

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

original

short name best effort

Toni_20120502_GM_Ecoli_01

..Ecoli_01

Toni_20120502_GM_Ecoli_02

..Ecoli_02

PAR: parameters

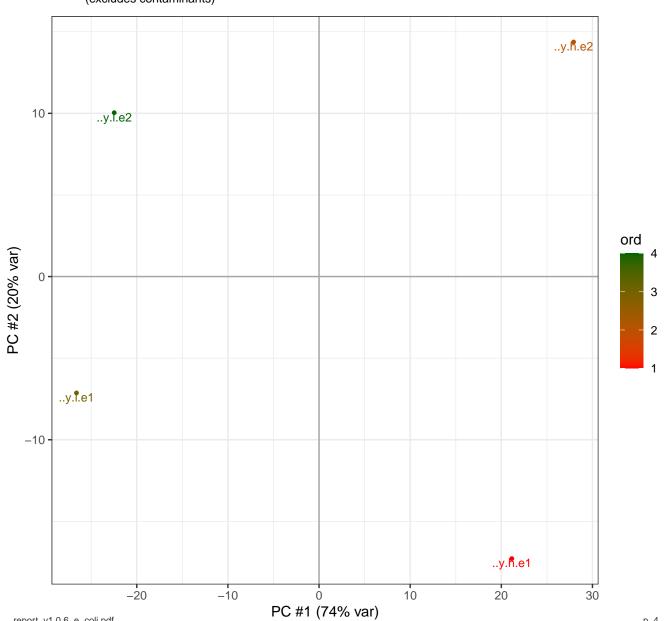
parameter	value	parameter	value
Advanced ratios	True	Min. score for modified pept	40
Alignment time window [min]	20	Modifications included in pr	Acetyl (Protein N-term) Oxidation (M)
Date of writing	11/13/2015 16:13:53	MS/MS tol. (FTMS)	20 ppm
Decoy mode	revert	MS/MS tol. (ITMS)	0.5 Da
Find dependent peptides	False	MS/MS tol. (TOF)	40 ppm
First pass AIF correlation	0.8	Peptides used for protein qu	Razor
Fixed modifications	Carbamidomethyl (C)	Protein FDR	0.01
Machine name	CD02-WIN7	Site tables	Oxidation (M)Sites.txt
Matching time window [min]	0.7	Special AAs	KR
Min. delta score for modifie	6	Top MS/MS peaks per 100 Da	12
Min. delta score for unmodif	0	Top MS/MS peaks per 100 Da	8
Min. peptide Length	7	Top MS/MS peaks per 100 Da	10
Min. peptides	1	User name	cbielow
Min. ratio count	2	Version	1.5.2.8

E_coli_k12.ASM584v1.16.pep.all.fasta

PG: PCA of 'raw intensity'



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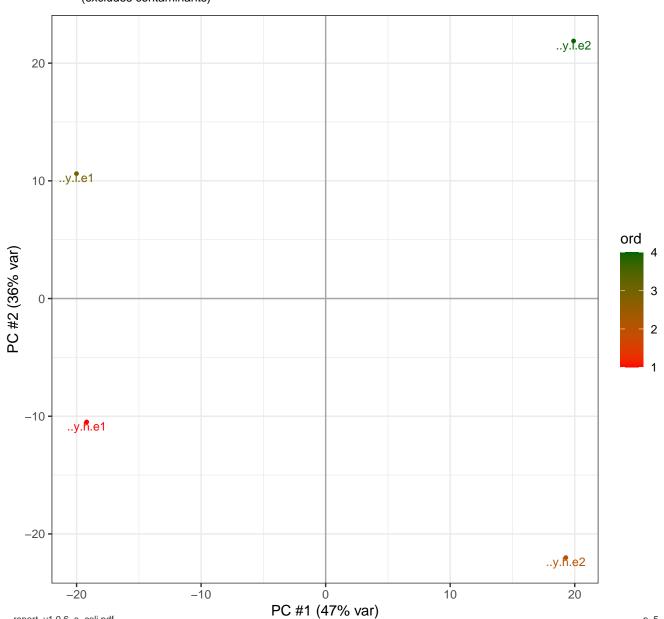


