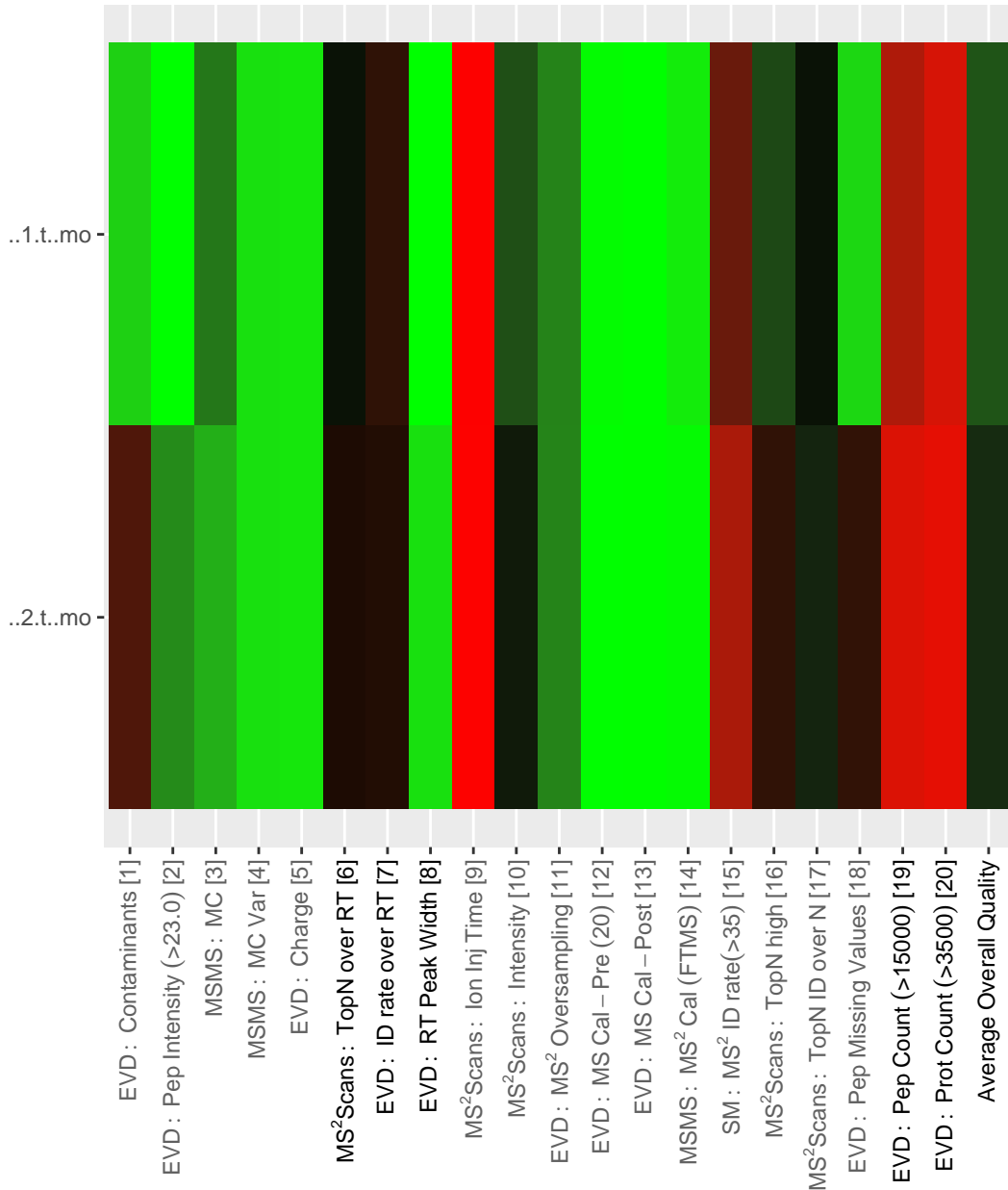


Performance overview

Raw file



score



Mapping of Raw files to their short names

Mapping source: automatic

original	short name	best effort
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Sample1.thermo	..1.t.mo
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Sample2.thermo	..2.t.mo
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PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	MS/MS deisotoping tolerance ..	7
Advanced site intensities	True	MS/MS deisotoping tolerance ..	ppm
Calculate peak properties	False	MS/MS dependent losses (FTMS..	True
Combined folder location		MS/MS dependent losses (ITMS..	True
Da interval. (FTMS)	100	MS/MS dependent losses (TOF)	True
Da interval. (ITMS)	100	MS/MS dependent losses (Unkn..	True
Da interval. (TOF)	100	MS/MS higher charges (FTMS)	True
Da interval. (Unknown)	100	MS/MS higher charges (ITMS)	True
Date of writing	10/21/2020 23:53:05	MS/MS higher charges (TOF)	True
Decoy mode	revert	MS/MS higher charges (Unknow..	True
Disable MD5	False	MS/MS recalibration (FTMS)	False
Discard unmodified counterpa..	False	MS/MS recalibration (ITMS)	False
Epsilon score for mutations		MS/MS recalibration (TOF)	False
Evaluate variant peptides se..	True	MS/MS recalibration (Unknown..	False
Find dependent peptides	False	MS/MS tol. (FTMS)	20 ppm
Fixed andromeda index folder		MS/MS tol. (ITMS)	0.5 Da
iBAQ	False	MS/MS tol. (TOF)	40 ppm
iBAQ log fit	False	MS/MS tol. (Unknown)	20 ppm
Include contaminants	True	MS/MS water loss (FTMS)	True
Label min. ratio count	2	MS/MS water loss (ITMS)	True
Machine name	vgcnbwc-compute-c20me-0593 .novalocal	MS/MS water loss (TOF)	True
Main search max. combination..	200	MS/MS water loss (Unknown)	True
Match between runs	False	Peptides used for protein qu..	Razor
Match unidentified features	False	Protein FDR	0.01
Max mods in site table	3	PSM FDR	0.01
Max. peptide length for unsp..	25	PSM FDR Crosslink	0.01

/data/dnb02/galaxy_db/files/022/443/dataset_22443304.dat

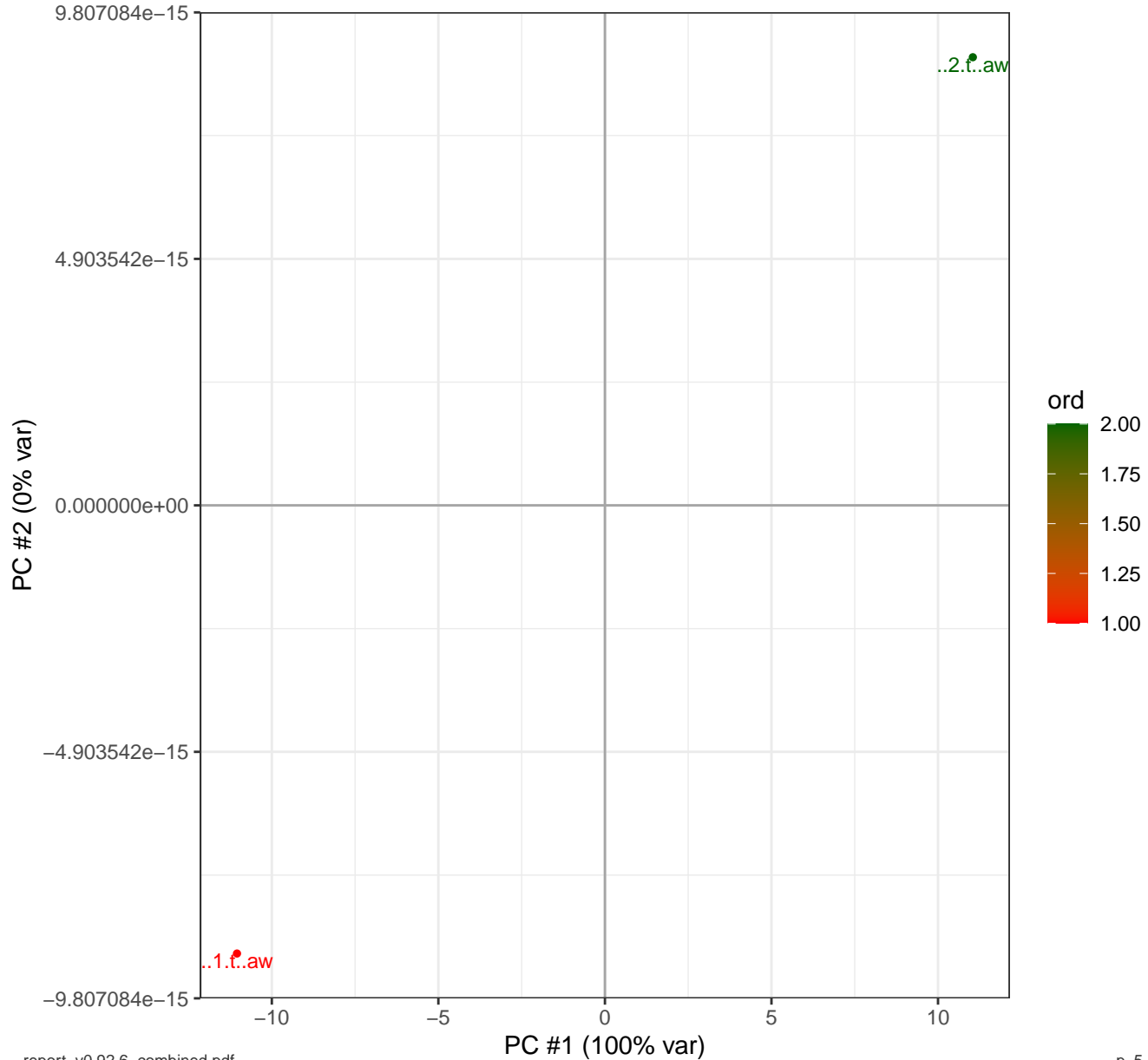
PAR: parameters

parameter	value	parameter	value
Max. peptide mass [Da]	4600	Razor protein FDR	True
Min. delta score for modifie..	6	Require MS/MS for LFQ compar..	True
Min. delta score for unmodif..	0	Second peptides	True
Min. peptide Length	7	Separate LFQ in parameter gr..	False
Min. peptide length for unsp..	8	Site FDR	0.01
Min. peptides	1	Site tables	
Min. razor peptides	1	Stabilize large LFQ ratios	True
Min. score for modified pept..	40	Temporary folder	
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	12
Min. unique peptides	1	Top MS/MS peaks per Da inter..	8
Modifications included in pr..	Acetyl (Protein N-term) Oxidation (M)	Top MS/MS peaks per Da inter..	10
MS/MS ammonia loss (FTMS)	True	Top MS/MS peaks per Da inter..	12
MS/MS ammonia loss (ITMS)	True	Use delta score	False
MS/MS ammonia loss (TOF)	True	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (Unknown)	True	Use only unmodified peptides..	True
MS/MS deisotoping (FTMS)	True	User name	galaxy
MS/MS deisotoping (ITMS)	False	Variation mode	None
MS/MS deisotoping (TOF)	True	Version	1.6.10.43
MS/MS deisotoping (Unknown)	True	Write accumulatedPasefMsmsSc.	True
MS/MS deisotoping tolerance ..	7	Write allPeptides table	True
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

