Performance overview

Raw file: ..qc_test3

score
- best
- under performing
- fail

Missing
- NA

Columns (x-axis):
- EVD : Contaminants [1]
- EVD : Peptide Intensity (>23.0) [2]
- EVD : Reporter intensity [3]
- MSMS : Missed Cleavages [4]
- MSMS : Missed Cleavages Var [5]
- EVD : Charge [6]
- MS²Scans : TopN over RT [7]
- EVD : ID rate over RT [8]
- EVD : RT Peak Width [9]
- MS²Scans : Ion Inj Time [10]
- MS²Scans : Intensity [11]
- EVD : MS² Oversampling [12]
- EVD : MS Cal−Pre (20) [13]
- EVD : MS Cal−Post [14]
- MSMS : MS² Cal (FTMS) [15]
- SM : MS² ID rate(>35) [16]
- MS²Scans : TopN high [17]
- MS²Scans : TopN ID over N [18]
- EVD : Peptide Count (>15000) [19]
- EVD : Protein Count (>3500) [20]
- Average Overall Quality [21]

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

original	short name	best effort
ptxqc_test3	..qc_test3	..qc_test3

PAR: parameters

parameter	value	parameter	value
Advanced ratios	True	Min. score for modified pept..	40
Calculate peak properties	False	Modifications included in pr..	Oxidation (M) Acetyl (Protein N–term)
Combined folder location		MS/MS deisotoping tolerance ..	ppm
Da interval. (FTMS)	100	MS/MS deisotoping tolerance ..	0.15
Date of writing	05/31/2021 17:30:36	MS/MS deisotoping tolerance ..	Da
Decoy mode	revert	MS/MS deisotoping tolerance ..	0.01
Label min. ratio count	2	MS/MS tol. (FTMS)	20 ppm
Machine name	DESKTOP–I3UDKML	MS/MS tol. (ITMS)	0.5 Da
Main search max. combination..	200	MS/MS tol. (TOF)	40 ppm
Max mods in site table	3	Peptides used for protein qu..	Razor
Max. peptide length for unsp..	25	Site tables	Oxidation (M)Sites.txt
Max. peptide mass [Da]	4600	Top MS/MS peaks per Da inter..	12
Min. delta score for modifie..	6	Top MS/MS peaks per Da inter..	10
Min. delta score for unmodif..	0	User name	niko
Min. peptide Length	7	Variation mode	None
Min. peptide length for unsp..	8	Version	1.6.10.43
Min. peptides	1	NA	NA

/tmp/tmpkt3o4xar/files/6/5/3/dataset_653c3e53–619f–40f4–a5c2–5f41c01e3406.dat

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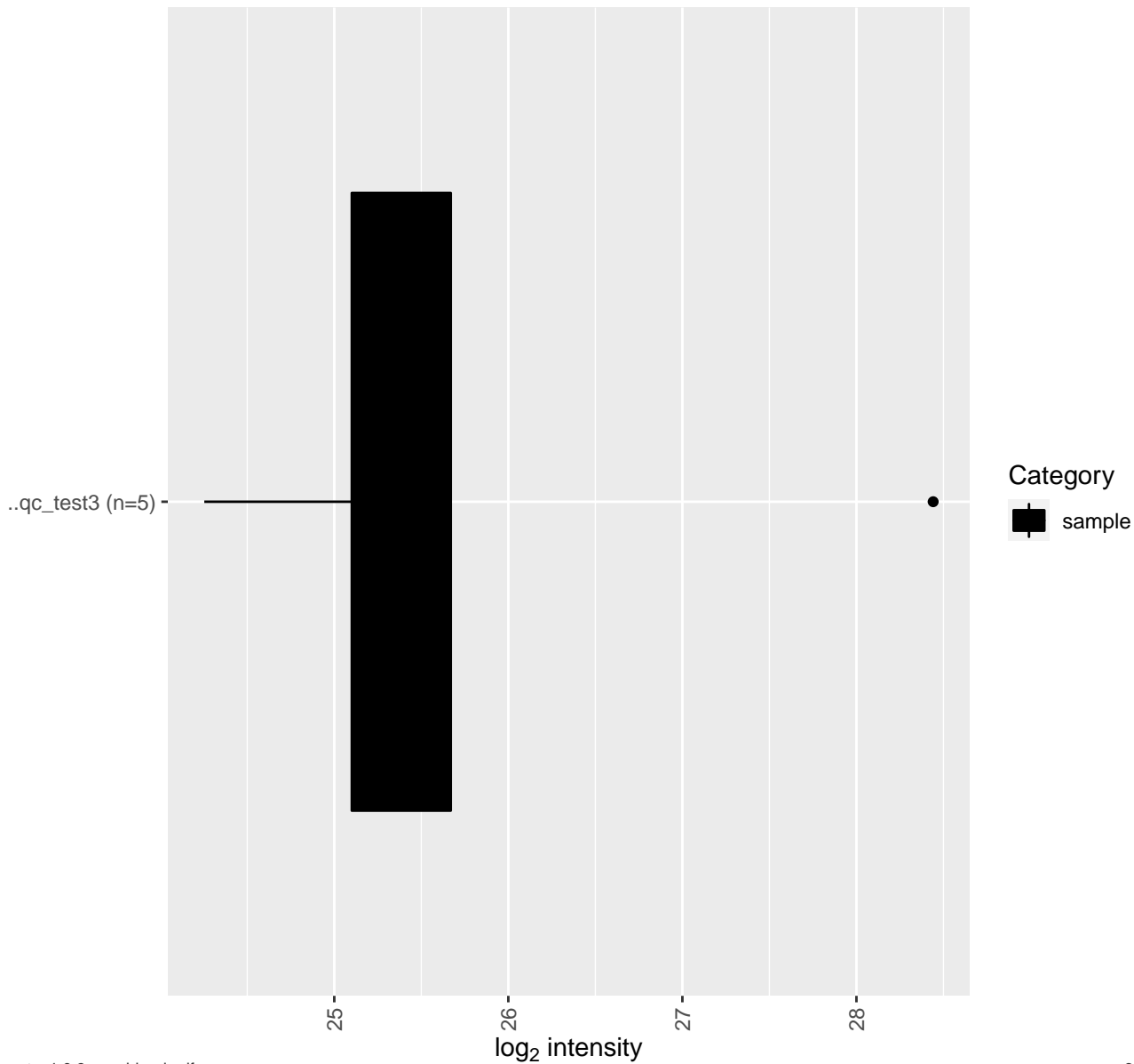
(excludes contaminants)
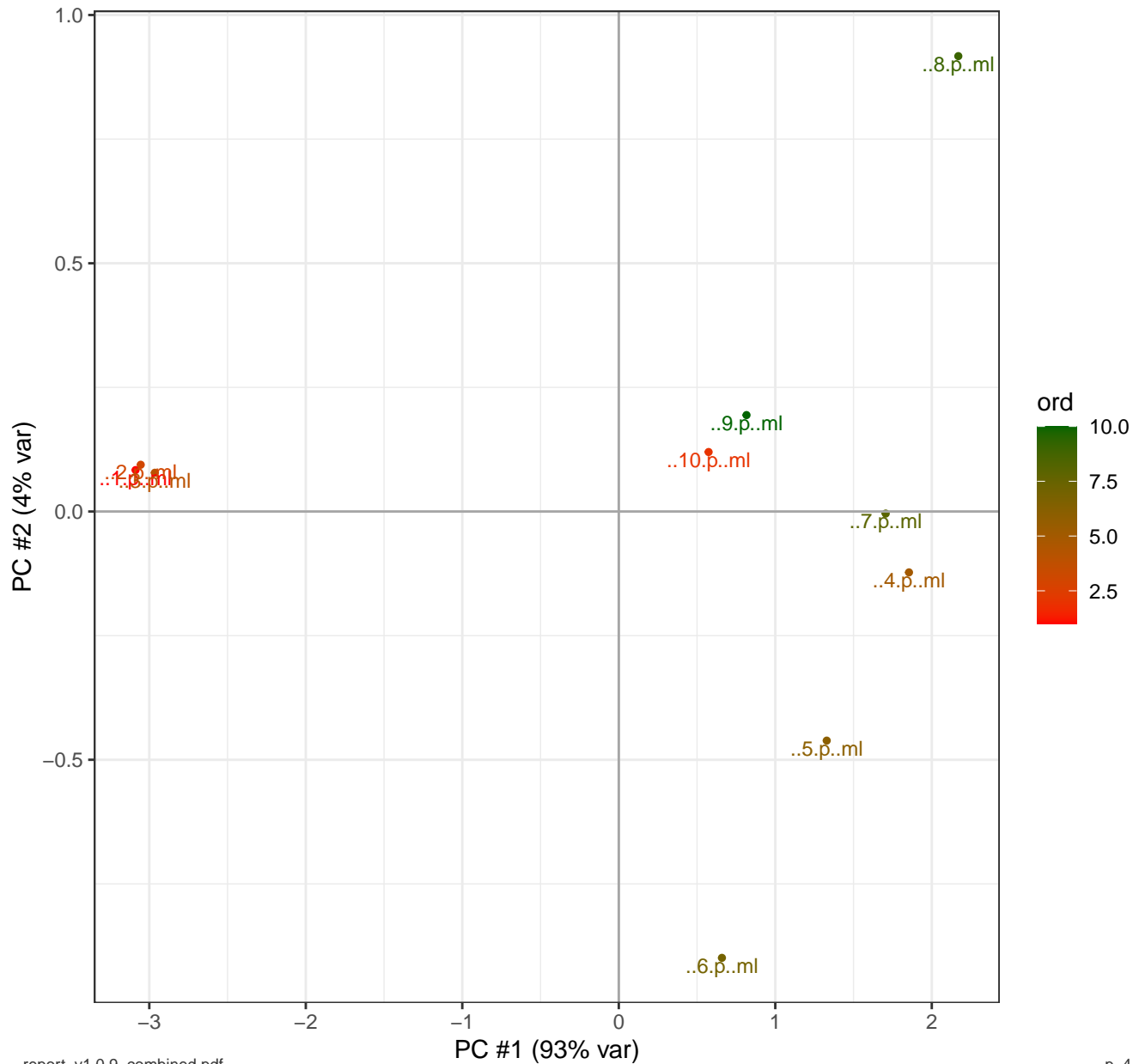
EVD: Top5 Contaminant per Raw file

No contaminants found in any sample.