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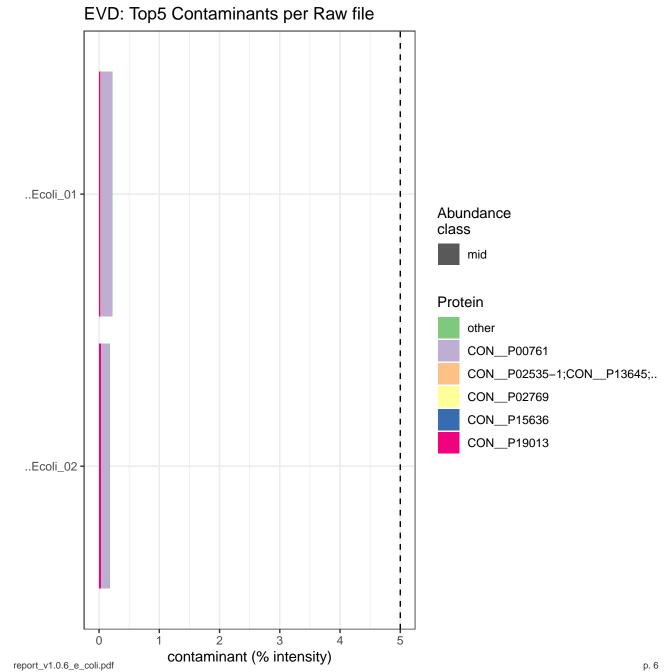
PG: PCA of 'Ifq intensity'

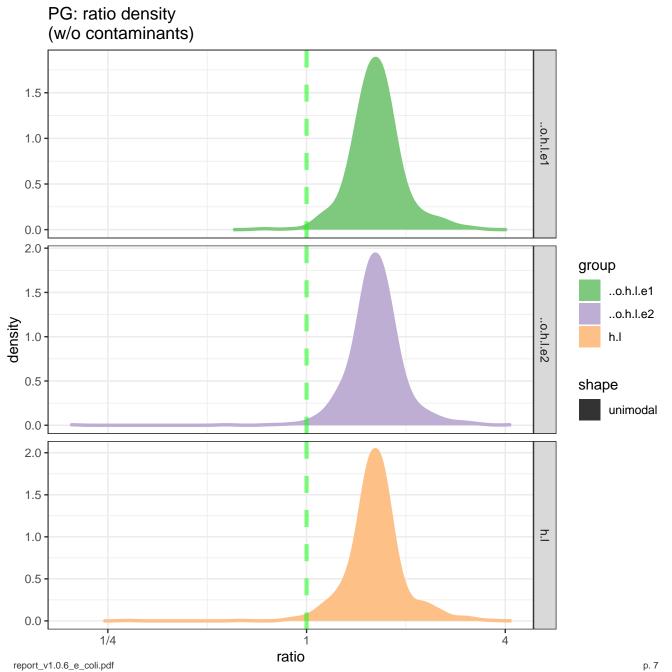
(excludes contaminants)

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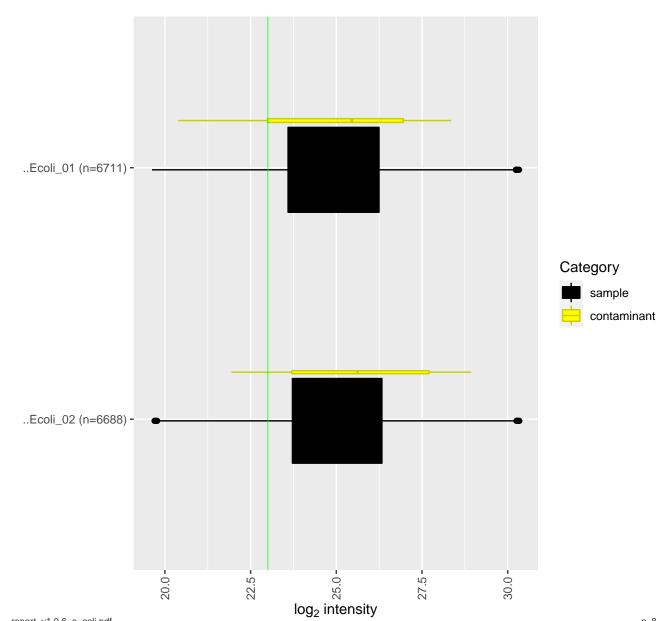