/data/dnb02/galaxy_db/files/022/443/dataset_22443304.dat

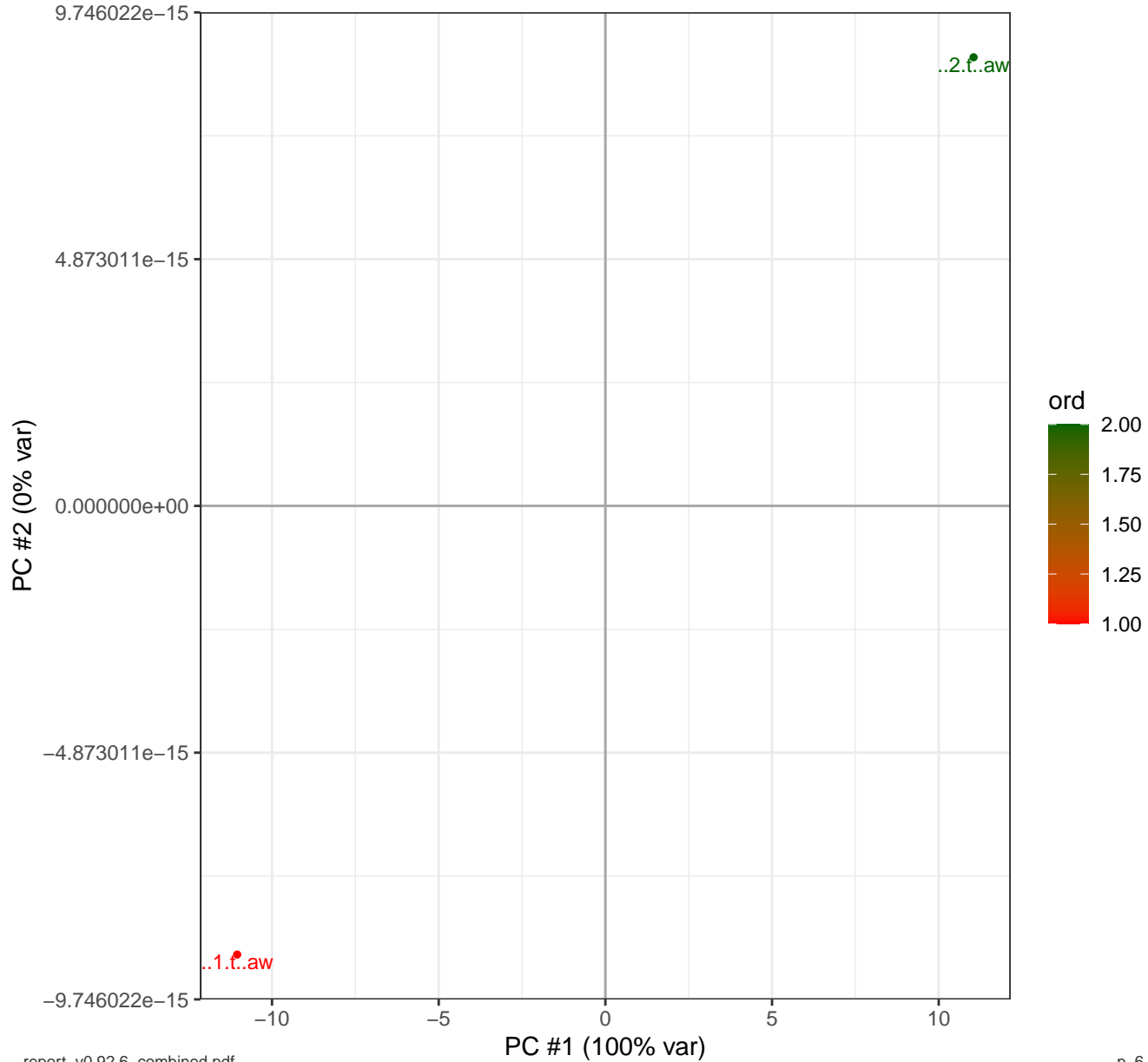
PG: PCA of 'raw intensity'

(excludes contaminants)

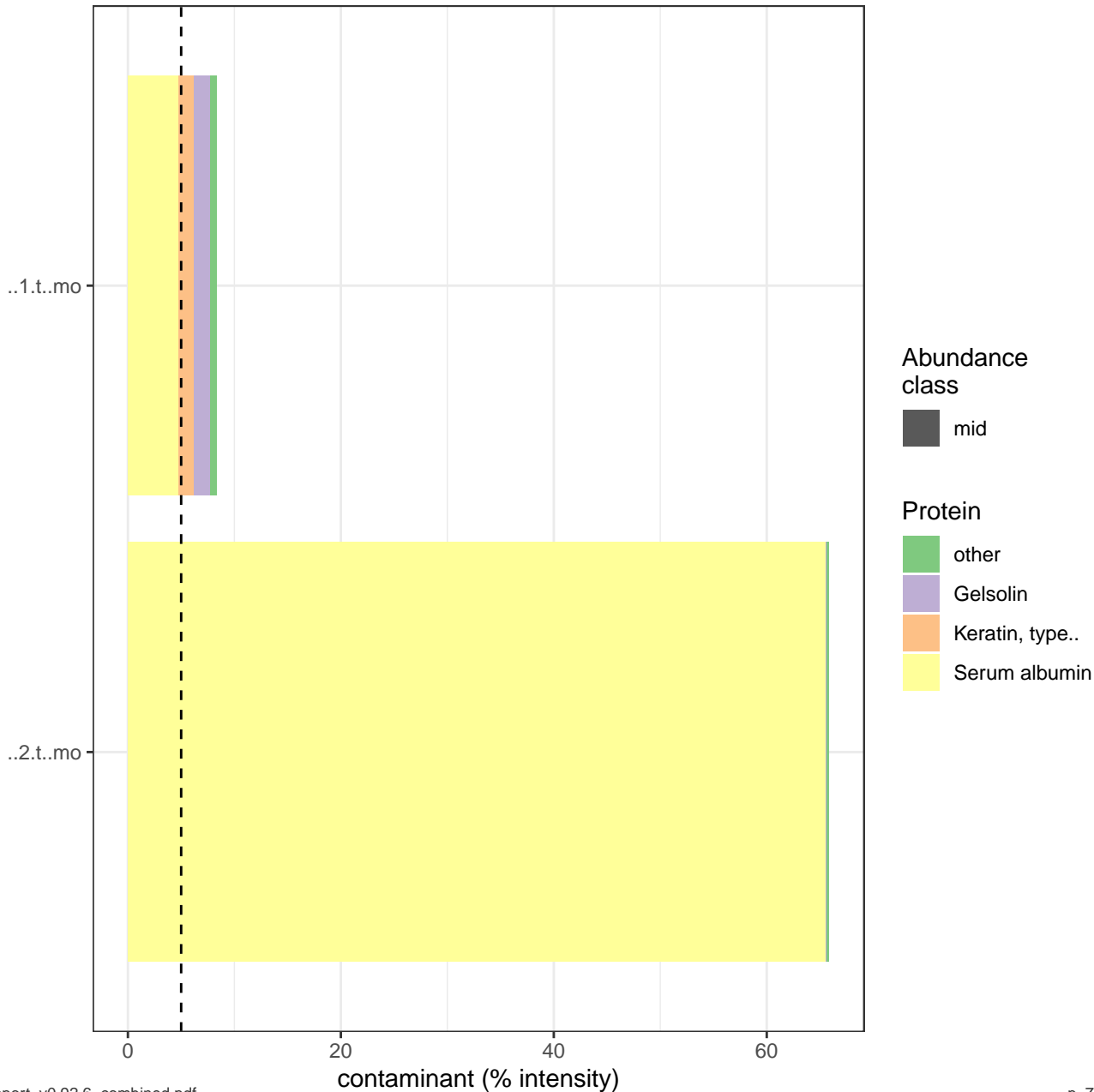


PG: PCA of 'lfq intensity'

(excludes contaminants)



EVD: Top5 Contaminants per Raw file



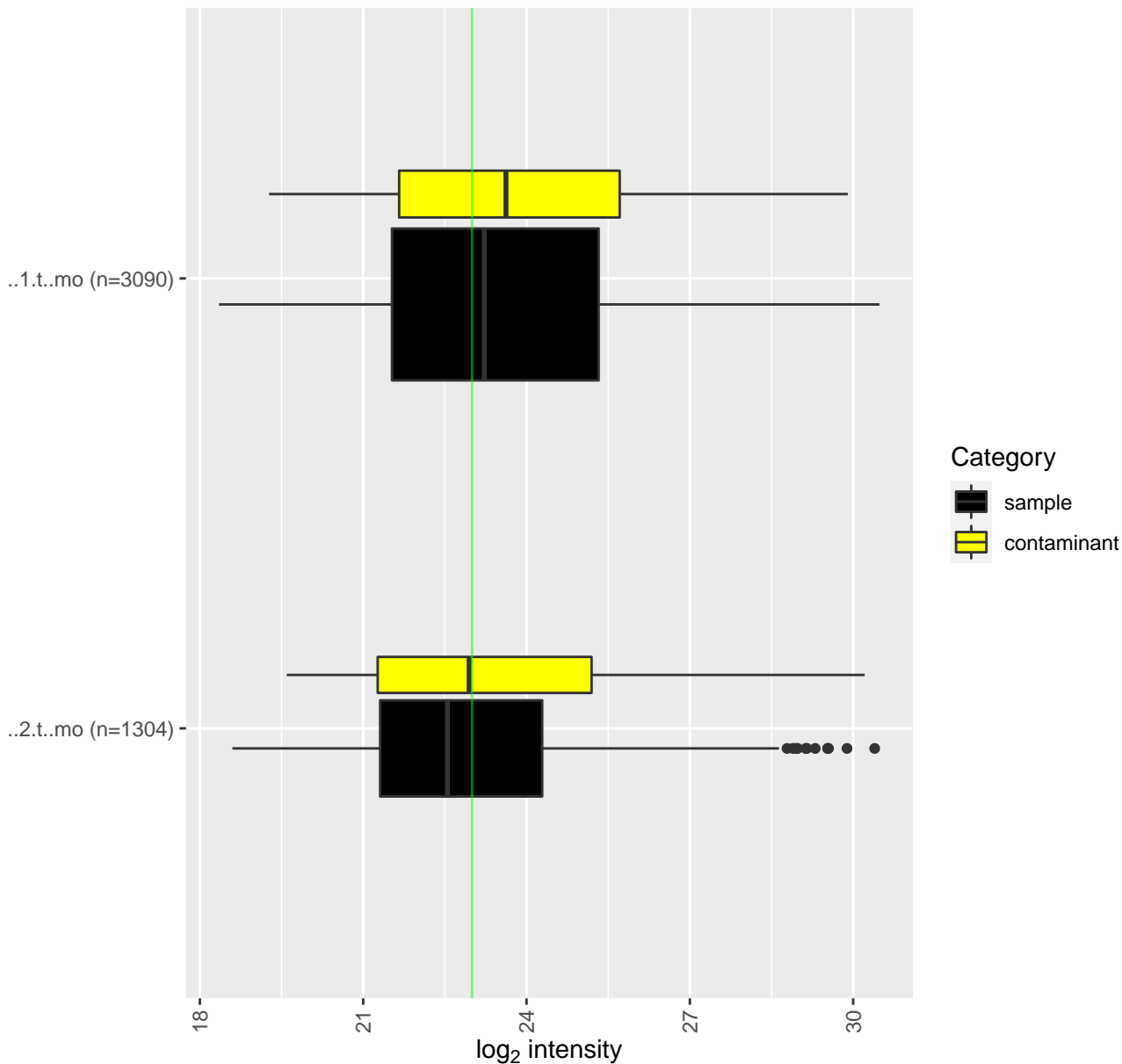
EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

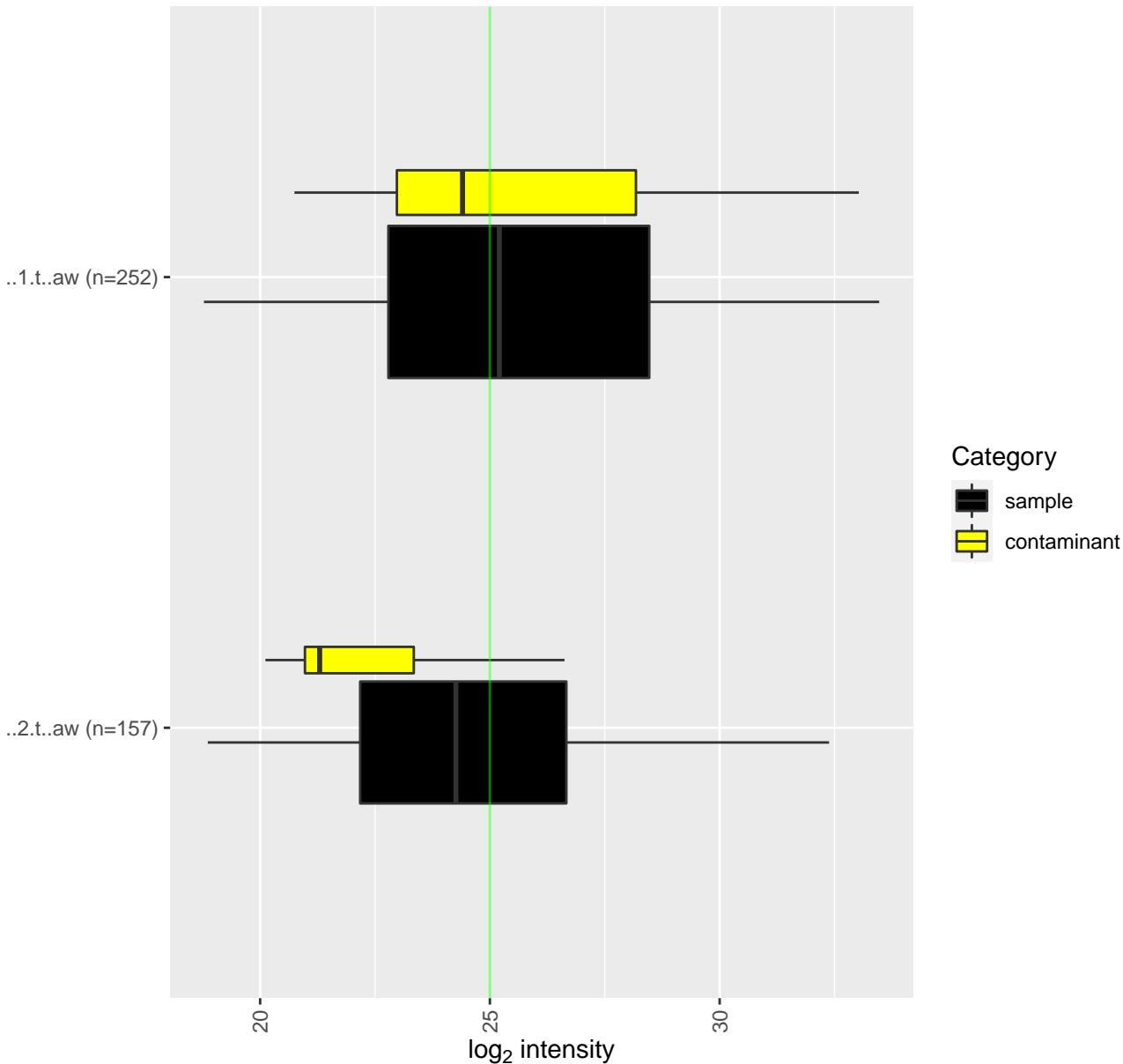
Did you use the correct database?

