

PAR: parameters

Version	1.4.1.2	Min. delta score for modifie..	17
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	Site quantification	Use least modified peptide
MS/MS deisotoping (ITMS)	False	Re-quantify	True
MS/MS tol. (TOF)	0.1 Da	Use delta score	False
Top MS/MS peaks per 100 Da. ..	10	iBAQ	False
MS/MS deisotoping (TOF)	False	iBAQ log fit	False
MS/MS tol. (Unknown)	0.5 Da	MS/MS recalibration	False
Top MS/MS peaks per 100 Da. ..	10	Match between runs	True
MS/MS deisotoping (Unknown)	False	Matching time window [min]	1
PSM FDR	0.01	Alignment time window [min]	100
Protein FDR	0.01	Find dependent peptides	False
Site FDR	0.01	Labeled amino acid filtering	True
Use Normalized Ratios For Oc..	True	Site tables	Oxidation (M)Sites.txt
Min. peptide Length	7	Cut peaks	True
Min. score for unmodified pe..	0	RT shift	False
Min. score for modified pept..	40	Advanced ratios	False
Min. delta score for unmodif..	0	First pass AIF correlation	0.8

uniprot_human_canonical_and_isoforms_20130513.fasta

Info: mapping of raw files to their short names
(automatic shortening of names was not sufficiently short – see 'best effort')

original	short name	best_effort
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Toni_20140521_GM_QC_01	f 1	521_GM_QC_01
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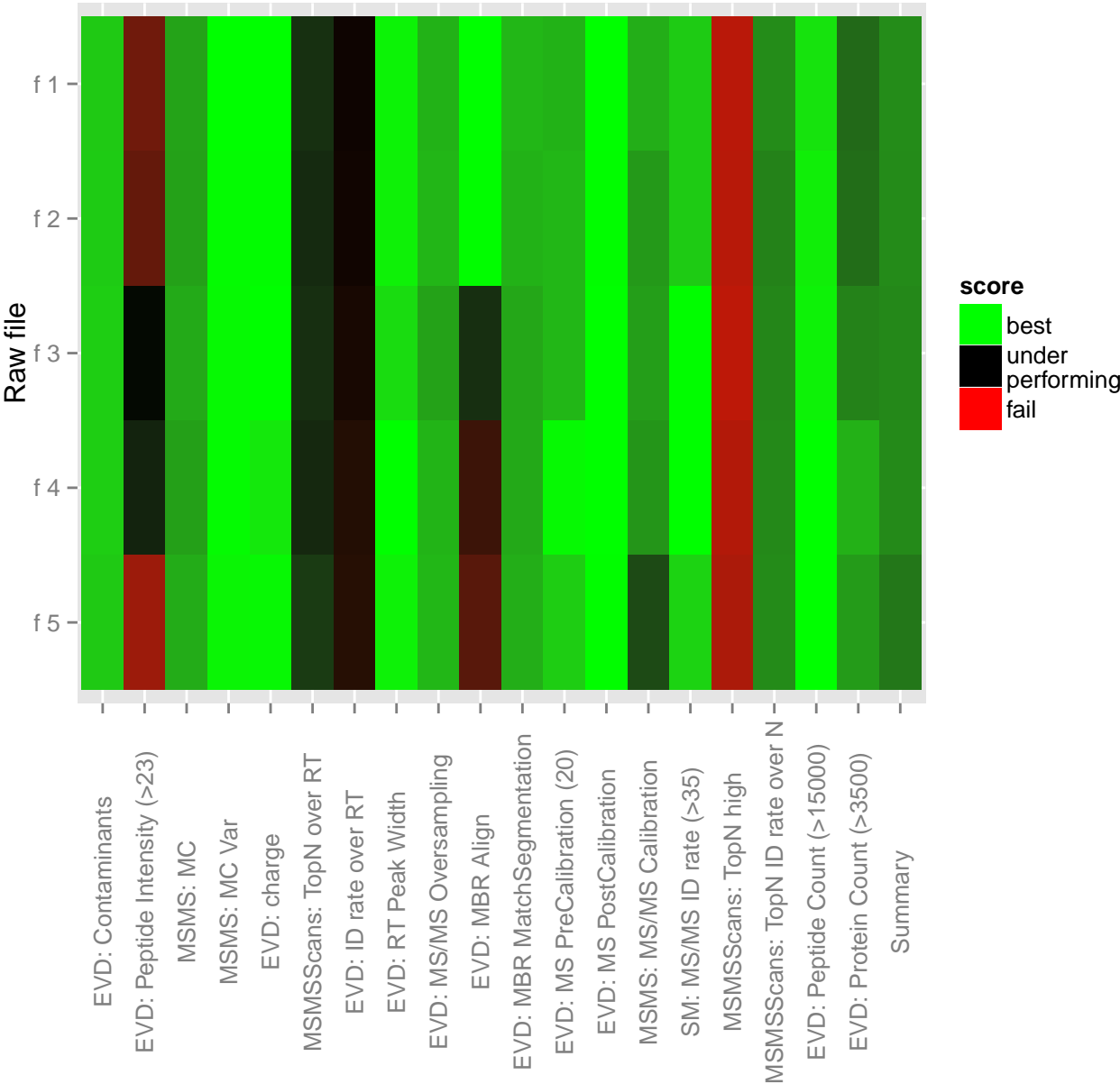
Toni_20140521_GM_QC_02	f 2	521_GM_QC_02
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Toni_20140522_GM_QC_01	f 3	522_GM_QC_01
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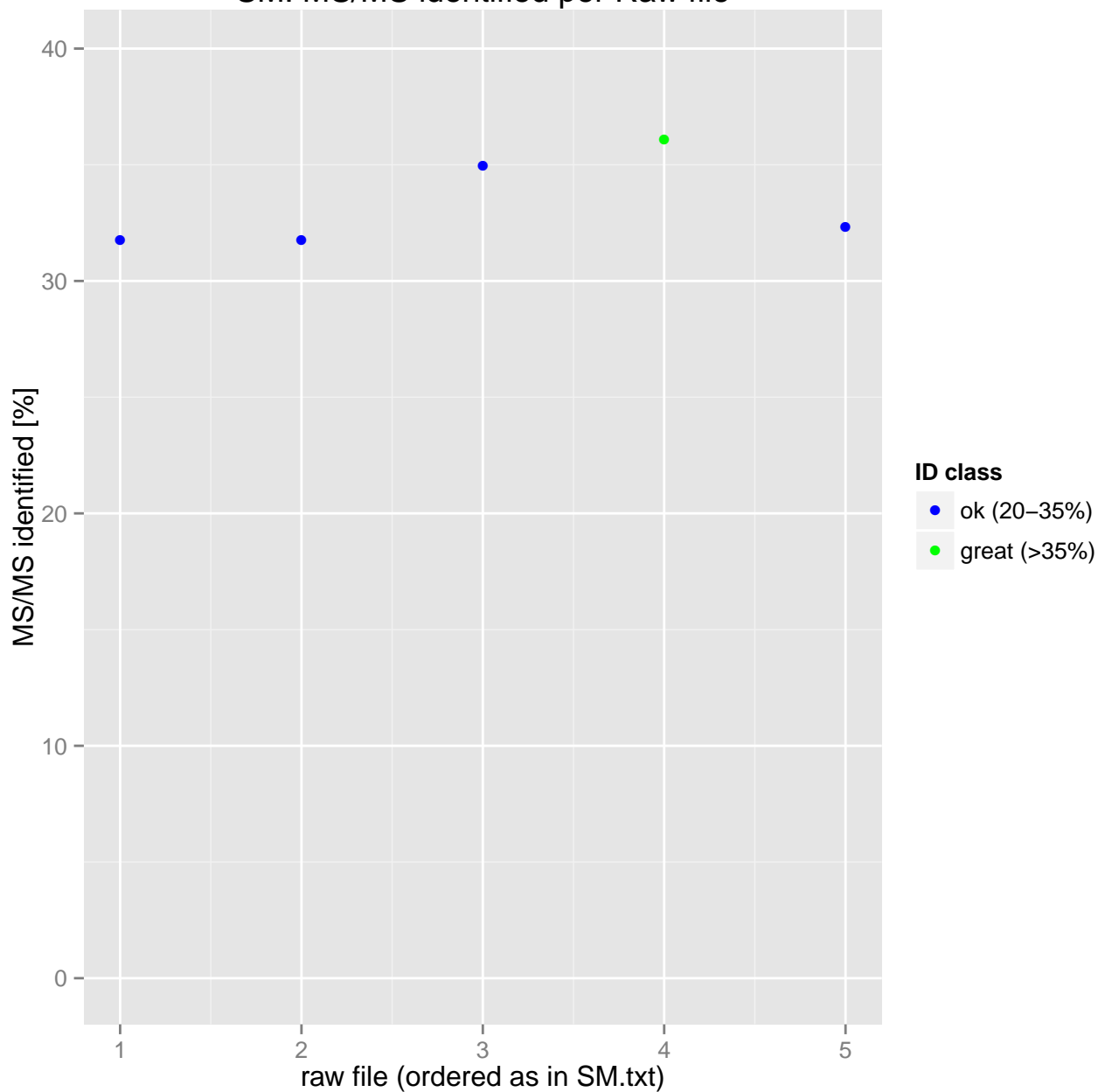
Toni_20140531_FB_QC_02	f 4	531_FB_QC_02
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Toni_20140608_FB_qc_01	f 5	608_FB_qc_01
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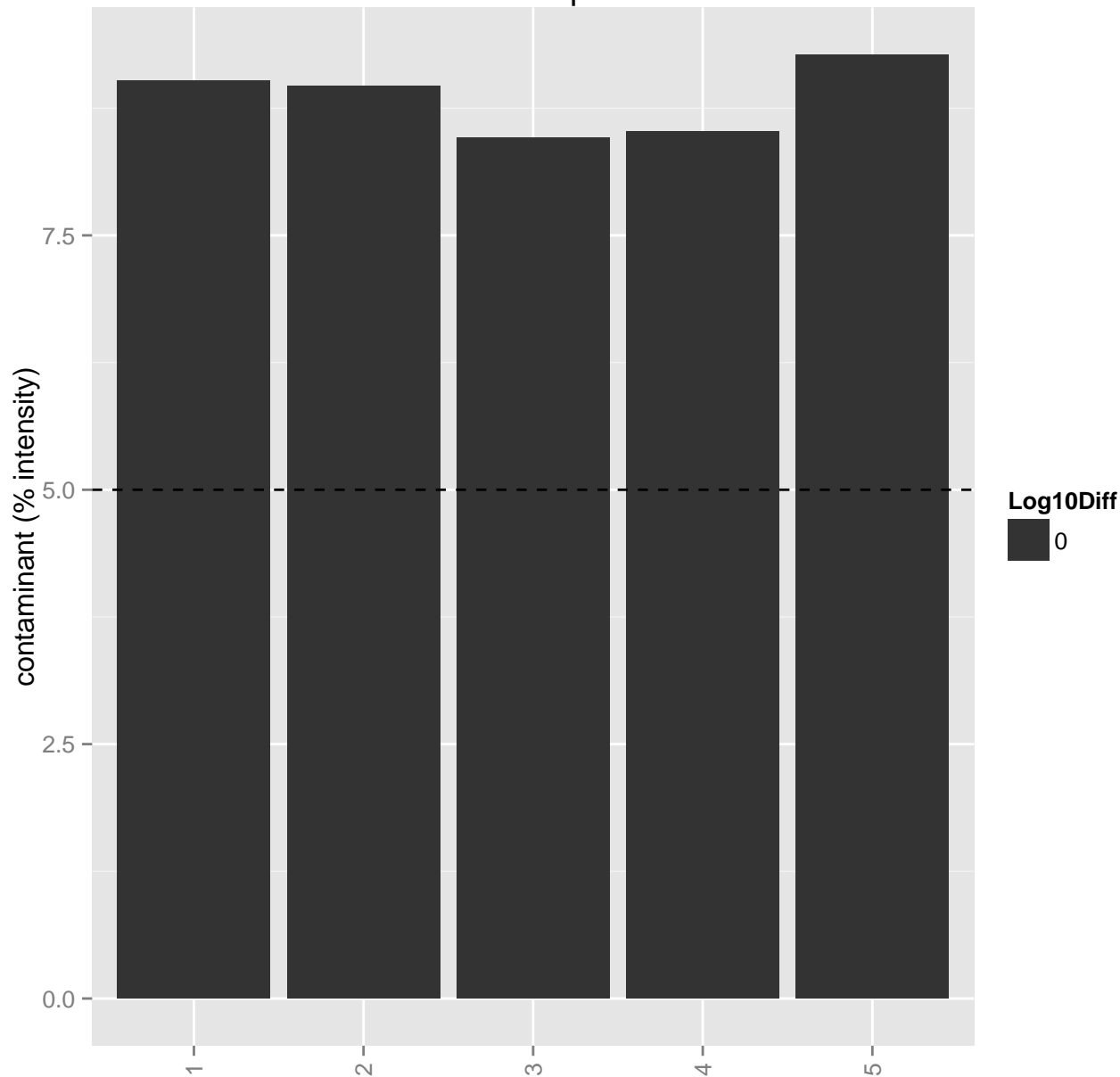
Performance overview



