Performance overview
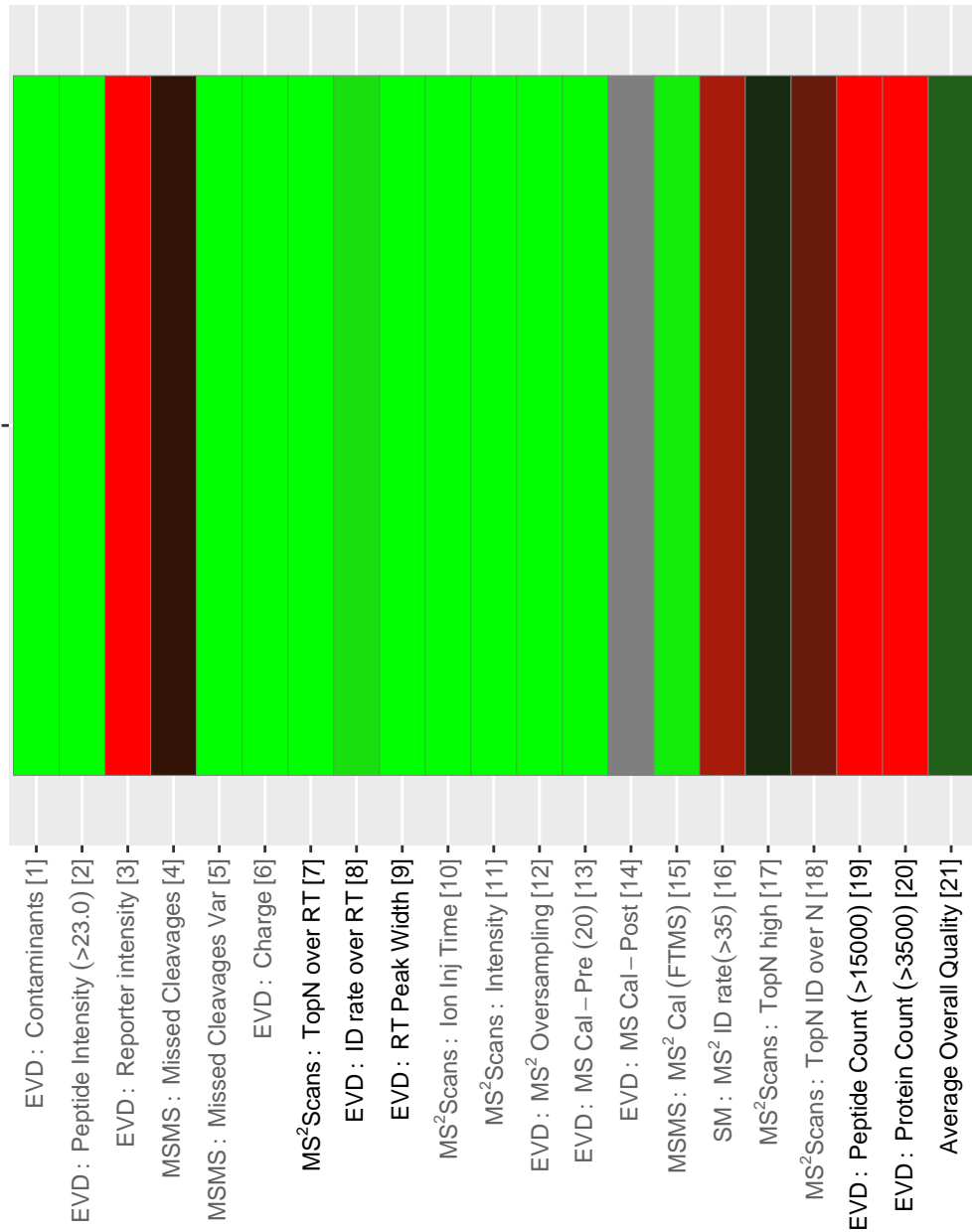
Mapping of Raw files to their short names
Mapping source: automatic

original	short name	best effort
ptxqc	ptxqc	ptxqc

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	06/19/2021 18:51:18	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	DESKTOP−I3UDKML	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

/tmp/tmp6otynggs/files/a/1/c/dataset_a1c72fbb−46f6−46be−ad77−0fc10d10b251.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	Oxidation (M)Sites.txt
Min. razor peptides	1	Stabilize large LFQ ratios	True
Min. score for modified pept..	40	Top MS/MS peaks per Da inter..	12
Min. score for unmodified pe..	0	Top MS/MS peaks per Da inter..	8
Min. unique peptides	0	Top MS/MS peaks per Da inter..	10
Modifications included in pr..	Oxidation (M) Acetyl (Protein N−term)	Top MS/MS peaks per Da inter..	12
MS/MS ammonia loss (FTMS)	True	Use delta score	False
MS/MS ammonia loss (ITMS)	True	Use Normalized Ratios For Oc..	True
MS/MS ammonia loss (TOF)	True	Use only unmodified peptides..	True
MS/MS ammonia loss (Unknown)	True	User name	niko
MS/MS deisotoping (FTMS)	True	Variation mode	None
MS/MS deisotoping (ITMS)	False	Version	1.6.17.0
MS/MS deisotoping (TOF)	True	Write accumulatedPasefMsmsSc..	False
MS/MS deisotoping (Unknown)	True	Write allPeptides table	True
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

/tmp/tmp6otynggs/files/a/1/c/dataset_a1c72fbb−46f6−46be−ad77−0fc10d10b251.dat

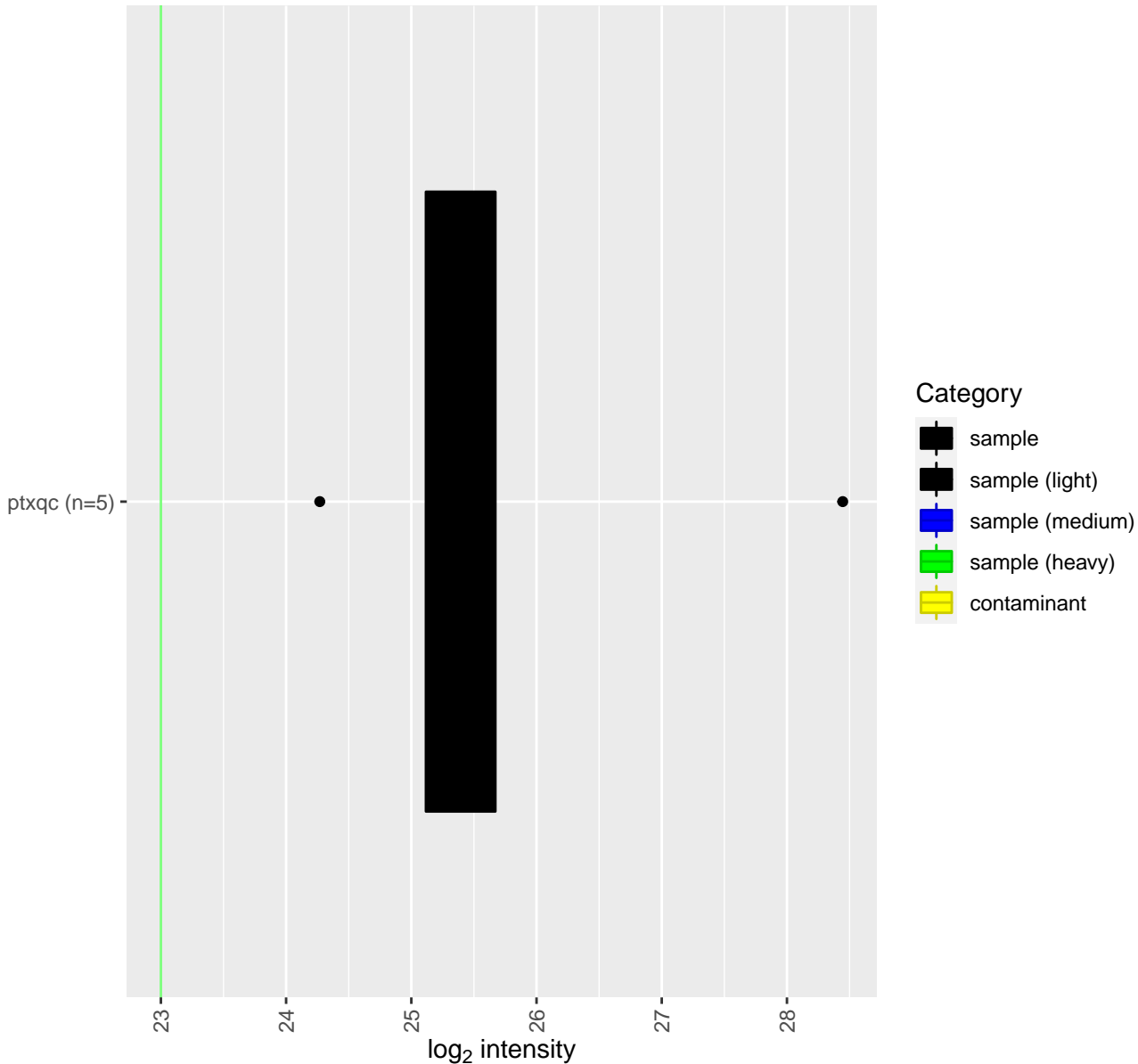# PG: PCA of 'reporter intensity'
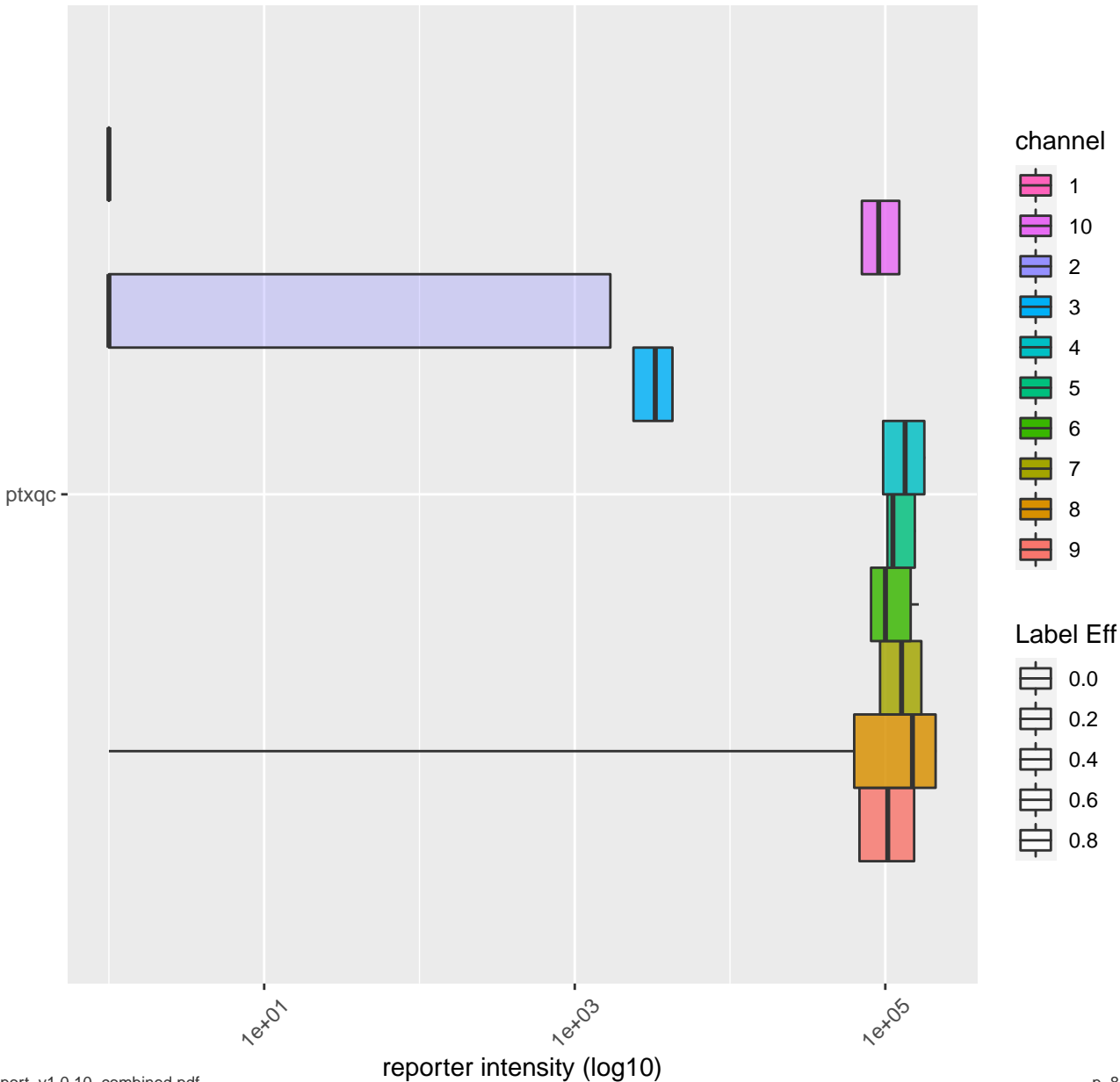## (excludes contaminants)
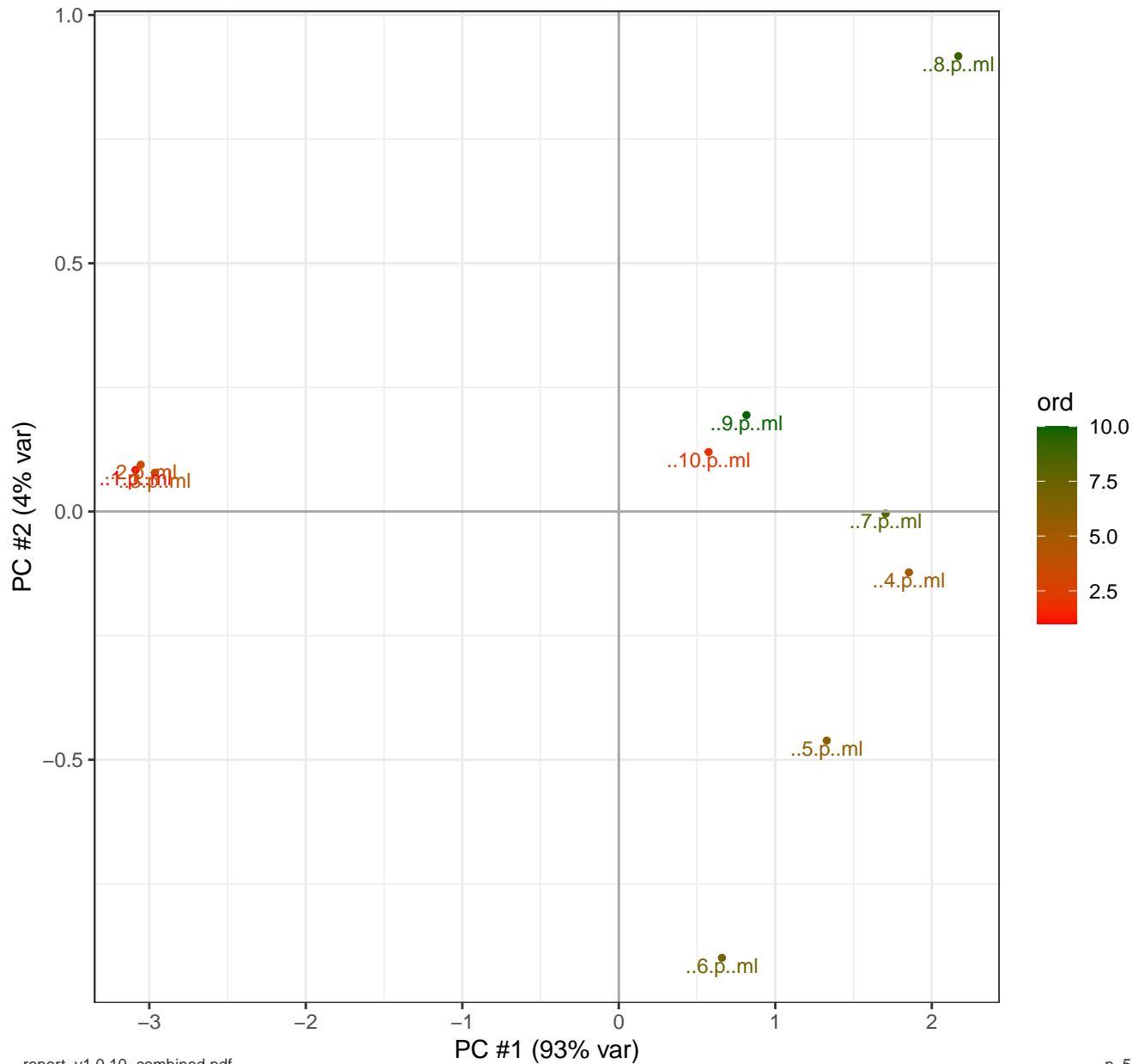
EVD: Top5 Contaminants per Raw file