EVD: peptide intensity distribution

RSD 1.9% (expected < 5%)



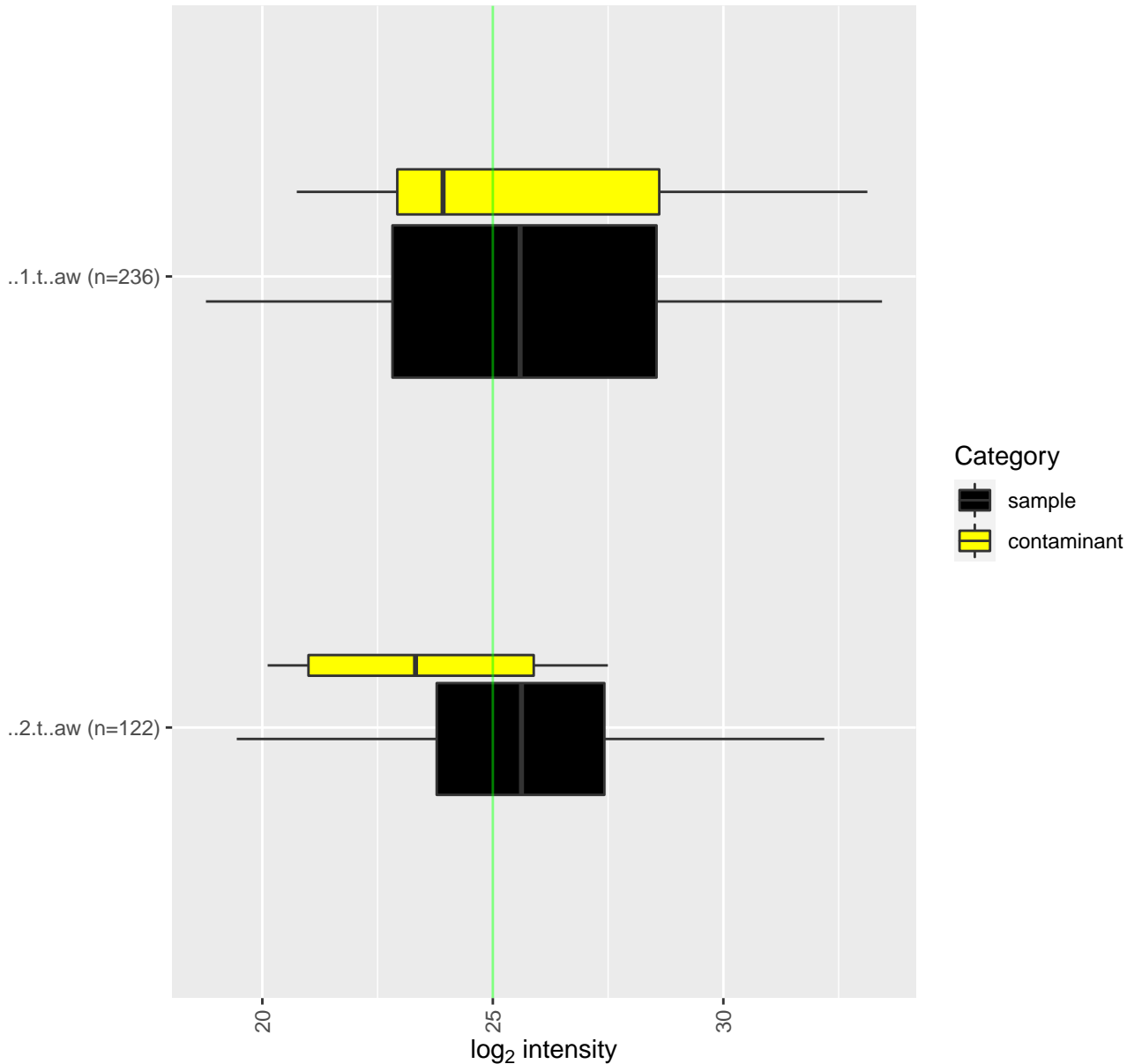
PG: intensity distribution
RSD 2.5% (w/o zero int.; expected < 5%)
RSD 10.5% [high RSD --> few peptides]



PG: LFQ intensity distribution

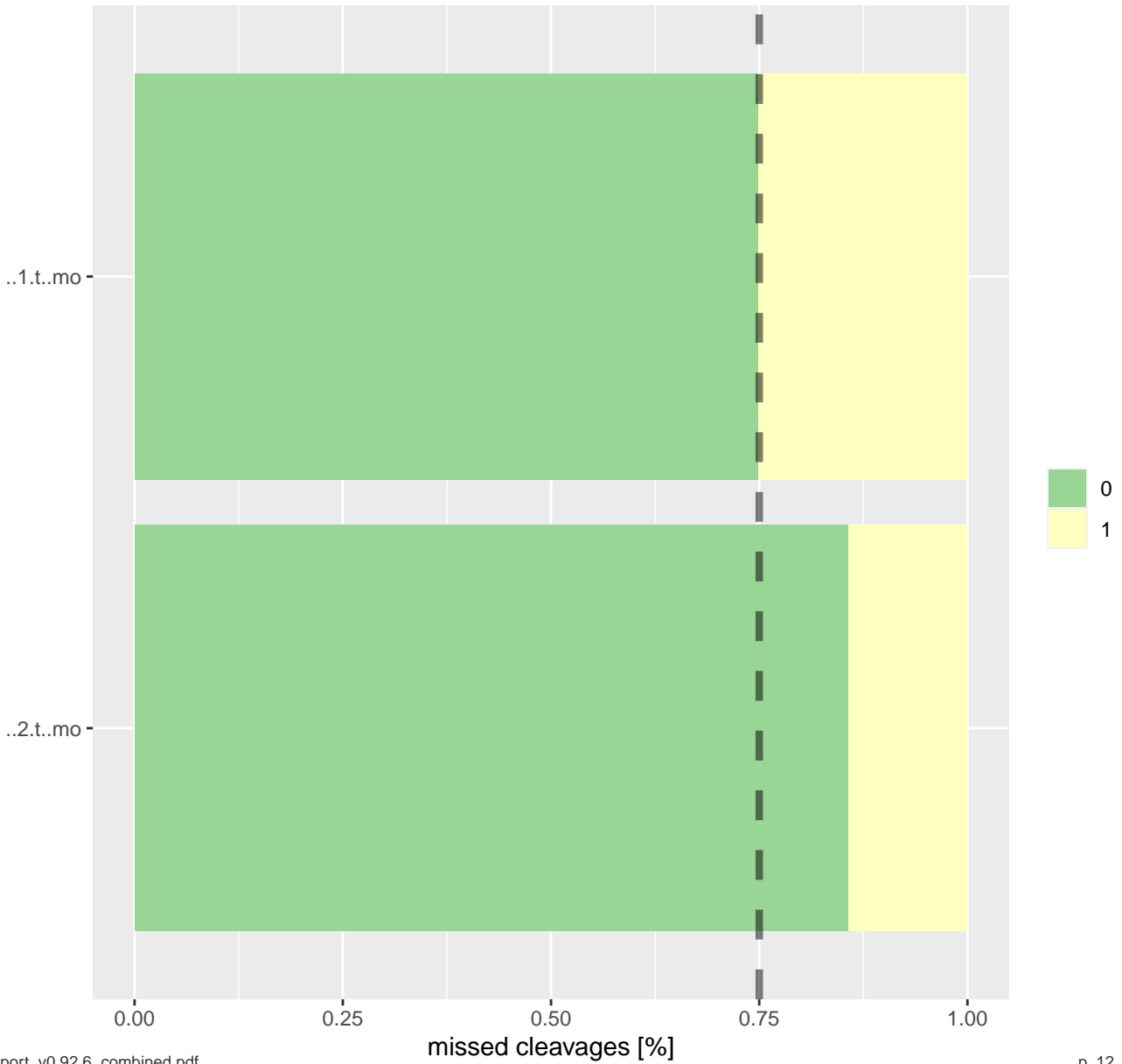
RSD 0.3% (w/o zero int.; expected < 5%)

RSD 141.4% [high RSD --> few peptides]

