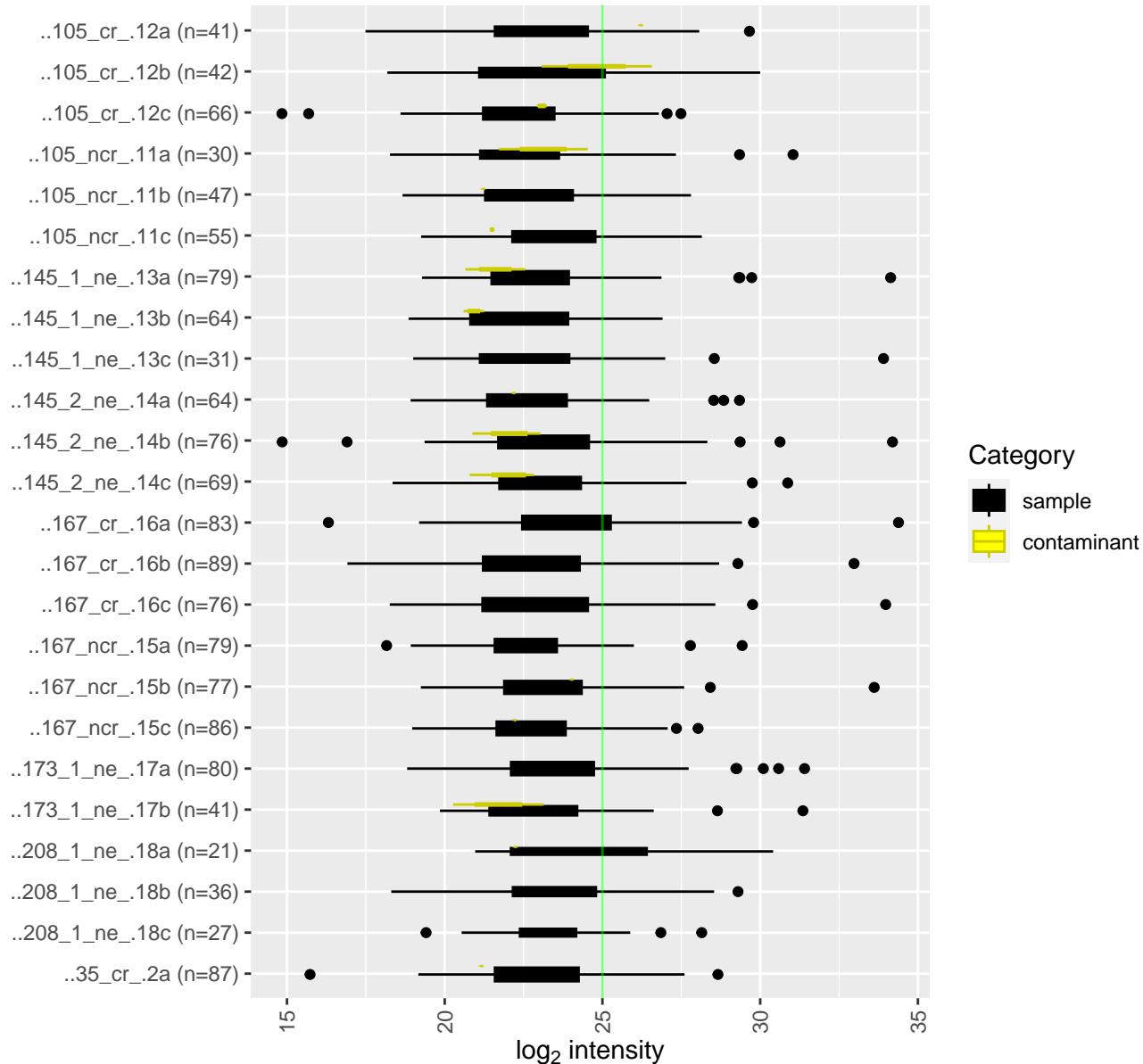
RSD 3.9% (expected < 5%)



# PG: intensity distribution

RSD 2.8% (w/o zero int.; expected < 5%)

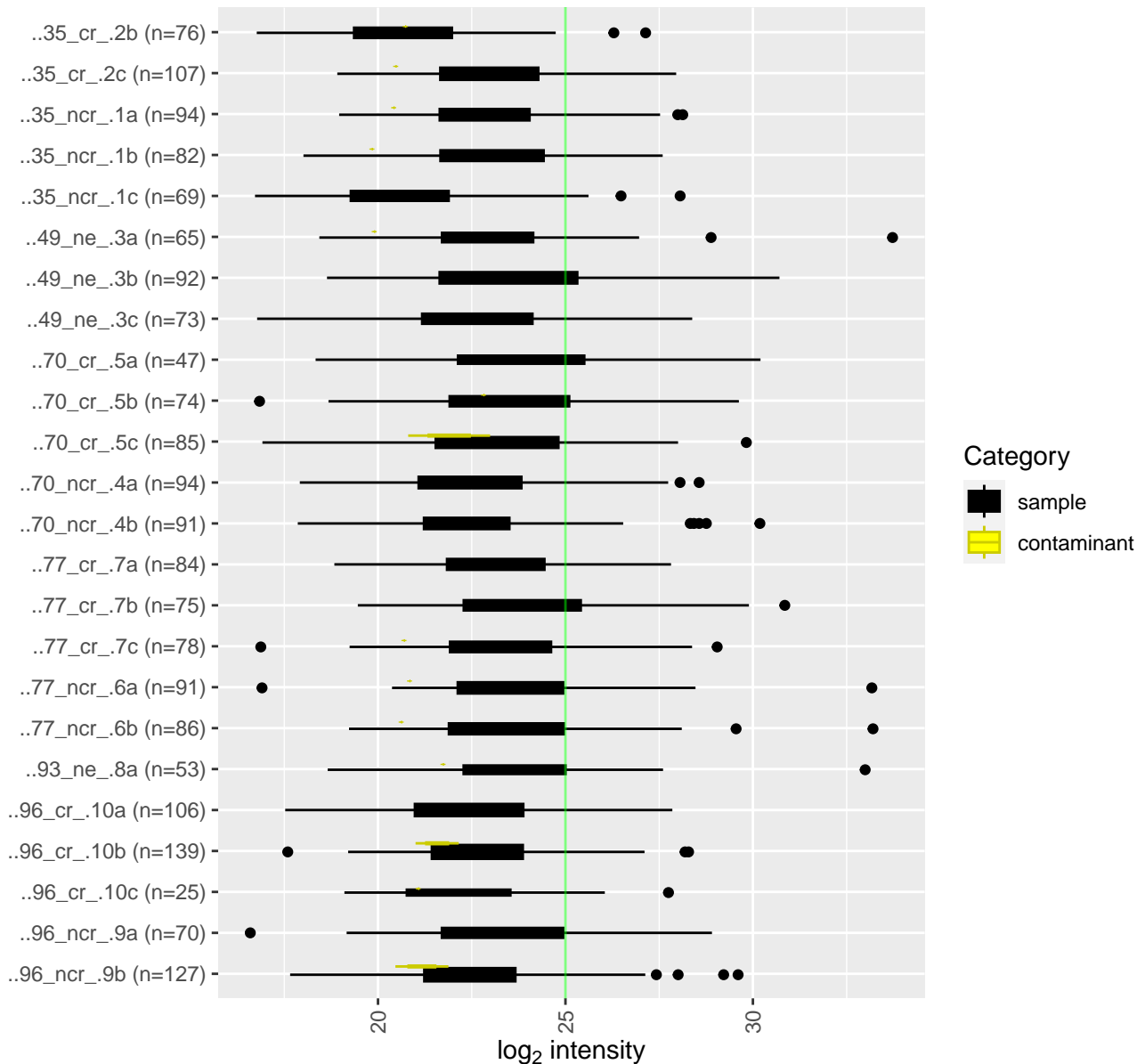
RSD NaN% [high RSD --> few peptides]



# PG: intensity distribution

RSD 2.8% (w/o zero int.; expected < 5%)

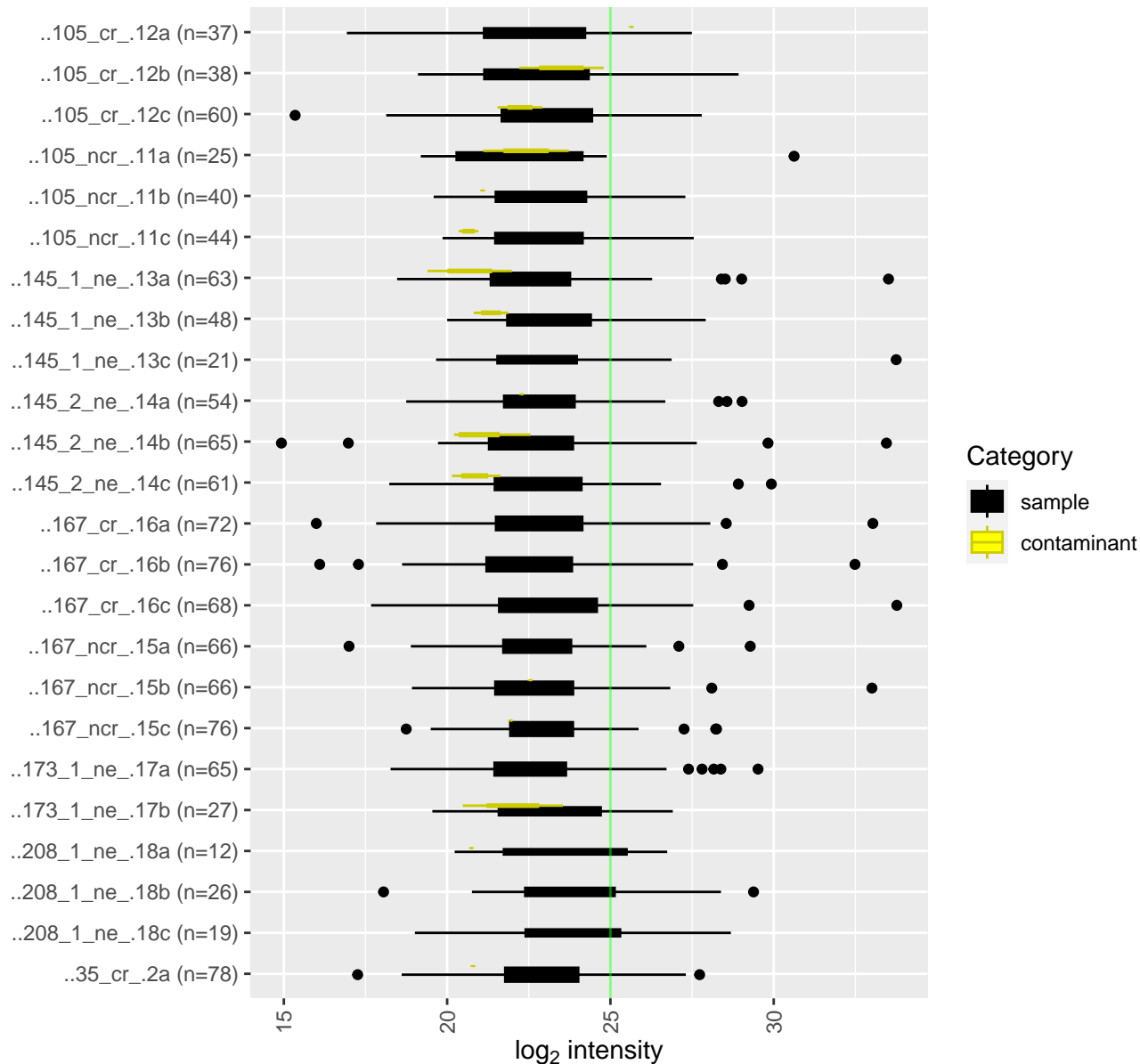
RSD NaN% [high RSD --> few peptides]



# PG: Lfq intensity distribution

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

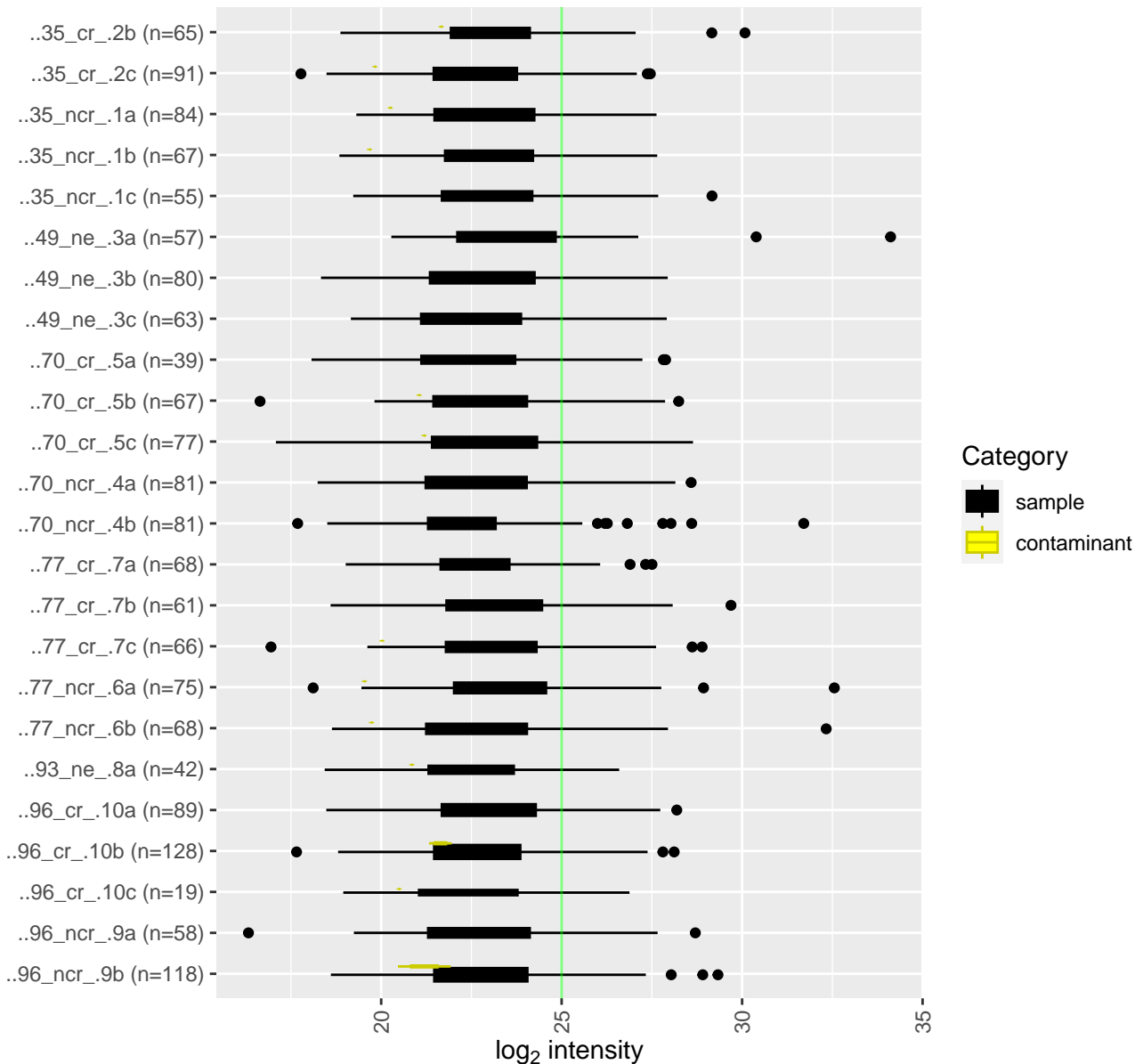
RSD NaN% [high RSD --> few peptides]



# PG: LFQ intensity distribution

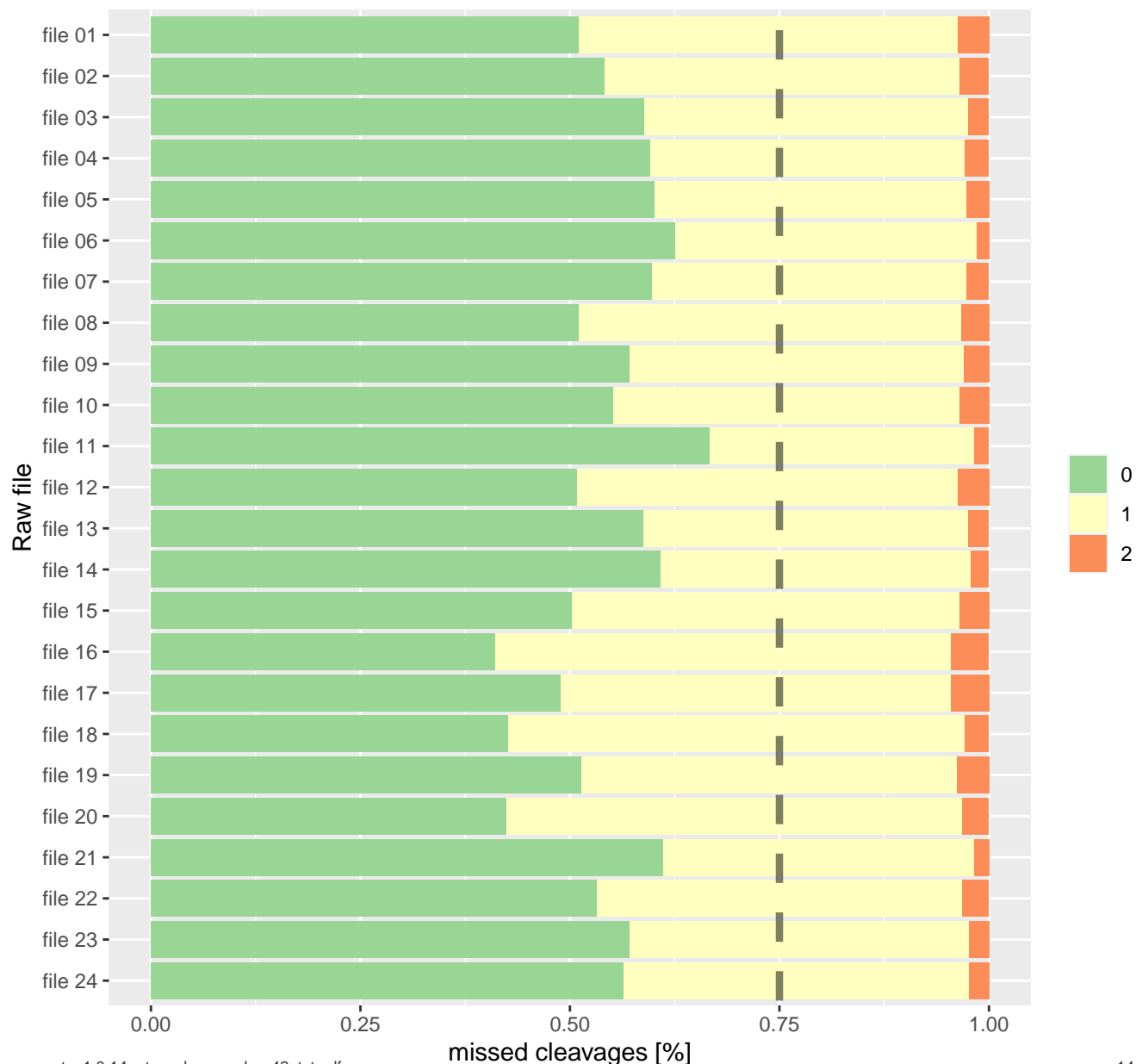
RSD 1.5% (w/o zero int.; expected < 5%)

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



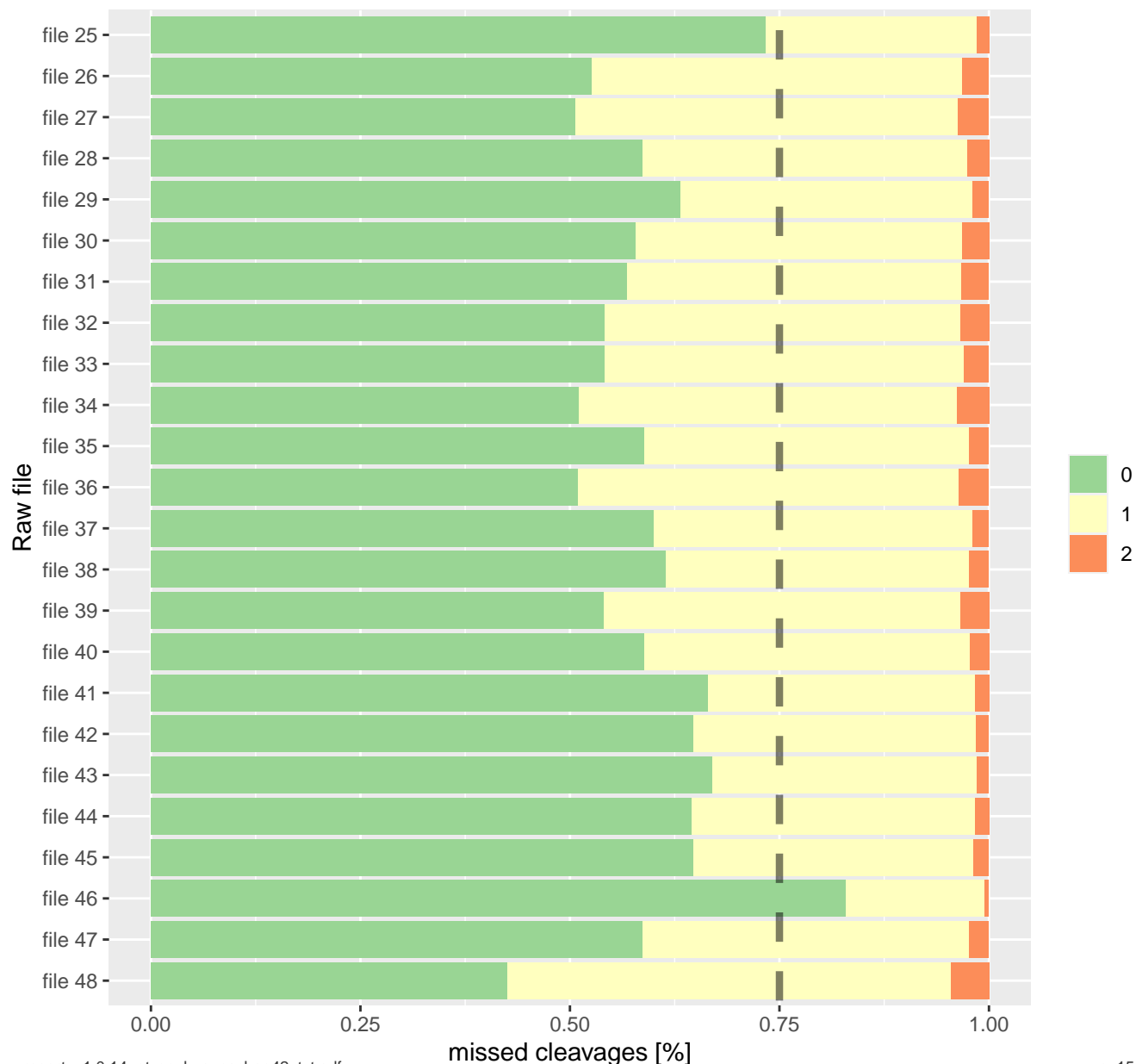
# MSMS: Missed cleavages per Raw file

(excludes contaminants)



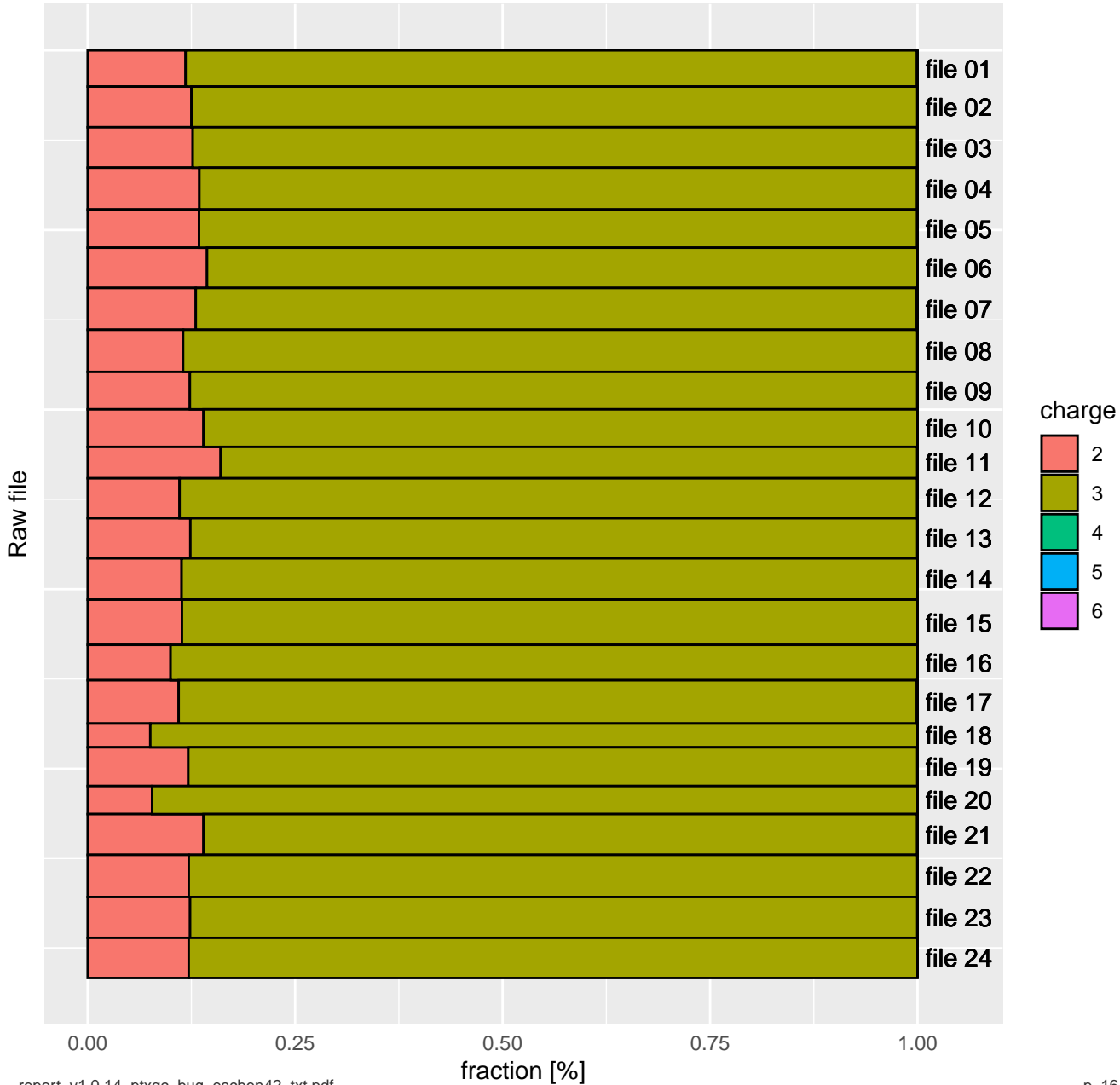
# MSMS: Missed cleavages per Raw file

(excludes contaminants)