Protein

CON__P20930

Abundance class

mid

ptxqc

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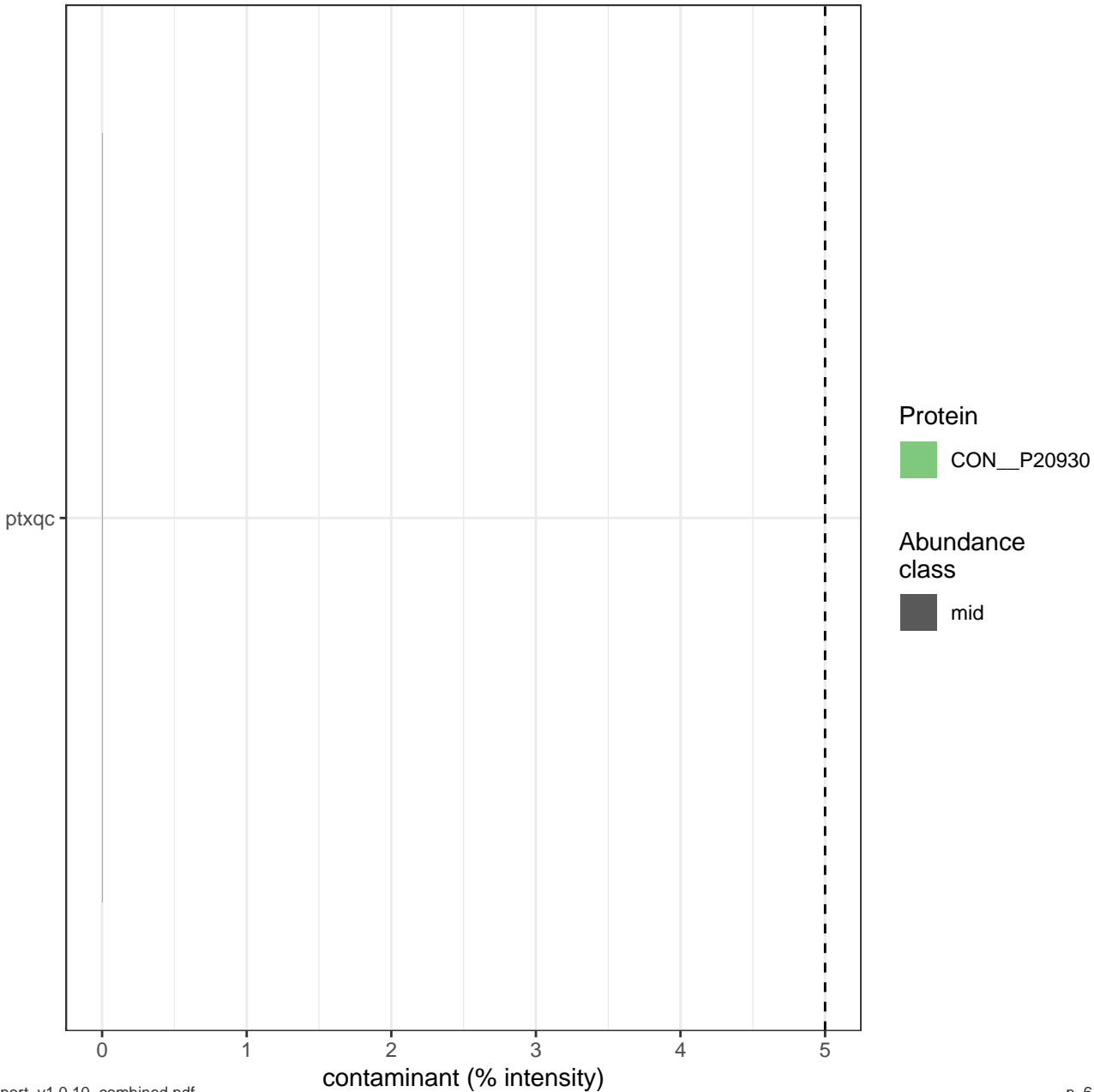
EVD: peptide intensity distribution
RSD NA% (expected < 5%)

EVD: Reporter label intensities

Warning: MaxQuant did NO isotope correction

reporter intensity (log10)

PG: intensity distribution

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

log$_2$ intensity

Category
- sample
- sample (light)
- sample (medium)
- sample (heavy)
- contaminant
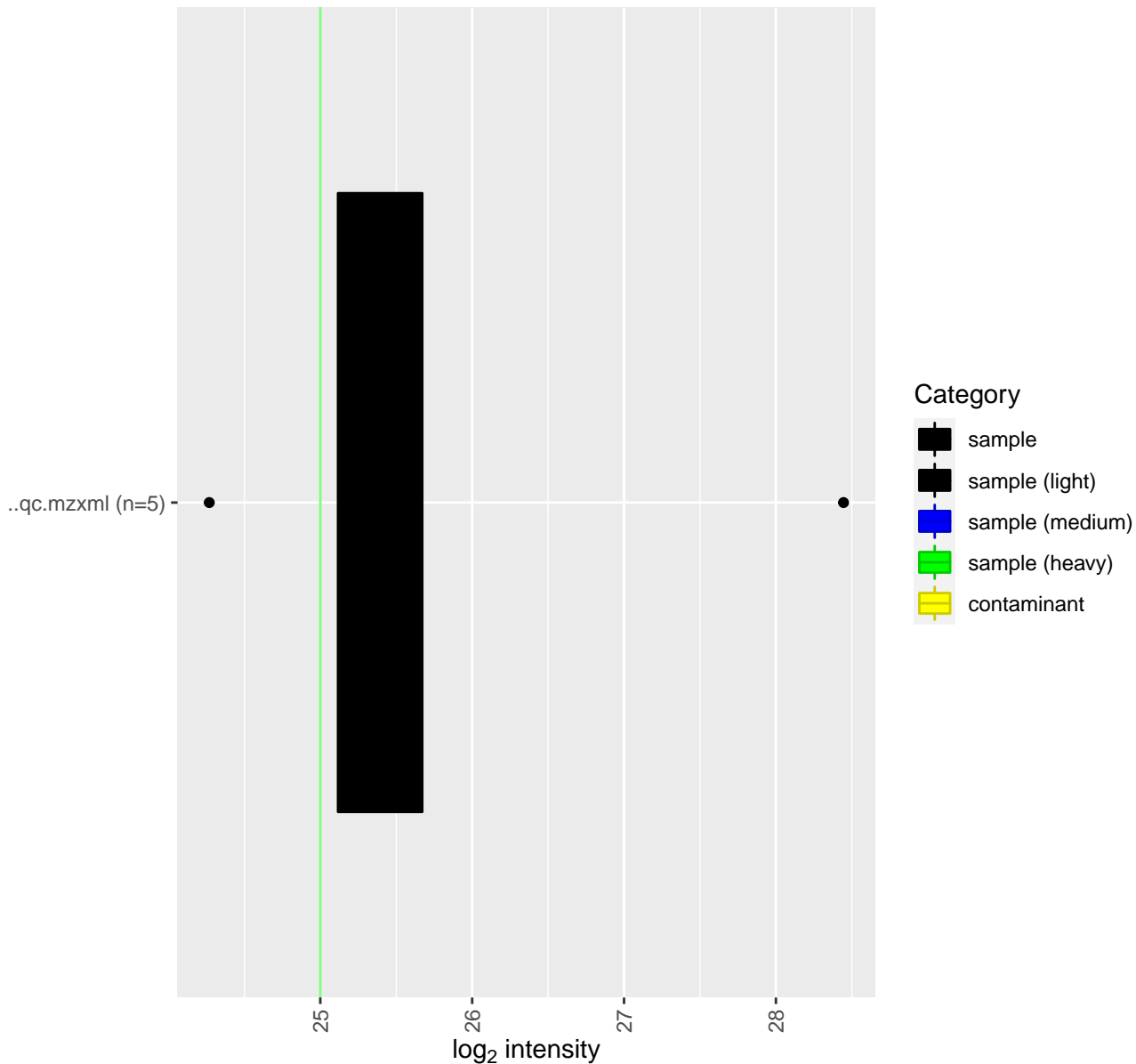
PG: reporter intensity distribution

