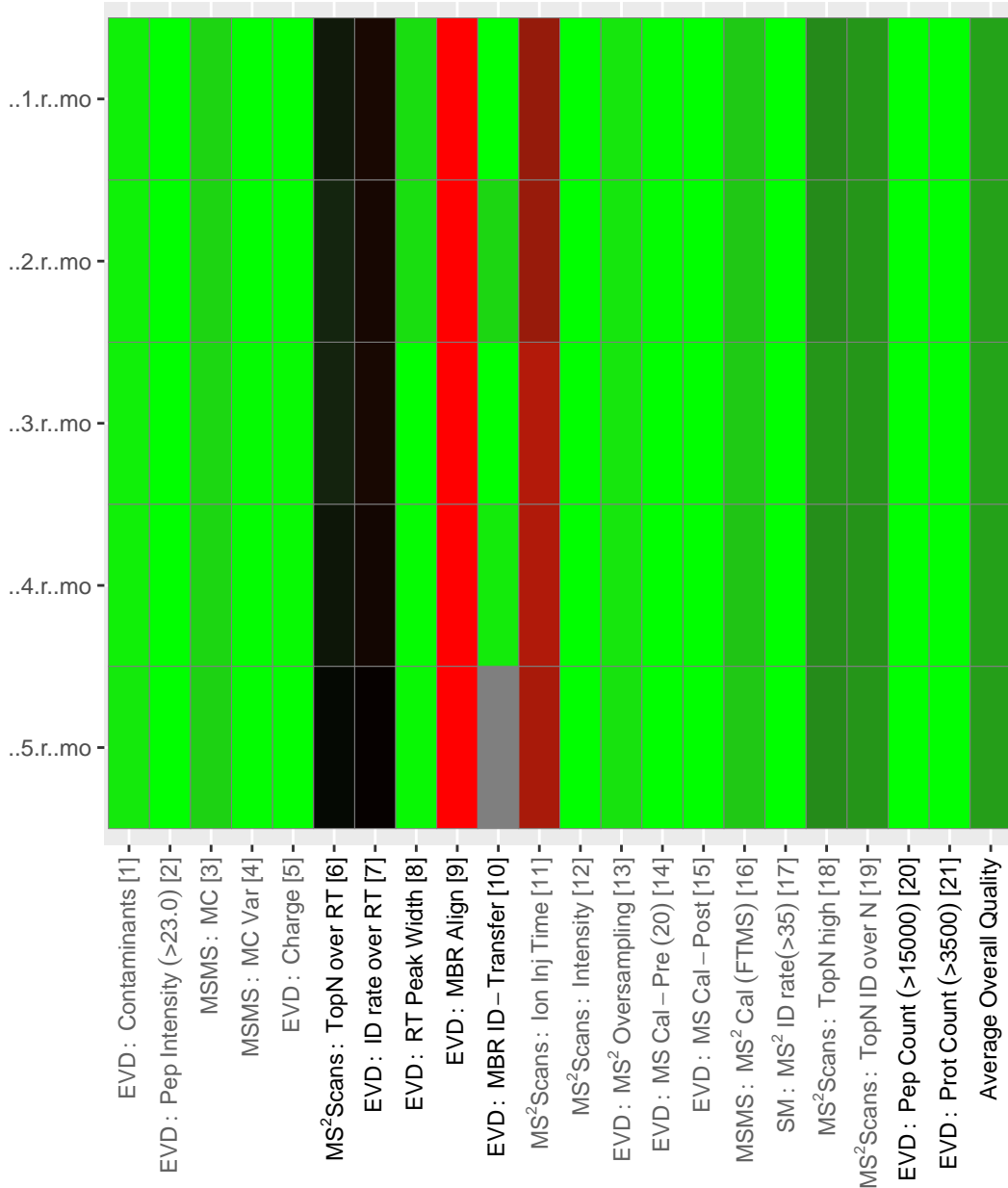


Performance overview

Raw file



score



Missing



Mapping of Raw files to their short names

Mapping source: automatic

original	short name	best effort
MST141.raw.thermo	..1.r.mo	
MST142.raw.thermo	..2.r.mo	
MST143.raw.thermo	..3.r.mo	
MST144.raw.thermo	..4.r.mo	
MST145.raw.thermo	..5.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..	0	MS/MS deisotoping tolerance ..	ppm
Alignment time window [min]	0	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	09/23/2020 23:57:19	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 (Unknow..	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	cn033.bi.uni-freiburg.de	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	PSM FDR	0.01
Match unidentified features	False	PSM FDR Crosslink	0.01

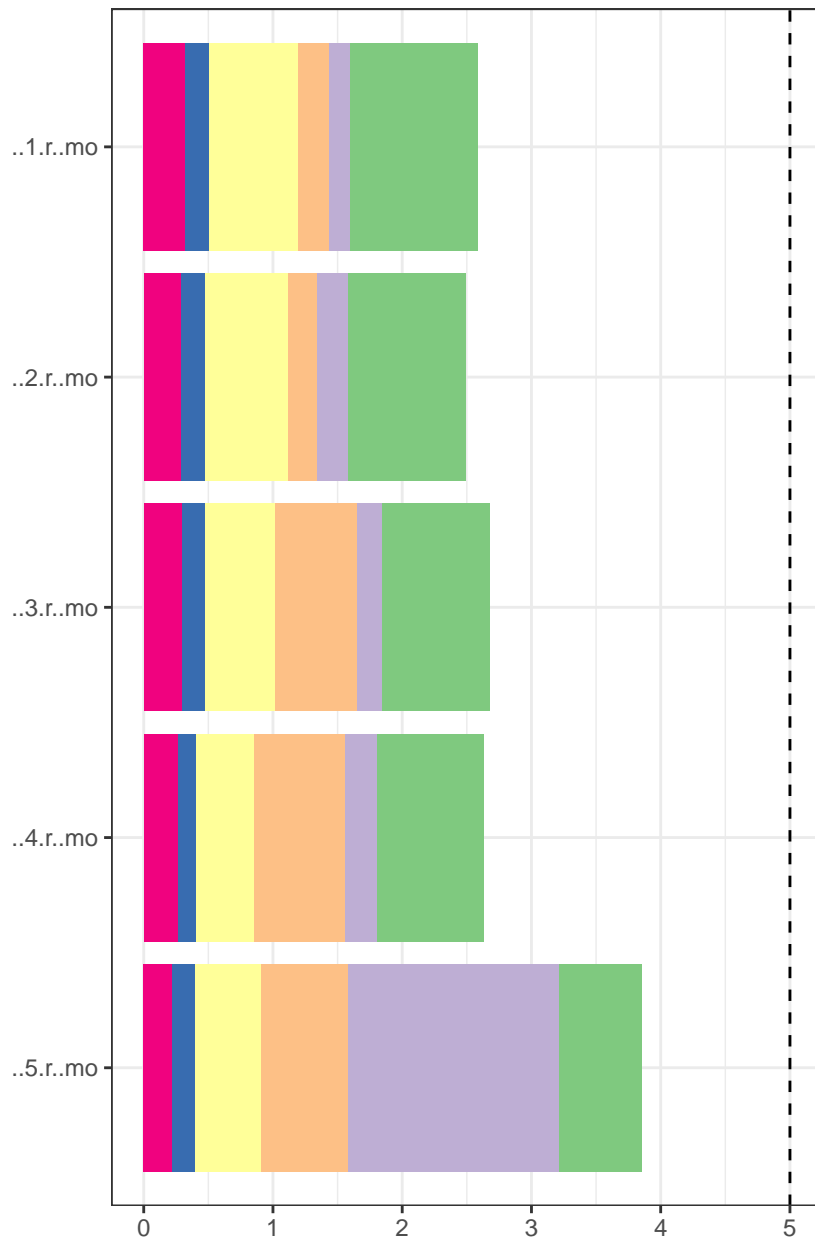
/data/dnb02/galaxy_db/files/018/324/dataset_18324059.dat

PAR: parameters

parameter	value	parameter	value
Matching time window [min]	0	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
Min. peptide Length	7	Stabilize large LFQ ratios	True
Min. peptide length for unsp..	8	Temporary folder	
Min. peptides	1	Top MS/MS peaks per Da inter..	12
Min. razor peptides	1	Top MS/MS peaks per Da inter..	8
Min. score for modified pept..	40	Top MS/MS peaks per Da inter..	10
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	12
Min. unique peptides	1	Use delta score	False
MS/MS ammonia loss (FTMS)	True	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (ITMS)	True	Use only unmodified peptides..	False
MS/MS ammonia loss (TOF)	True	User name	galaxy
MS/MS ammonia loss (Unknown)	True	Variation mode	None
MS/MS deisotoping (FTMS)	True	Version	1.6.10.43
MS/MS deisotoping (ITMS)	False	Write accumulatedPasefMsmsSc.	True
MS/MS deisotoping (TOF)	True	Write allPeptides table	True
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		

/data/dnb02/galaxy_db/files/018/324/dataset_18324059.dat

EVD: Top5 Contaminants per Raw file



Abundance class

mid

Protein

other

CON__P00761

CON__P15636

sp|P04264|K2C...;CON__P04264

sp|P13645|K1C...;CON__P13645

sp|P35527|K1C...;CON__P35527

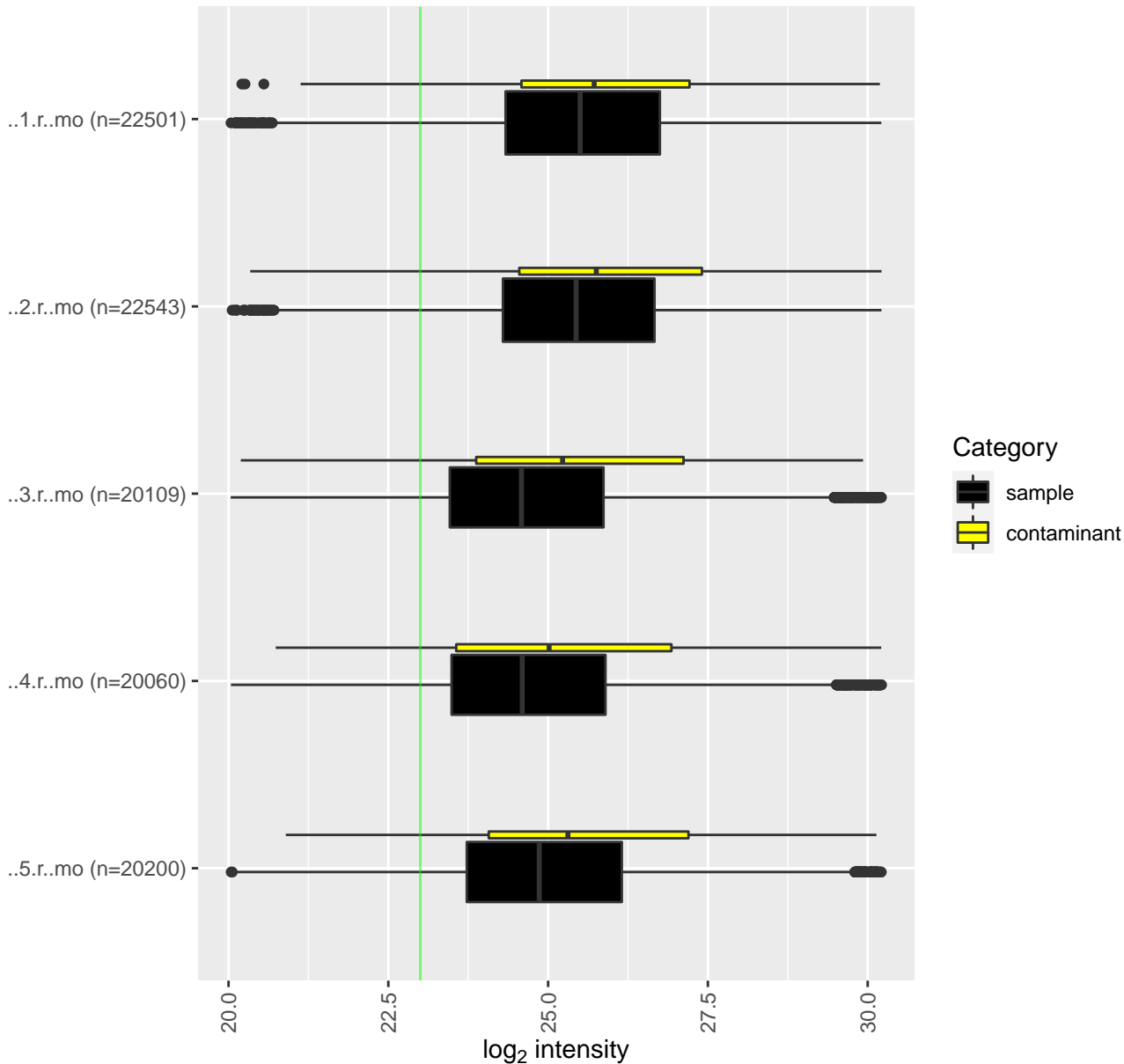
EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