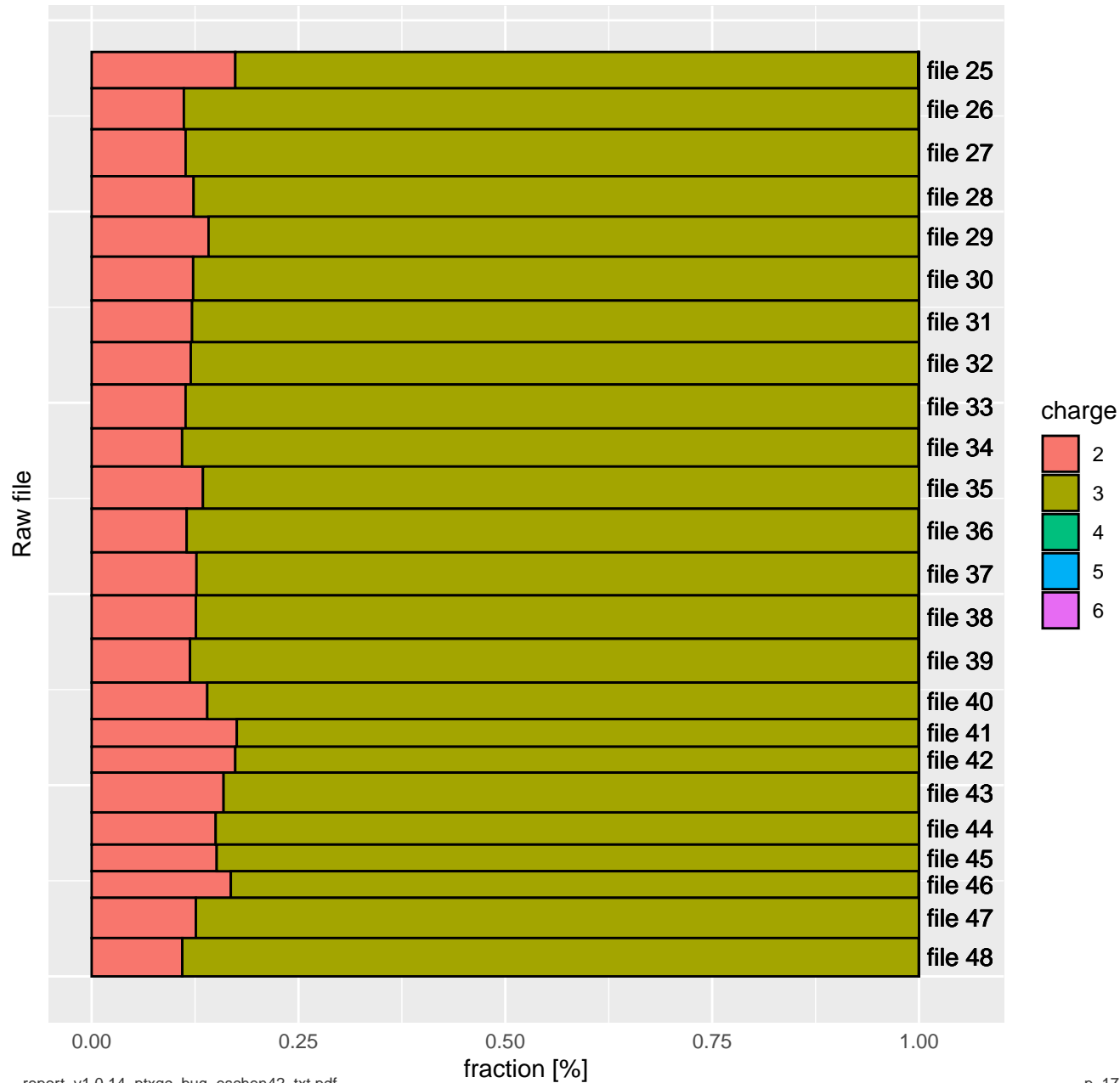




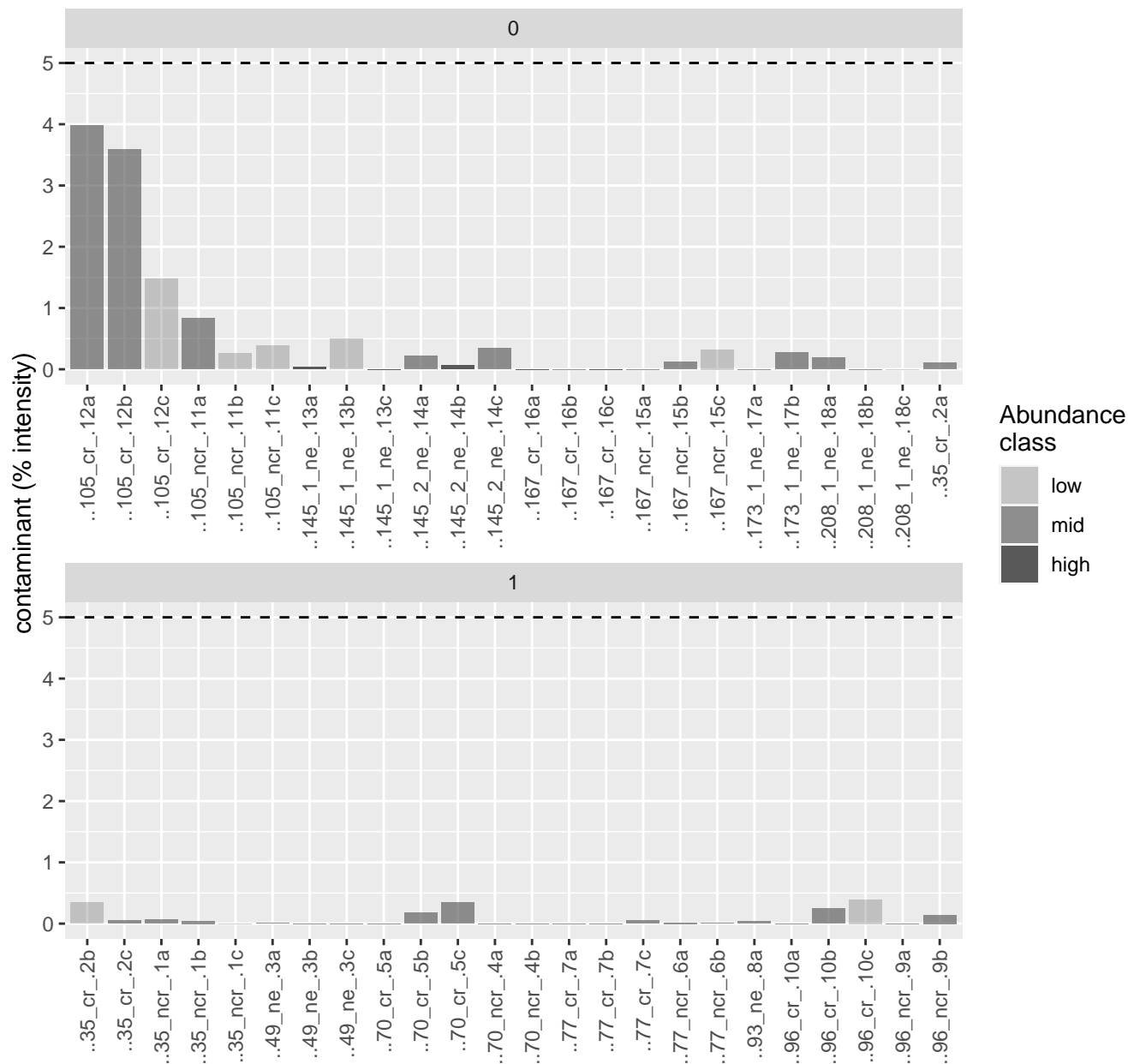
# EVD: charge distribution



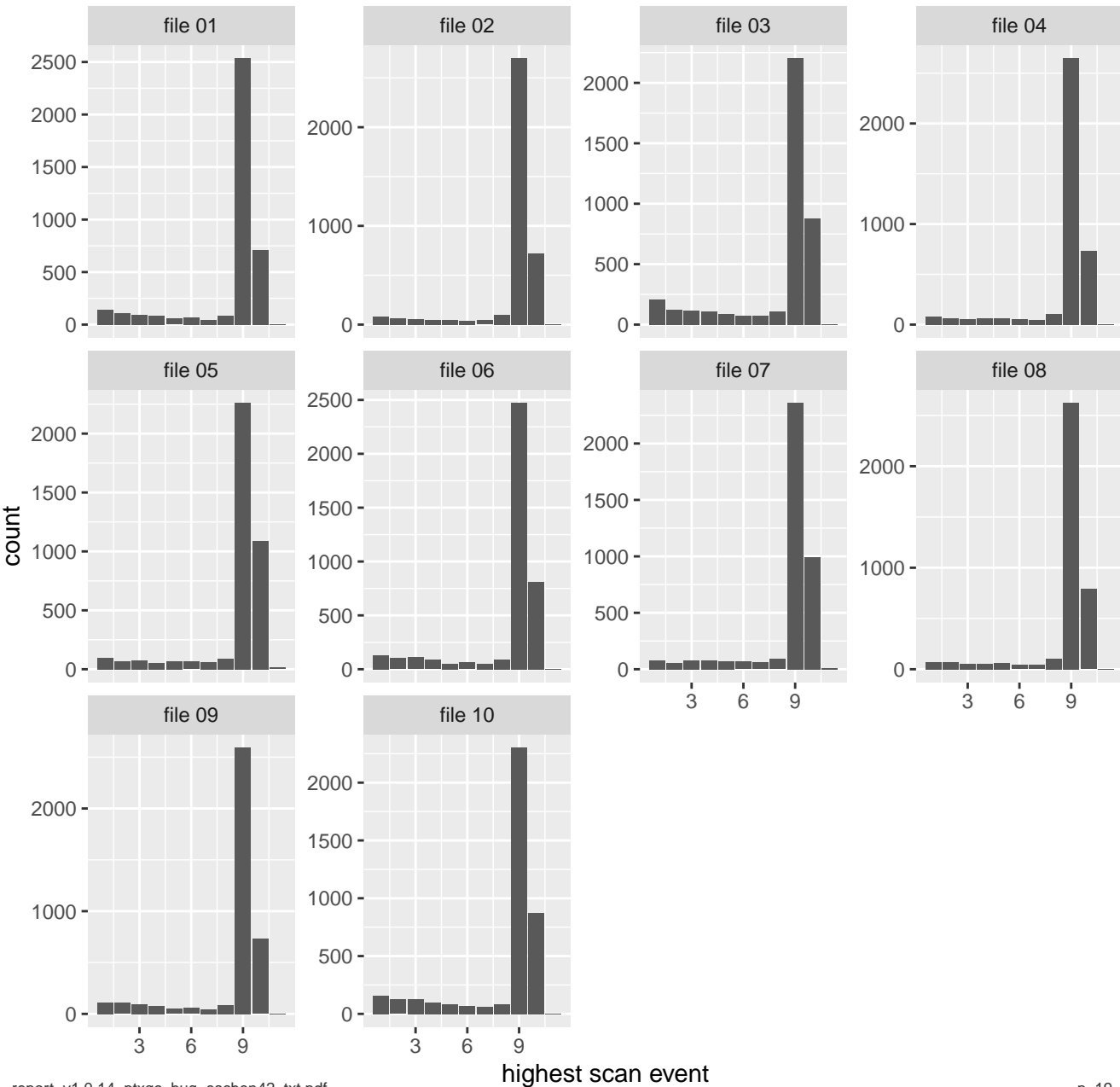
# EVD: charge distribution



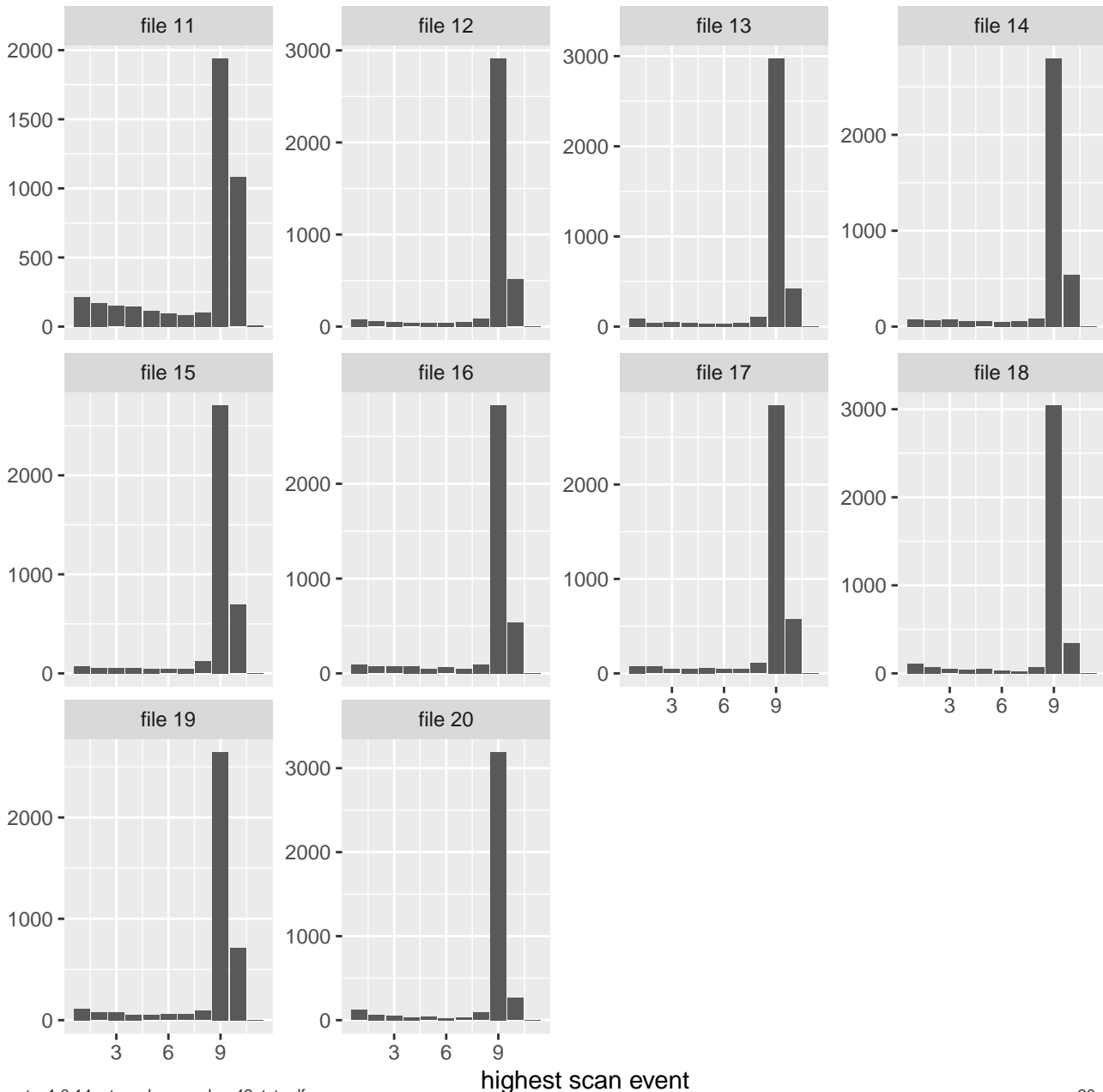
# PG: Contaminant per condition



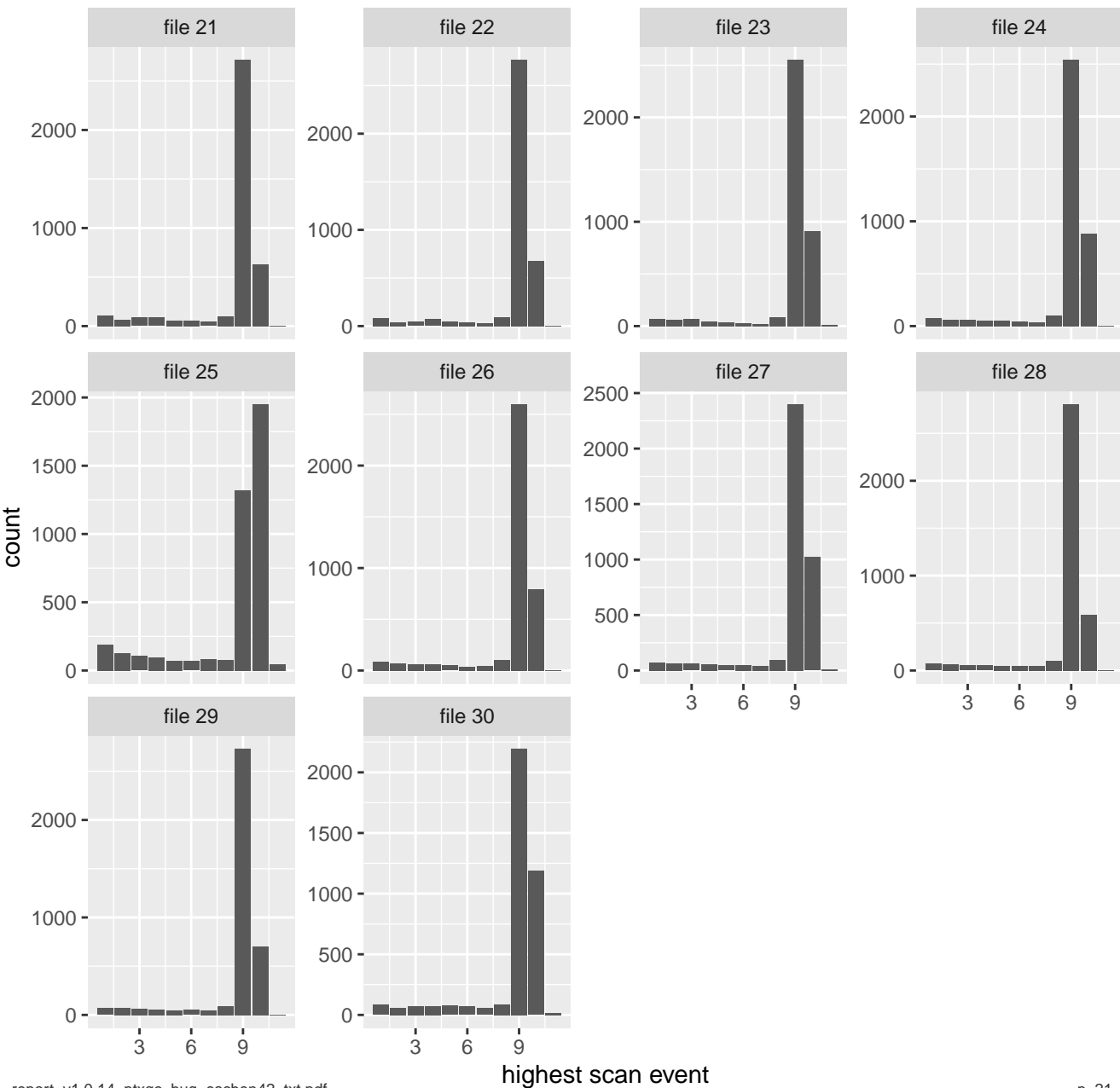
# MSMSscans: TopN



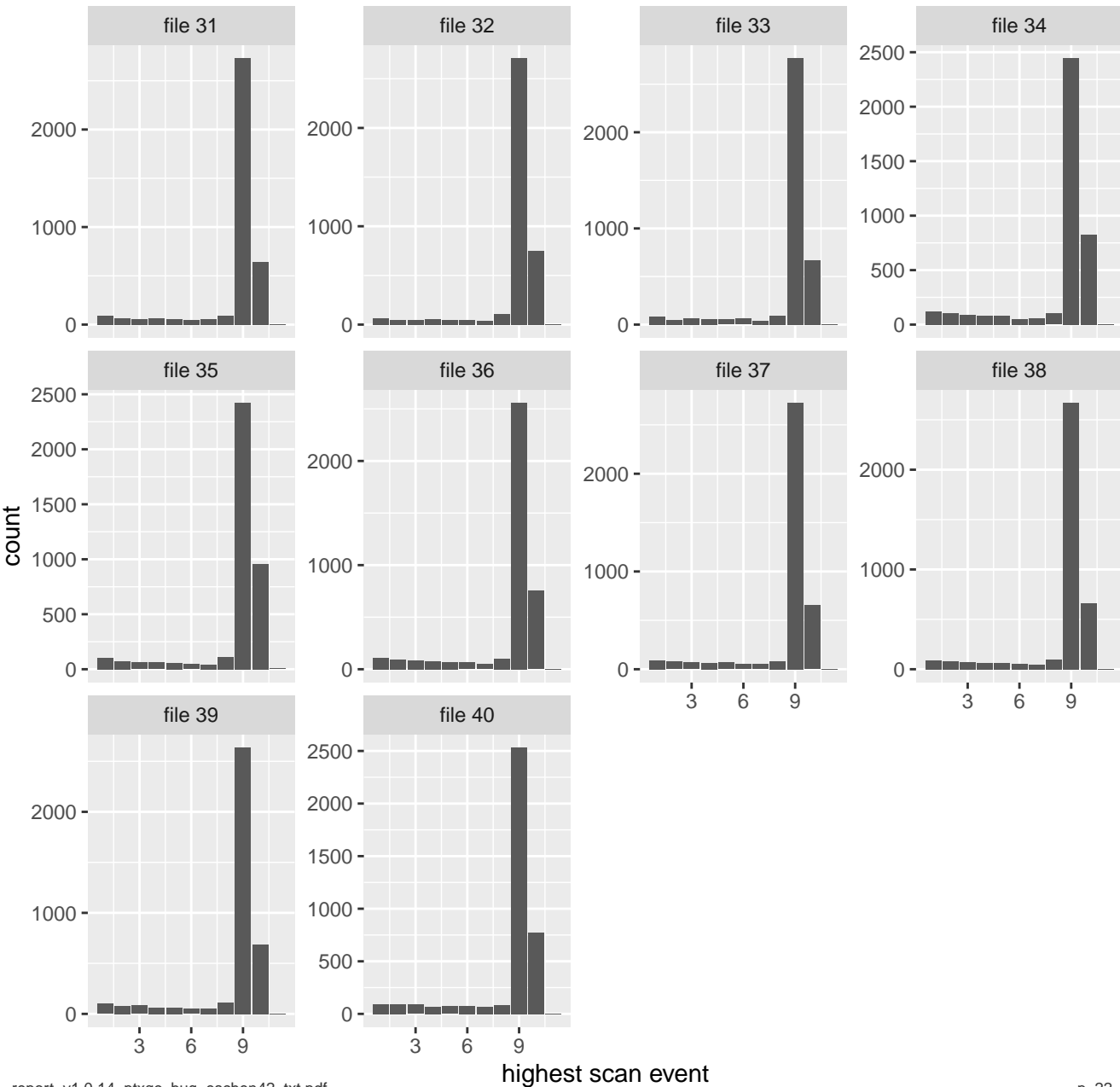
# MSMSscans: TopN



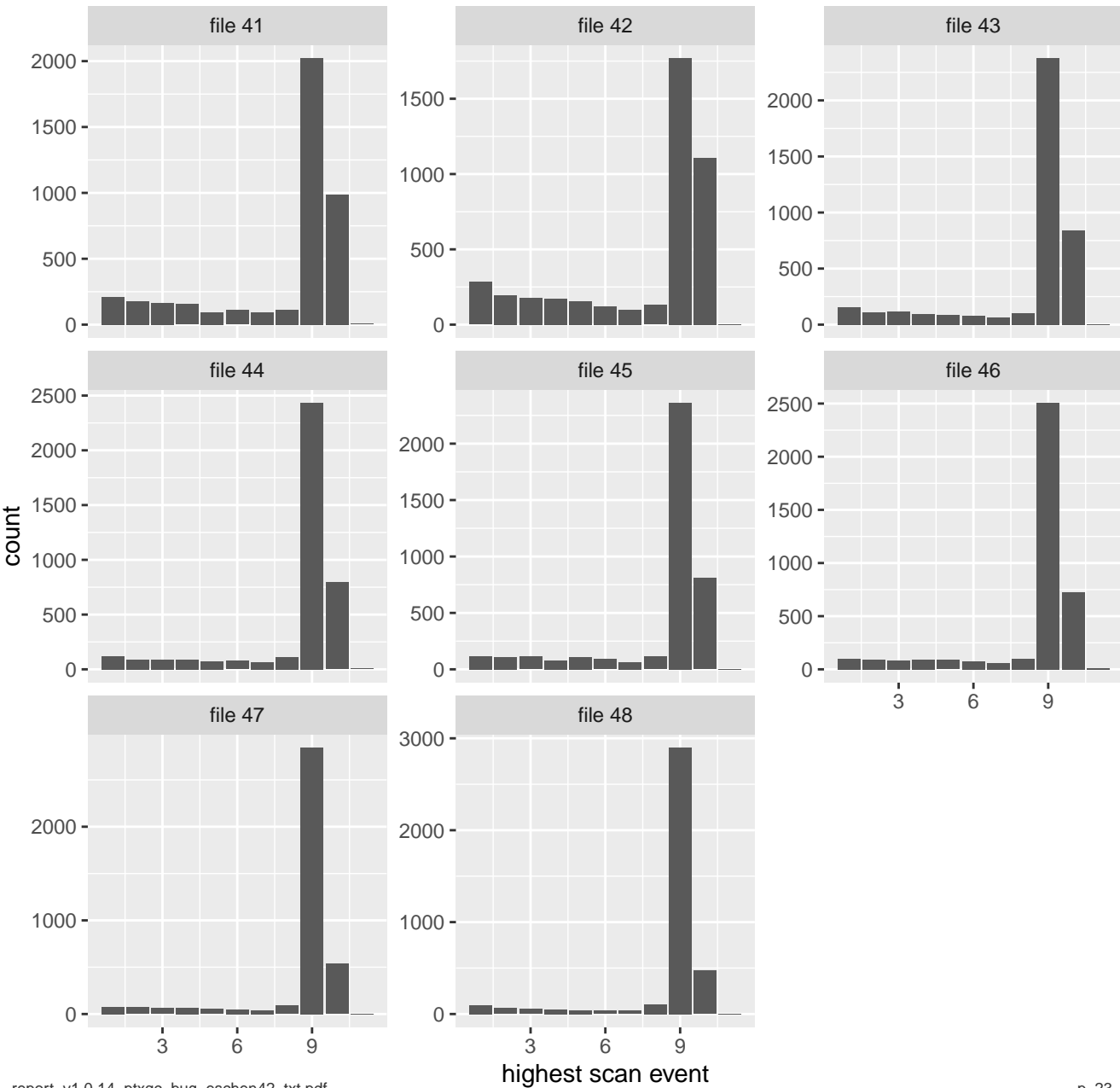
# MSMScans: TopN



# MSMSScans: TopN

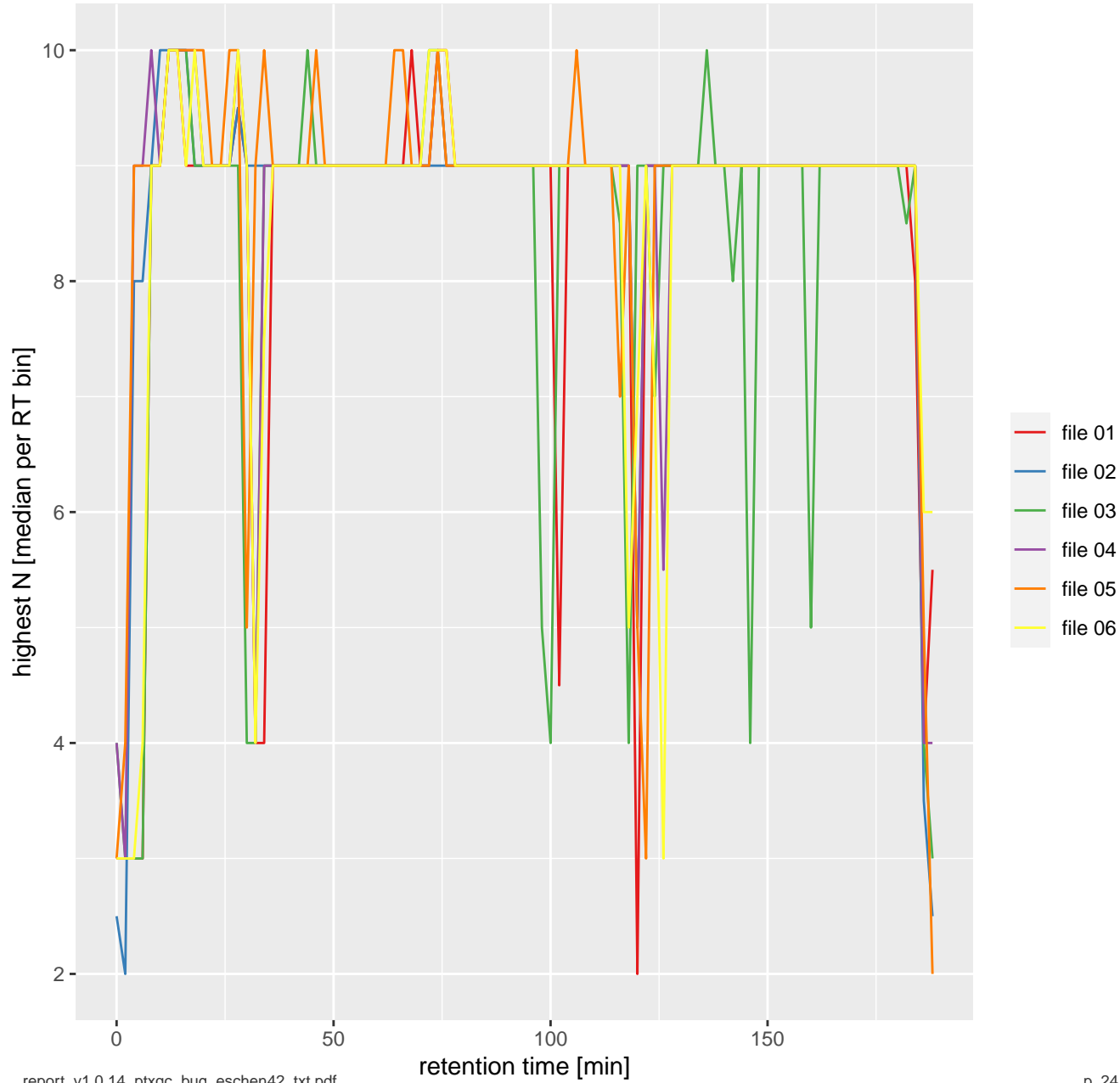


# MSMSscans: TopN

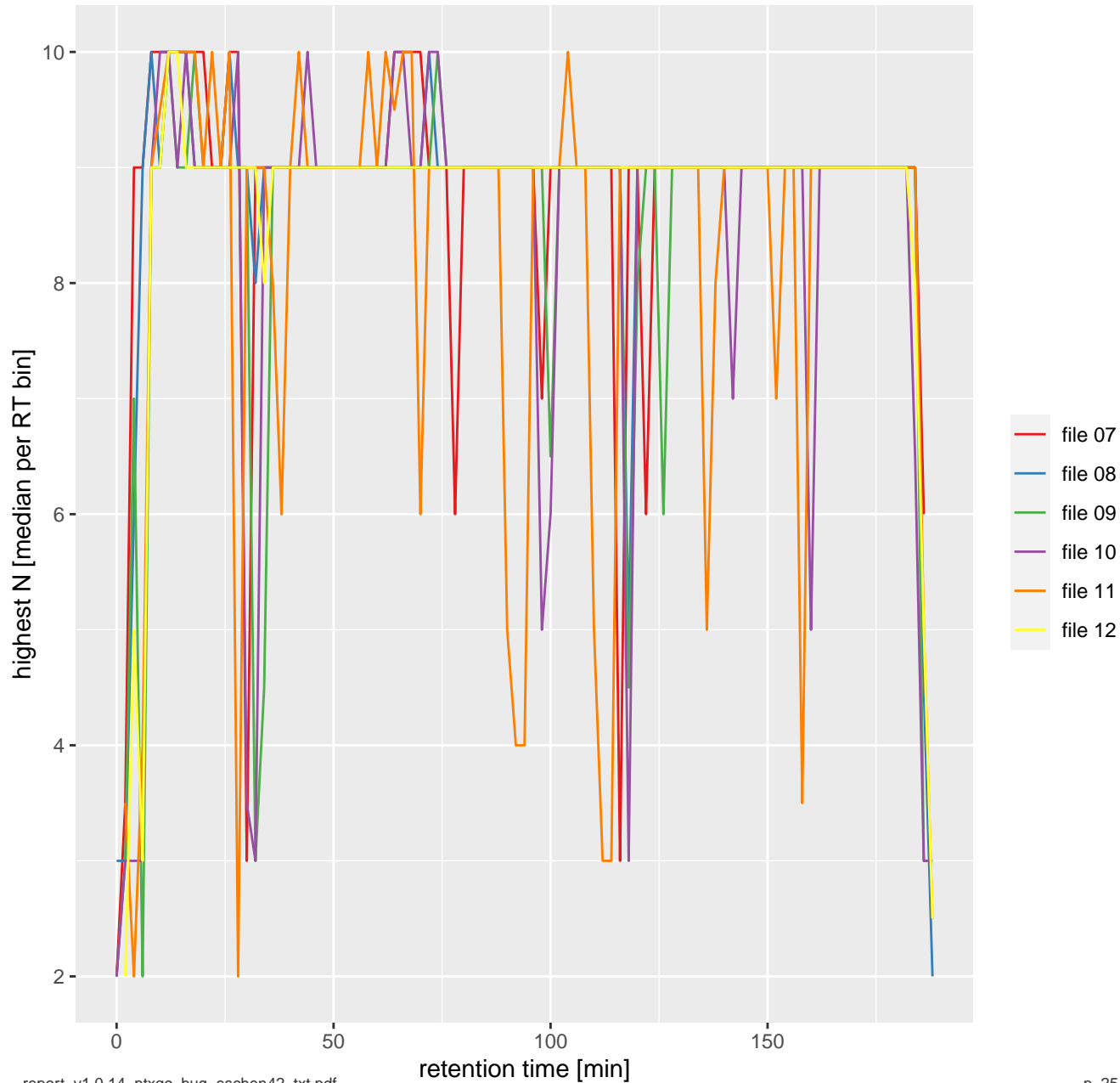




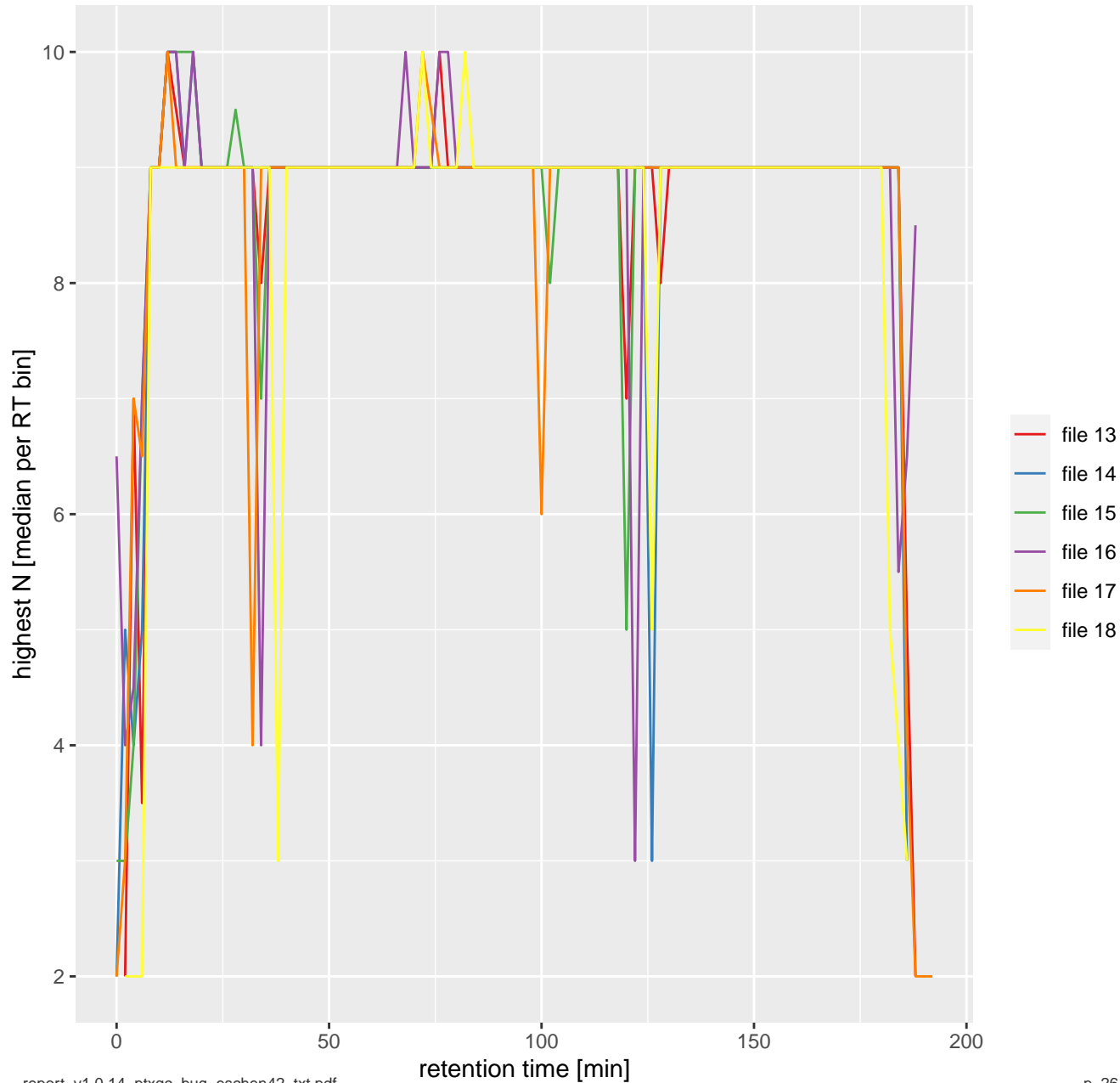
# MSMSscans: TopN over RT



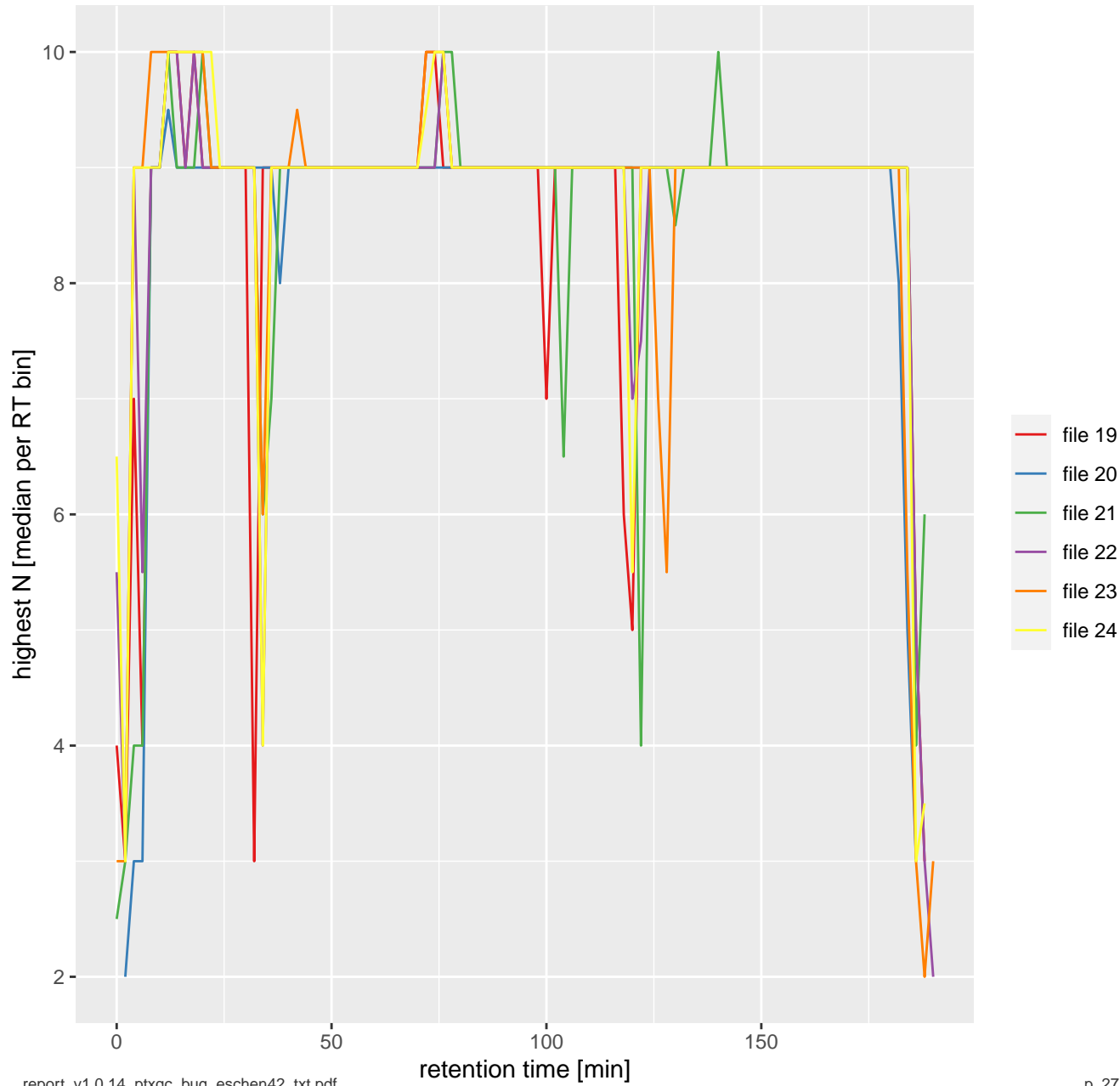
# MSMSscans: TopN over RT



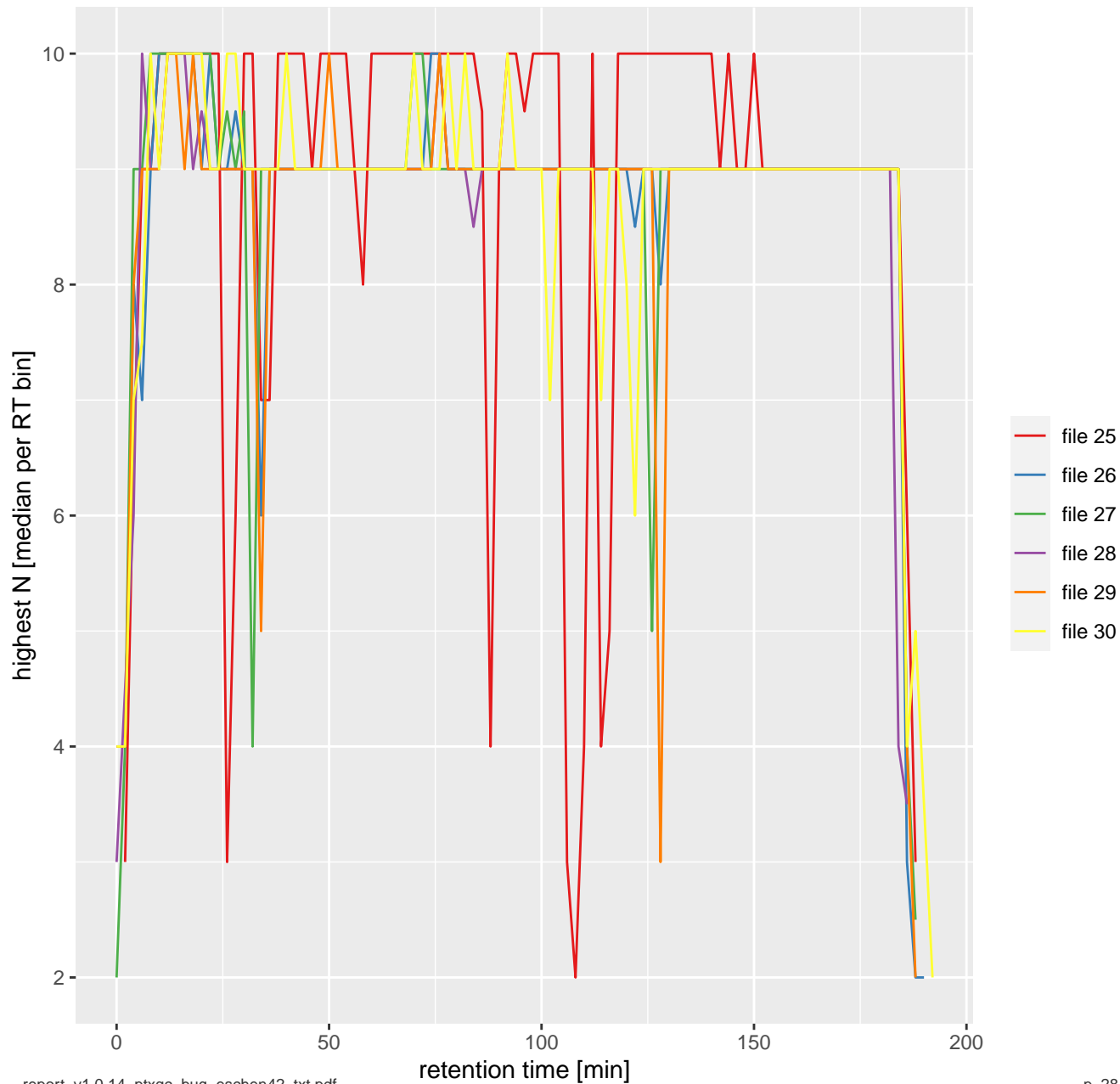
# MSMSscans: TopN over RT



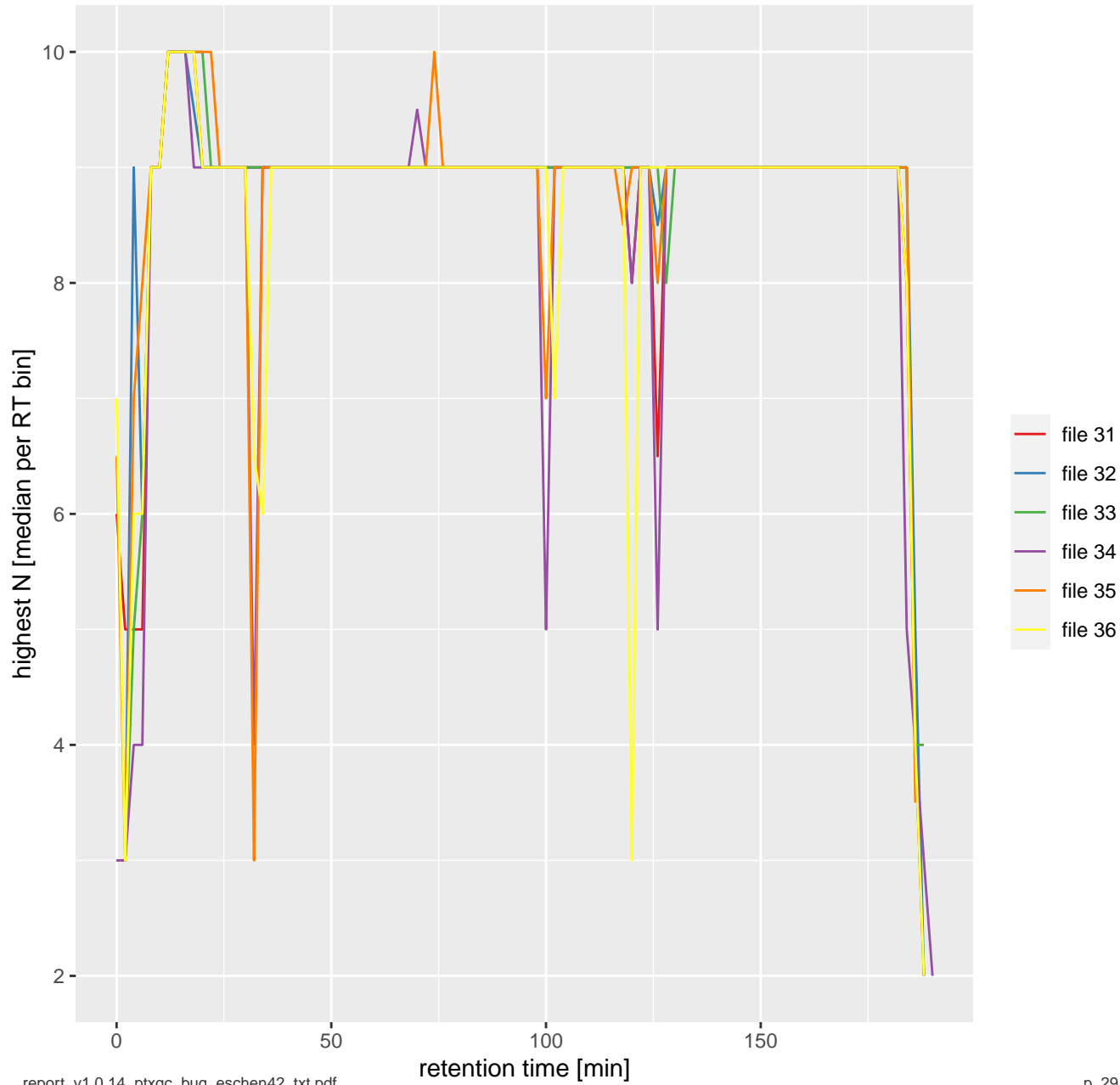
# MSMSscans: TopN over RT



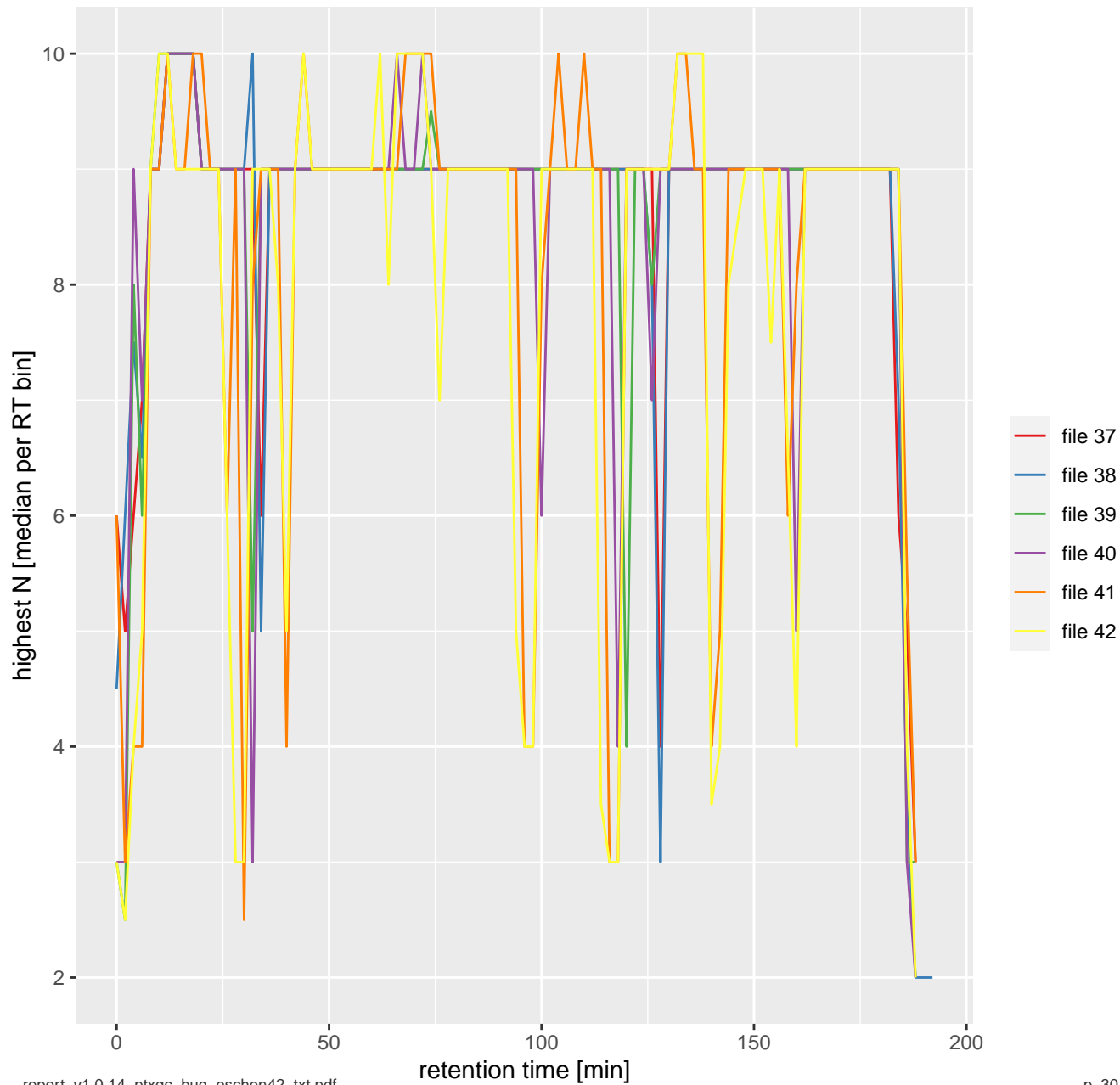
