

PAR: parameters

Version	1.5.2.8	Min. score for unmodified pe..	0
User name	cbielow	Min. score for modified pept..	40
Machine name	CD02-WIN7	Min. delta score for unmodif..	0
Date of writing	08/05/2015 14:17:27	Min. delta score for modifie..	6
Fixed modifications	Carbamidomethyl (C)	Min. unique peptides	0
Decoy mode	revert	Min. razor peptides	1
Special AAs	KR	Min. peptides	1
Include contaminants	True	Use only unmodified peptides..	True
MS/MS tol. (FTMS)	20 ppm	Modifications included in pr..	Acetyl (Protein N-term) Oxidation (M)
Top MS/MS peaks per 100 Da. ..	12	Peptides used for protein qu..	Razor
MS/MS deisotoping (FTMS)	True	Discard unmodified counterpa..	True
MS/MS tol. (ITMS)	0.5 Da	Min. ratio count	2
Top MS/MS peaks per 100 Da. ..	8	Re-quantify	False
MS/MS deisotoping (ITMS)	False	Use delta score	False
MS/MS tol. (TOF)	40 ppm	iBAQ	False
Top MS/MS peaks per 100 Da. ..	10	iBAQ log fit	False
MS/MS deisotoping (TOF)	True	Match between runs	True
MS/MS tol. (Unknown)	0.5 Da	Matching time window [min]	0.7
Top MS/MS peaks per 100 Da. ..	8	Alignment time window [min]	100
MS/MS deisotoping (Unknown)	False	Find dependent peptides	False
PSM FDR	0.01	Labeled amino acid filtering	True
Protein FDR	0.01	Site tables	Oxidation (M)Sites.txt
Site FDR	0.01	RT shift	False
Use Normalized Ratios For Oc..	True	Advanced ratios	True
Min. peptide Length	7	First pass AIF correlation	0.8
crap_withMycoplasma.fasta			
uniprot_human_canonical_and_isoforms_20130513.fasta			

Mapping of Raw files to their short names

Mapping source: file (user-defined)

original	short name
----------	---------------

QC_20140521_1	..140521_1
---------------	------------

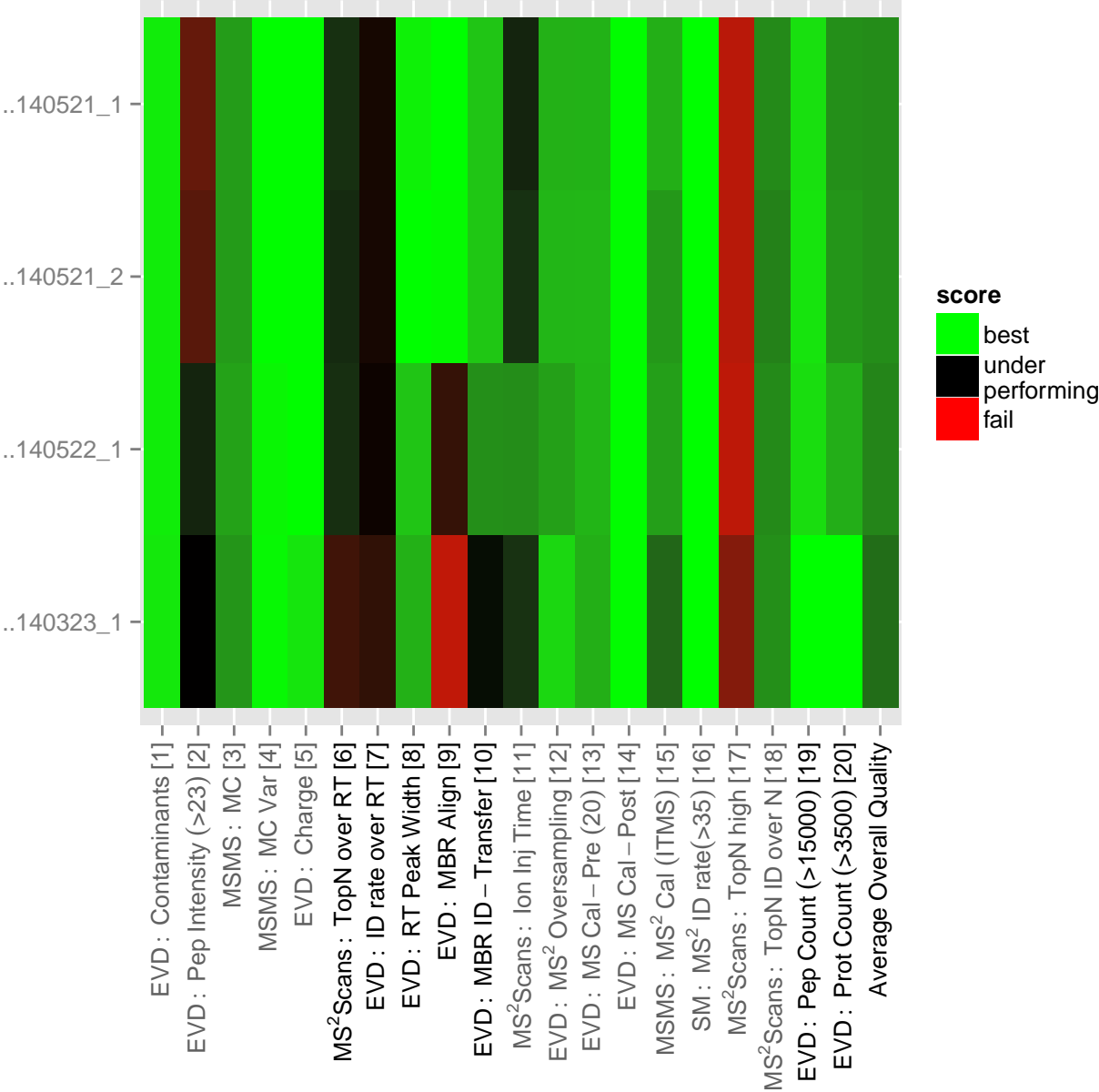
QC_20140521_2	..140521_2
---------------	------------

QC_20140522_1	..140522_1
---------------	------------

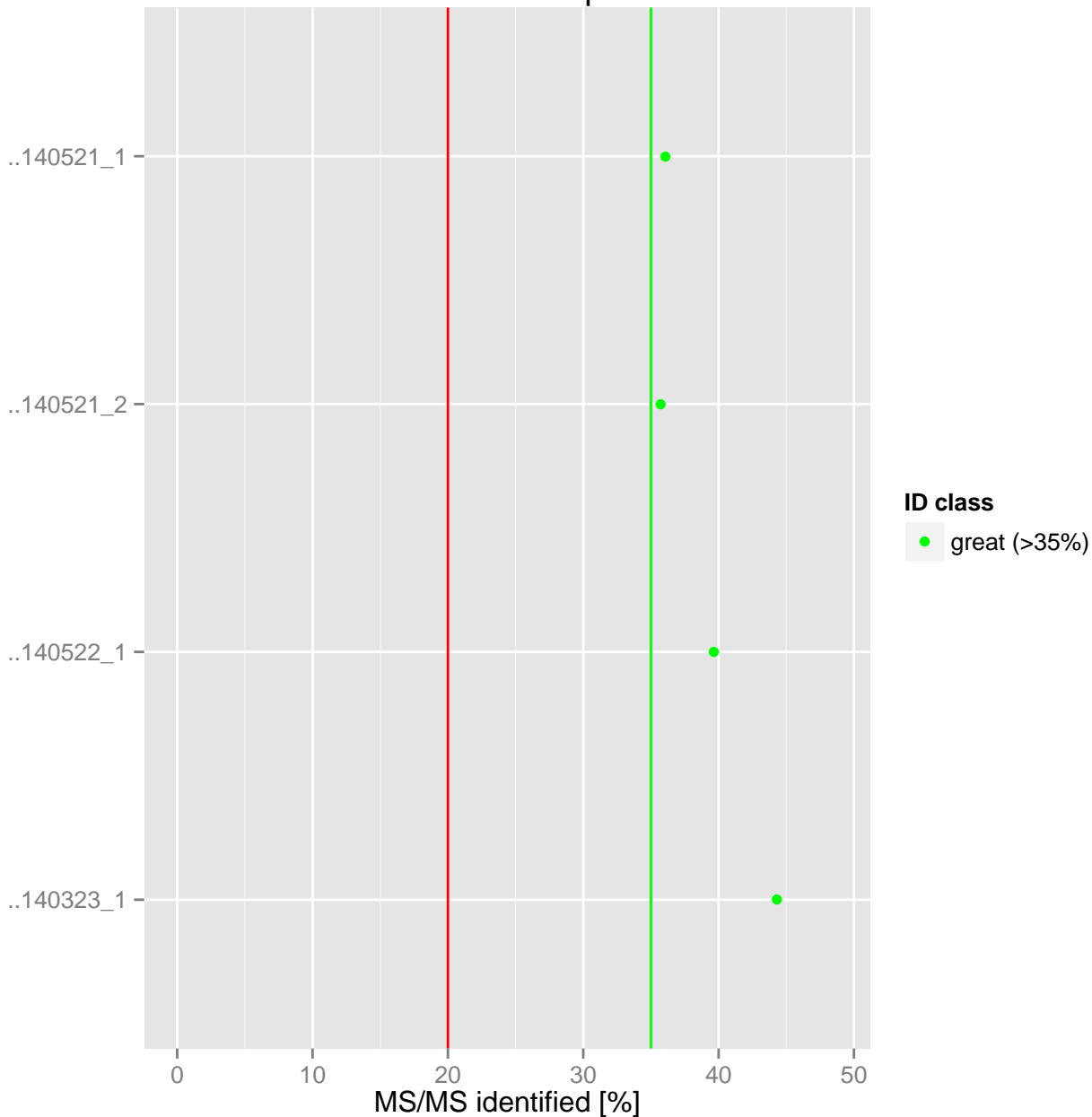
QC_20140323_1	..140323_1
---------------	------------

