

Performance overview

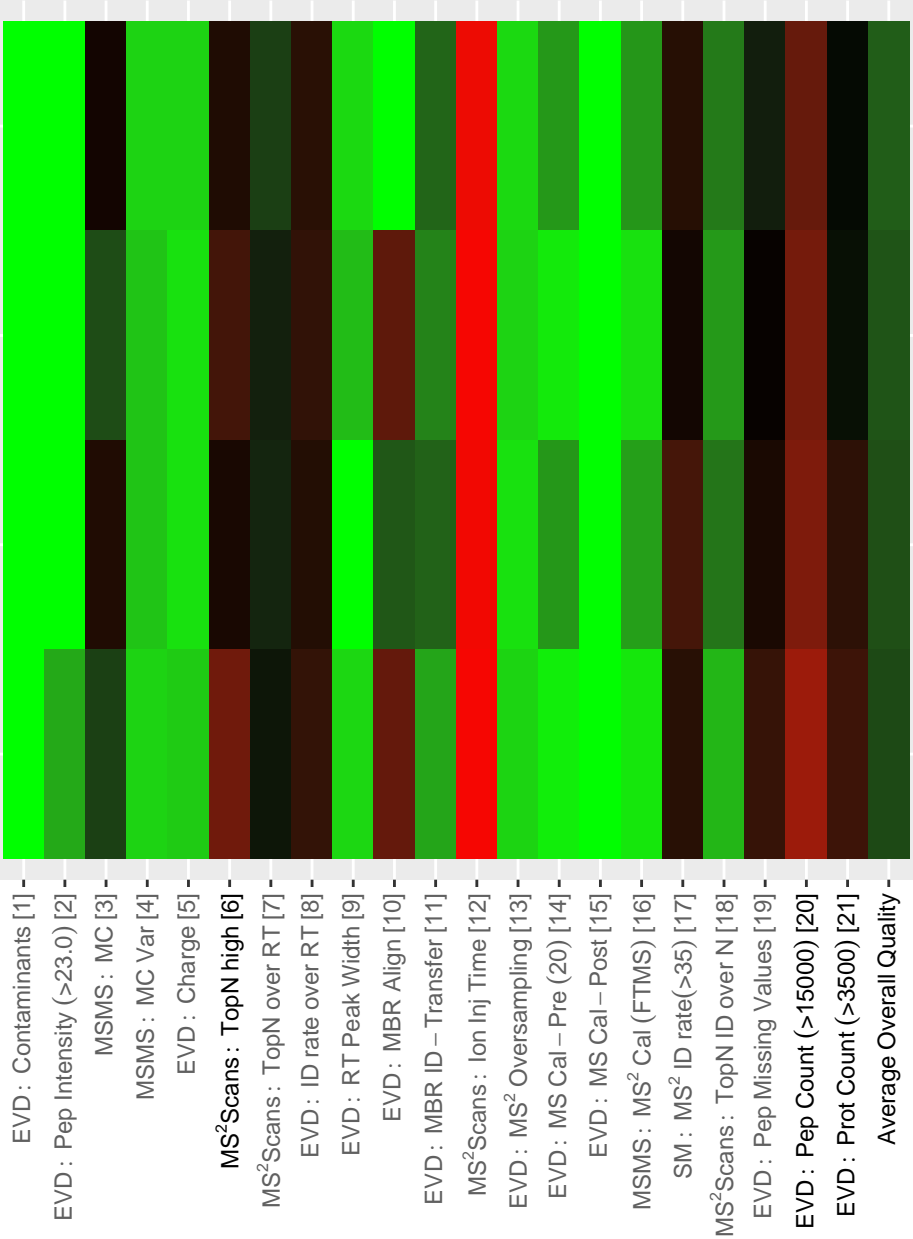
Raw file

PSB100 (2)

PSB100

PSB250-1

PSB250-2



Mapping of Raw files to their short names

Mapping source: automatic

(automatic shortening of names was not sufficiently short – see 'best effort')

original	short name	best effort
PSB100 (2)	PSB100 (2)	PSB100 (2)
PSB100	PSB100	PSB100
PSB250-1	PSB250-1	PSB250-1
PSB250-2	PSB250-2	PSB250-2

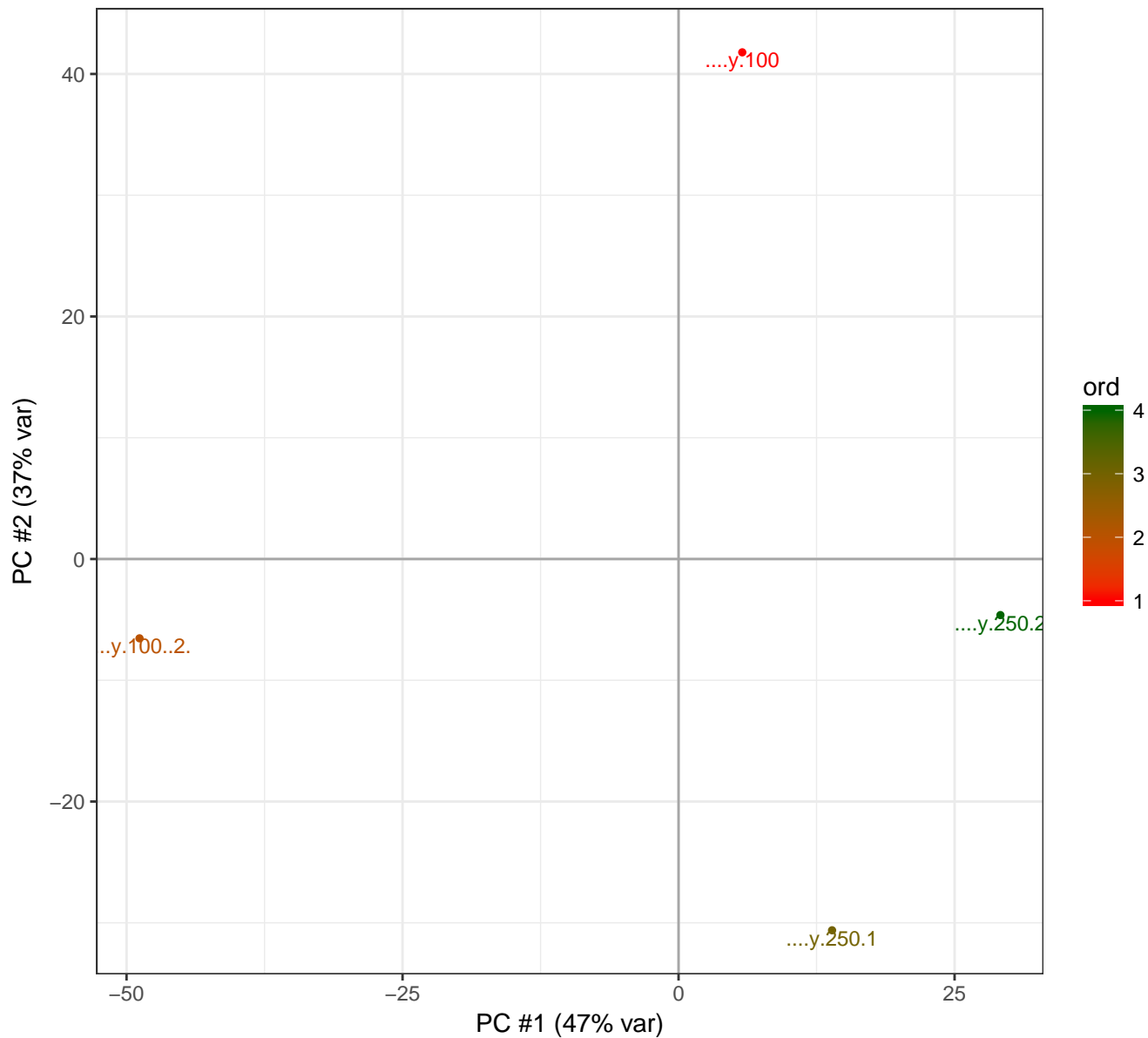
PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	MS/MS deisotoping (FTMS)	True
Alignment time window [min]	20	MS/MS deisotoping (ITMS)	False
Date of writing	01/21/2017 13:22:40	MS/MS deisotoping (TOF)	True
Decoy mode	revert	MS/MS deisotoping (Unknown)	False
Discard unmodified counterpa..	True	MS/MS tol. (FTMS)	20 ppm
Find dependent peptides	False	MS/MS tol. (ITMS)	0.5 Da
First pass AIF correlation	0.8	MS/MS tol. (TOF)	40 ppm
Fixed modifications	Carbamidomethyl (C)	MS/MS tol. (Unknown)	0.5 Da
iBAQ	False	Peptides used for protein qu..	Razor
iBAQ log fit	False	Protein FDR	0.01
Include contaminants	True	PSM FDR	0.01
Labeled amino acid filtering	True	Re-quantify	False
Machine name	W7DELLT340002	RT shift	False
Match between runs	True	Site FDR	0.01
Matching time window [min]	0.7	Site tables	Oxidation (M)Sites.txt Phospho (STY)Sites.txt
Min. delta score for modifie..	6	Special AAs	KR
Min. delta score for unmodif..	0	Top MS/MS peaks per 100 Da. ...	12
Min. peptide Length	7	Top MS/MS peaks per 100 Da. ...	8
Min. peptides	1	Top MS/MS peaks per 100 Da. ...	10
Min. ratio count	1	Top MS/MS peaks per 100 Da. ...	8
Min. razor peptides	1	Use delta score	False
Min. score for modified pept..	40	Use Normalized Ratios For Oc..	True
Min. score for unmodified pe..	0	Use only unmodified peptides..	True
Min. unique peptides	0	User name	mubeen
Modifications included in pr..	Acetyl (Protein N-term) Oxidation (M) Phospho (STY)	Version	1.5.2.8

uniprot-taxonomy%3A-Arabidopsis+%5B3701%5D-.fasta

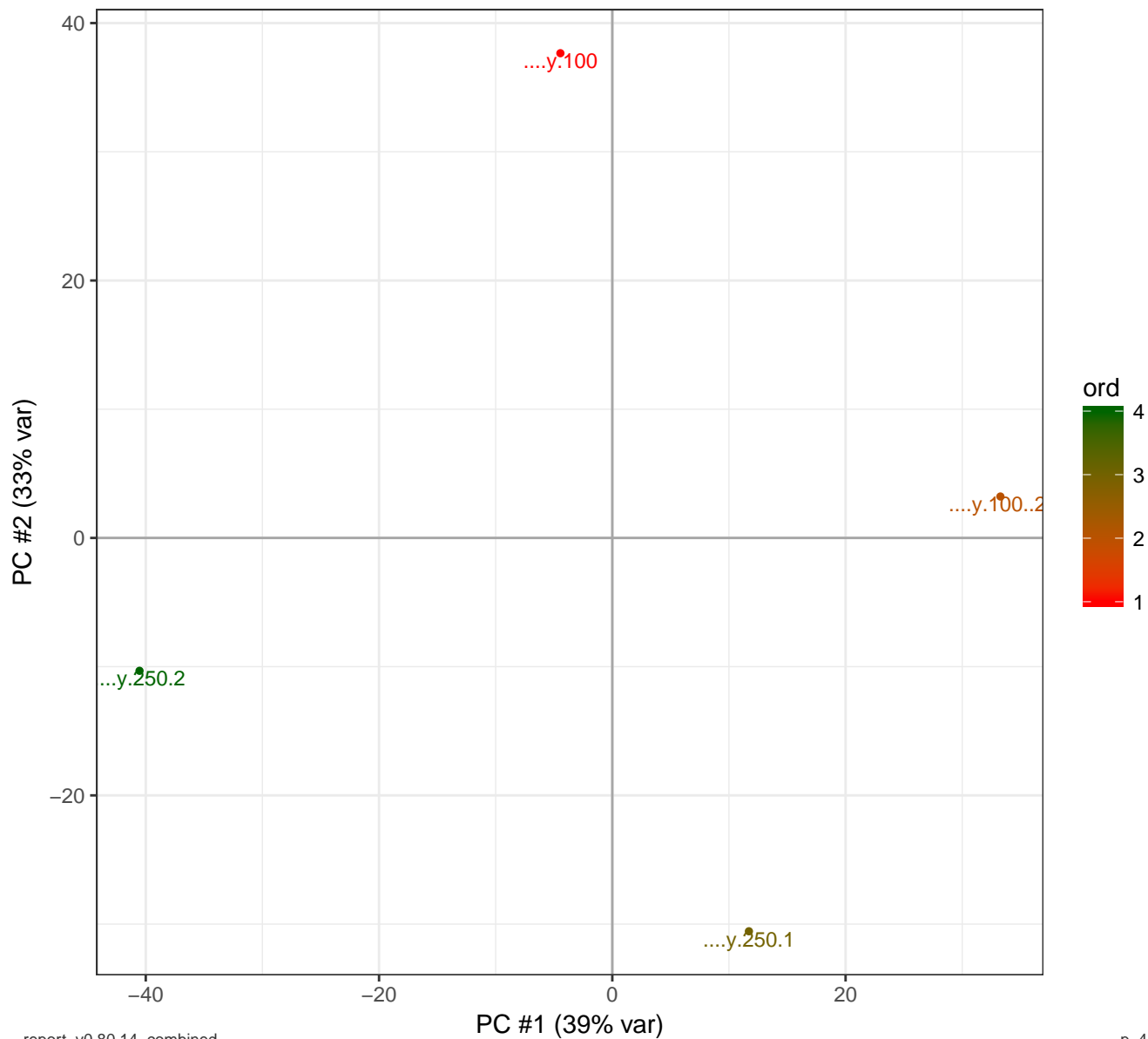
PG: PCA of 'raw intensity'

(excludes contaminants)