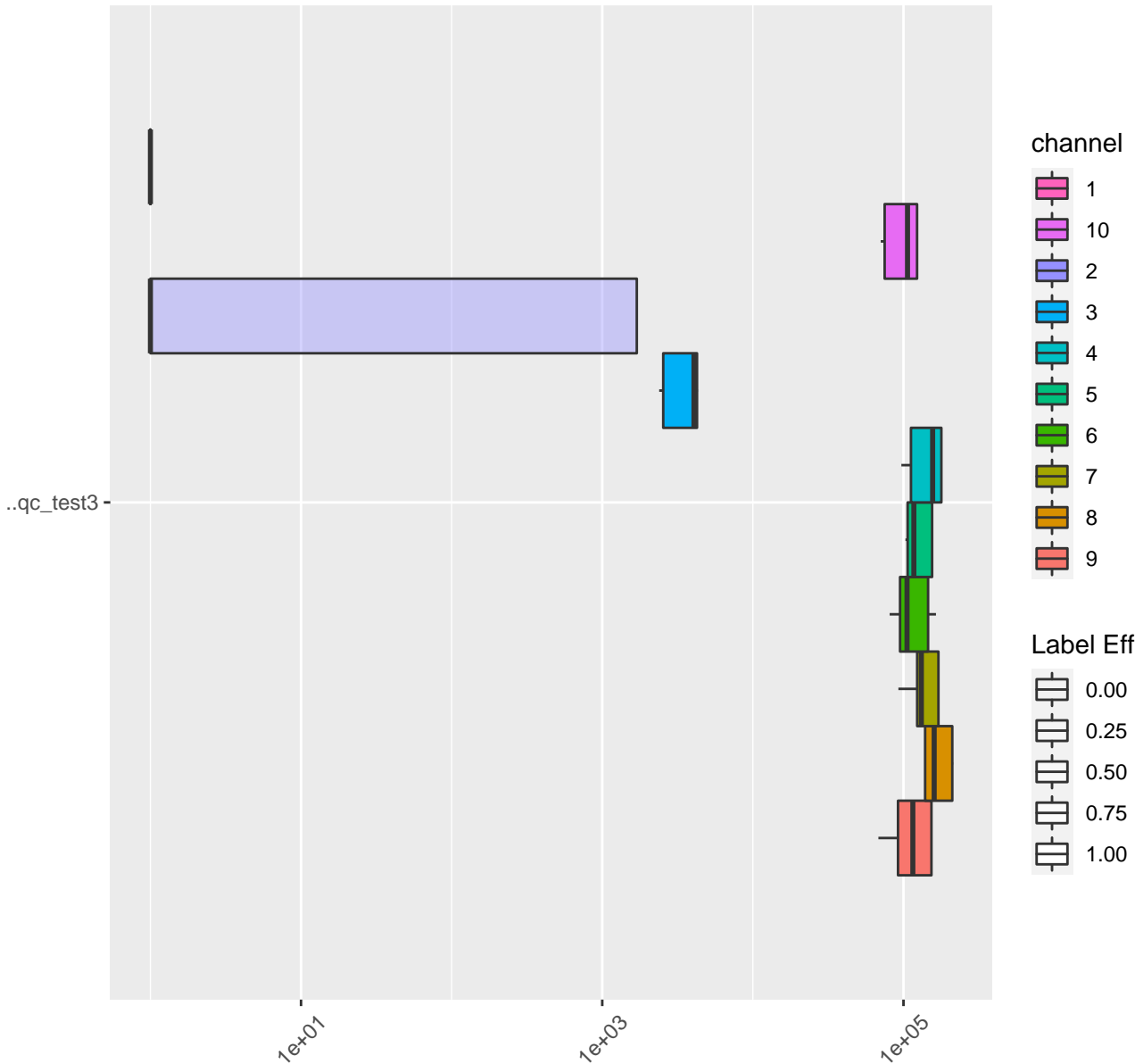Incorporating contaminants during search is highly recommended!

EVD: peptide intensity distribution

RSD NA% (expected < 5%)

