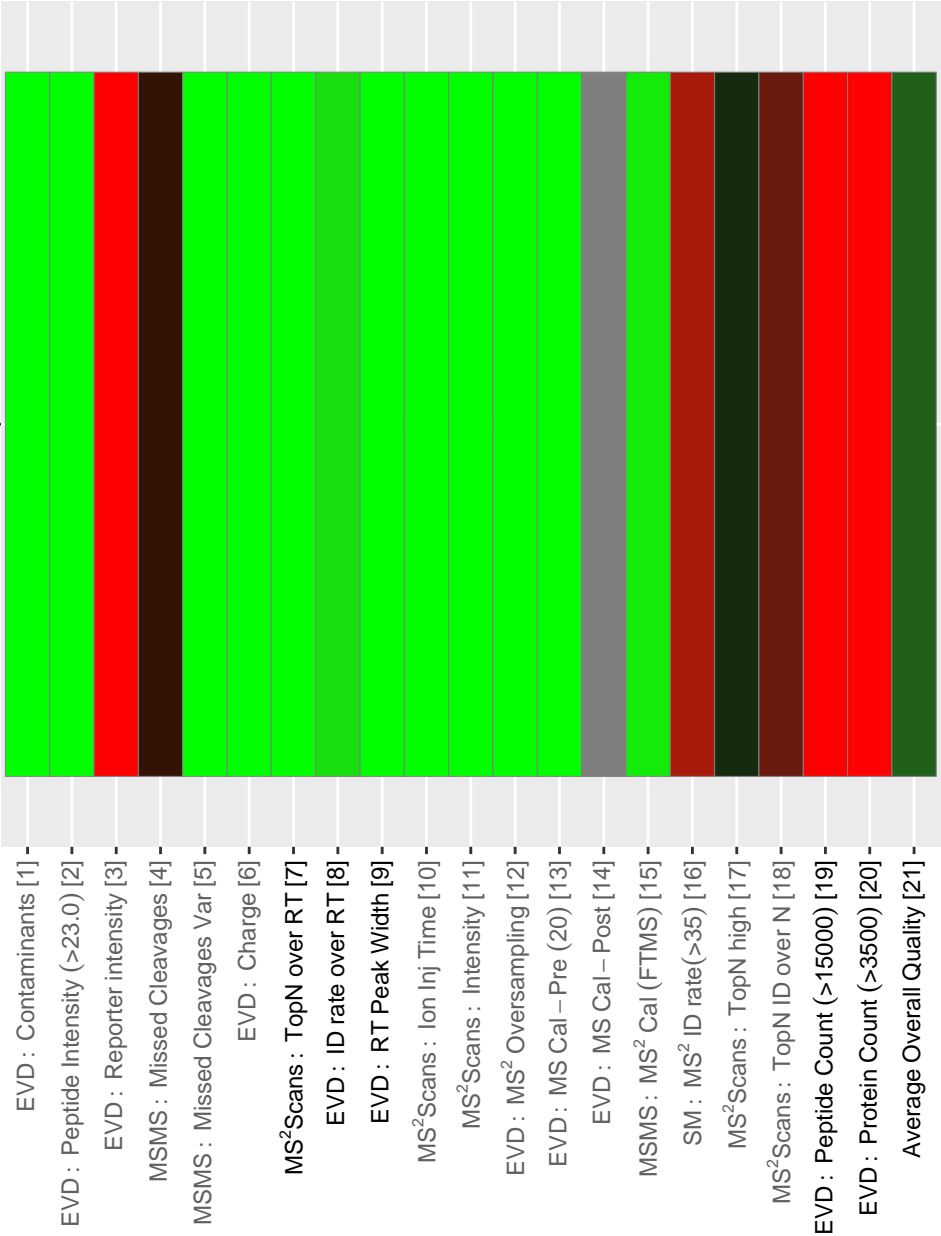


Performance overview

Raw file

tmt_data -



Missing

NA

score

best

under performing

fail

Mapping of Raw files to their short names

Mapping source: automatic

original	short name	best effort
----------	---------------	----------------

tmt_data	tmt_data	tmt_data
----------	----------	----------

PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	MS/MS deisotoping tolerance ..	ppm
Advanced site intensities	True	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	04/27/2023 14:54:17	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..	False	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	mthang-sandpit.qfab.org	MS/MS water loss (Unknown)	True
Main search max. combination..	200	Peptides used for protein qu..	Razor
Match between runs	False	Protein FDR	0.01
Match unidentified features	False	PSM FDR	0.01
Max mods in site table	3	PSM FDR Crosslink	0.01
Max. peptide length for unsp..	25	Razor protein FDR	True

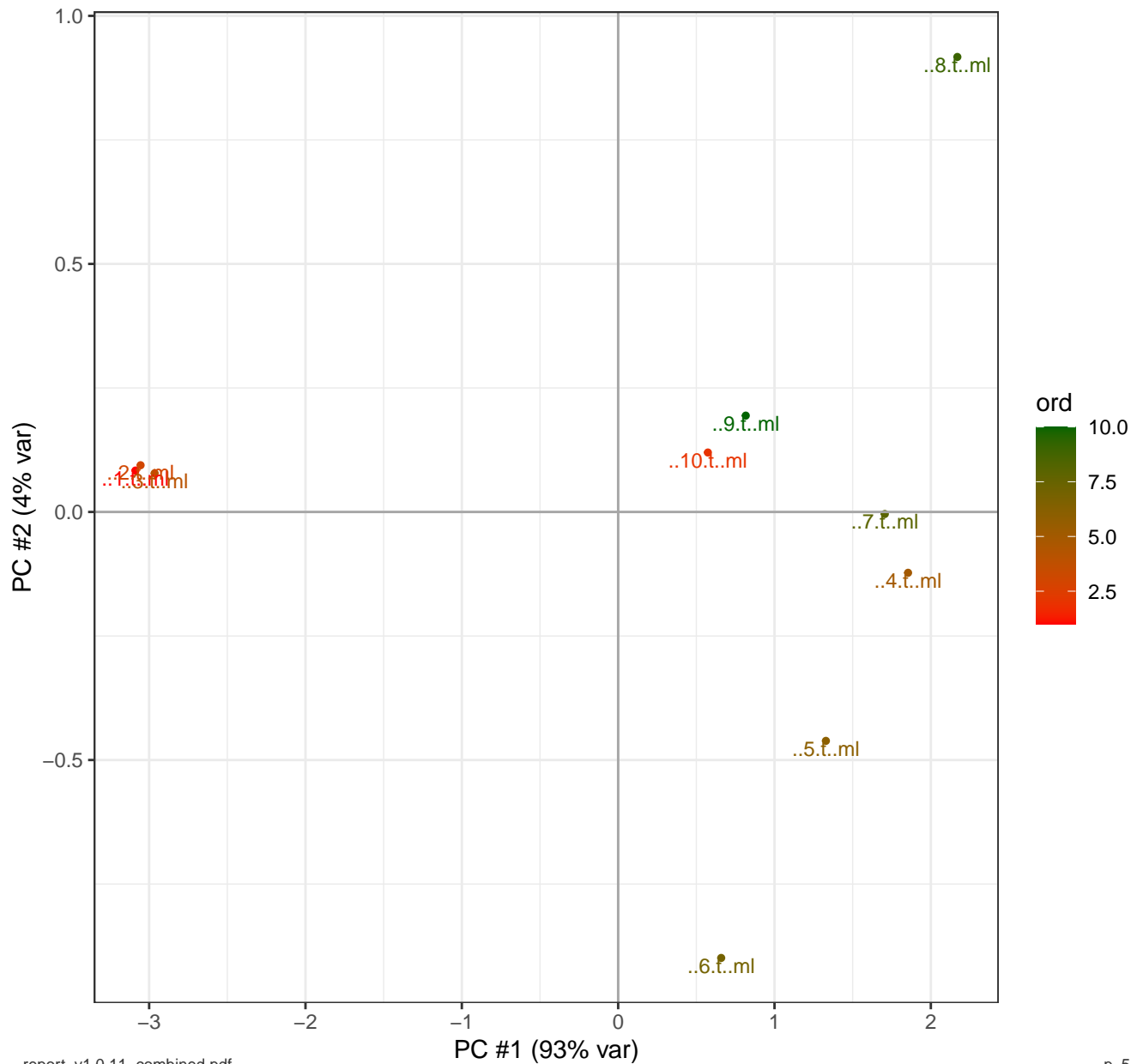
/tmp/tmpuhlzy3c0/files/0/7/5/dataset_07512022-d1df-45a6-a62a-7603afe38d6b.dat

PAR: parameters

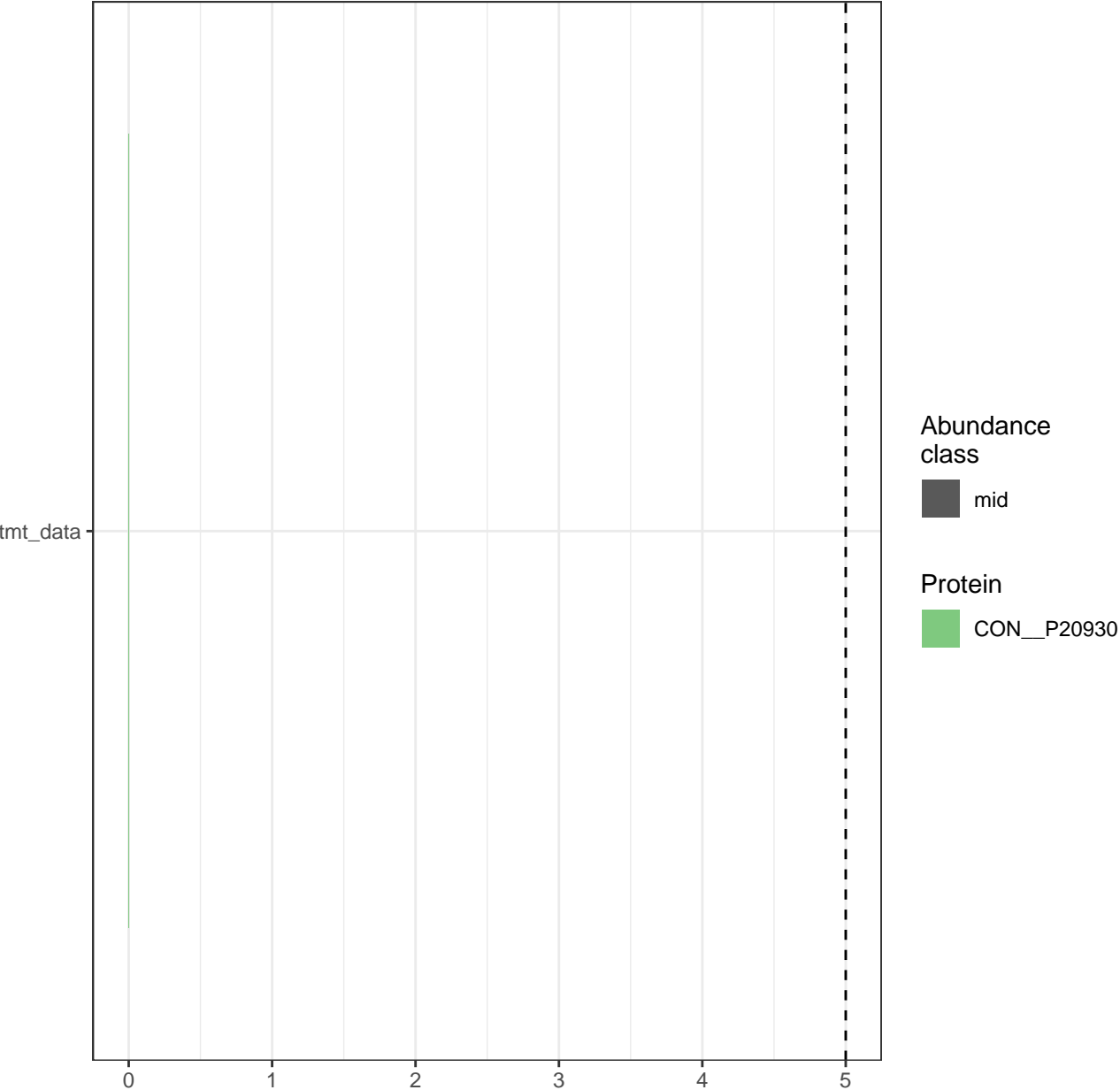
parameter	value	parameter	value
Max. peptide mass [Da]	4600	Require MS/MS for LFQ compar..	True
Min. delta score for modifie..	6	Second peptides	True
Min. delta score for unmodif..	0	Separate LFQ in parameter gr..	False
Min. peptide Length	7	Site FDR	0.01
Min. peptide length for unsp..	8	Site tables	Oxidation (M)Sites.txt
Min. peptides	1	Stabilize large LFQ ratios	True
Min. razor peptides	1	Top MS/MS peaks per Da inter..	12
Min. score for modified pept..	40	Top MS/MS peaks per Da inter..	8
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	10
Min. unique peptides	0	Top MS/MS peaks per Da inter..	12
Modifications included in pr..	Oxidation (M) Acetyl (Protein N-term)	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..	True
MS/MS ammonia loss (TOF)	True	User name	m.thang
MS/MS ammonia loss (Unknown)	True	Variation mode	None
MS/MS deisotoping (FTMS)	True	Version	2.0.3.0
MS/MS deisotoping (ITMS)	False	Write accumulatedMsmsScans t..	True
MS/MS deisotoping (TOF)	True	Write allPeptides table	True
MS/MS deisotoping (Unknown)	True	Write DIA fragments quant ta..	False
MS/MS deisotoping tolerance ..	7	Write DIA fragments table	False
MS/MS deisotoping tolerance ..	ppm	Write ms3Scans table	True
MS/MS deisotoping tolerance ..	0.15	Write msmsScans table	True
MS/MS deisotoping tolerance ..	Da	Write msScans table	False
MS/MS deisotoping tolerance ..	0.01	Write mzRange table	True
MS/MS deisotoping tolerance ..	Da	Write pasefMsmsScans table	True
MS/MS deisotoping tolerance ..	7		