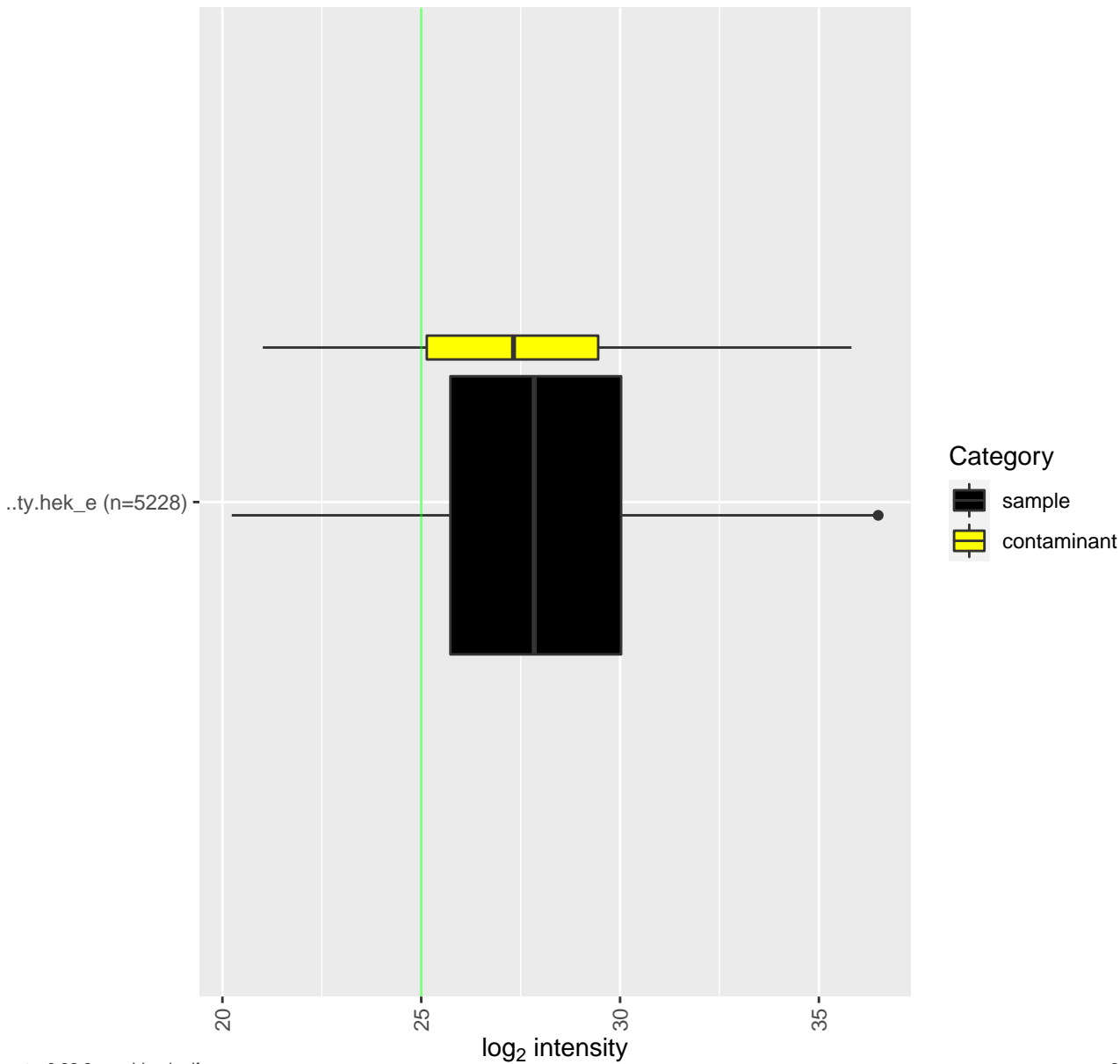
Did you use the correct database?

EVD: peptide intensity distribution

RSD 1.8% (expected < 5%)

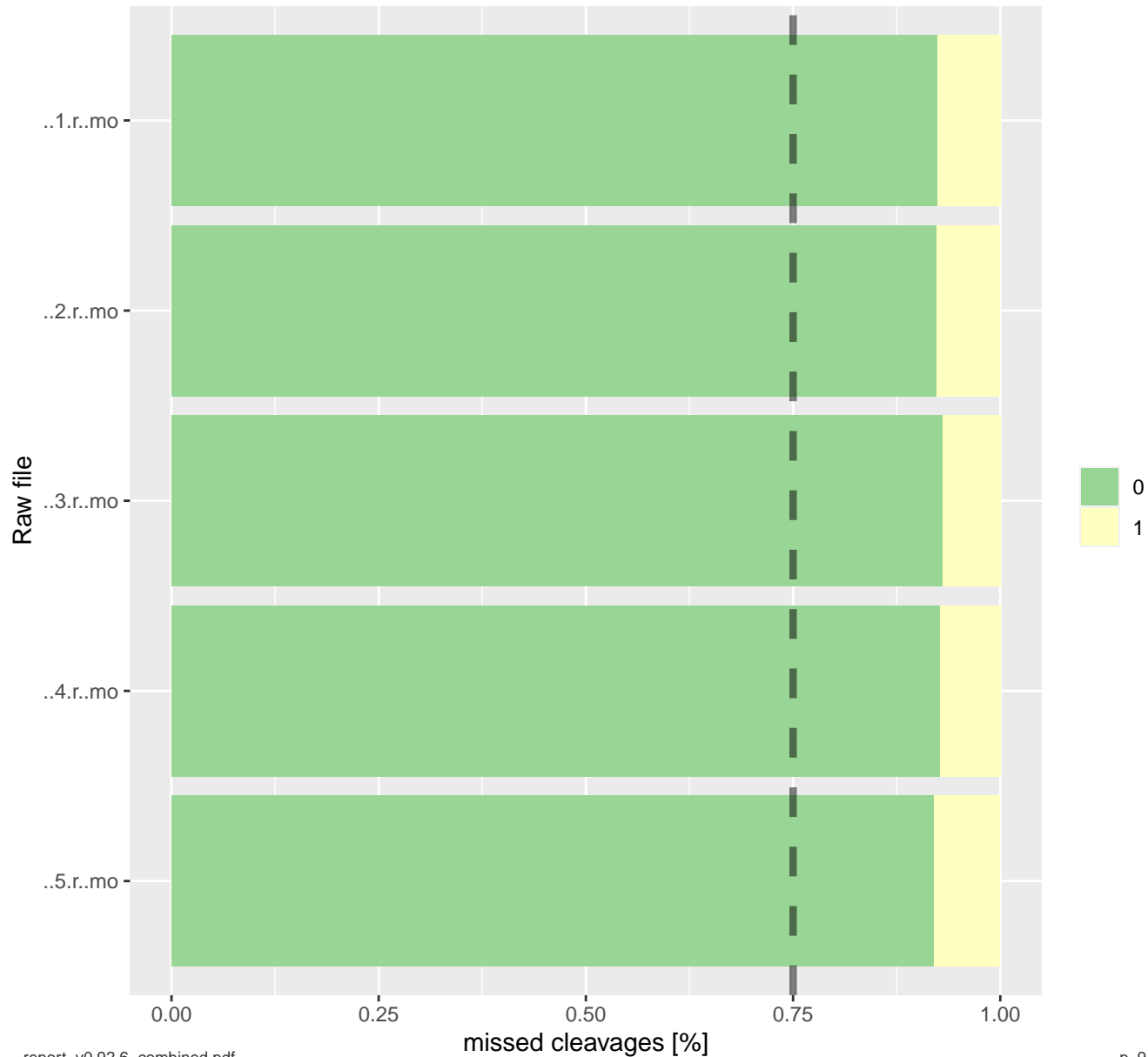


PG: intensity distribution
RSD NA% (w/o zero int.; expected < 5%)
RSD NA% [high RSD --> few peptides]