# MSMScans: TopN over RT



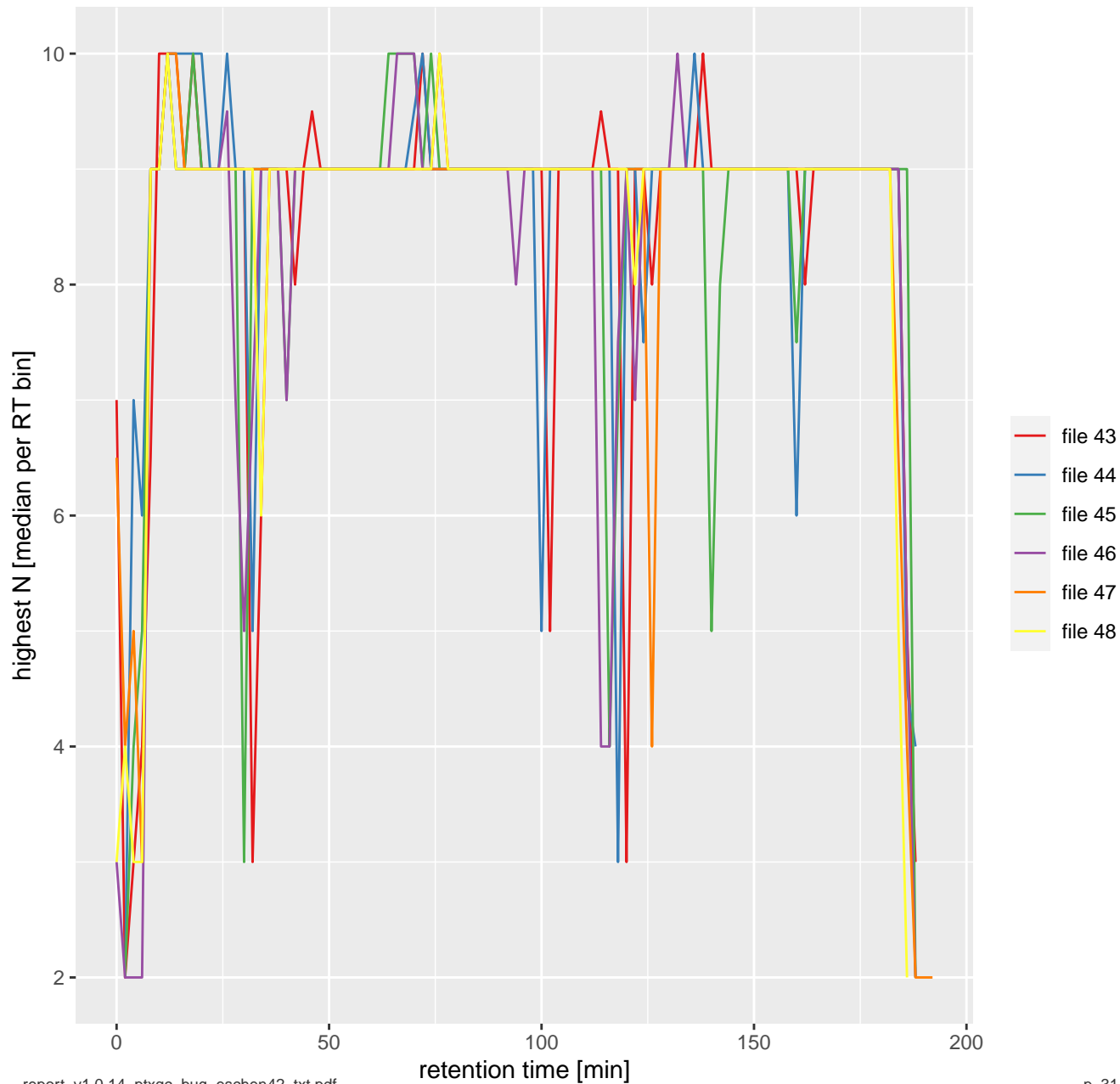
# MSMSscans: TopN over RT



# MSMSscans: TopN over RT

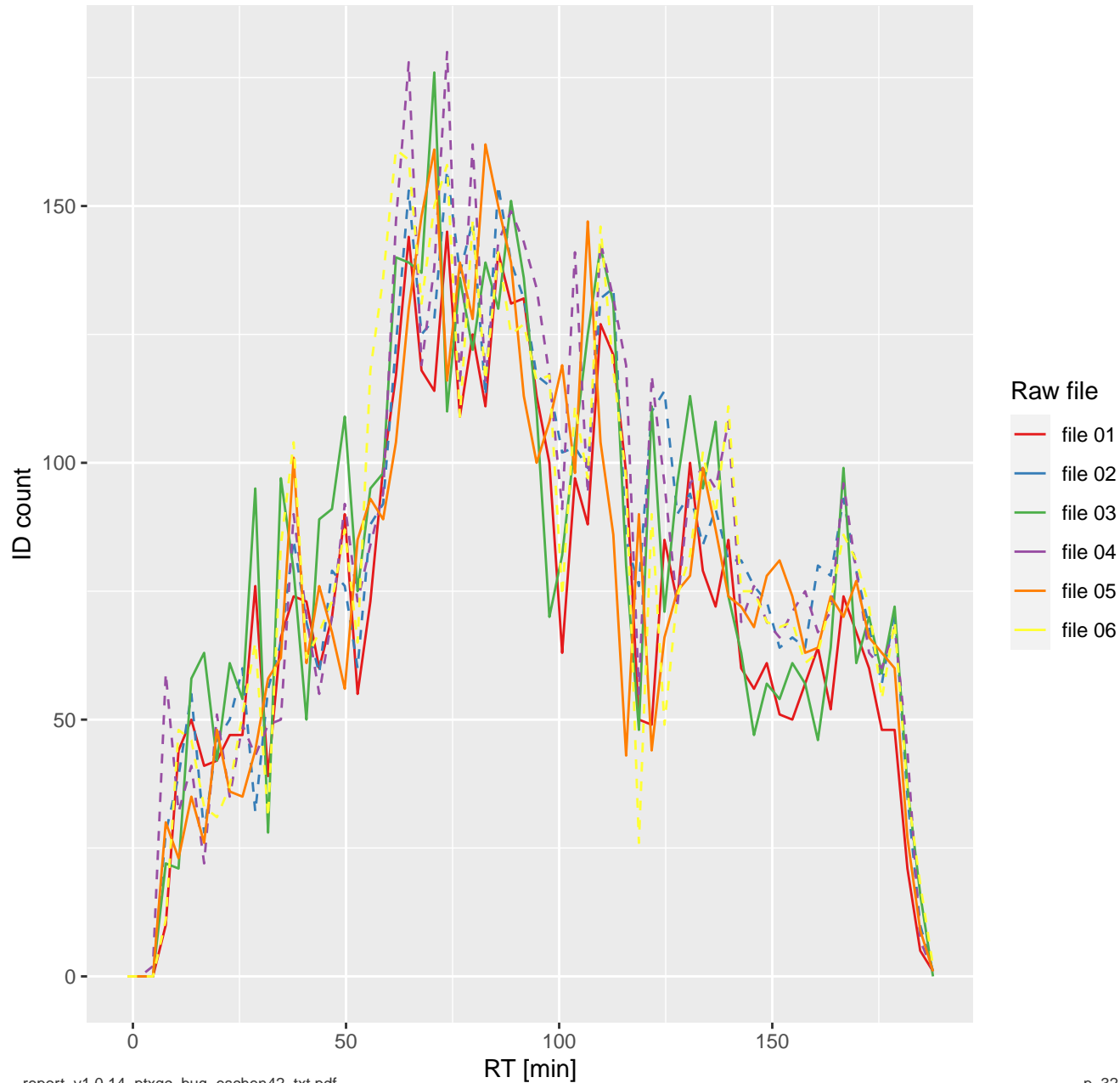


# MSMSscans: TopN over RT

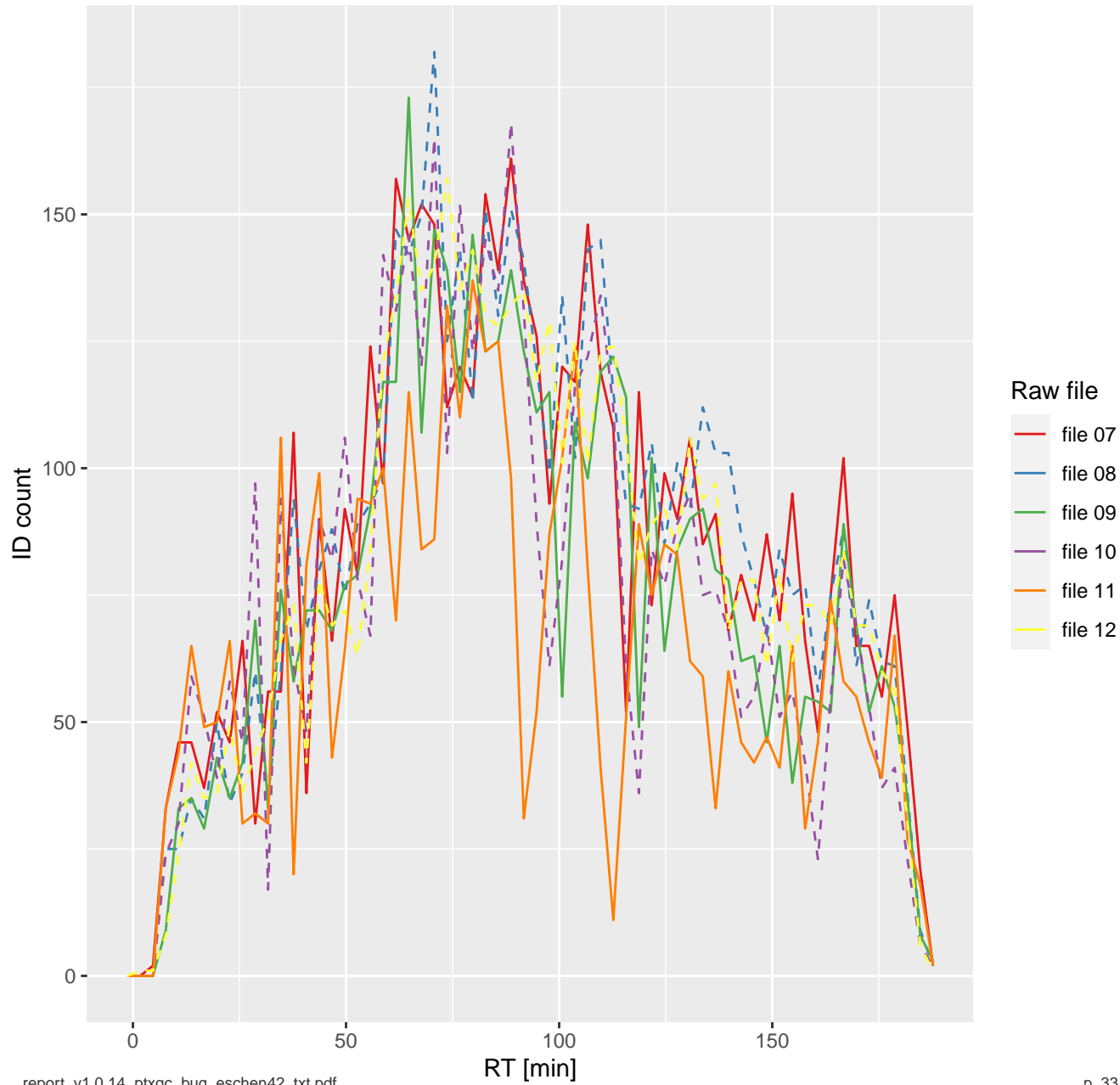




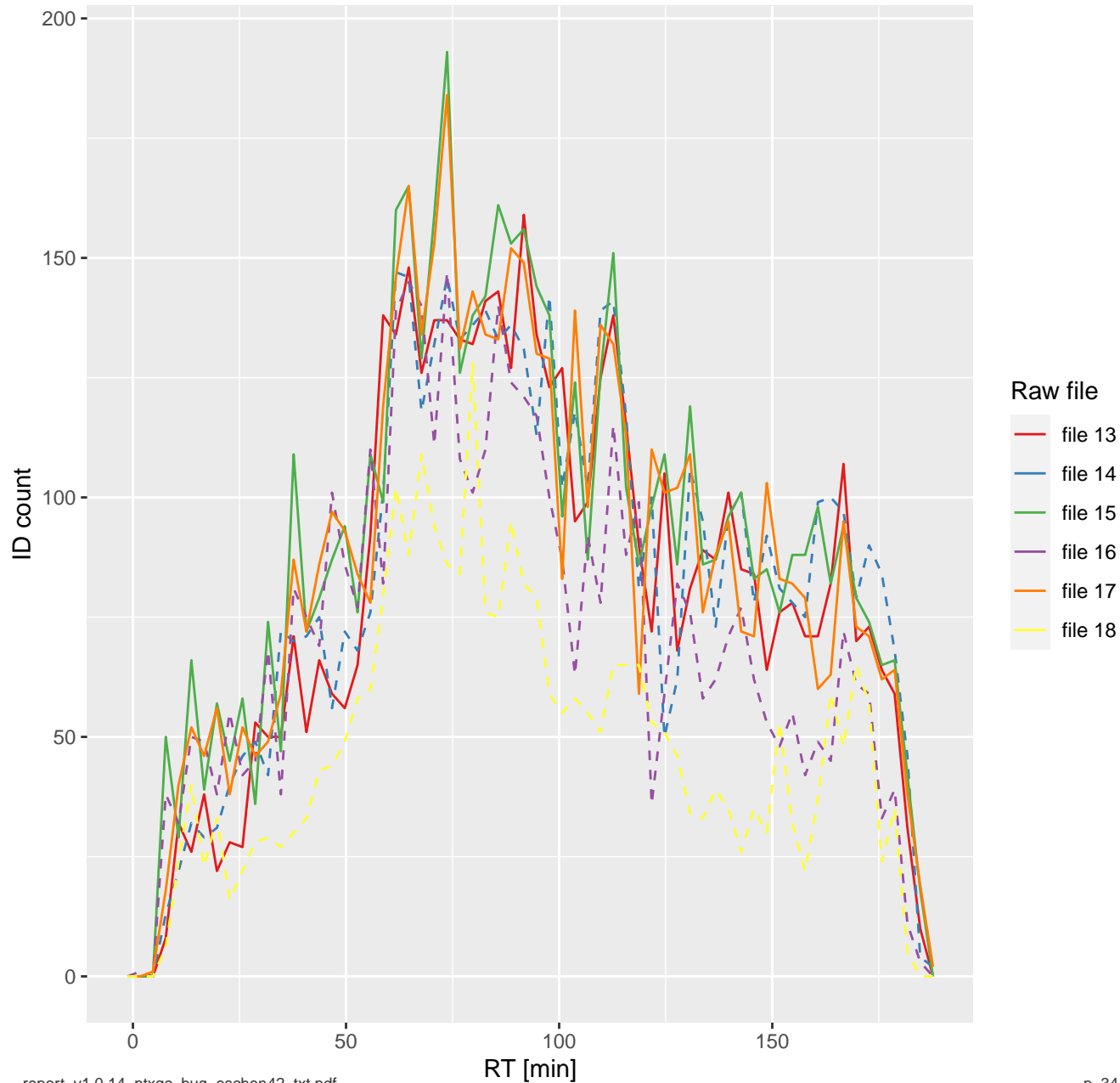
# EVD: IDs over RT



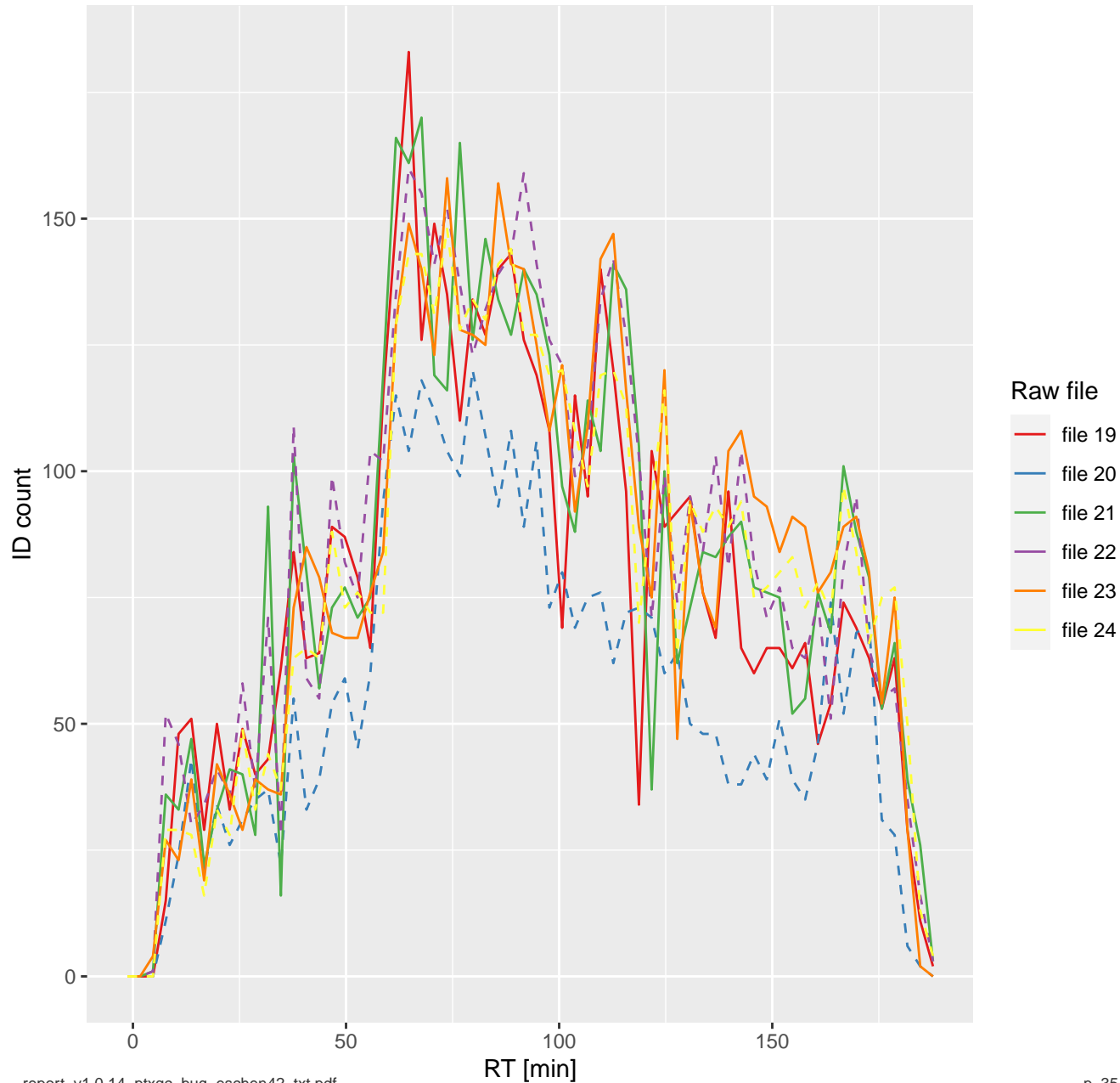
# EVD: IDs over RT



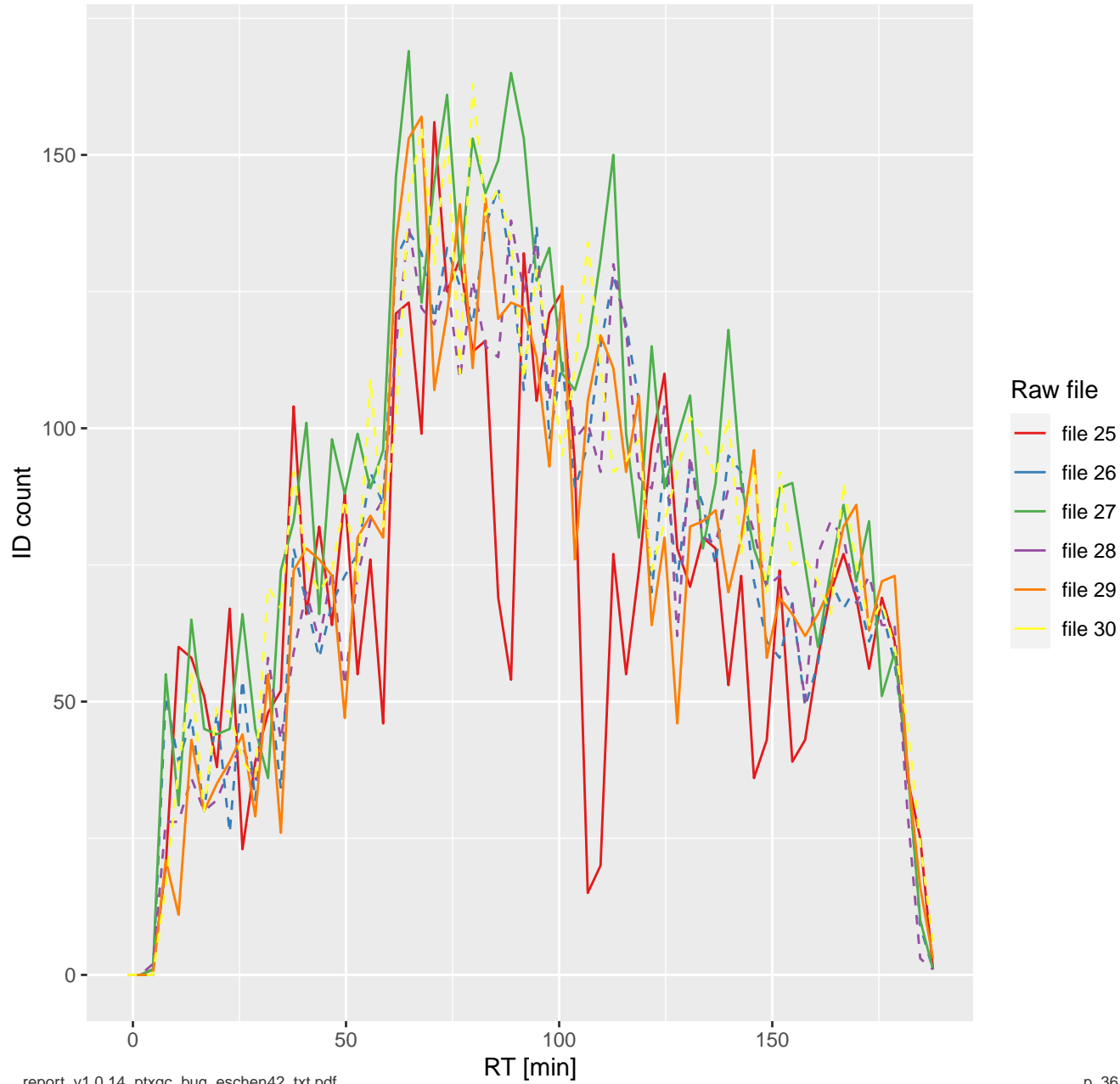
# EVD: IDs over RT



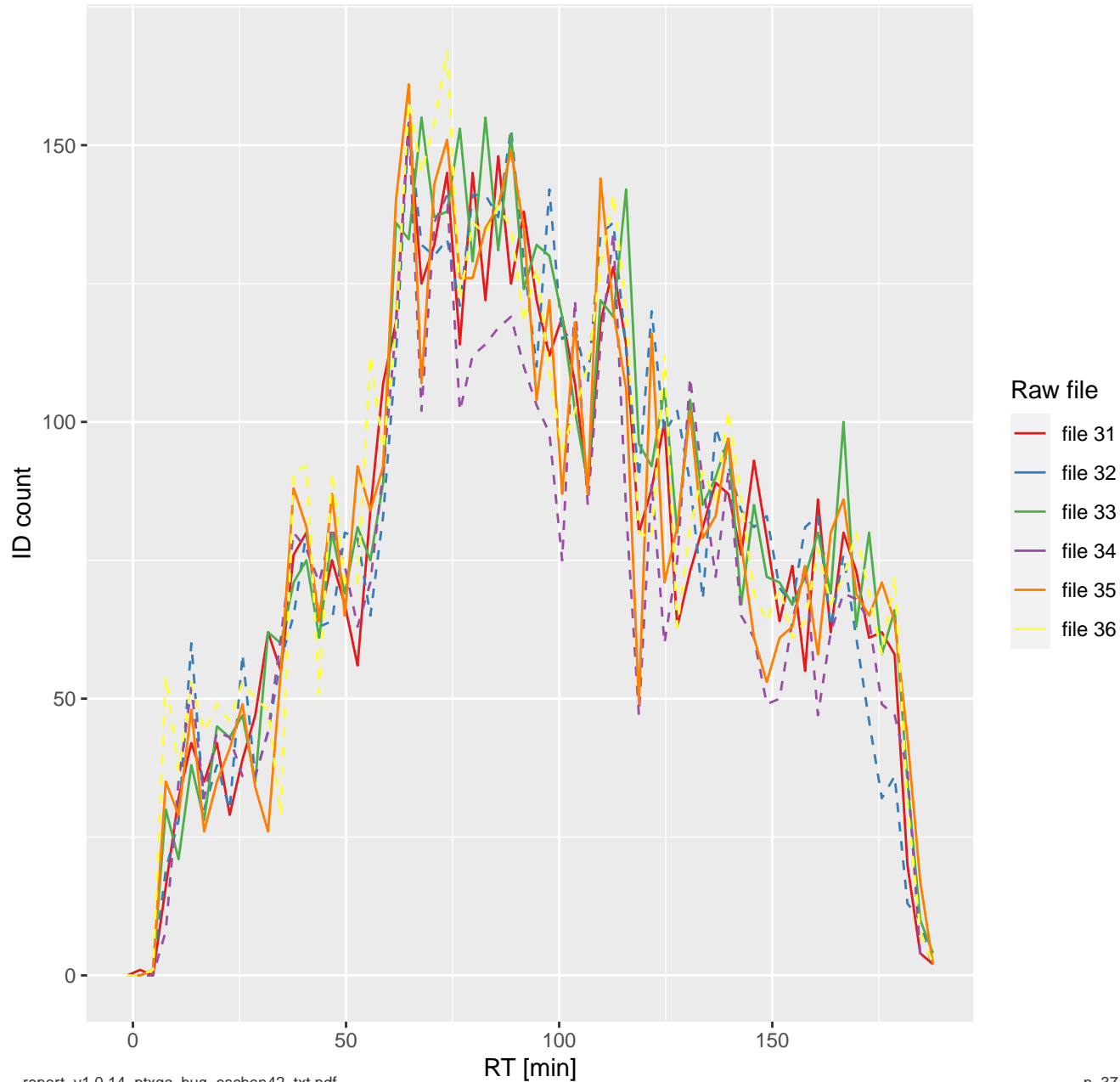
# EVD: IDs over RT



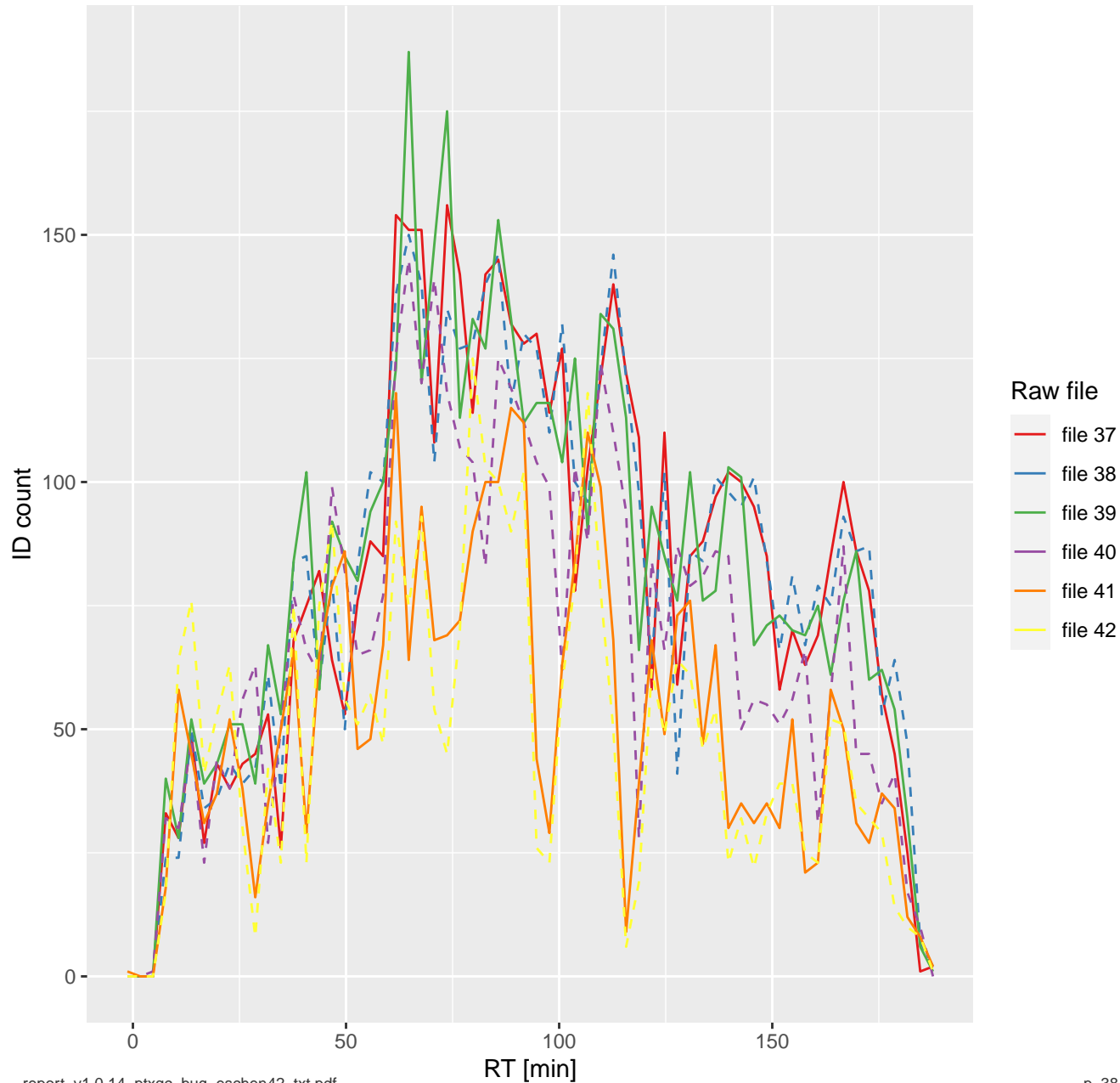
# EVD: IDs over RT



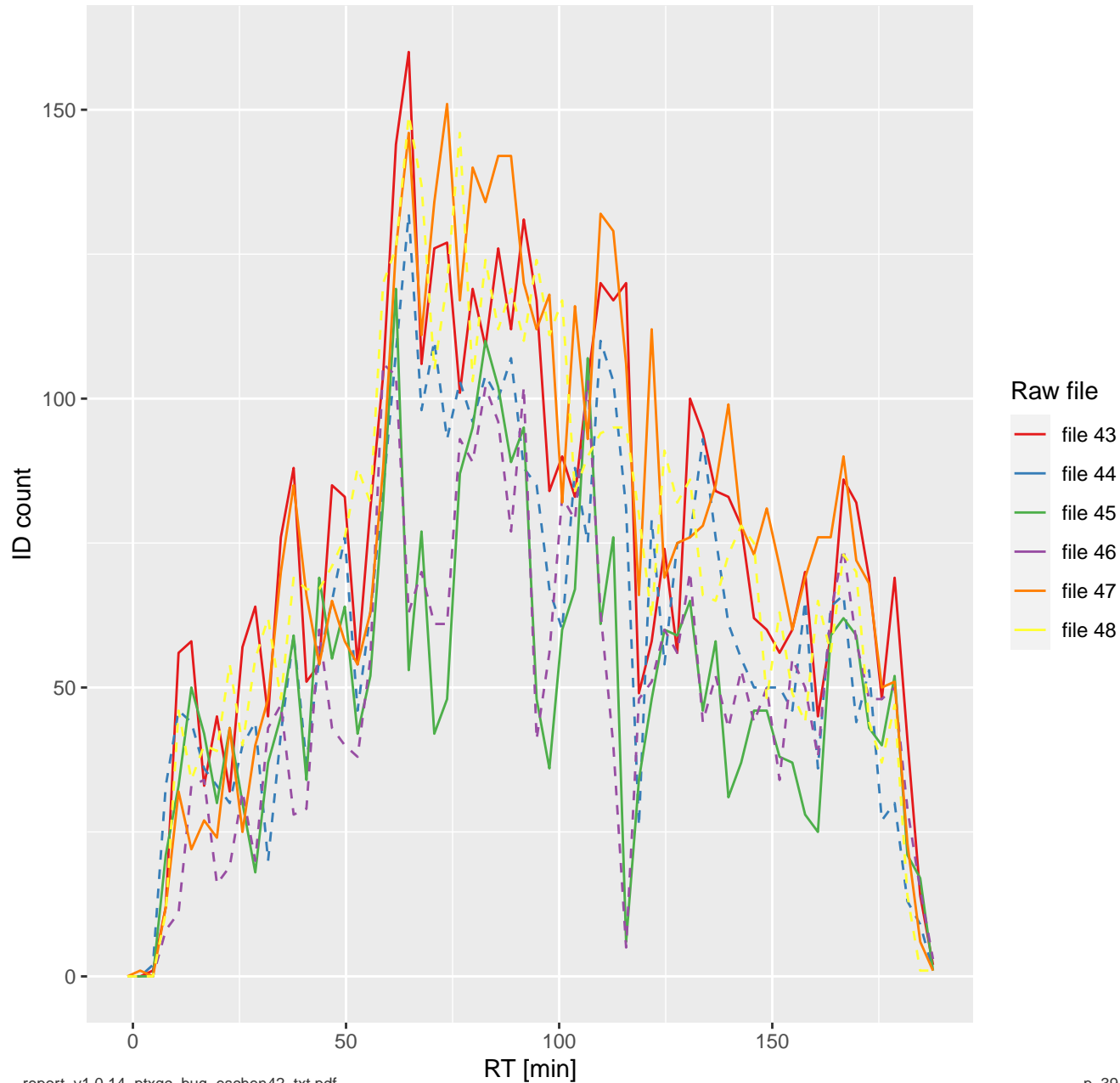
# EVD: IDs over RT



# EVD: IDs over RT

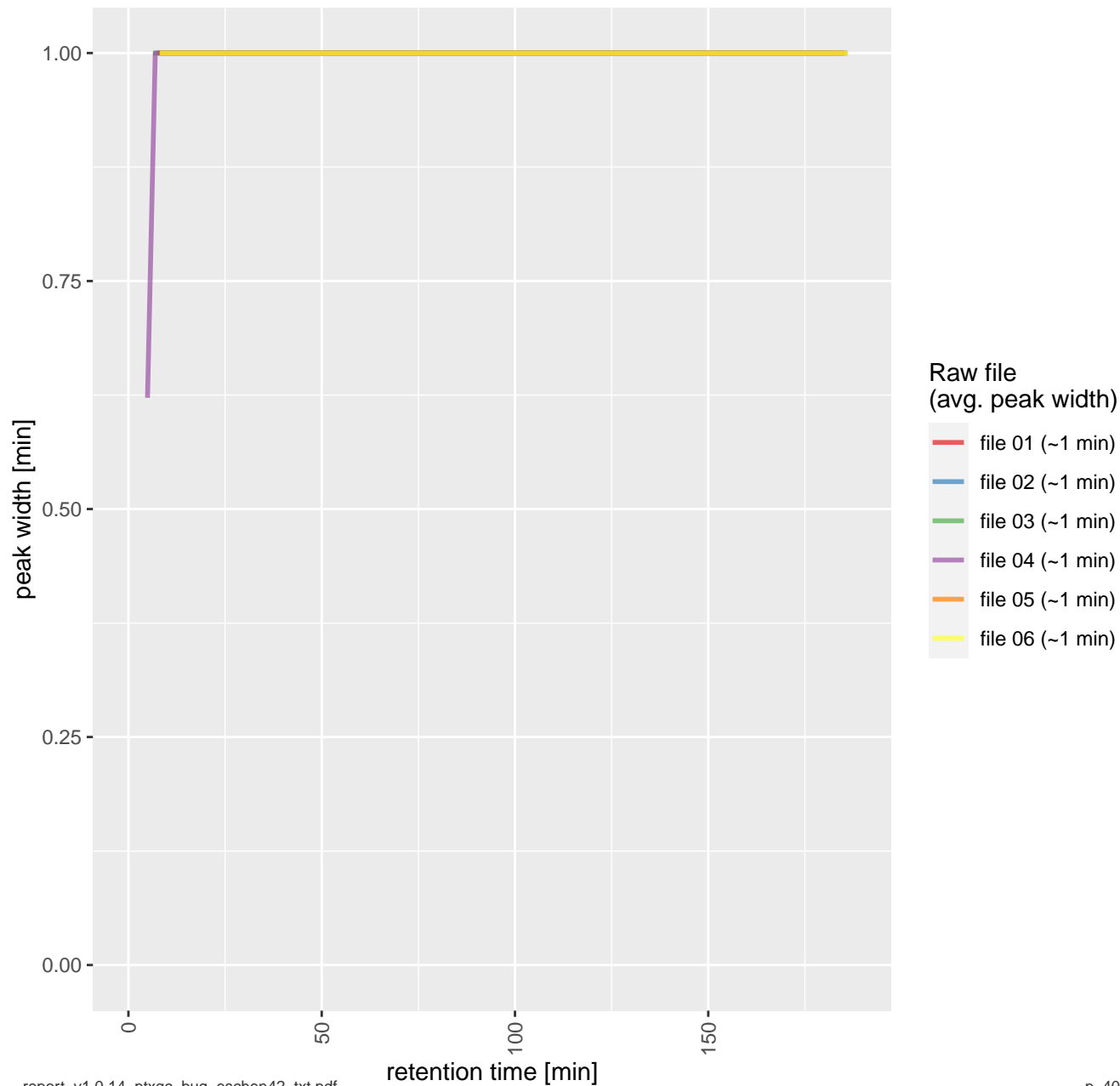


# EVD: IDs over RT

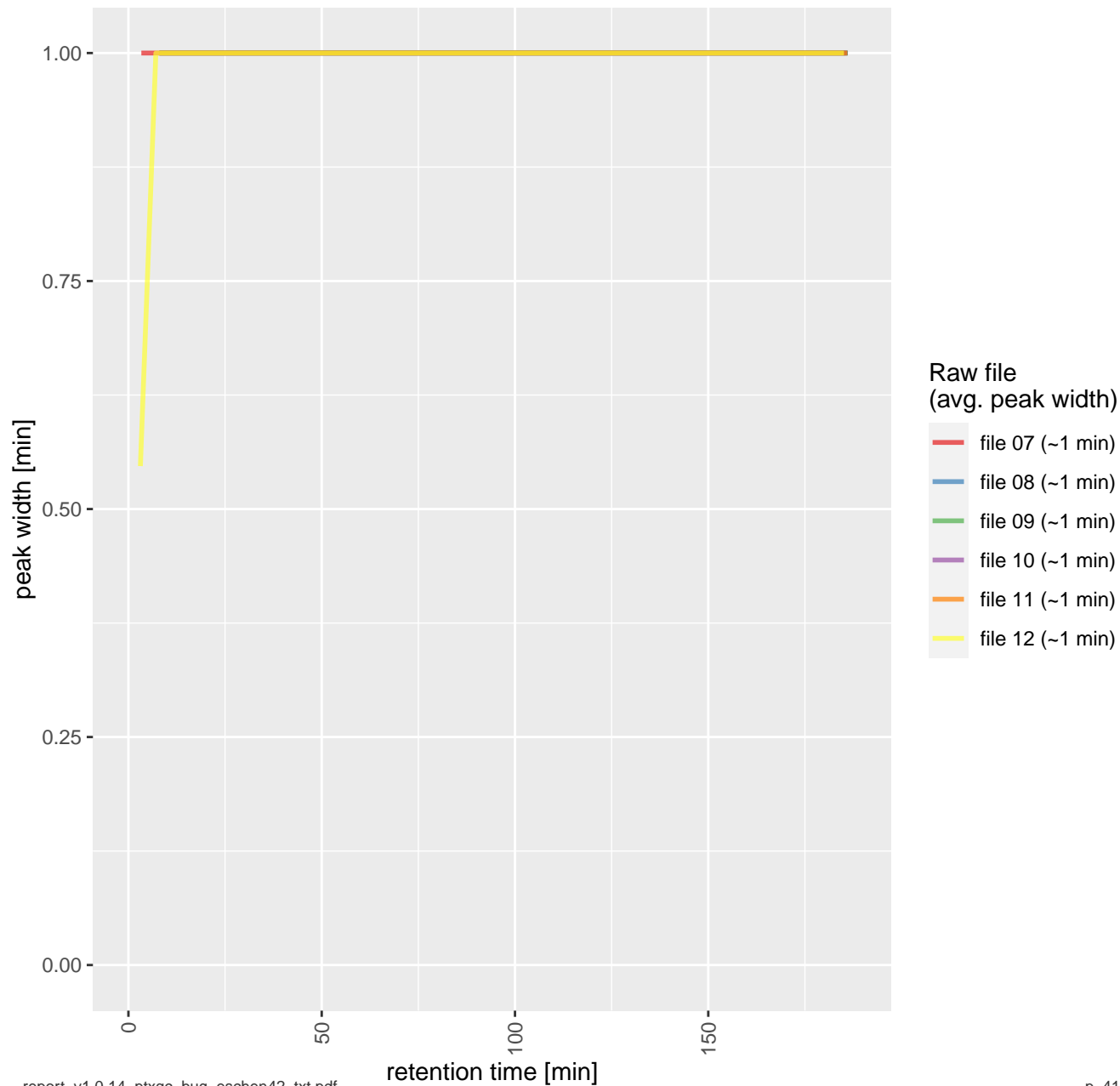




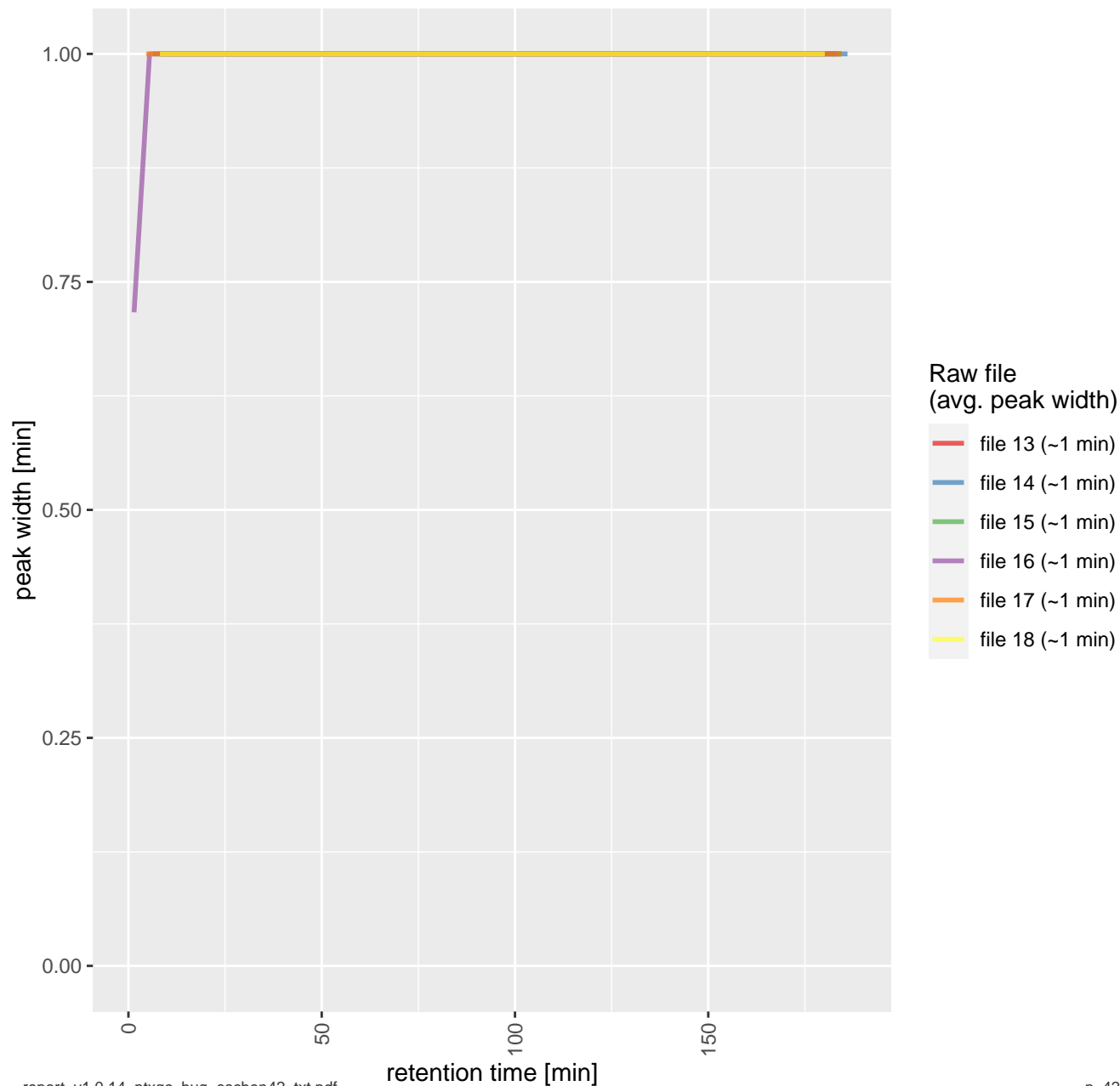
# EVD: Peak width over RT



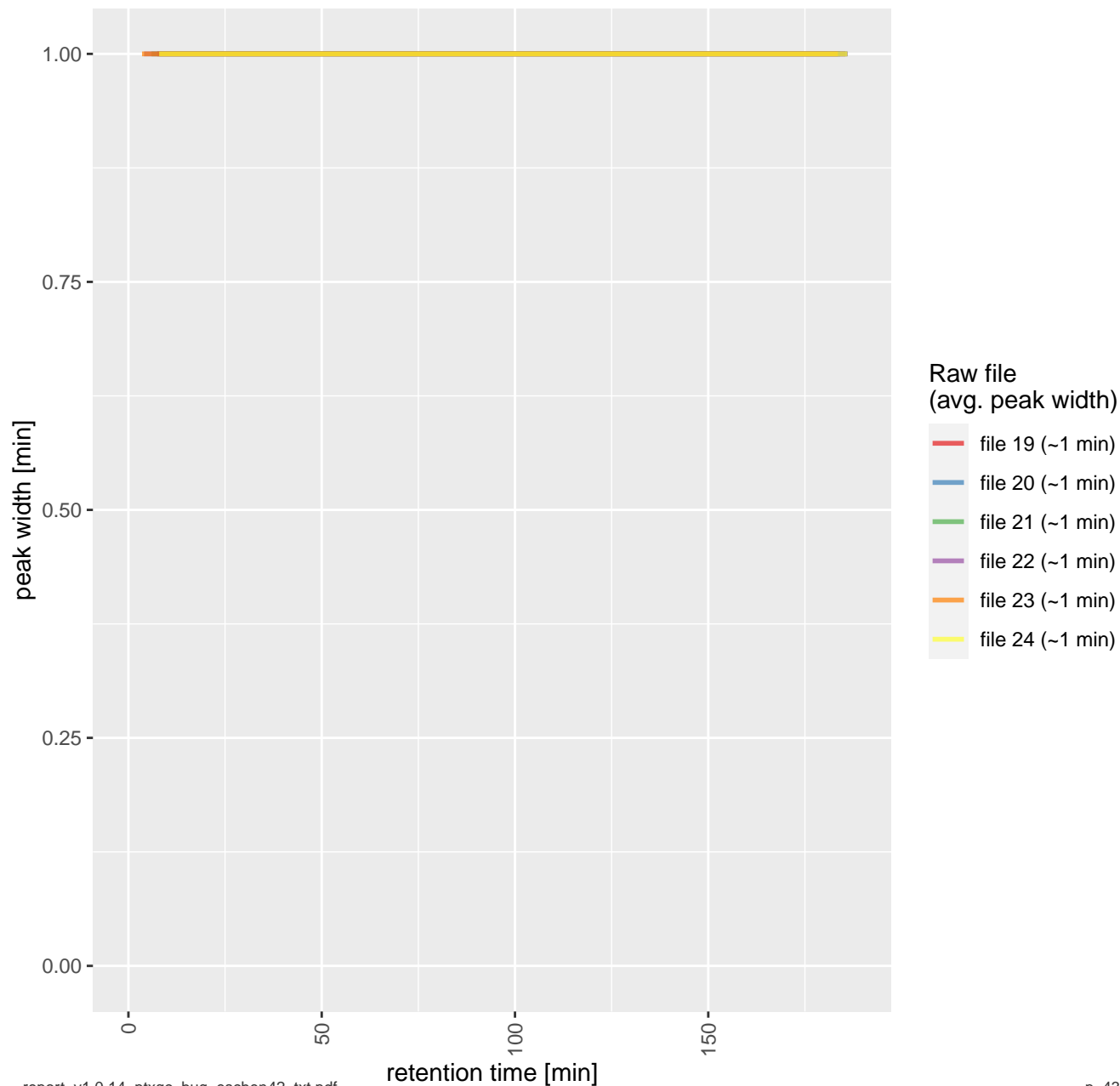