SM: MS/MS identified per Raw file



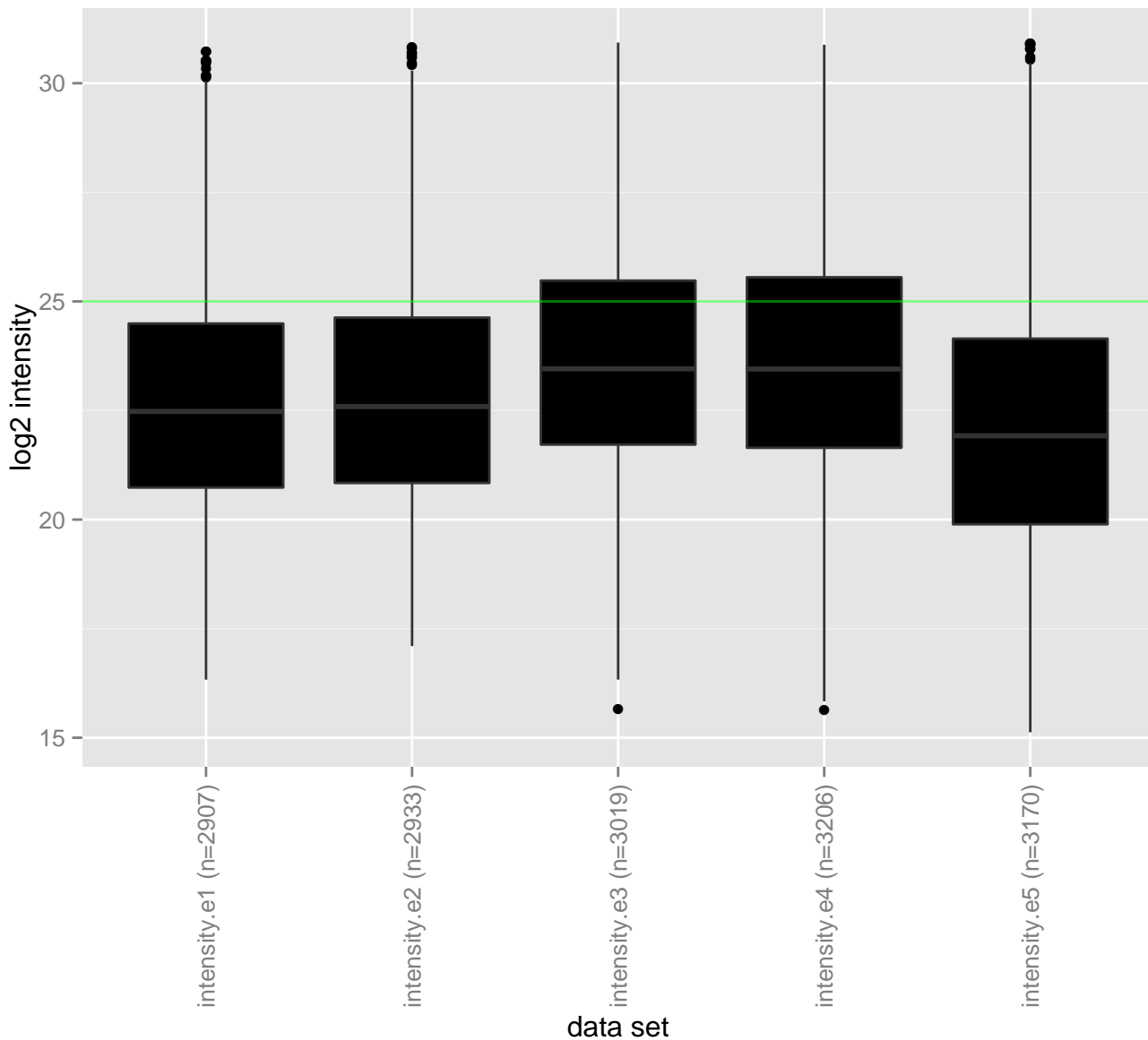
PG: Contaminant per condition



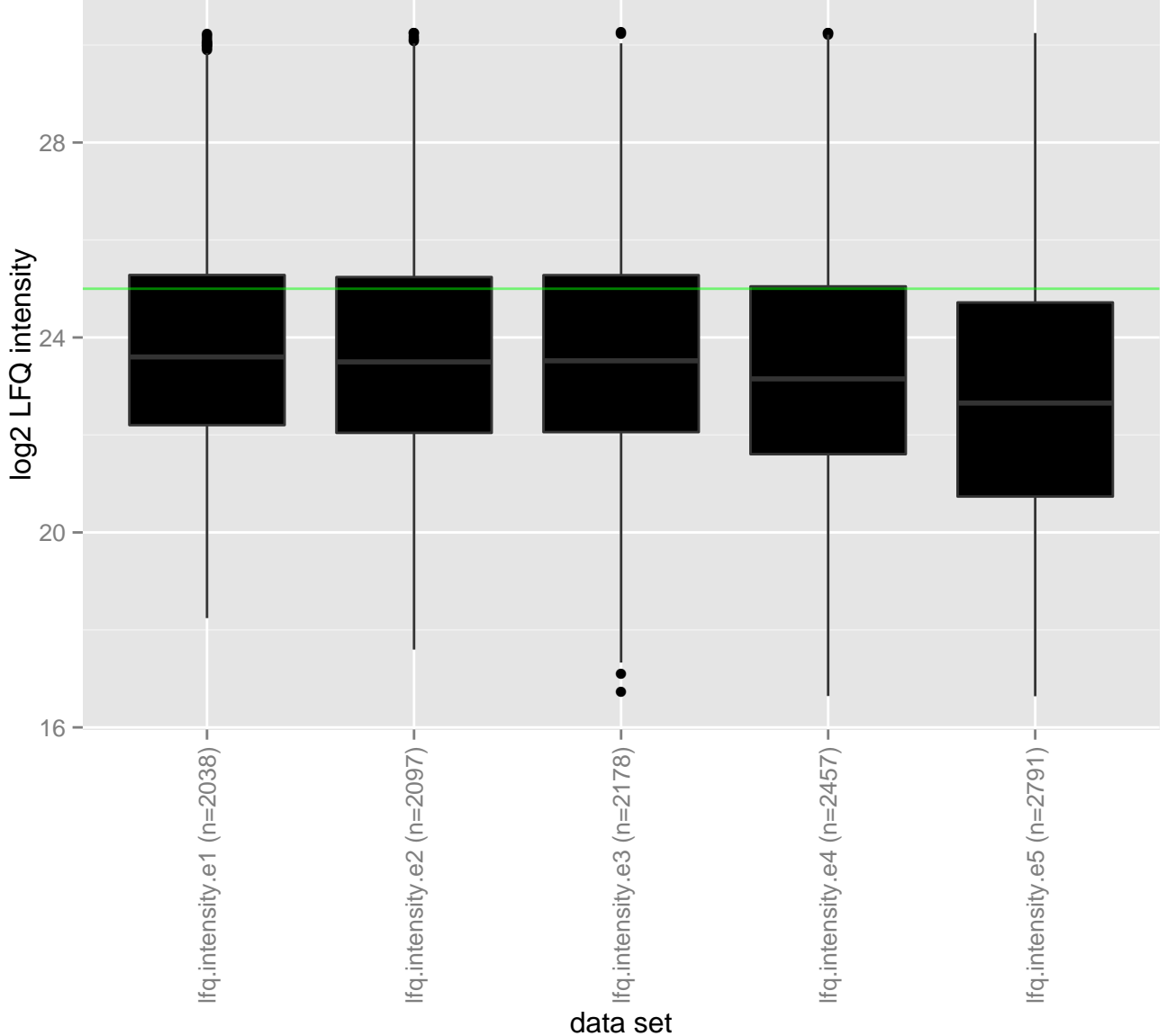
PG: intensity distribution

RSD 3% (should be < 5%)