RSD 14.9% (w/o zero int.; expected < 5%)
RSD 54.2% [high RSD −−> few peptides])

$\log_2$ reporter intensity

Category
- sample
- sample (light)
- sample (medium)
- sample (heavy)
- contaminant
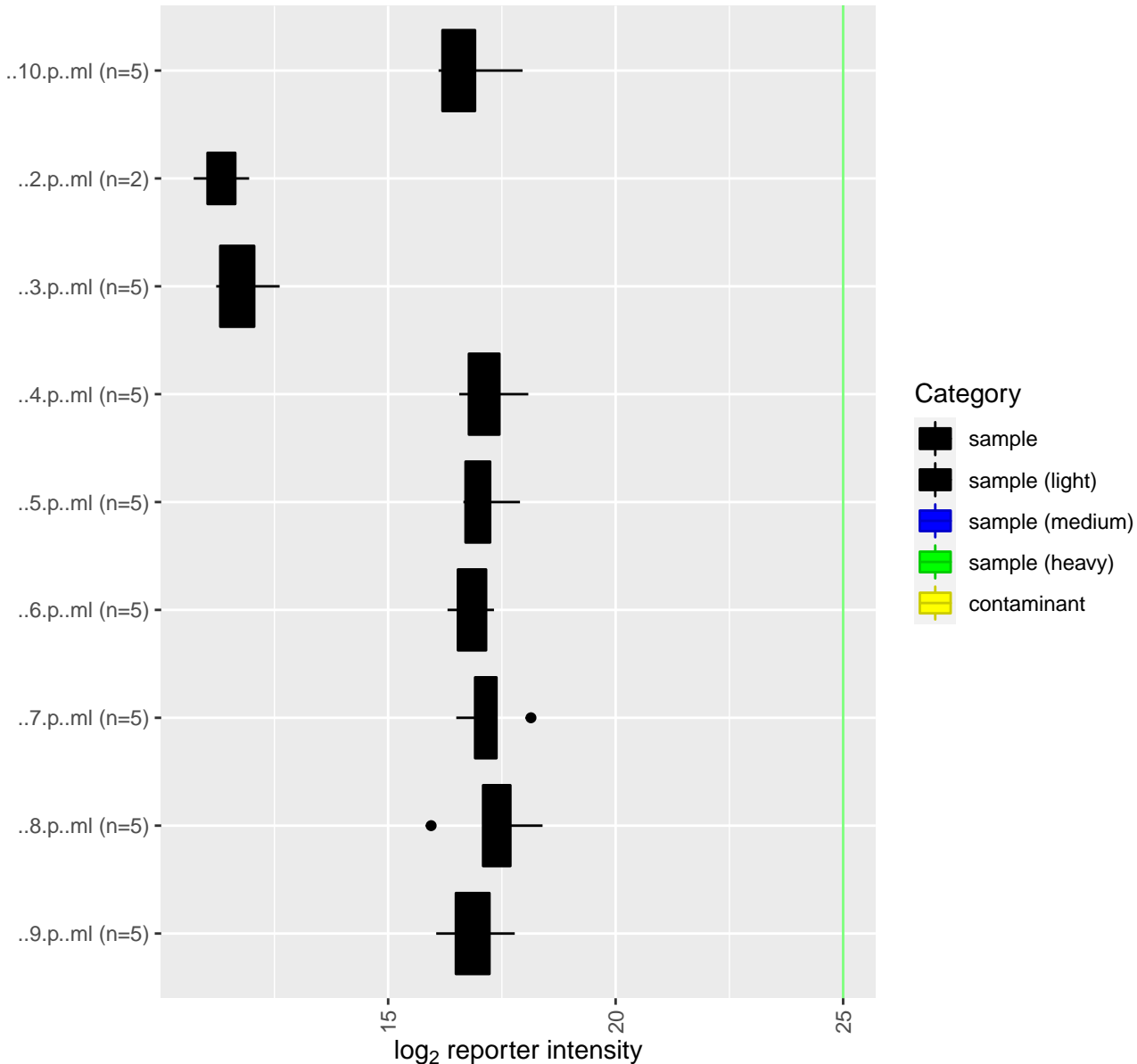
MSMS: Missed cleavages per Raw file
(excludes contaminants)
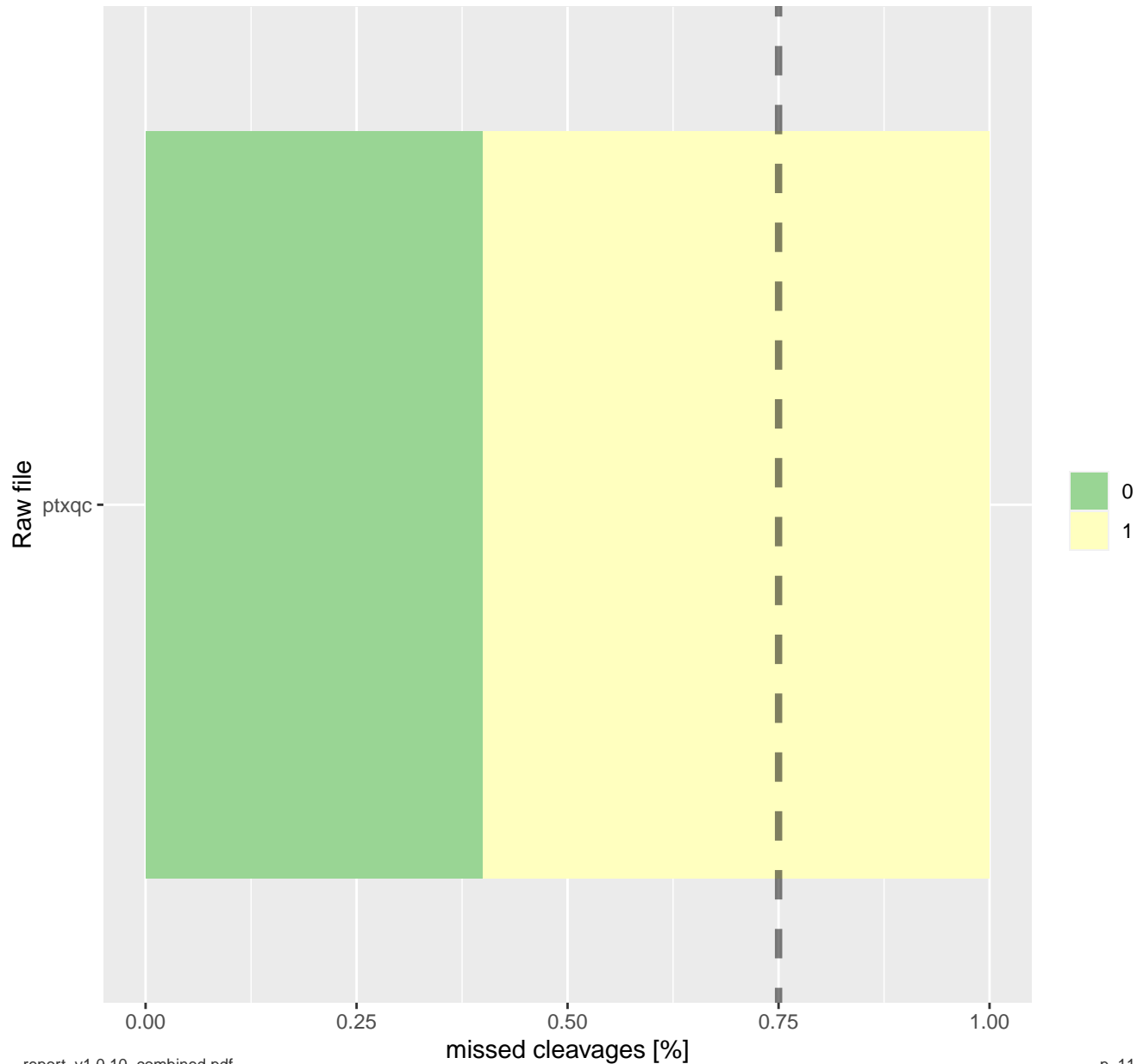
EVD: charge distribution
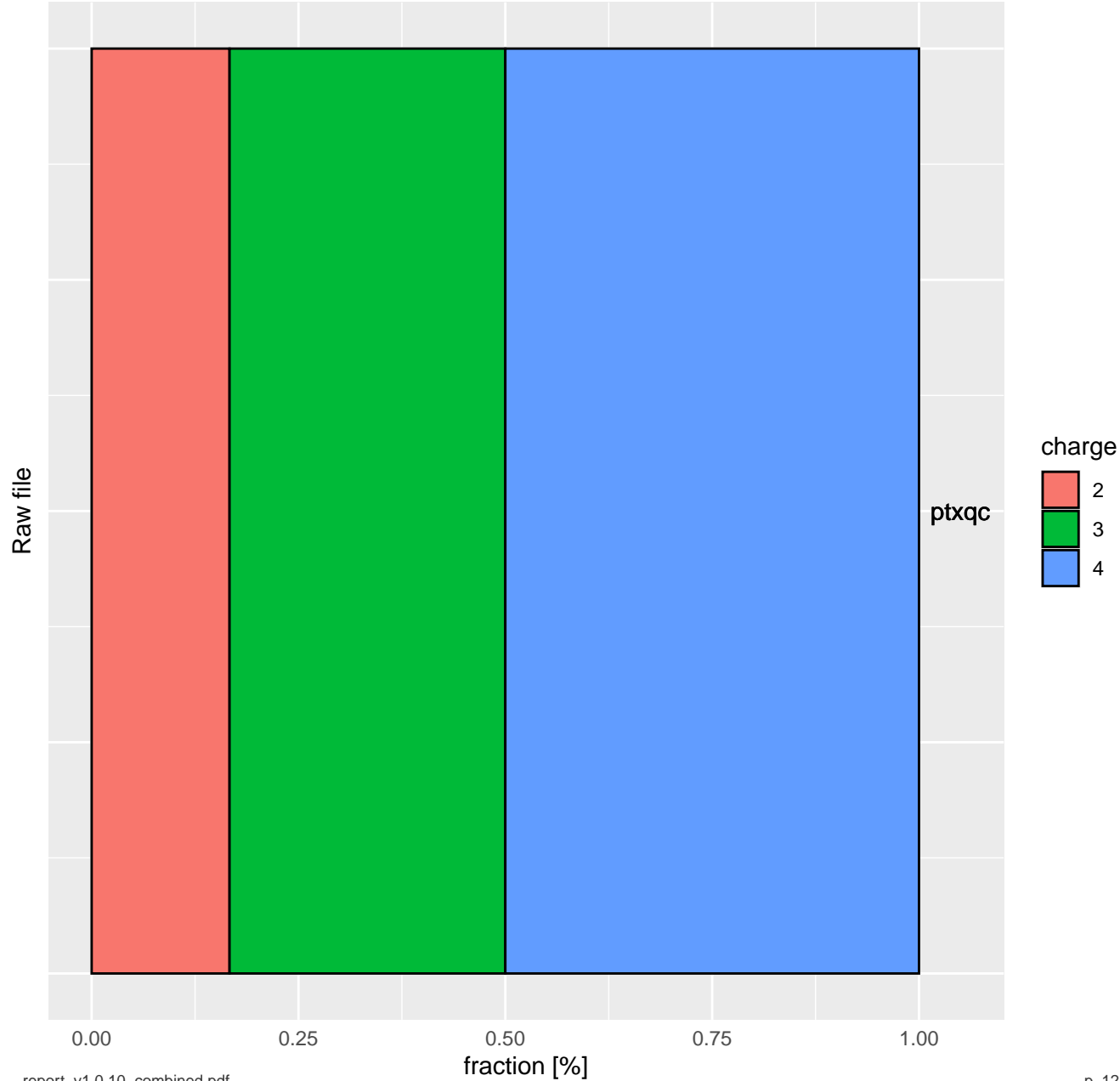
PG: Contaminant per condition