/tmp/tmpuhlzy3c0/files/0/7/5/dataset_07512022-d1df-45a6-a62a-7603afe38d6b.dat

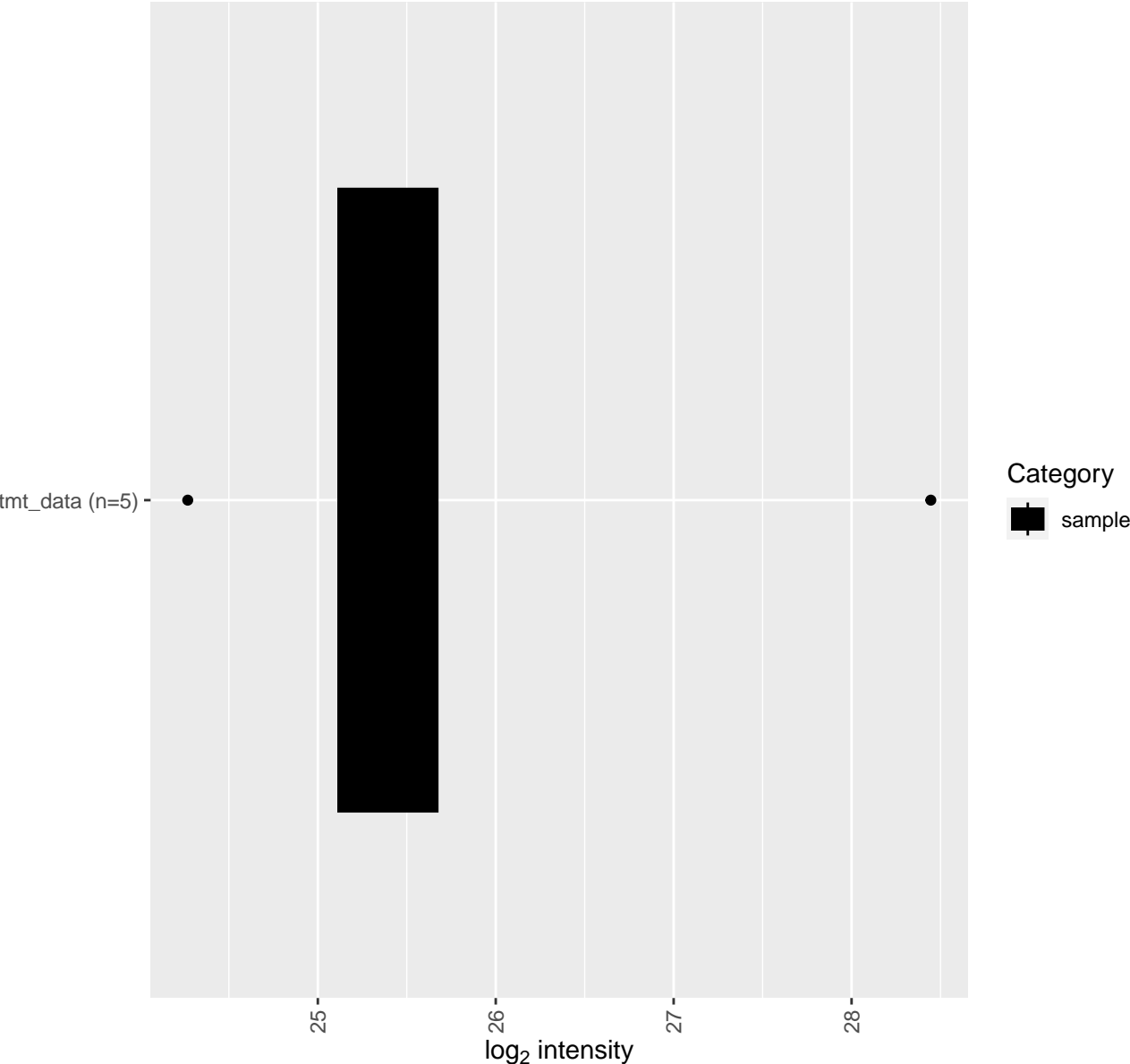
PG: PCA of 'reporter intensity'
(excludes contaminants)



EVD: Top5 Contaminants per Raw file

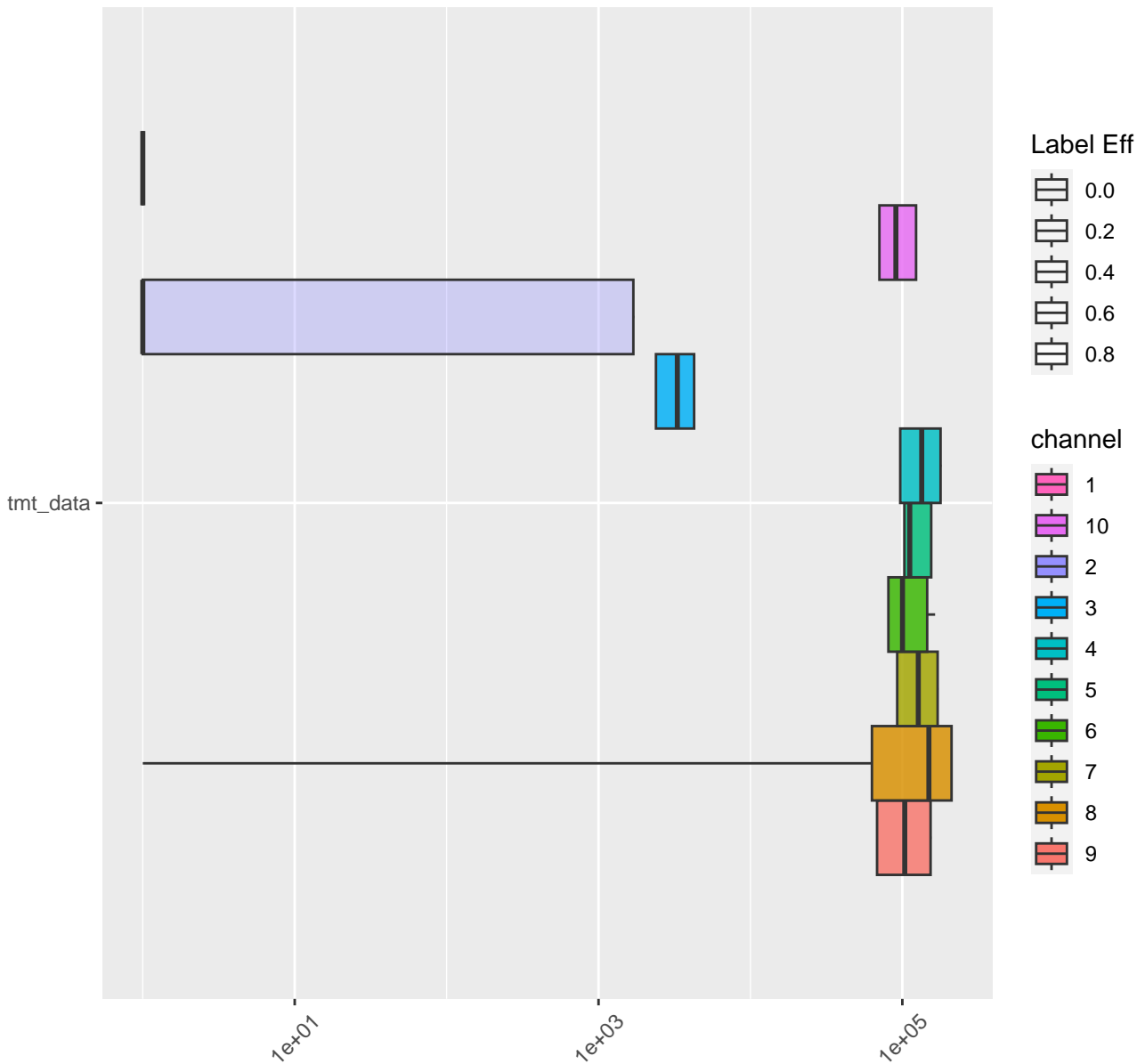


EVD: peptide intensity distribution
RSD NA% (expected < 5%)