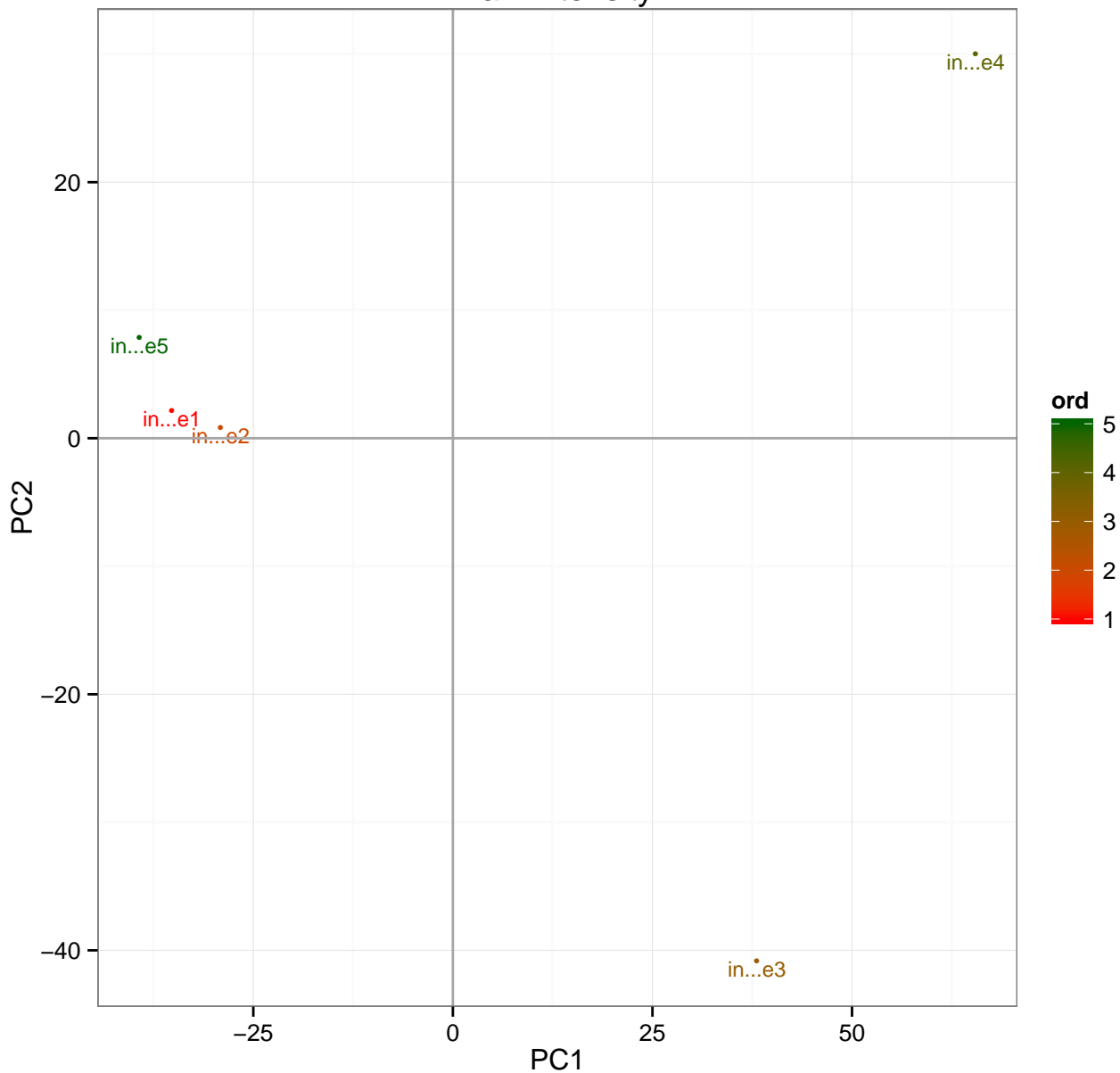
RSD 3.2% (with 0's remaining) [high RSD indicates few peptides]



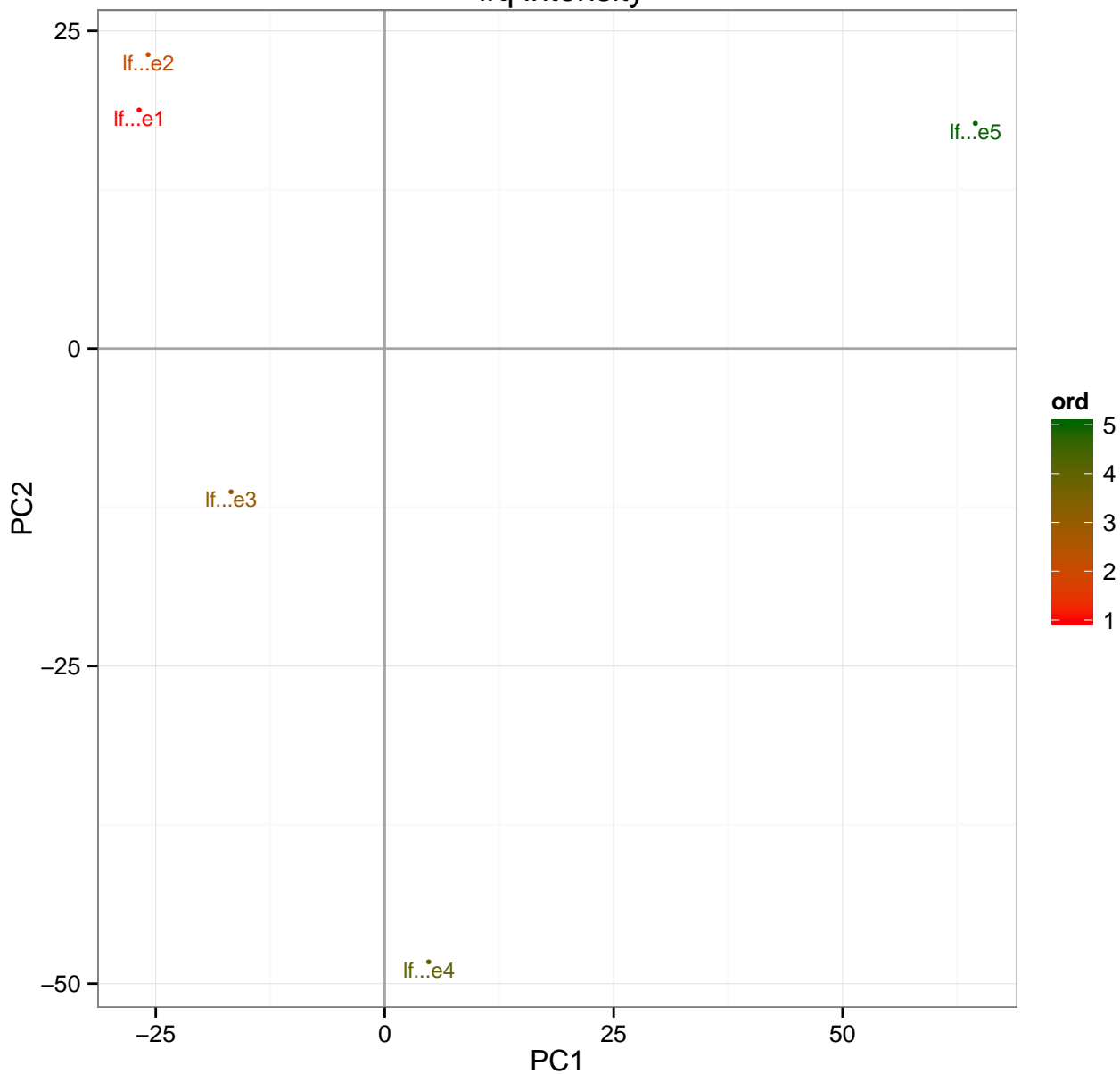
PG: LFQ intensity distribution
RSD 1.7% (should be < 5%)
RSD 0.5% (with 0's remaining) [high RSD indicates few peptides]



