

PAR: parameters

Version	1.5.1.2	Min. score for unmodified pe..	0
User name	cbielow	Min. score for modified pept..	40
Machine name	KEMPA31	Min. delta score for unmodif..	0
Date of writing	12/02/2014 18:00:57	Min. delta score for modifie..	6
Fixed modifications	Carbamidomethyl (C)	Min. unique peptides	0
Decoy mode	revert	Min. razor peptides	1
Special AAs	KR	Min. peptides	1
Include contaminants	True	Use only unmodified peptides..	True
MS/MS tol. (FTMS)	20 ppm	Modifications included in pr..	Acetyl (Protein N-term) Oxidation (M)
Top MS/MS peaks per 100 Da. ..	12	Peptides used for protein qu..	Razor
MS/MS deisotoping (FTMS)	True	Discard unmodified counterpa..	True
MS/MS tol. (ITMS)	0.5 Da	Min. ratio count	2
Top MS/MS peaks per 100 Da. ..	8	Re-quantify	False
MS/MS deisotoping (ITMS)	False	Use delta score	False
MS/MS tol. (TOF)	40 ppm	iBAQ	False
Top MS/MS peaks per 100 Da. ..	10	iBAQ log fit	False
MS/MS deisotoping (TOF)	True	Match between runs	True
MS/MS tol. (Unknown)	0.5 Da	Matching time window [min]	0.7
Top MS/MS peaks per 100 Da. ..	8	Alignment time window [min]	20
MS/MS deisotoping (Unknown)	False	Find dependent peptides	False
PSM FDR	0.01	Labeled amino acid filtering	True
Protein FDR	0.01	Site tables	Oxidation (M)Sites.txt
Site FDR	0.01	RT shift	False
Use Normalized Ratios For Oc..	True	Advanced ratios	True
Min. peptide Length	7	First pass AIF correlation	0.8

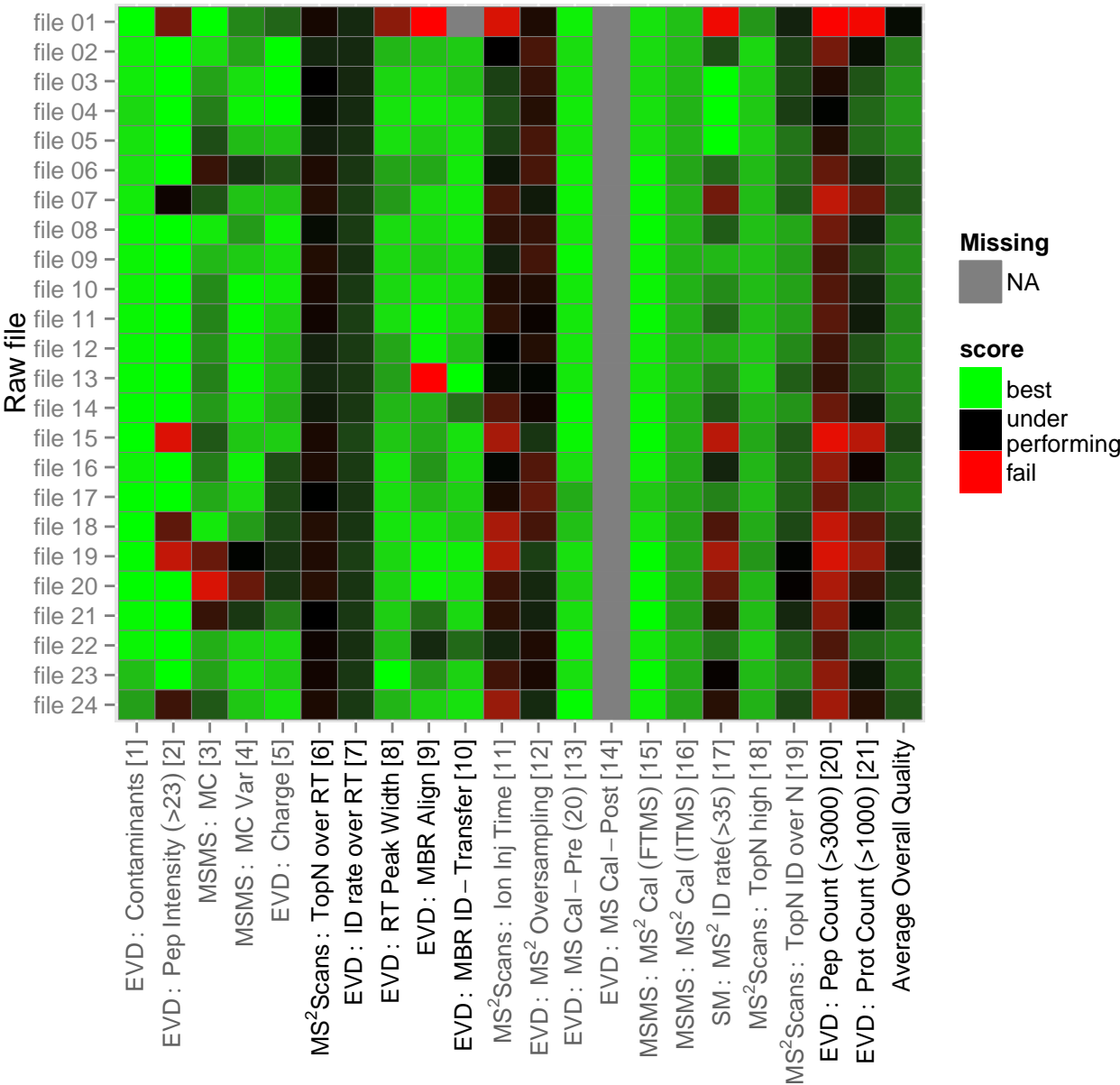
uniprot_human_canonical_and_isoforms_20130513.fasta

Mapping of Raw files to their short names

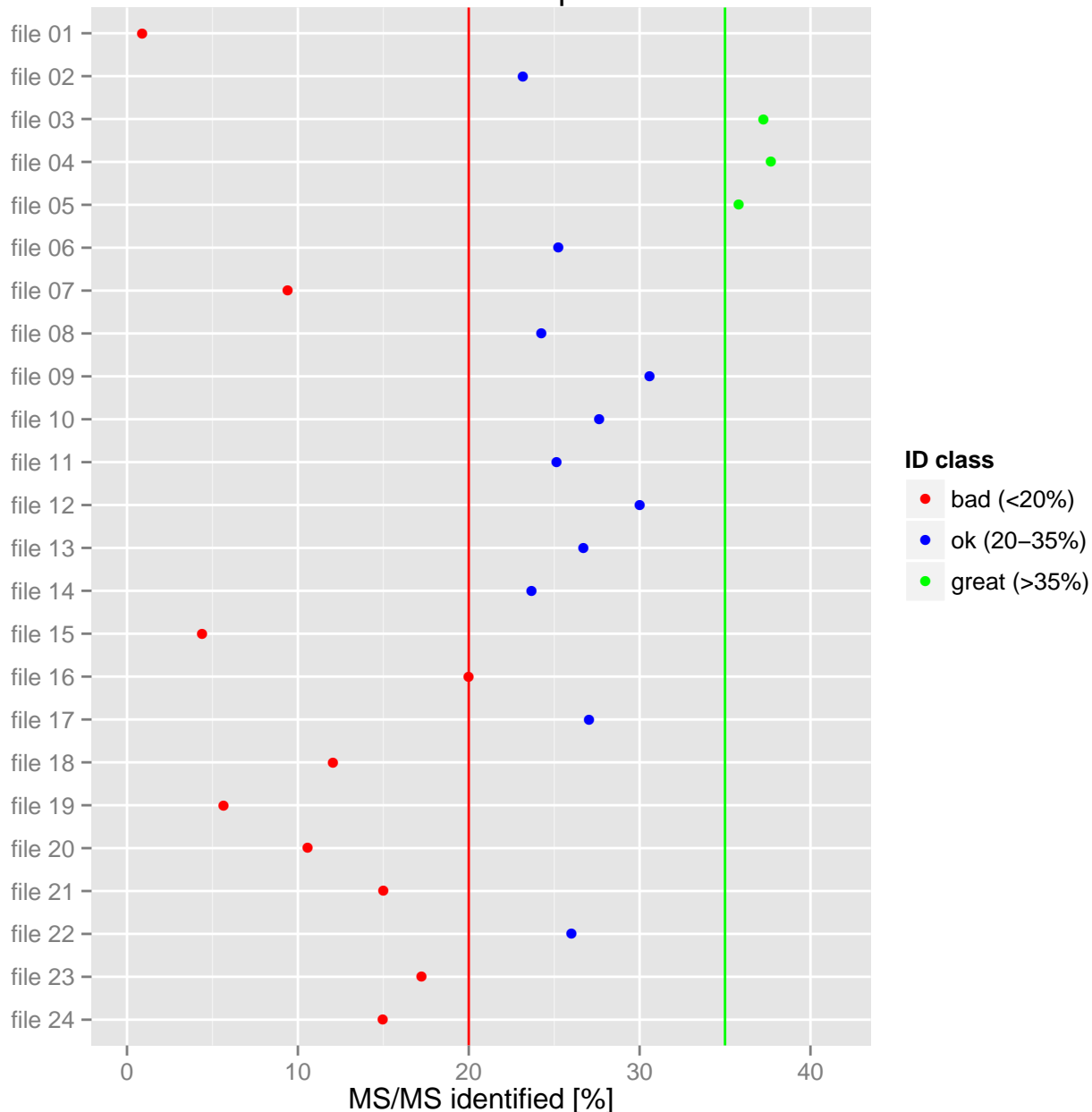
Mapping source: file (user-defined)

original	short name
2011_05_30_ALH_OT_21_VIL_TMT_FR01	file 01
2011_05_30_ALH_OT_22_VIL_TMT_FR02	file 02
2011_05_30_ALH_OT_23_VIL_TMT_FR03	file 03
2011_05_30_ALH_OT_24_VIL_TMT_FR04	file 04
2011_05_30_ALH_OT_25_VIL_TMT_FR05	file 05
2011_05_30_ALH_OT_26_VIL_TMT_FR06	file 06
2011_05_30_ALH_OT_28_VIL_TMT_FR07	file 07
2011_05_30_ALH_OT_29_VIL_TMT_FR08	file 08
2011_05_30_ALH_OT_30_VIL_TMT_FR09	file 09
2011_05_30_ALH_OT_31_VIL_TMT_FR10	file 10
2011_05_30_ALH_OT_32_VIL_TMT_FR11	file 11
2011_05_30_ALH_OT_33_VIL_TMT_FR12	file 12
2011_05_30_ALH_OT_35_VIL_TMT_FR13	file 13
2011_05_30_ALH_OT_36_VIL_TMT_FR14	file 14
2011_05_30_ALH_OT_37_VIL_TMT_FR15	file 15
2011_05_30_ALH_OT_38_VIL_TMT_FR16	file 16
2011_05_30_ALH_OT_39_VIL_TMT_FR17	file 17
2011_05_30_ALH_OT_40_VIL_TMT_FR18	file 18
2011_05_30_ALH_OT_42_VIL_TMT_FR19	file 19
2011_05_30_ALH_OT_43_VIL_TMT_FR20	file 20
2011_05_30_ALH_OT_44_VIL_TMT_FR21	file 21
2011_05_30_ALH_OT_45_VIL_TMT_FR22	file 22
2011_05_30_ALH_OT_46_VIL_TMT_FR23	file 23
2011_05_30_ALH_OT_47_VIL_TMT_FR24	file 24

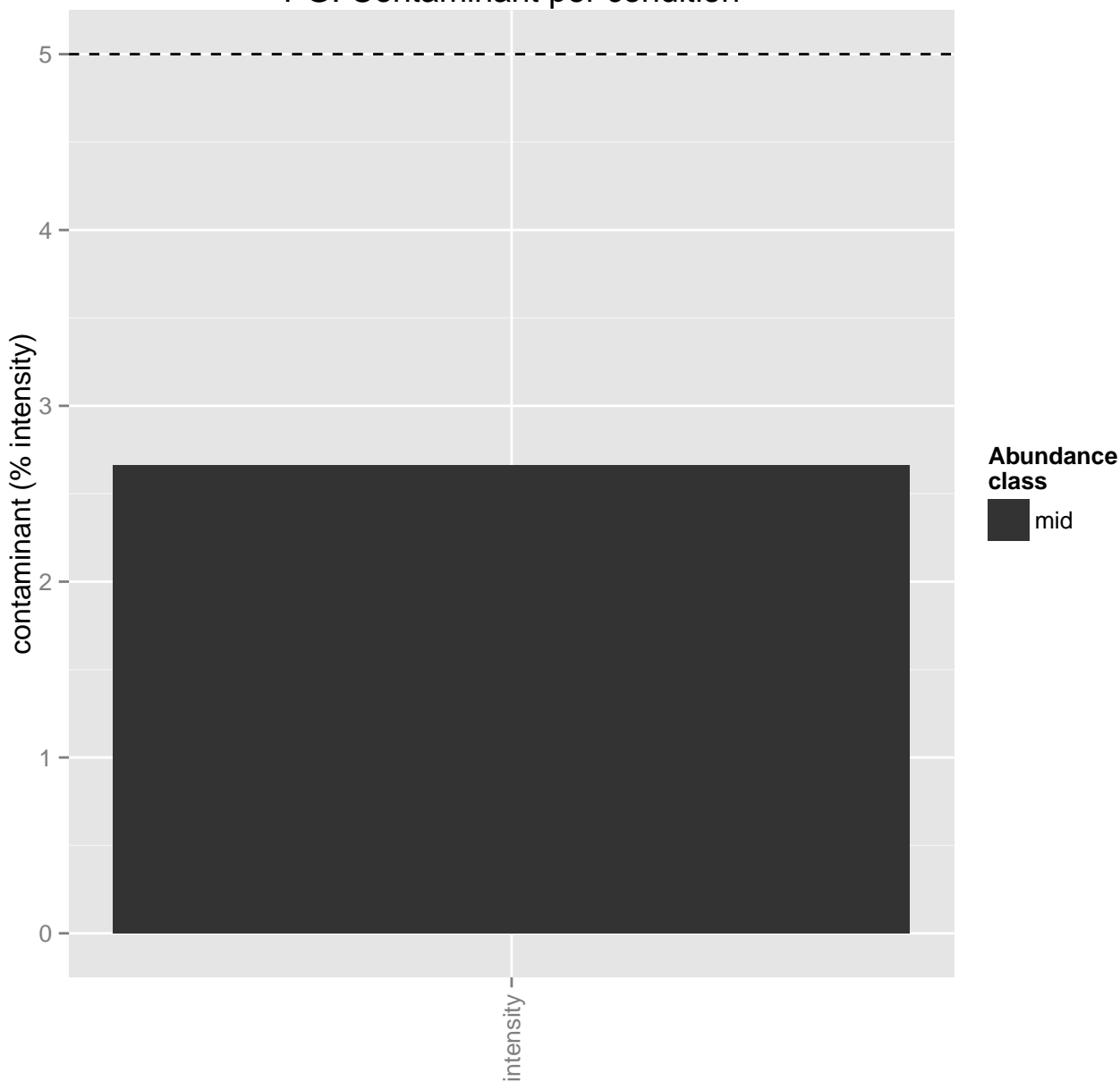
Performance overview



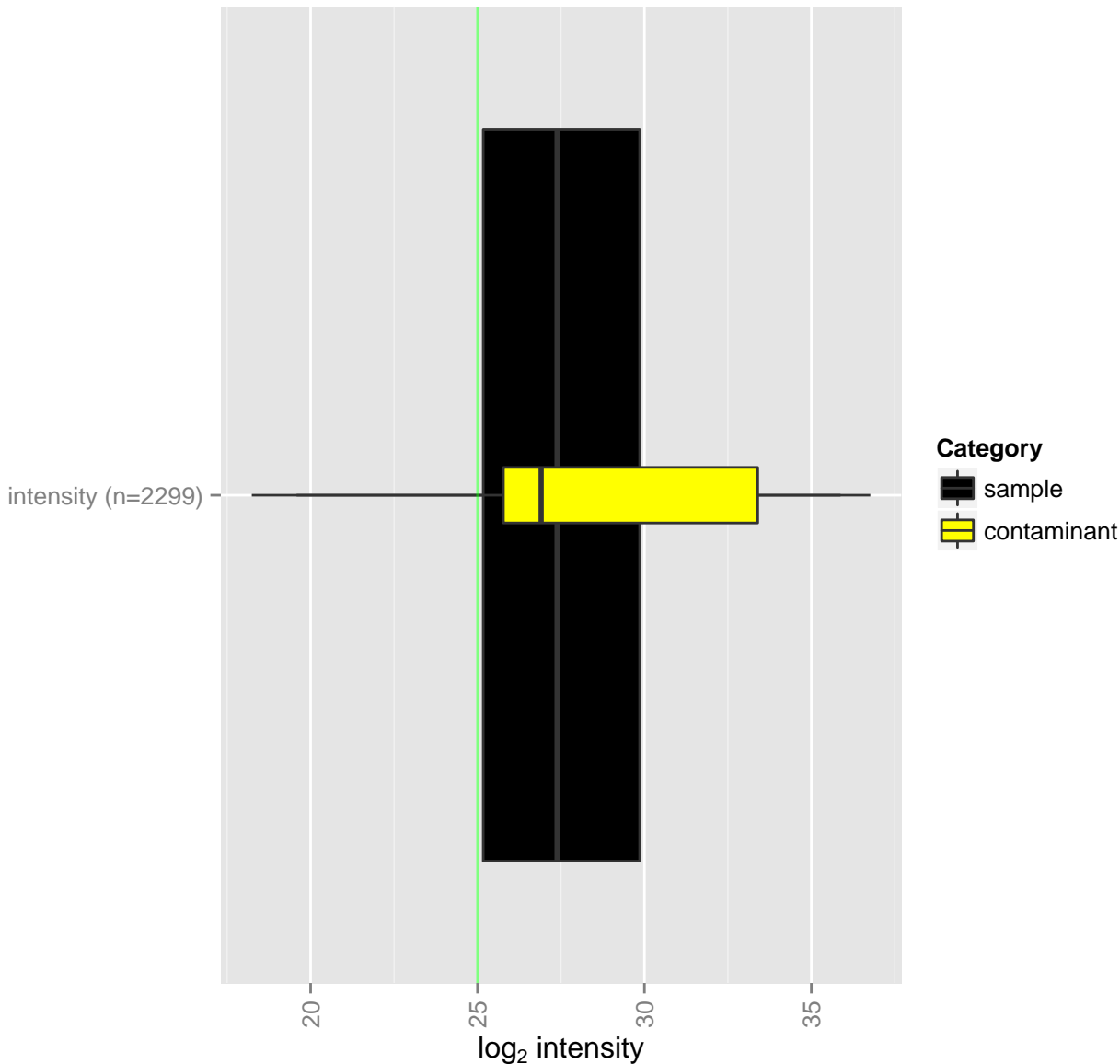
SM: MS/MS identified per Raw file



PG: Contaminant per condition



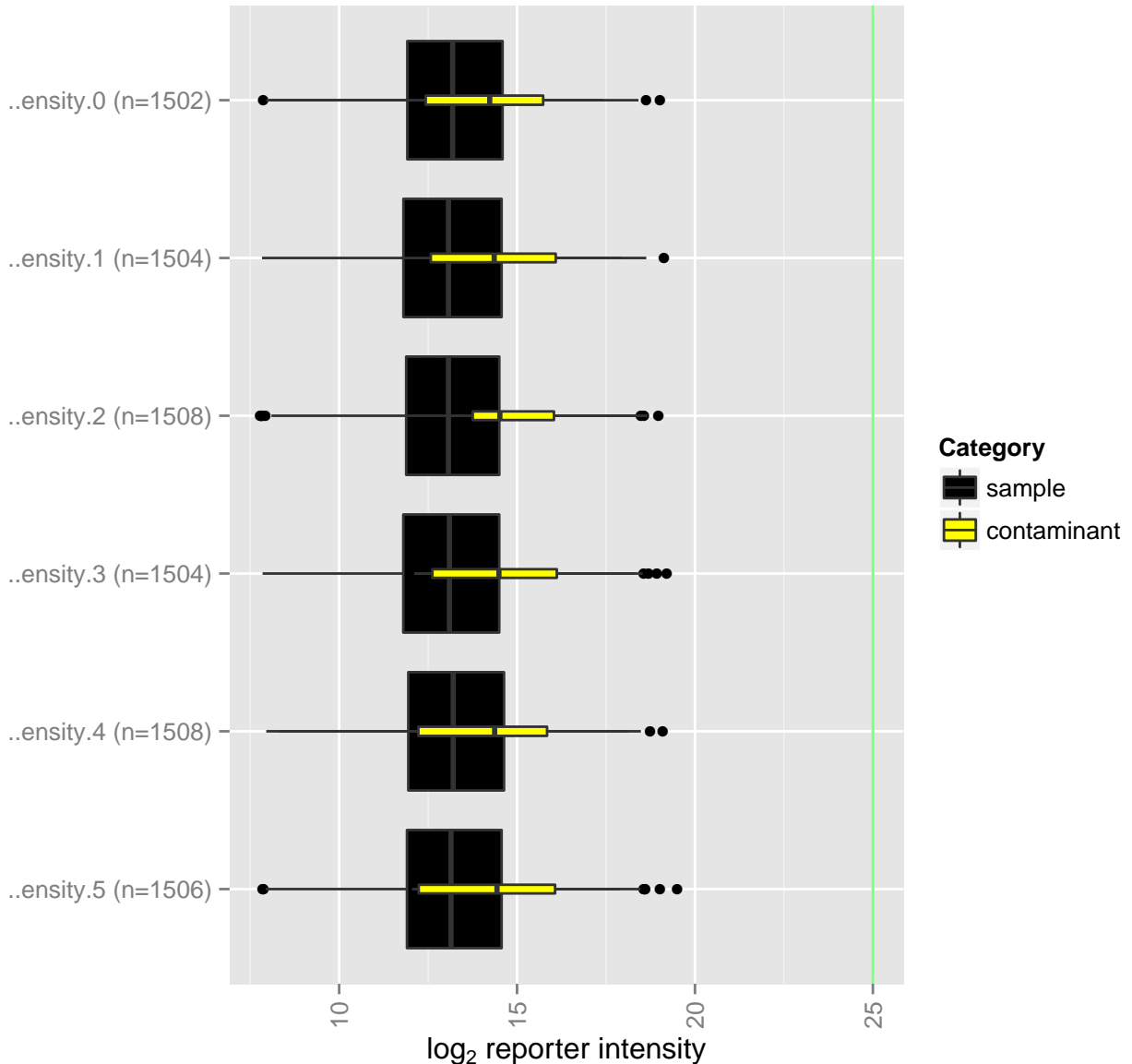
PG: intensity distribution
RSD NA% (w/o zero int.; expected < 5%)
RSD NA% [high RSD --> few peptides]