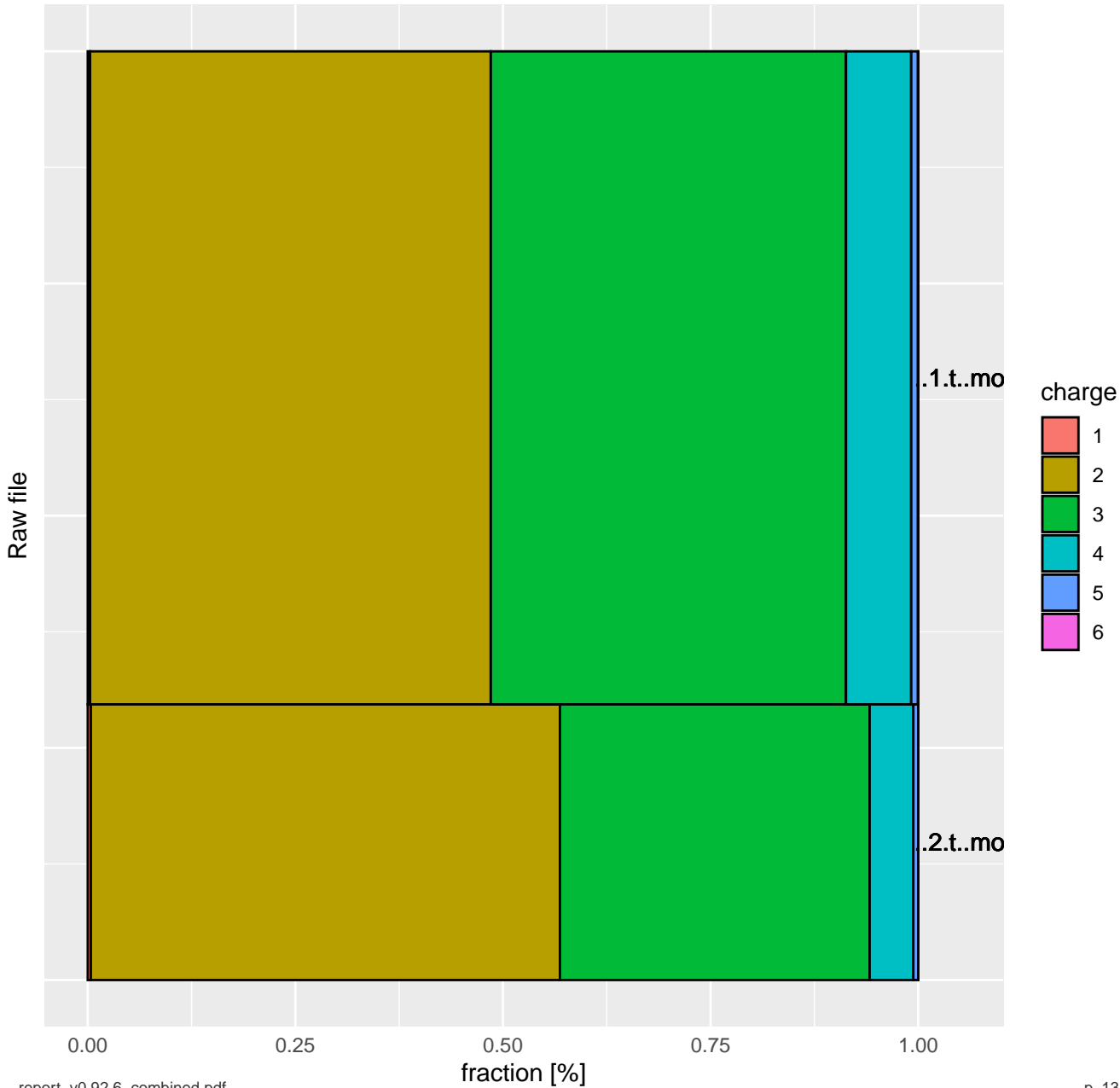


MSMS: Missed cleavages per Raw file

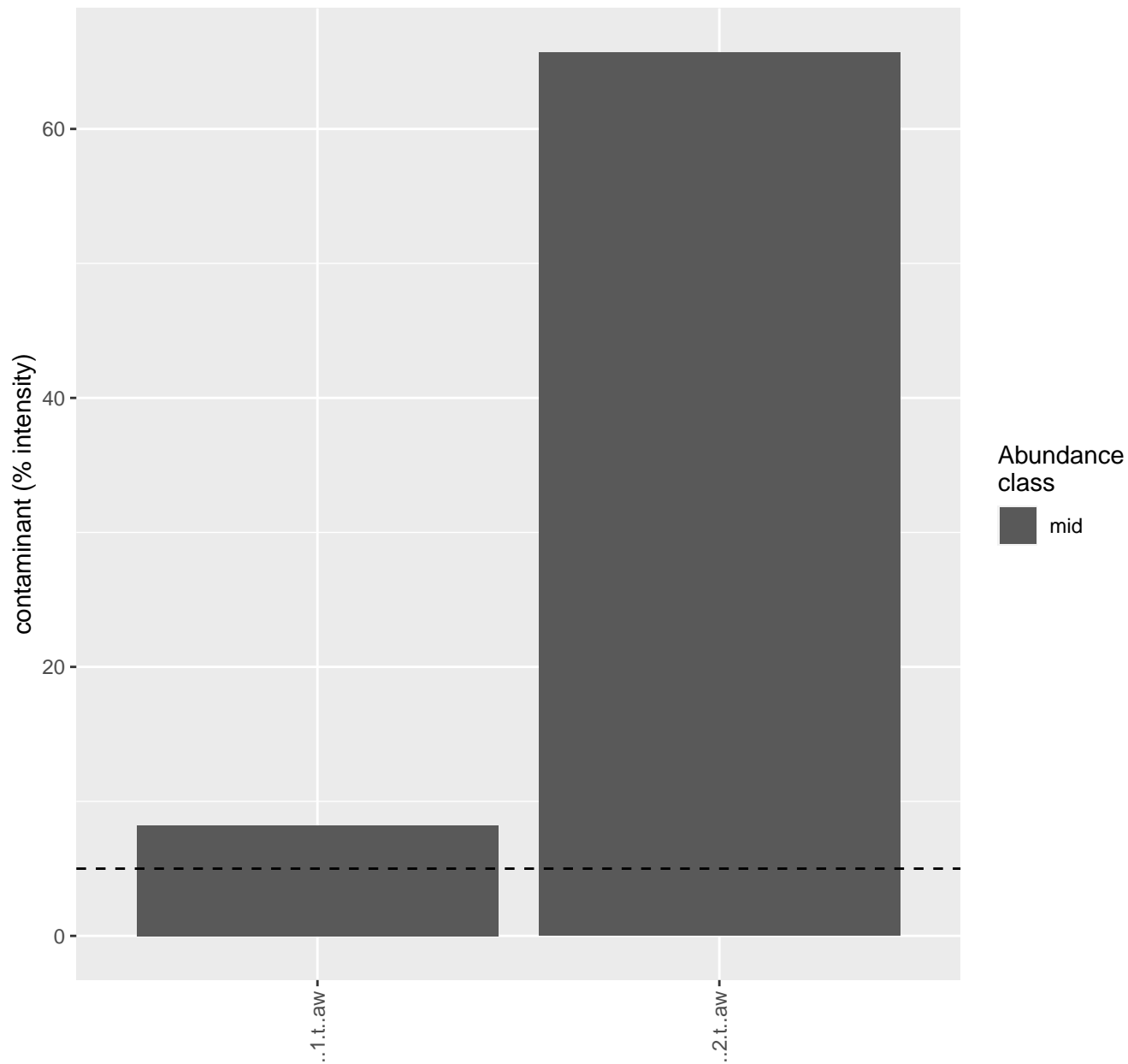
(excludes contaminants)



