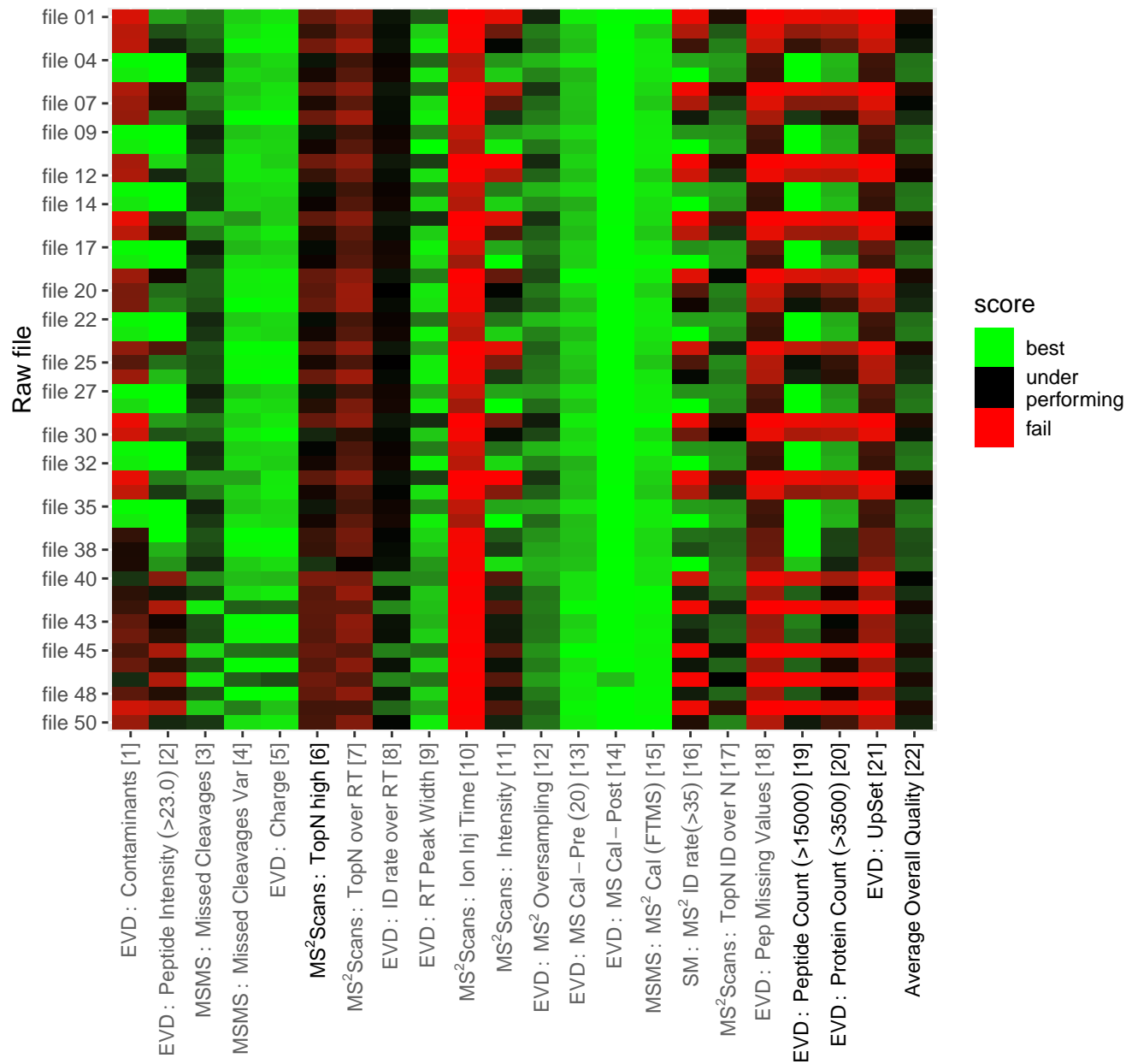


# Performance overview



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

original	short name	best effort
10_DMSO_SDS_3	file 01	10_DMSO_SDS_....._3
10_DMSO_SDS_3_5uL_20200612085223	file 02	10_DMSO_SDS_3_5uL_....._20200612085223
10_insol_WT	file 03	10_insol_....._WT
11_Cpt_wcl_3	file 04	11_Cpt_wcl_....._3
11_WCL_ATM	file 05	11_WCL_....._ATM
12_Cpt_SDS_3	file 06	12_Cpt_SDS_....._3
12_Cpt_SDS_3_5uL	file 07	12_Cpt_SDS_3_....._5uL
12_insol_ATM	file 08	12_insol_....._ATM
13_DMSO_wcl_4	file 09	13_DMSO_wcl_....._4
13_WCL_WT	file 10	13_WCL_....._WT
14_DMSO_SDS_4	file 11	14_DMSO_SDS_....._4
14_DMSO_SDS_4_5uL	file 12	14_DMSO_SDS_4_....._5uL
15_Cpt_wcl_4	file 13	15_Cpt_wcl_....._4
15_WCT_ATM	file 14	15_WCT_....._ATM
16_Cpt_SDS_4	file 15	16_Cpt_SDS_....._4
16_Cpt_SDS_4_5uL	file 16	16_Cpt_SDS_4_....._5uL
1_DMSO_wcl_1	file 17	1_DMSO_wcl_....._1

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

original	short name	best effort
1_WCL_WT	file 18	1_WCL_...._WT
2_DMSO_SDS_1	file 19	2_DMSO_SDS_...._1
2_DMSO_SDS_1_5uL	file 20	2_DMSO_SDS_1_...._5uL
2_insol_WT	file 21	2_insol_...._WT
3_Cpt_wcl_1	file 22	3_Cpt_wcl_...._1
3_WCL_ATM	file 23	3_WCL_...._ATM
4_cpt_SDS_1	file 24	4_cpt_SDS_...._1
4_cpt_SDS_1_5uL	file 25	4_cpt_SDS_1_...._5uL
4_insol_ATM	file 26	4_insol_...._ATM
5_DMSO_wcl_2	file 27	5_DMSO_wcl_...._2
5_WCL_WT_20200702083455	file 28	5_WCL_WT_...._20200702083455
6_DMSO_SDS_2	file 29	6_DMSO_SDS_...._2
6_DMSO_SDS_2_5uL	file 30	6_DMSO_SDS_2_...._5uL
7_Cpt_wcl_2	file 31	7_Cpt_wcl_...._2
7_WCL_ATM	file 32	7_WCL_...._ATM
8_Cpt_SDS_2	file 33	8_Cpt_SDS_...._2
8_Cpt_SDS_2_5uL	file 34	8_Cpt_SDS_2_...._5uL

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

original	short name	best effort
9_DMSO_wcl_3	file 35	9_DMSO_wcl.....3
9_WCL_WT	file 36	9_WCL.....WT
insol_ATM_1	file 37	insol_ATM.....1
insol_ATM_2	file 38	insol_ATM.....2
insol_ATM_3	file 39	insol_ATM.....3
insol_ATM_3_20200725191715	file 40	insol_ATM_3....._20200725191715
insol_ATM_3_20200727092836	file 41	insol_ATM_3....._20200727092836
insol_ATM_4	file 42	insol_ATM.....4
insol_ATM_4_20200729233315	file 43	insol_ATM_4....._20200729233315
insol_WT_1_20200727152510	file 44	insol_WT_1....._20200727152510
insol_WT_2	file 45	insol_WT.....2
insol_WT_2_20200727173305	file 46	insol_WT_2....._20200727173305
insol_WT_3	file 47	insol_WT.....3
insol_WT_3_20200727194055	file 48	insol_WT_3....._20200727194055
insol_WT_4	file 49	insol_WT.....4
insol_WT_4_20200727214846	file 50	insol_WT_4....._20200727214846

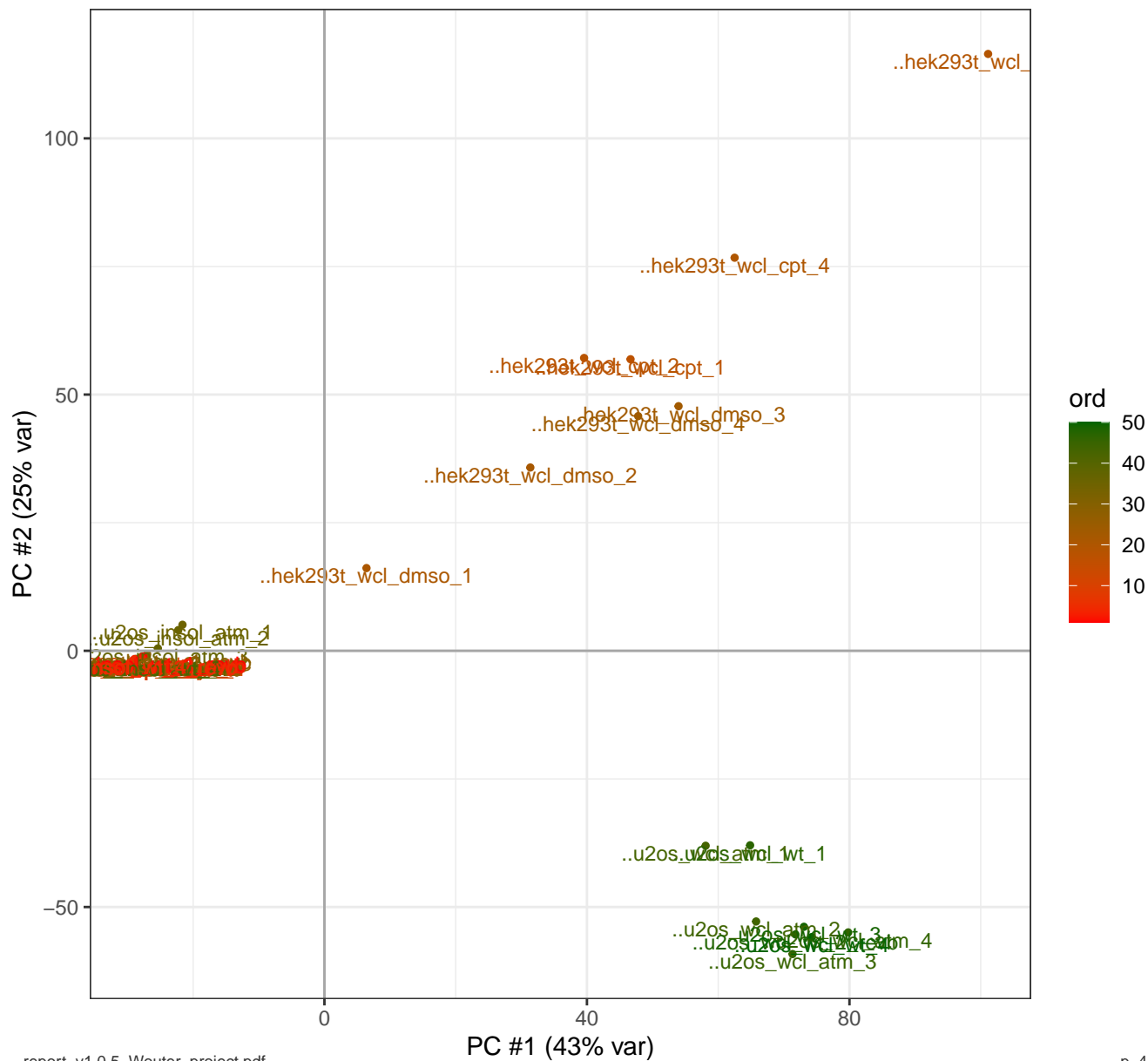
## PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	Min. score for modified pept..	40
Calculate peak properties	False	Modifications included in pr..	Oxidation (M) Acetyl (Protein N-term)
Combined folder location	C:\Users\lacav\Desktop\MQ\Wouter_project	MS/MS deisotoping tolerance ..	ppm
Da interval. (FTMS)	100	MS/MS deisotoping tolerance ..	0.15
Date of writing	09/21/2020 12:23:37	MS/MS deisotoping tolerance ..	Da
Decoy mode	revert	MS/MS deisotoping tolerance ..	0.01
Fixed andromeda index folder	C:\Users\lacav\Desktop\MQ\Andromeda	MS/MS tol. (FTMS)	20 ppm
Label min. ratio count	2	MS/MS tol. (ITMS)	0.5 Da
Machine name	DESKTOP-OMCDT80	MS/MS tol. (TOF)	40 ppm
Main search max. combination..	200	Peptides used for protein qu..	Razor
Max mods in site table	3	Site tables	Oxidation (M)Sites.txt Phospho (STY)Sites.txt
Max. peptide length for unsp..	25	Temporary folder	C:\Users\lacav\Desktop\MQ\Temp
Max. peptide mass [Da]	4600	Top MS/MS peaks per Da inter..	12
Min. delta score for modifie..	6	Top MS/MS peaks per Da inter..	10
Min. delta score for unmodif..	0	User name	lacav
Min. peptide Length	7	Variation mode	None
Min. peptide length for unsp..	8	Version	1.6.7.0
Min. peptides	1	NA	NA

uniprot-proteome\_up000005640+AND+reviewed\_yes.fasta

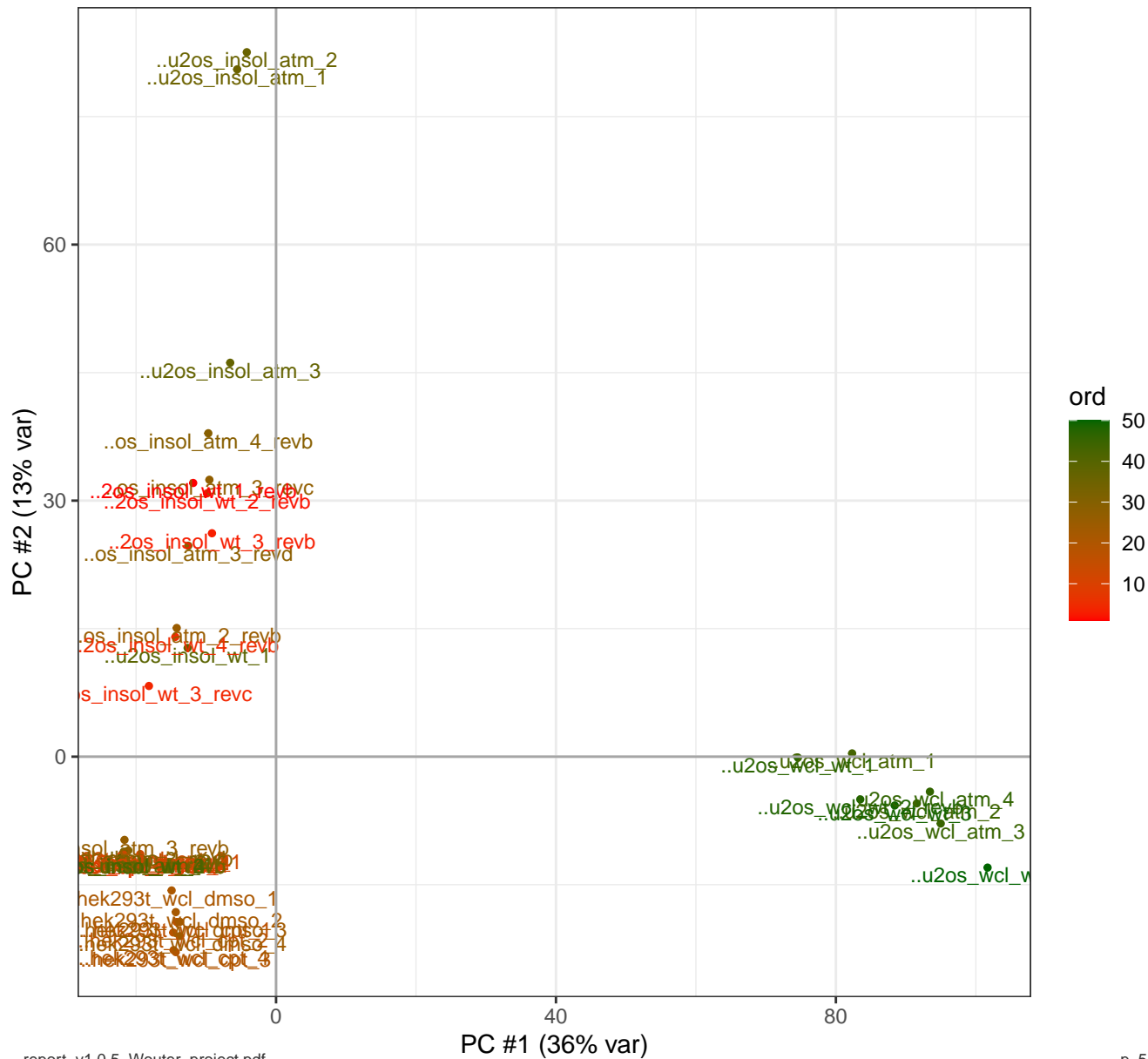
# PG: PCA of 'raw intensity'

(excludes contaminants)

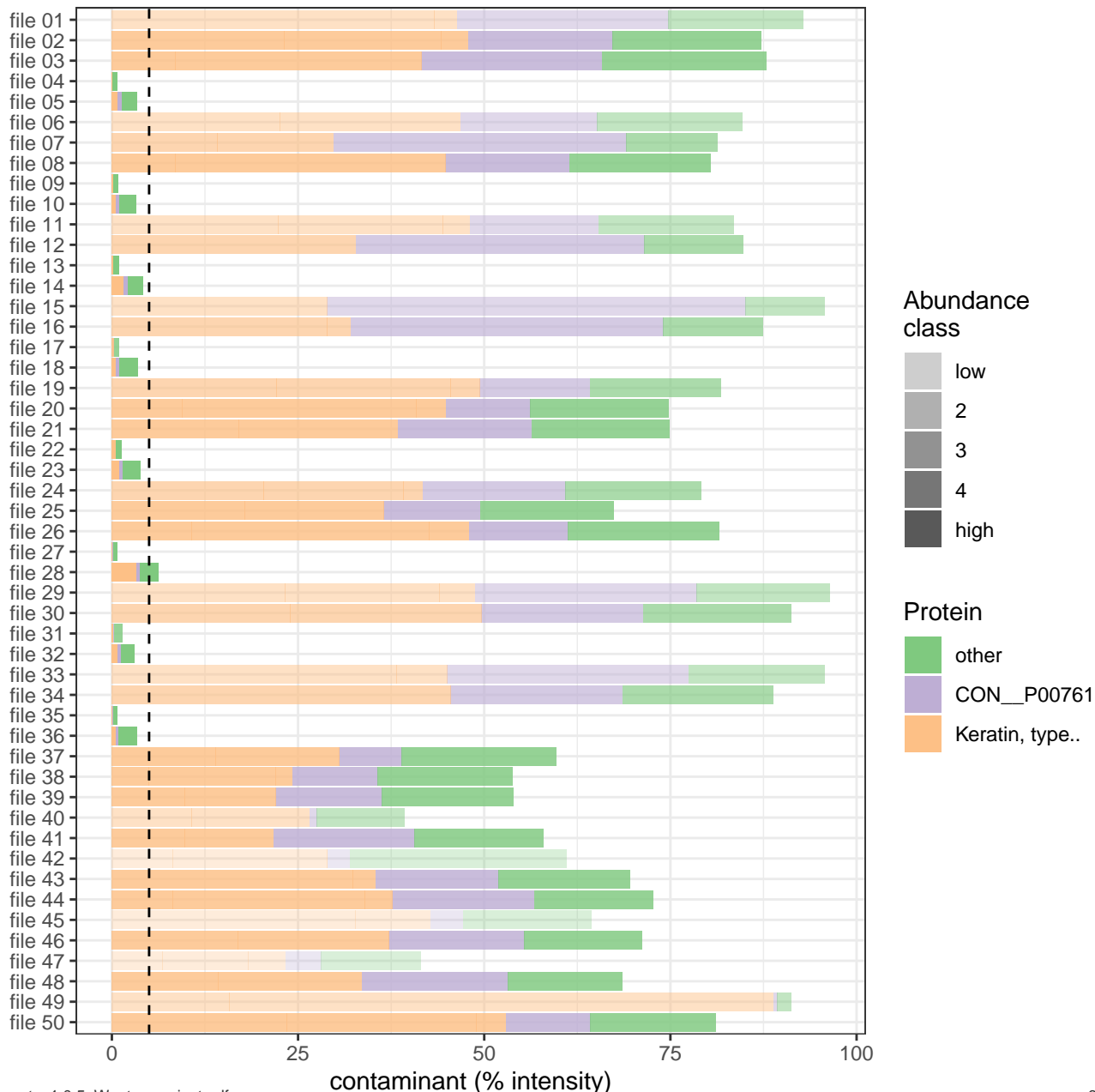


## PG: PCA of 'lfq intensity'

(excludes contaminants)



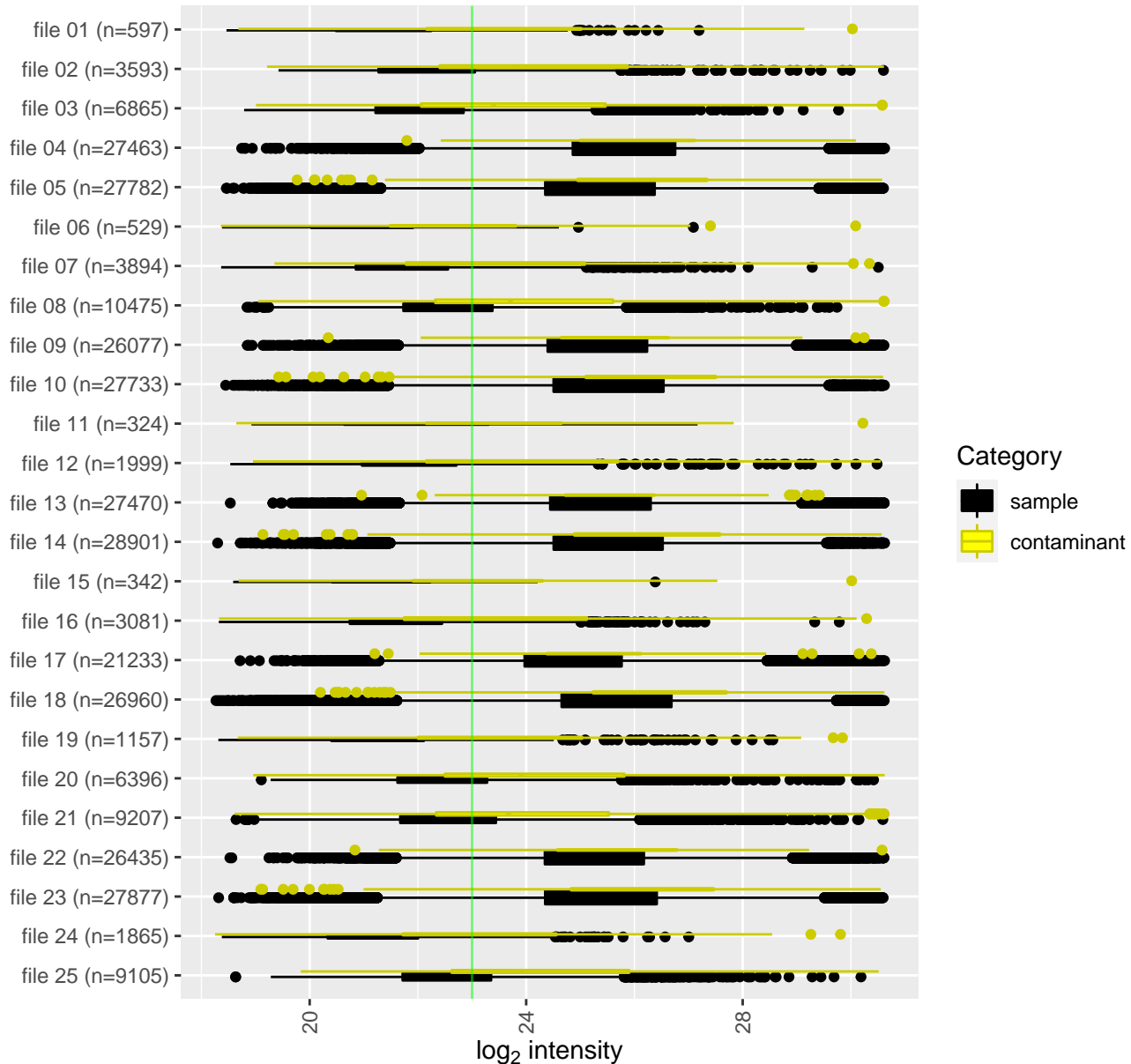
# EVD: Top5 Contaminants per Raw file





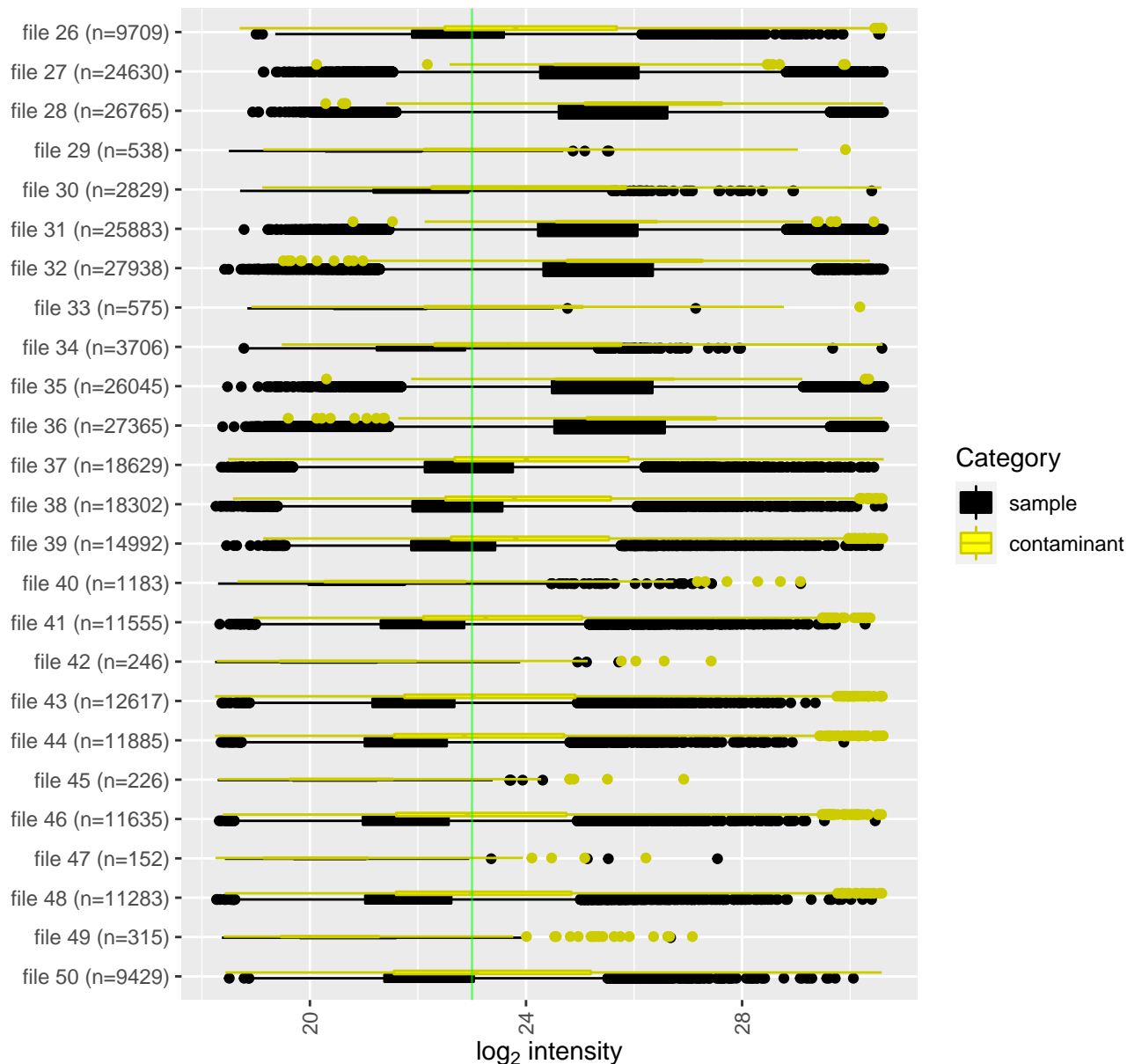
# EVD: peptide intensity distribution

RSD 7.4% (expected < 5%)



# EVD: peptide intensity distribution

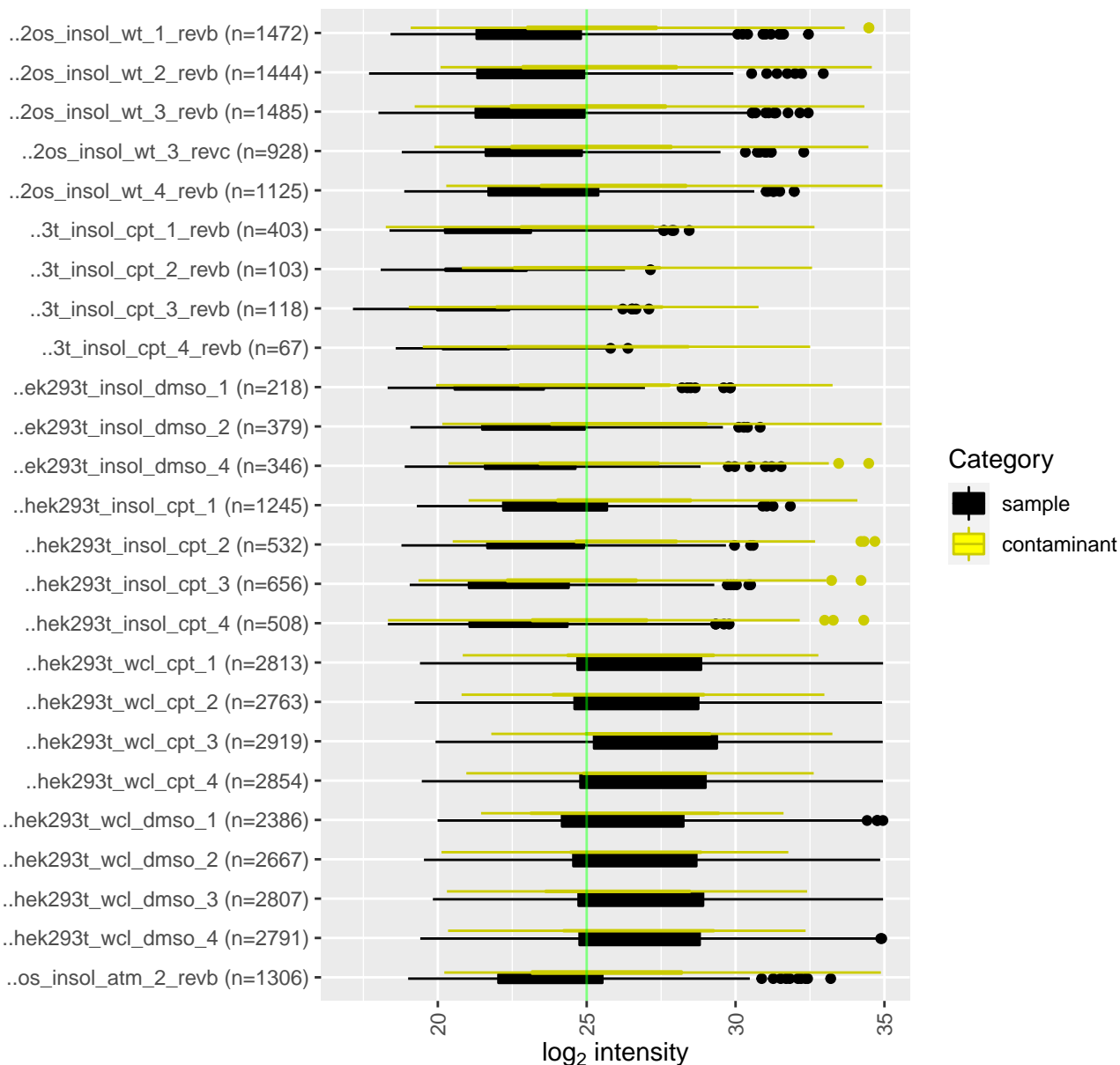
RSD 7.4% (expected < 5%)



# PG: intensity distribution

RSD 9.2% (w/o zero int.; expected < 5%)

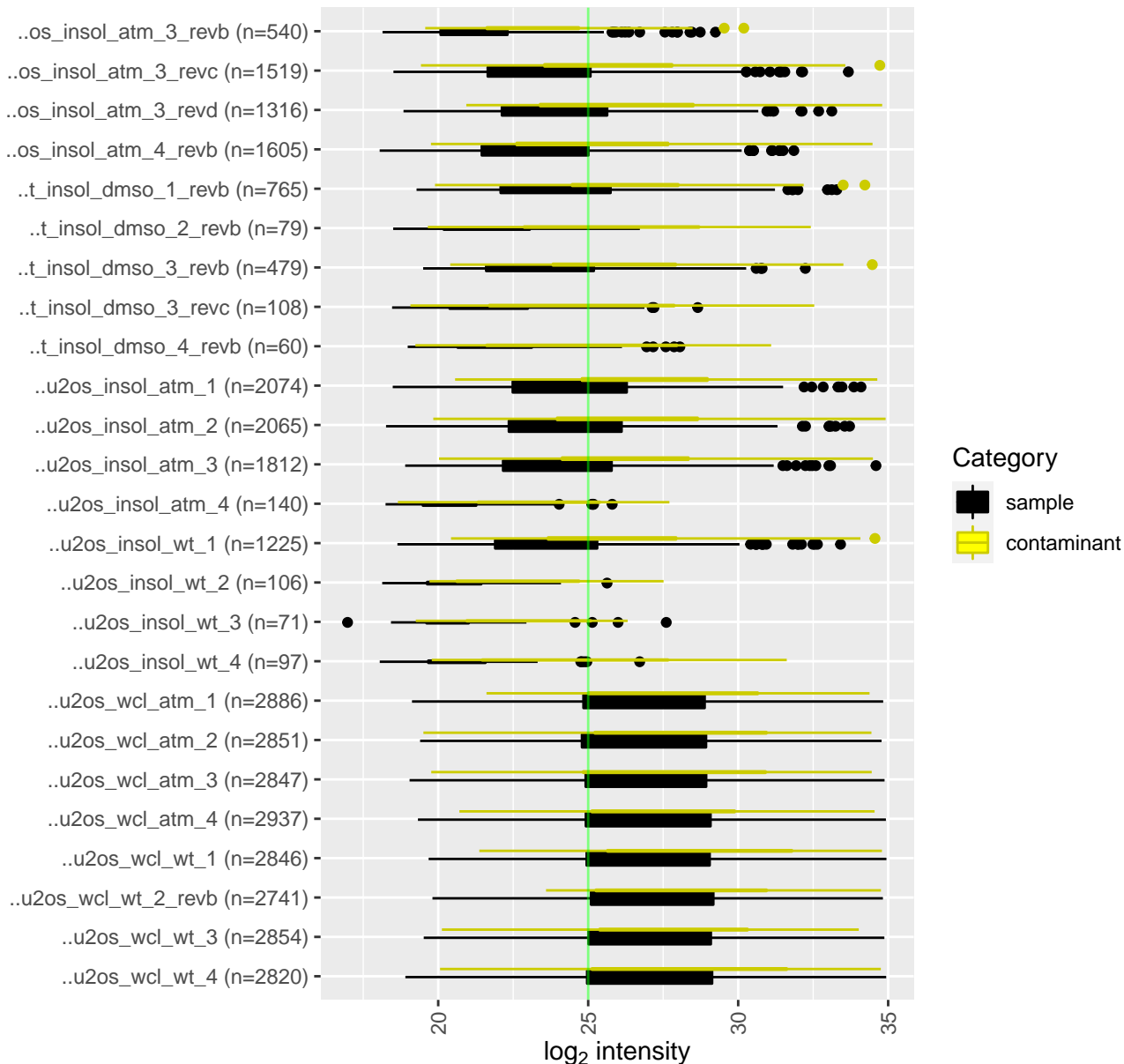
RSD 147.3% [high RSD --> few peptides])



# PG: intensity distribution

RSD 9.2% (w/o zero int.; expected < 5%)

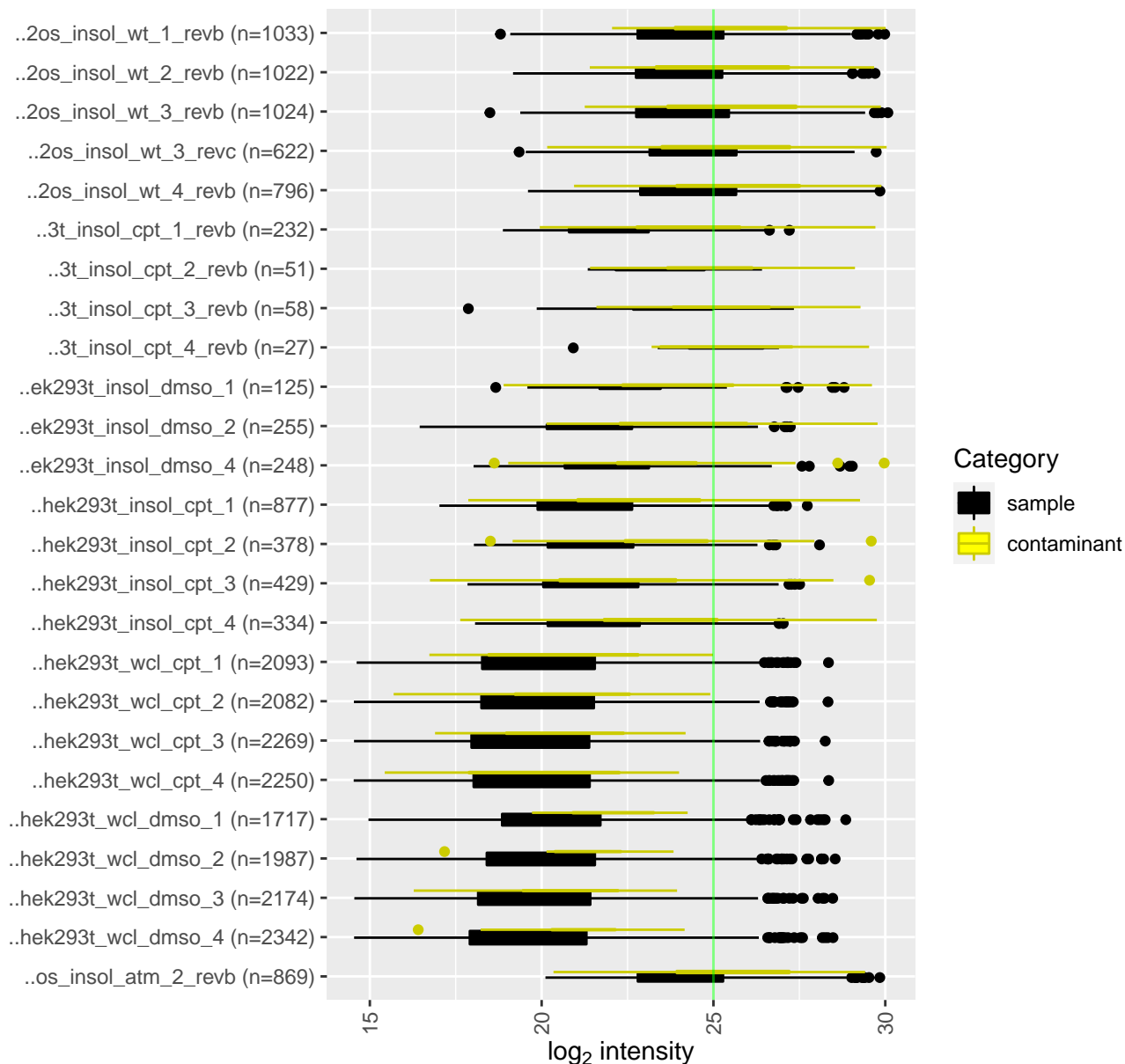
RSD 147.3% [high RSD --> few peptides])



# PG: LFQ intensity distribution

RSD 7.7% (w/o zero int.; expected < 5%)

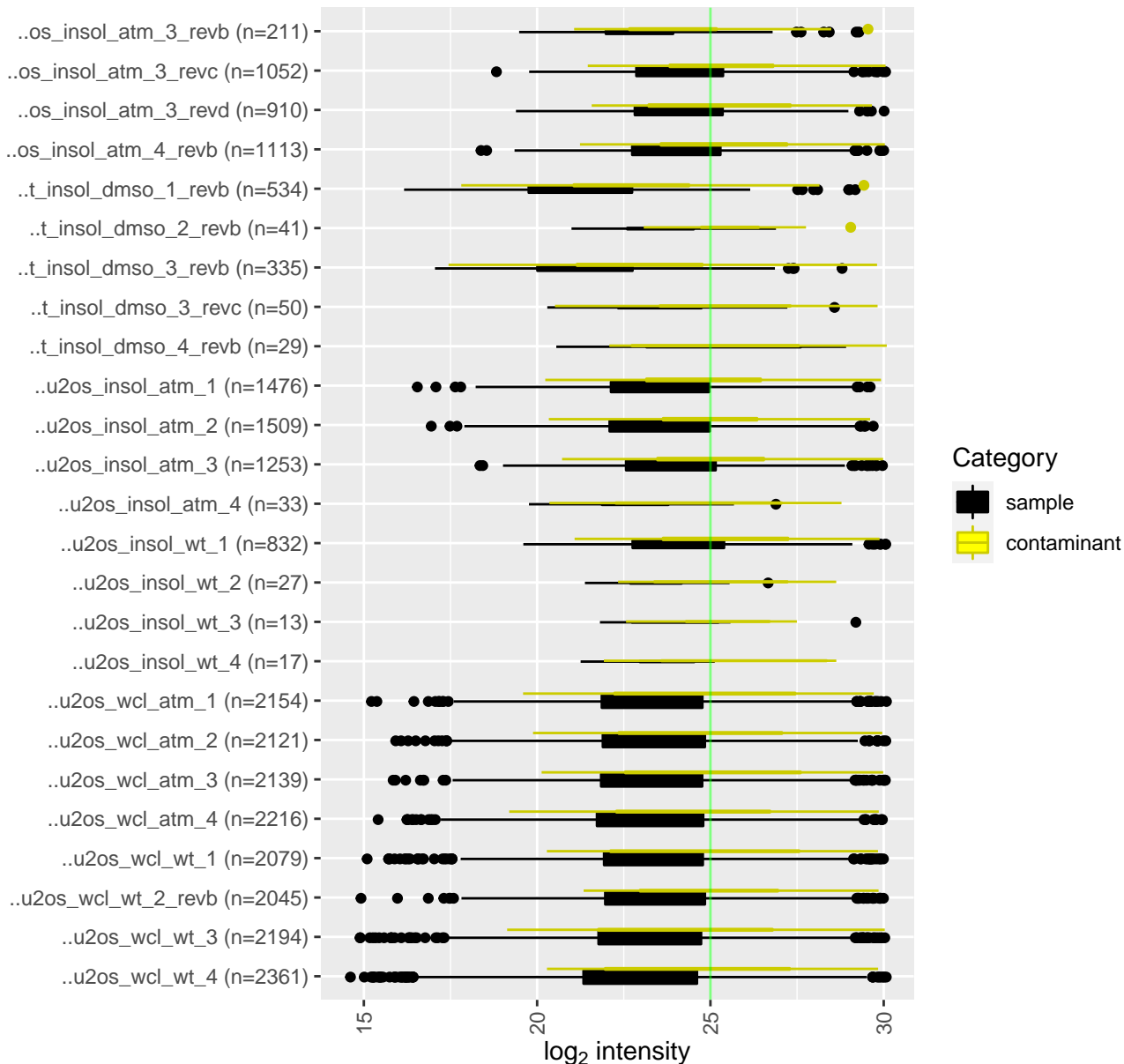
RSD 345.2% [high RSD --> few peptides]