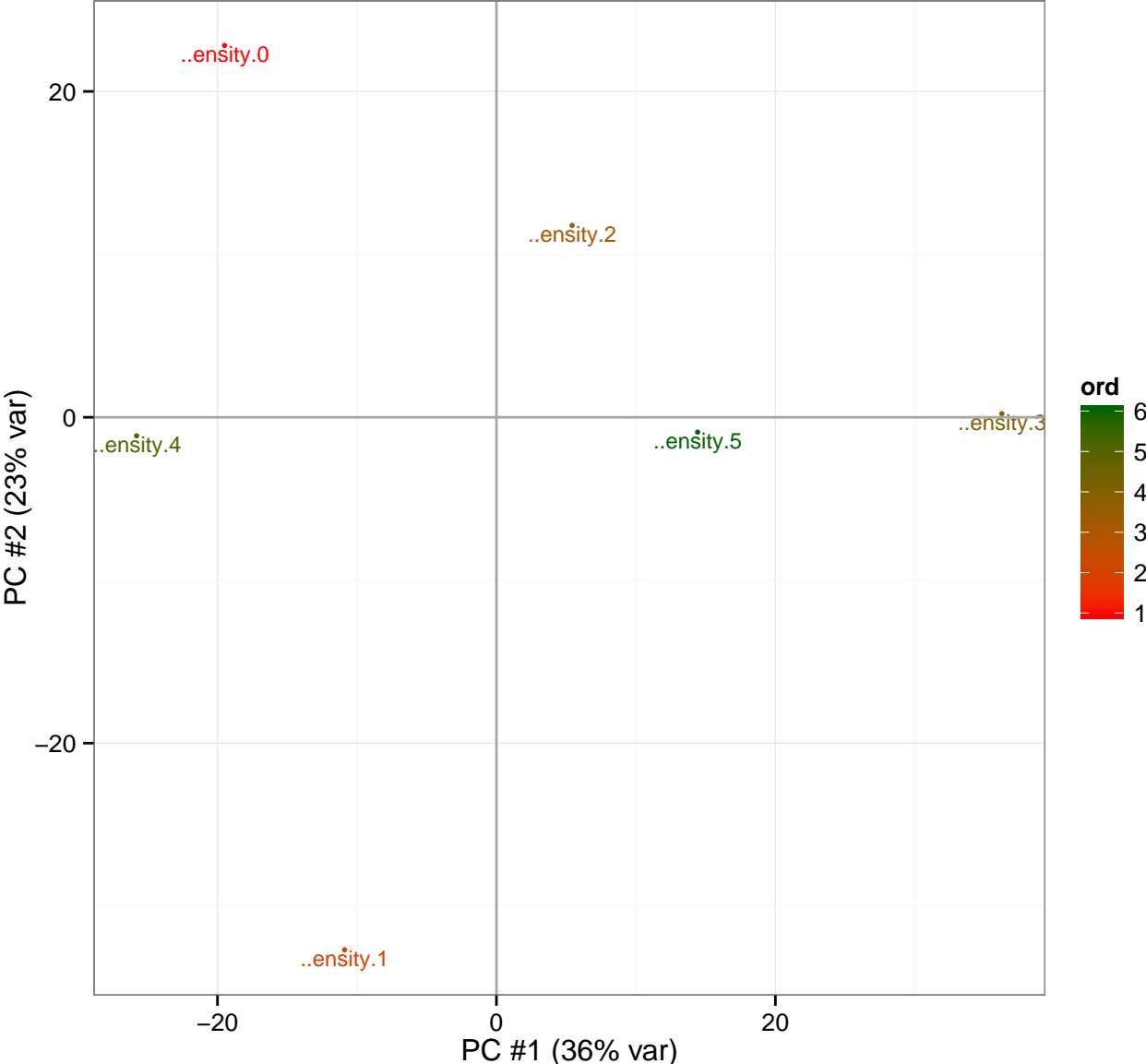
PG: reporter intensity distribution

RSD 0.4% (w/o zero int.; expected < 5%)

RSD 0.3% [high RSD --> few peptides]

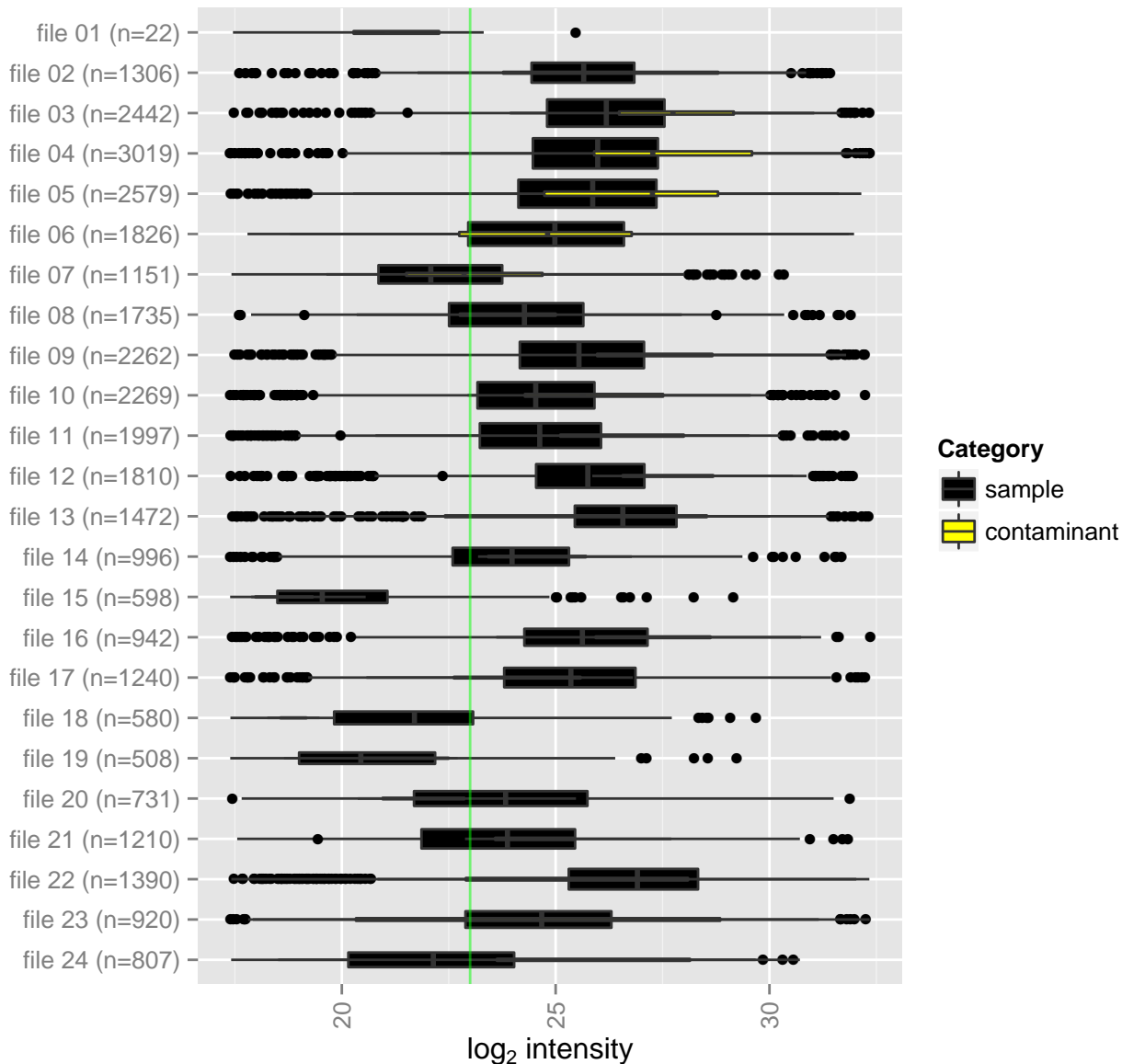


PG: PCA of 'reporter intensity'
(excludes contaminants)



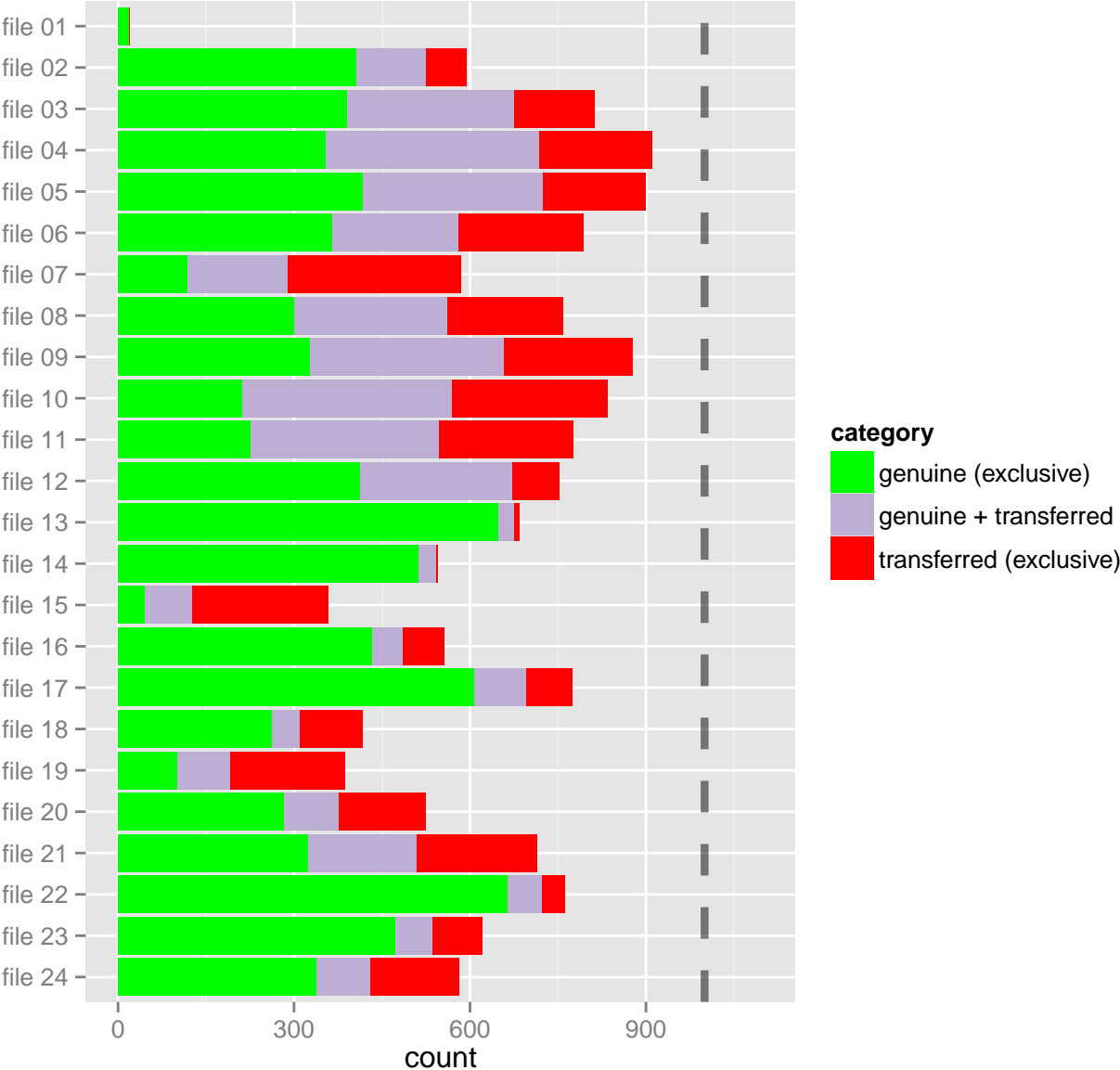
EVD: peptide intensity distribution

RSD 9% (expected < 5%)