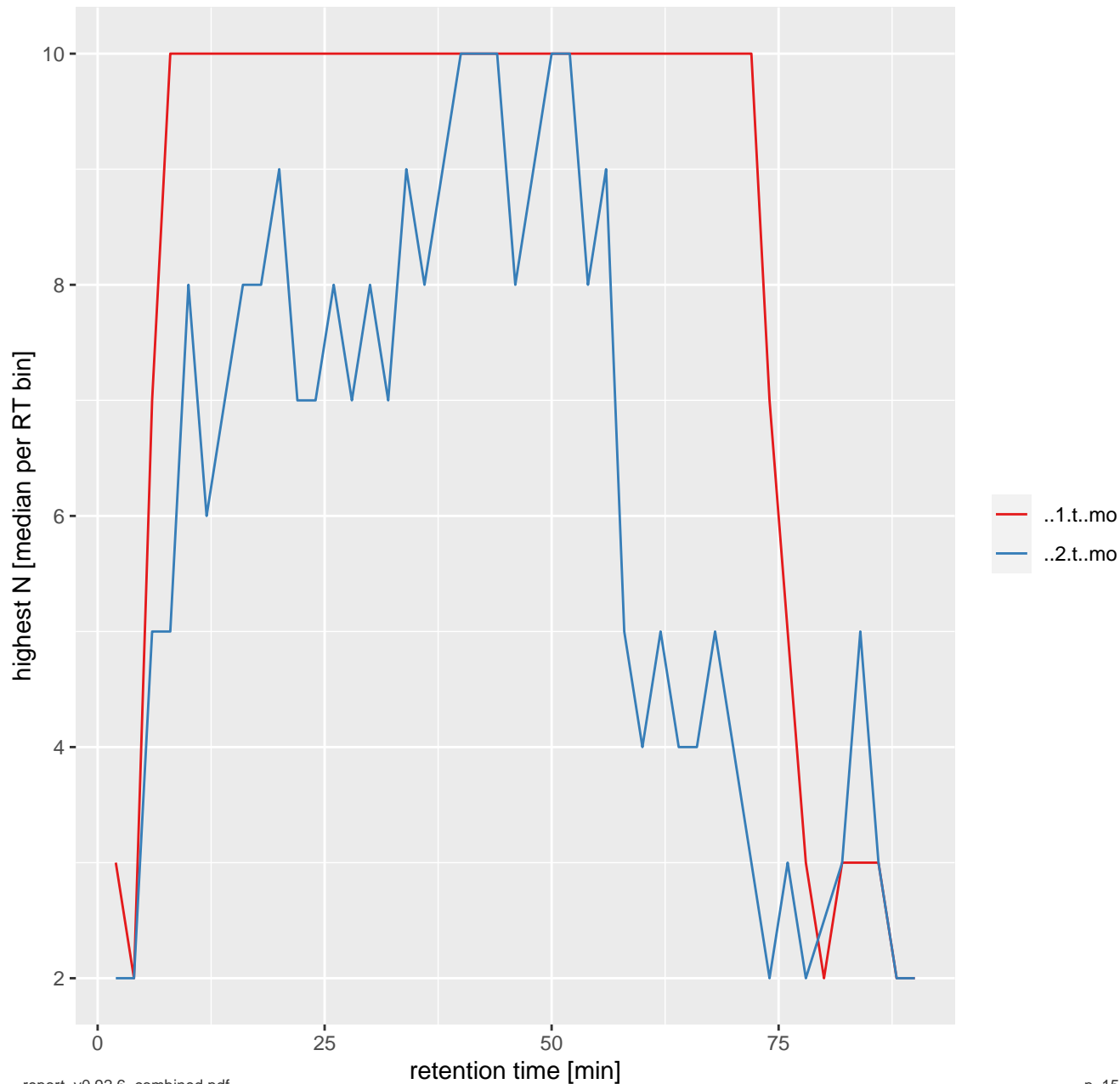
EVD: charge distribution



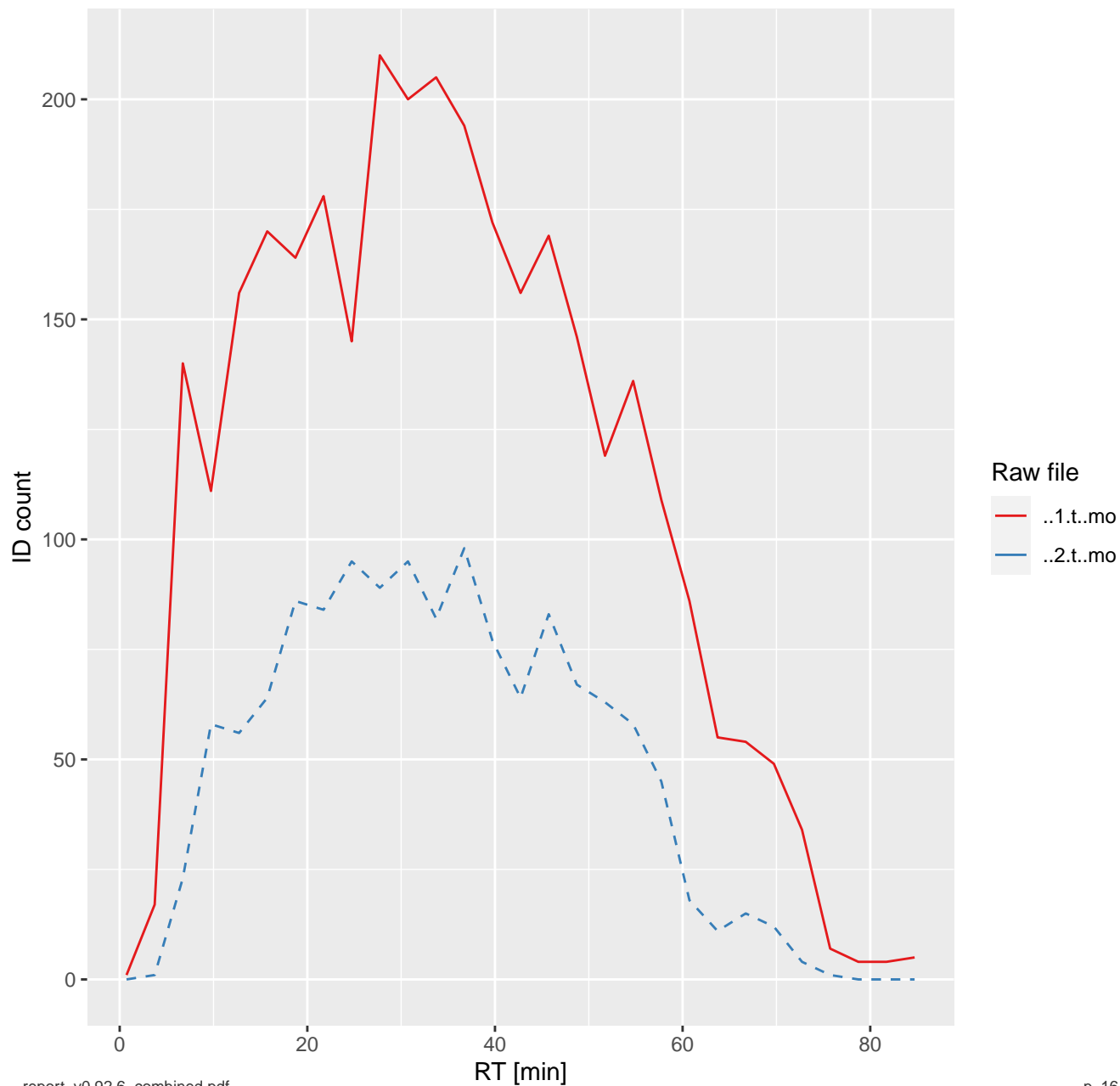
PG: Contaminant per condition



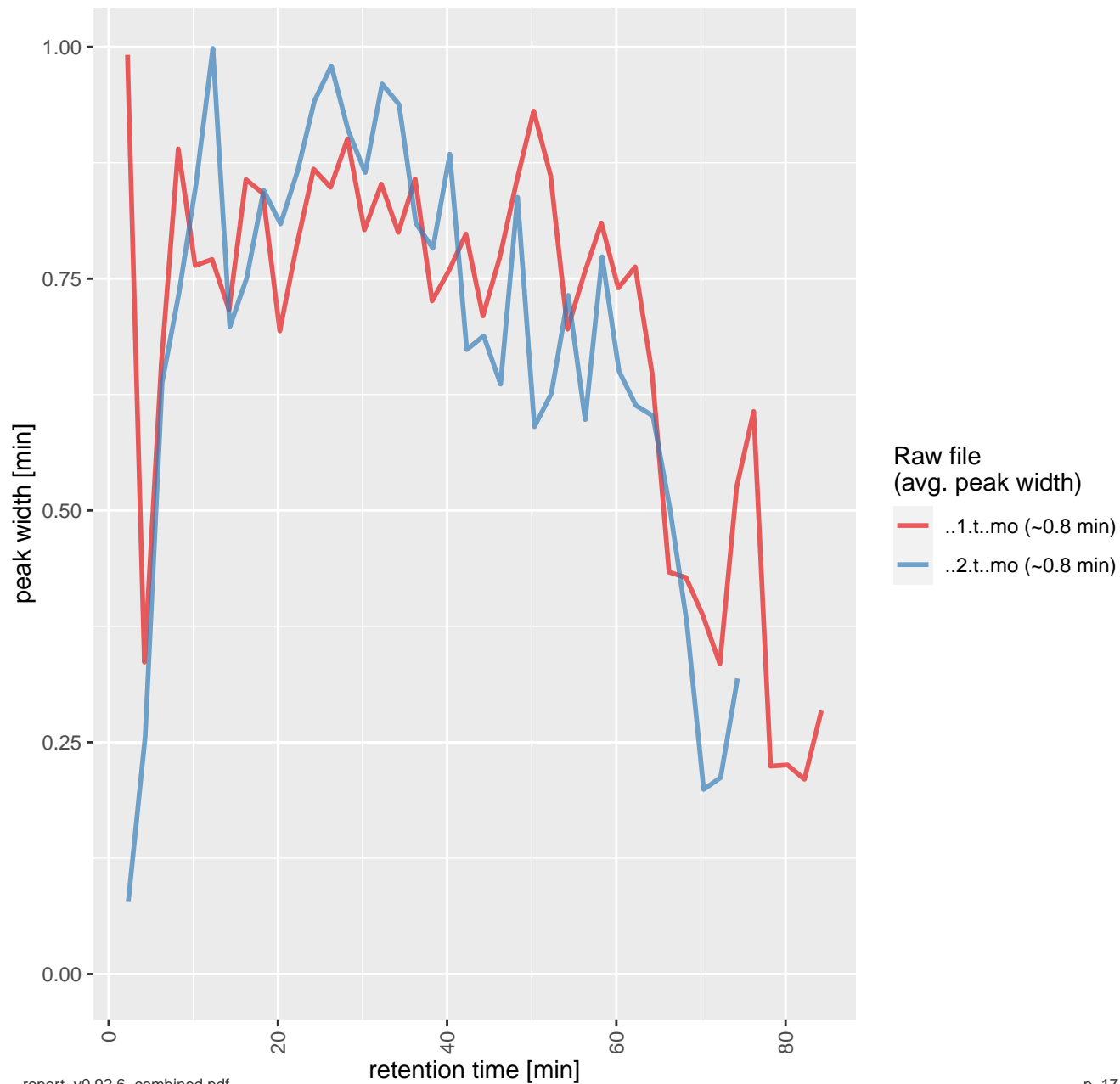
MSMSscans: TopN over RT



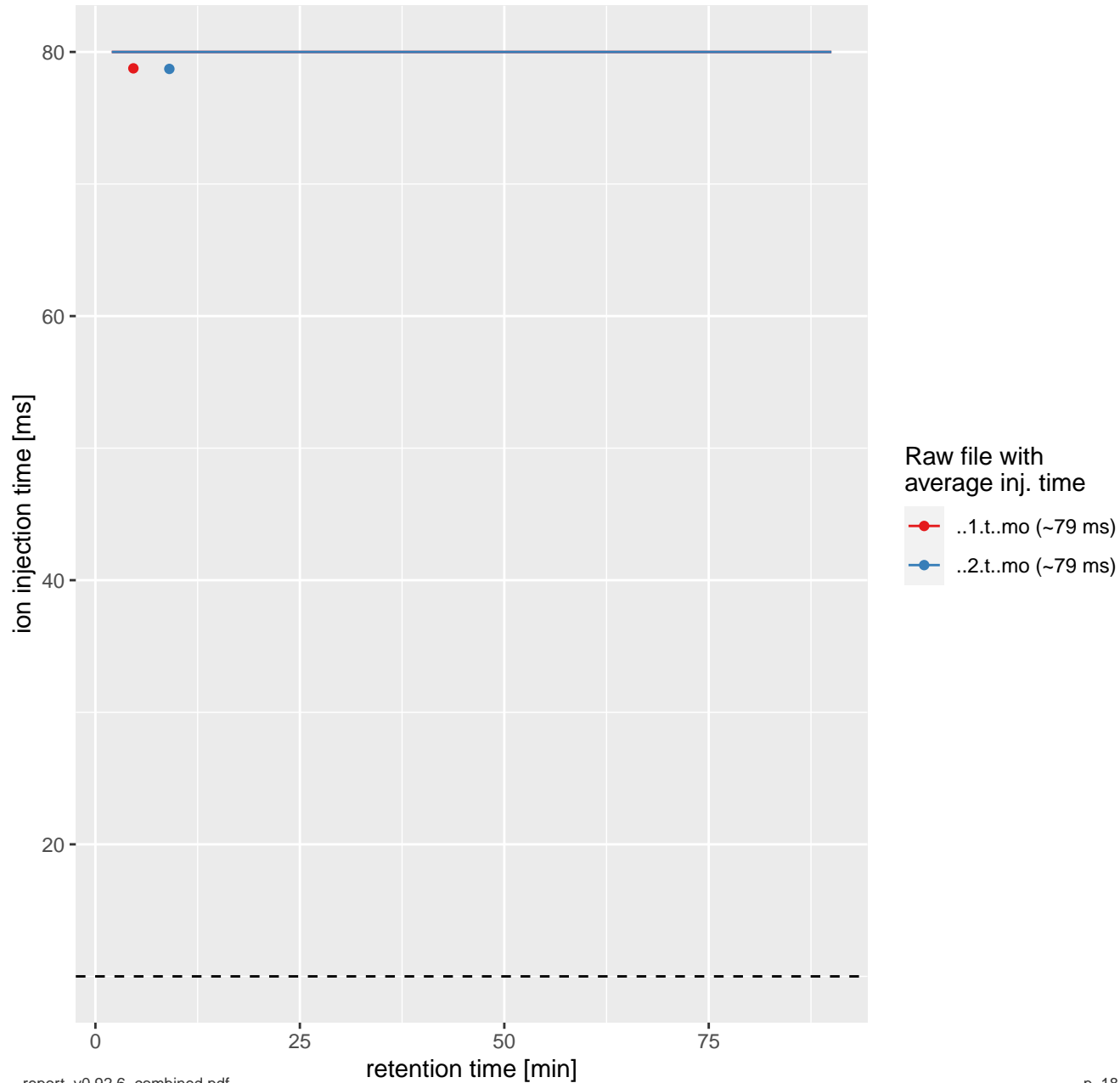
EVD: IDs over RT



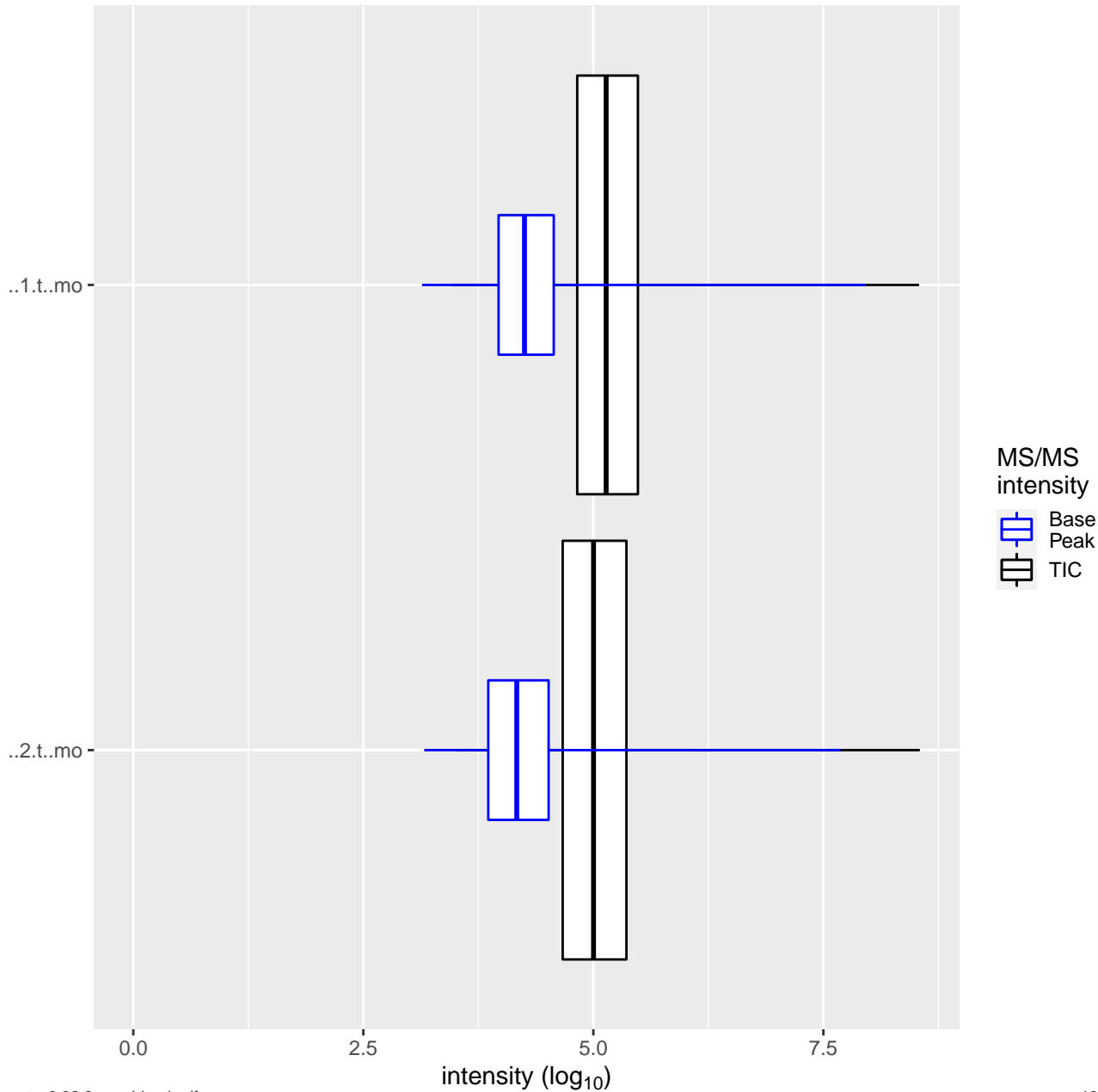