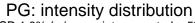
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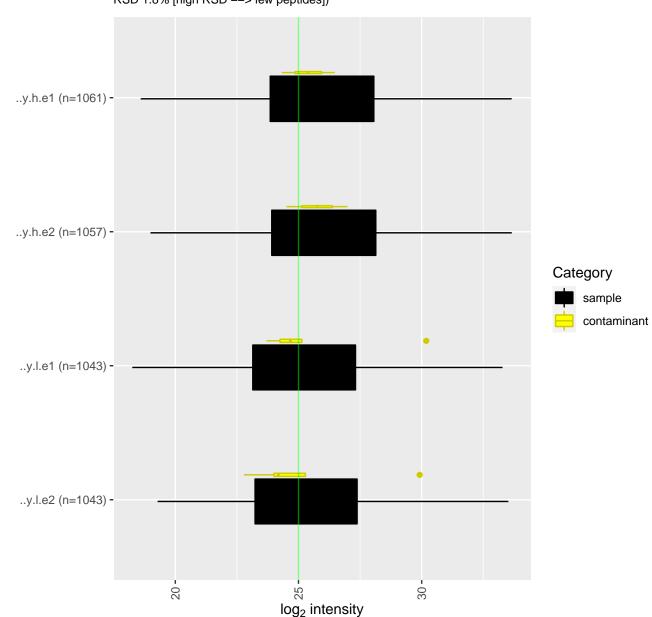


EVD: peptide intensity distribution RSD 0.3% (expected < 5%)



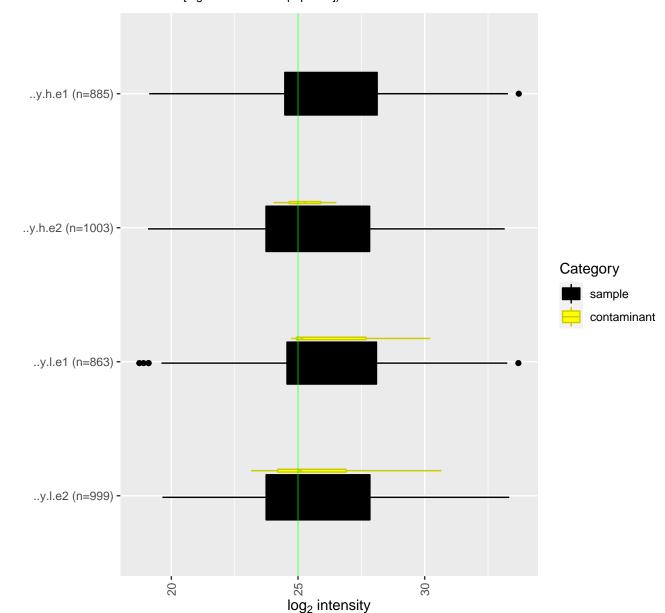


RSD 1.8% (w/o zero int.; expected < 5%) RSD 1.8% [high RSD --> few peptides])

