# Performance overview



Legend — score:
- best (green)
- under performing (black)
- fail (red)

Columns (x-axis):
EVD : Contaminants [1], EVD : Pep Intensity (>23.0) [2], MSMS : MC [3], MSMS : MC Var [4], EVD : Charge [5], MS²Scans : TopN high [6], MS²Scans : TopN over RT [7], EVD : ID rate over RT [8], EVD : RT Peak Width [9], EVD : MBR Align [10], EVD : MBR ID – Transfer [11], MS²Scans : Ion Inj Time [12], MS²Scans : Intensity [13], EVD : MS² Oversampling [14], EVD : MS Cal – Pre (20) [15], EVD : MS Cal – Post [16], MSMS : MS² Cal (ITMS) [17], SM : MS² ID rate(>35) [18], MS²Scans : TopN ID over N [19], EVD : Pep Missing Values [20], EVD : Pep Count (>15000) [21], EVD : Prot Count (>3500) [22], Average Overall Quality
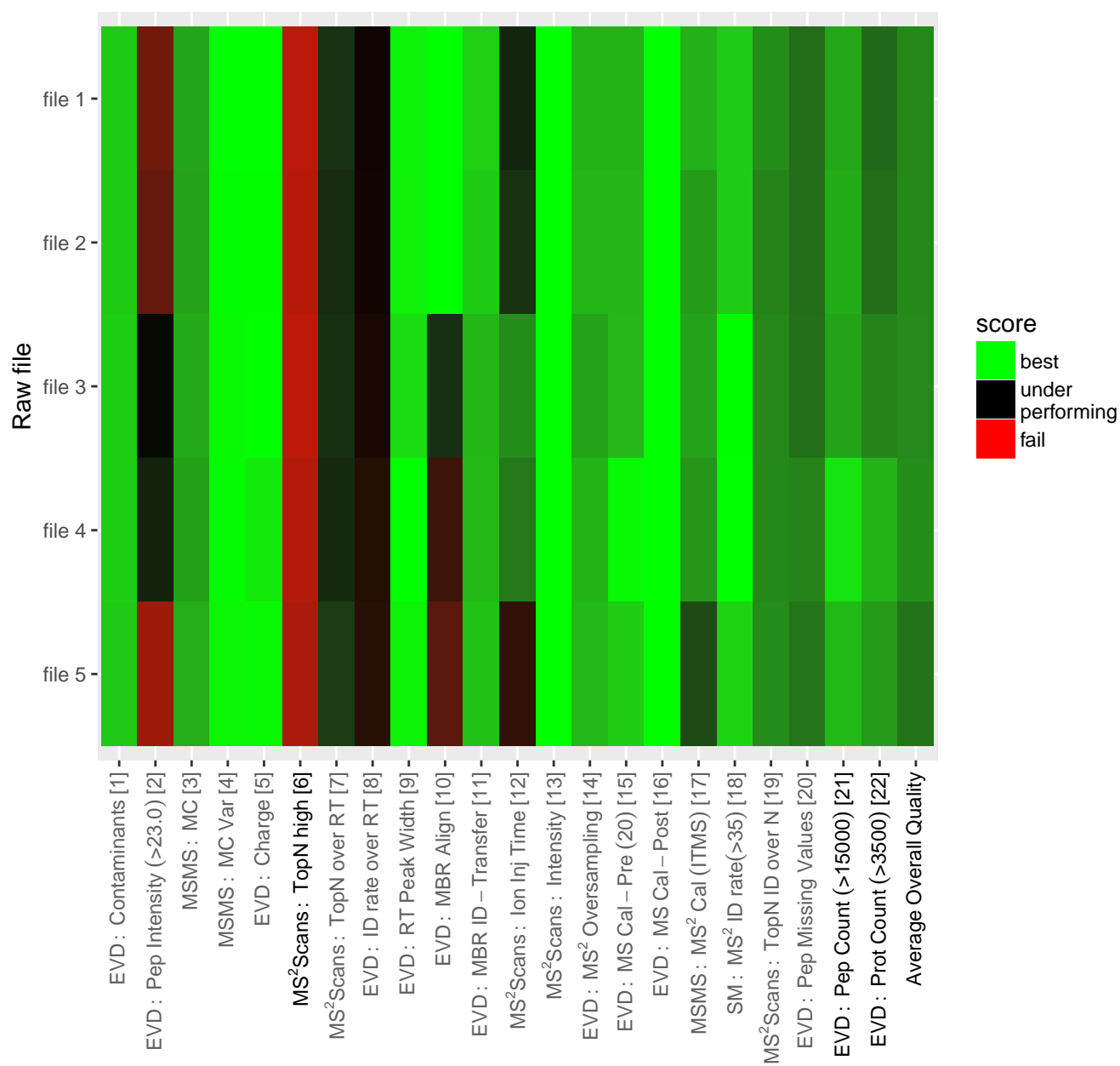
Rows (y-axis, Raw file): file 1, file 2, file 3, file 4, file 5

# Mapping of Raw files to their short names
## Mapping source: automatic
(automatic shortening of names was not sufficient – see 'best effort')

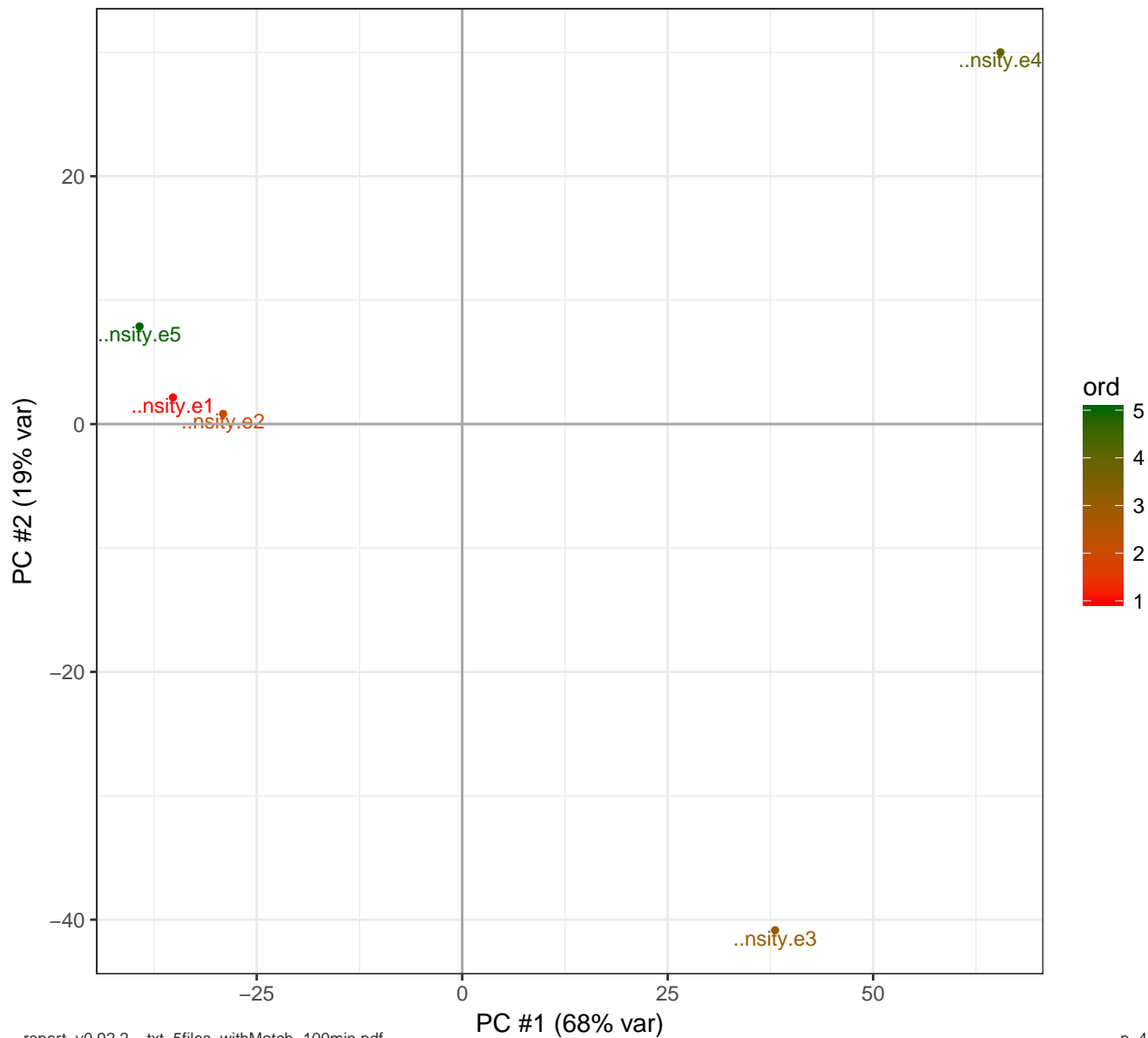| original | short name | best effort |
|---|---|---|
| Toni_20140521_GM_QC_01 | file 1 | ..521_GM_QC_01 |
| Toni_20140521_GM_QC_02 | file 2 | ..521_GM_QC_02 |
| Toni_20140522_GM_QC_01 | file 3 | ..522_GM_QC_01 |
| Toni_20140531_FB_QC_02 | file 4 | ..531_FB_QC_02 |
| Toni_20140608_FB_qc_01 | file 5 | ..608_FB_qc_01 |

# PAR: parameters

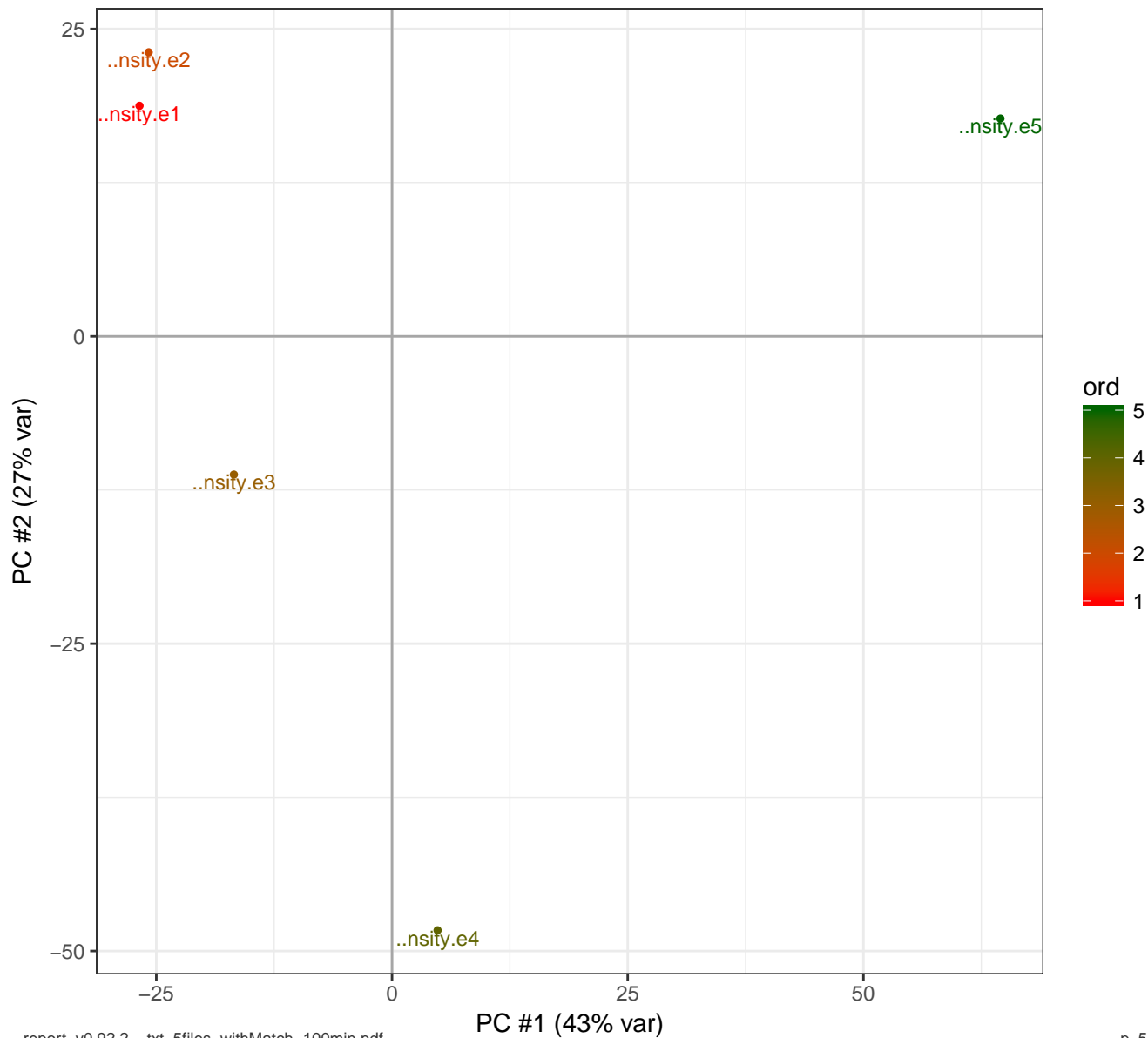| parameter | value | parameter | value |
|---|---|---|---|
| Advanced ratios | False | MS/MS deisotoping (ITMS) | False |
| Alignment time window [min] | 100 | MS/MS deisotoping (TOF) | False |
| Cut peaks | True | MS/MS deisotoping (Unknown) | False |
| Decoy mode | revert | MS/MS recalibration | False |
| 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) | 0.1 Da |
| 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 | True |
| Match between runs | True | RT shift | False |
| Matching time window [min] | 1 | Site FDR | 0.01 |
| Min. delta score for modifie.. | 17 | Site quantification | Use least modified peptide |
| Min. delta score for unmodif.. | 0 | Site tables | Oxidation (M)Sites.txt |
| Min. peptide Length | 7 | Special AAs | KR |
| Min. peptides | 1 | Top MS/MS peaks per 100 Da. .. | 12 |
| Min. ratio count | 2 | Top MS/MS peaks per 100 Da. .. | 8 |
| Min. razor peptides | 1 | Top MS/MS peaks per 100 Da. .. | 10 |
| Min. score for modified pept.. | 40 | Top MS/MS peaks per 100 Da. .. | 10 |
| Min. score for unmodified pe.. | 0 | Use delta score | False |
| Min. unique peptides | 0 | Use Normalized Ratios For Oc.. | True |
| Modifications included in pr.. | Acetyl (Protein N−term) Oxidation (M) | Use only unmodified peptides.. | True |
| MS/MS deisotoping (FTMS) | True | Version | 1.4.1.2 |