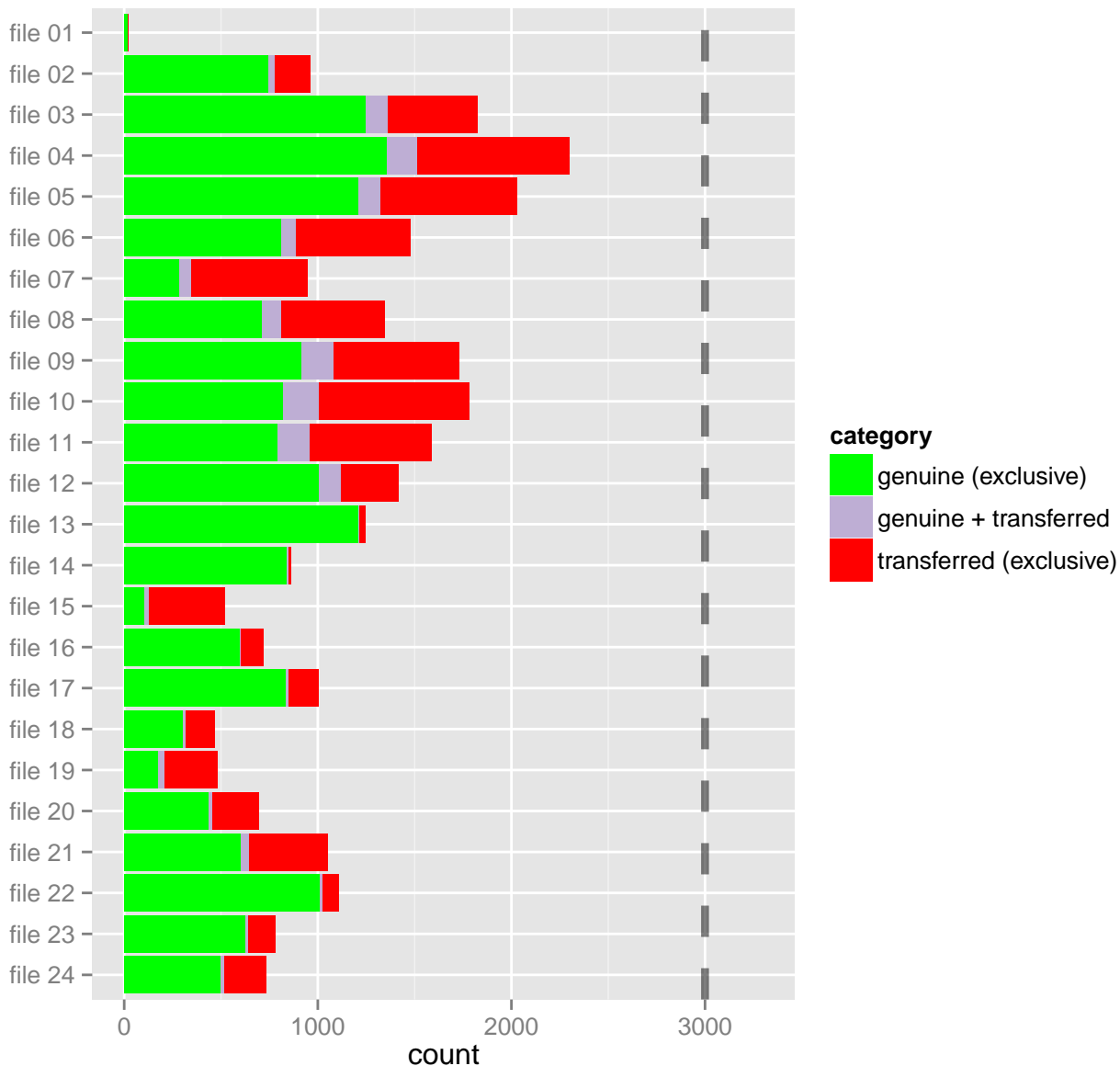
EVD: ProteinGroups count

MBR gain: +36%

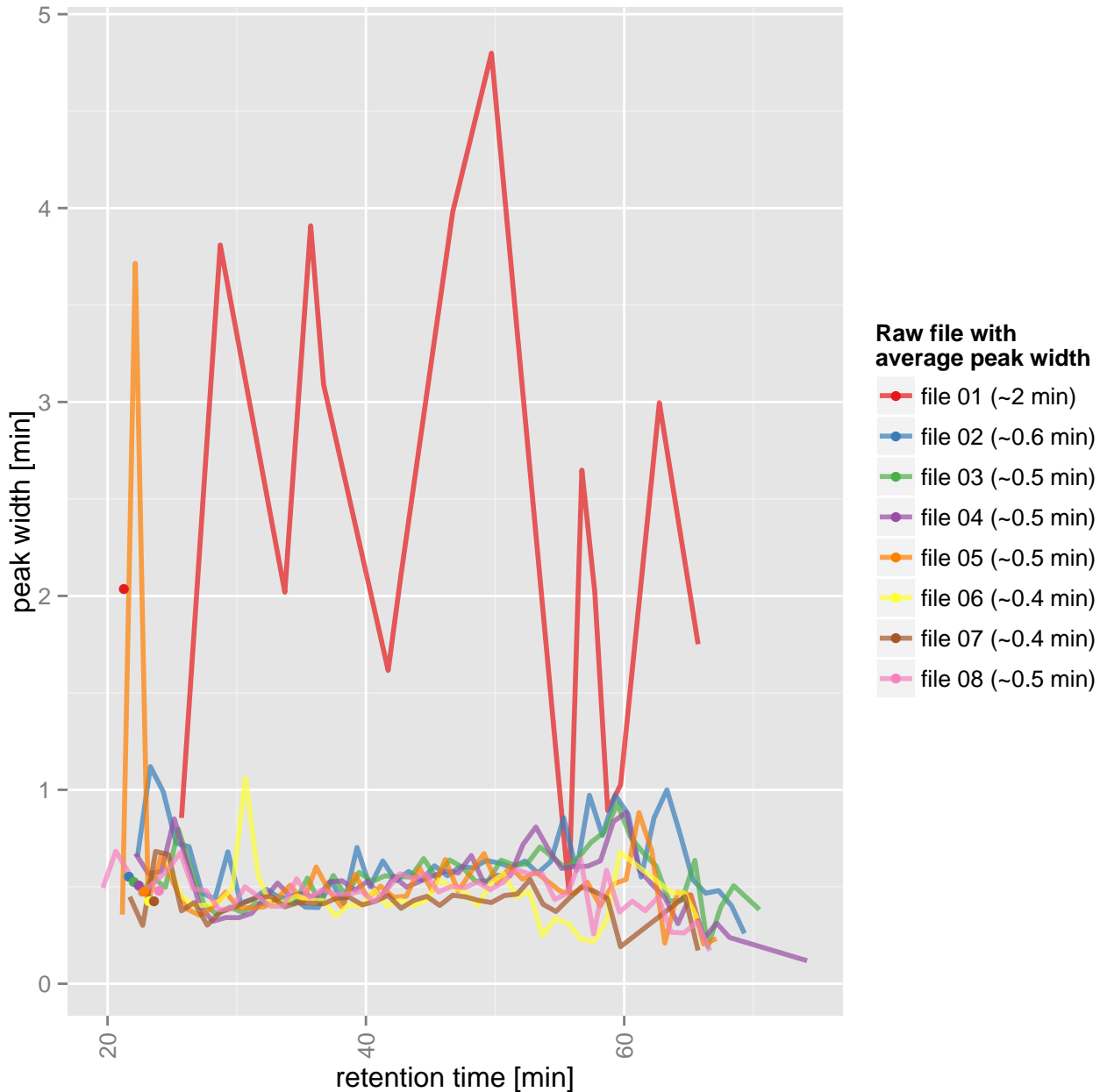


EVD: Peptide ID count

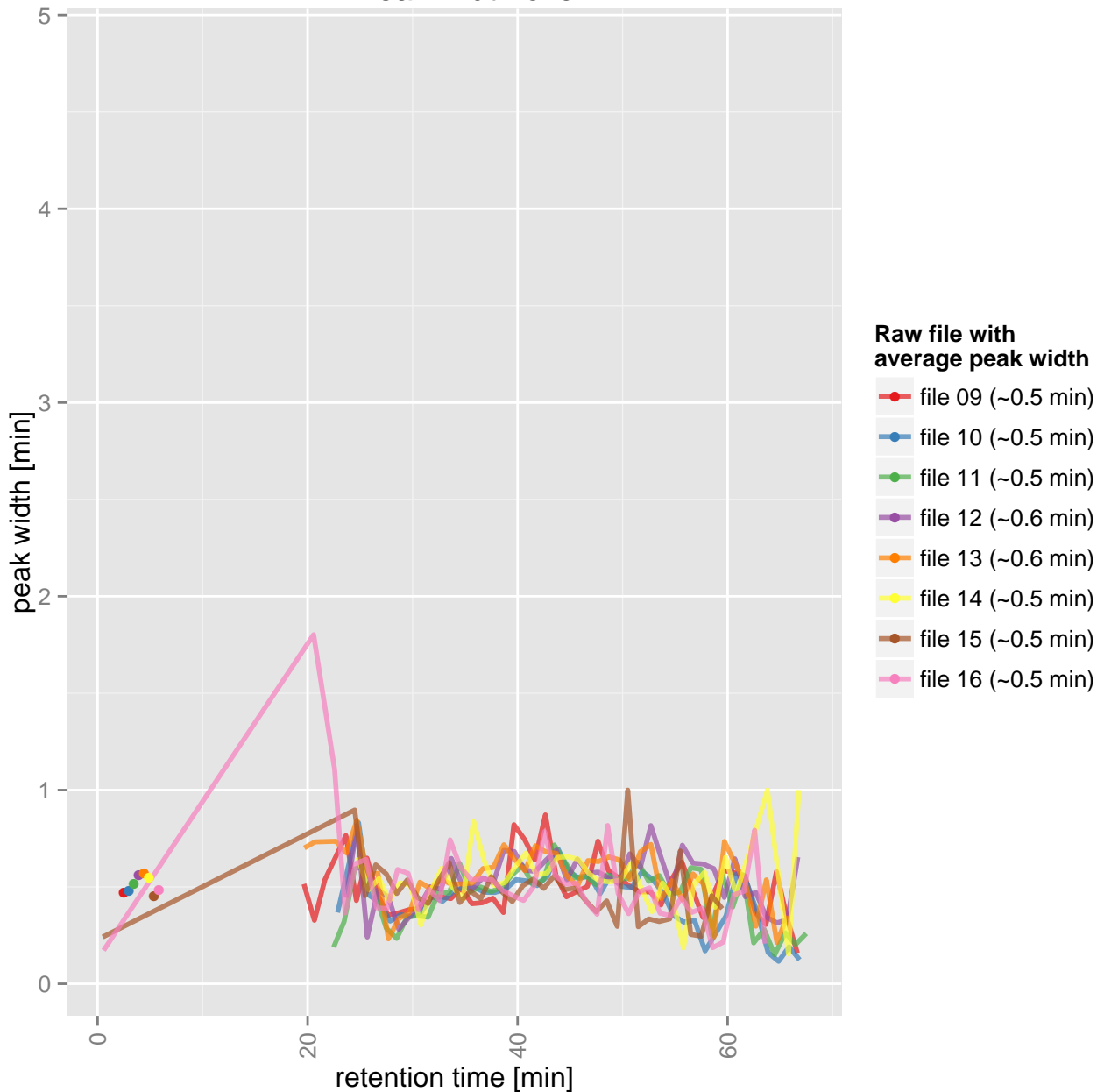
MBR gain: +58%



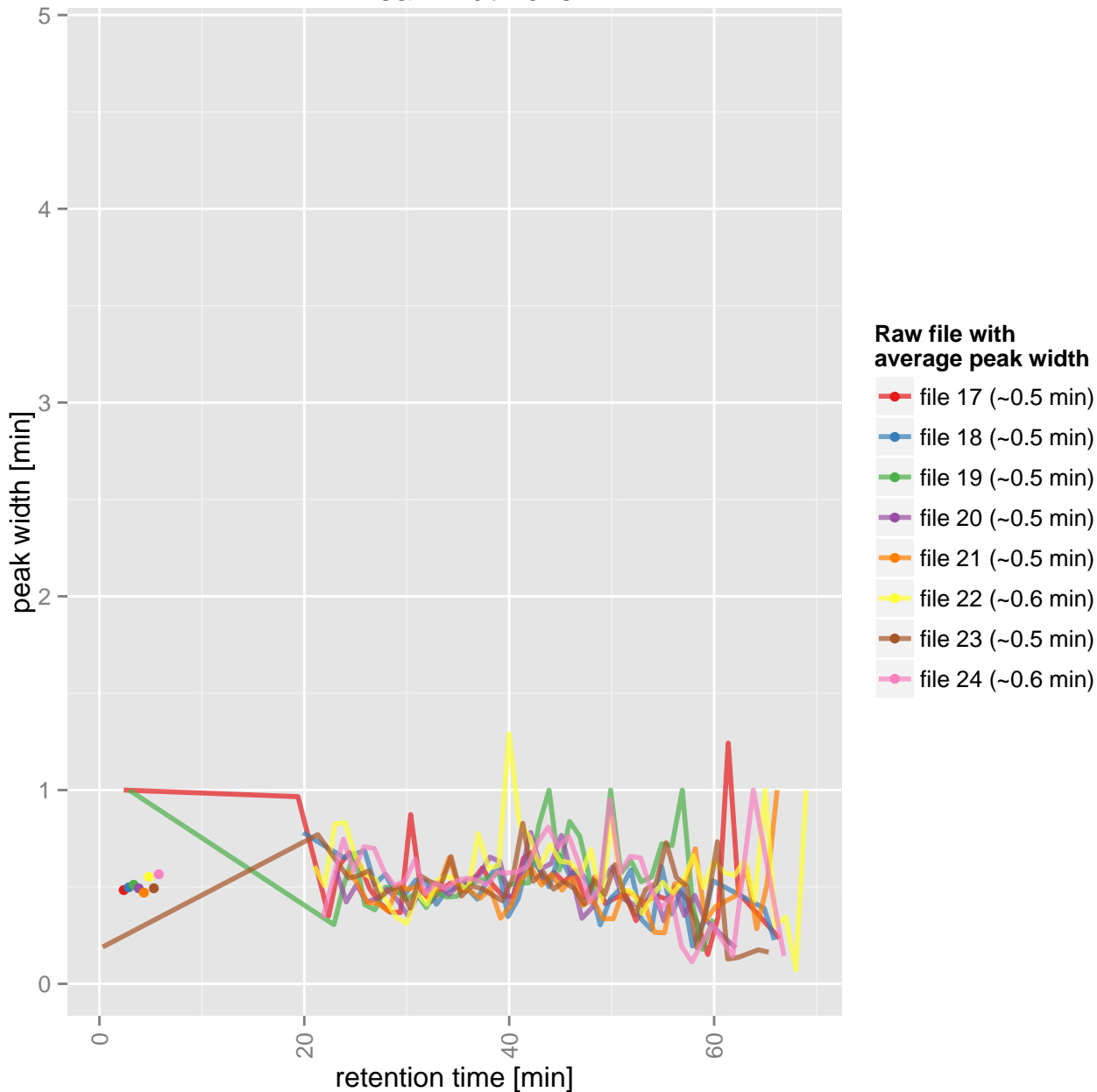
EVD: Peak width over RT



EVD: Peak width over RT

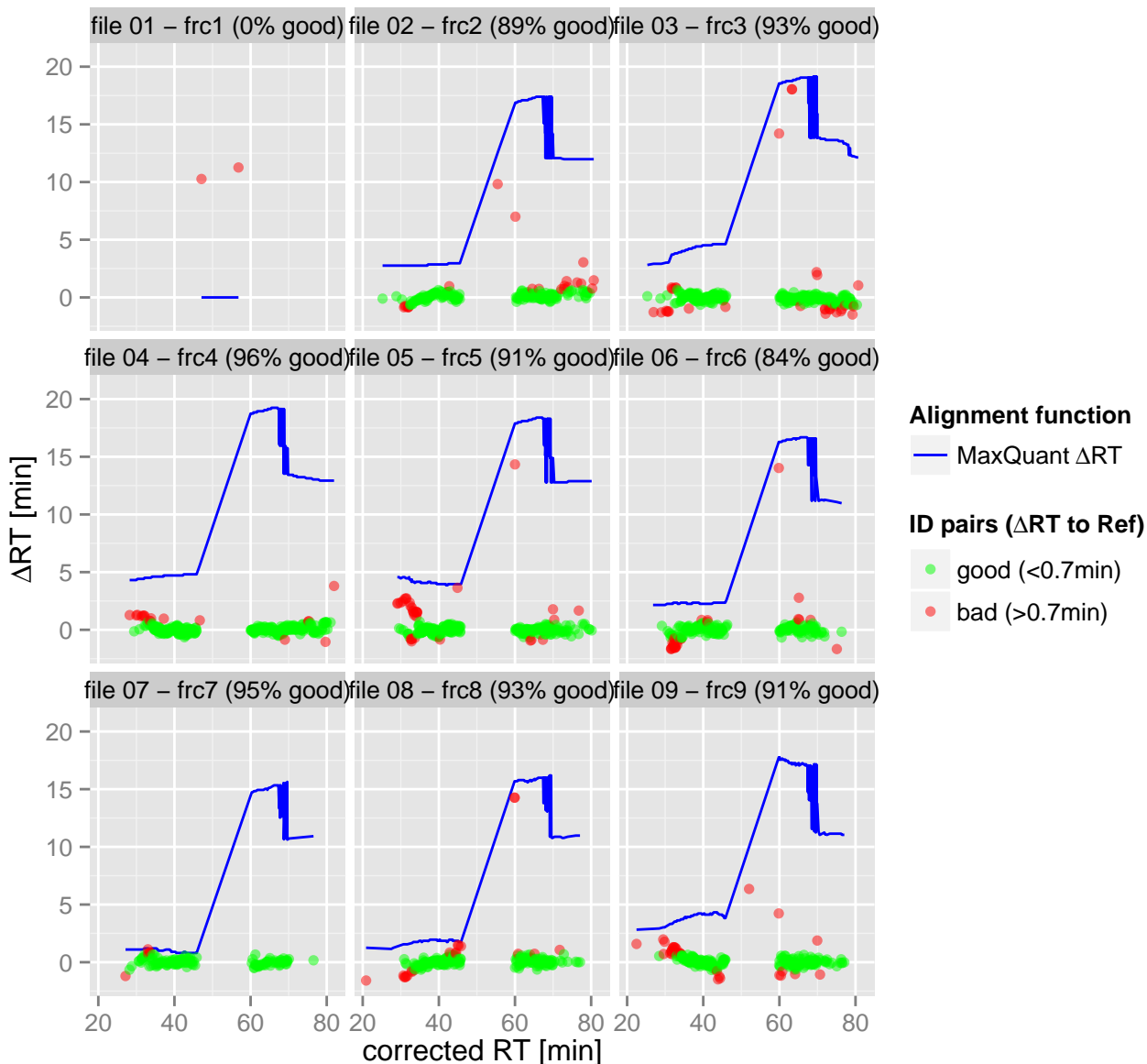


EVD: Peak width over RT



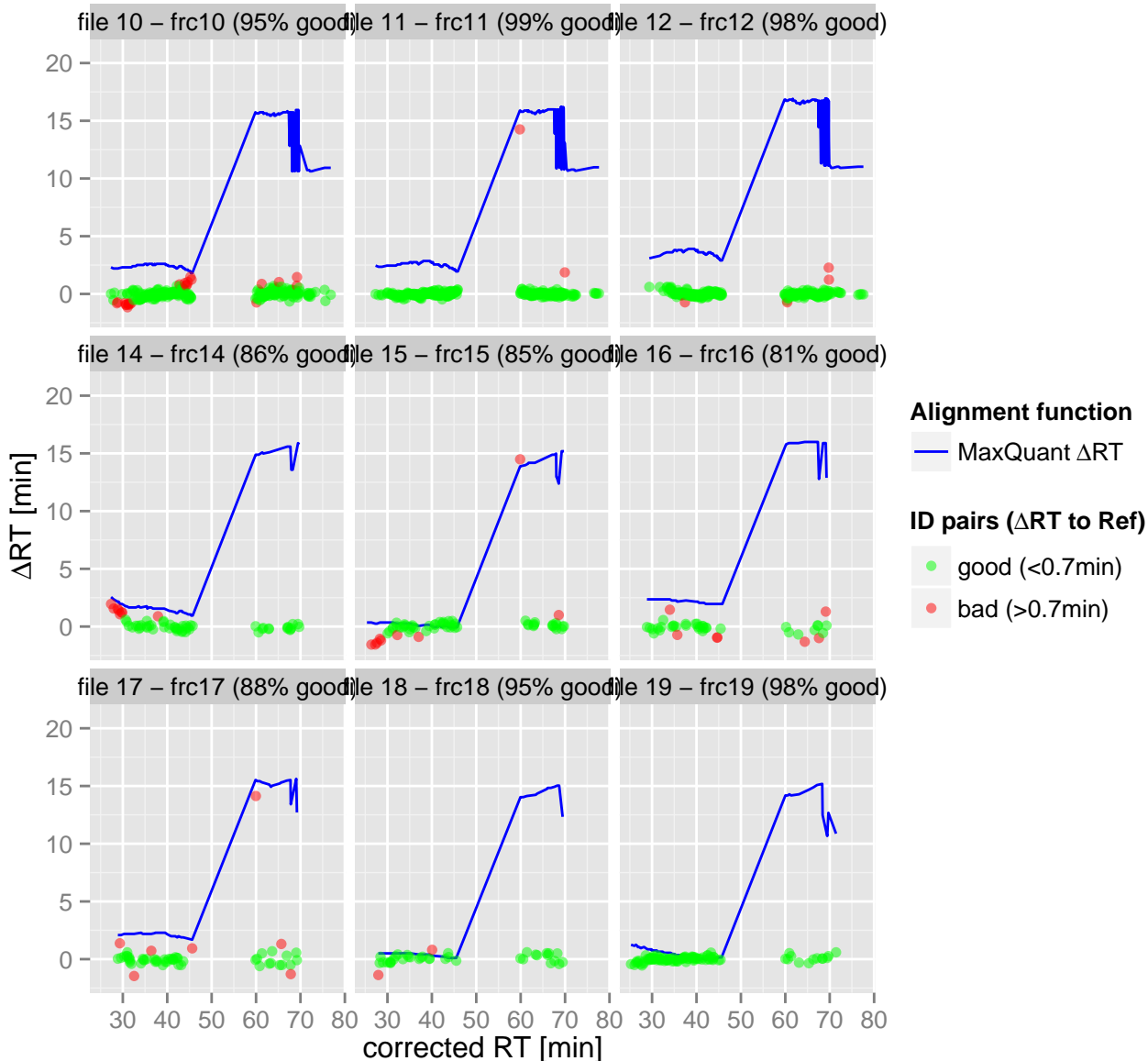
EVD: MBR – alignment