# EVD: Peak width over RT



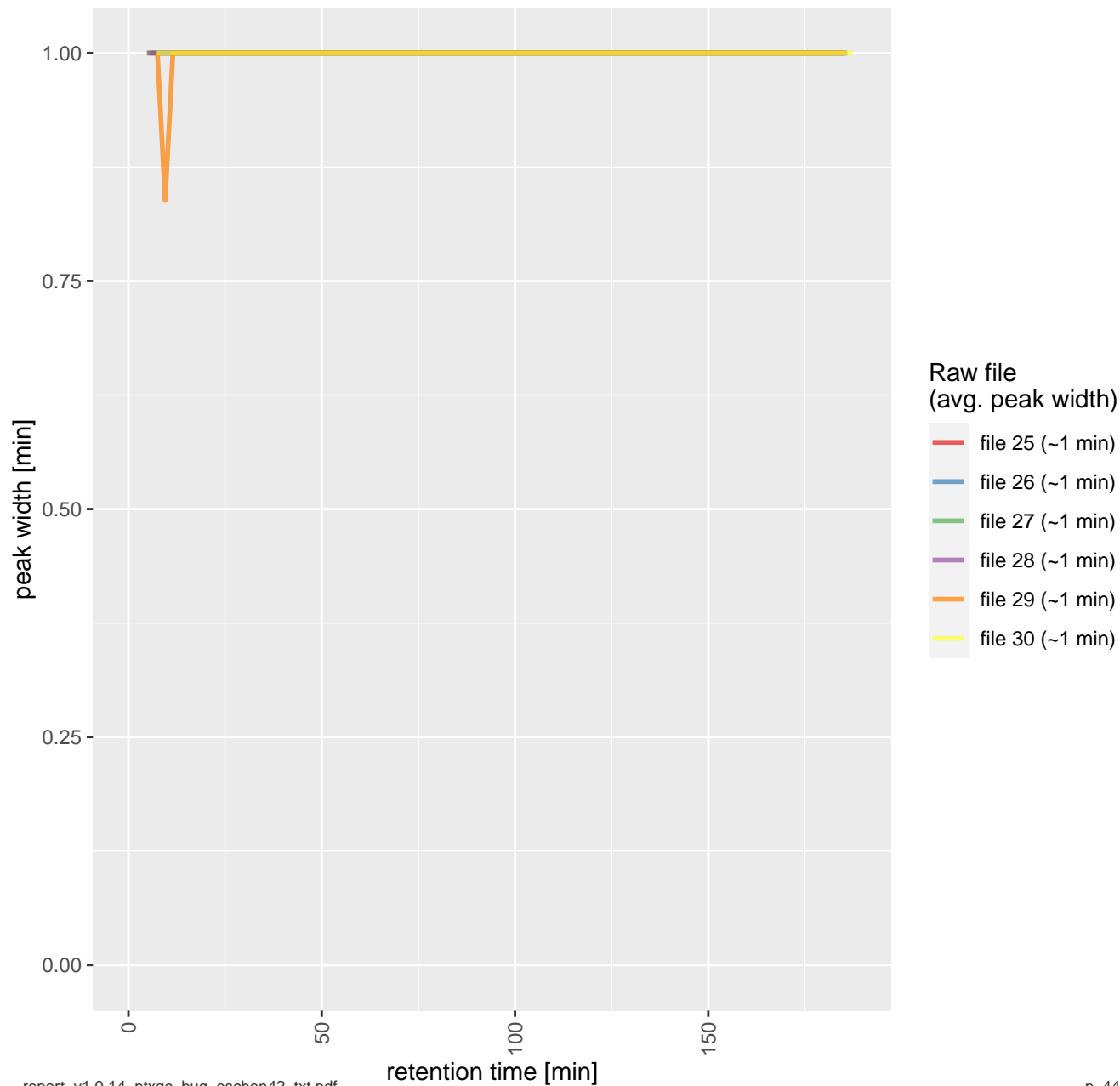
# EVD: Peak width over RT



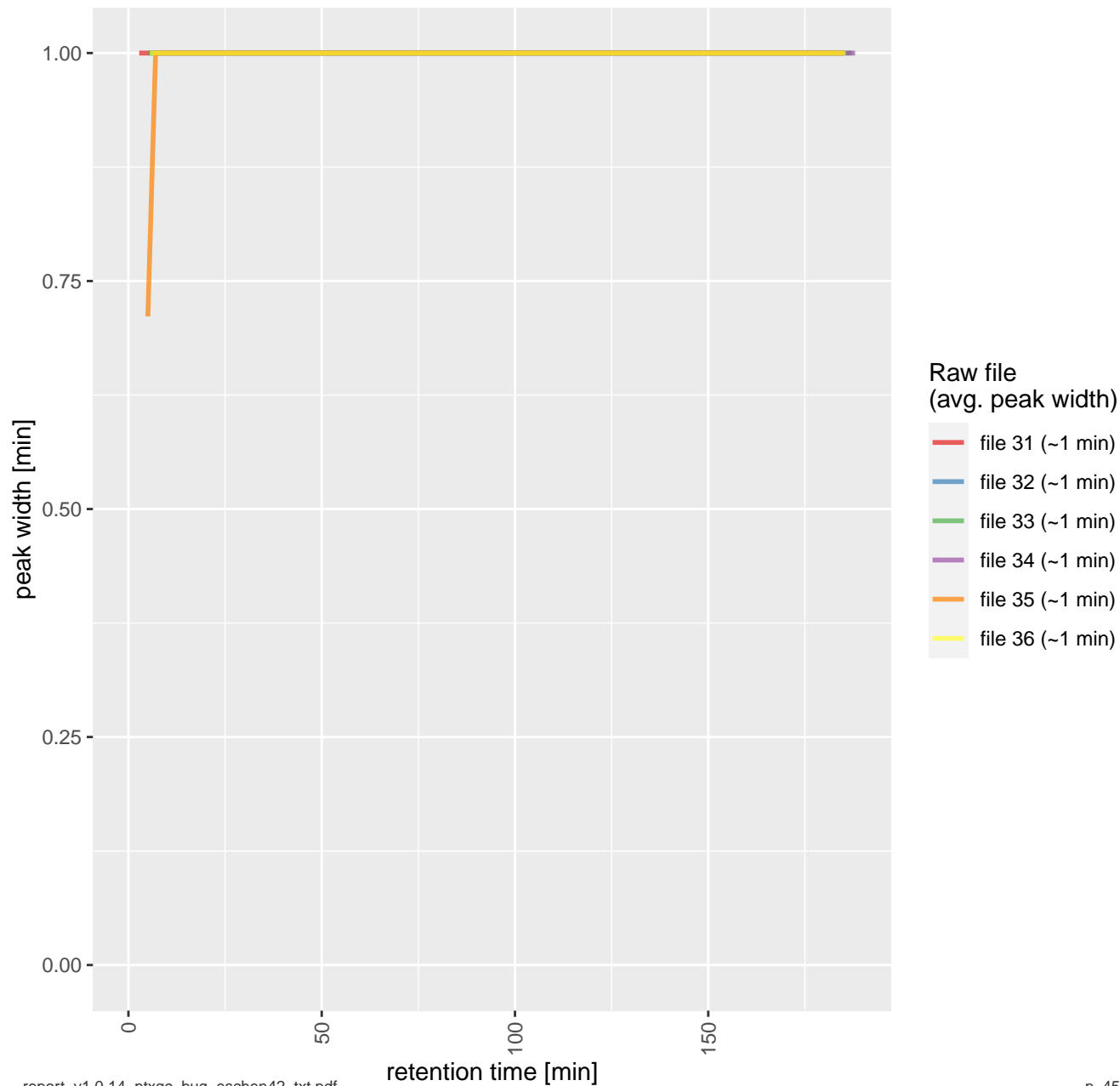
# EVD: Peak width over RT



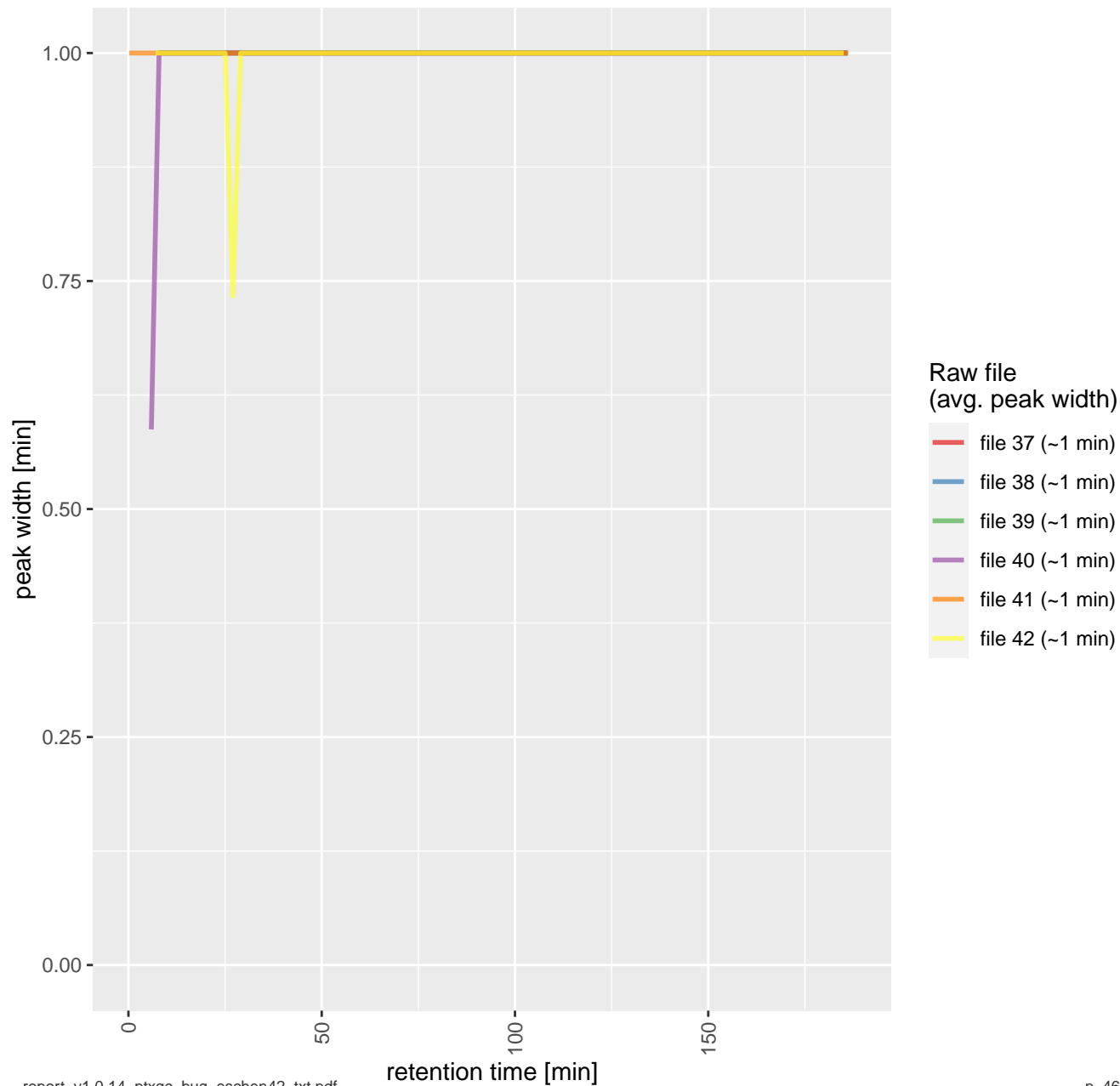
# EVD: Peak width over RT



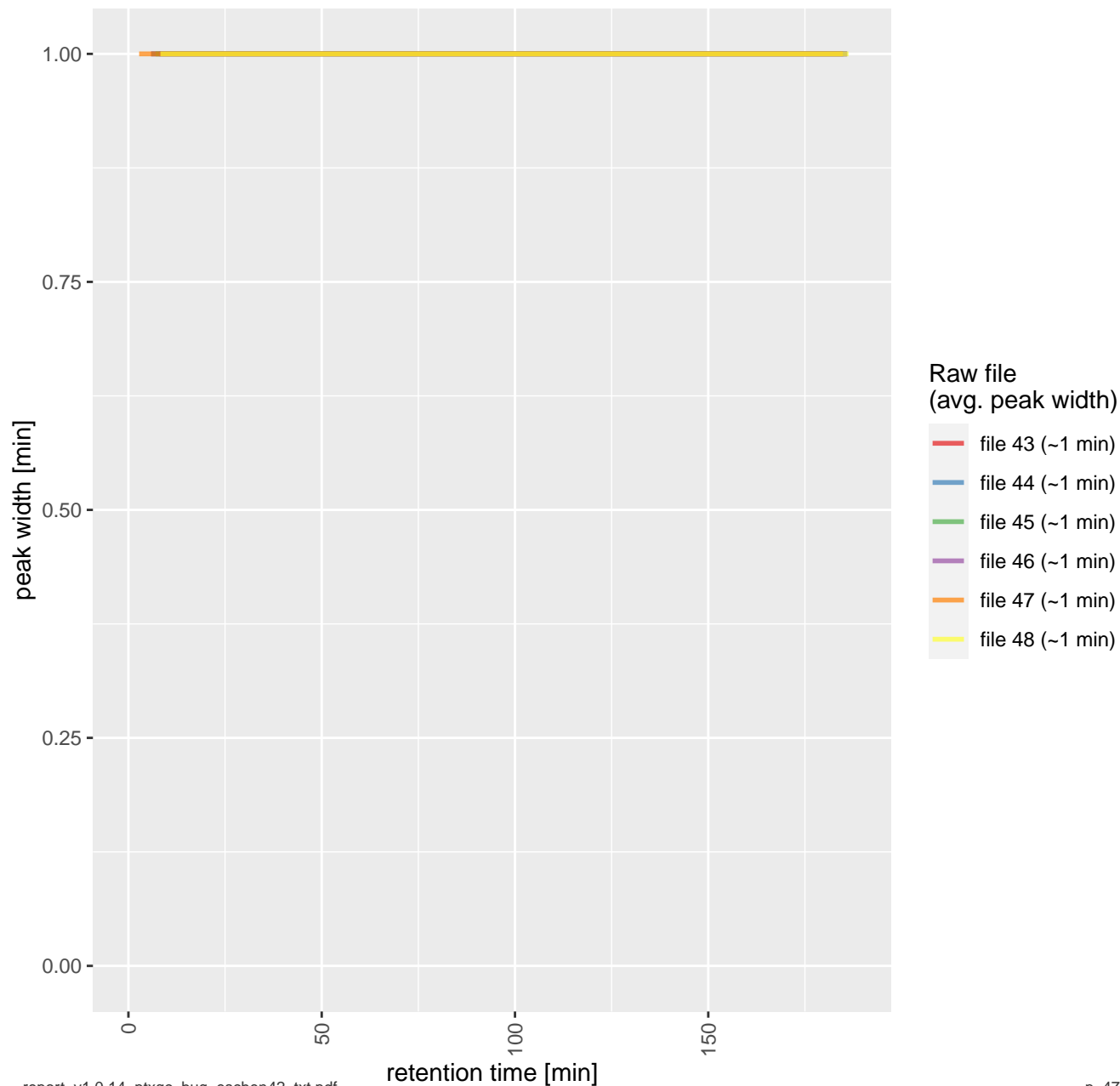
# EVD: Peak width over RT



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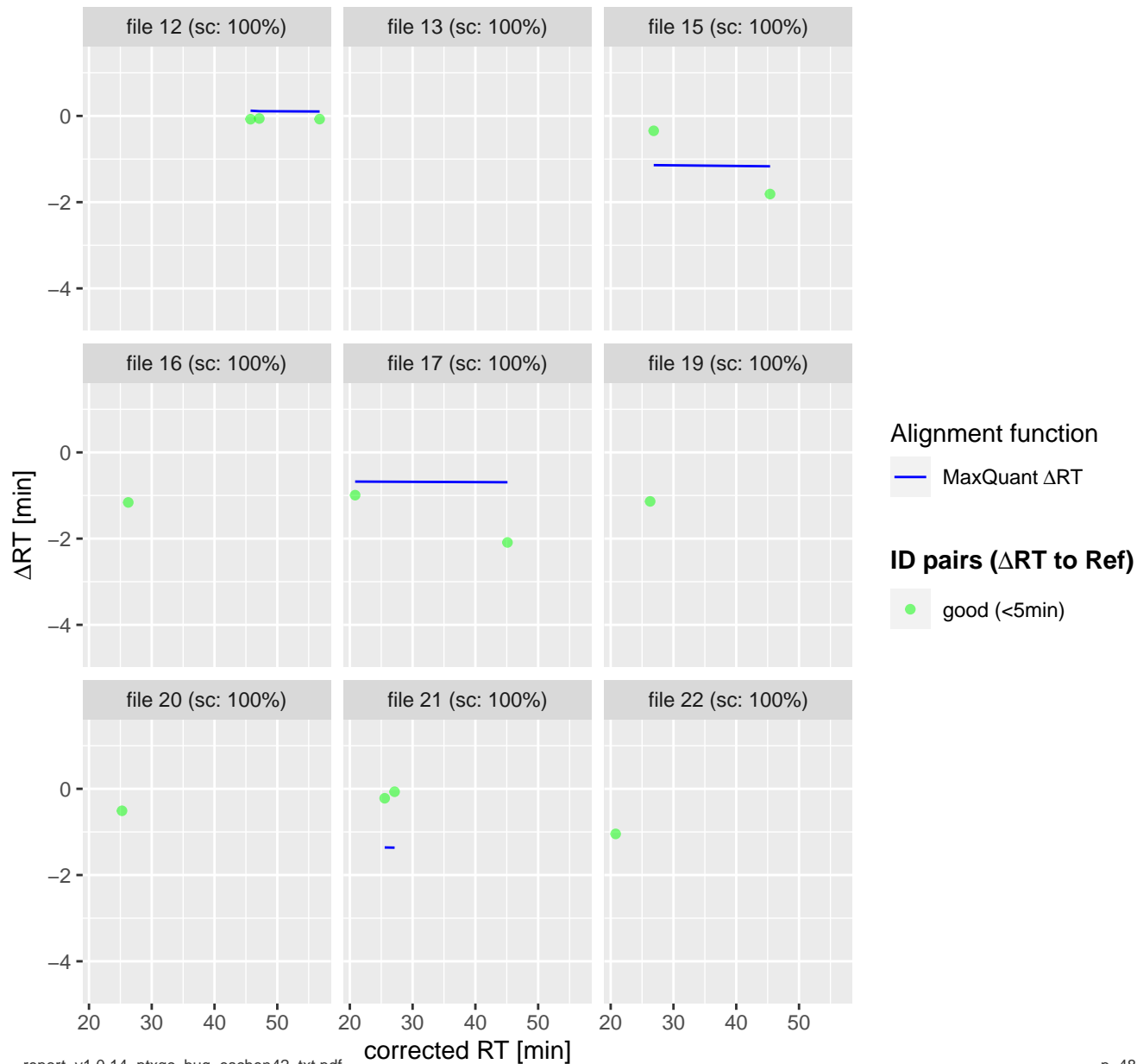
# EVD: Peak width over RT





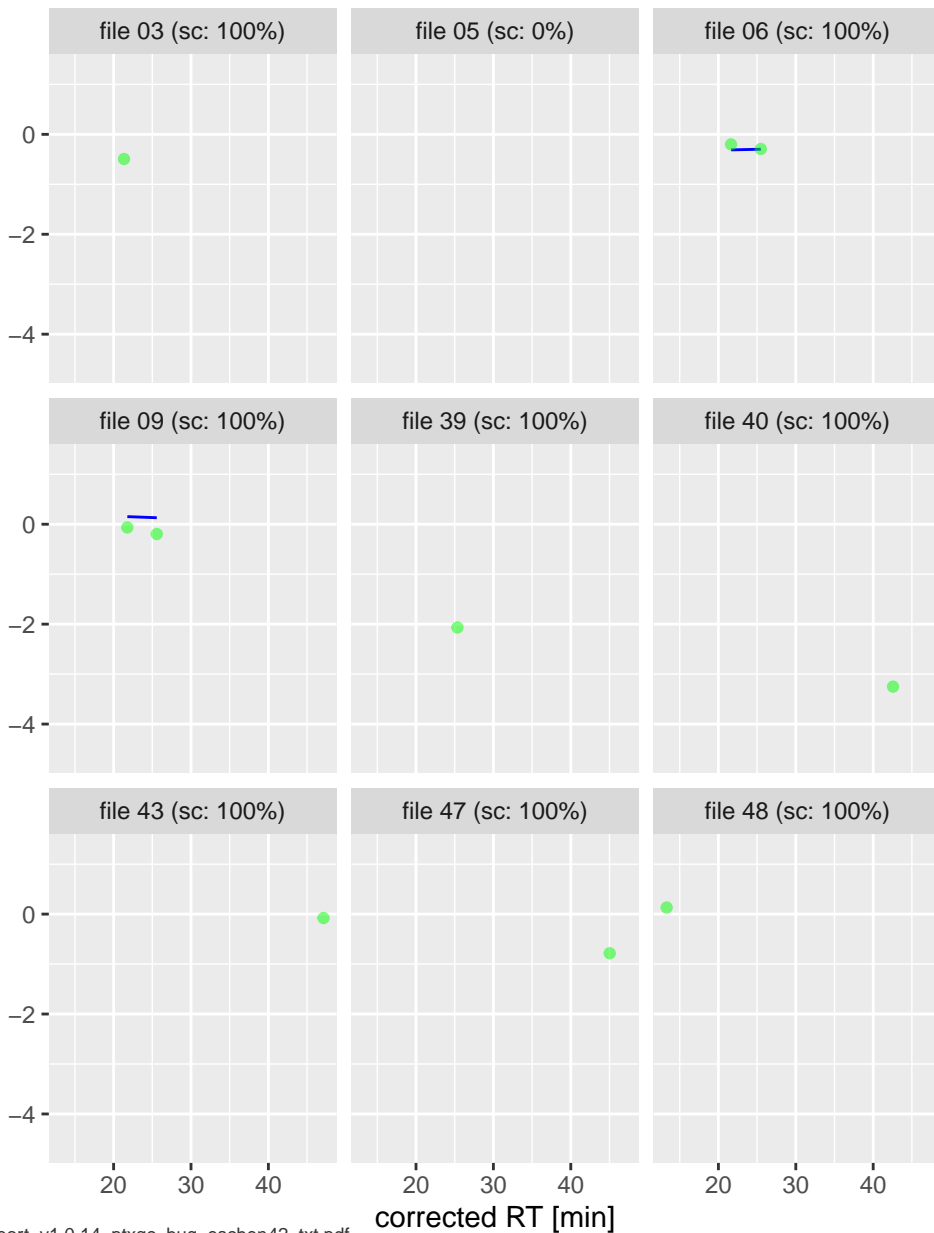
# EVD: MBR – alignment

alignment reference: jdrake\_zsychev\_18366\_20211124\_FAIMS\_totalPr\_26\_s96\_3408.raw.therm



# EVD: MBR – alignment

alignment reference: jdrake\_zsychev\_18366\_20211124\_FAIMS\_totalPr\_26\_s96\_3408.raw.therm



Alignment function

MaxQuant  $\Delta RT$

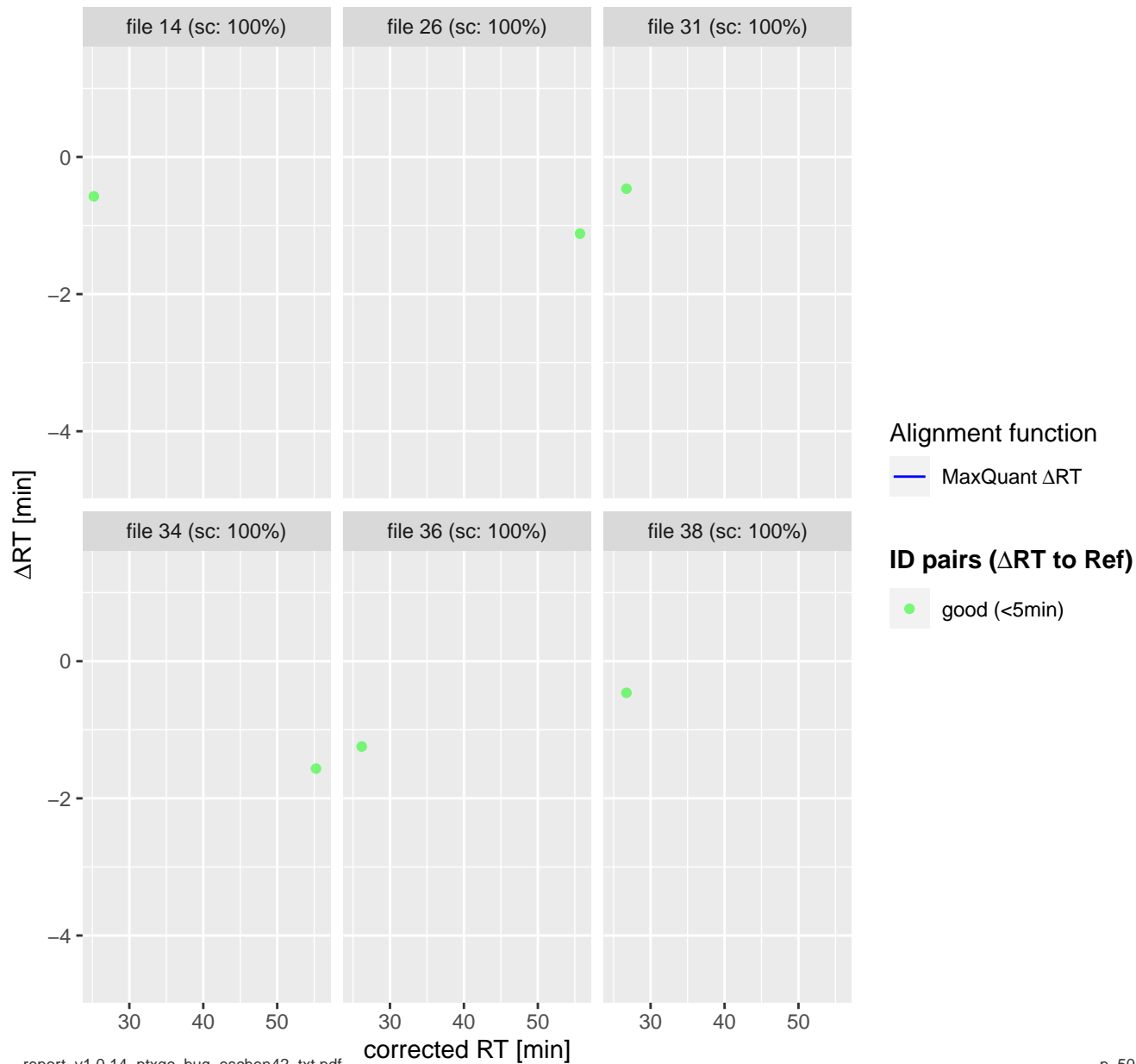
**ID pairs ( $\Delta RT$  to Ref)**

good ( $< 5$ min)

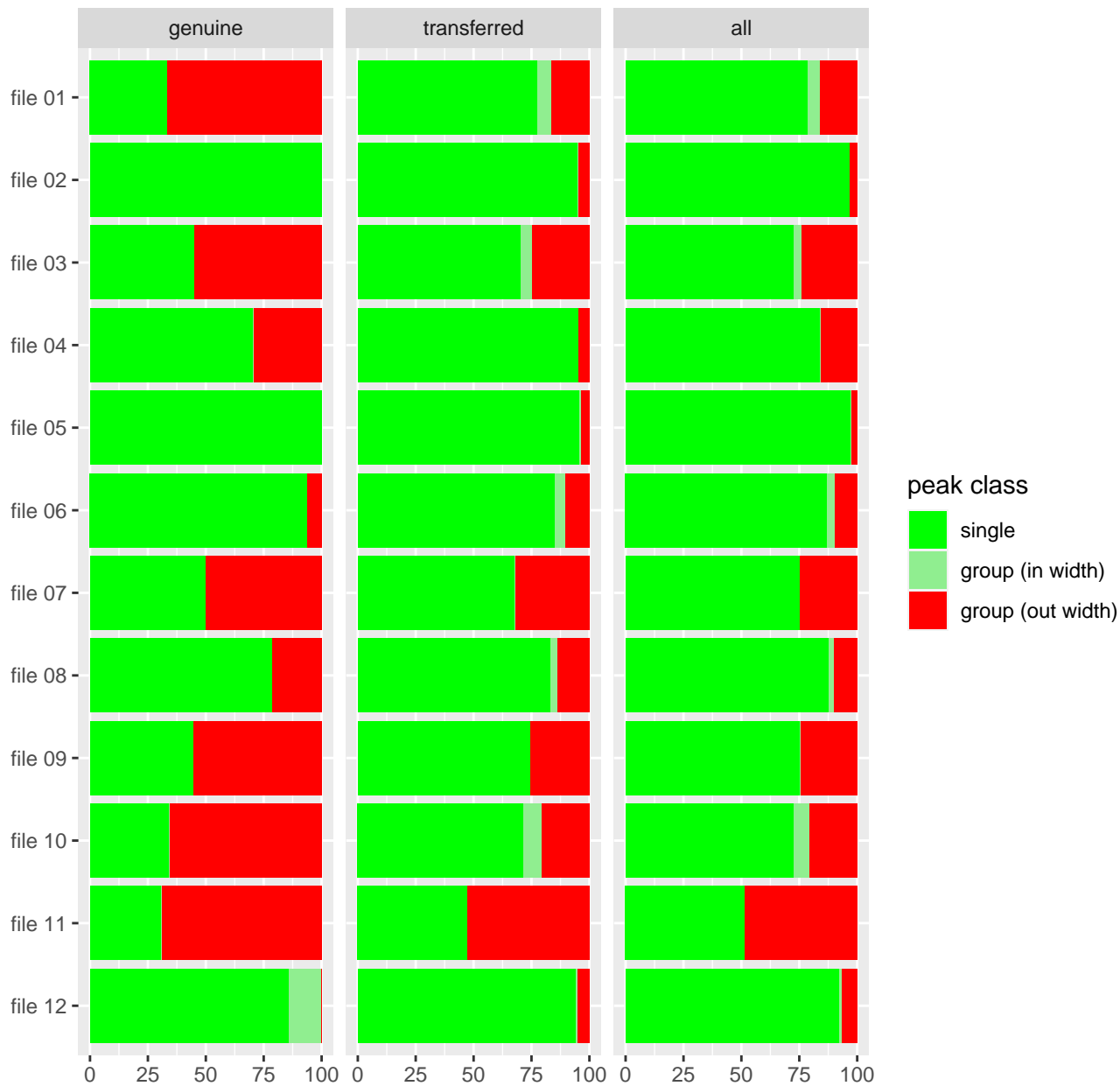
bad ( $> 5$ min)