uniprot_human_canonical_and_isoforms_20130513.fasta
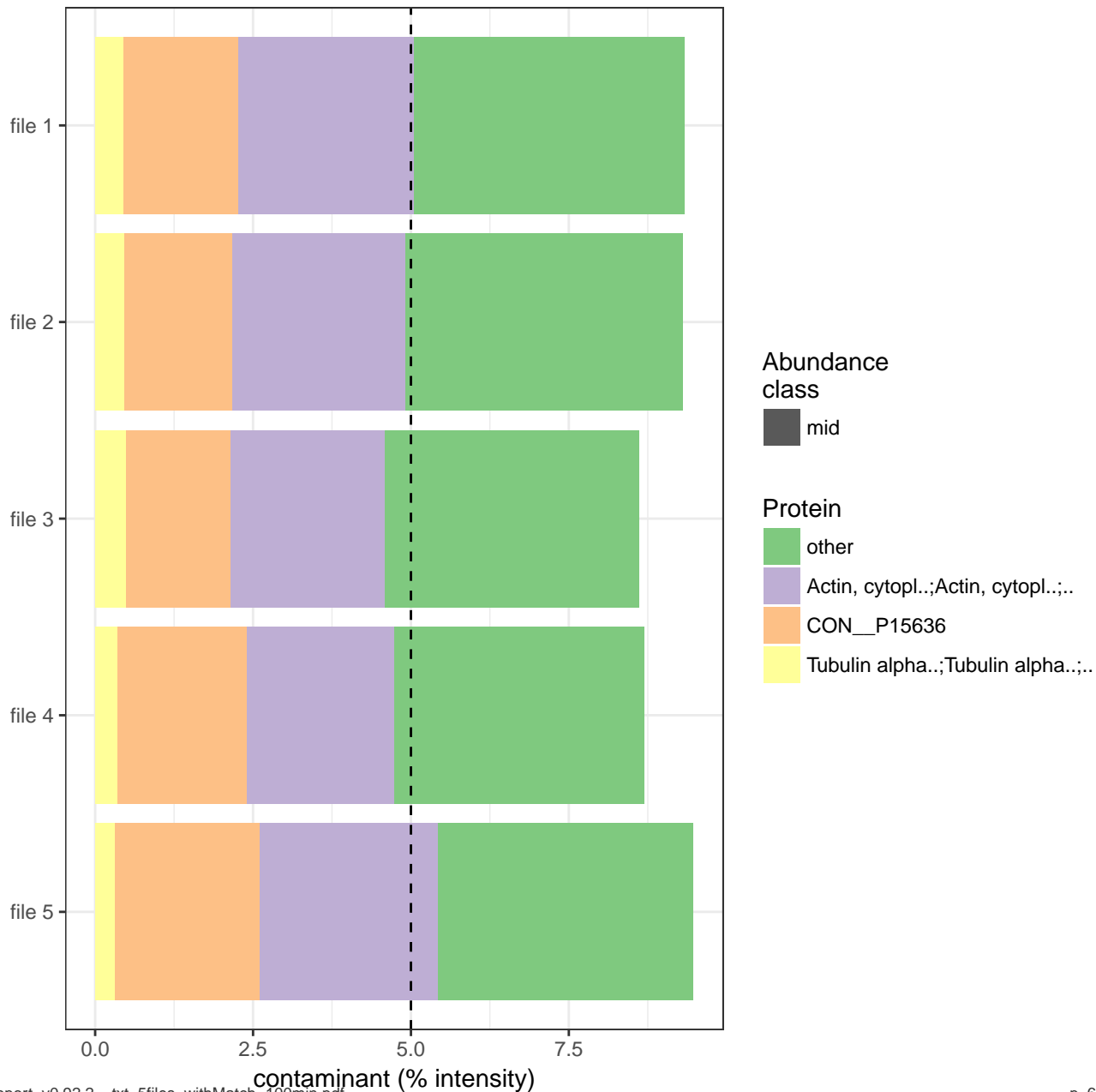
# PG: PCA of 'raw intensity'

(excludes contaminants)

# PG: PCA of 'lfq intensity'

## (excludes contaminants)

# EVD: Top5 Contaminants per Raw file

**Abundance class**
- mid

**Protein**
- other
- Actin, cytopl..;Actin, cytopl..;..
- CON__P15636
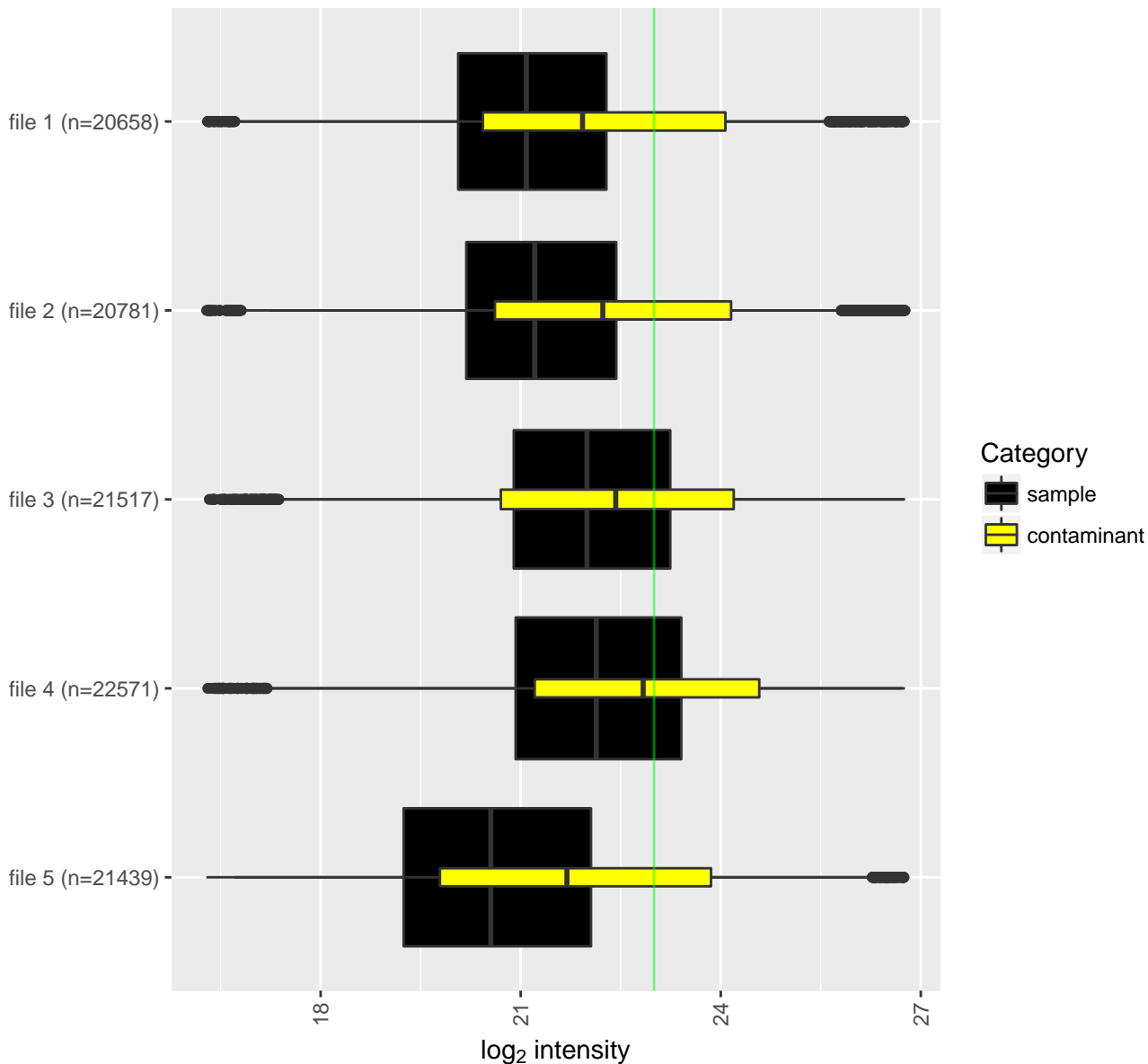- Tubulin alpha..;Tubulin alpha..;..

contaminant (% intensity)

# EVD: Contaminants

Contaminant 'MYCOPLASMA' was not found in any sample.

Did you use the correct database?

# EVD: peptide intensity distribution
### RSD 3.2% (expected < 5%)

file 1 (n=20658)

file 2 (n=20781)

file 3 (n=21517)

file 4 (n=22571)

file 5 (n=21439)

Category

■ sample

▭ contaminant

$\log_2$ intensity

18    21    24    27

PG: intensity distribution
RSD 3% (w/o zero int.; expected < 5%)
RSD 3.2% [high RSD −−> few peptides])
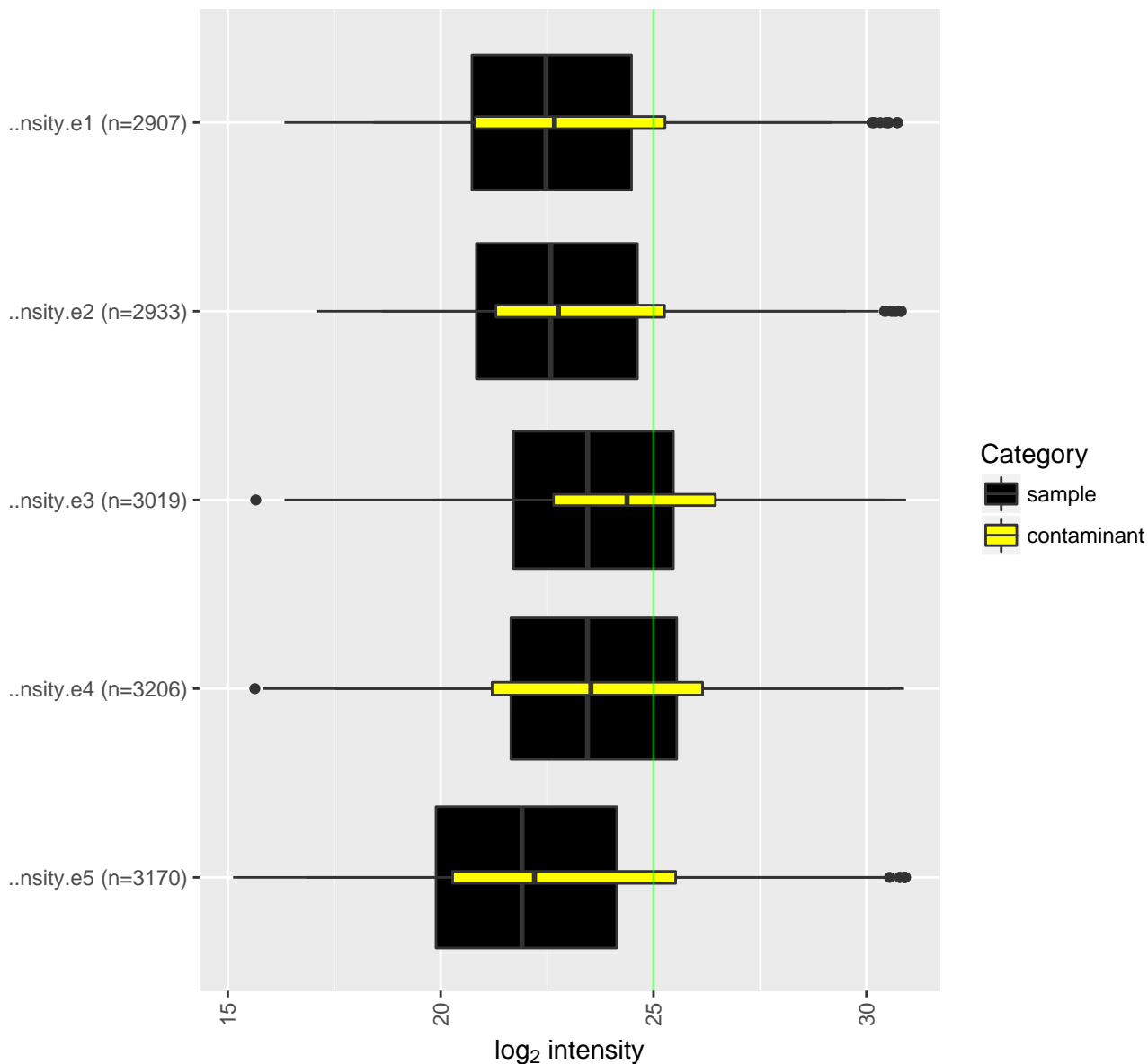
# PG: LFQ intensity distribution
RSD 1.7% (w/o zero int.; expected < 5%)
RSD 0.5% [high RSD ––> few peptides])



Category
- sample
- contaminant
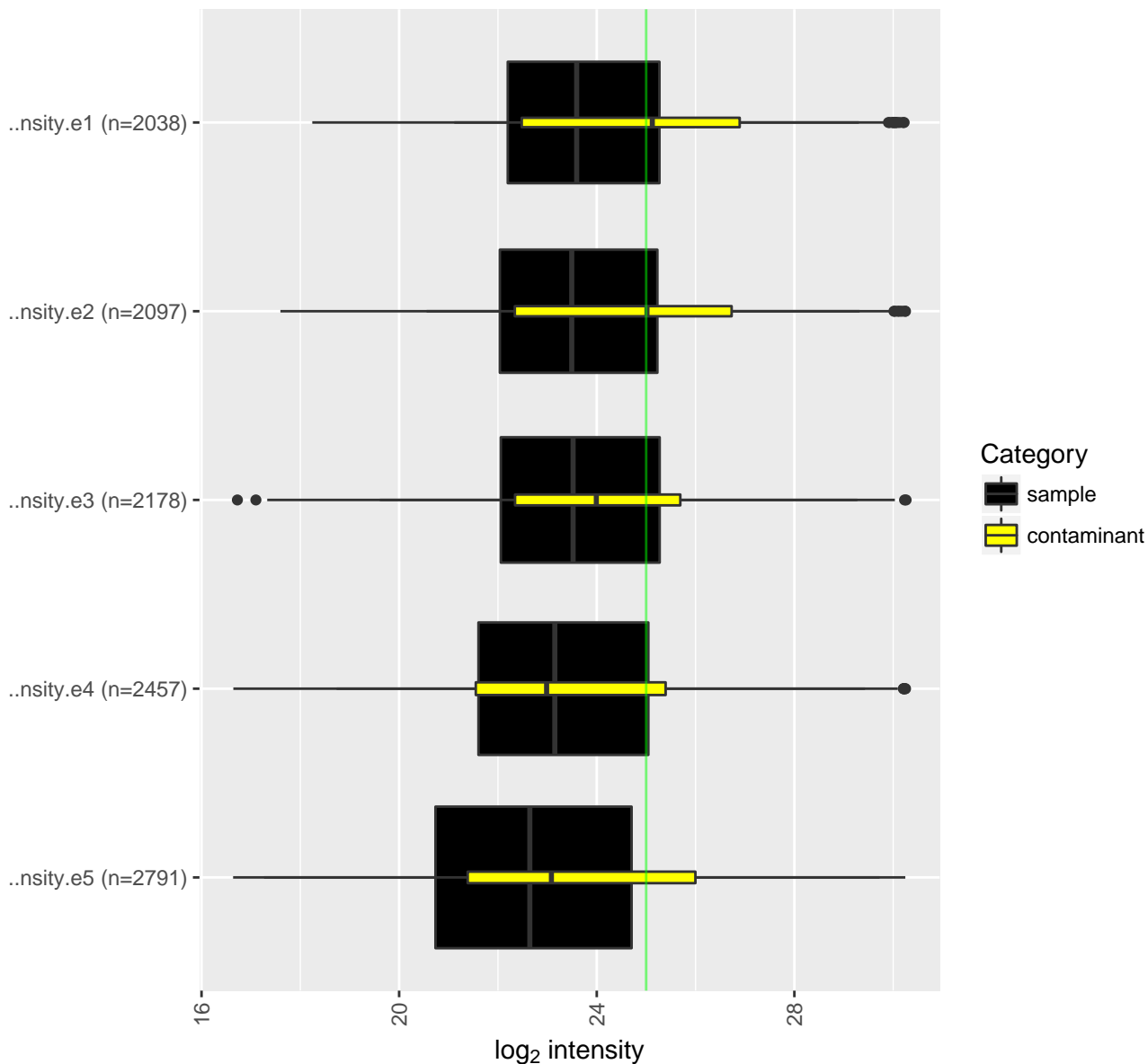
# MSMS: Missed cleavages per Raw file