fraction: neighbour comparison



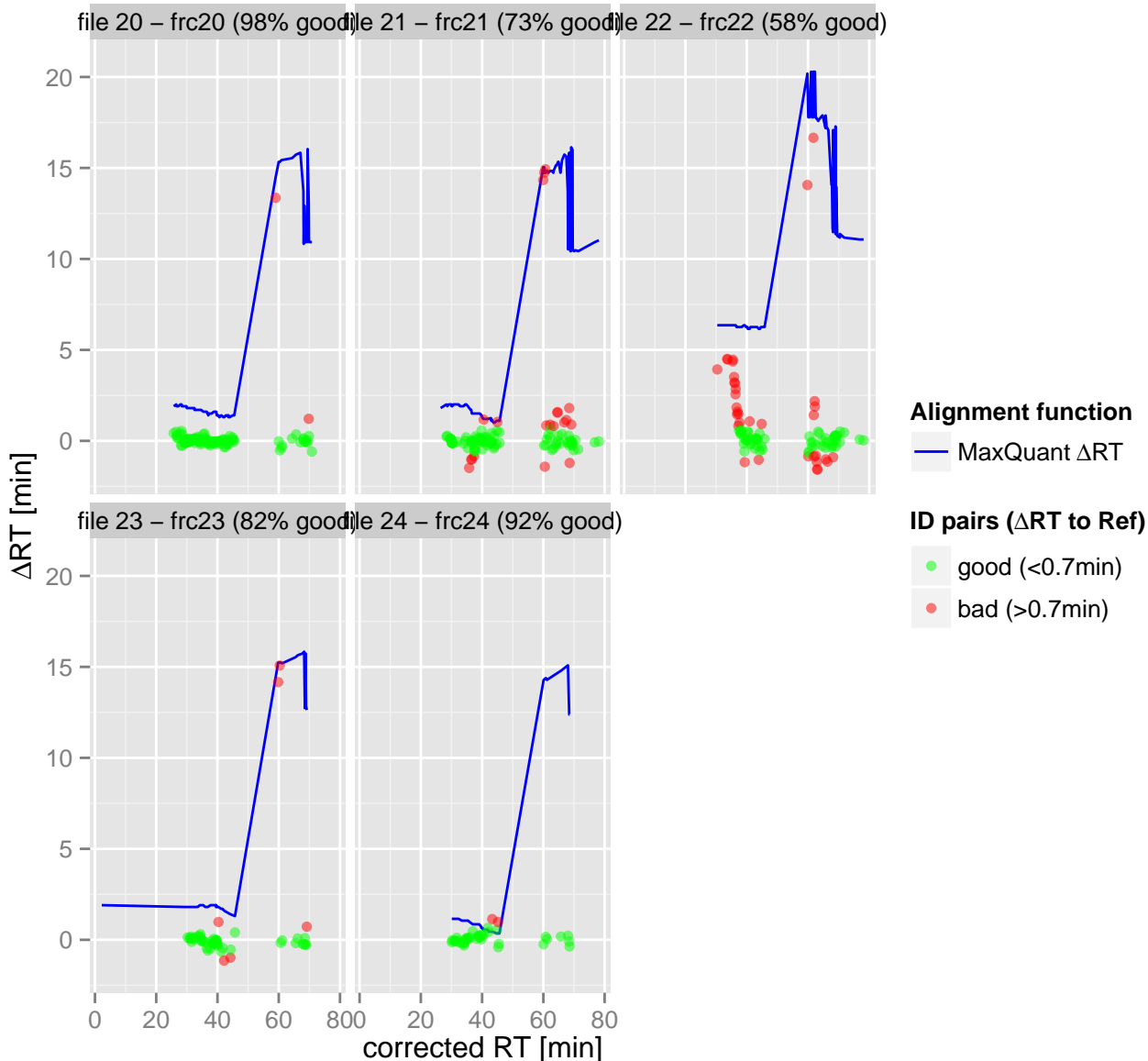
EVD: MBR – alignment

fraction: neighbour comparison

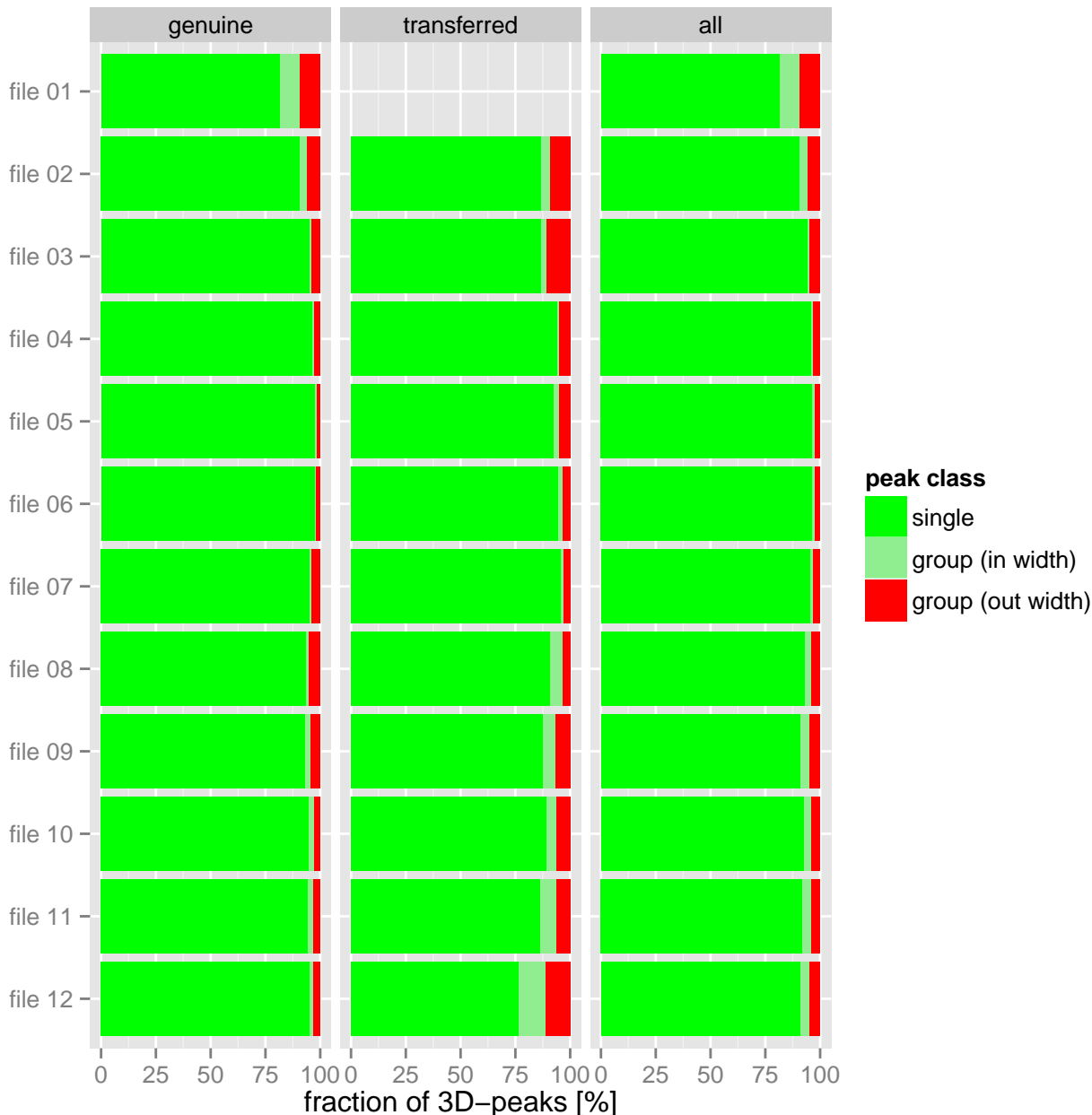


EVD: MBR – alignment

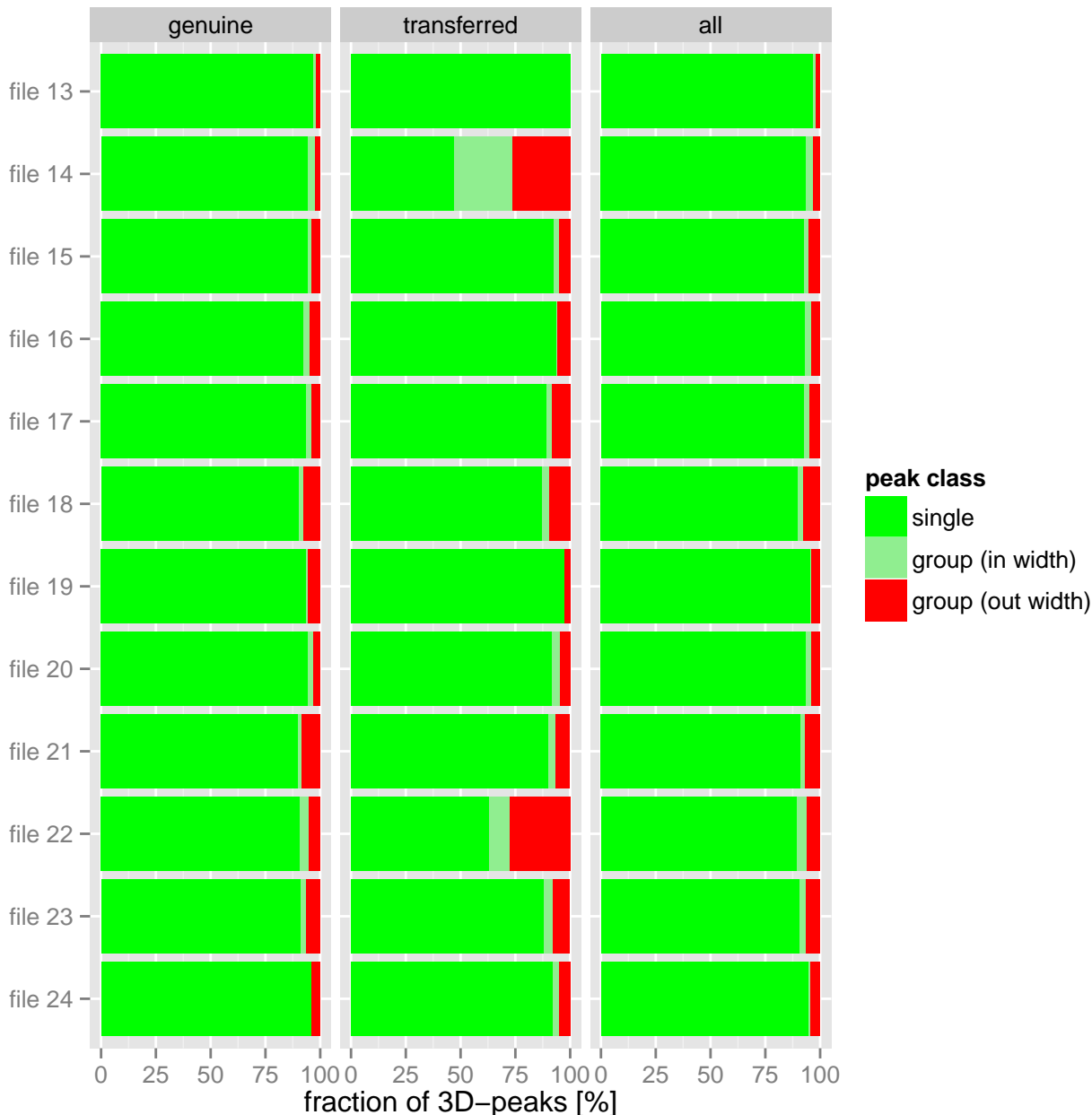
fraction: neighbour comparison



EVD: MBR – ID Transfer

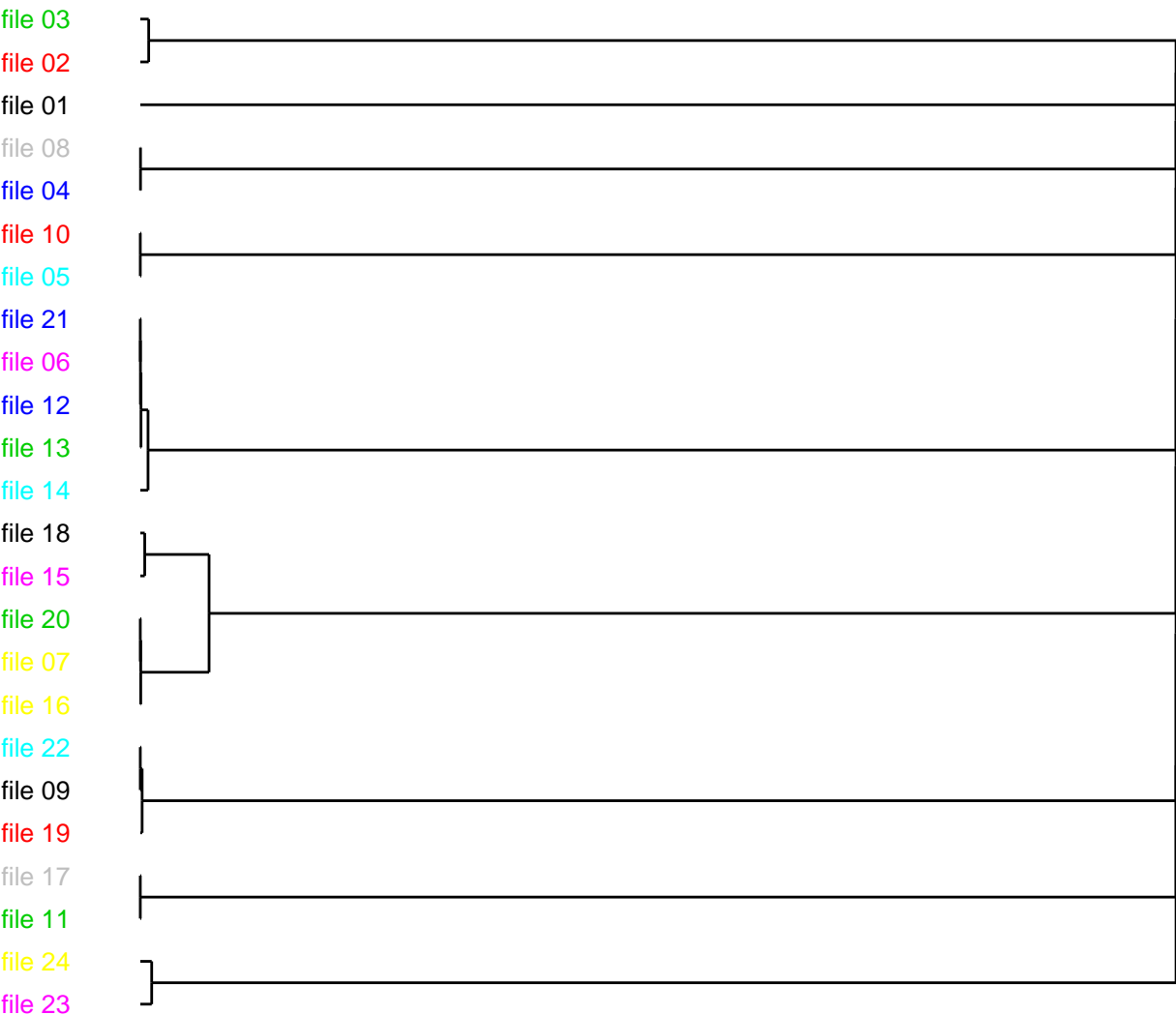


EVD: MBR – ID Transfer



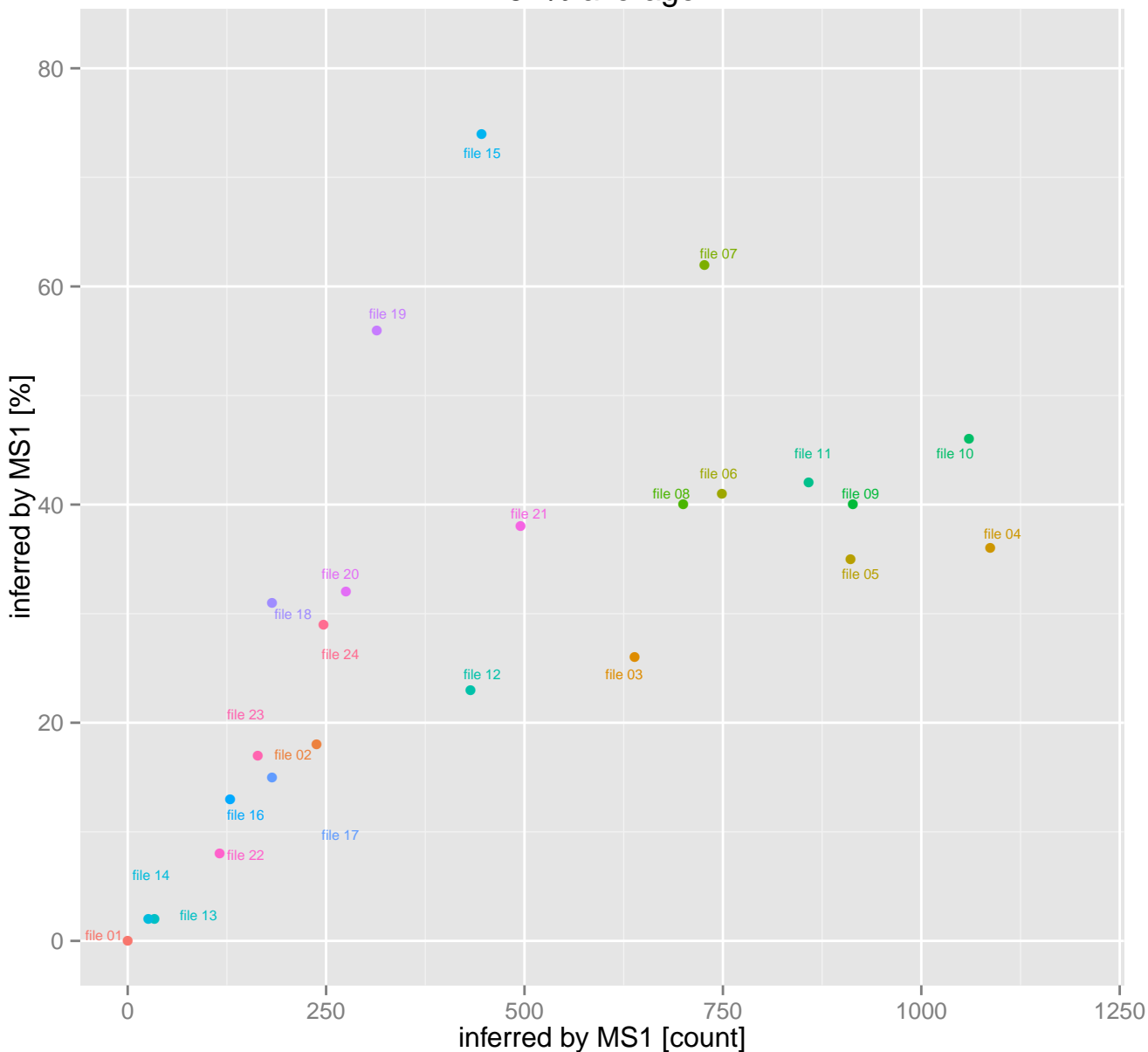
[experimental] EVD: Clustering Tree of Raw files