Performance overview

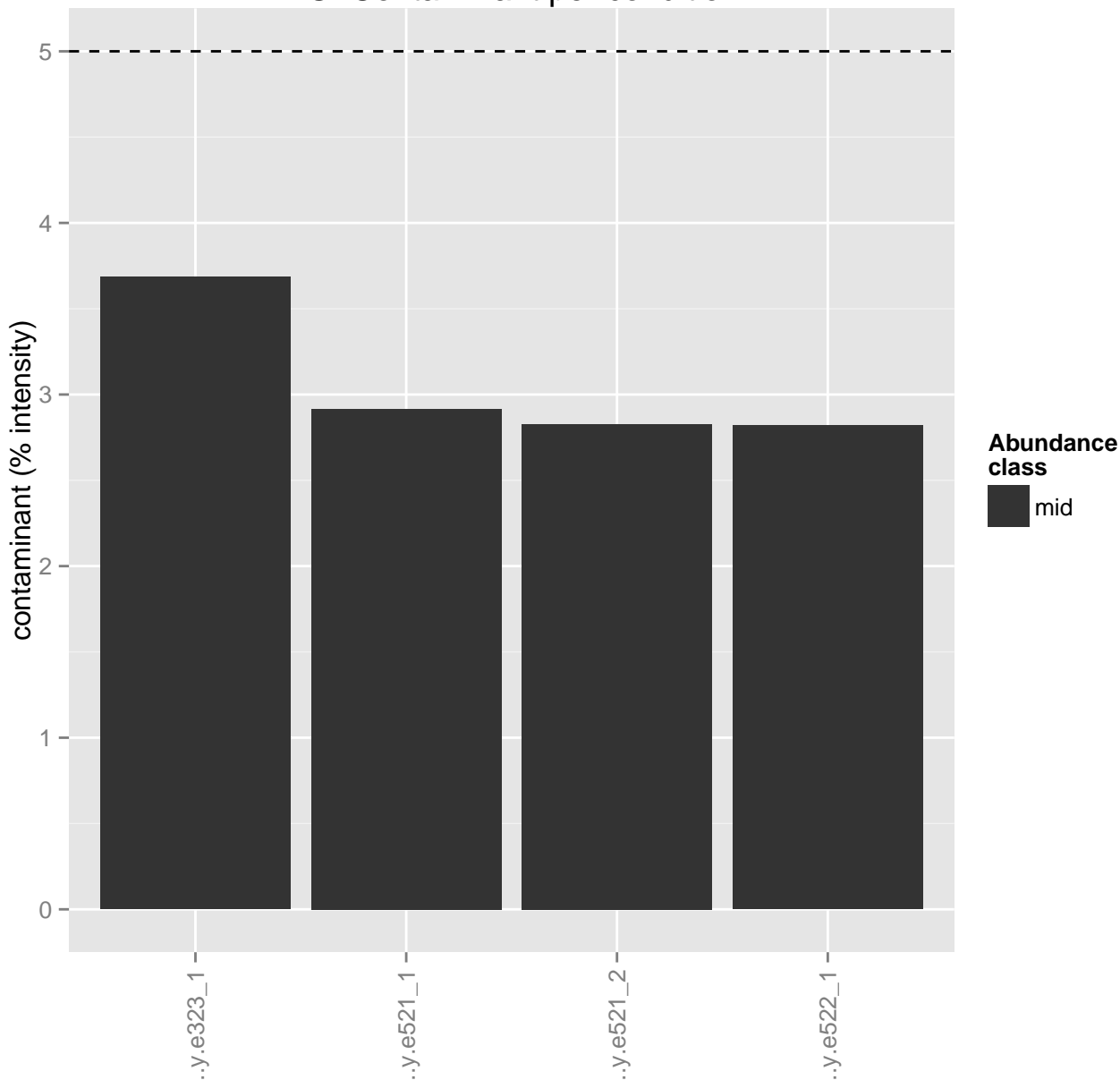
Raw file



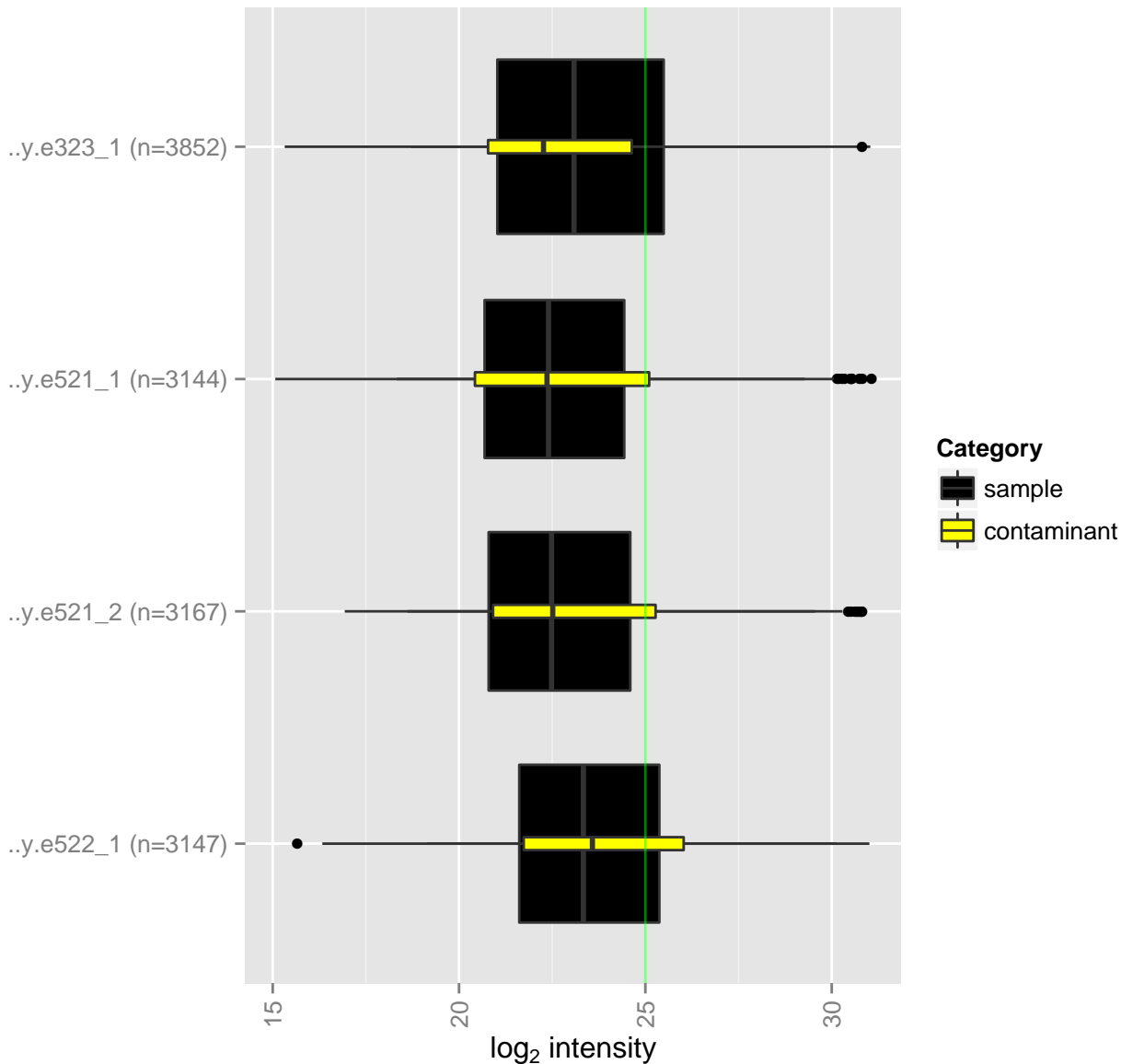
SM: MS/MS identified per Raw file



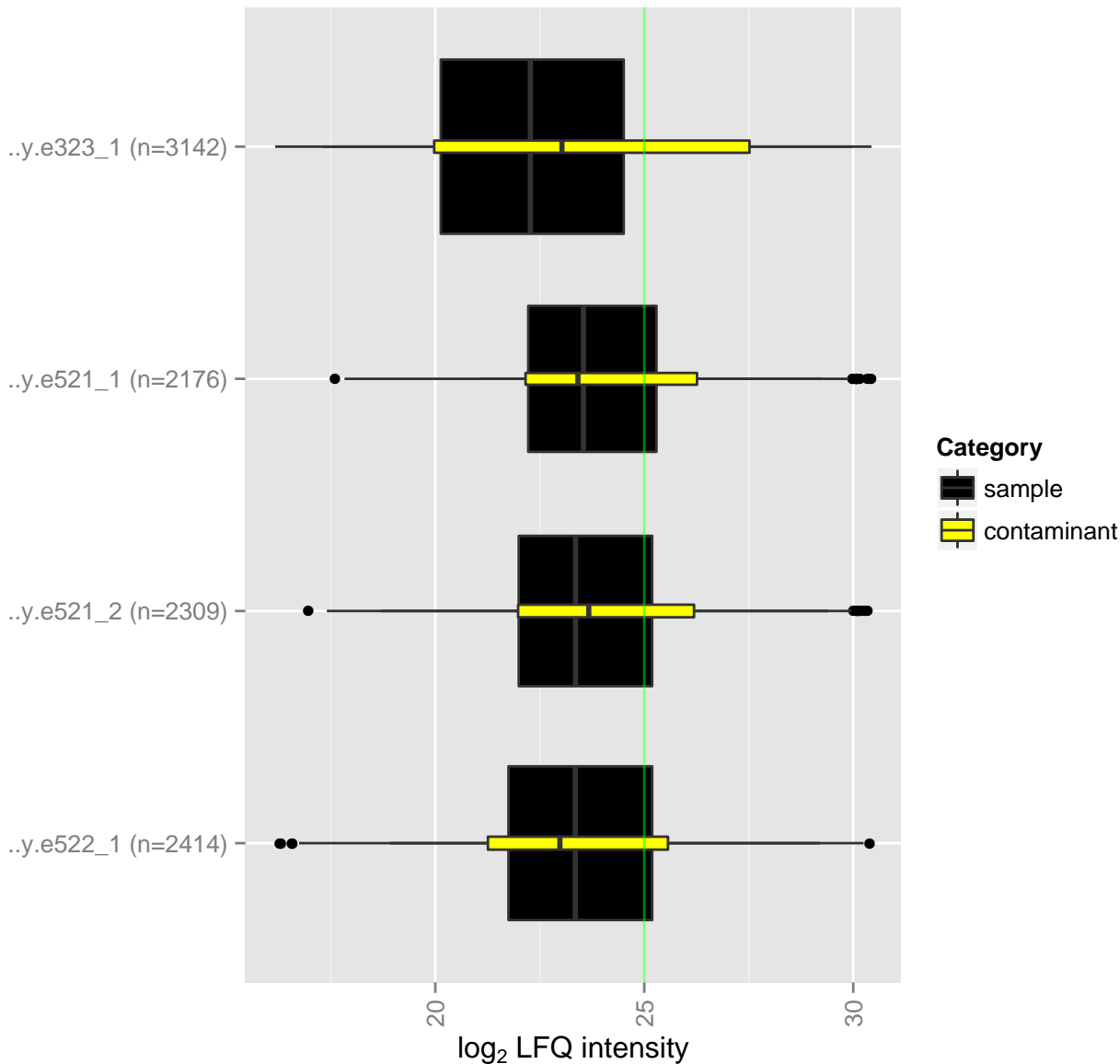
PG: Contaminant per condition



PG: intensity distribution
RSD 2% (w/o zero int.; expected < 5%)
RSD 3.1% [high RSD ---> few peptides]

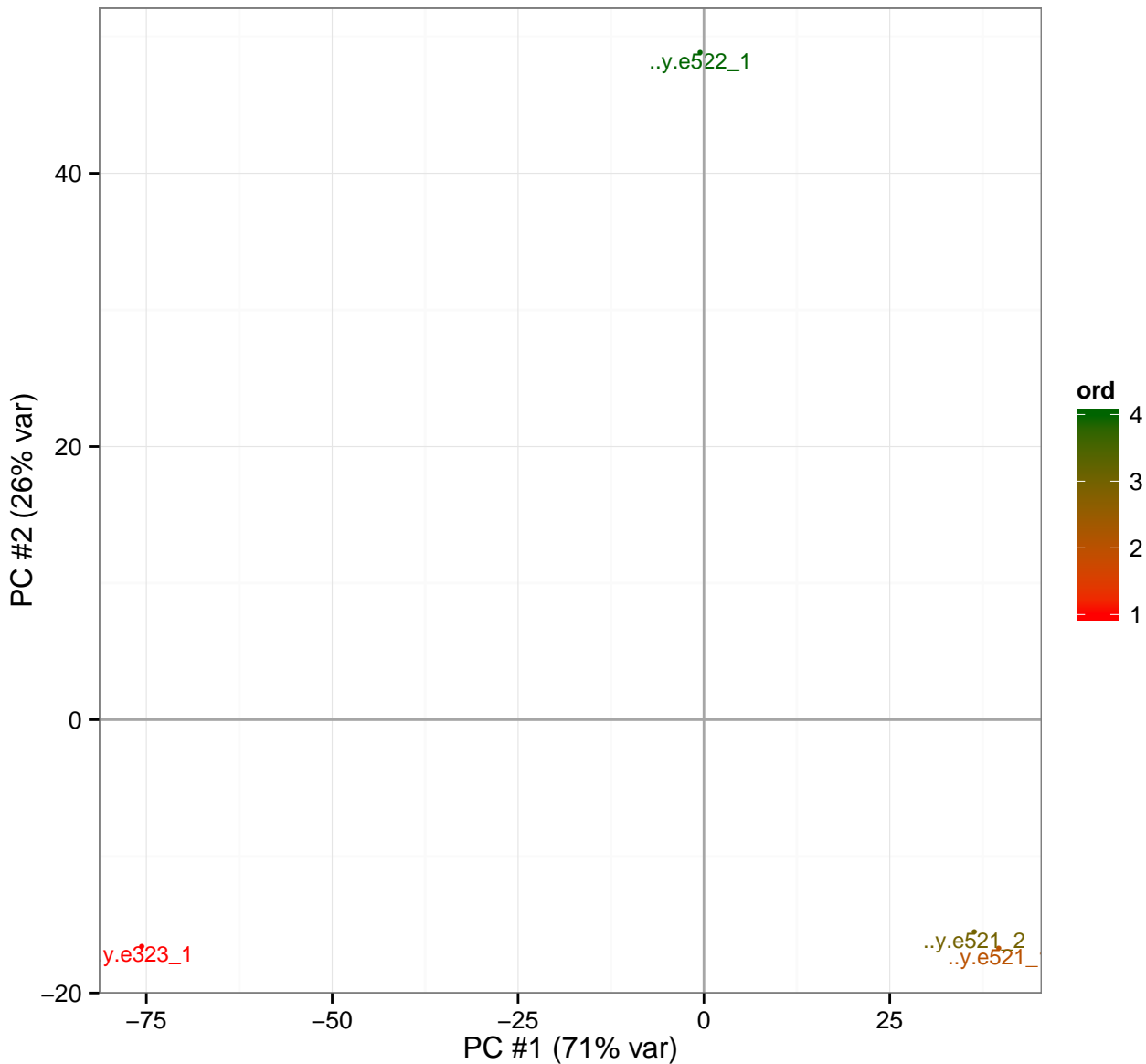


PG: LFO intensity distribution
RSD 2.7% (w/o zero int., expected < 5%)
RSD 0.6% [high RSD --> few peptides]