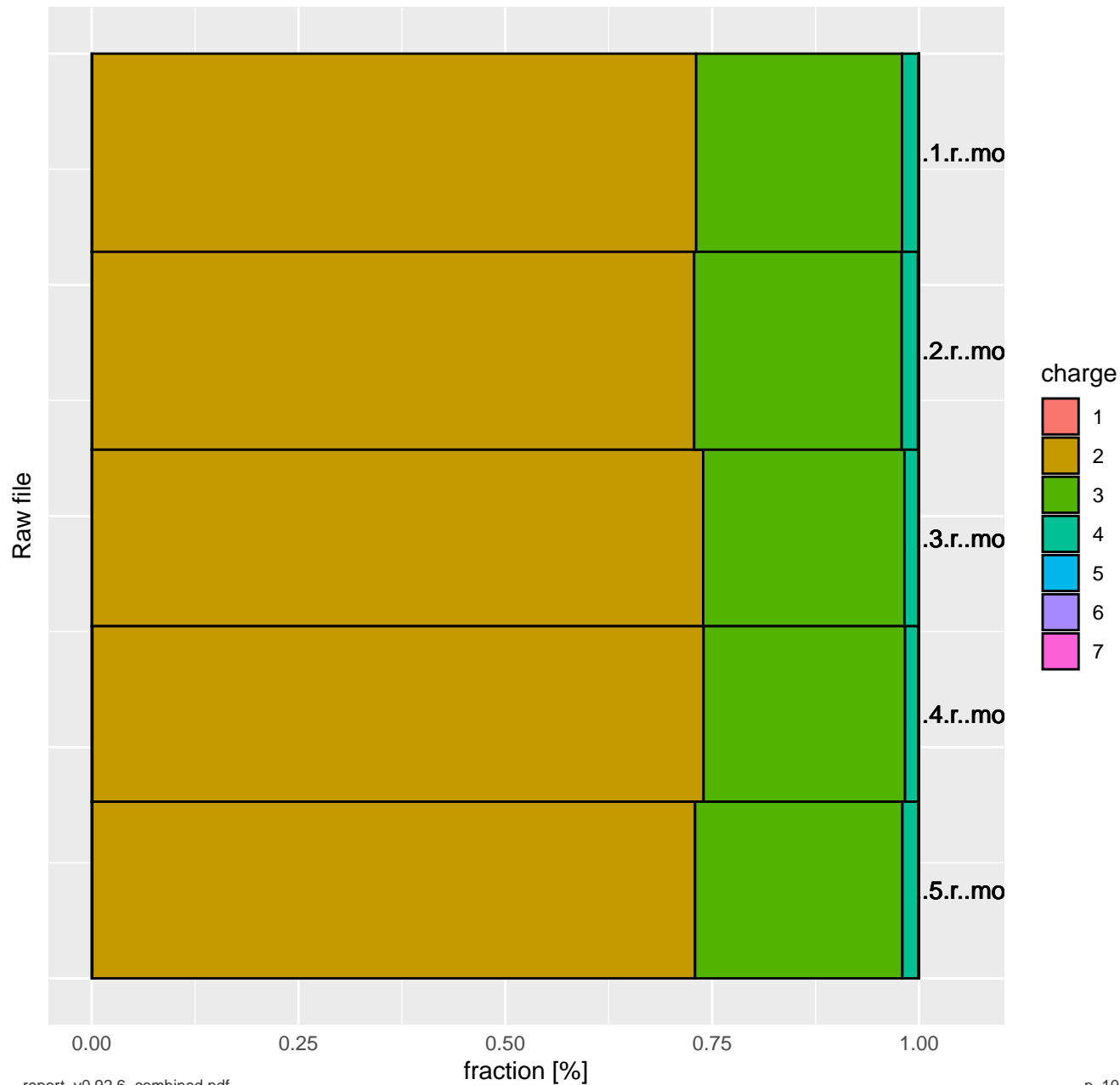


MSMS: Missed cleavages per Raw file

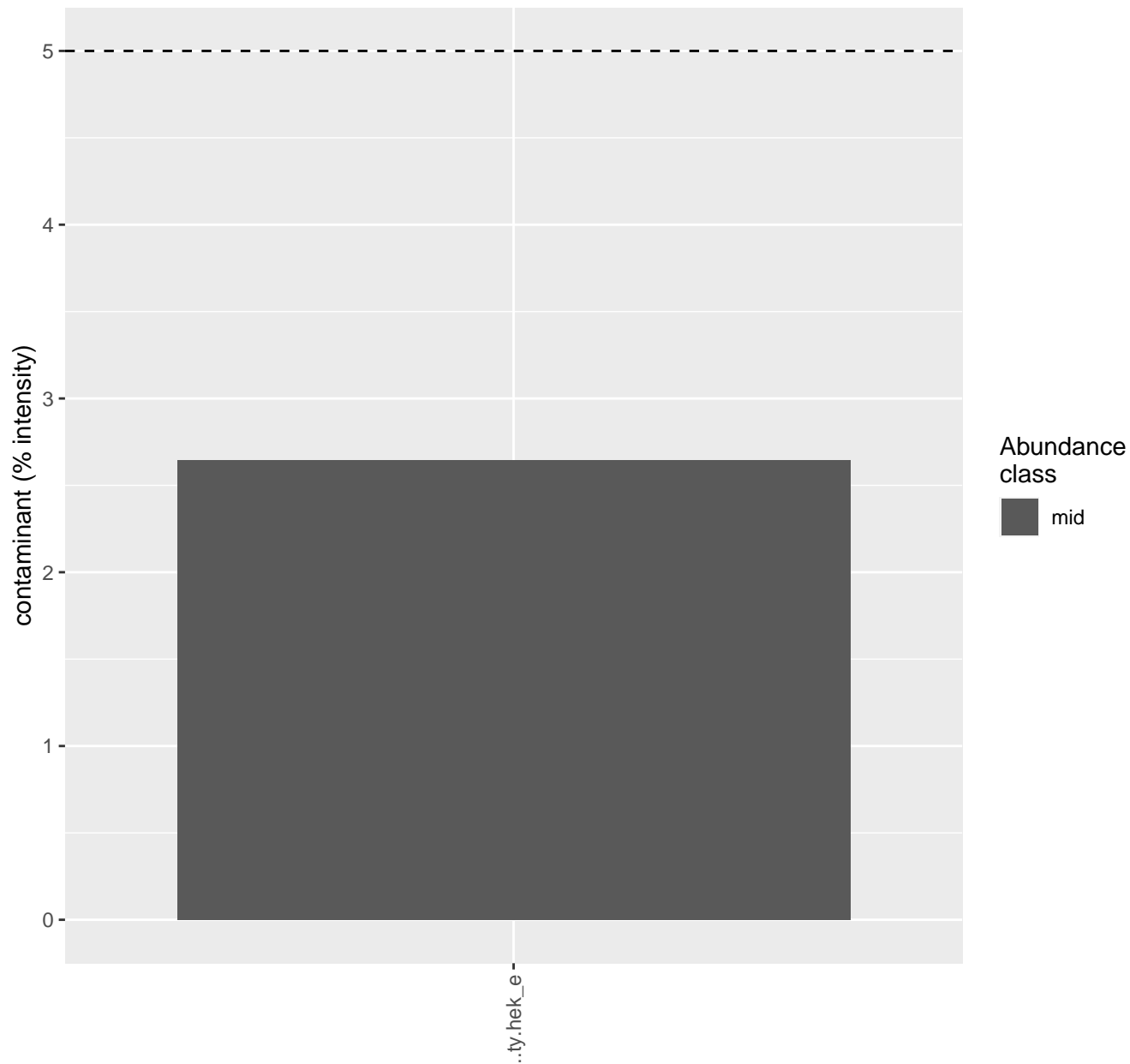
(excludes contaminants)