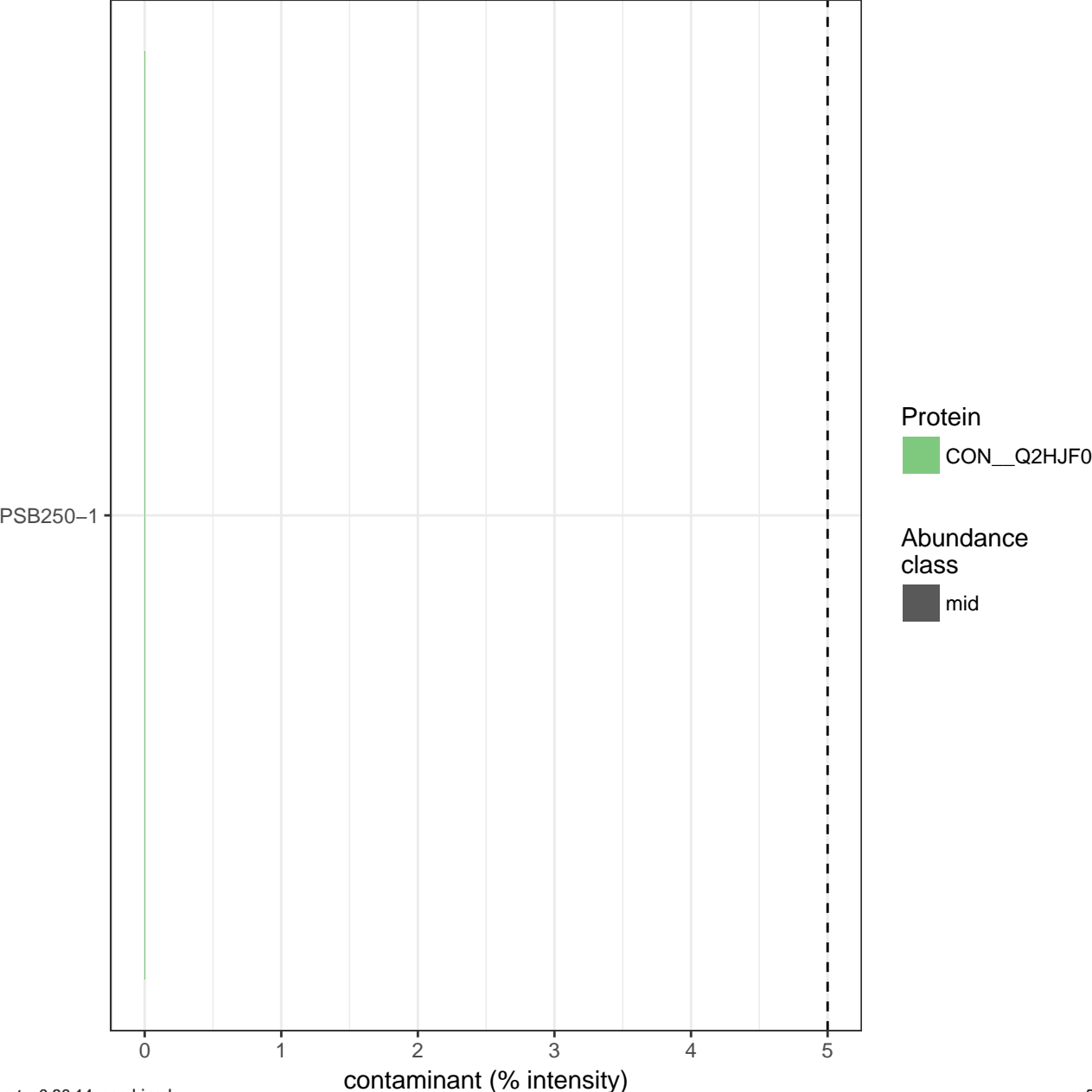


PG: PCA of 'lfq intensity'

(excludes contaminants)



EVD: Top5 Contaminants per Raw file



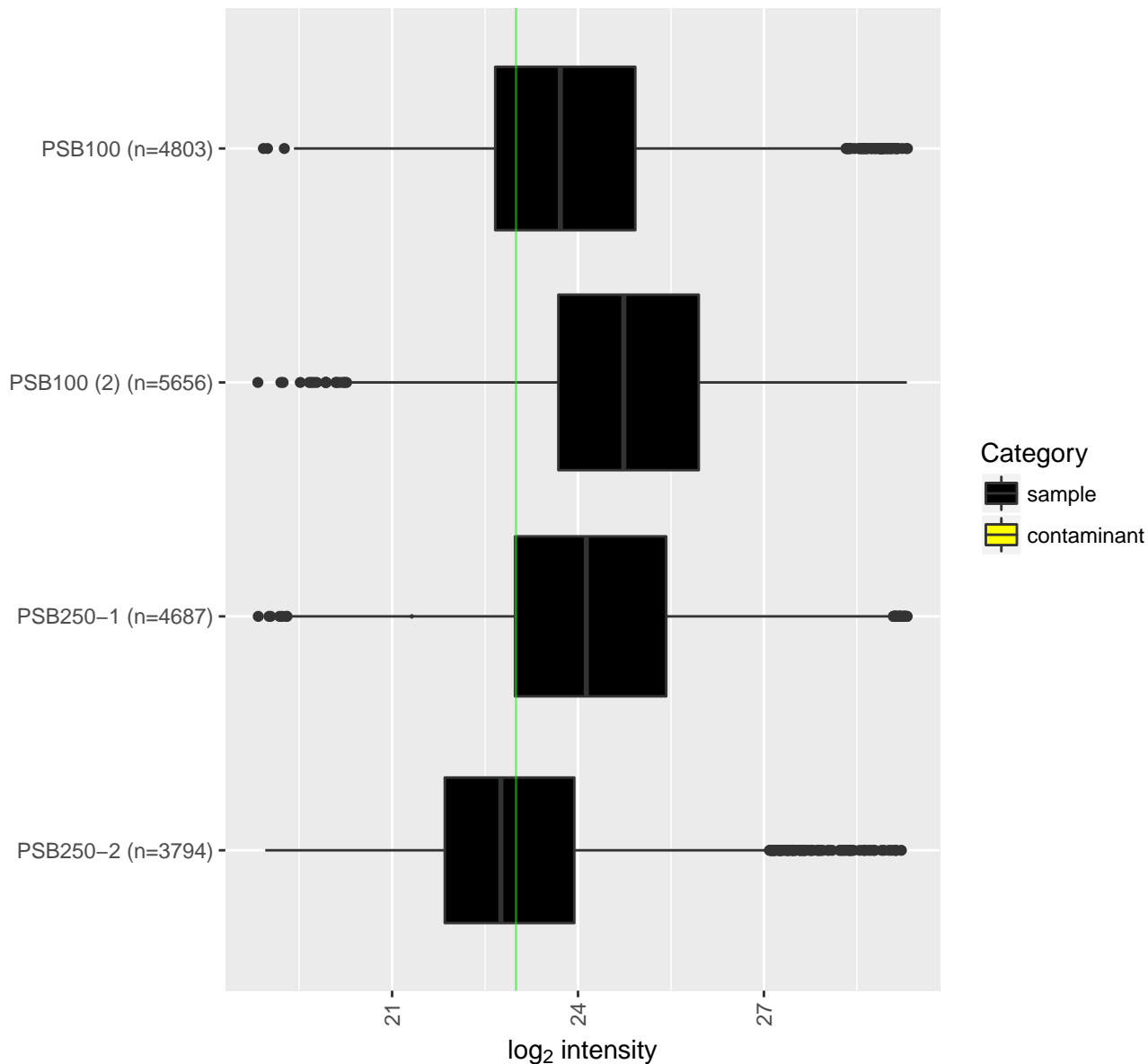
EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

Did you use the correct database?

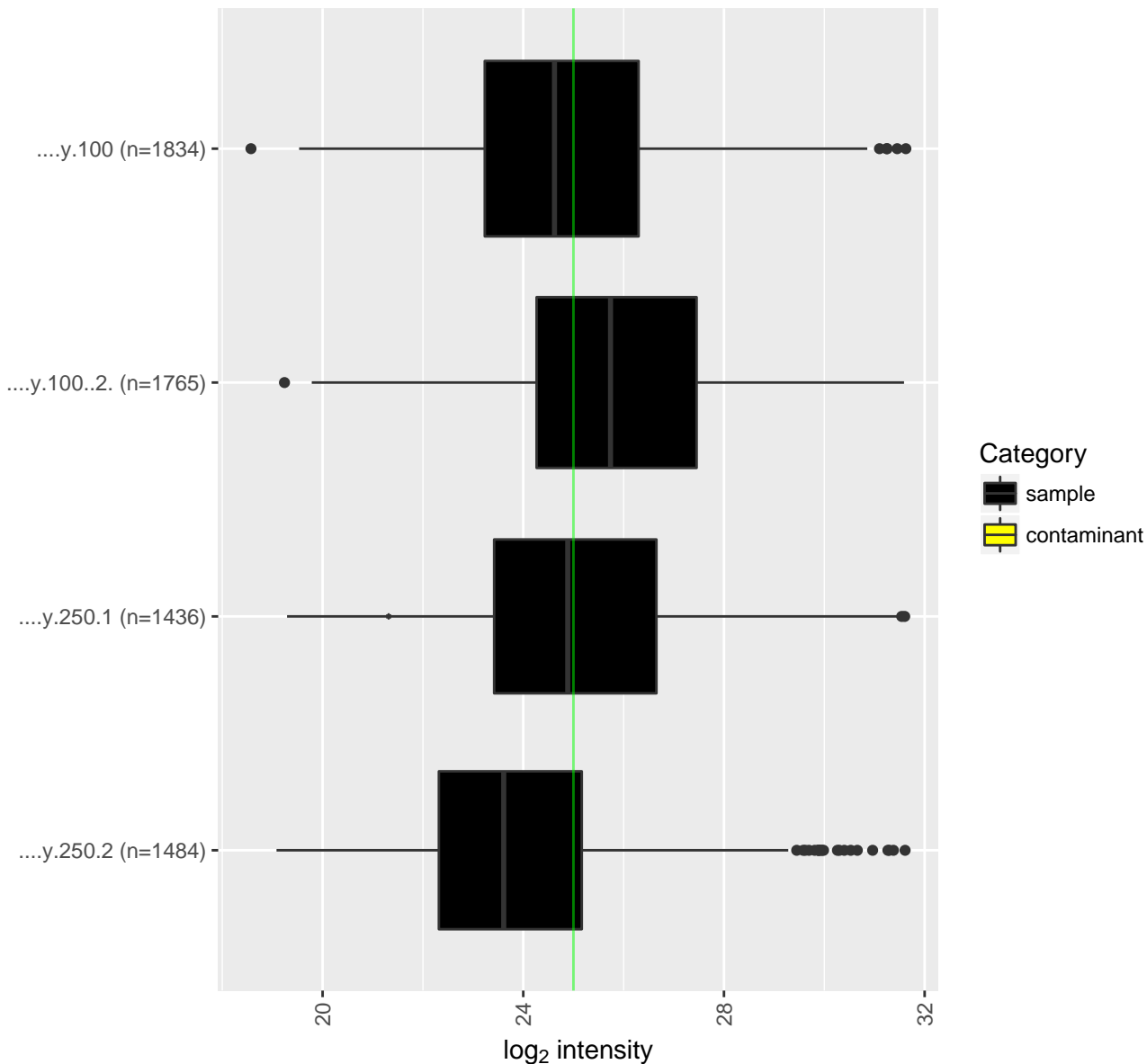
EVD: peptide intensity distribution

RSD 3.6% (expected < 5%)



PG: intensity distribution

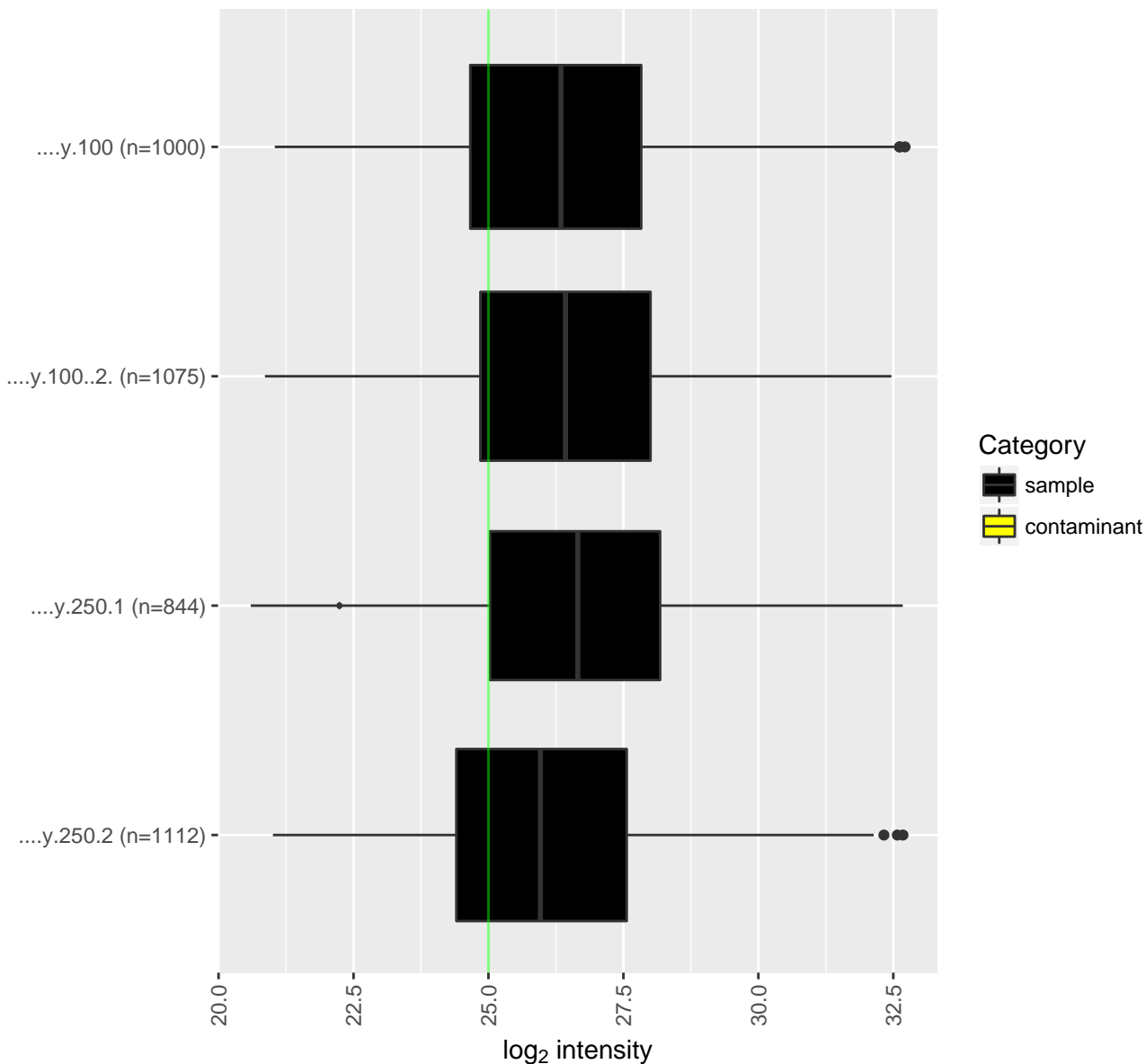
RSD 3.7% (w/o zero int.; expected < 5%)
RSD 5.3% [high RSD --> few peptides])