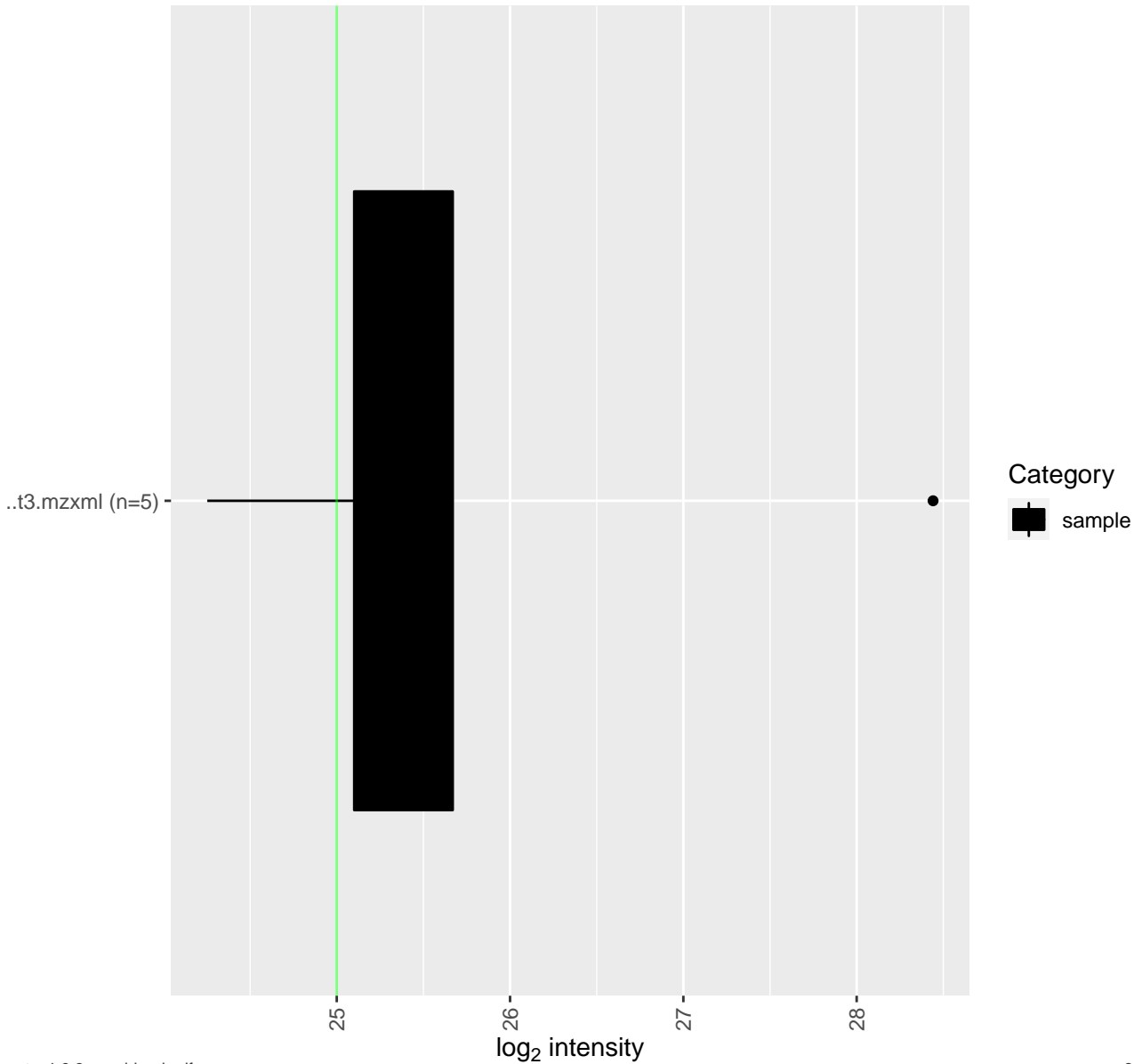# EVD: Reporter label intensities

Warning: MaxQuant did NO isotope correction

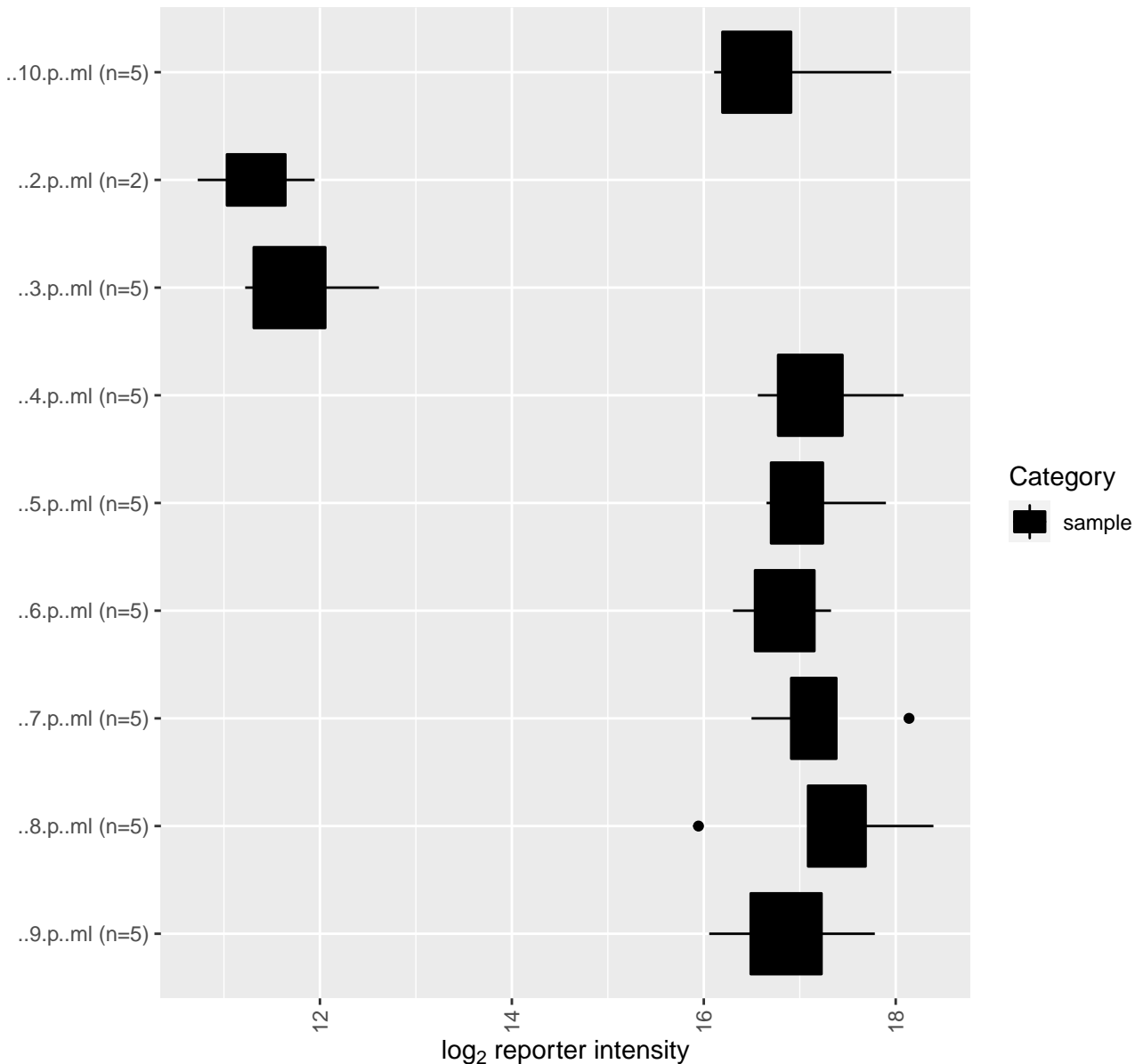# PG: intensity distribution

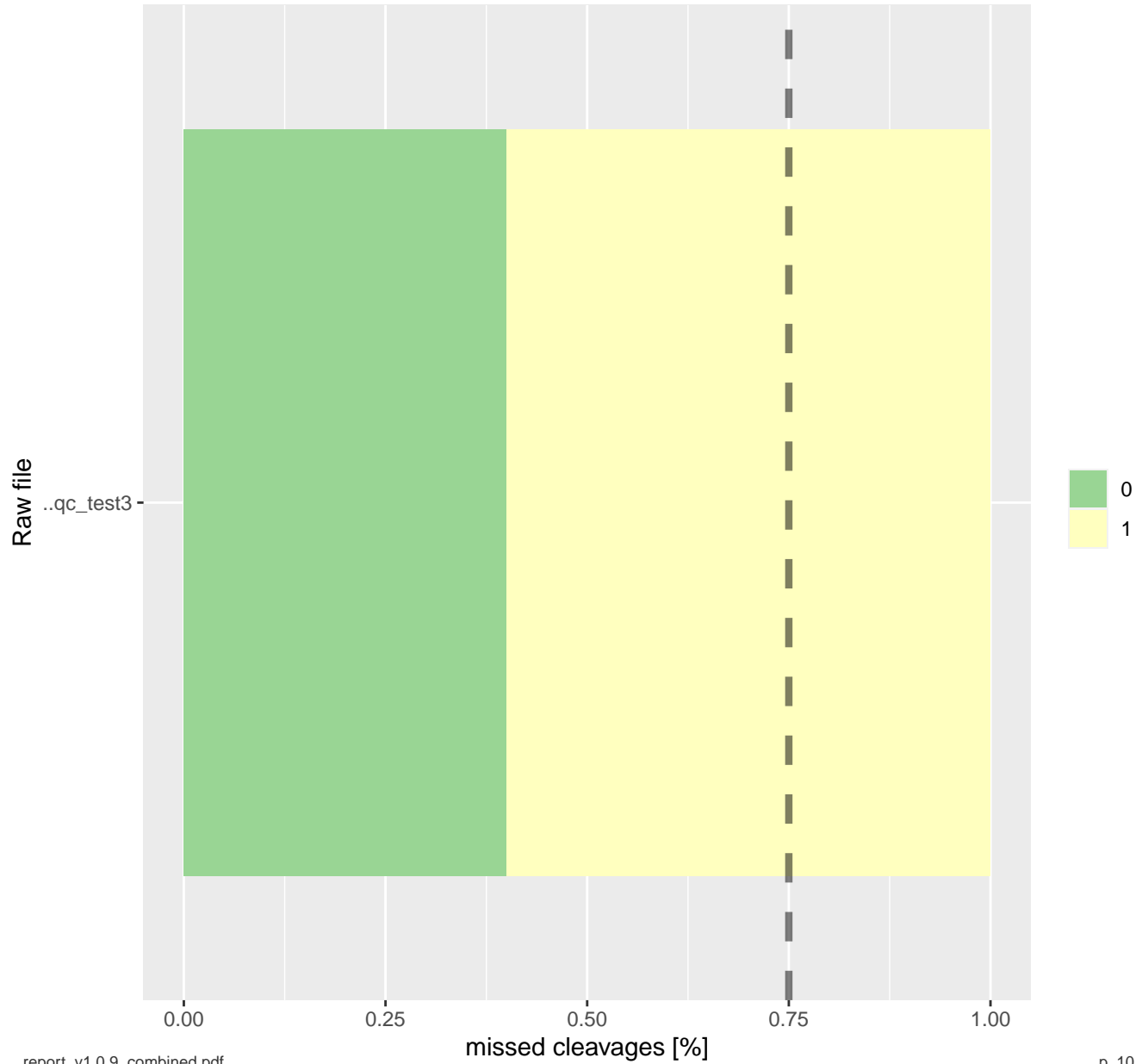RSD NA% (w/o zero int.; expected < 5%)
RSD NA% [high RSD ––> few peptides])

Category

sample

$\log_2$ intensity

..t3.mzxml (n=5)

PG: reporter intensity distribution

RSD 14.9% (w/o zero int.; expected < 5%)
RSD 54% [high RSD ––> few peptides])

$\log_2$ reporter intensity

MSMS: Missed cleavages per Raw file
(excludes contaminants)

EVD: charge distribution
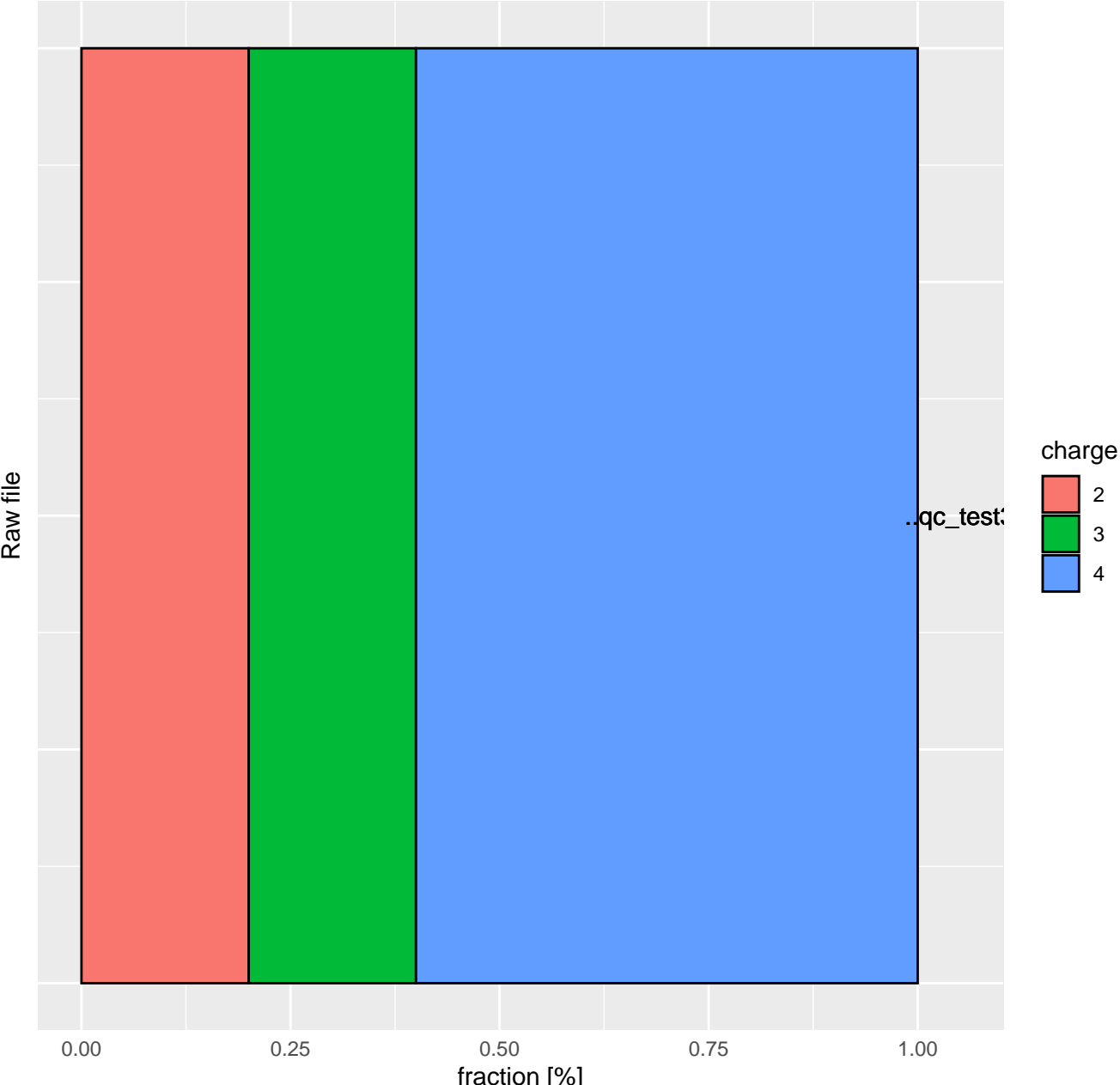
PG: Contaminant per condition

contaminant (% intensity)

5 ‐

4

3

2

1

0

..t3.mzxml

Abundance class

■ mid

MSMSscans: TopN over RT

.. qc_test3

highest N [median per RT bin]