EVD: Peak width over RT



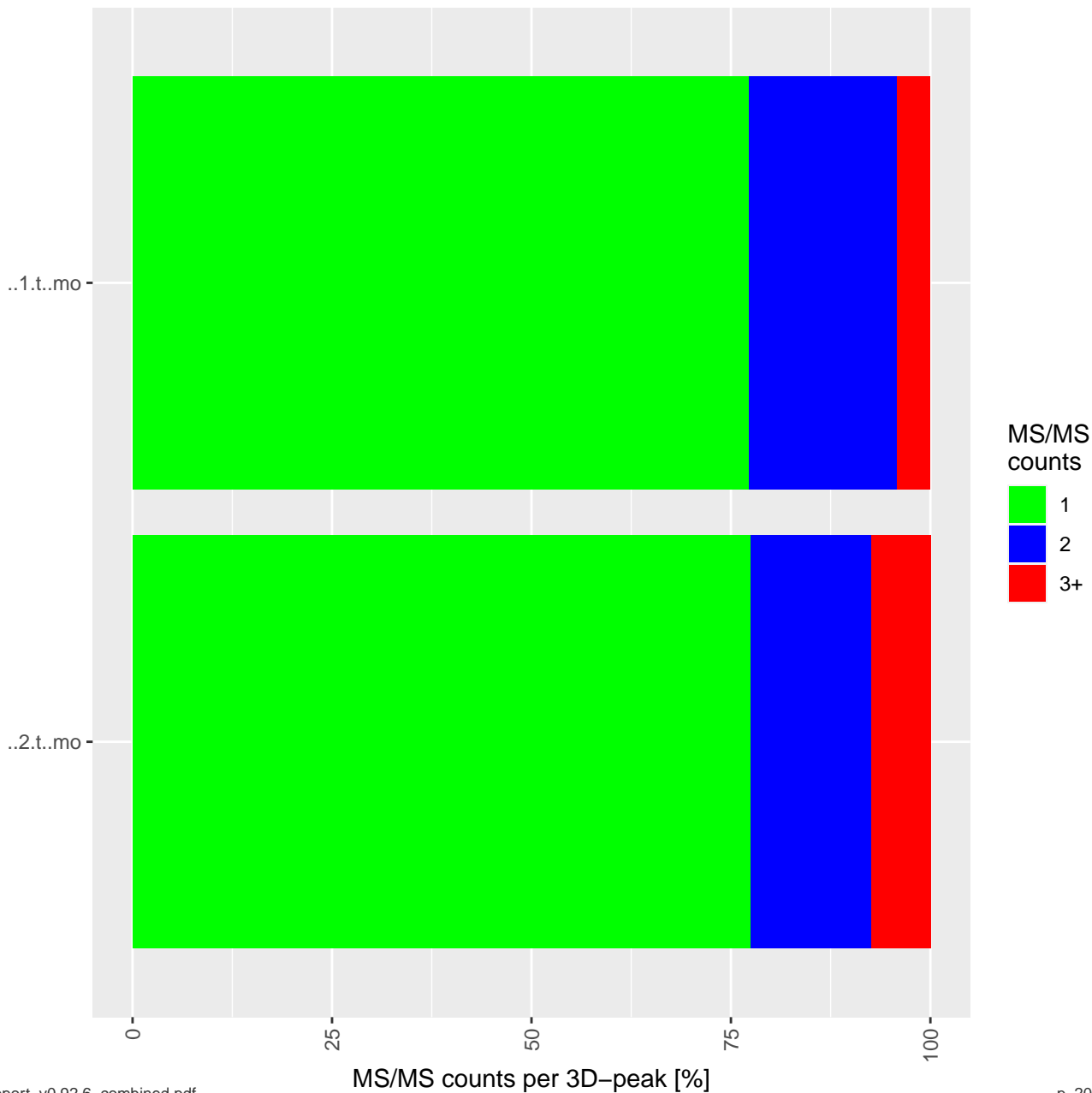
MSMSscans: Ion Injection Time over RT



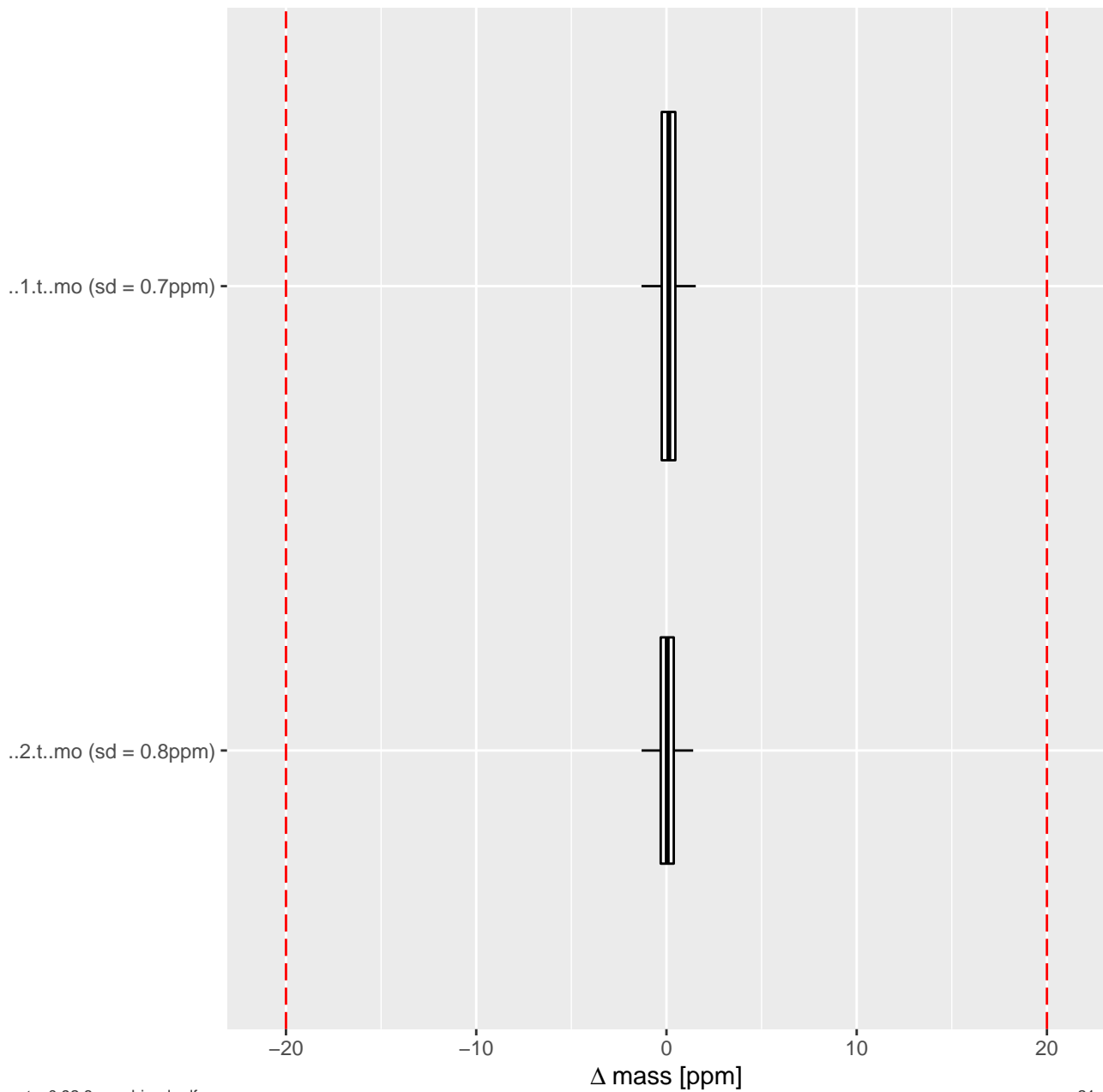
[experimental] MSMSscans: MS/MS intensity



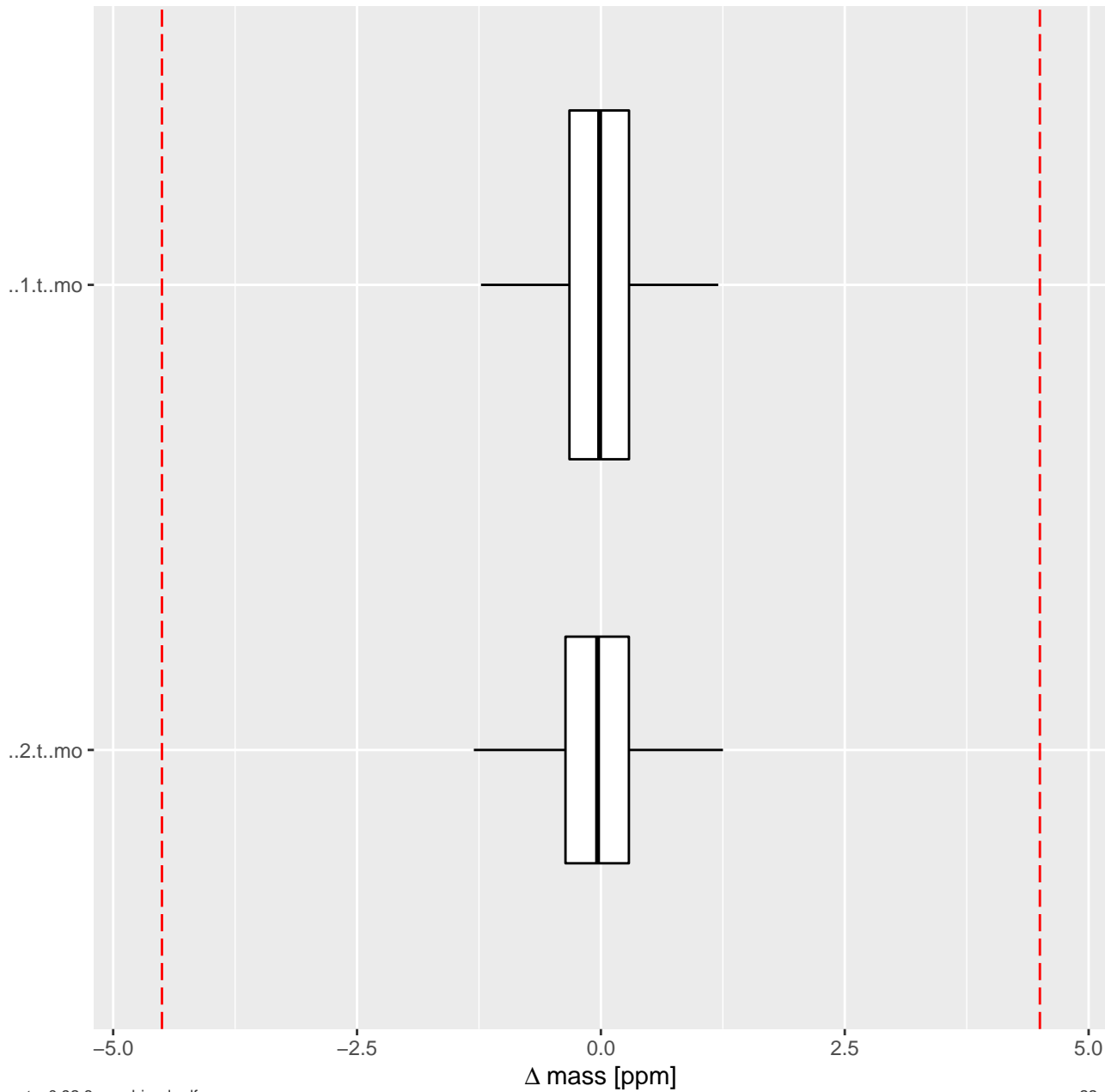
EVD: Oversampling (MS/MS counts per 3D-peak)