by Correlation of Corrected Retention Times



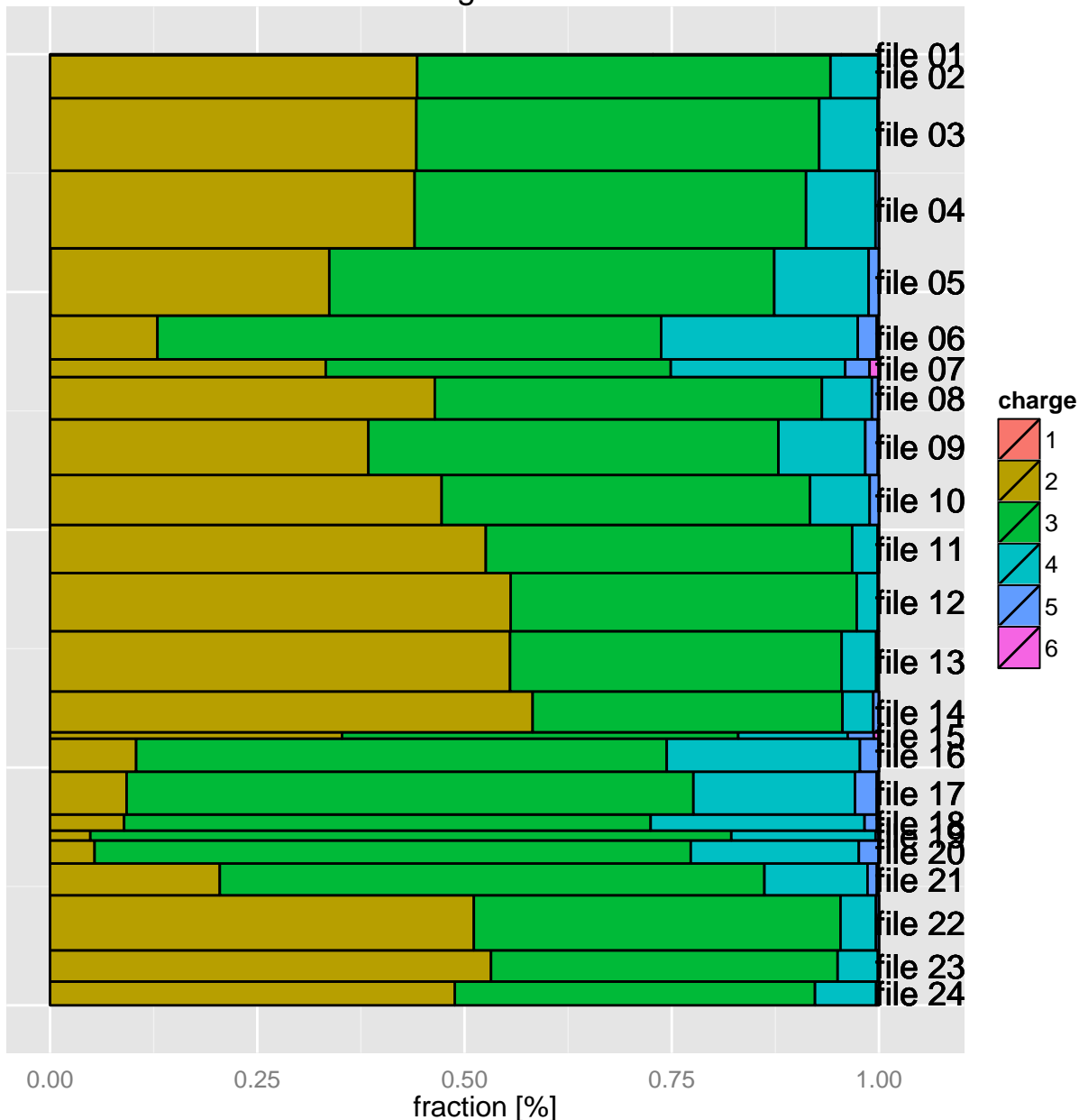
EVD: Peptides inferred by AMT-matching

31% average

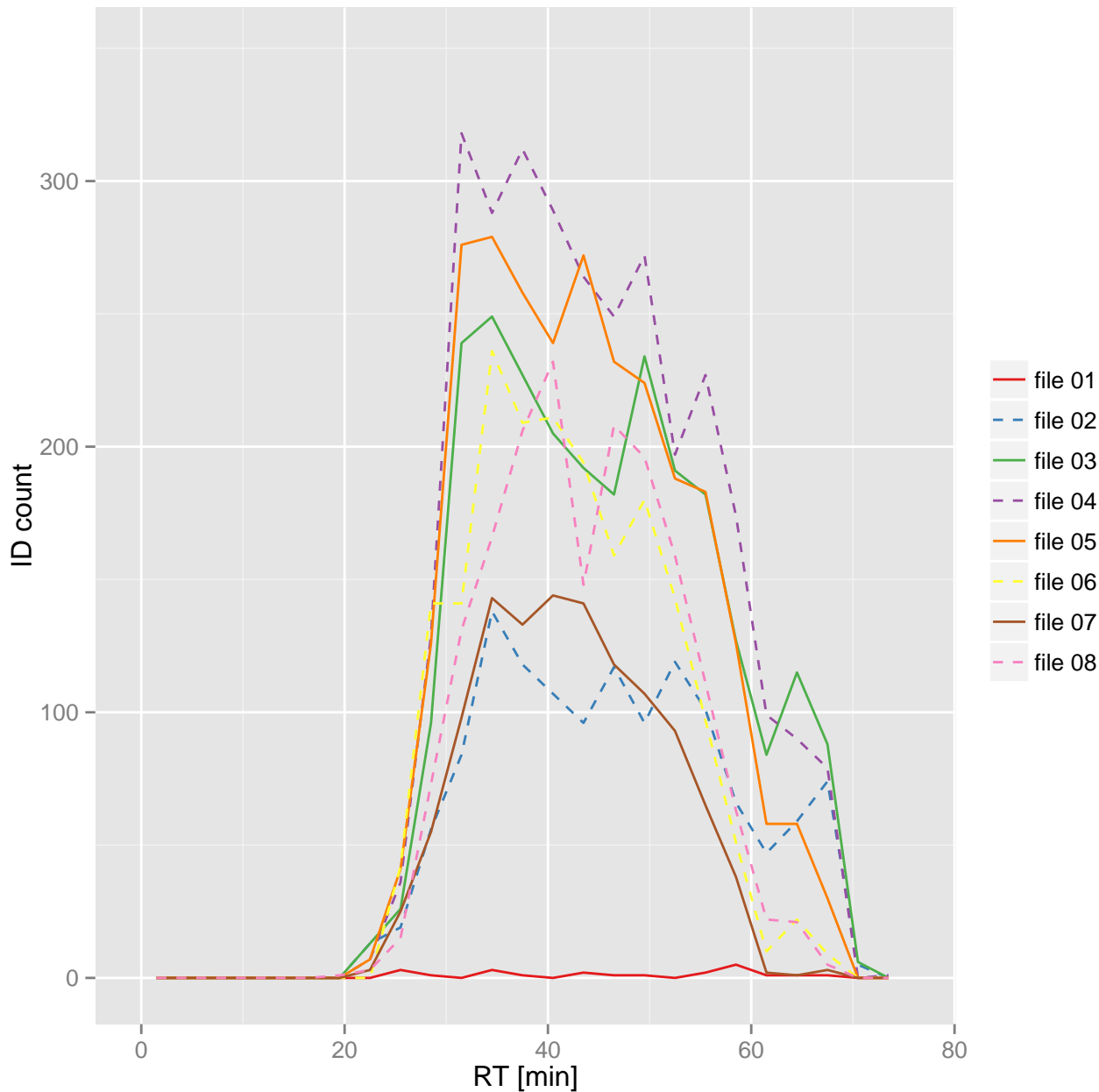


EVD: charge distribution

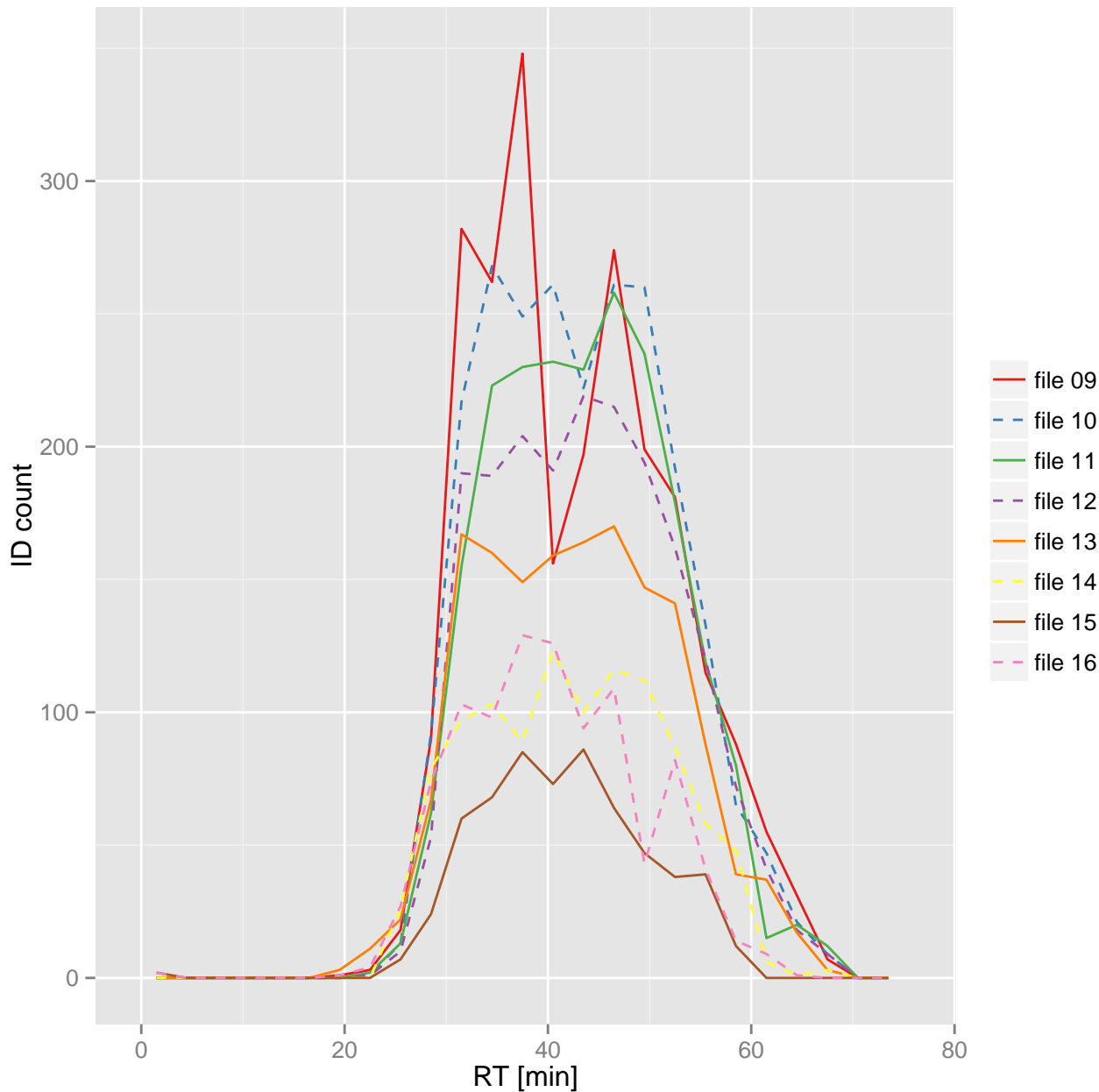
Raw file



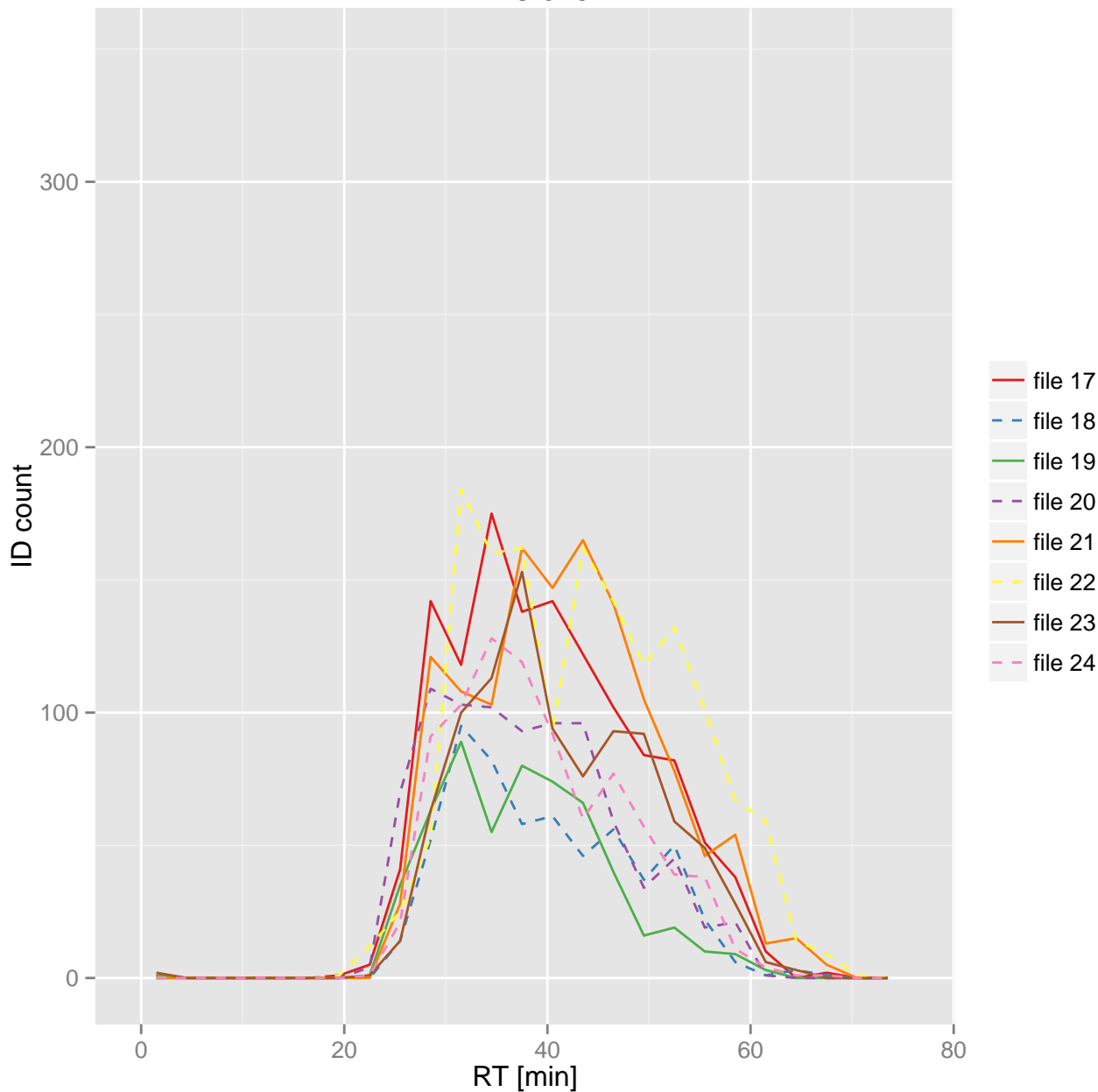
EVD: IDs over RT



EVD: IDs over RT

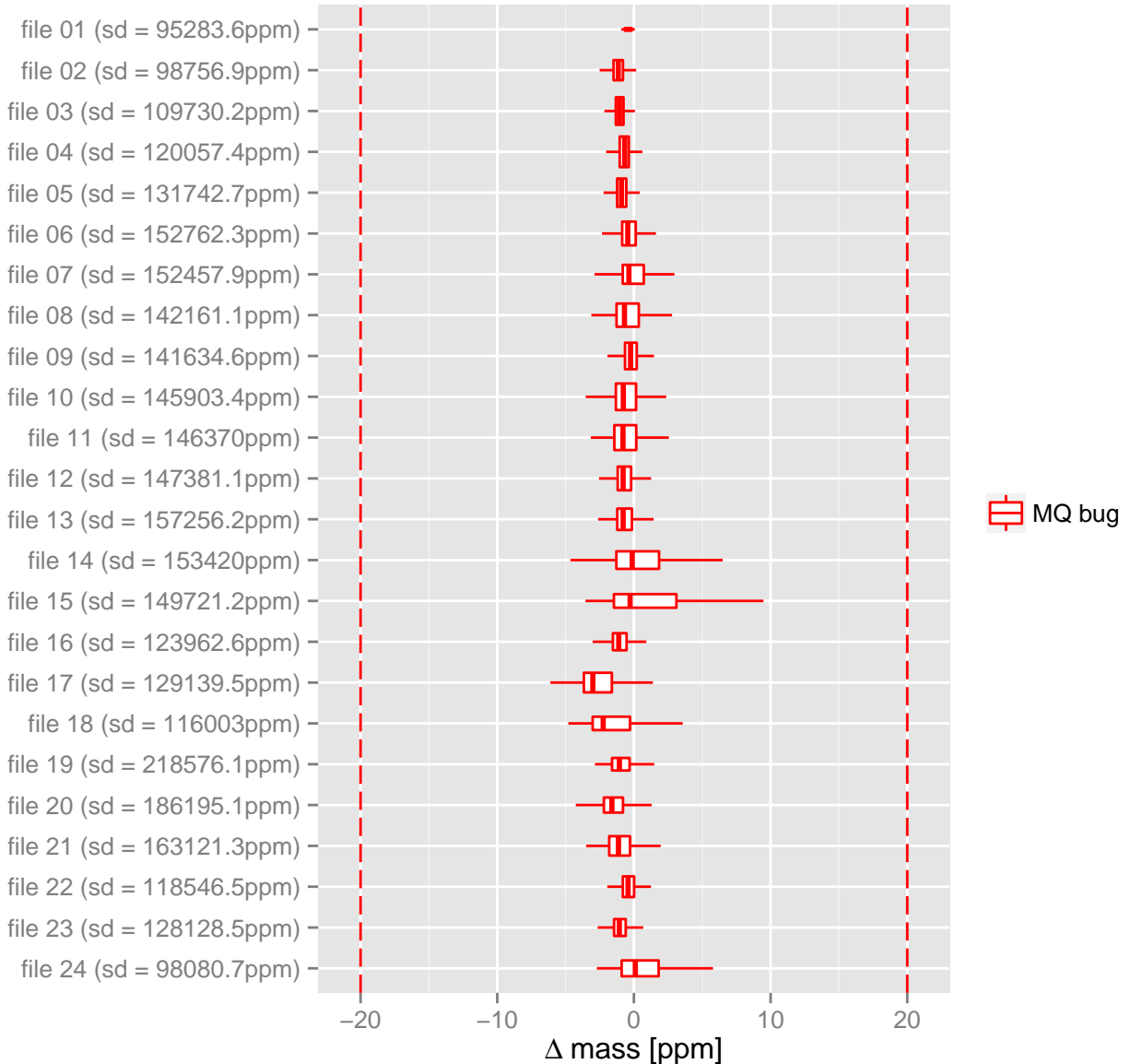


EVD: IDs over RT