EVD: Reporter label intensities

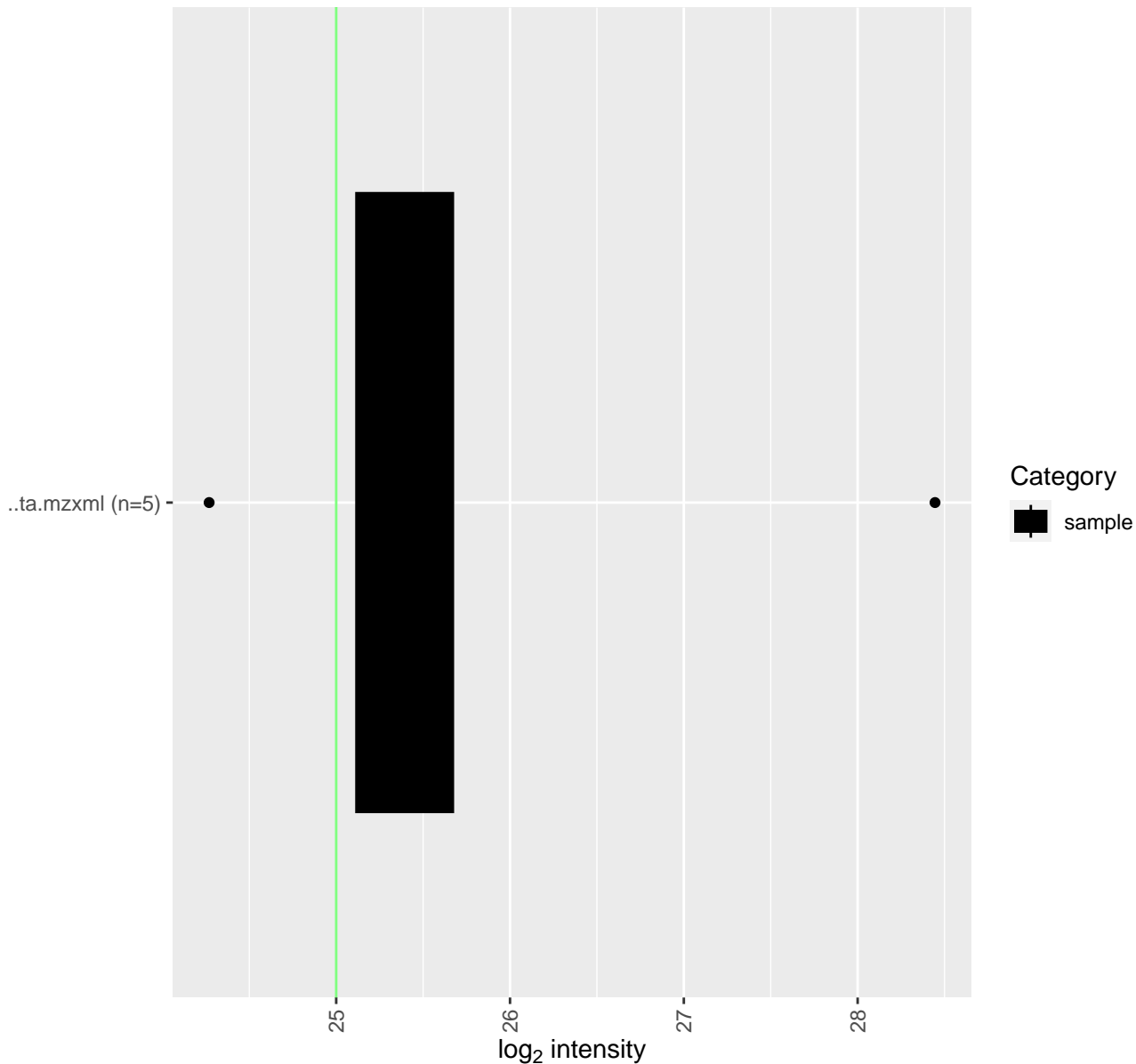
Warning: MaxQuant did NO isotope correction



PG: intensity distribution

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

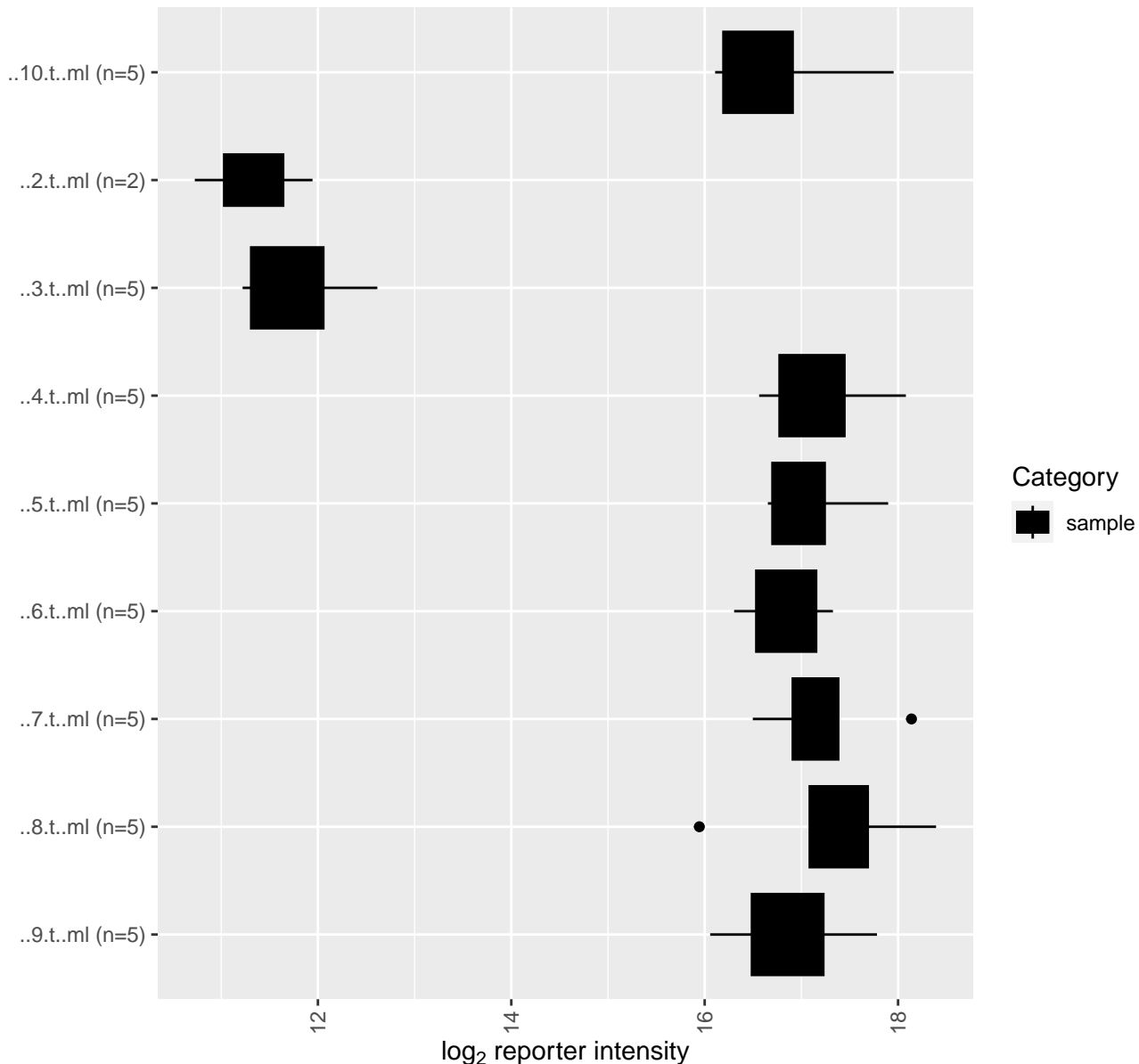
RSD NA% [high RSD --> few peptides]



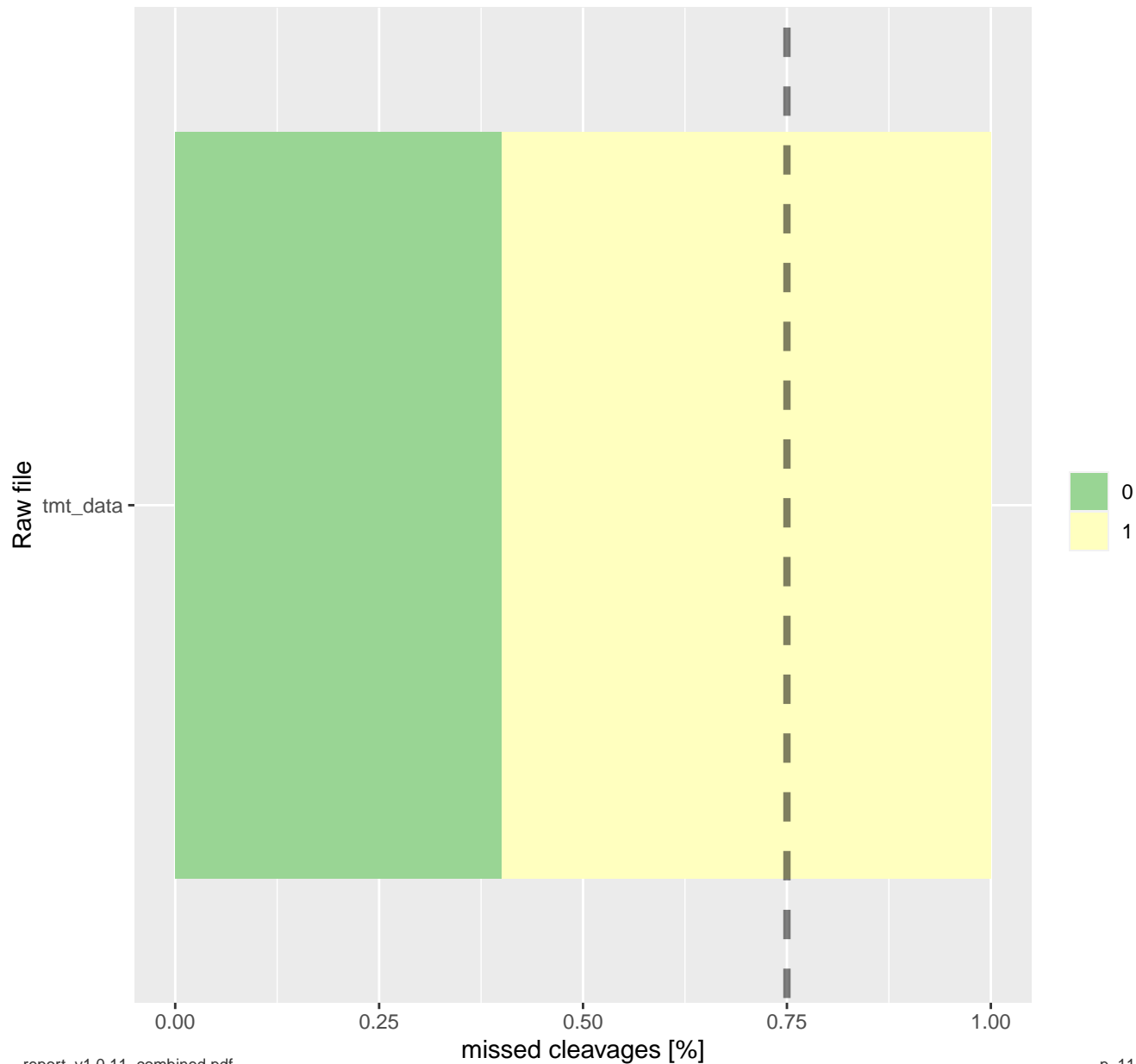
PG: reporter intensity distribution

RSD 14.9% (w/o zero int.; expected < 5%)

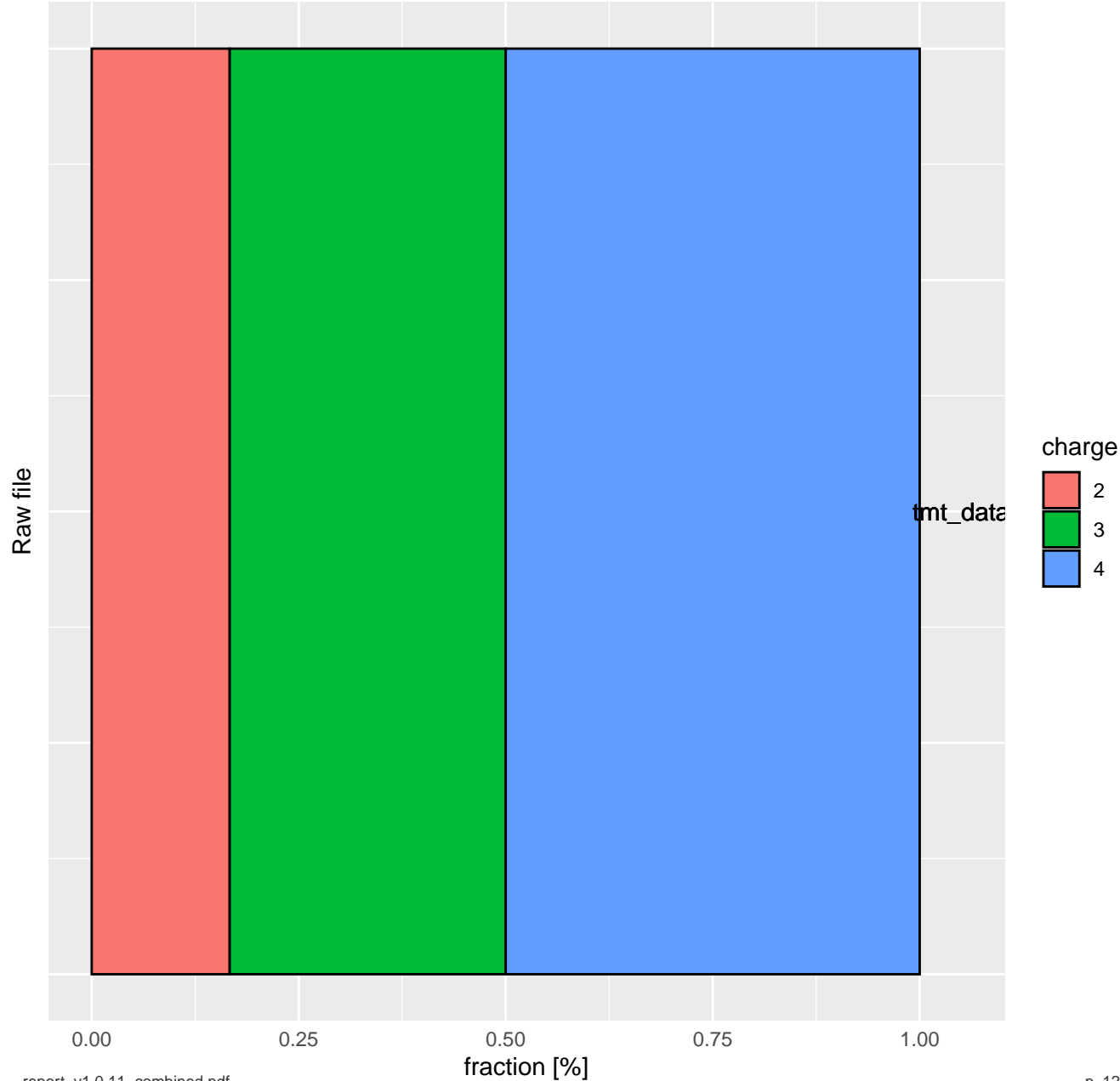
RSD 54.2% [high RSD --> few peptides])