PG: PCA
raw intensity



PG: PCA
lfq intensity

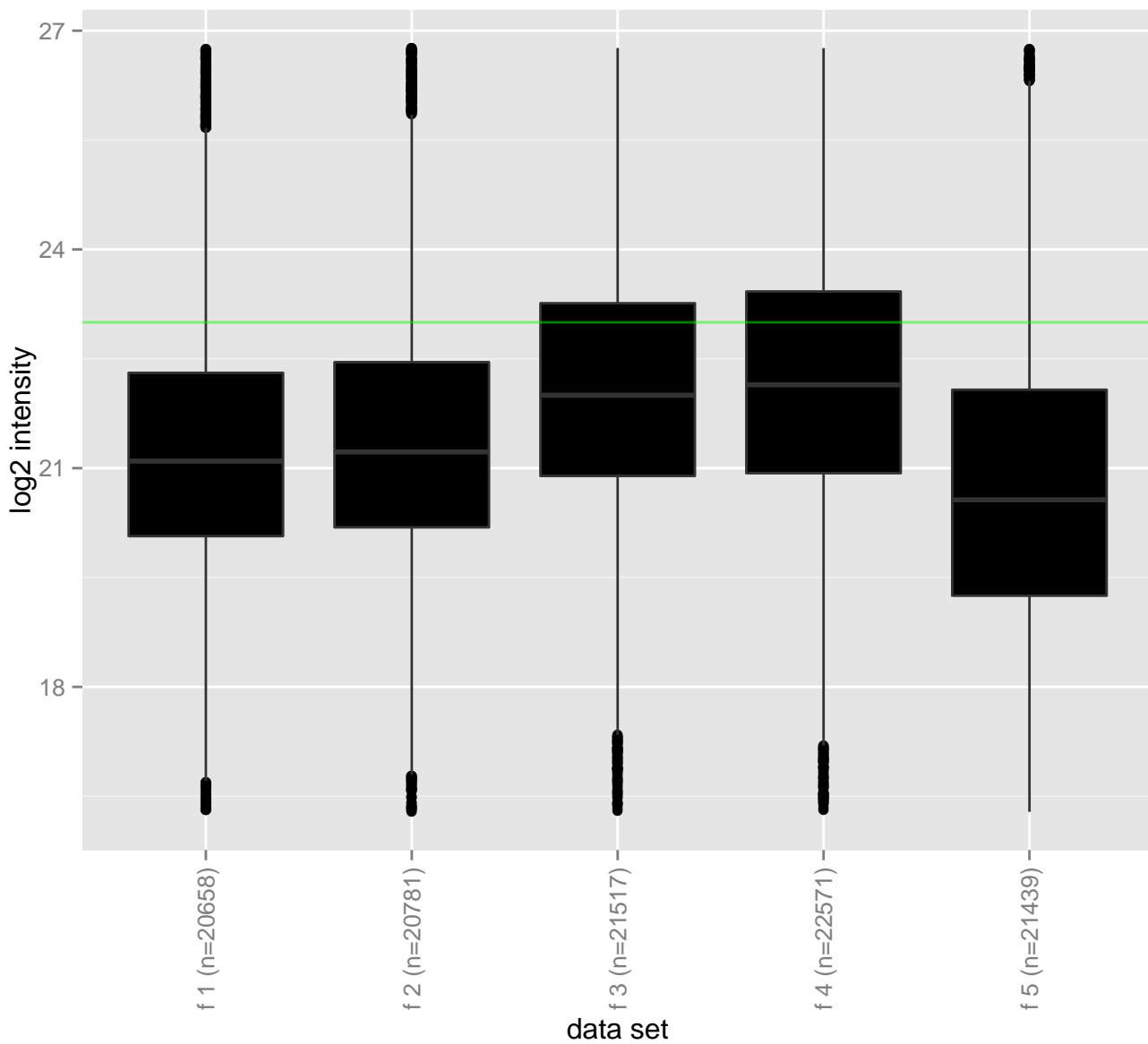


PG: Contaminants

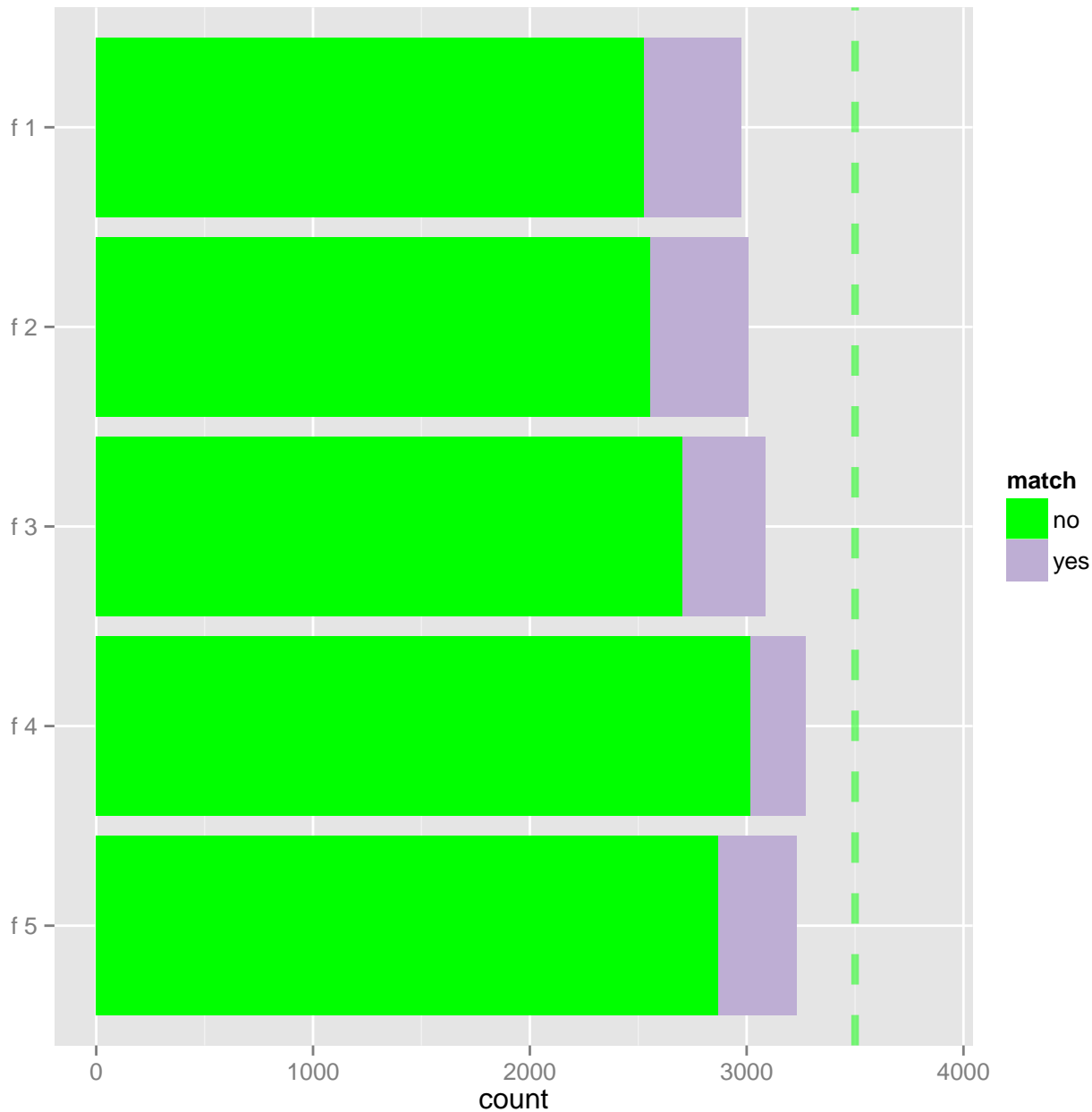
Contaminant 'MYCOPLASMA' was not found in any sample

Did you use the correct database?

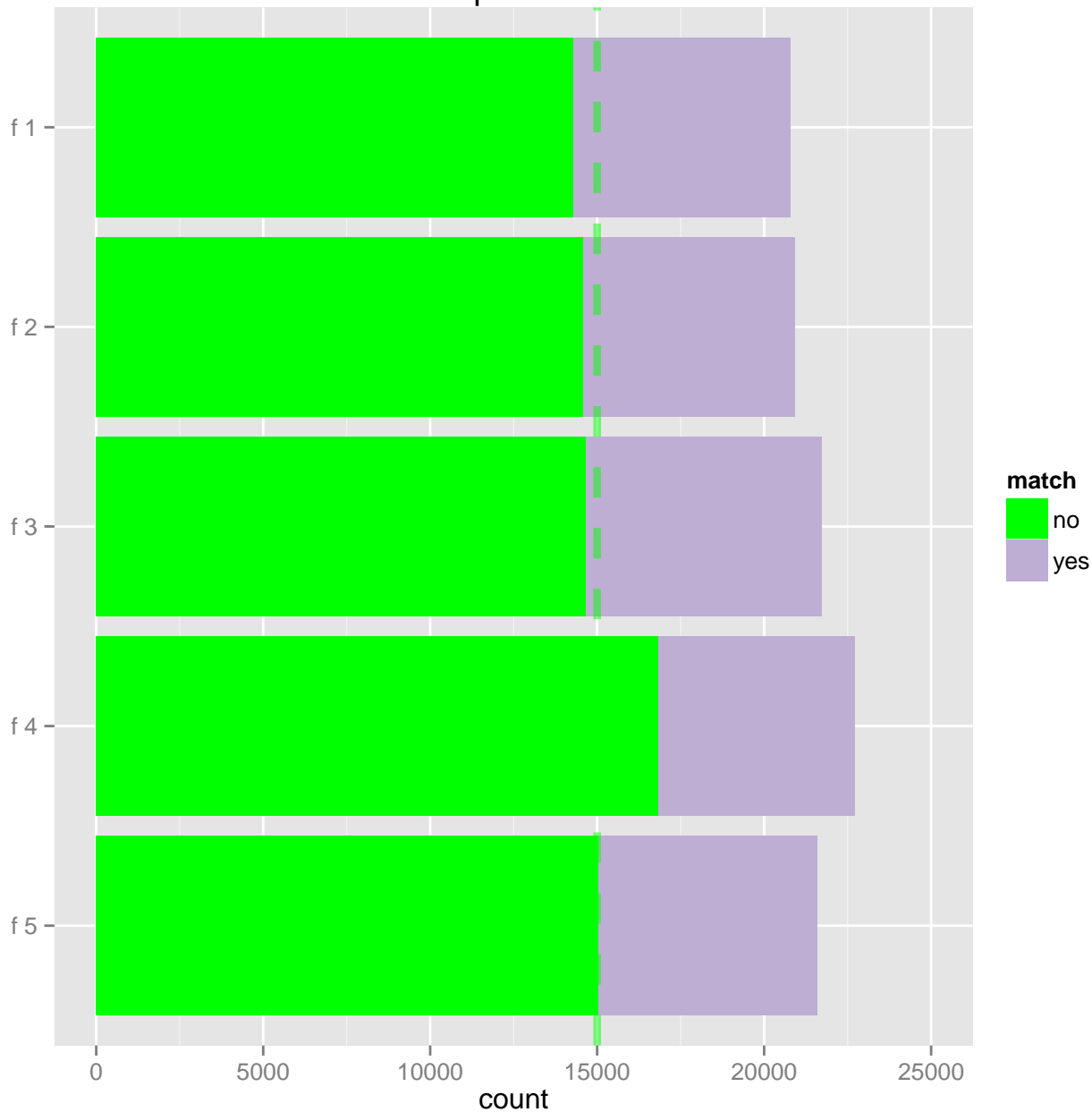
RSD 3.2% (should be < 5%)