retention time [min]
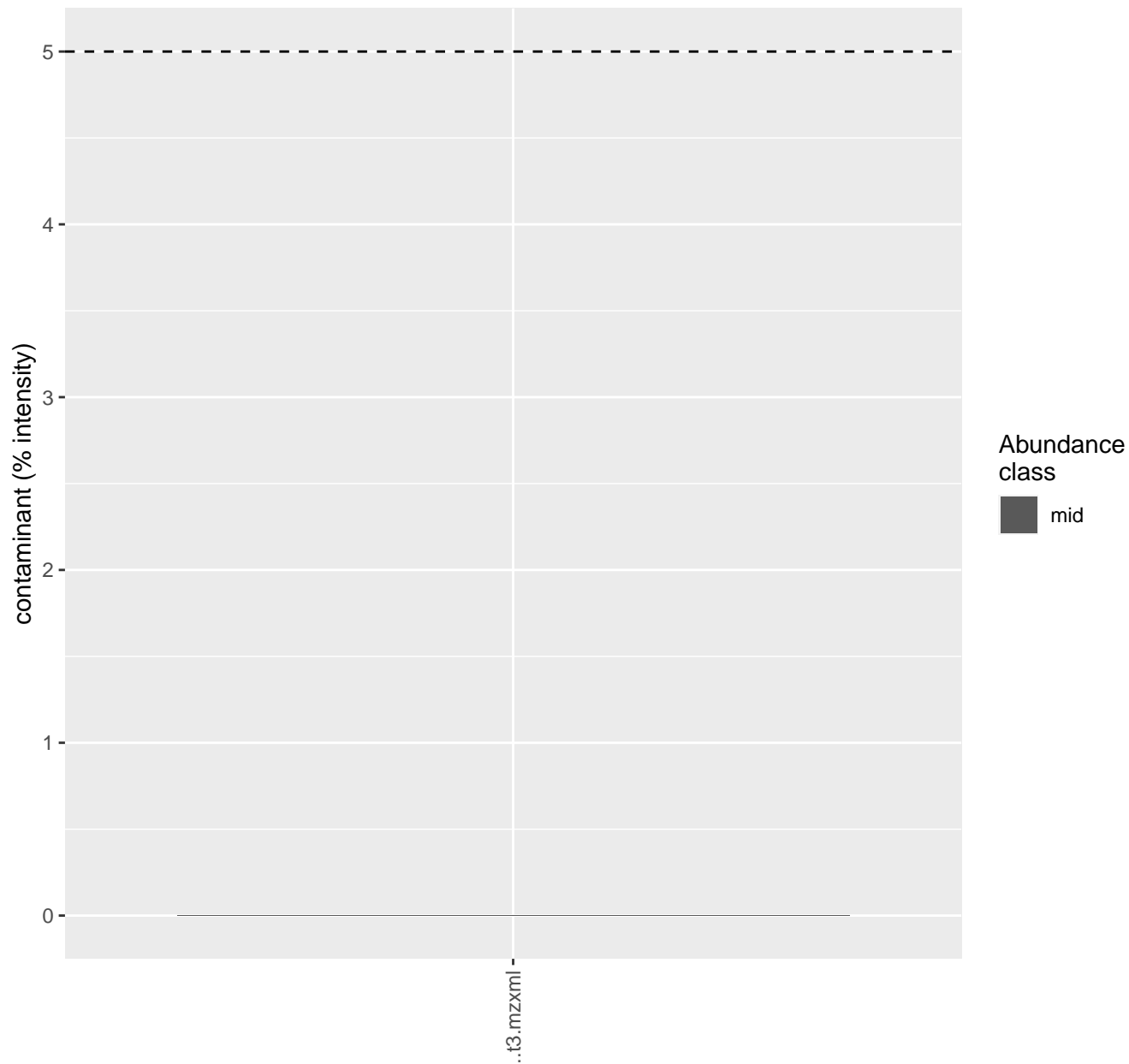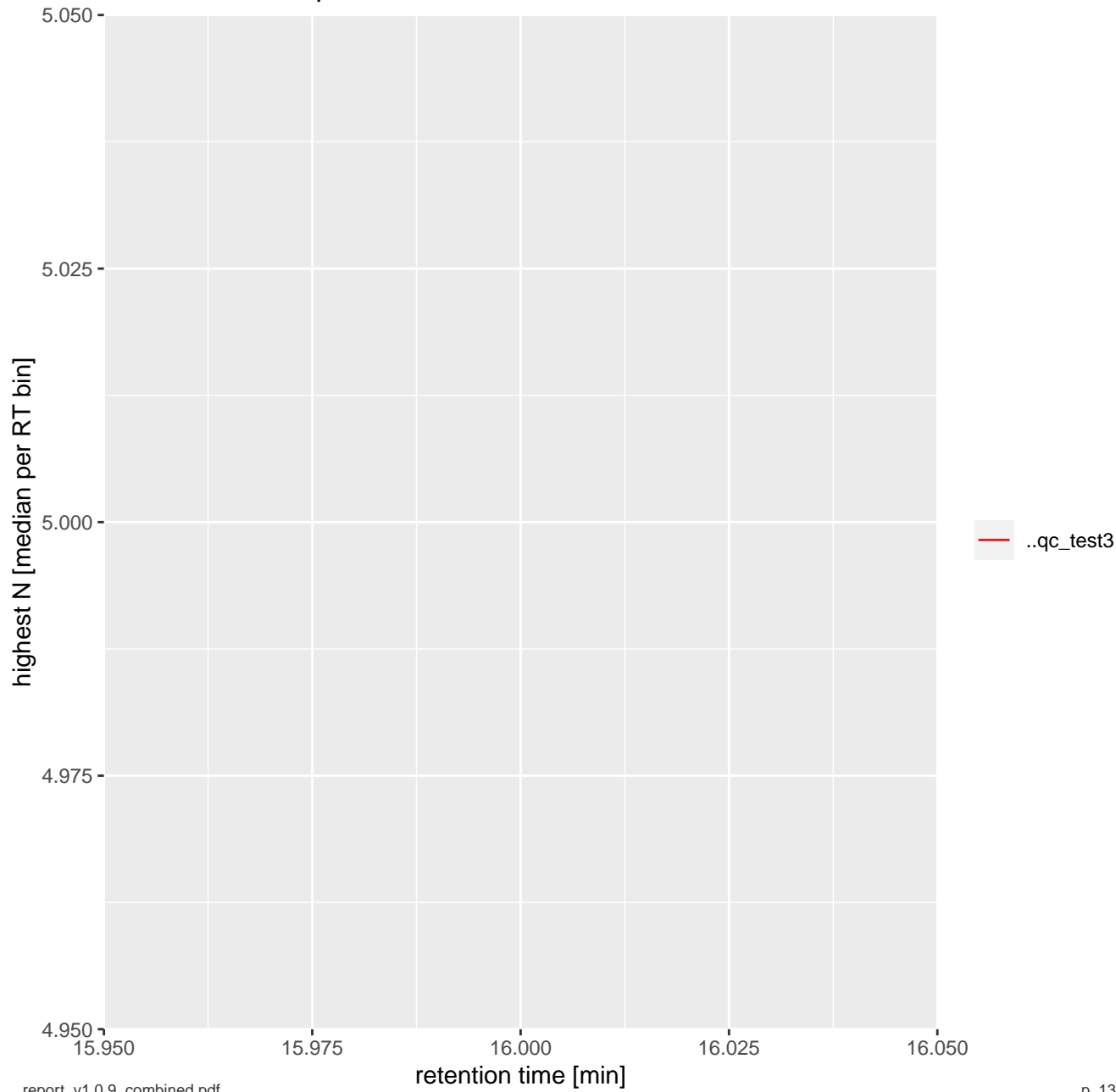
EVD: IDs over RT

EVD: Peak width over RT

peak width [min]

retention time [min]

Raw file
(avg. peak width)

— ..qc_test3 (~0.2 min)
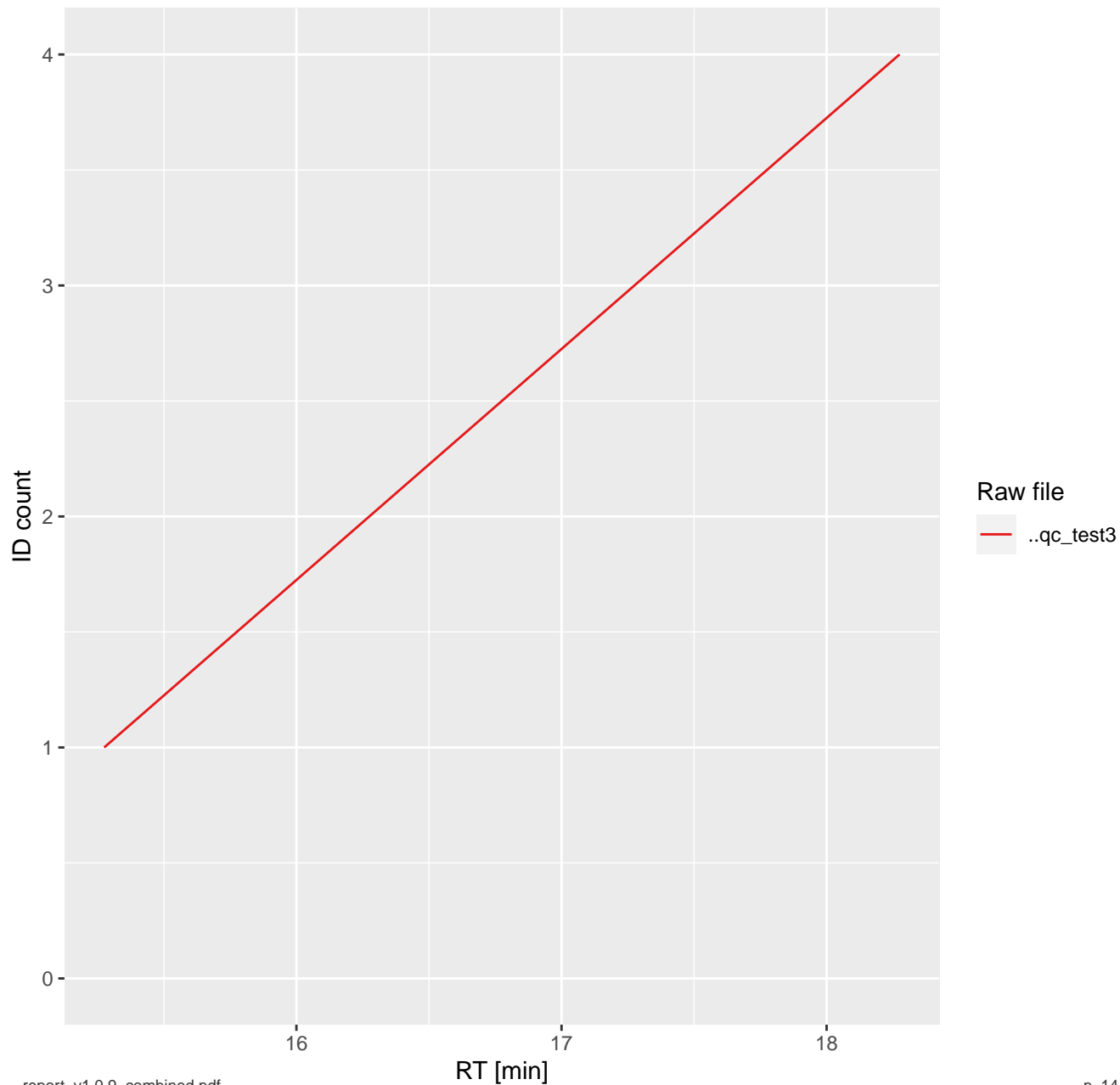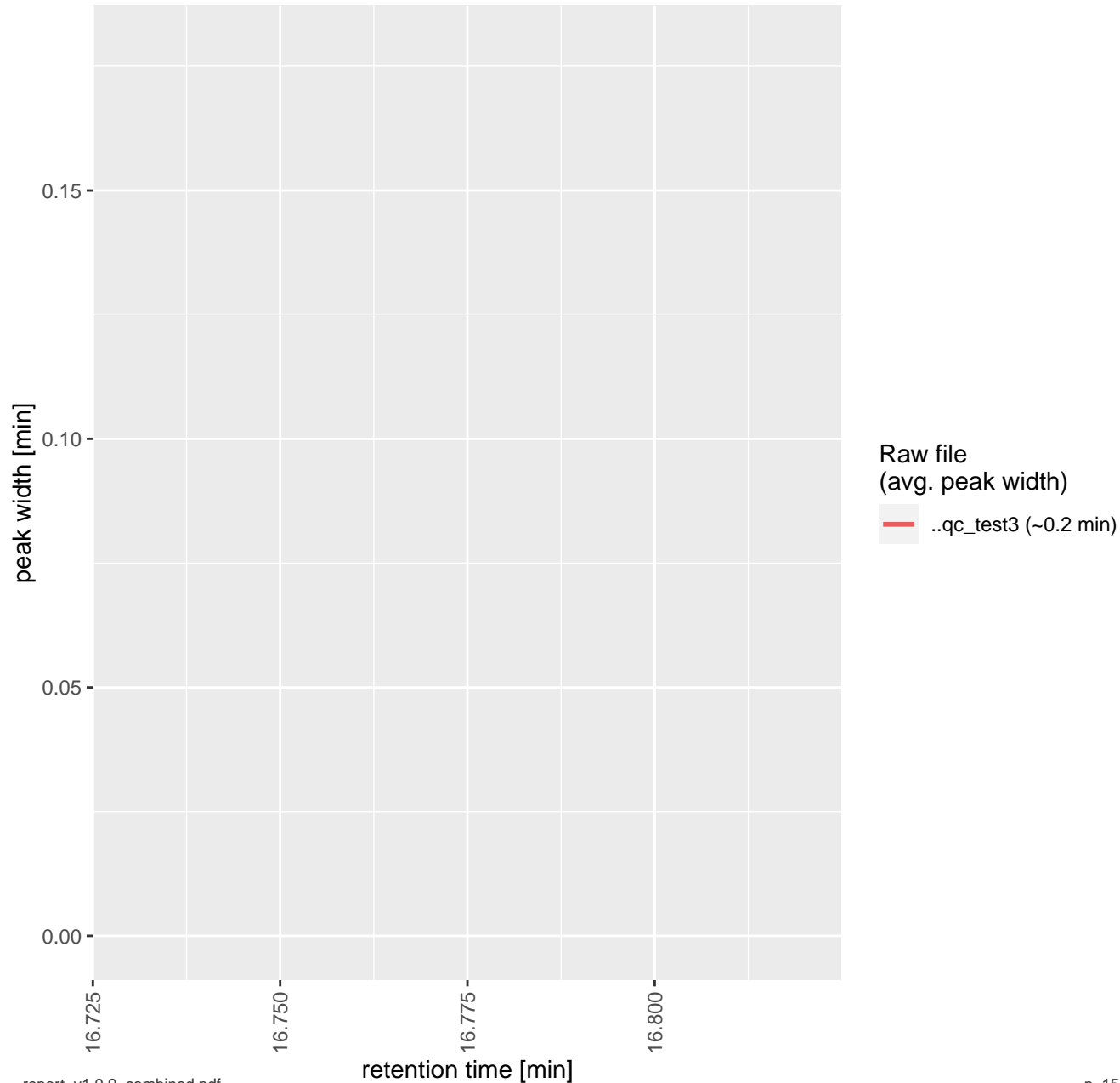
MSMSscans: Ion Injection Time over RT