# PG: LFQ intensity distribution

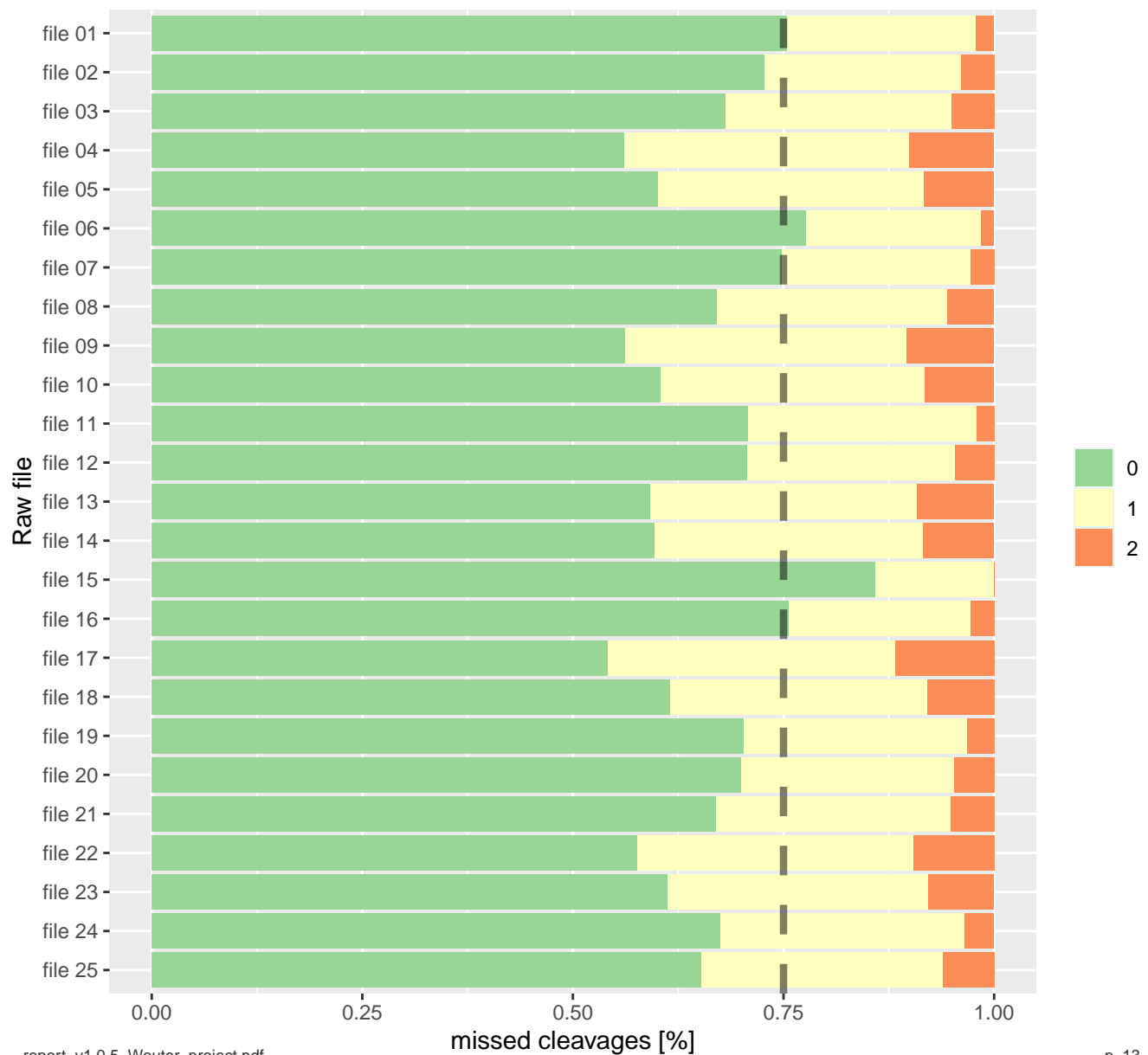
RSD 7.7% (w/o zero int.; expected < 5%)

RSD 345.2% [high RSD --> few peptides])



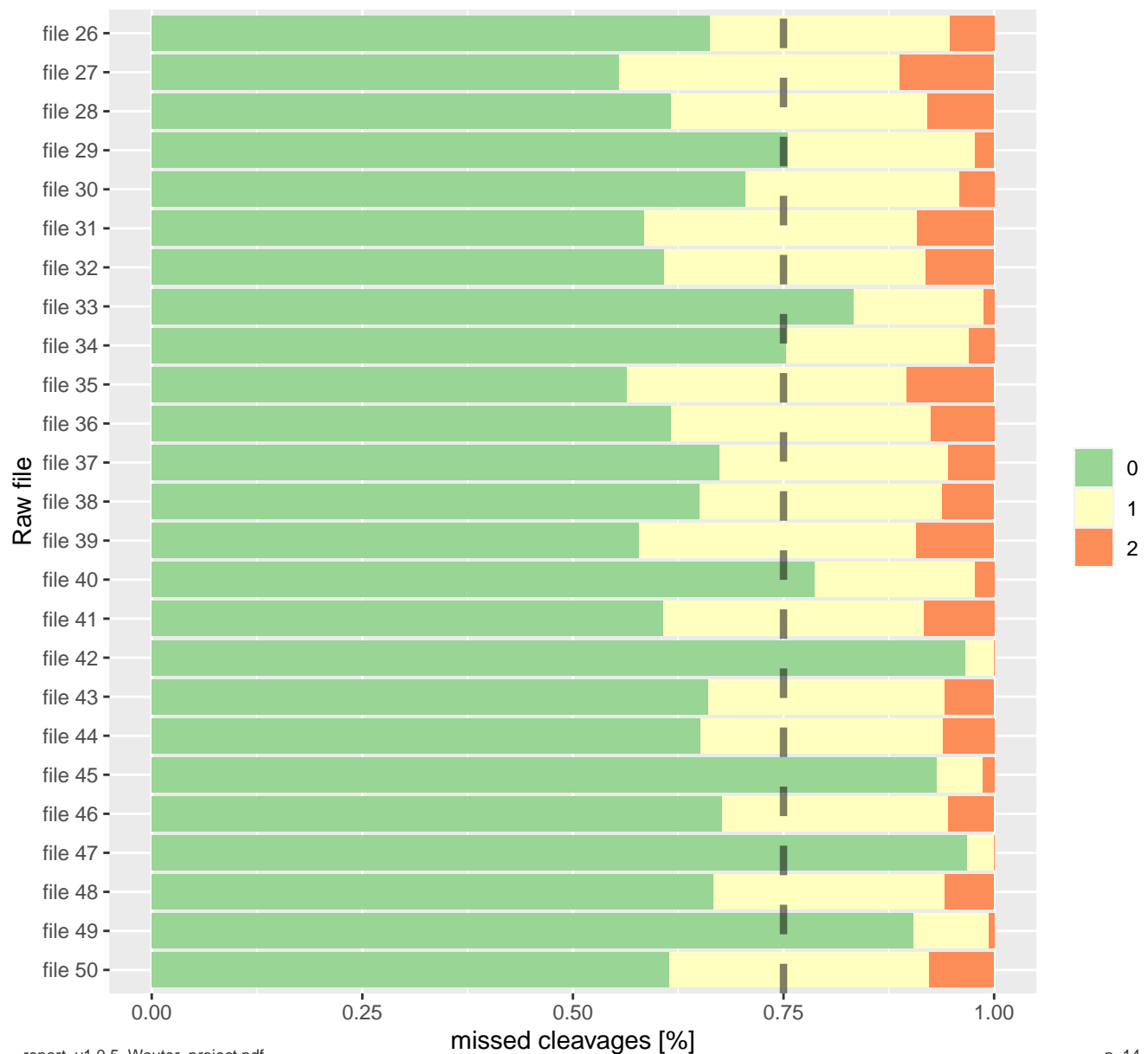
# MSMS: Missed cleavages per Raw file

(excludes contaminants)



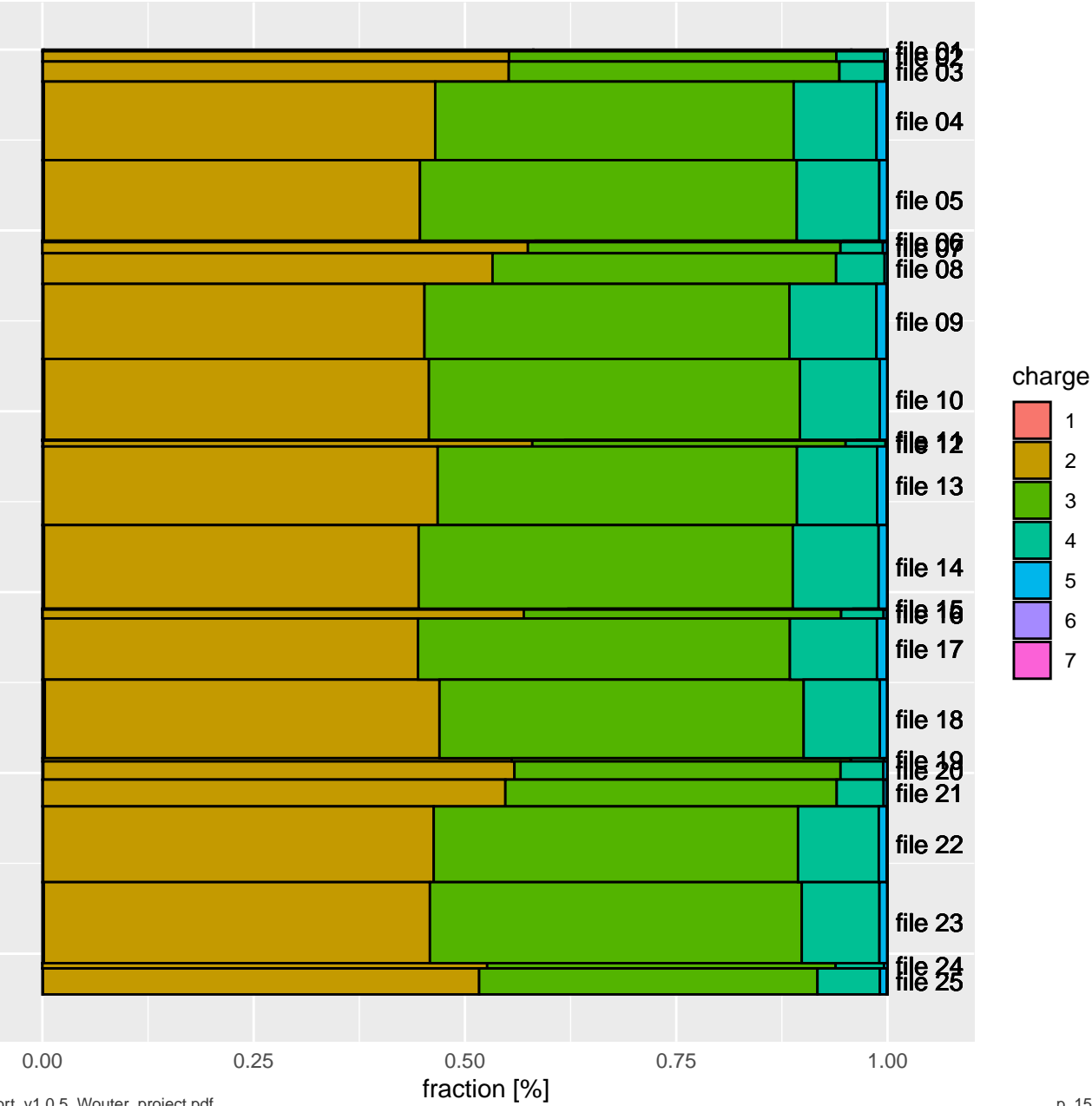
# MSMS: Missed cleavages per Raw file

(excludes contaminants)