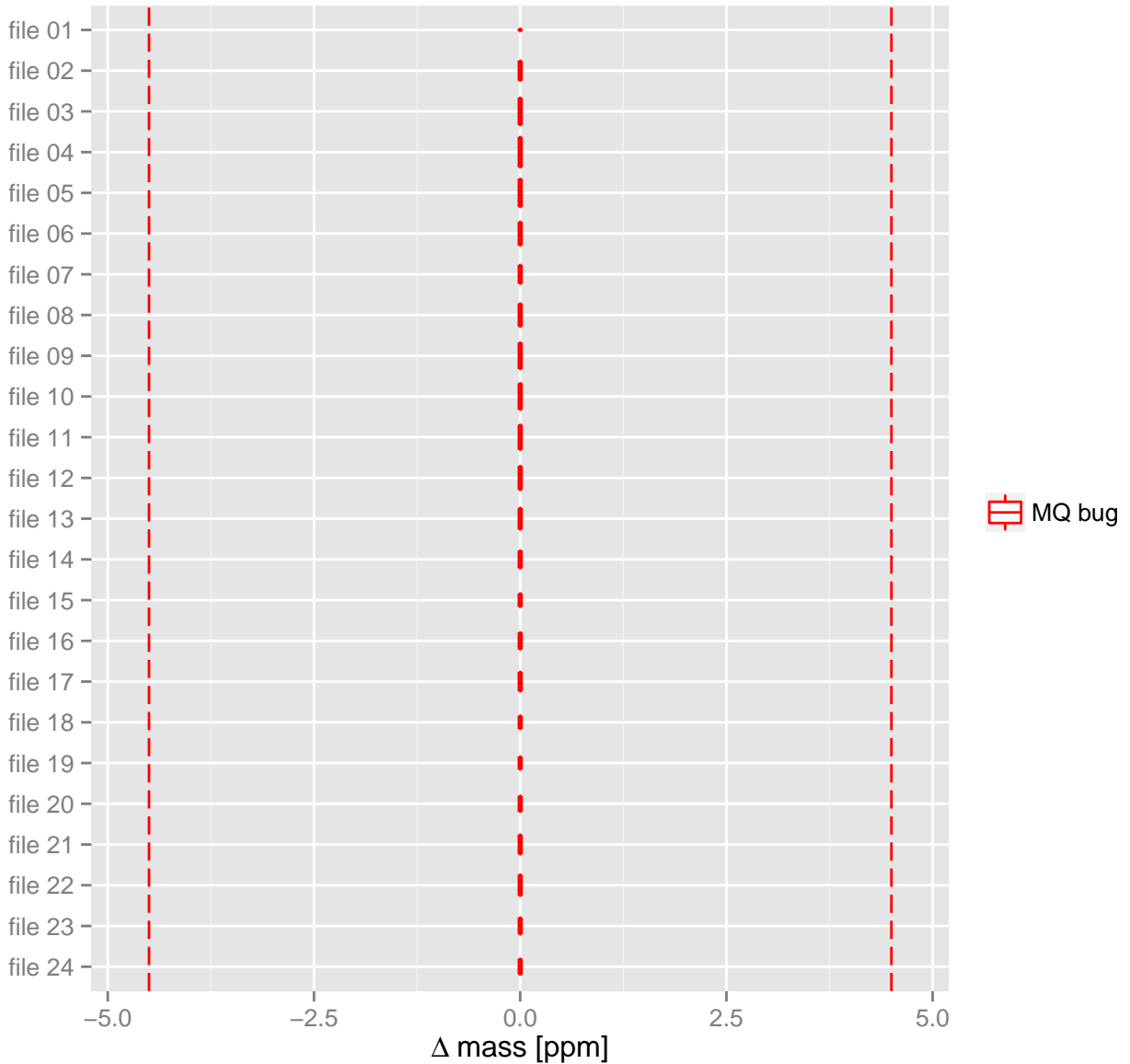
EVD: Uncalibrated mass error

MQ bug: data rescued

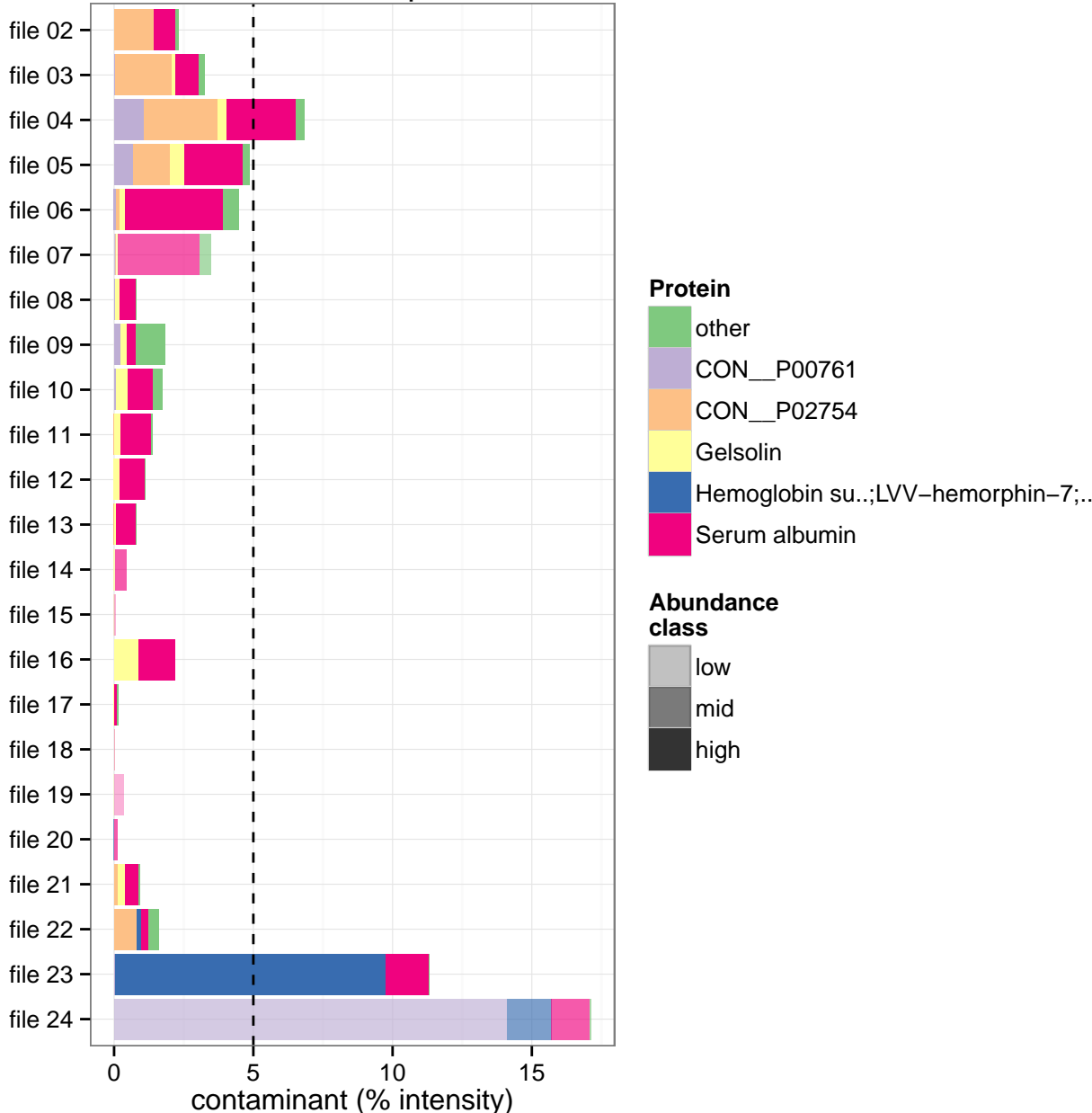


EVD: Calibrated mass error

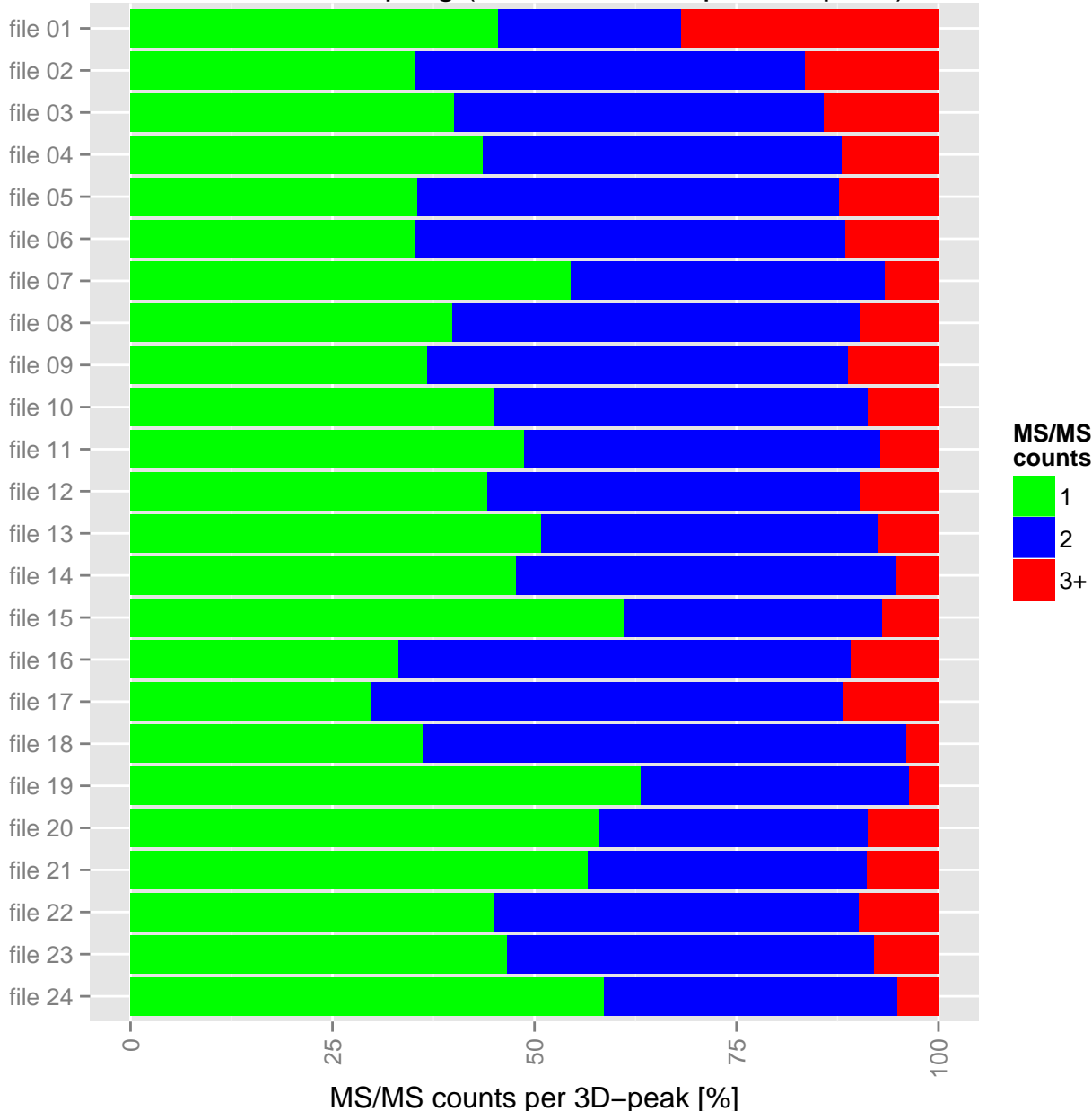
MQ bug: data cannot be rescued



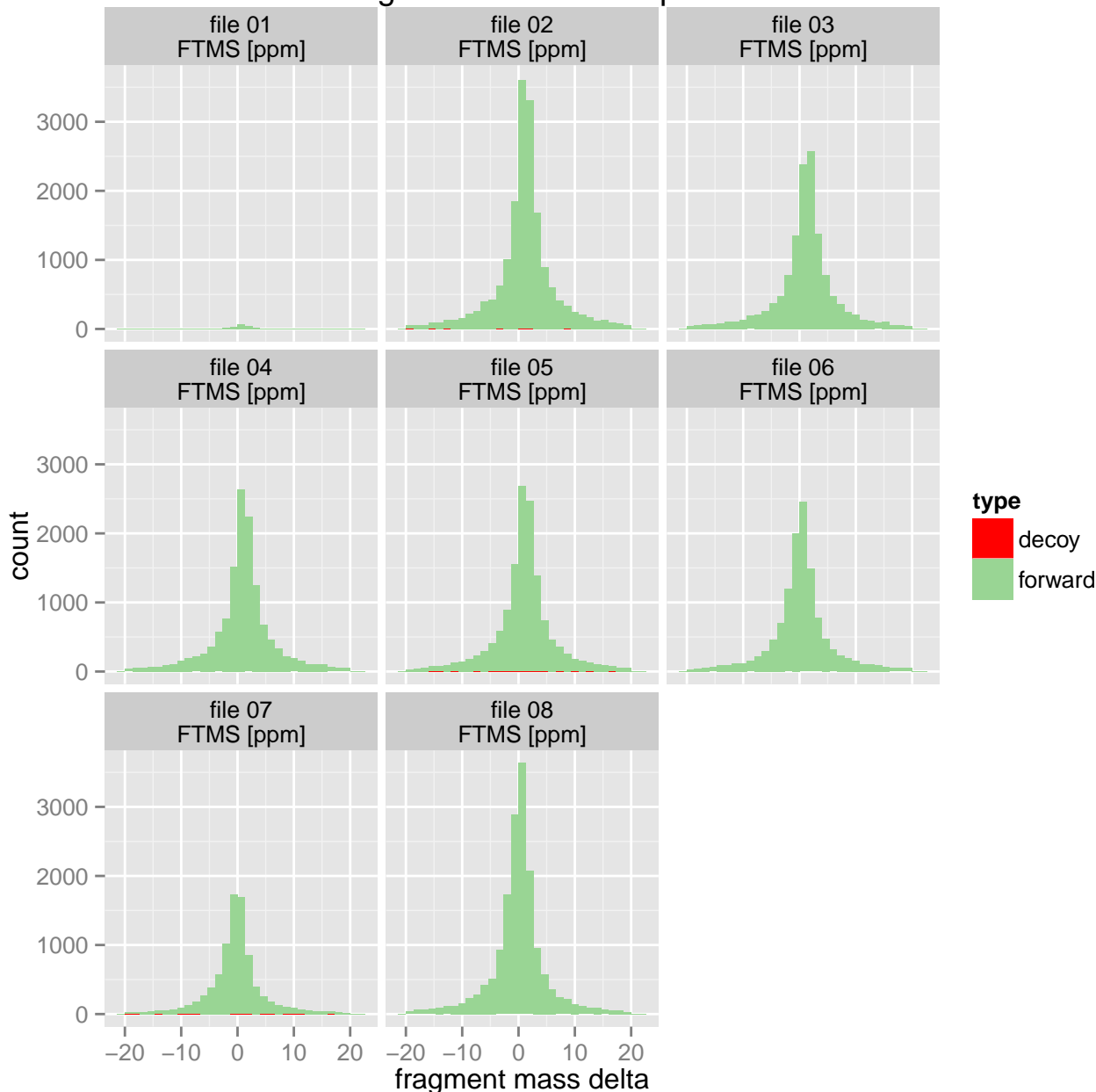
EVD: Contaminant per Raw file



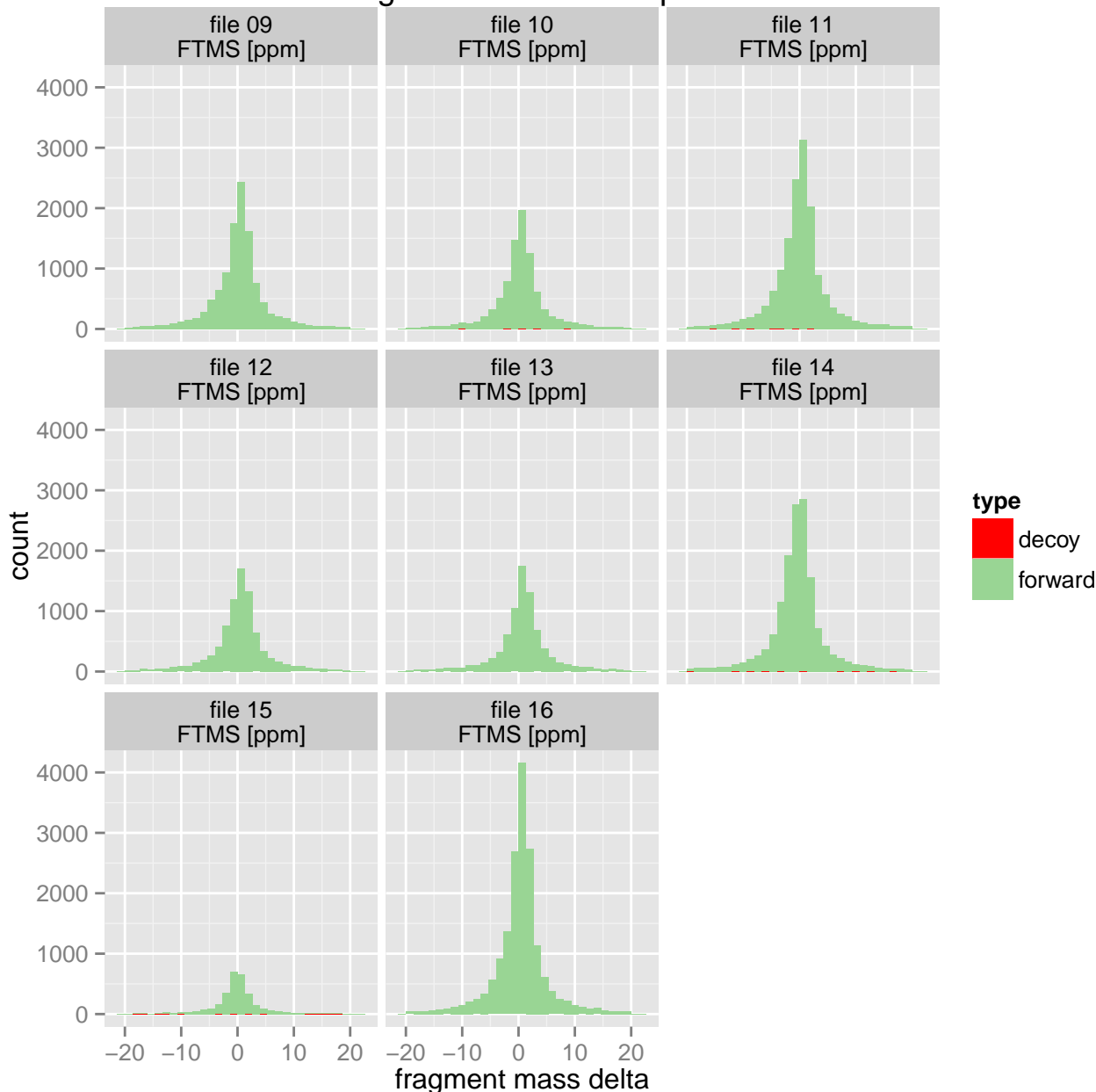
EVD: Oversampling (MS/MS counts per 3D-peak)