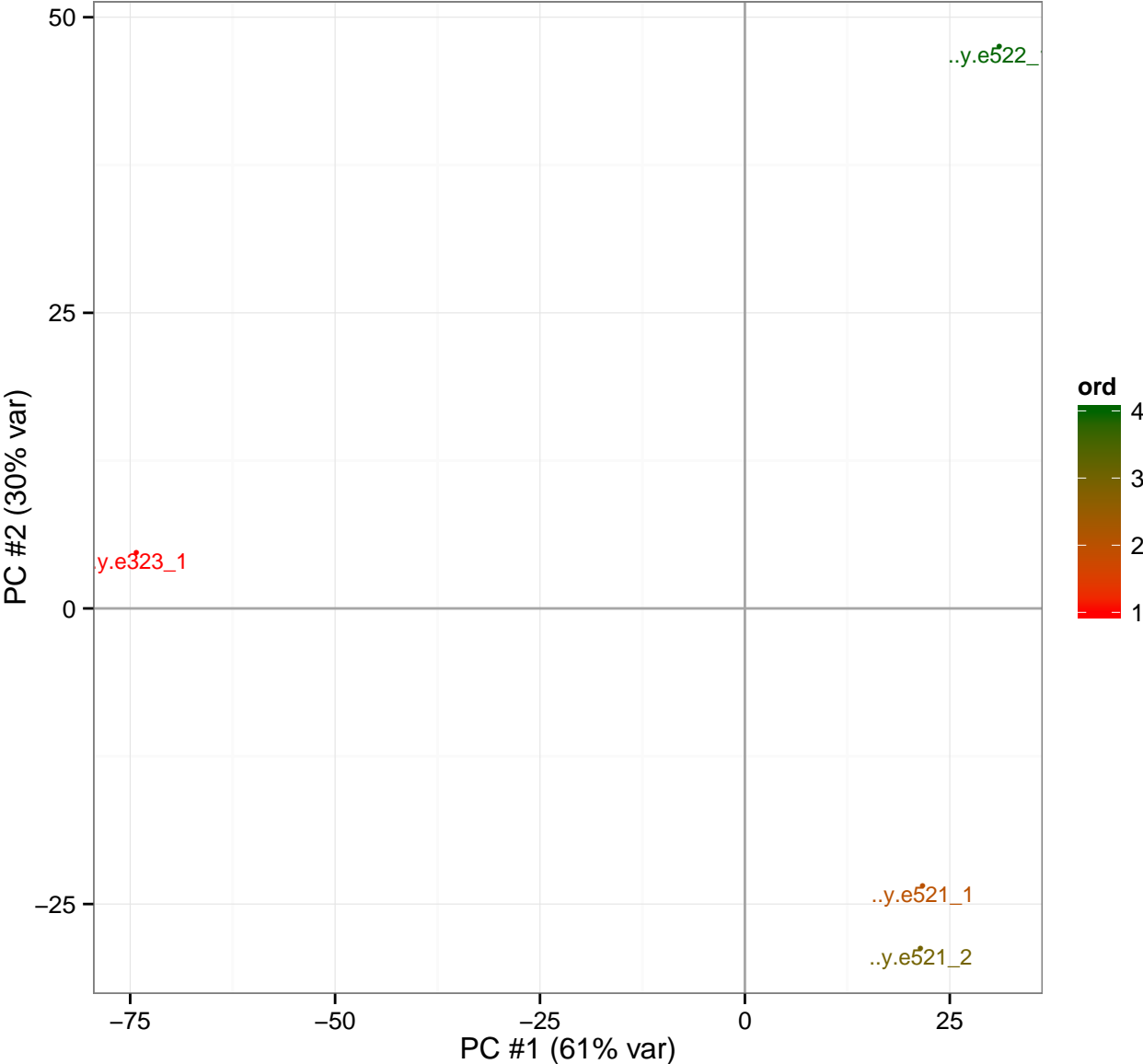


PG: PCA of 'raw intensity'

(excludes contaminants)

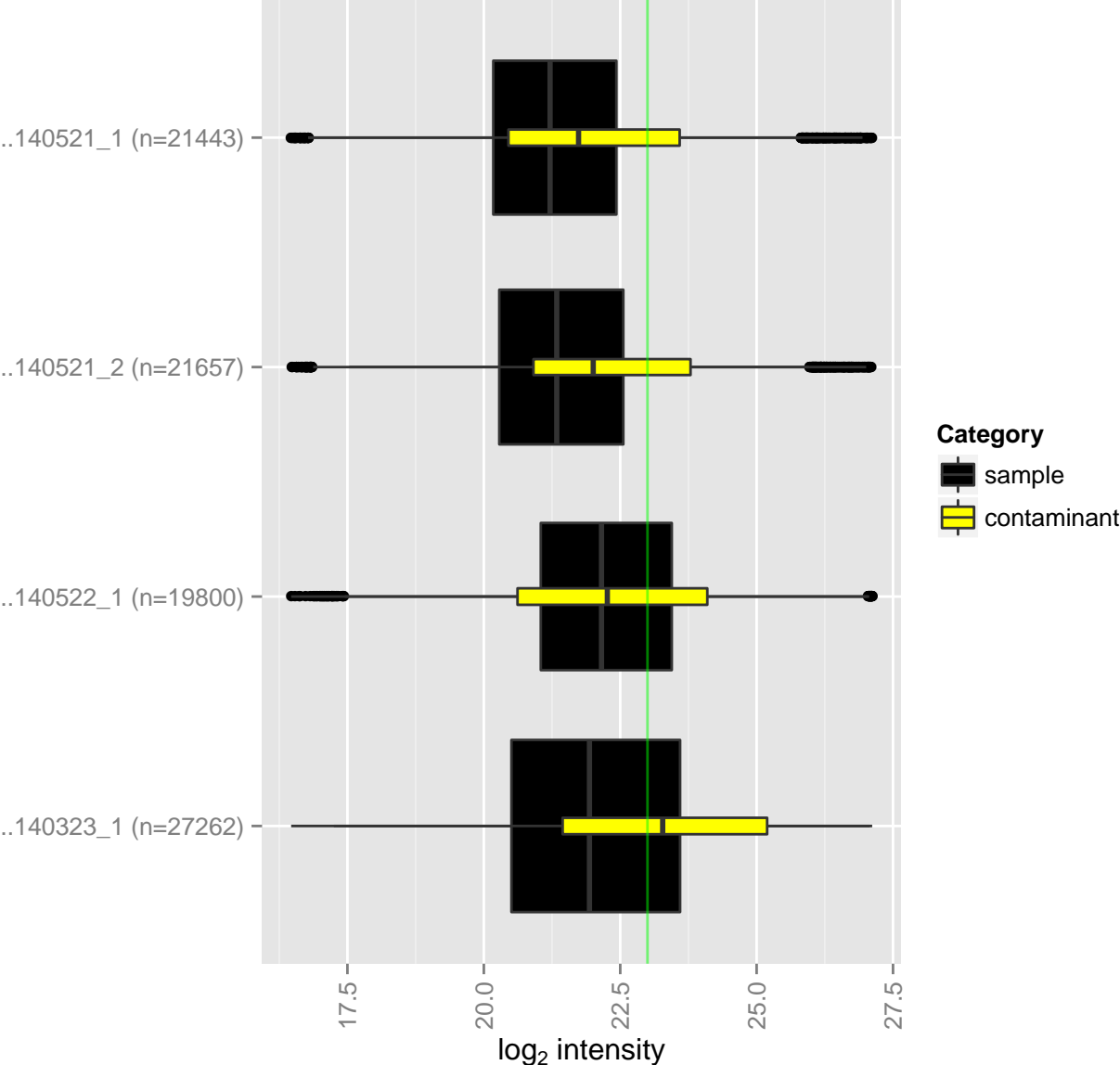


PG: PCA of 'lfq intensity'
(excludes contaminants)



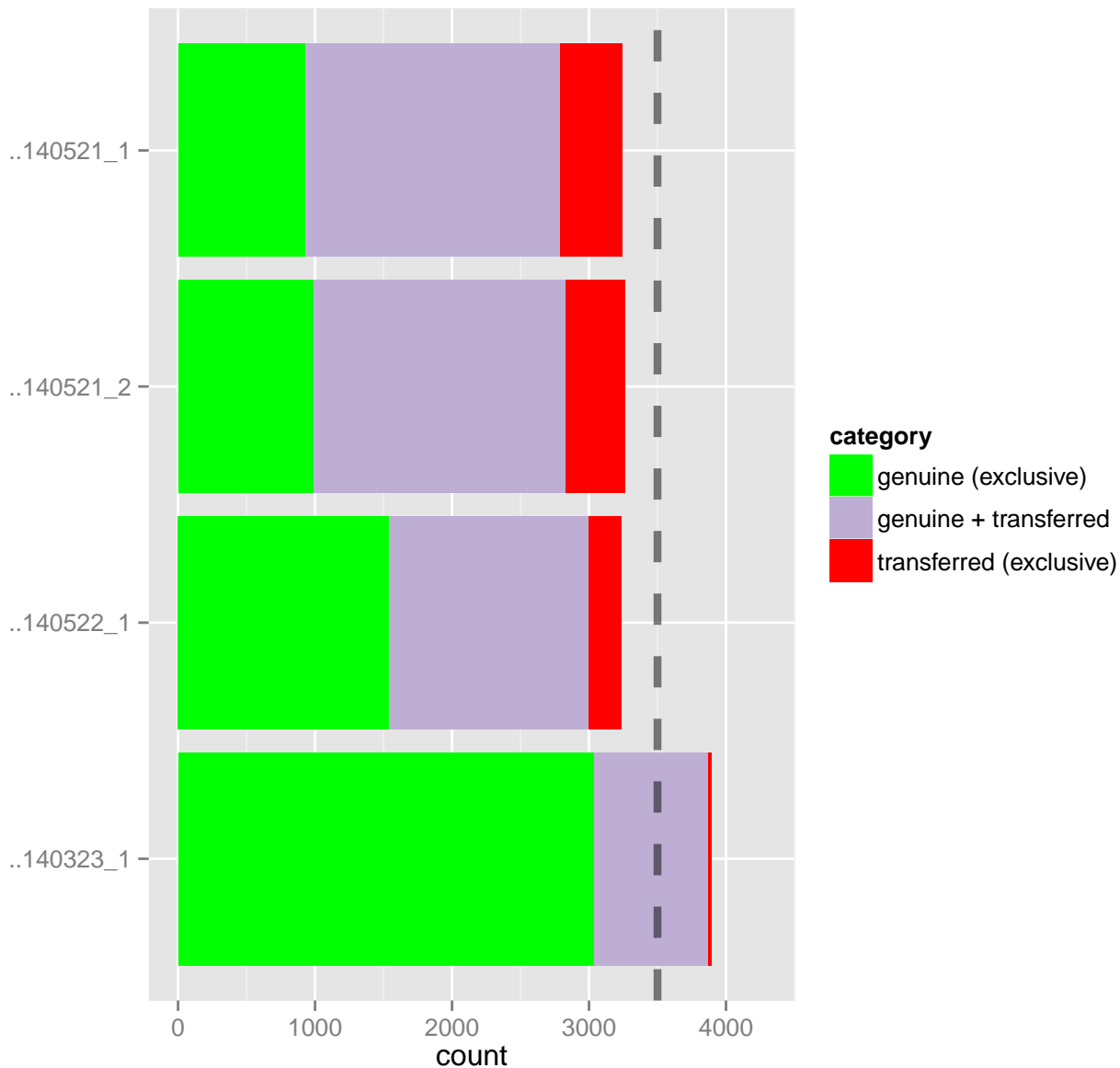
EVD: peptide intensity distribution

RSD 2.2% (expected < 5%)