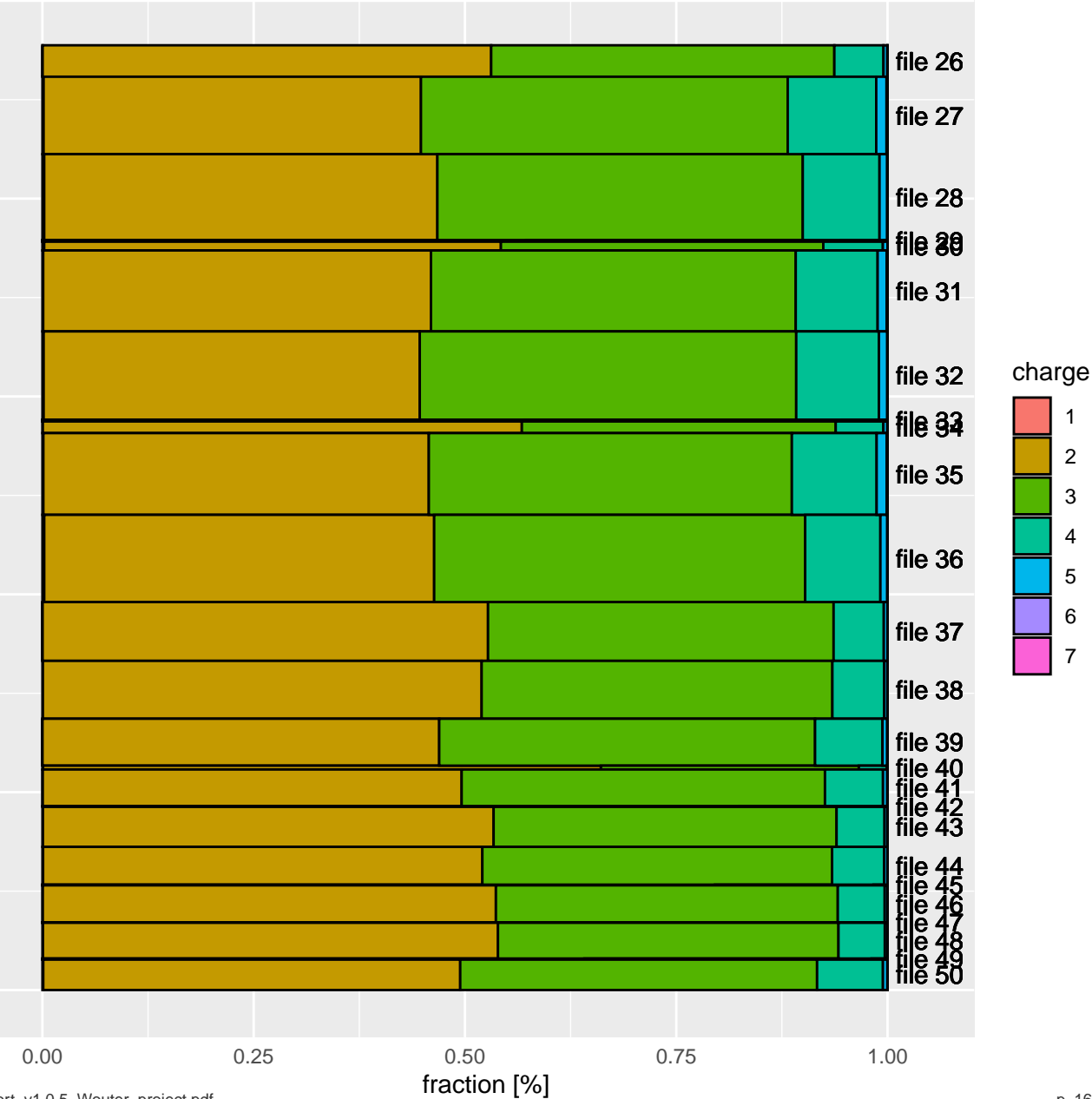




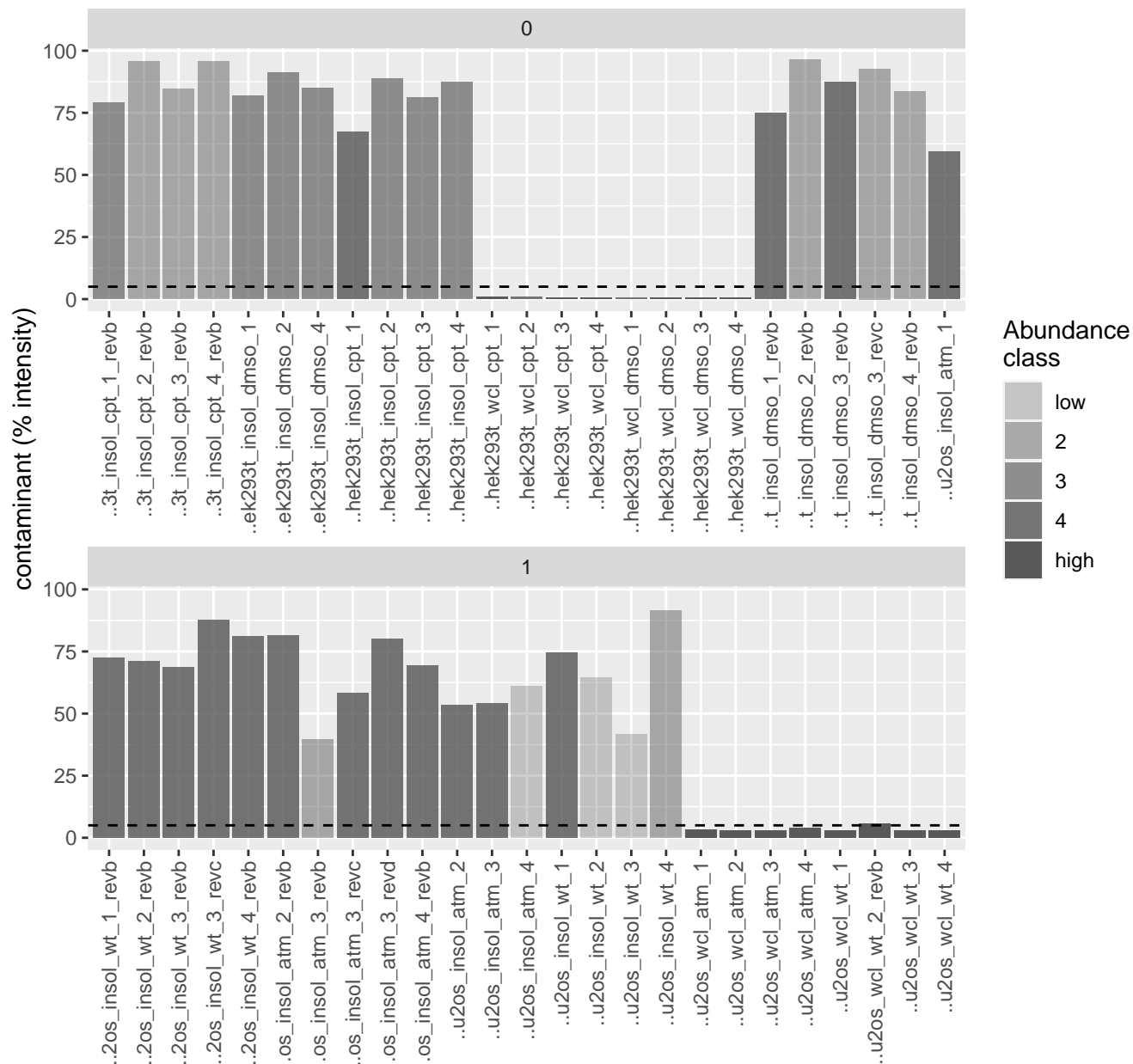
EVD: charge distribution



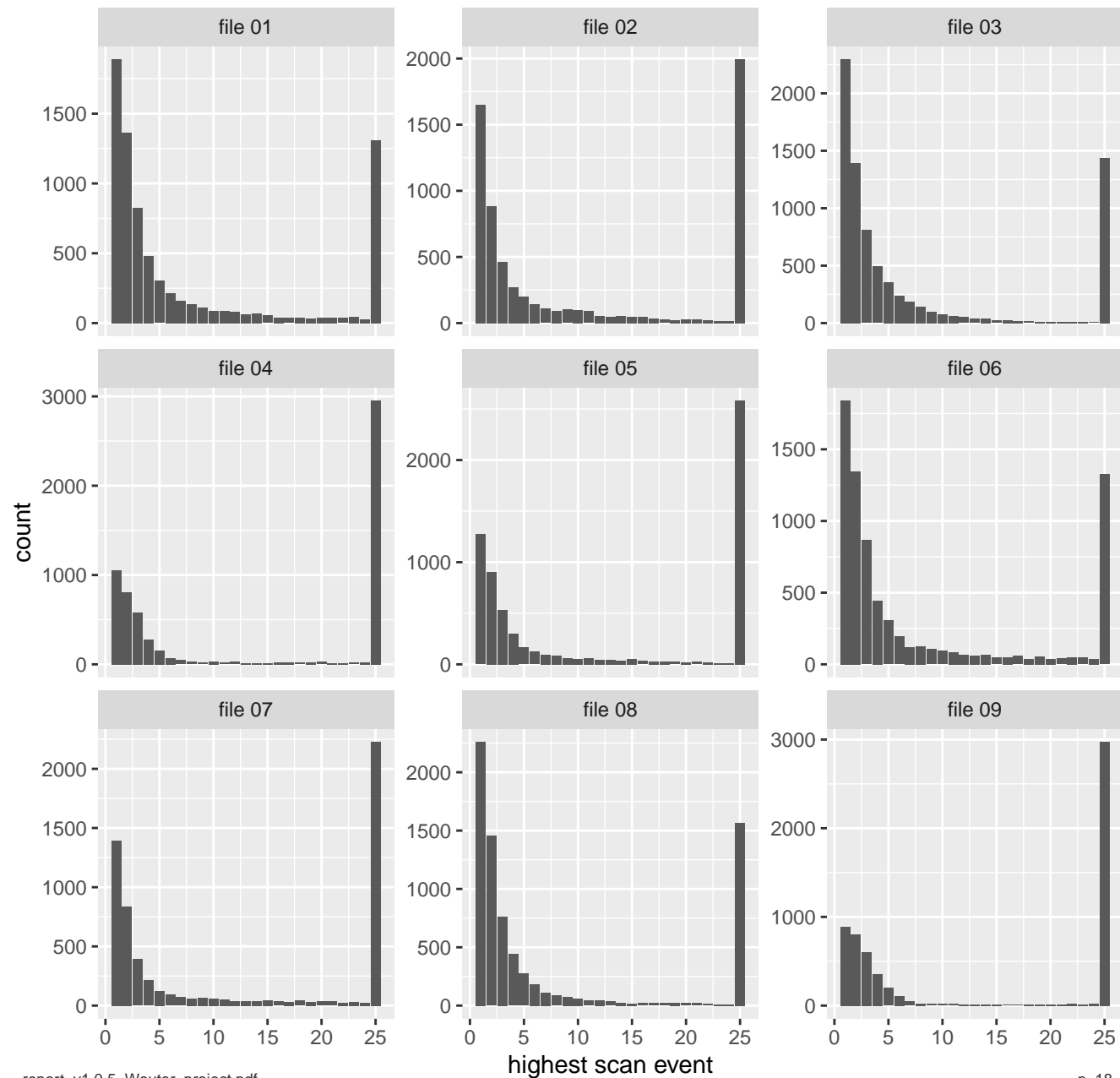
EVD: charge distribution



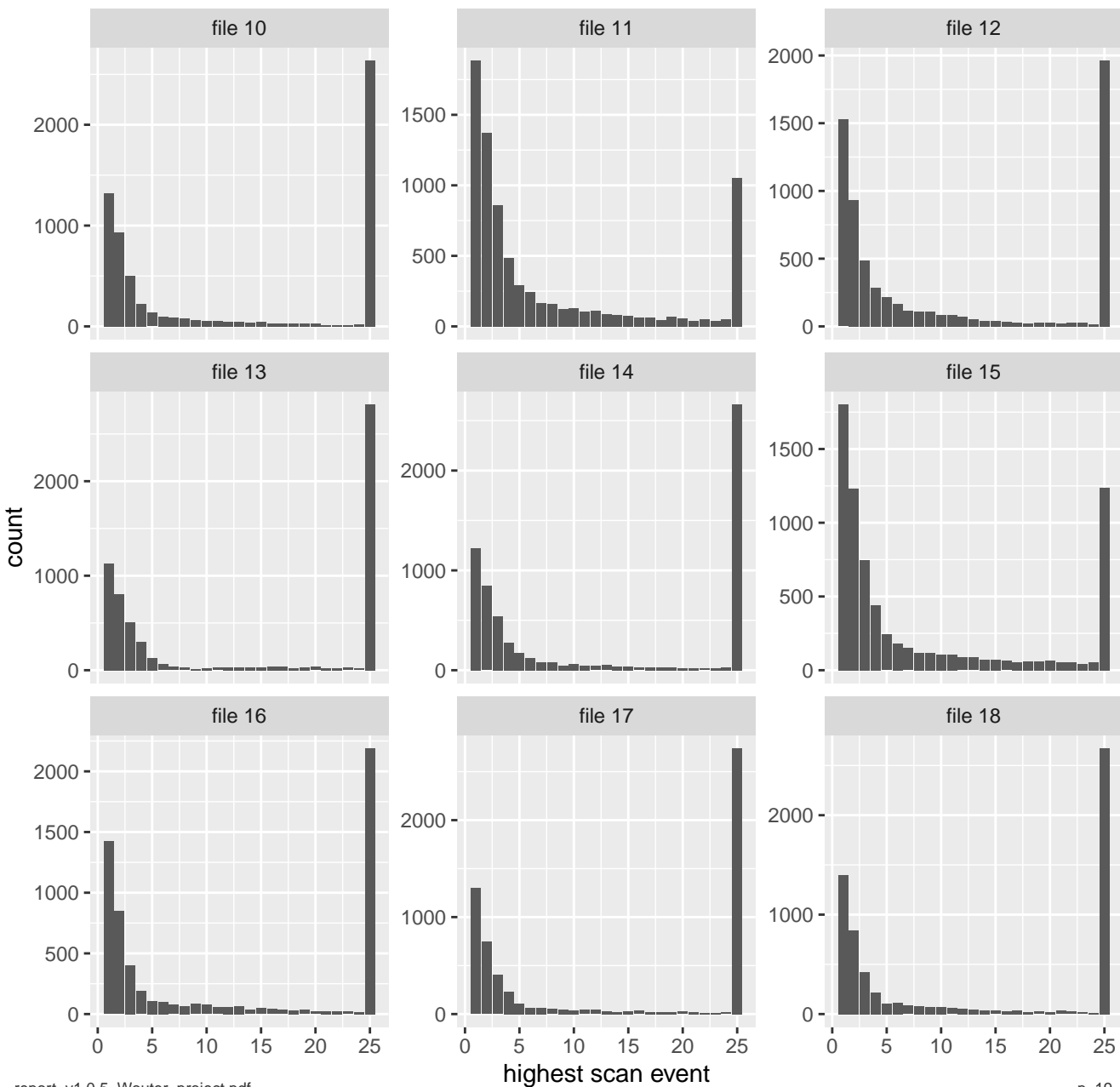
# PG: Contaminant per condition



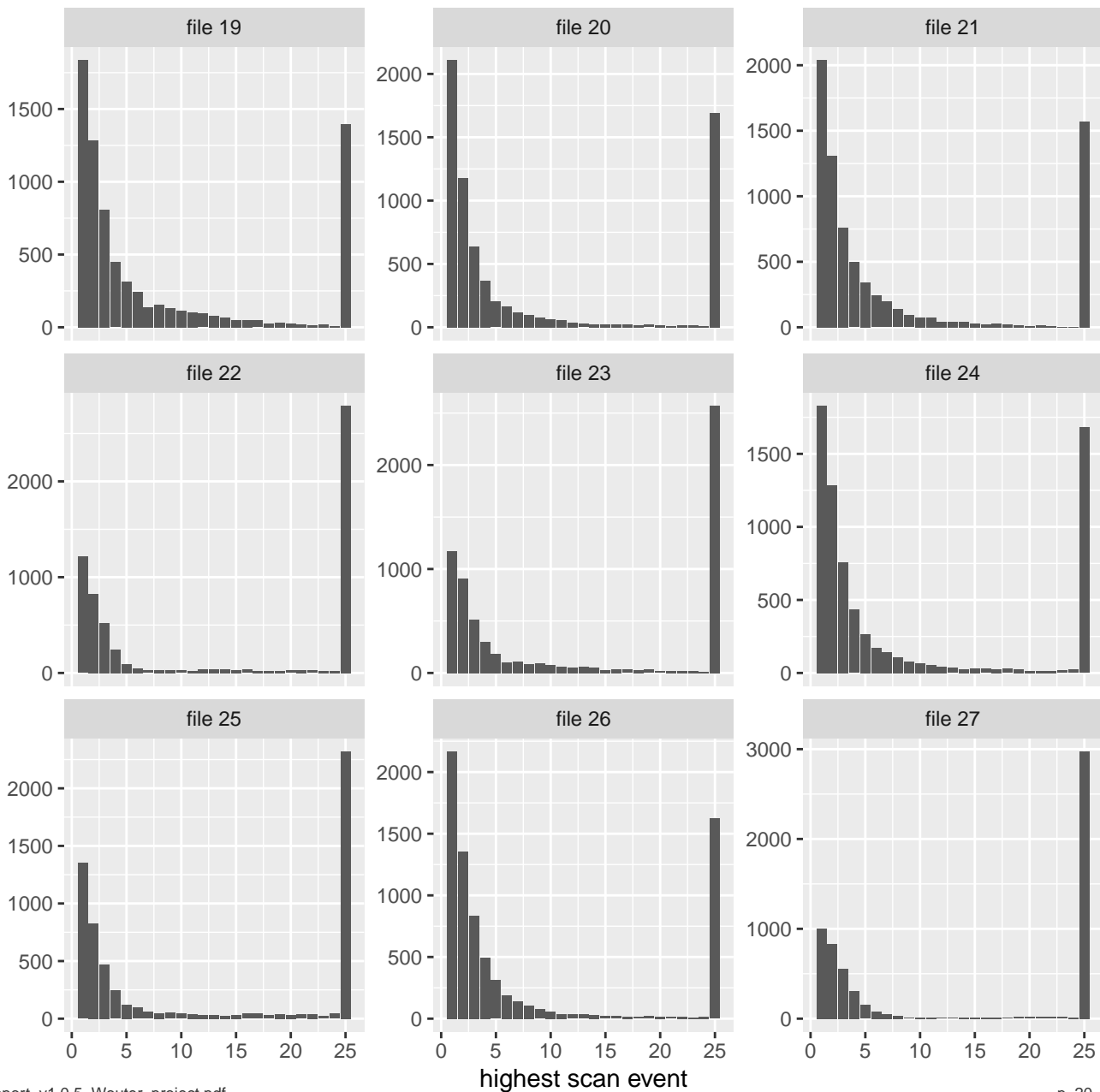
# MSMSScans: TopN



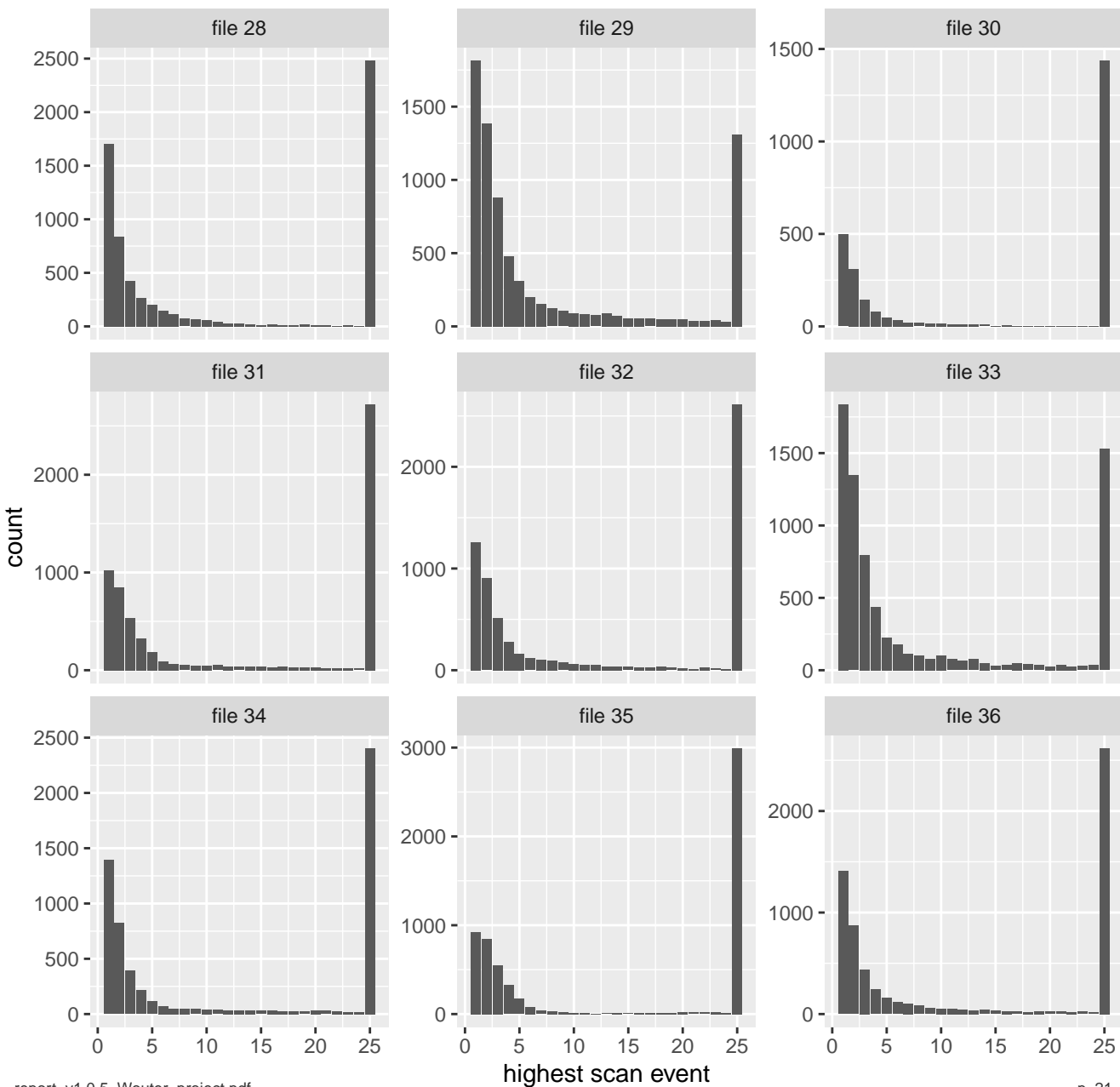
# MSMSscans: TopN



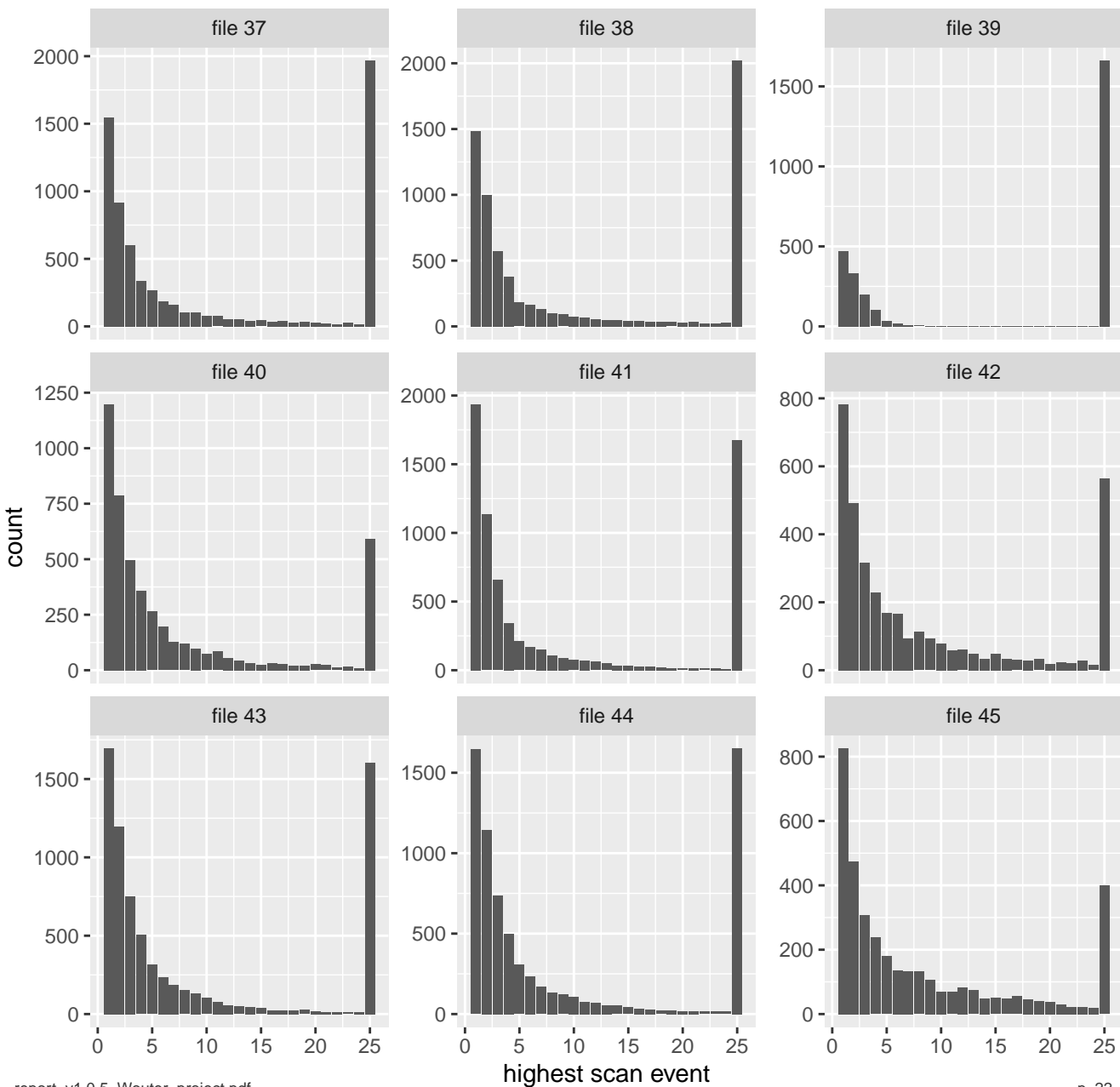
# MSMSScans: TopN



# MSMSScans: TopN

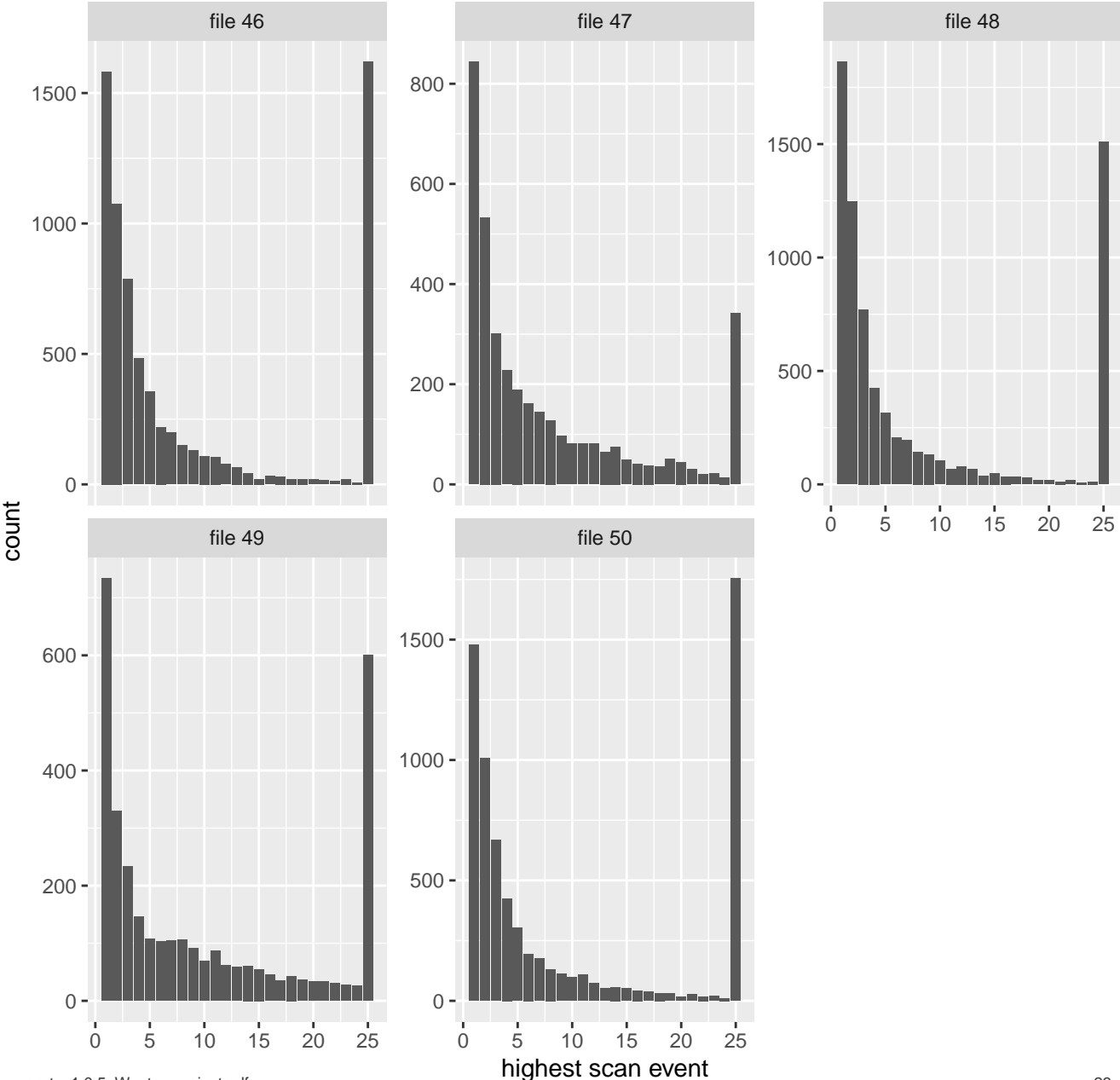


# MSMSscans: TopN

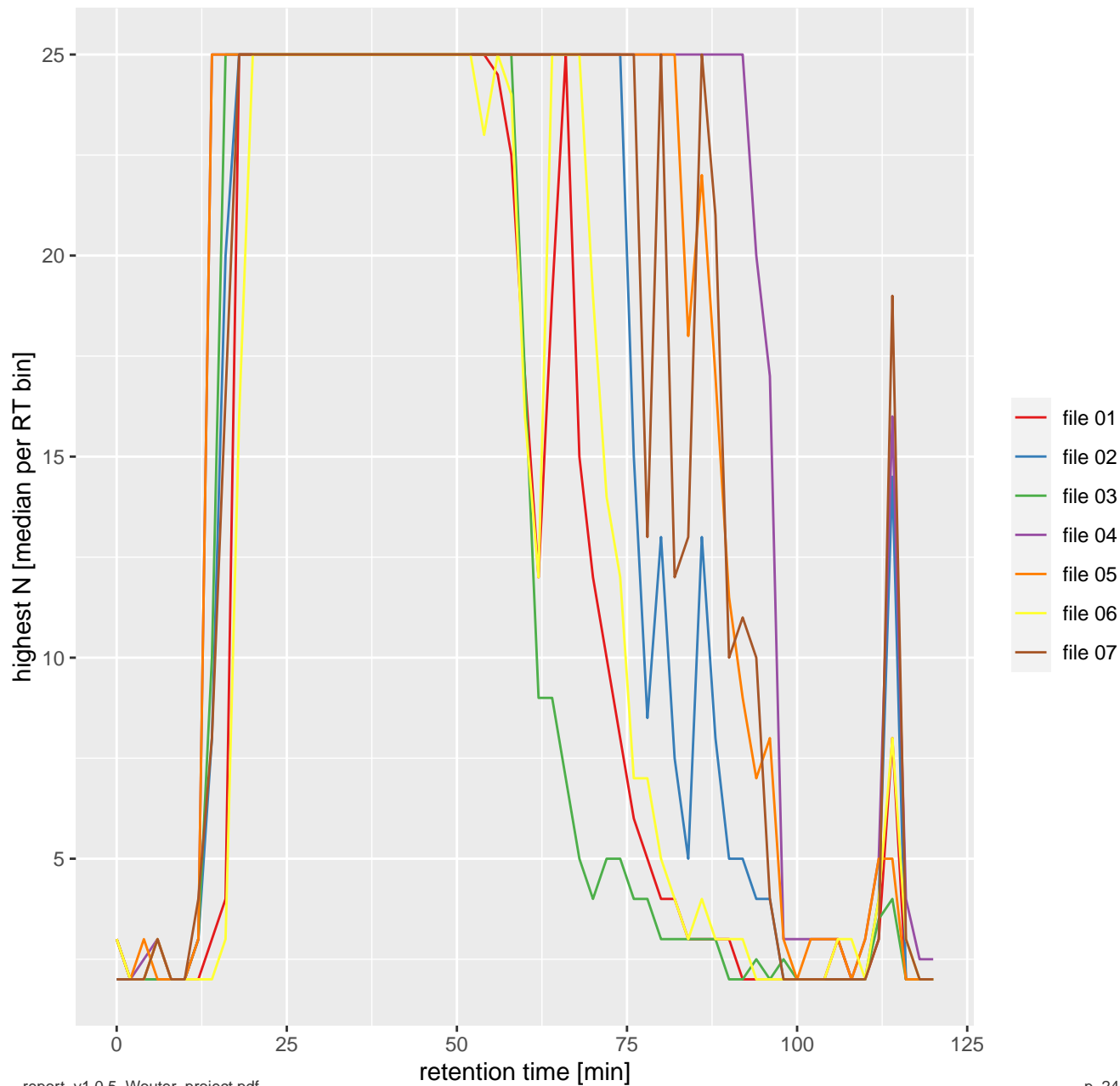




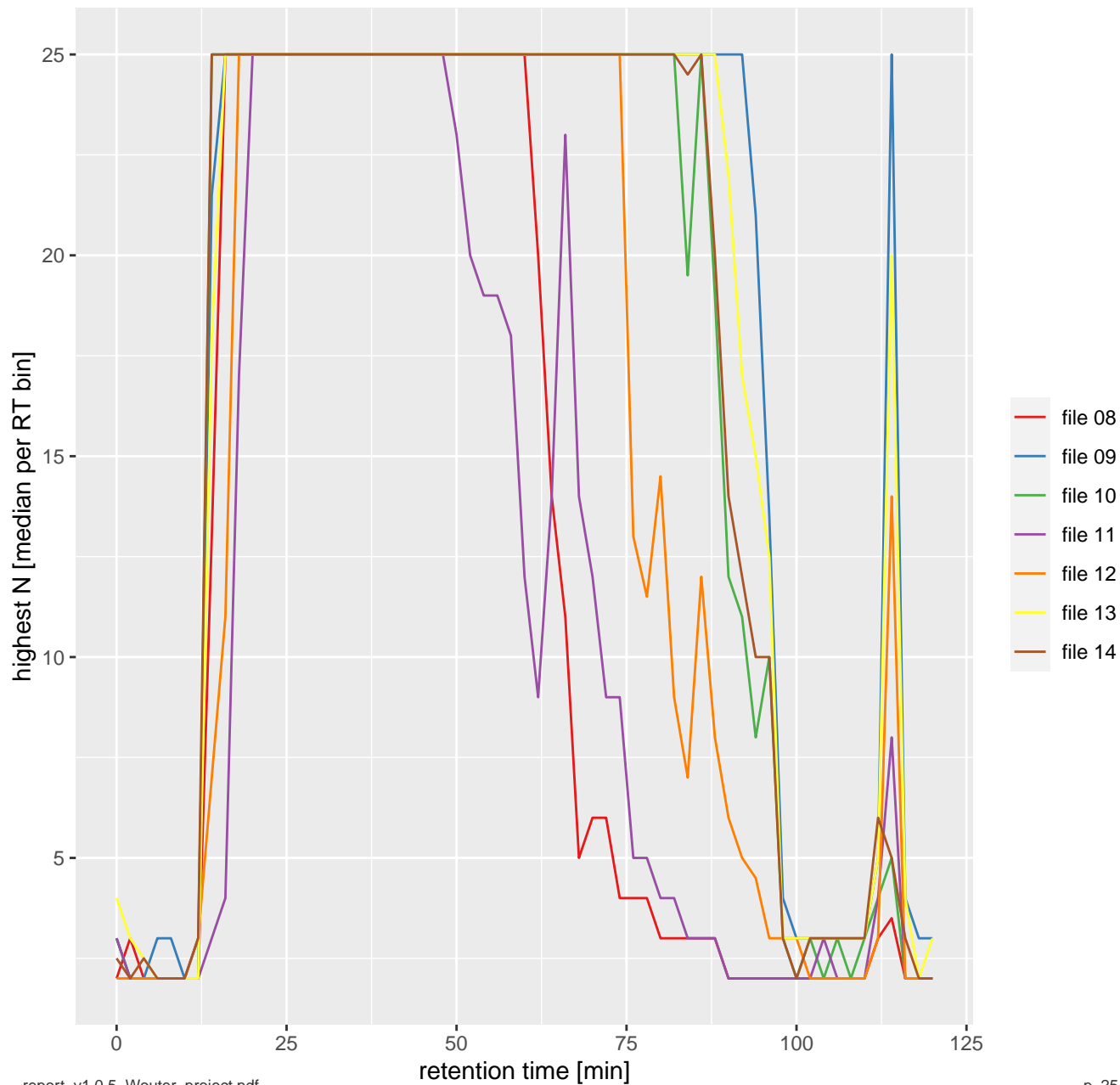
# MSMSscans: TopN



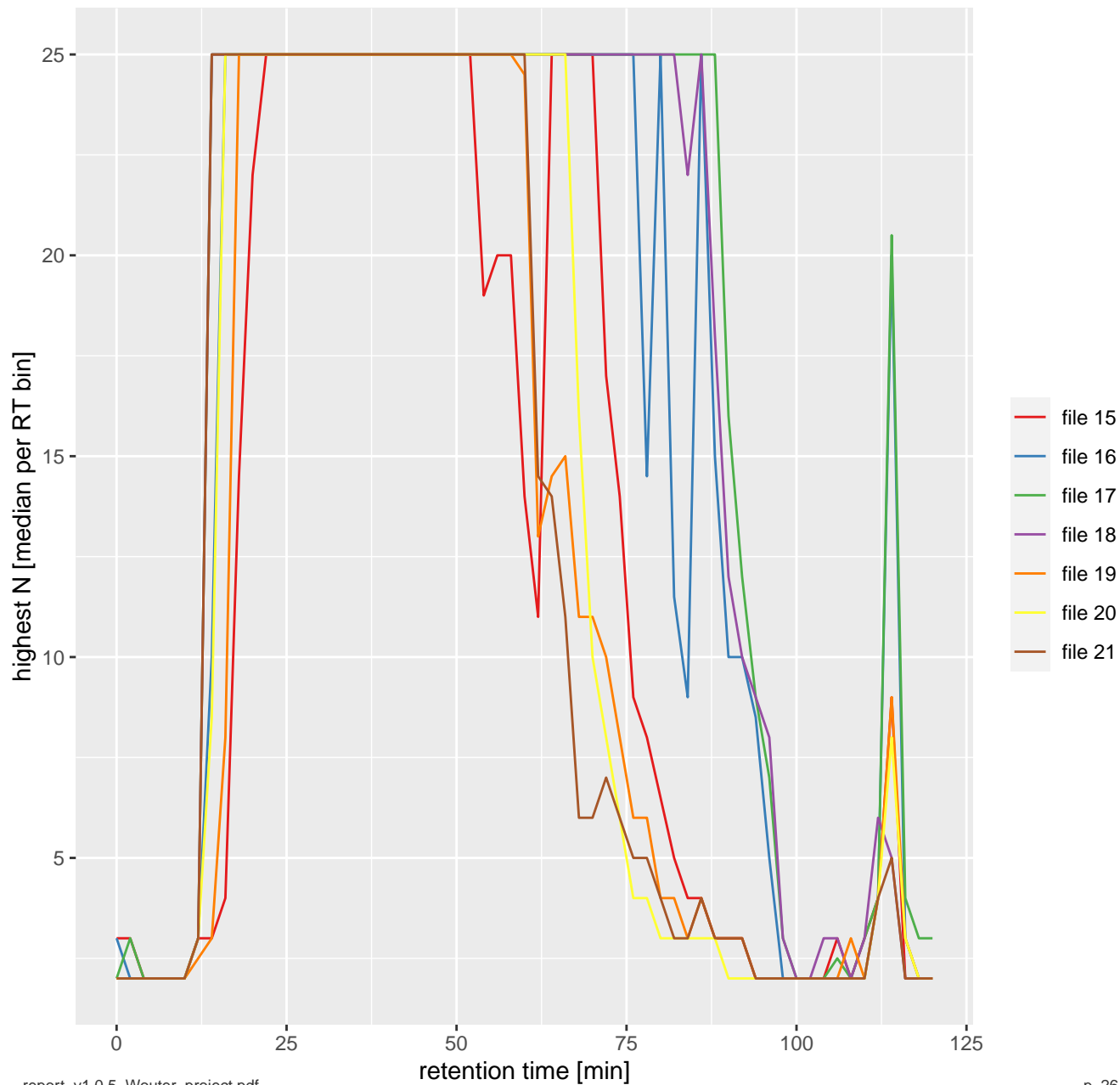
# MSMSscans: TopN over RT



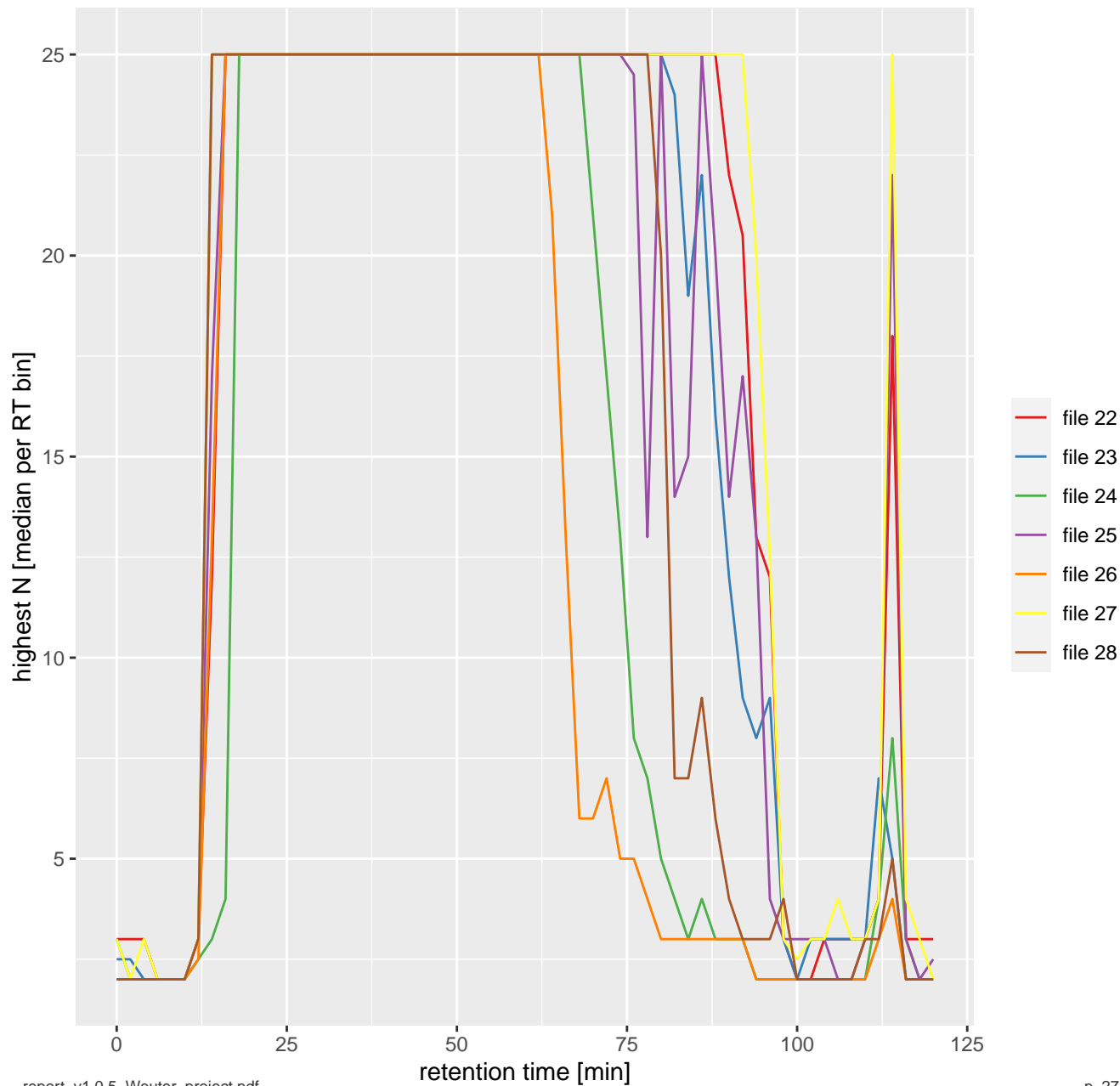
# MSMSscans: TopN over RT



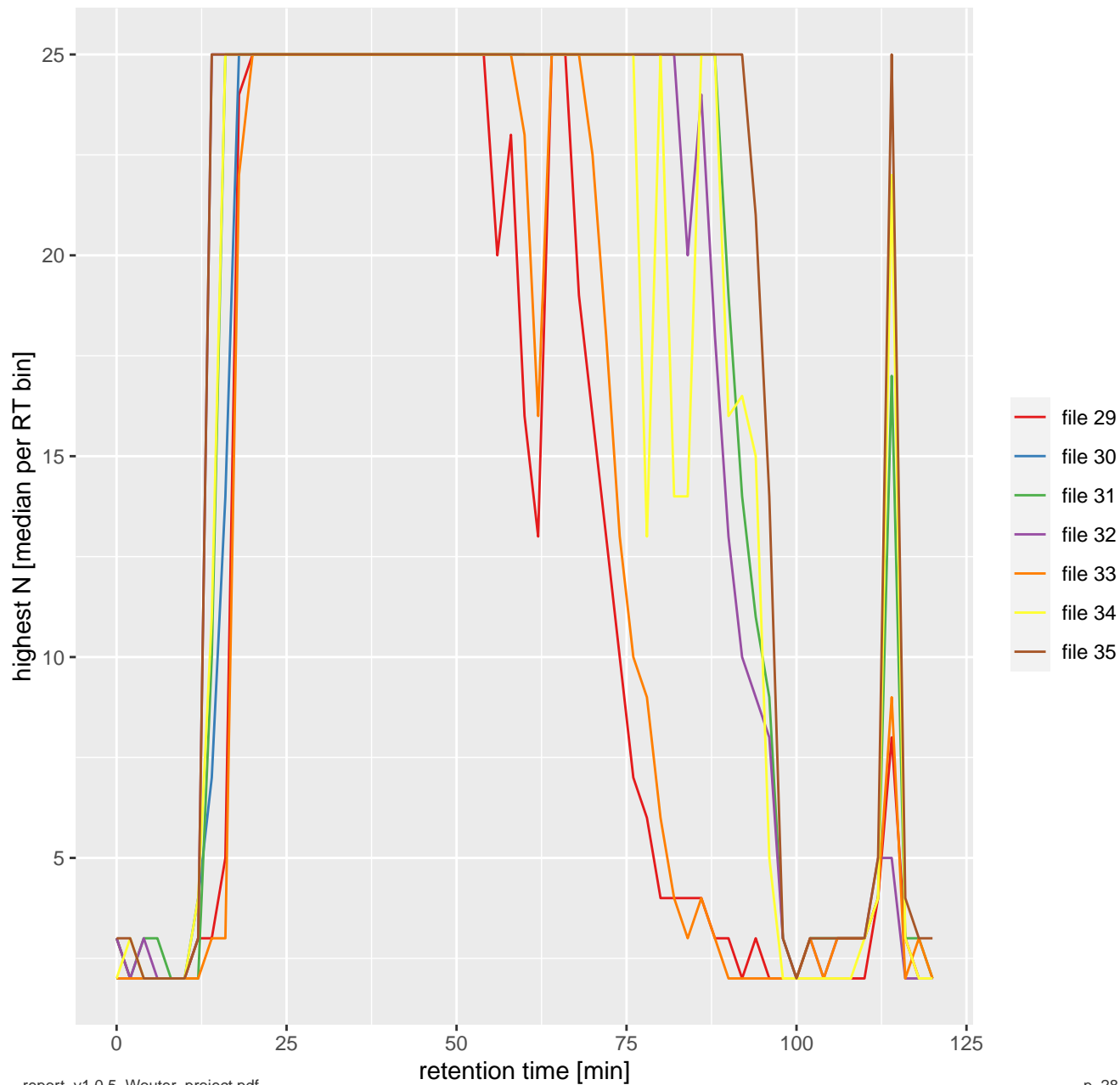
# MSMSscans: TopN over RT



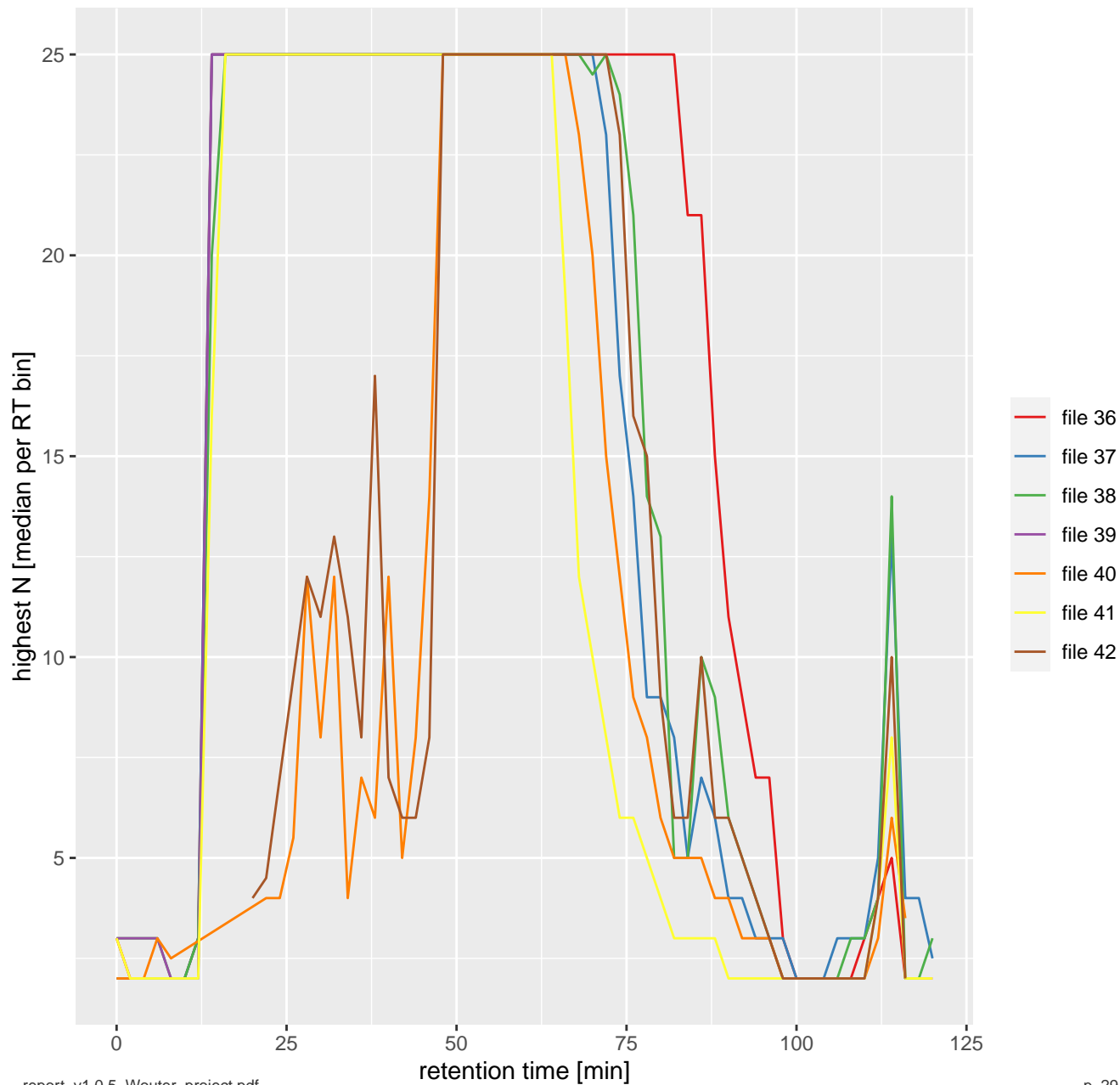
# MSMSscans: TopN over RT



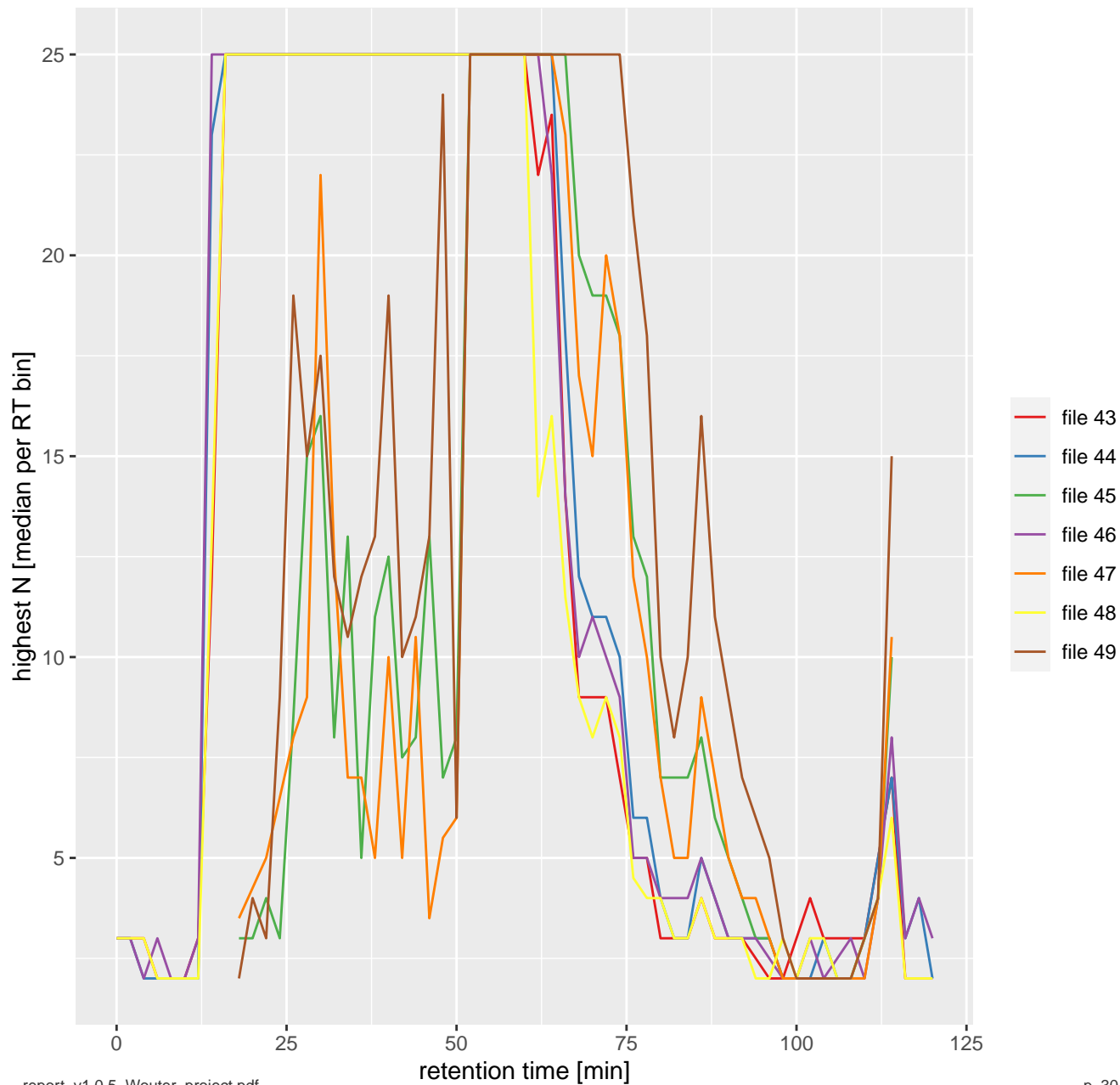
# MSMSscans: TopN over RT



# MSMSScans: TopN over RT

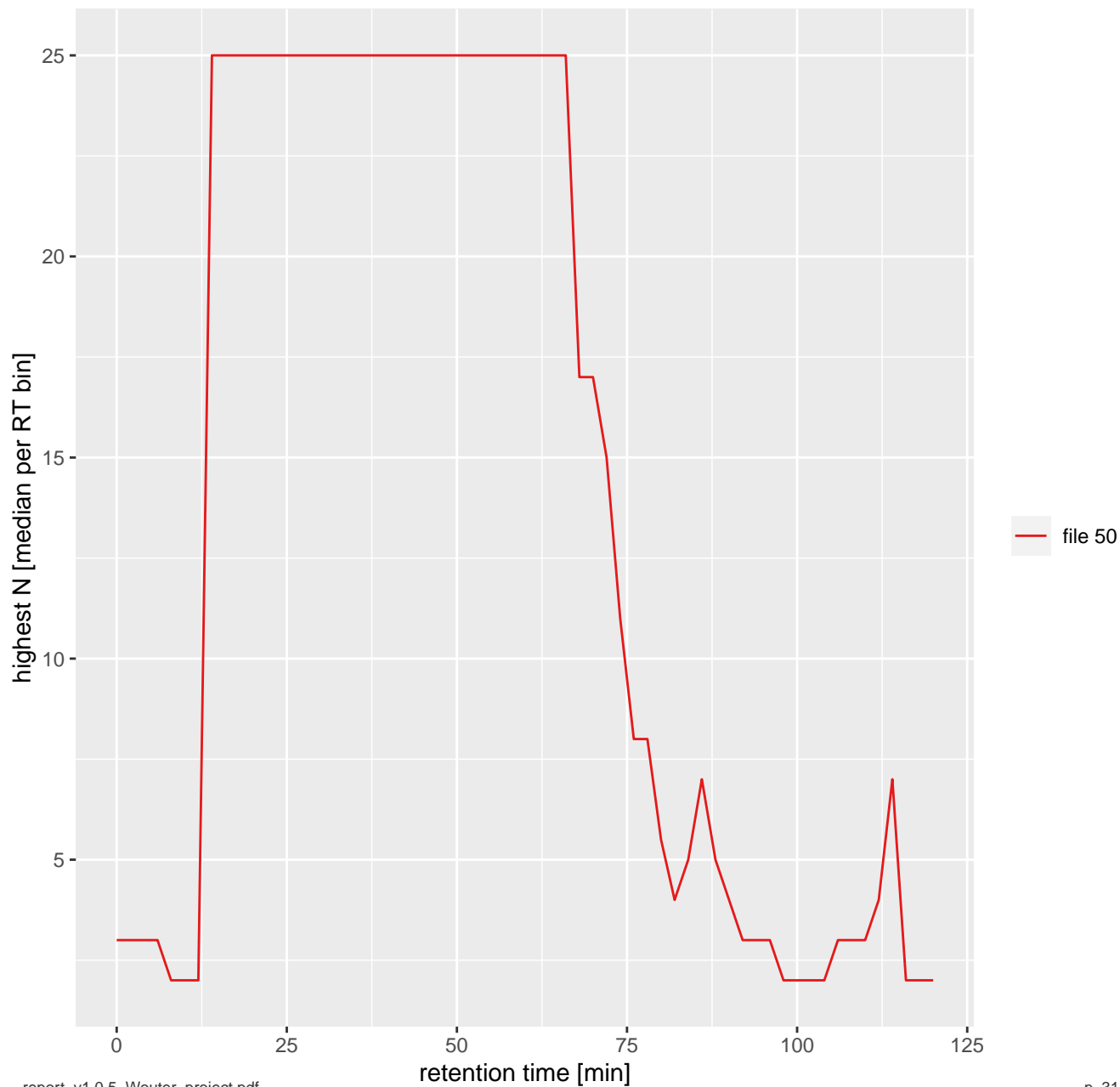