Raw file with
average inj. time

─●─ ..qc_test3 (~−1 ms)
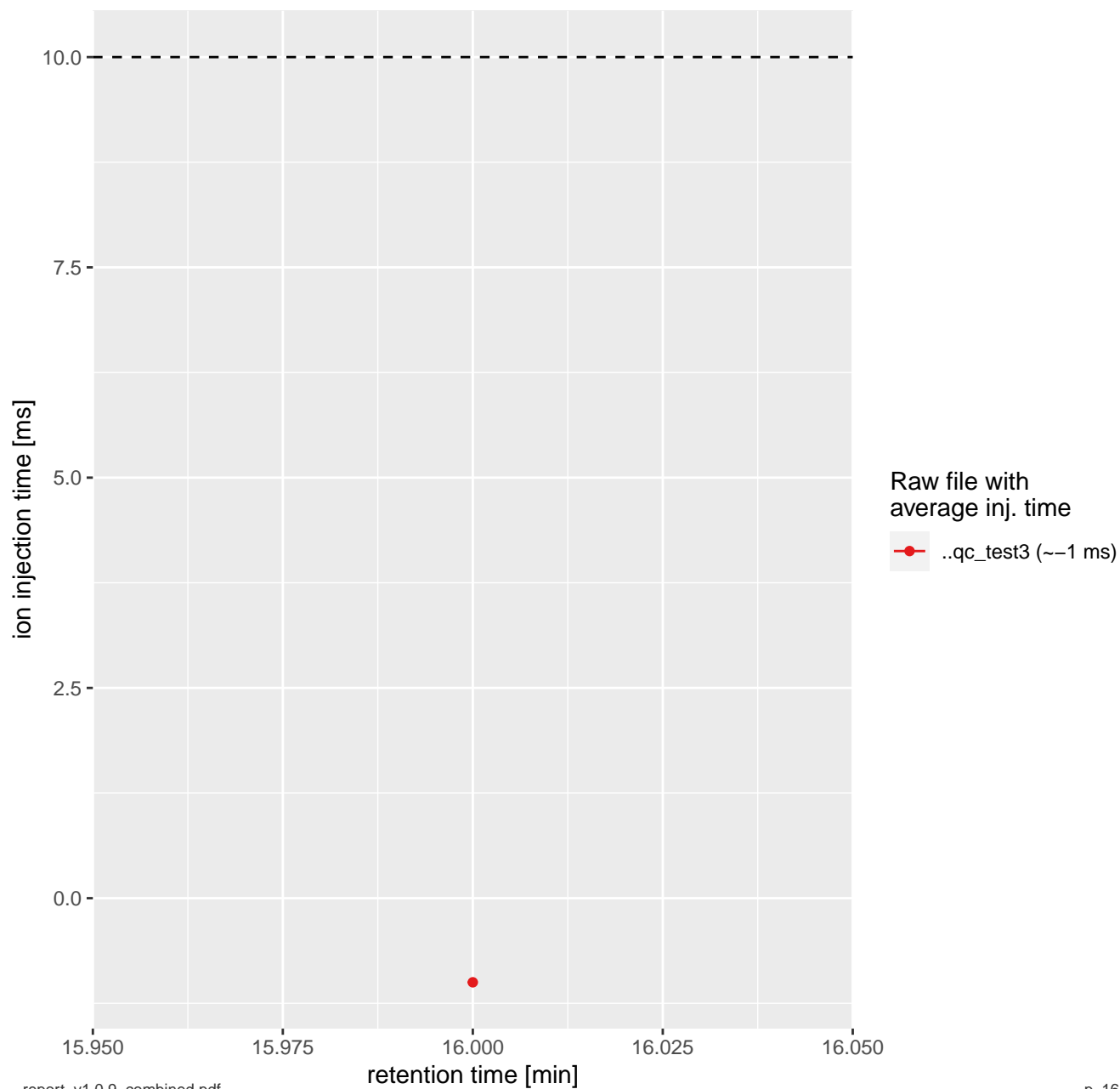
[experimental] MSMSscans: MS/MS intensity

intensity ($\log_{10}$)

MS/MS
intensity

Base
Peak

TIC

..qc_test3
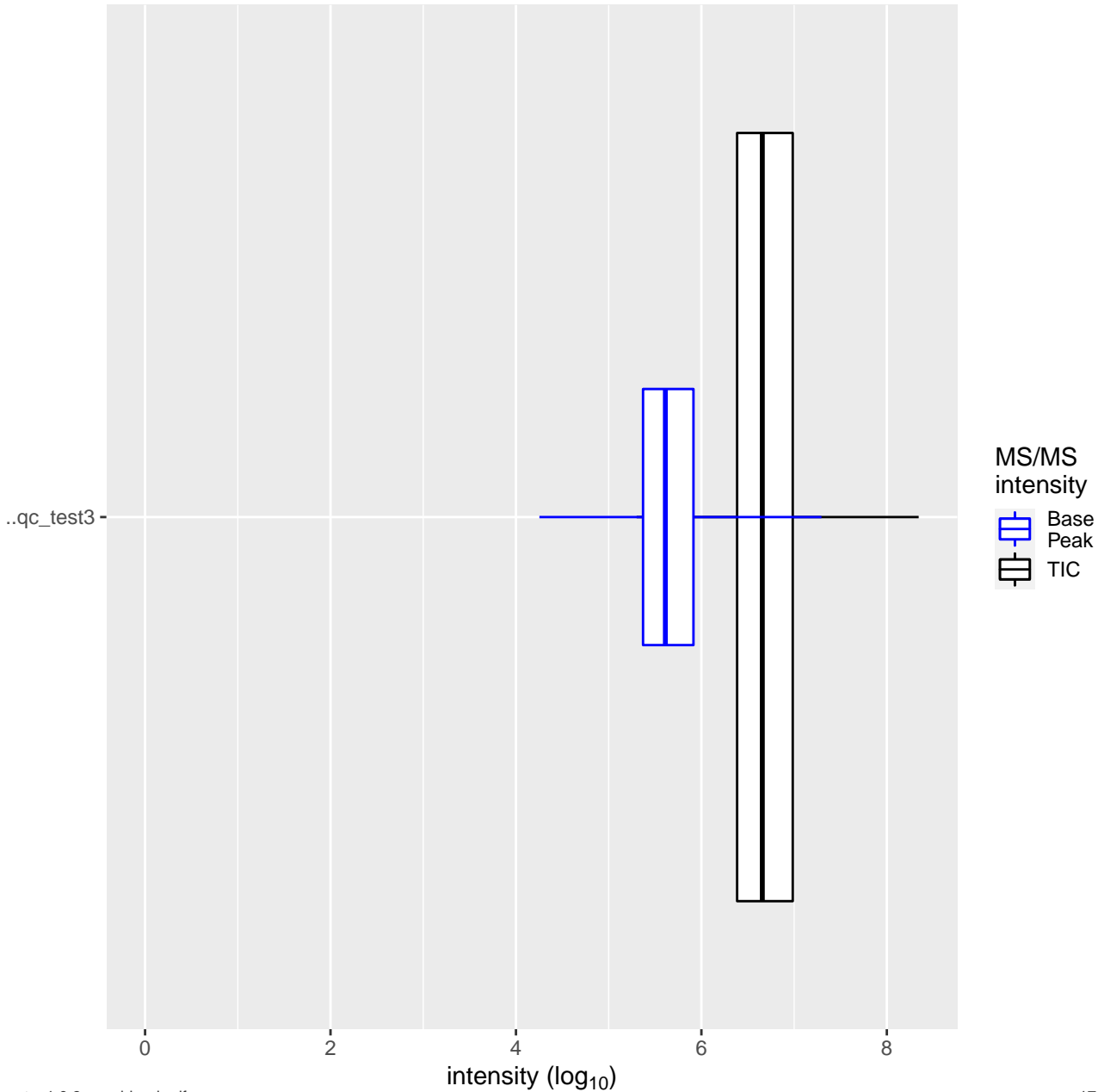
EVD: Oversampling (MS/MS counts per 3D−peak)