PG: LFQ intensity distribution

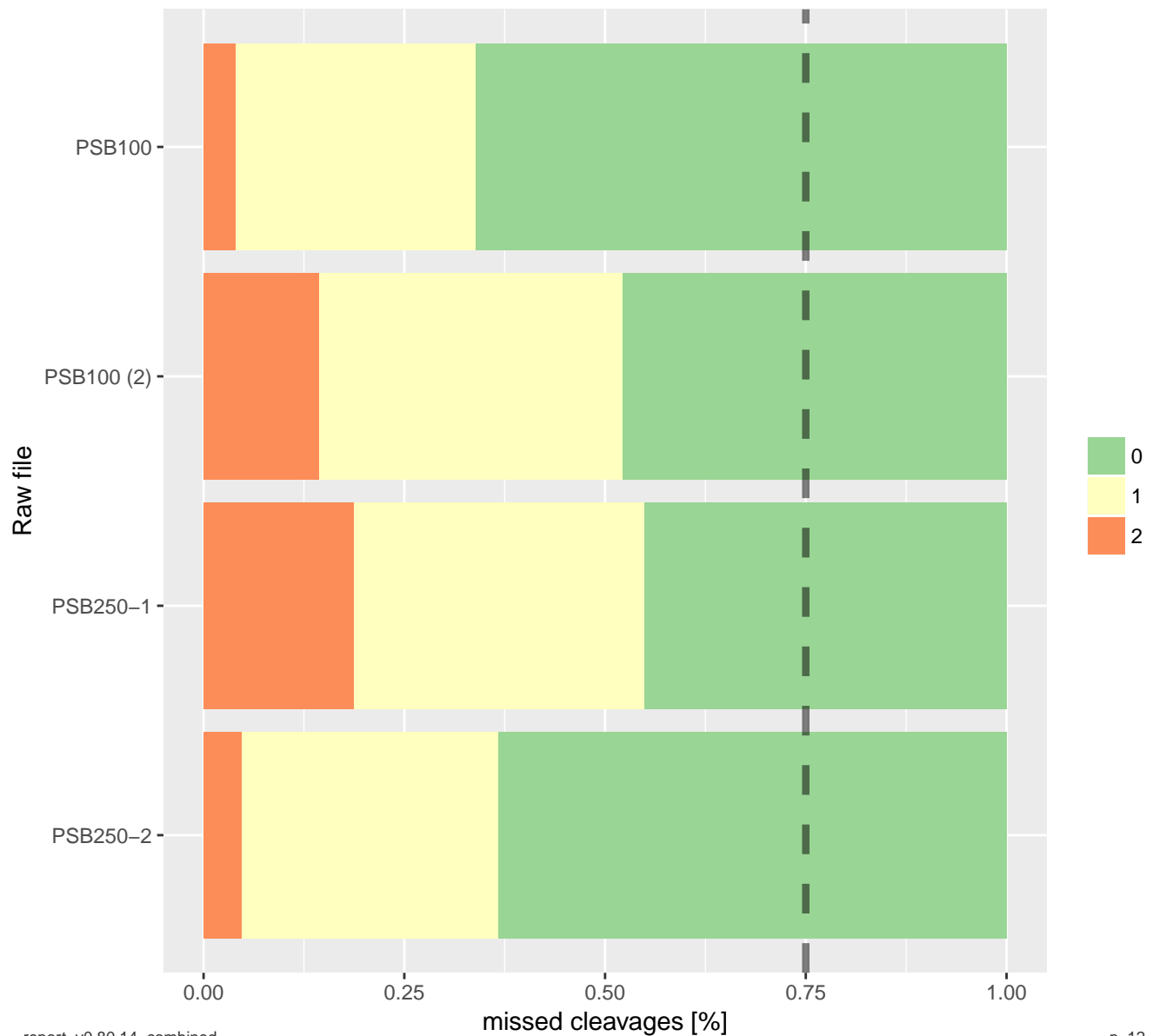
RSD 1.2% (w/o zero int.; expected < 5%)

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

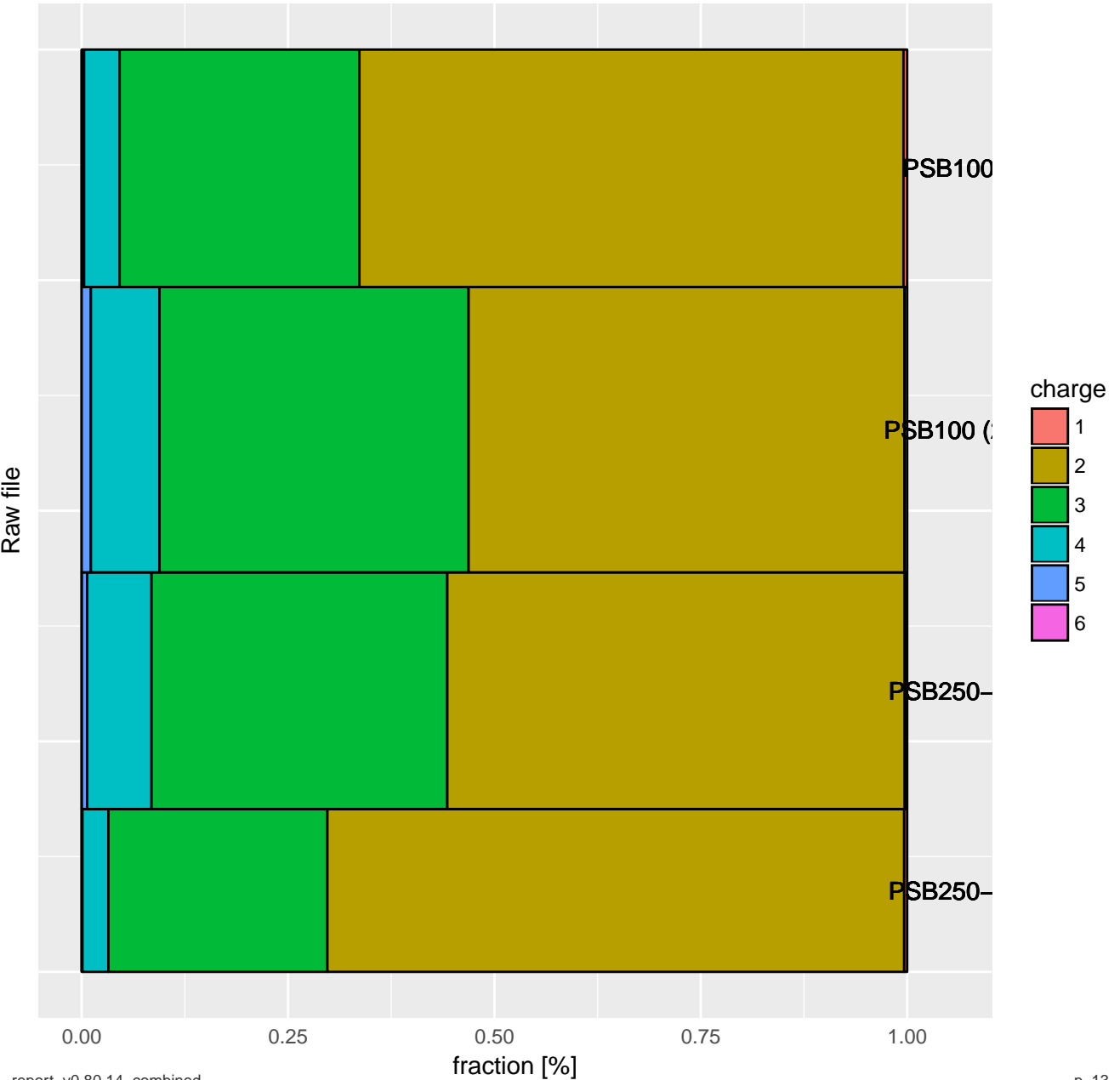


MSMS: Missed cleavages per Raw file

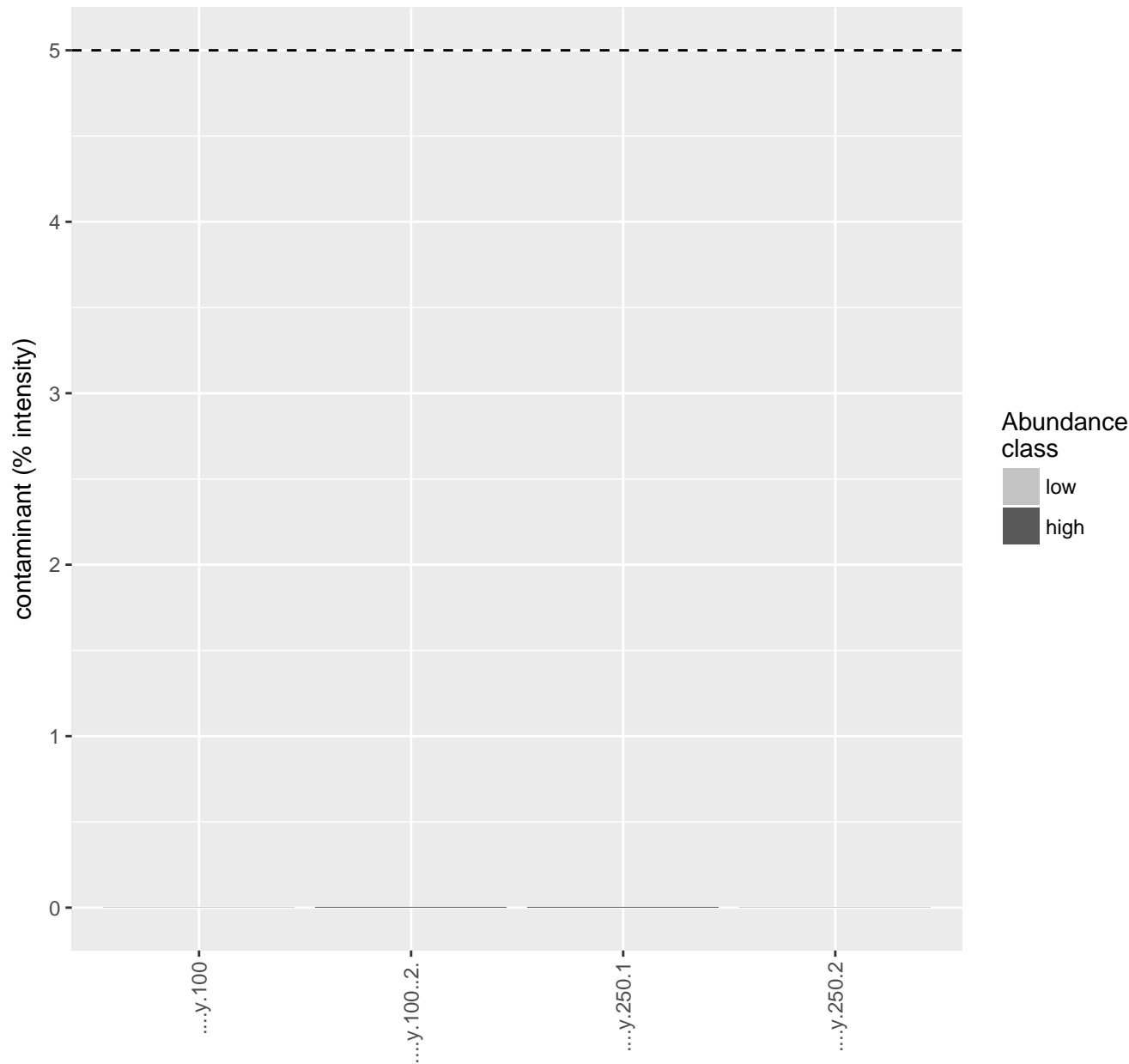
(excludes contaminants)