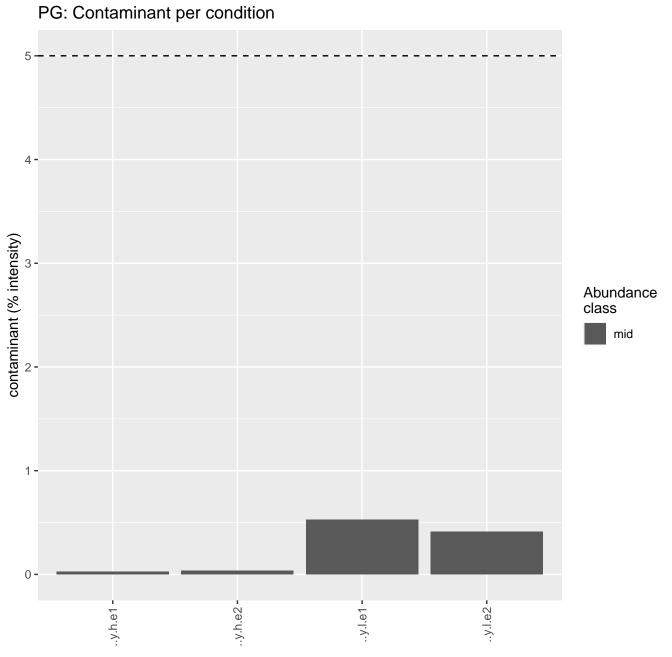


PG: LFQ intensity distribution

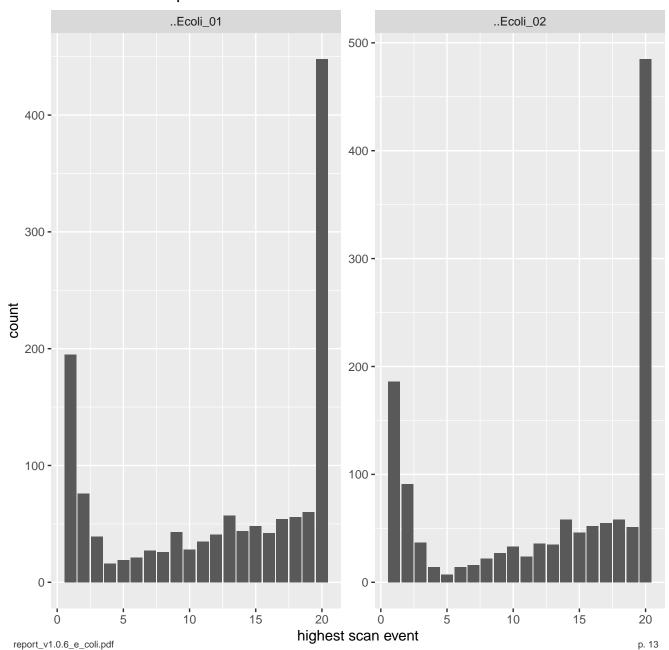
RSD 1.1% (w/o zero int.; expected < 5%) RSD 0.1% [high RSD --> few peptides])