# EVD: MBR – alignment

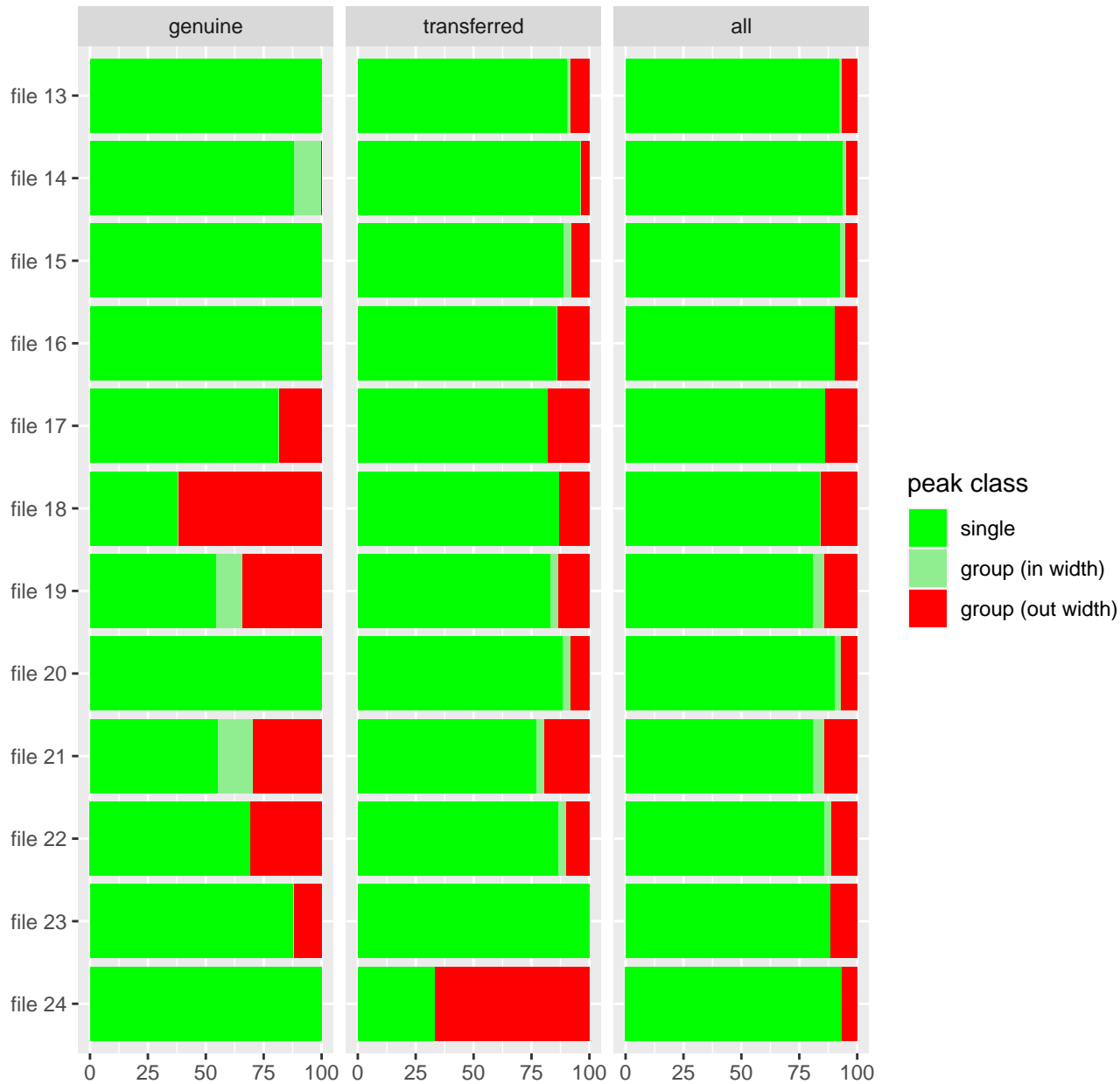
alignment reference: jdrake\_zsychev\_18366\_20211124\_FAIMS\_totalPr\_26\_s96\_3408.raw.therm



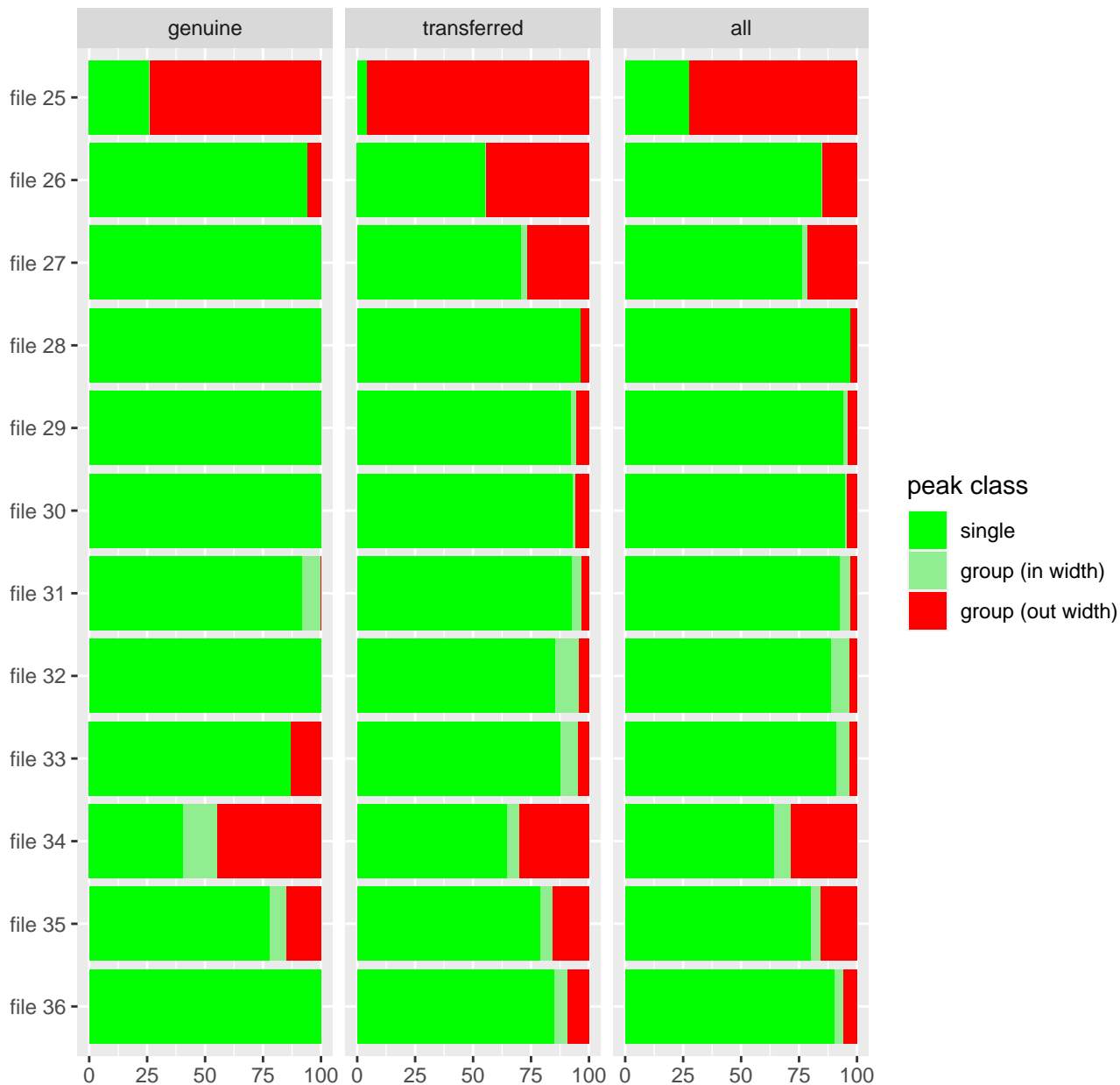
# EVD: MBR – ID Transfer



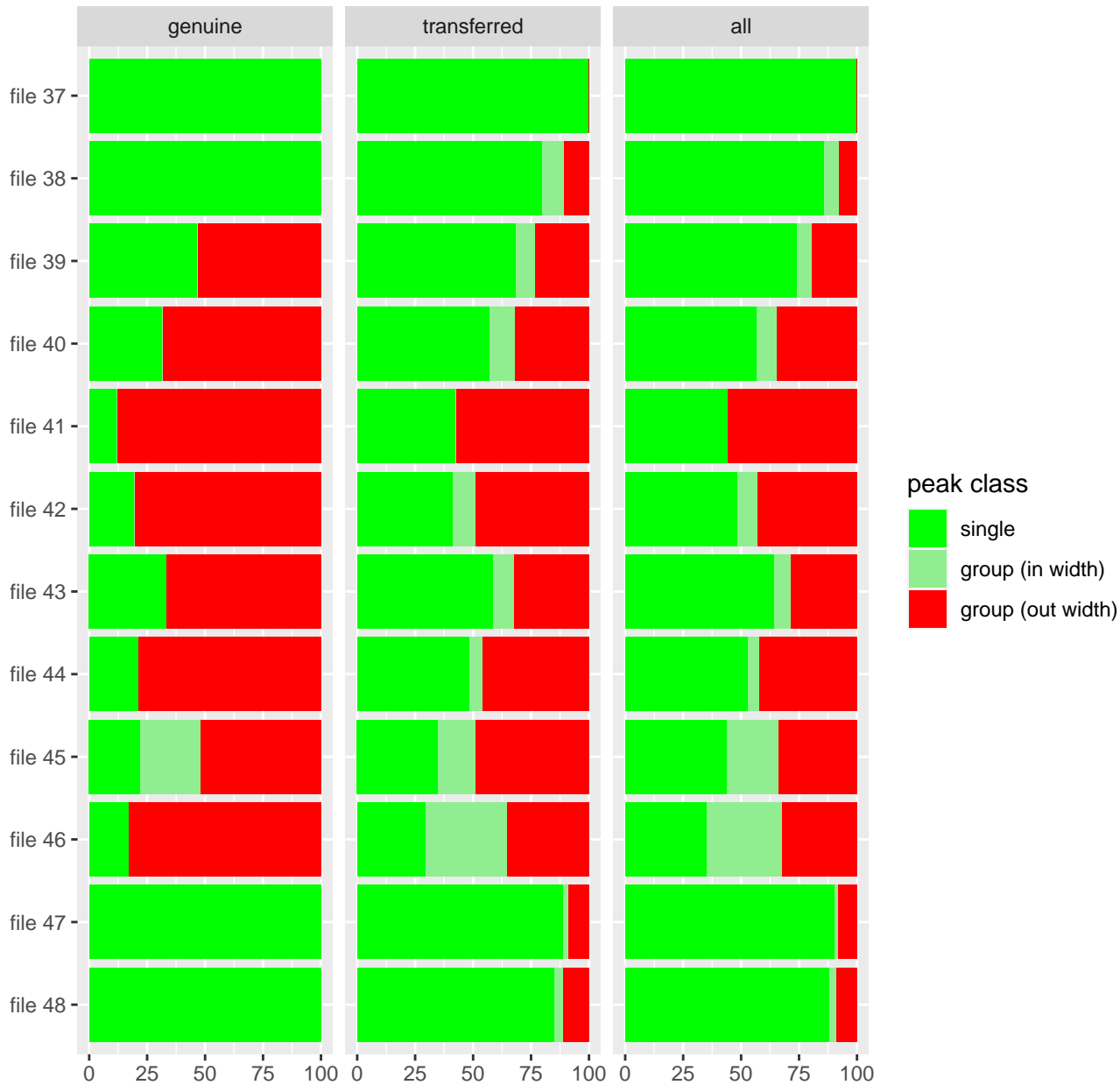
# EVD: MBR – ID Transfer



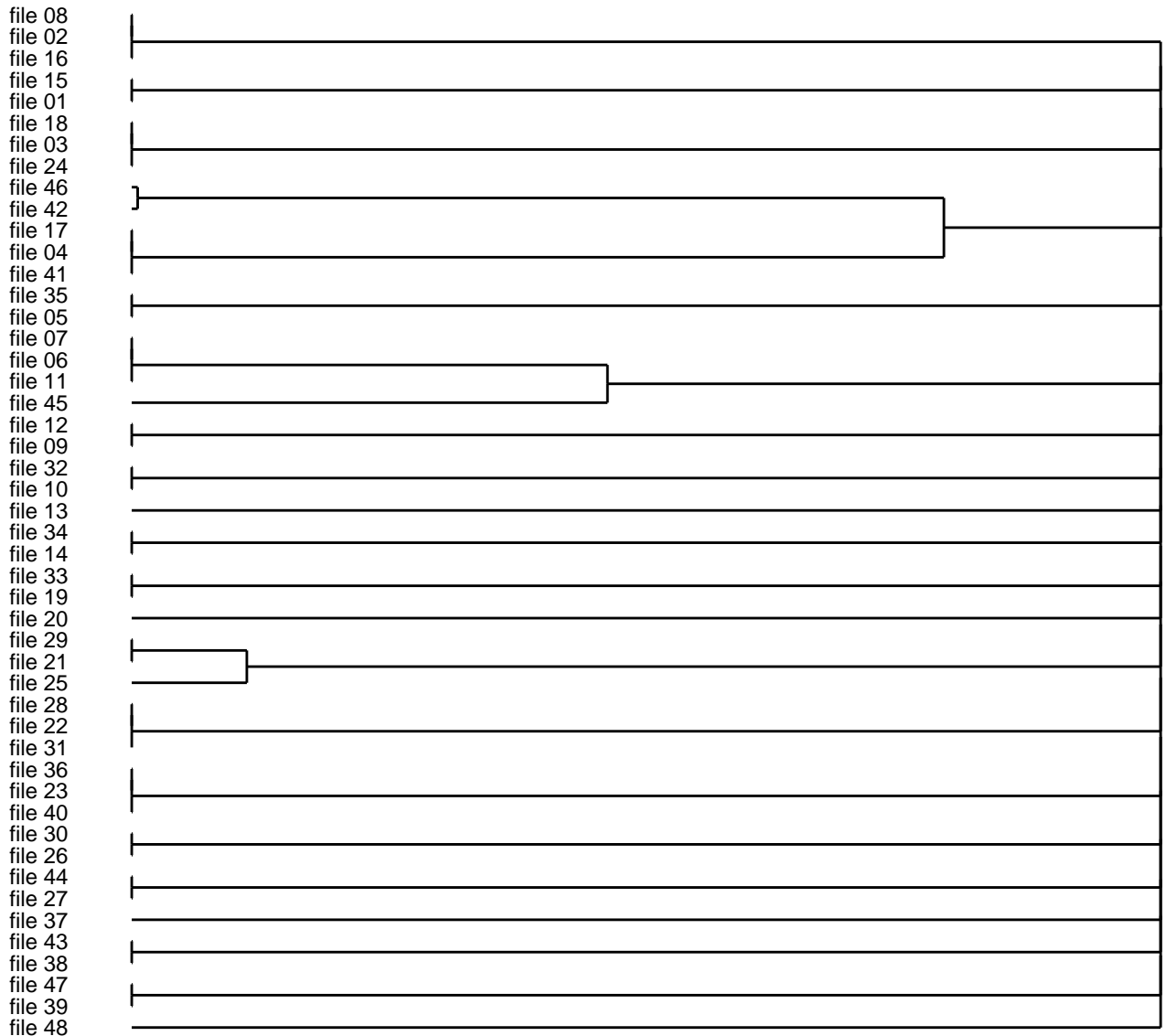
# EVD: MBR – ID Transfer



# EVD: MBR – ID Transfer

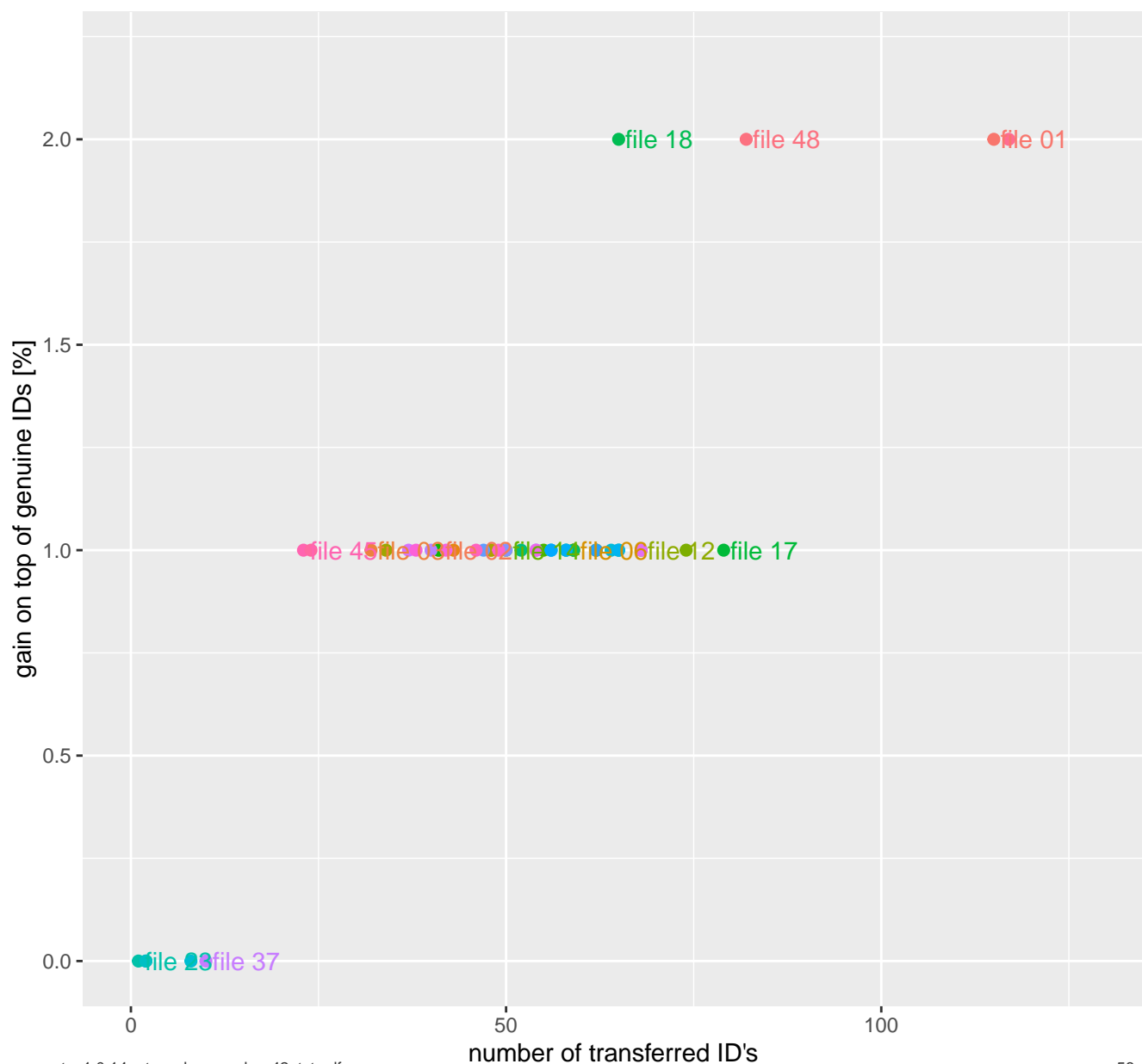


# [experimental] EVD: Clustering Tree of Raw files by Correlation of Corrected Retention Times

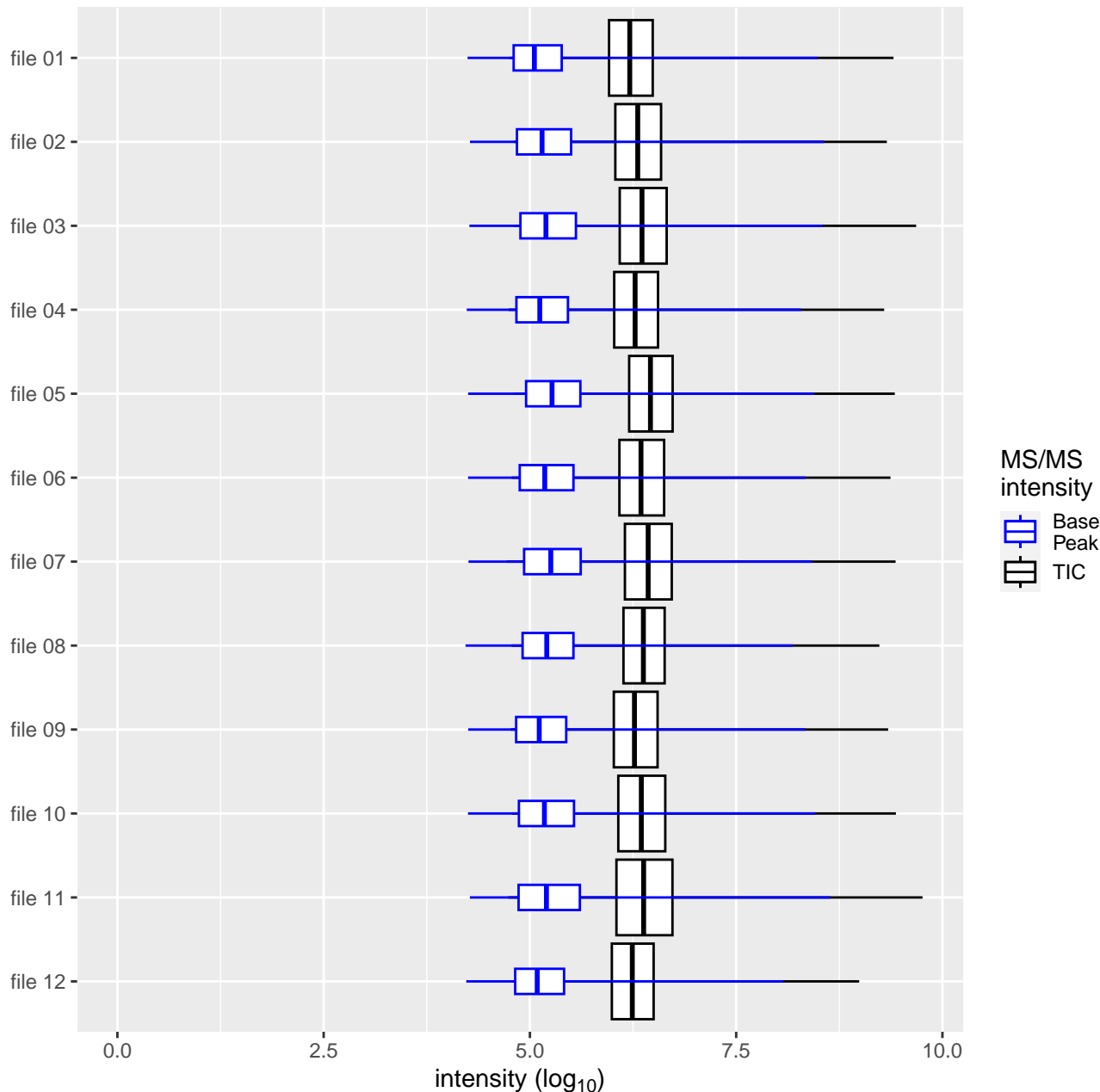




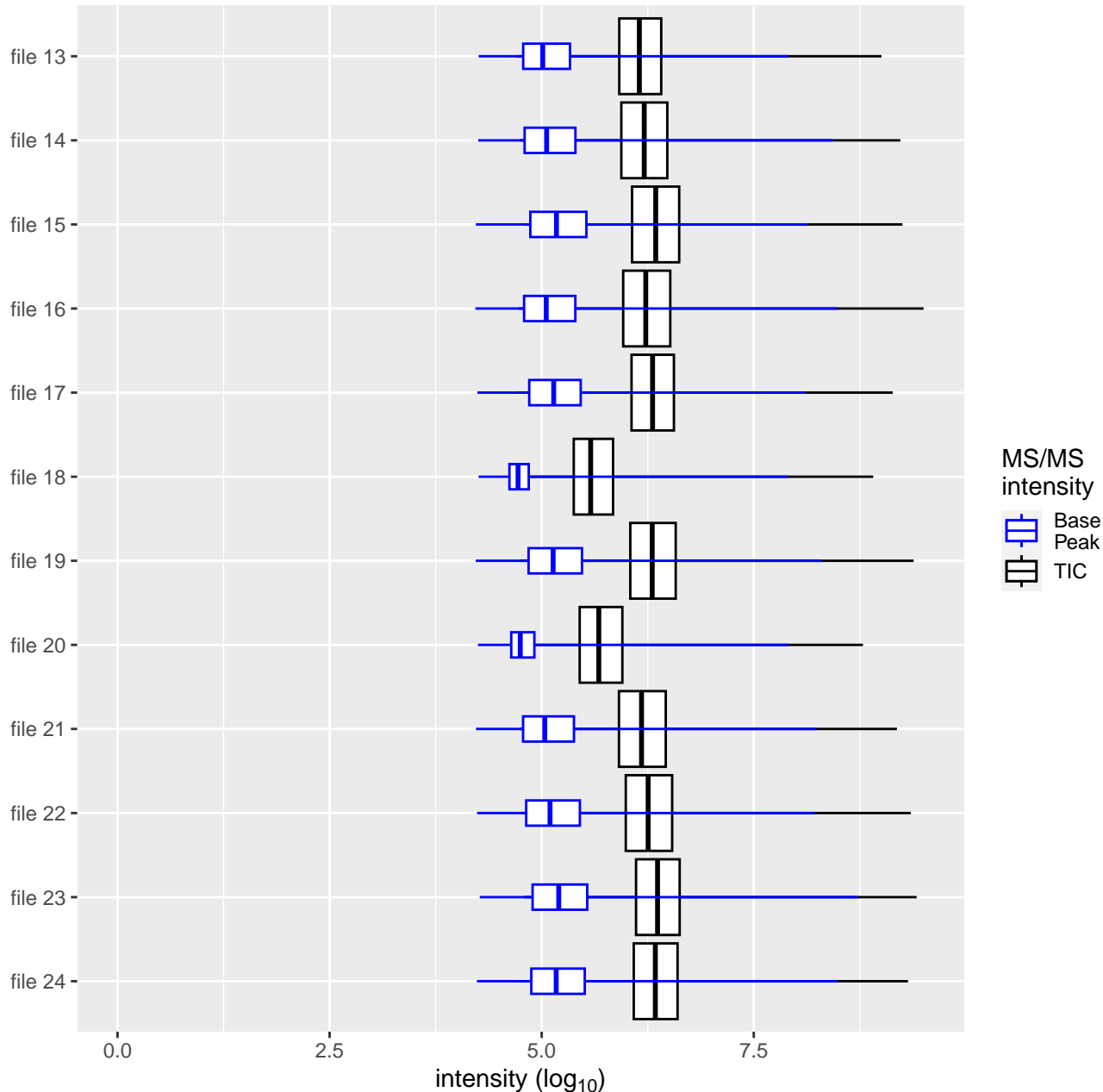
# EVD: Peptides inferred by MBR



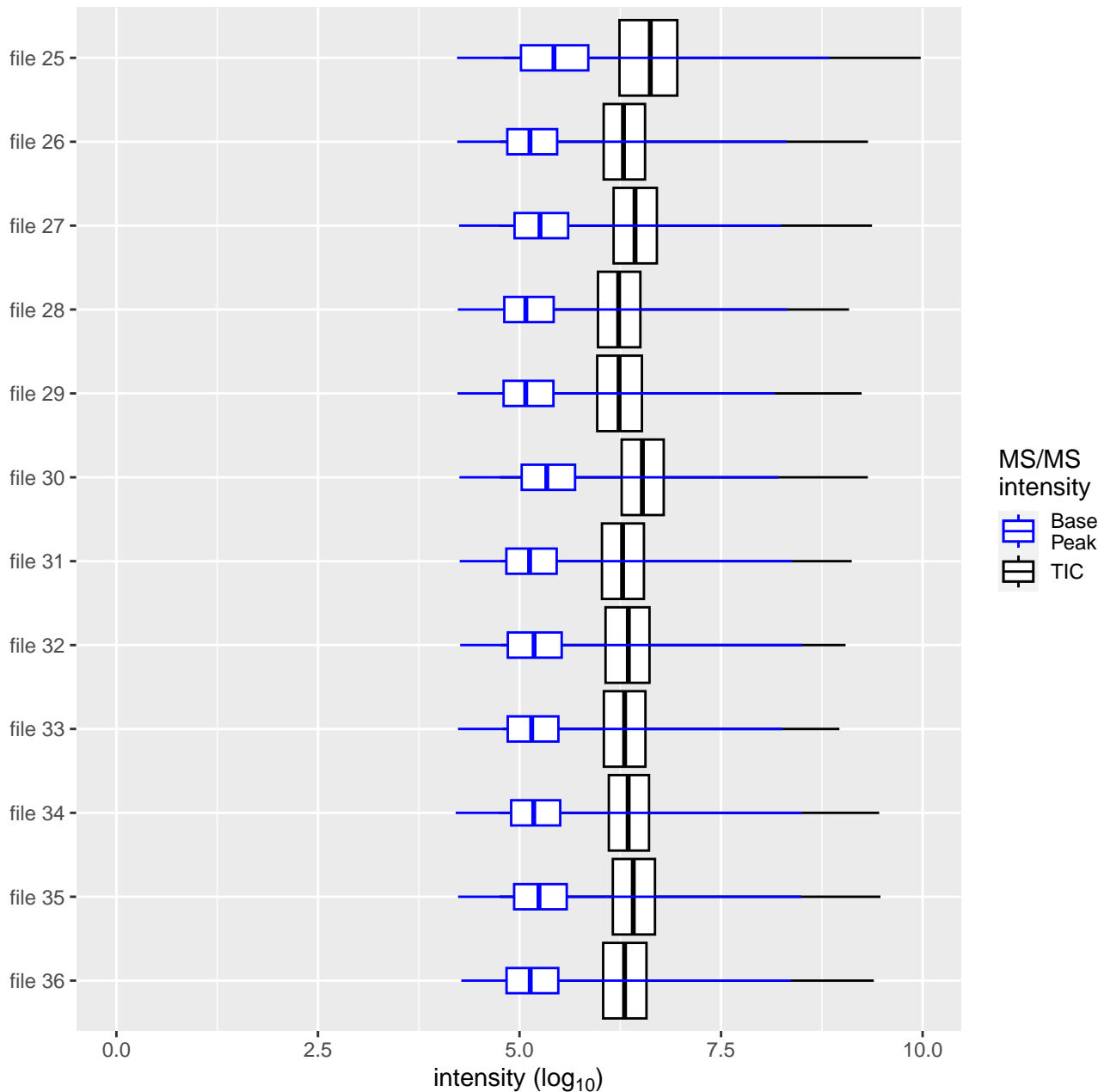
# [experimental] MSMSscans: MS/MS intensity



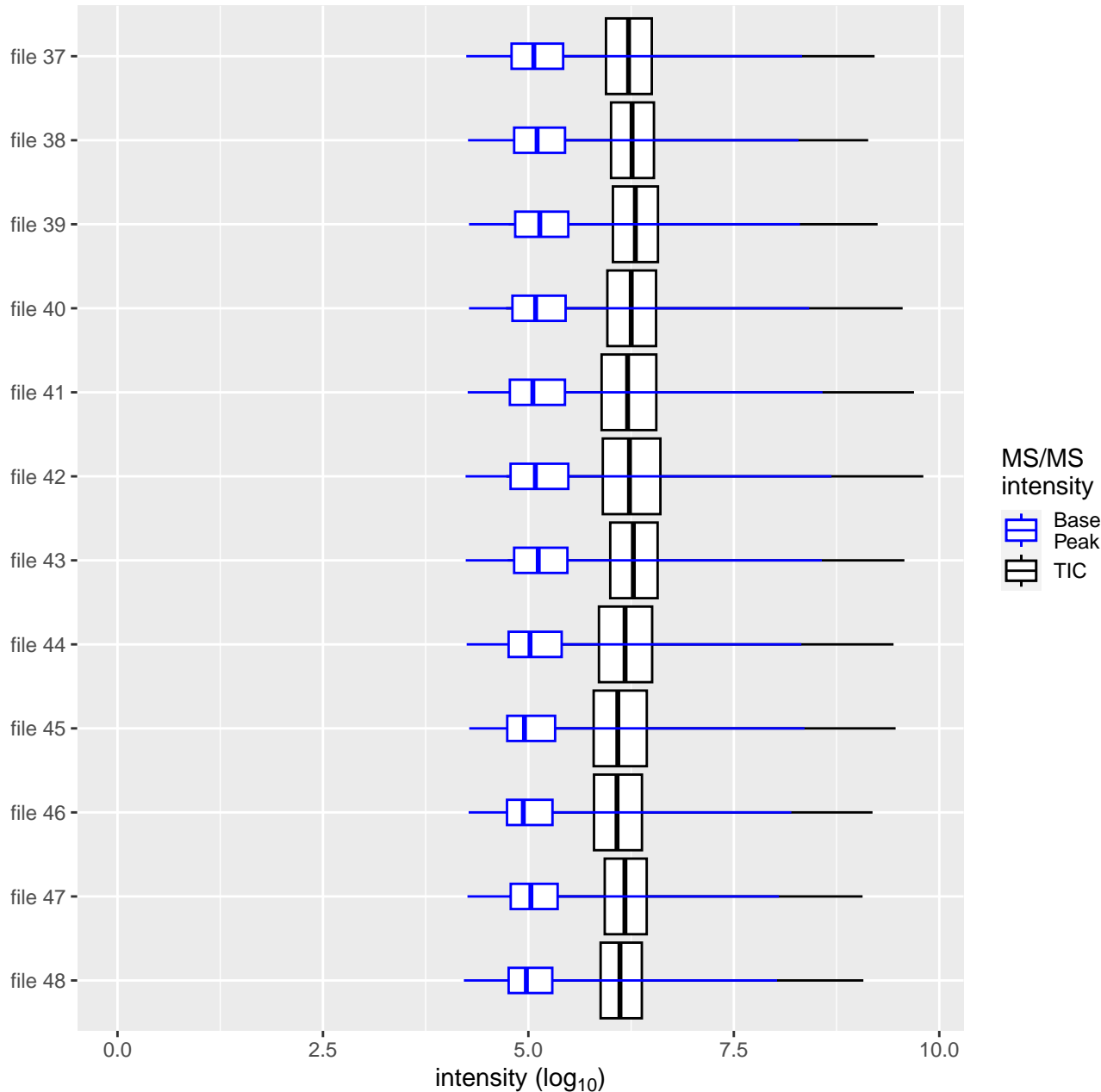
# [experimental] MSMSscans: MS/MS intensity



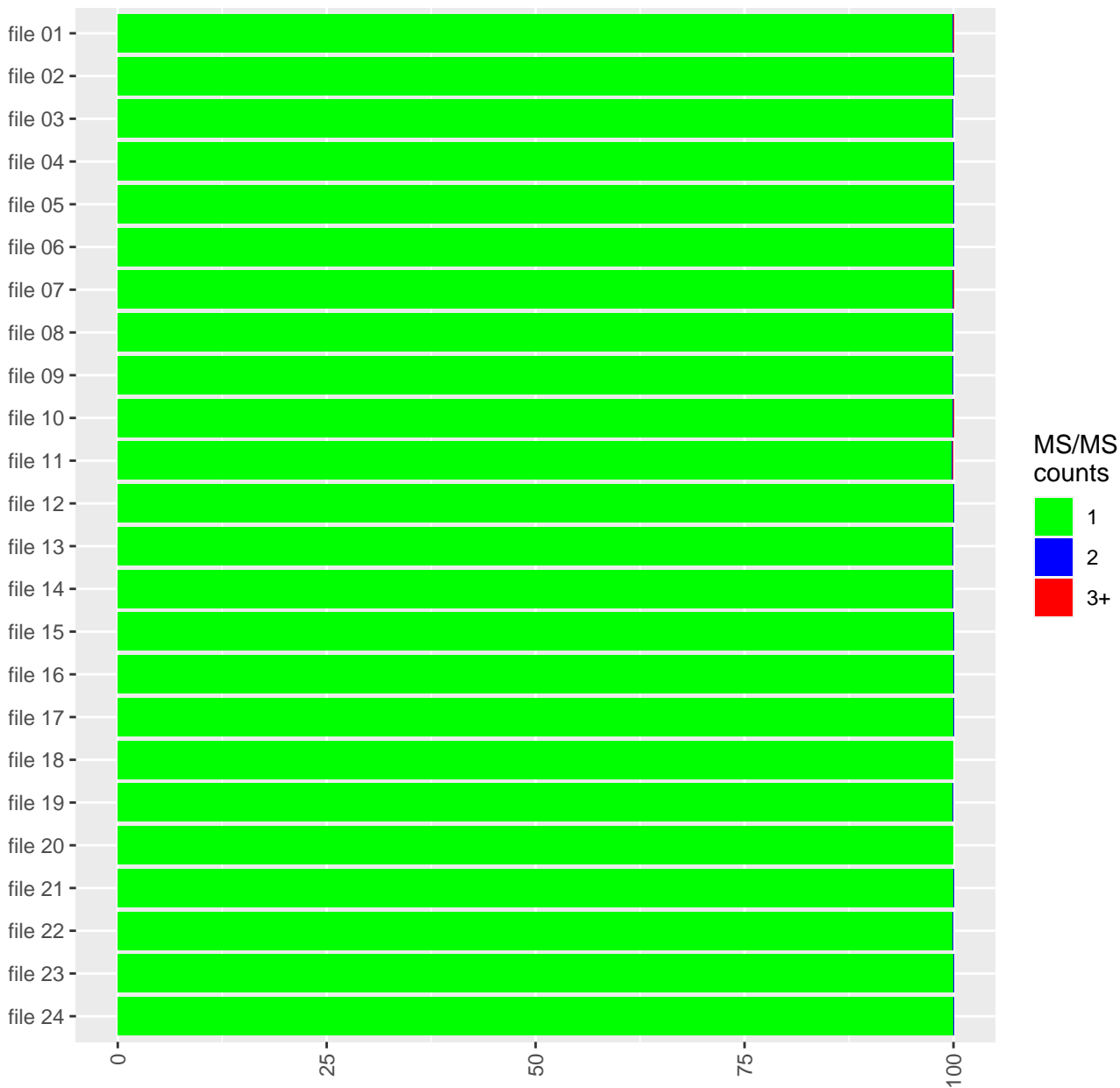
# [experimental] MSMSscans: MS/MS intensity