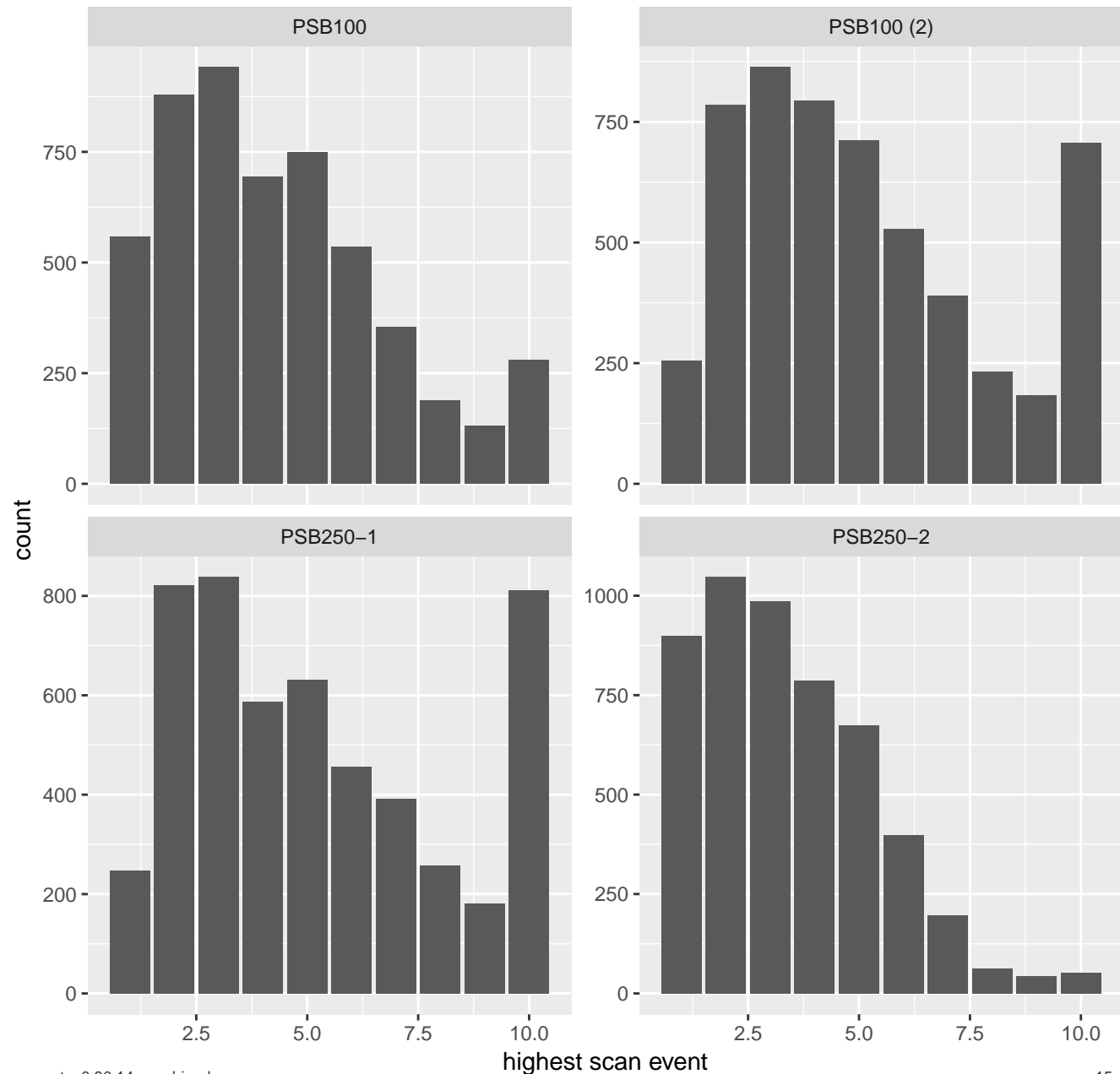
EVD: charge distribution



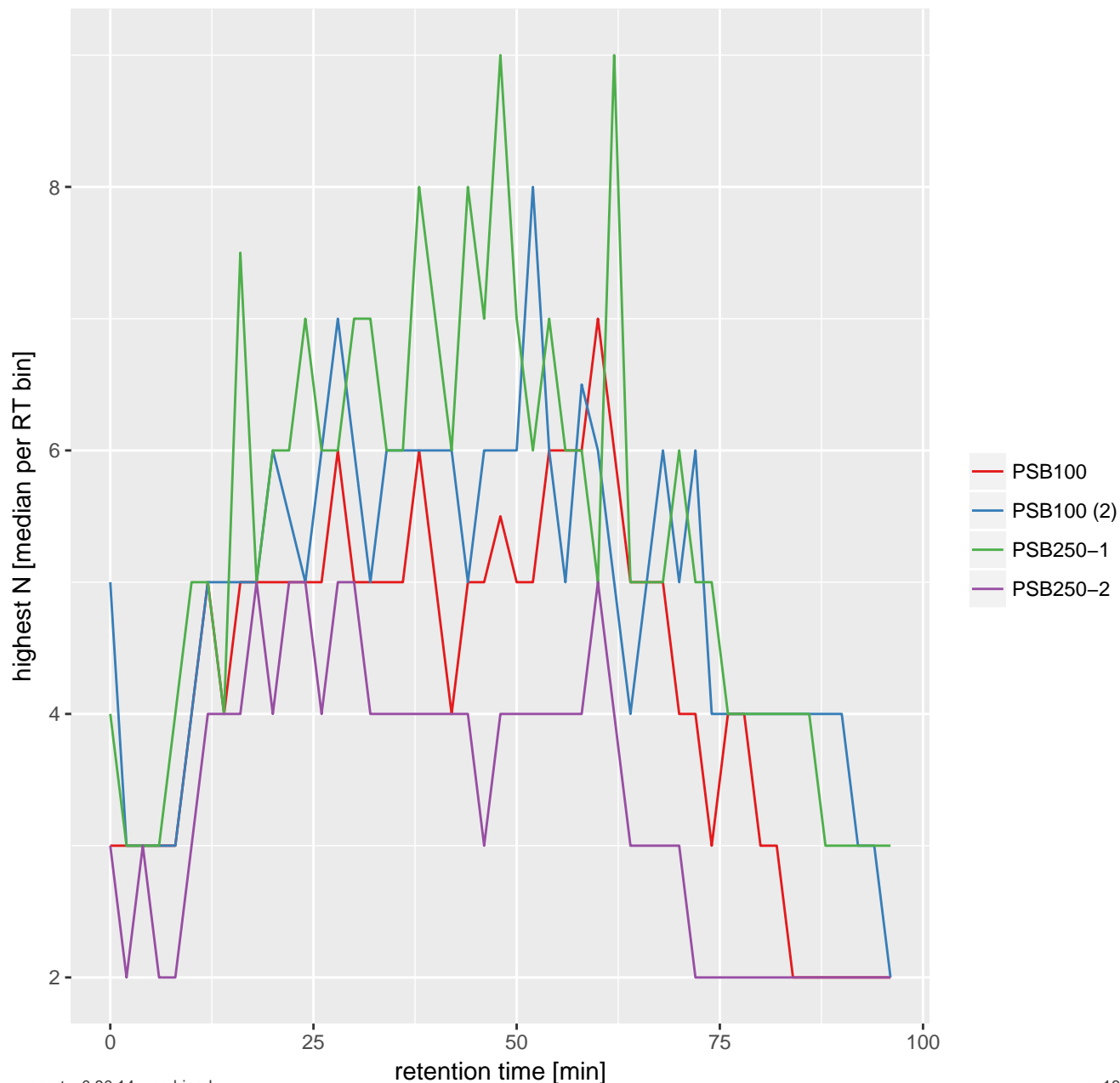
PG: Contaminant per condition



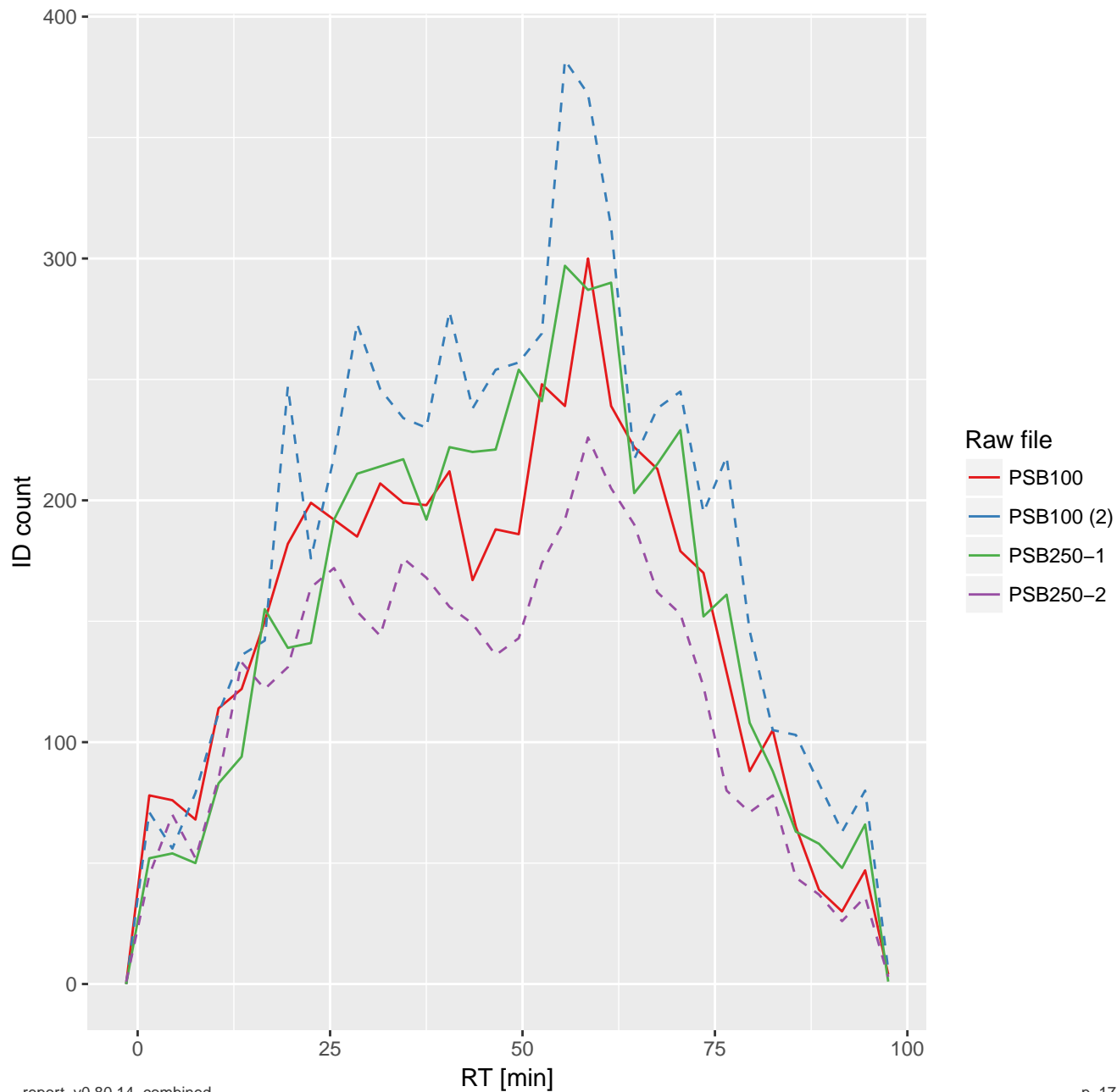
MSMSScans: TopN



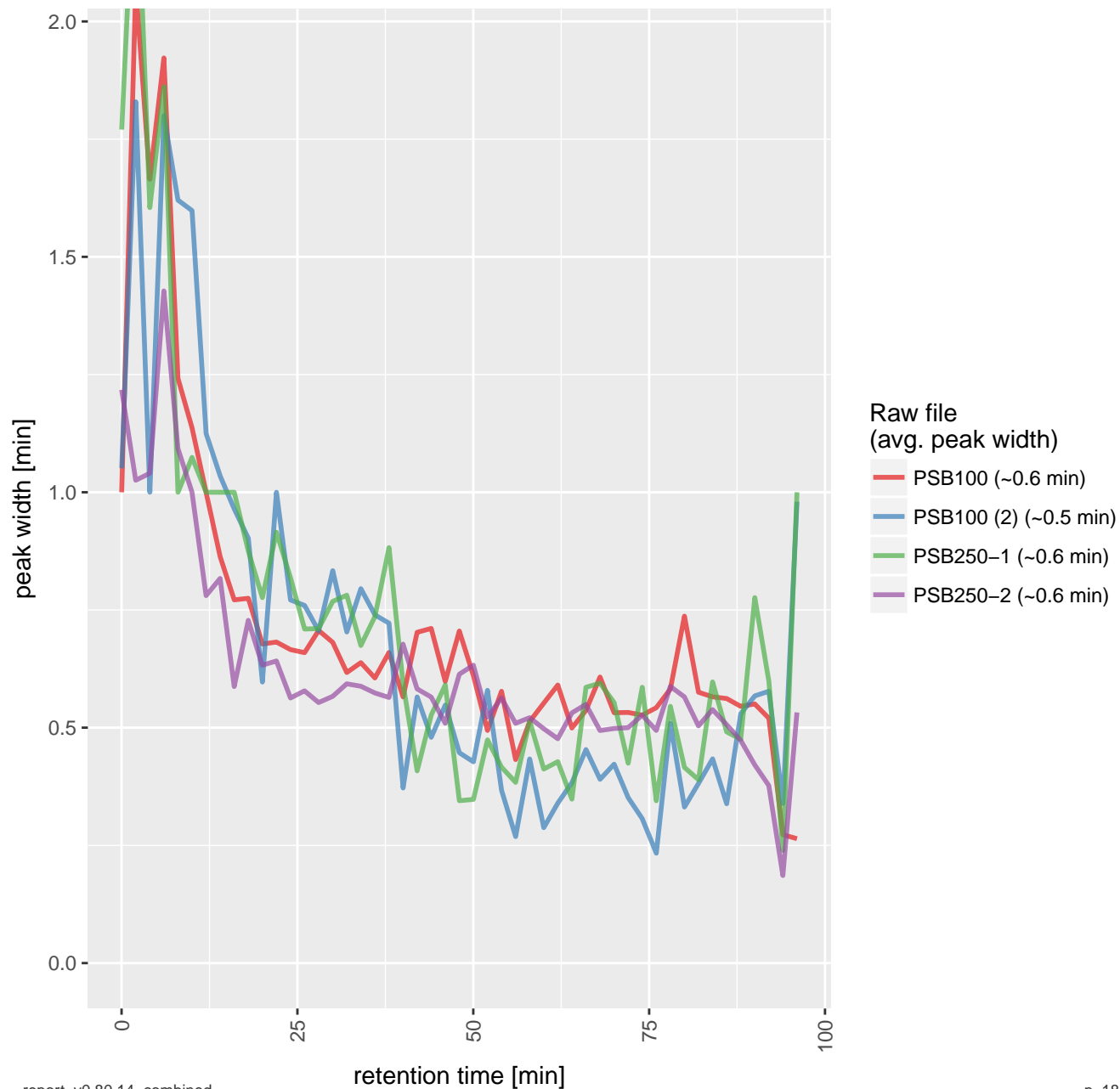
MSMSscans: TopN over RT



EVD: IDs over RT

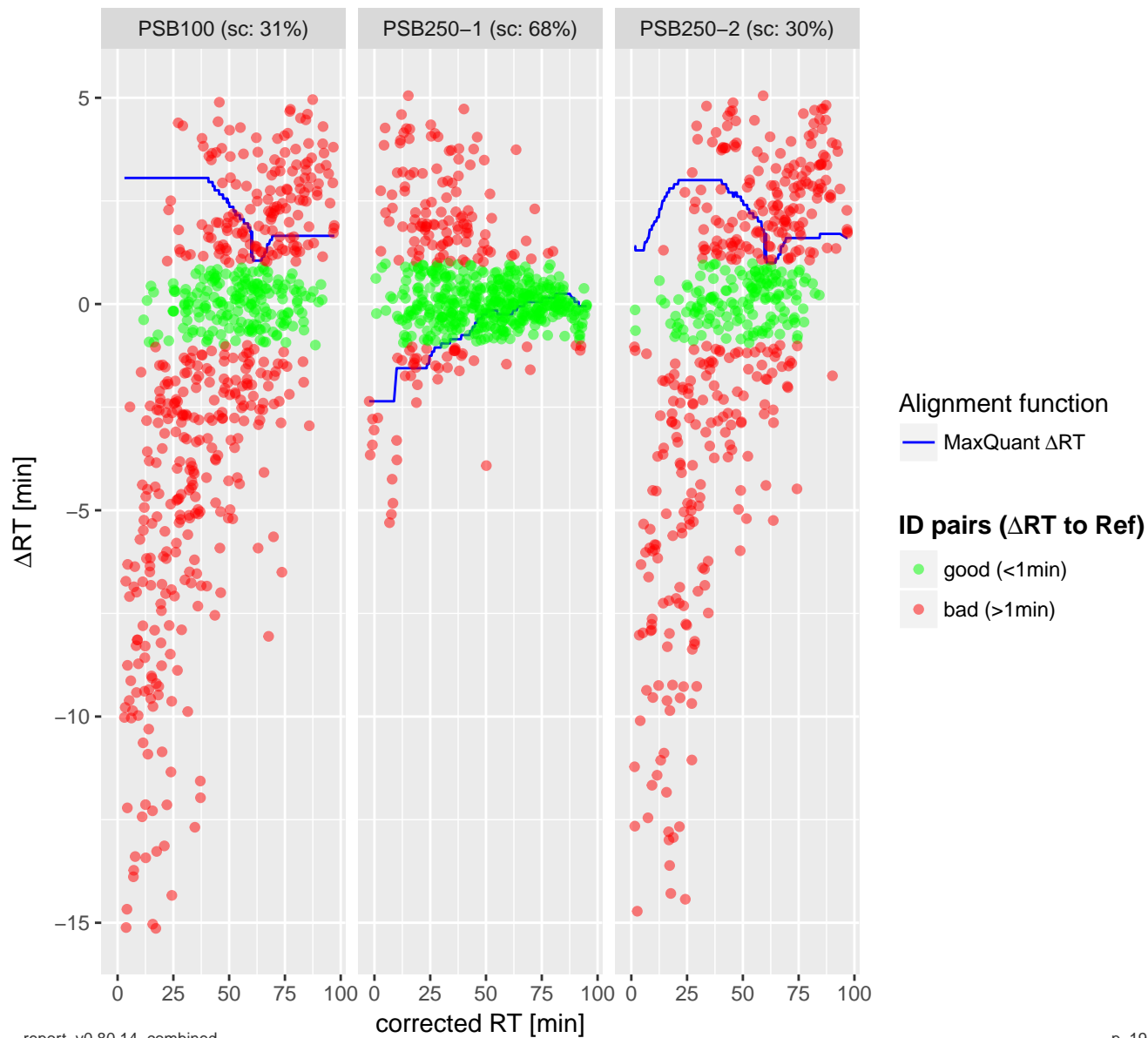


EVD: Peak width over RT

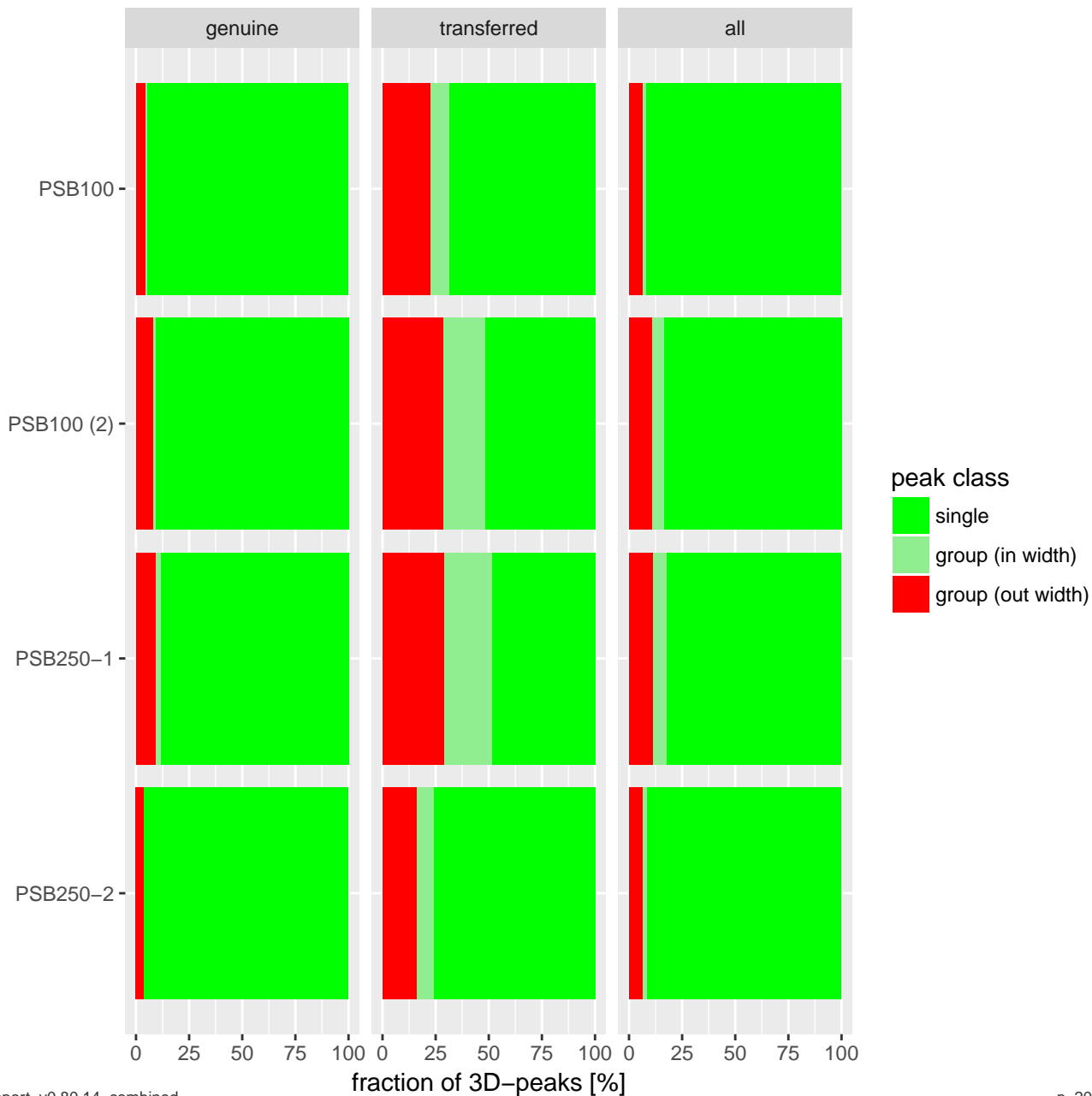


EVD: MBR – alignment

alignment reference: PSB100 (2)