# MSMSscans: TopN over RT

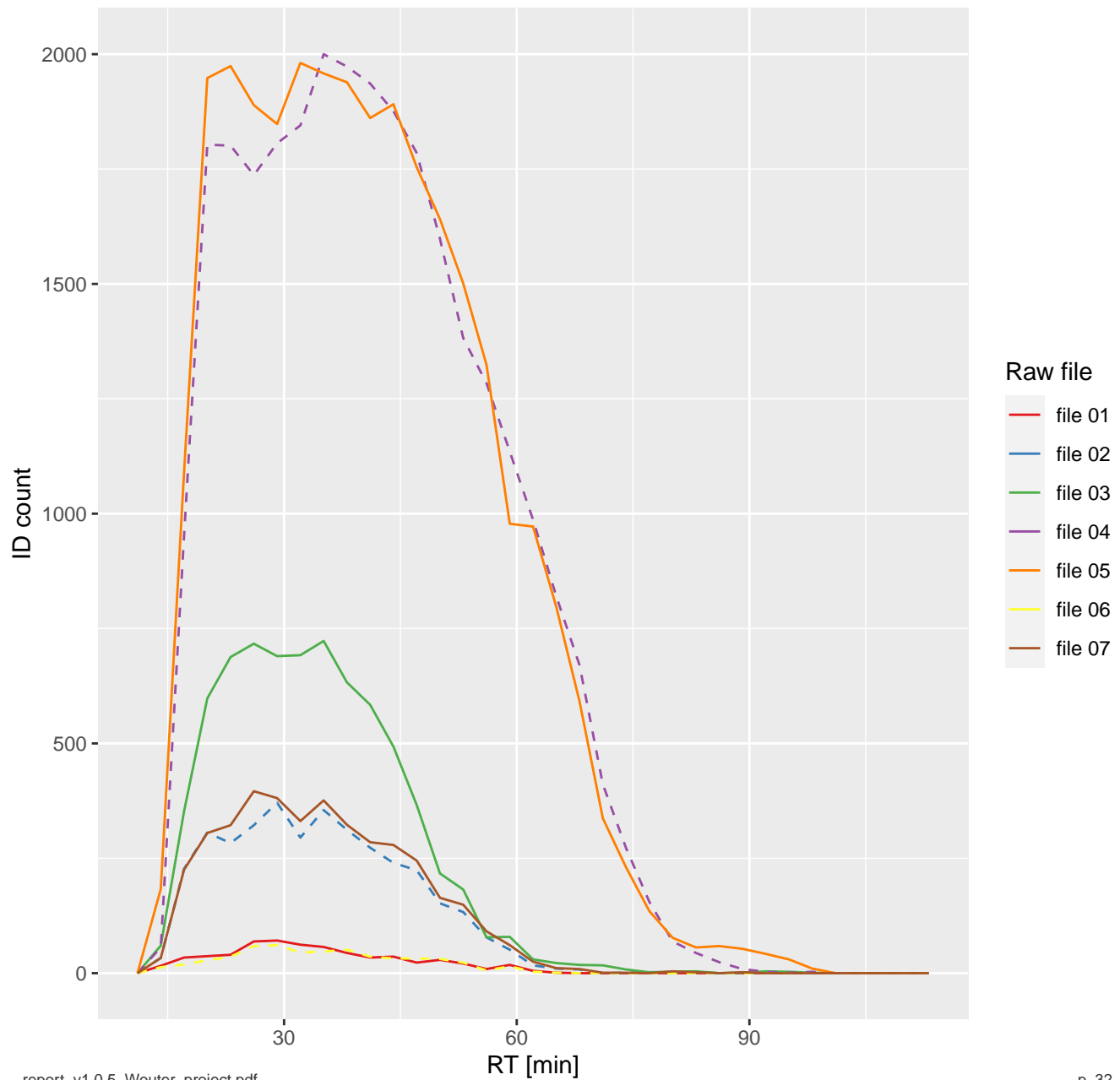




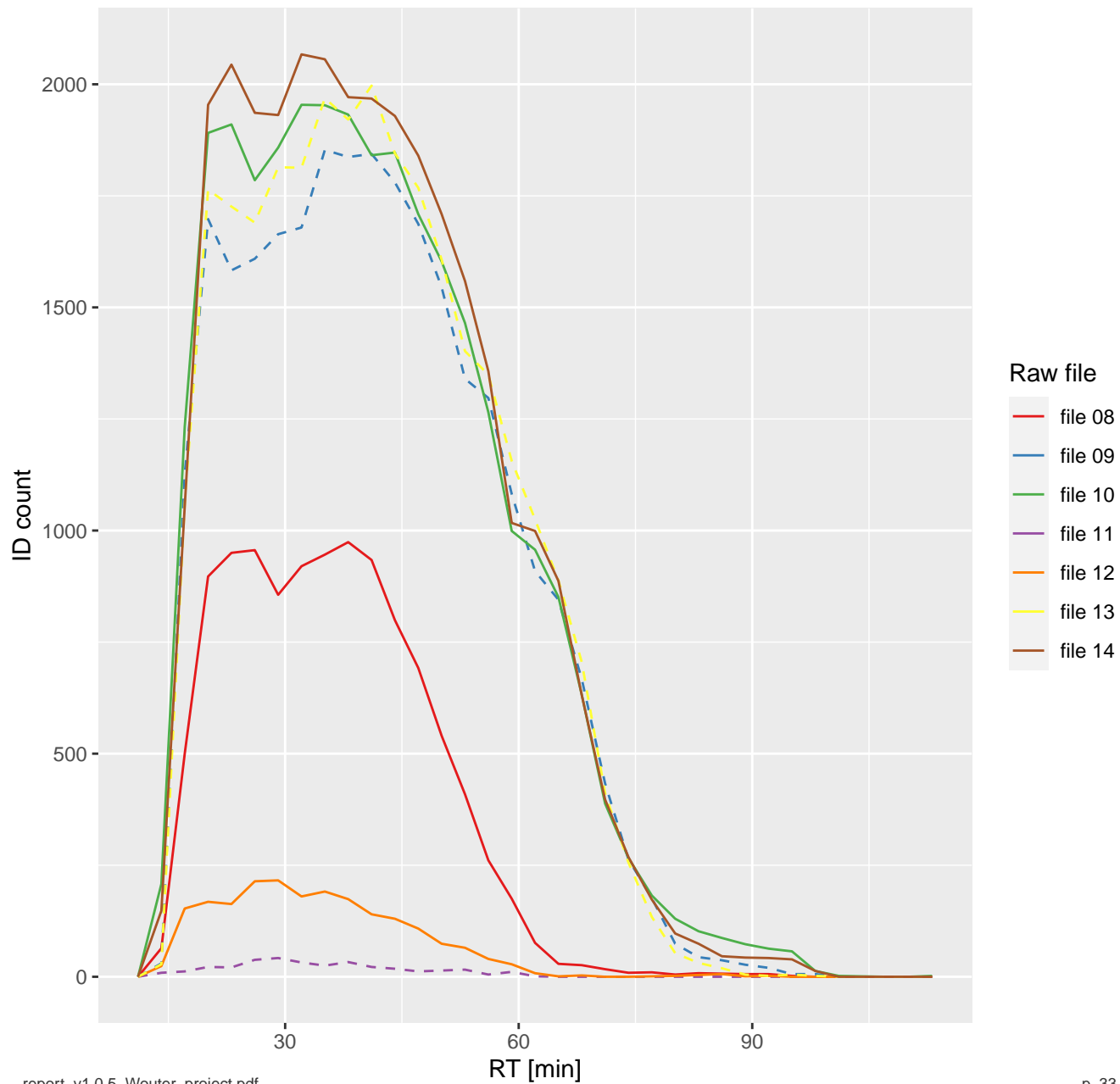
# MSMSscans: TopN over RT



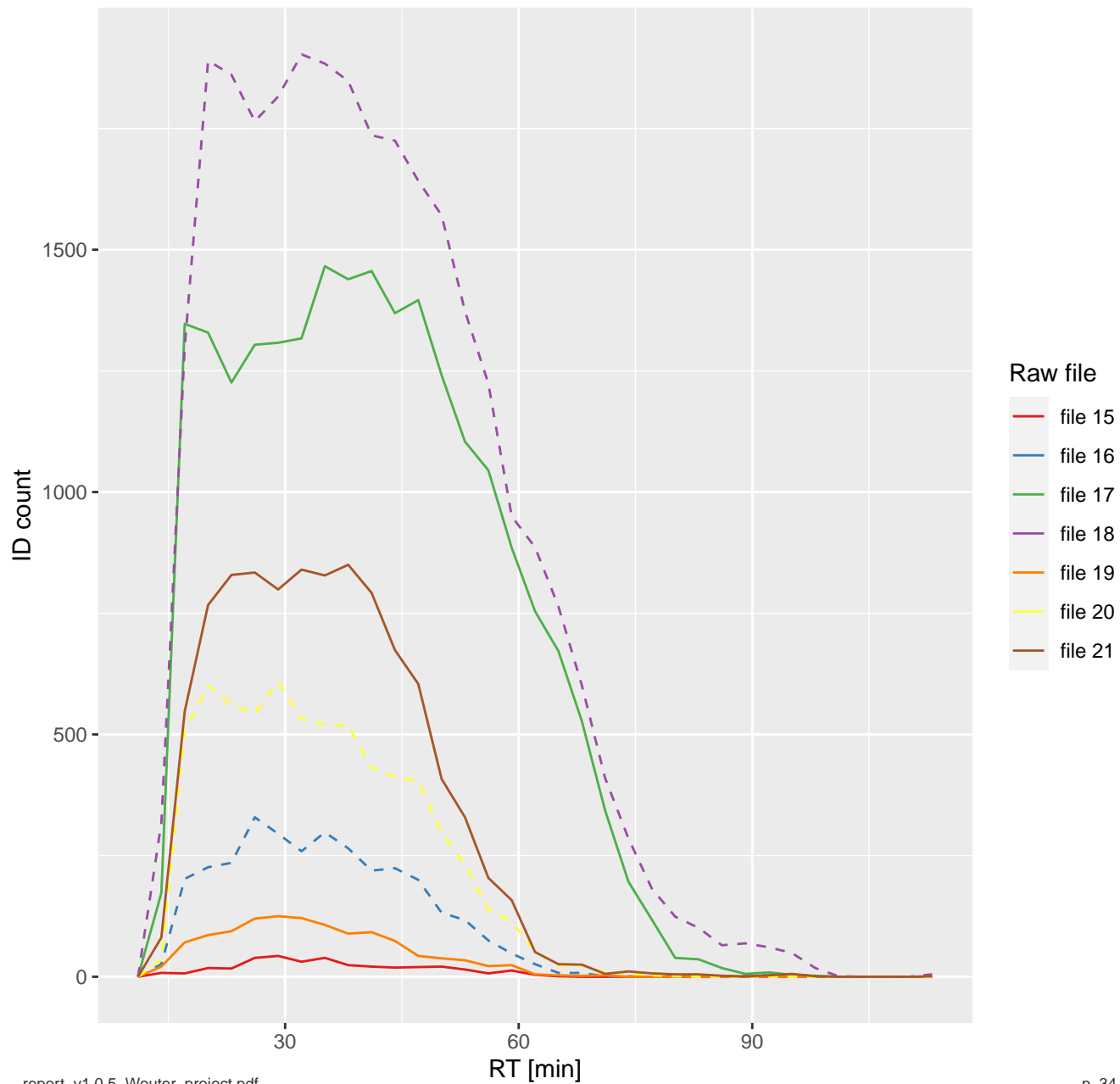
# EVD: IDs over RT



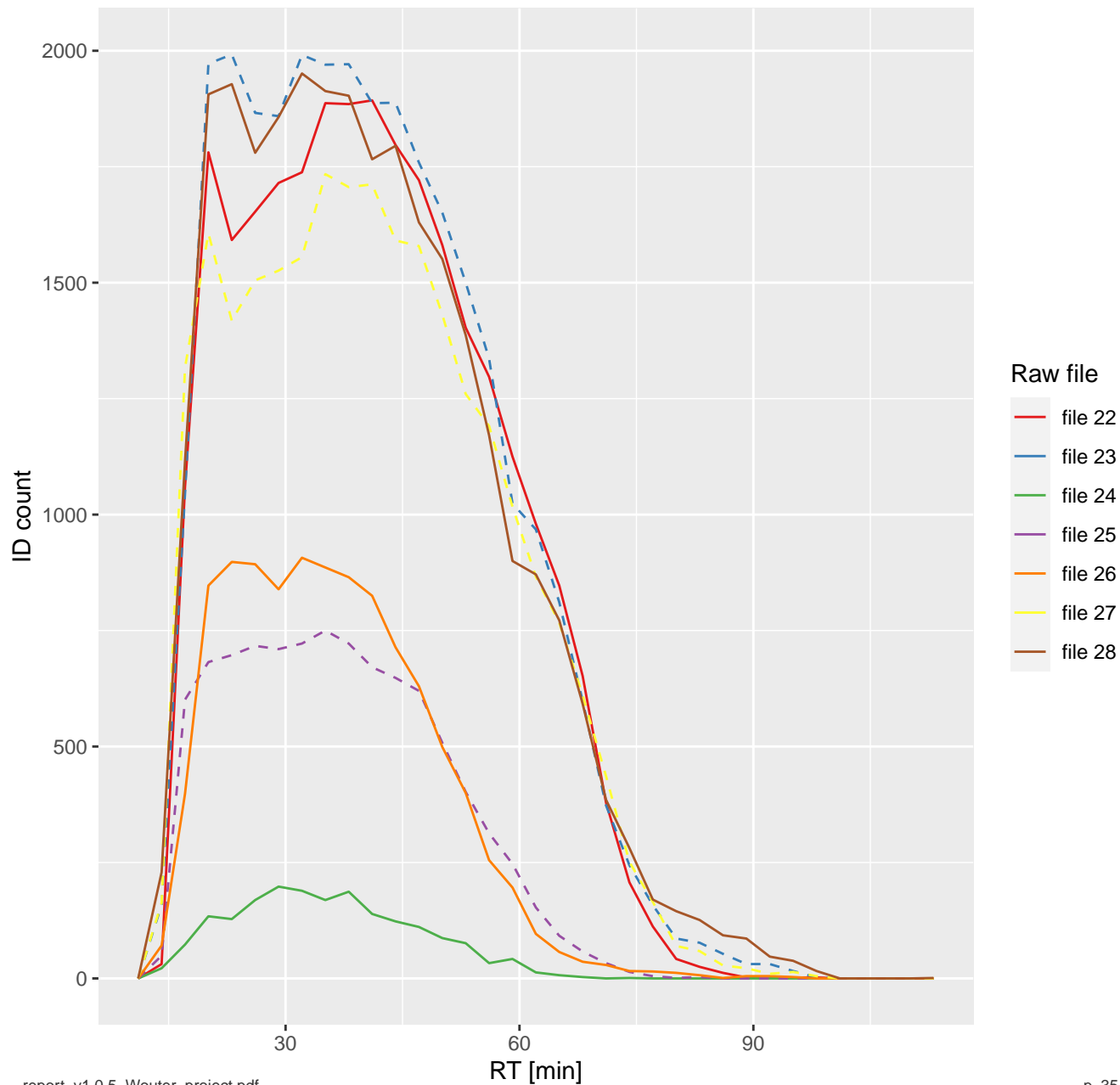
# EVD: IDs over RT



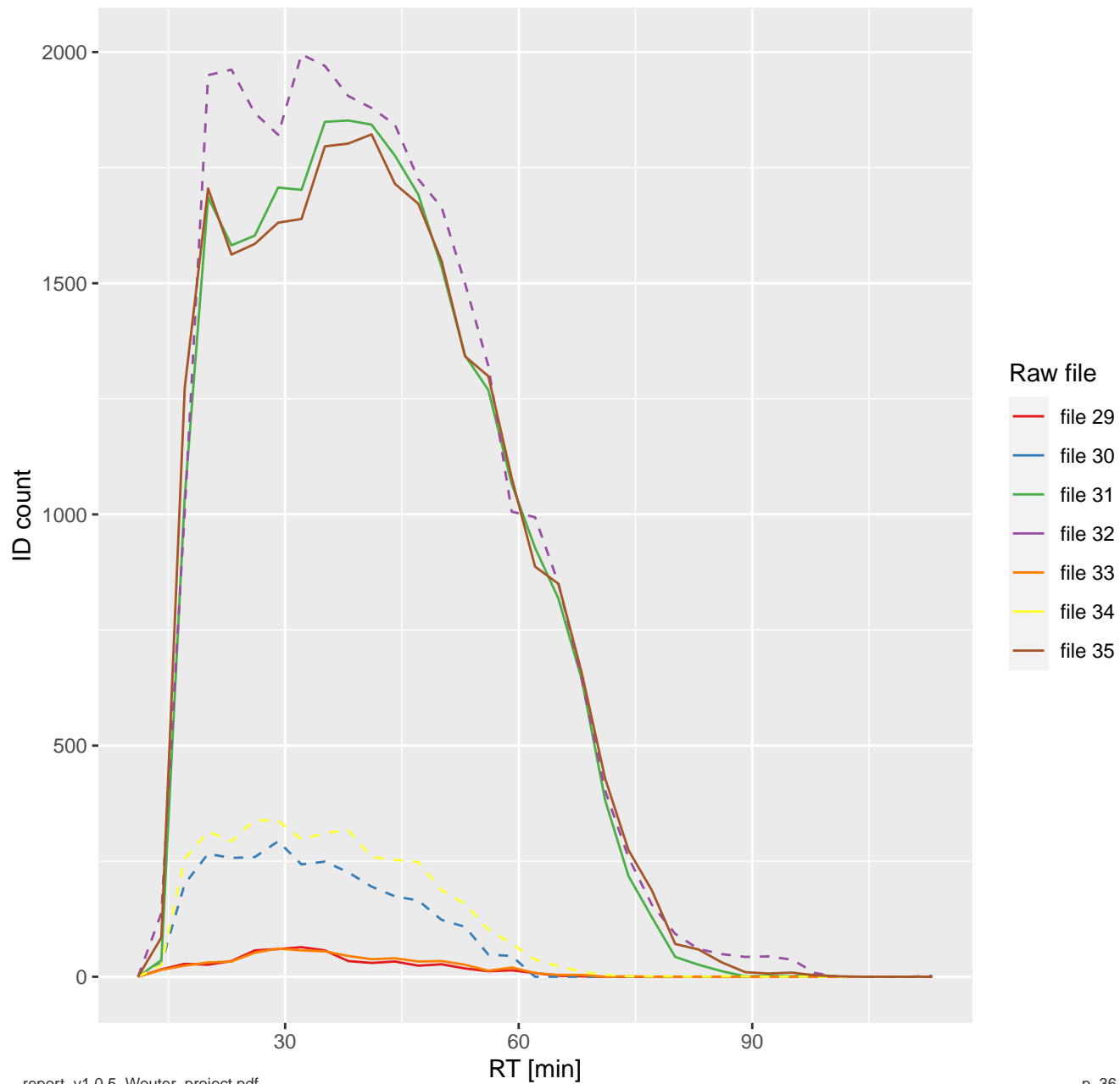
# EVD: IDs over RT



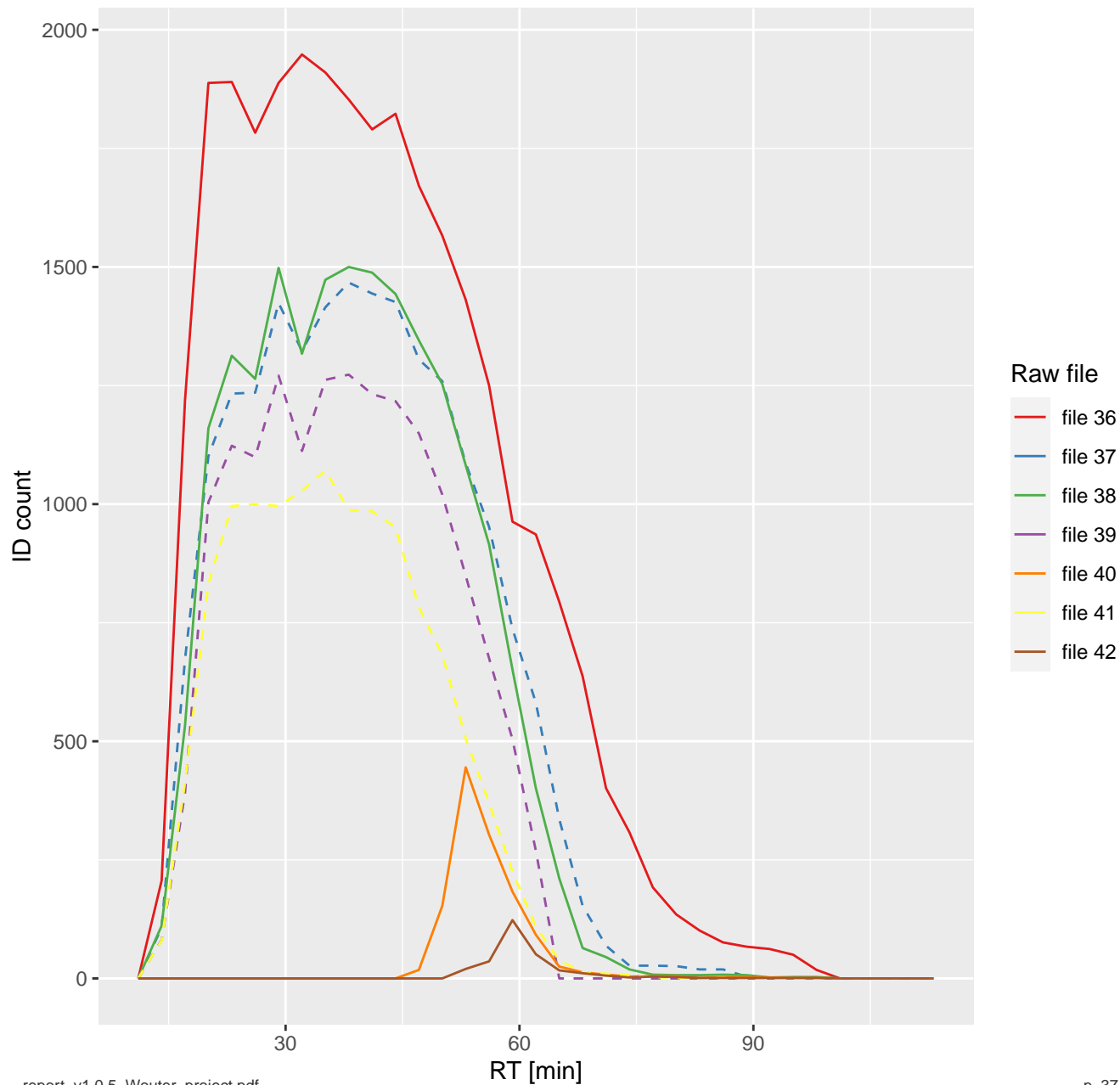
# EVD: IDs over RT



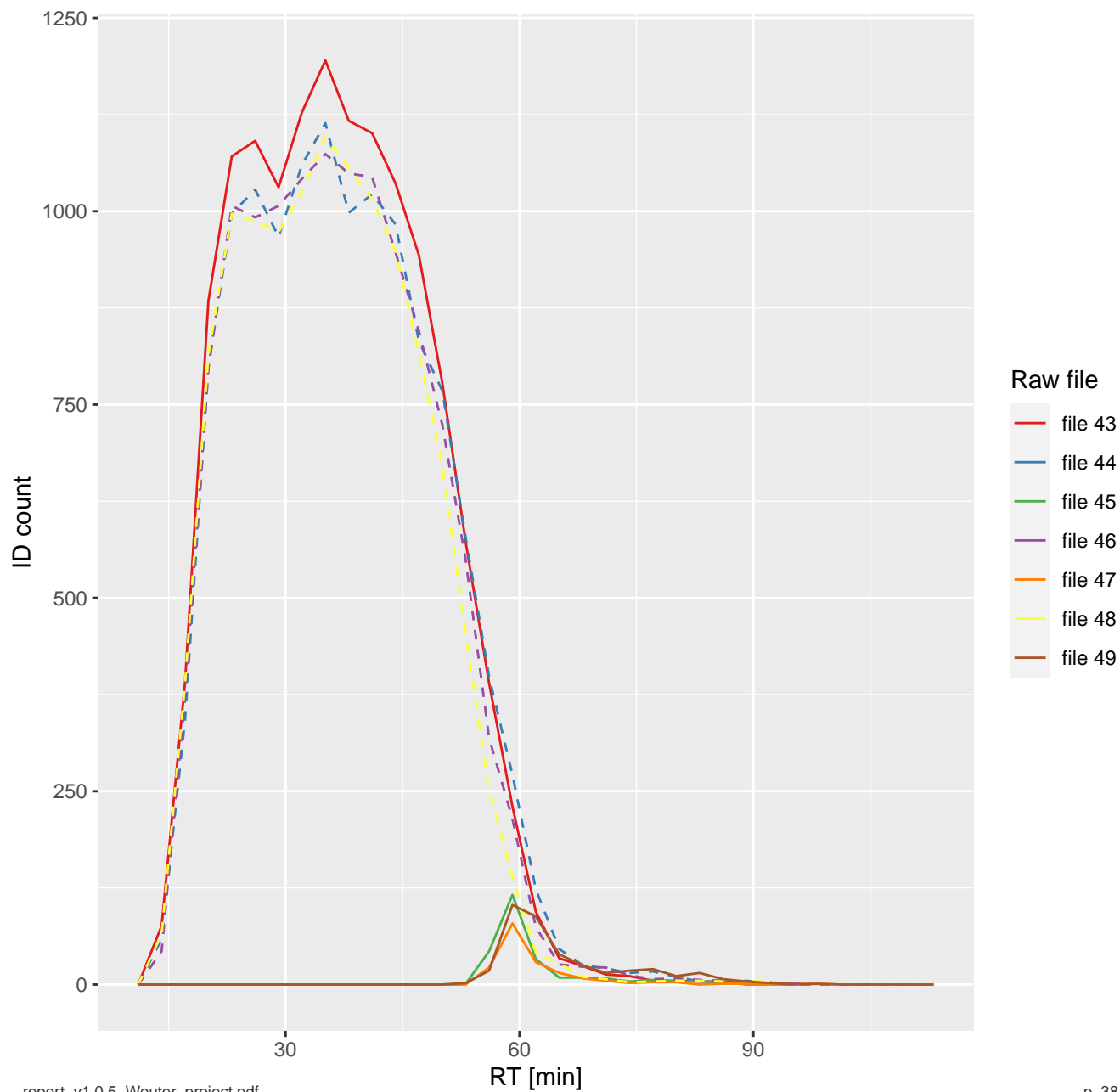
# EVD: IDs over RT



# EVD: IDs over RT

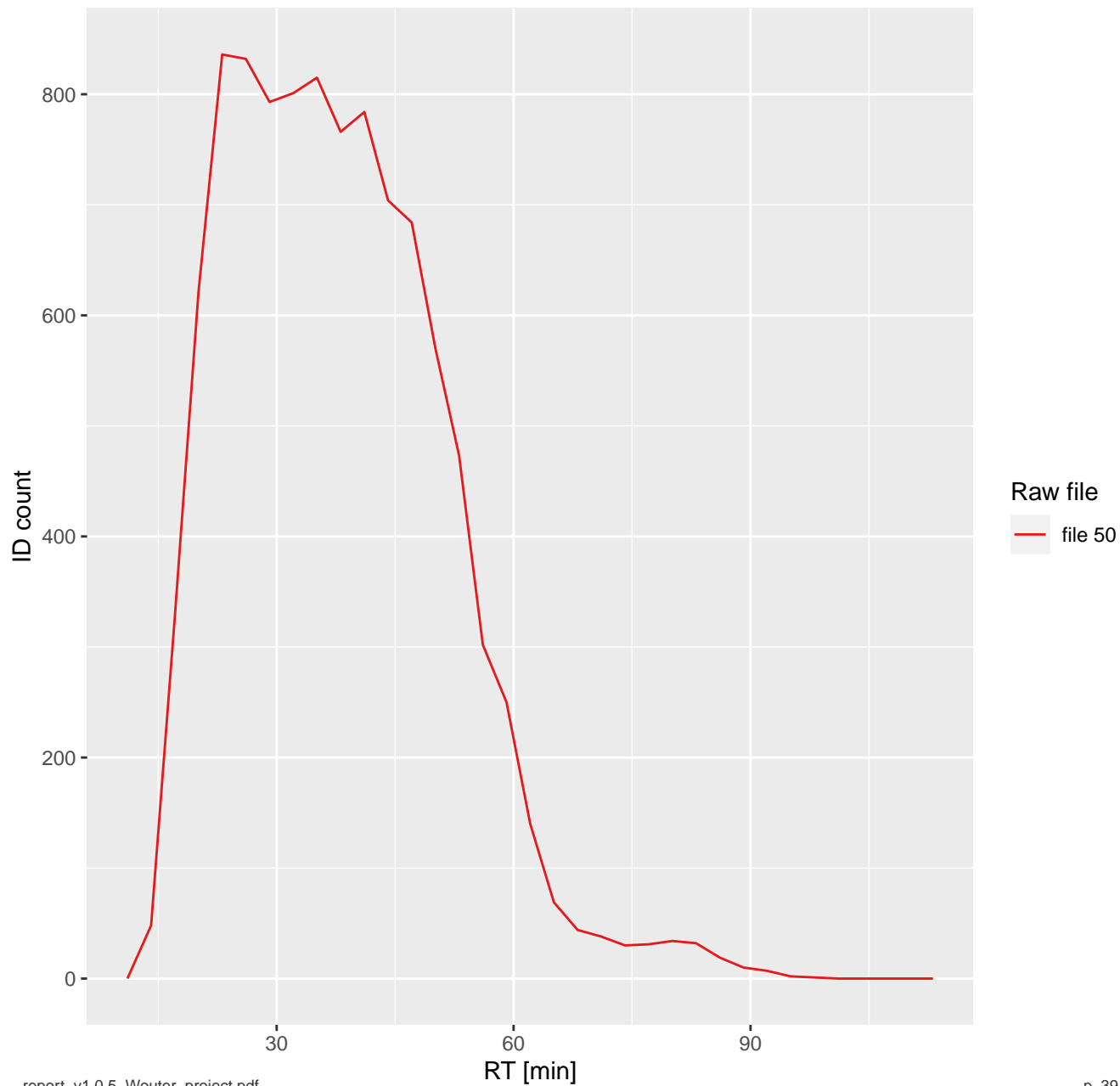


# EVD: IDs over RT

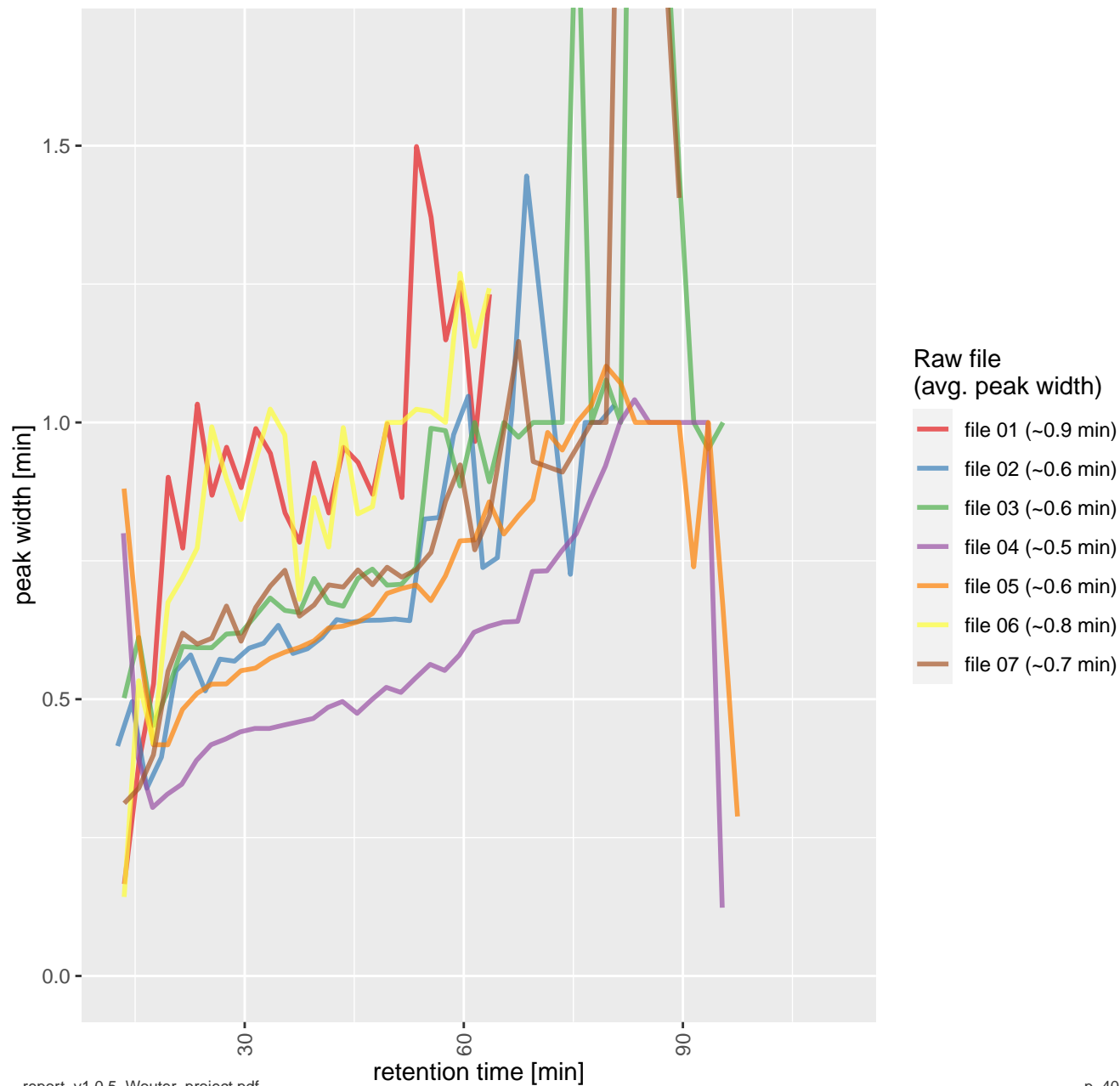




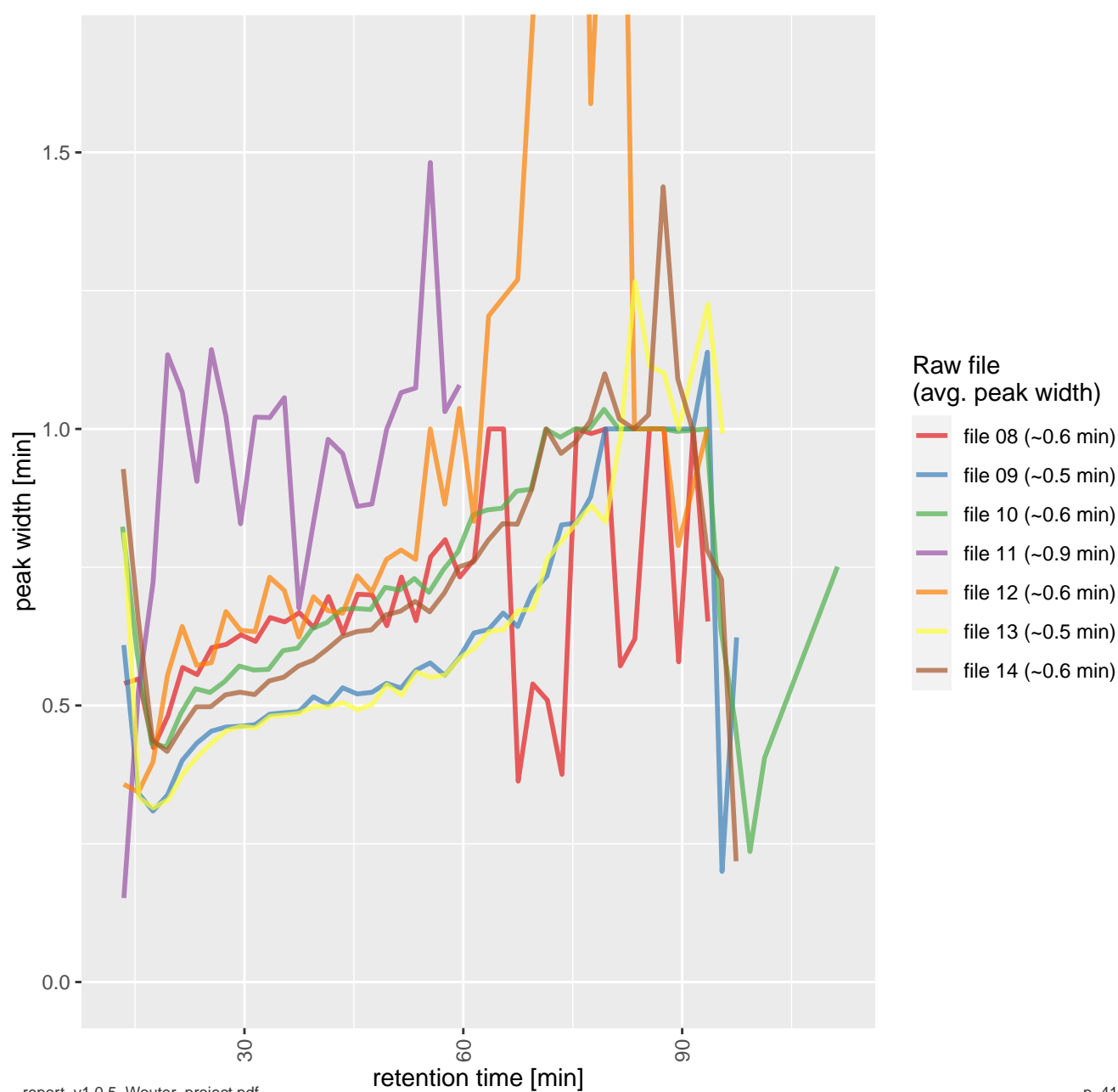
# EVD: IDs over RT



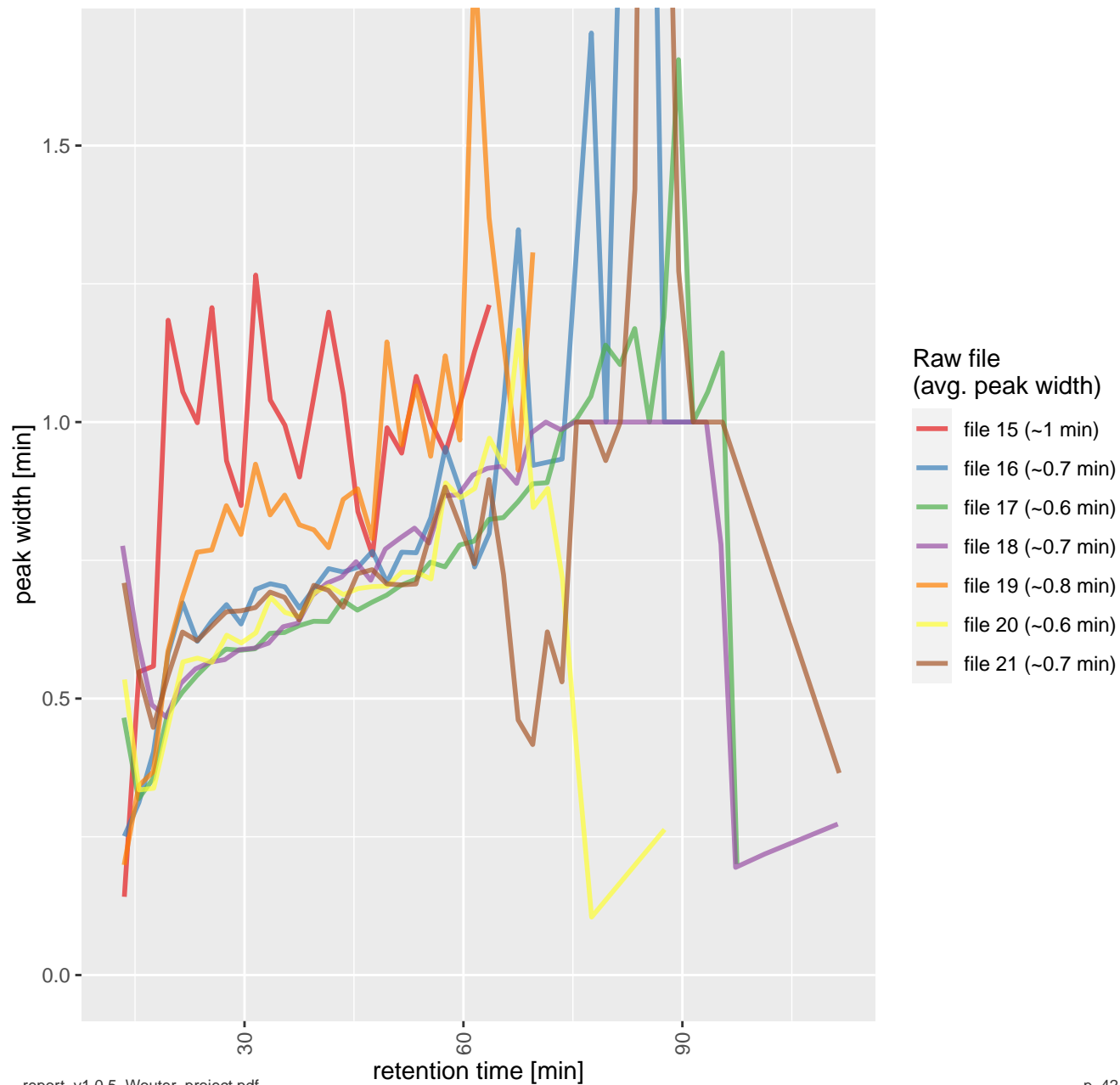
## EVD: Peak width over RT



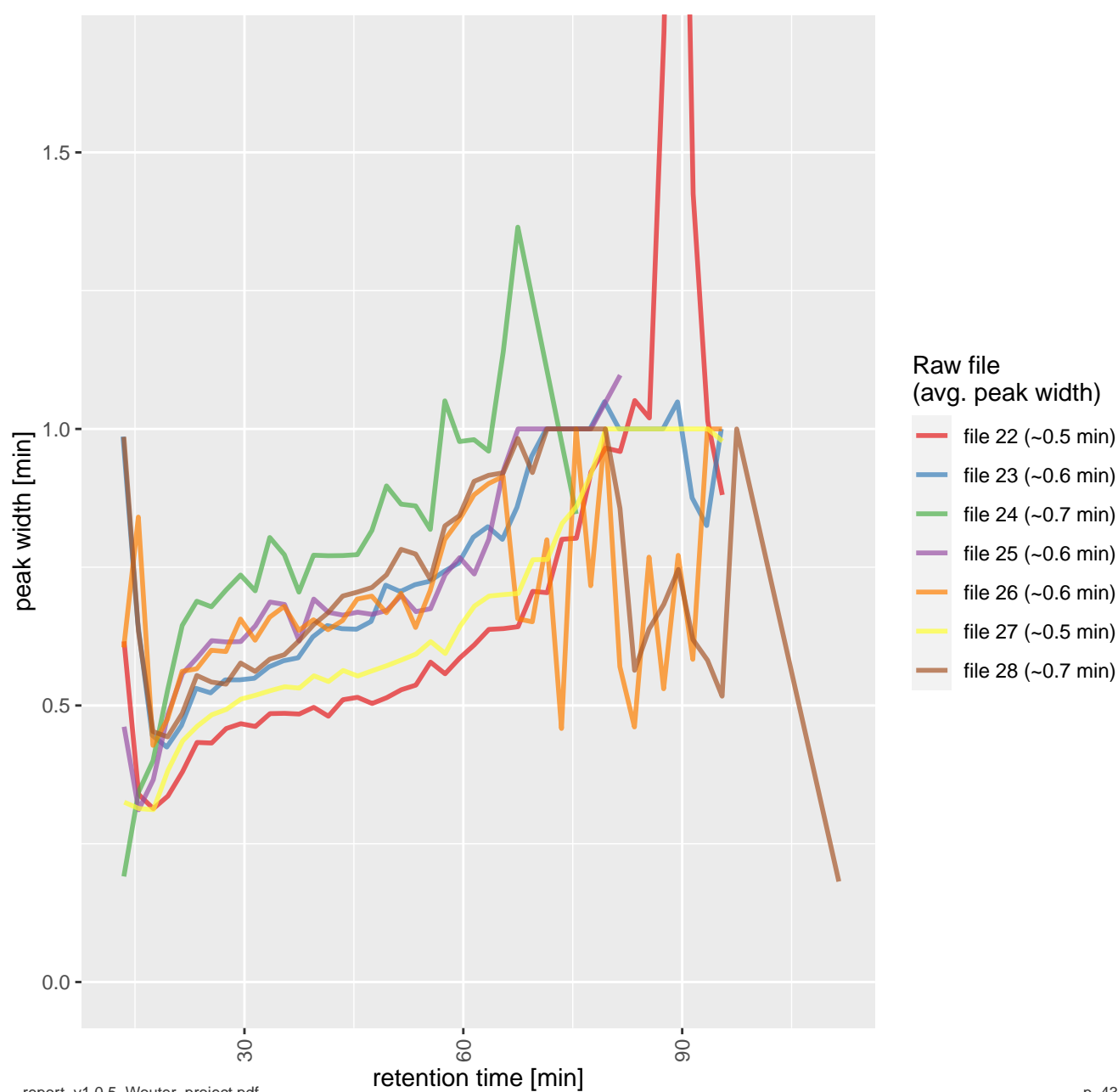
# EVD: Peak width over RT



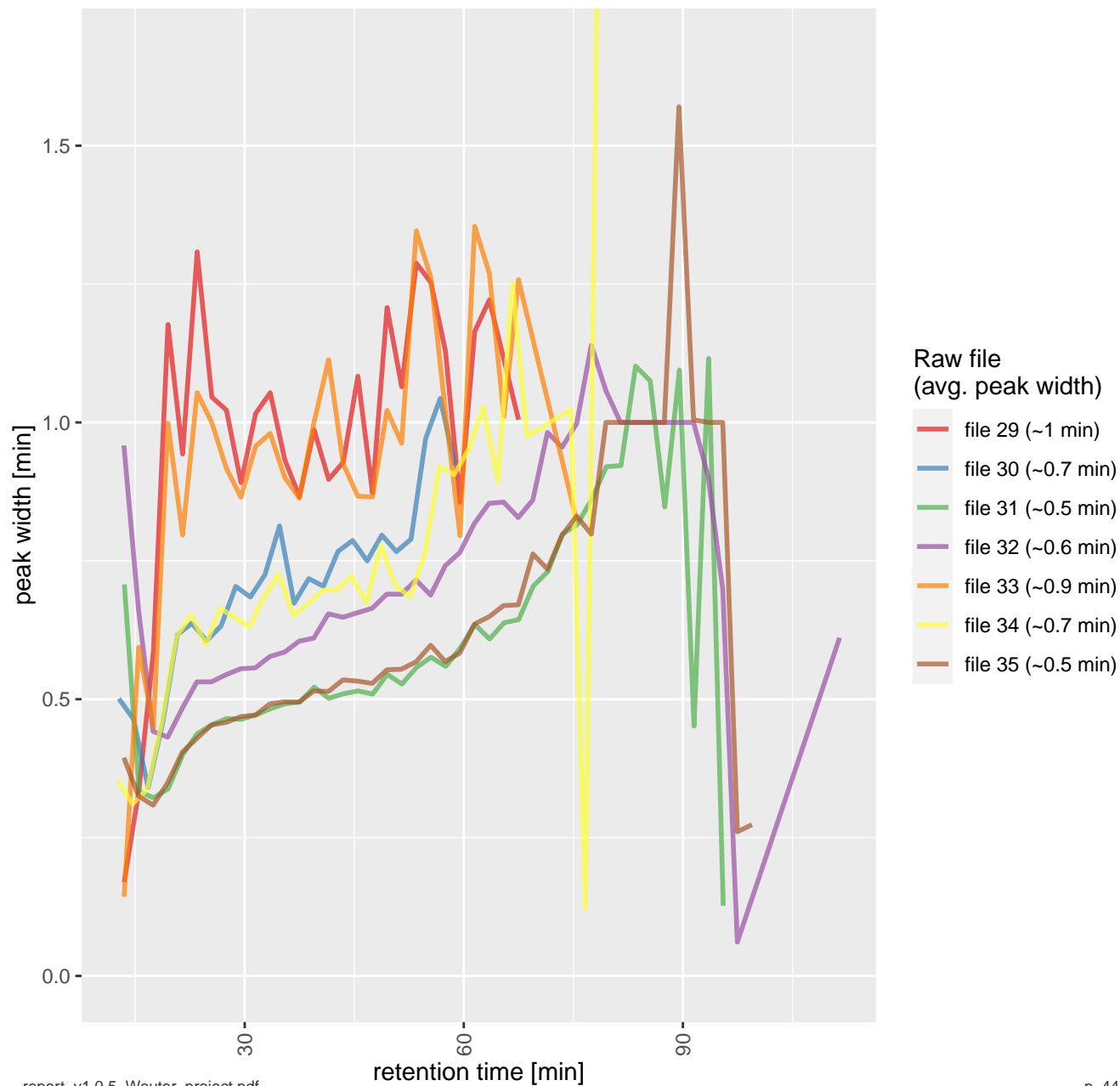
## EVD: Peak width over RT



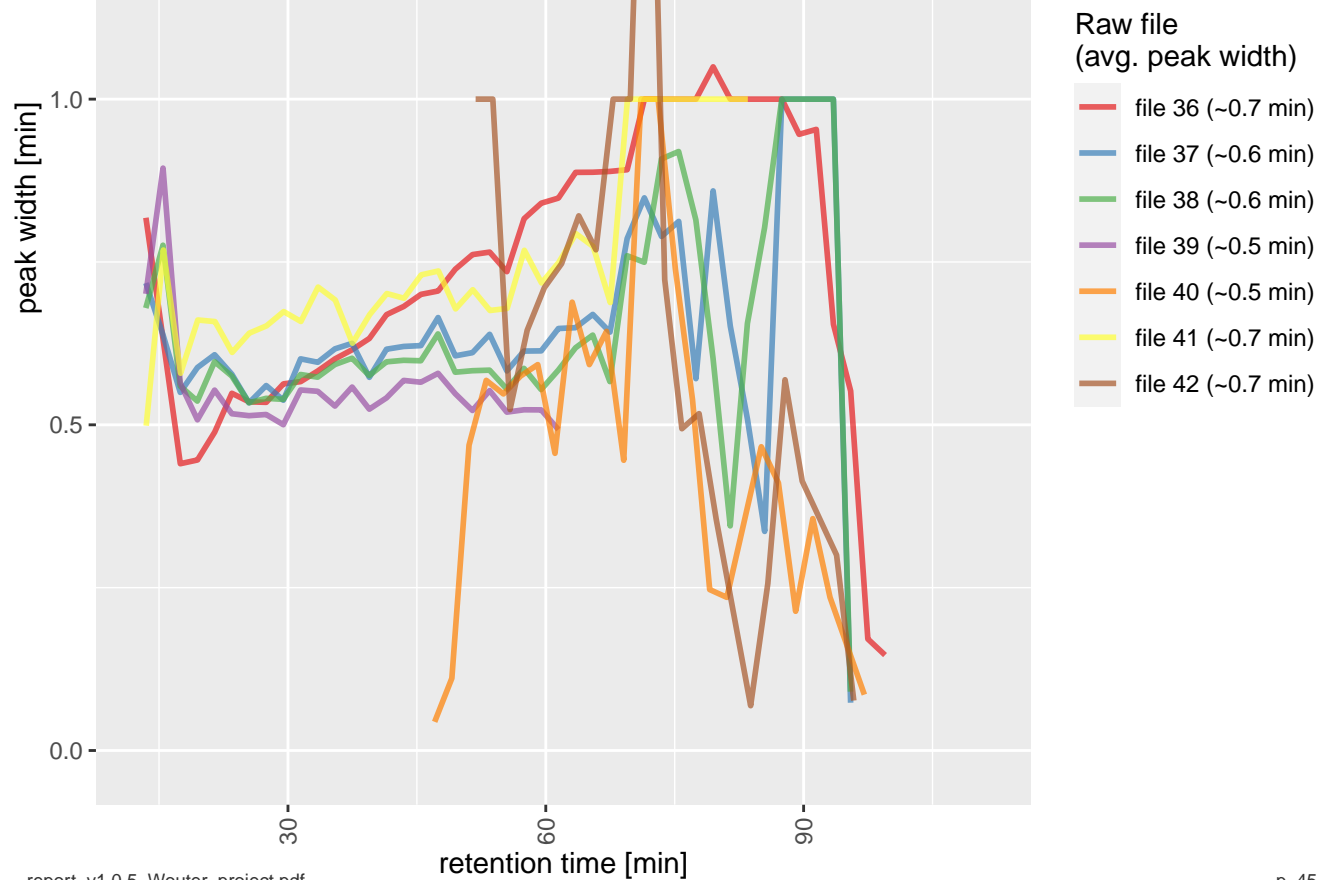
# EVD: Peak width over RT



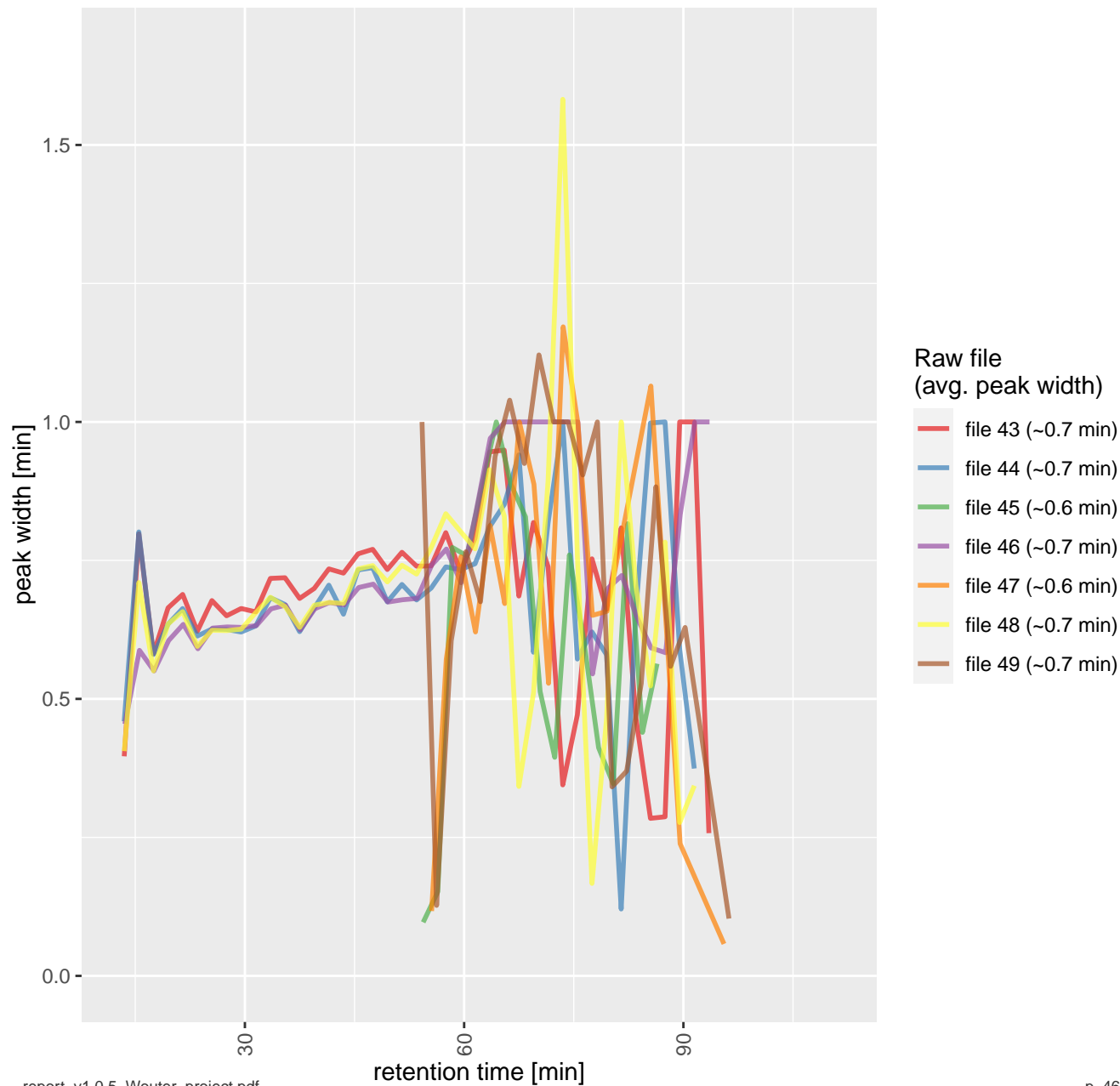
## EVD: Peak width over RT



## EVD: Peak width over RT

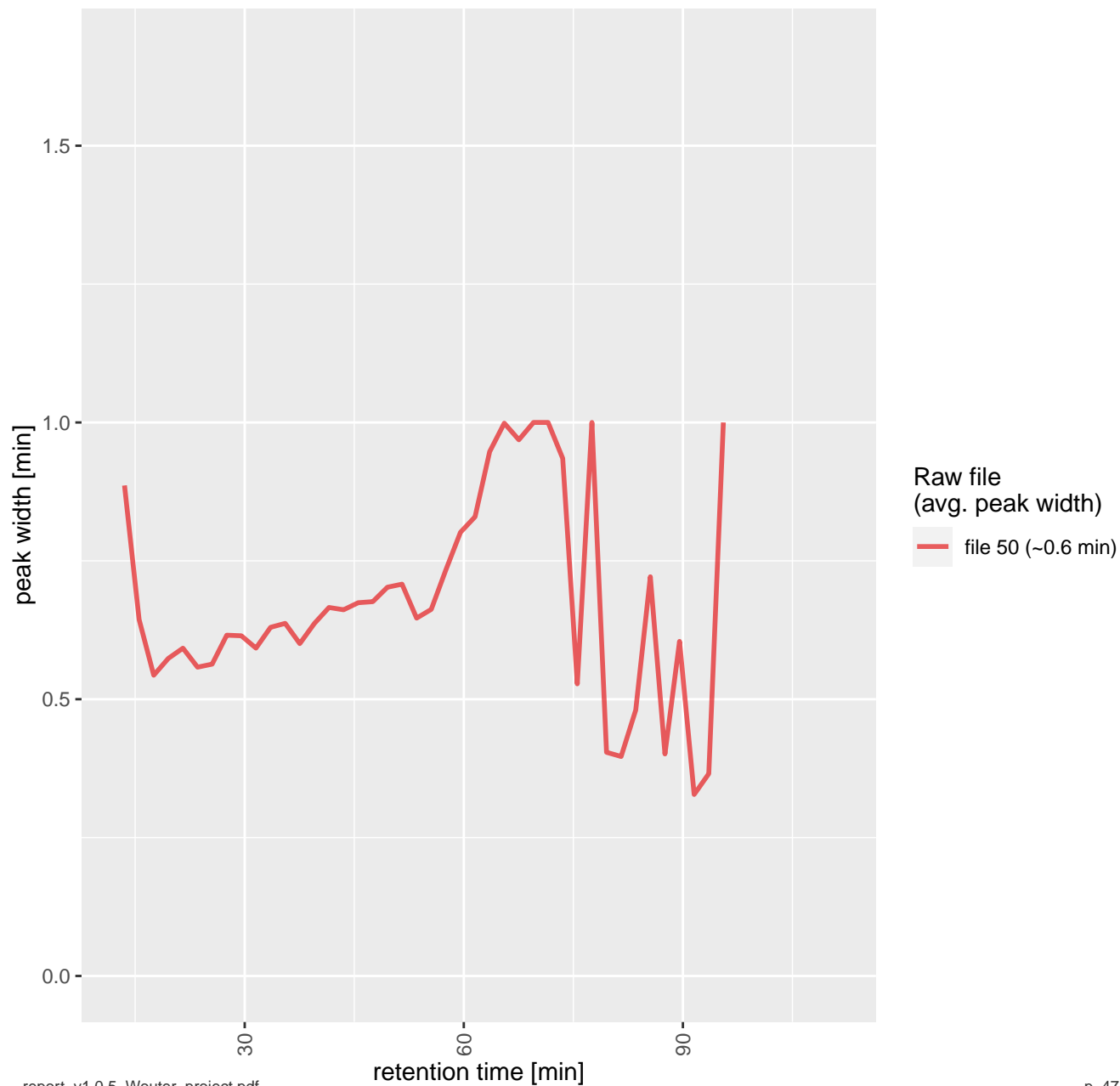