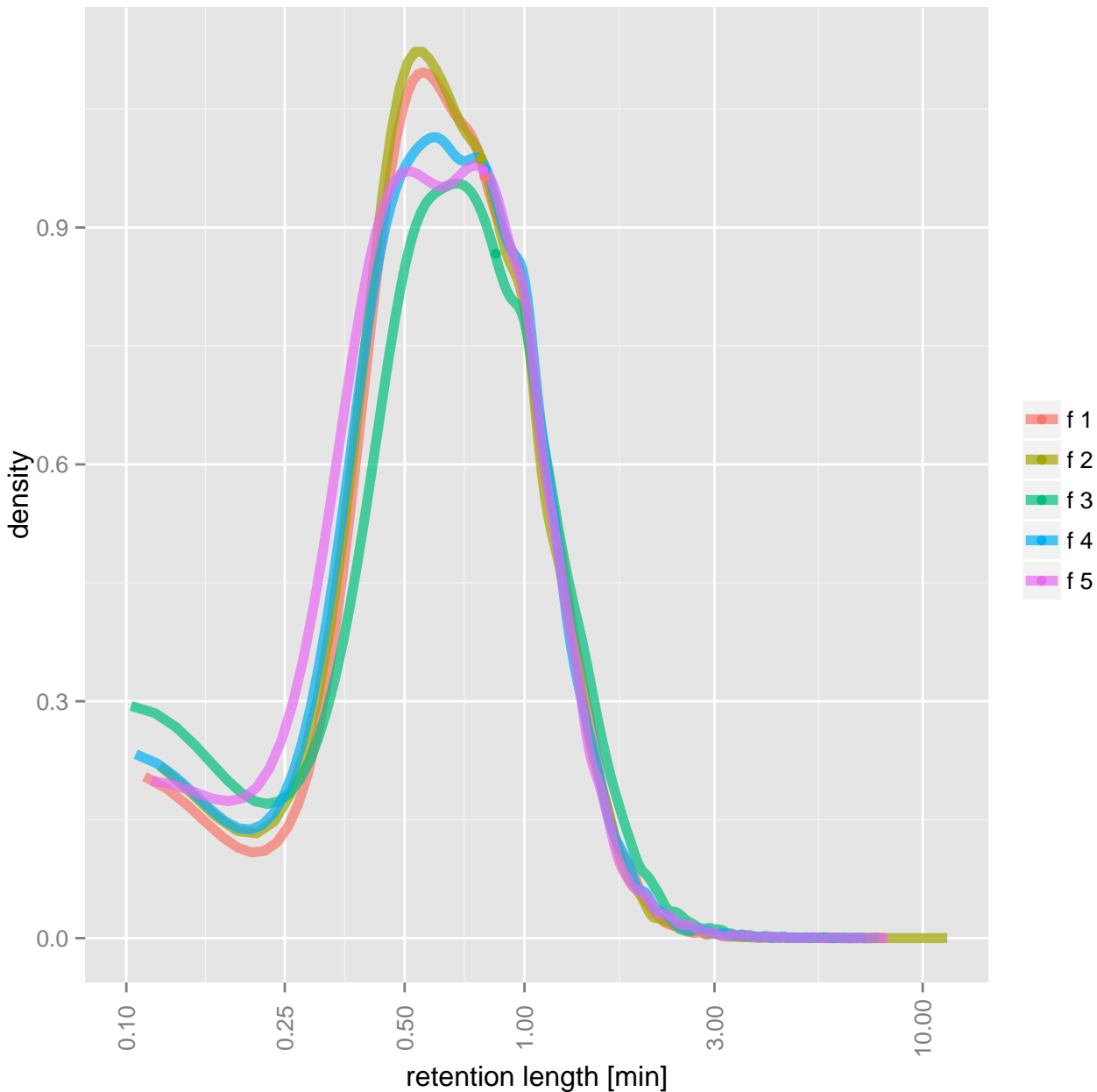
EVD: Protein ID count



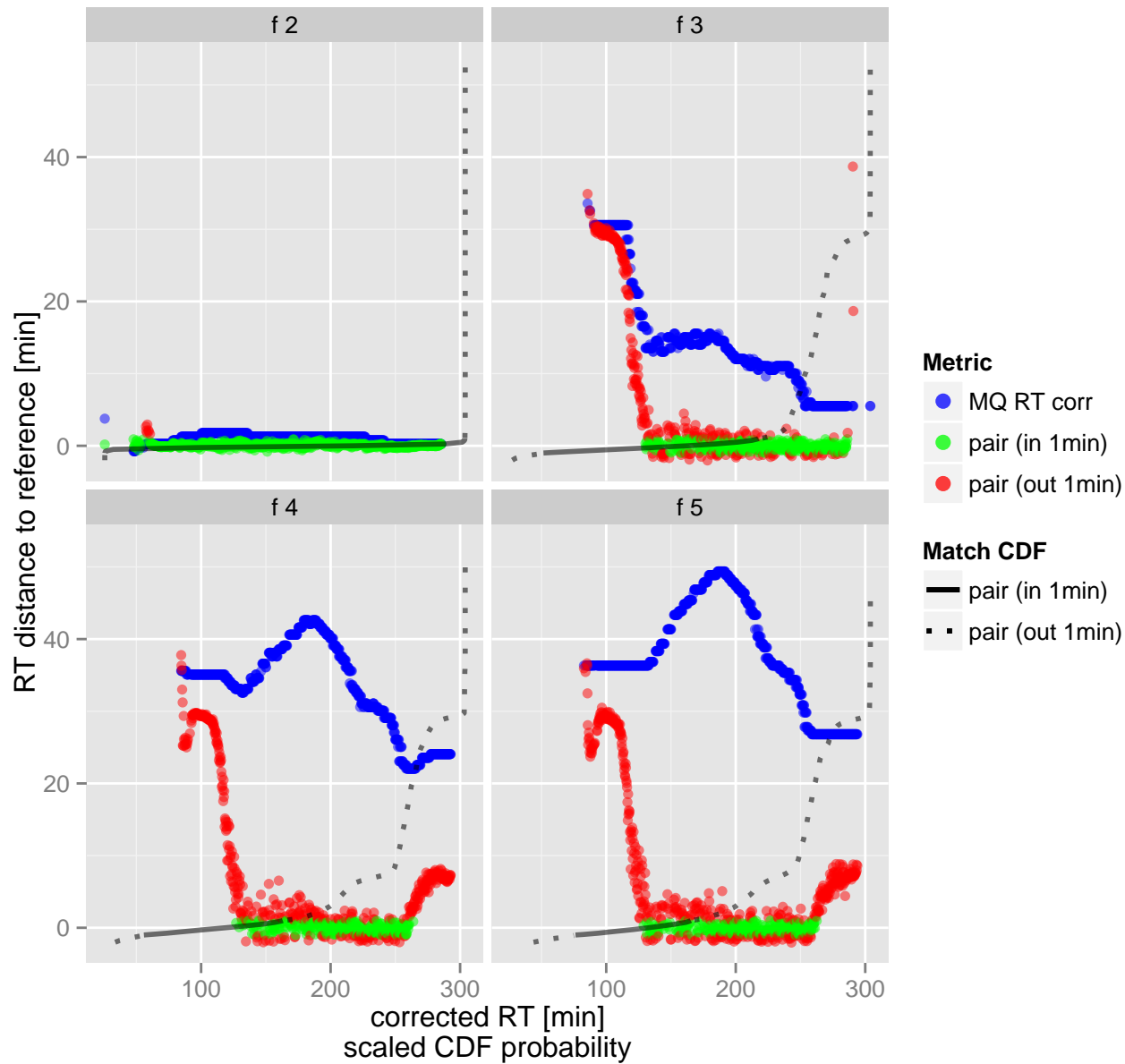
EVD: Peptide ID count



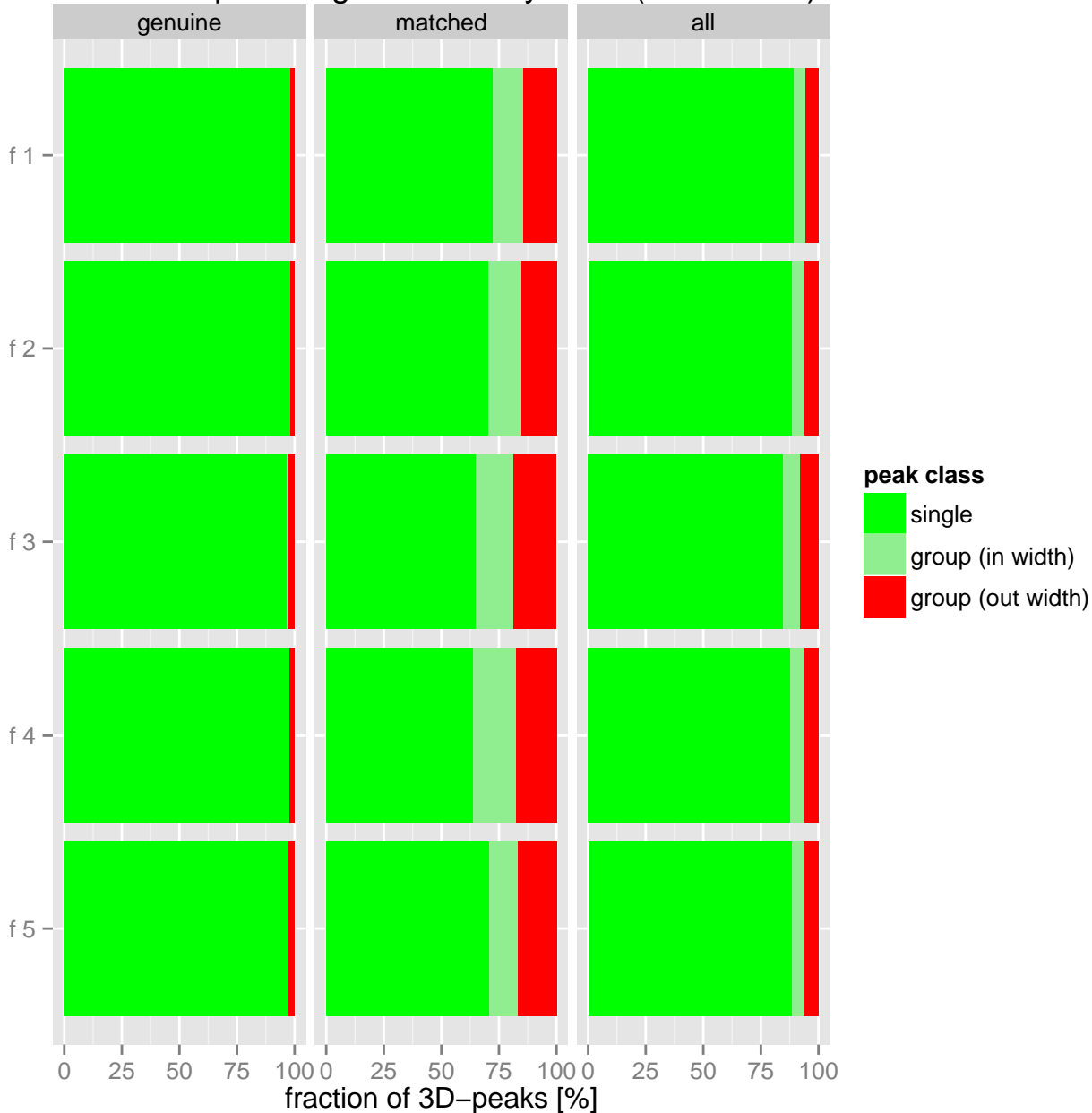
EVD: Peak width distribution



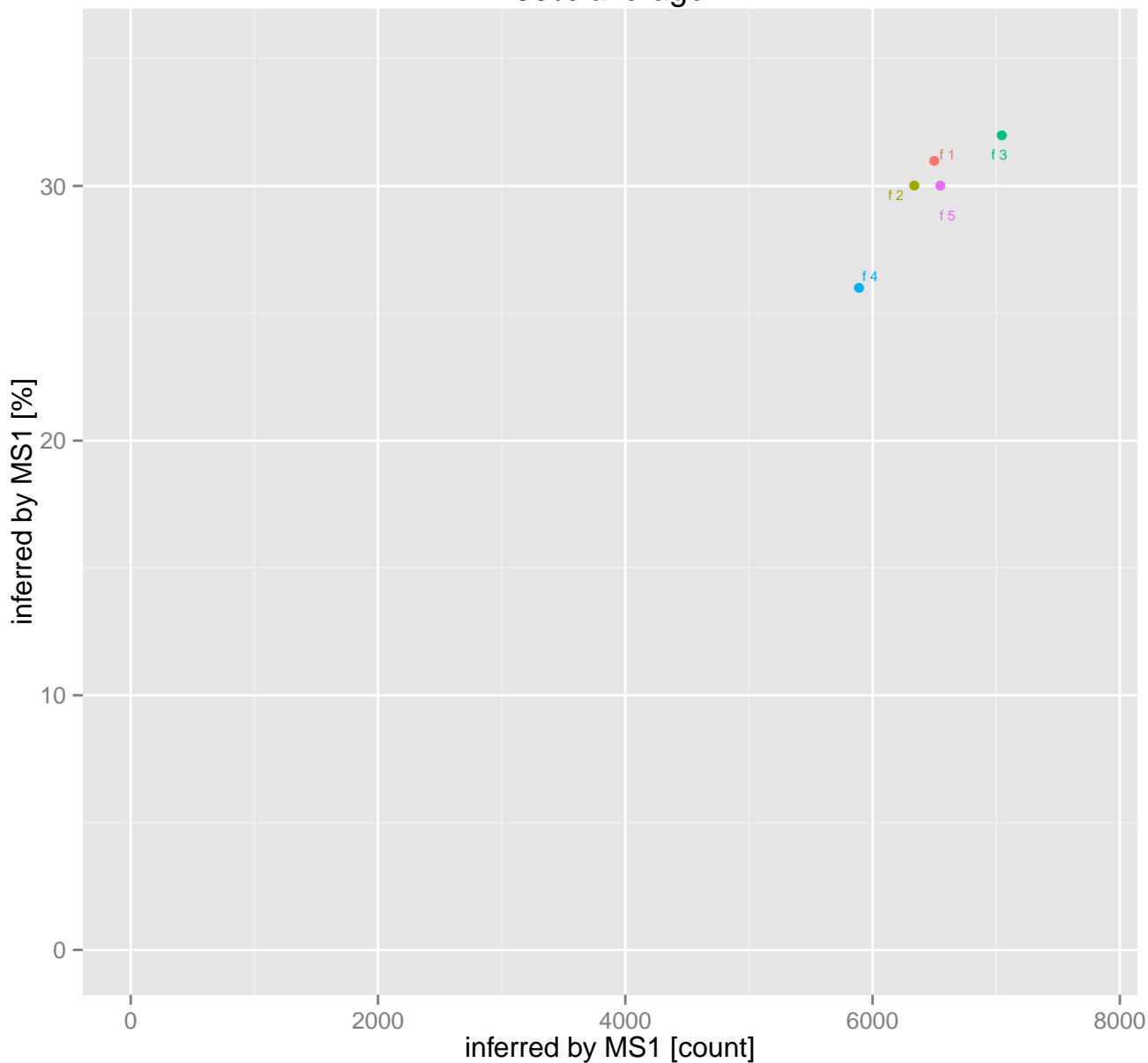
EVD: RT distance of genuine peptides to reference after alignment



EVD: 3D-peak segmentation by MBR (ID Transfer)