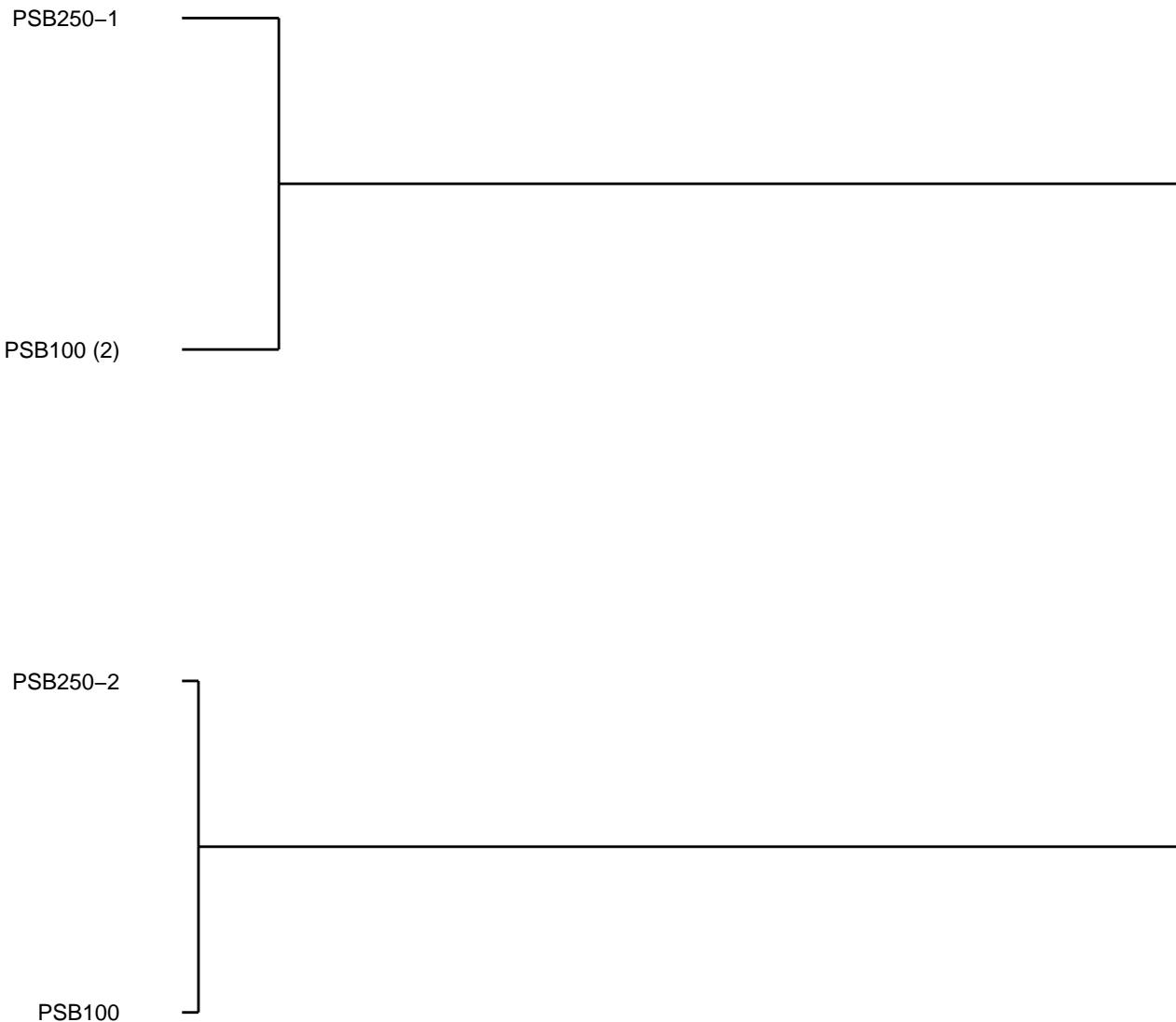


EVD: MBR – ID Transfer

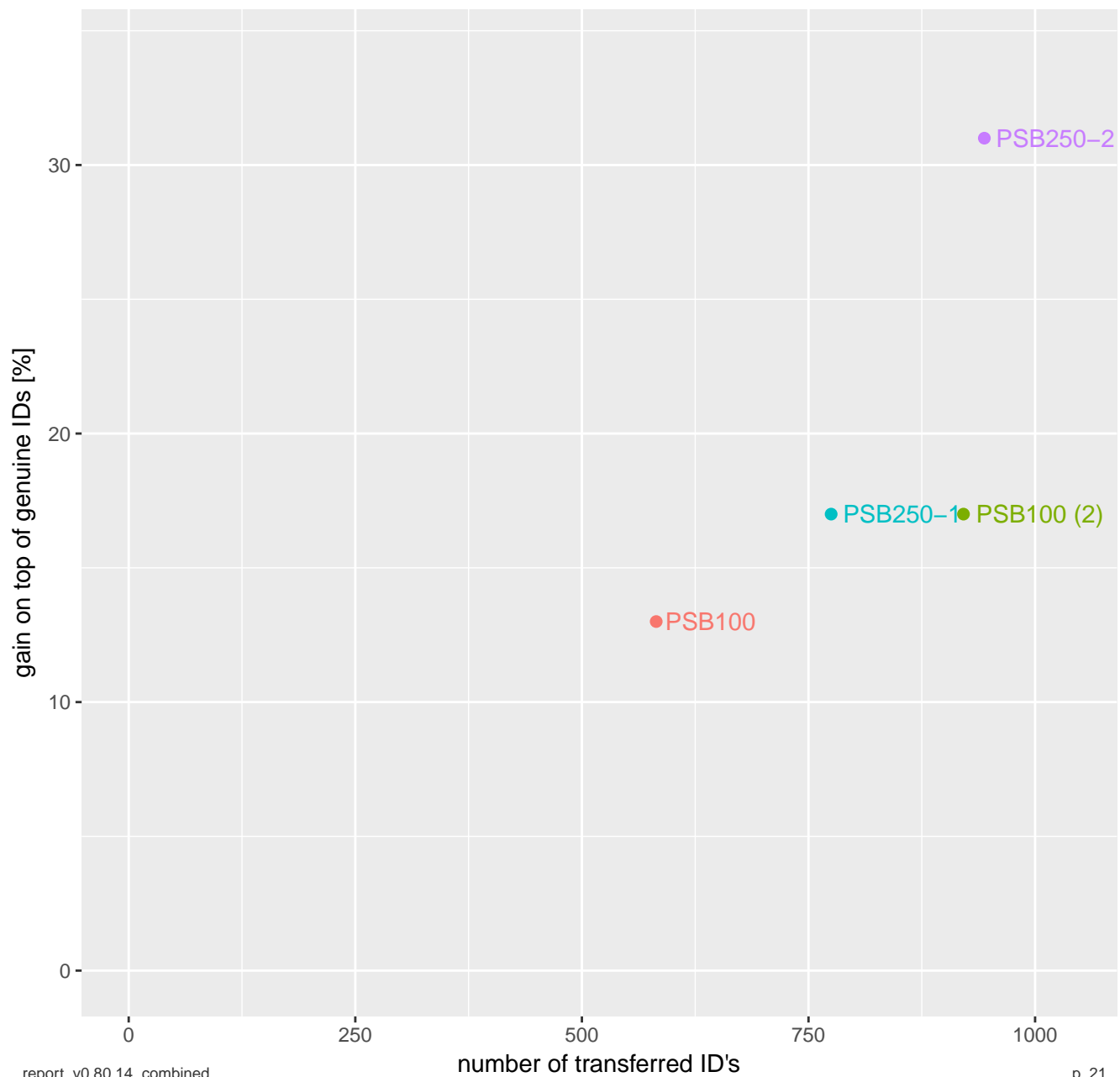


[experimental] EVD: Clustering Tree of Raw files

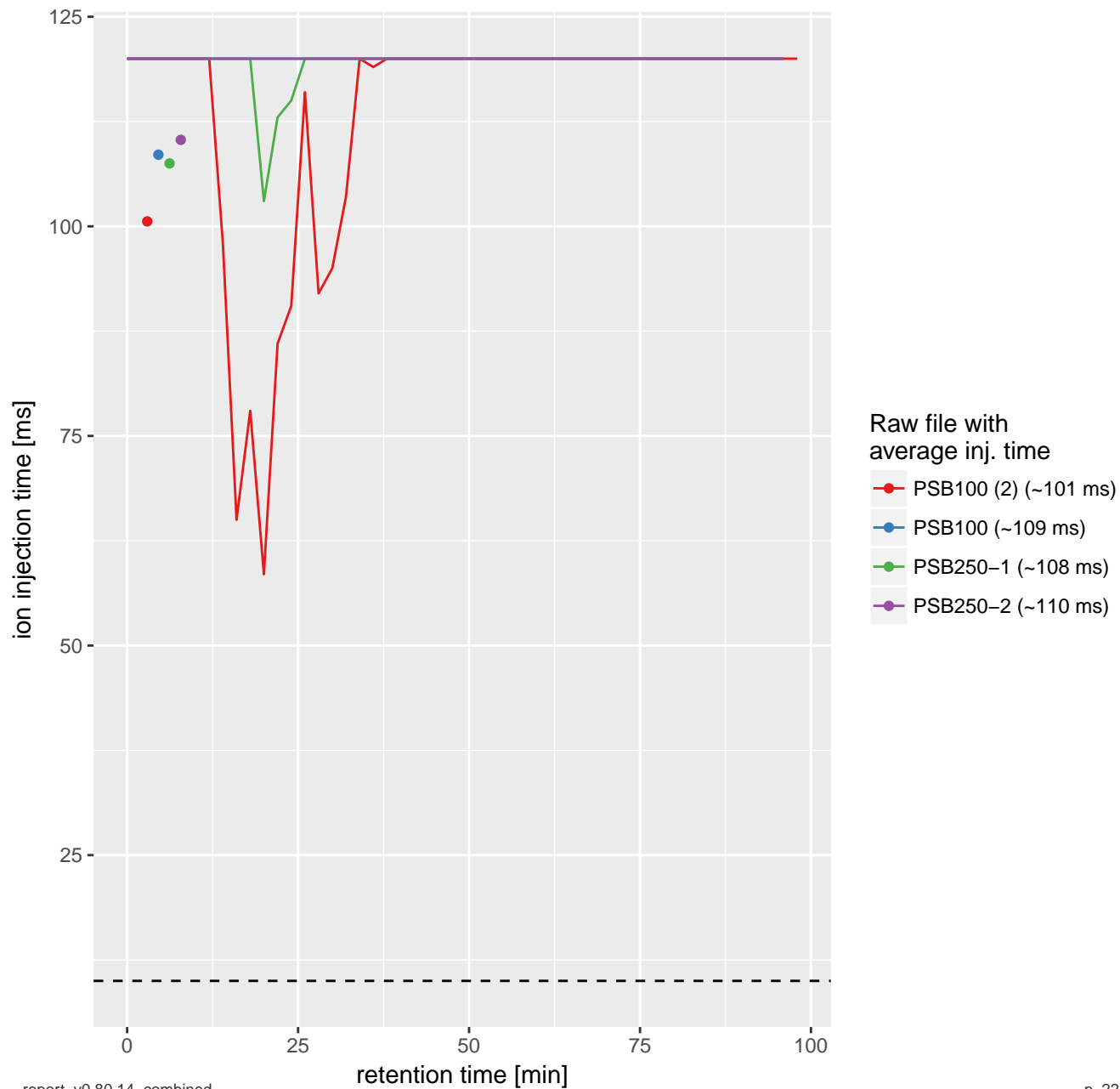
by Correlation of Corrected Retention Times