(excludes contaminants)
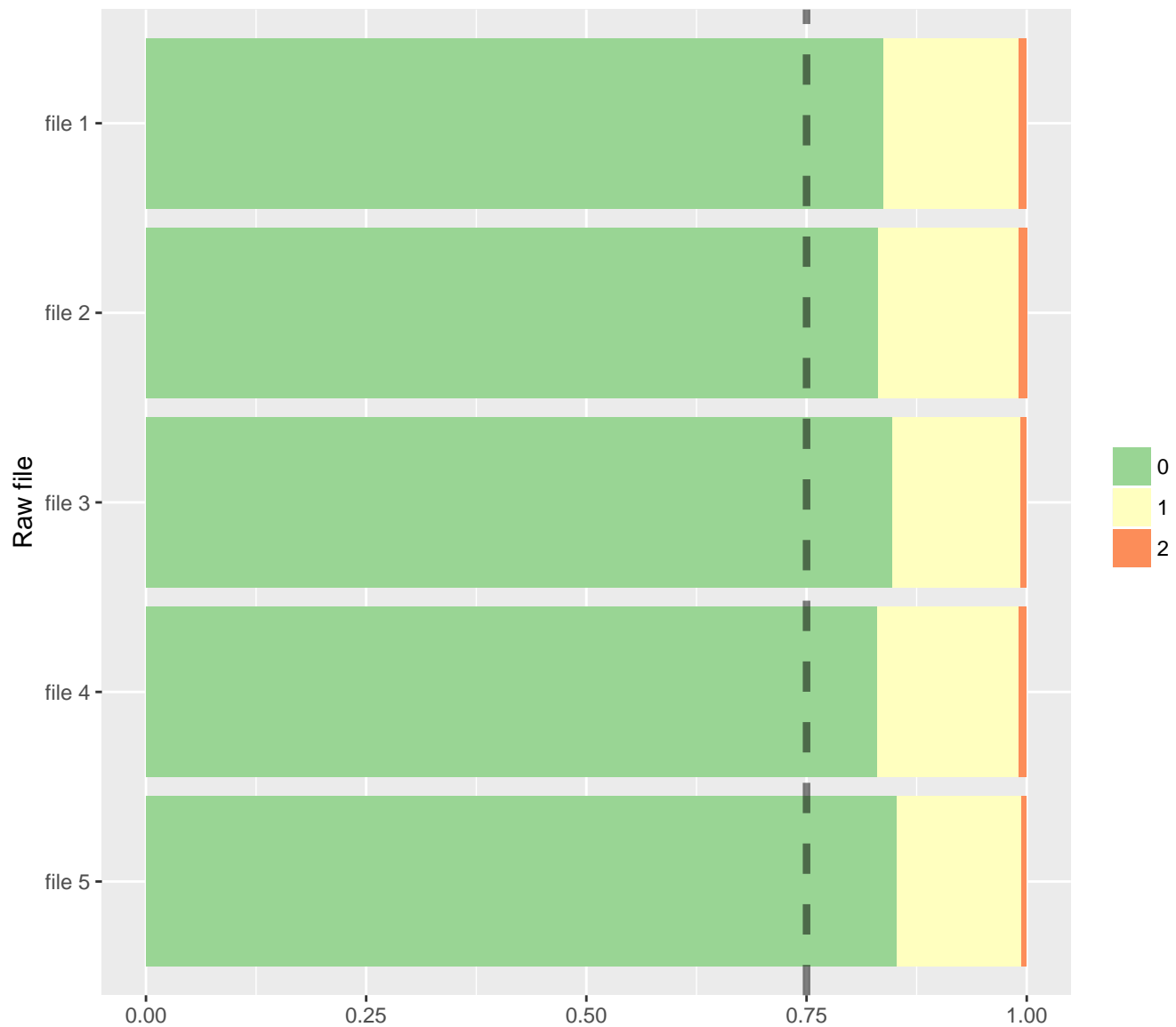
# EVD: charge distribution
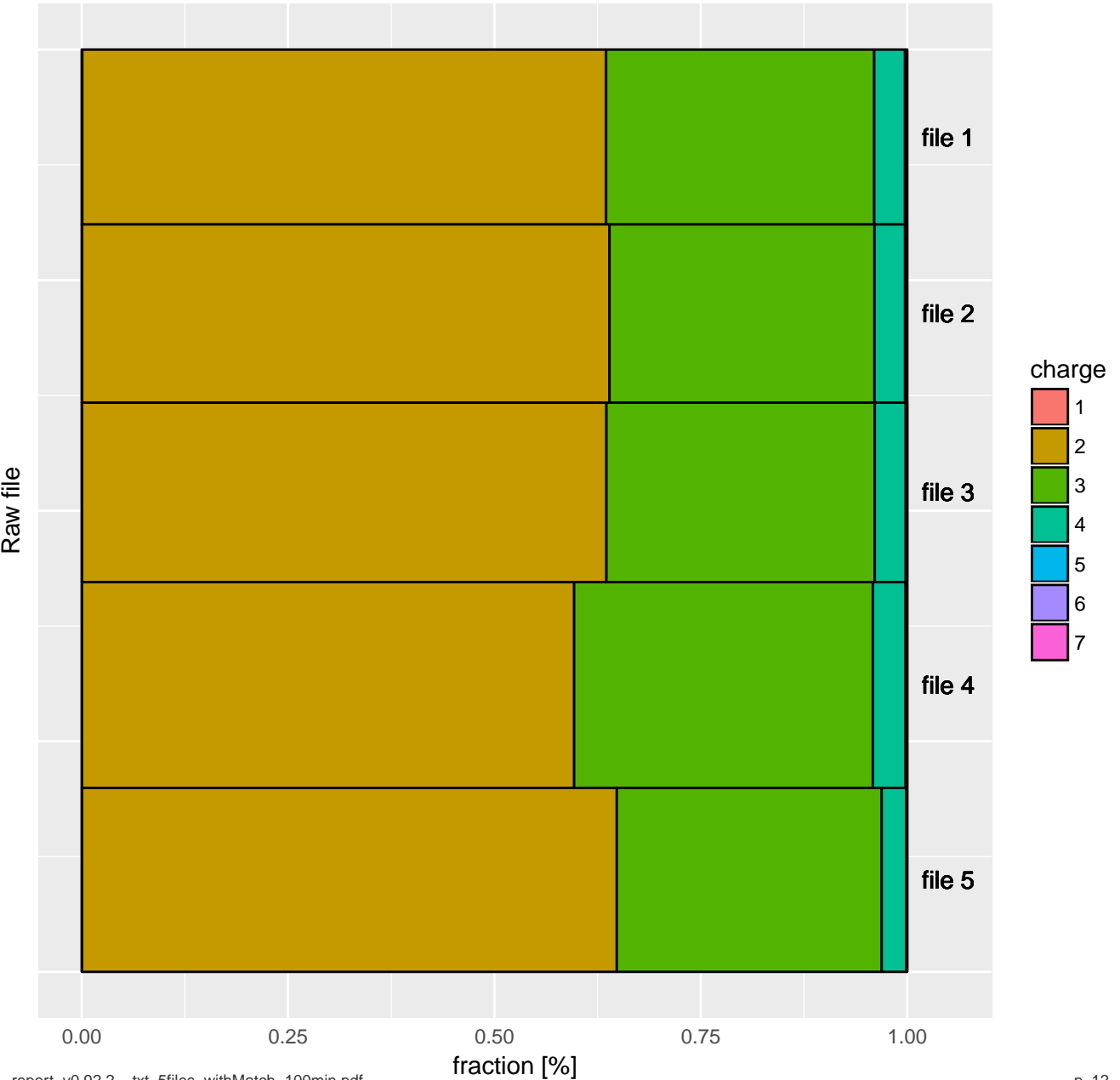
# PG: Contaminant per condition
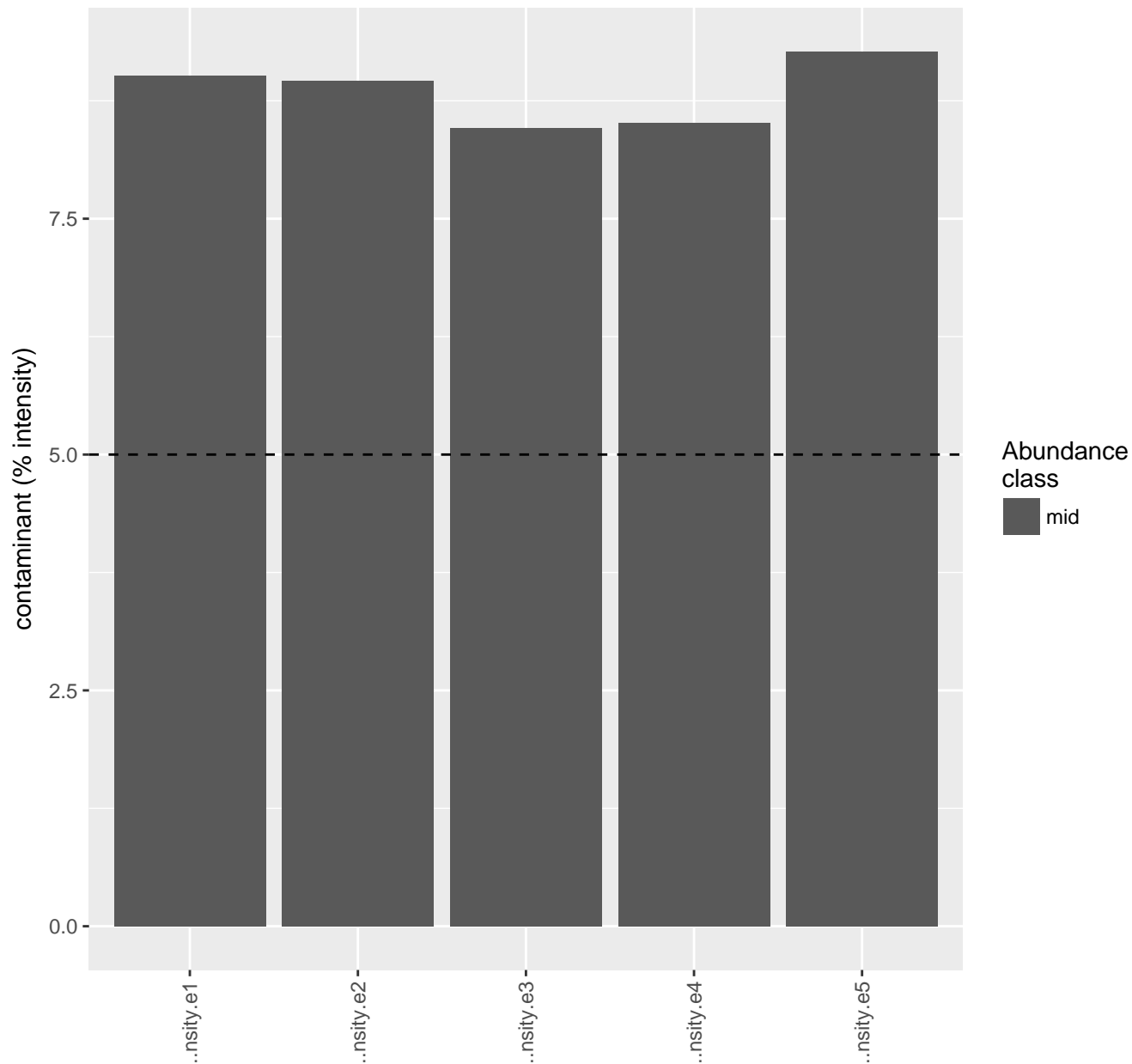
# MSMSscans: TopN

# MSMSscans: TopN over RT



Figure axes: retention time [min] (x-axis), highest N [median per RT bin] (y-axis)

Legend: file 1, file 2, file 3, file 4, file 5
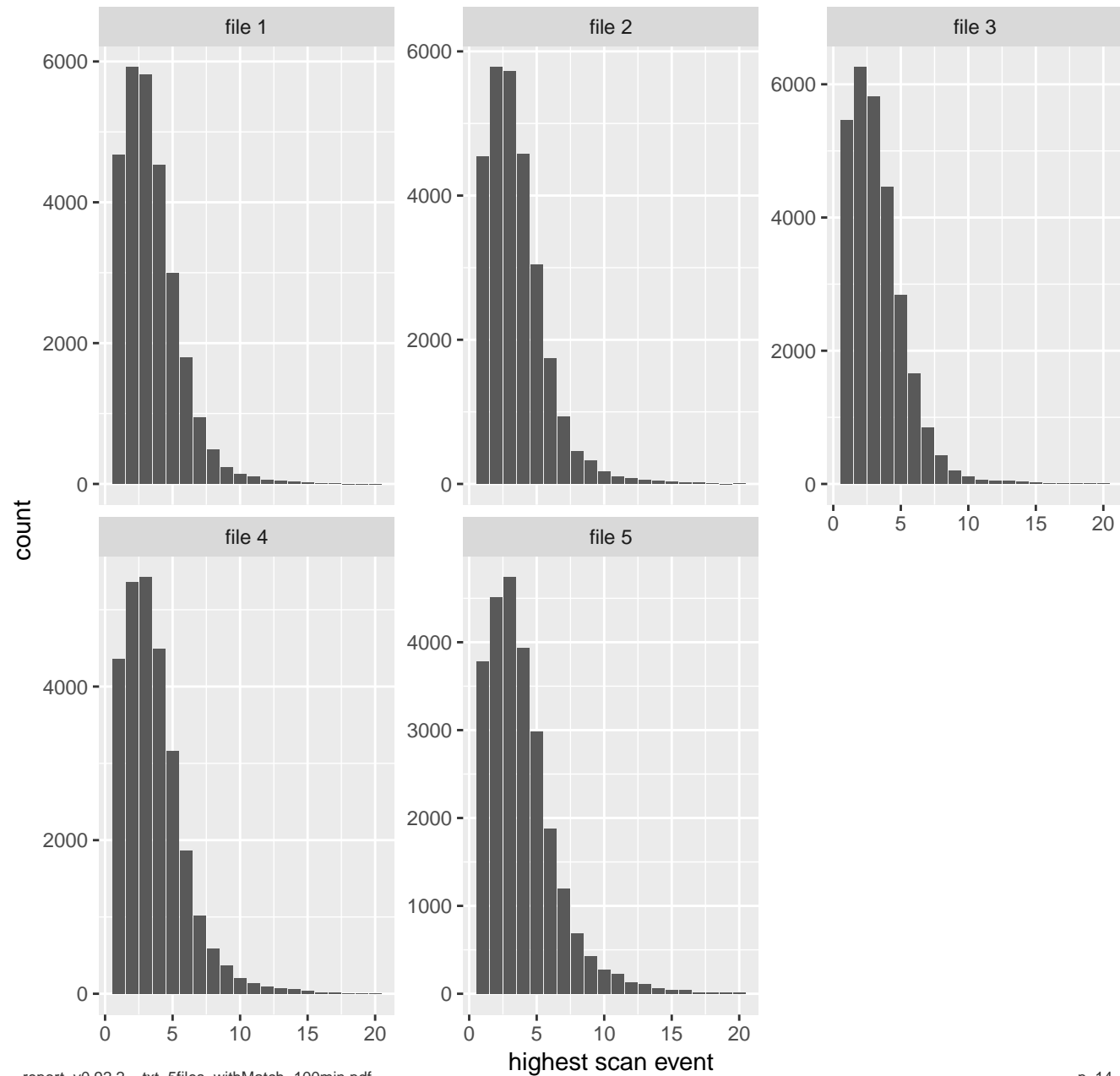
# EVD: IDs over RT