EVD: Peptides inferred by AMT-matching 30% average



EVD: charge distribution

Raw file

f 1

f 2

f 3

f 4

f 5

charge



0.00

0.25

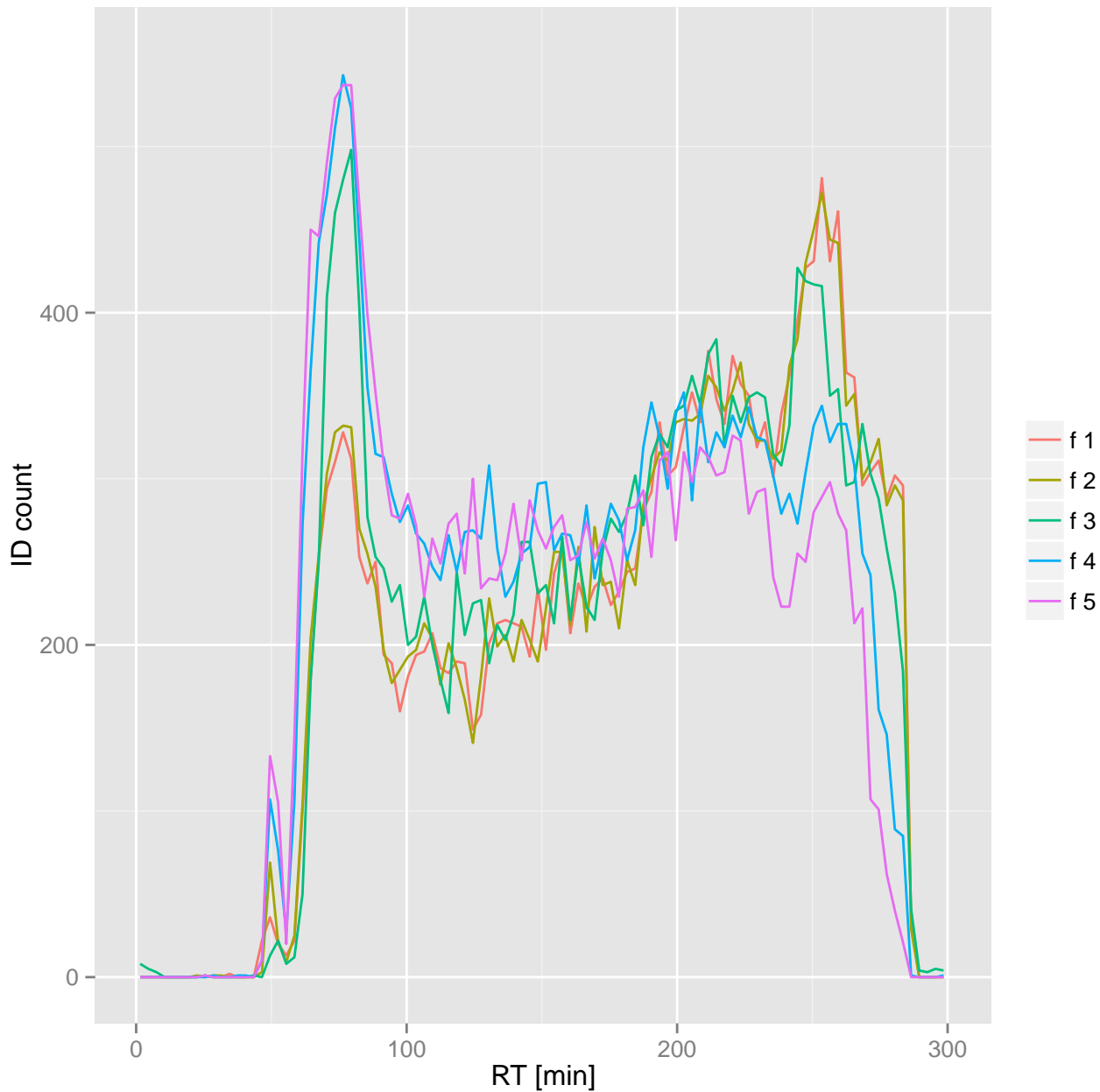
0.50

0.75

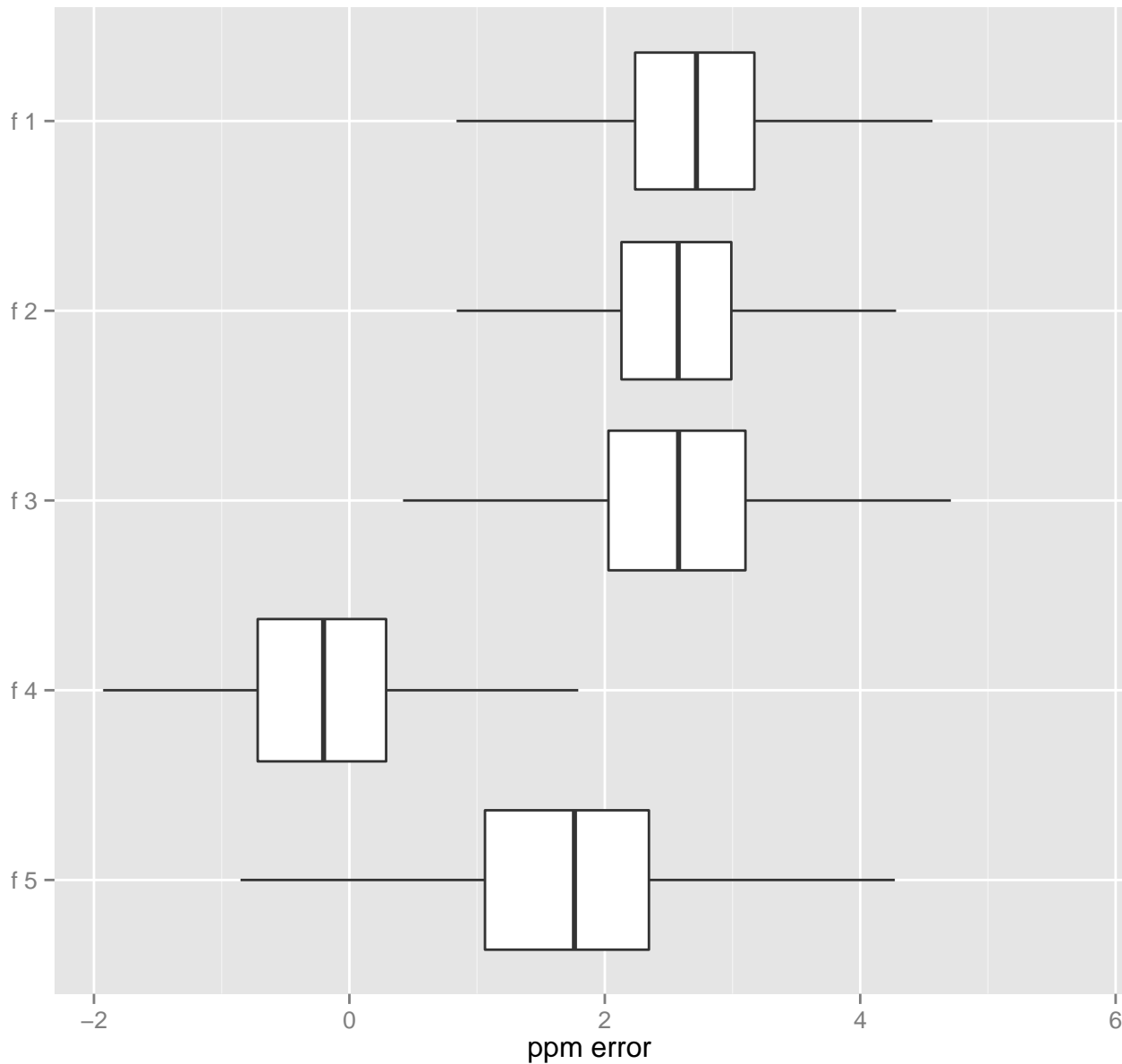
1.00

fraction [%]