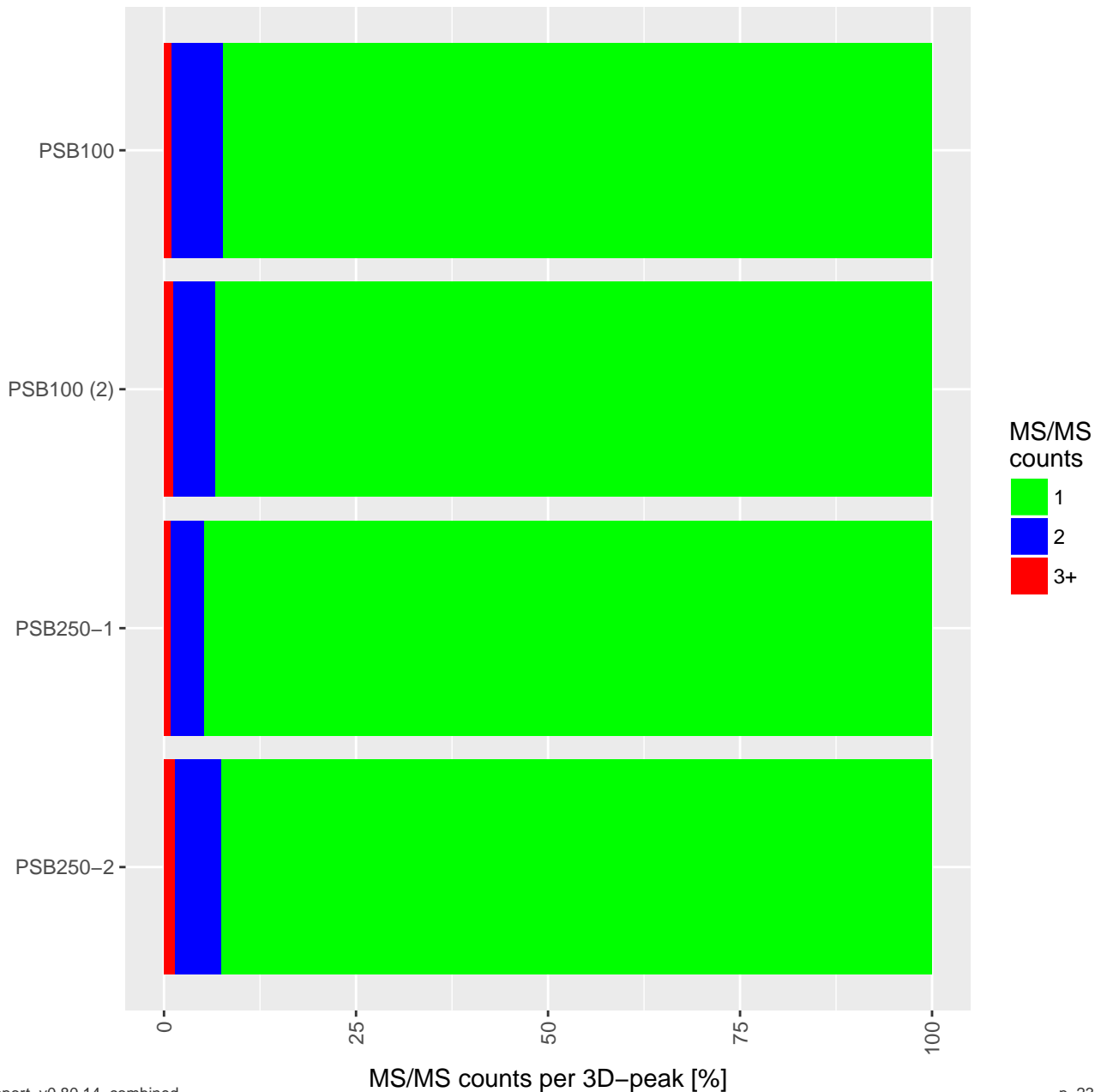
EVD: Peptides inferred by MBR



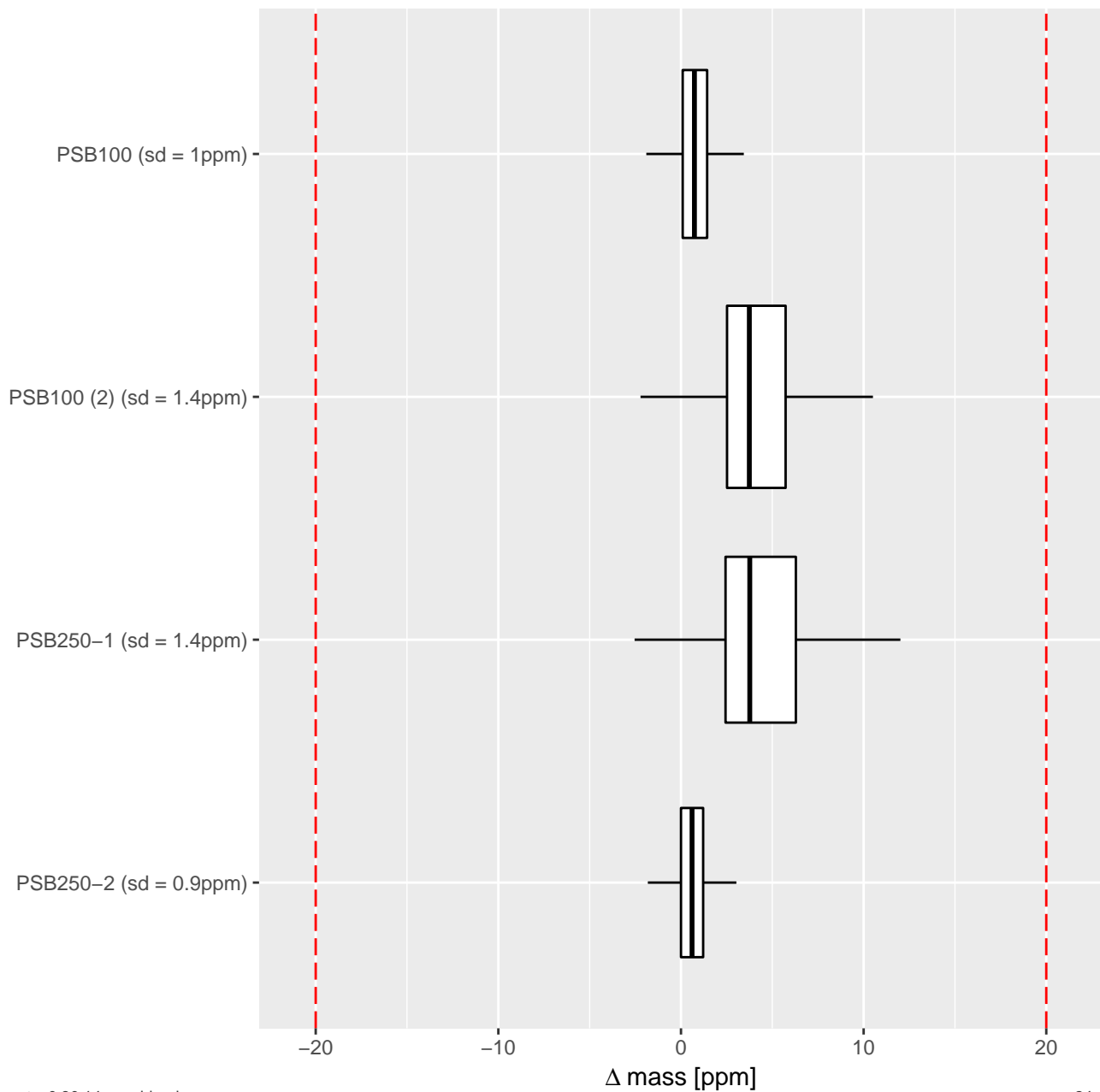
MSMSscans: Ion Injection Time over RT



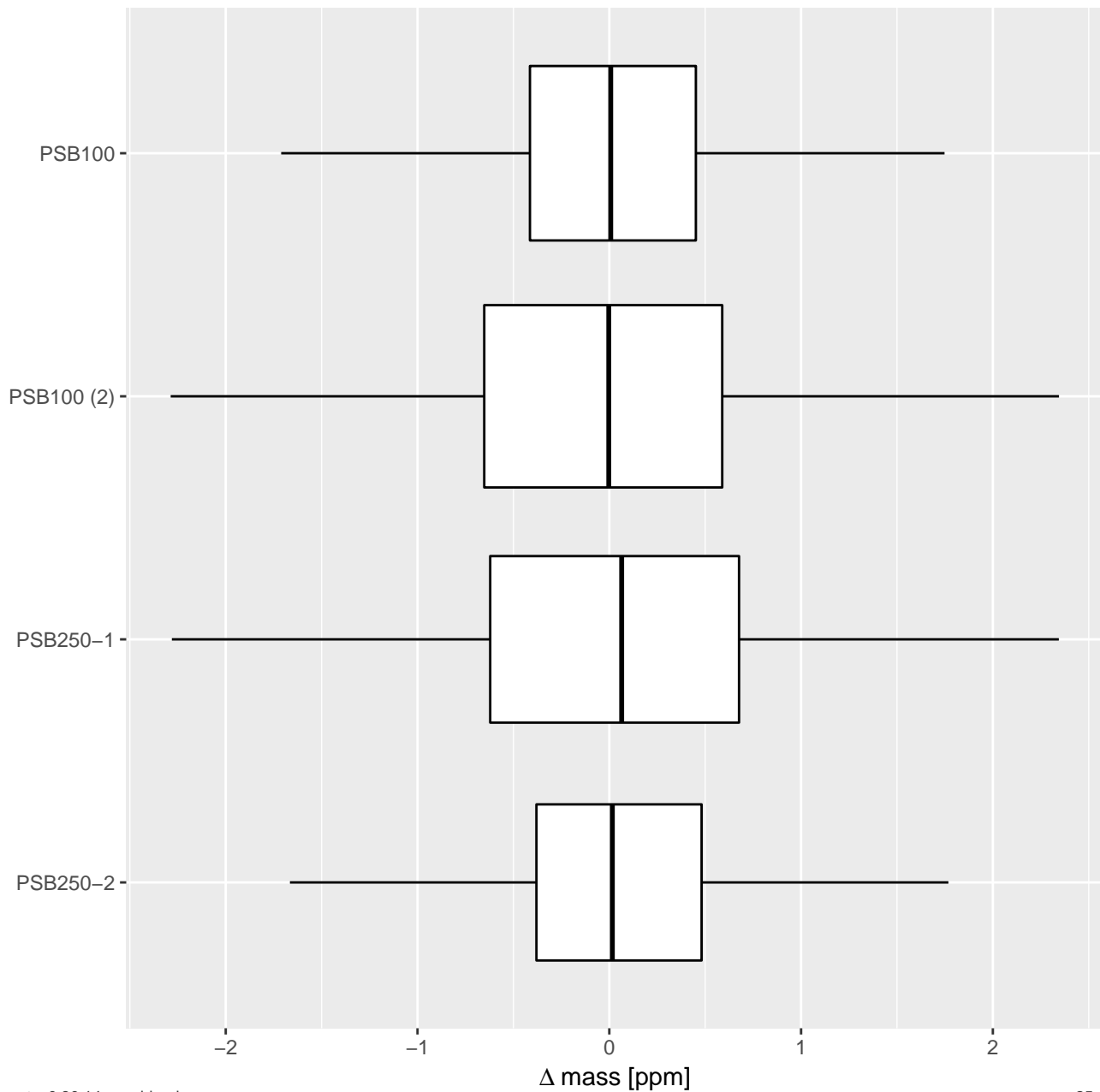
EVD: Oversampling (MS/MS counts per 3D-peak)