Raw file
— file 1
— file 2
— file 3
-- file 4
— file 5
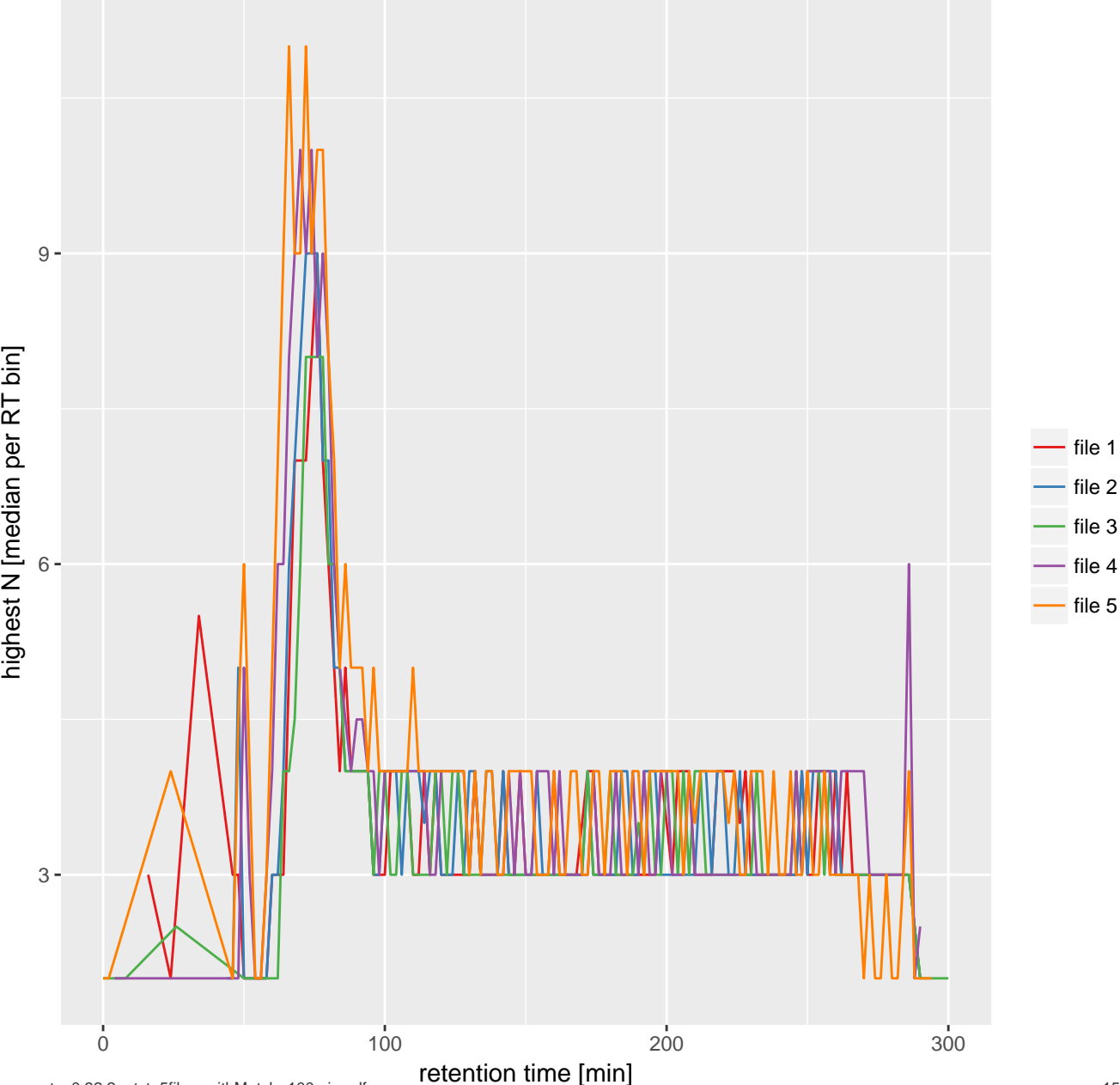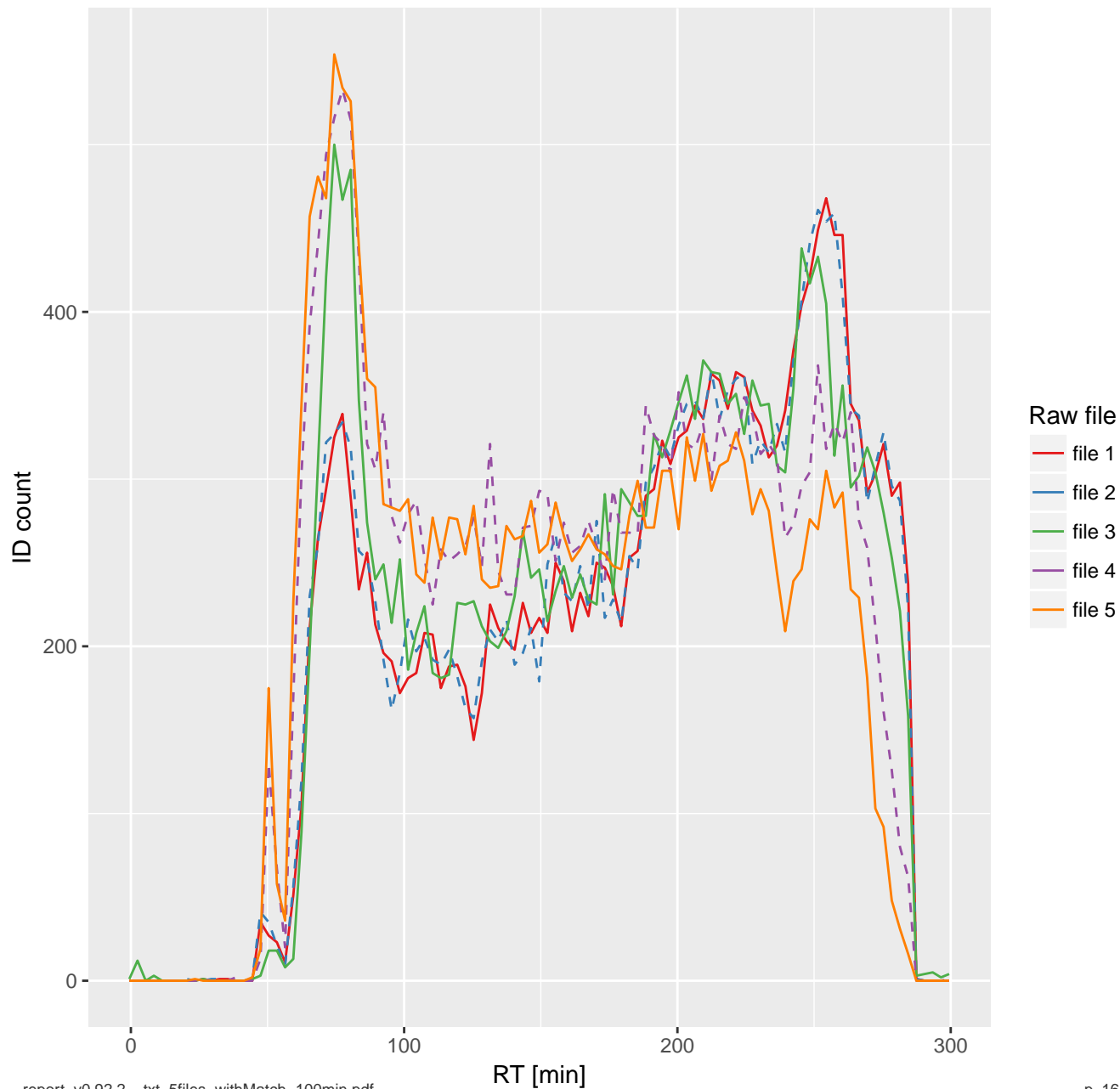
# EVD: Peak width over RT
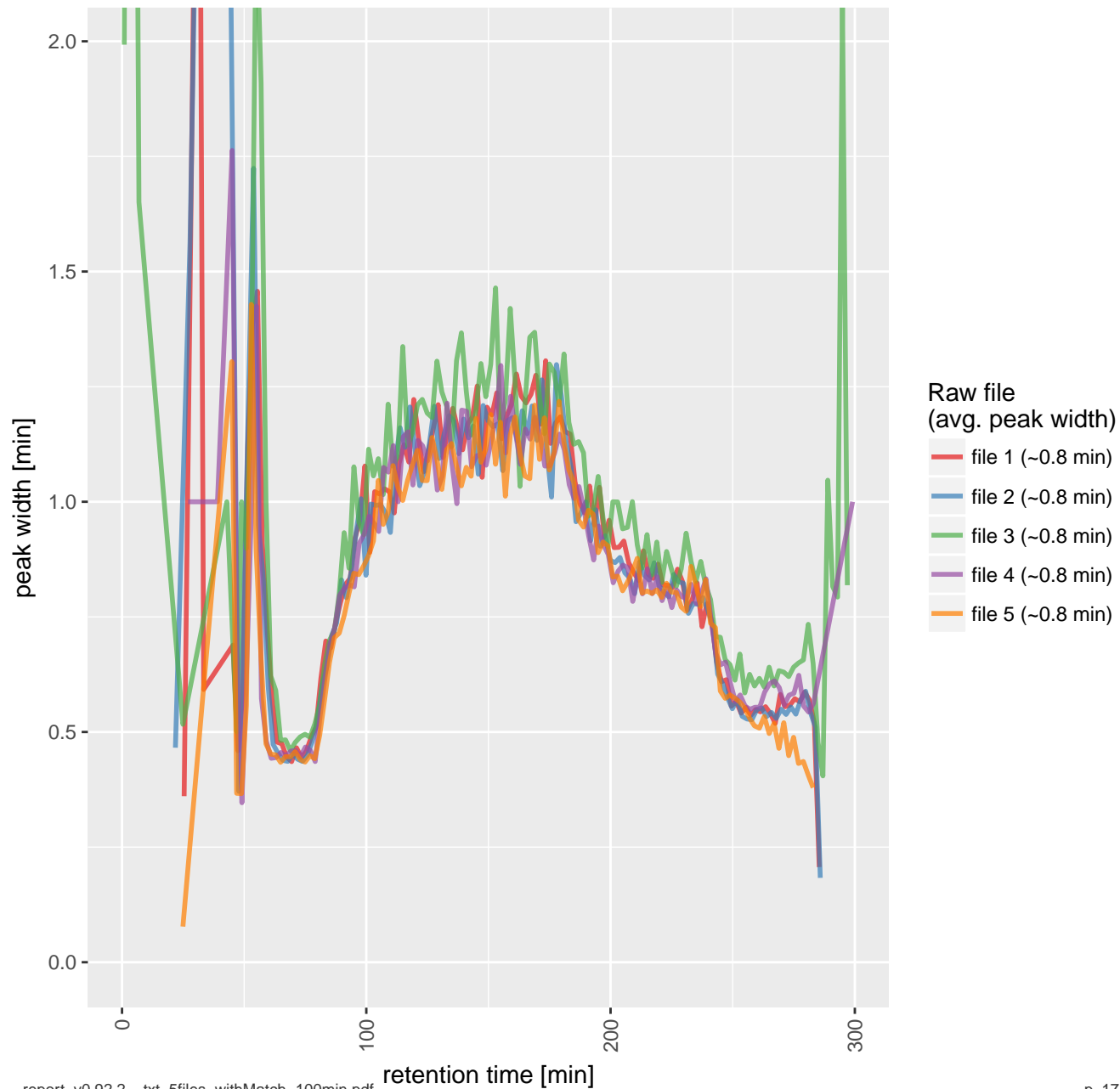
# EVD: MBR – alignment