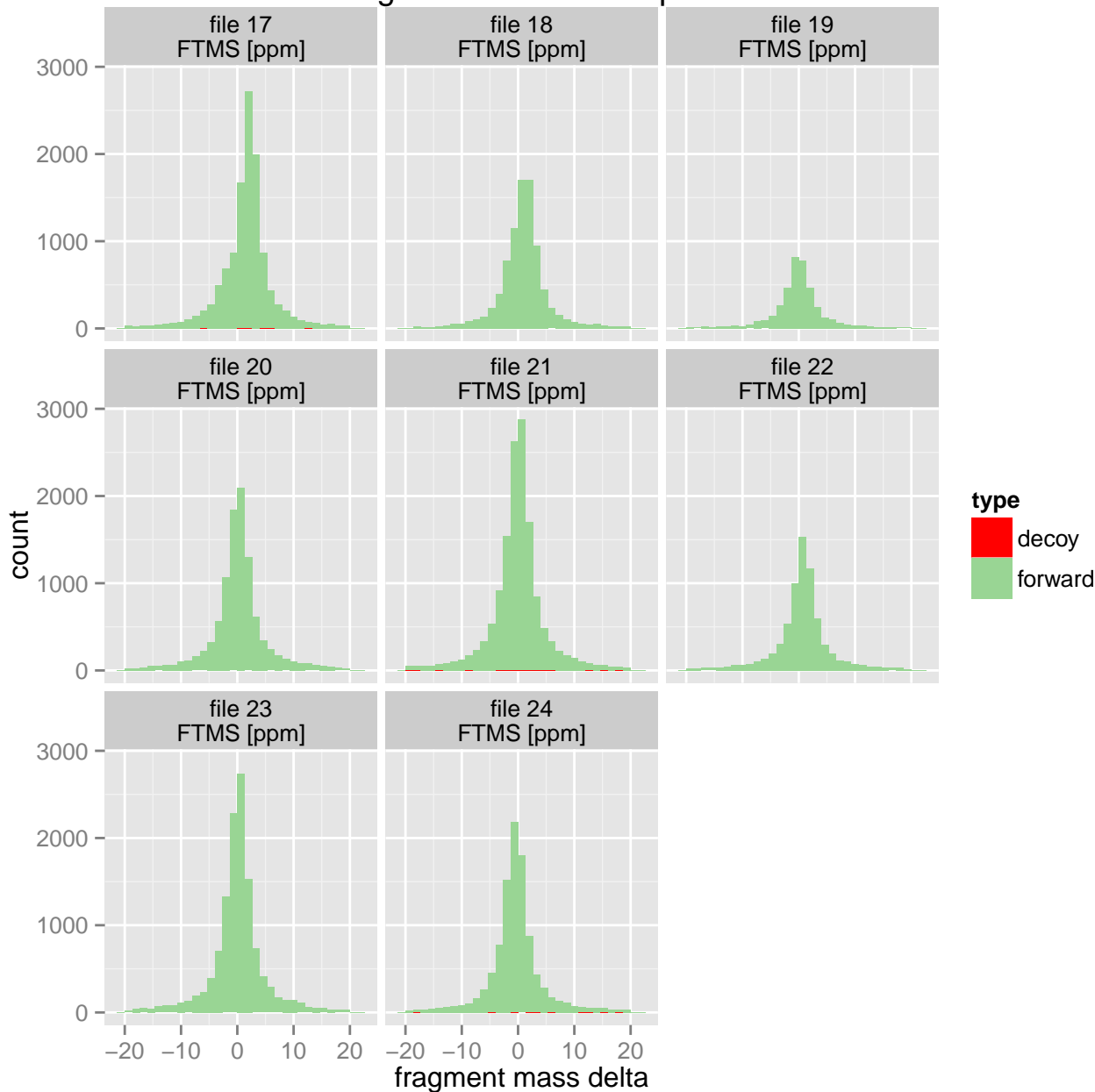
MSMS: Fragment mass errors per Raw file



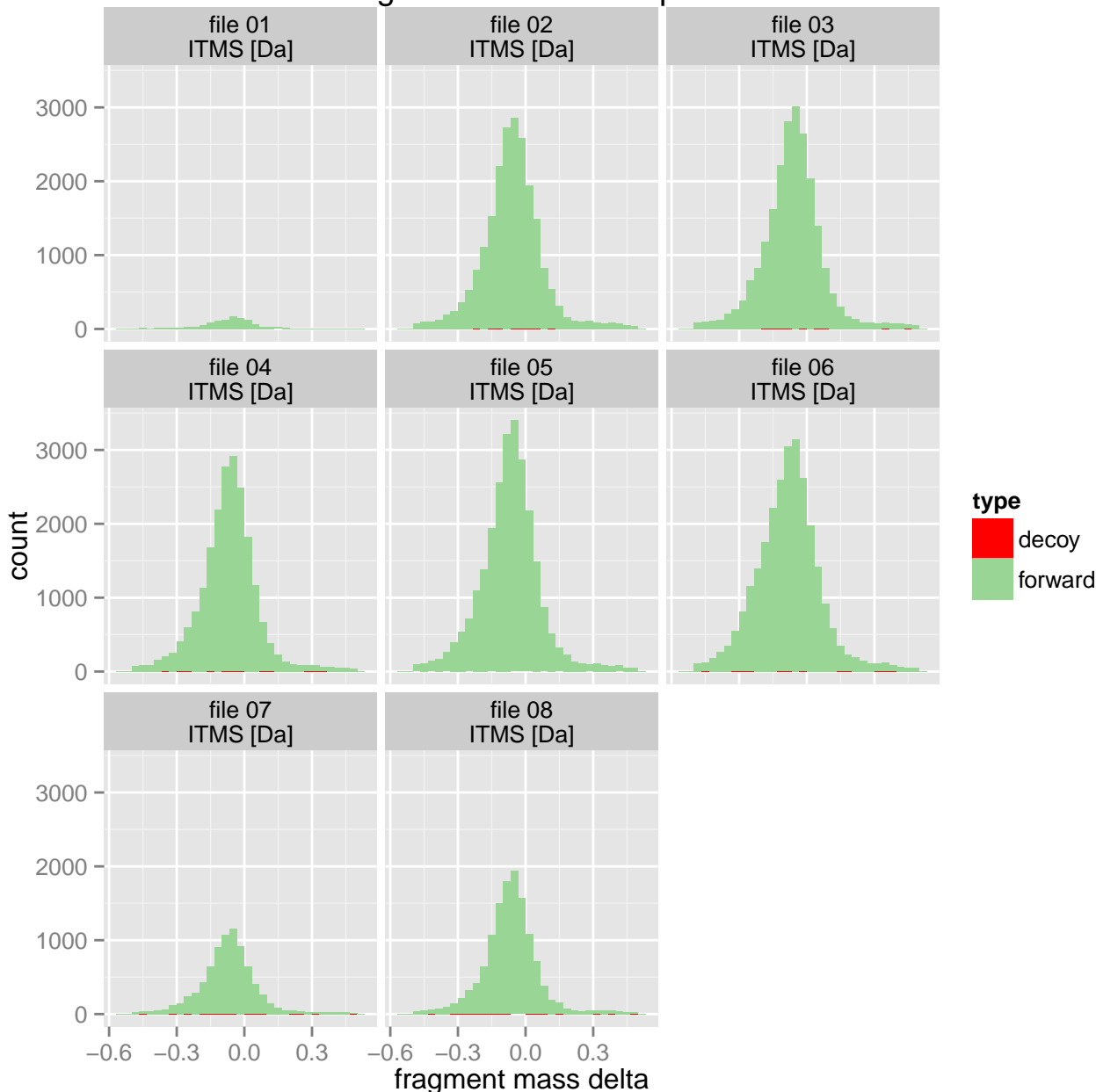
MSMS: Fragment mass errors per Raw file



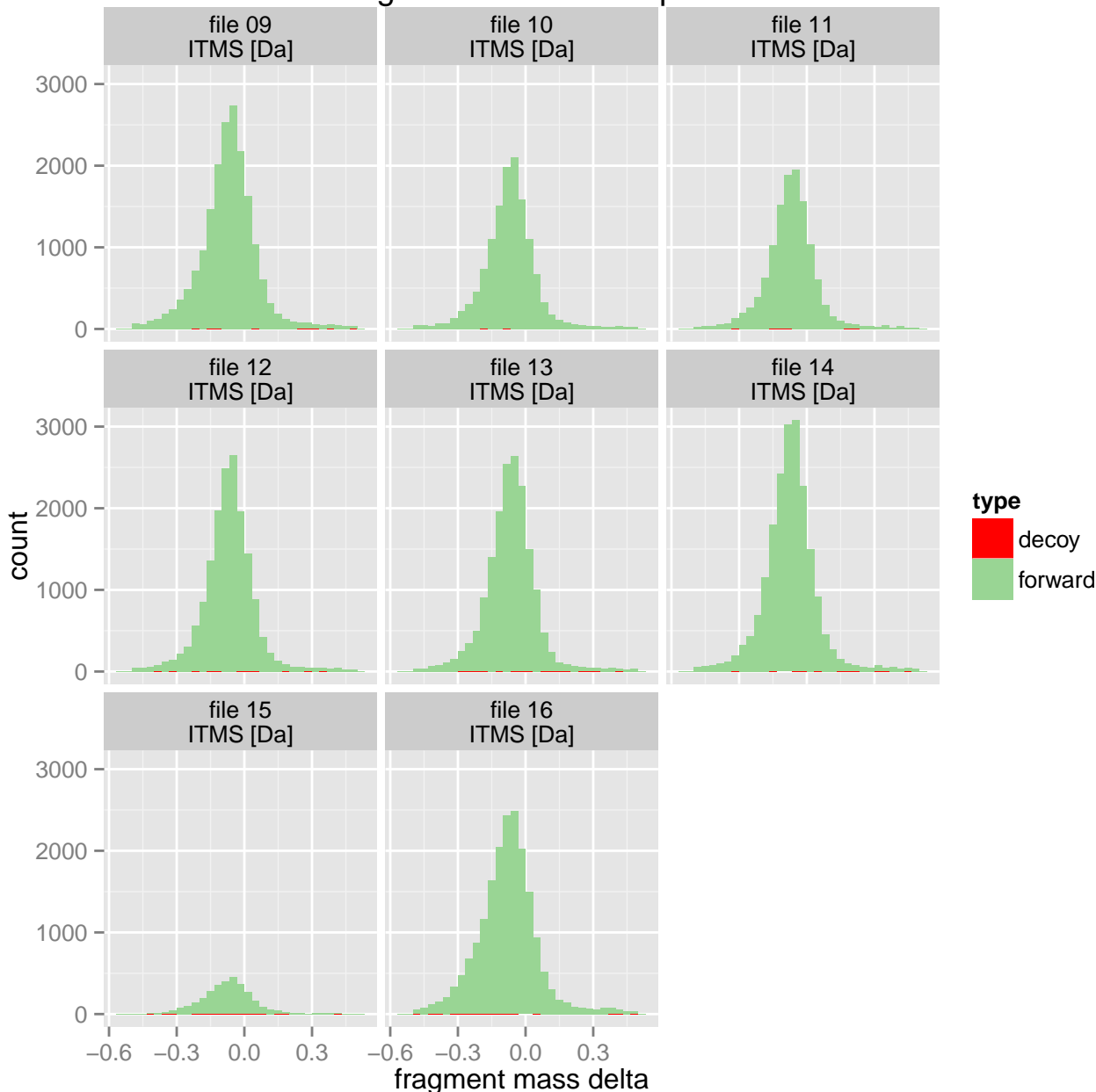
MSMS: Fragment mass errors per Raw file



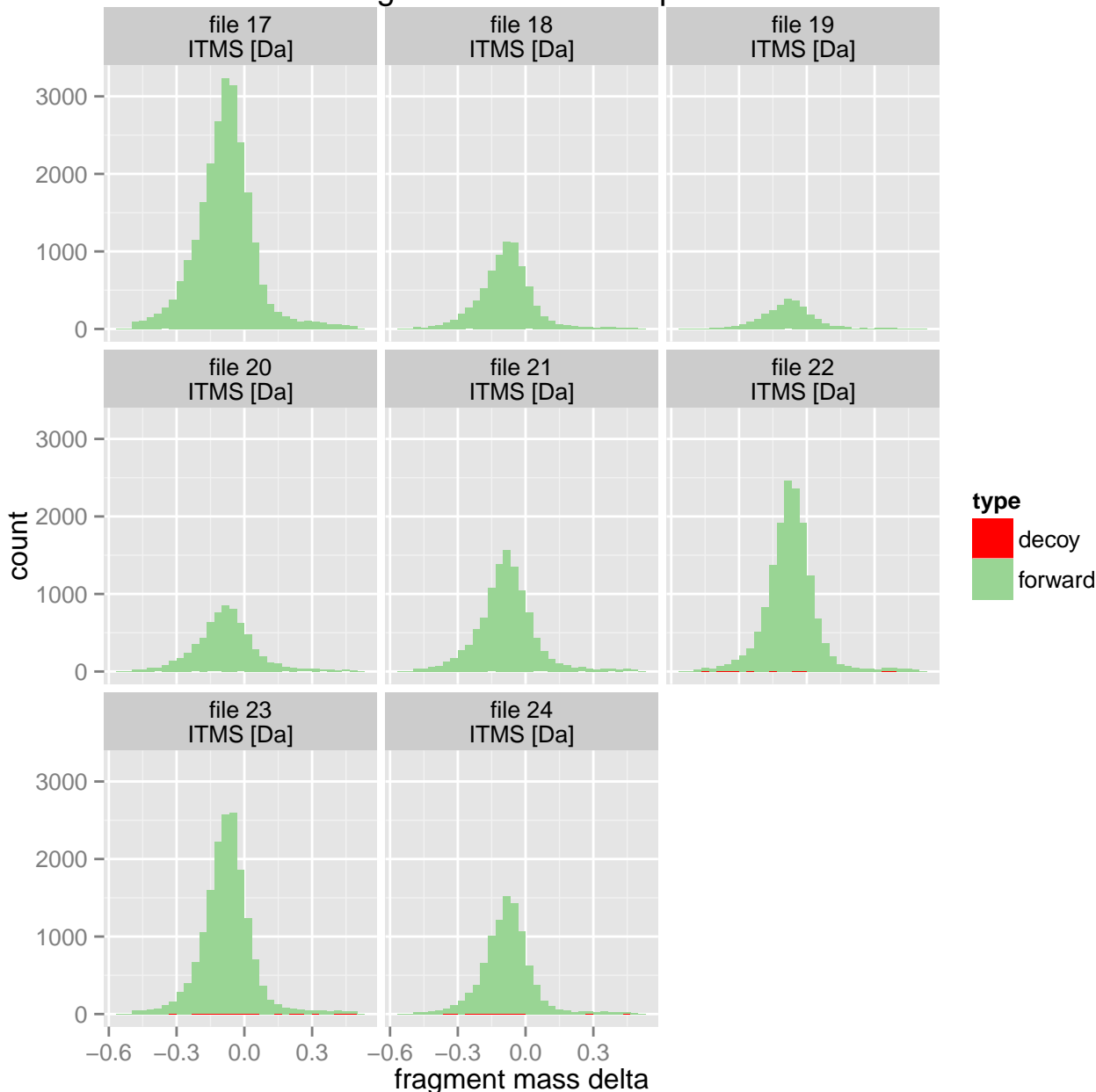
MSMS: Fragment mass errors per Raw file



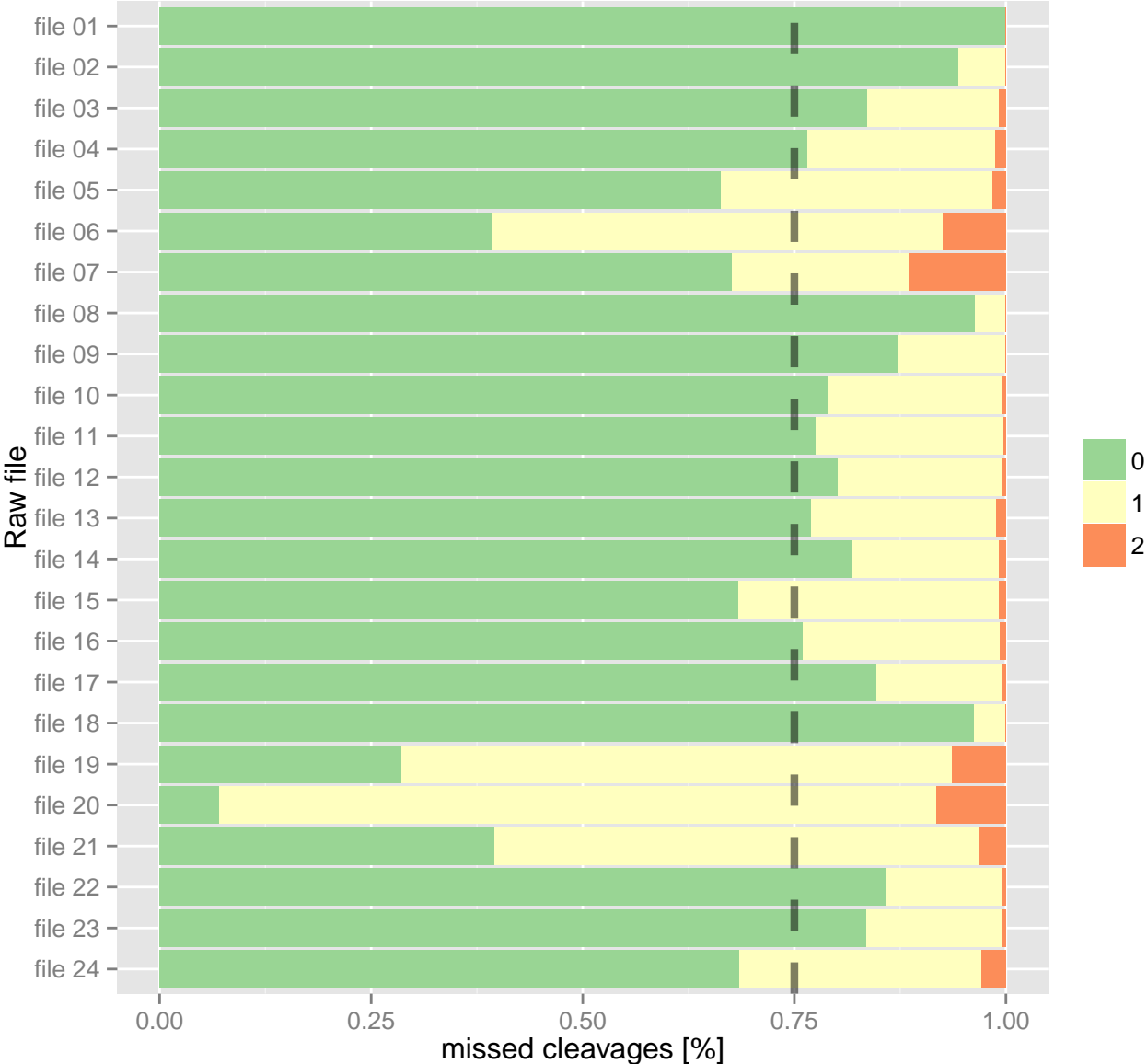
MSMS: Fragment mass errors per Raw file



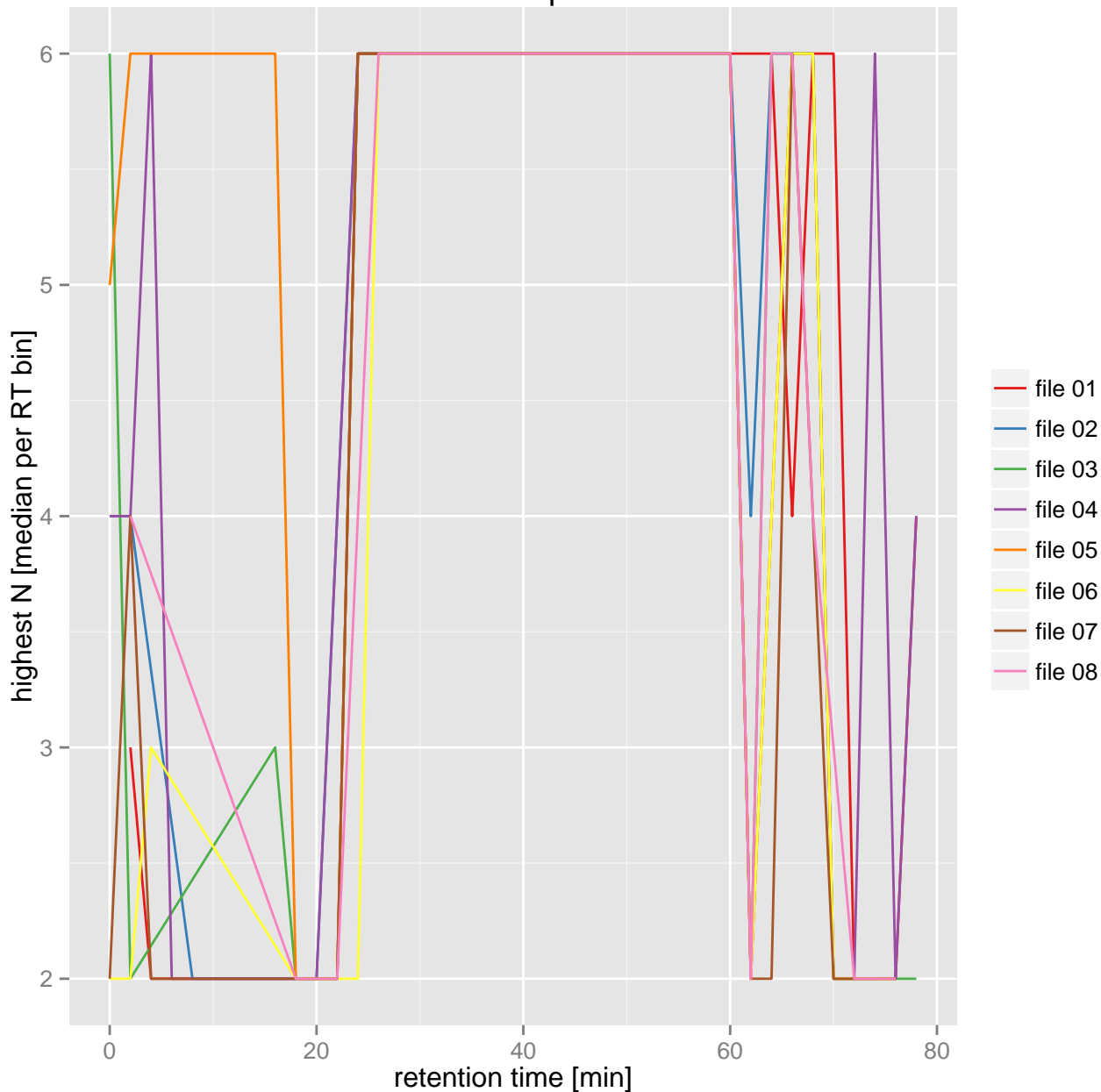
MSMS: Fragment mass errors per Raw file



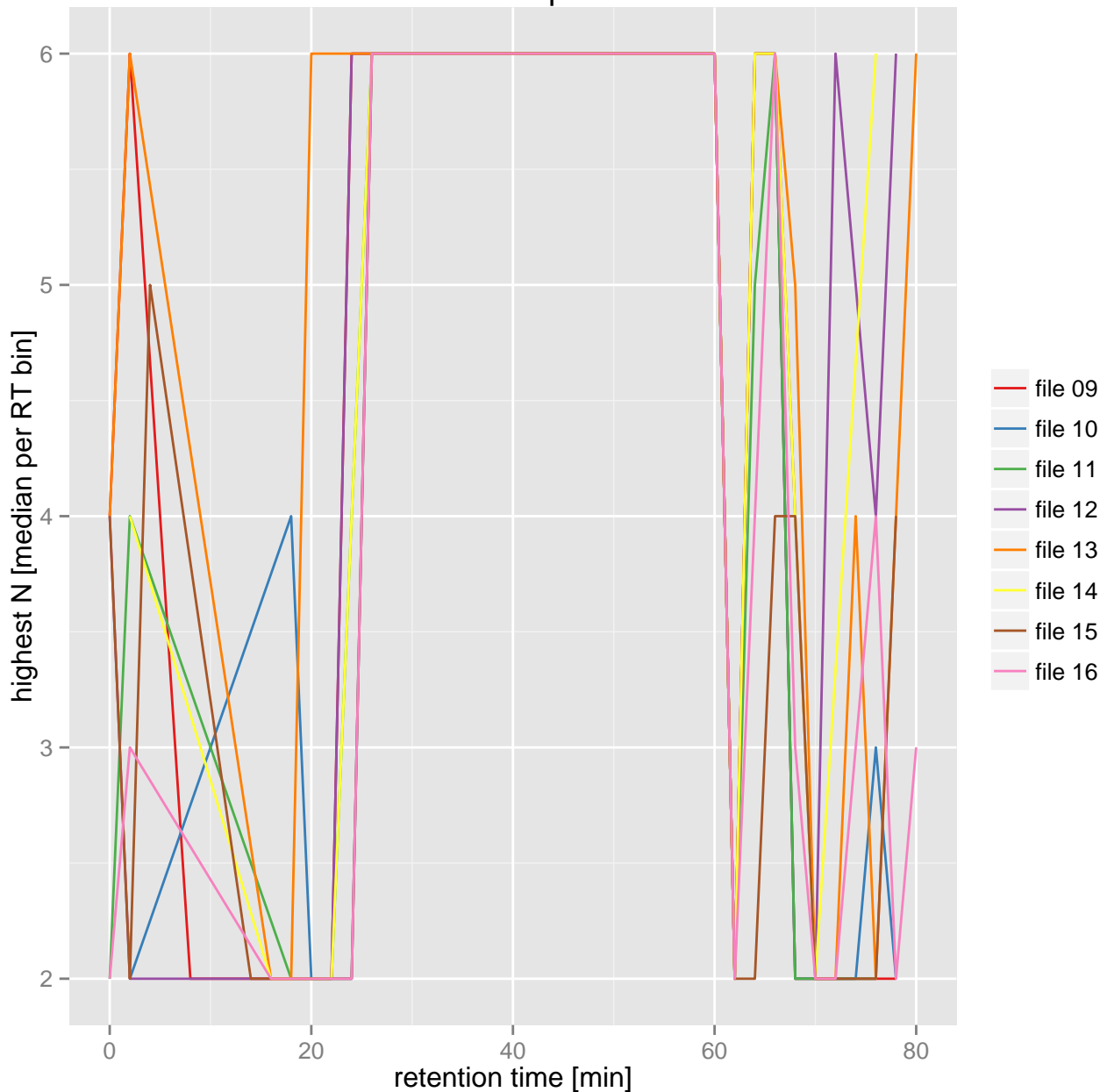
MSMS: Missed cleavages per Raw file
(excludes contaminants)