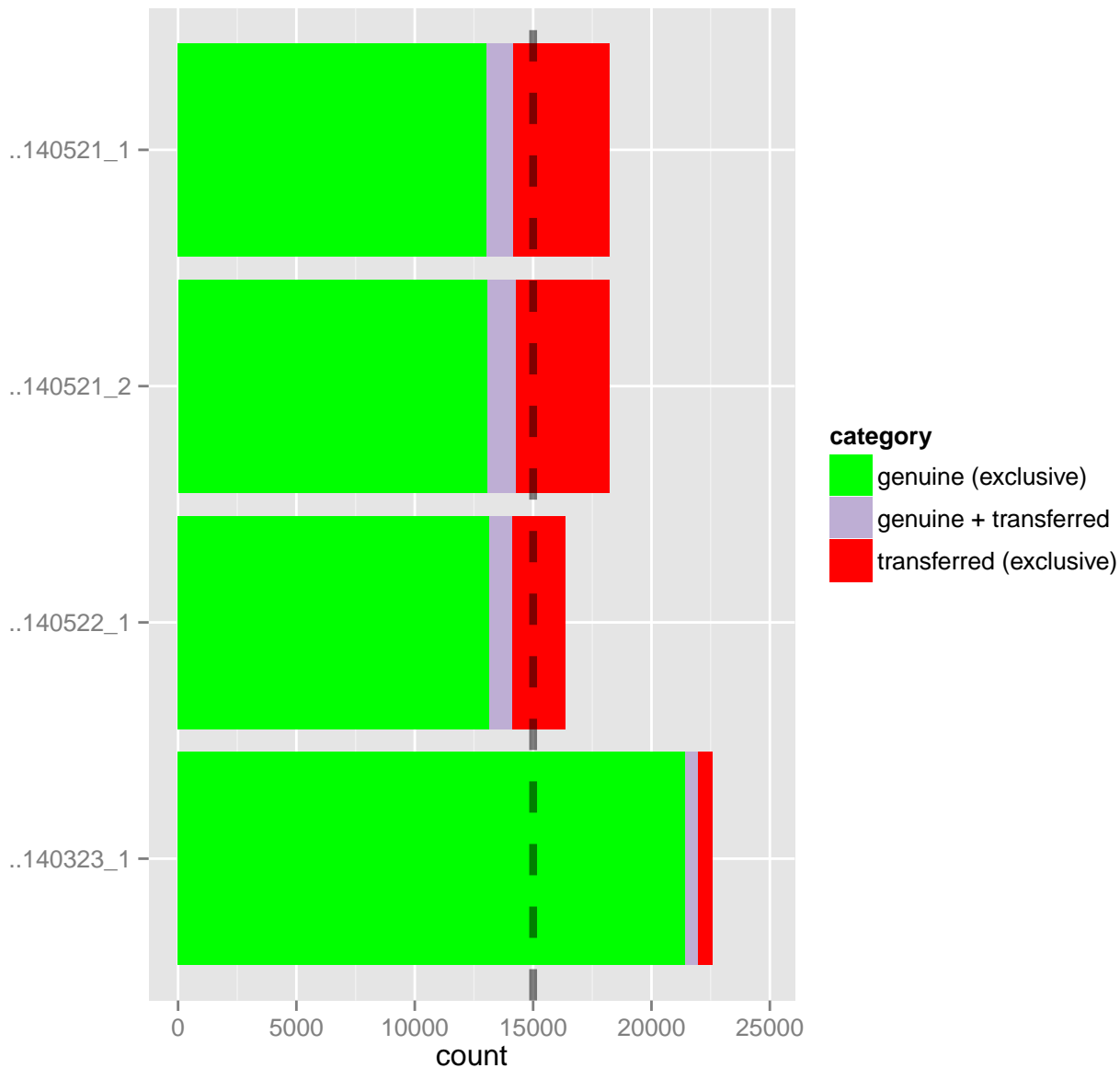
EVD: ProteinGroups count

MBR gain: +10%

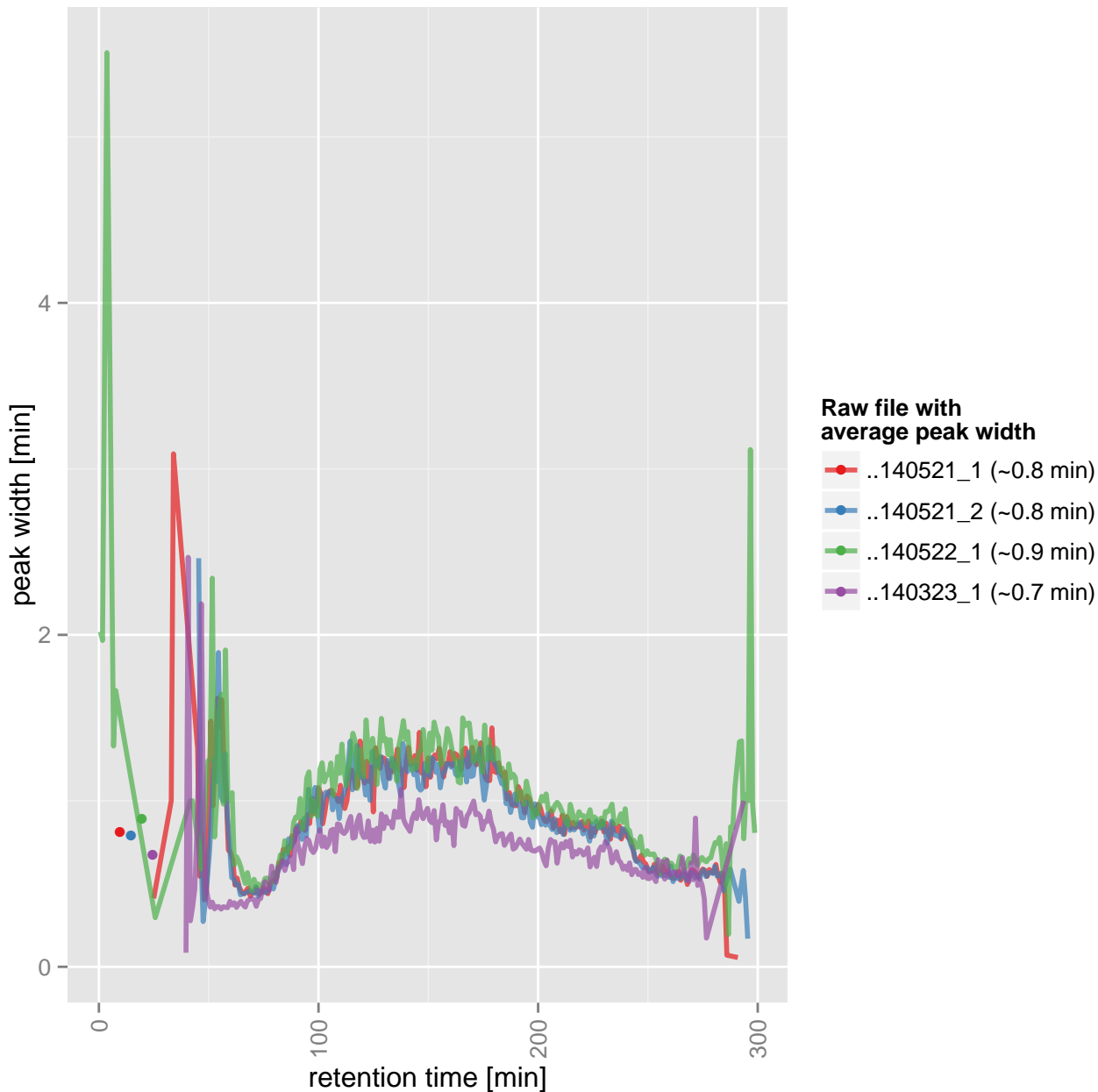


EVD: Peptide ID count

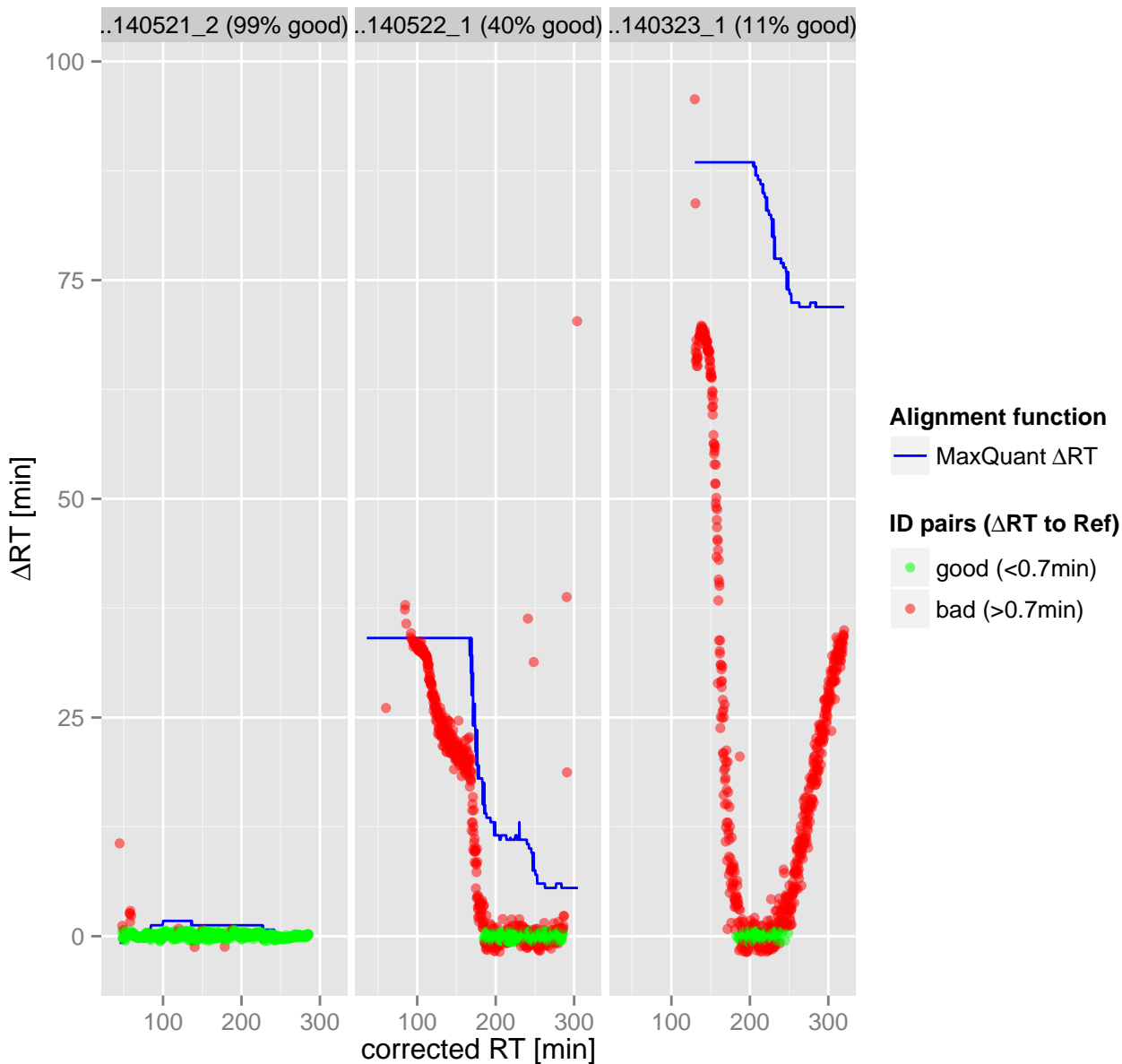
MBR gain: +19%



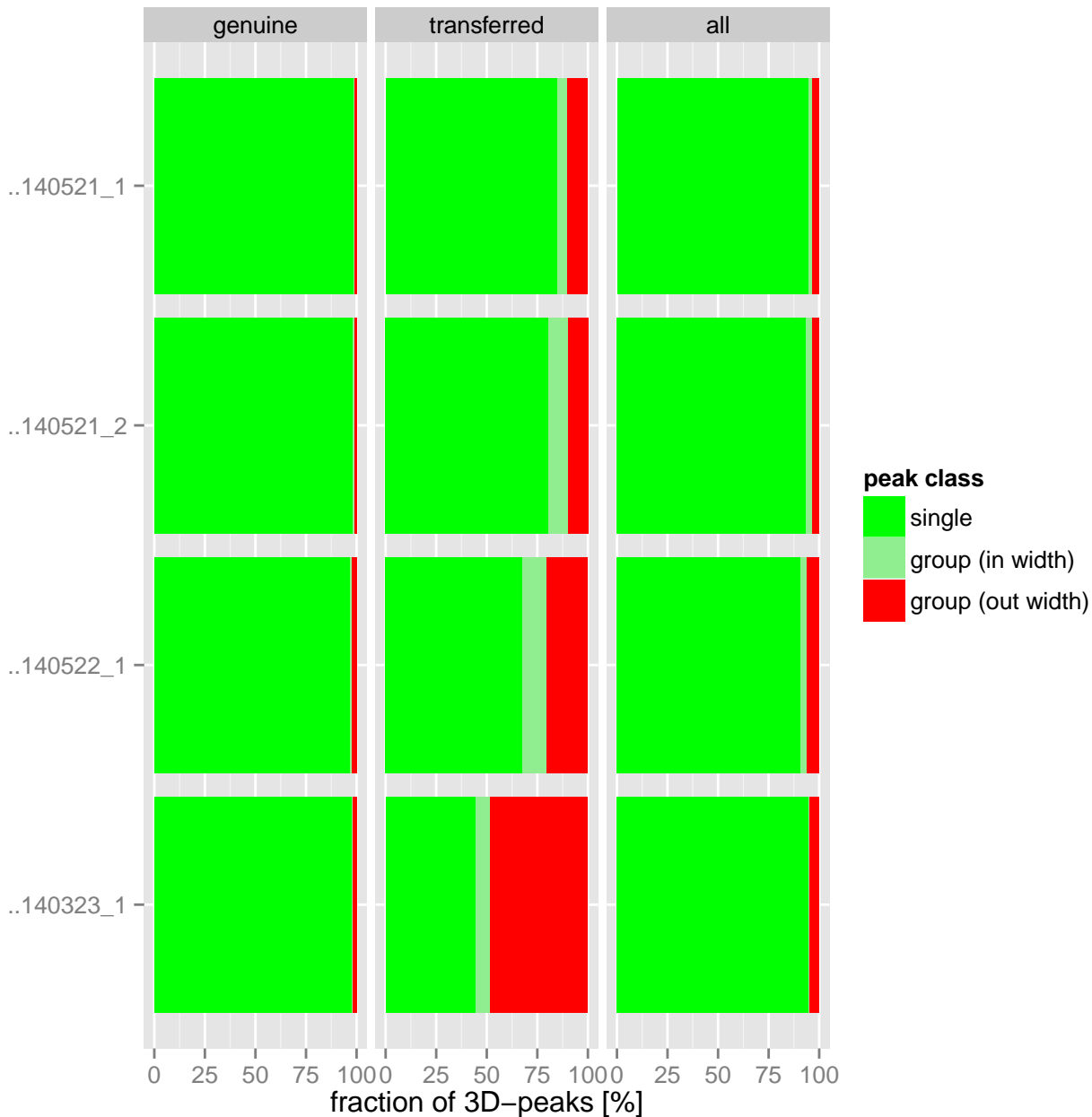
EVD: Peak width over RT