EVD: Peak width over RT

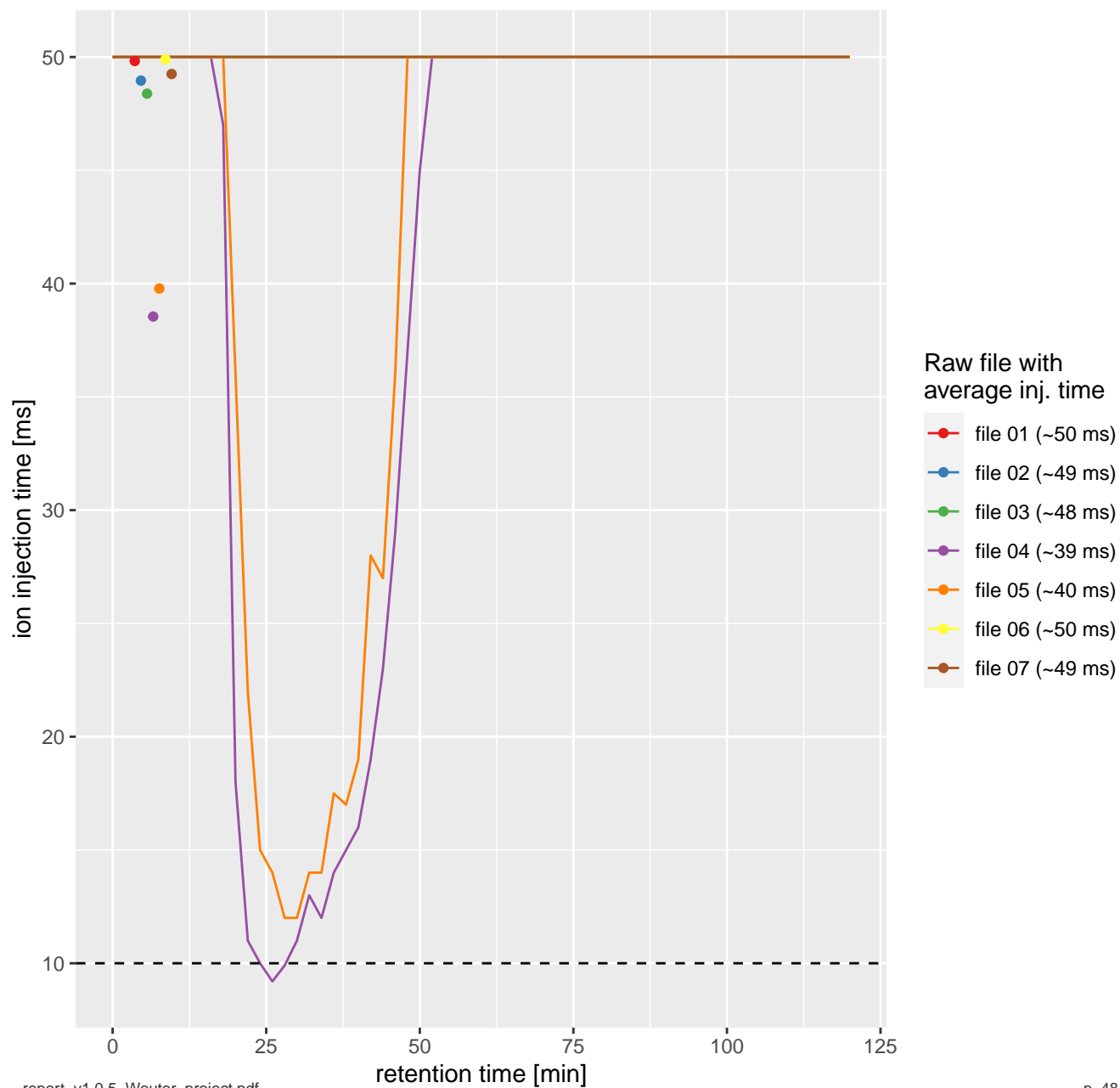




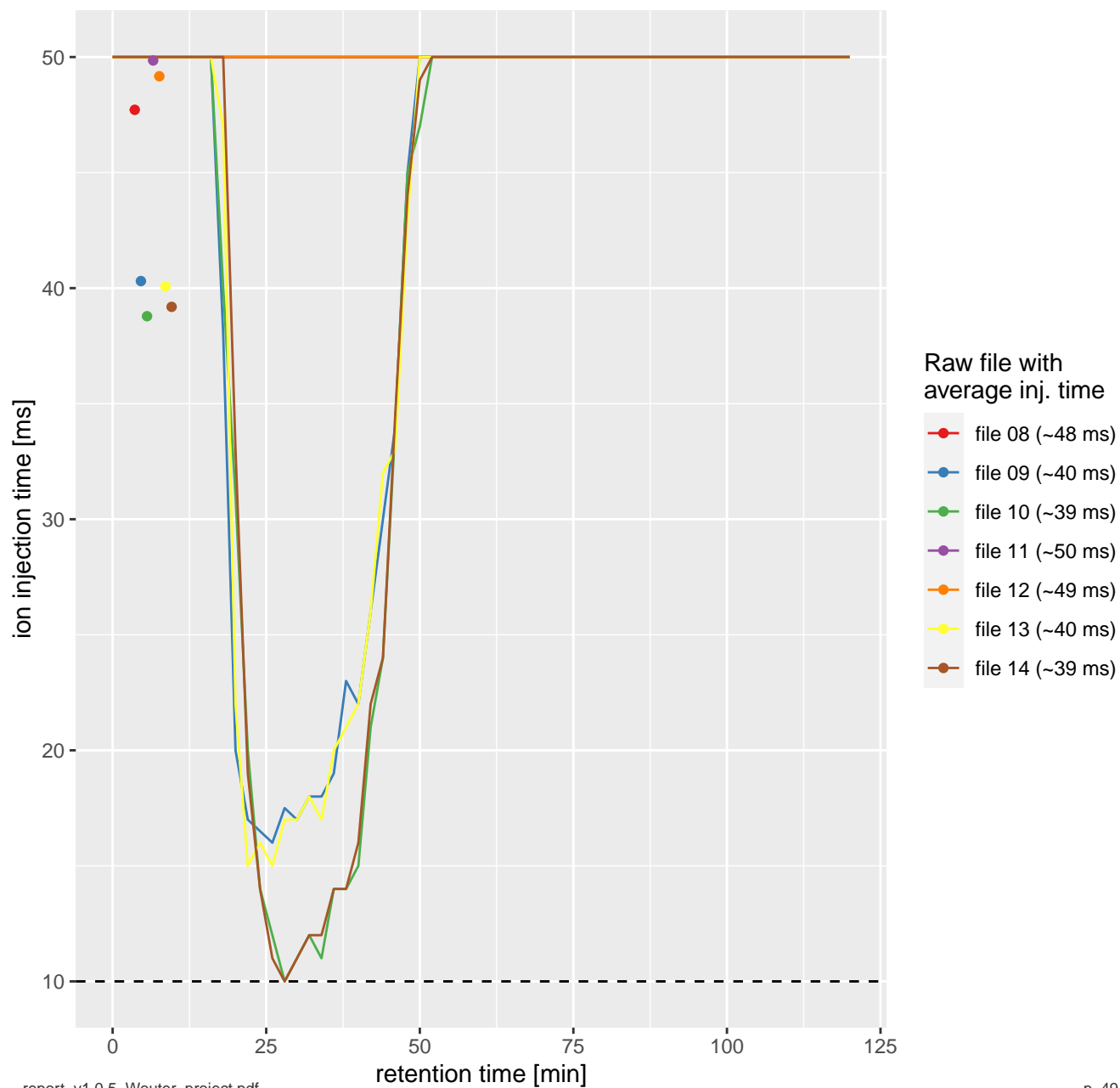
## EVD: Peak width over RT



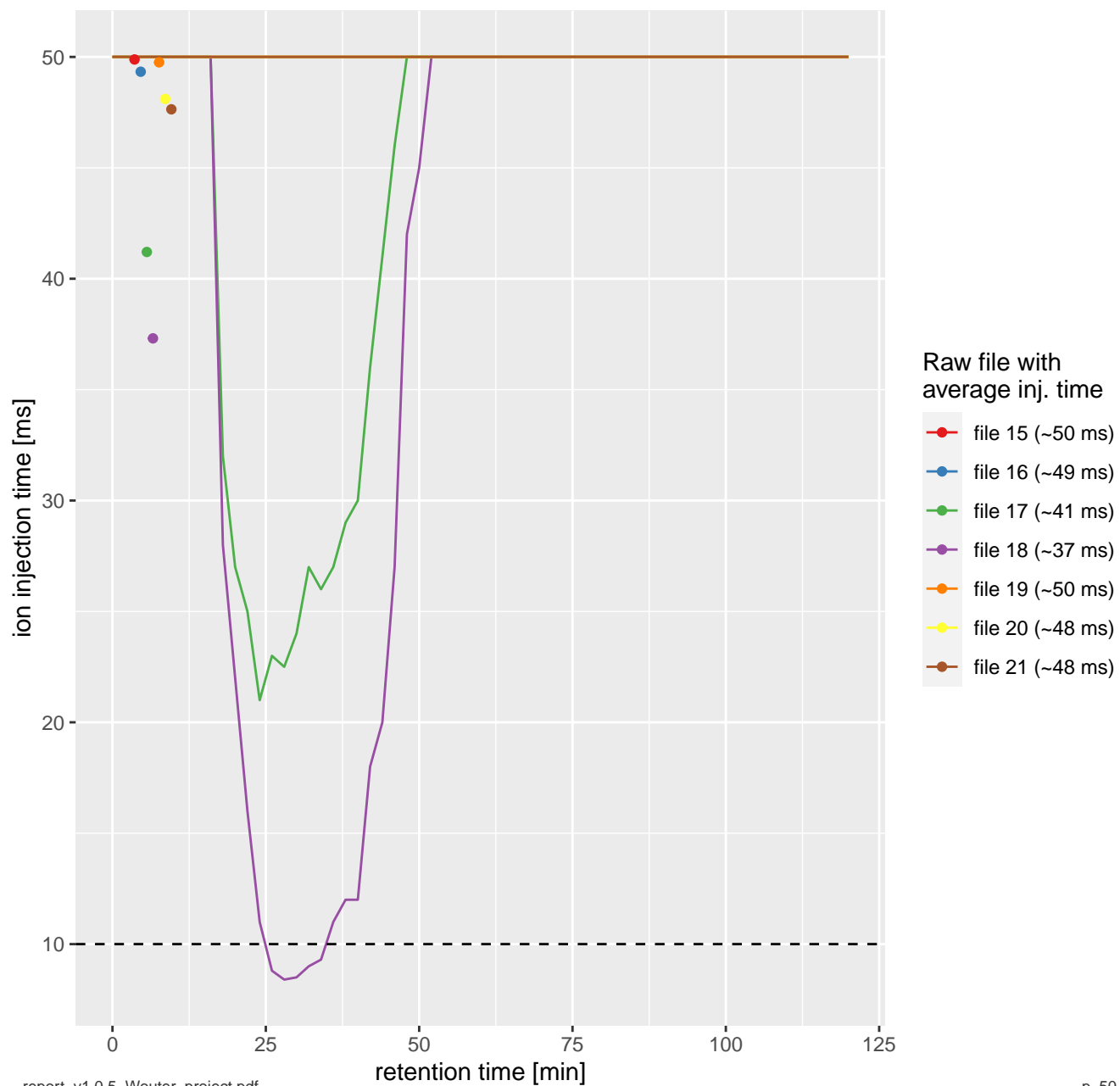
# MSMSscans: Ion Injection Time over RT



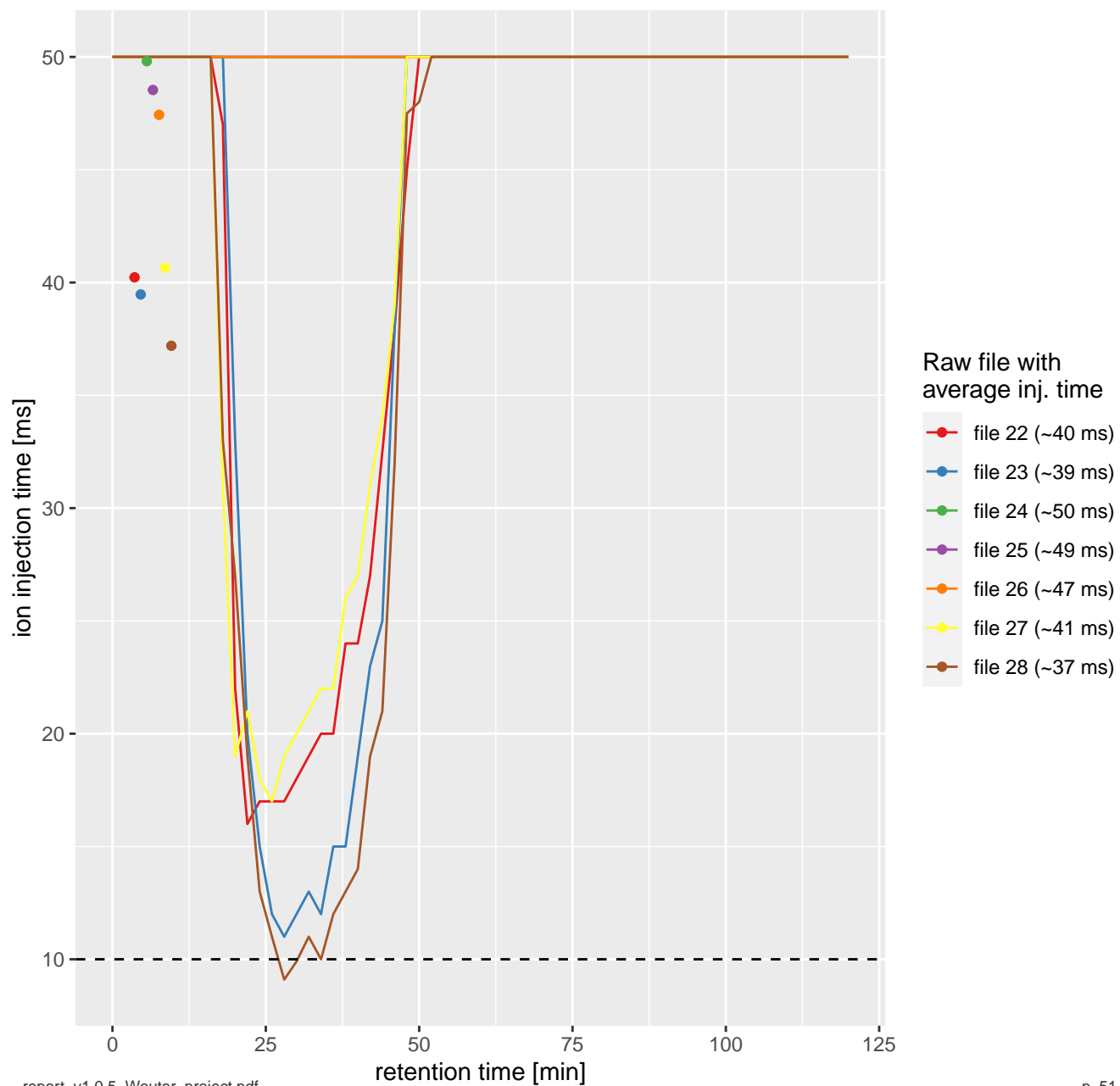
# MSMSscans: Ion Injection Time over RT



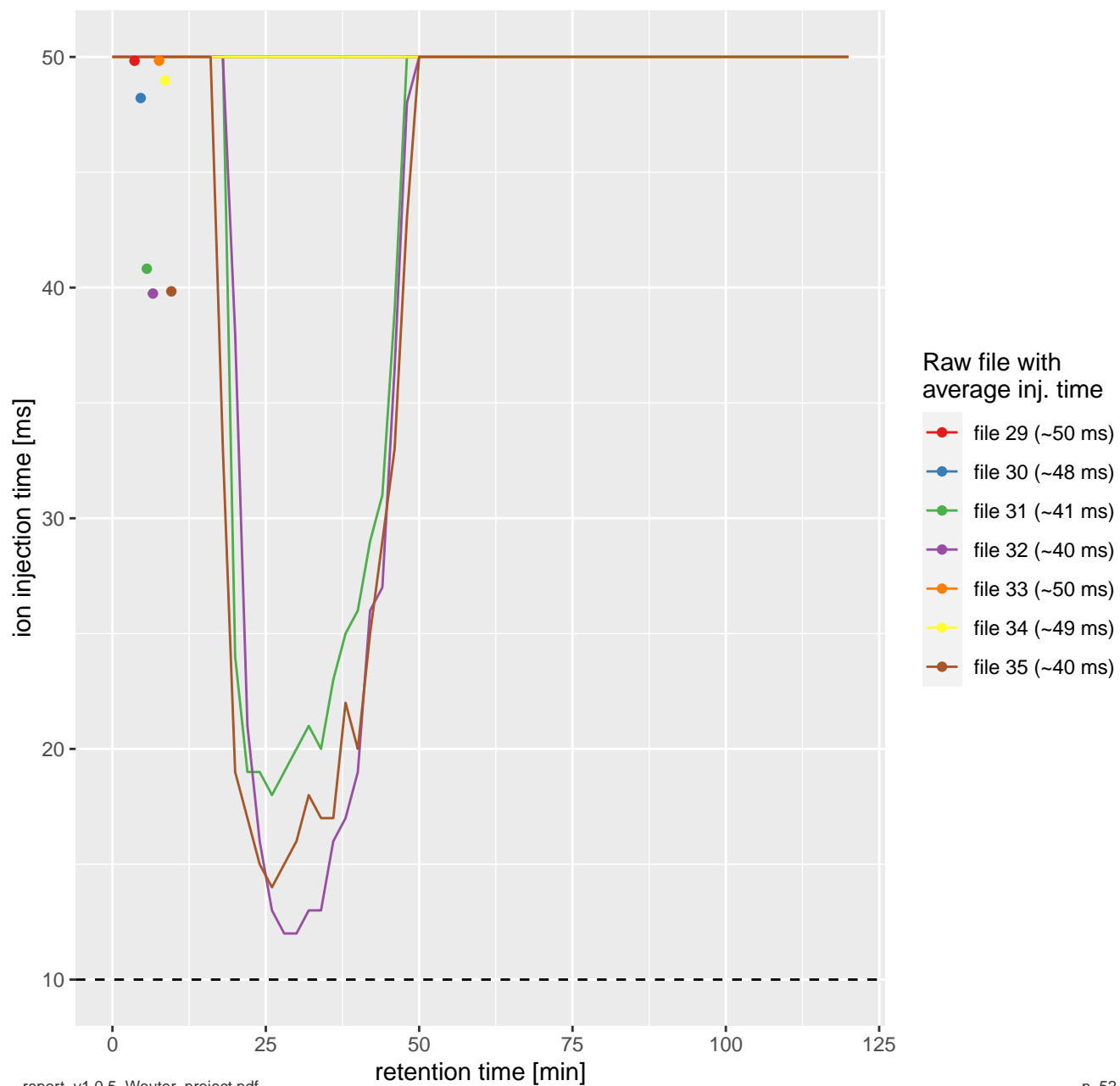
# MSMSscans: Ion Injection Time over RT



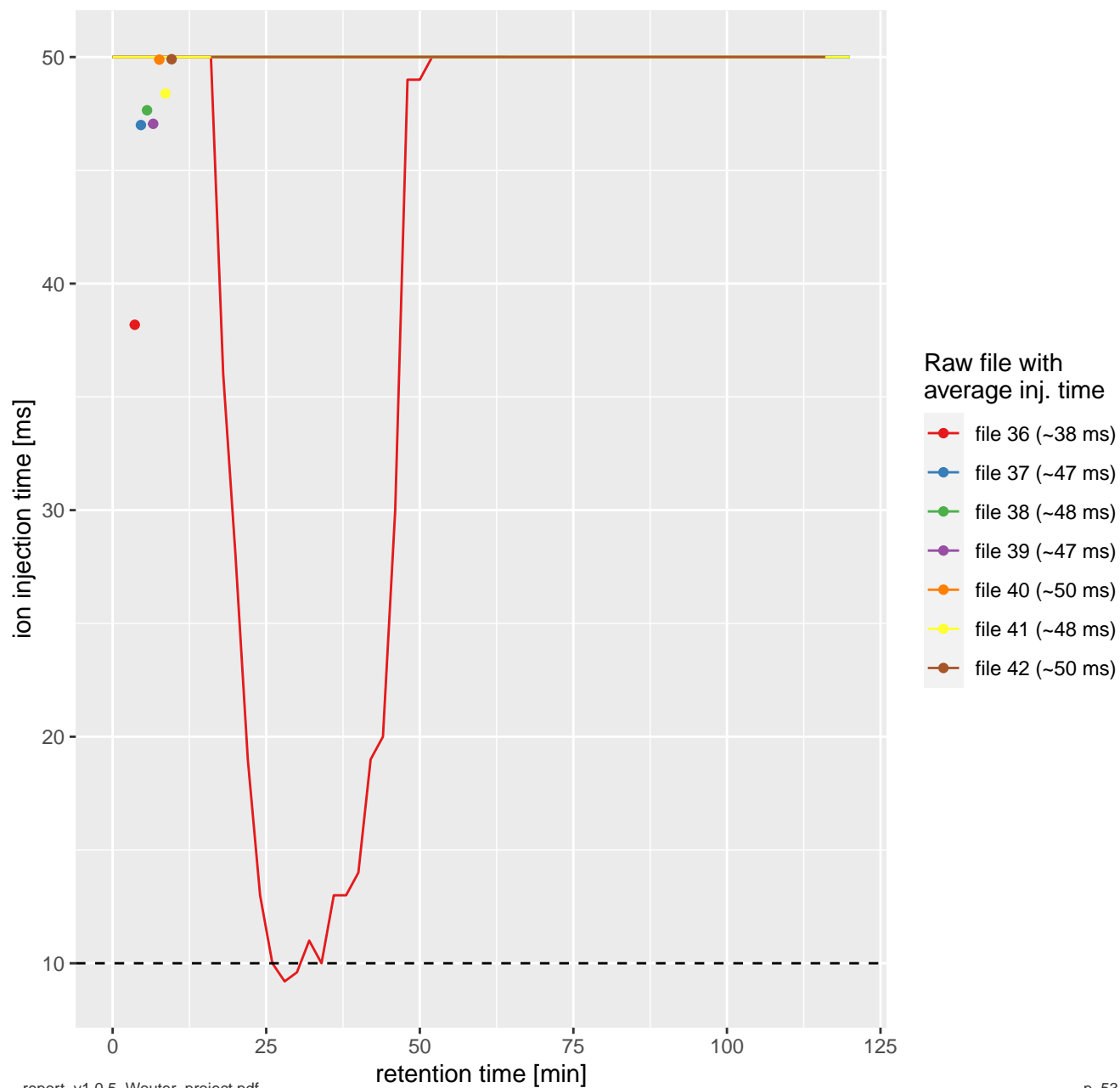
# MSMSscans: Ion Injection Time over RT



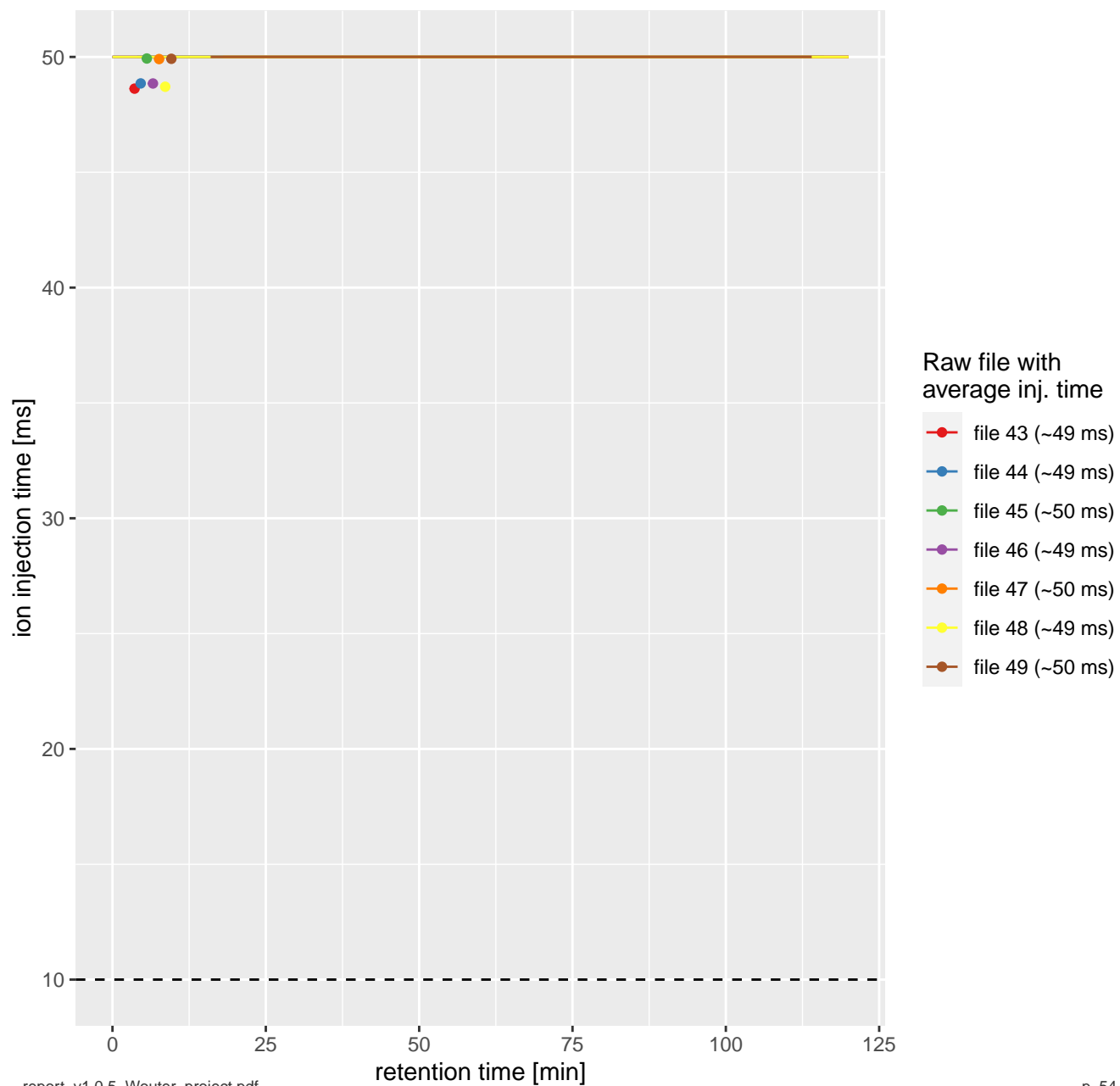
# MSMSscans: Ion Injection Time over RT



# MSMSscans: Ion Injection Time over RT

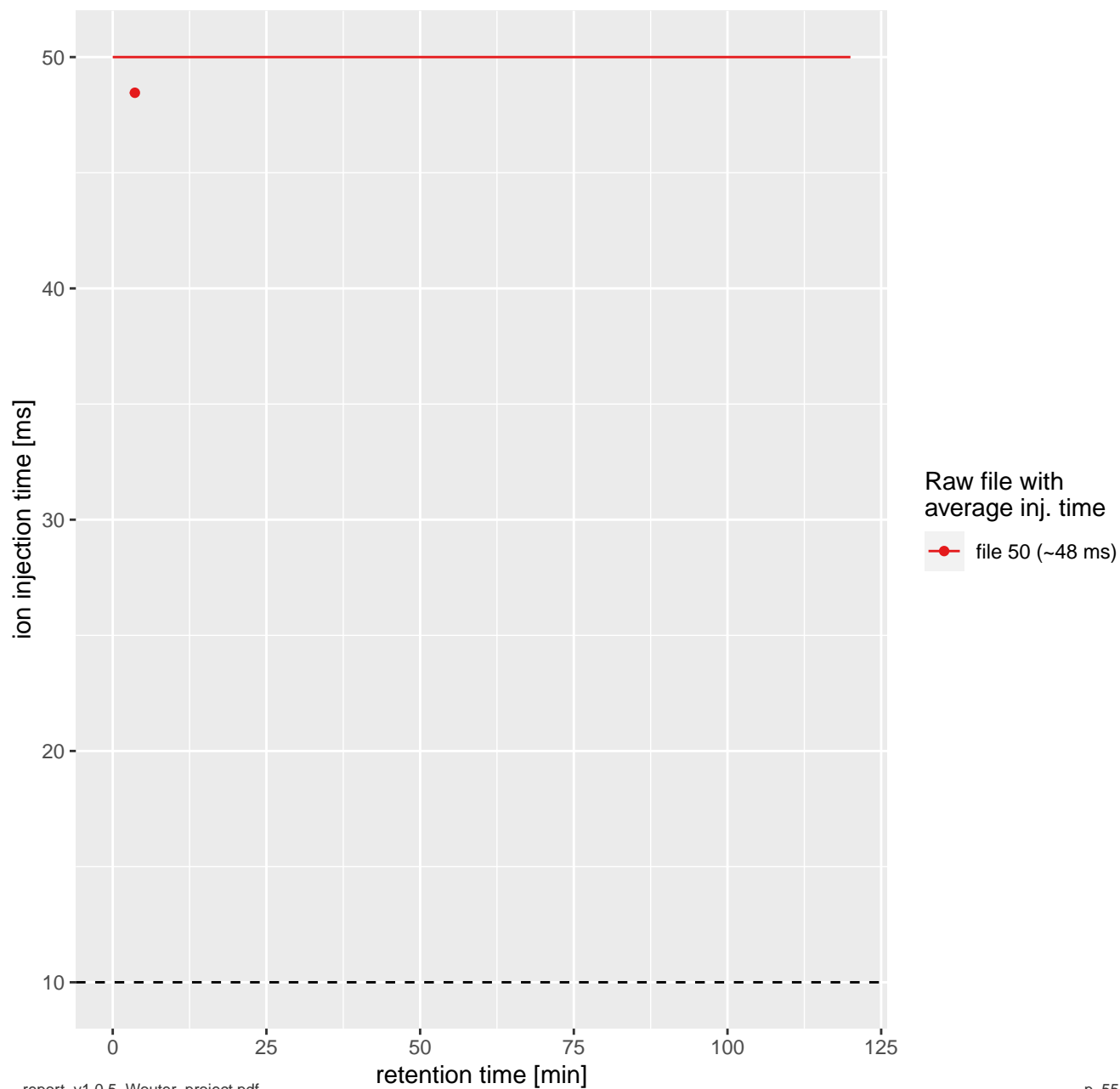


# MSMSscans: Ion Injection Time over RT

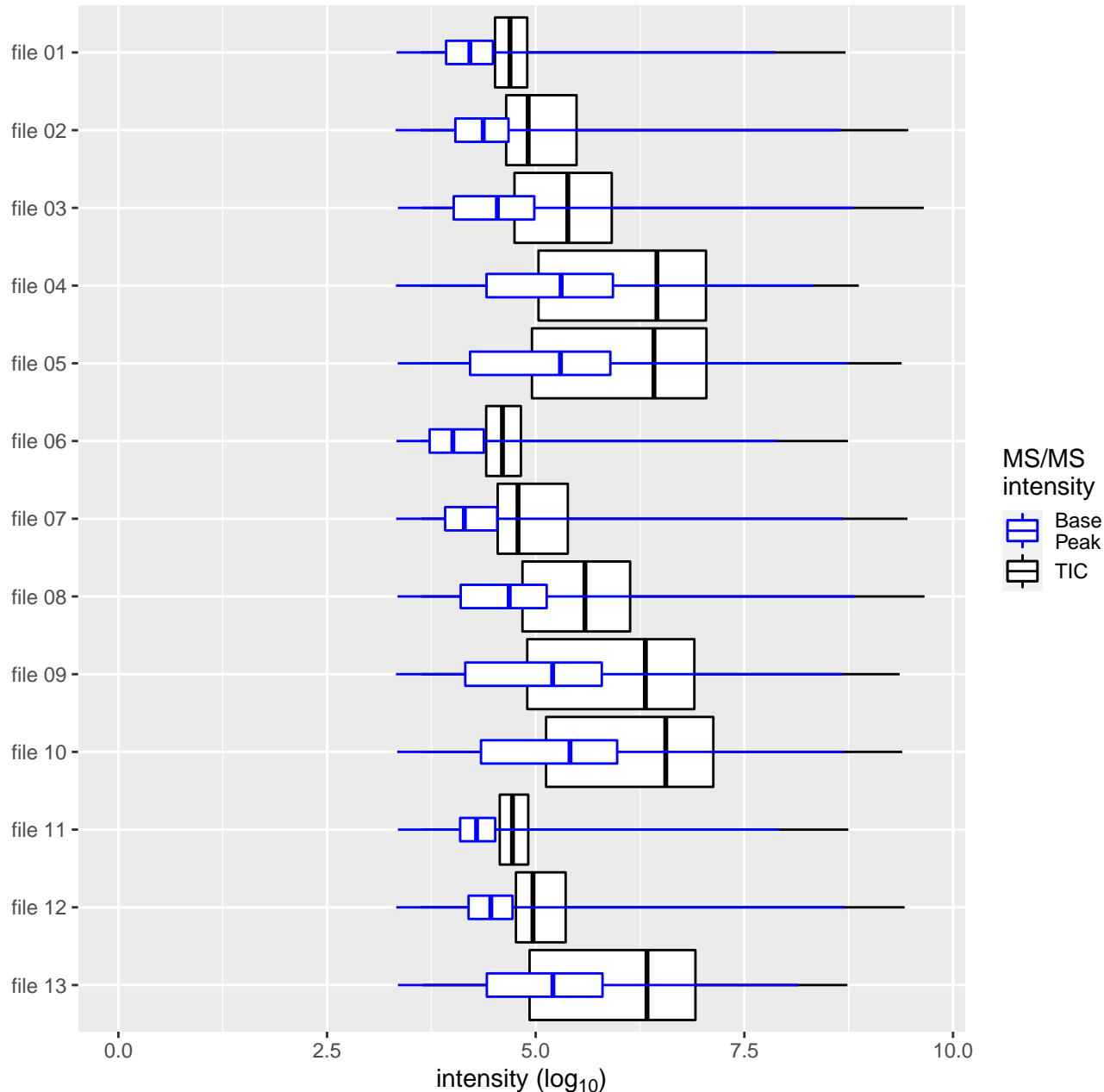




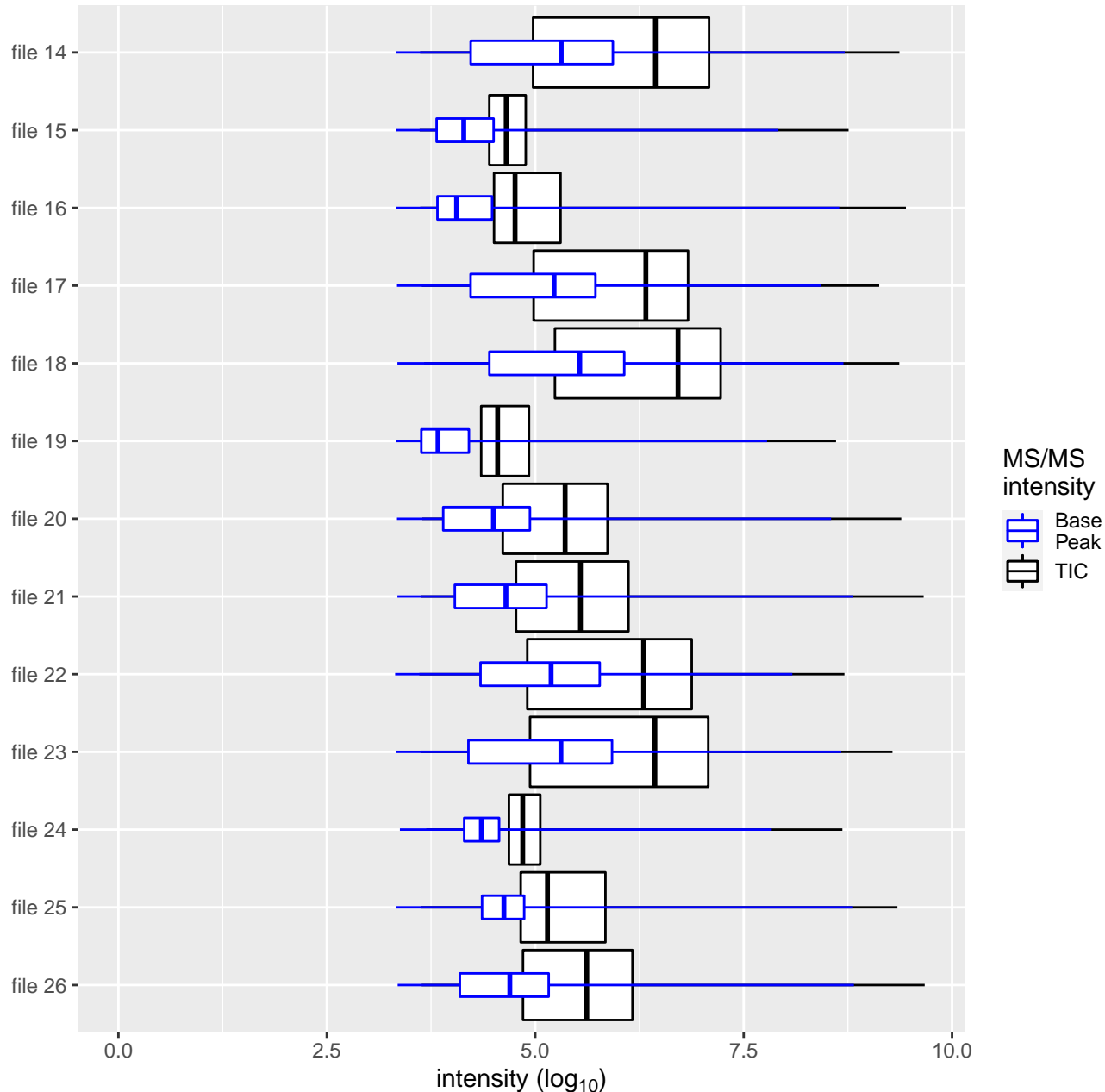
# MSMSscans: Ion Injection Time over RT



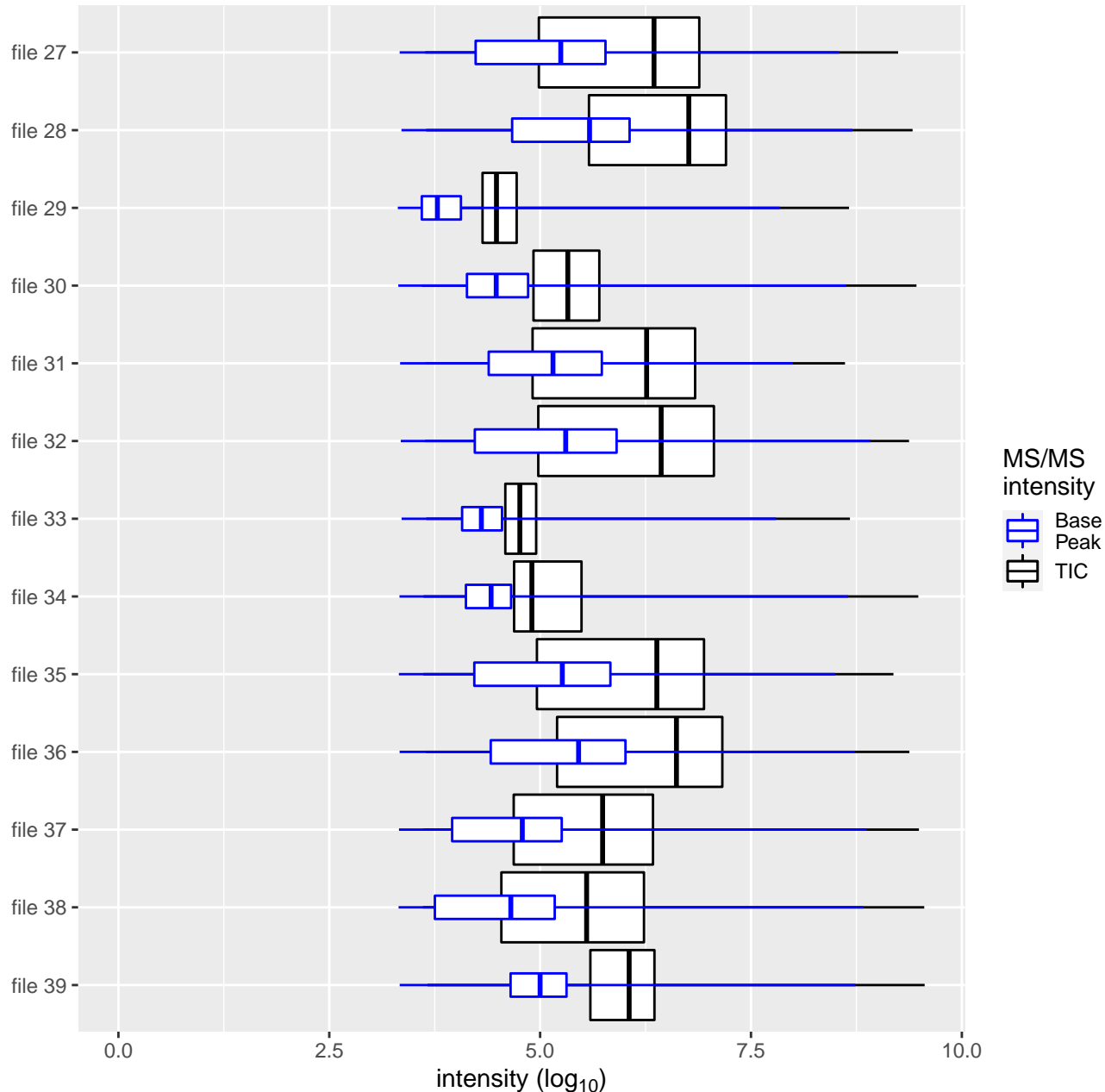
# [experimental] MSMSscans: MS/MS intensity



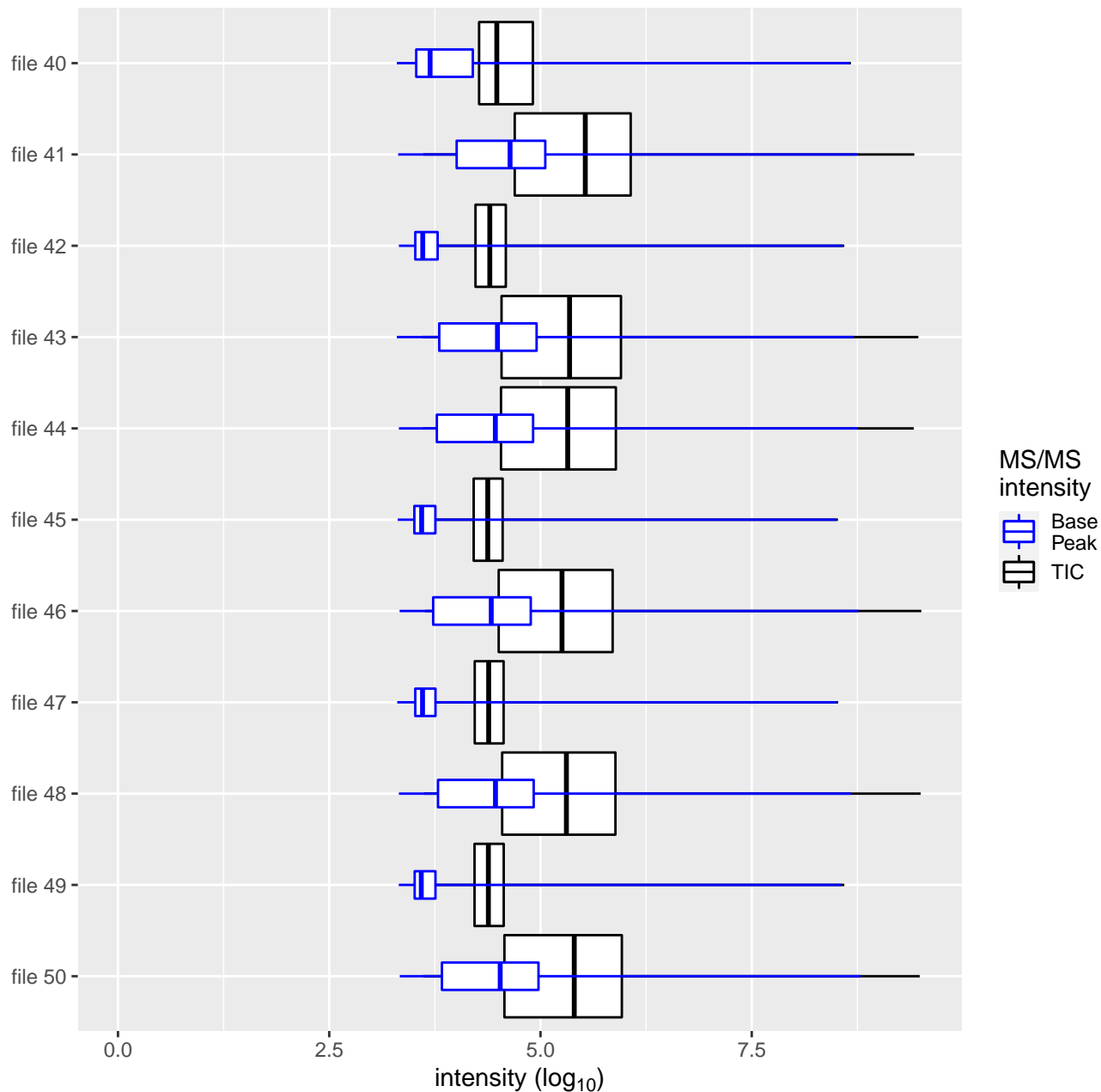
# [experimental] MSMSscans: MS/MS intensity



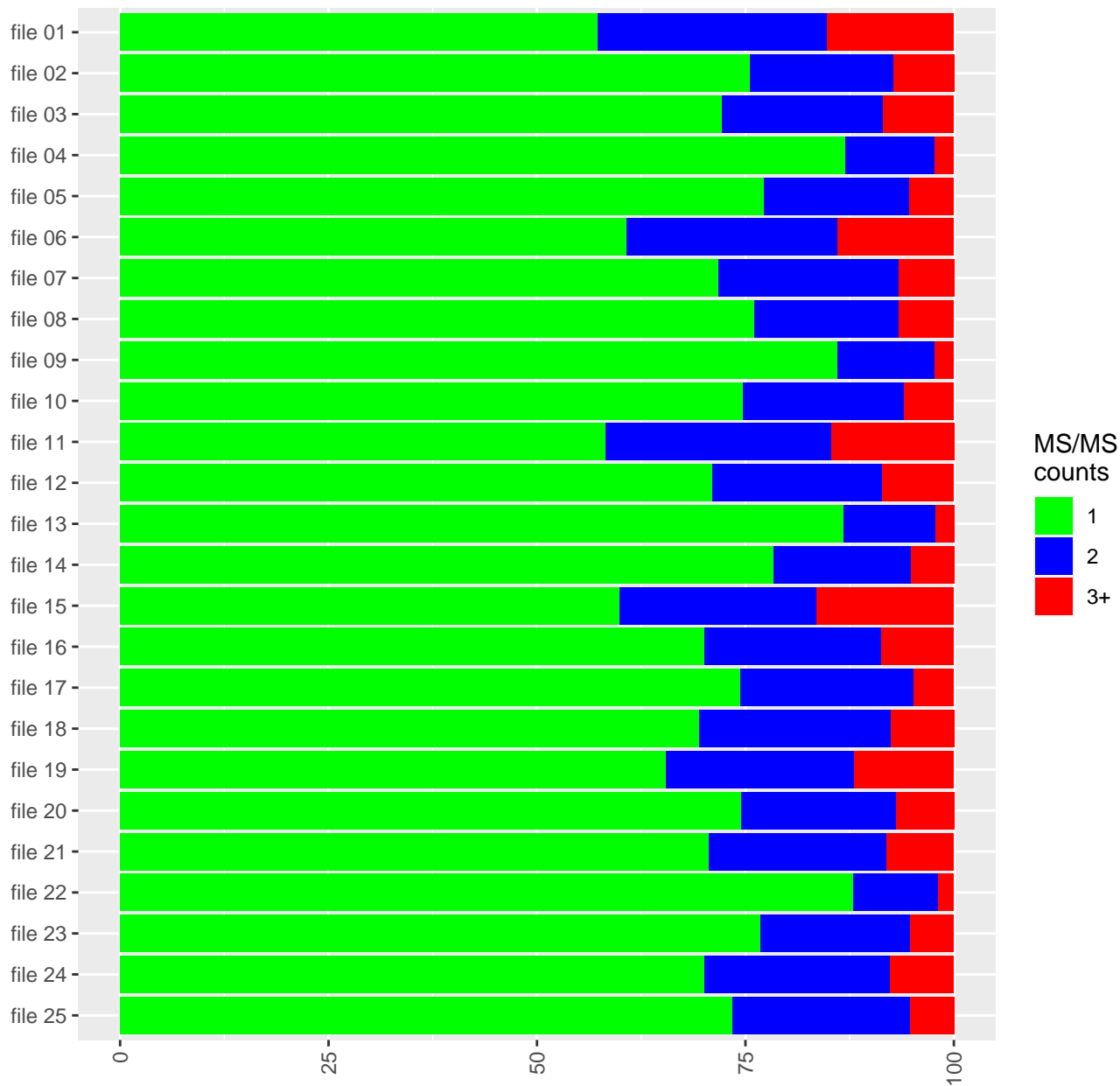
# [experimental] MSMSscans: MS/MS intensity