..qc_test3

MS/MS counts

1

MS/MS counts per 3D−peak [%]
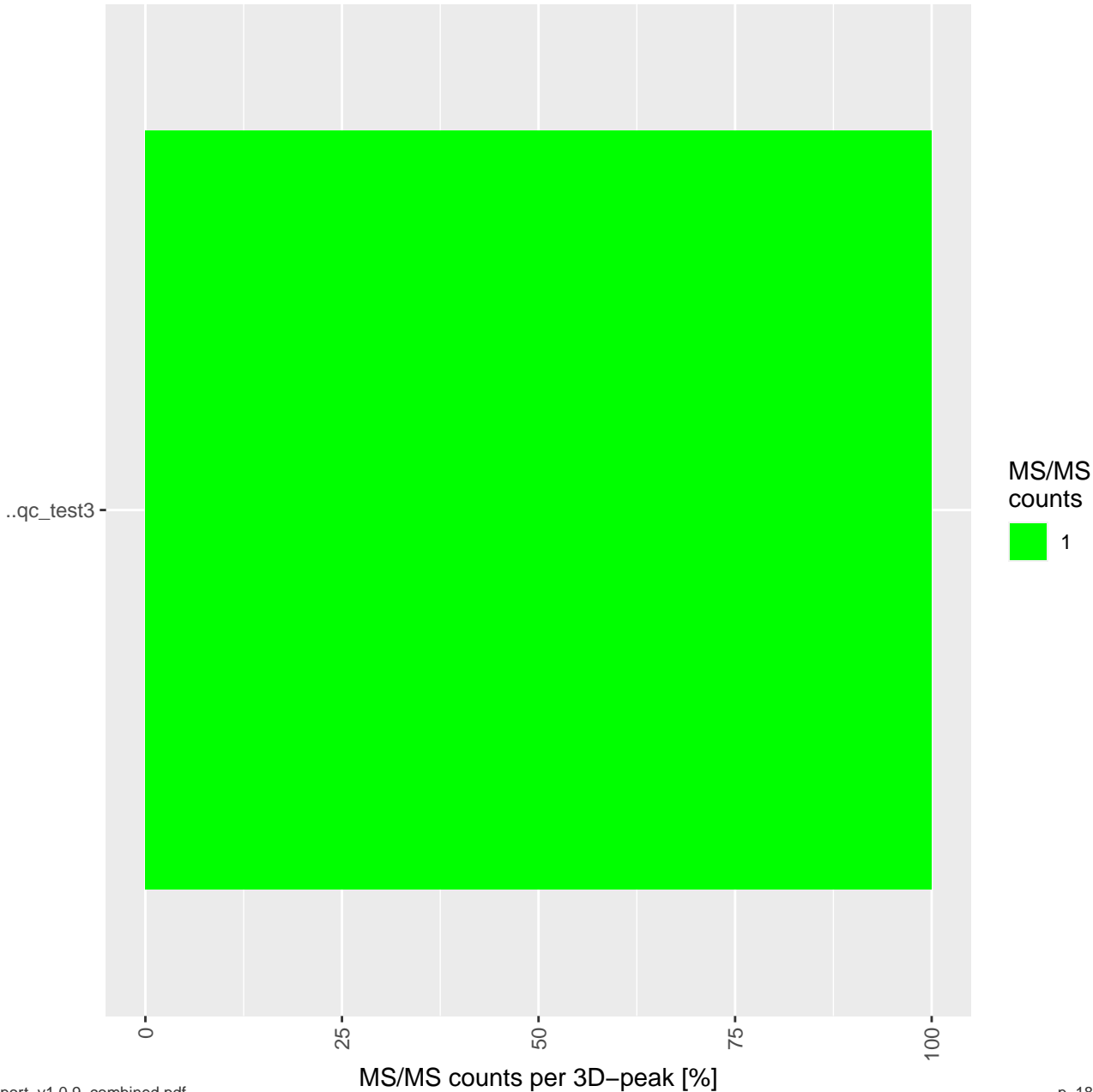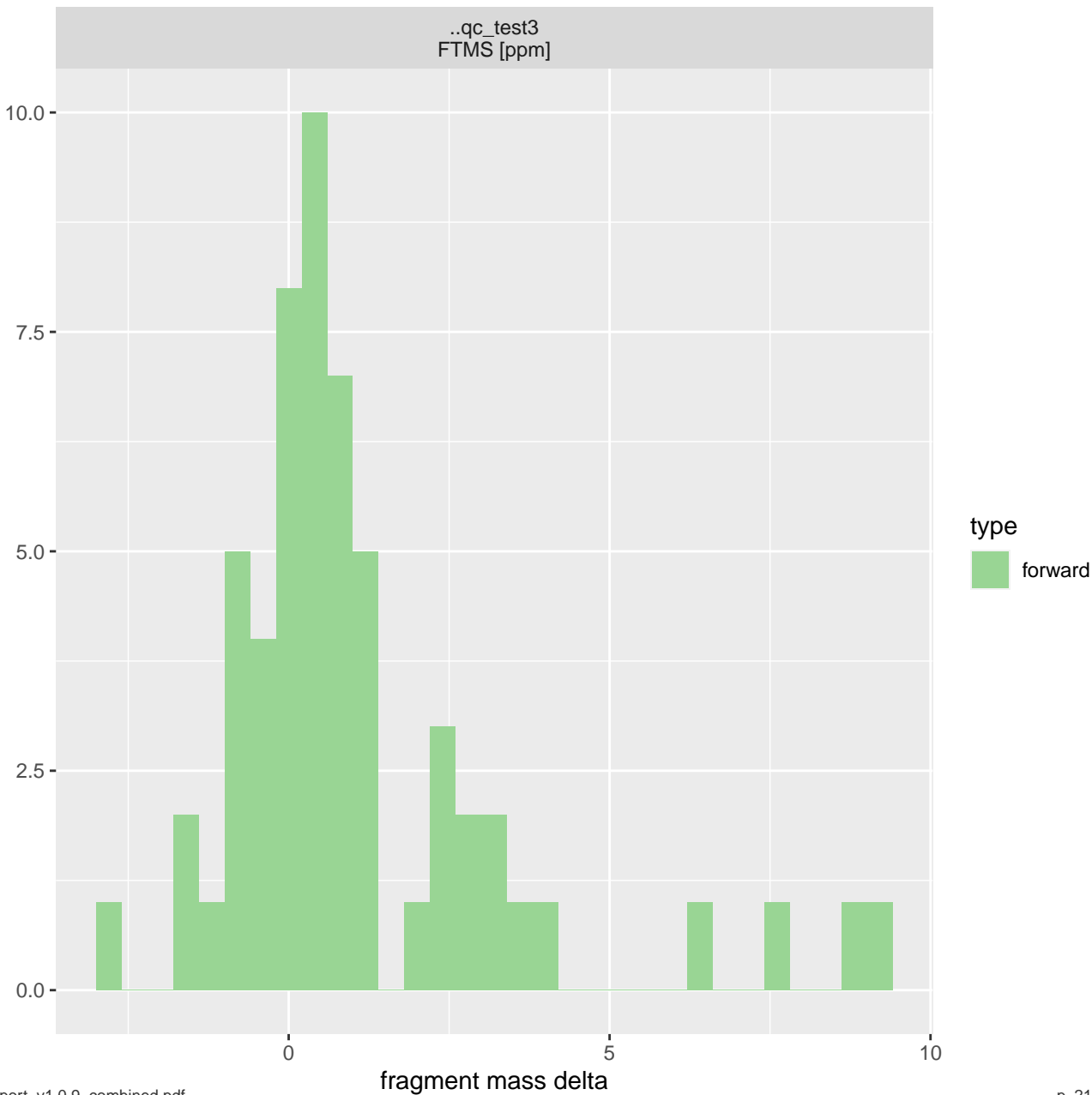
EVD: Uncalibrated mass error
MQ bug: data rescued
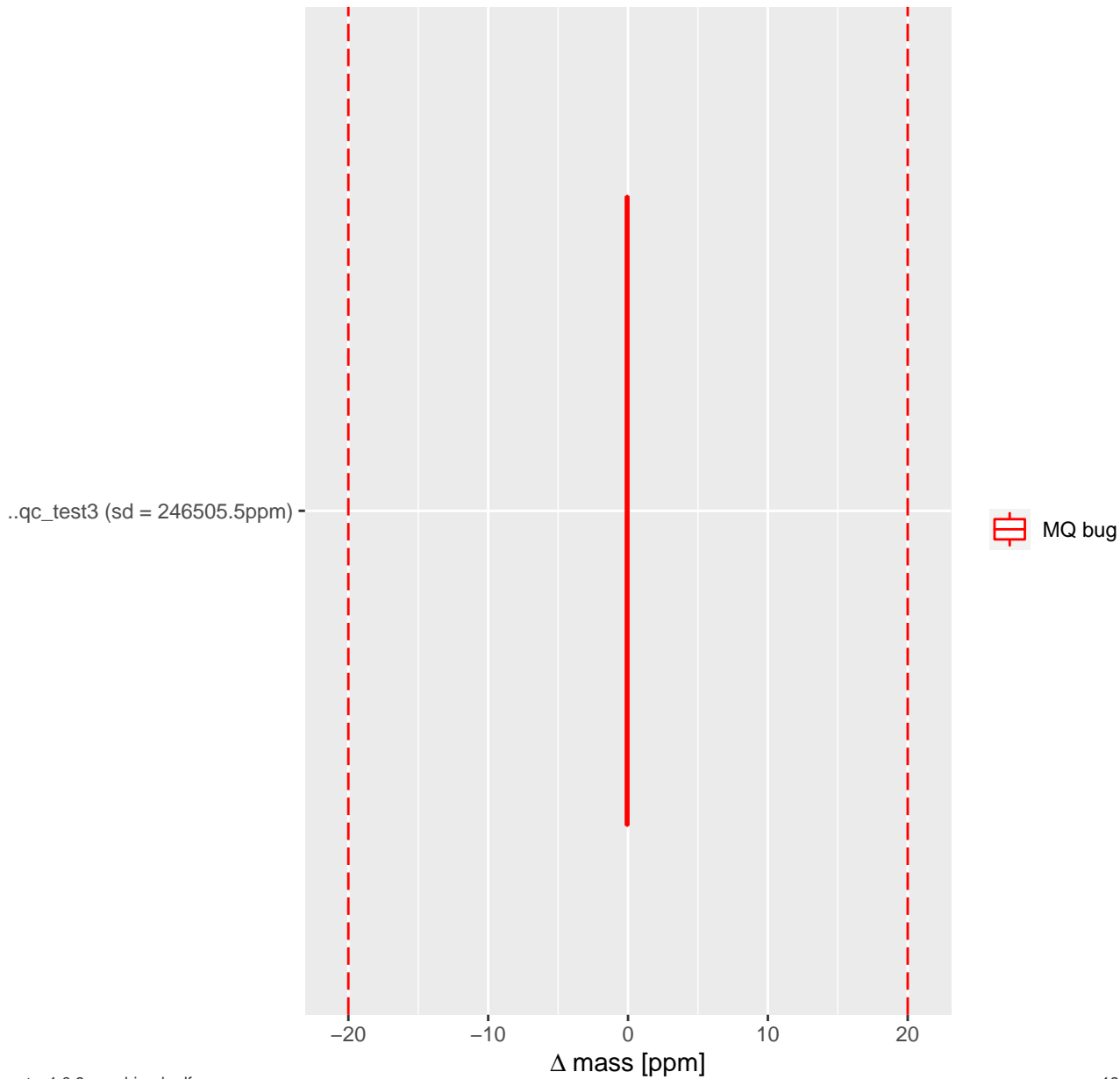
EVD: Calibrated mass error
MQ bug: data cannot be rescued
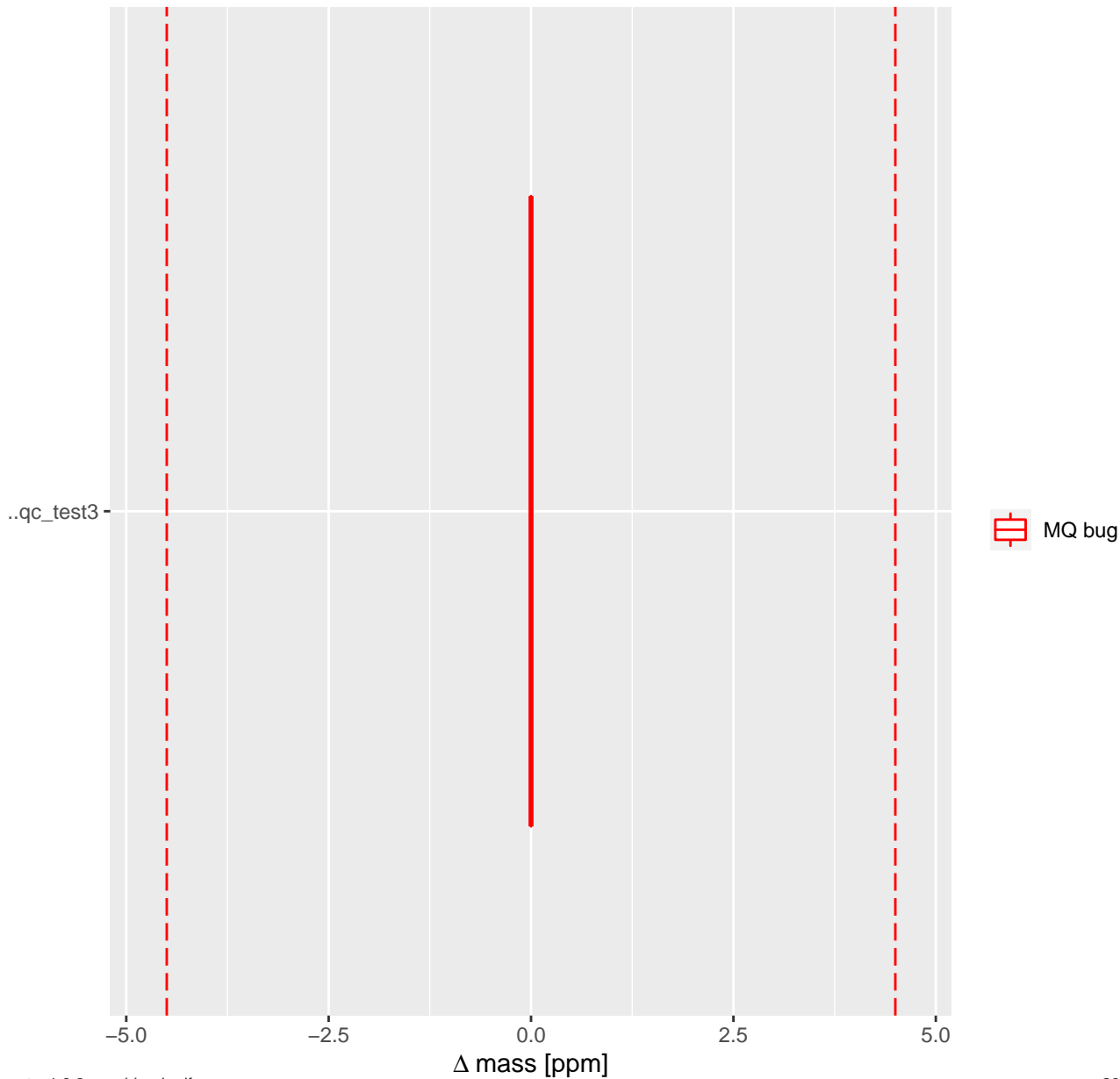
MSMS: Fragment mass errors per Raw file
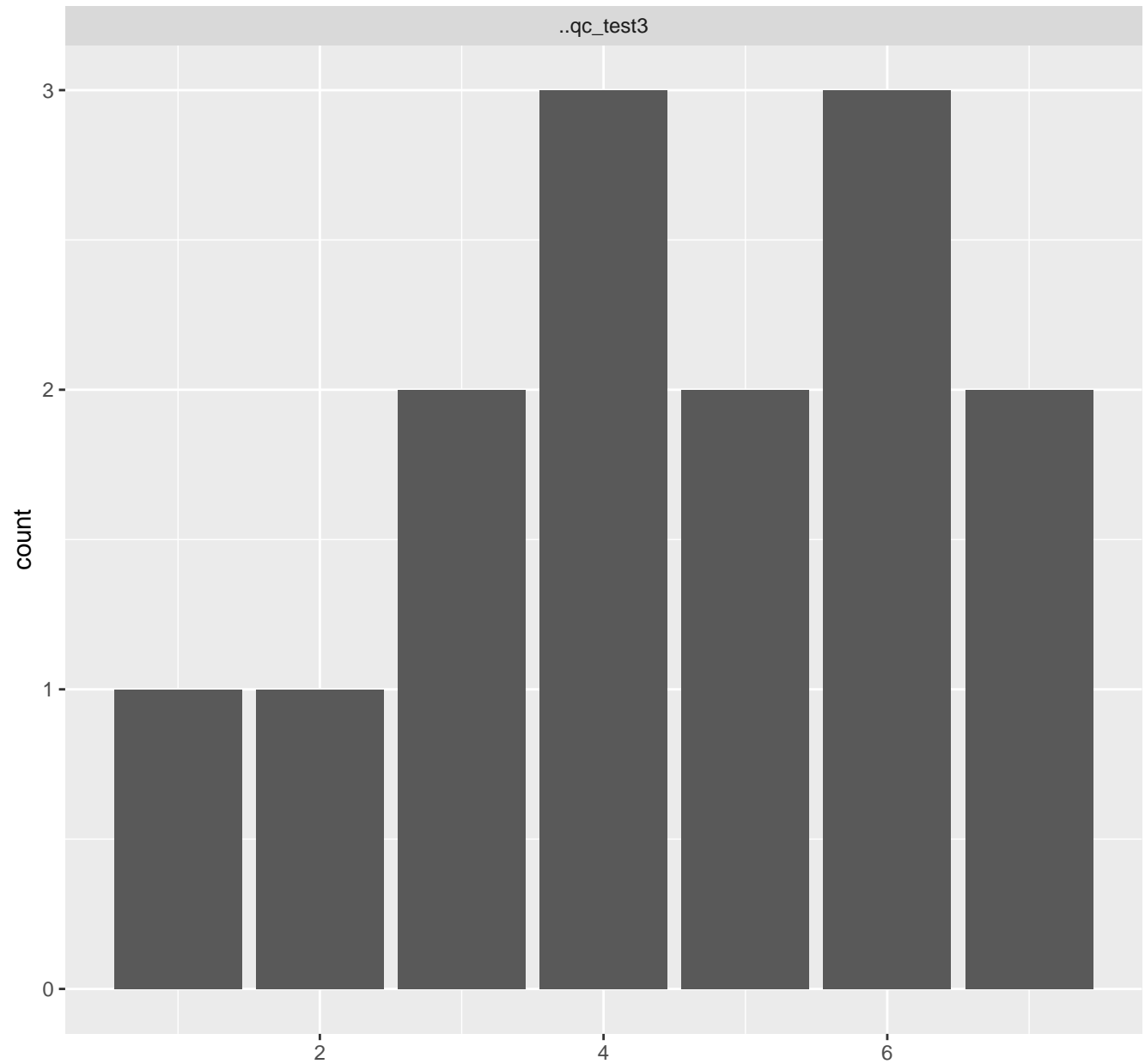
SM: MS/MS identified per Raw file