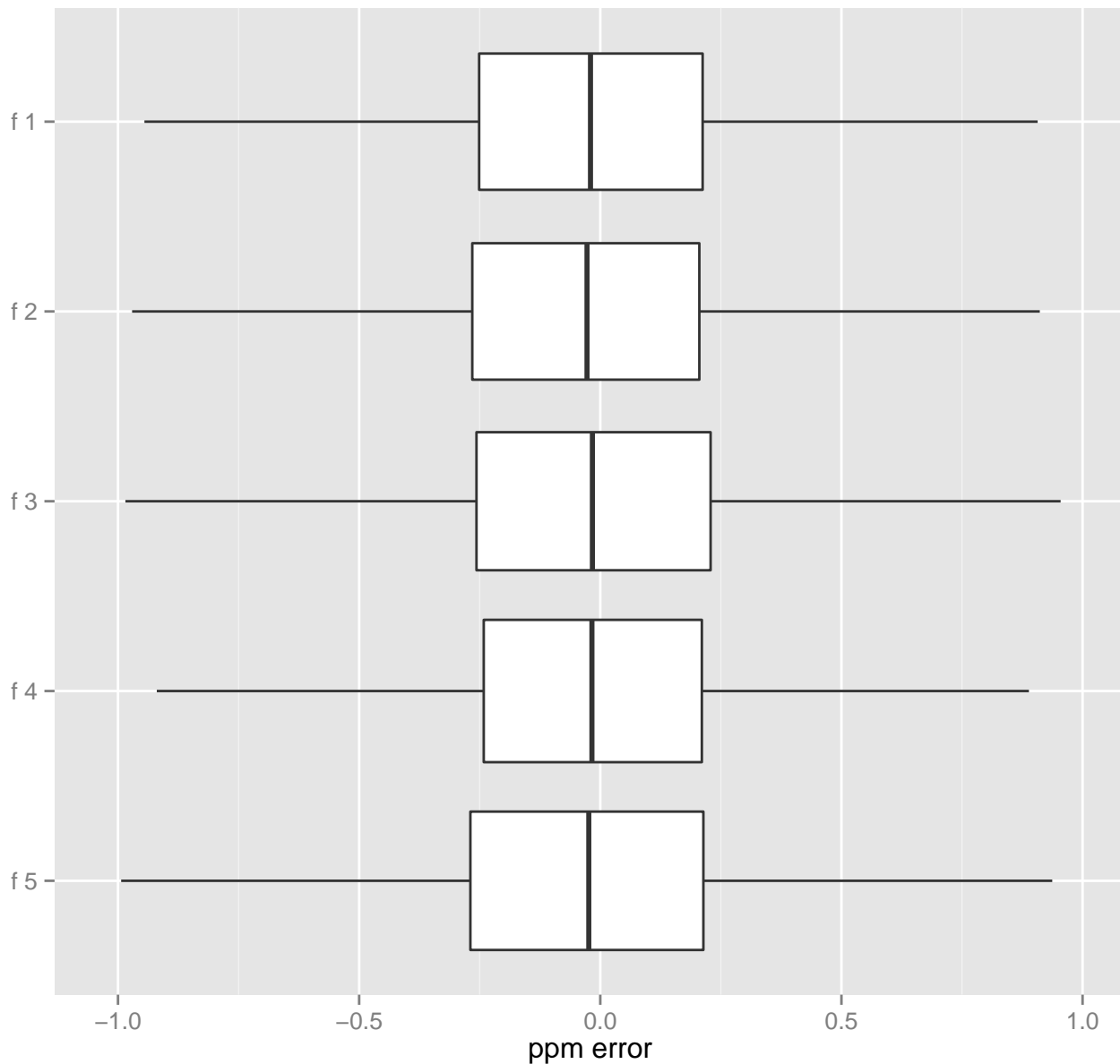
EVD: IDs over RT



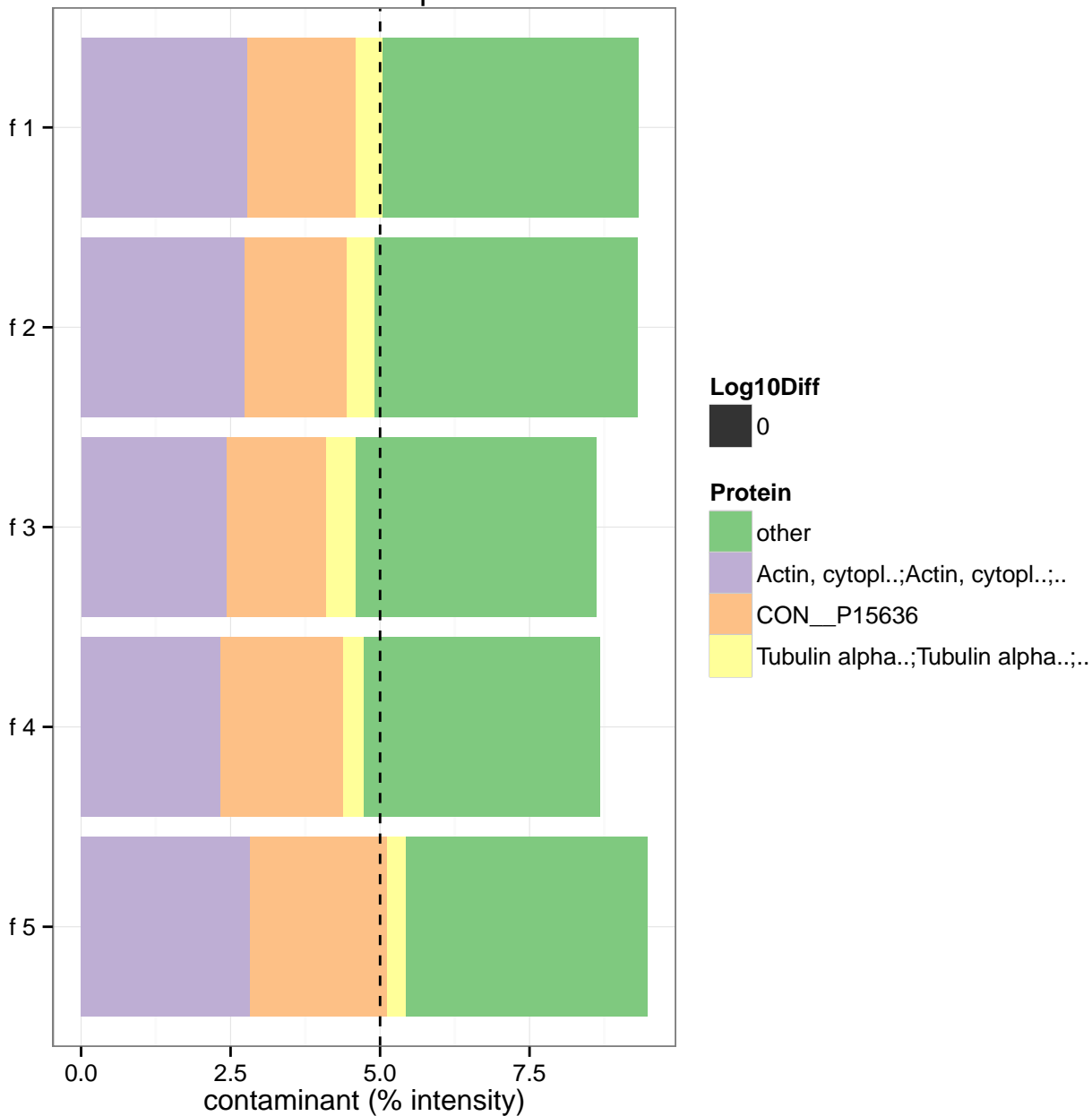
EVD: Uncalibrated mass error



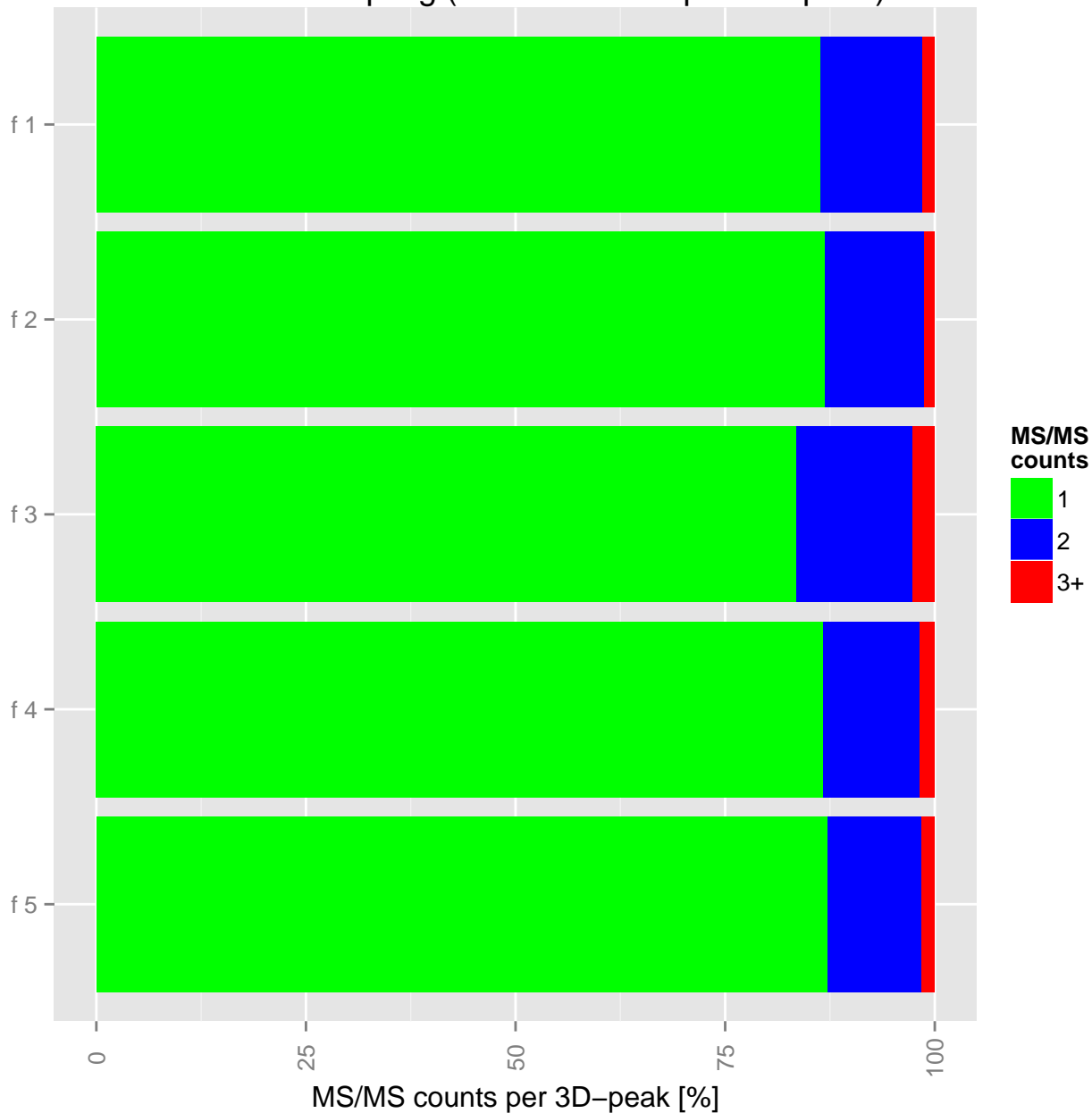
EVD: Calibrated mass error



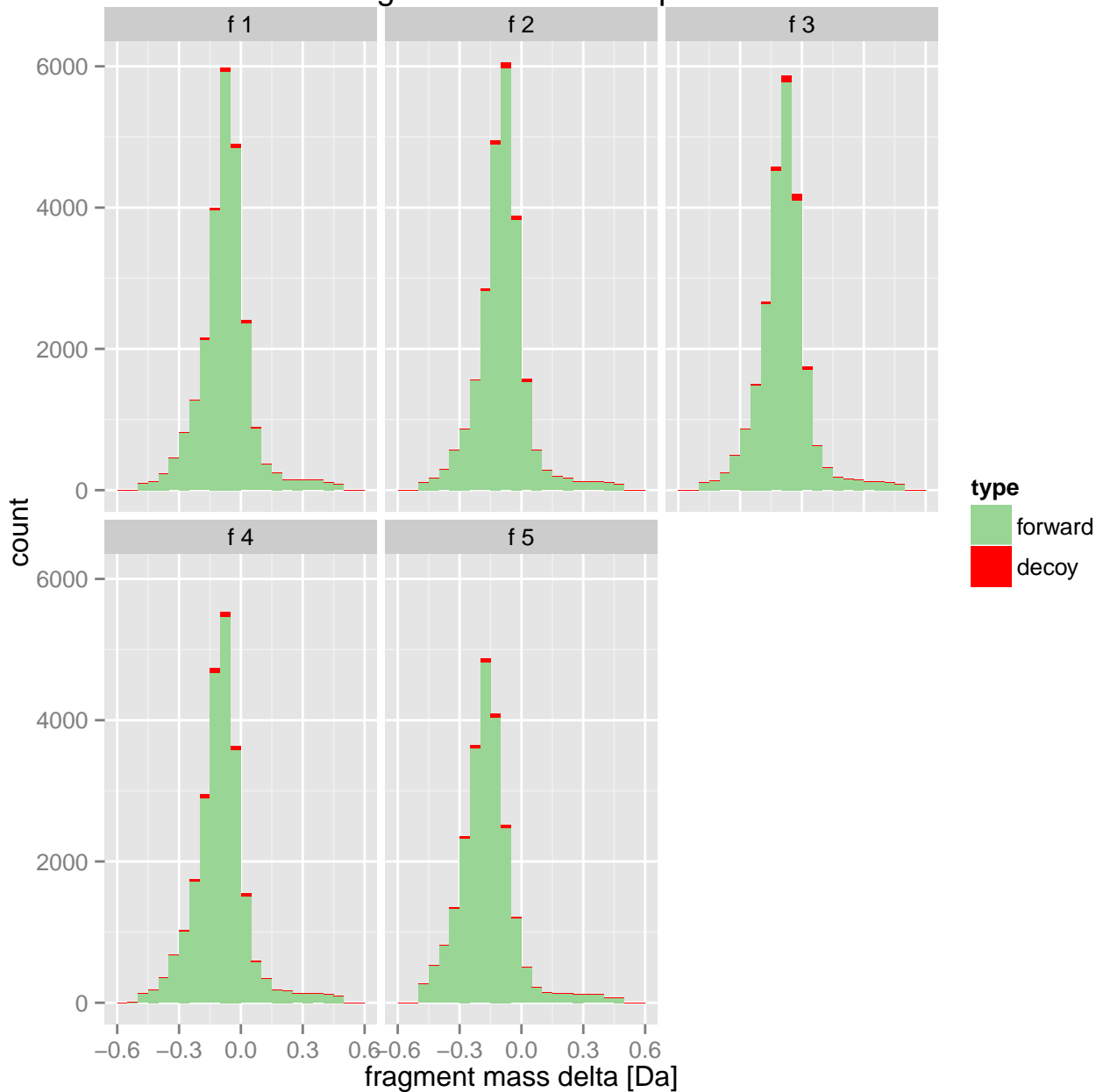
EVD: Contaminant per Raw file



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