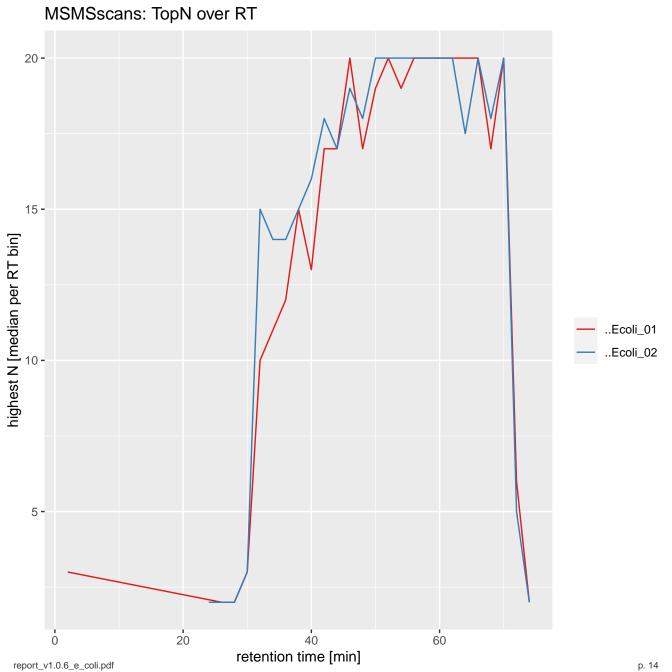


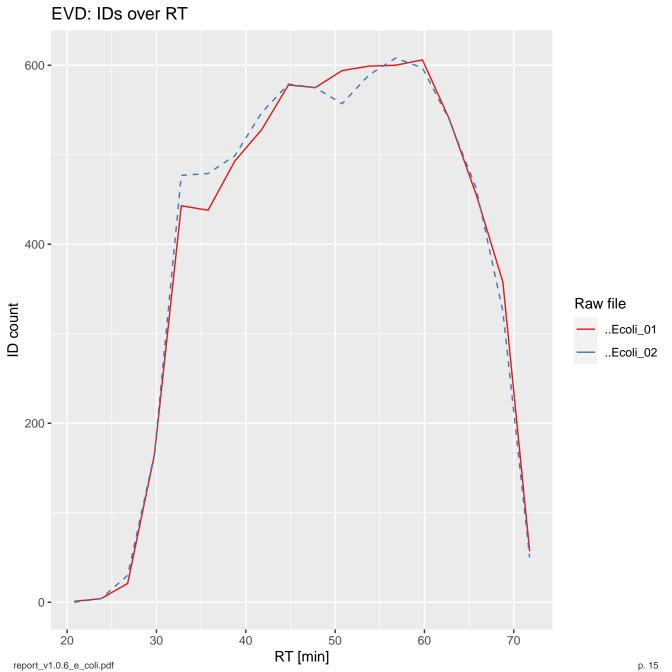
EVD: charge distribution .Ecoli_0 charge Raw file 2 5 .Ecoli_0: 0.50 0.00 0.25 0.75 1.00 fraction [%] report_v1.0.6_e_coli.pdf p. 11