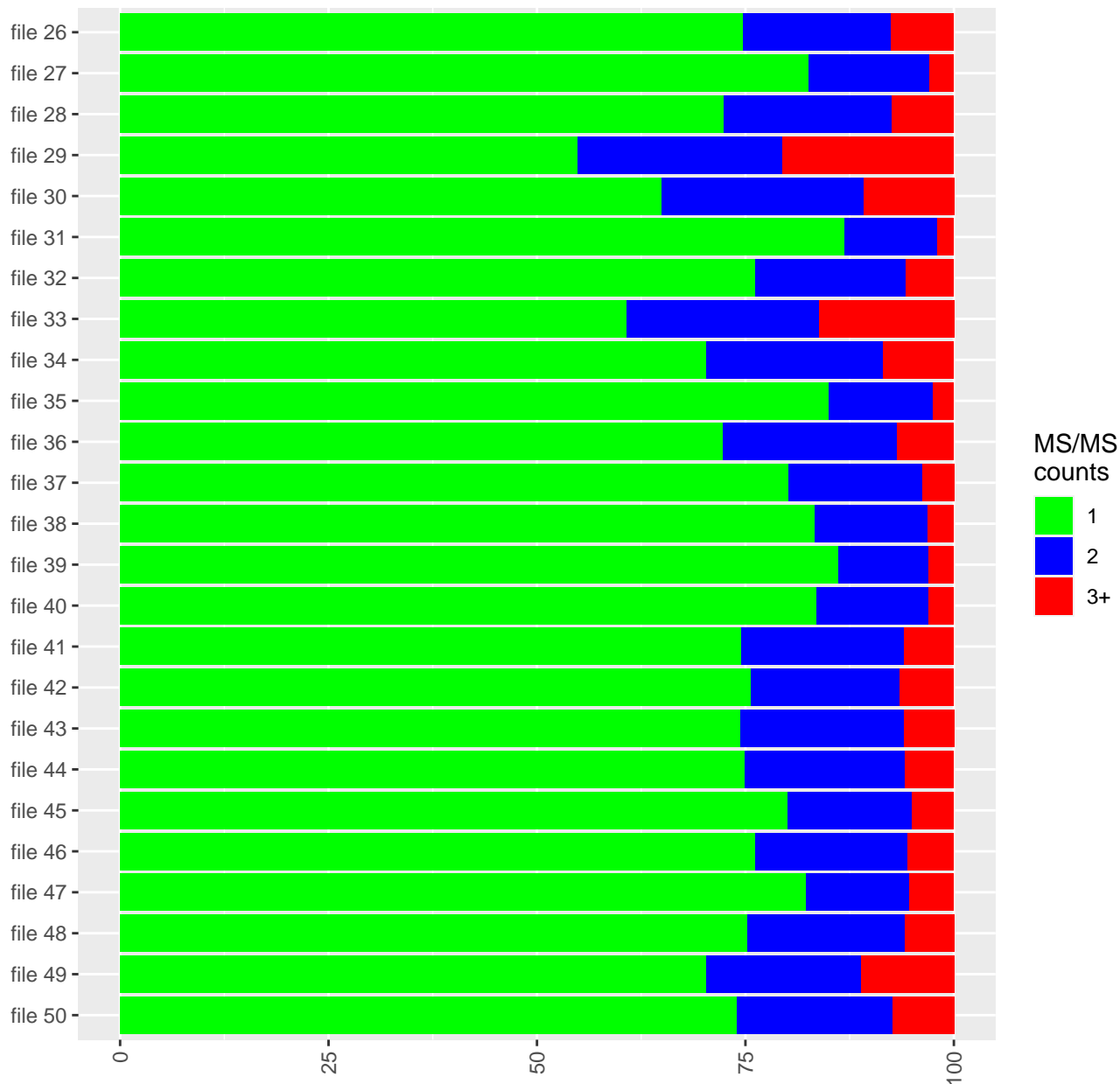
# [experimental] MSMSscans: MS/MS intensity



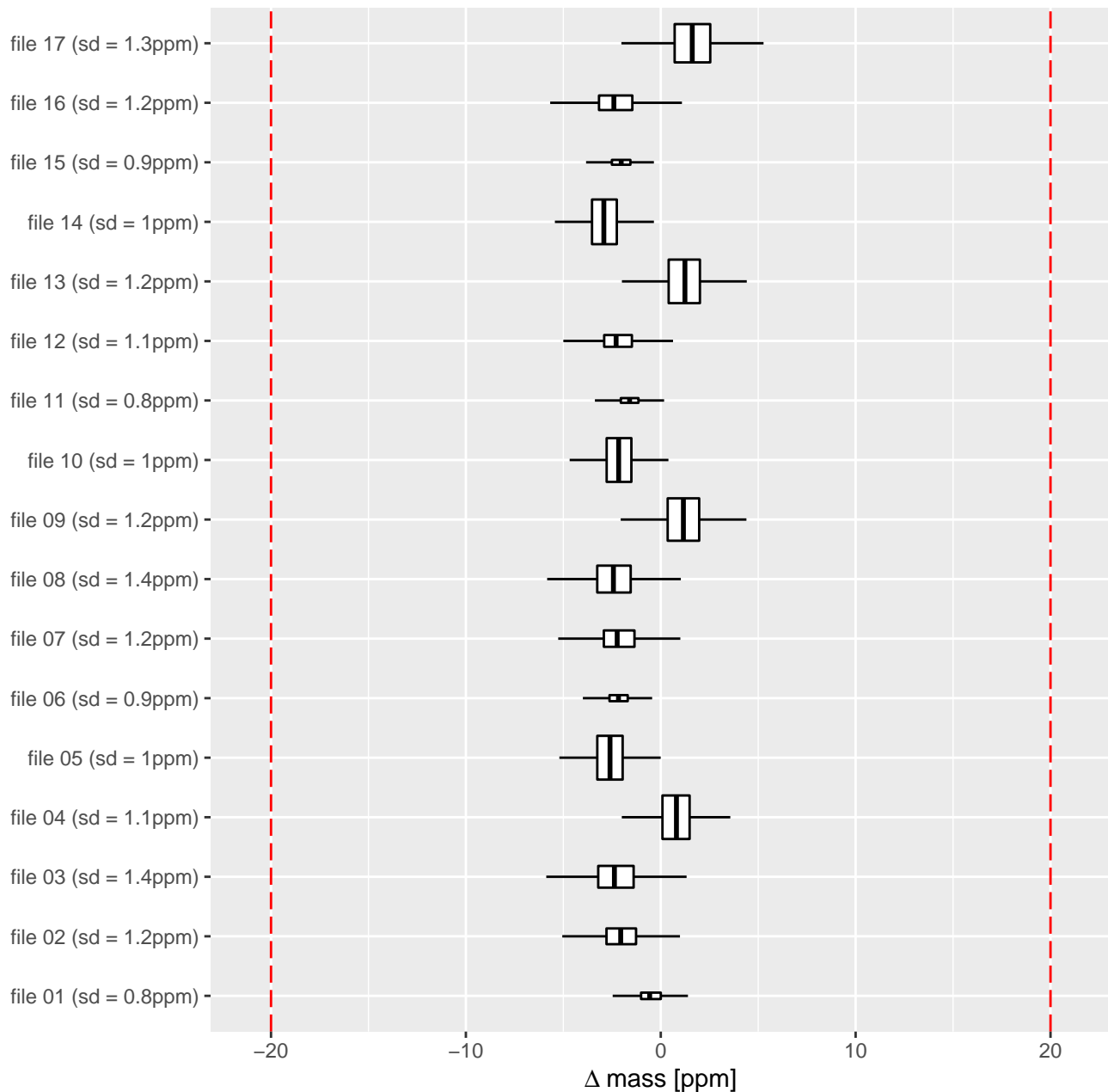
# EVD: Oversampling (MS/MS counts per 3D-peak)



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

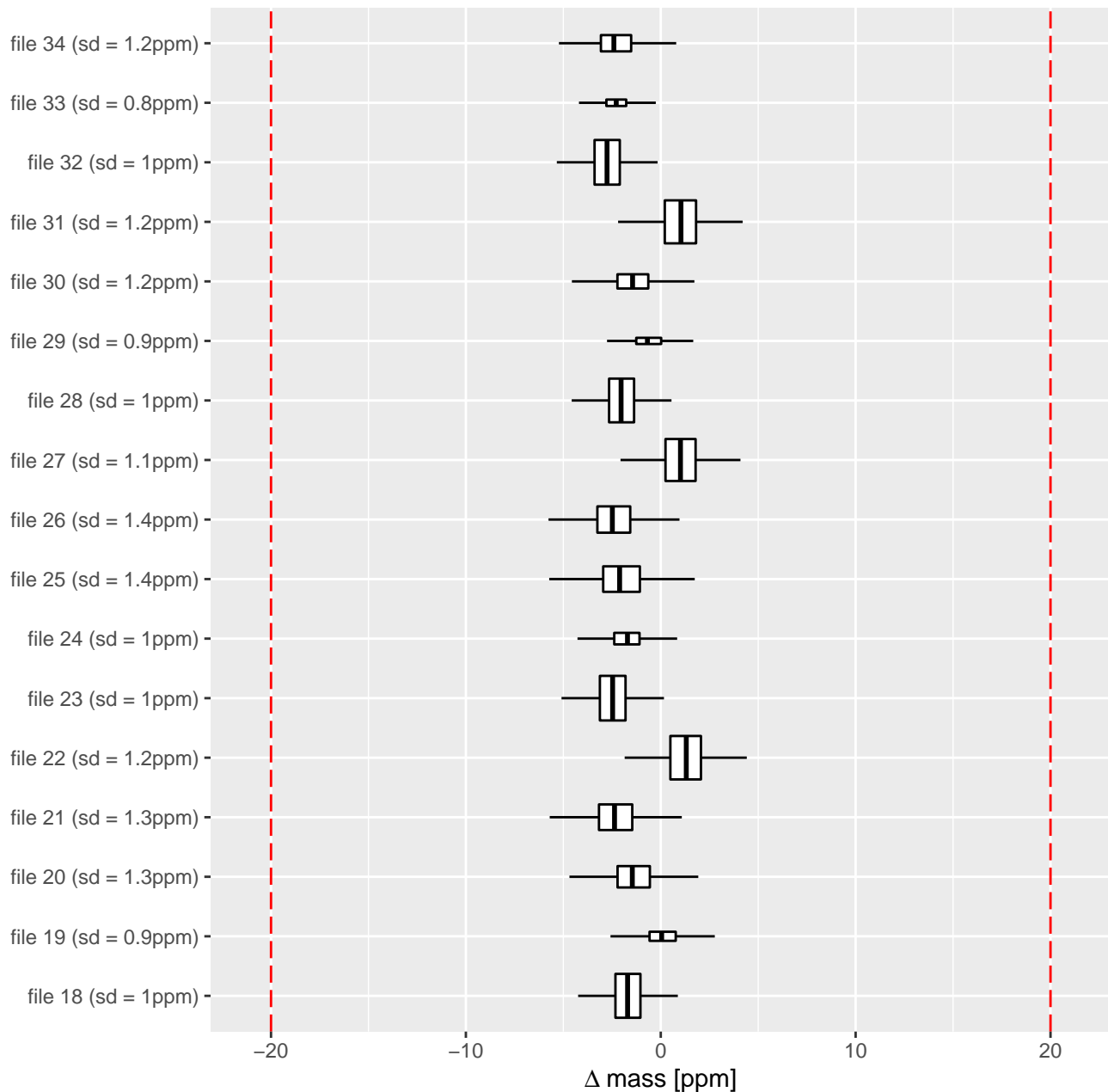


## EVD: Uncalibrated mass error

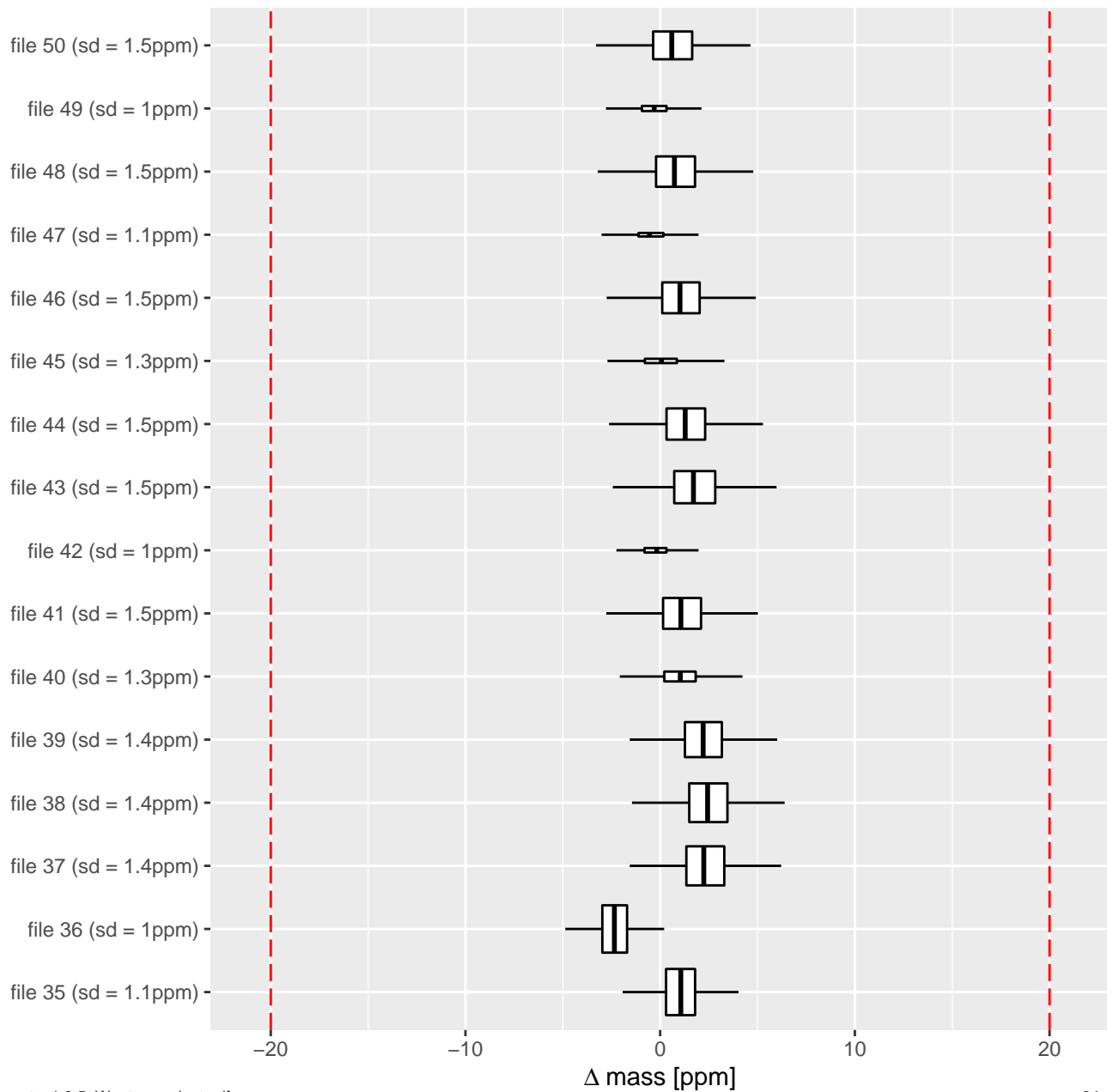




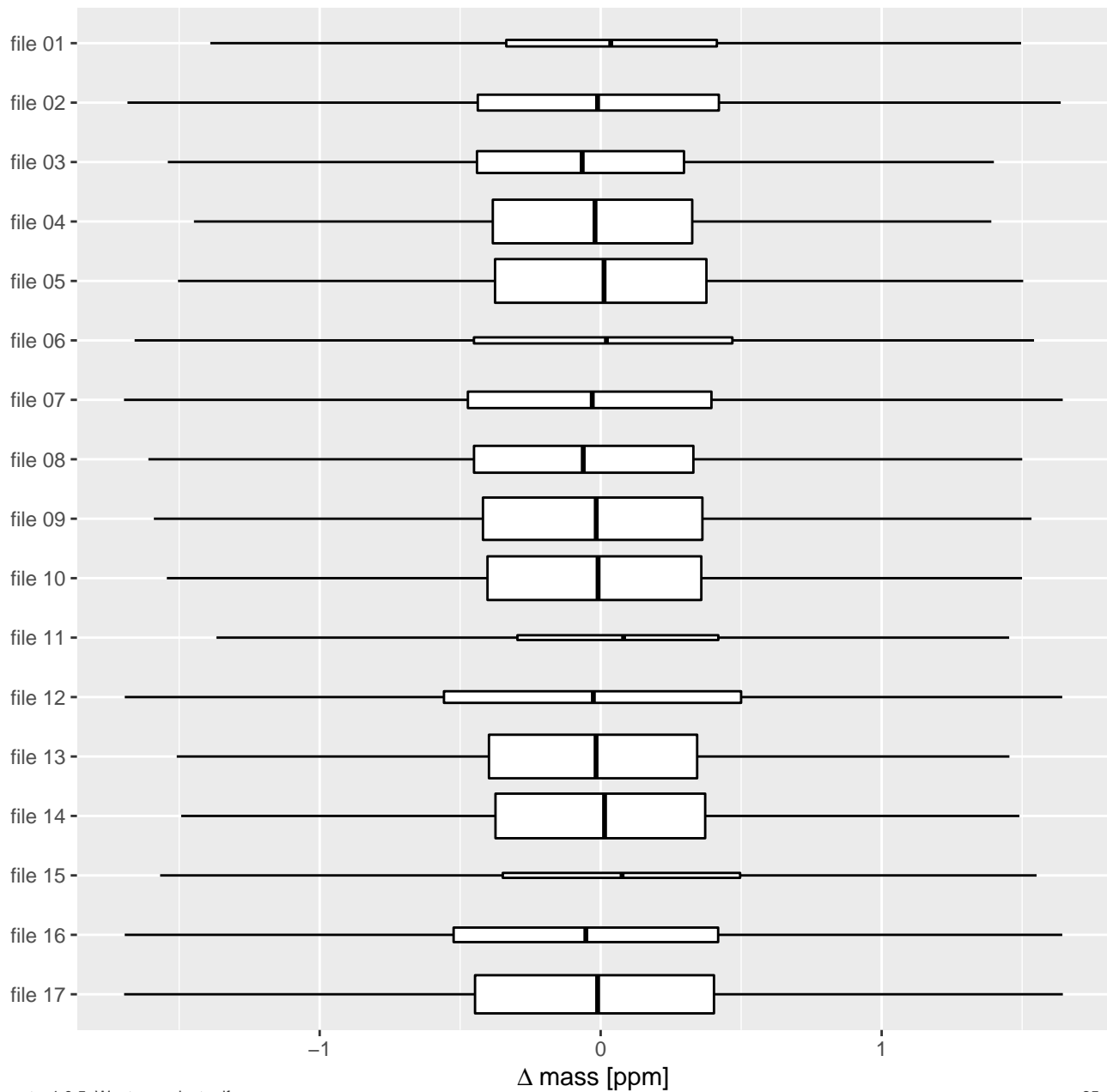
## EVD: Uncalibrated mass error



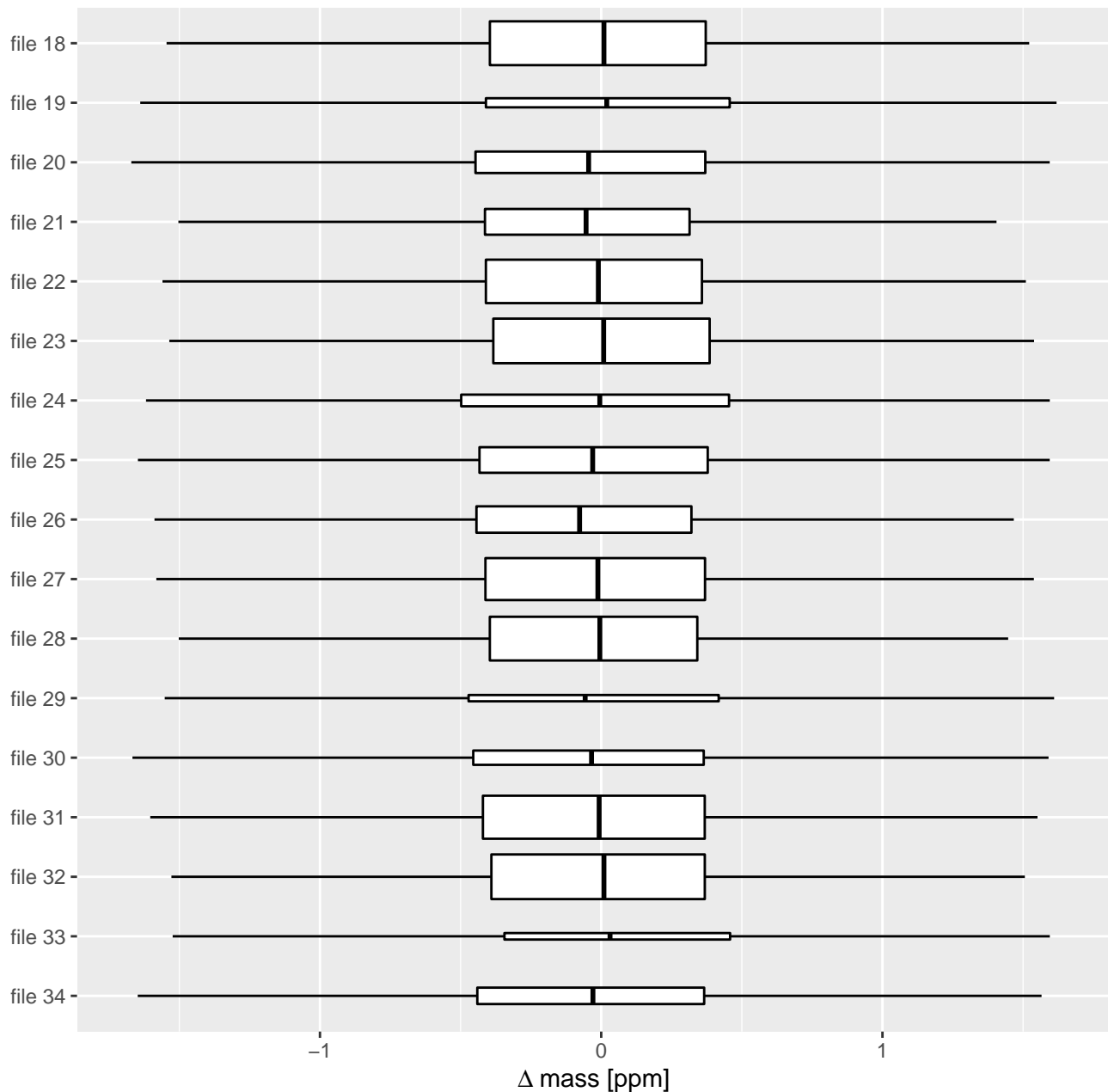
## EVD: Uncalibrated mass error



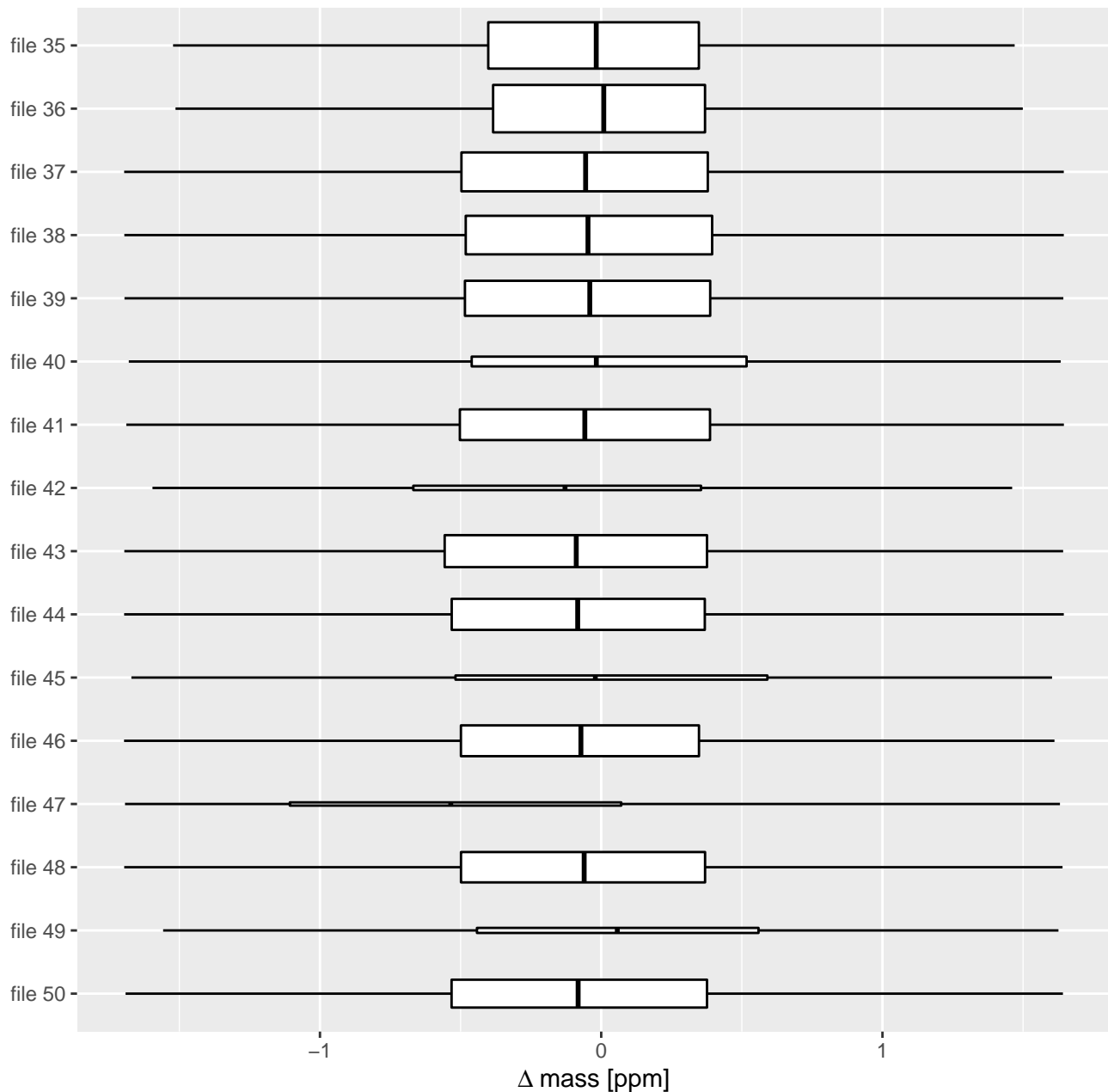
# EVD: Calibrated mass error



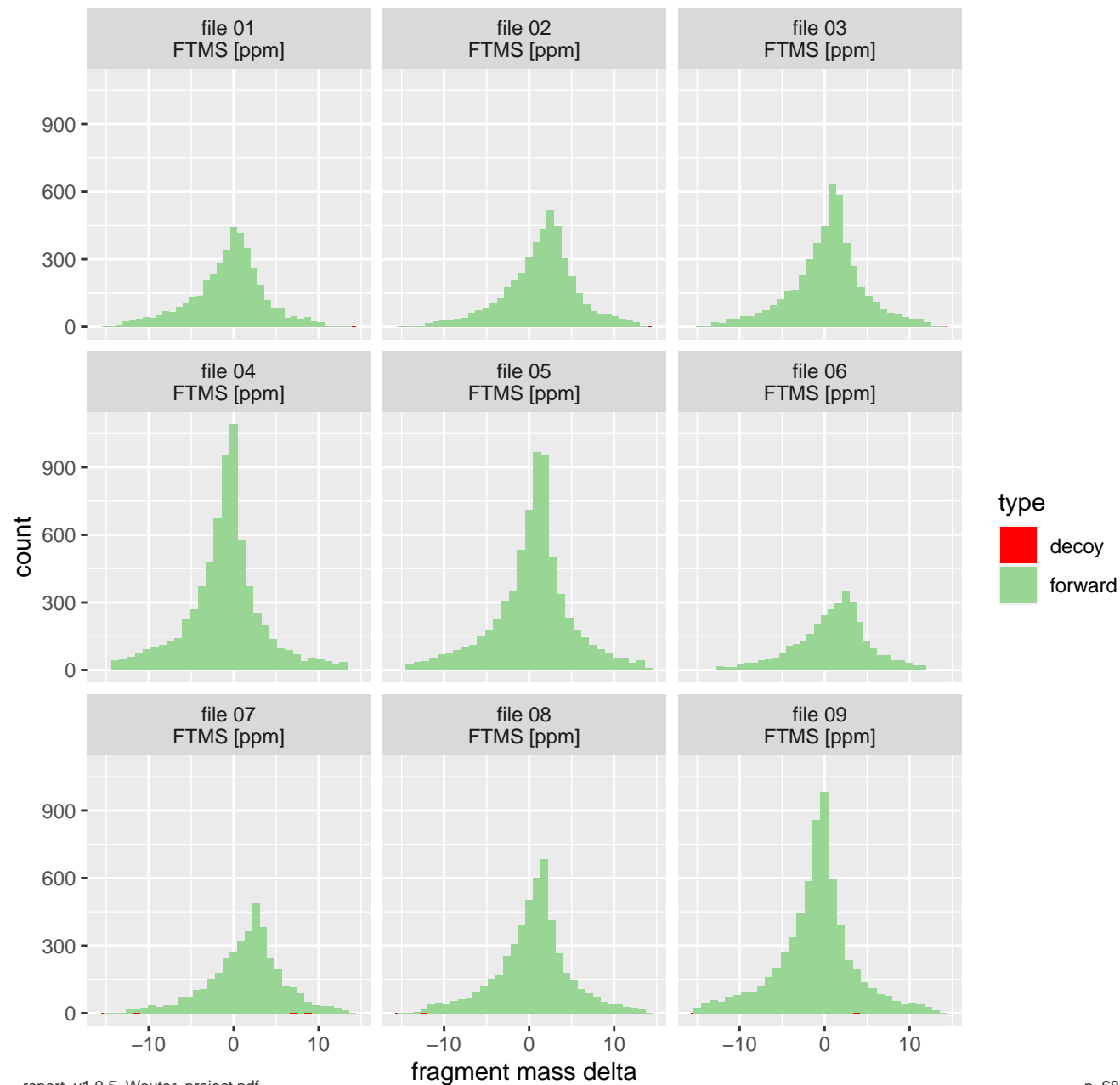
# EVD: Calibrated mass error



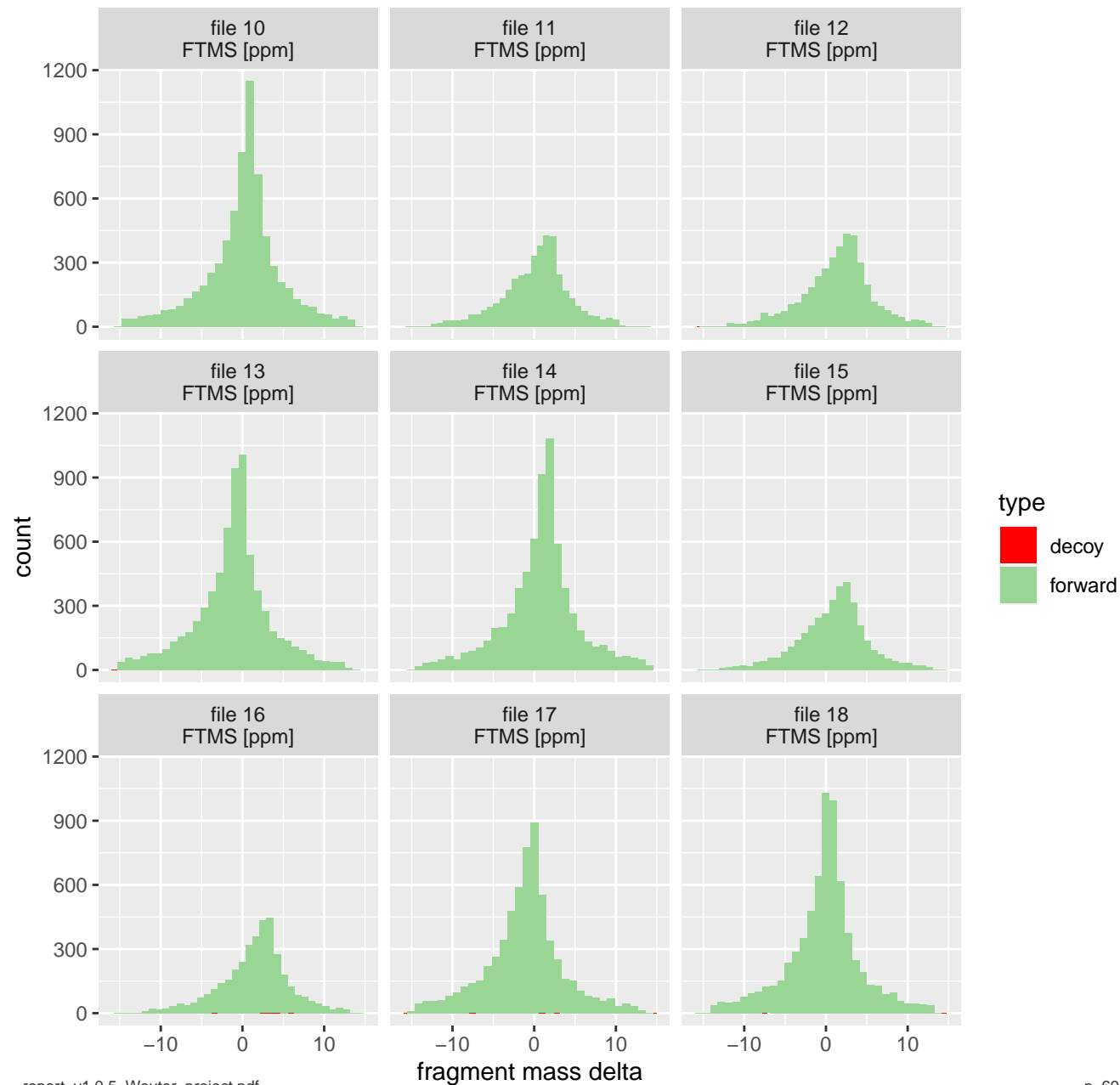
# EVD: Calibrated mass error



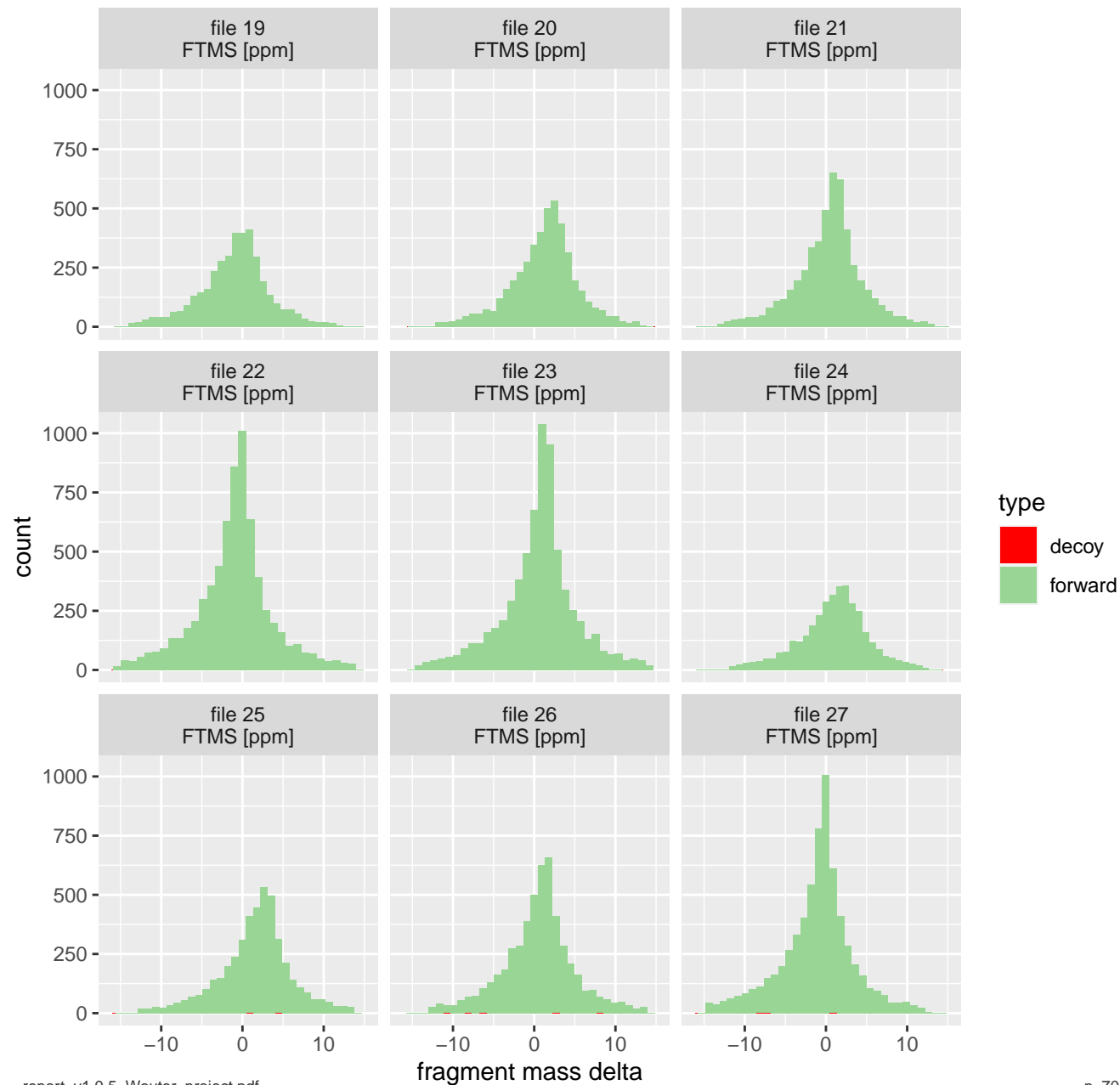
# MSMS: Fragment mass errors per Raw file



# MSMS: Fragment mass errors per Raw file

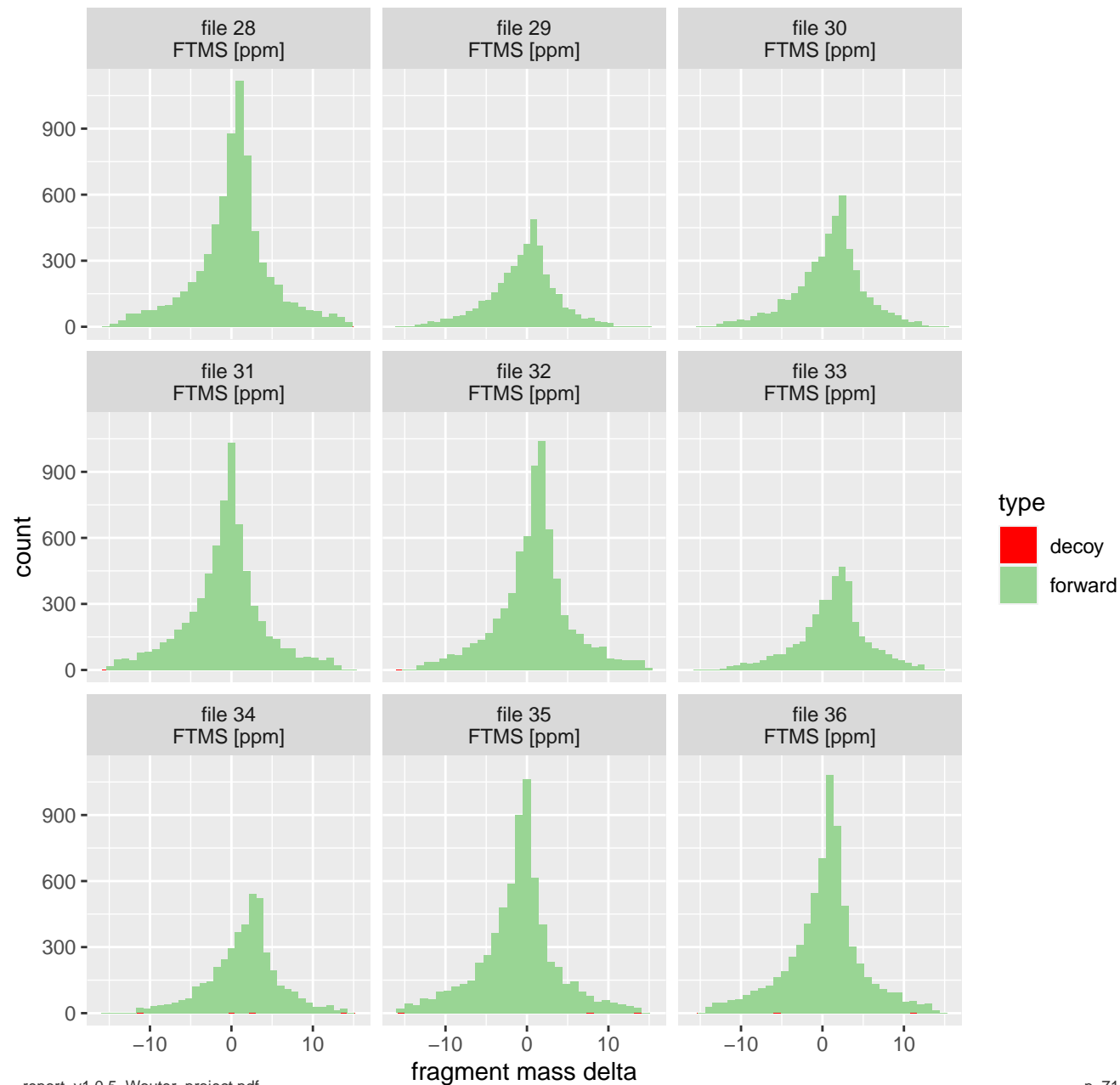


# MSMS: Fragment mass errors per Raw file

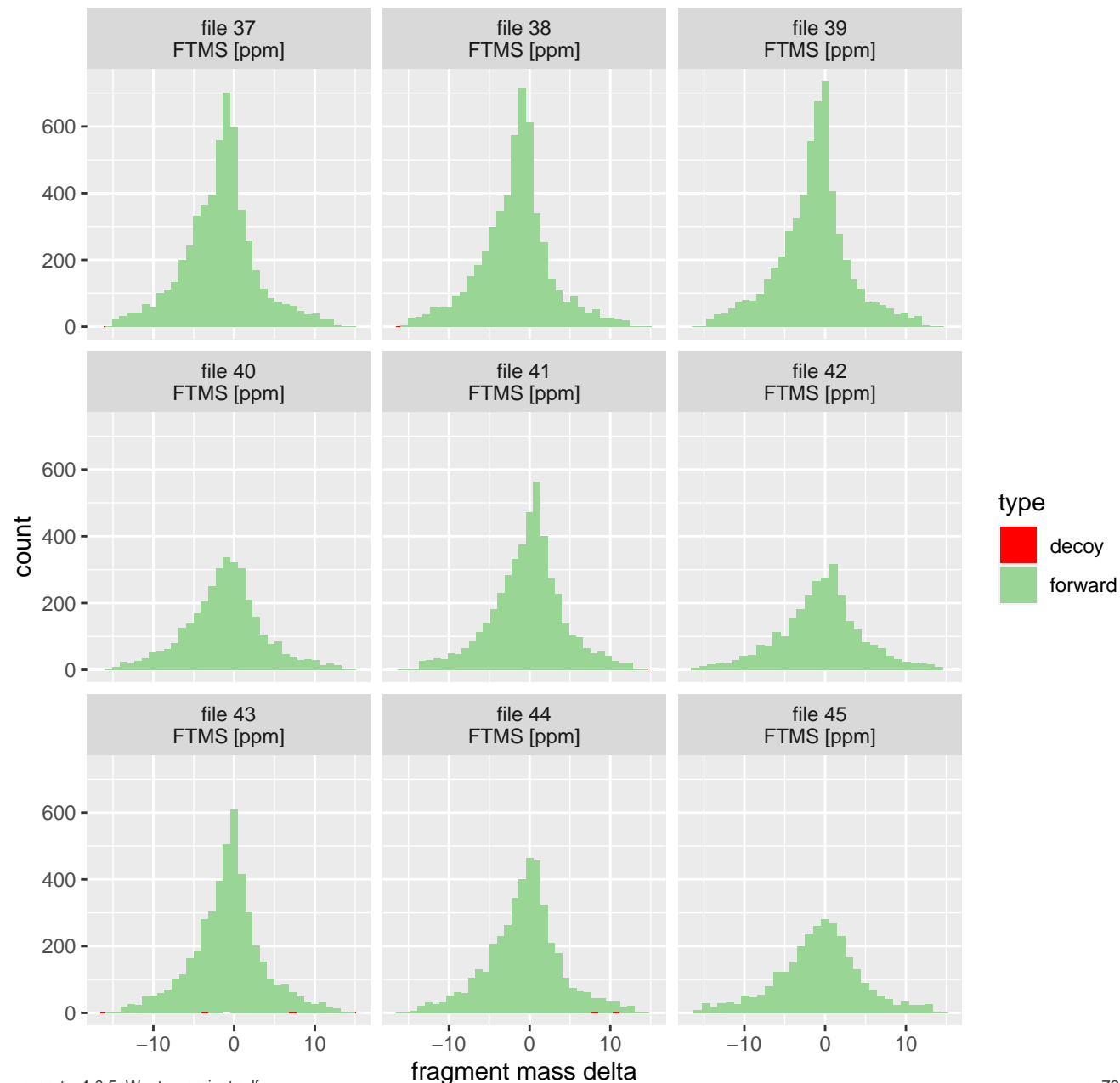




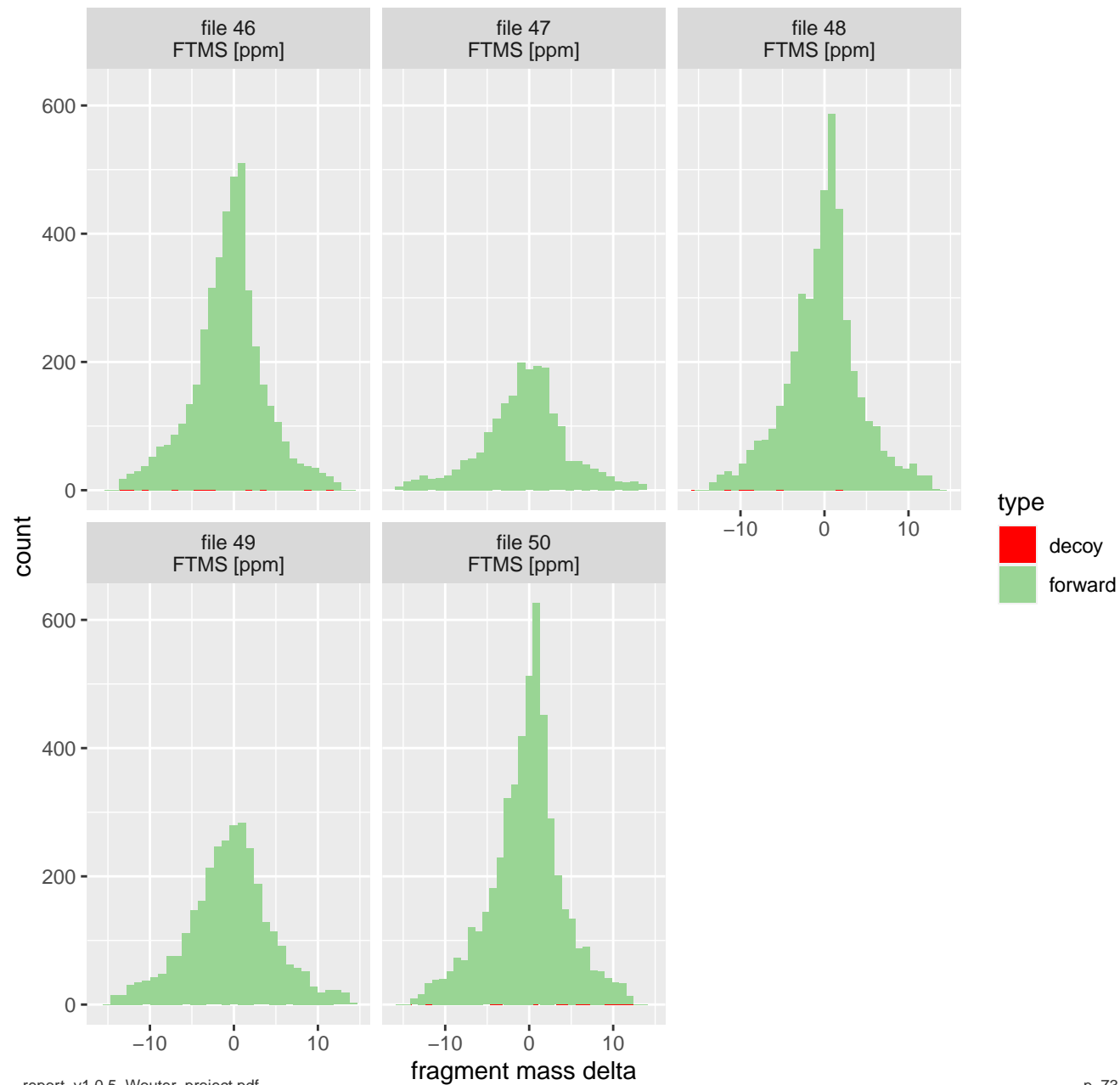
# MSMS: Fragment mass errors per Raw file