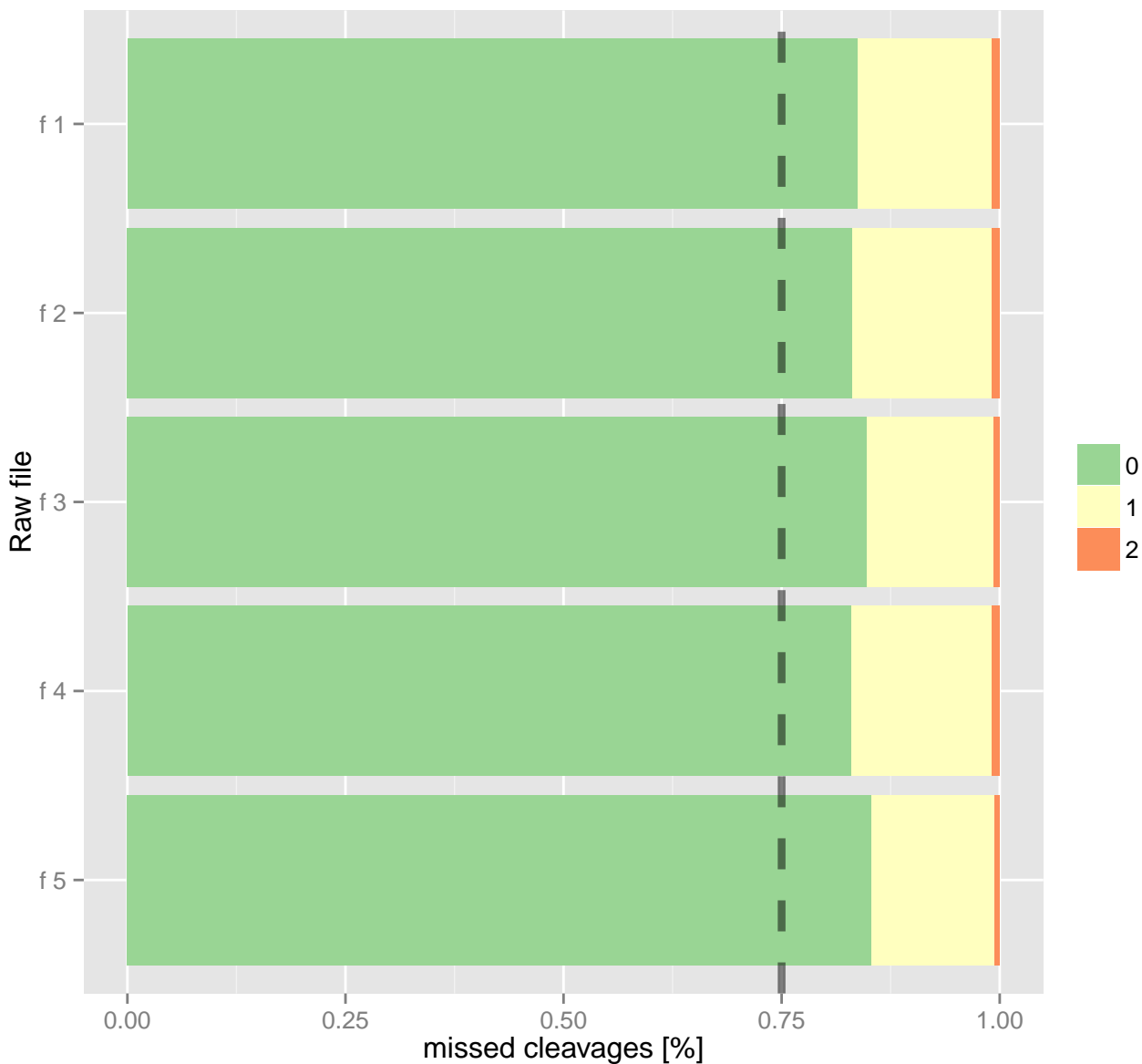


MSMS: Fragment mass errors per Raw file

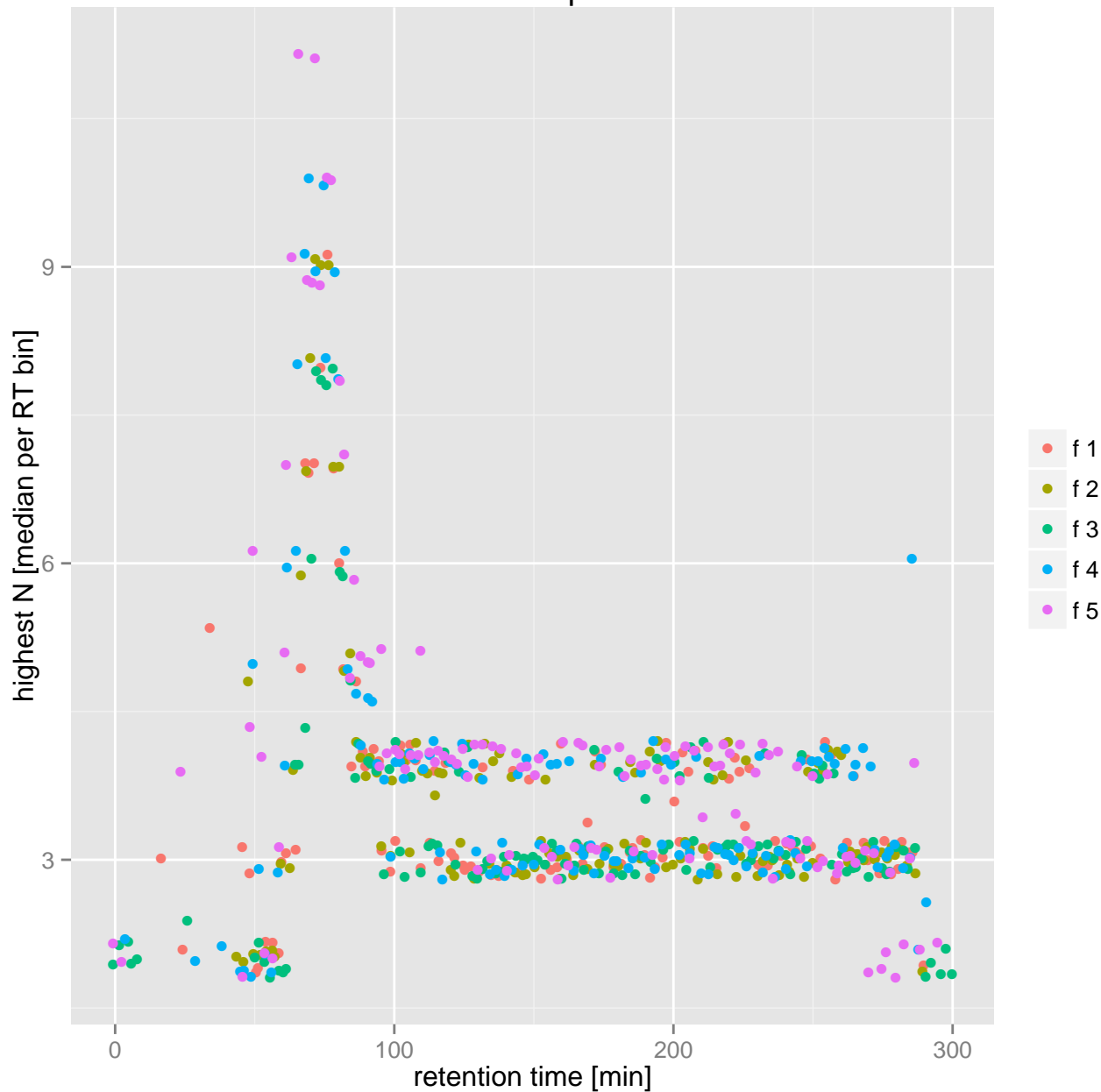


MSMS: Missed cleavages per Raw file

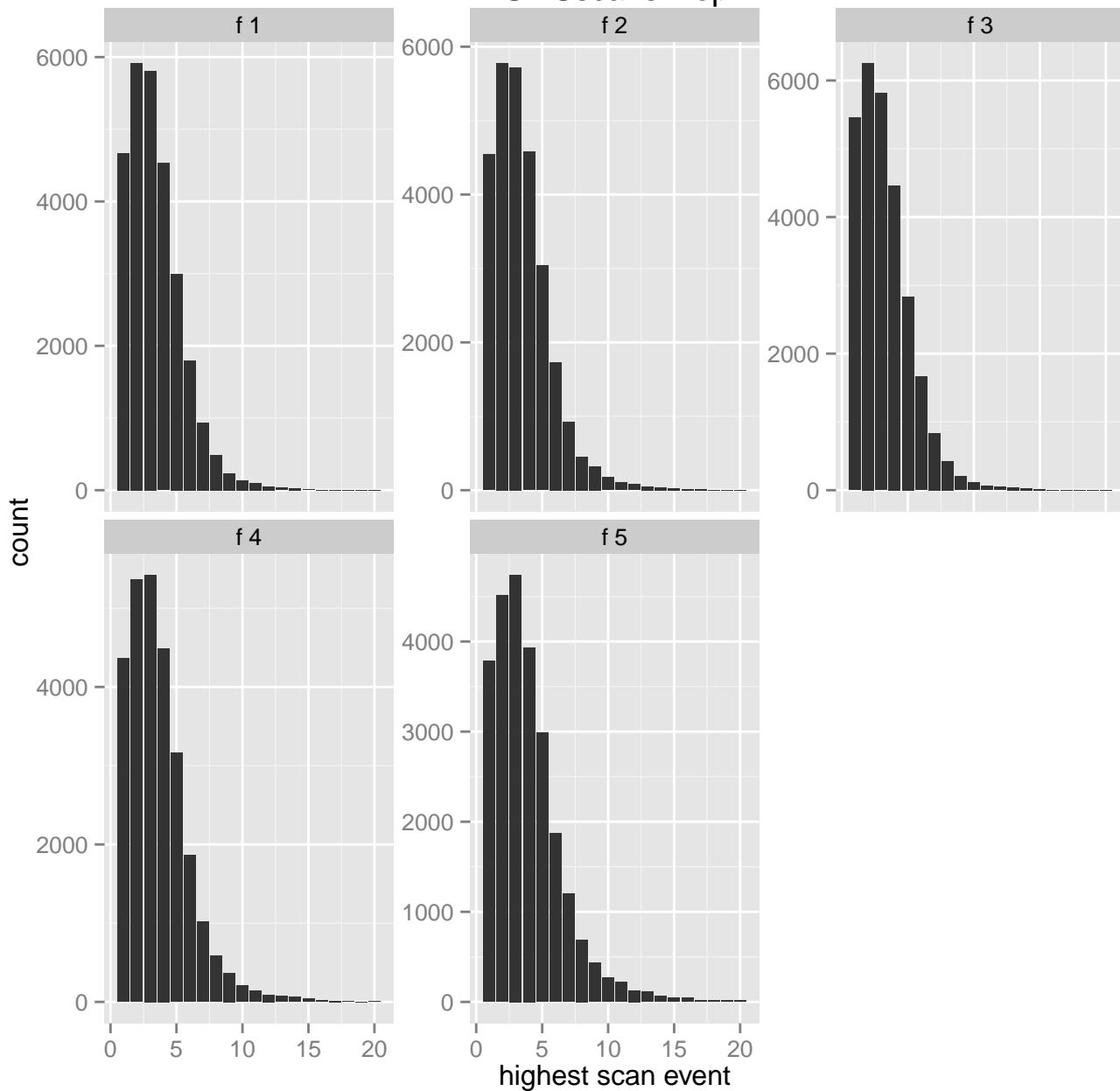
(excludes contaminants)



MSMSscans: TopN over RT



MSMSscans: TopN



MSMSscans: TopN % identified over N