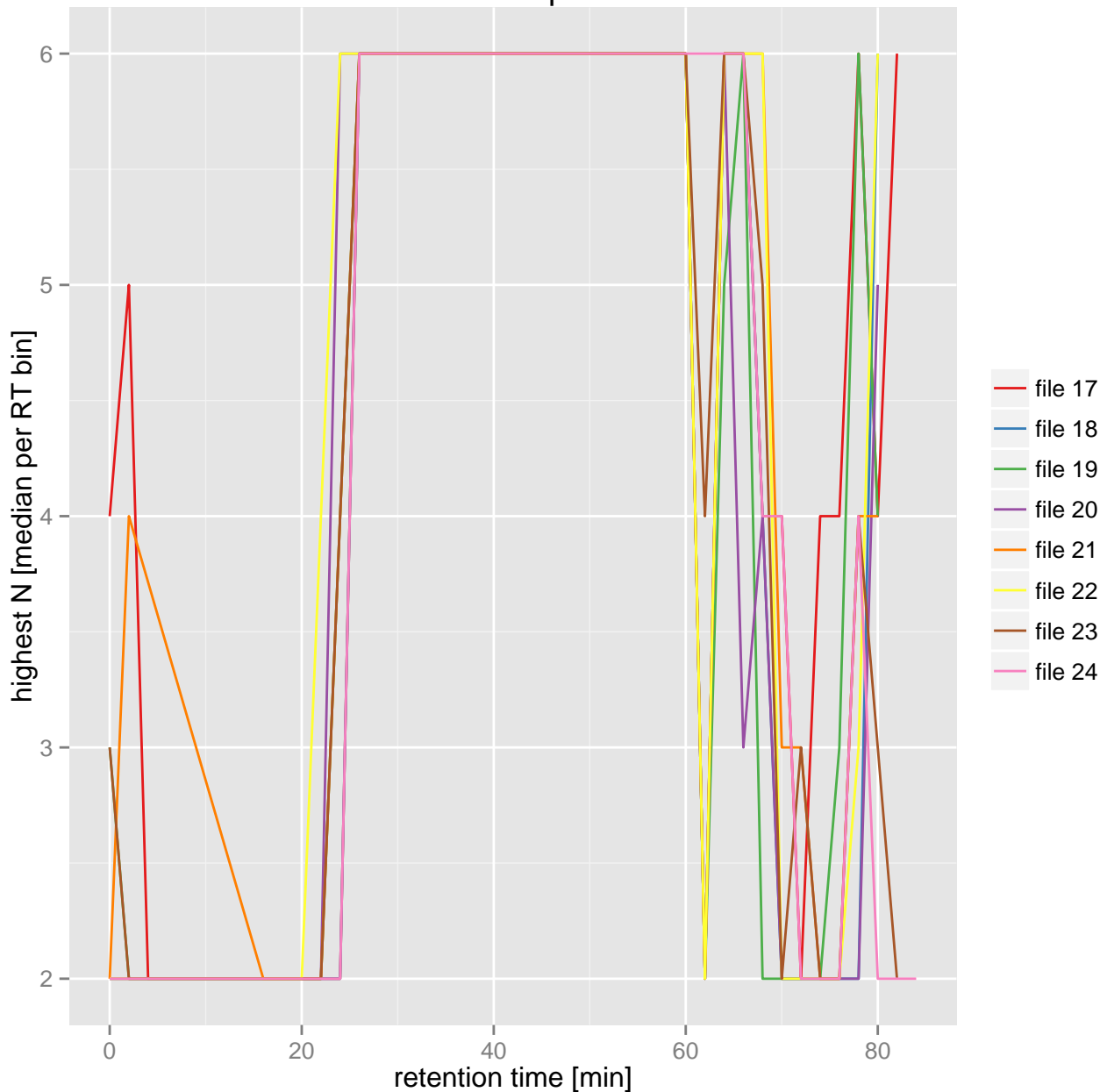
MSMSscans: TopN over RT



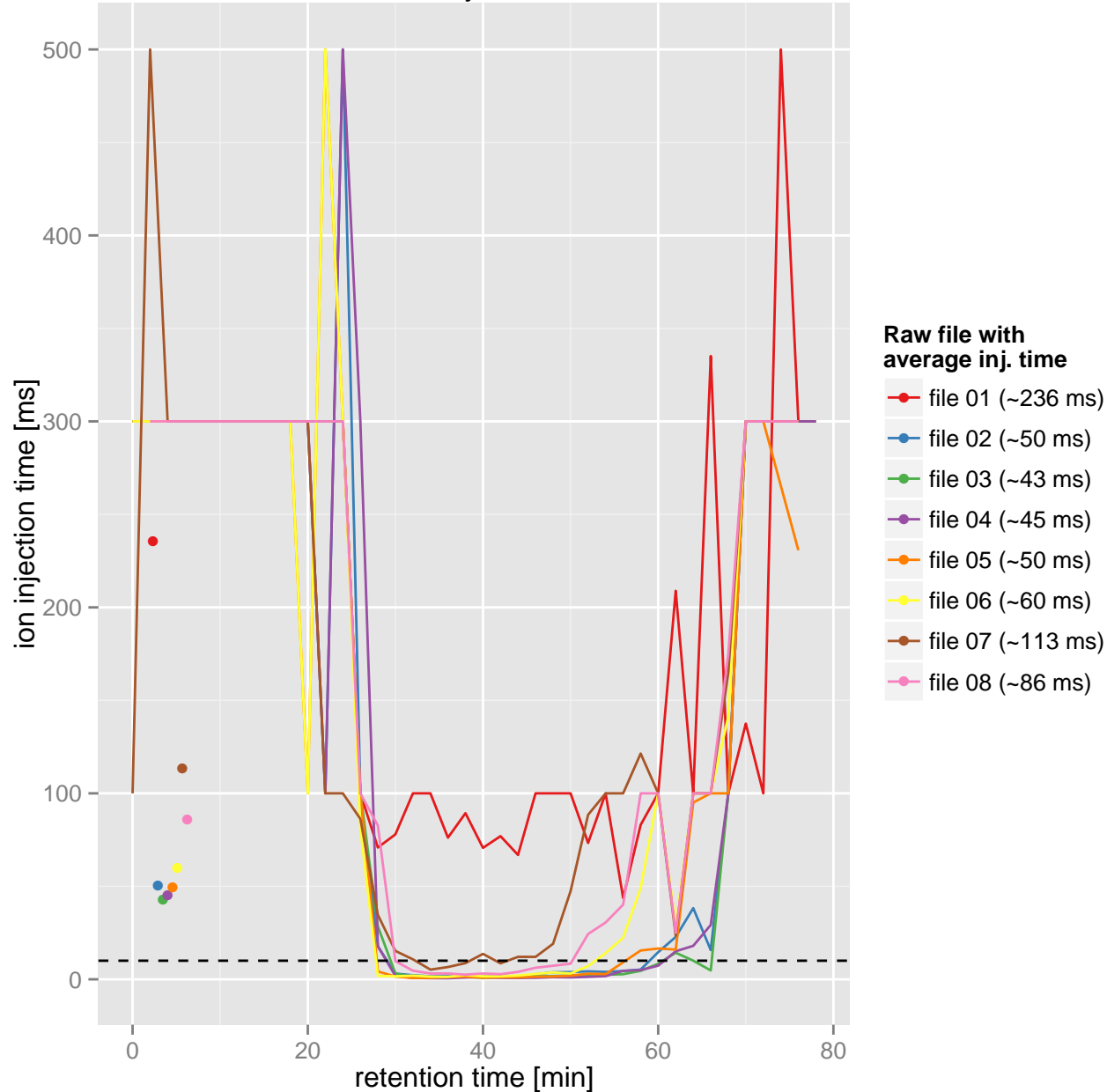
MSMSscans: TopN over RT



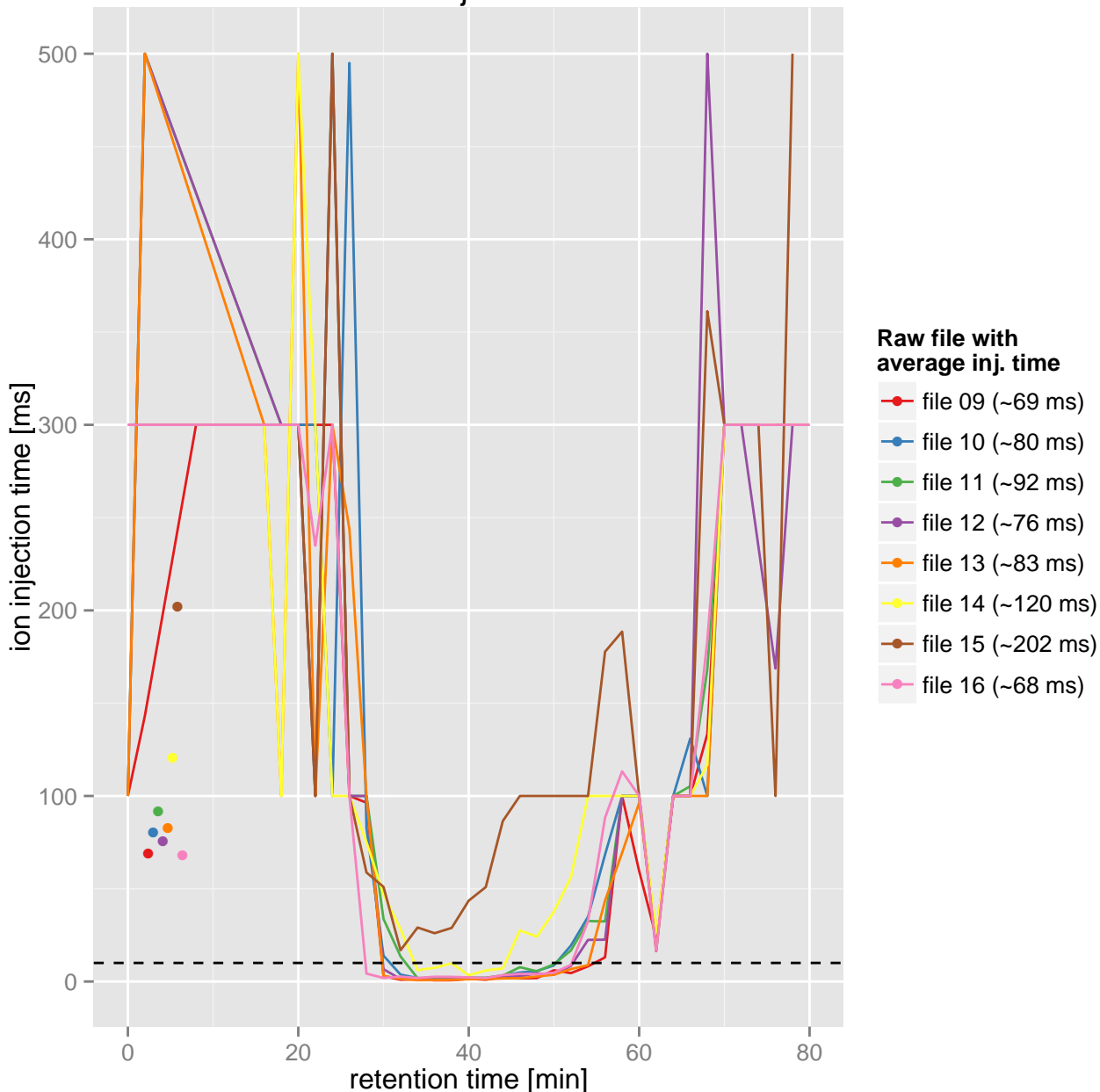
MSMSscans: TopN over RT



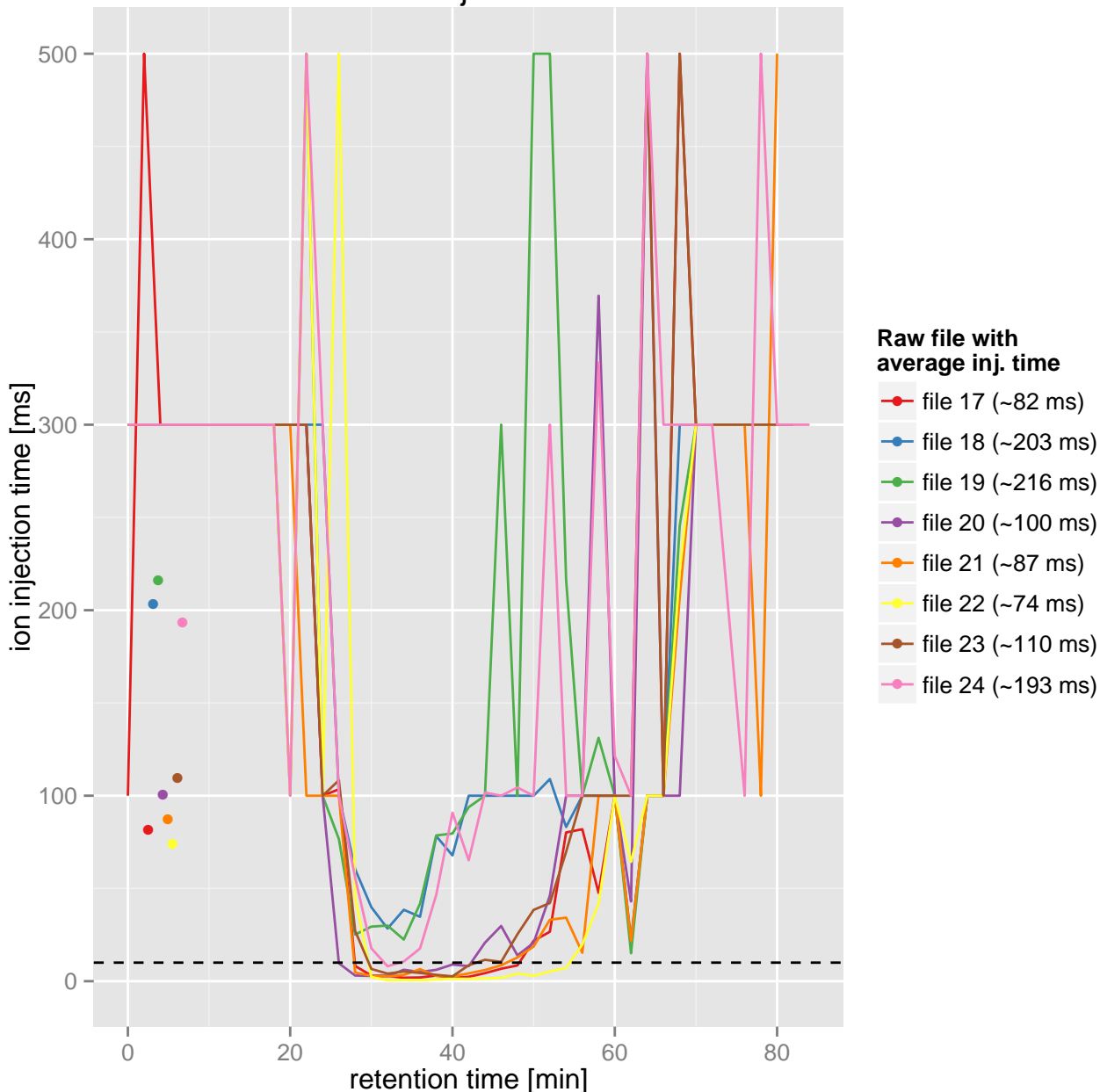
MSMSscans: Ion Injection Time over RT



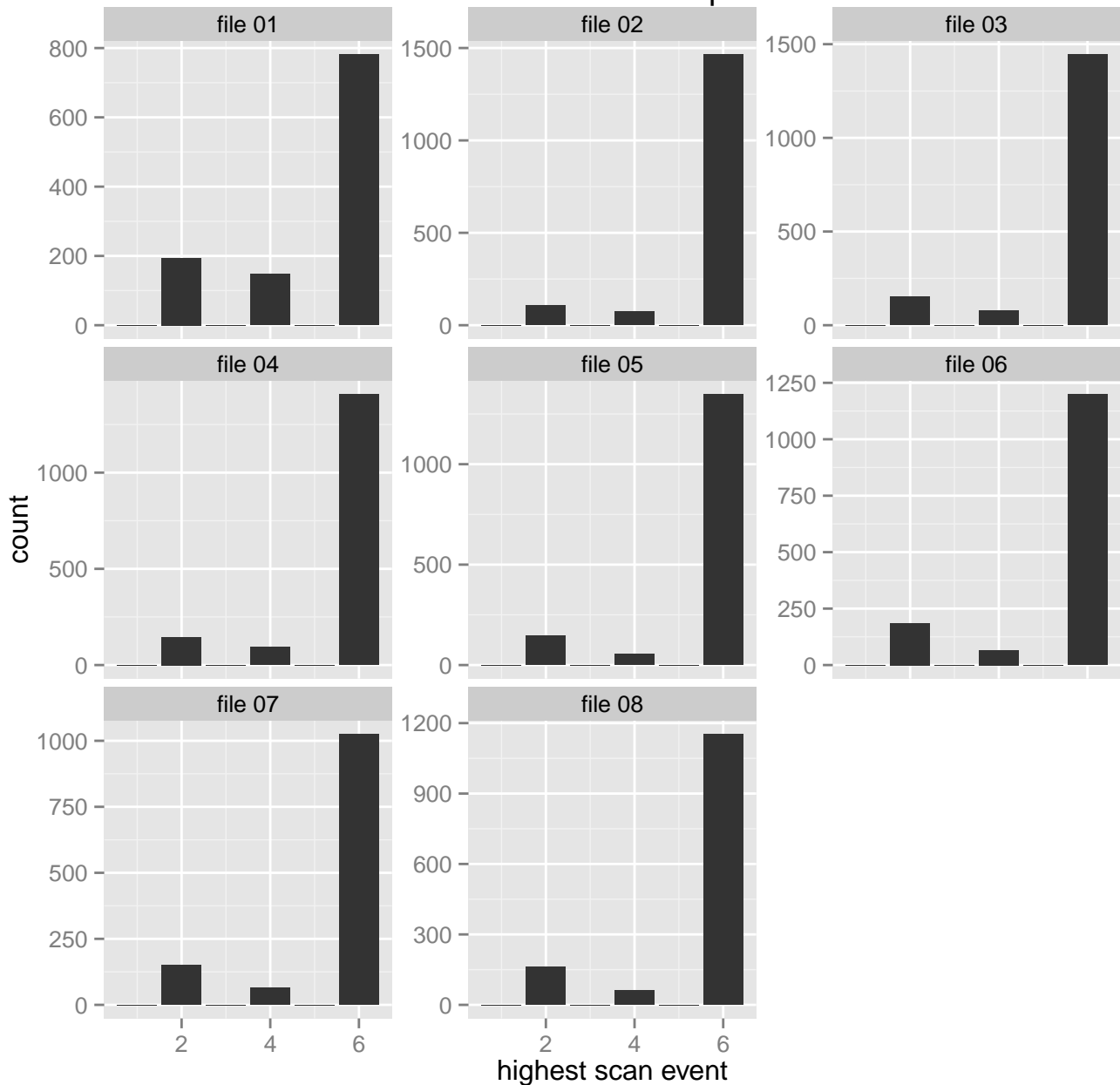
MSMSscans: Ion Injection Time over RT



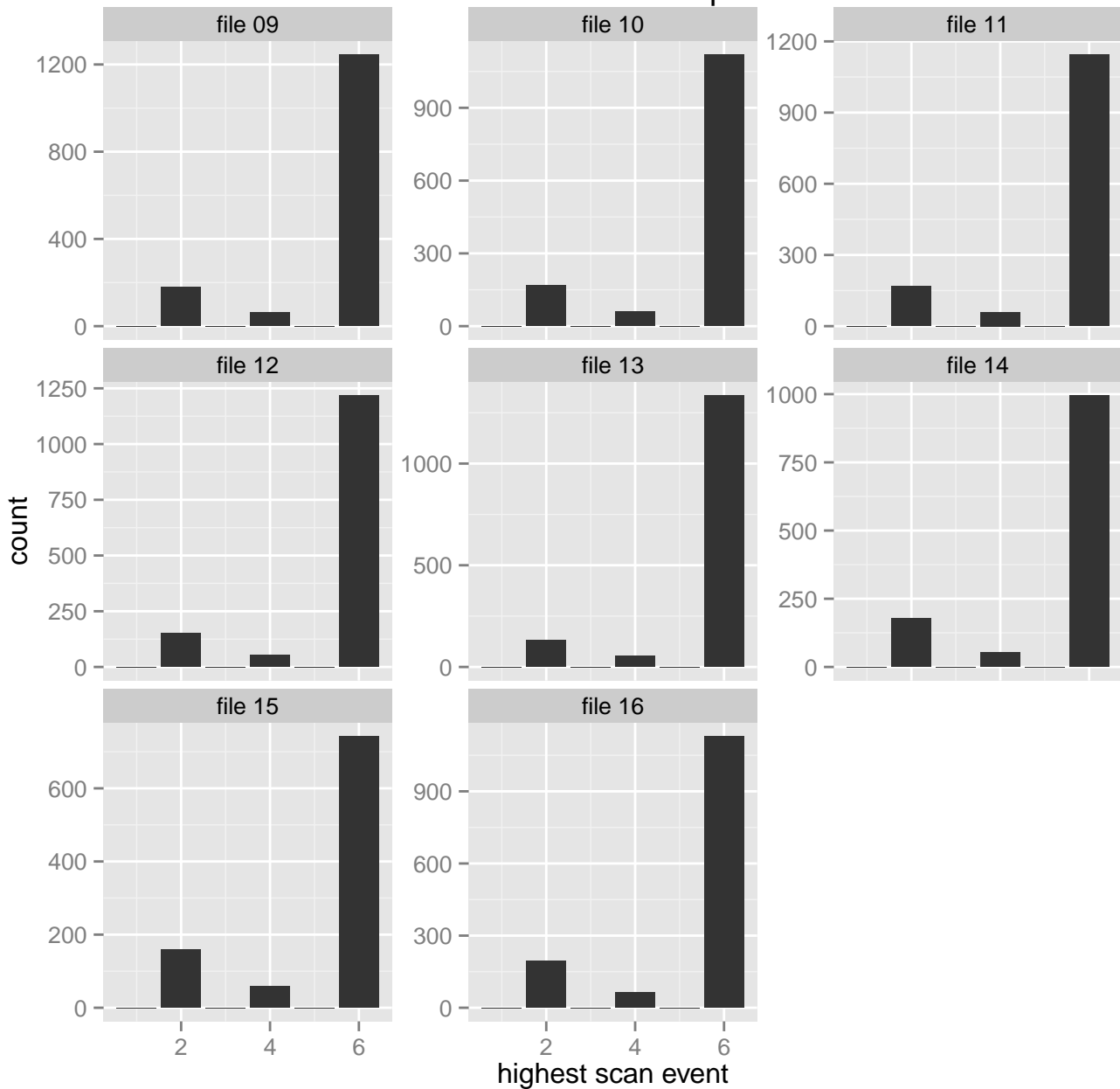
MSMSscans: Ion Injection Time over RT



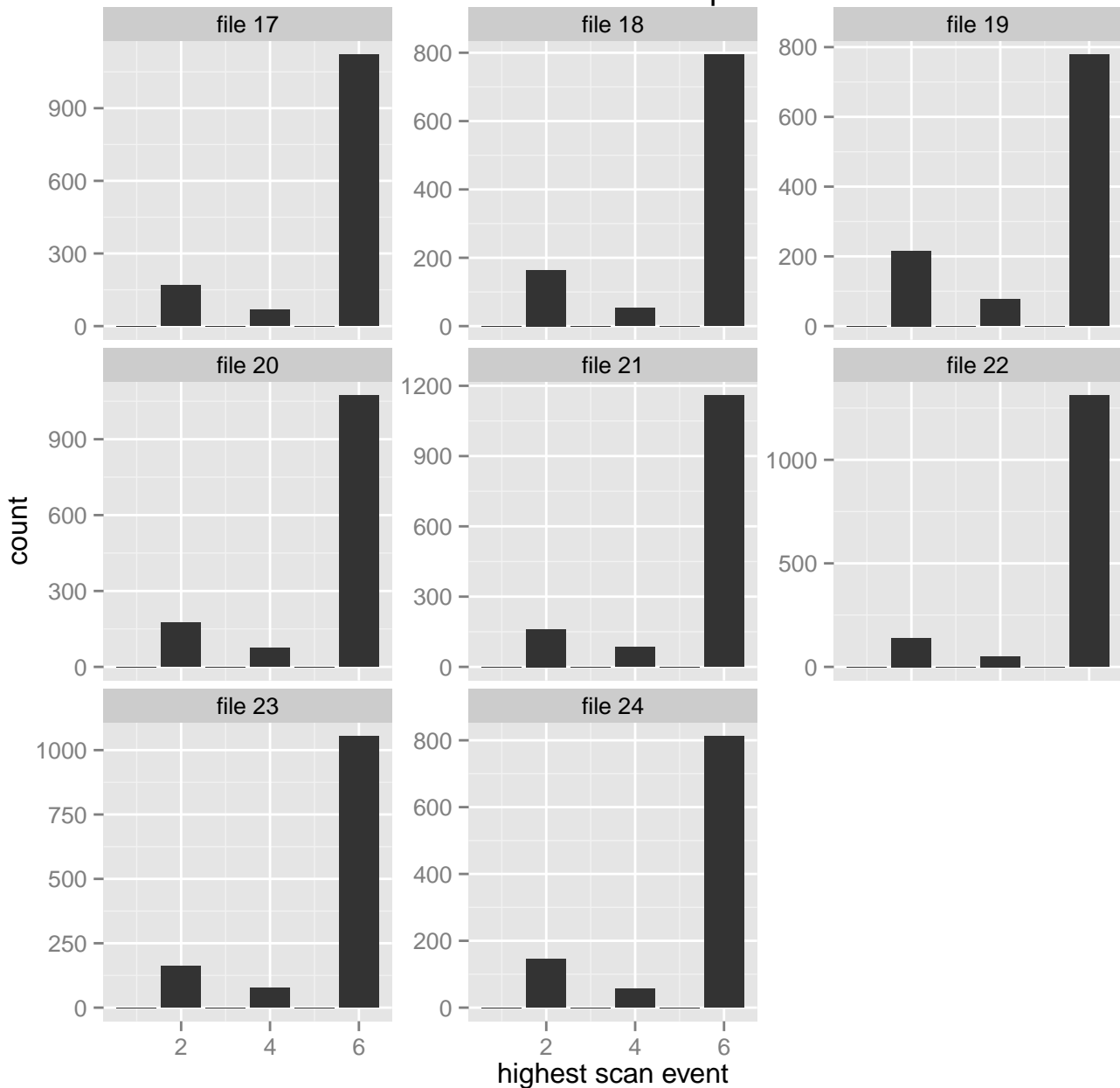
MSMSscans: TopN



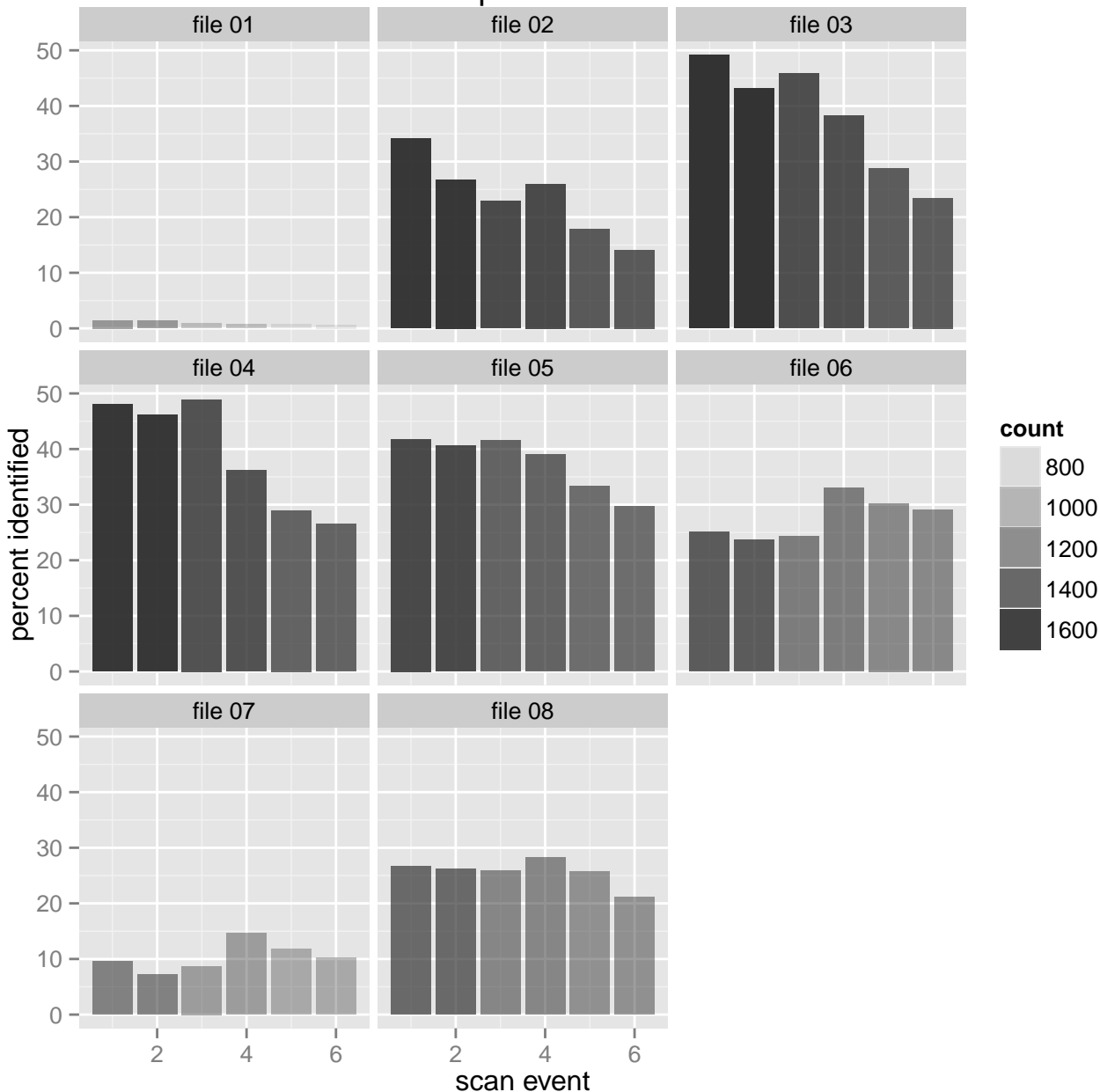
MSMScans: TopN



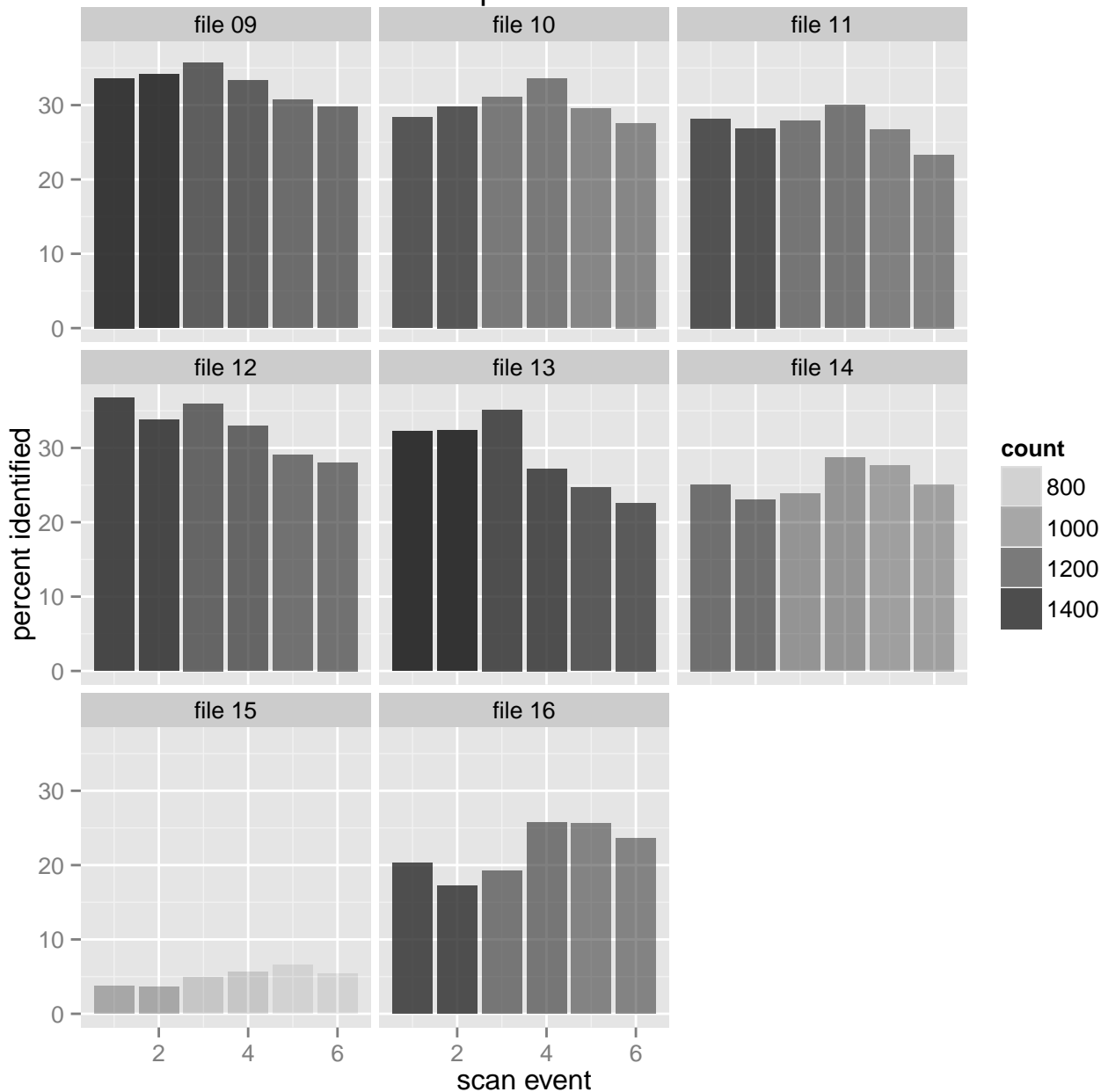
MSMScans: TopN



MSMSscans: TopN % identified over N



MSMSScans: TopN % identified over N



MSMSscans: TopN % identified over N