alignment reference: Toni_20140521_GM_QC_01

# EVD: MBR – ID Transfer



fraction of 3D−peaks [%]
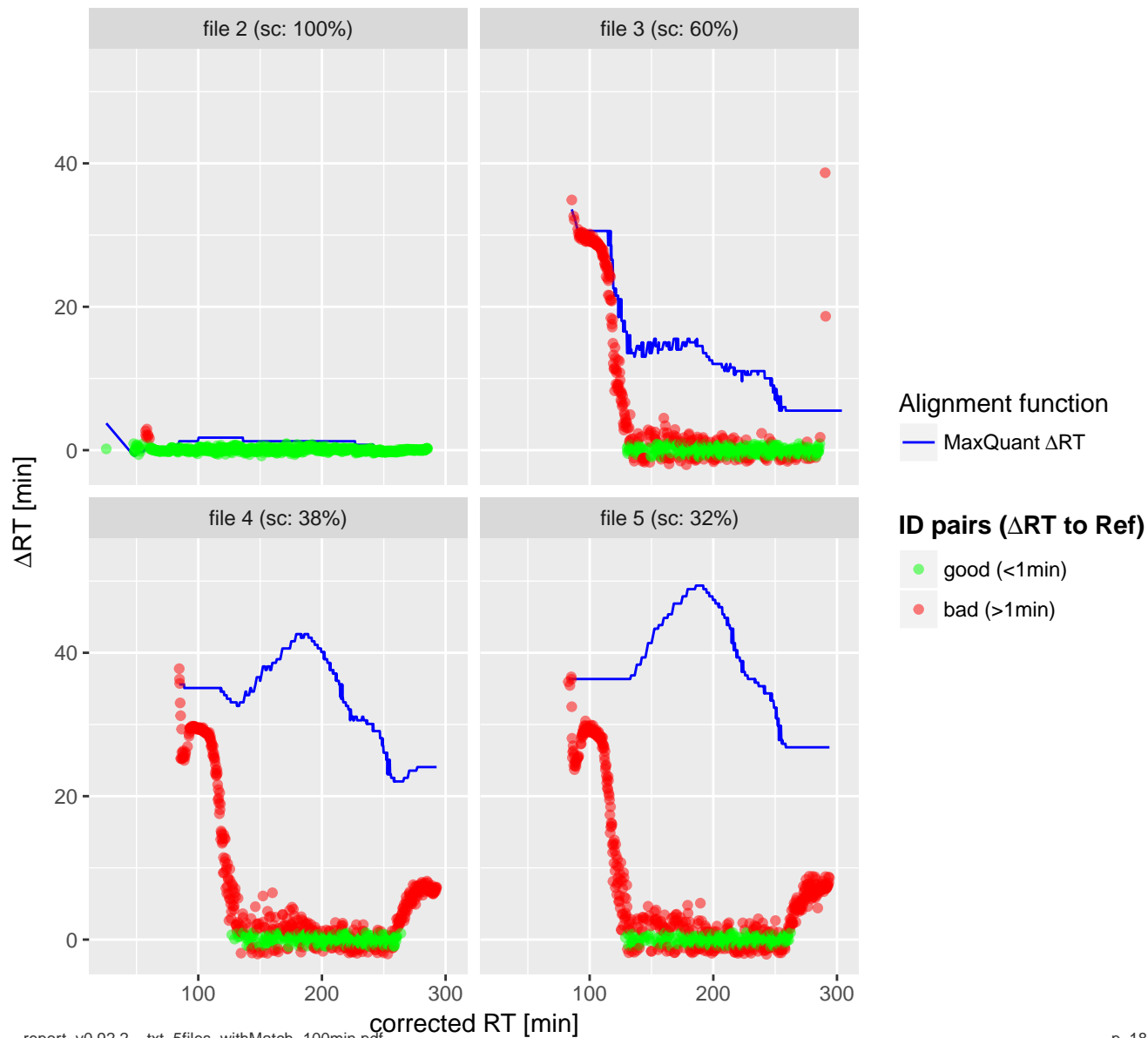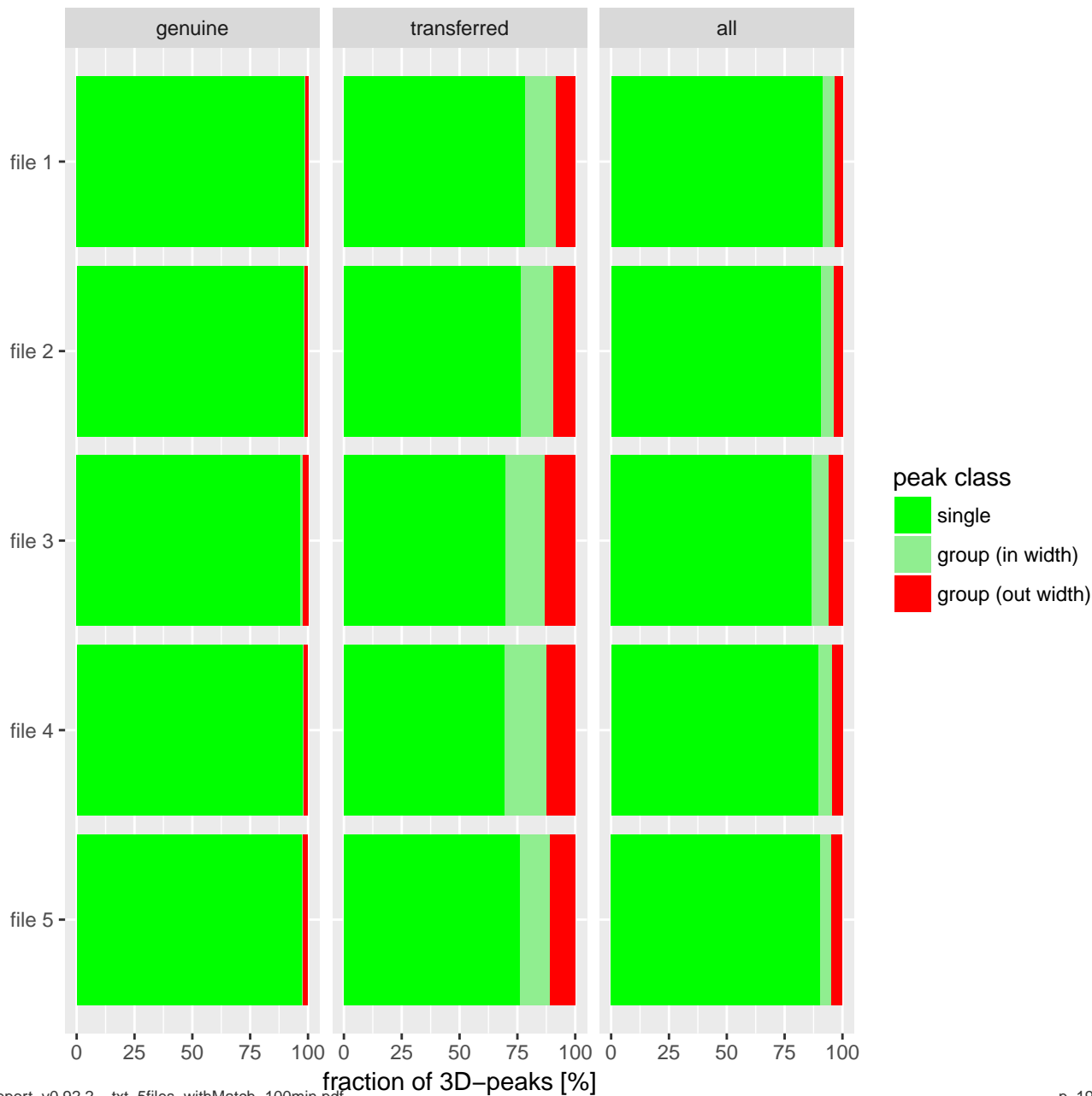
# [experimental] EVD: Clustering Tree of Raw files

by Correlation of Corrected Retention Times

file 5

file 4

file 3

file 2

file 1
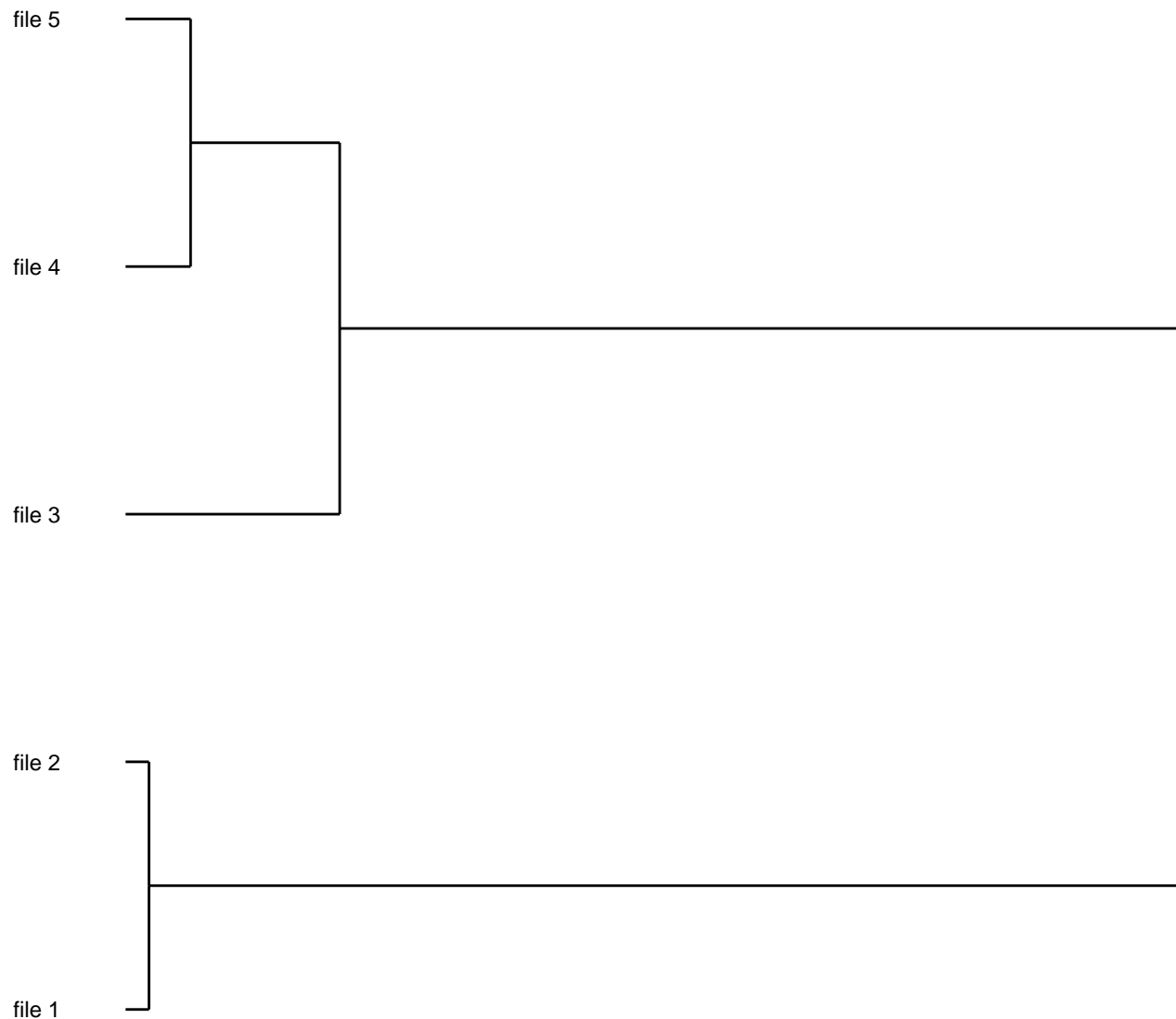
# EVD: Peptides inferred by MBR
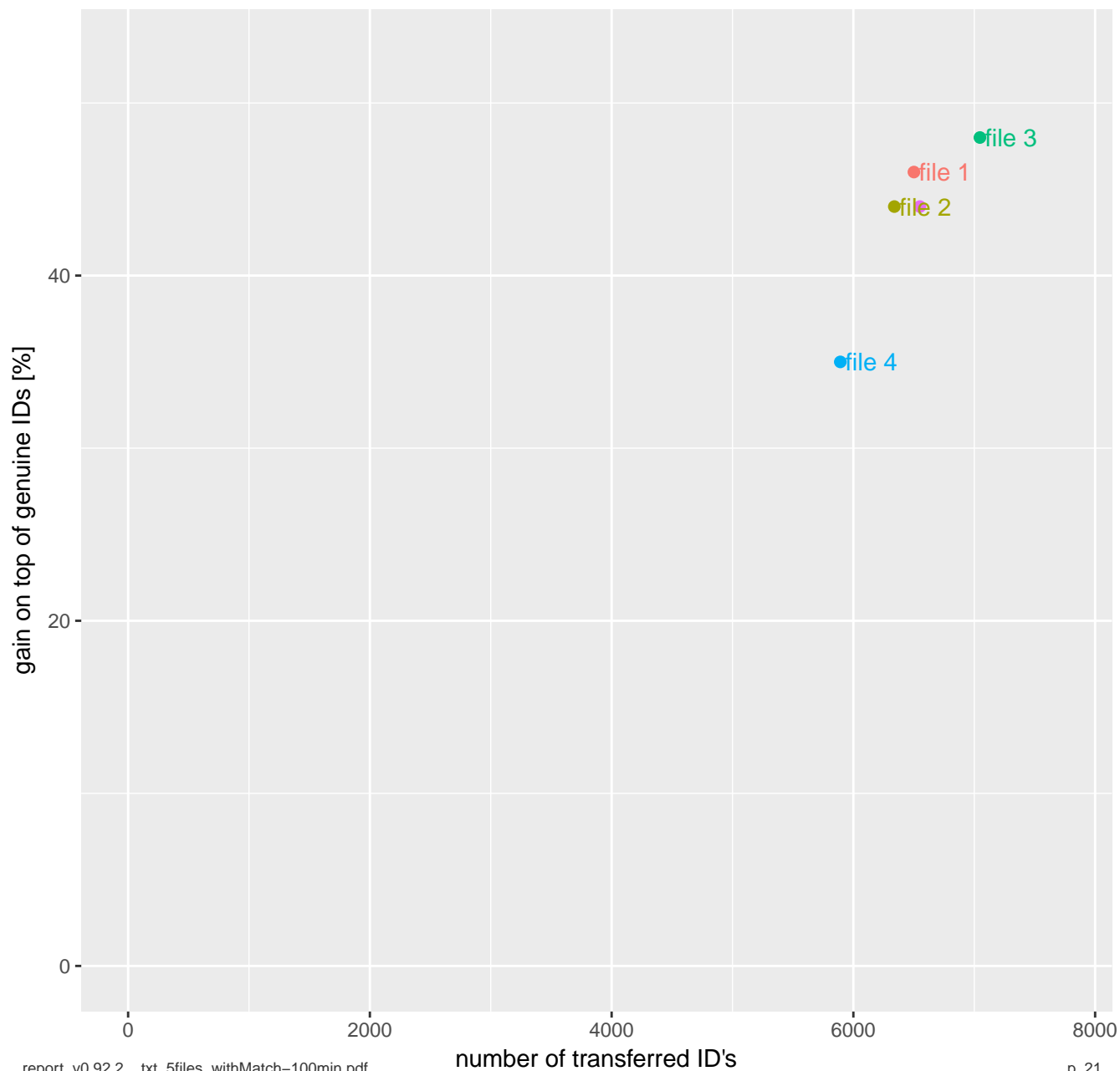
MSMSscans: Ion Injection Time over RT