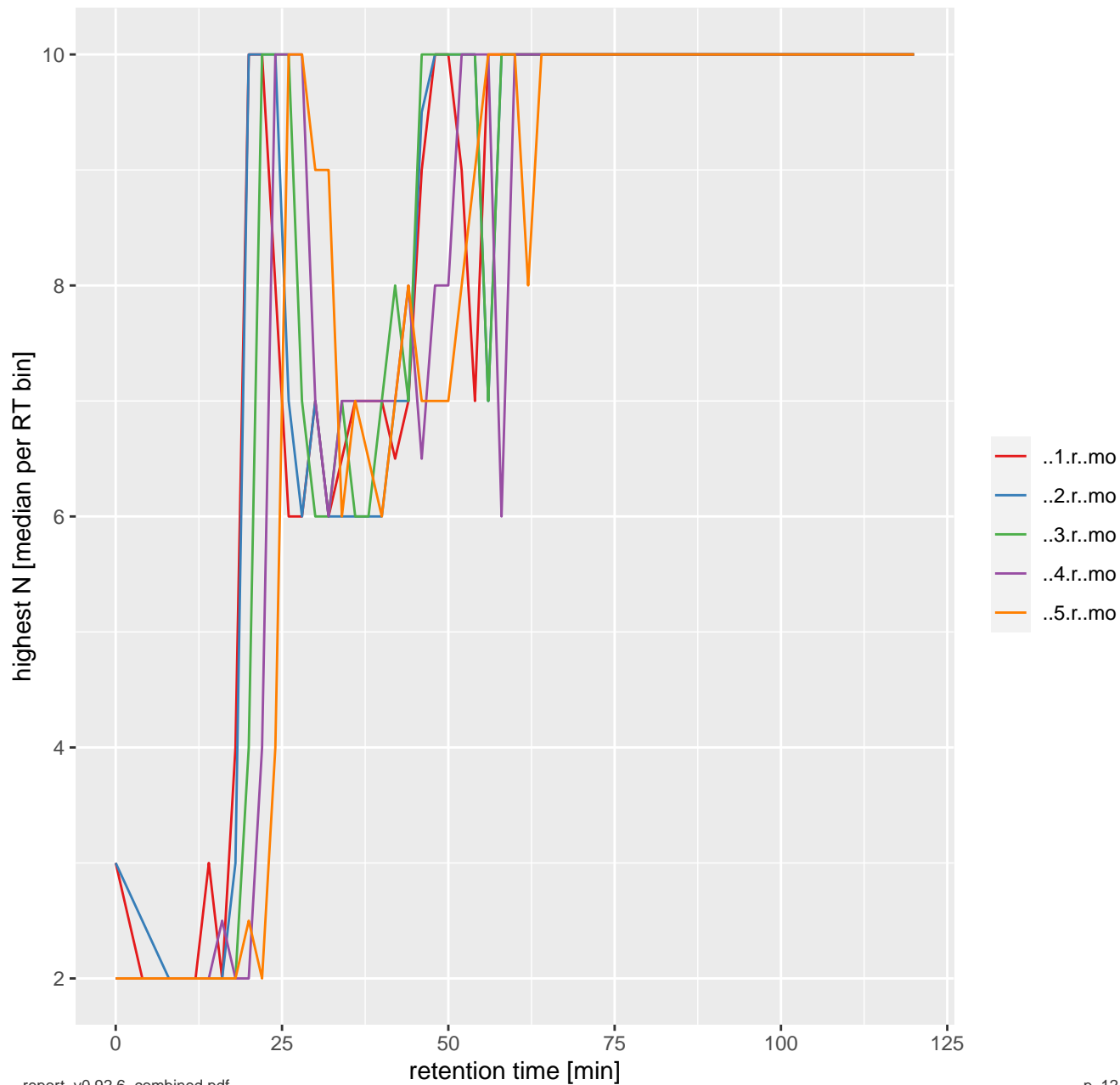
EVD: charge distribution



PG: Contaminant per condition



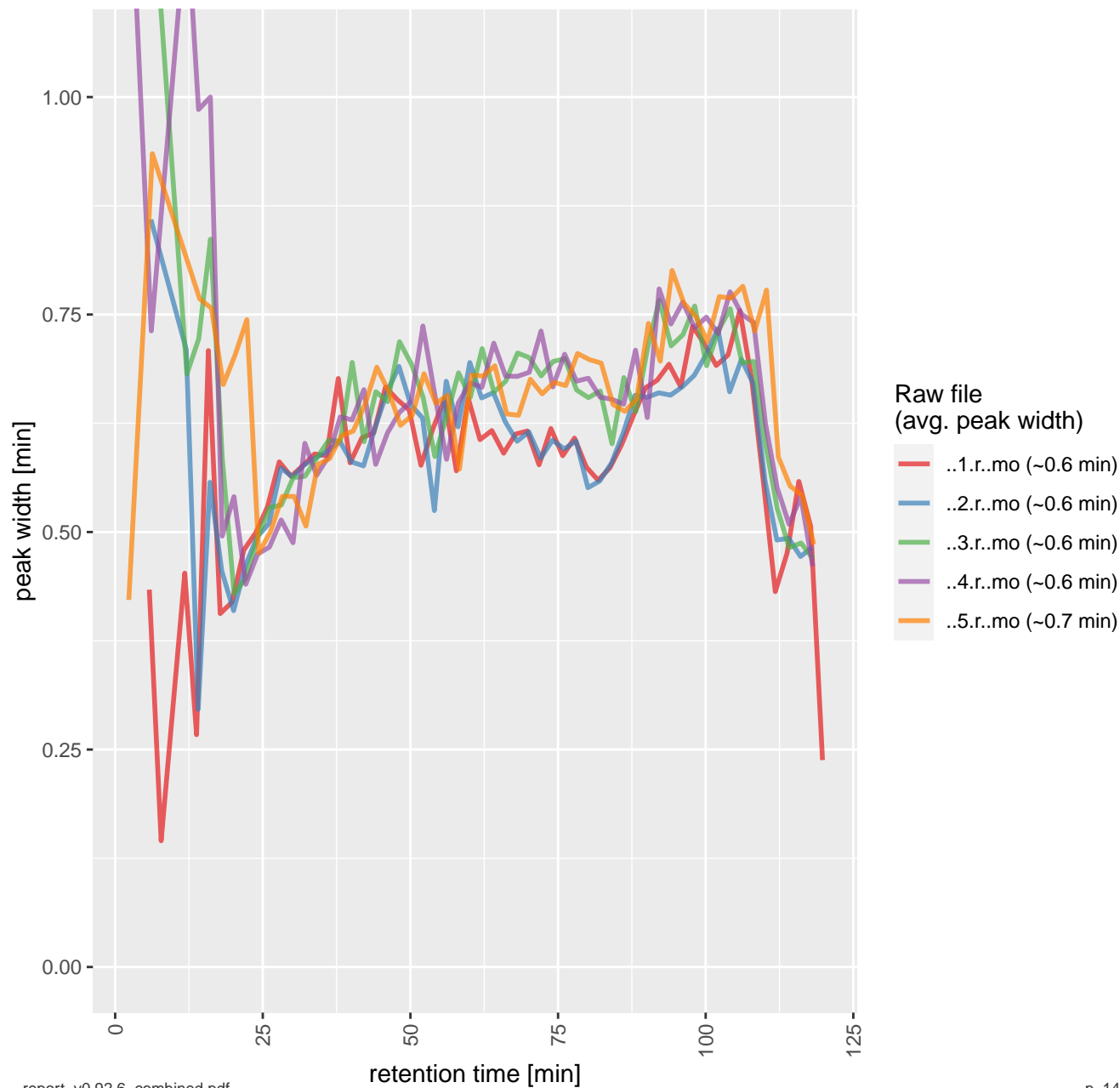
MSMSscans: TopN over RT



EVD: IDs over RT

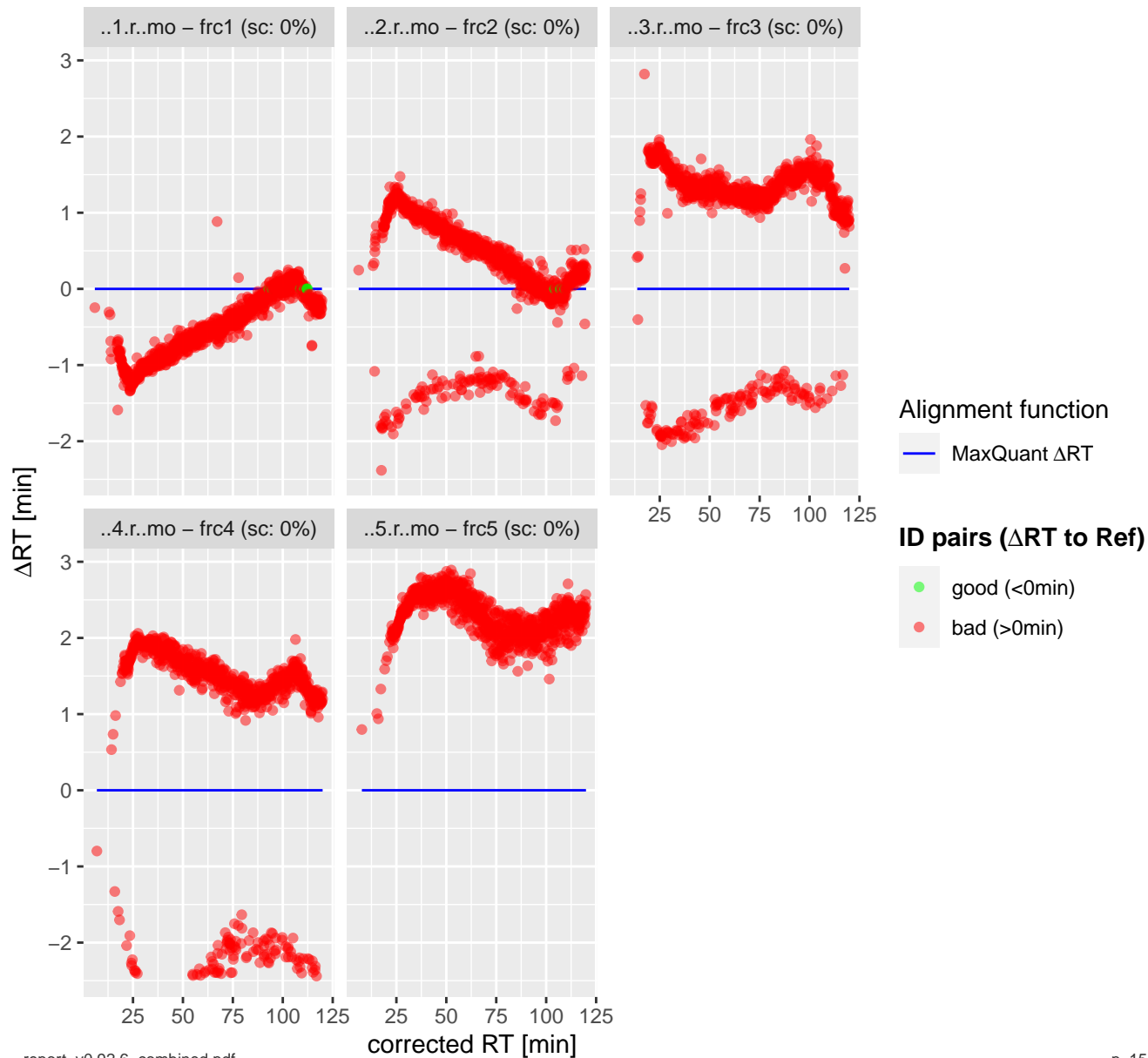


EVD: Peak width over RT

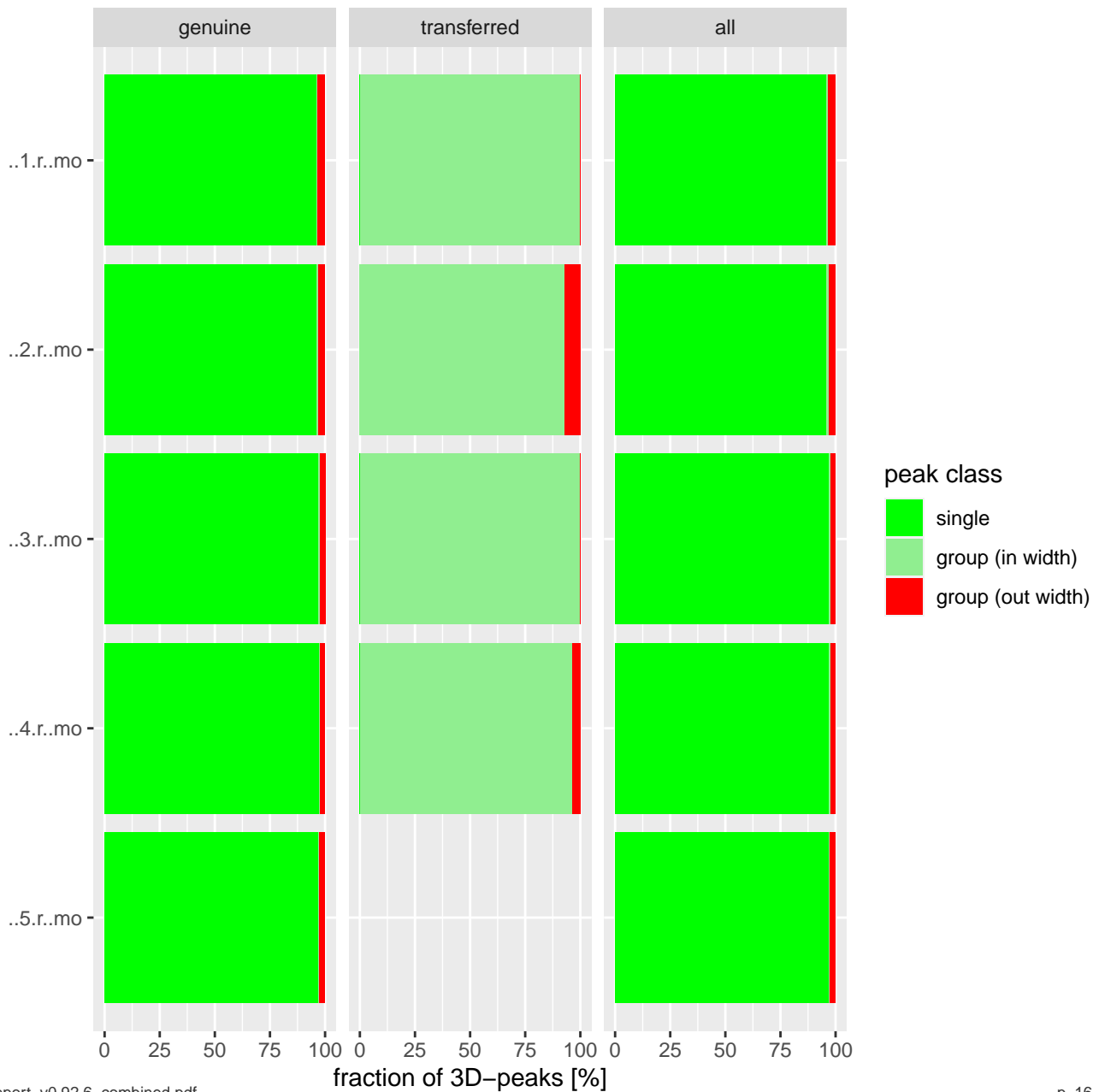