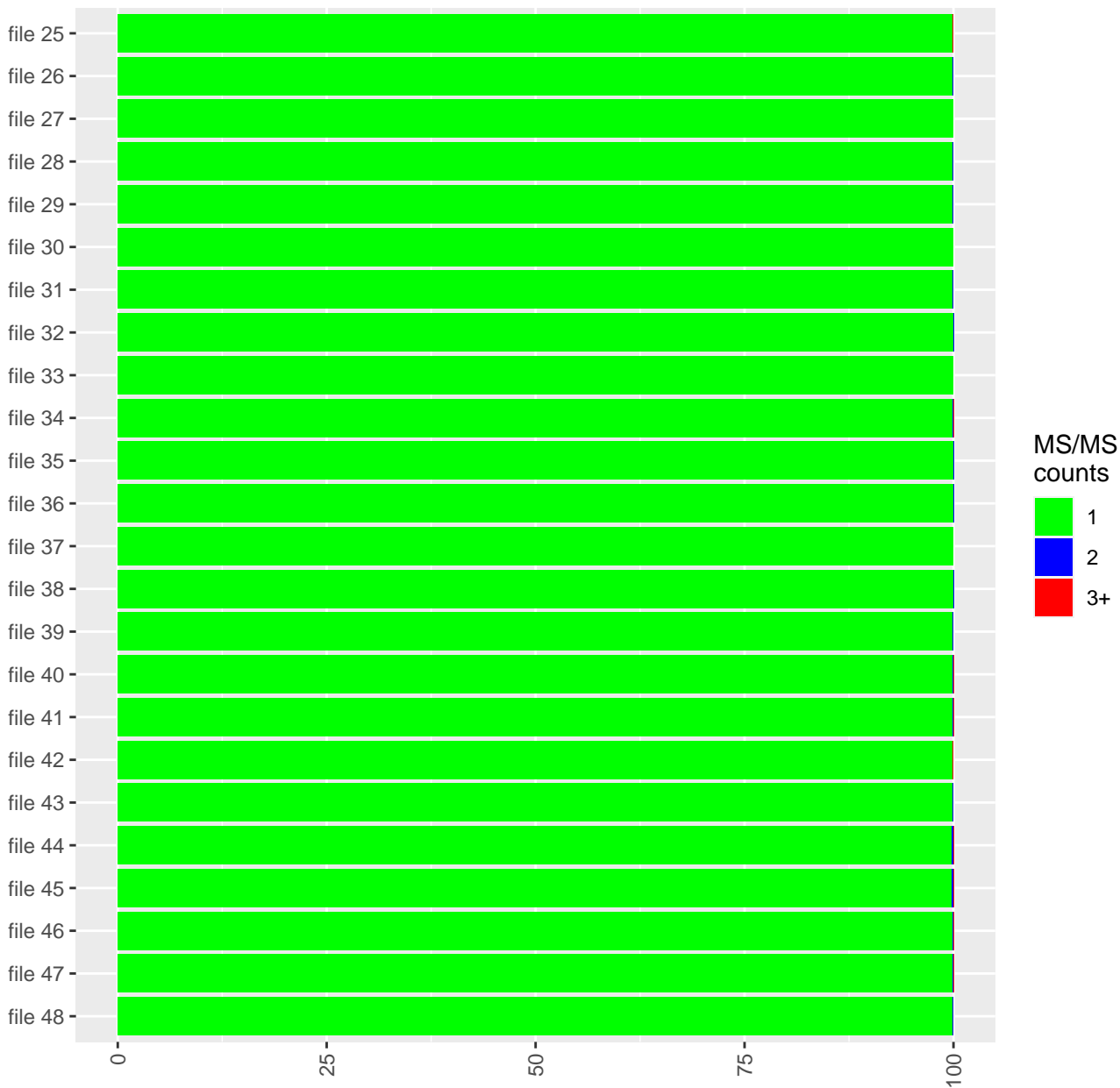
# [experimental] MSMSscans: MS/MS intensity



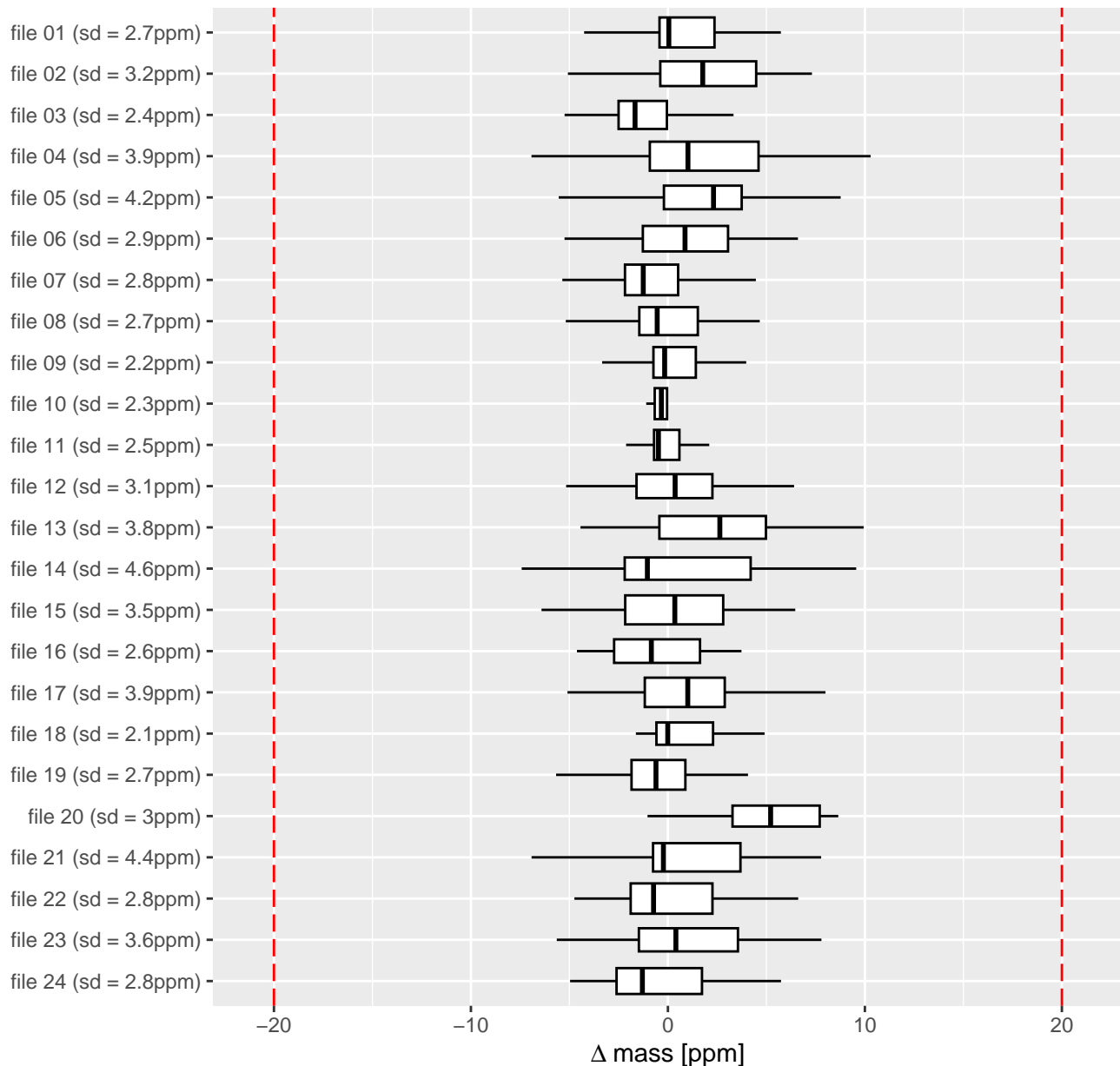
# EVD: Oversampling (MS/MS counts per 3D-peak)



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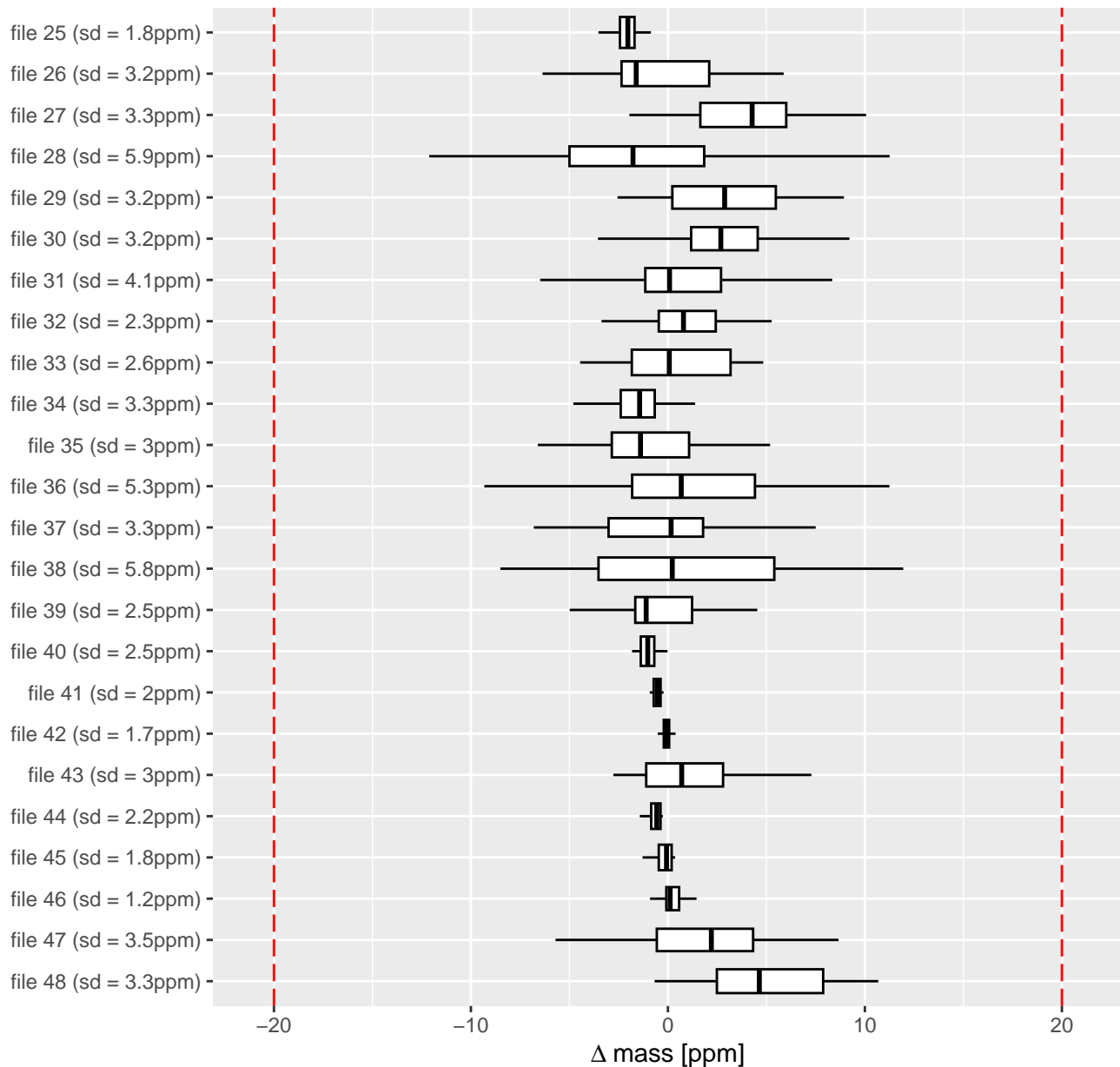


# EVD: Uncalibrated mass error

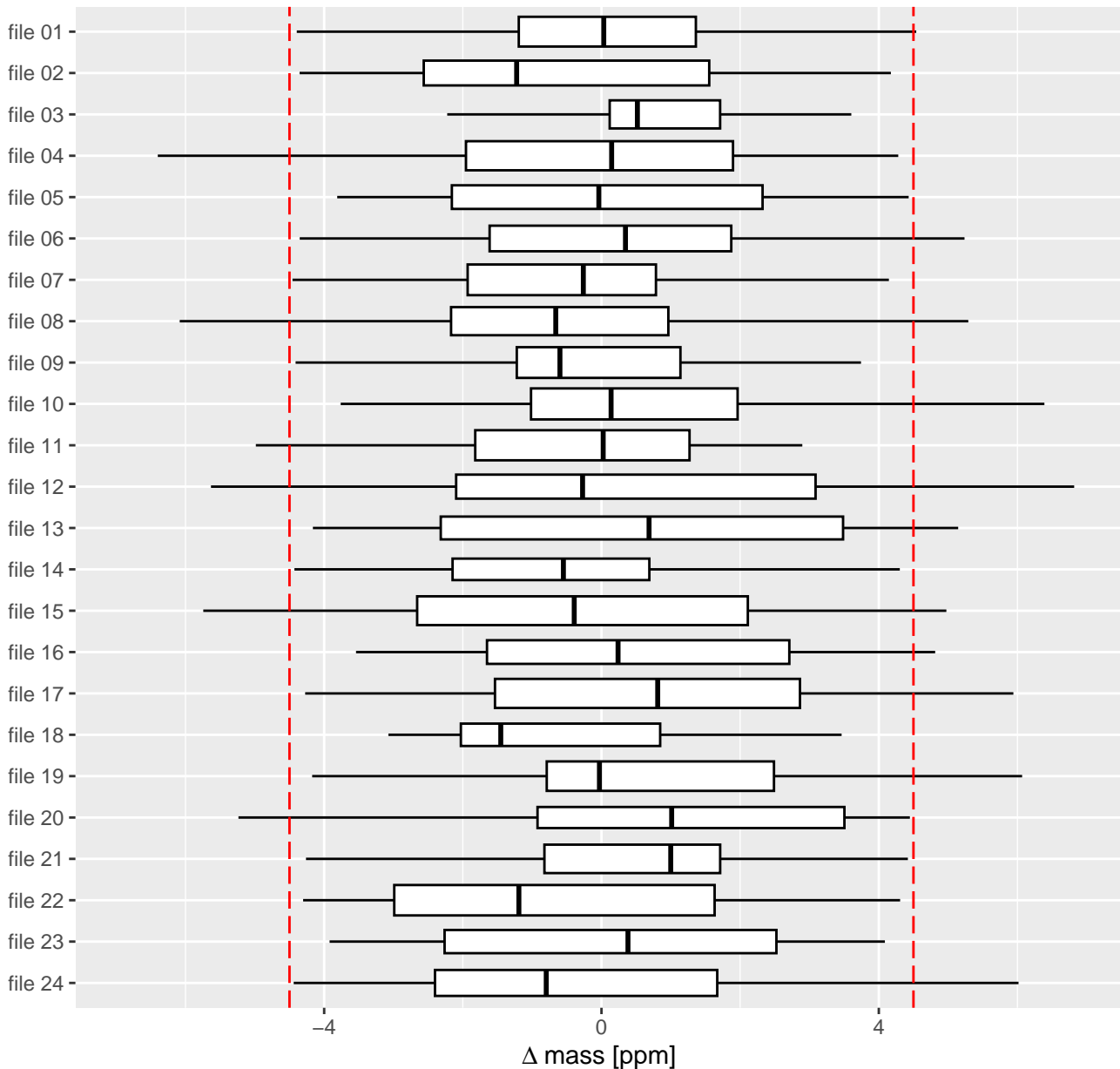




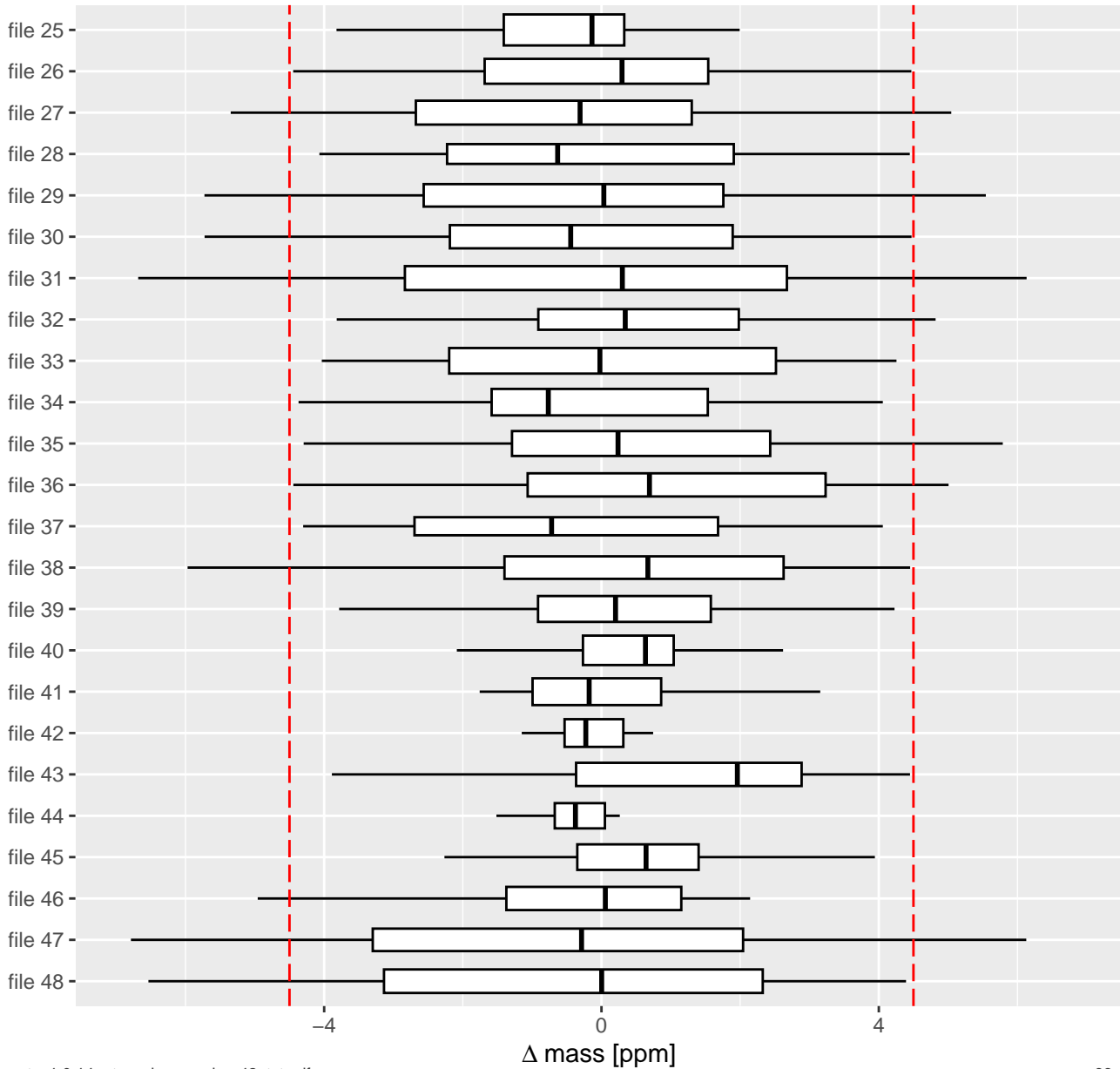
# EVD: Uncalibrated mass error



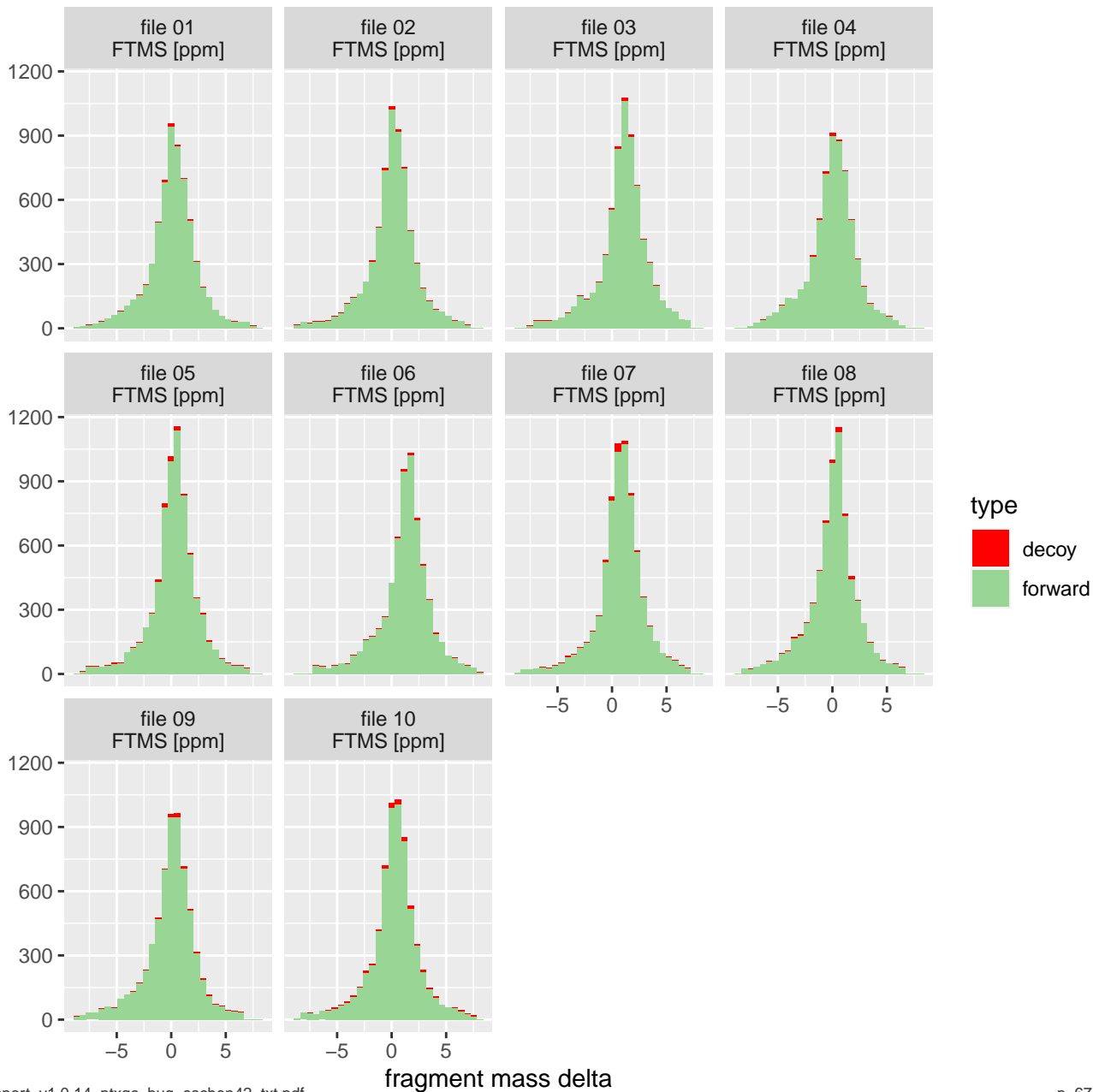
# EVD: Calibrated mass error



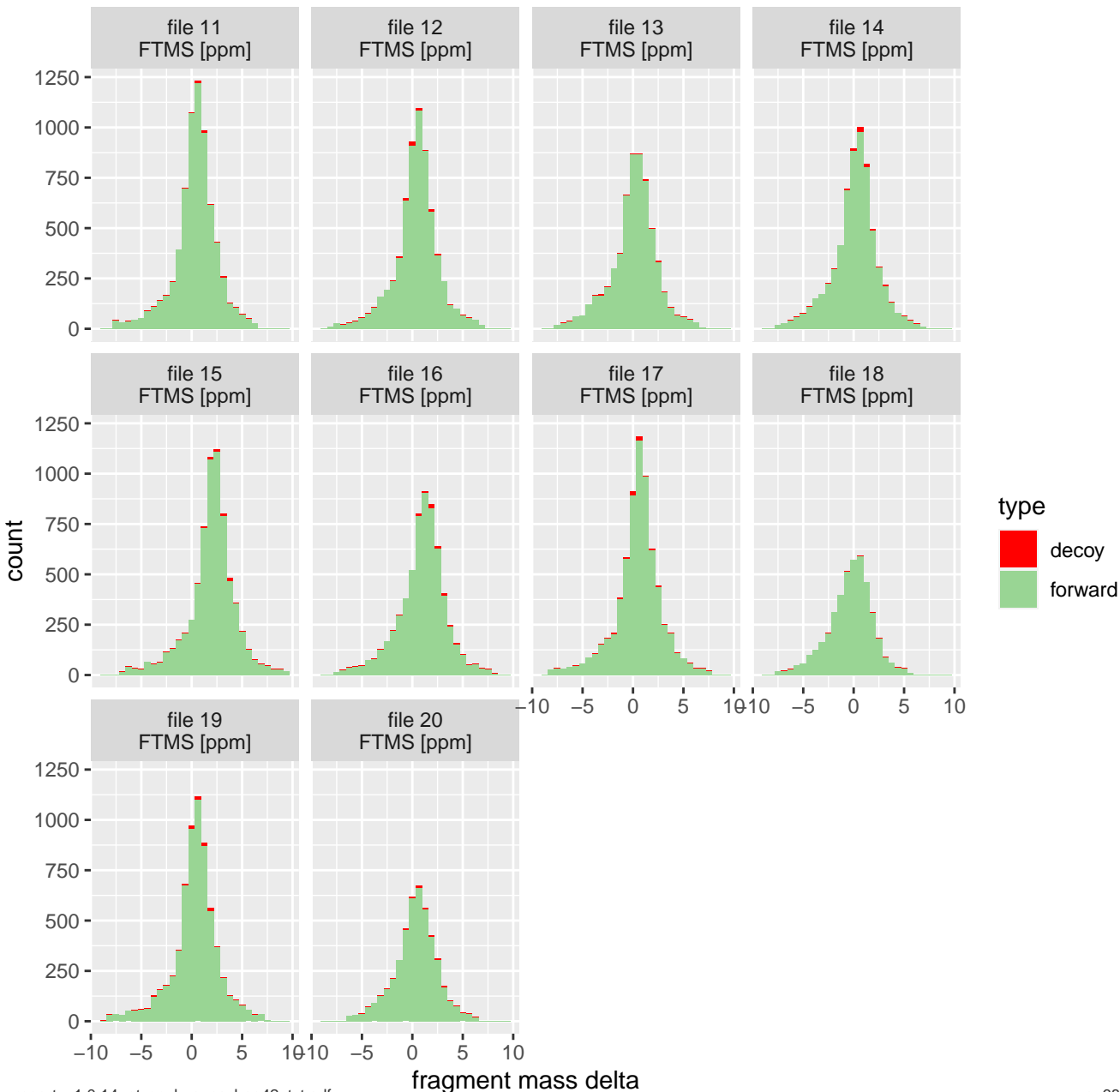
# EVD: Calibrated mass error



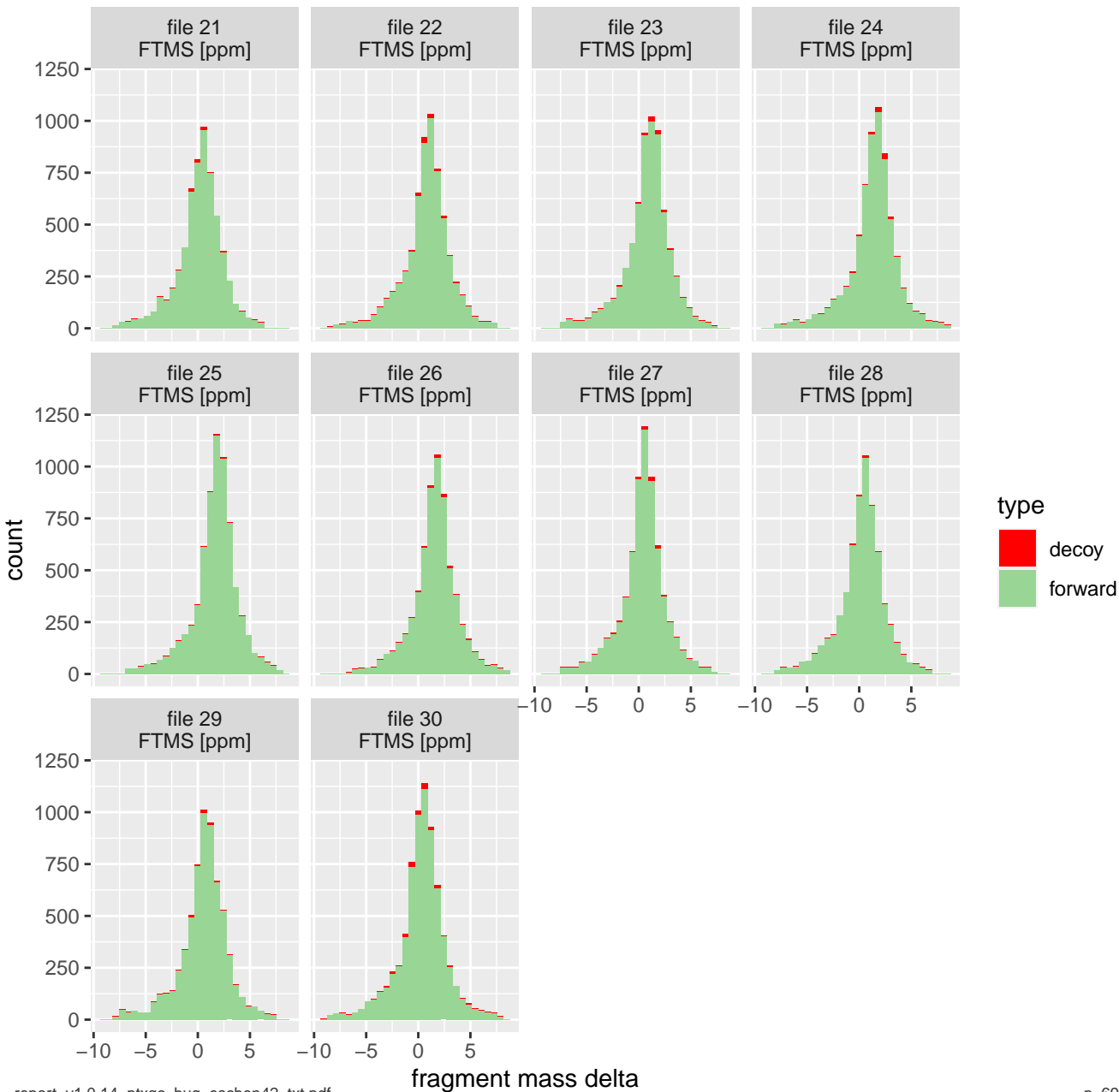
# MSMS: Fragment mass errors per Raw file



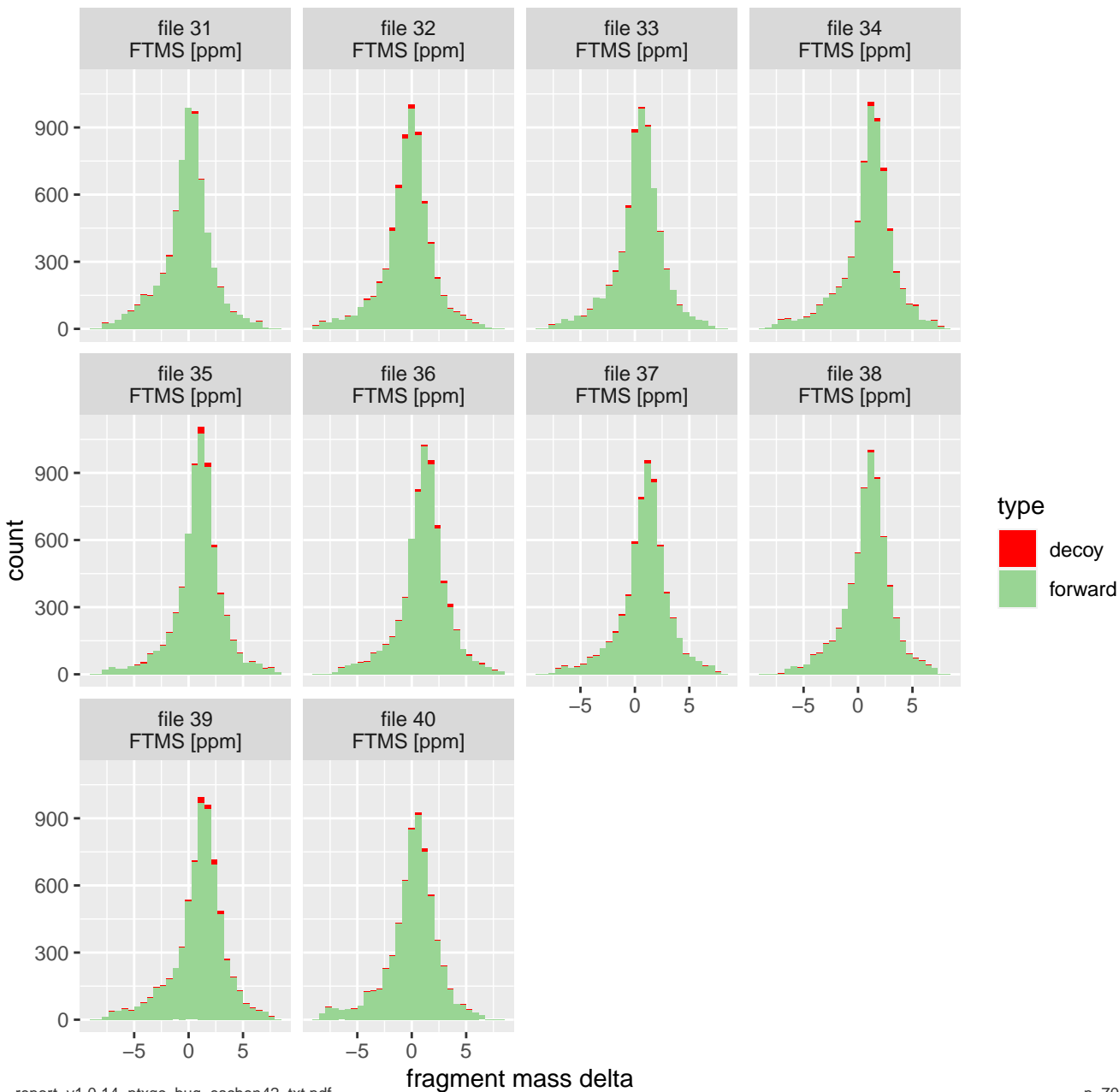
# MSMS: Fragment mass errors per Raw file



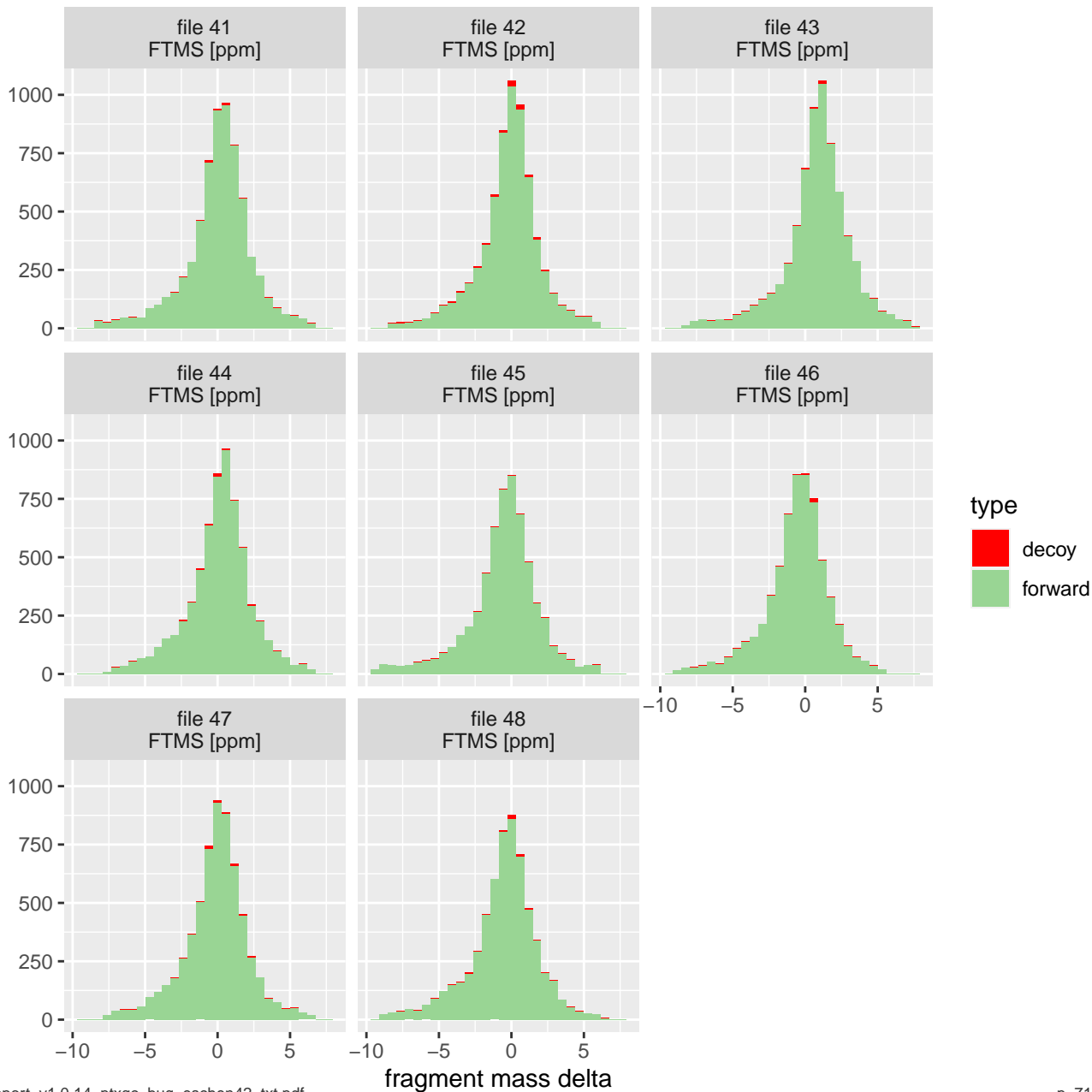
# MSMS: Fragment mass errors per Raw file



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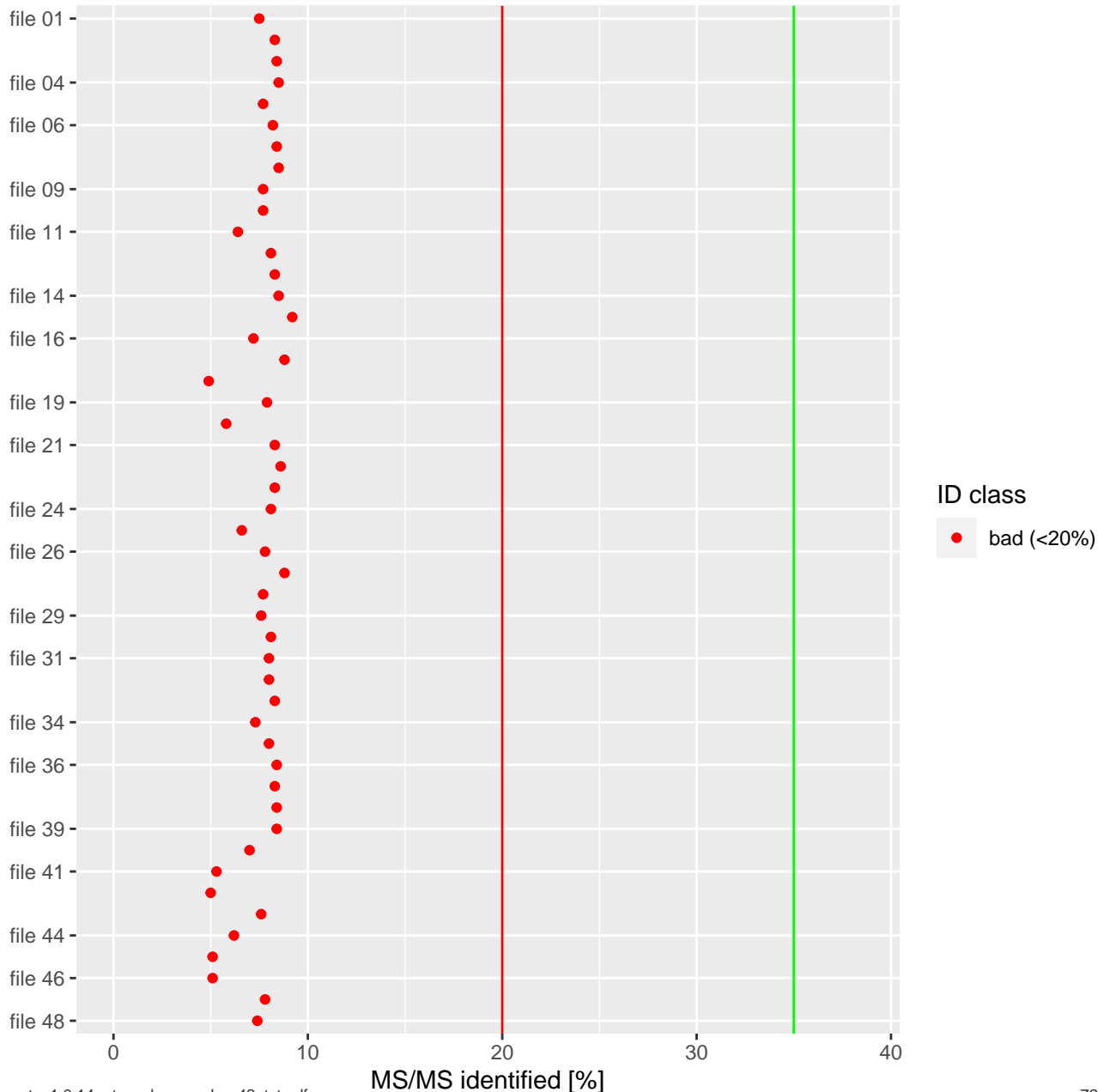