EVD: MBR – alignment

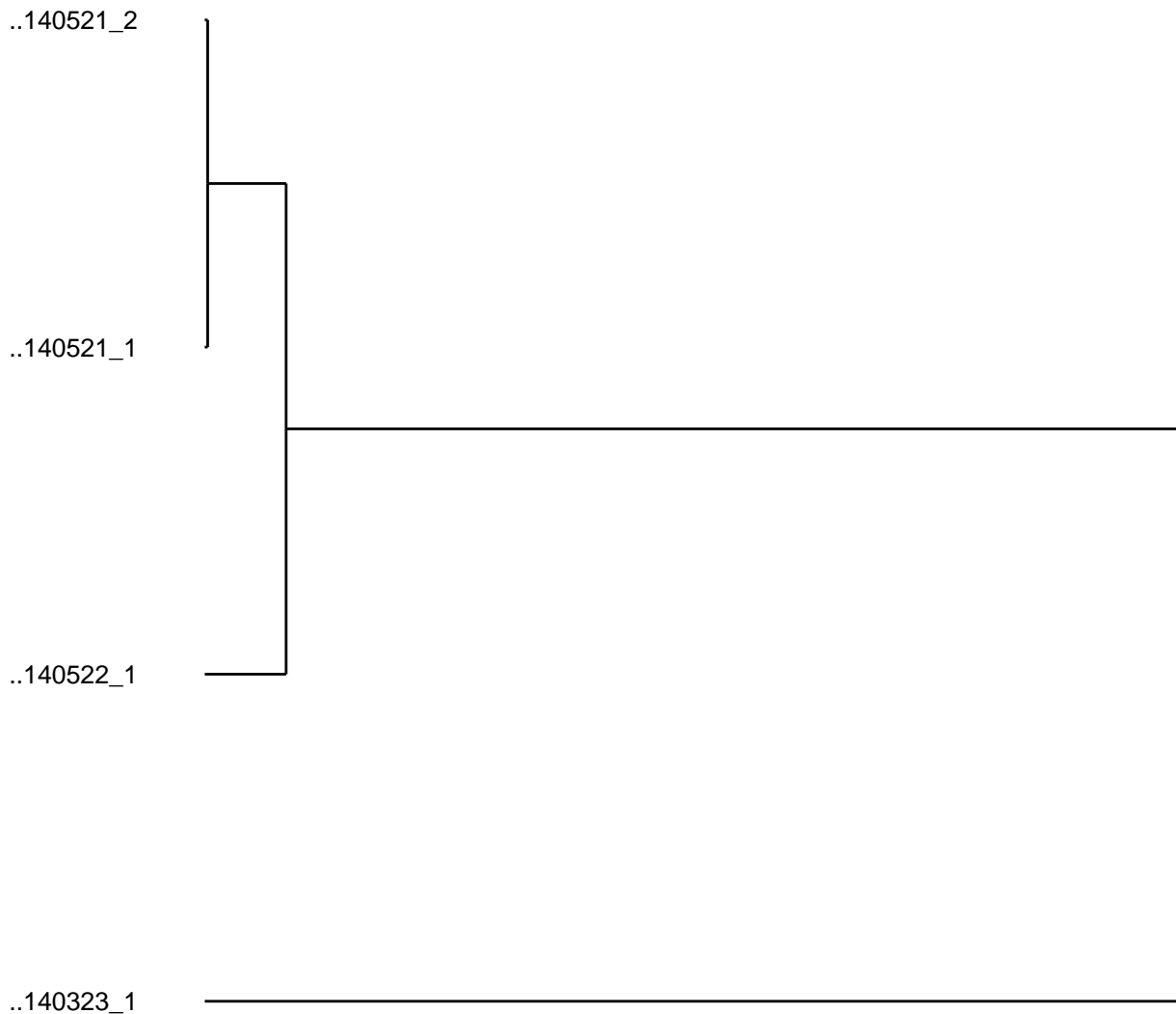


EVD: MBR – ID Transfer

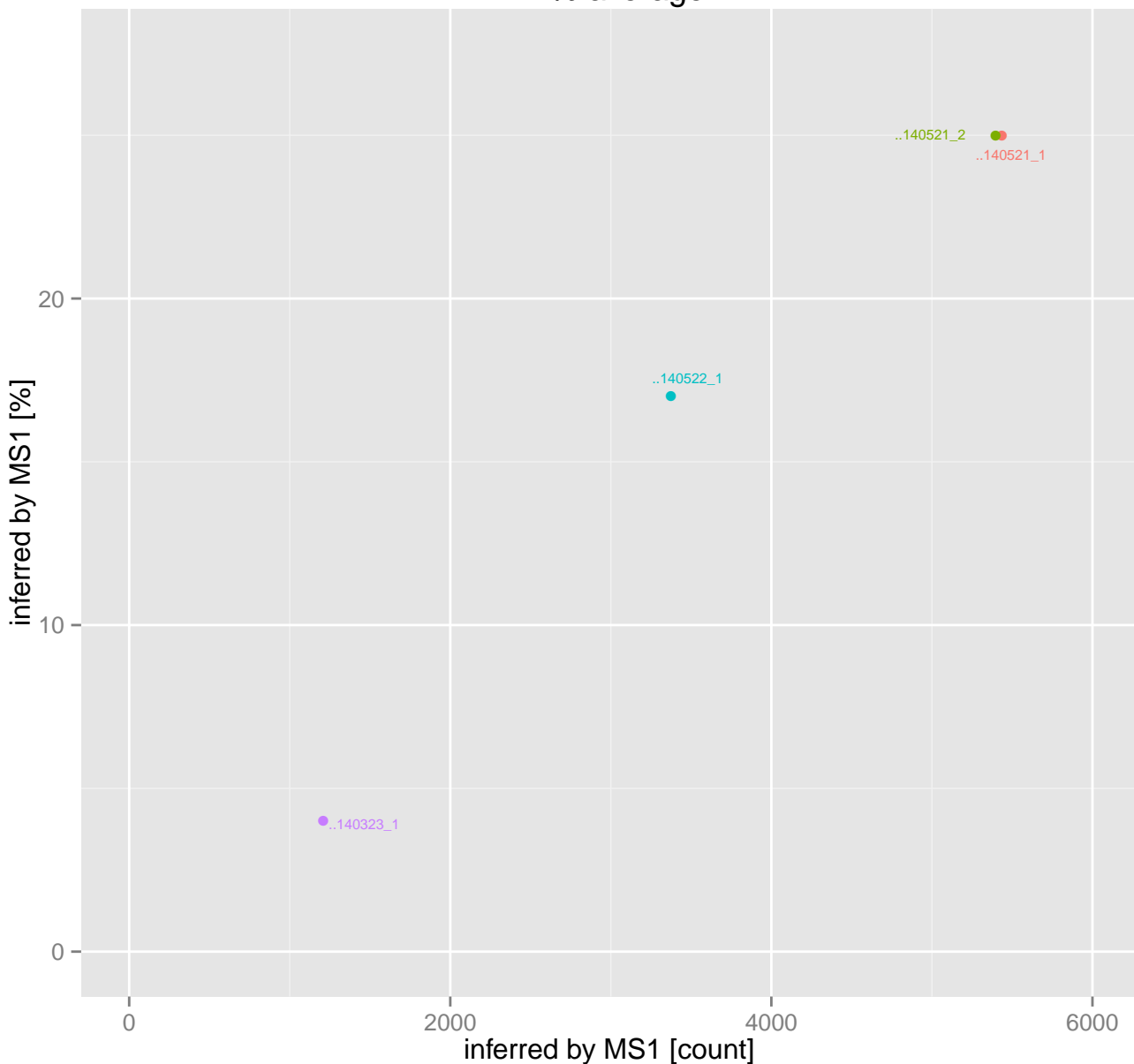


[experimental] EVD: Clustering Tree of Raw files

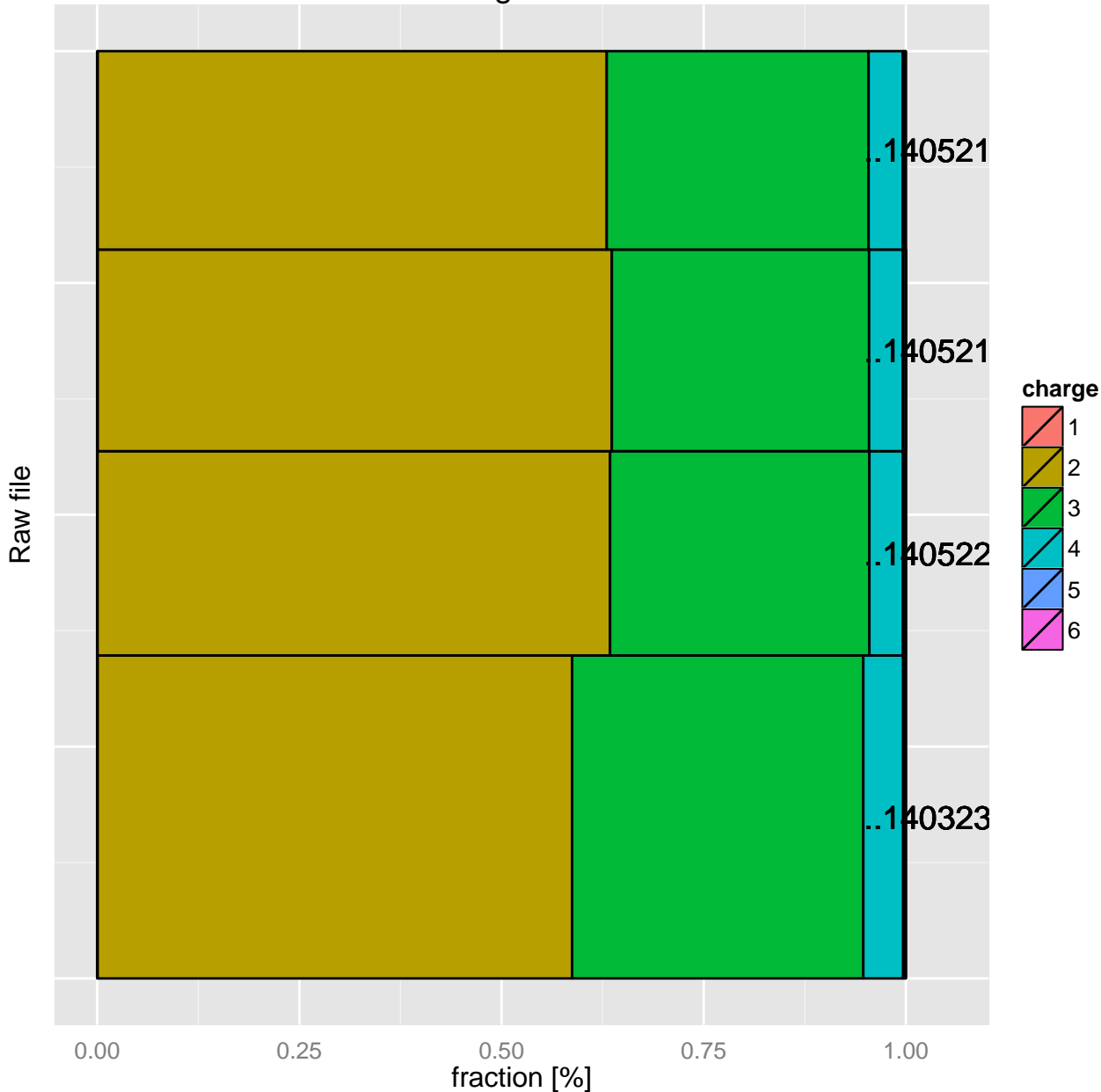
by Correlation of Corrected Retention Times