MSMSscans: TopN over RT

highest N [median per RT bin]

5.050 —
5.025 —
5.000 — ——— ptxqc
4.975 —
4.950 —

retention time [min]

15.950　　15.975　　16.000　　16.025　　16.050
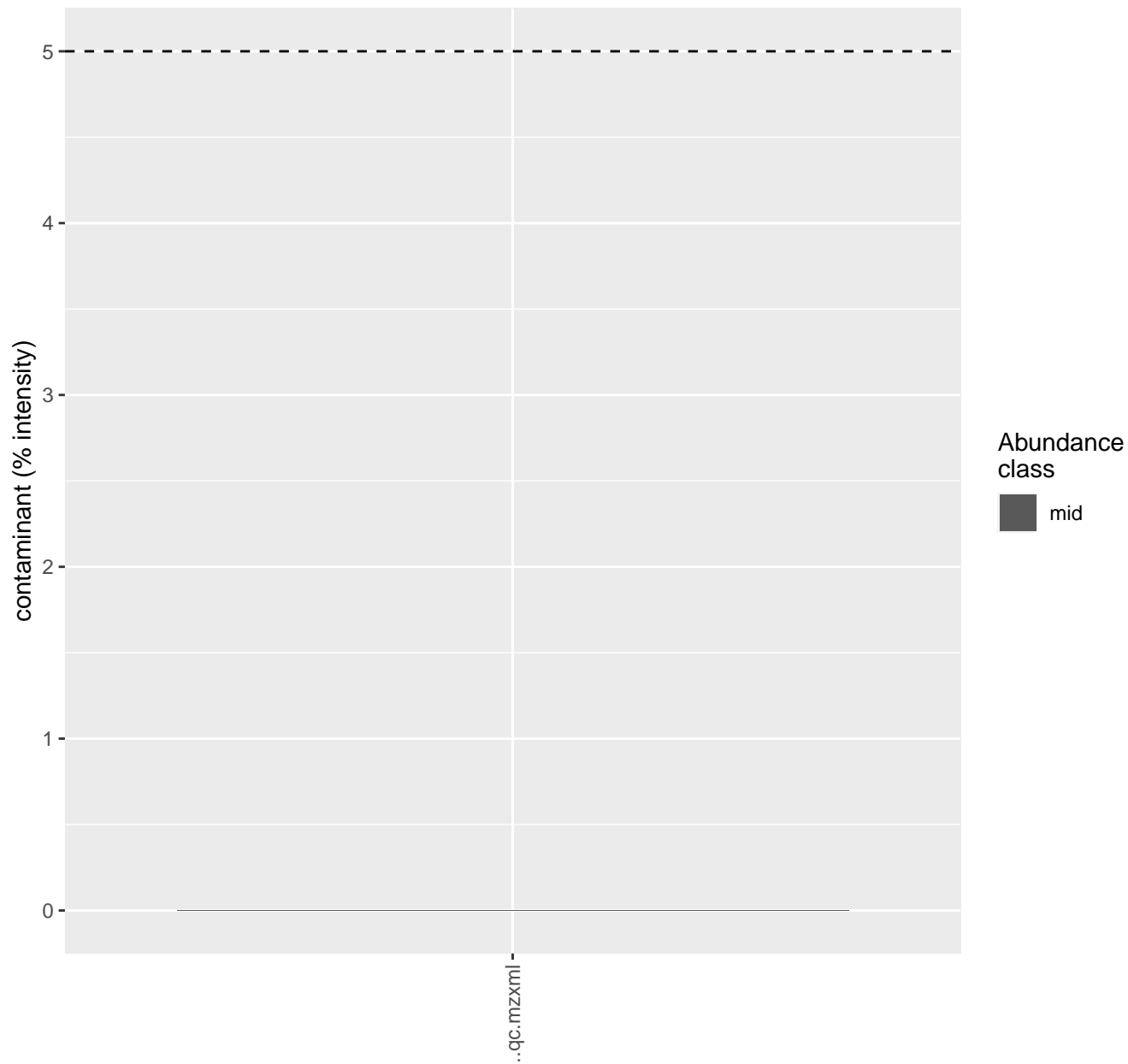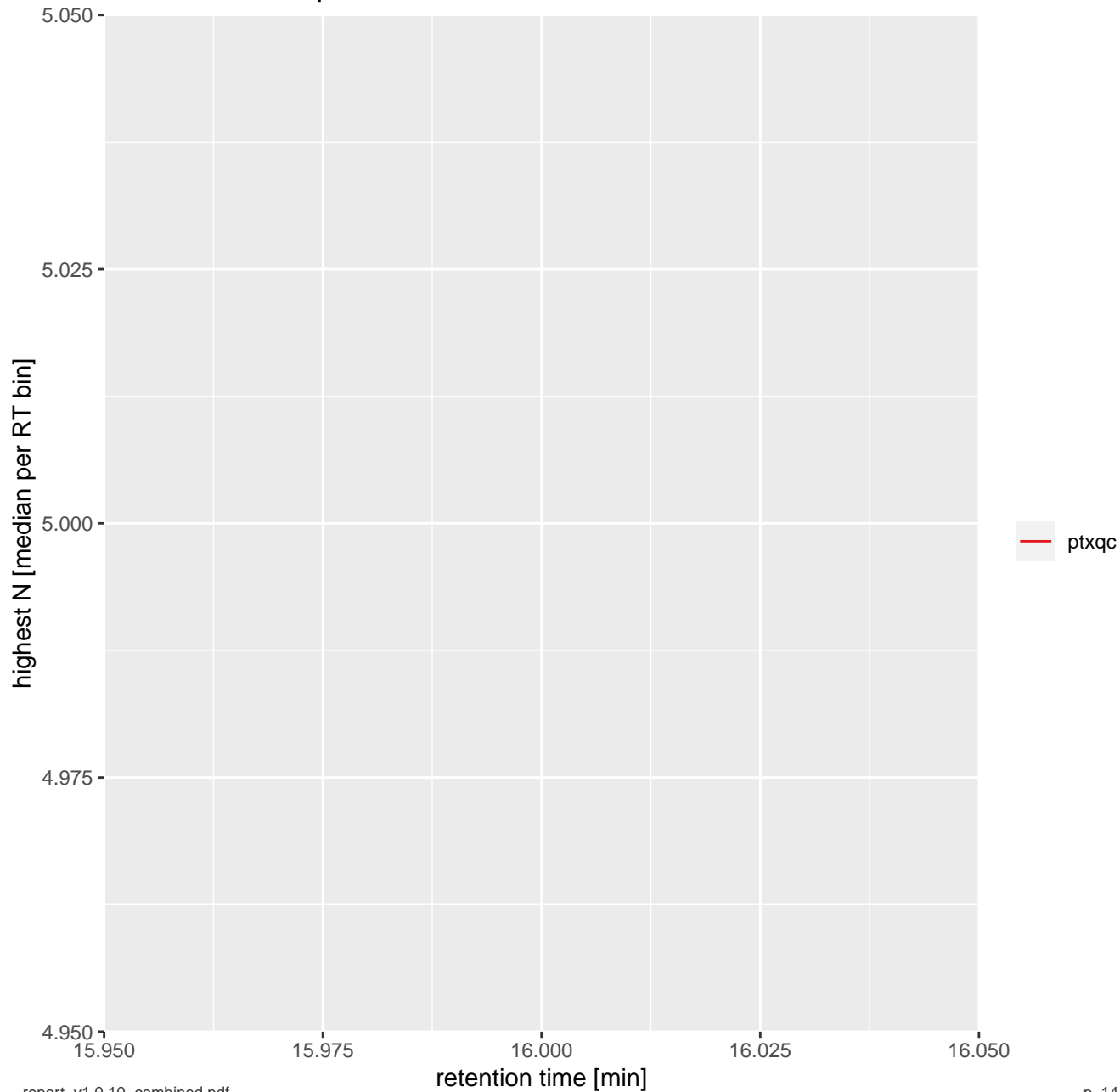
EVD: IDs over RT

EVD: Peak width over RT

peak width [min]

retention time [min]

Raw file
(avg. peak width)