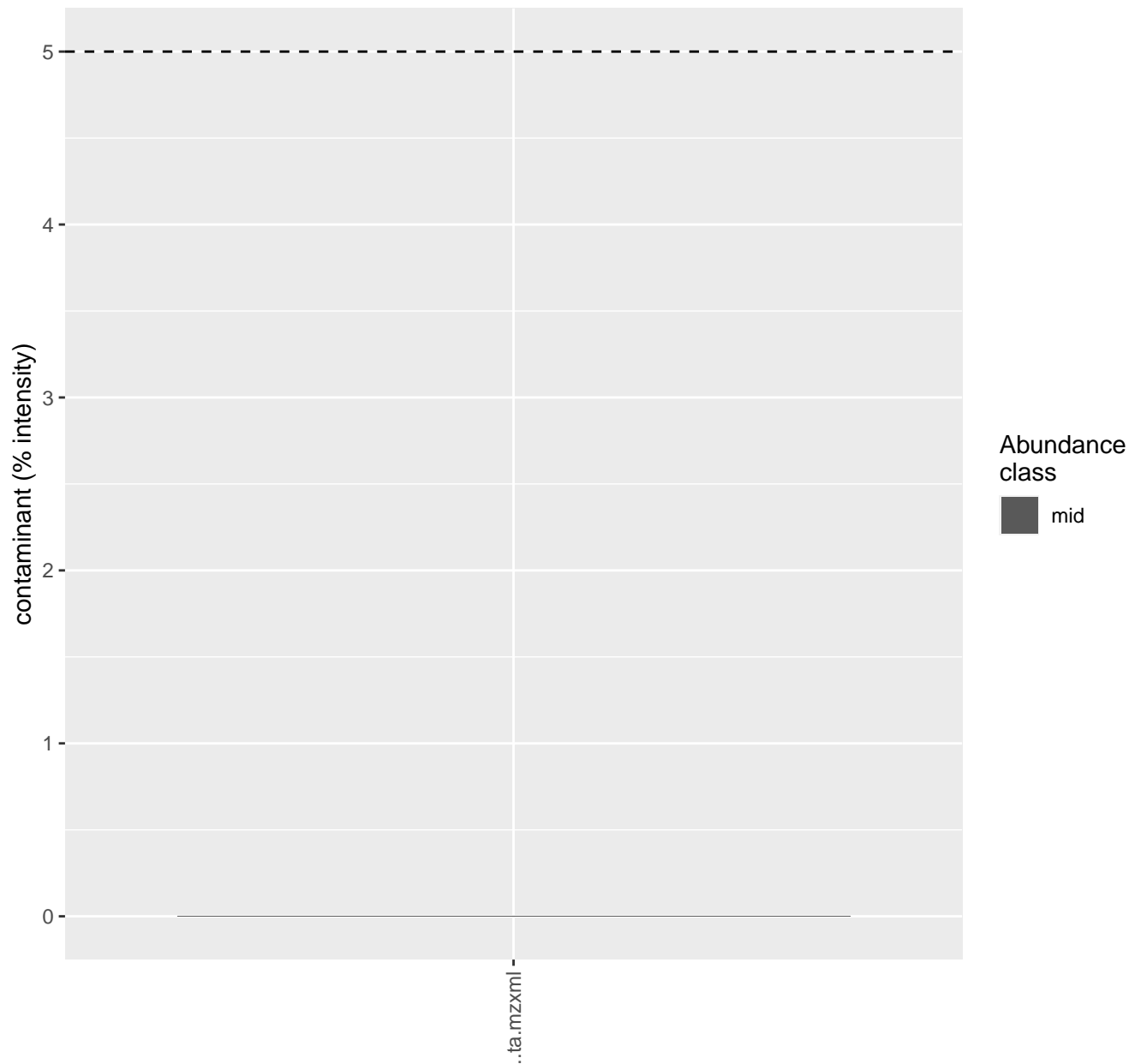
MSMS: Missed cleavages per Raw file (excludes contaminants)