EVD: MBR – alignment

fraction: neighbour comparison

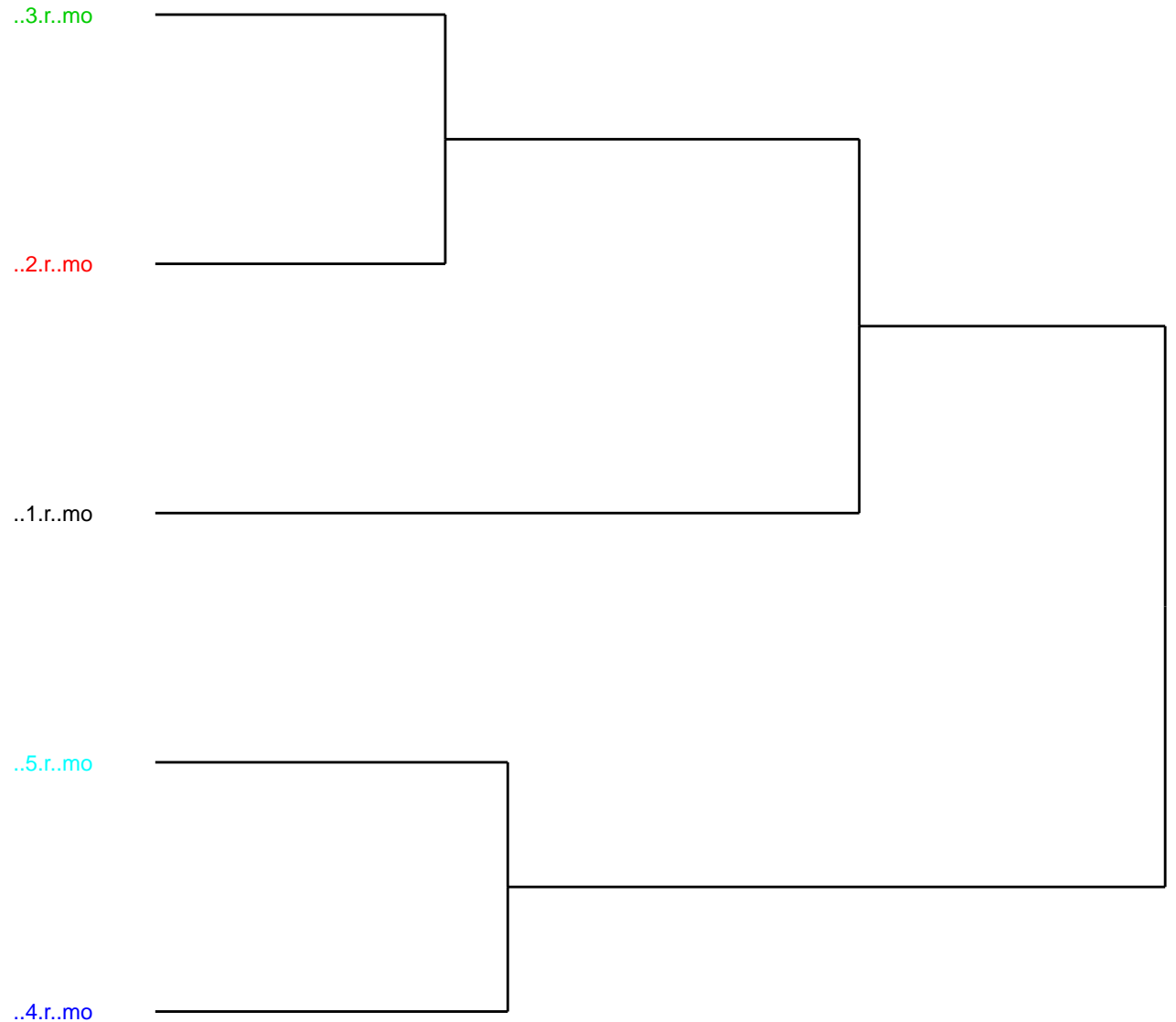


EVD: MBR – ID Transfer

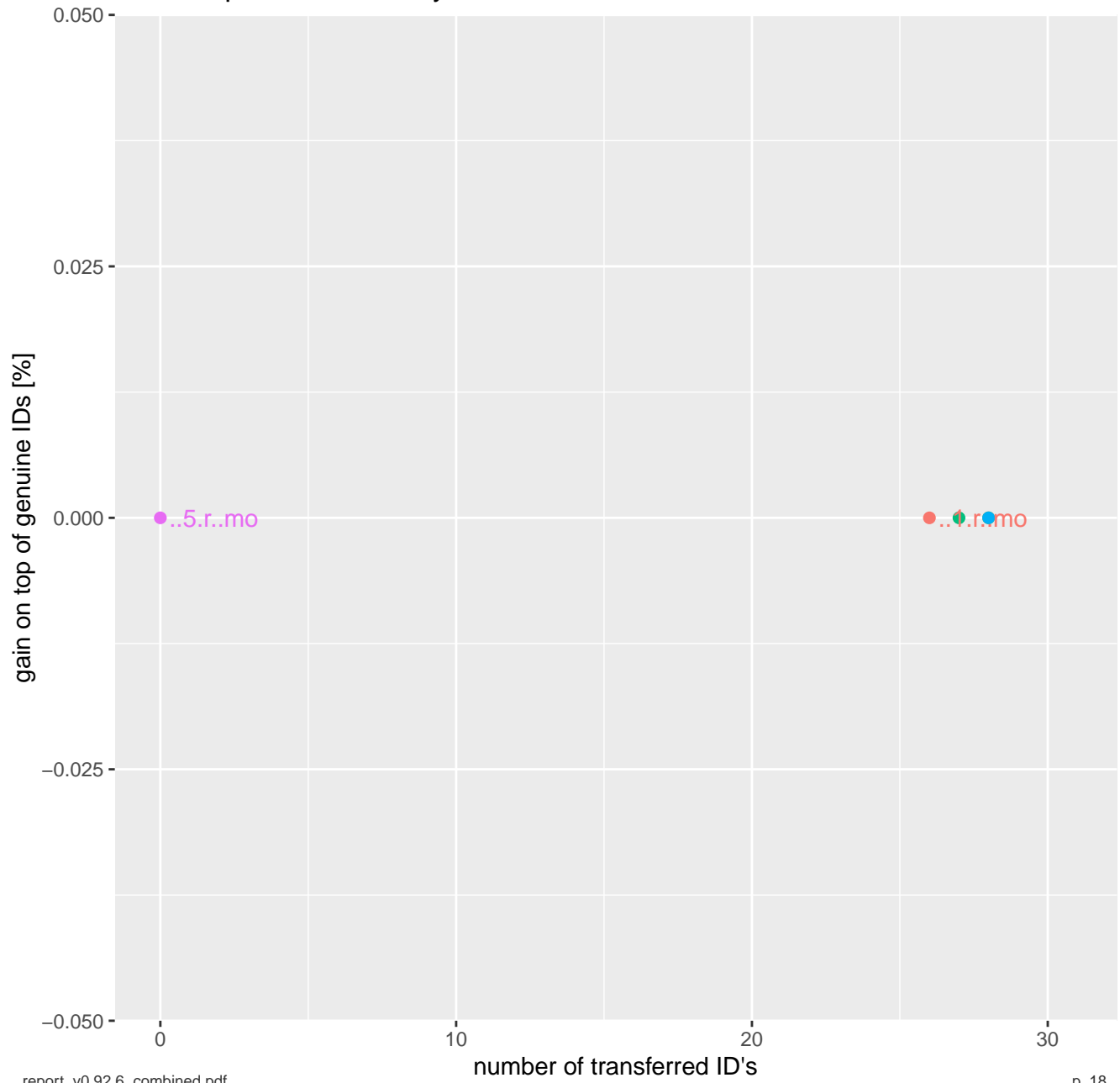


[experimental] EVD: Clustering Tree of Raw files

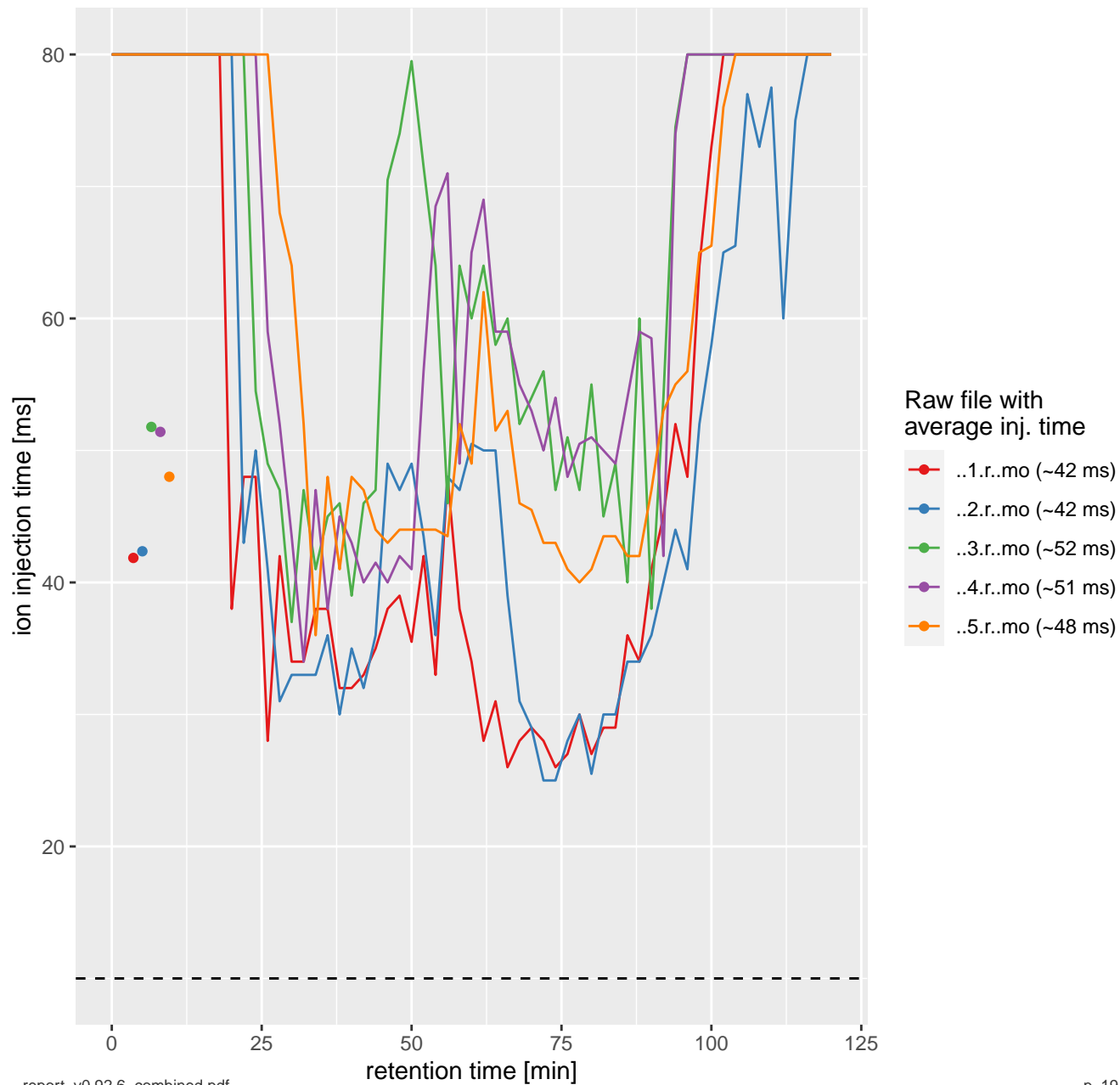
by Correlation of Corrected Retention Times