ID class

● bad (<20%)
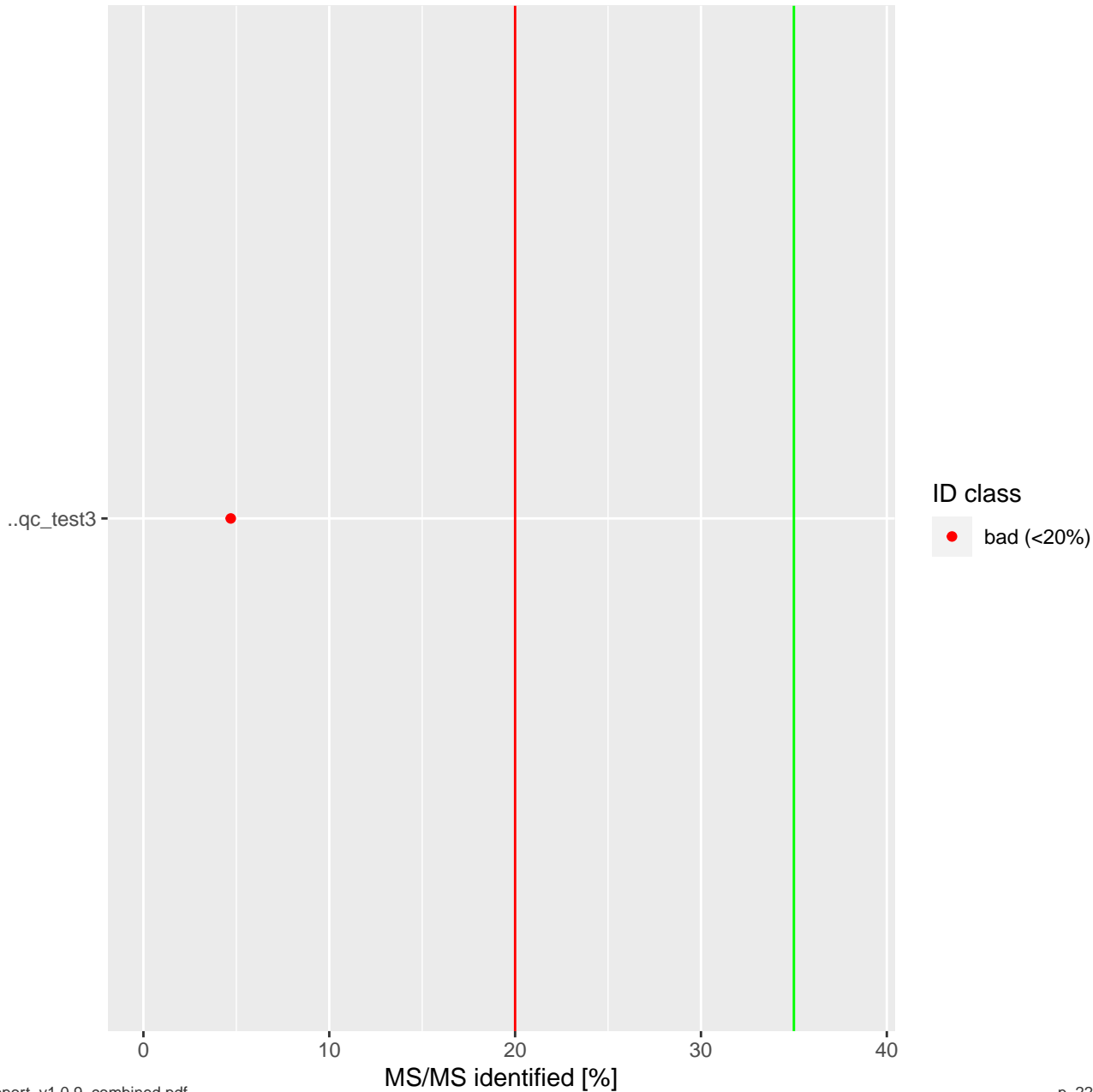
MS/MS identified [%]