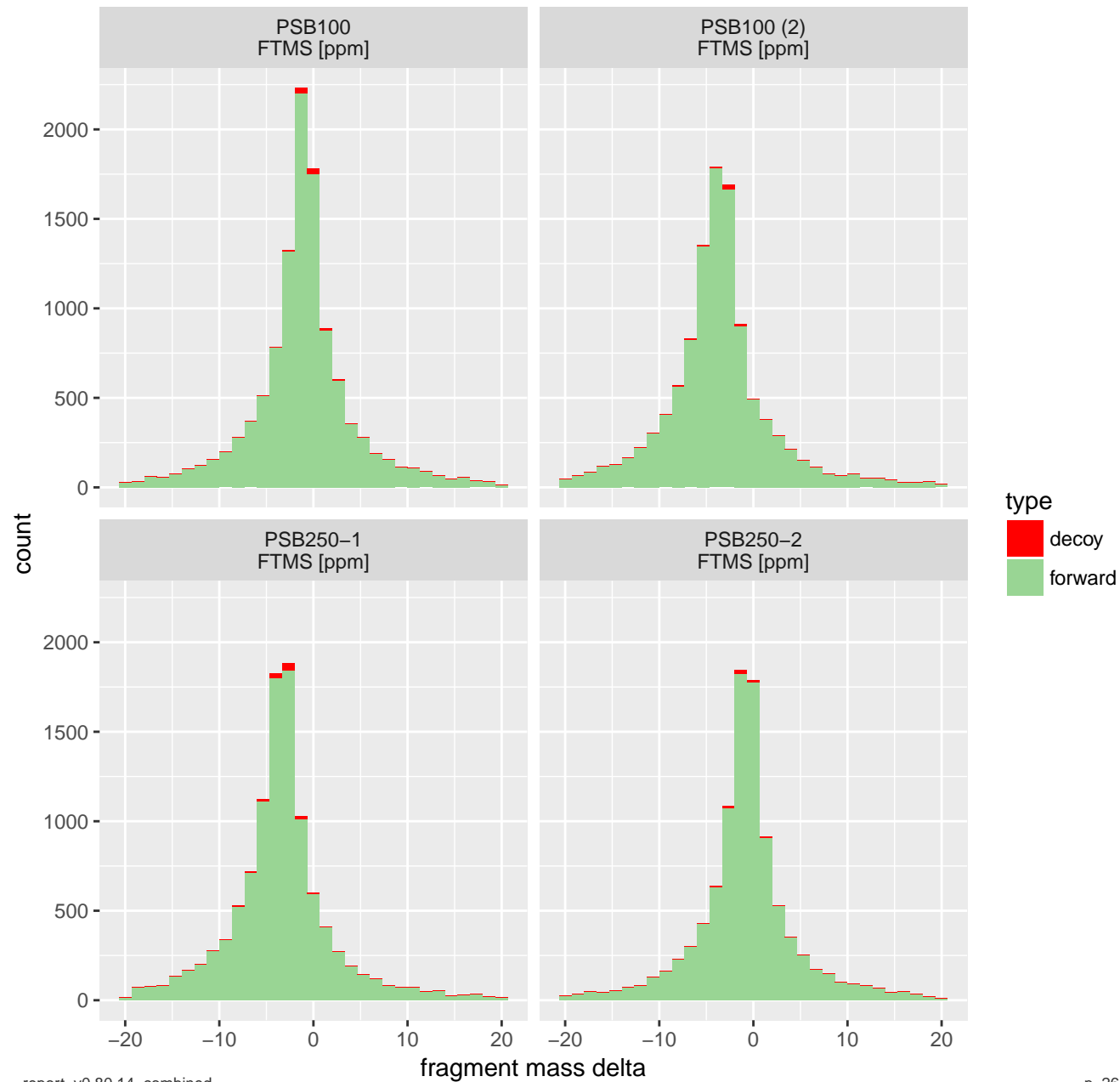
EVD: Uncalibrated mass error



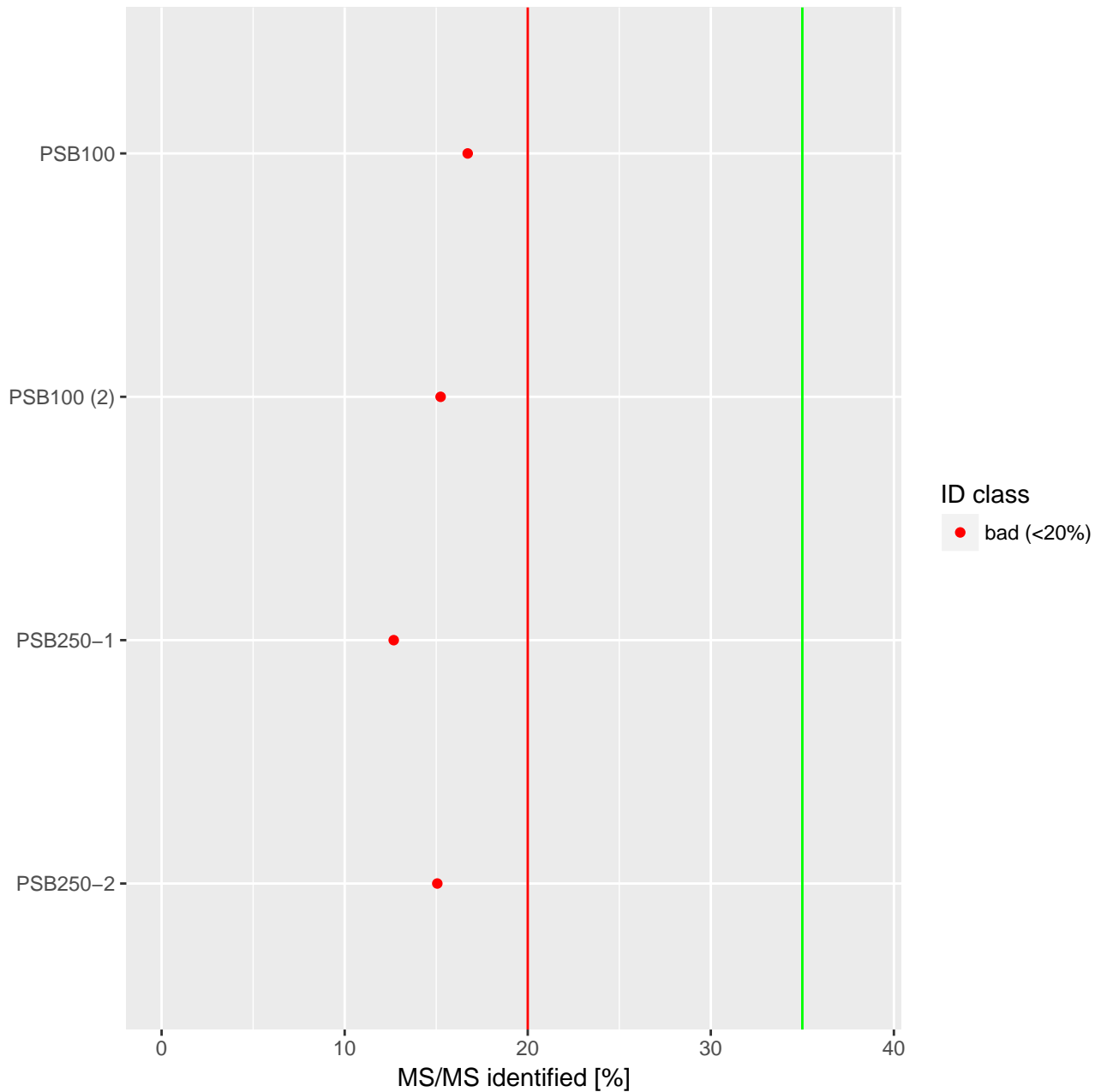
EVD: Calibrated mass error



MSMS: Fragment mass errors per Raw file



SM: MS/MS identified per Raw file

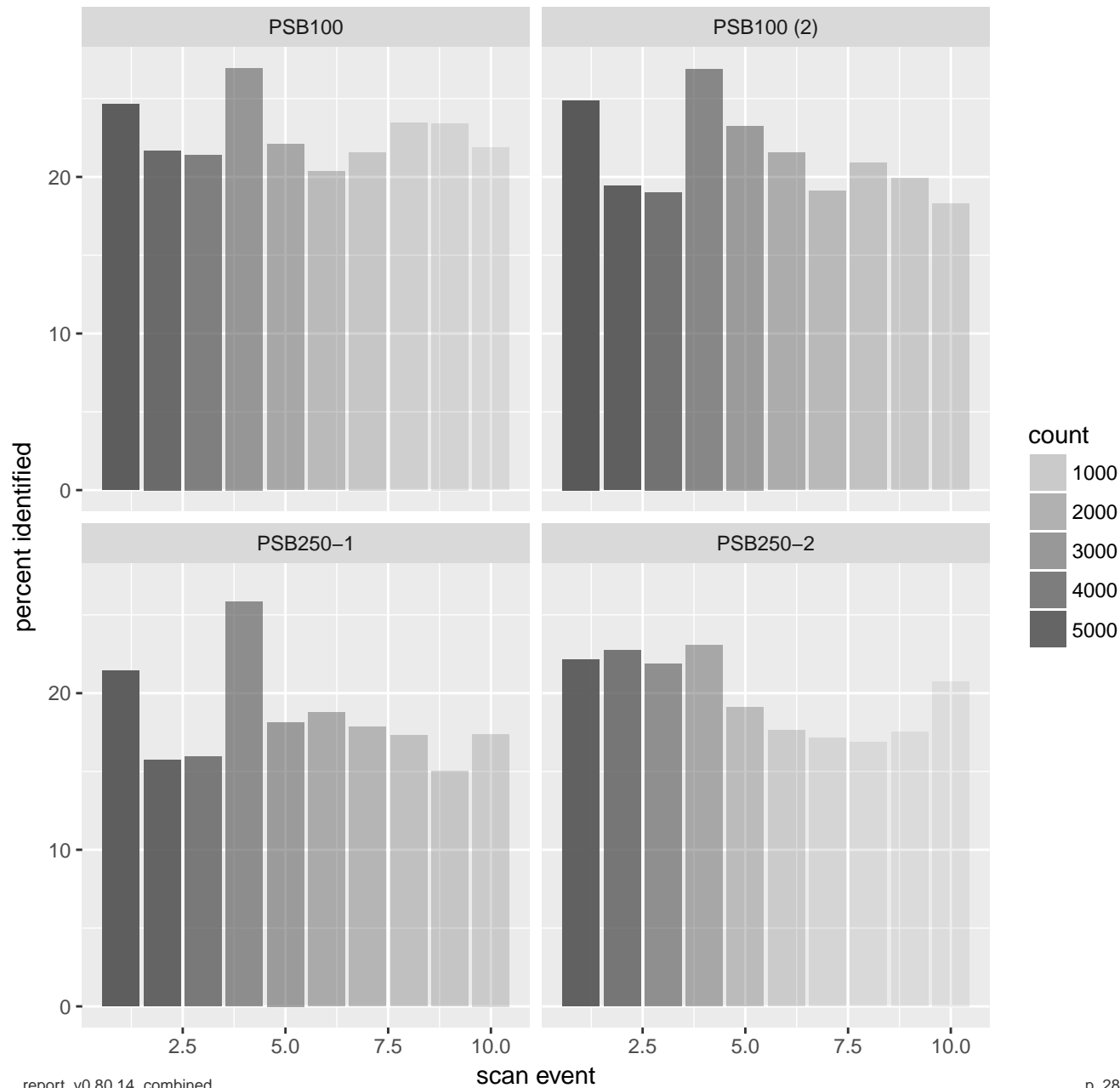


SM: Files with 'red' ID rate

Raw file	% identified
PSB100 (2)	15.24
PSB100	16.72
PSB250-1	12.68
PSB250-2	15.06