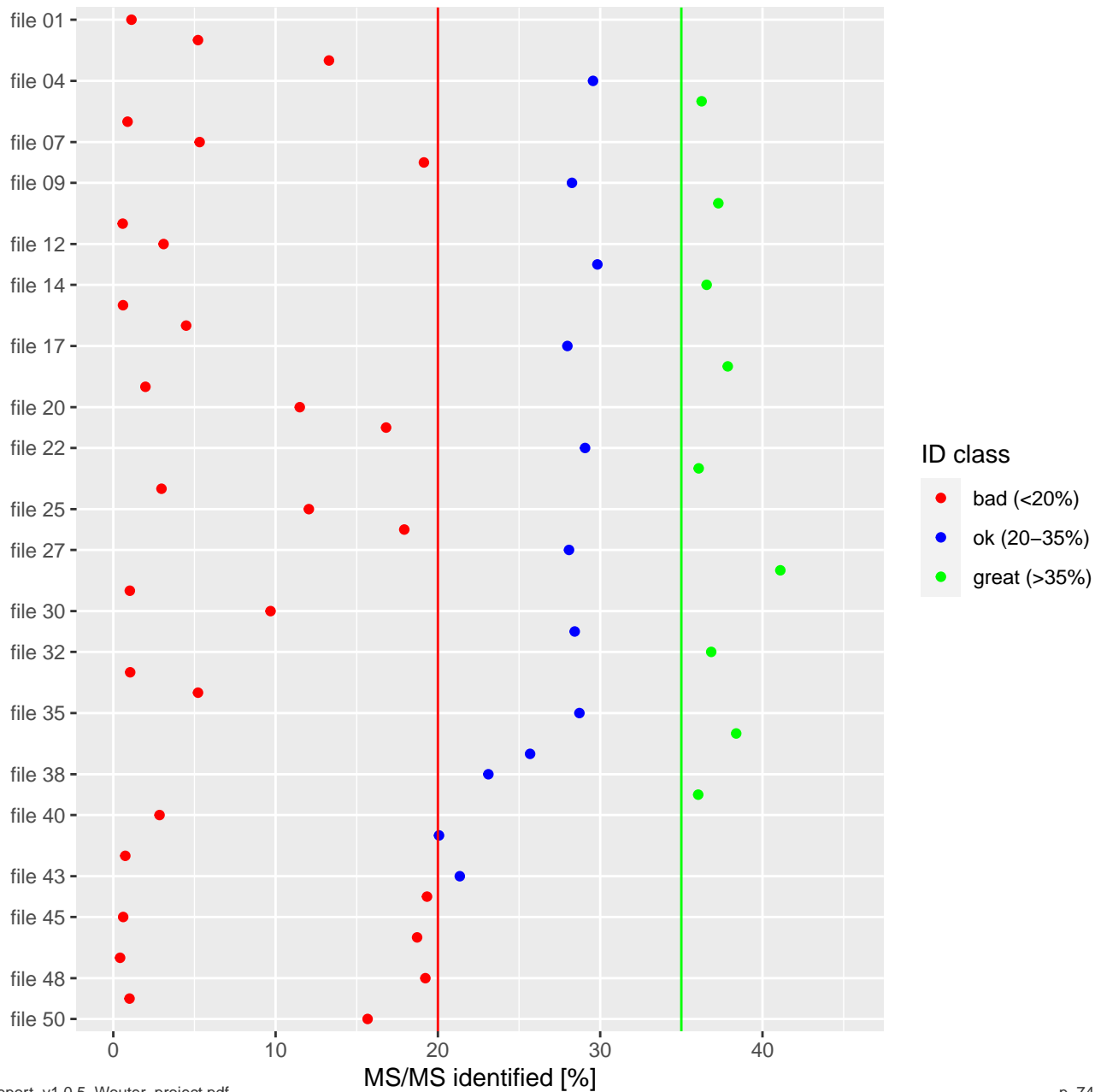
# MSMS: Fragment mass errors per Raw file



# MSMS: Fragment mass errors per Raw file



# SM: MS/MS identified per Raw file

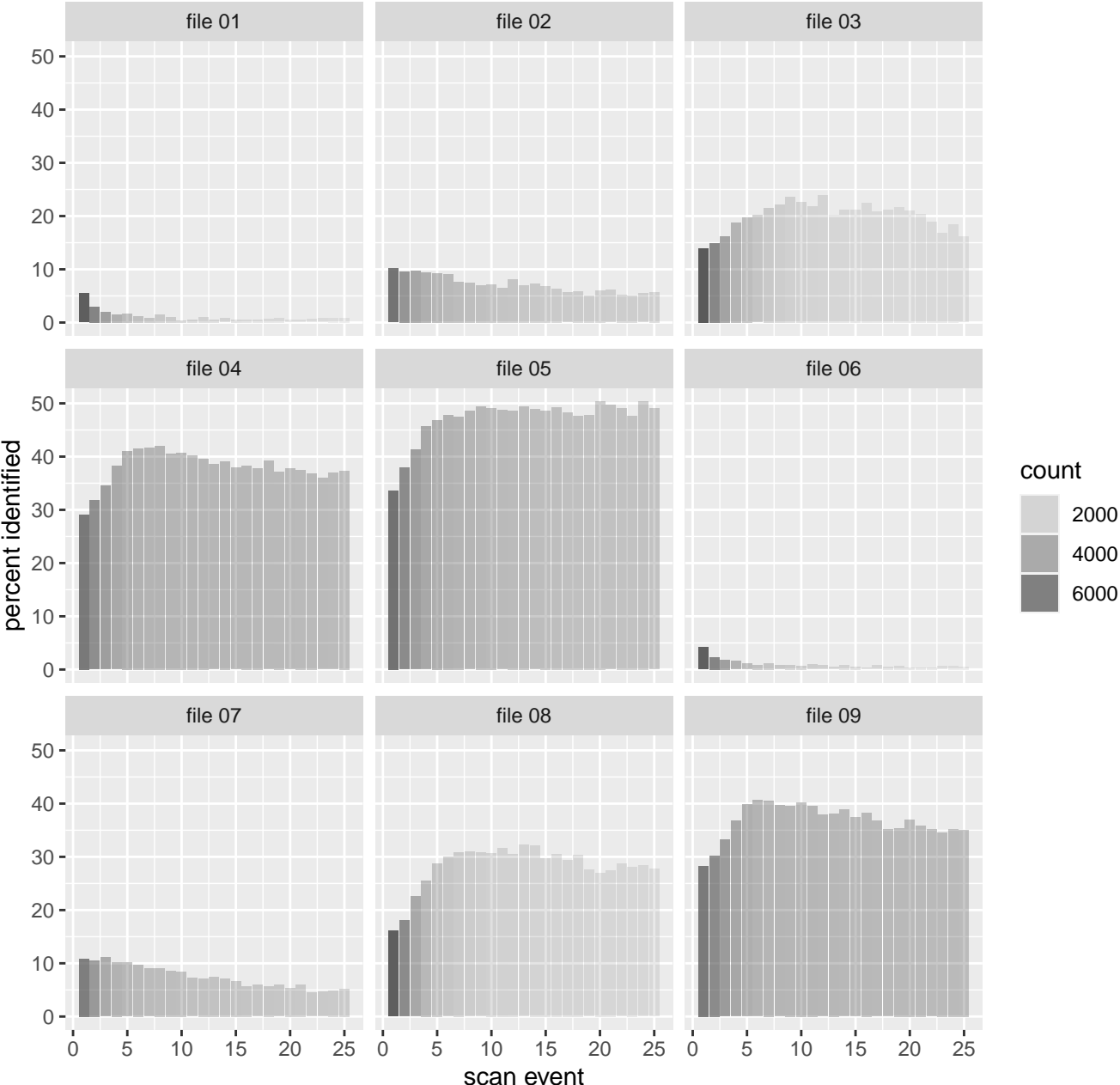


SM: Files with 'red' ID rate

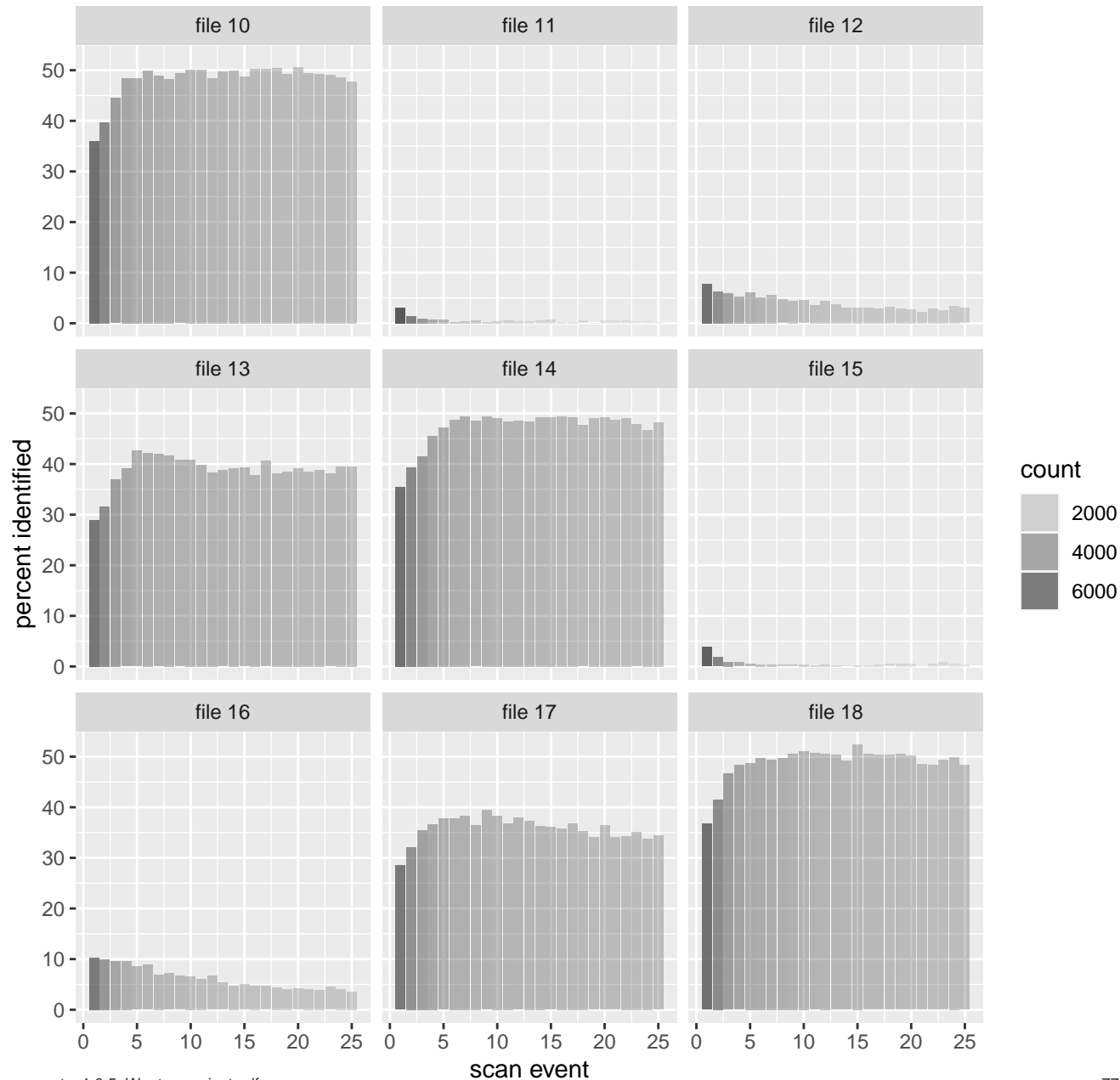
Raw file	% identified
10_DMSO_SDS_3	1.12
10_DMSO_SDS_3_5uL_20200612085223	5.22
10_insol_WT	13.29
12_Cpt_SDS_3	0.88
12_Cpt_SDS_3_5uL	5.32
12_insol_ATM	19.14
14_DMSO_SDS_4	0.58
14_DMSO_SDS_4_5uL	3.10
16_Cpt_SDS_4	0.60
16_Cpt_SDS_4_5uL	4.49
2_DMSO_SDS_1	1.98
2_DMSO_SDS_1_5uL	11.49
2_insol_WT	16.81
4_cpt_SDS_1	2.97
4_cpt_SDS_1_5uL	12.05
4_insol_ATM	17.93
6_DMSO_SDS_2	1.02
6_DMSO_SDS_2_5uL	9.69
8_Cpt_SDS_2	1.04
8_Cpt_SDS_2_5uL	5.22
insol_ATM_3_20200725191715	2.85
insol_ATM_4	0.74
insol_WT_1_20200727152510	19.33
insol_WT_2	0.61
insol_WT_2_20200727173305	18.72
insol_WT_3	0.42
insol_WT_3_20200727194055	19.23
insol_WT_4	1.00
insol_WT_4_20200727214846	15.67

58% of samples)

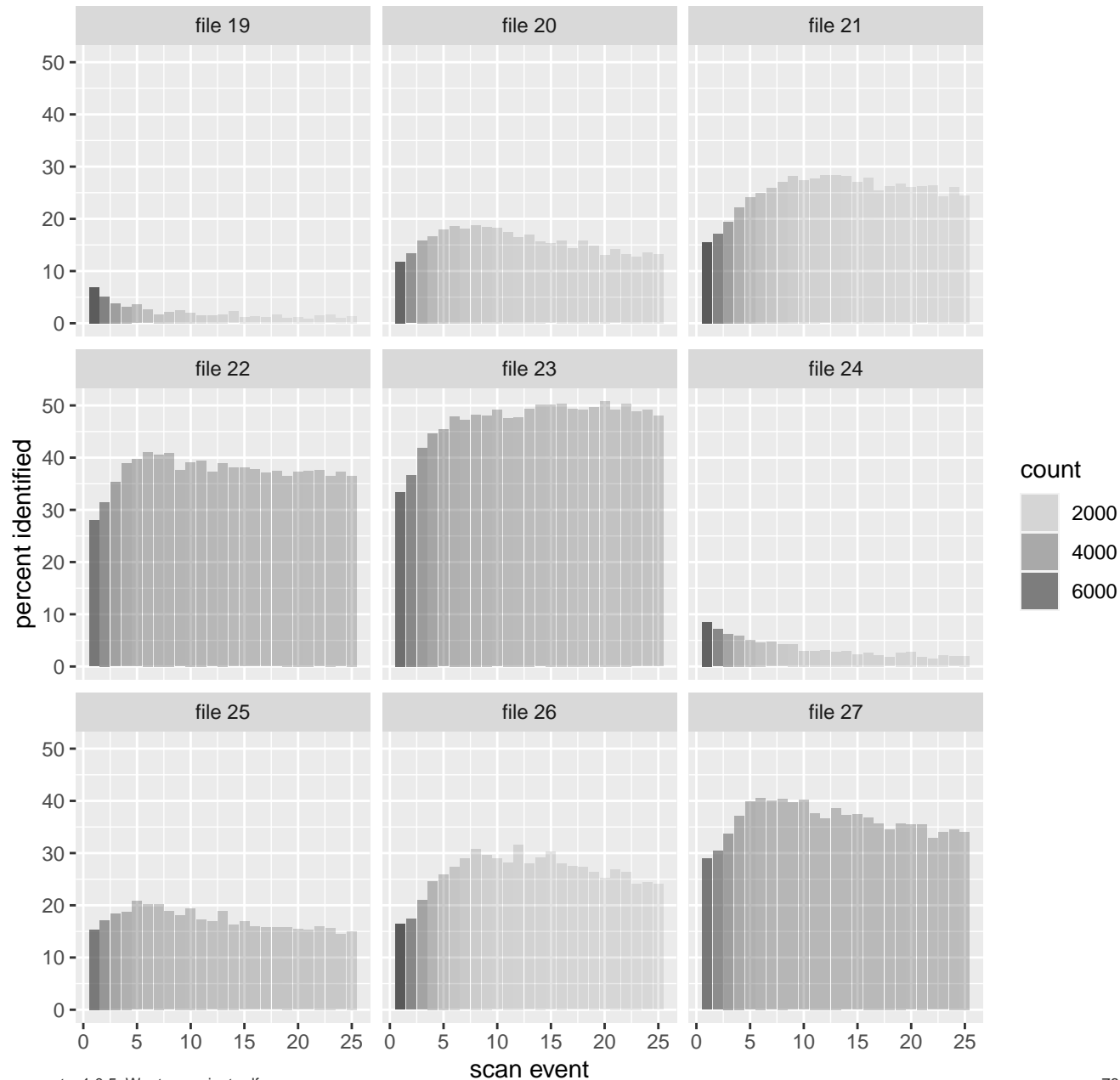
# MSMSscans: TopN % identified over N



# MSMSscans: TopN % identified over N

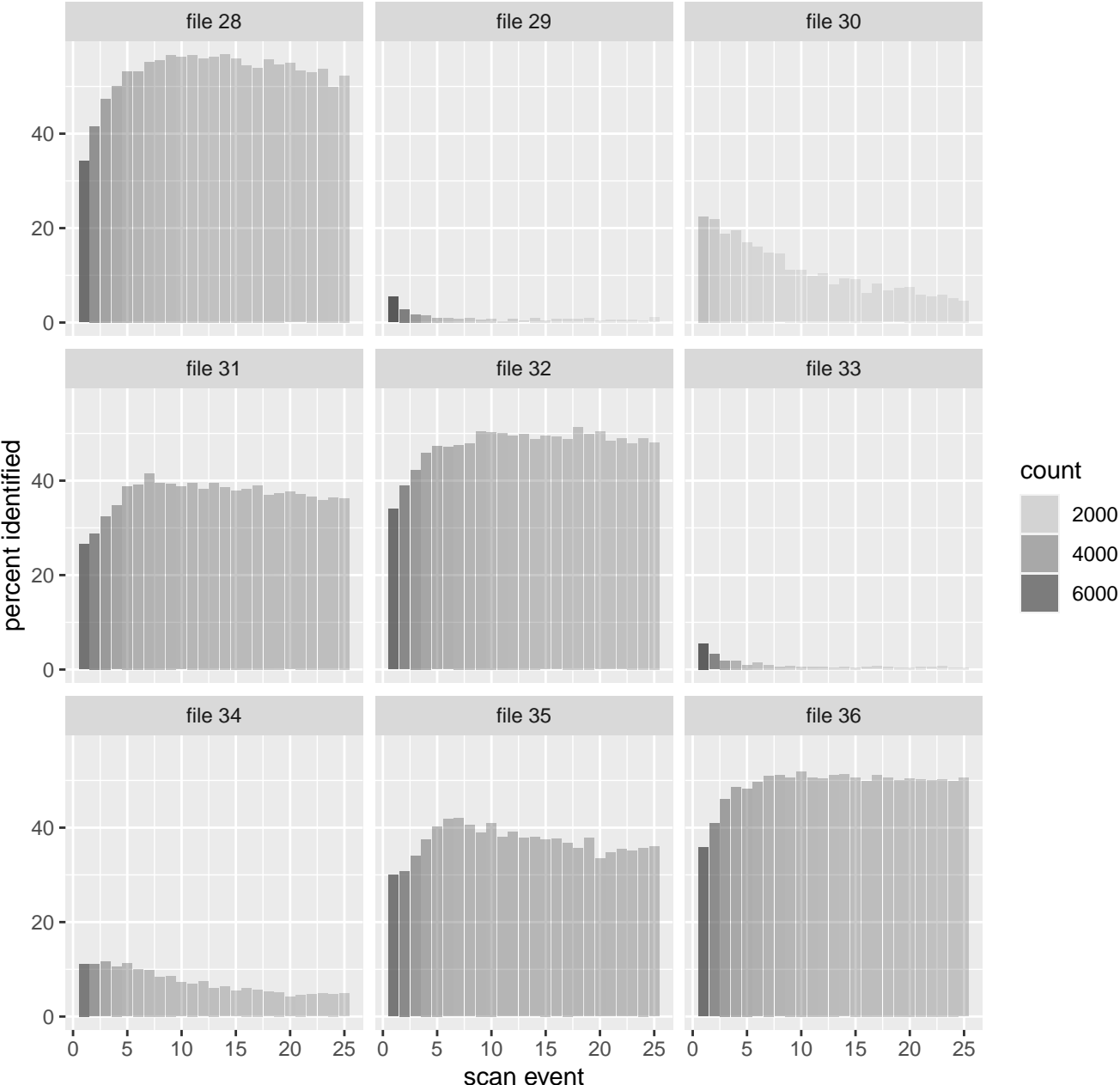


# MSMSscans: TopN % identified over N

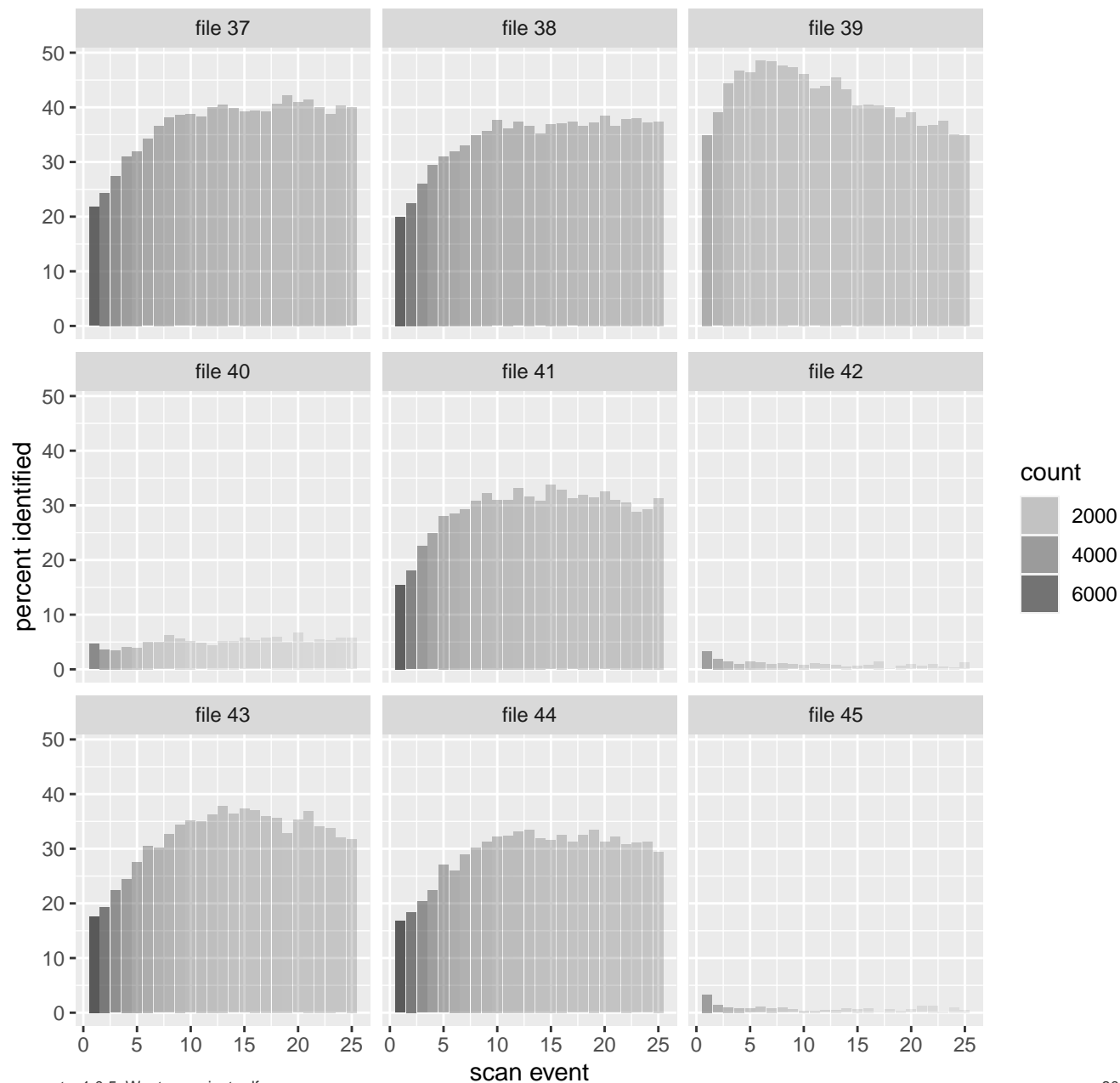




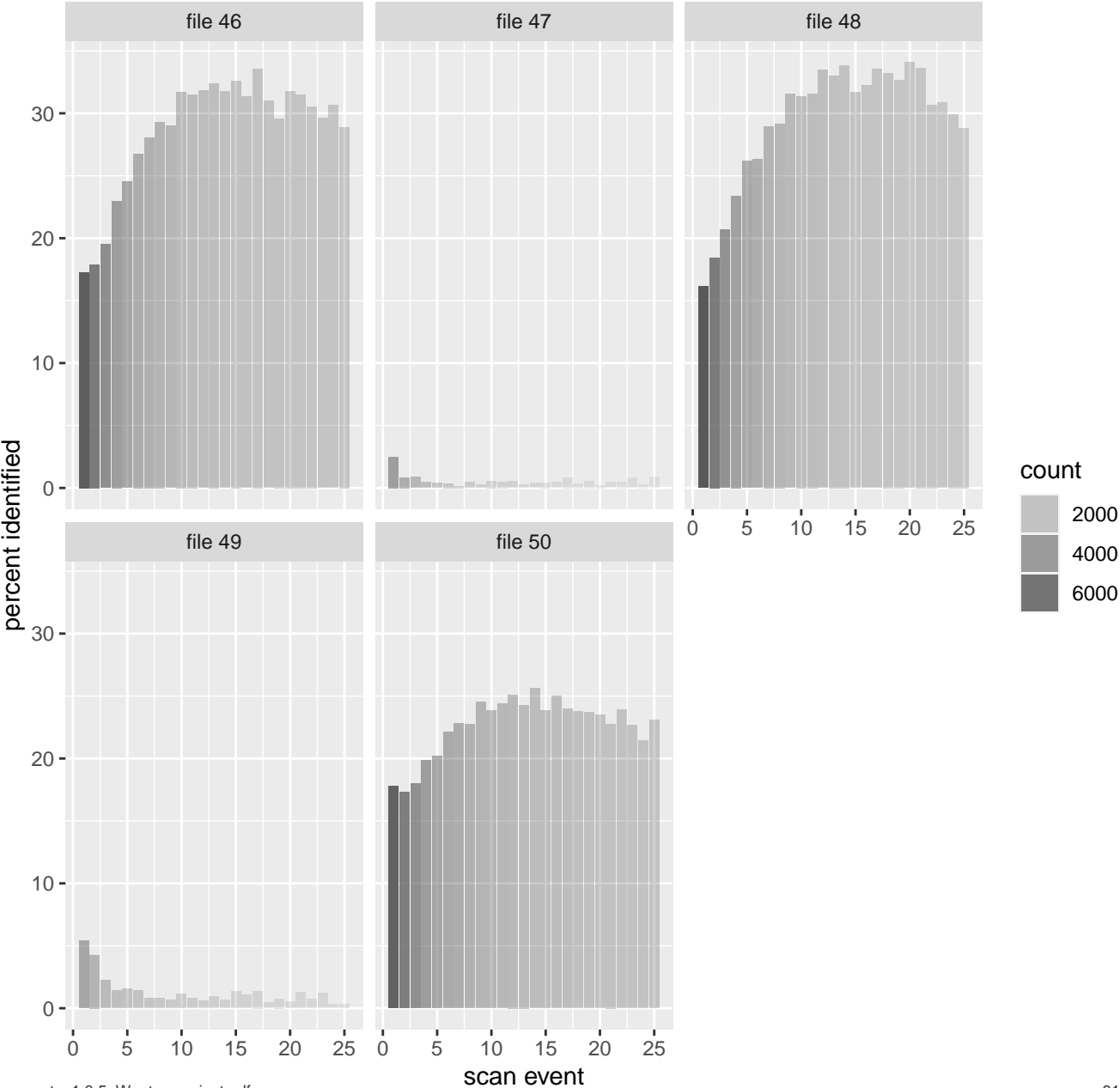
MSMSScans: TopN % identified over N



# MSMSscans: TopN % identified over N

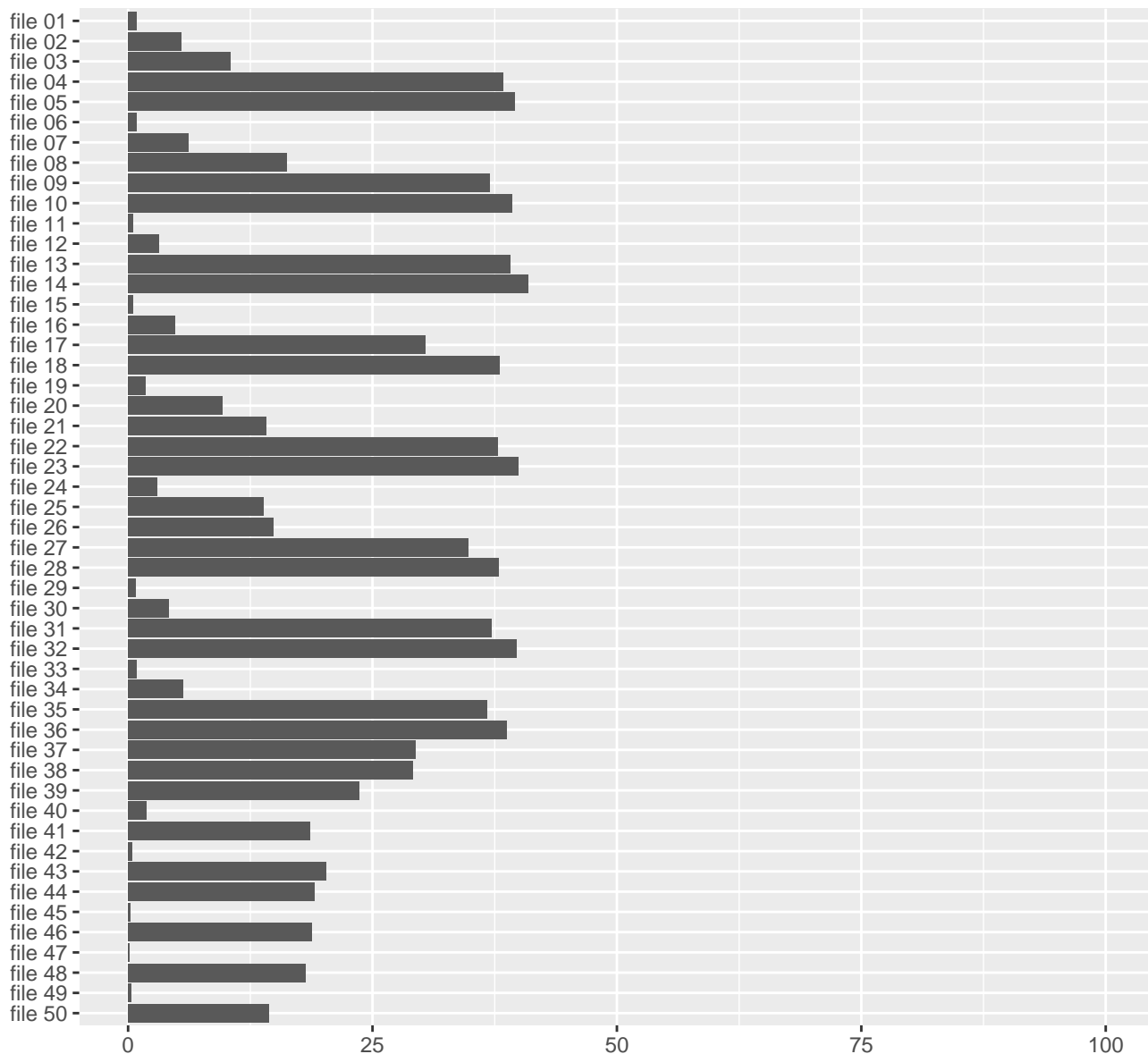


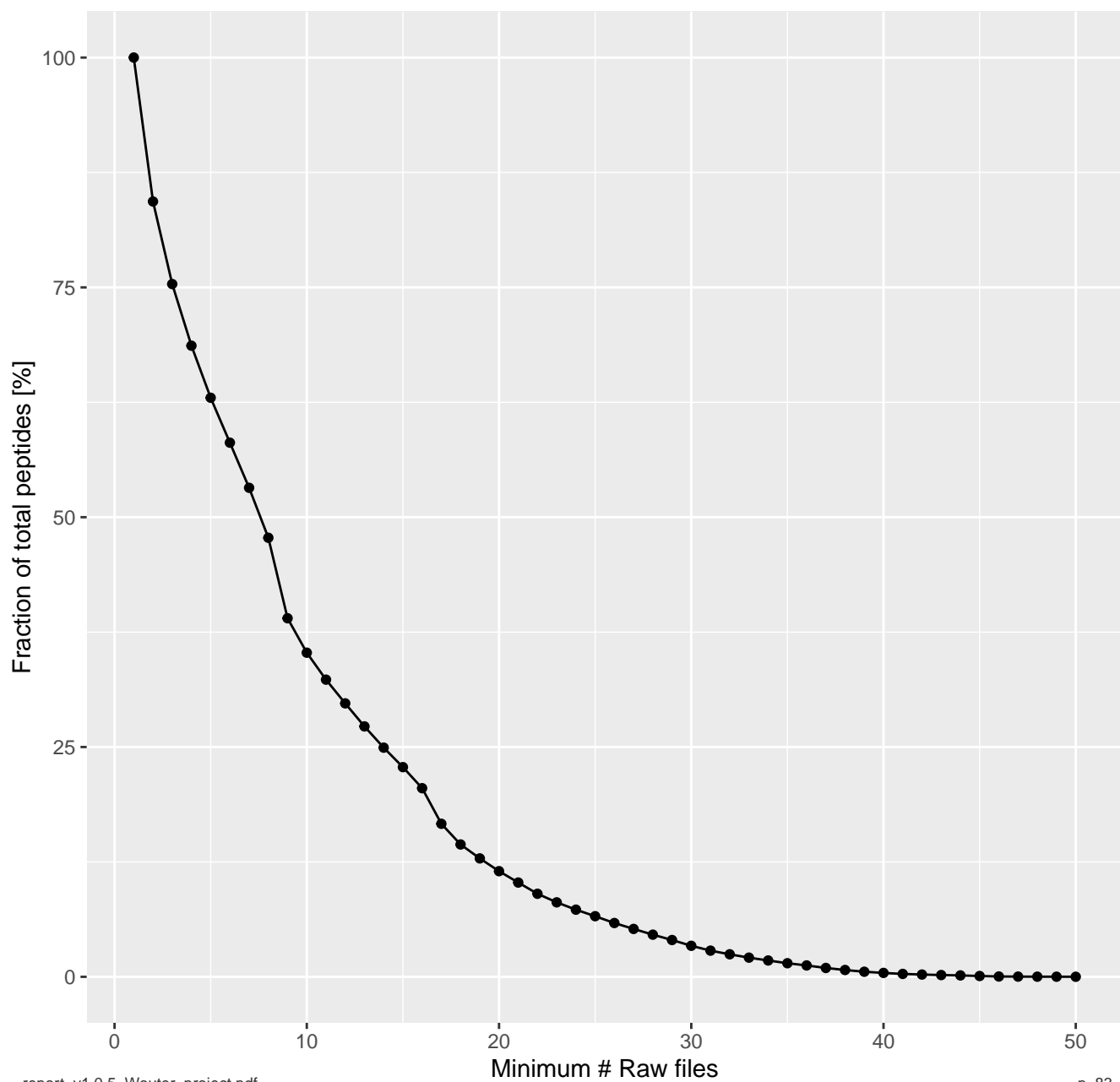
MSMSscans: TopN % identified over N



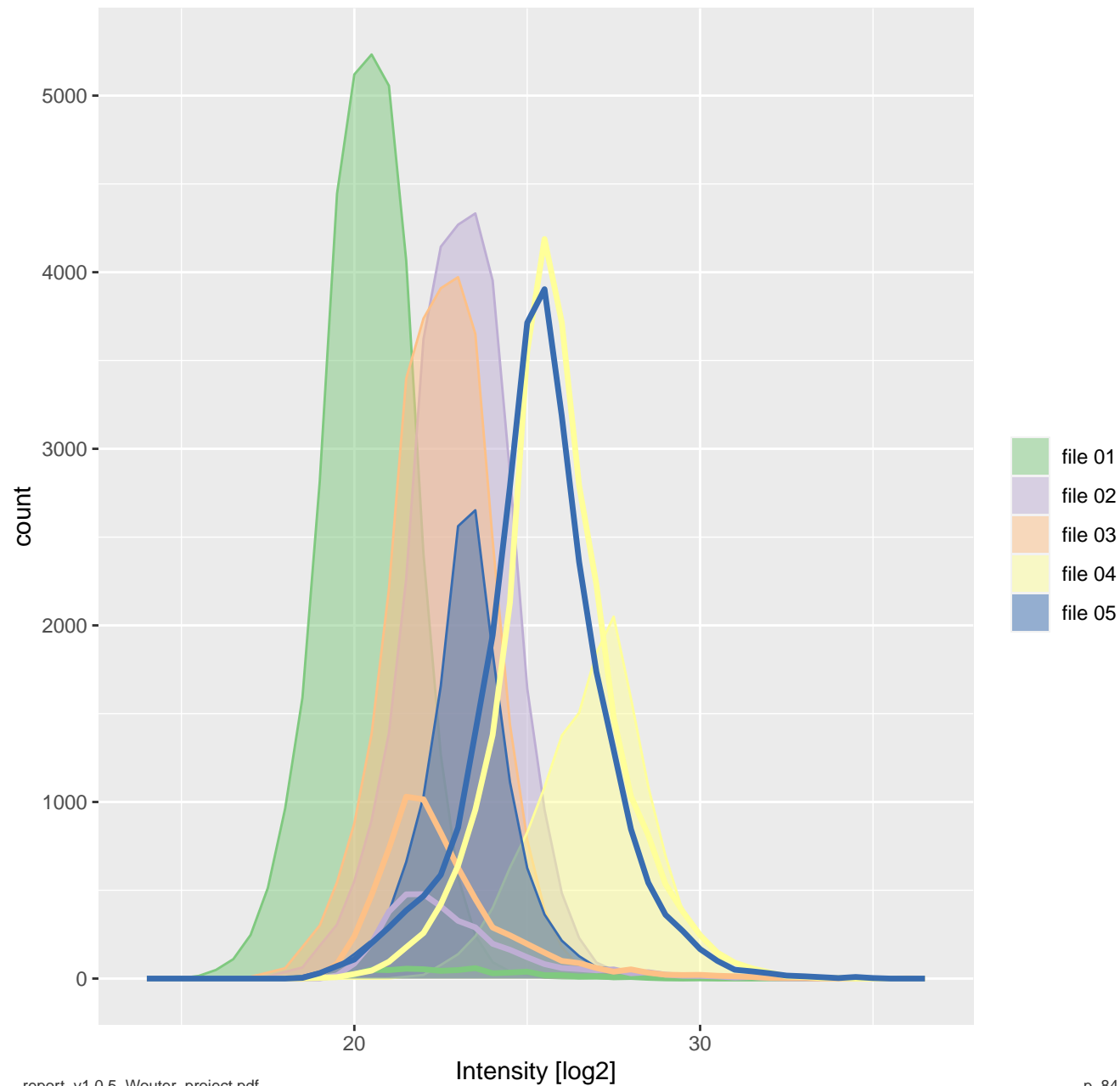
# [experimental] EVD: Non-Missing Peptides