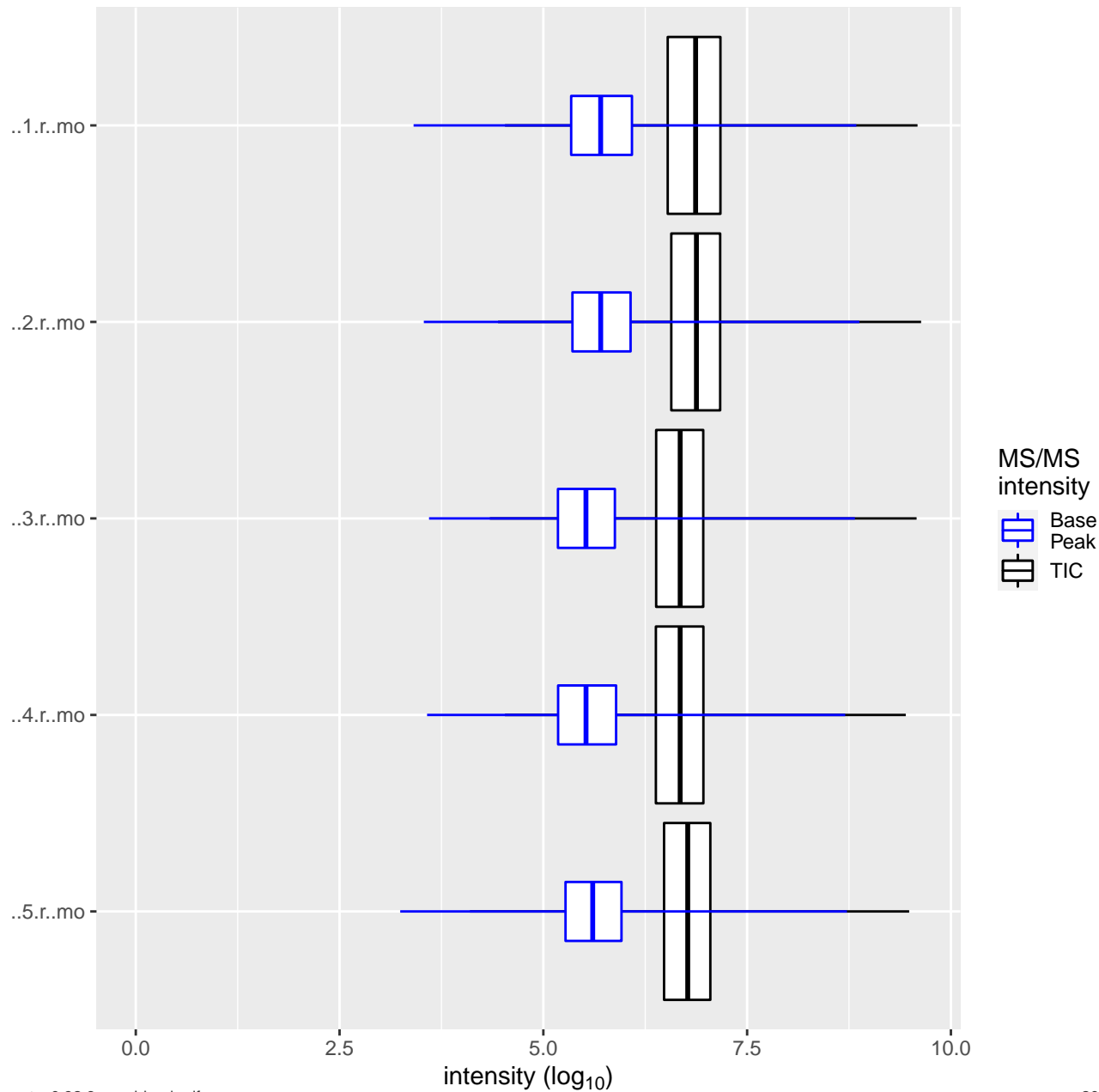
EVD: Peptides inferred by MBR



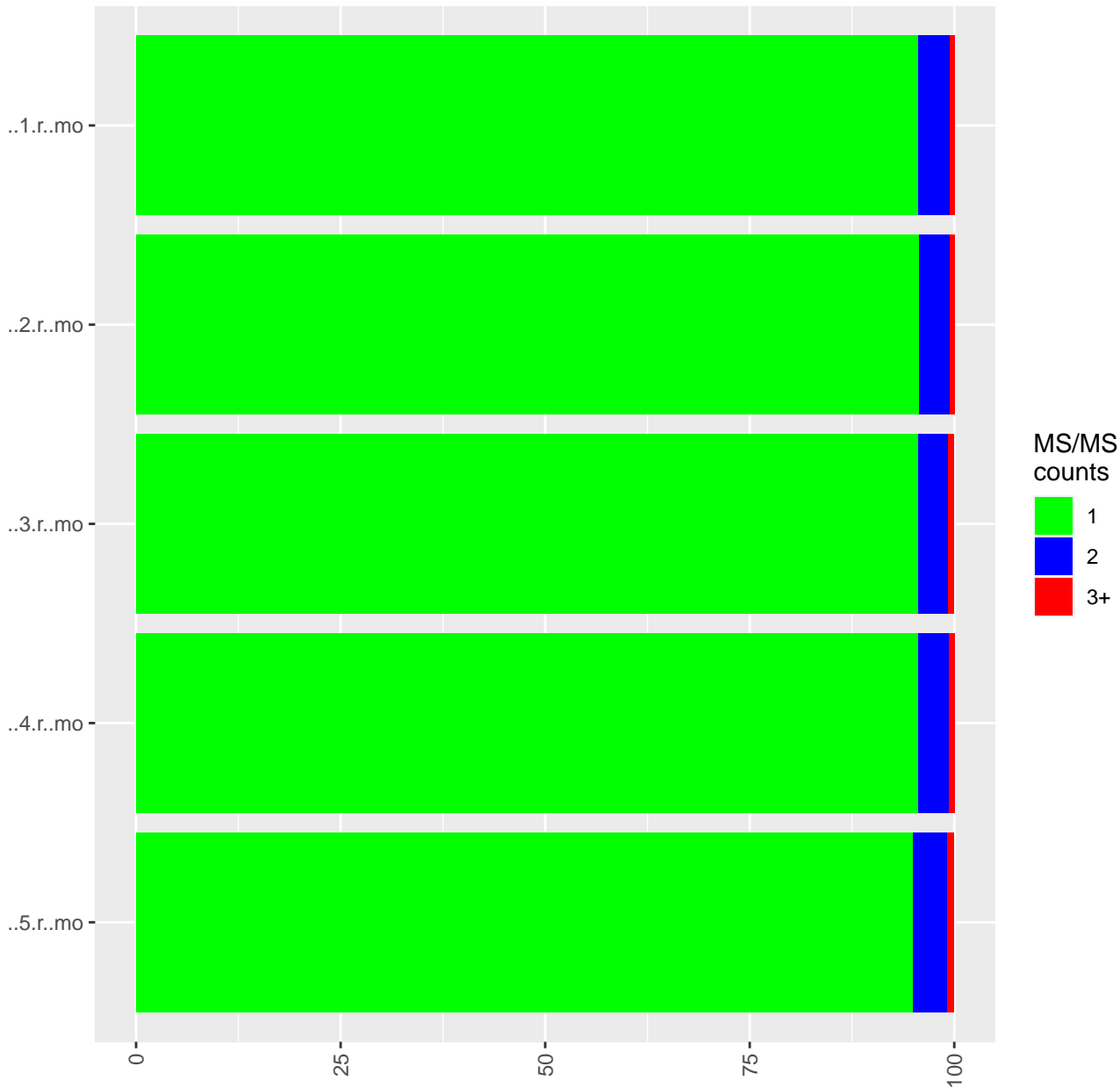
MSMSscans: Ion Injection Time over RT



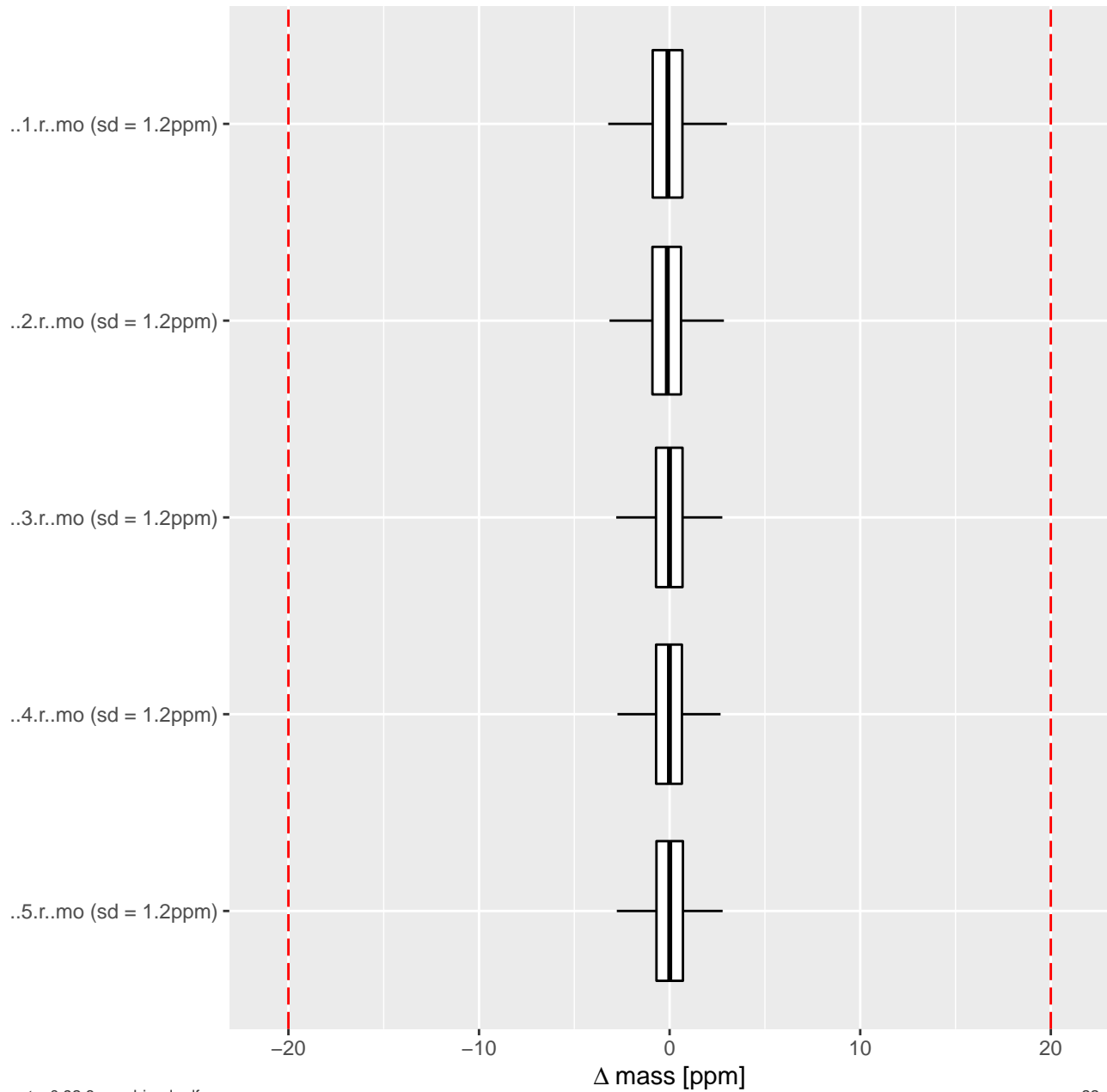
[experimental] MSMSscans: MS/MS intensity