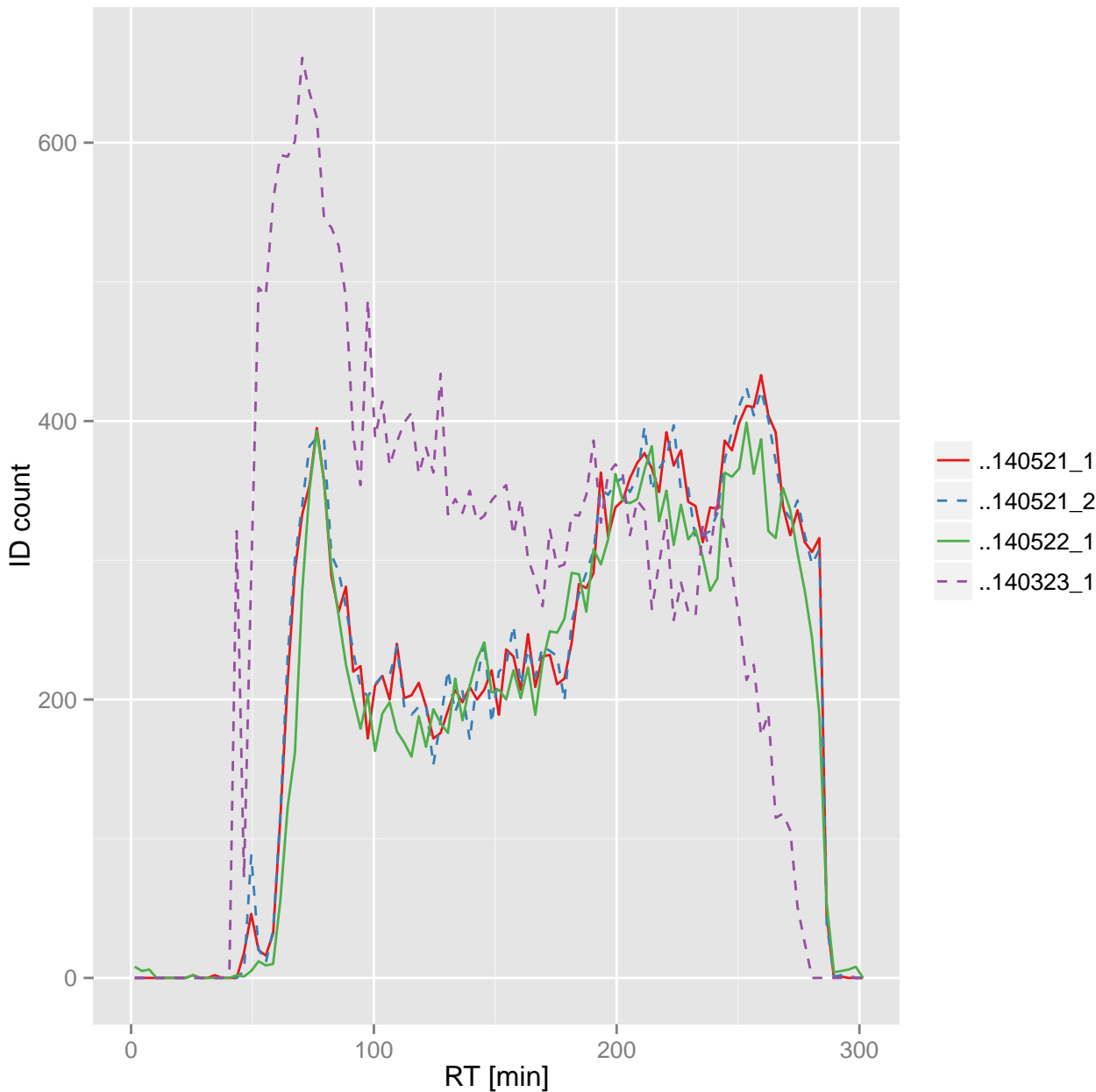
EVD: Peptides inferred by AMT-matching 17% average