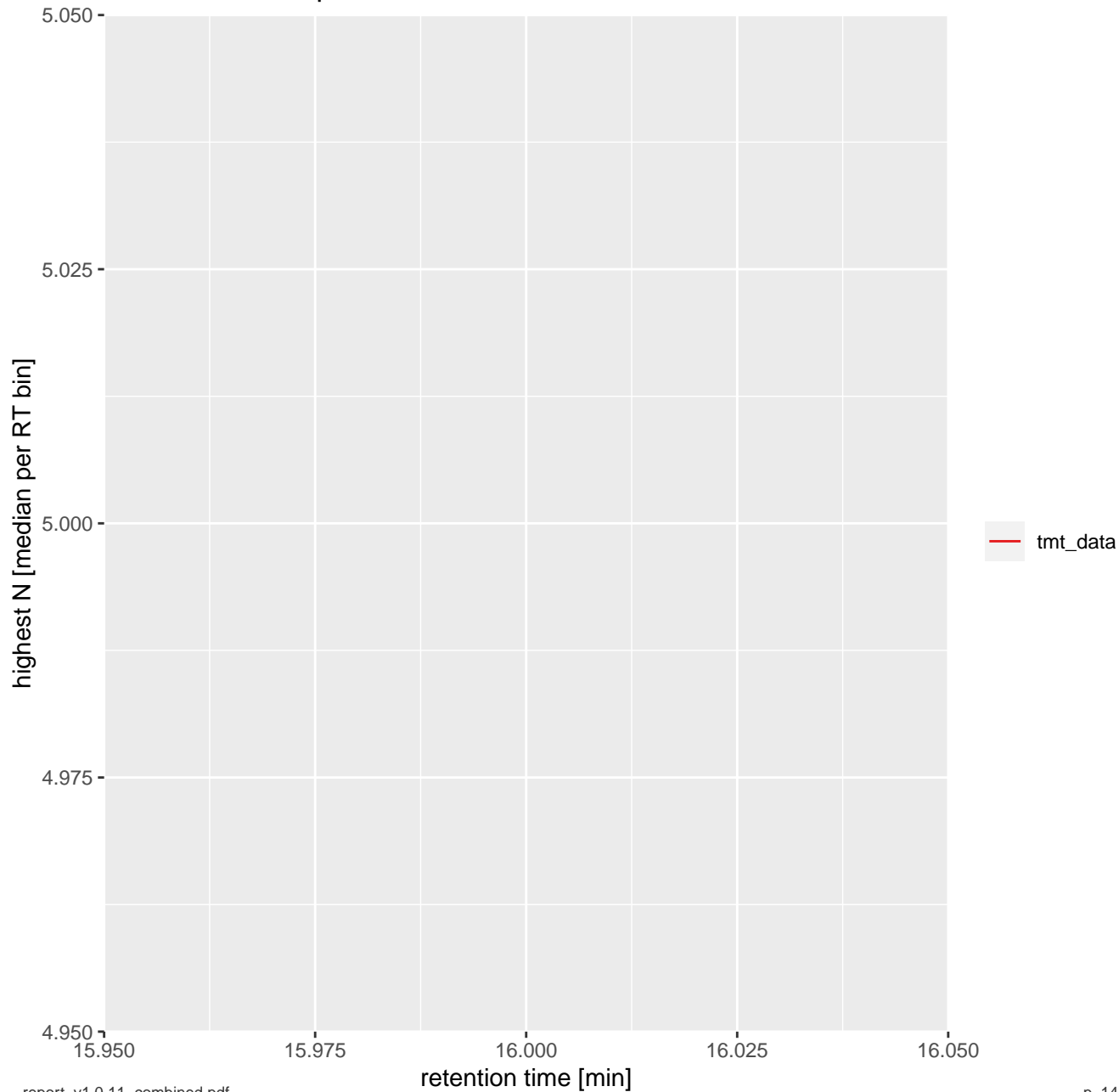
EVD: charge distribution



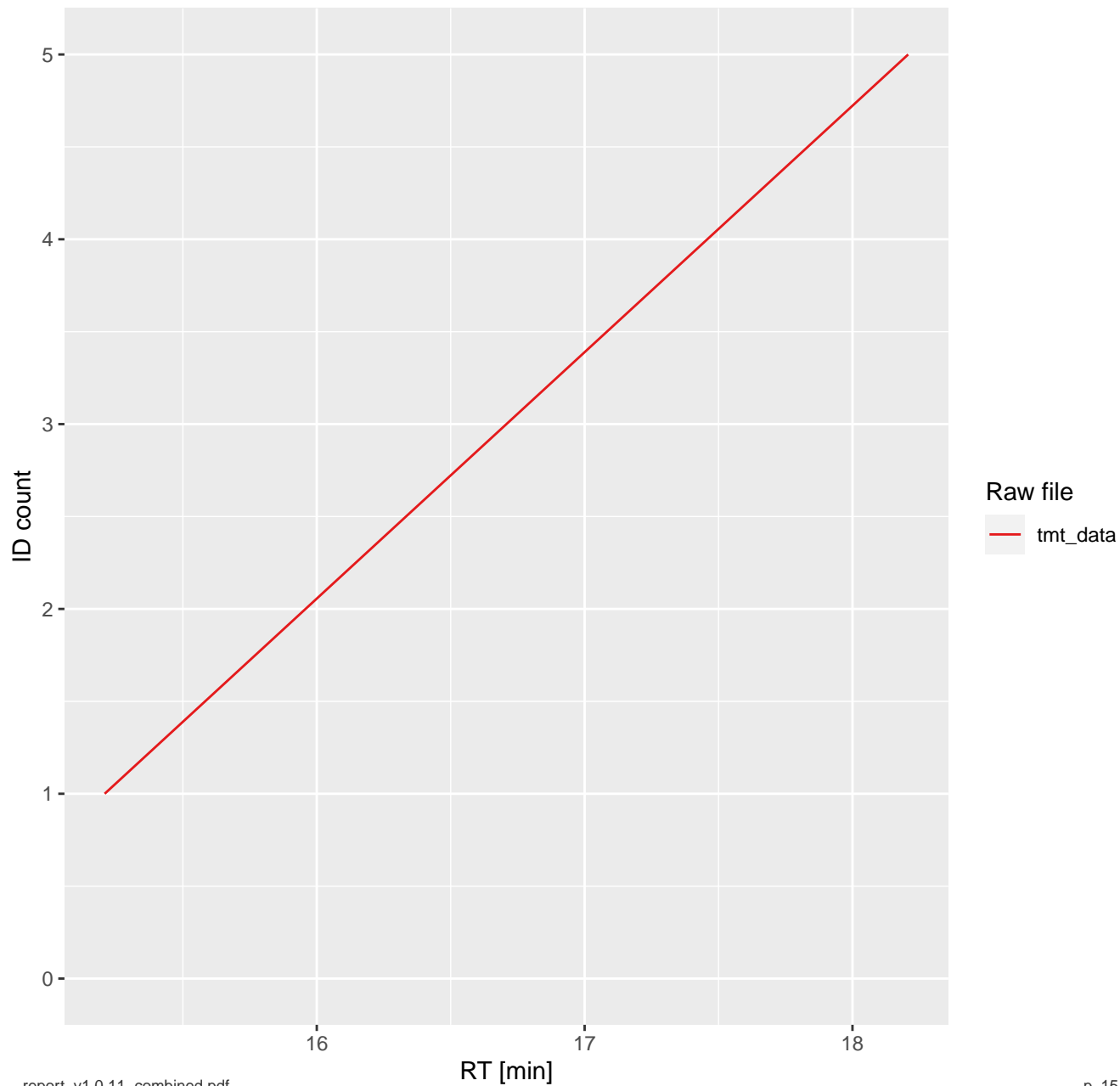
PG: Contaminant per condition



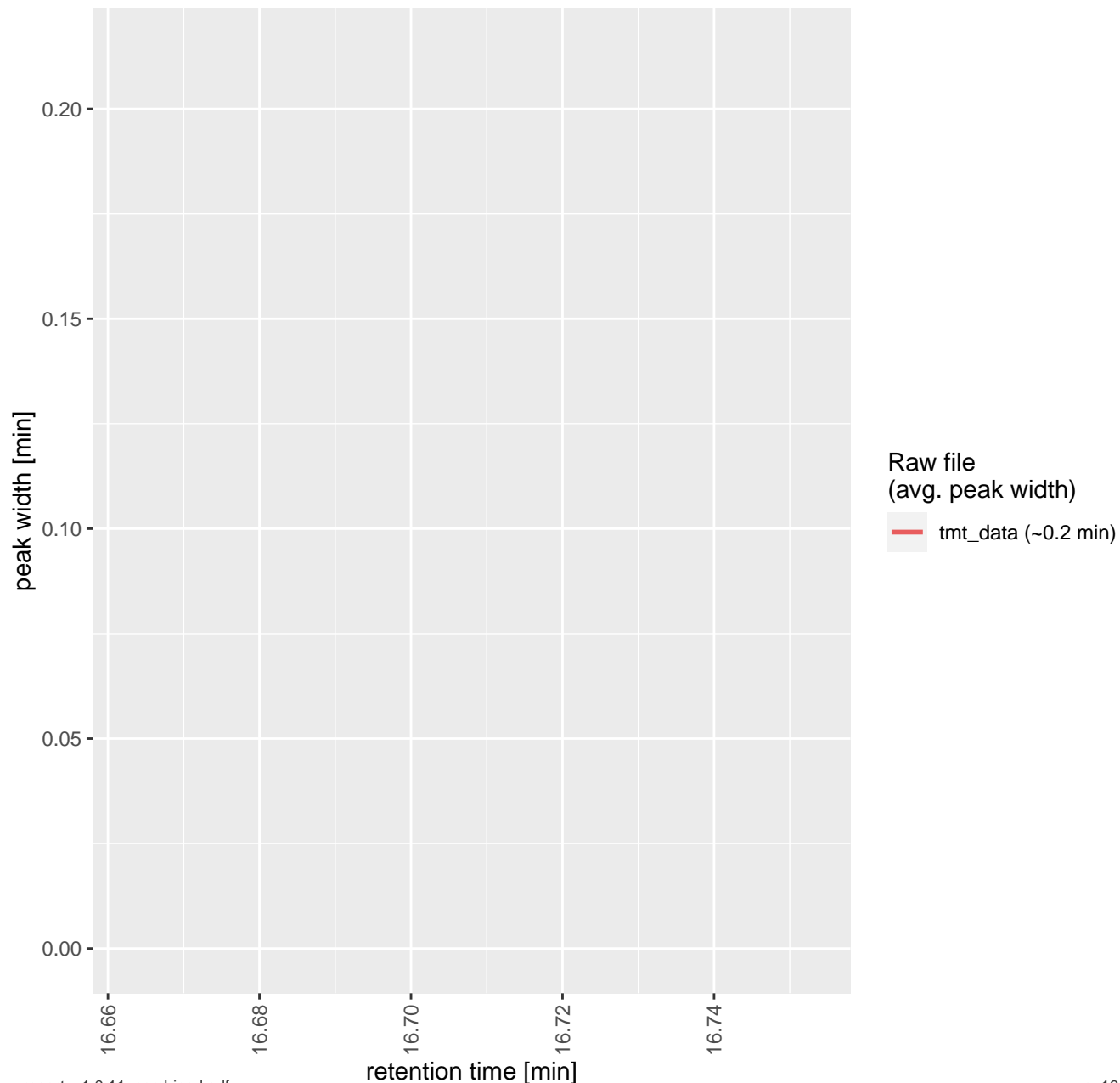
MSMSscans: TopN over RT



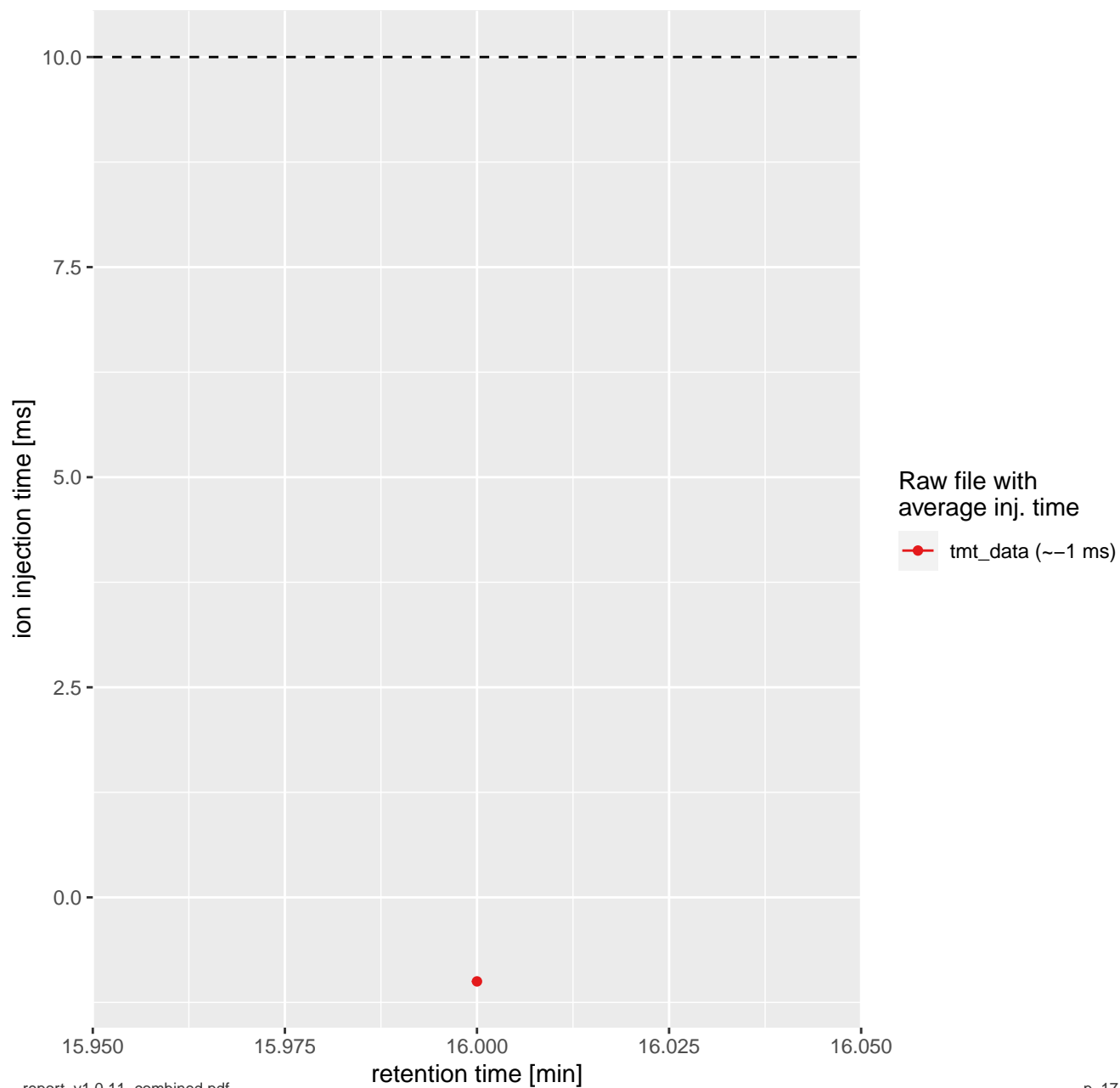