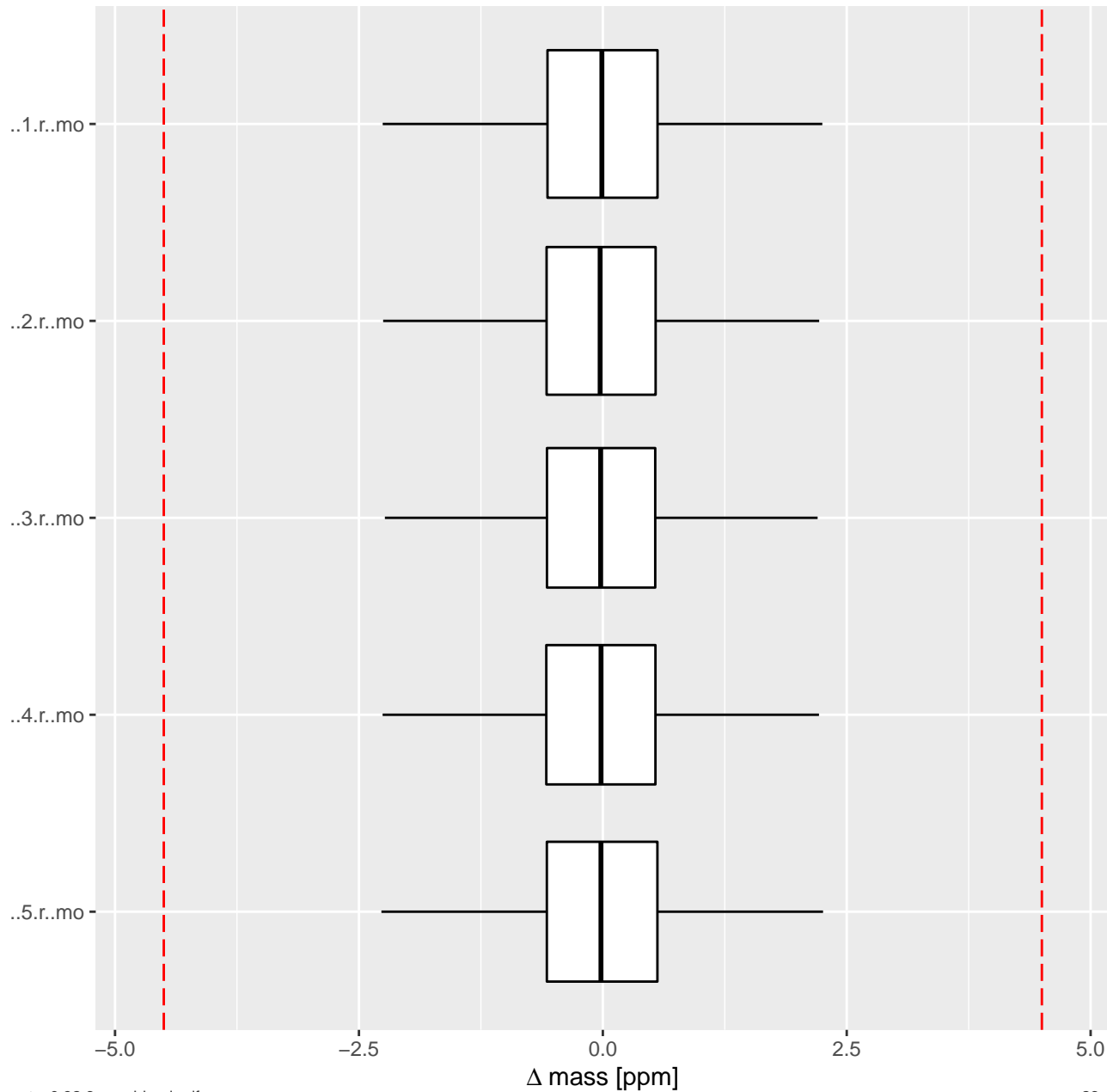
EVD: Oversampling (MS/MS counts per 3D-peak)