Raw file with average inj. time
- file 1 (~12 ms)
- file 2 (~11 ms)
- file 3 (~7 ms)
- file 4 (~9 ms)
- file 5 (~20 ms)
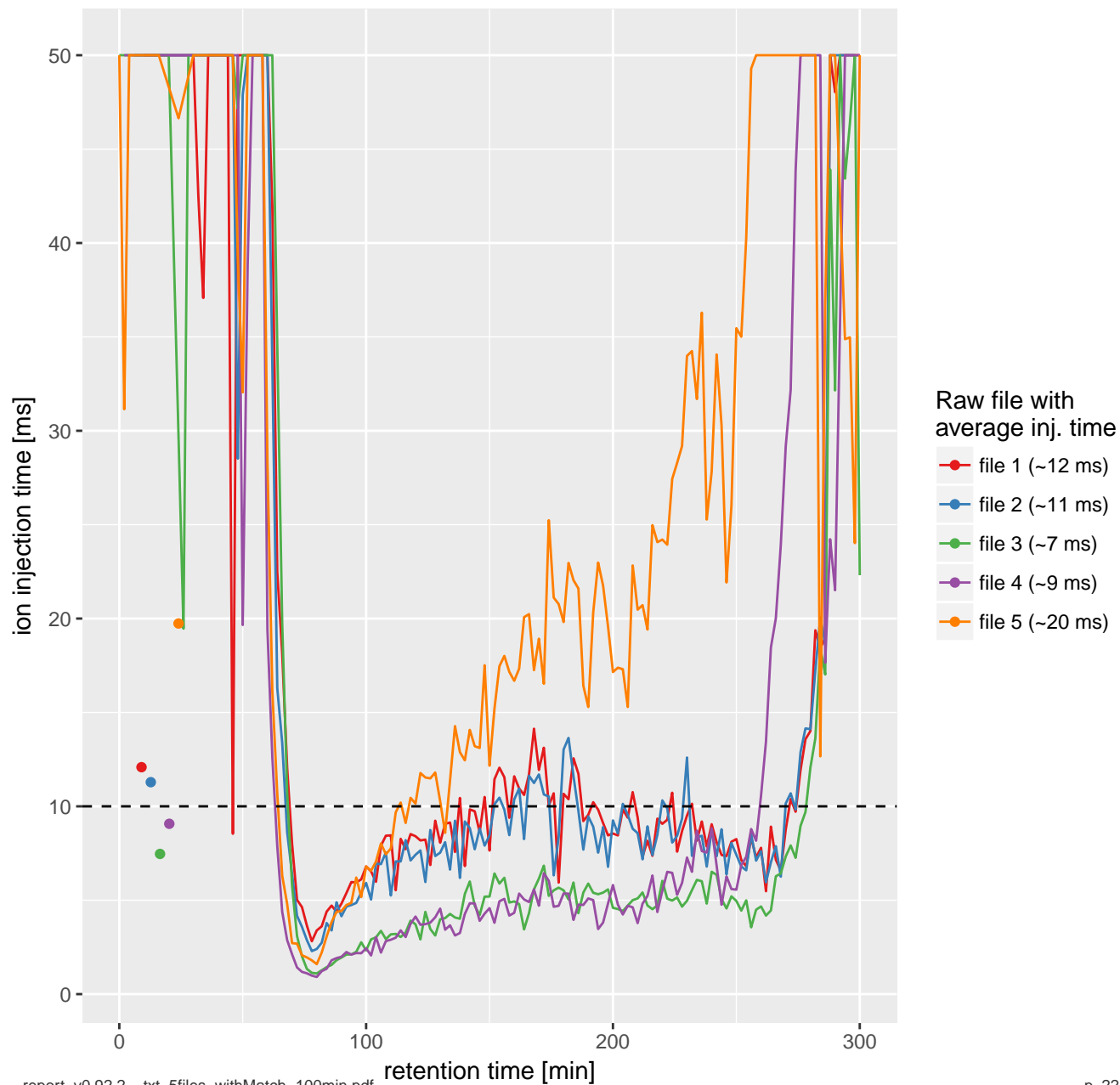
# [experimental] MSMSscans: MS/MS intensity



intensity ($\log_{10}$)