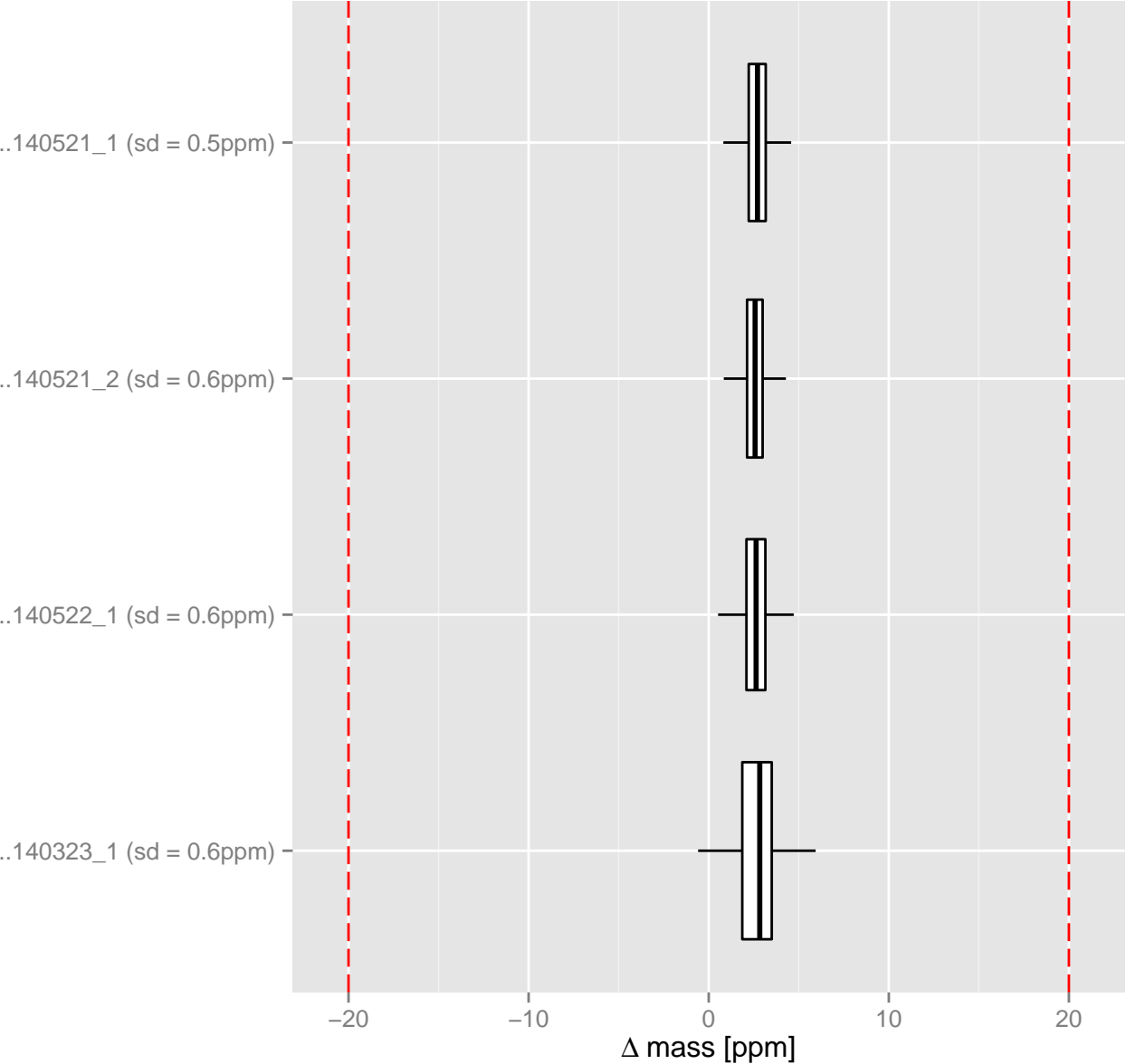
EVD: charge distribution



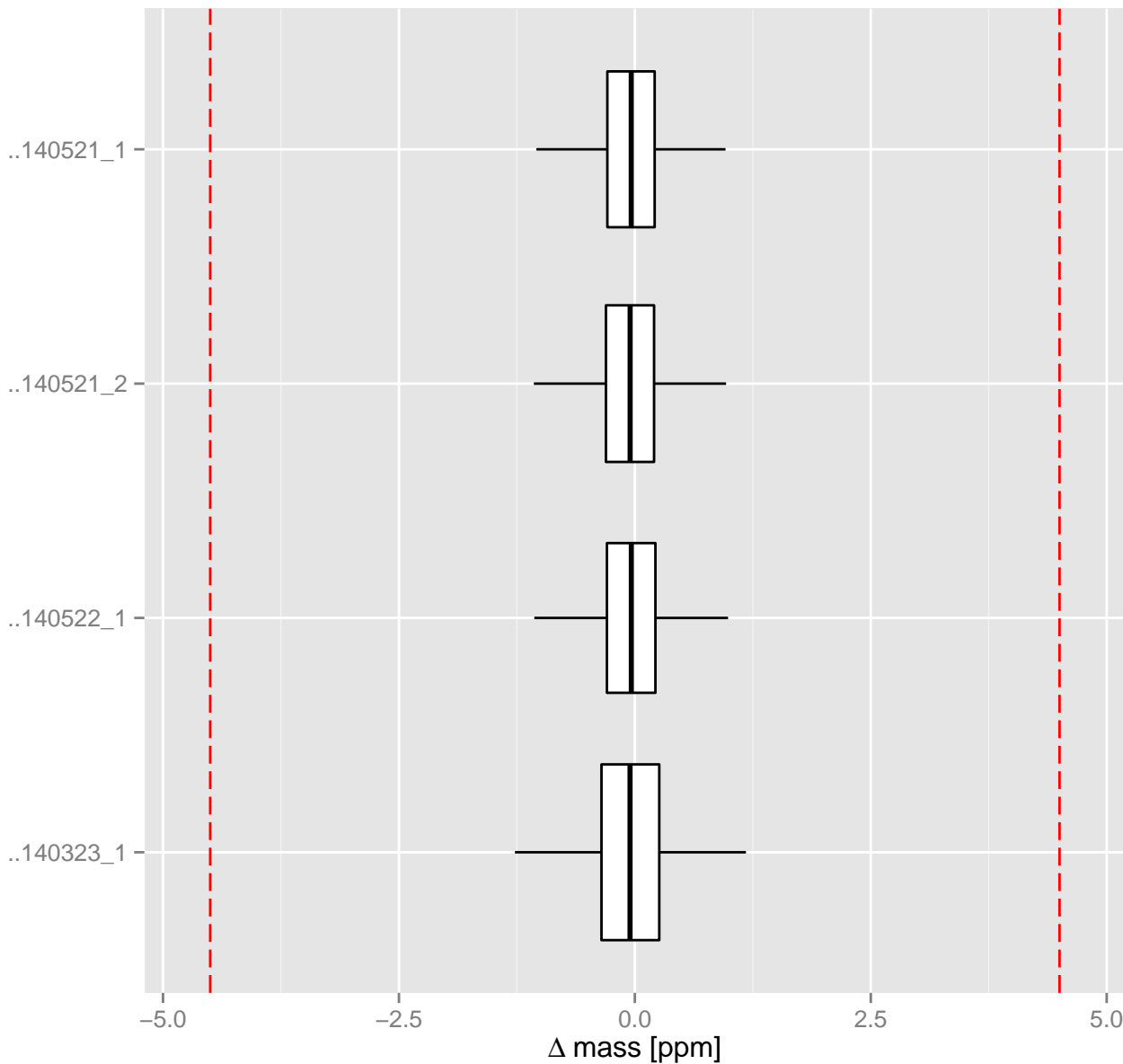
EVD: IDs over RT



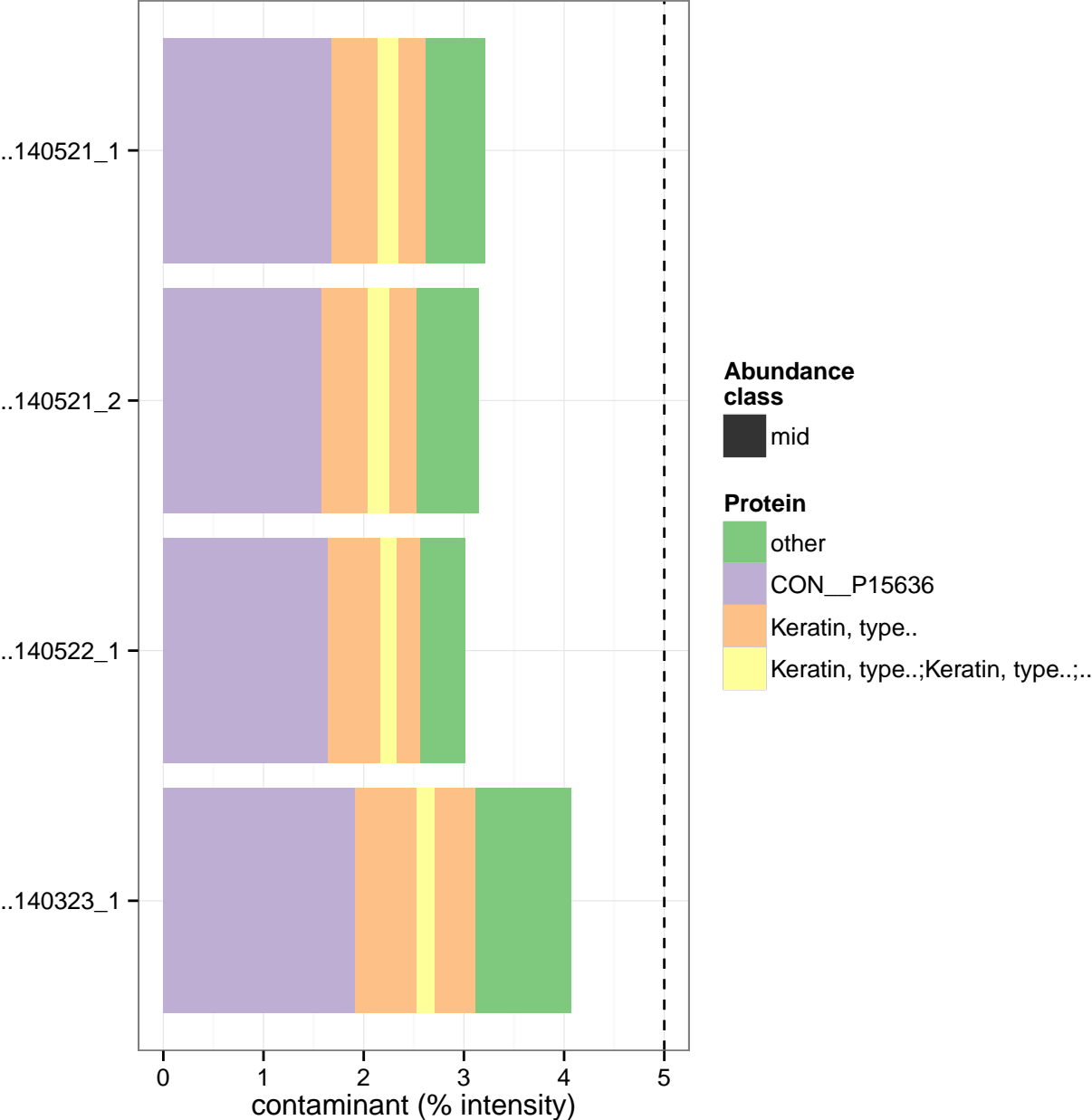
EVD: Uncalibrated mass error



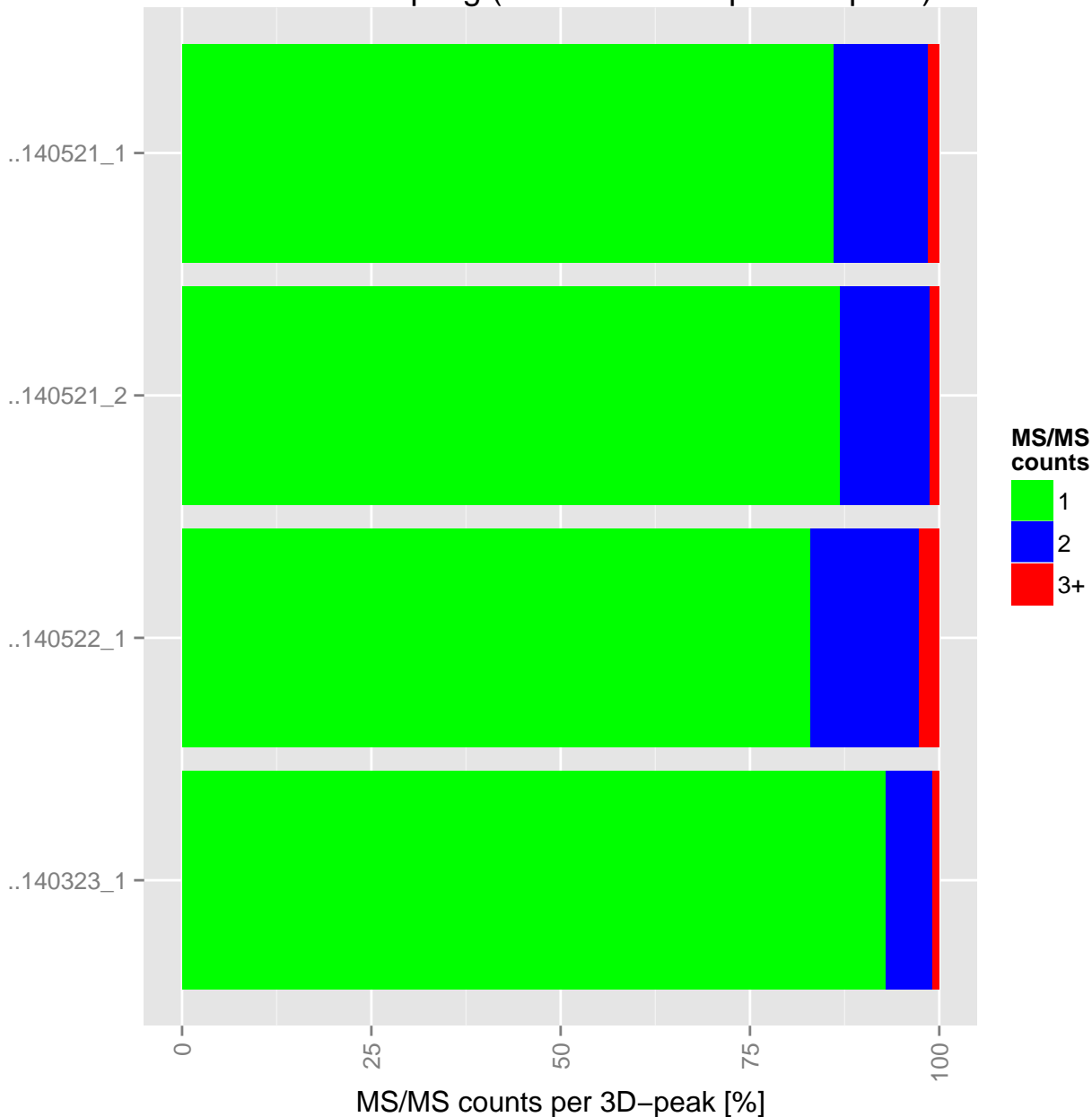
EVD: Calibrated mass error



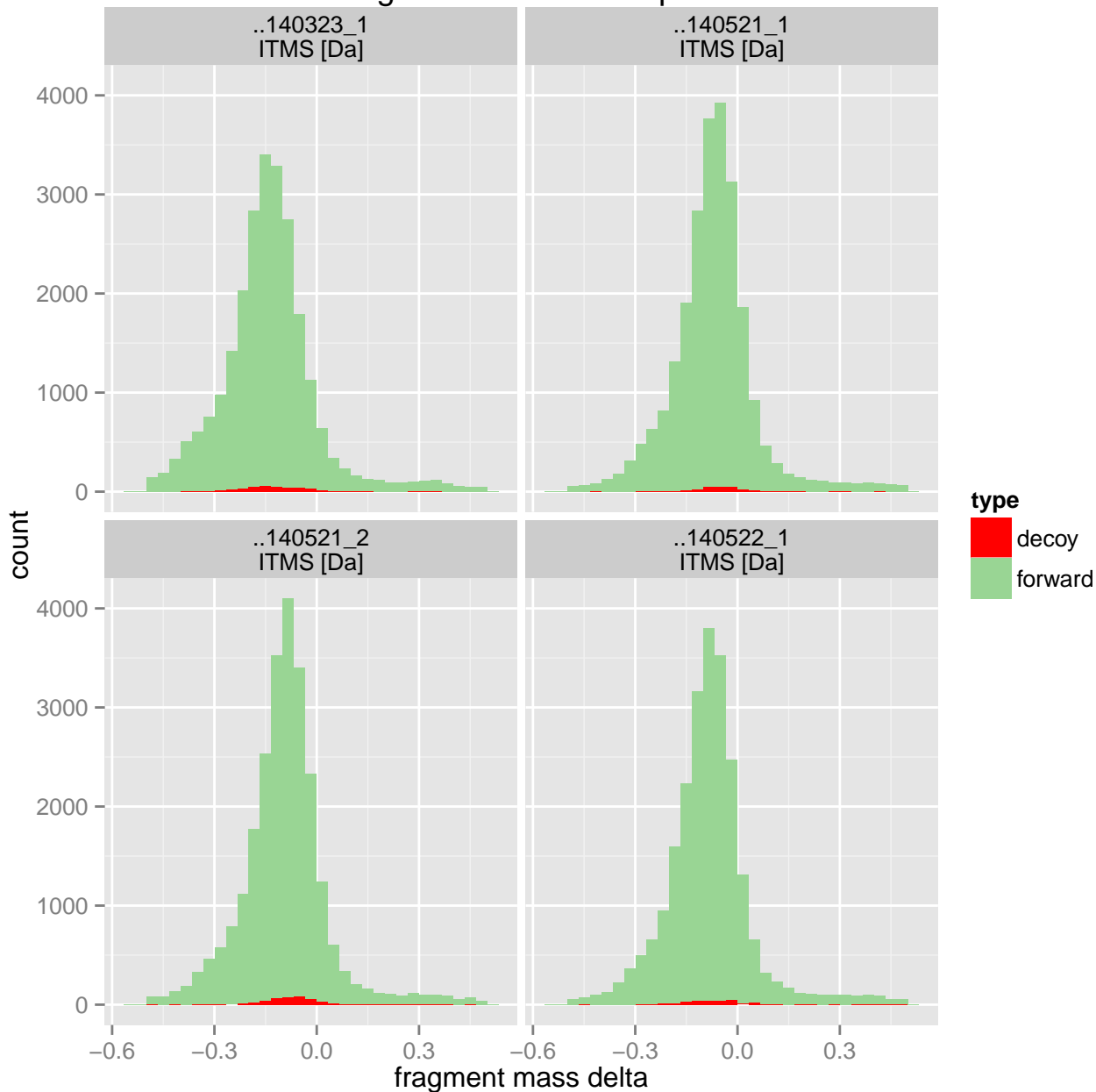
EVD: Contaminant per Raw file



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