# MSMS: Fragment mass errors per Raw file





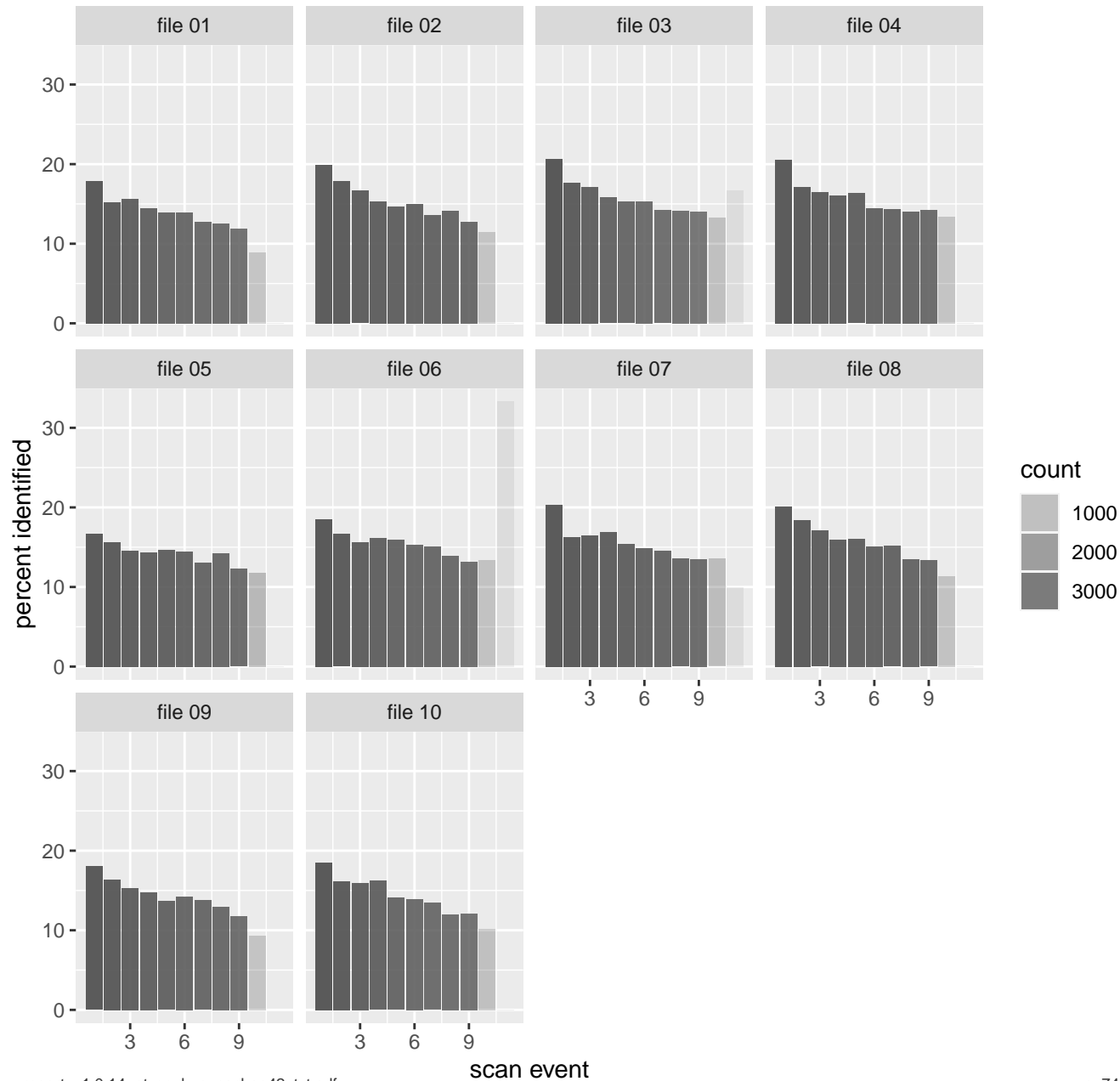
# SM: MS/MS identified per Raw file



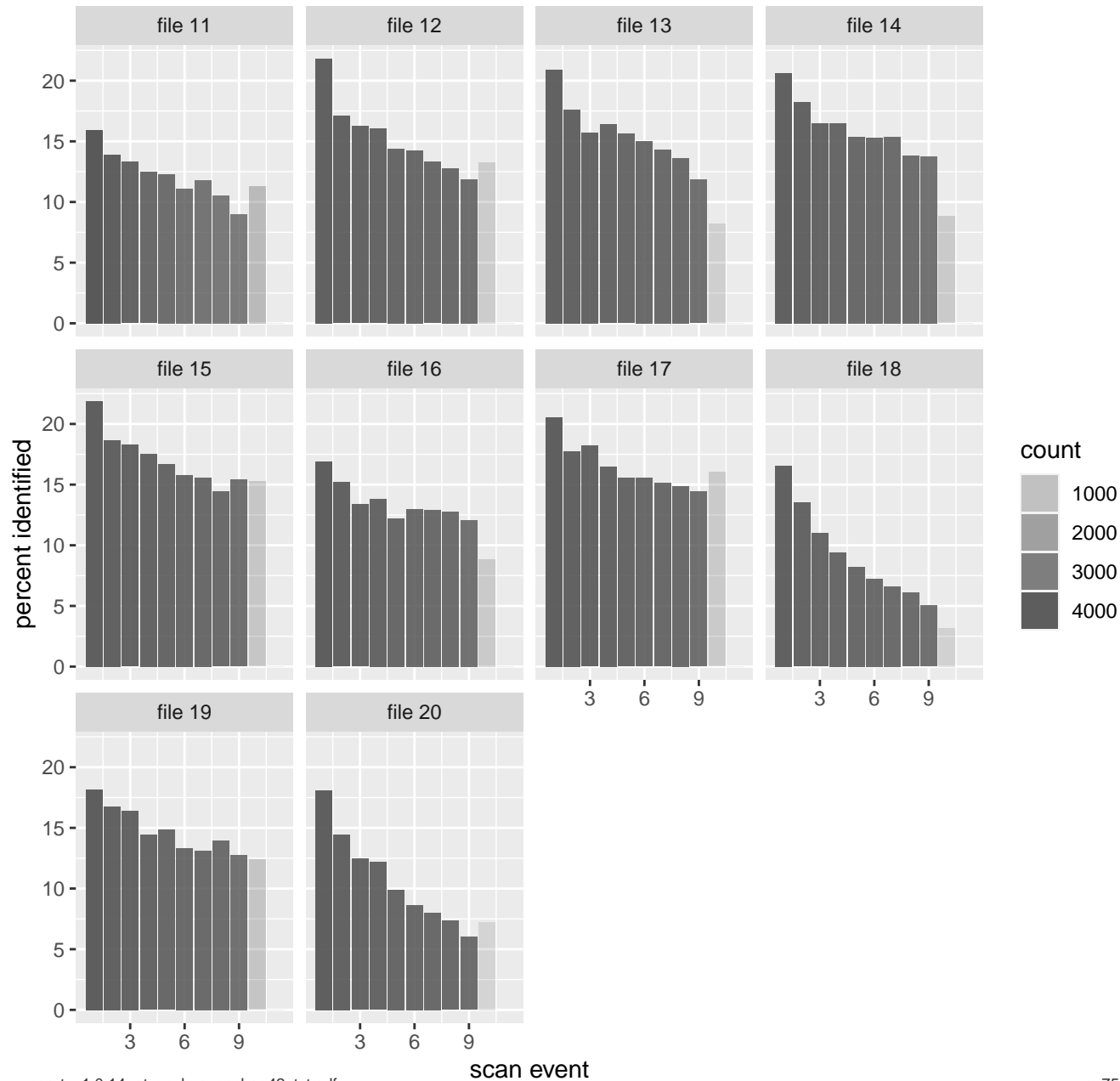
# SM: Files with 'red' ID rate

Raw file	% identified
jdrake_zsychev_18366_20211124_FAIMS_totalPr_26_s96_3408.raw.thermo	7.5
jdrake_zsychev_18366_20211124_FAIMS_totalPr_25_s96_2583.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_24_s93_4571.raw.thermo	8.4
jdrake_zsychev_18366_20211124_FAIMS_totalPr_21_s77CR_5496.raw.thermo	8.5
jdrake_zsychev_18366_20211124_FAIMS_totalPr_20_s77CR_2042.raw.thermo	7.7
jdrake_zsychev_18366_20211124_FAIMS_totalPr_19_s77CR_1018.raw.thermo	8.2
jdrake_zsychev_18366_20211124_FAIMS_totalPr_18_s77_4327.raw.thermo	8.4
jdrake_zsychev_18366_20211124_FAIMS_totalPr_16_s77_949.raw.thermo	8.5
jdrake_zsychev_18366_20211124_FAIMS_totalPr_15_s70CR_6134.raw.thermo	7.7
jdrake_zsychev_18366_20211124_FAIMS_totalPr_14_s70CR_5206.raw.thermo	7.7
jdrake_zsychev_18366_20211124_FAIMS_totalPr_13_s70CR_1015.raw.thermo	6.4
jdrake_zsychev_18366_20211124_FAIMS_totalPr_11_s70_2099.raw.thermo	8.1
jdrake_zsychev_18366_20211124_FAIMS_totalPr_10_s70_1205.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_9_s49_6052.raw.thermo	8.5
jdrake_zsychev_18366_20211124_FAIMS_totalPr_08_s49_4385.raw.thermo	9.2
jdrake_zsychev_18366_20211124_FAIMS_totalPr_07_s49_1261.raw.thermo	7.2
jdrake_zsychev_18366_20211124_FAIMS_totalPr_06_s35CR_6378.raw.thermo	8.8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_05_s35CR_5490.raw.thermo	4.9
jdrake_zsychev_18366_20211124_FAIMS_totalPr_04_s35CR_1339.raw.thermo	7.9
jdrake_zsychev_18366_20211124_FAIMS_totalPr_03_s35_3853.raw.thermo	5.8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_02_s35_2564.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_01_s35_810.raw.thermo	8.6
jdrake_zsychev_18366_20211124_FAIMS_totalPr_54_s208_1_6719.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_53_s208_1_4865.raw.thermo	8.1
jdrake_zsychev_18366_20211124_FAIMS_totalPr_52_s208_1_4107.raw.thermo	6.6
jdrake_zsychev_18366_20211124_FAIMS_totalPr_50_s173_1_2824.raw.thermo	7.8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_49_s173_1_2032.raw.thermo	8.8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_48_s167CR_4675.raw.thermo	7.7
jdrake_zsychev_18366_20211124_FAIMS_totalPr_47_s167CR_1732.raw.thermo	7.6
jdrake_zsychev_18366_20211124_FAIMS_totalPr_46_s167CR_964.raw.thermo	8.1
jdrake_zsychev_18366_20211124_FAIMS_totalPr_45_s167_4895.raw.thermo	8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_44_s167_2473.raw.thermo	8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_43_s167_1532.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_42_s145_2_2467.raw.thermo	7.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_41_s145_2_1396.raw.thermo	8
jdrake_zsychev_18366_20211124_FAIMS_totalPr_40_s145_2_829.raw.thermo	8.4
jdrake_zsychev_18366_20211124_FAIMS_totalPr_39_s145_1_2519.raw.thermo	8.3
jdrake_zsychev_18366_20211124_FAIMS_totalPr_38_s145_1_1709.raw.thermo	8.4
jdrake_zsychev_18366_20211124_FAIMS_totalPr_37_s145_1_1003.raw.thermo	8.4
9 more ...	

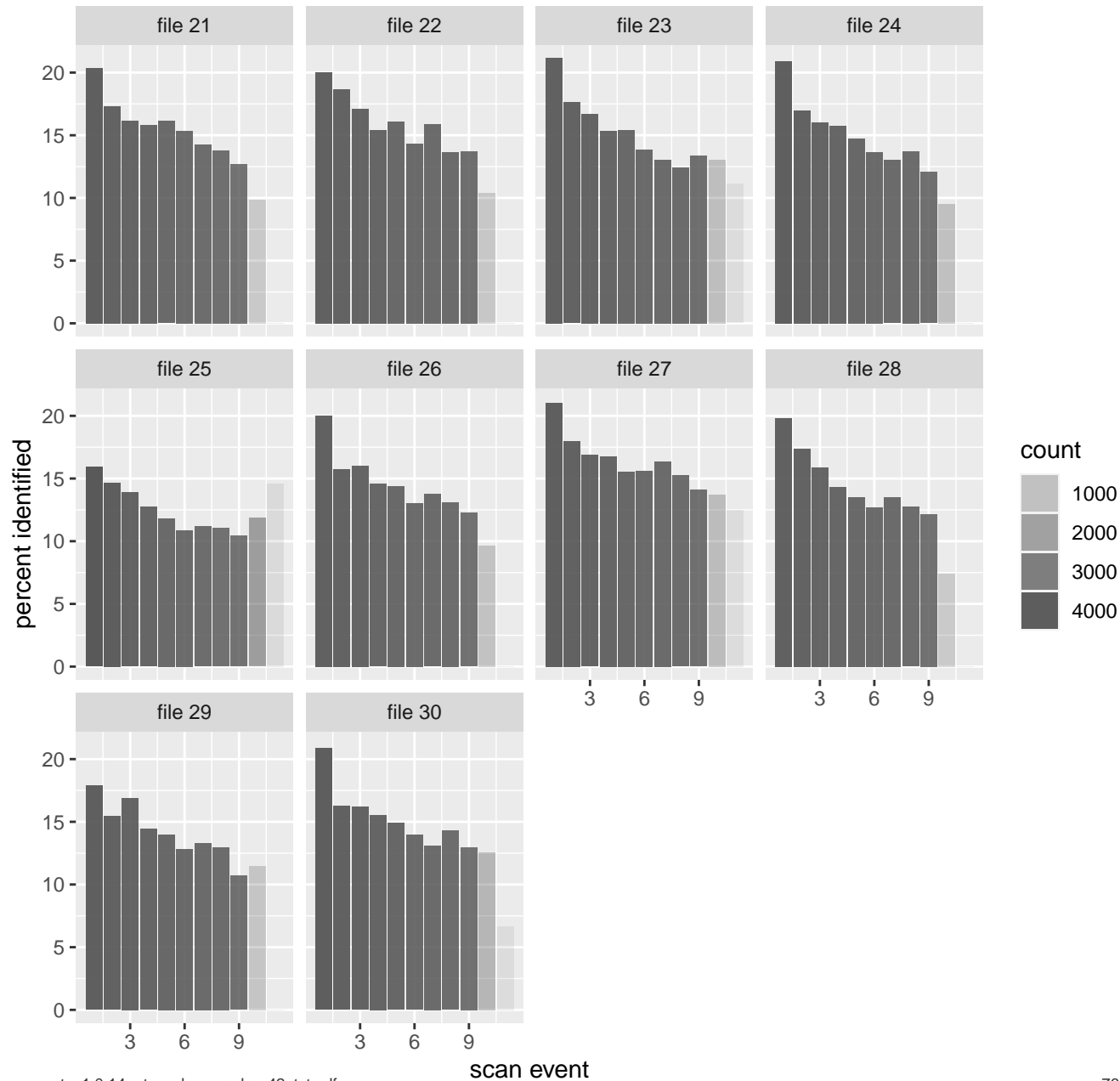
# MSMSscans: TopN % identified over N



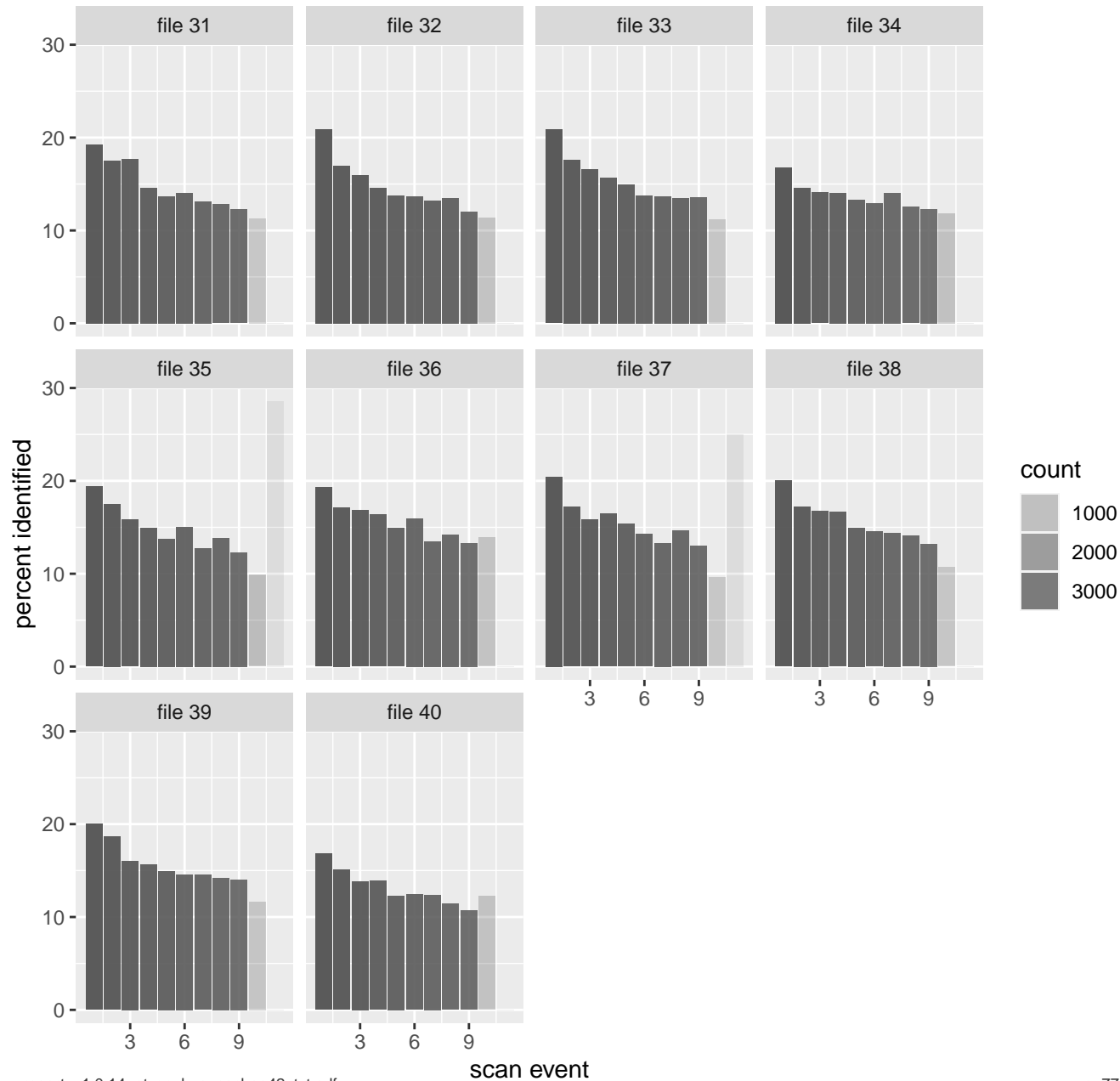
# MSMSscans: TopN % identified over N



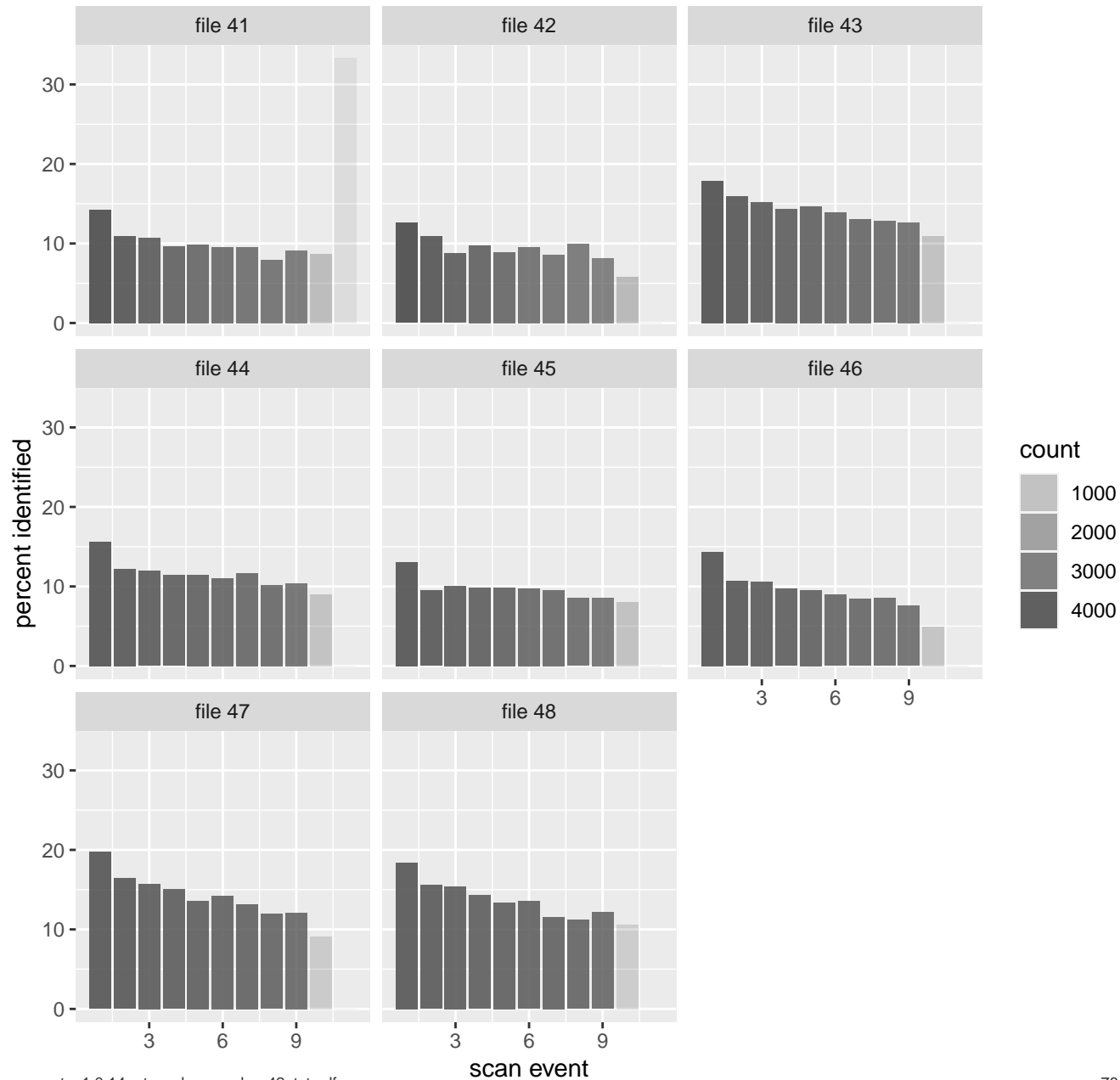
# MSMSscans: TopN % identified over N



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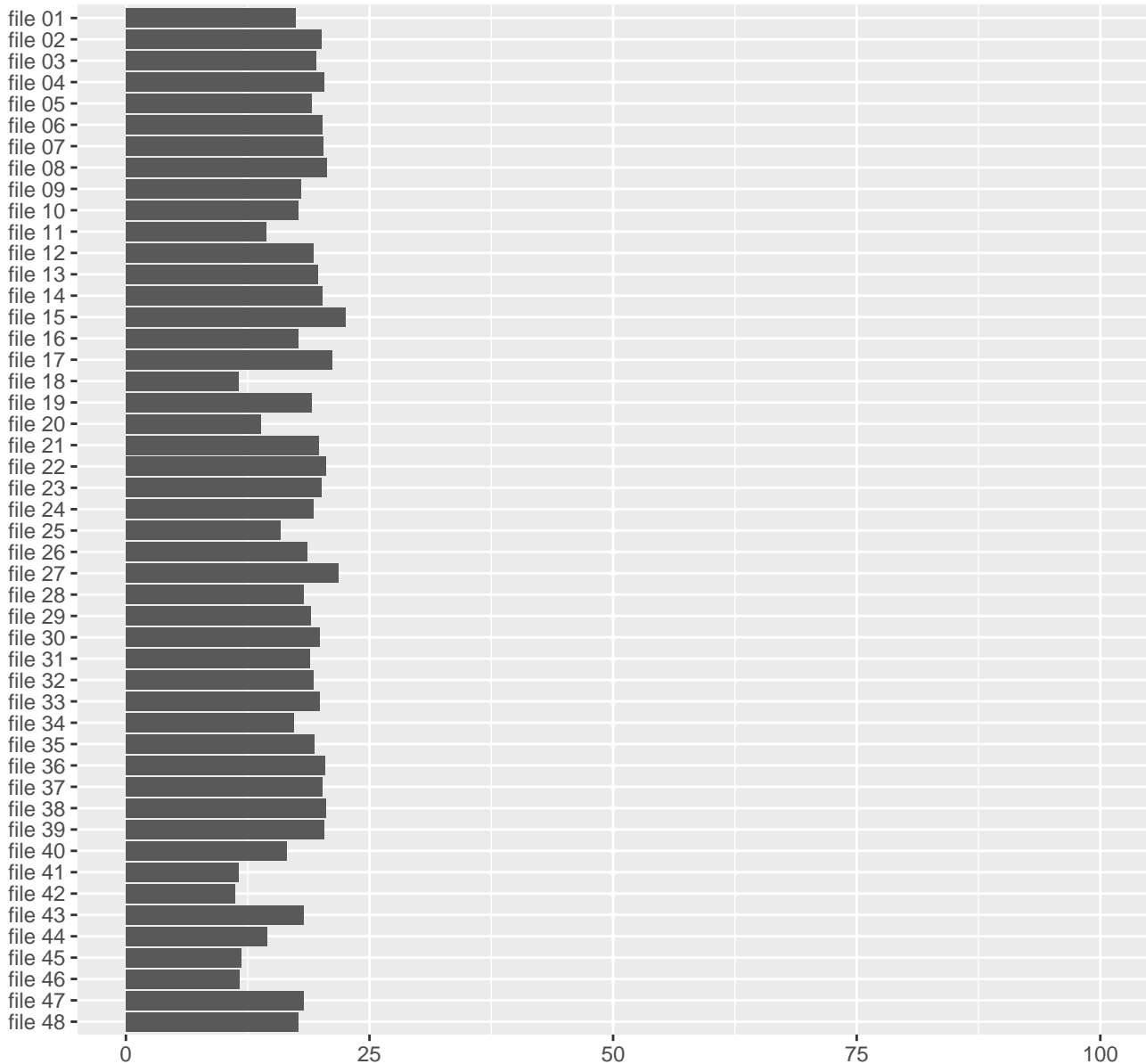


# MSMSscans: TopN % identified over N



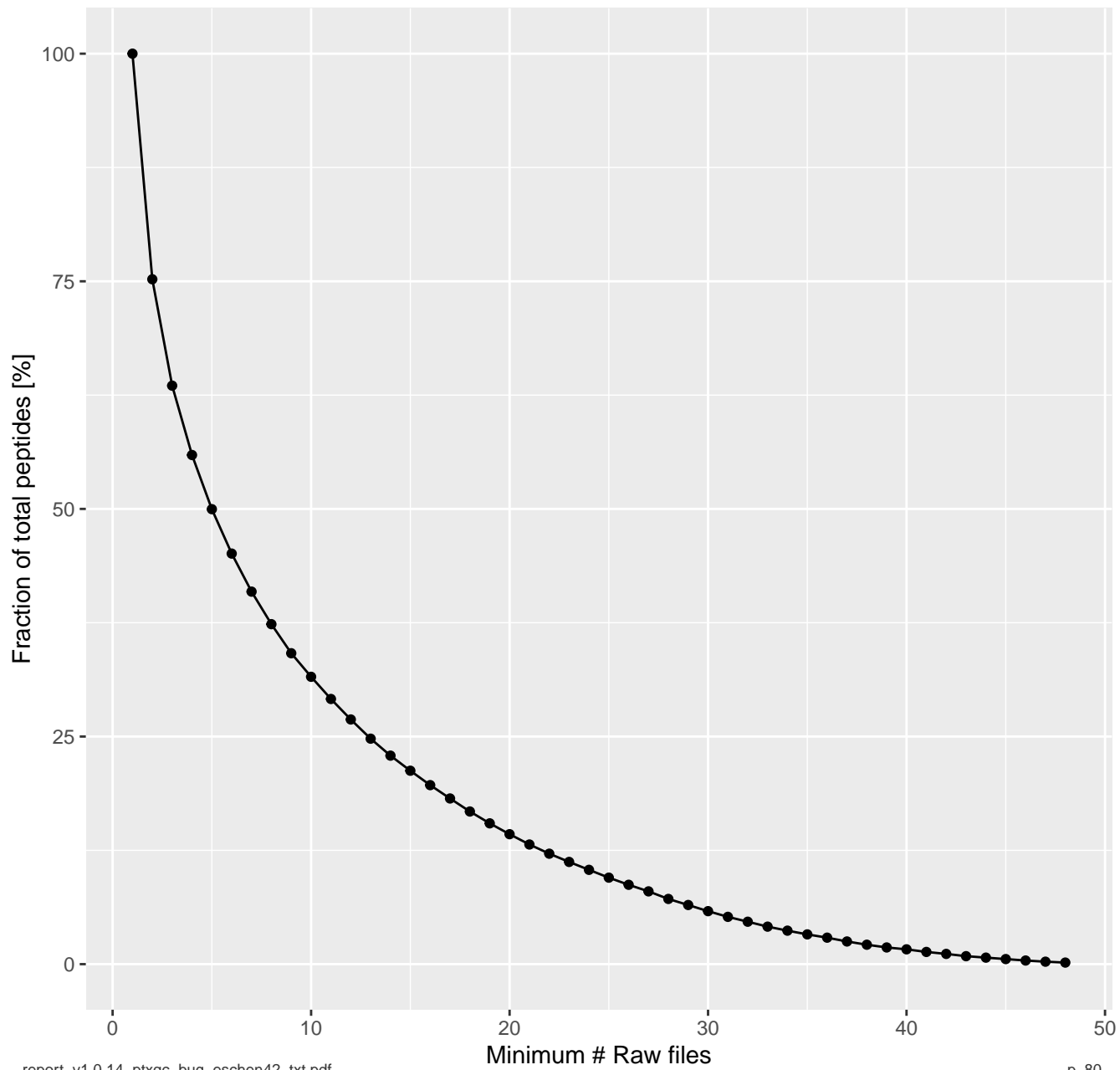
# [experimental] EVD: Non-Missing Peptides

compared to all peptides seen in experiment

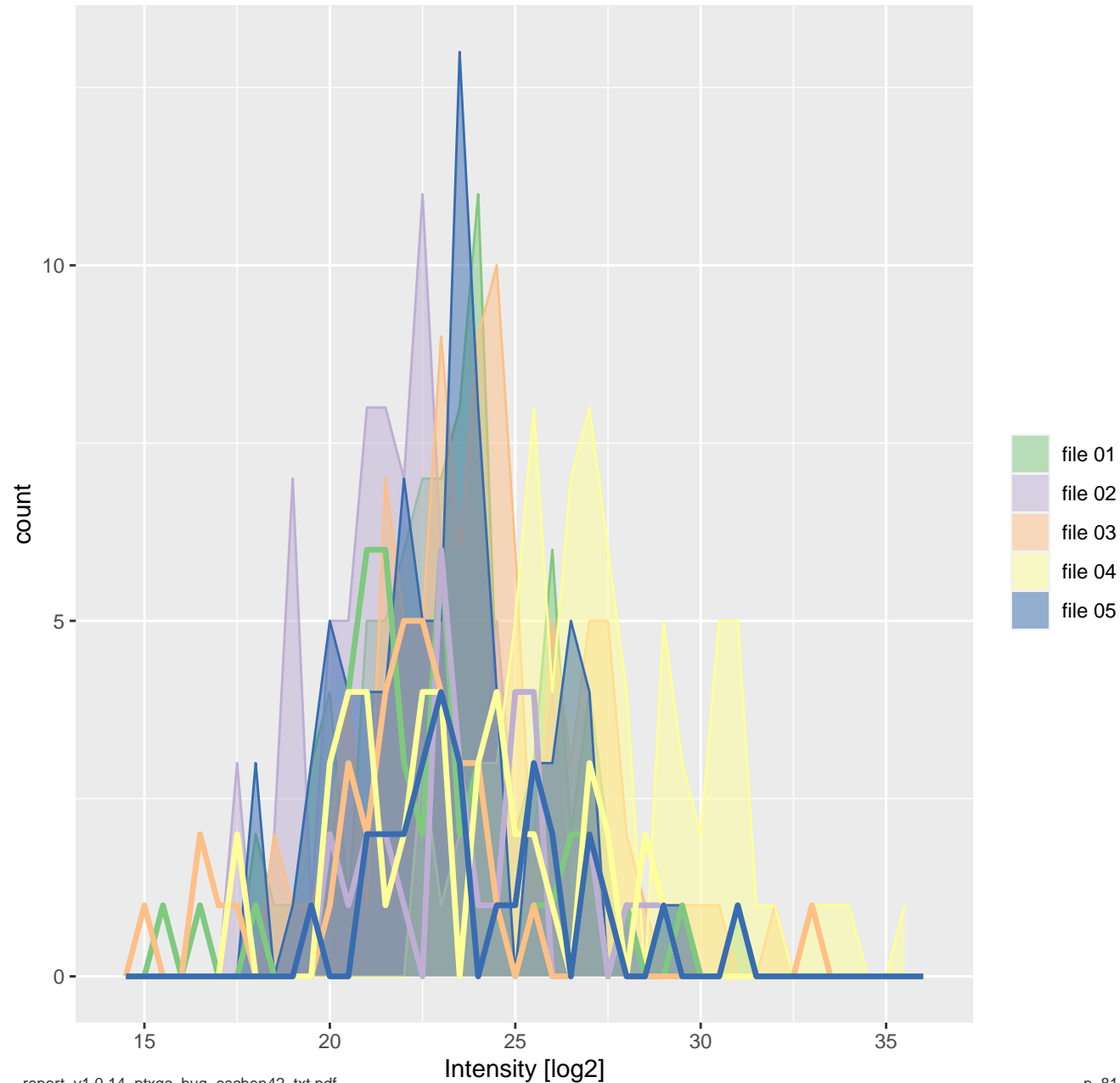




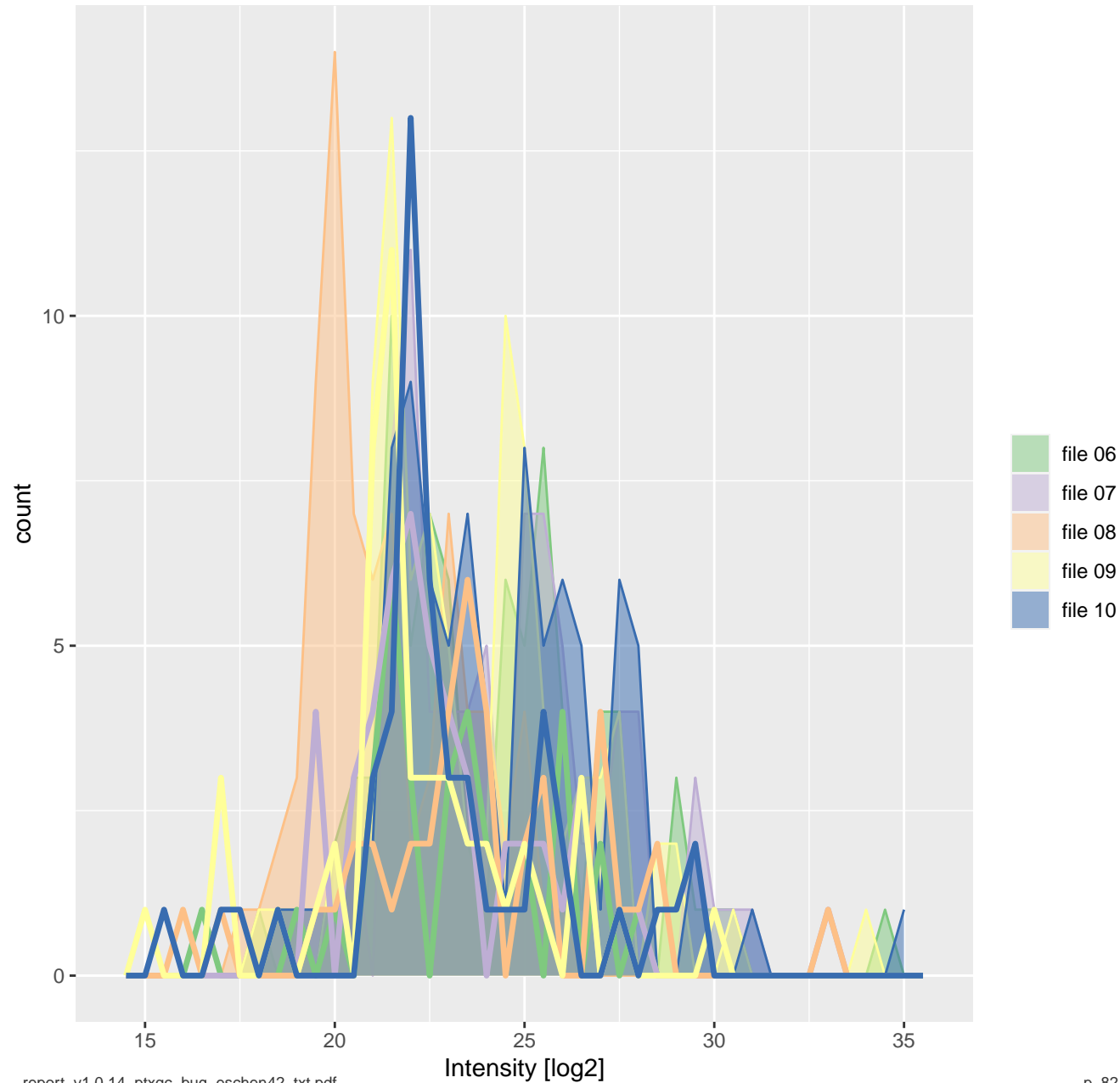
# [experimental] EVD: Non-missing by set