EVD: IDs over RT

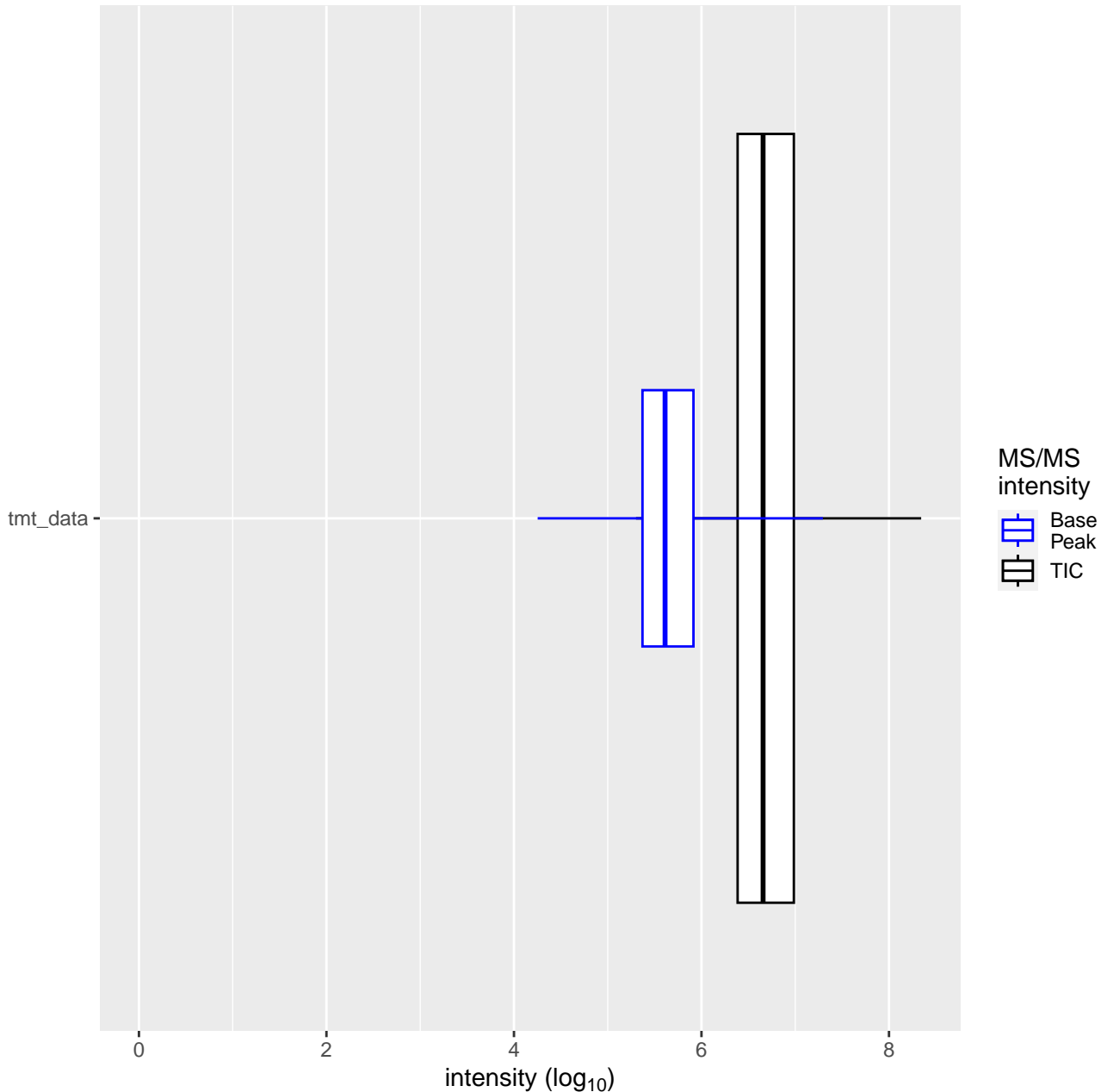


EVD: Peak width over RT

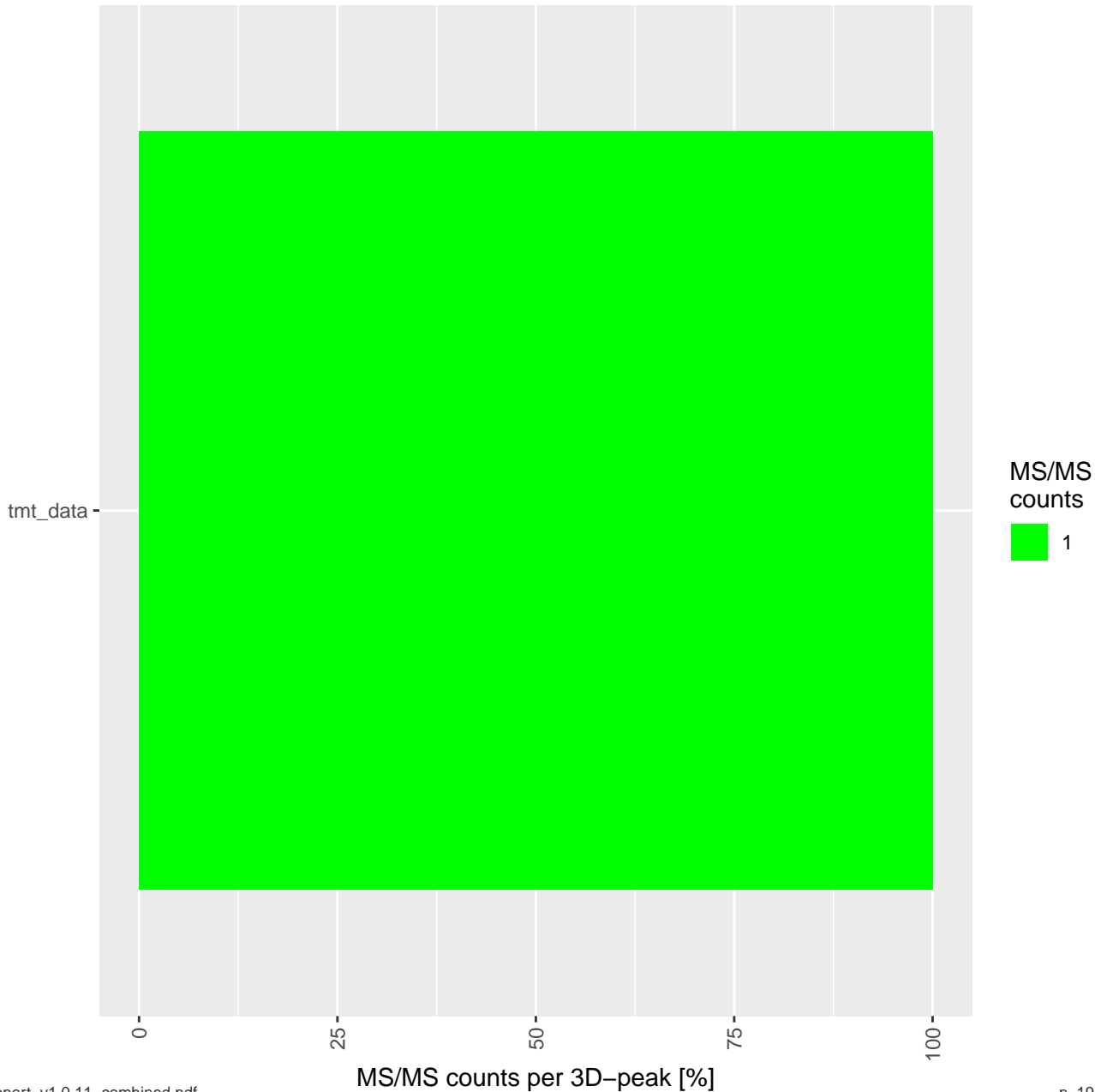


MSMSscans: Ion Injection Time over RT



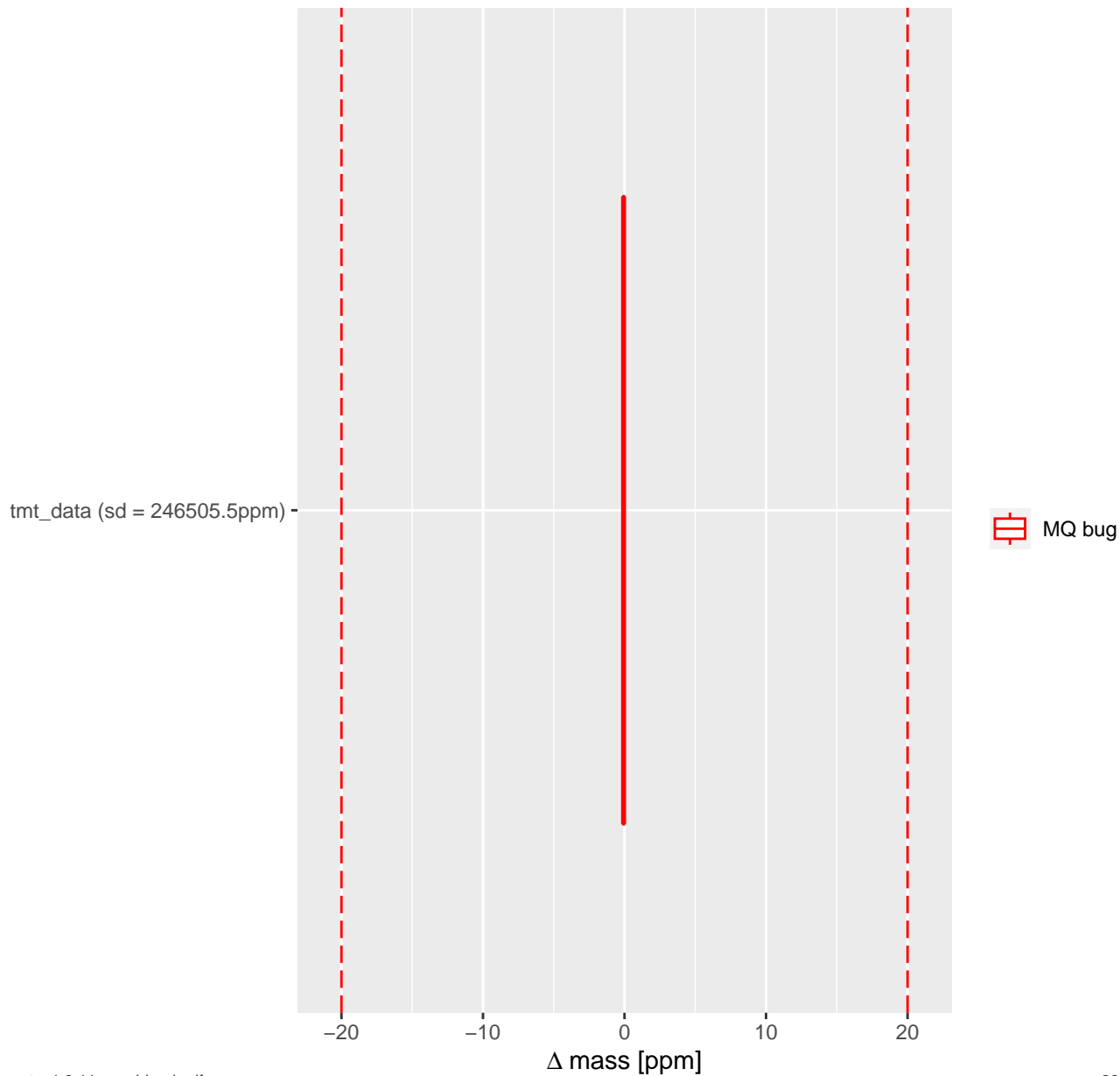


EVD: Oversampling (MS/MS counts per 3D-peak)