SM: Files with 'red' ID rate
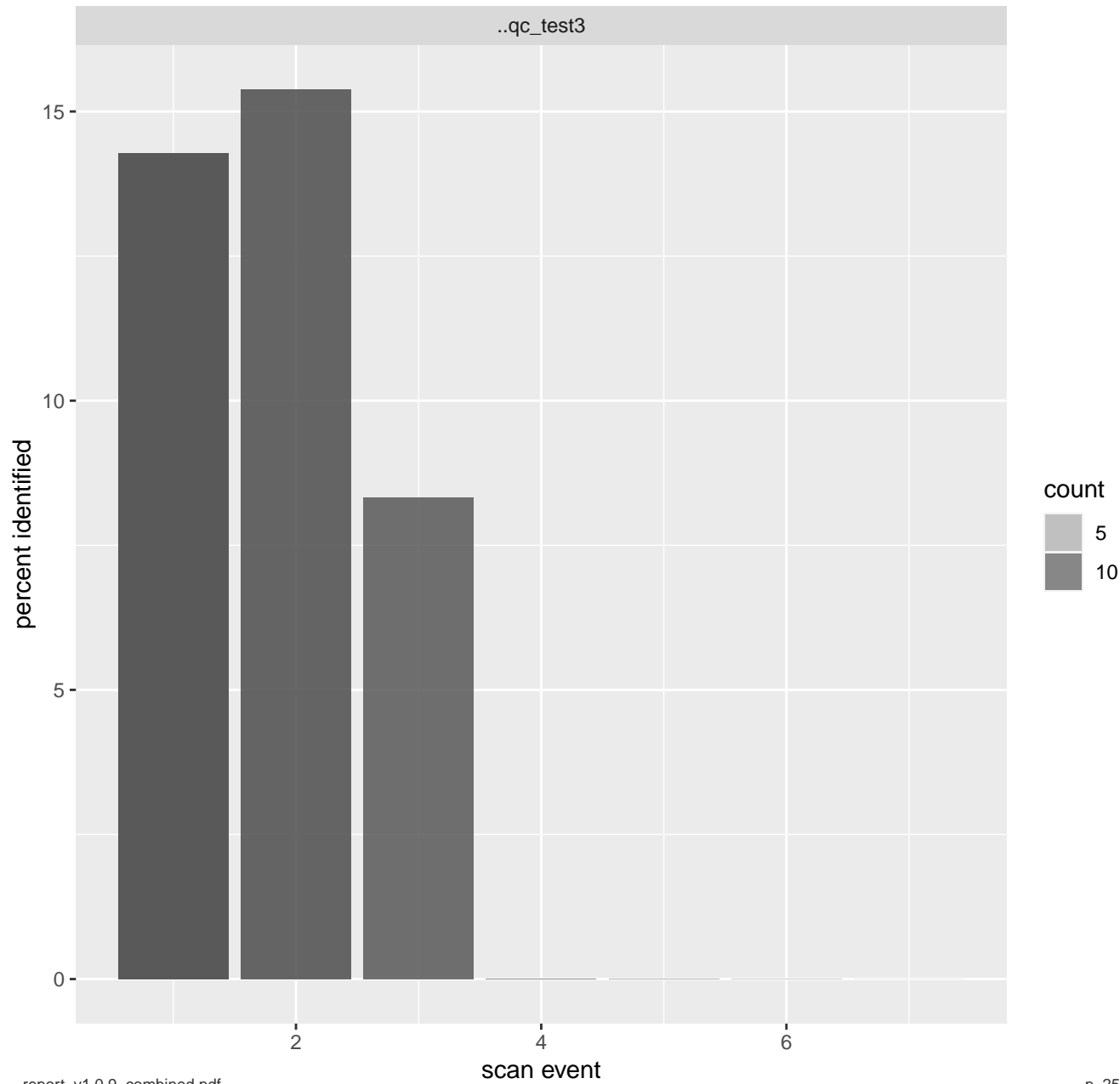
Raw file	% identified
ptxqc_test3	4.7

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
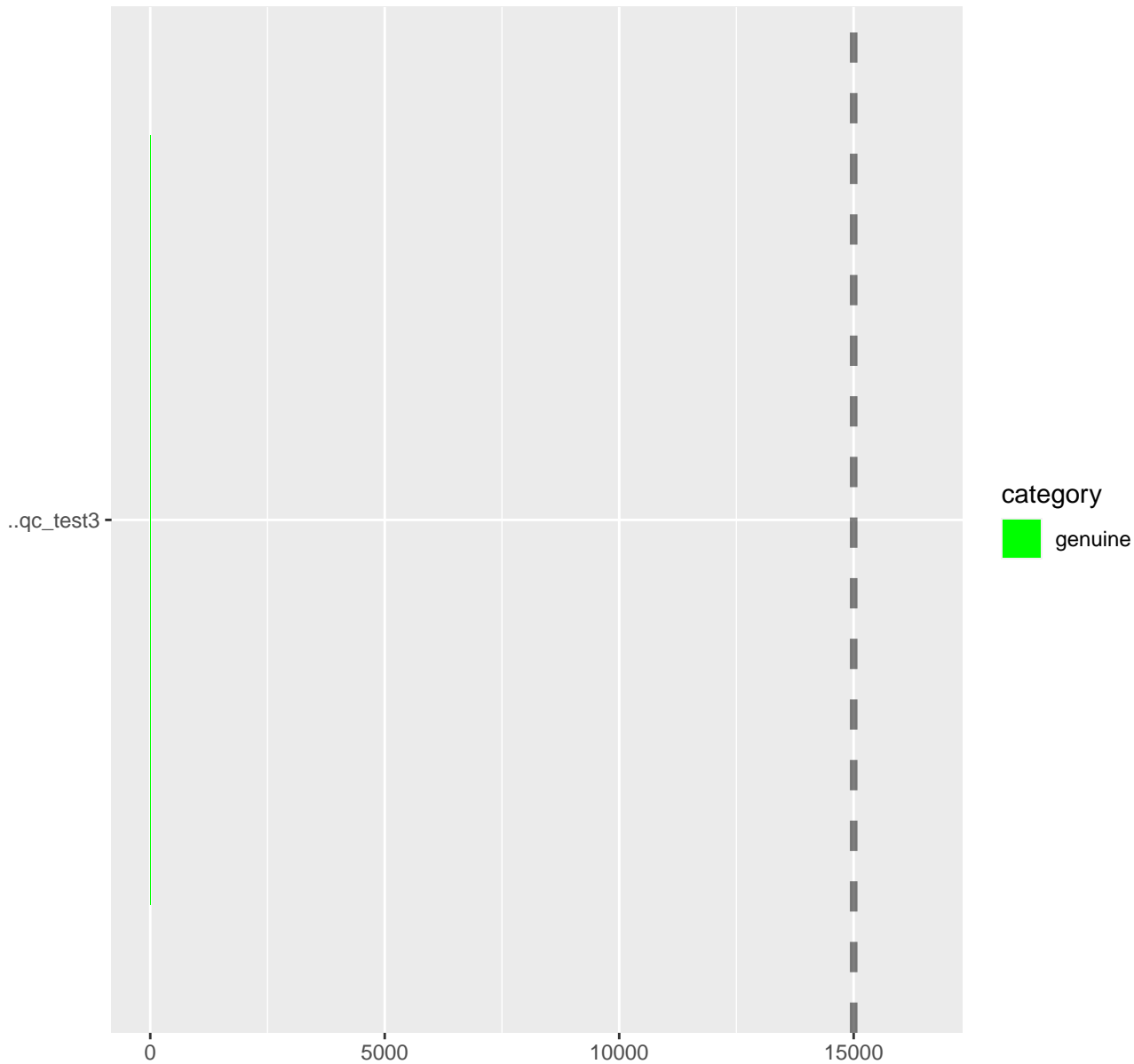
EVD: ProteinGroups count
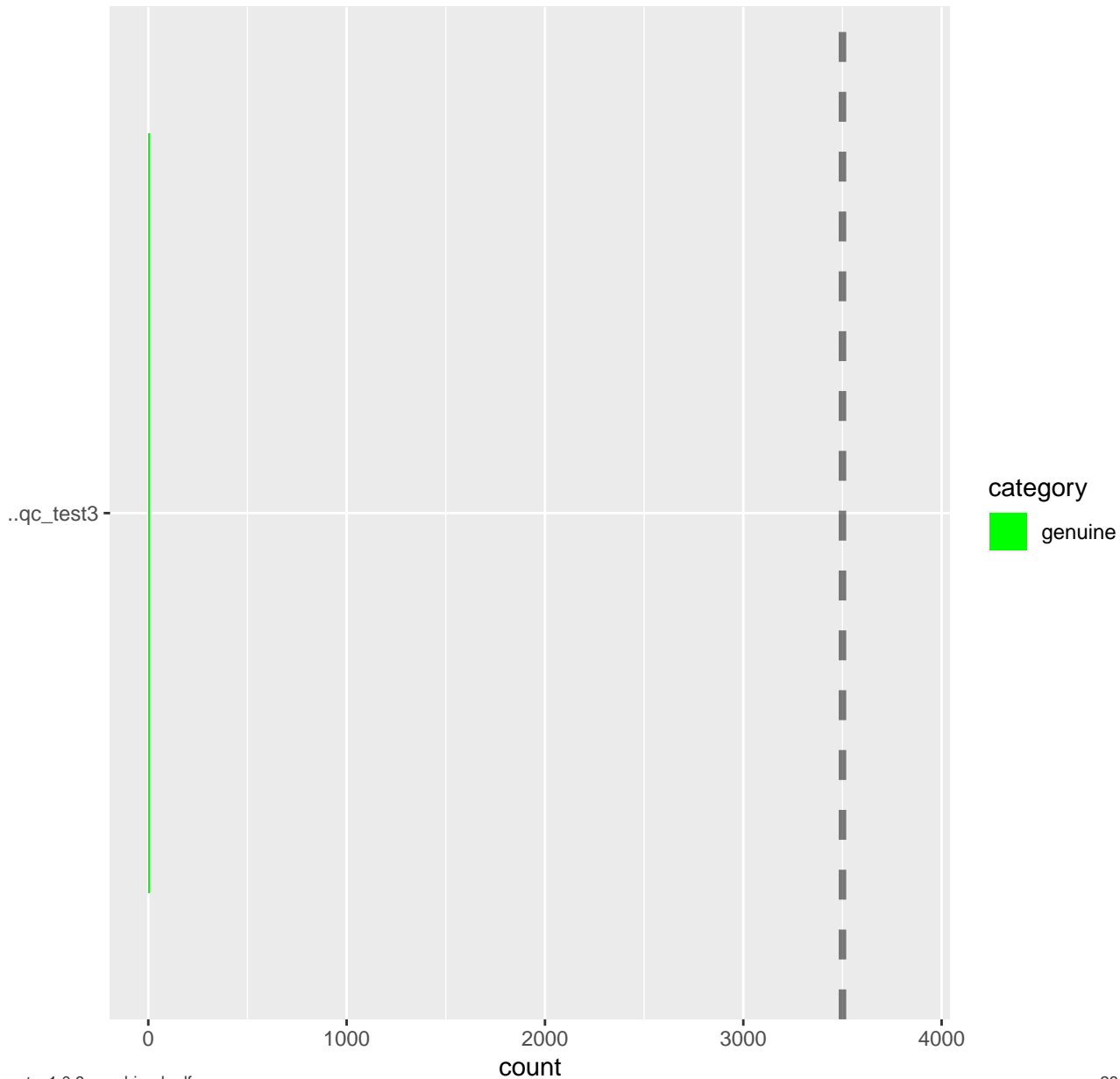
UpSetR

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