— ptxqc (~0.2 min)
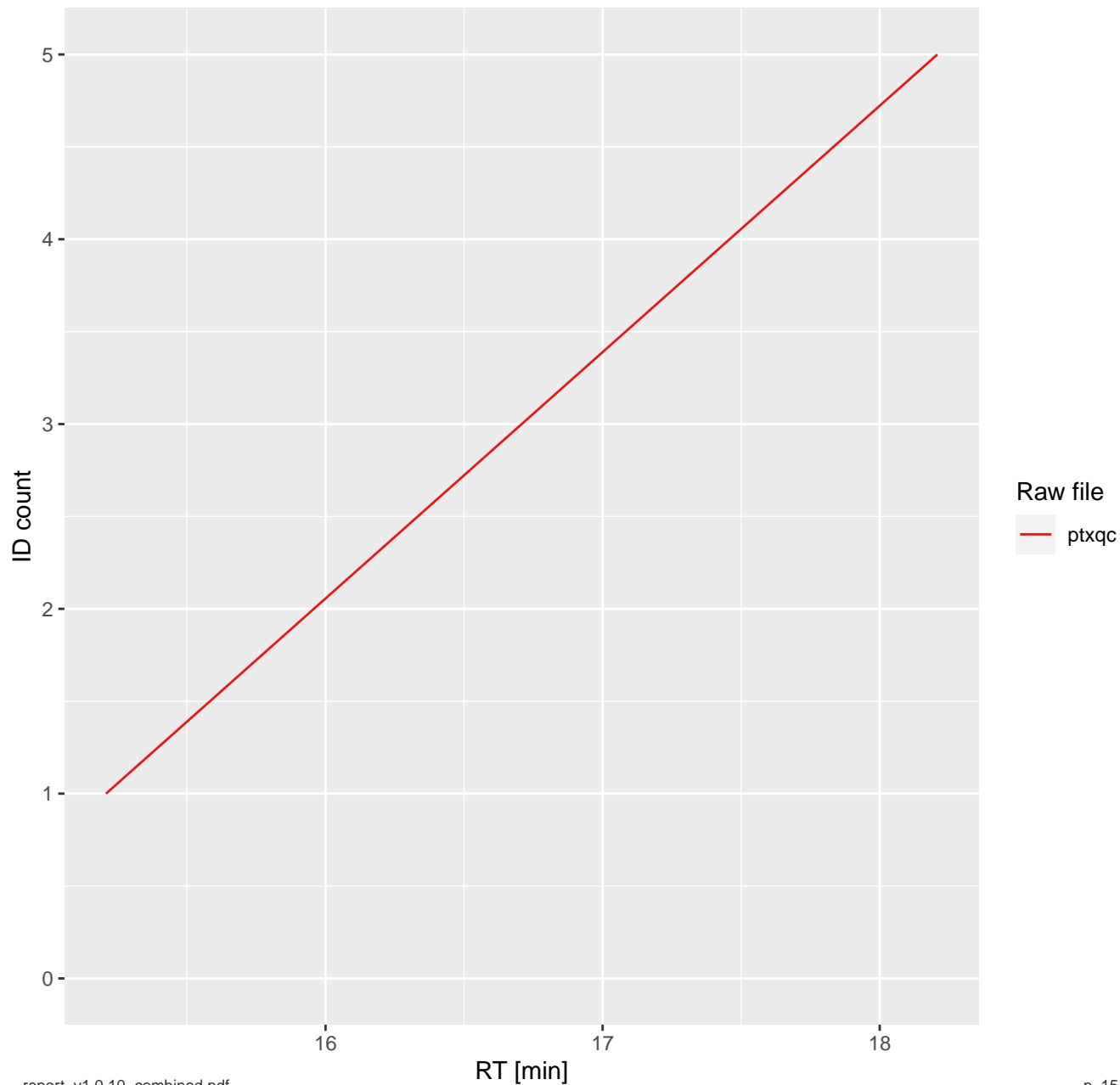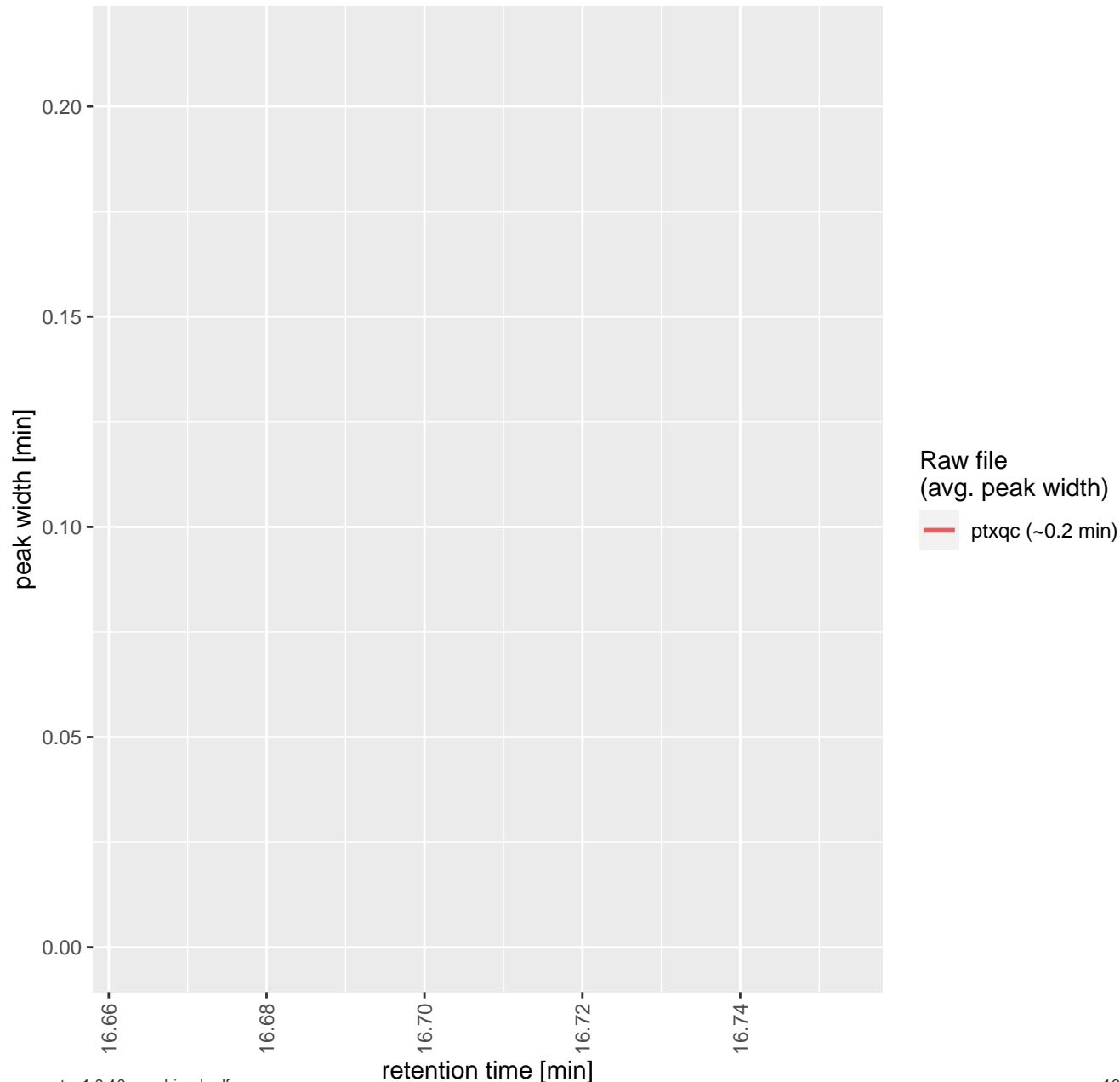
MSMSscans: Ion Injection Time over RT

ion injection time [ms]

retention time [min]

Raw file with
average inj. time

●— ptxqc (~−1 ms)
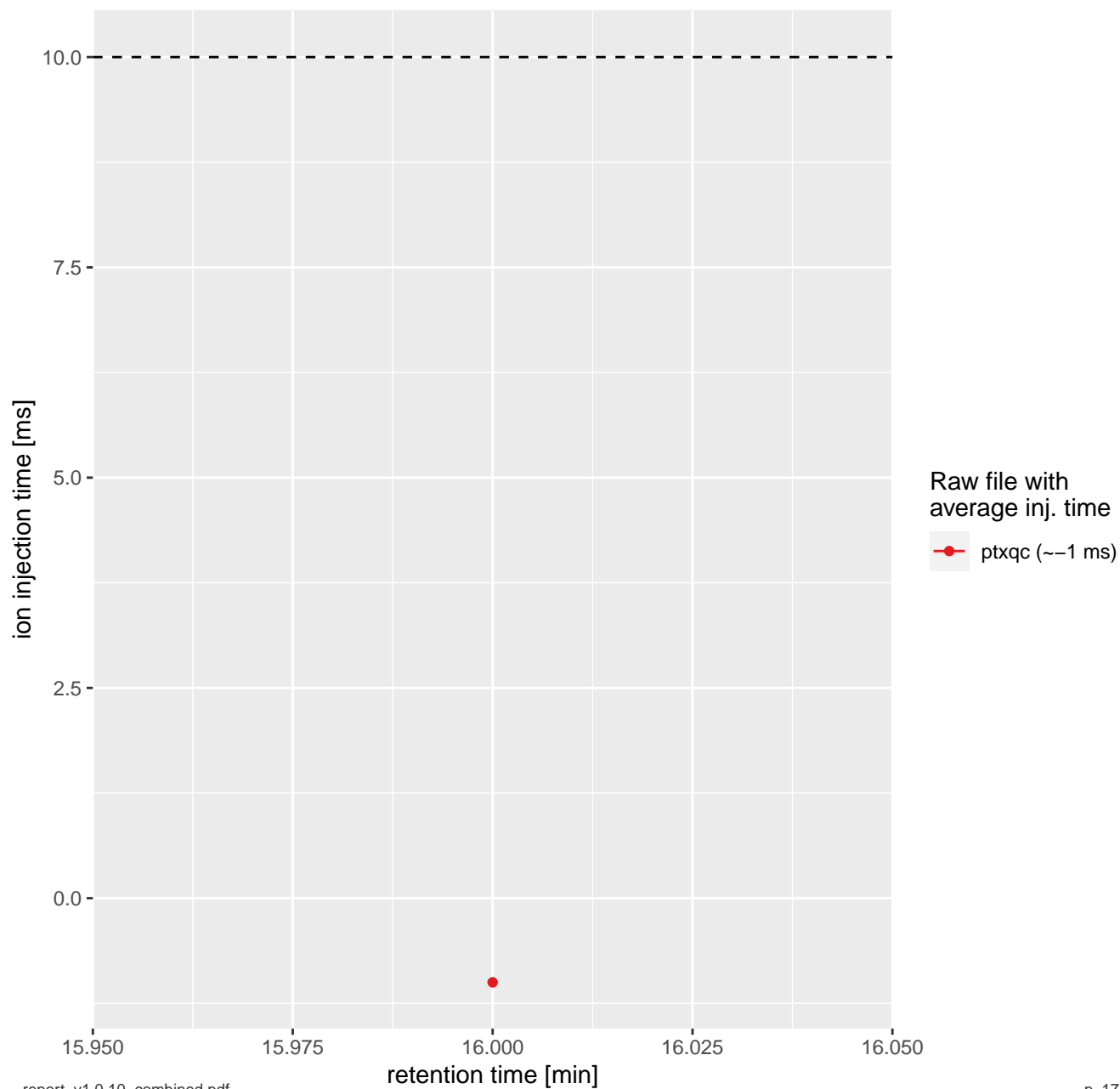
[experimental] MSMSscans: MS/MS intensity

MS/MS intensity

- TIC
- Base Peak

intensity ($\log_{10}$)
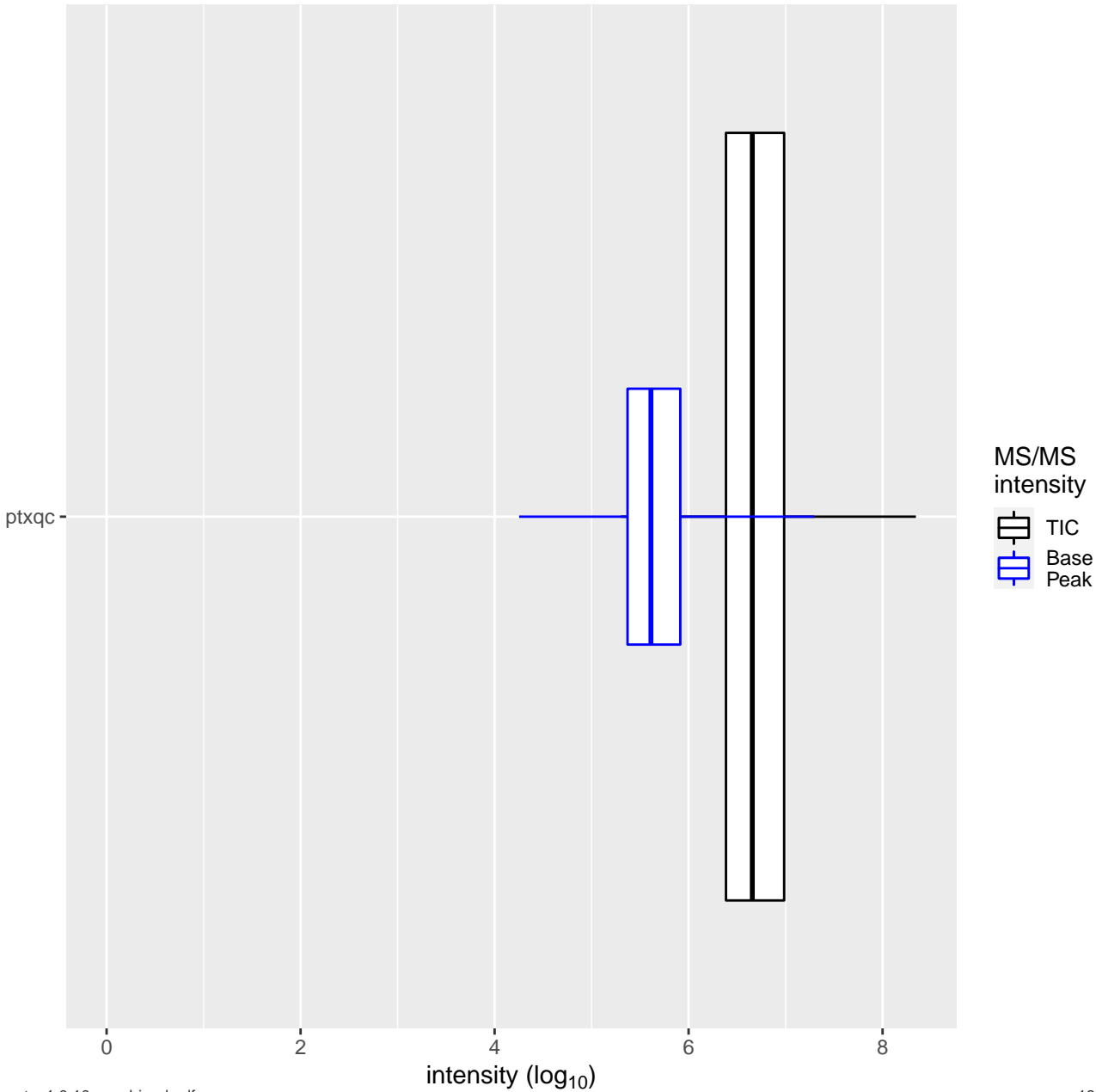
EVD: Oversampling (MS/MS counts per 3D−peak)