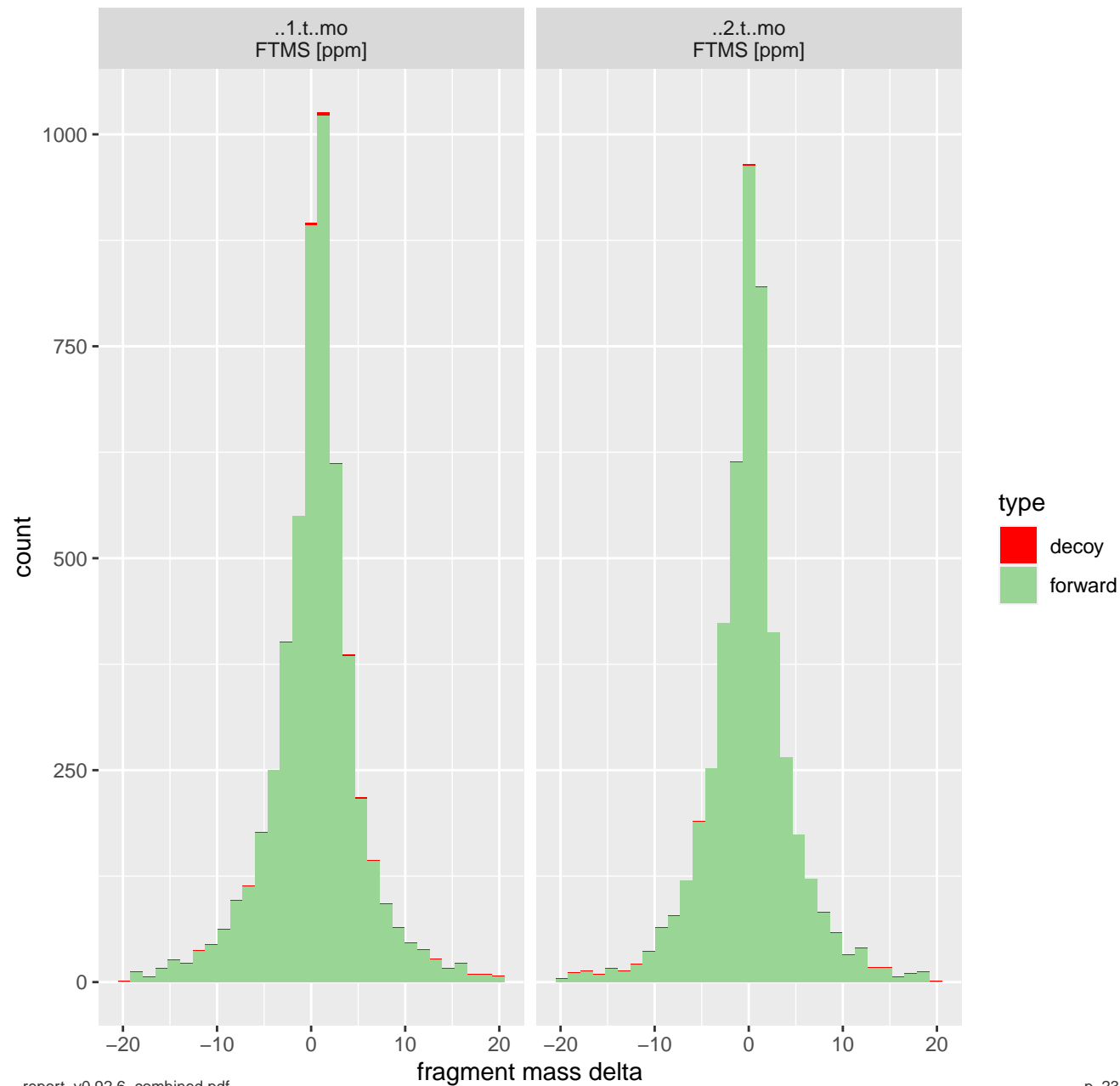
EVD: Uncalibrated mass error



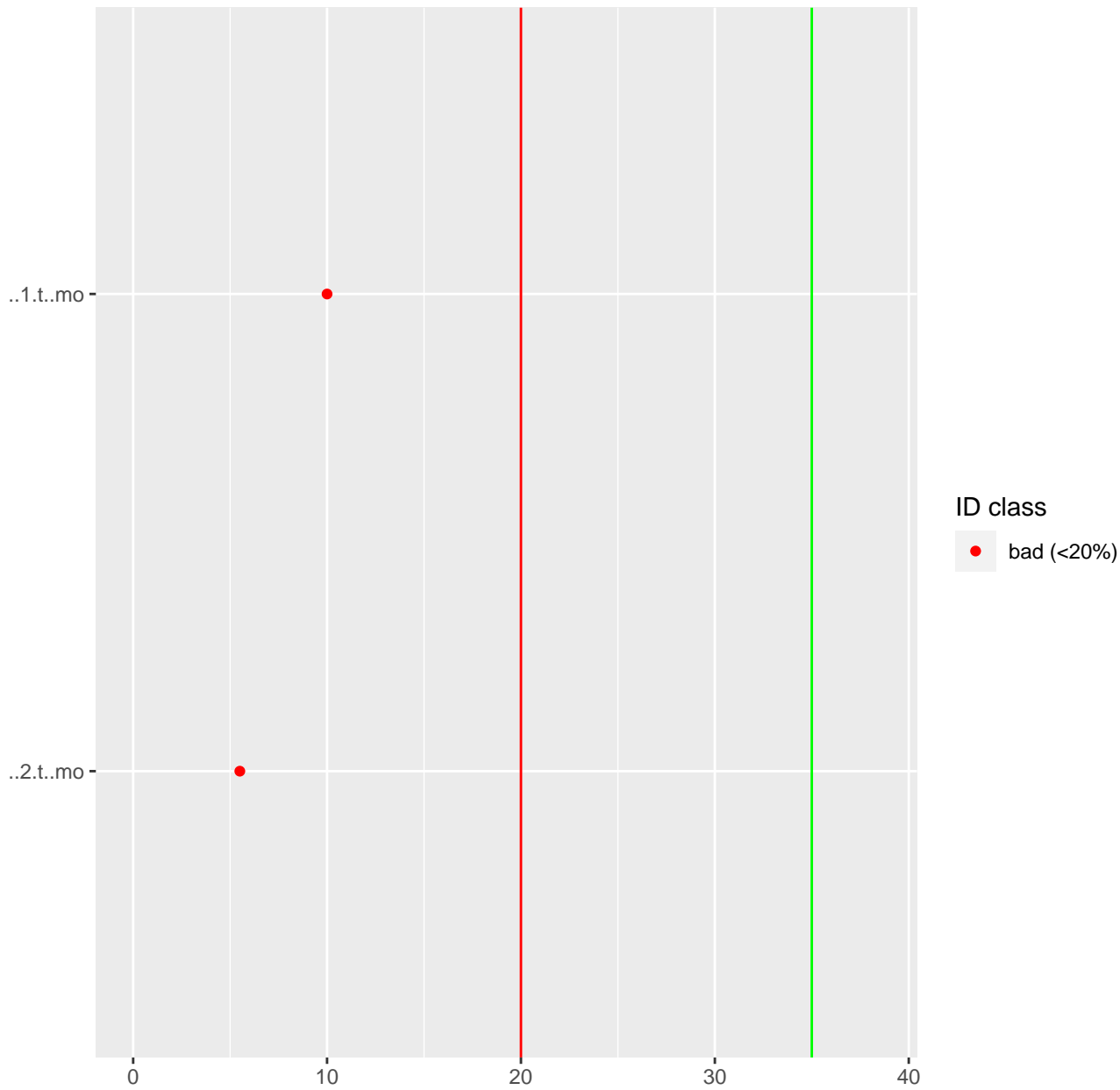
EVD: Calibrated mass error



MSMS: Fragment mass errors per Raw file



SM: MS/MS identified per Raw file

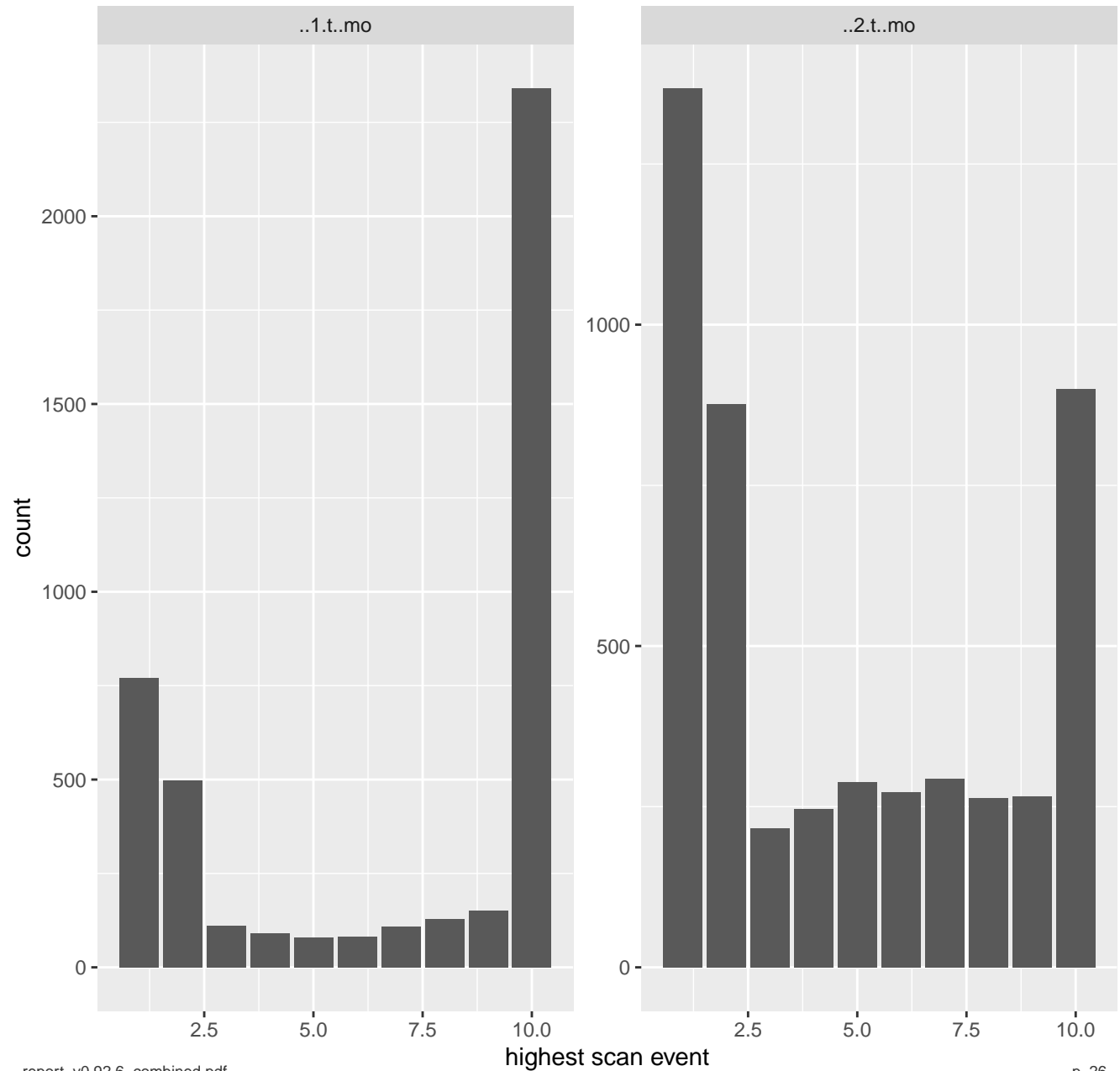


SM: Files with 'red' ID rate

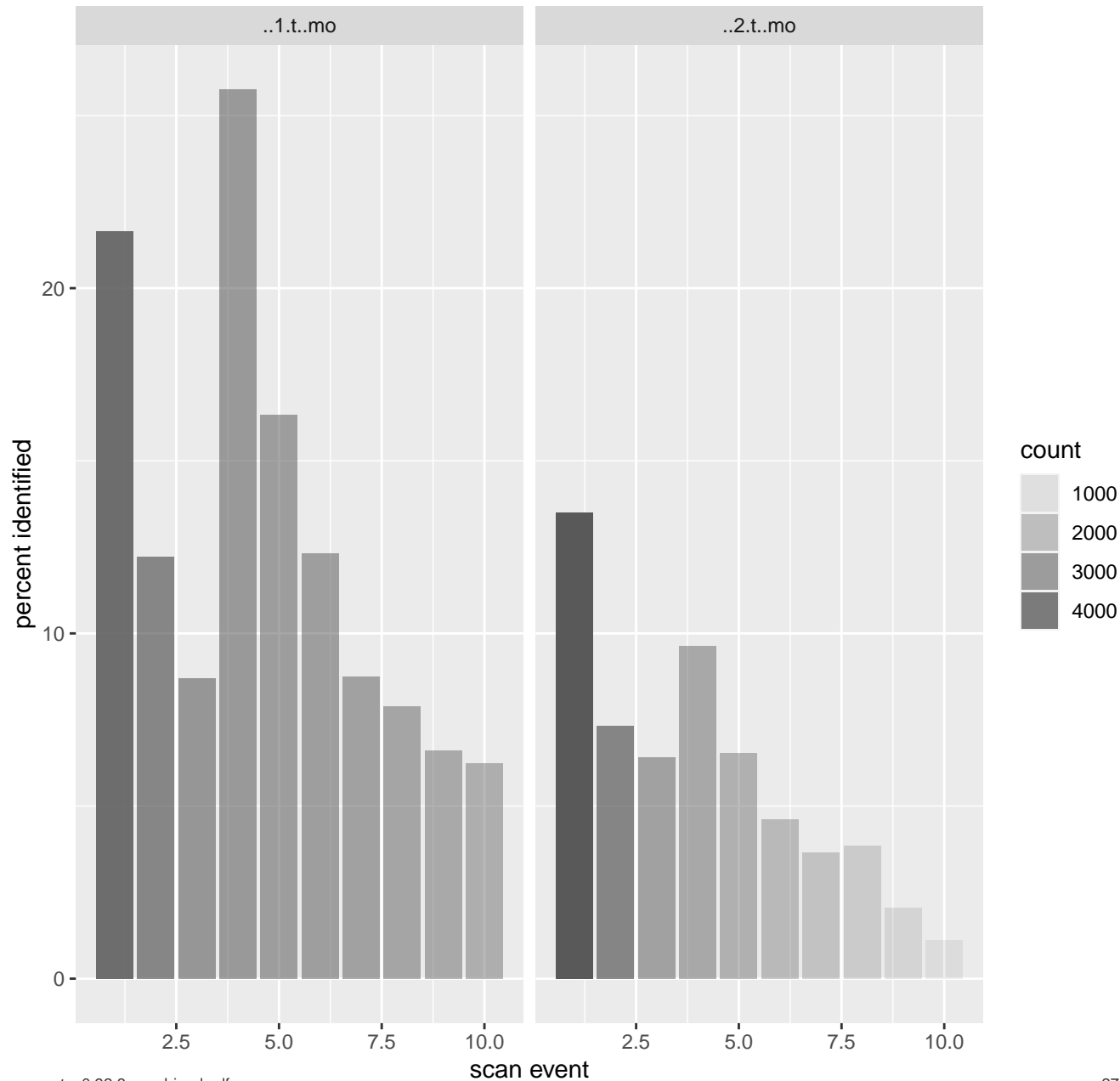
Raw file	% identified
Sample1.thermo	10.0
Sample2.thermo	5.5

100% of samples)