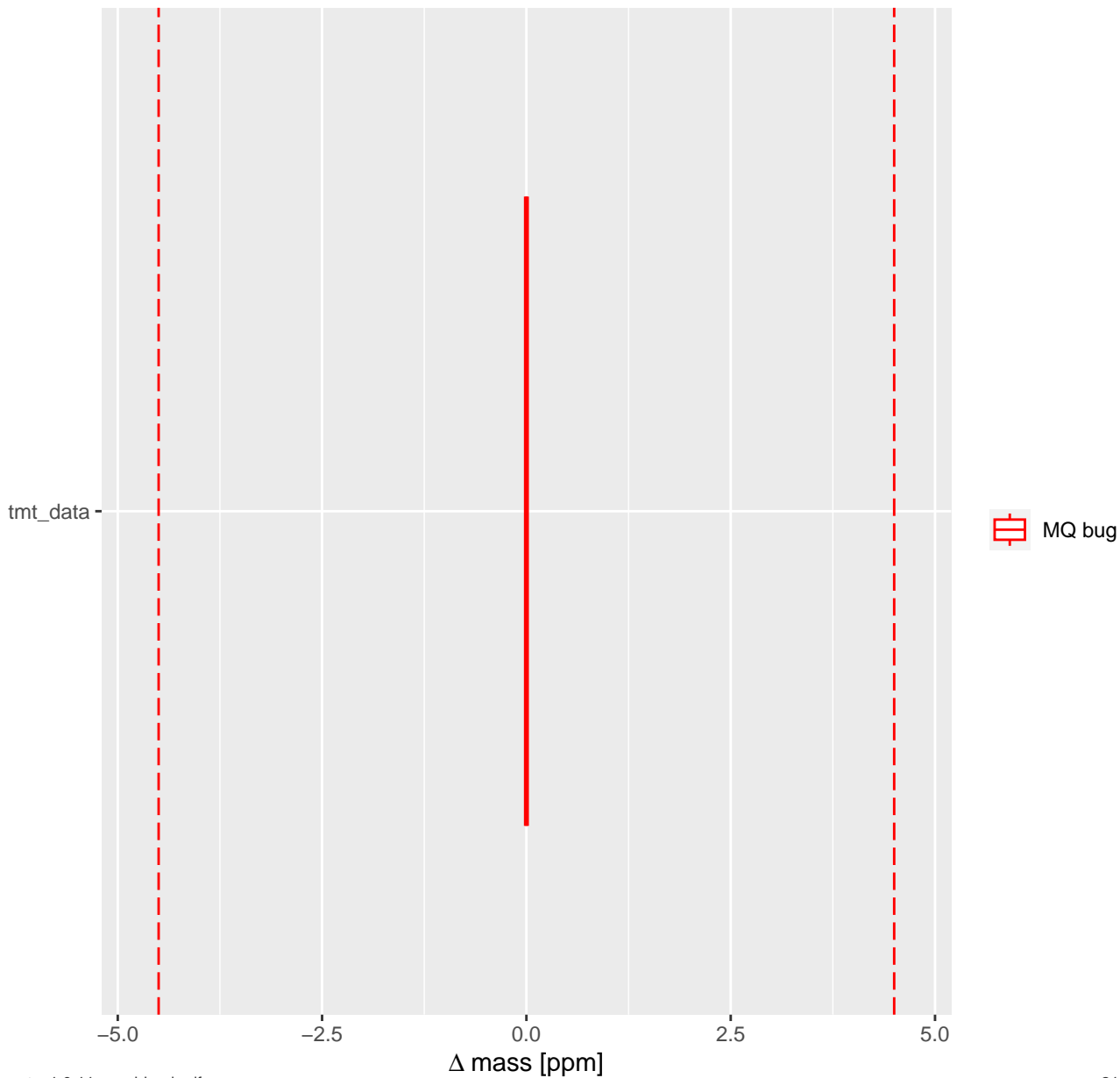
EVD: Uncalibrated mass error

MQ bug: data rescued

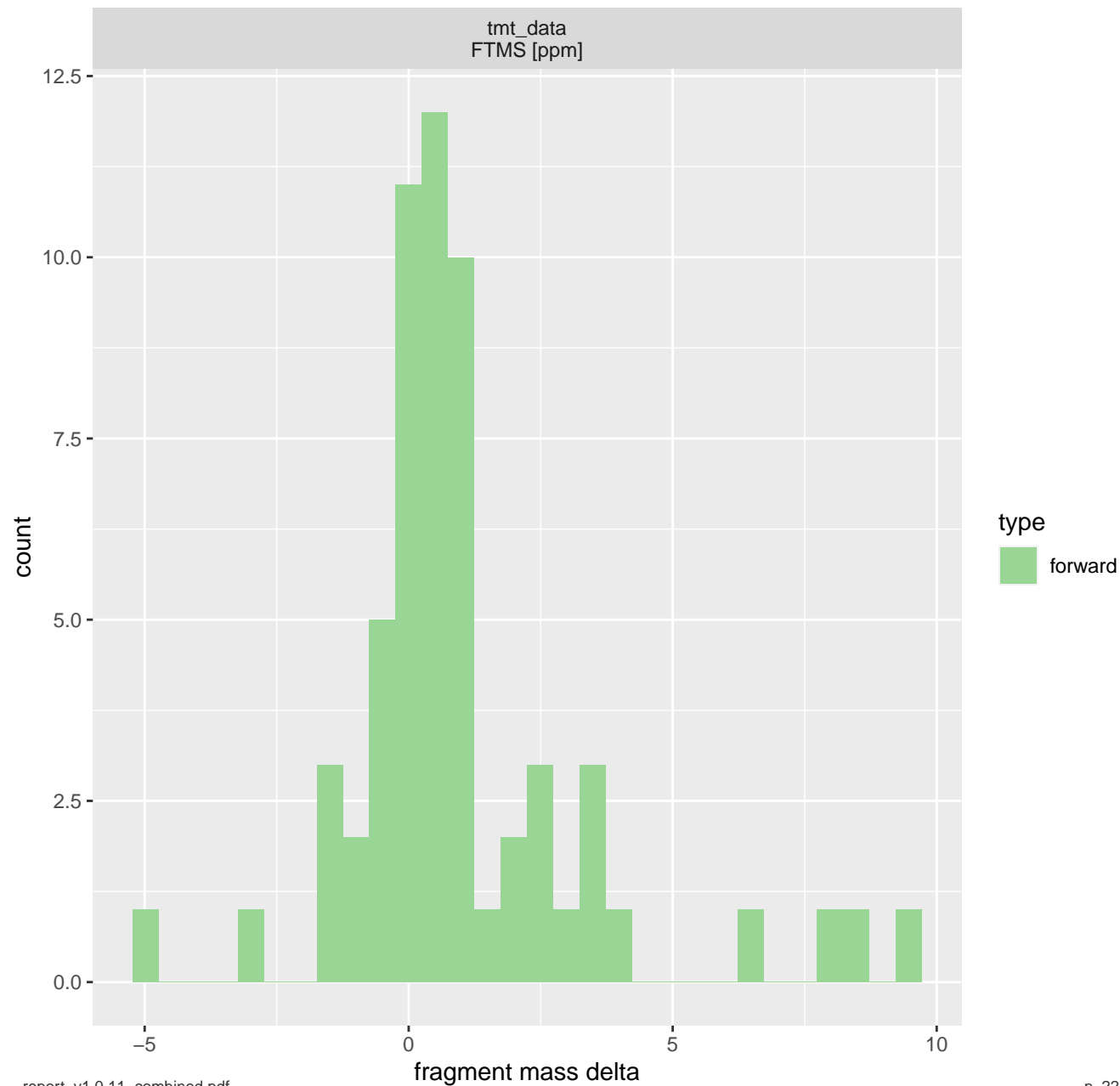


EVD: Calibrated mass error

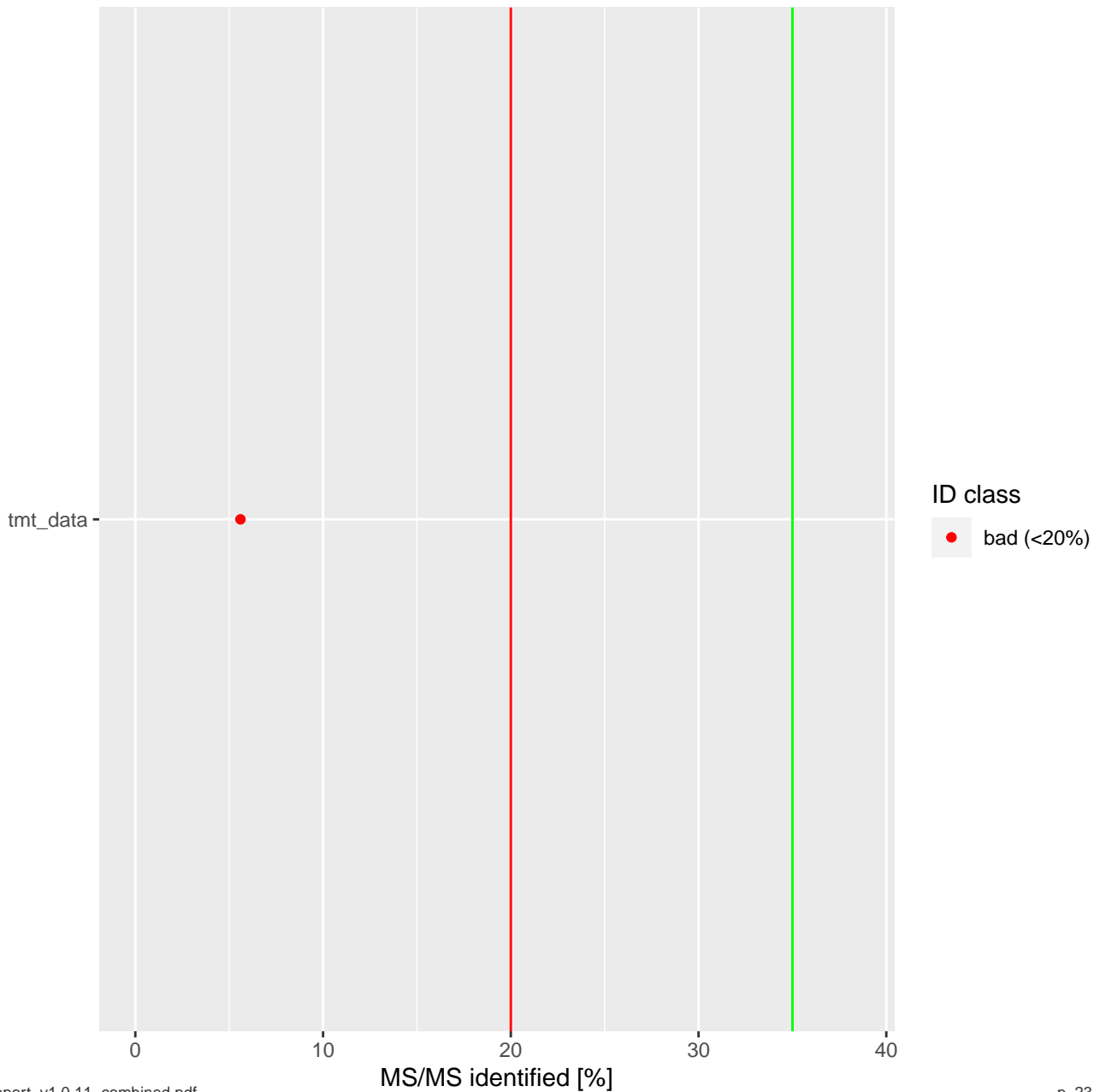
MQ bug: data cannot be rescued



MSMS: Fragment mass errors per Raw file



SM: MS/MS identified per Raw file

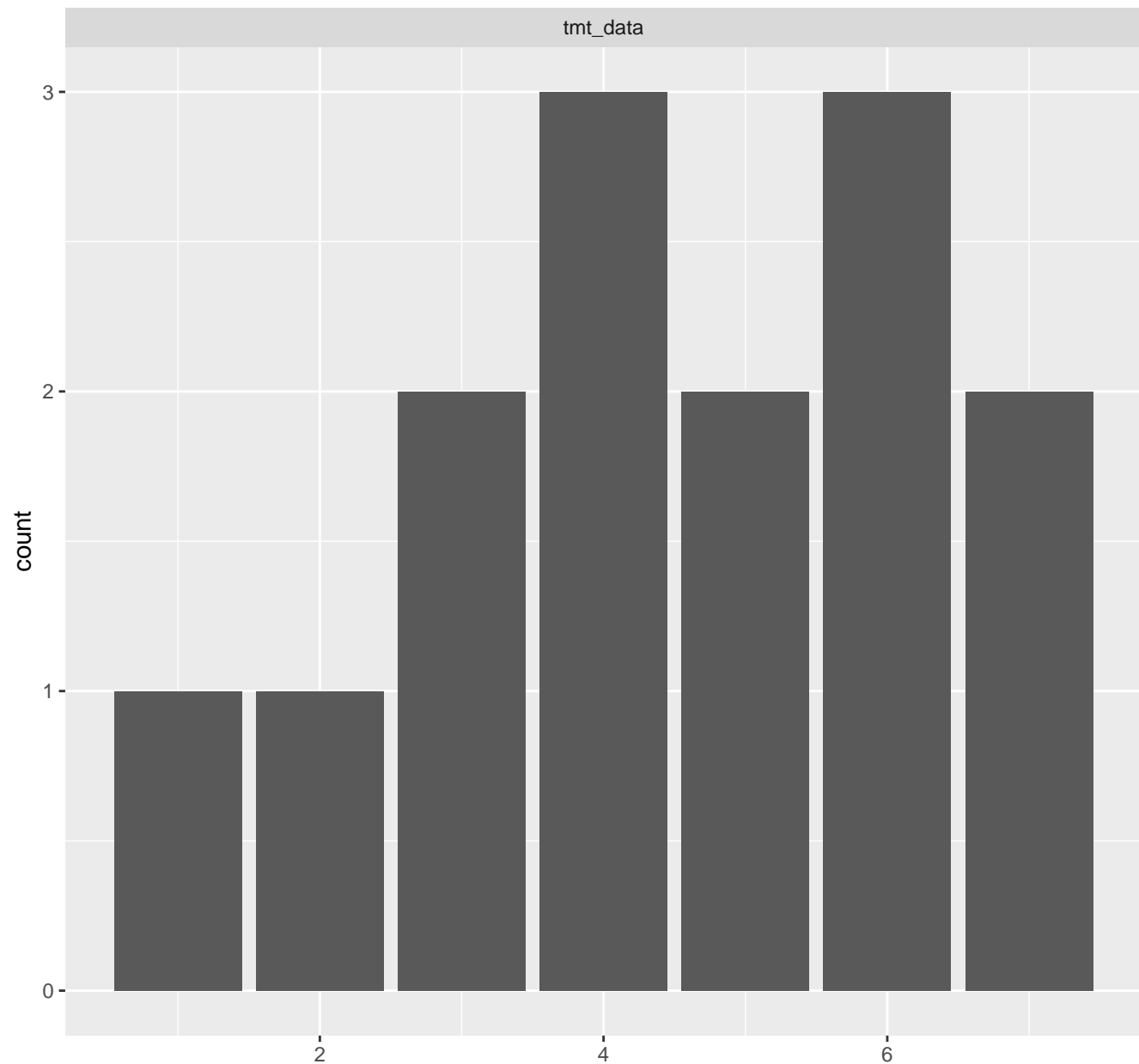


SM: Files with 'red' ID rate