MS/MS
counts

■ 1

ptxqc

MS/MS counts per 3D−peak [%]
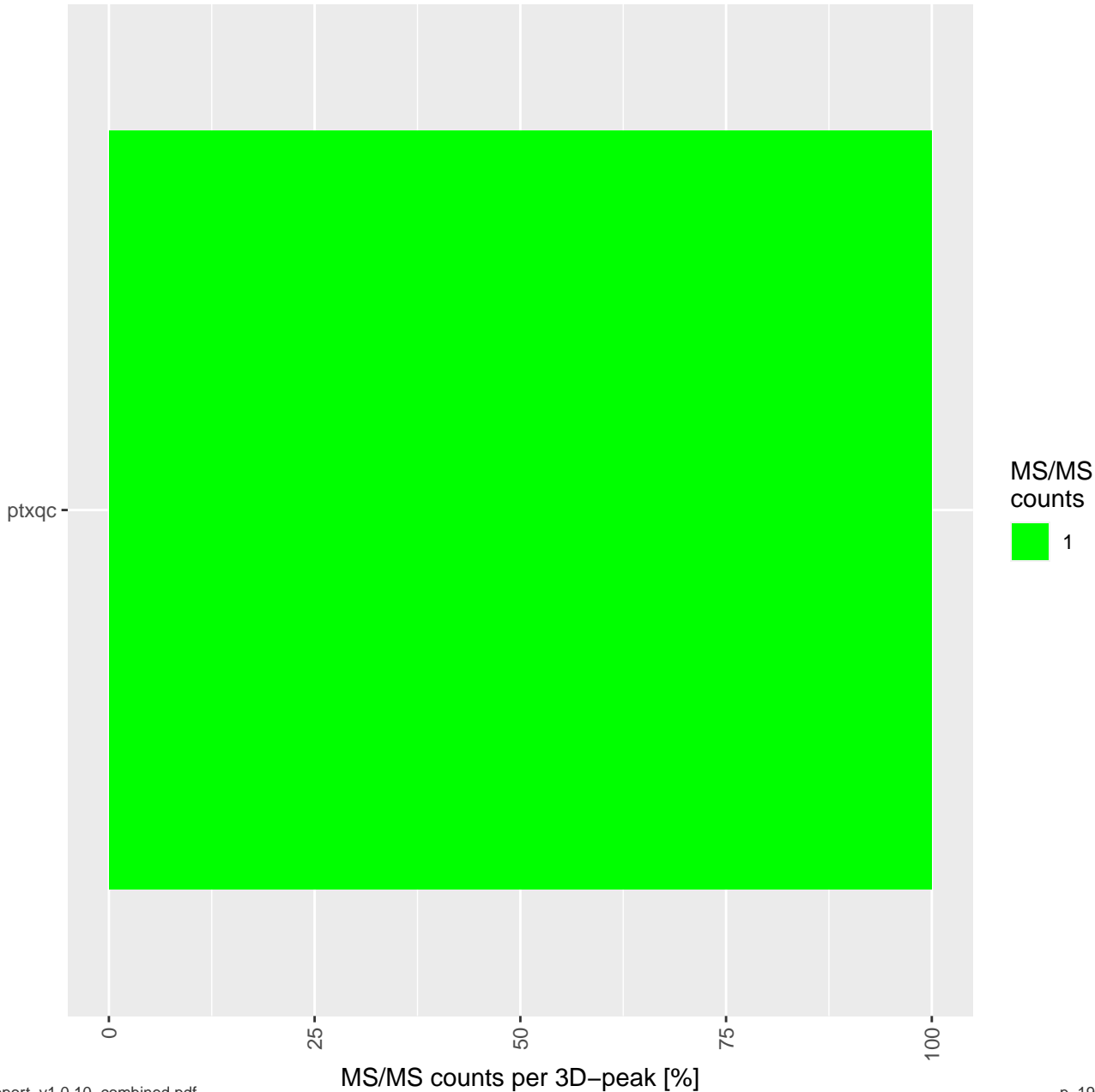
EVD: Uncalibrated mass error

MQ bug: data rescued
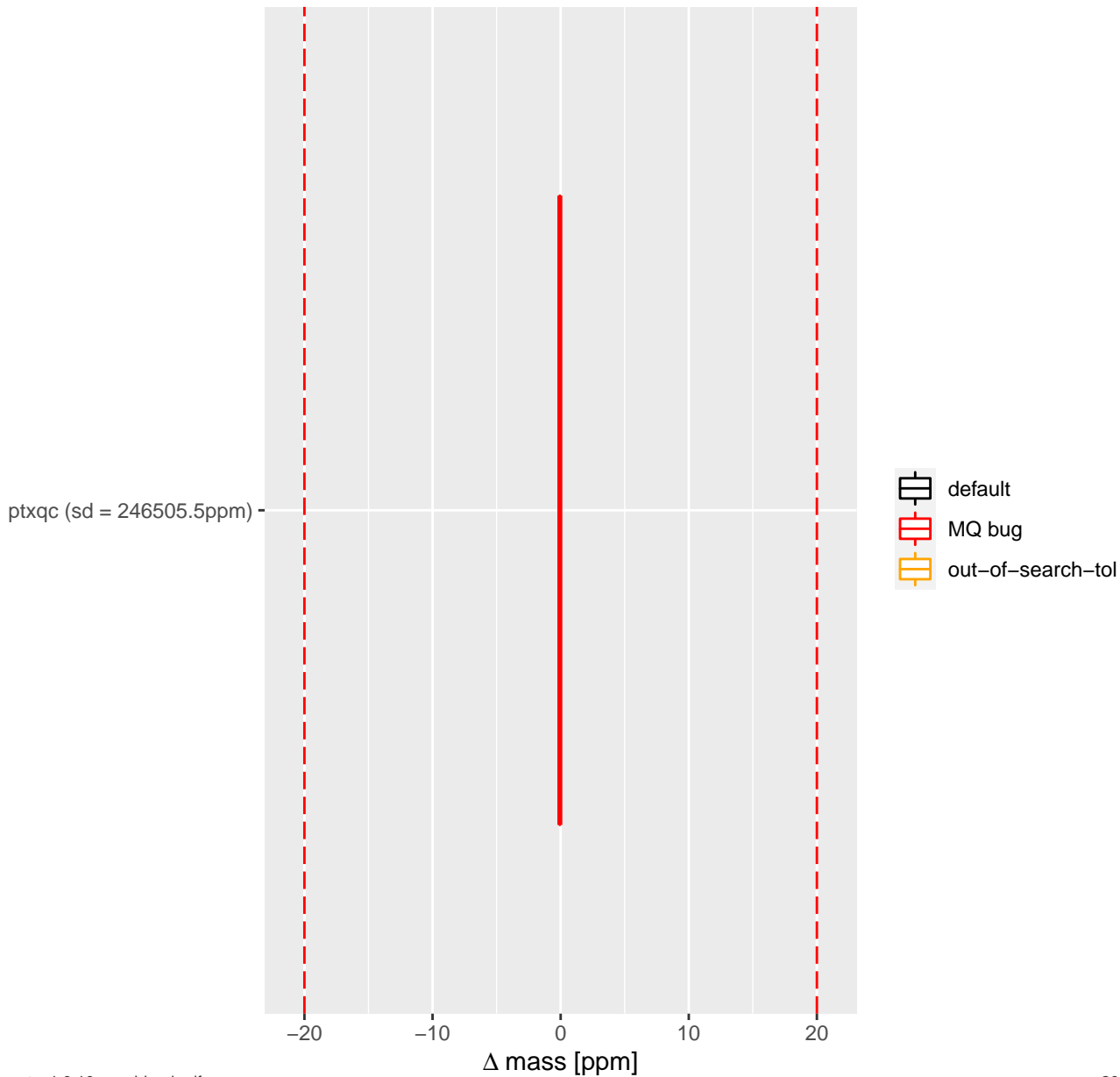
EVD: Calibrated mass error