MSMSscans: TopN

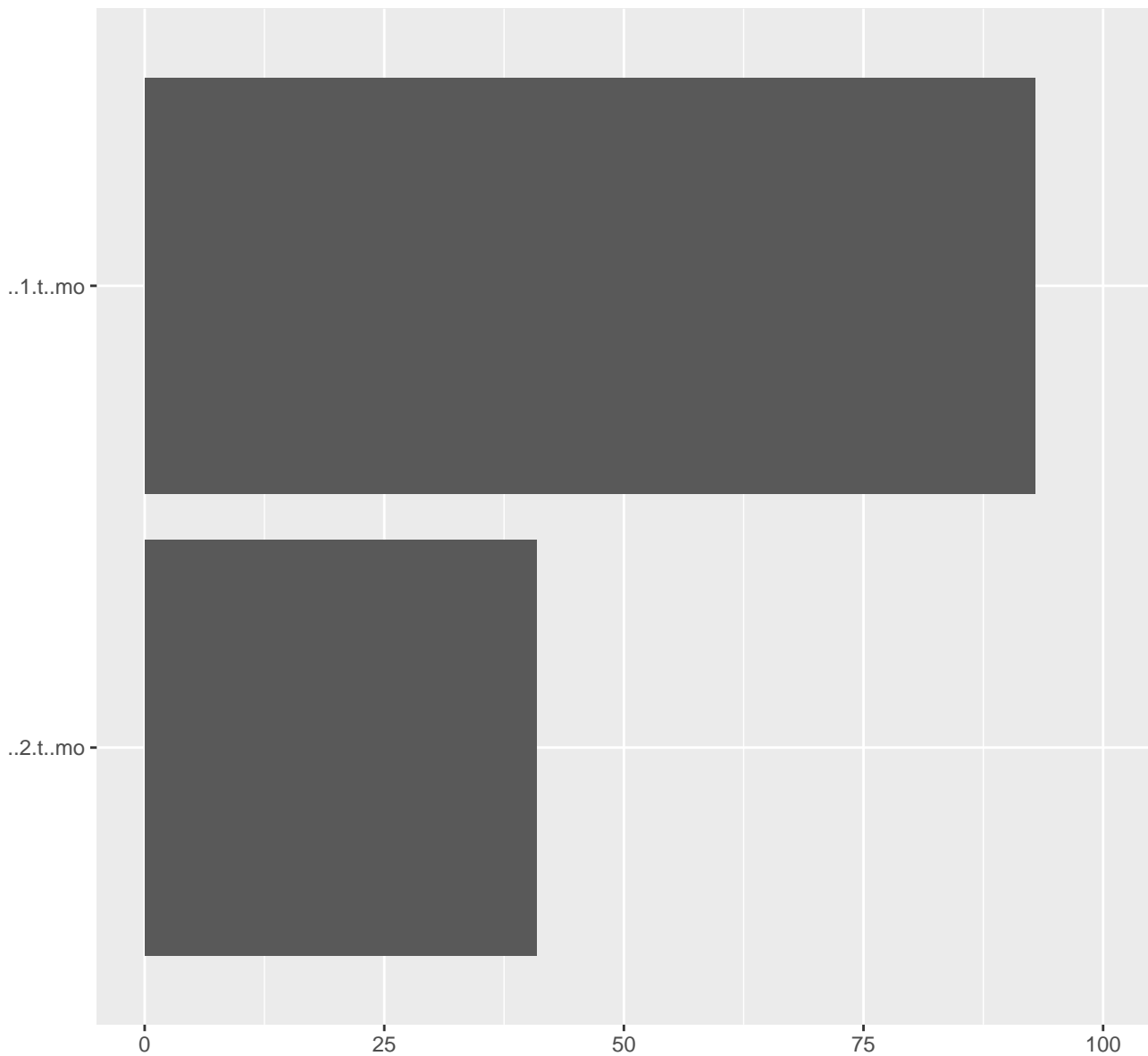


MSMSscans: TopN % identified over N

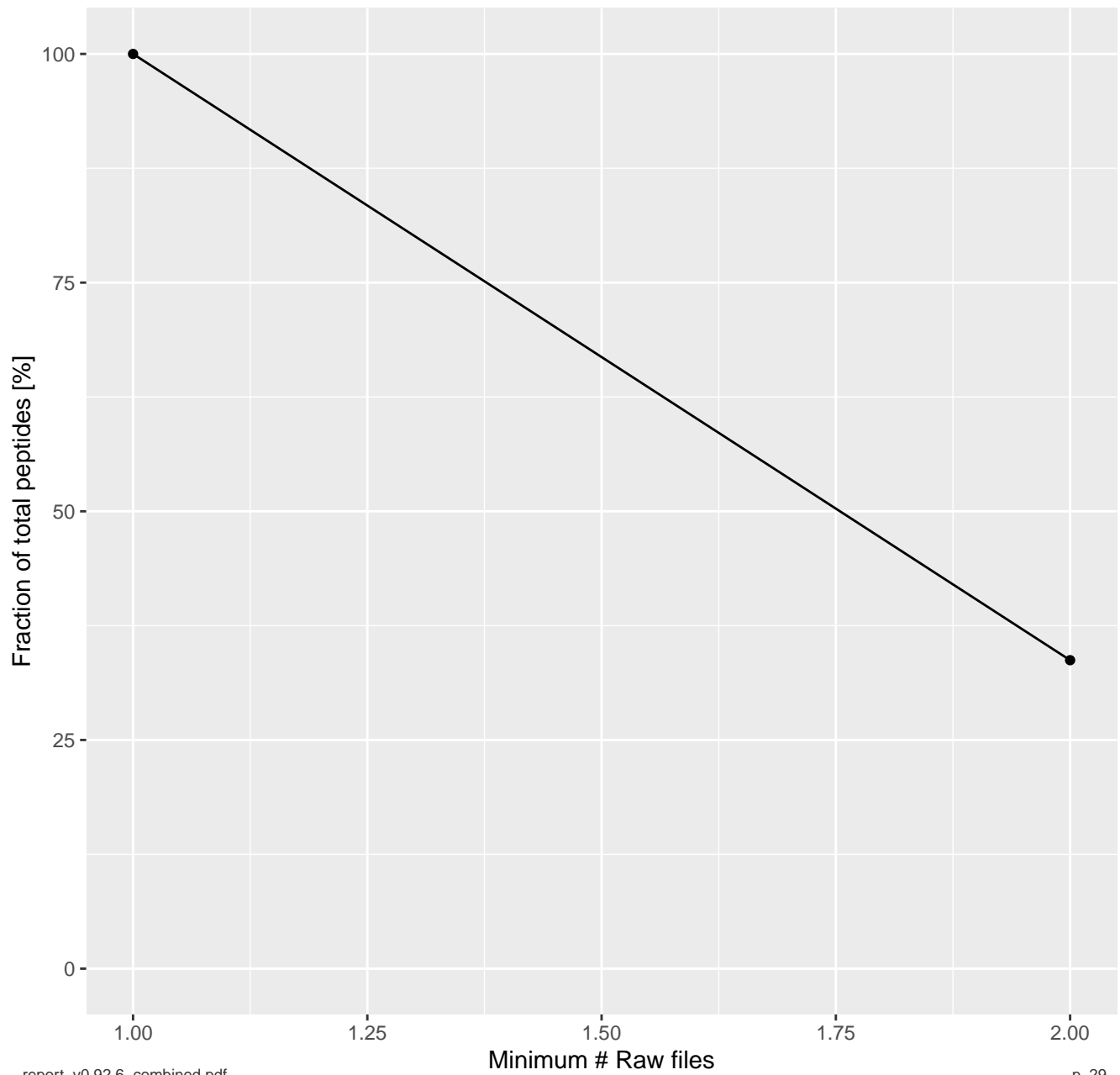


[experimental] EVD: Non-Missing Peptides

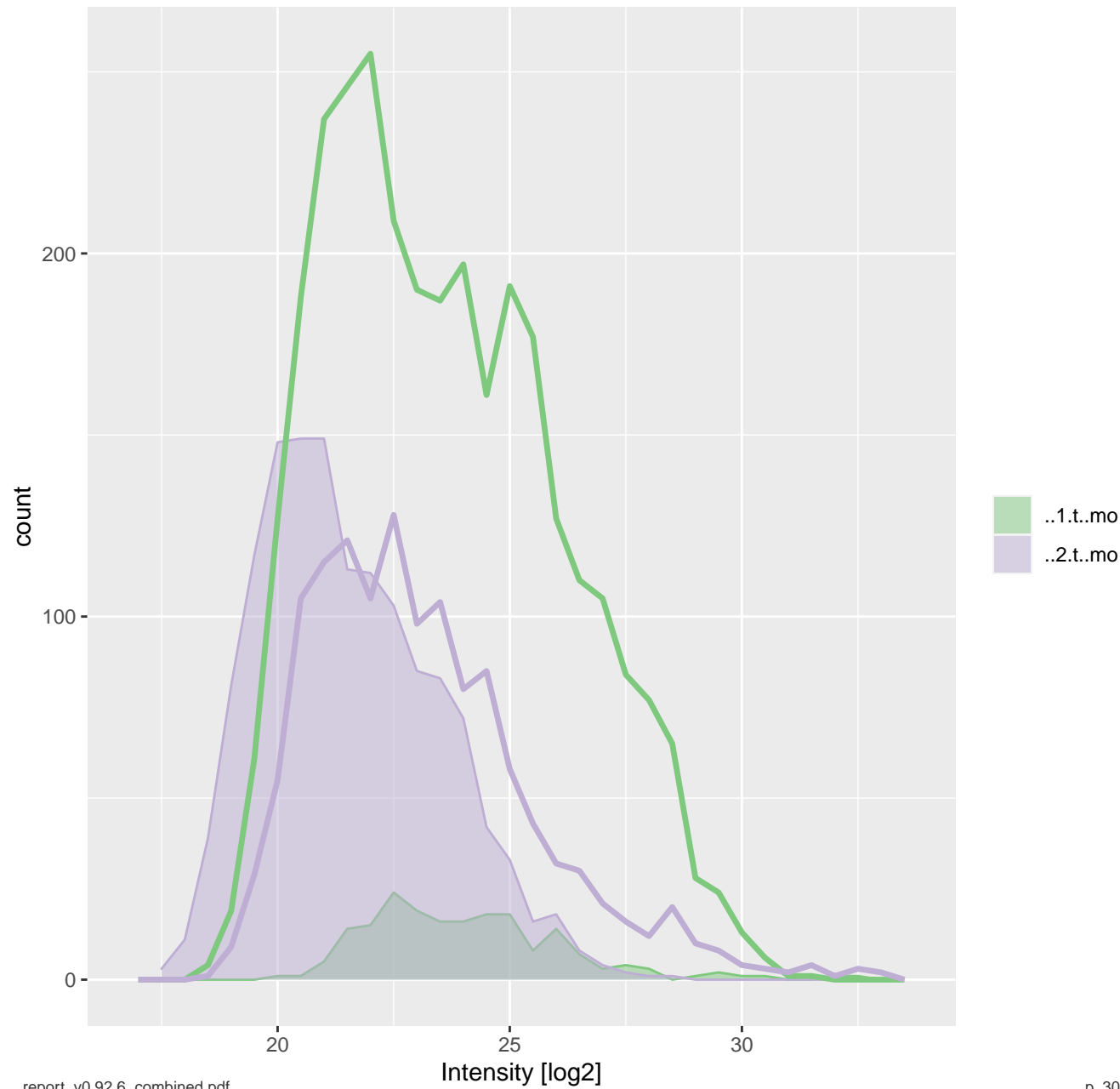
compared to all peptides seen in experiment



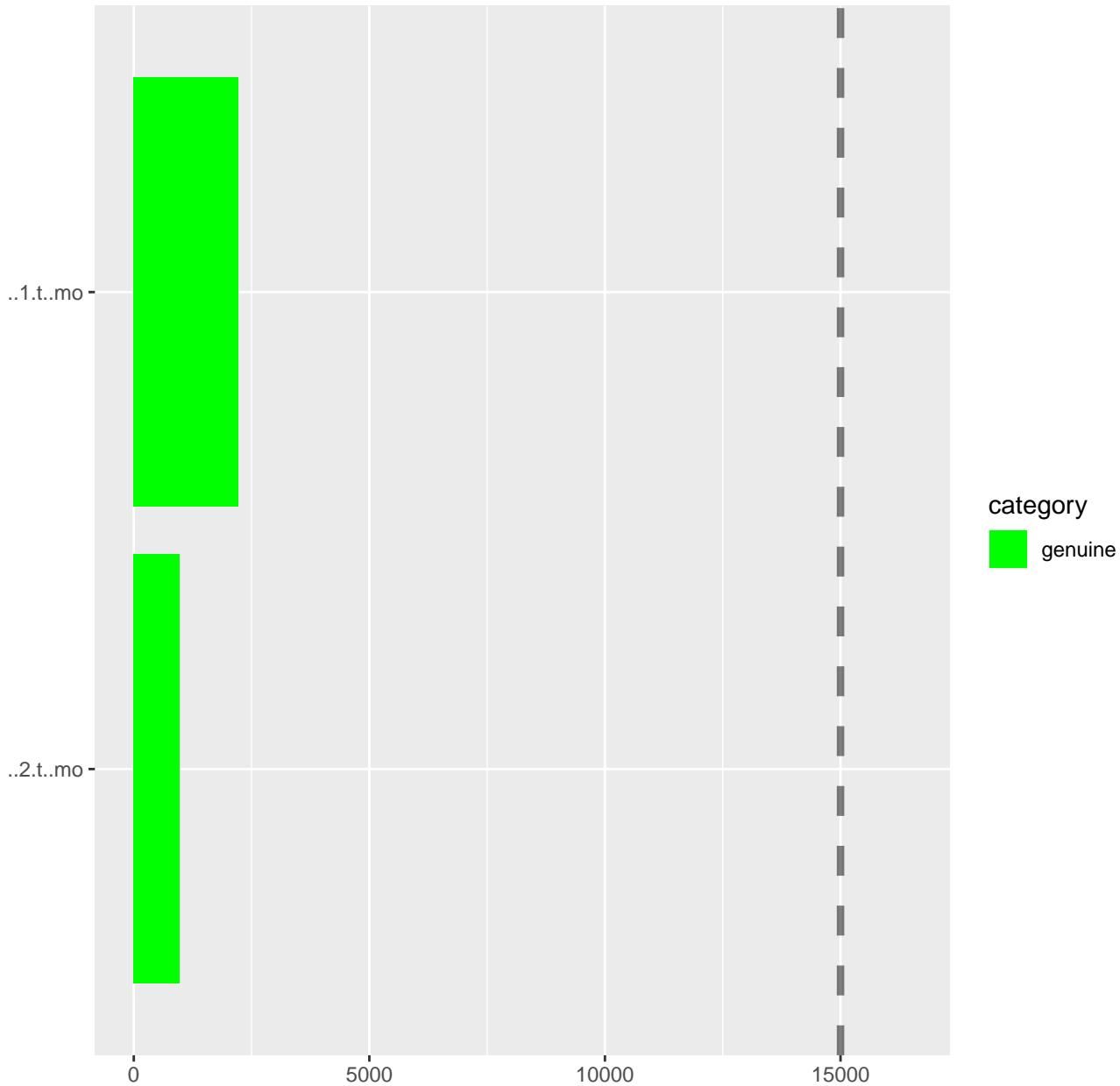
[experimental] EVD: Non-missing by set



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



EVD: Peptide ID count



EVD: ProteinGroups count