Legend: MS/MS intensity — Base Peak, TIC
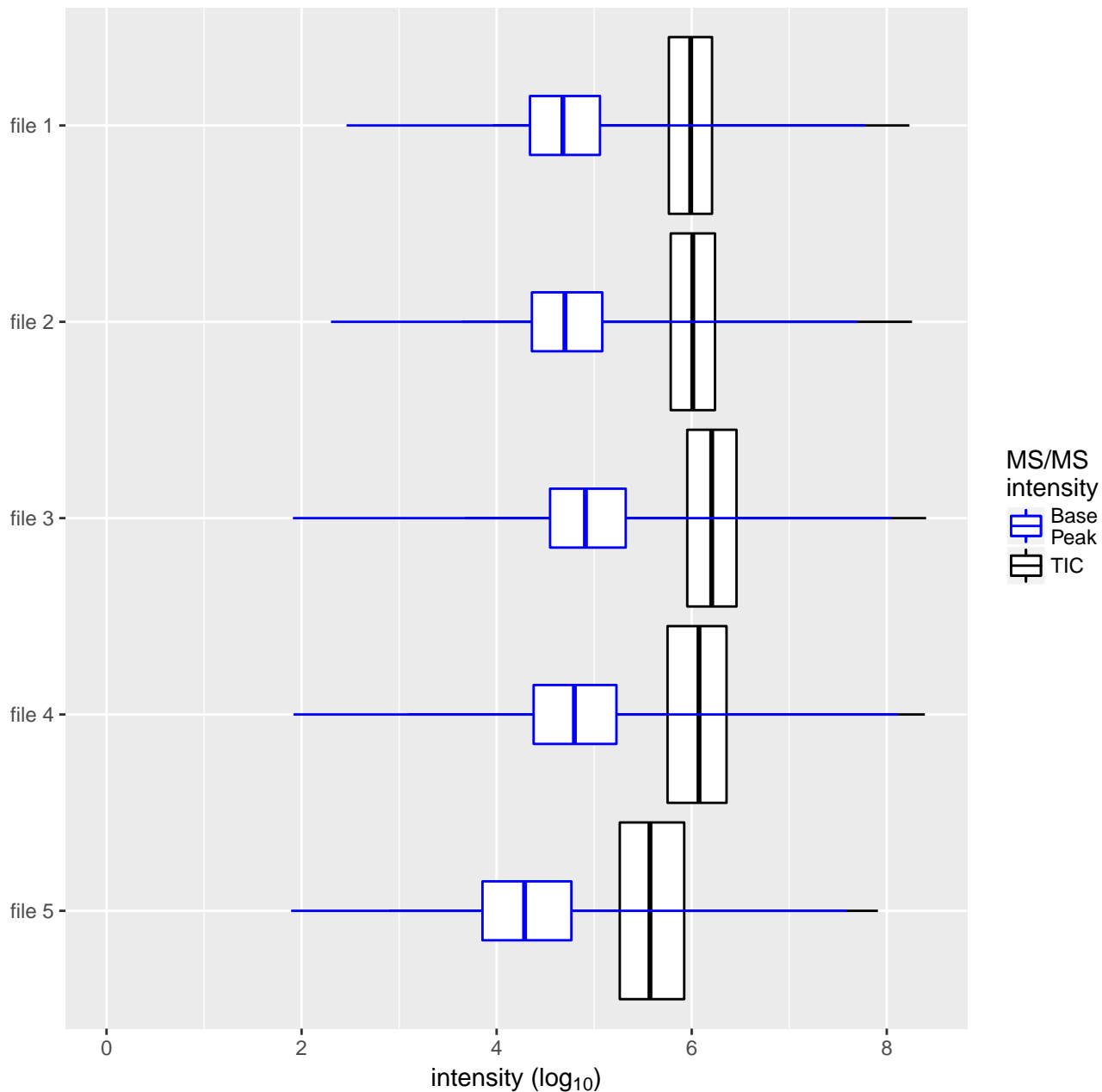
# EVD: Oversampling (MS/MS counts per 3D−peak)
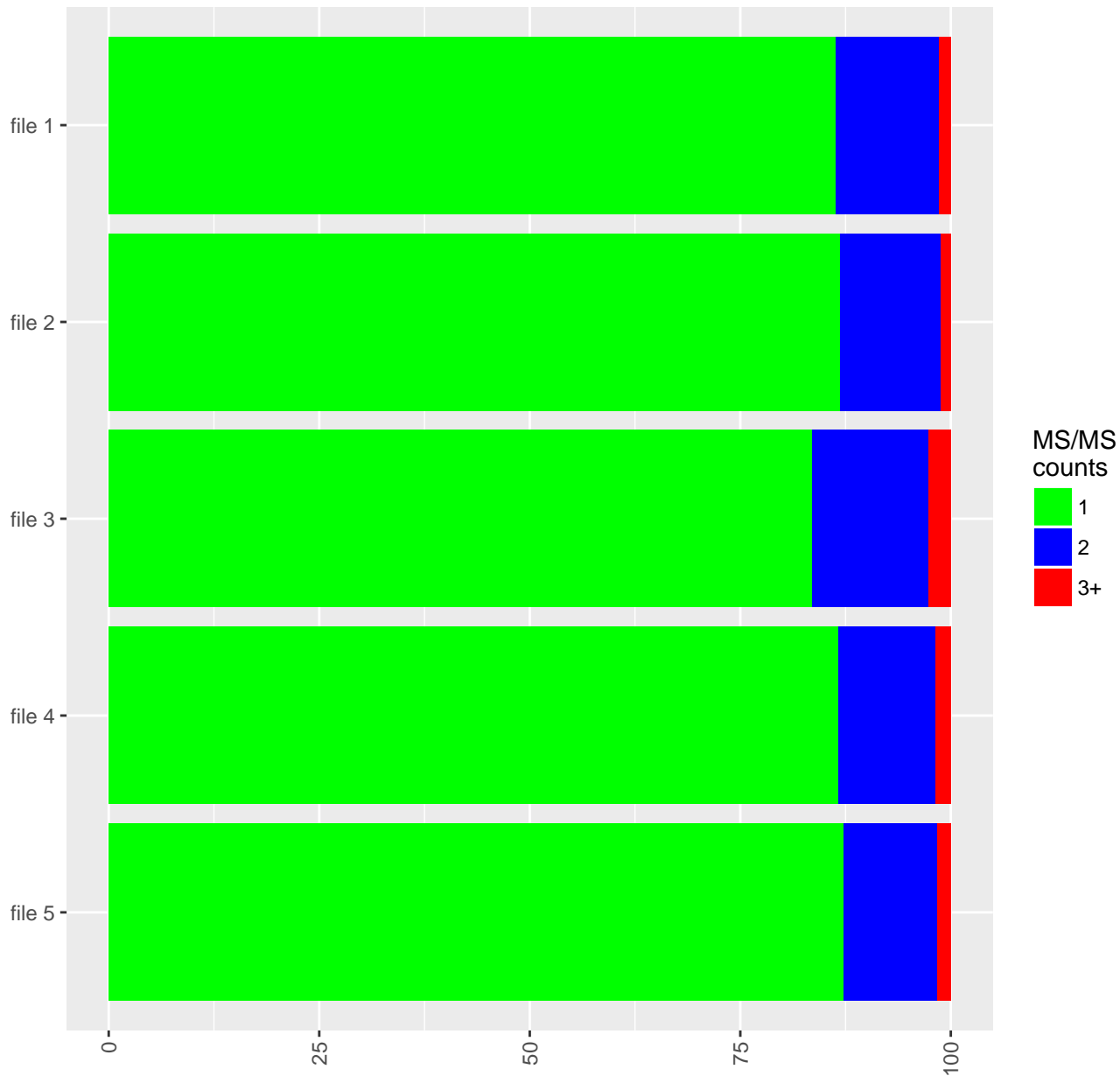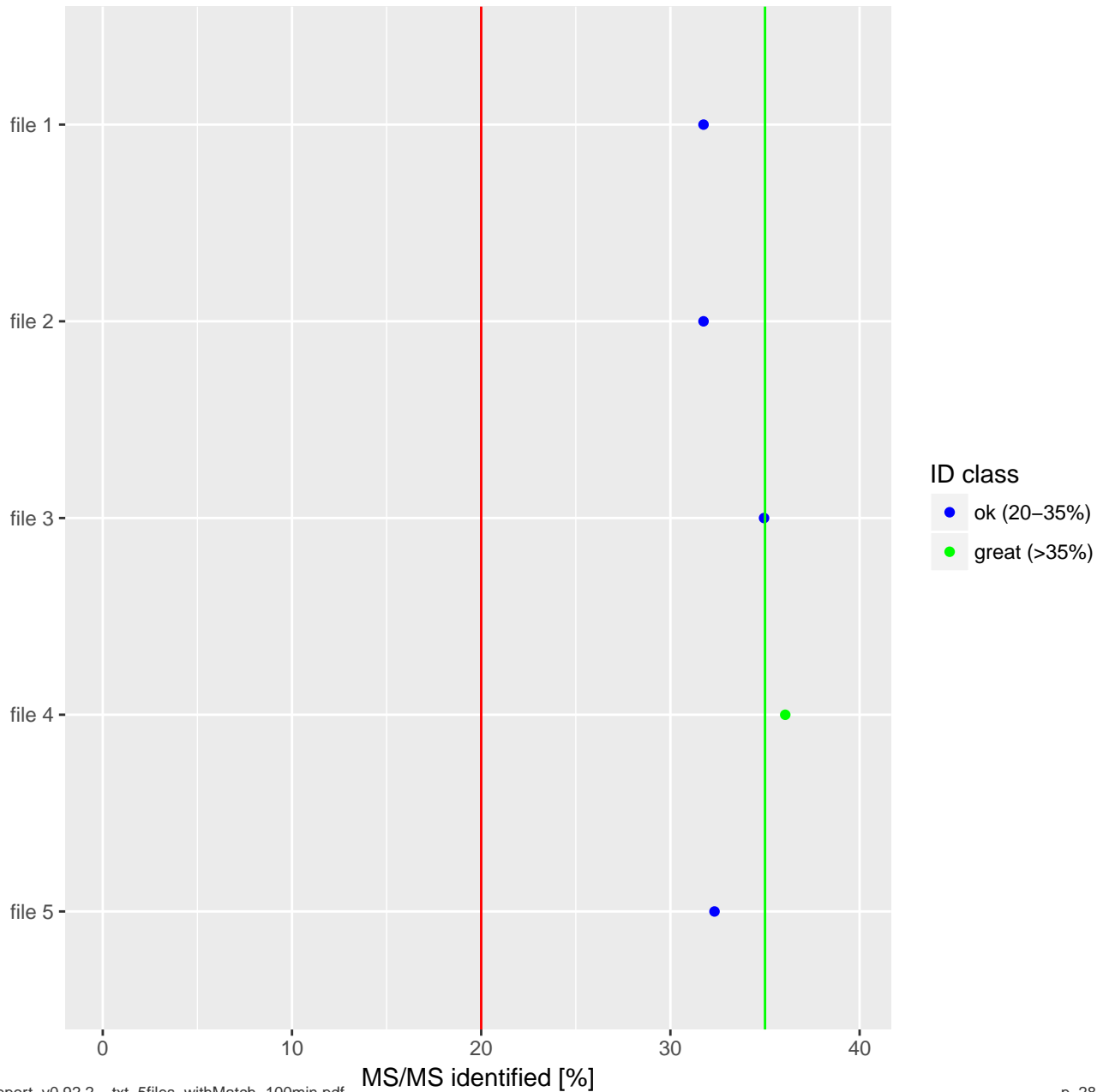
# EVD: Uncalibrated mass error
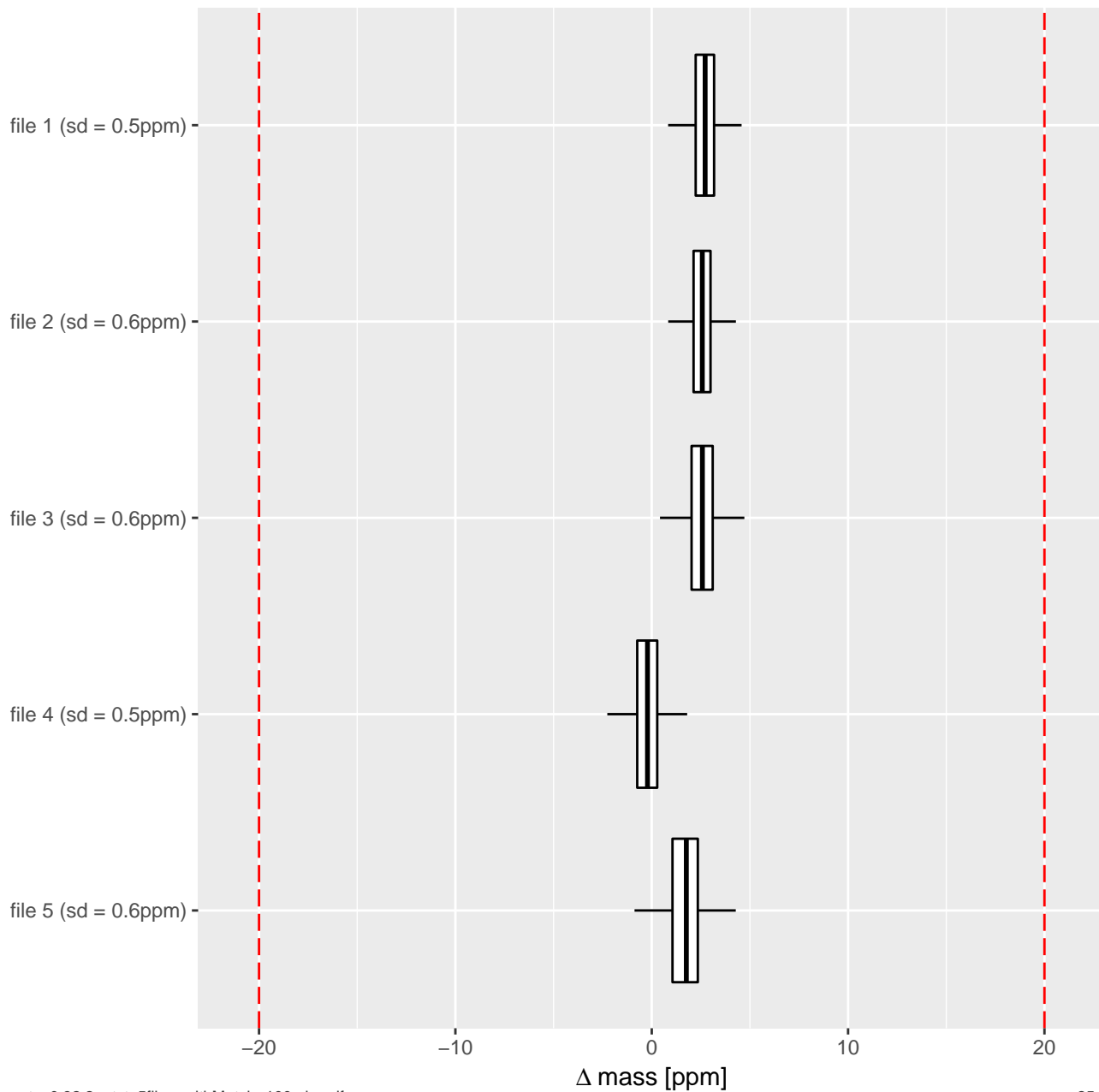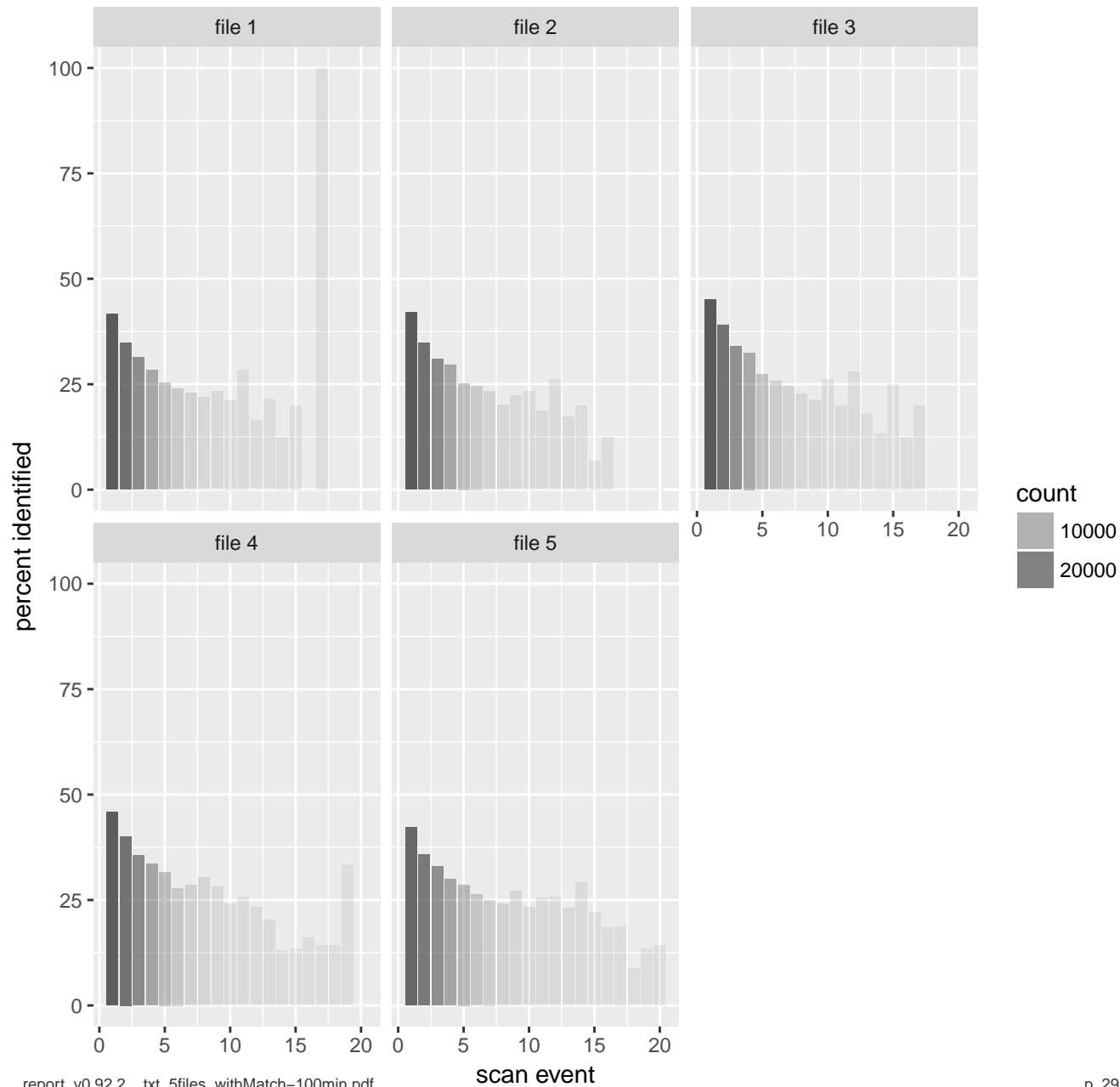
# EVD: Calibrated mass error
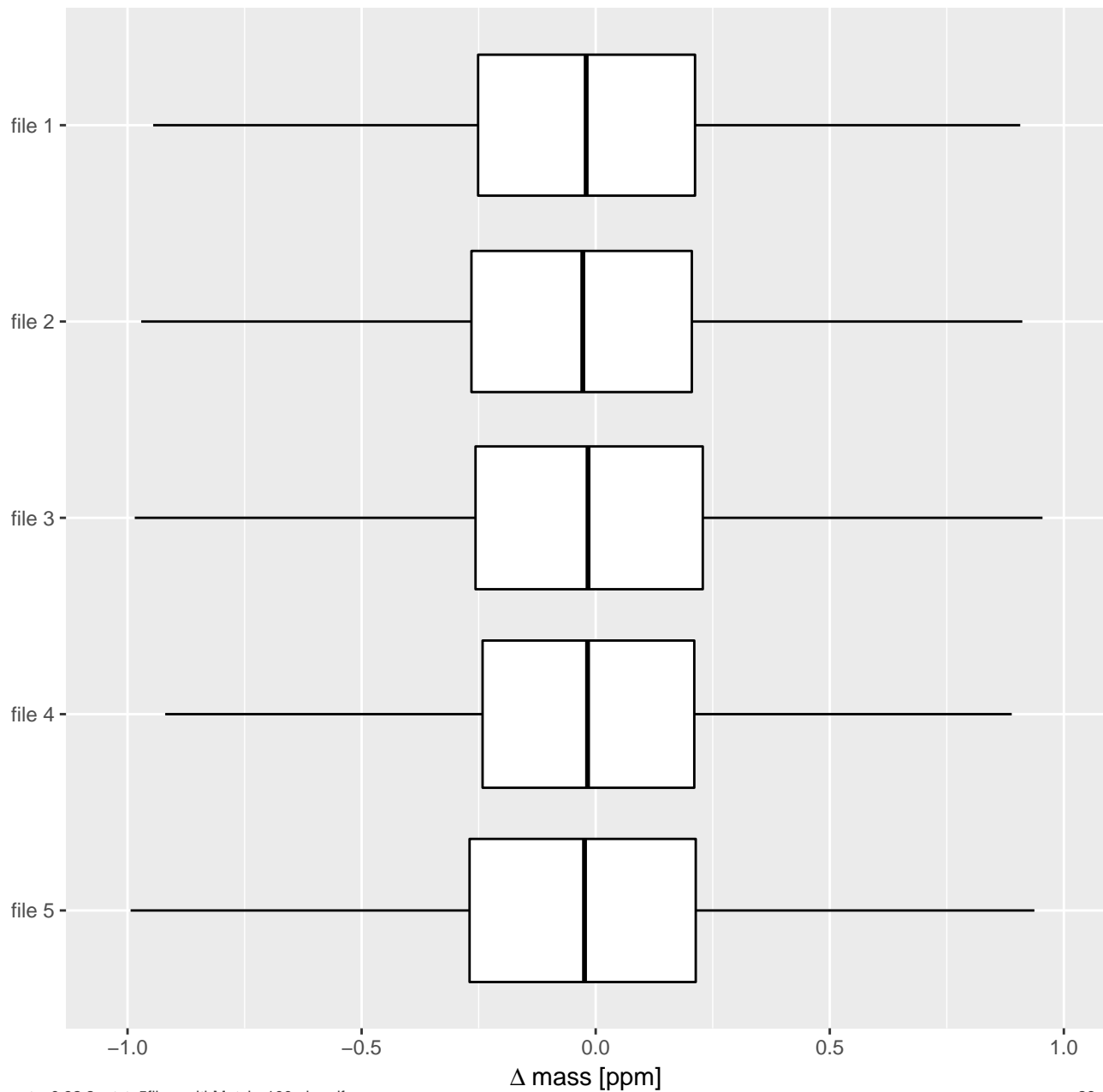
# MSMS: Fragment mass errors per Raw file
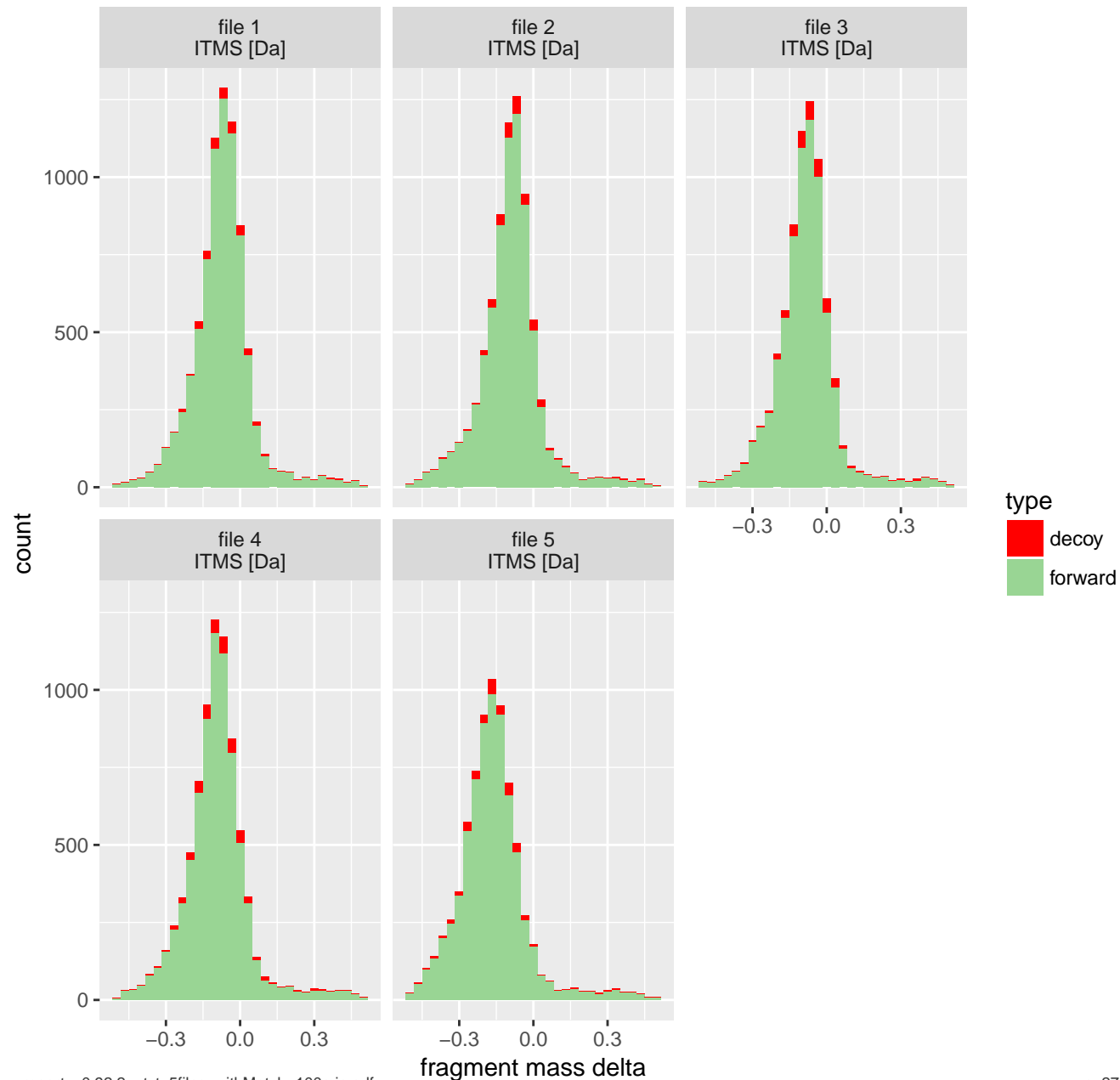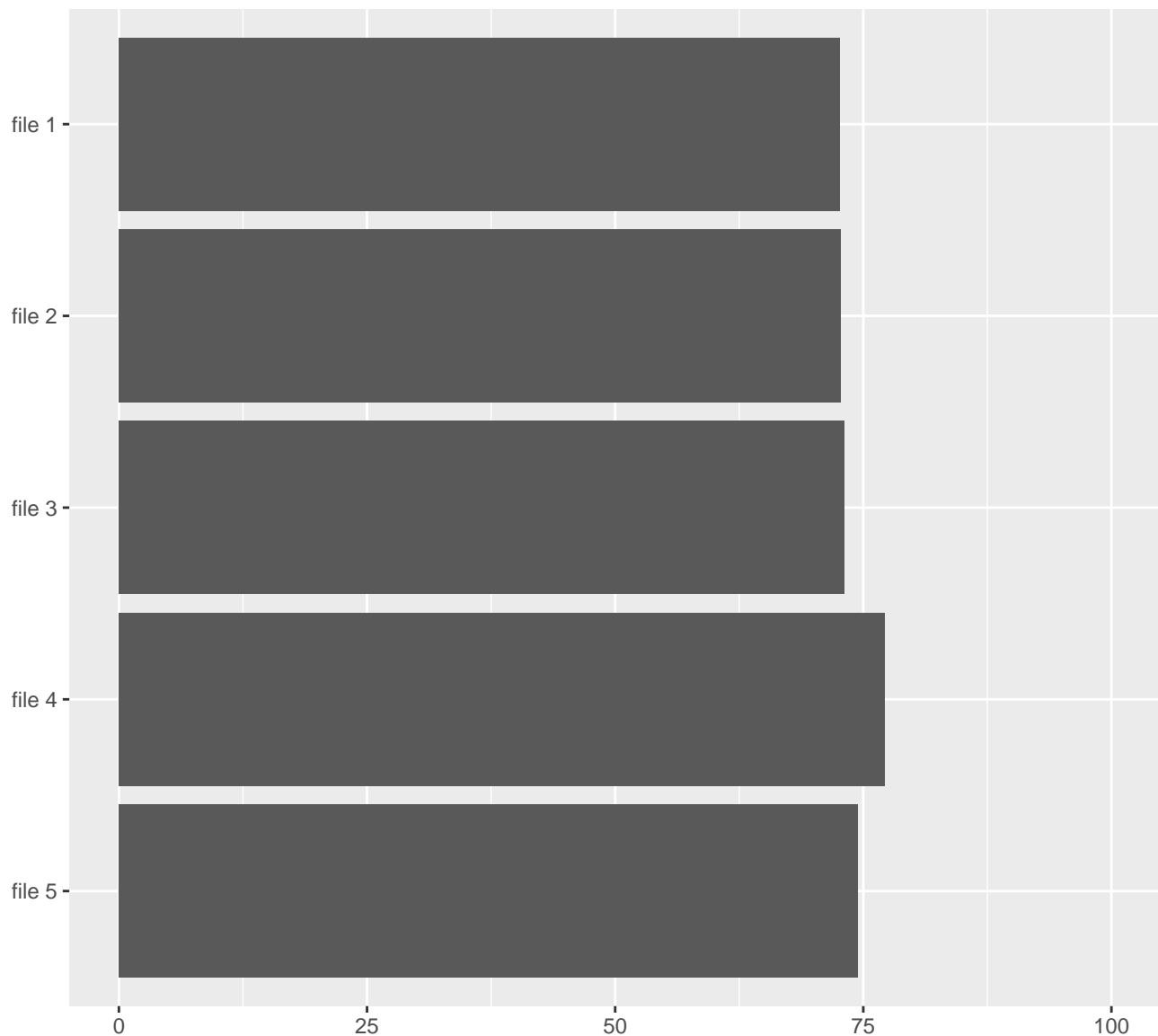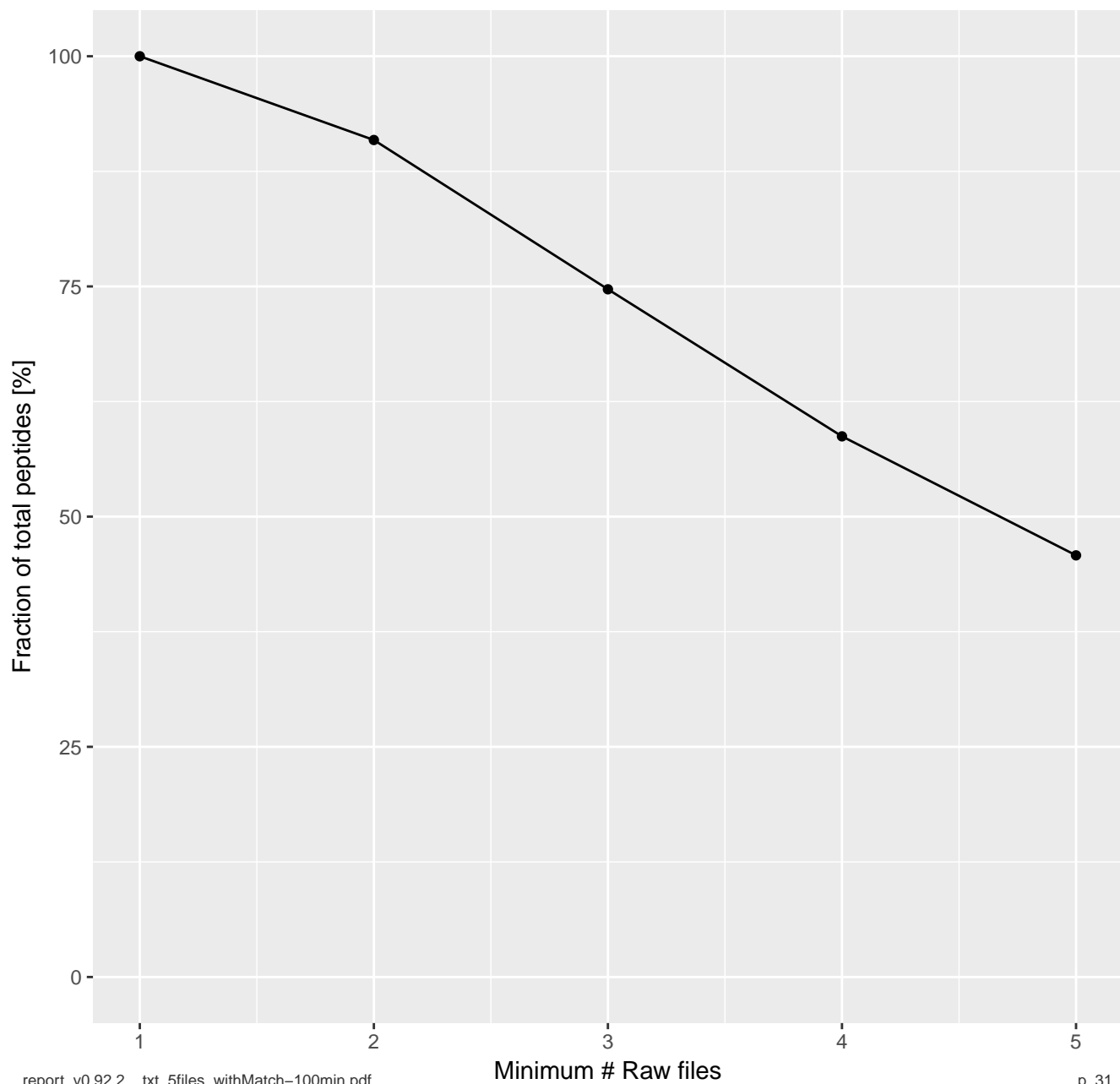
# SM: MS/MS identified per Raw file