MQ bug: data cannot be rescued
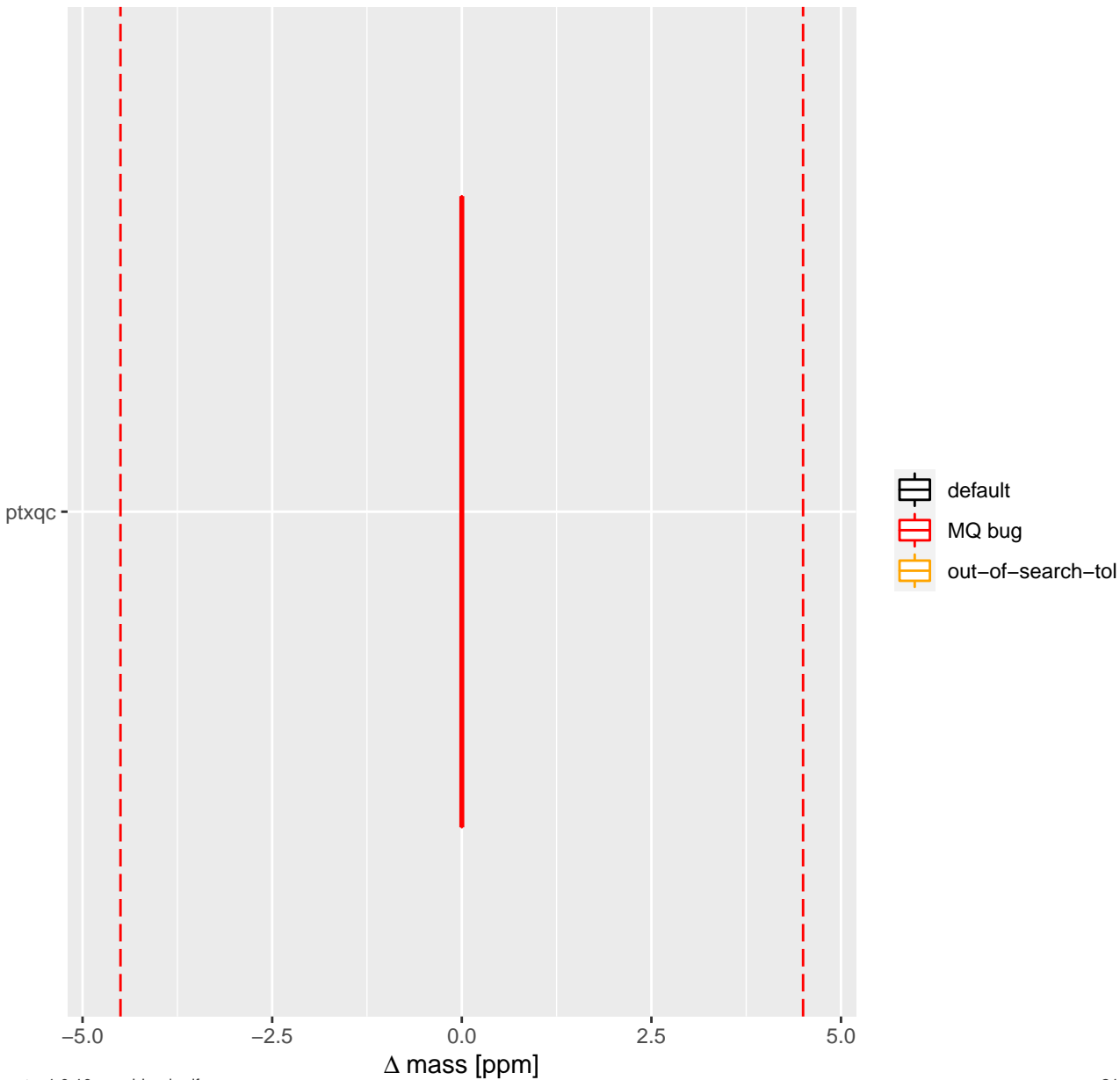
MSMS: Fragment mass errors per Raw file
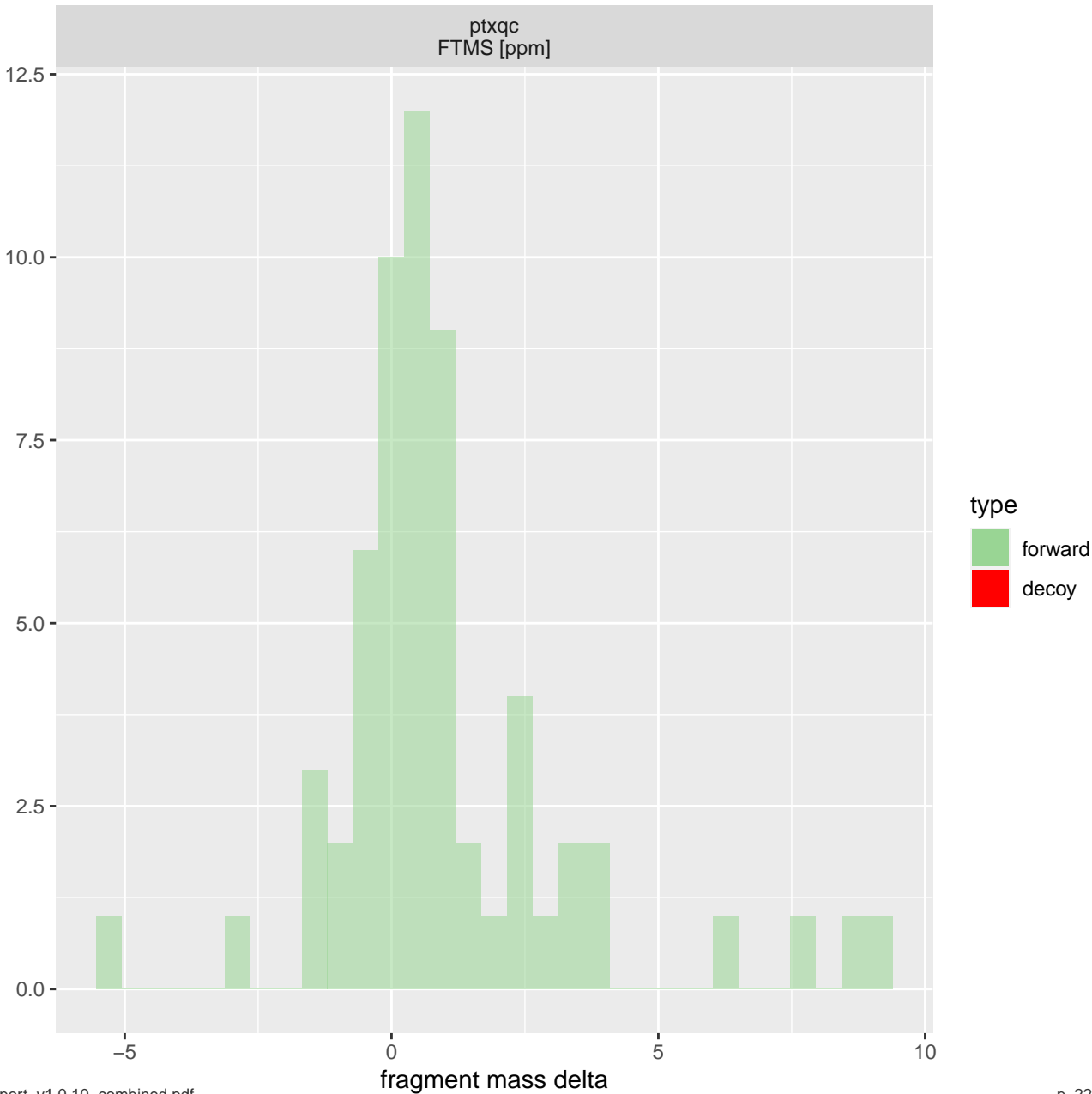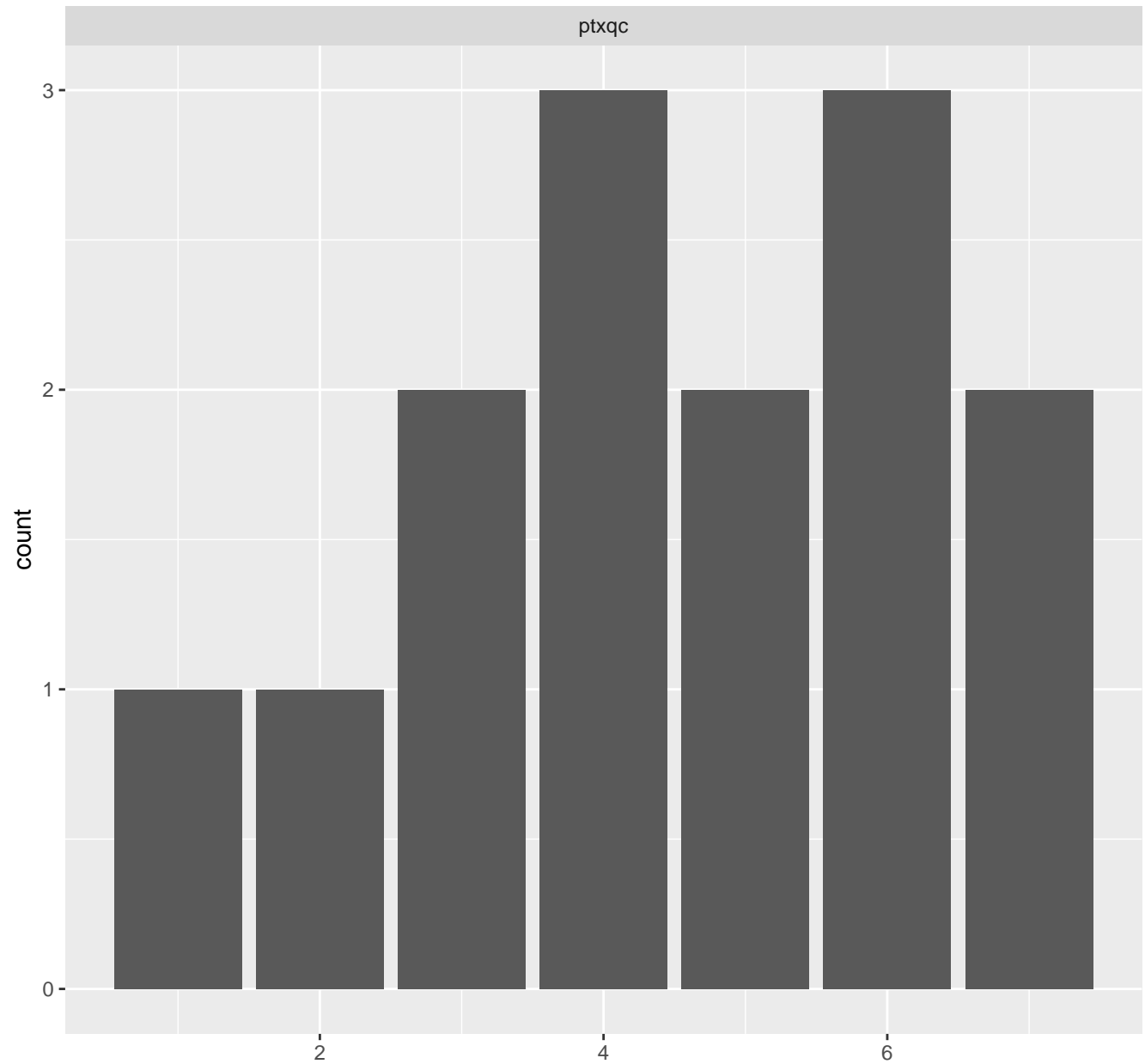
SM: MS/MS identified per Raw file

ID class
- ● bad (<20%)
- ● ok (20–35%)
- ● great (>35%)
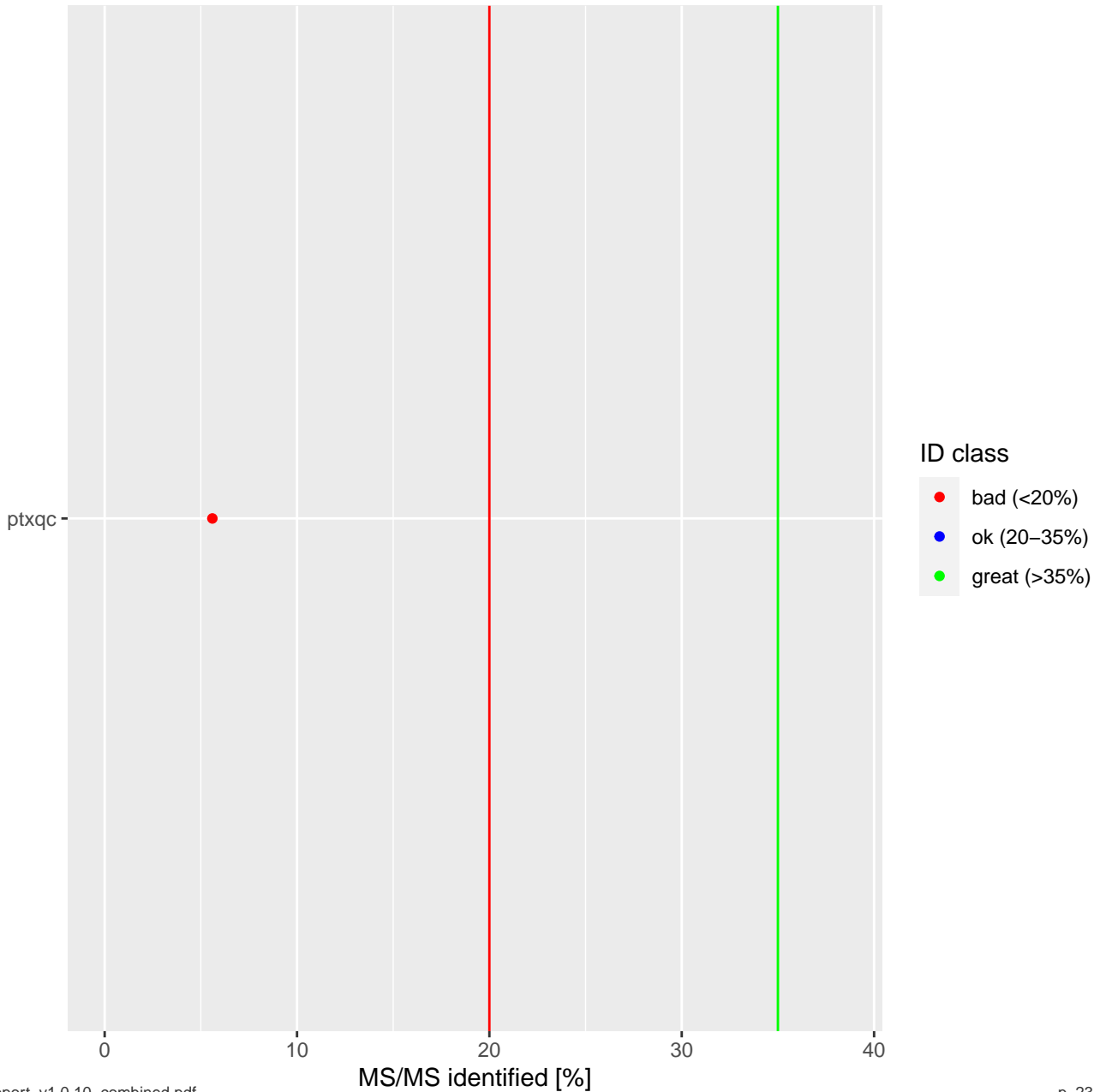
MS/MS identified [%]