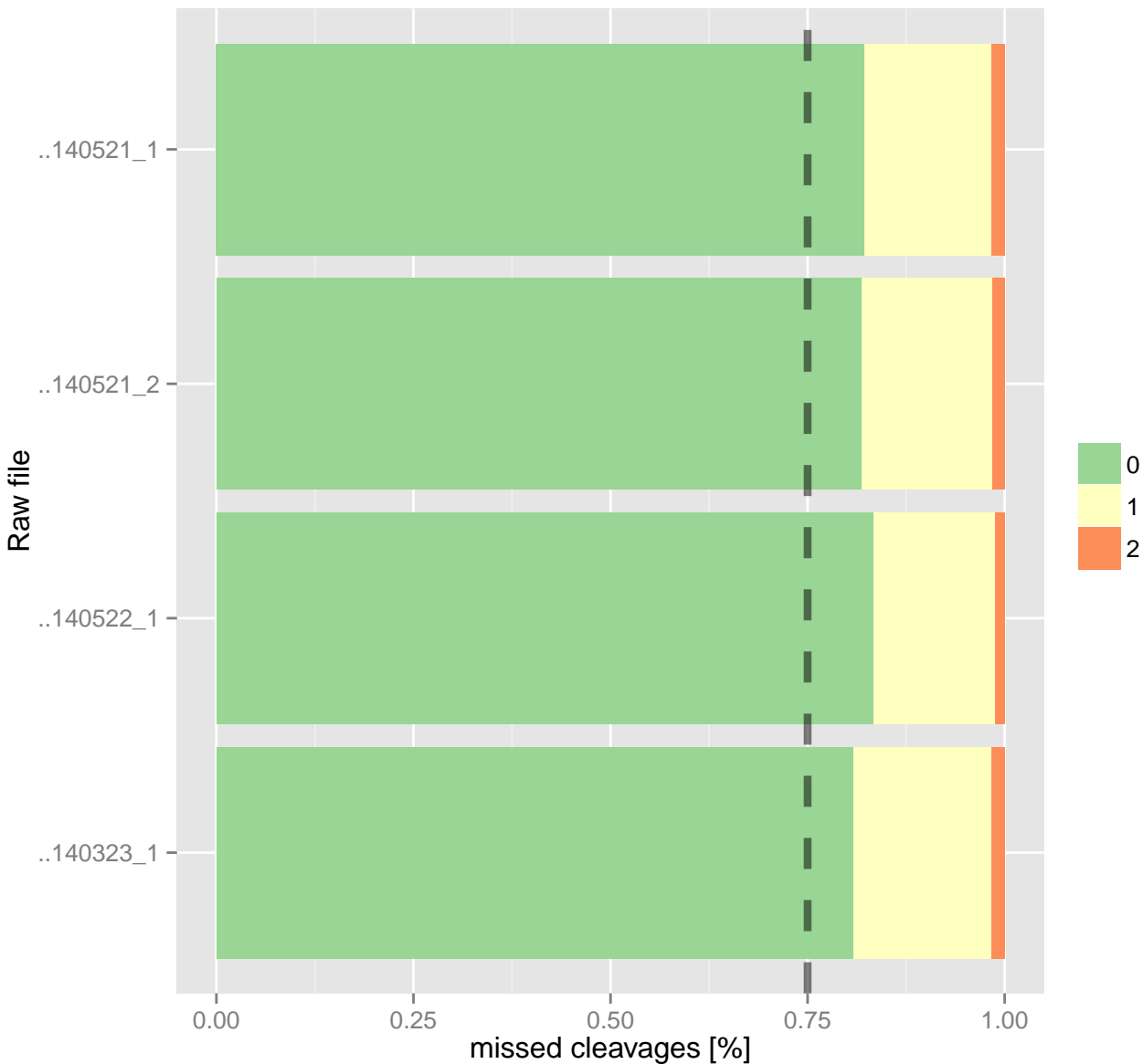


MSMS: Fragment mass errors per Raw file

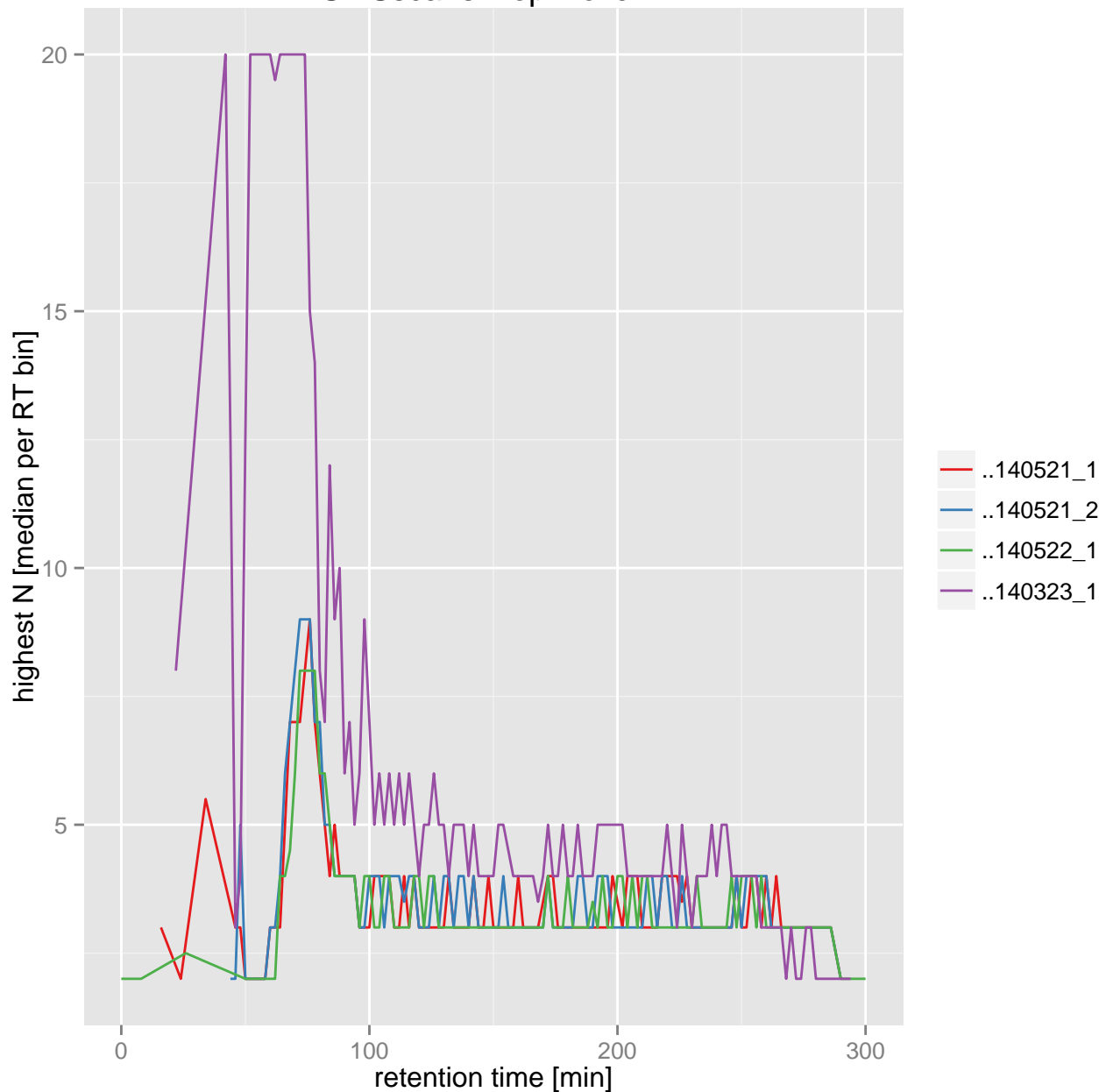


MSMS: Missed cleavages per Raw file

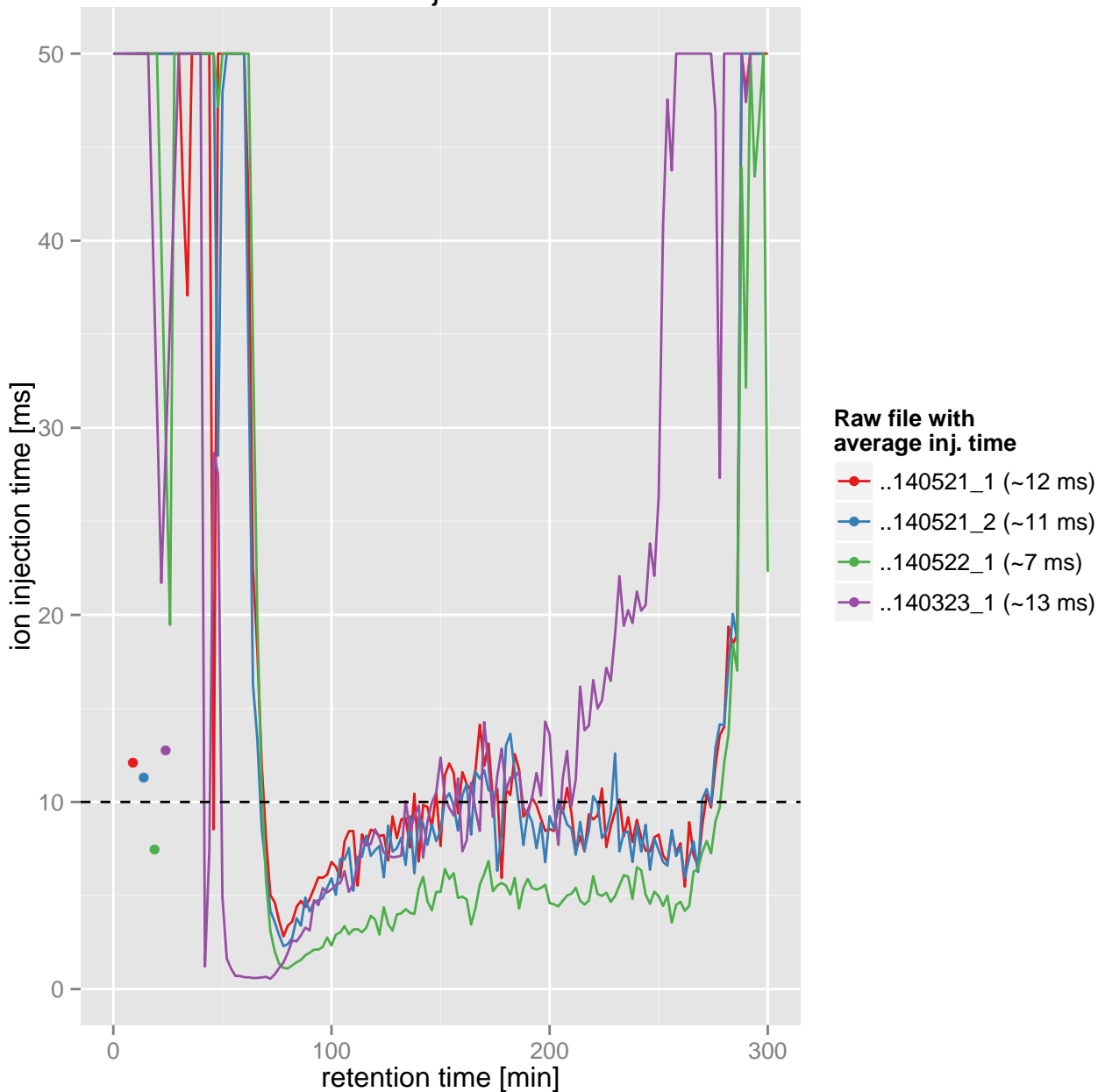
(excludes contaminants)



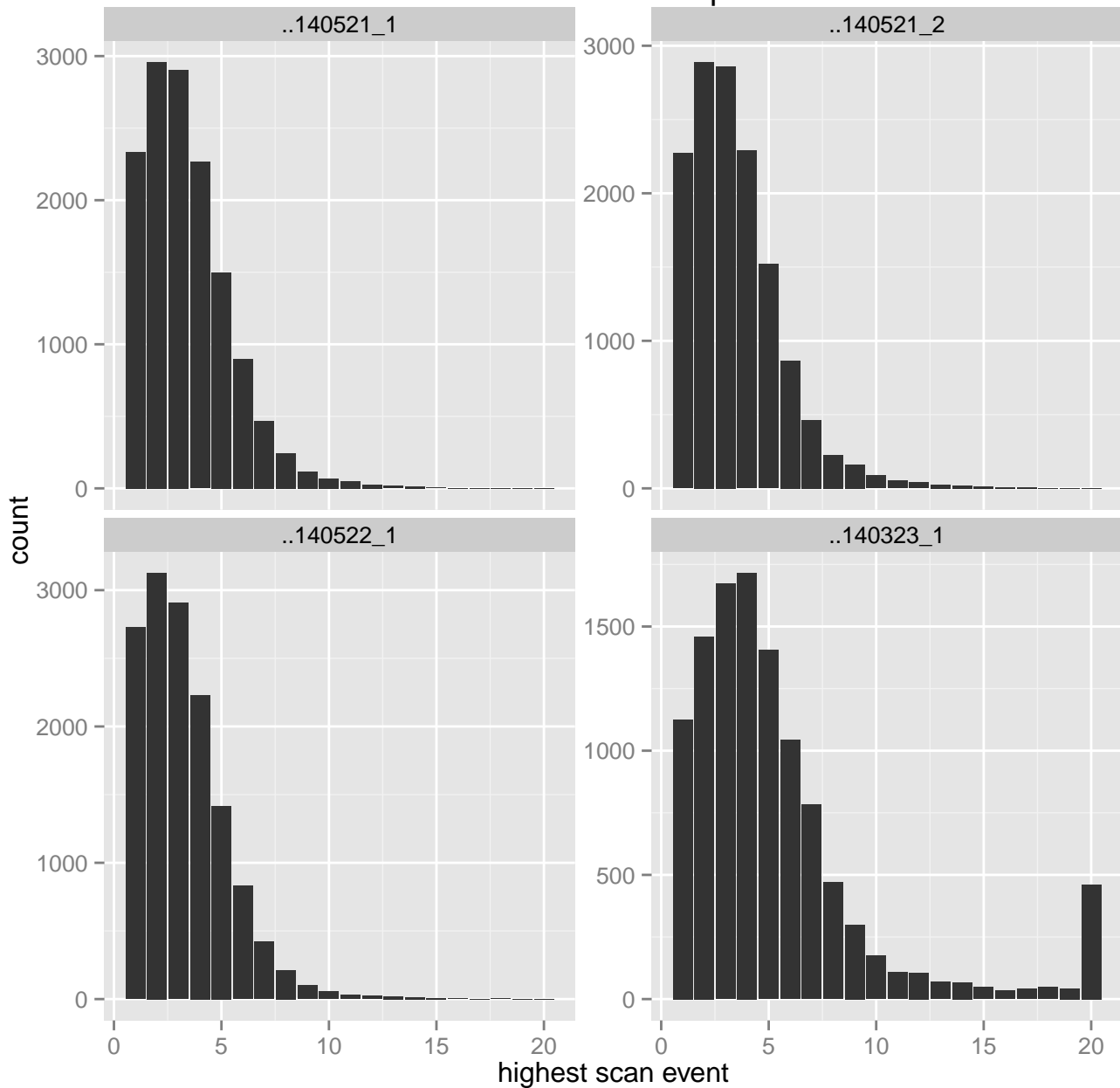
MSMSscans: TopN over RT



MSMSScans: Ion Injection Time over RT



MSMSscans: TopN



MSMSscans: TopN % identified over N