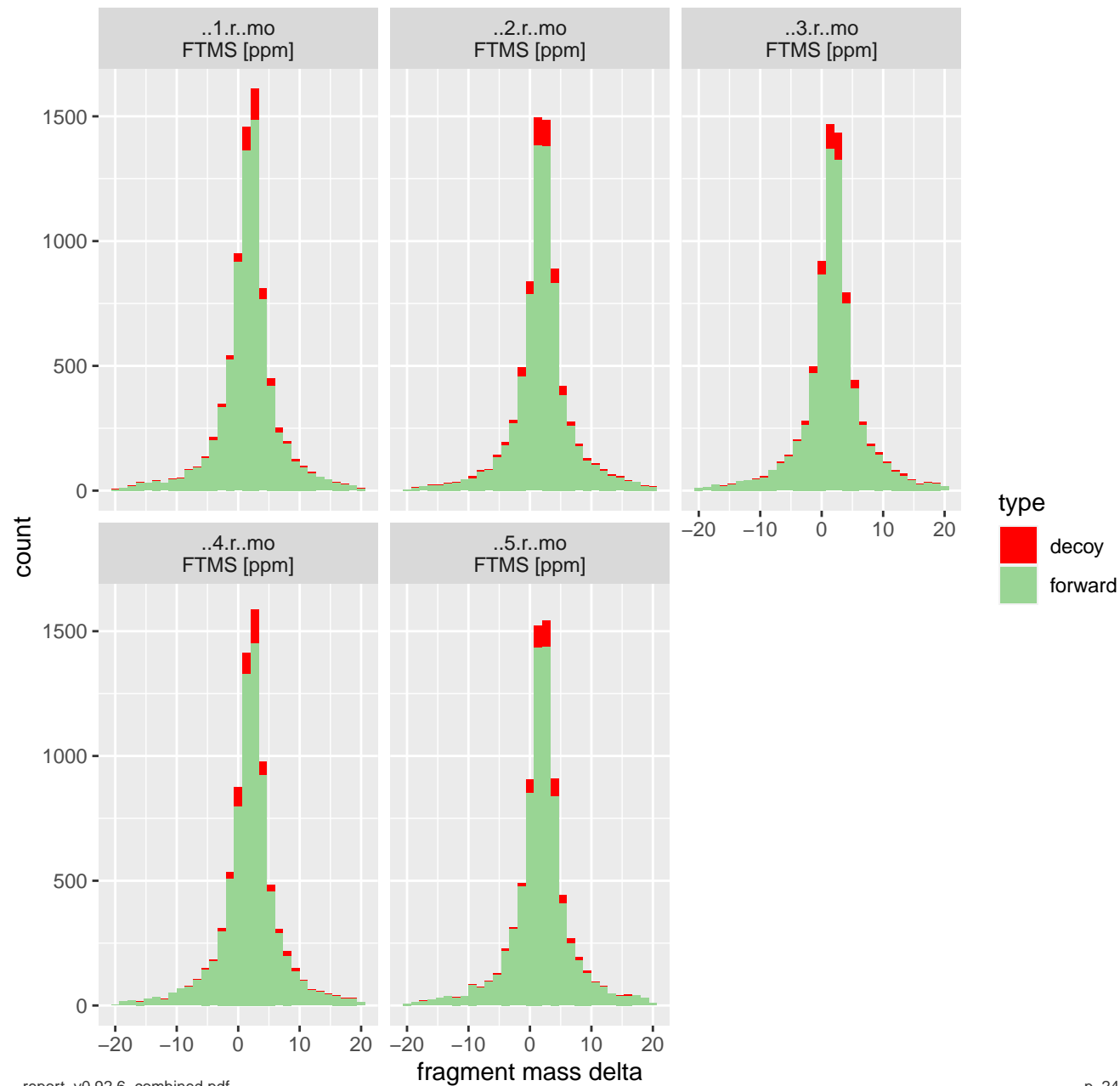
EVD: Uncalibrated mass error



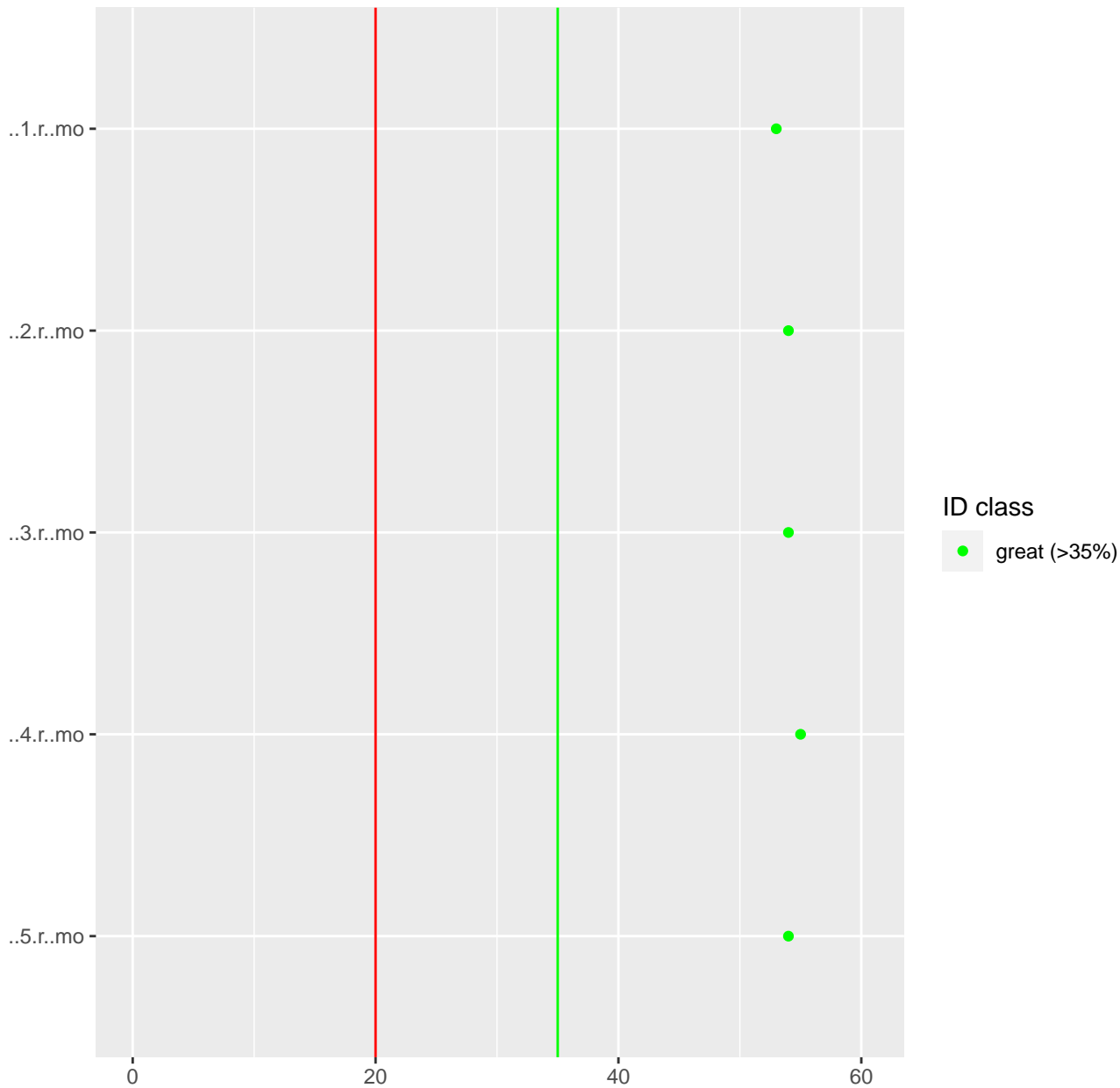
EVD: Calibrated mass error



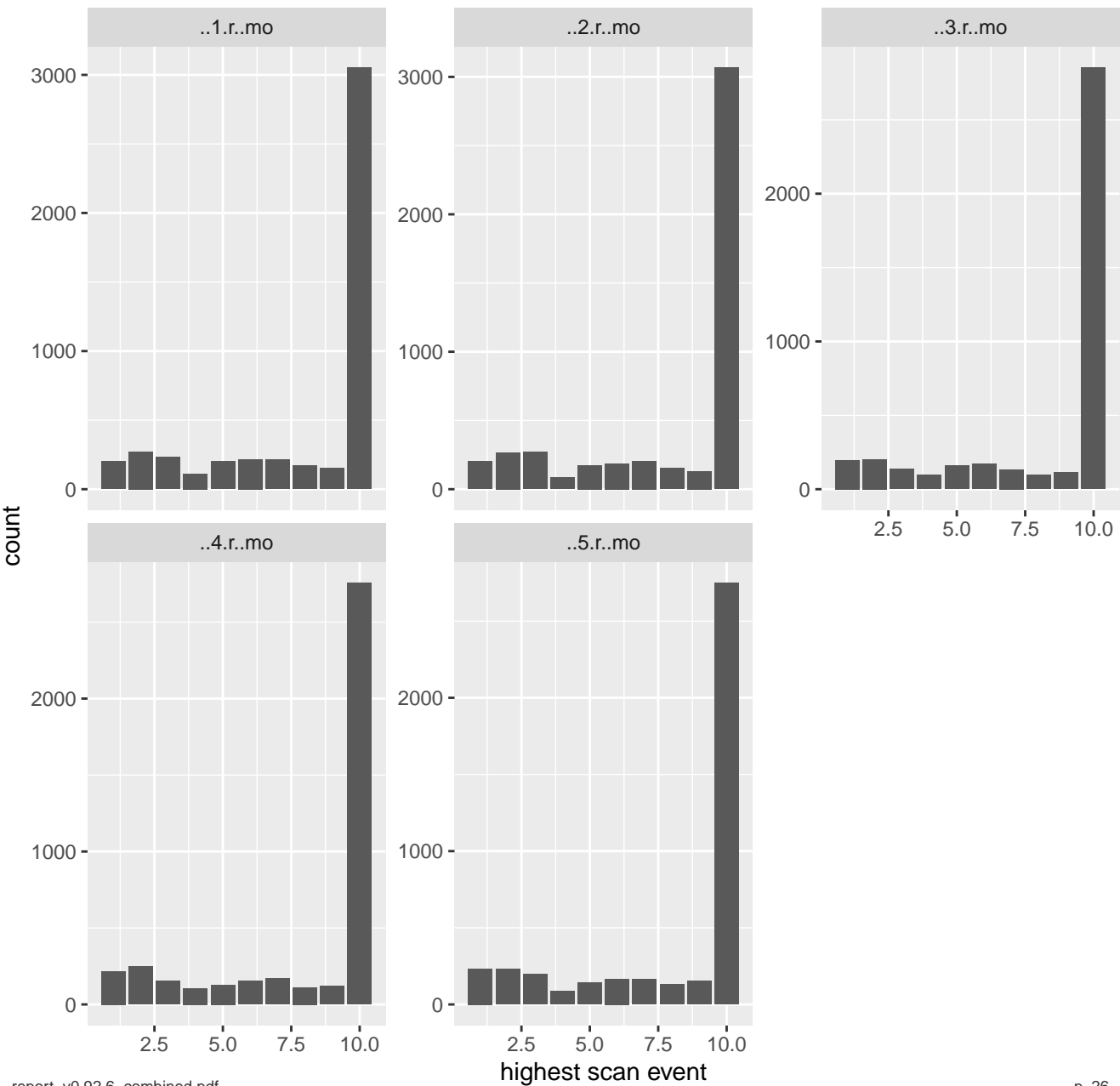
MSMS: Fragment mass errors per Raw file



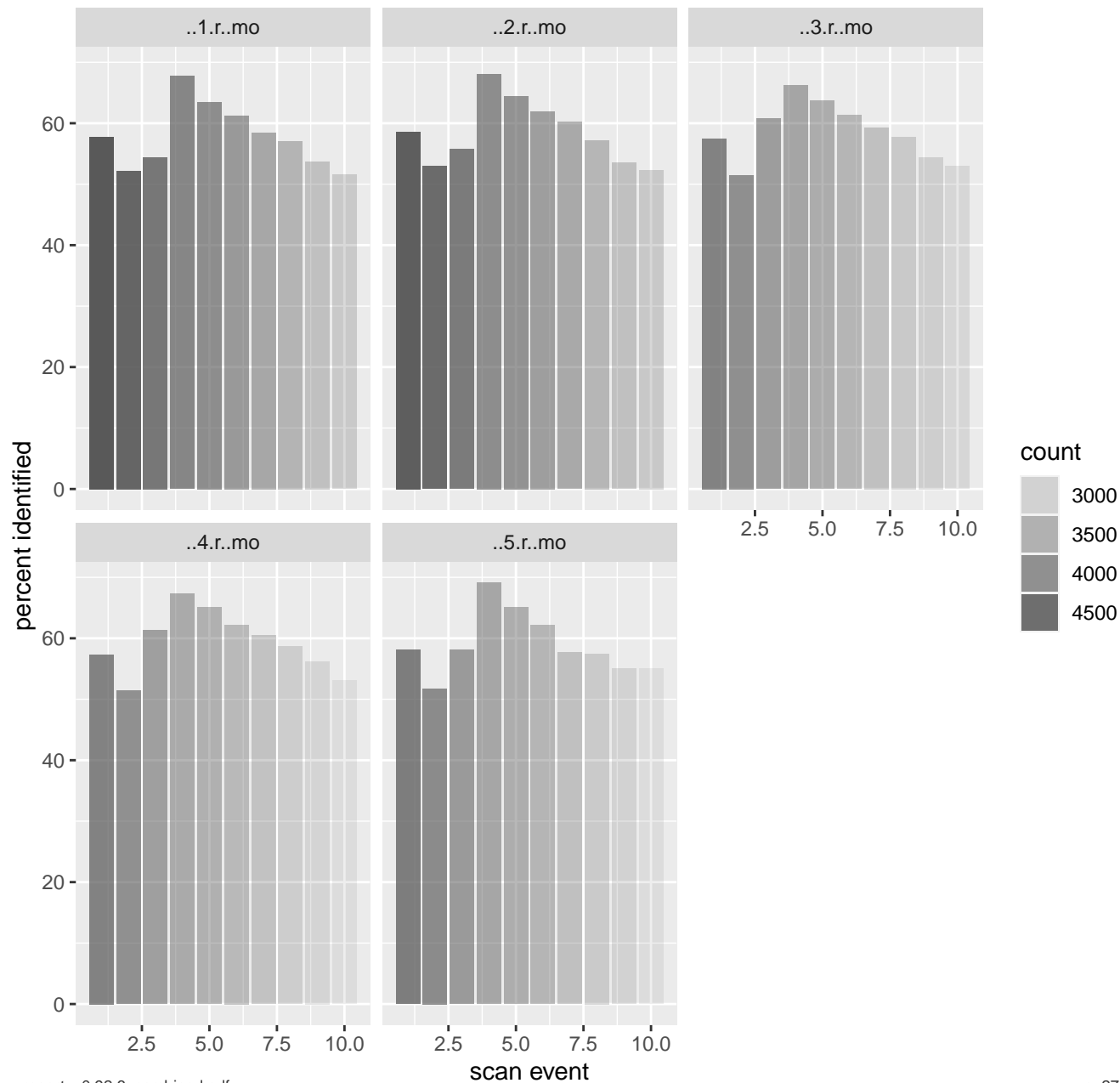
SM: MS/MS identified per Raw file



MSMSscans: TopN



MSMSscans: TopN % identified over N

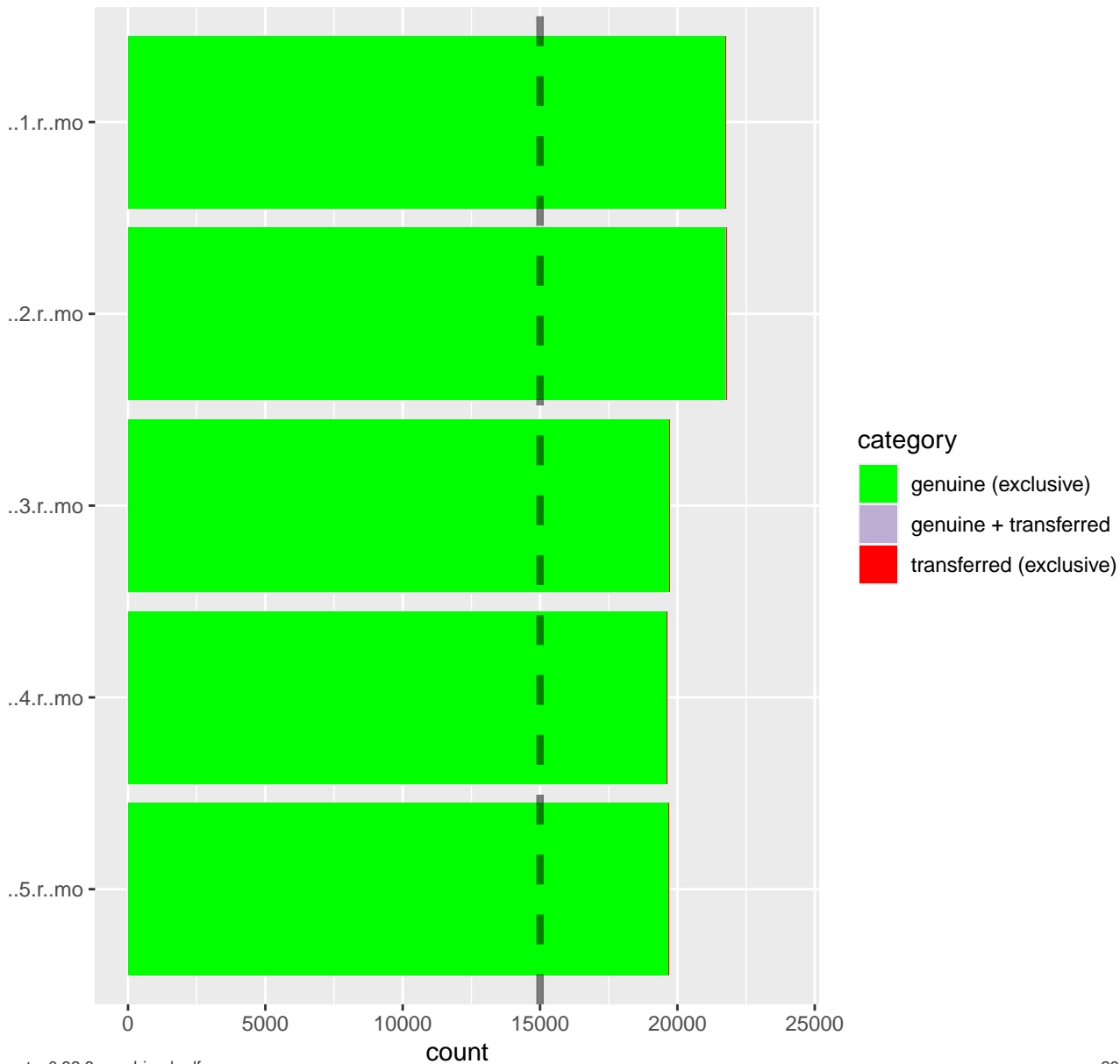


Missing Values Skipped

Missing values calculation skipped. Fractionated data detected!

EVD: Peptide ID count

MBR gain: +0%



EVD: ProteinGroups count

MBR gain: +0%