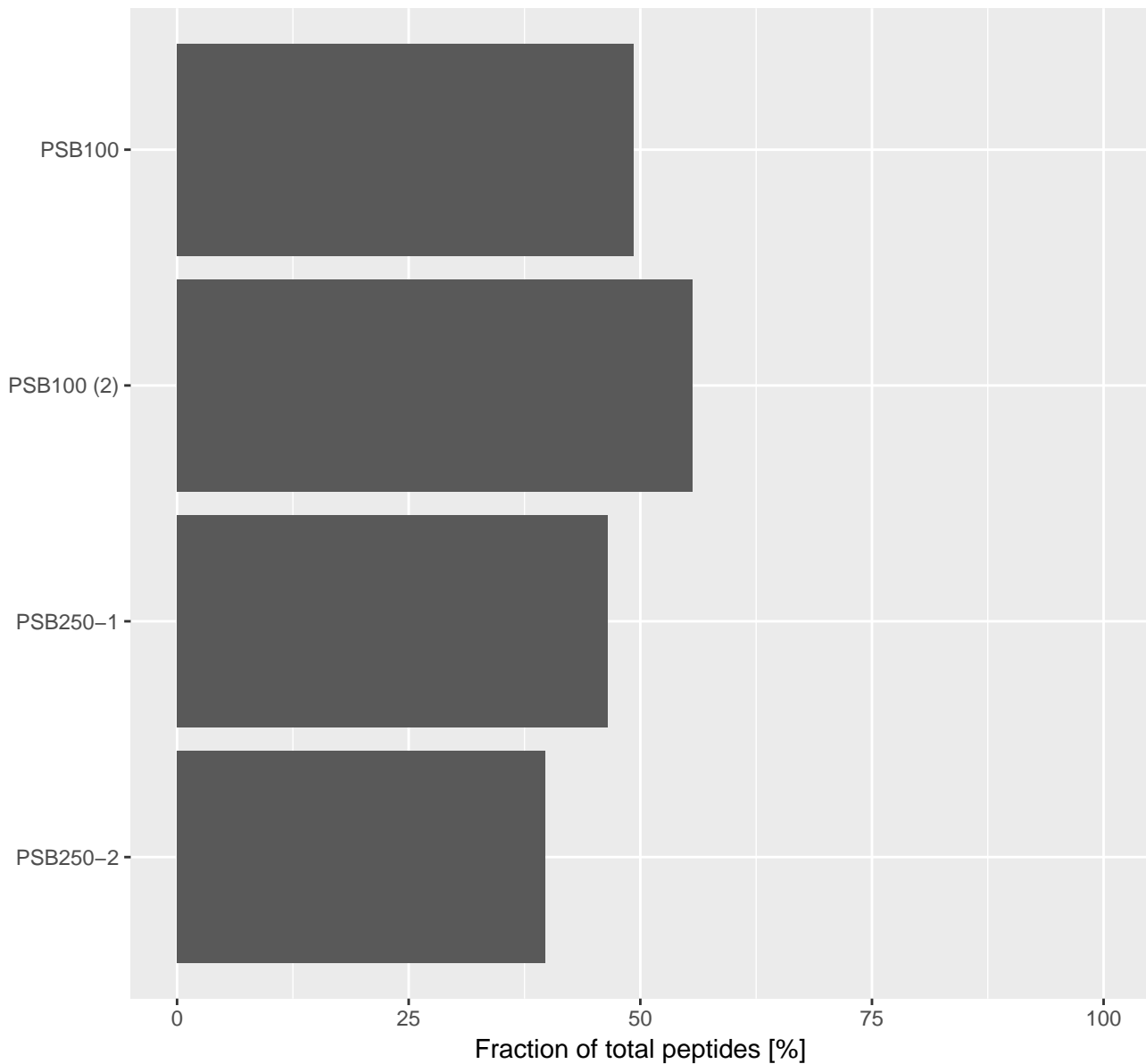
100% of samples)

MSMSscans: TopN % identified over N

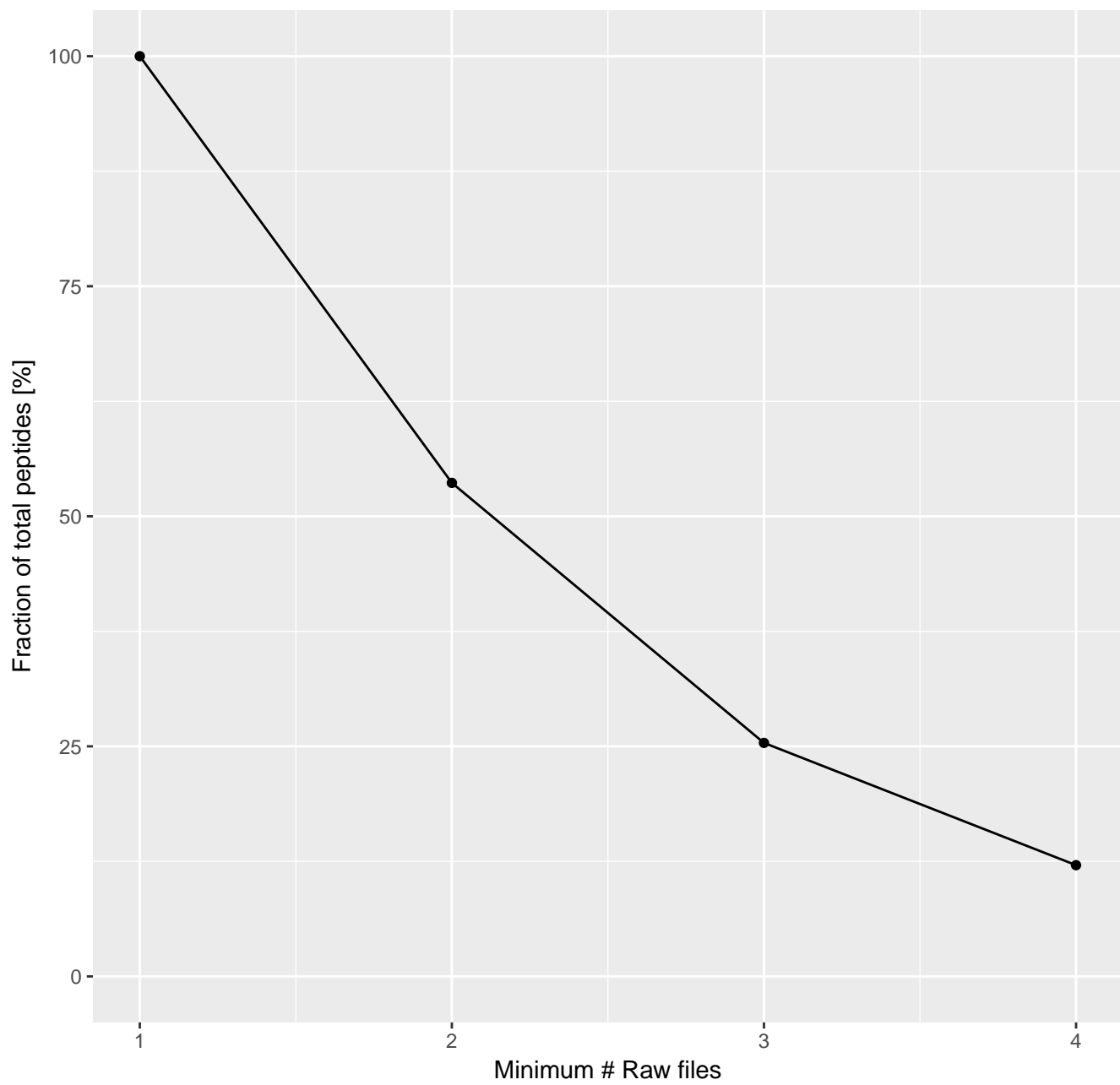


[experimental] EVD: Non-Missing Peptides

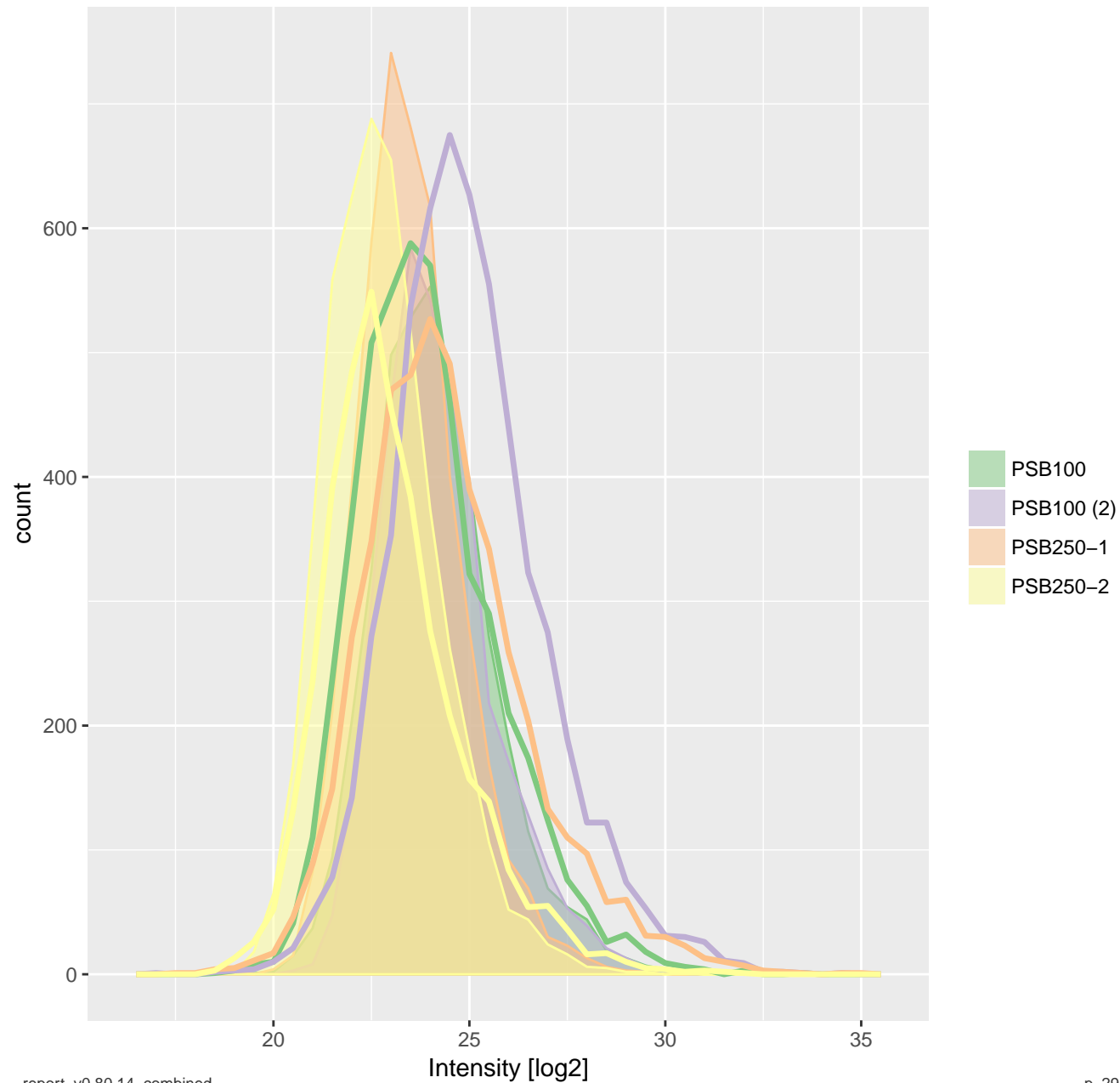
compared to all peptides seen in experiment



[experimental] EVD: Non-missing by set

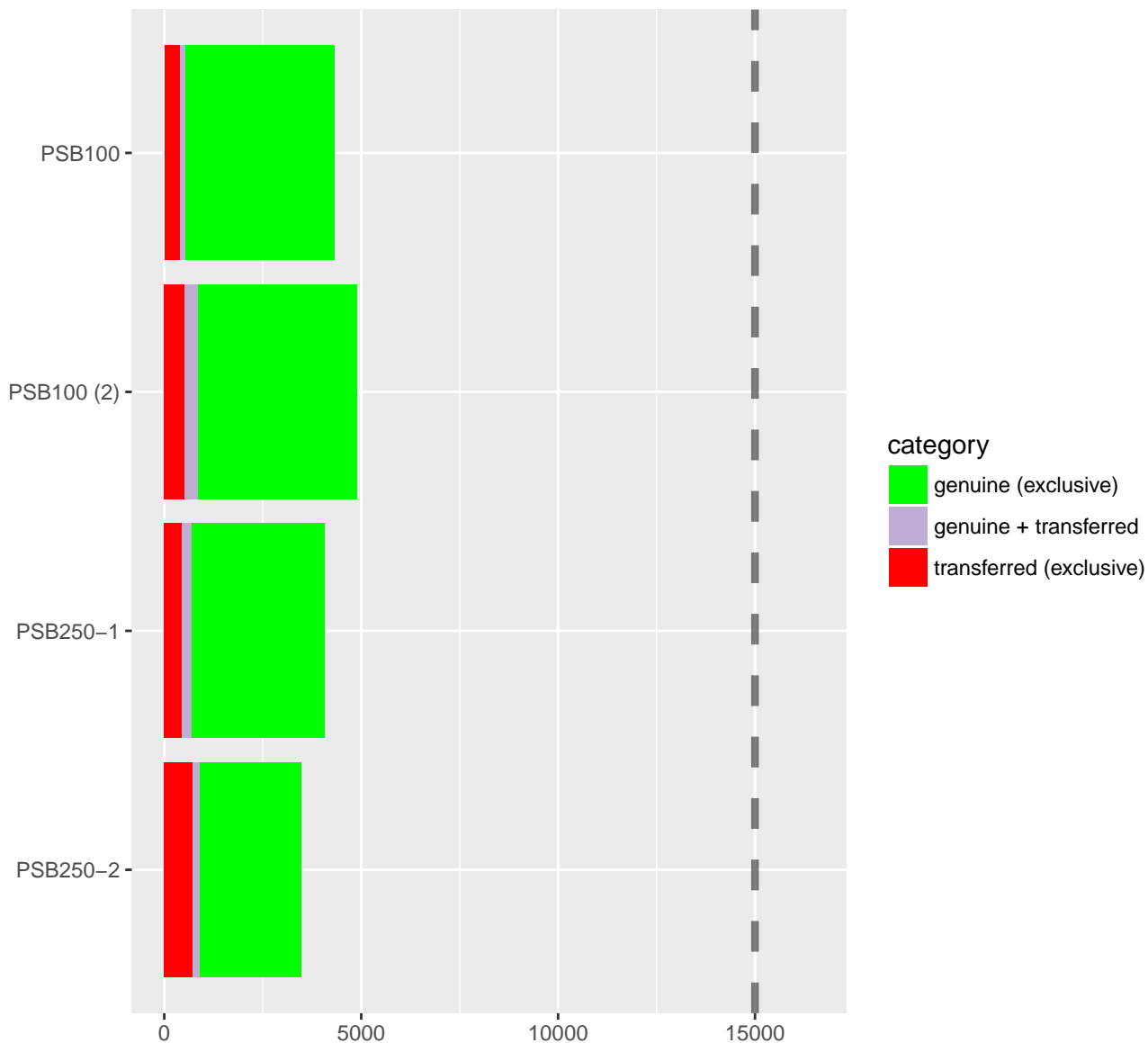


[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



EVD: Peptide ID count

MBR gain: +15%



EVD: ProteinGroups count

MBR gain: +9%