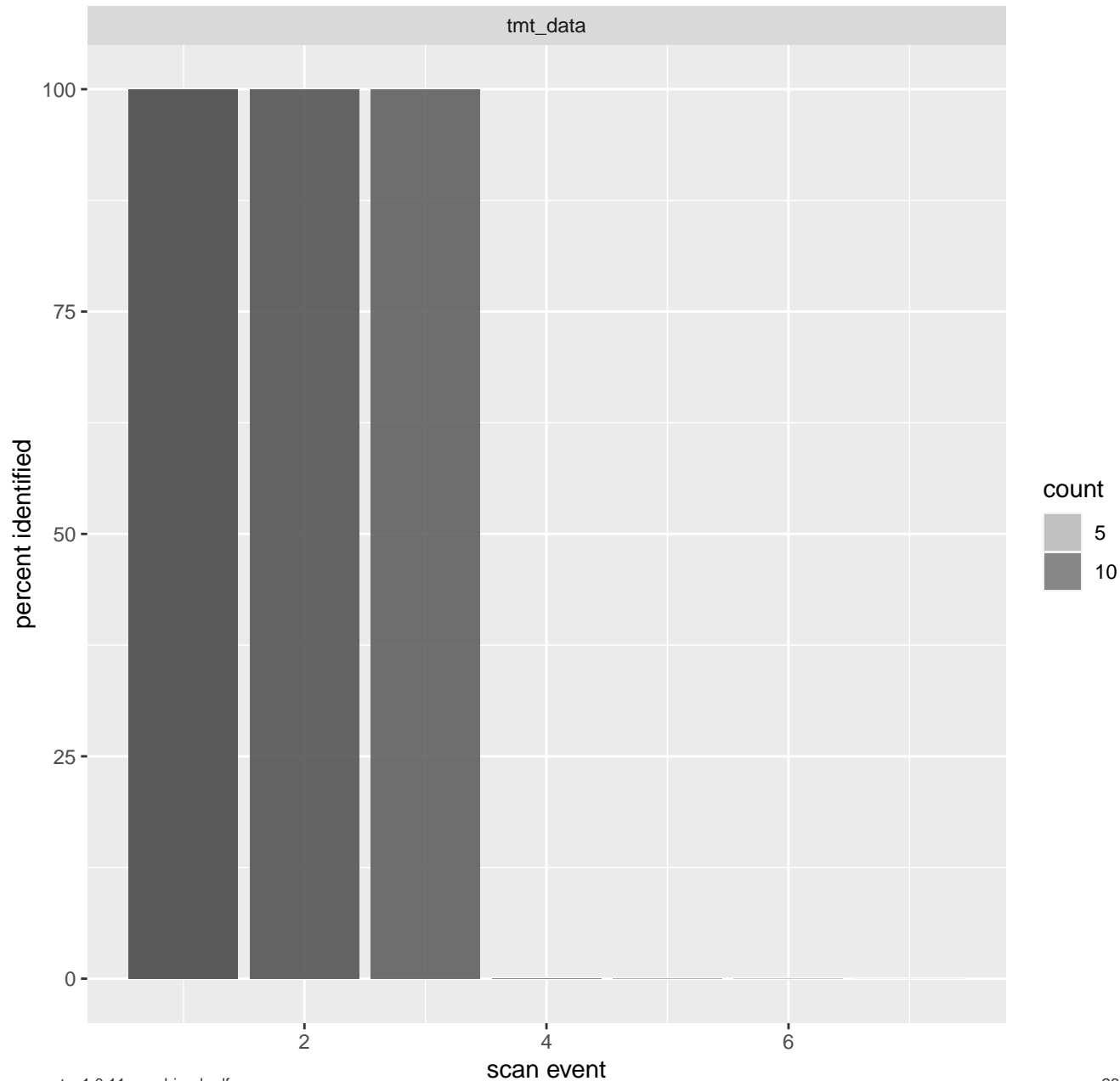
Raw file	% identified
tmt_data	5.6

100% of samples)

MSMSscans: TopN



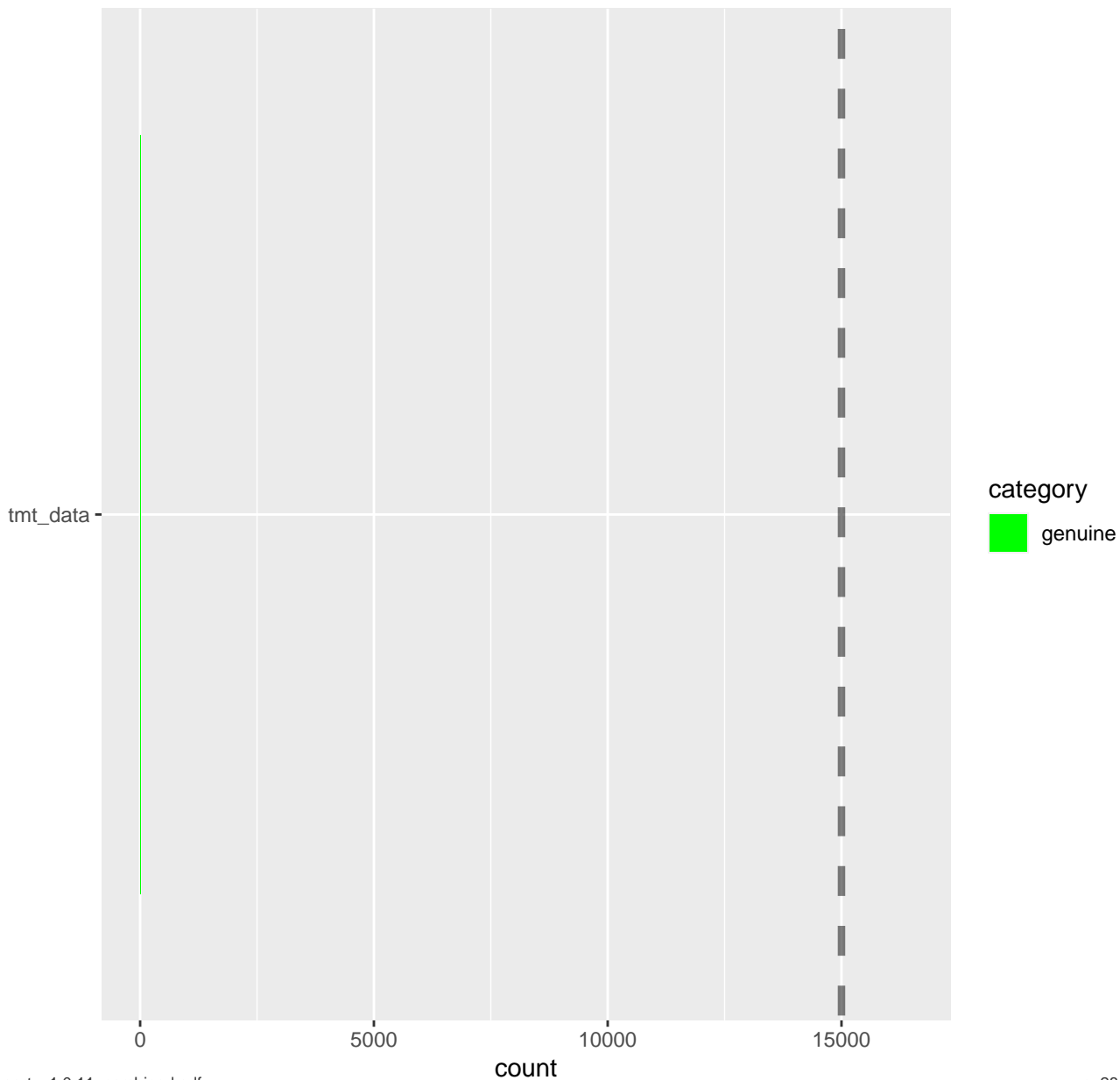
MSMSscans: TopN % identified over N



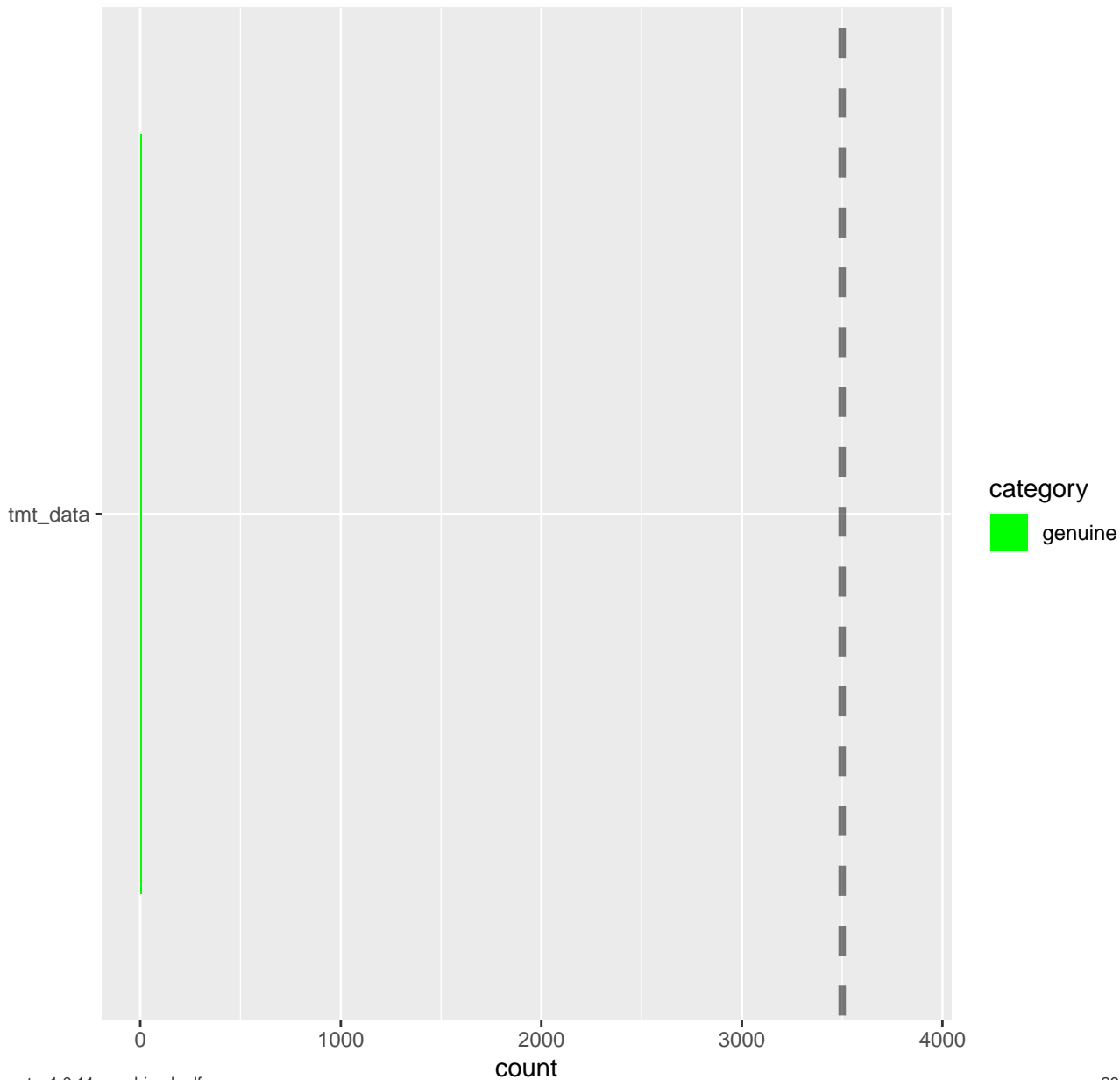
Missing Values Skipped

Need more than one Raw file!

EVD: Peptide ID count



EVD: ProteinGroups count



UpSetR

Only single Raw file detected. Cannot compute unions/intersections.