SM: Files with 'red' ID rate

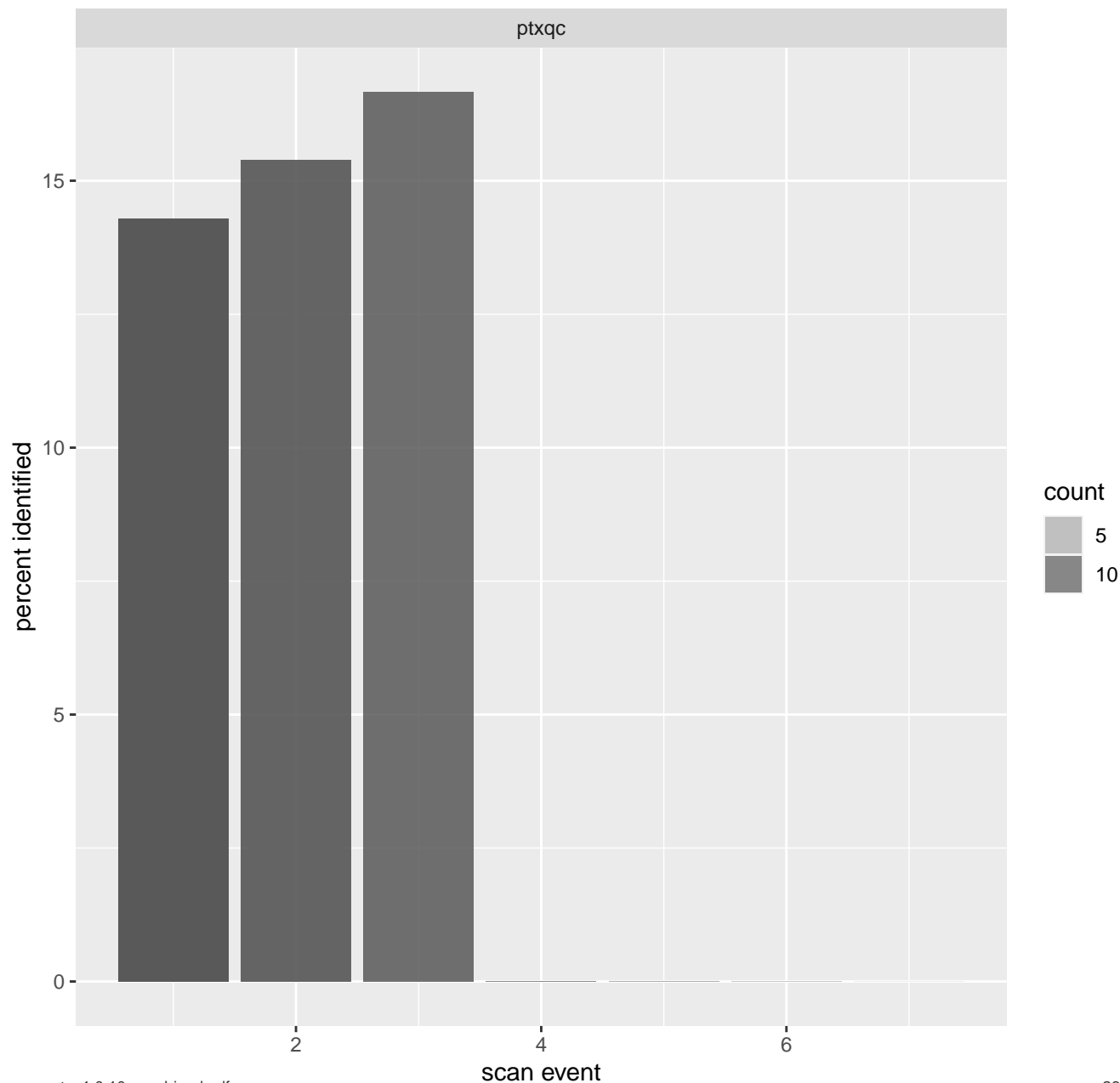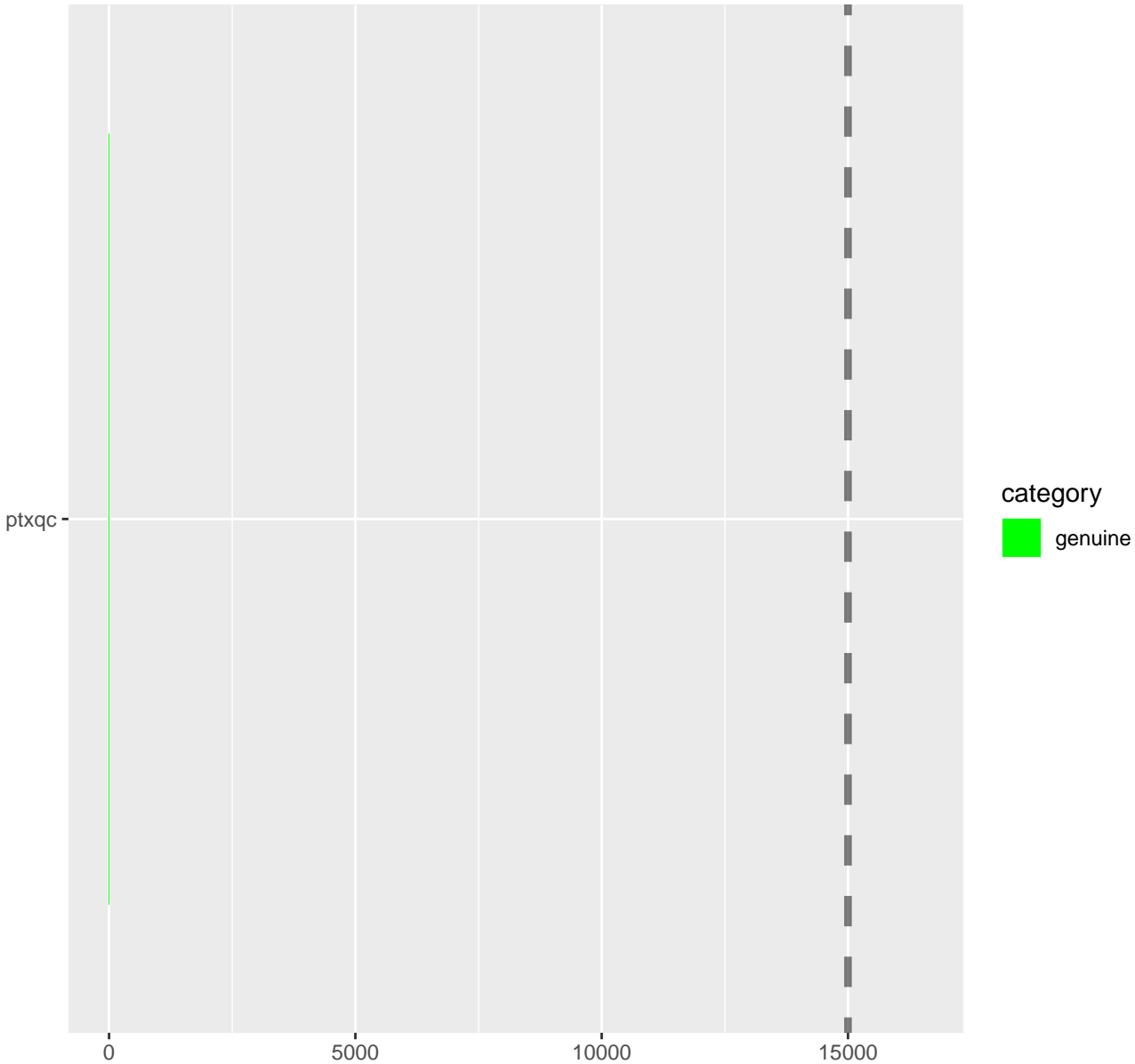| Raw file	% identified
ptxqc	5.6

100% of samples)

MSMSscans: TopN

MSMSscans: TopN % identified over N

Missing Values Skipped

Need more than one Raw file!

EVD: Peptide ID count

category

■ genuine

EVD: ProteinGroups count
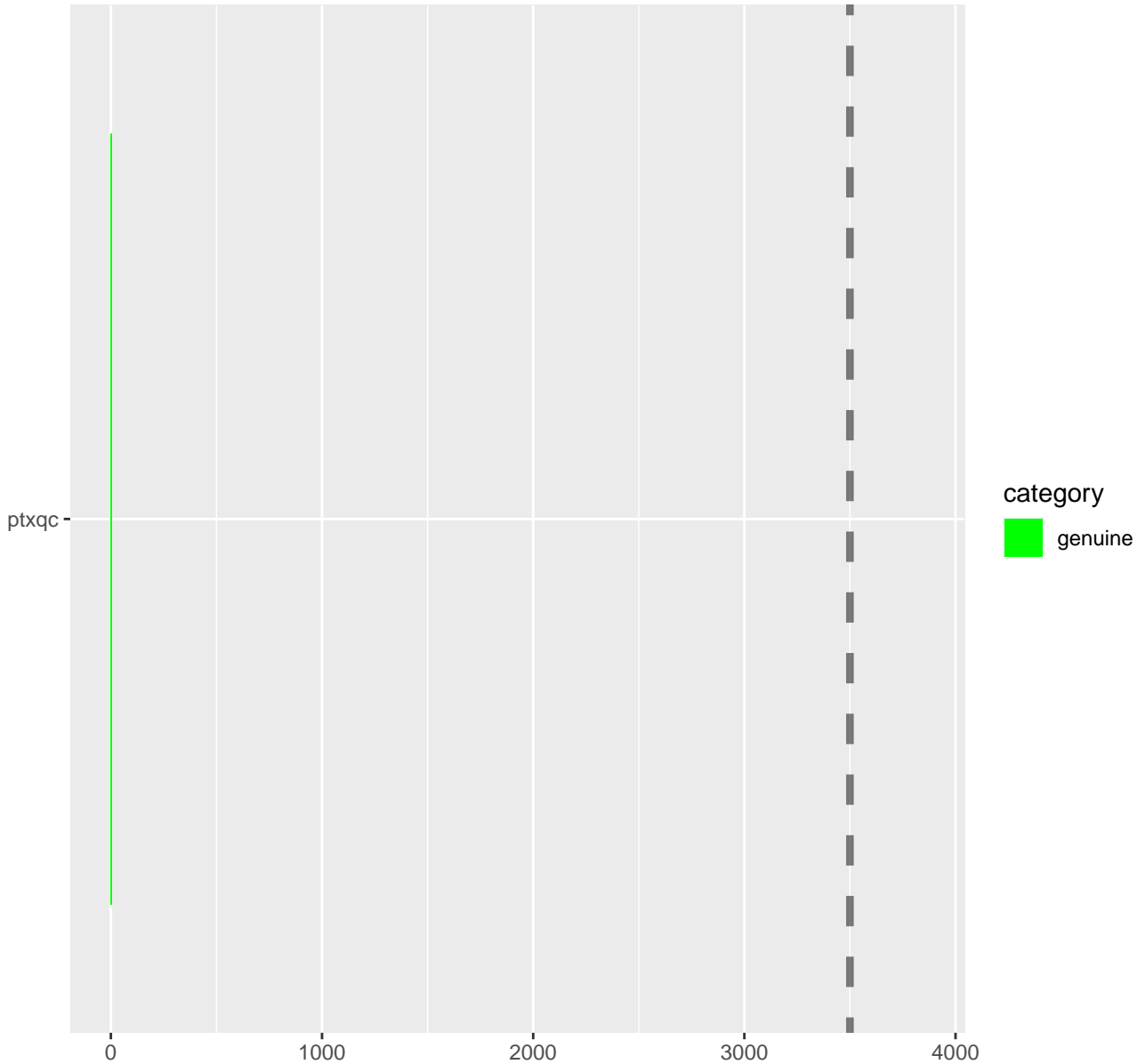
UpSetR

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