# MSMSscans: TopN % identified over N

# [experimental] EVD: Non−Missing Peptides

compared to all peptides seen in experiment



Fraction of total peptides [%]

# [experimental] EVD: Non−missing by set

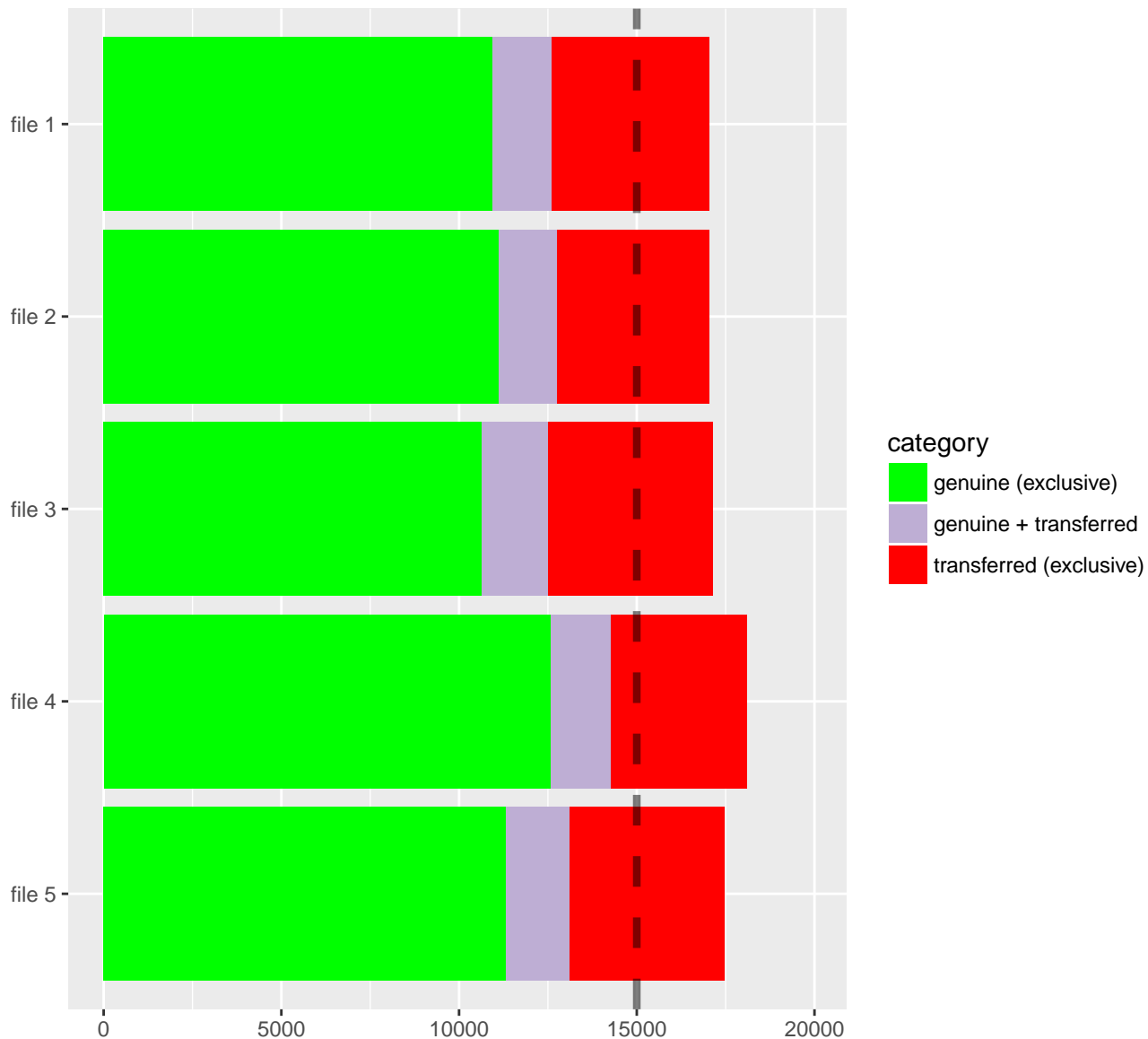Fraction of total peptides [%]

Minimum # Raw files

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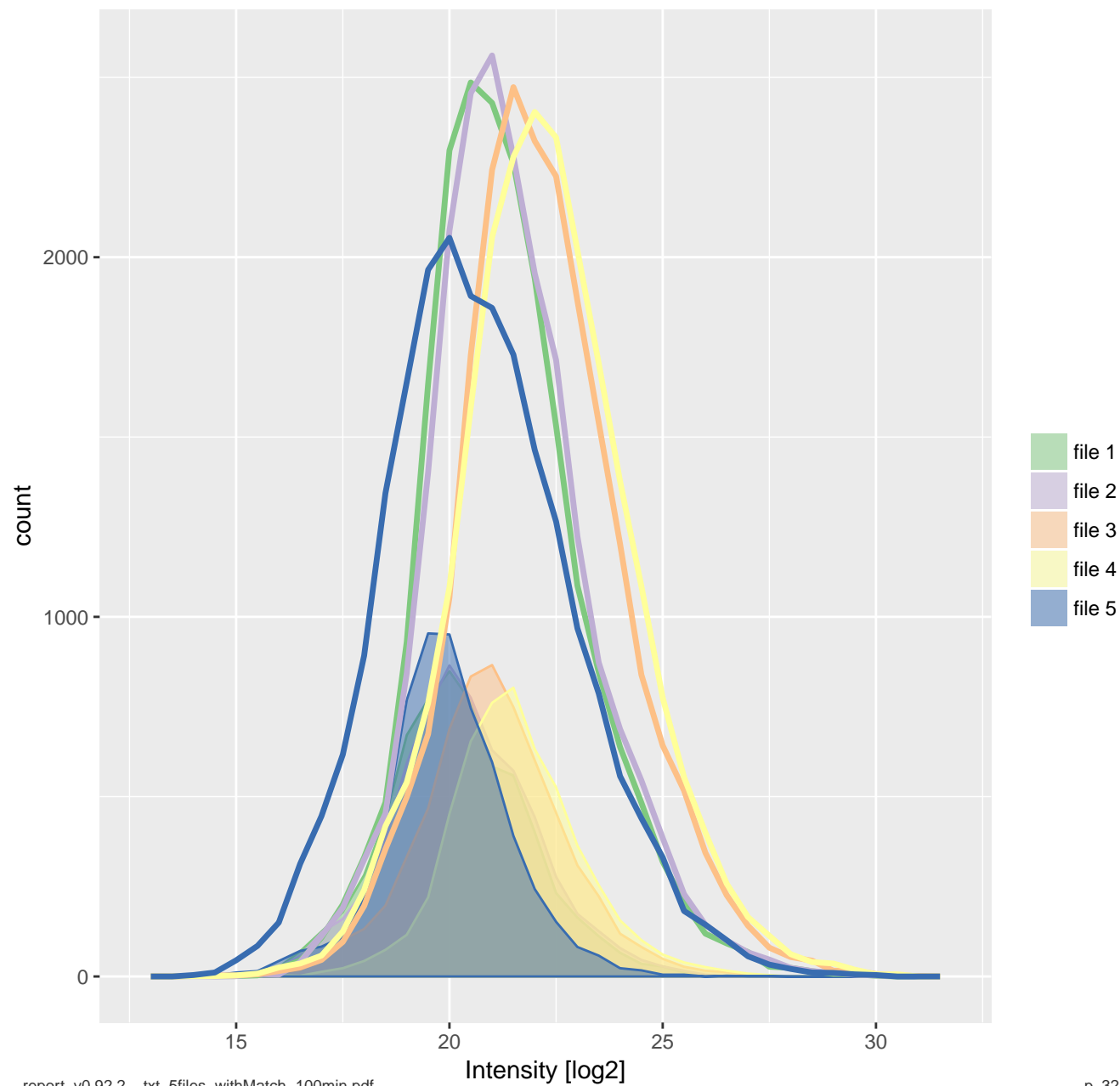
# EVD: Peptide ID count

MBR gain: +33%

# EVD: ProteinGroups count

MBR gain: +14%