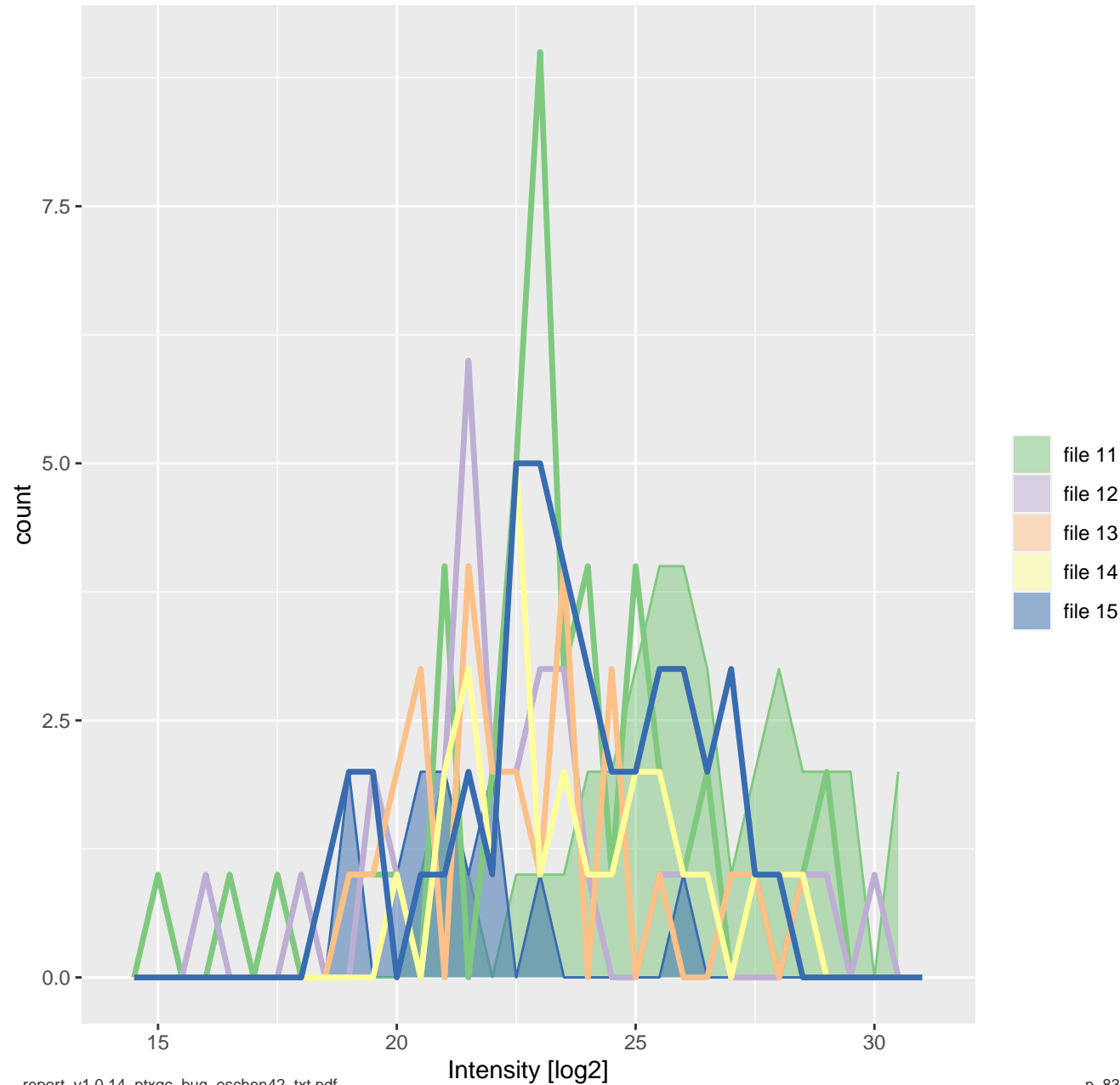
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



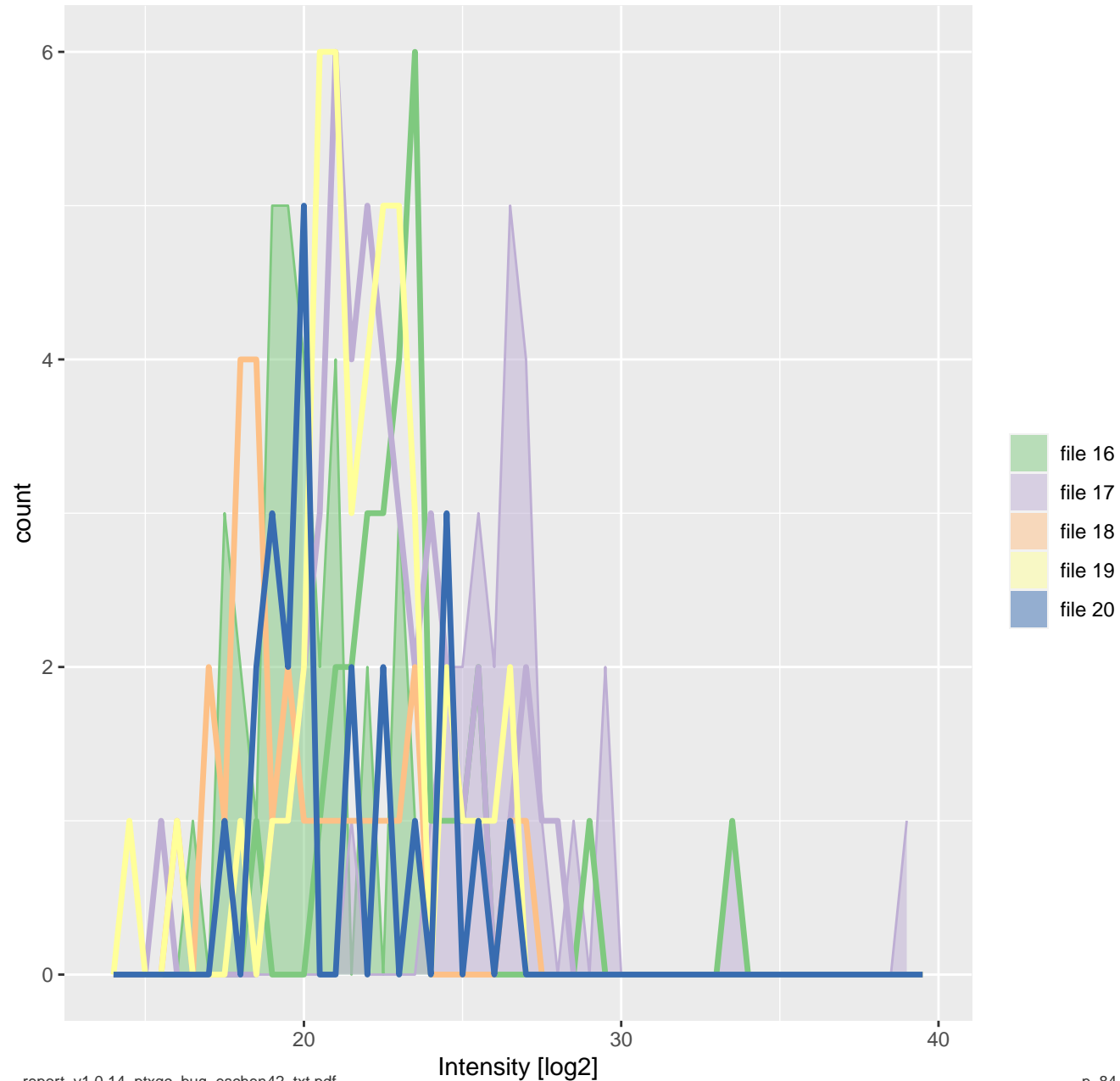
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



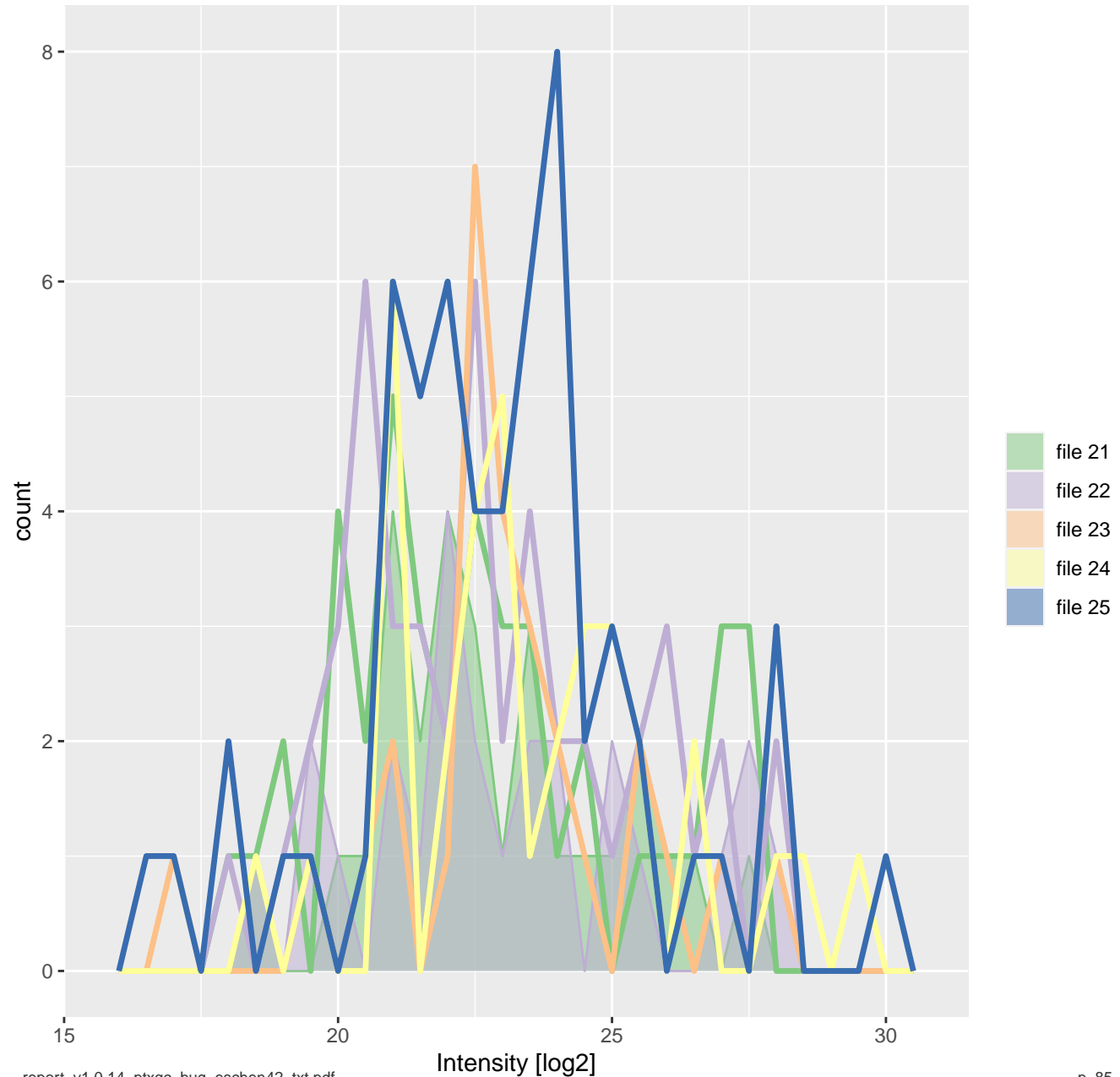
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



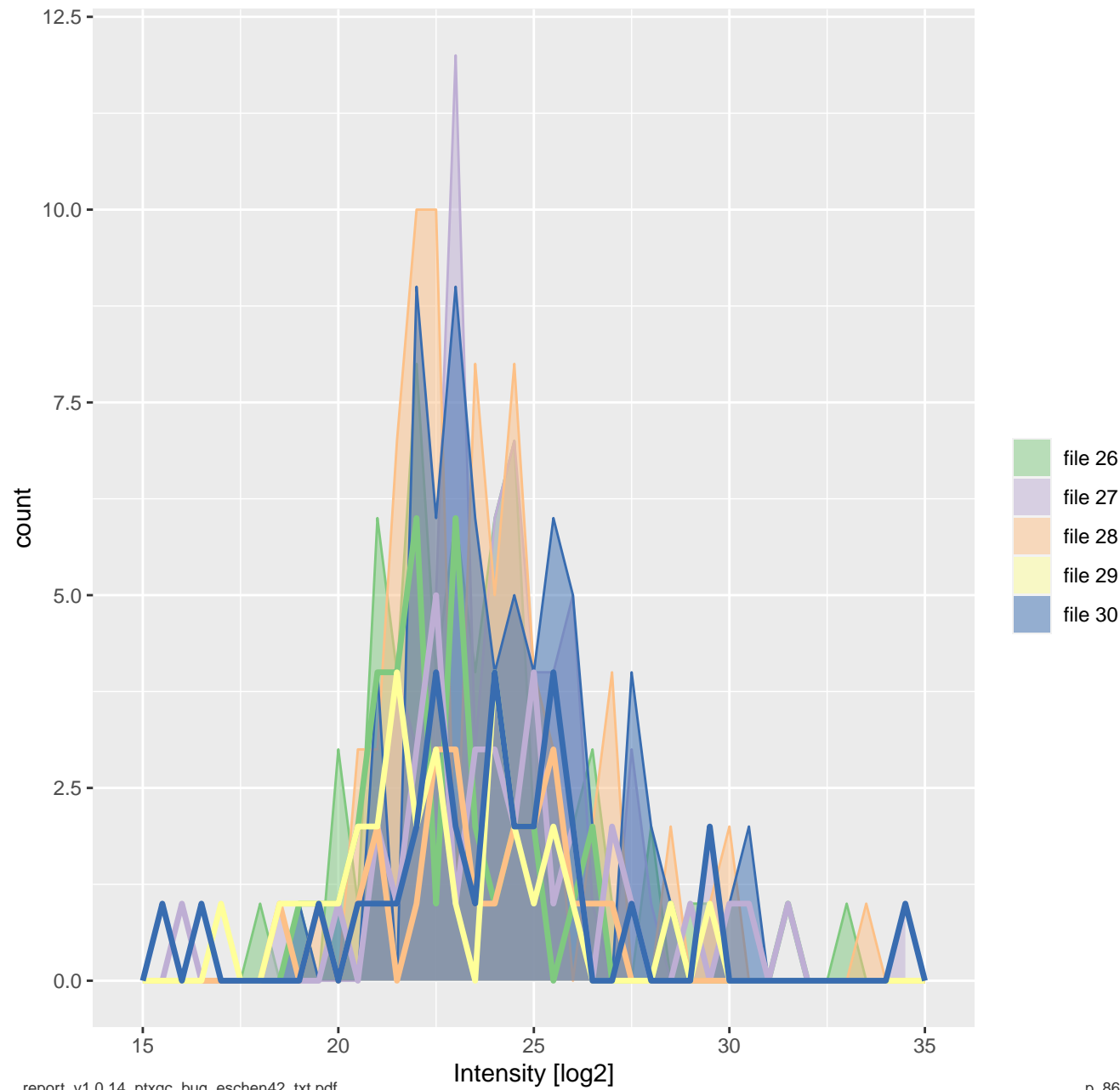
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



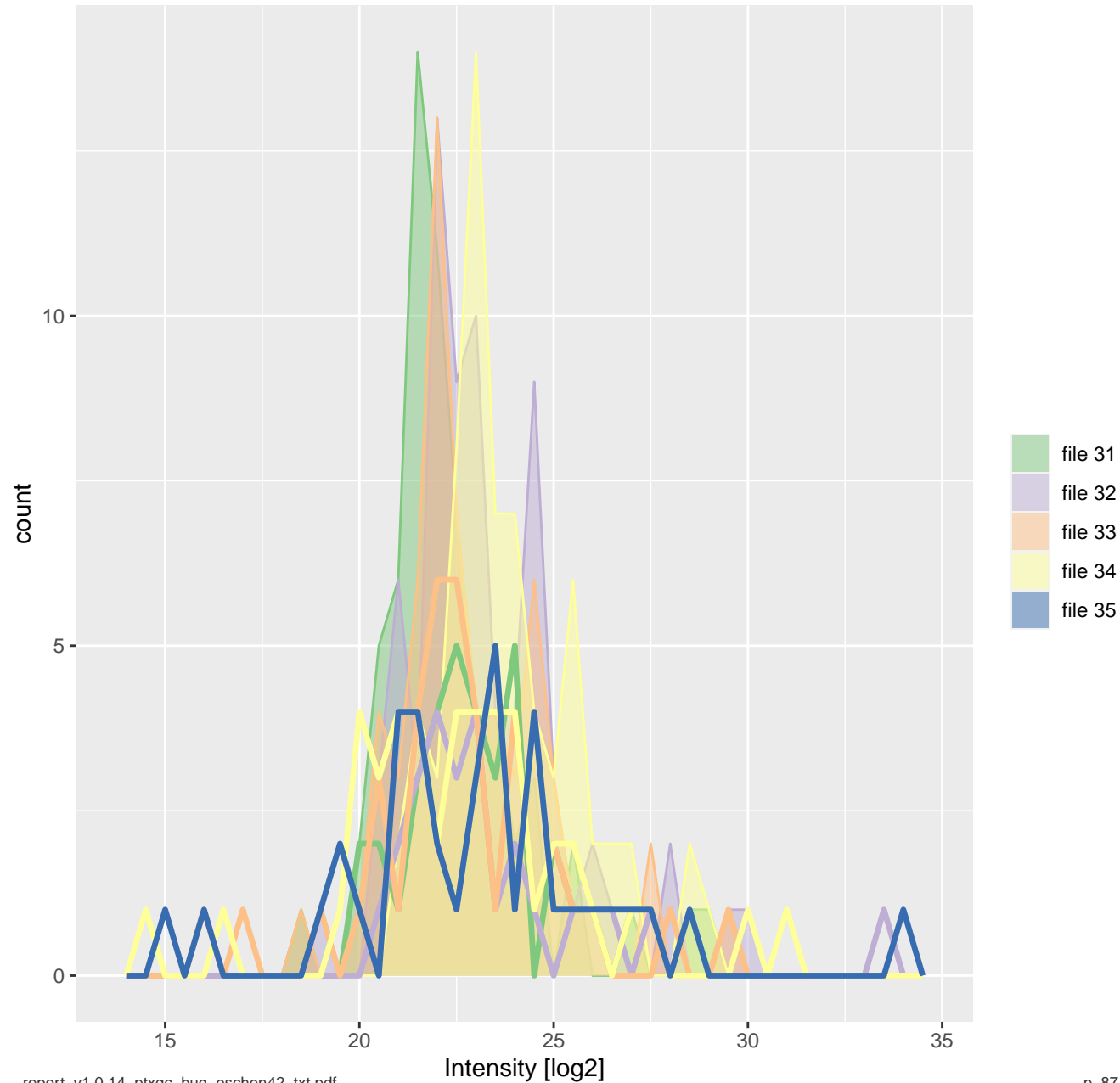
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



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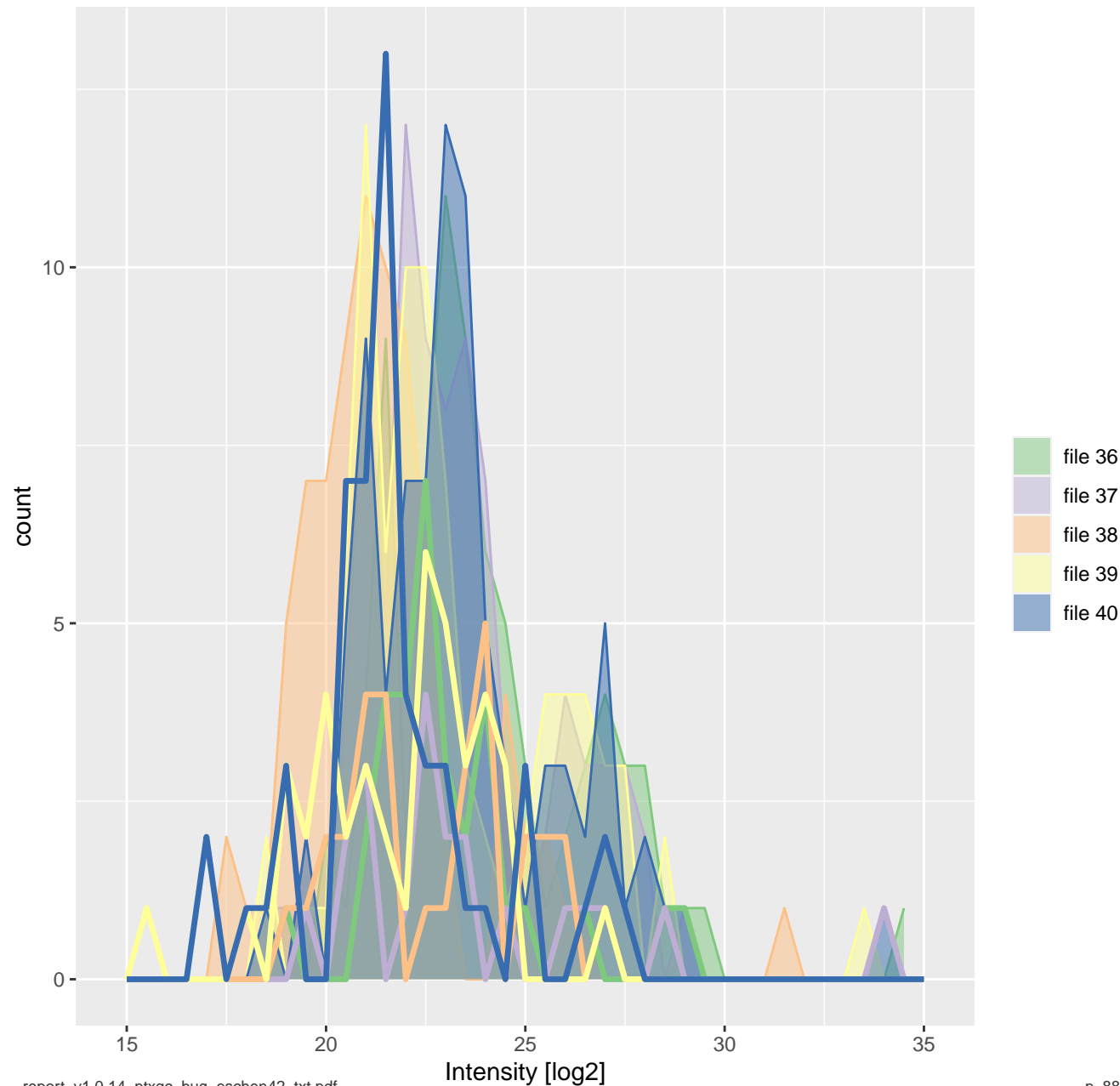


# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values

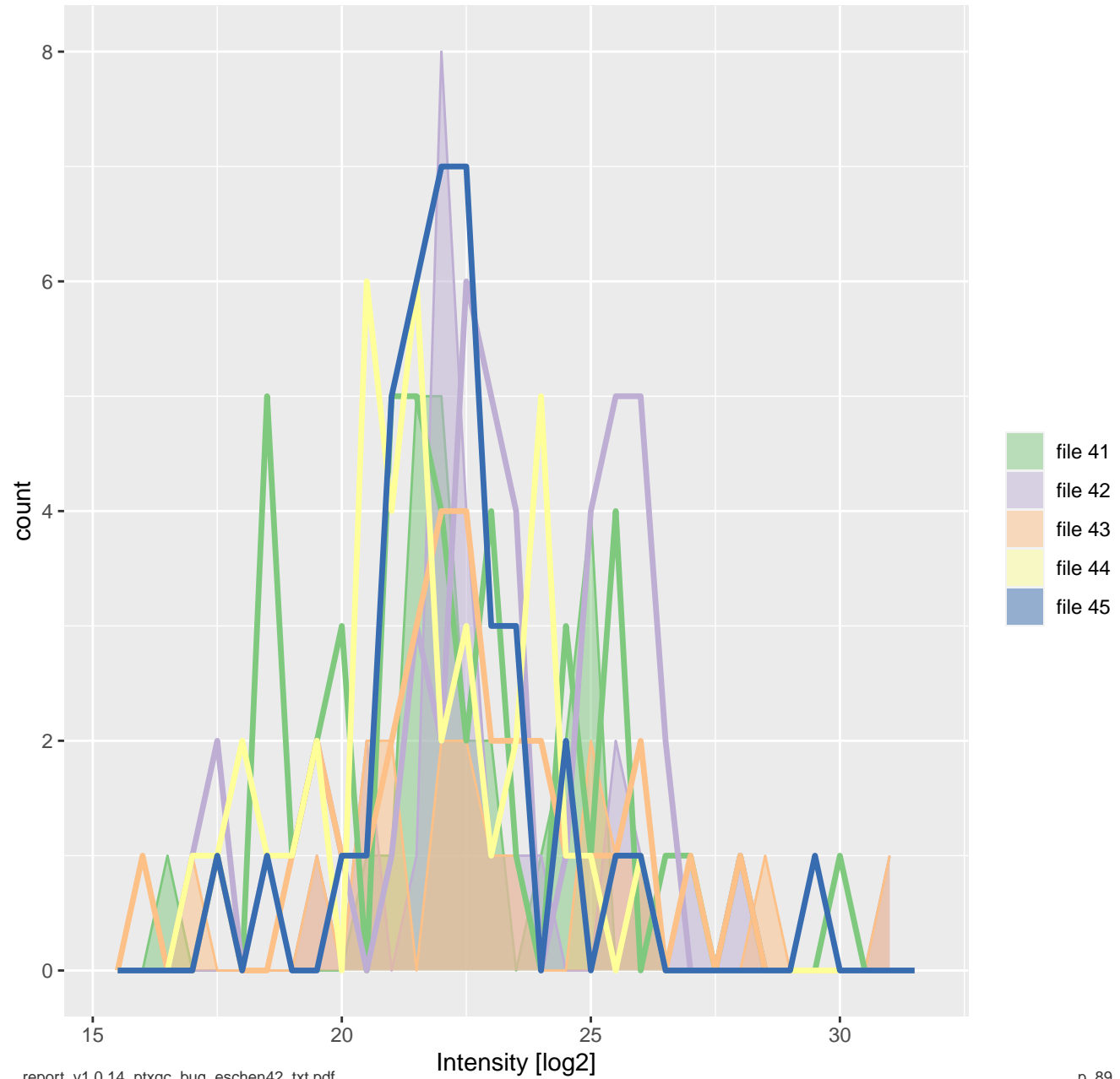




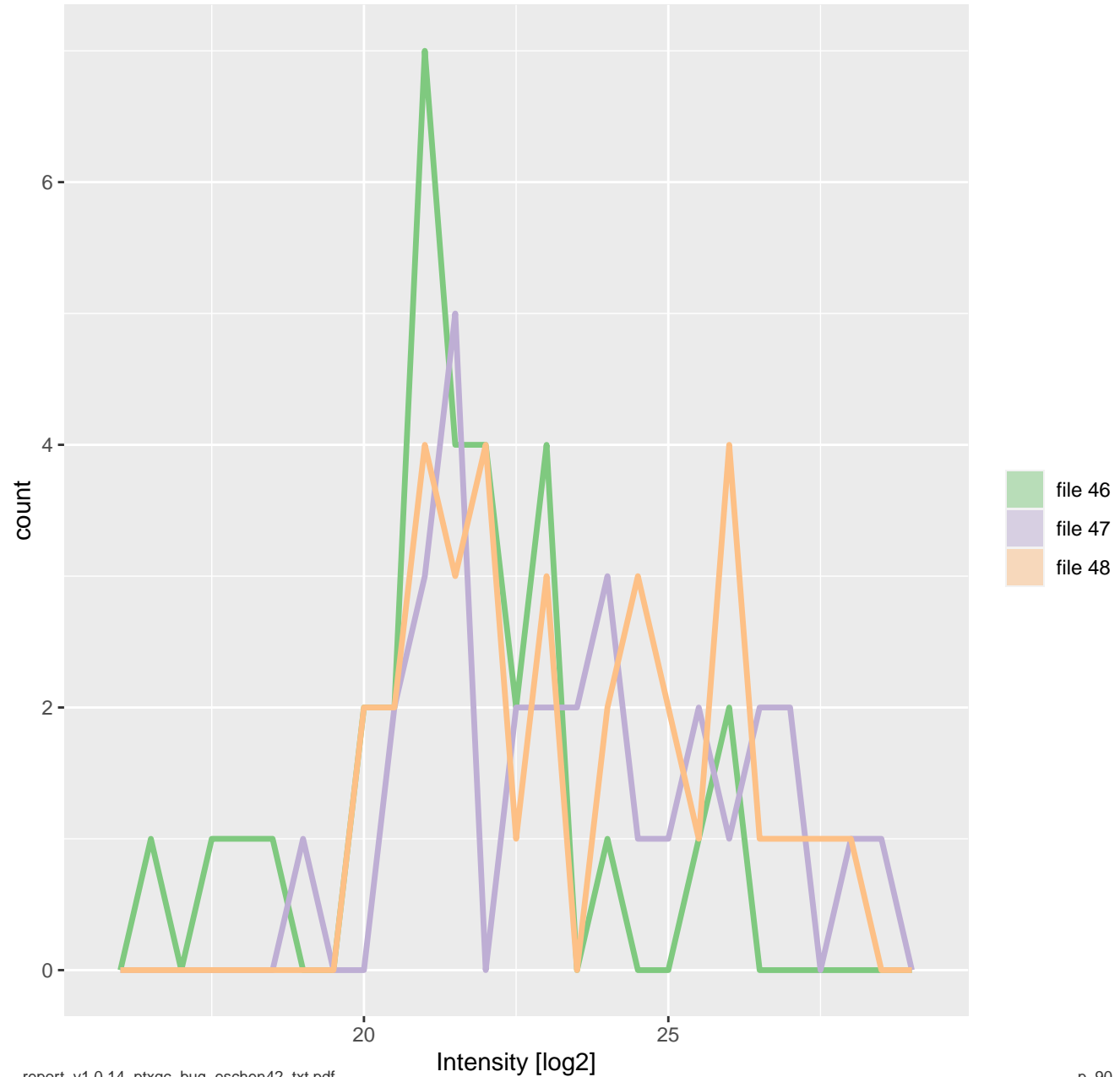
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



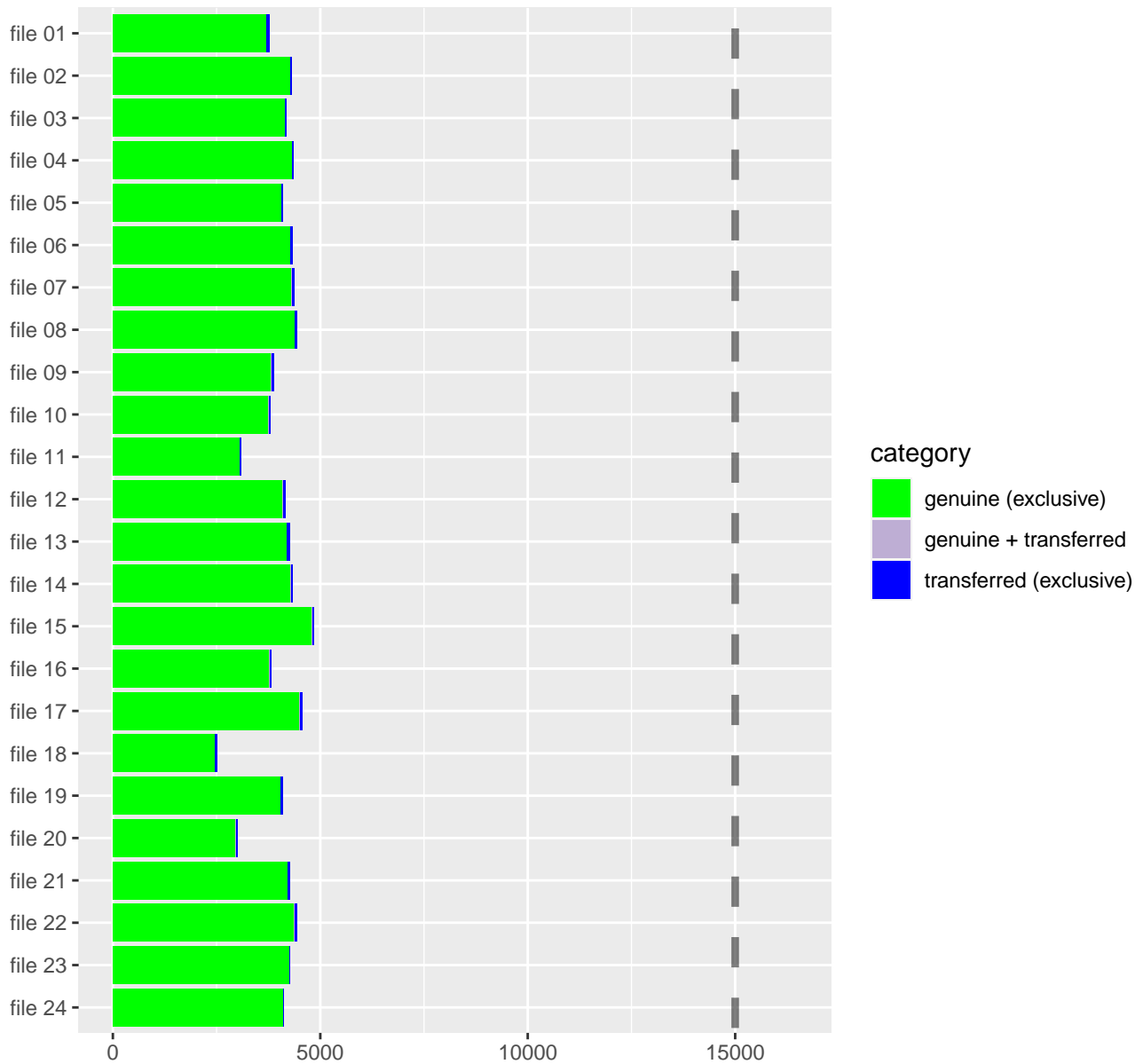
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



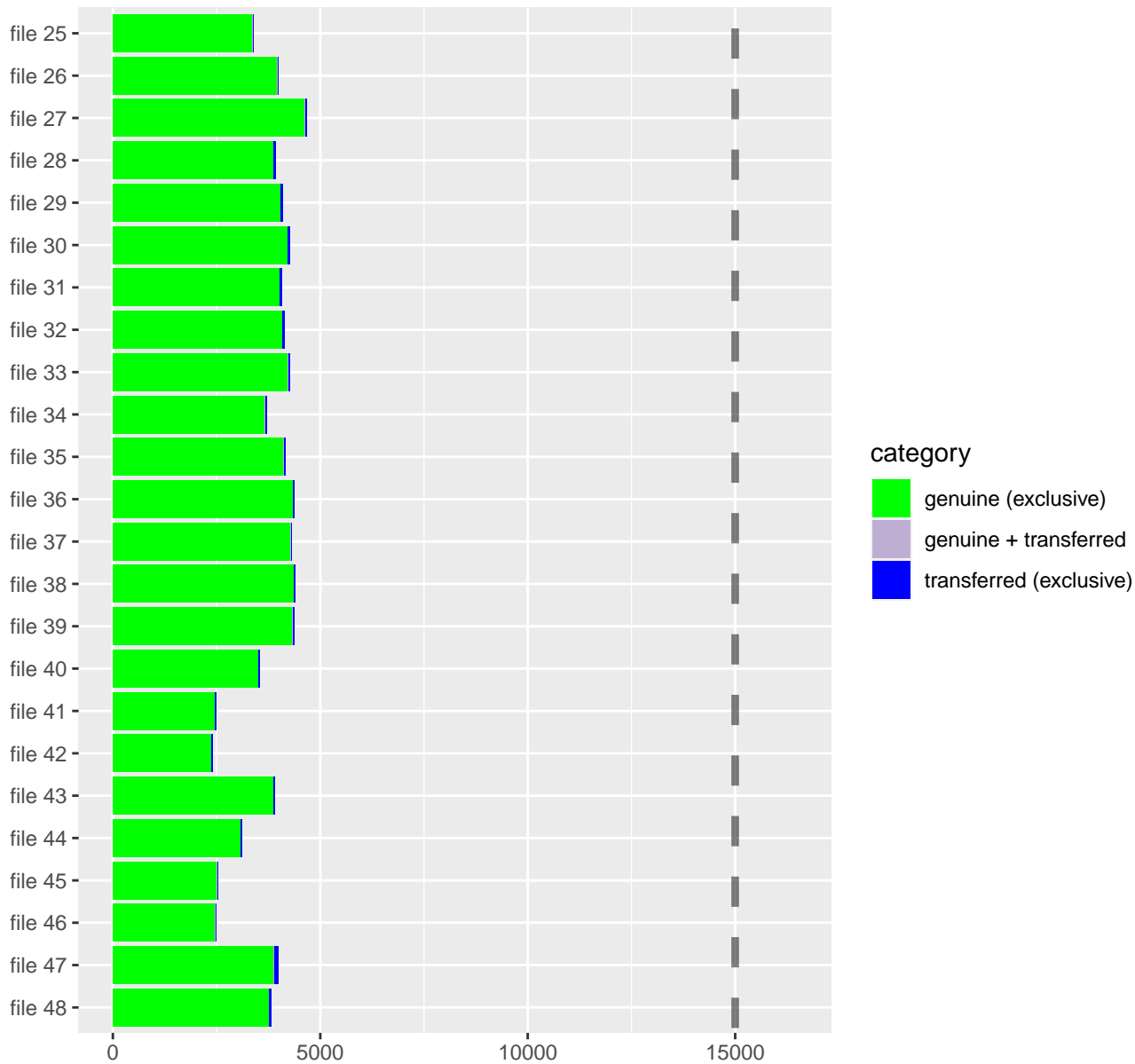
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



# EVD: Peptide ID count

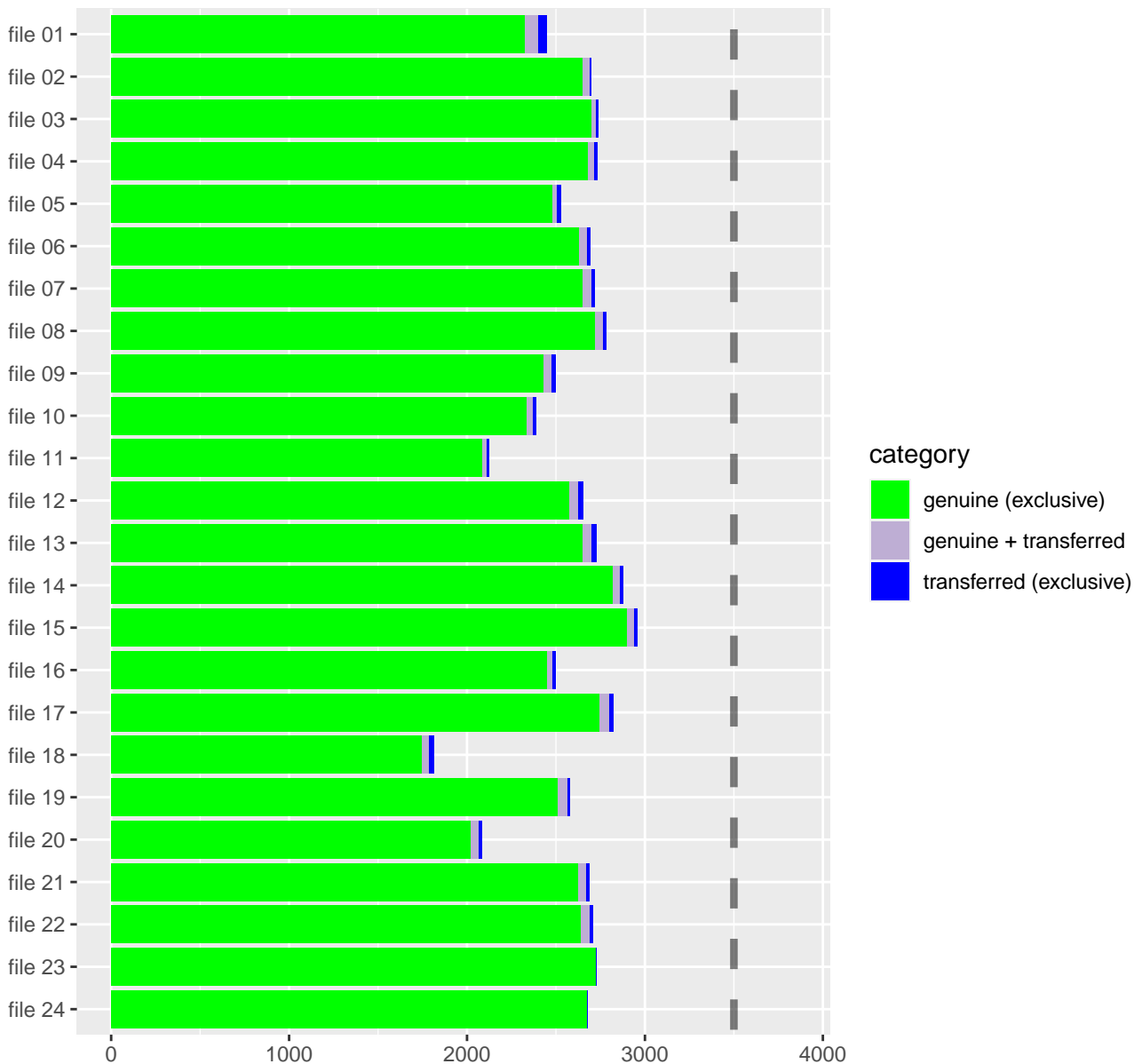


# EVD: Peptide ID count



# EVD: ProteinGroups count

MBR gain: +1%



# EVD: ProteinGroups count

MBR gain: +1%