compared to all peptides seen in experiment

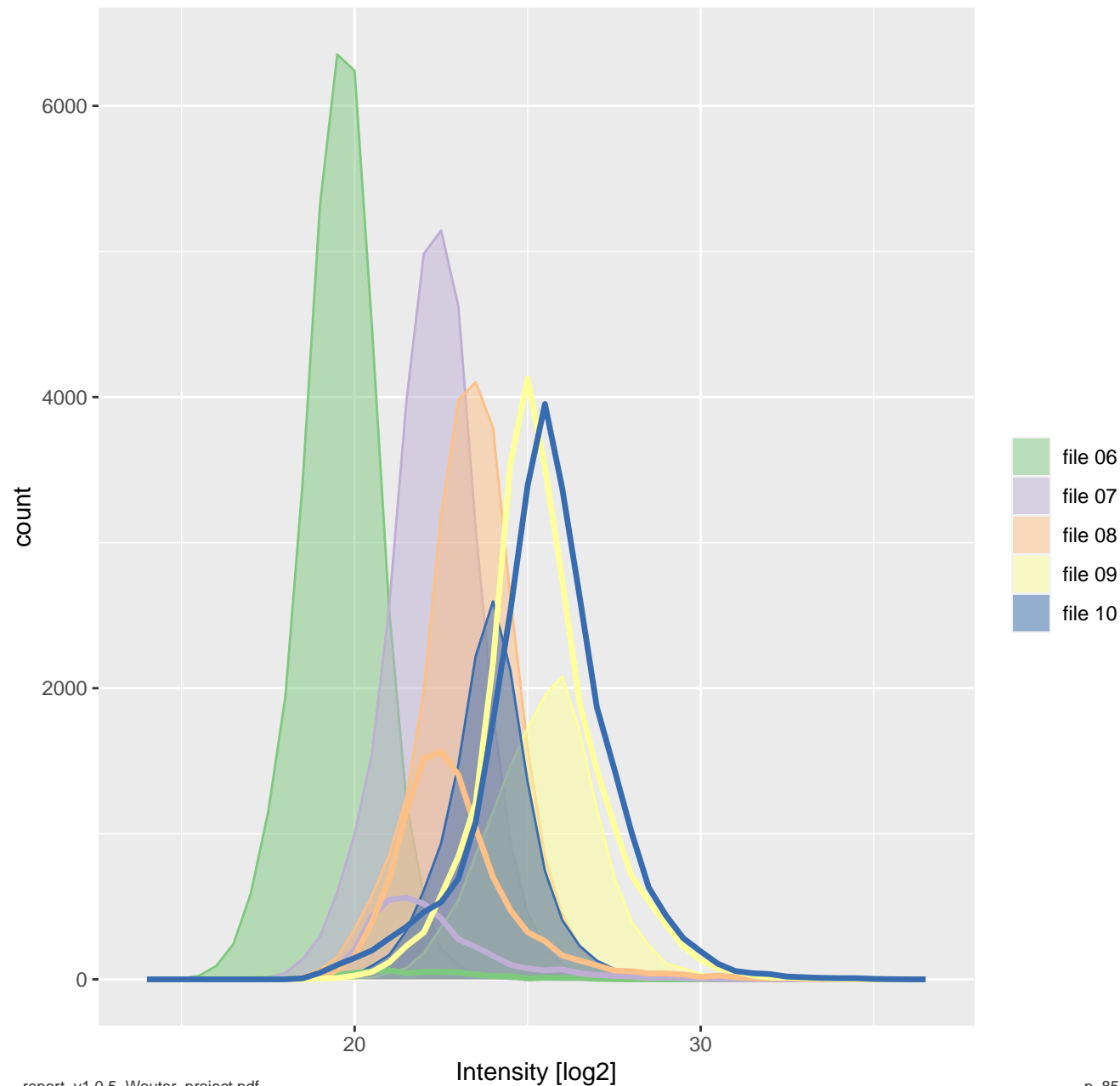




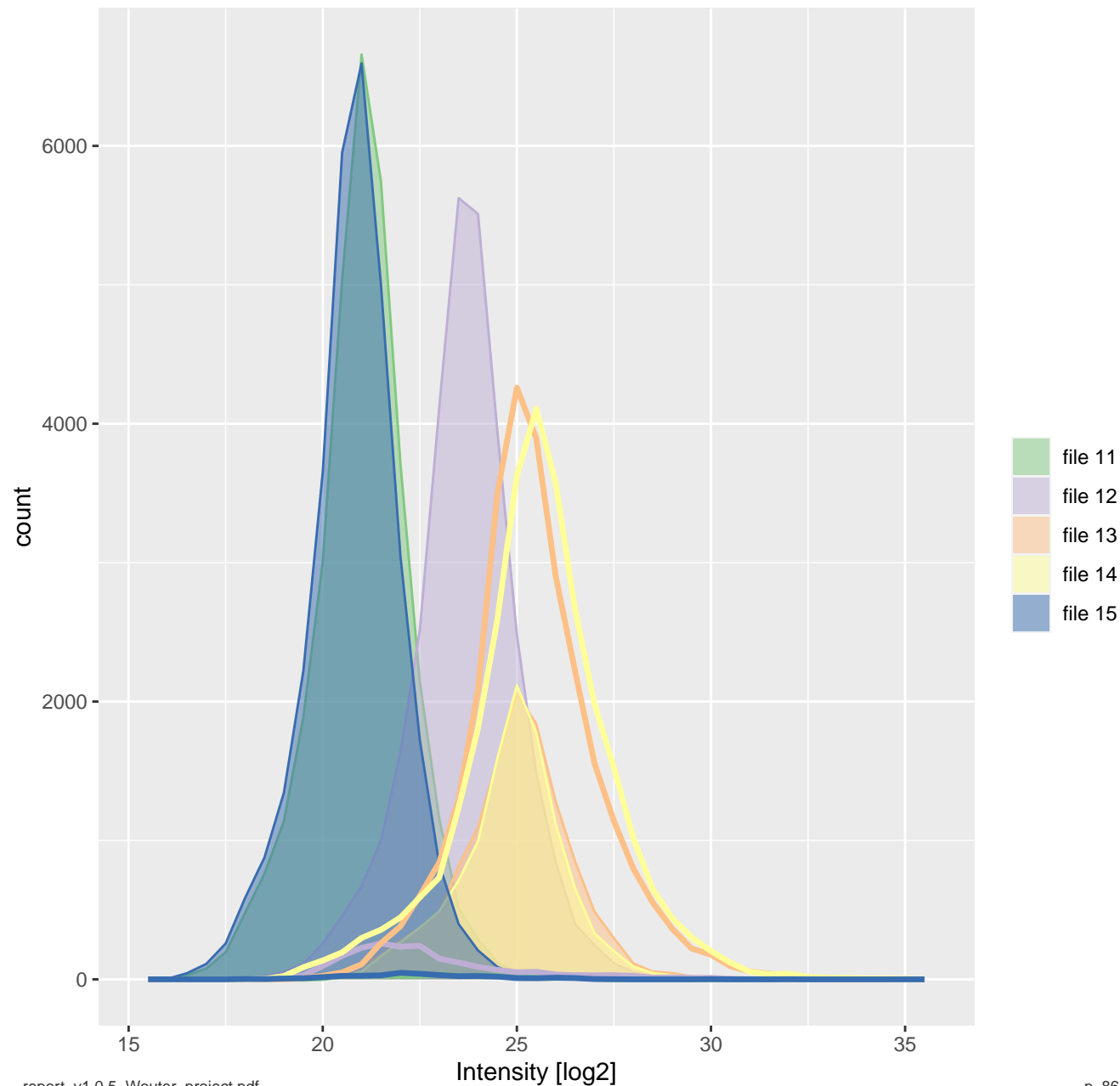
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



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

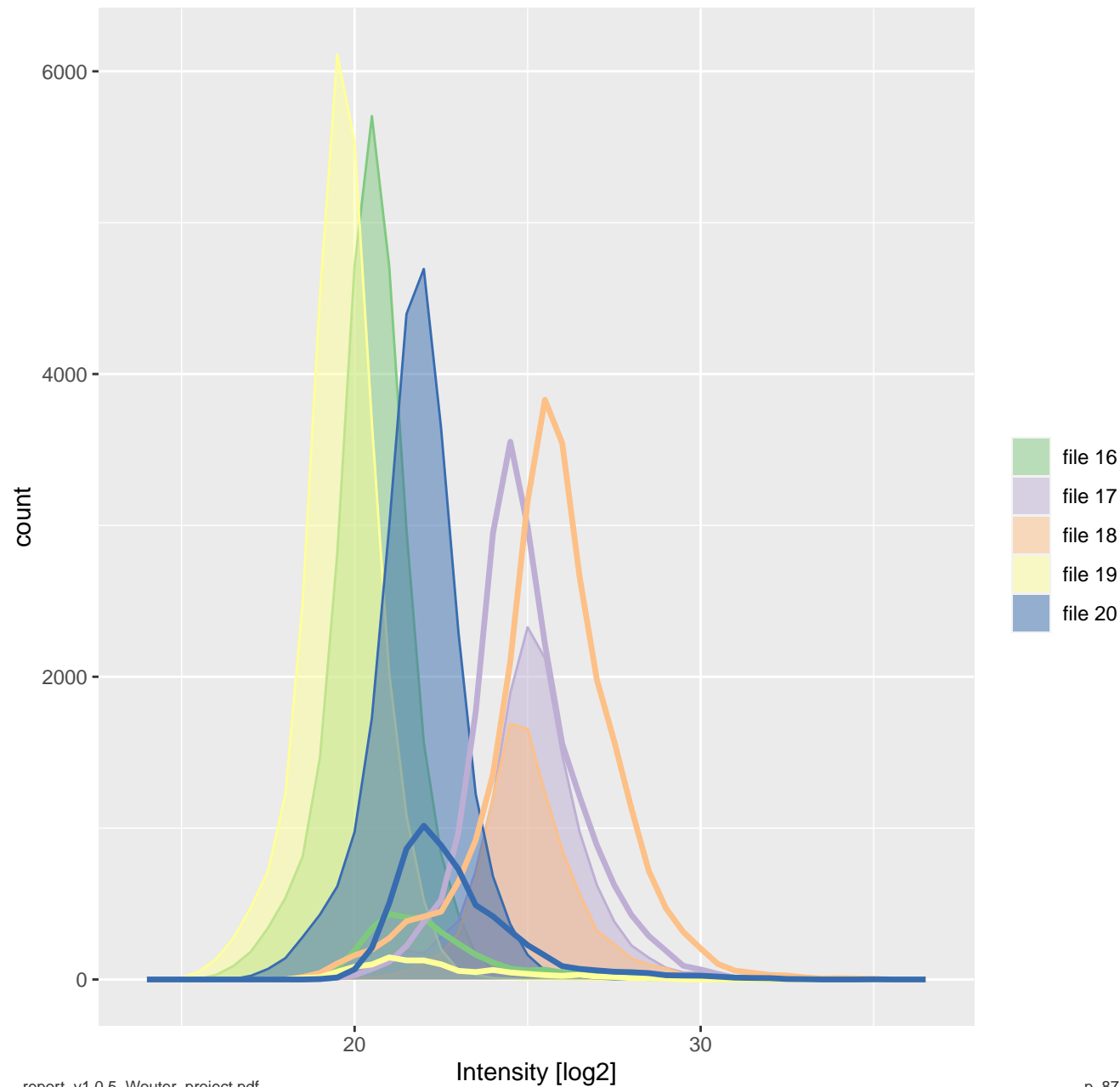


# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values

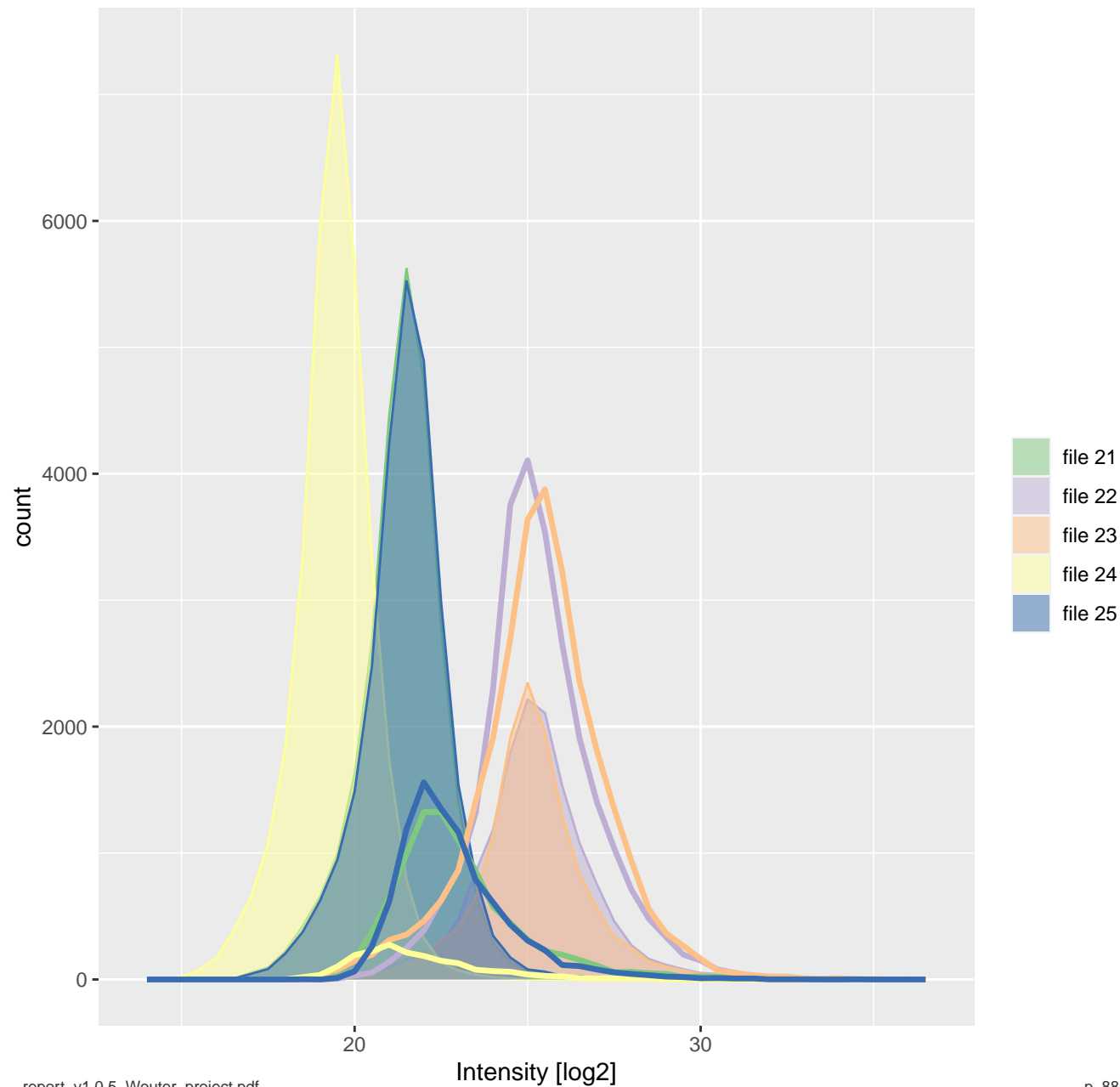




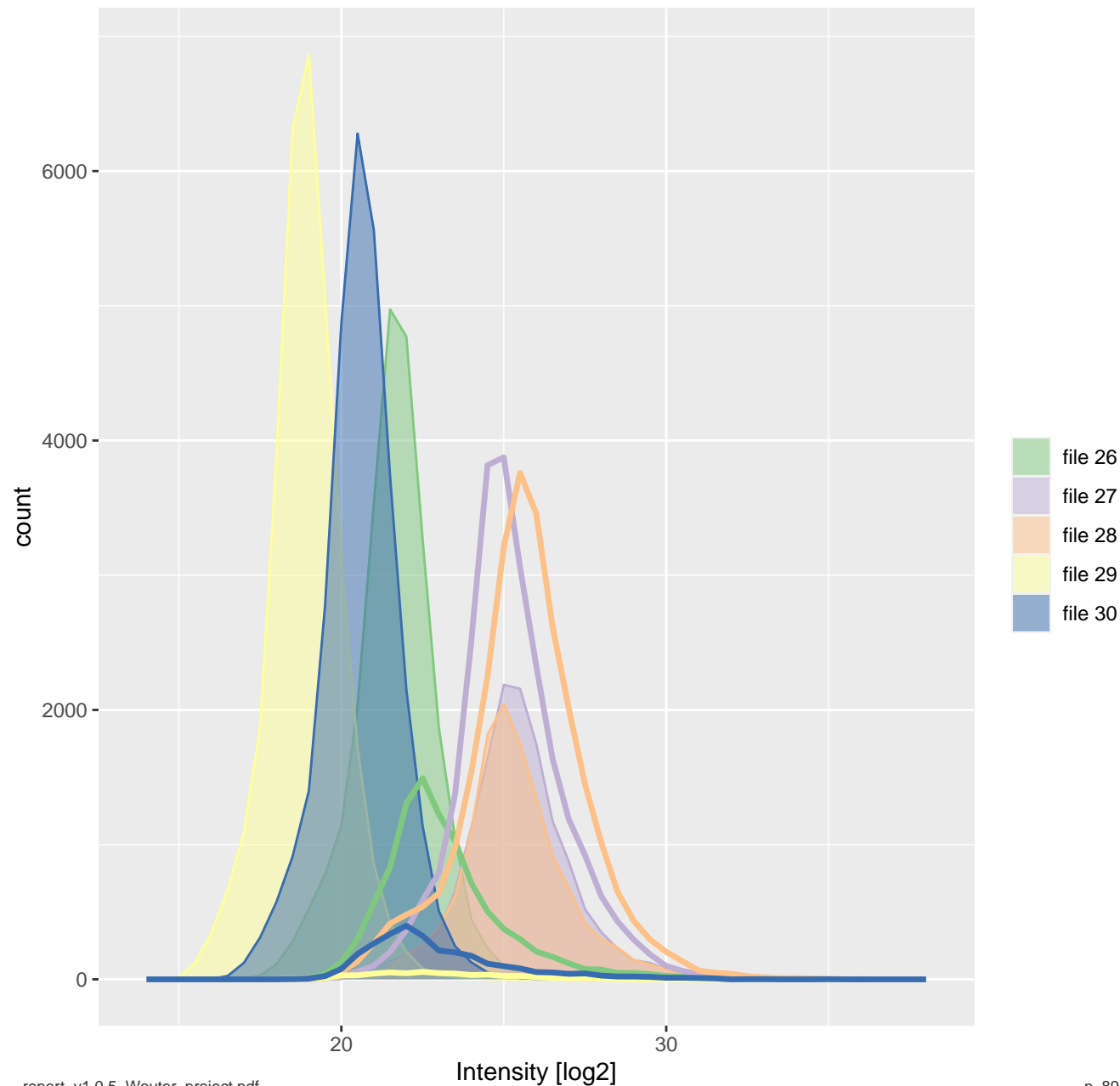
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



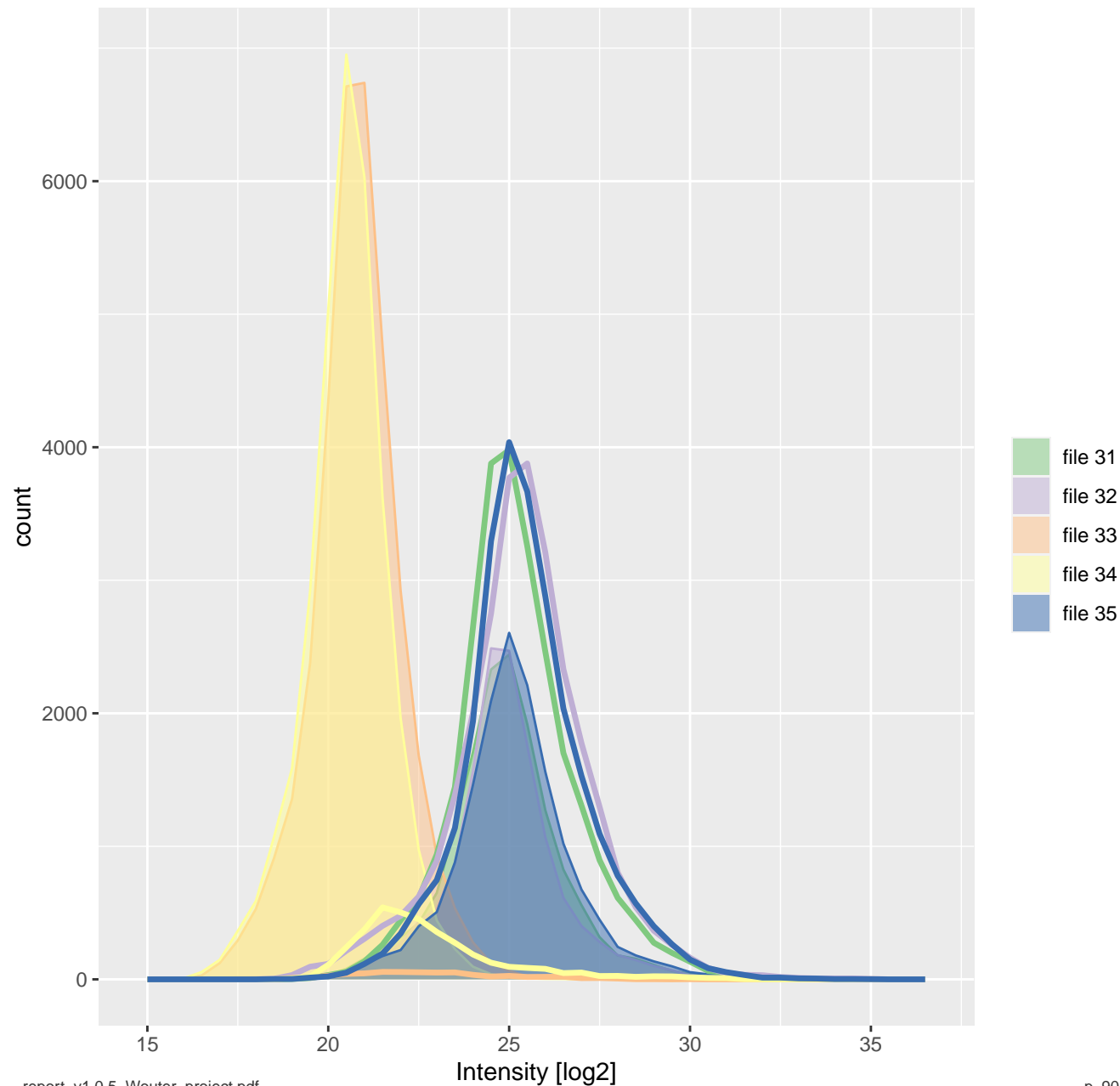
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



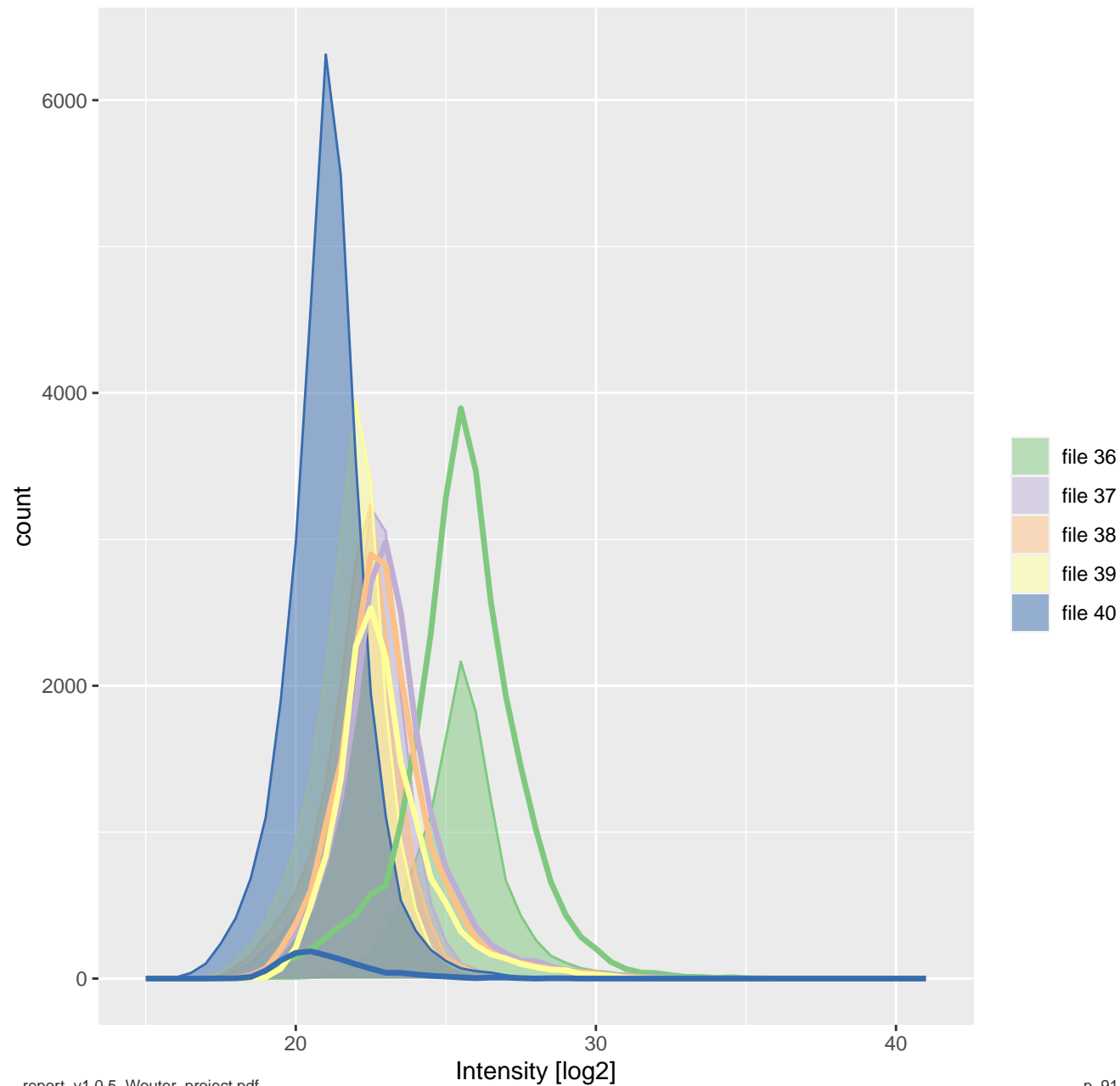
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



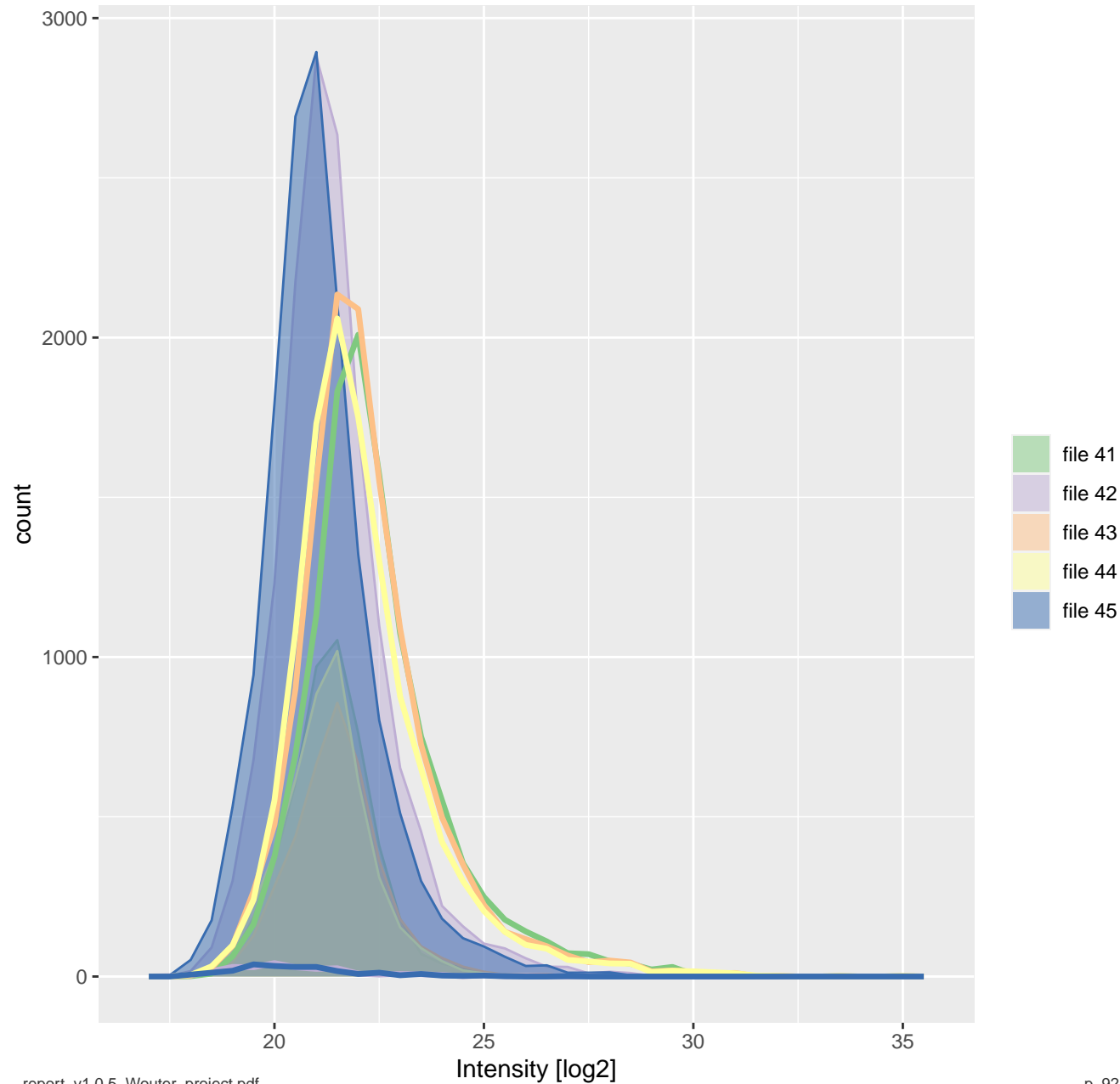
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



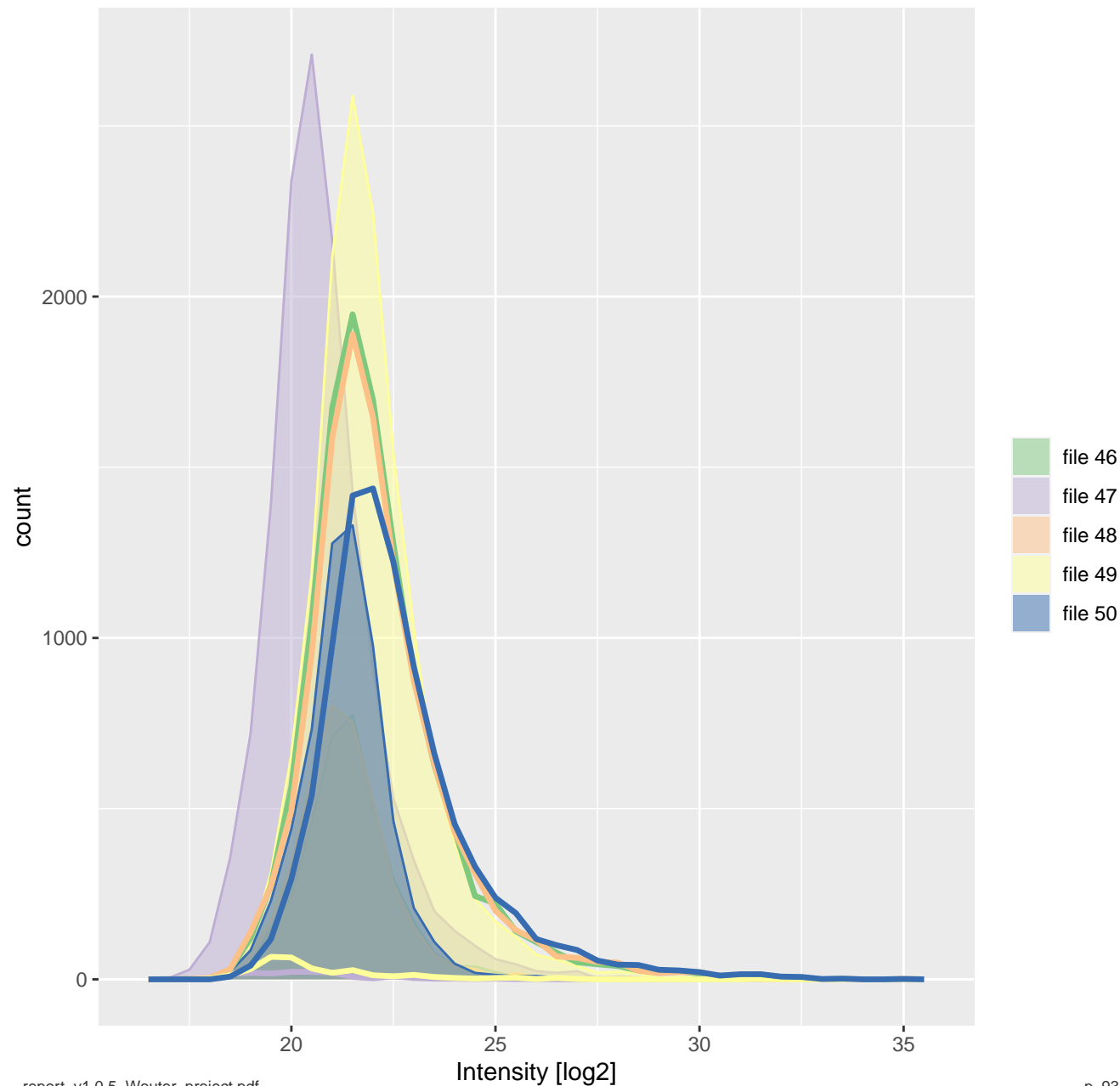
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



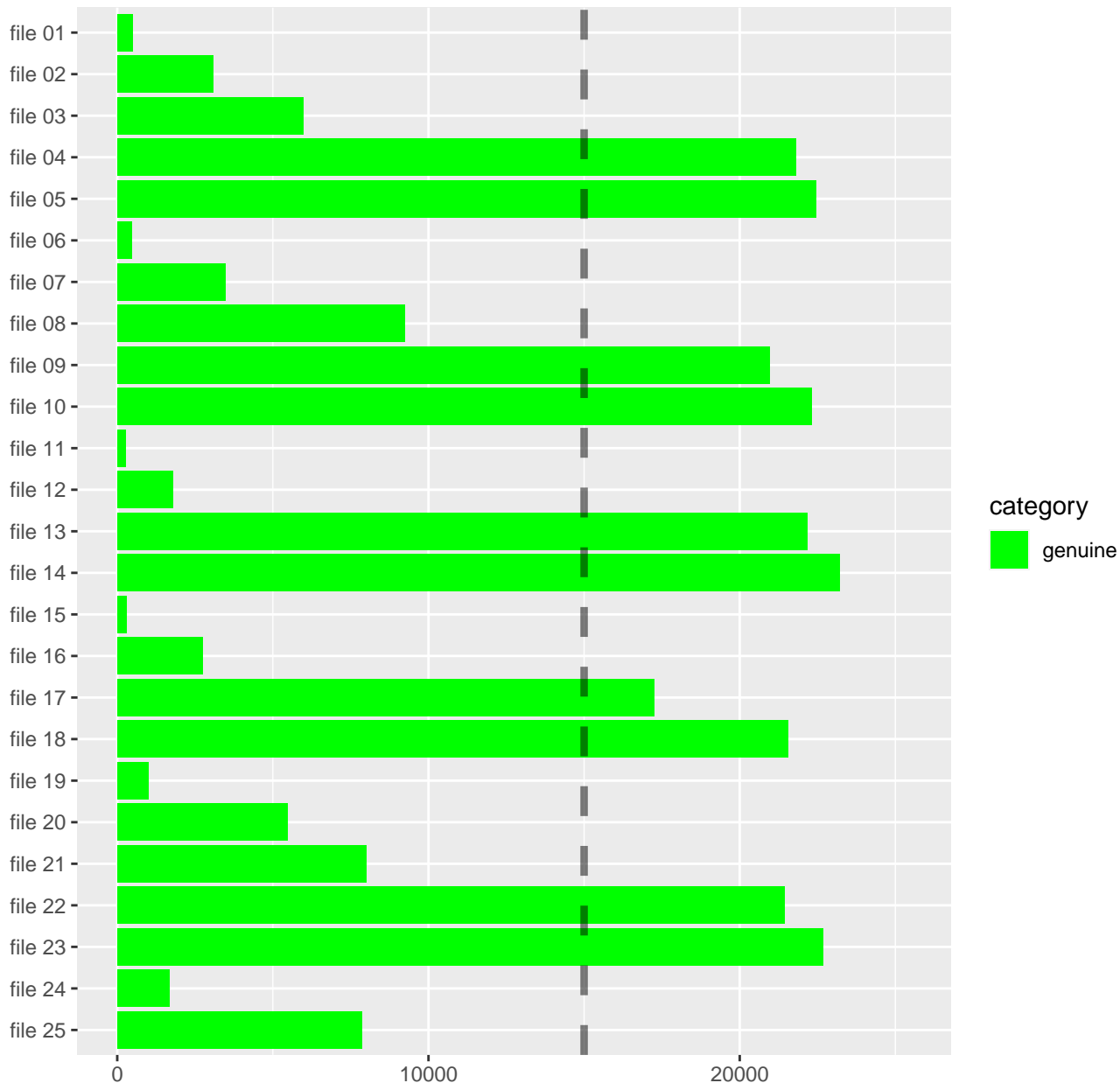
# [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



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

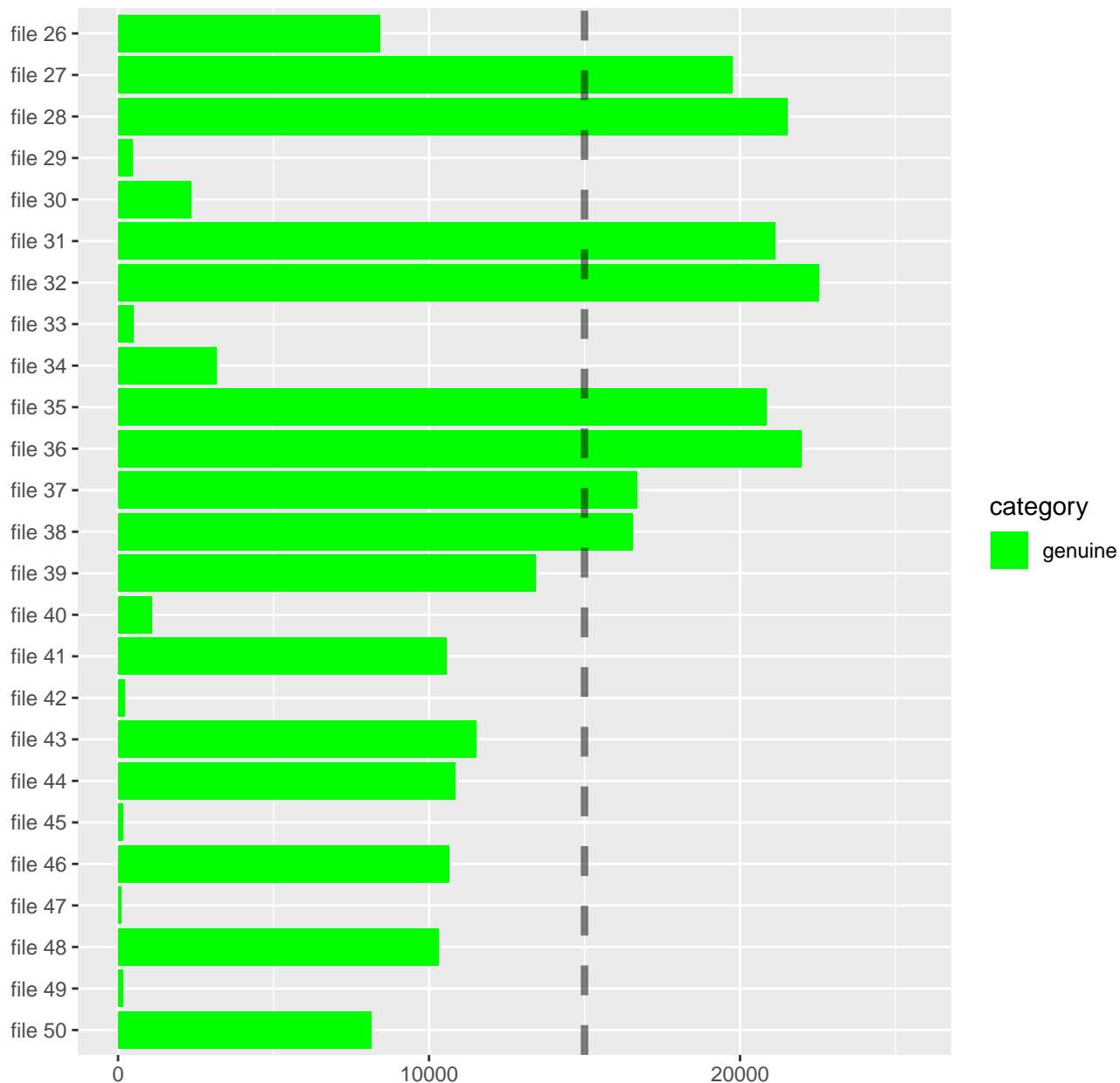


## EVD: Peptide ID count

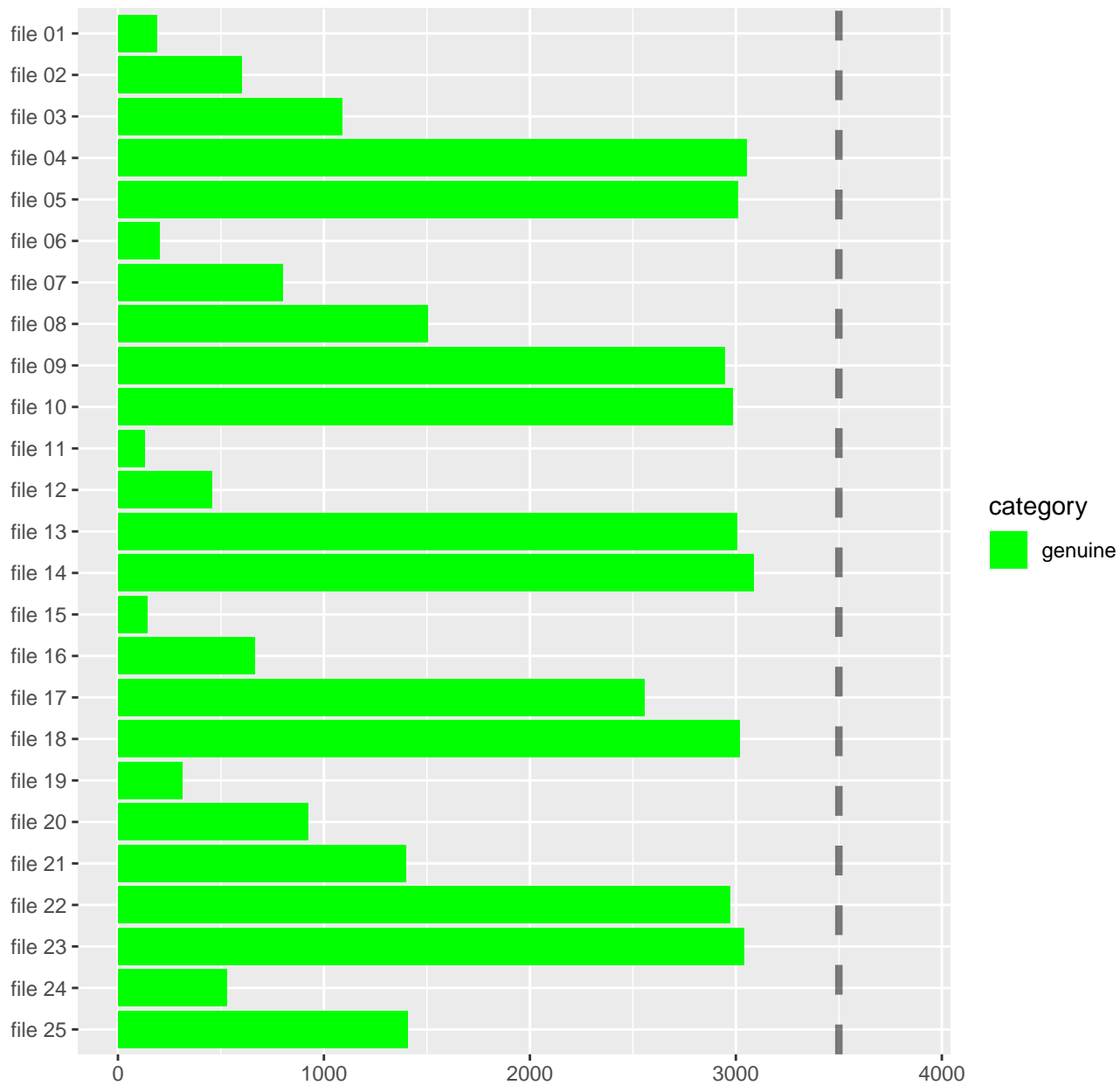




## EVD: Peptide ID count



## EVD: ProteinGroups count



## EVD: ProteinGroups count