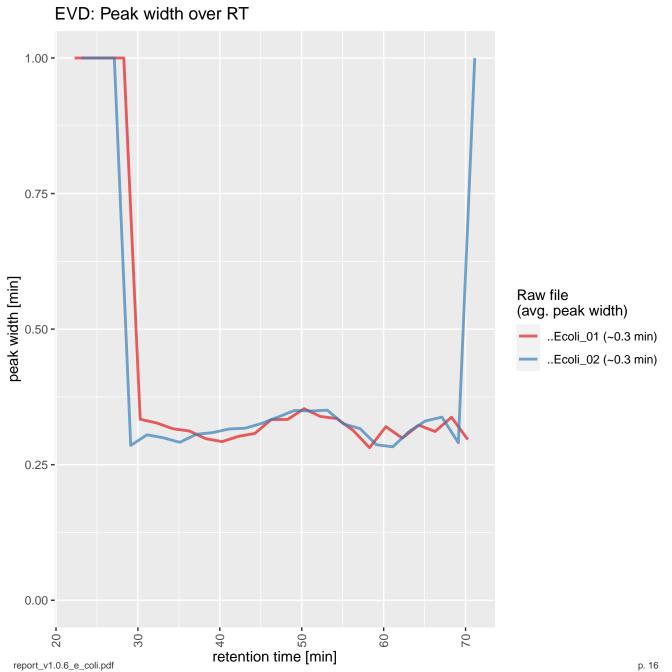


MSMSscans: TopN



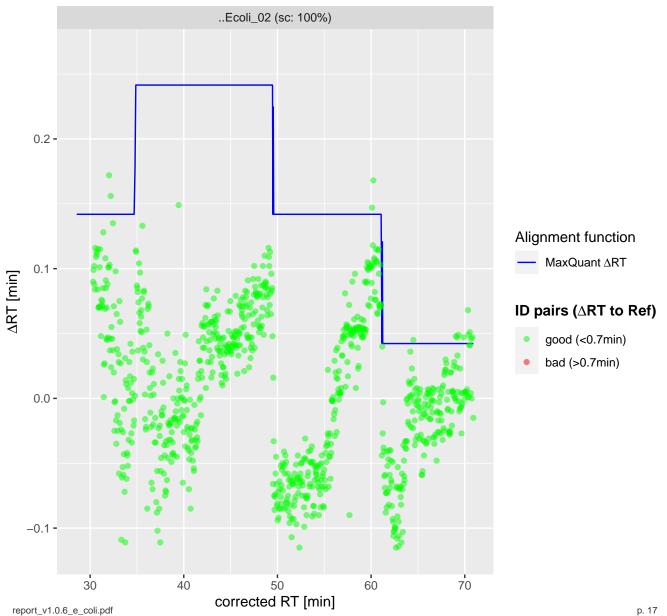




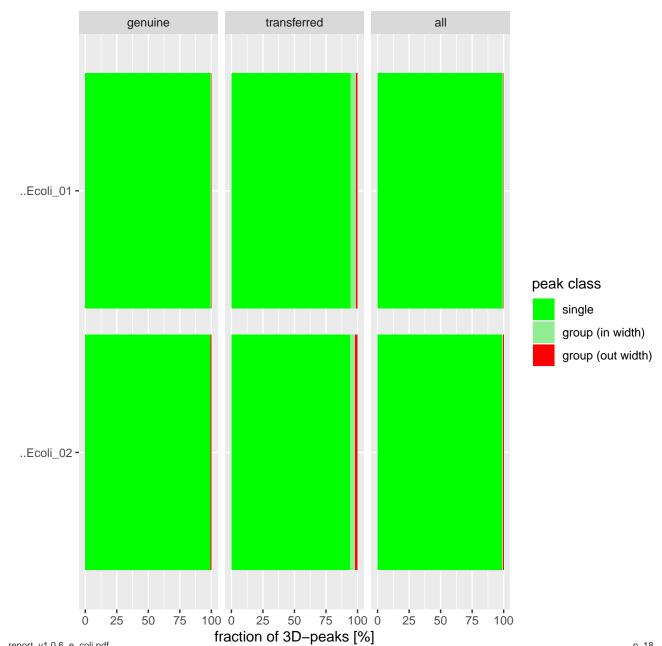


EVD: MBR – alignment

alignment reference: Toni_20120502_GM_Ecoli_01

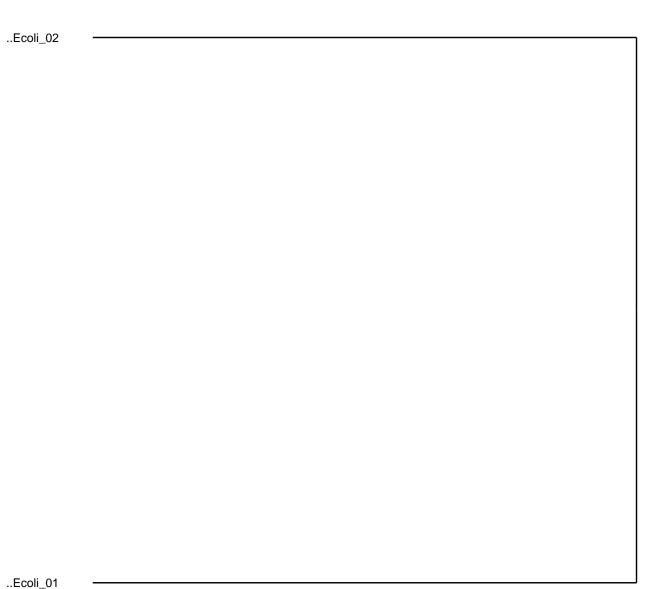


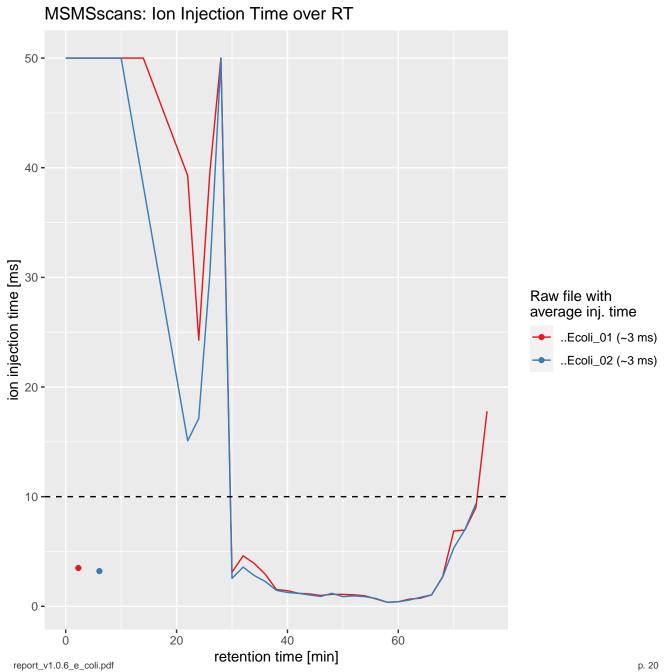
EVD: MBR - ID Transfer

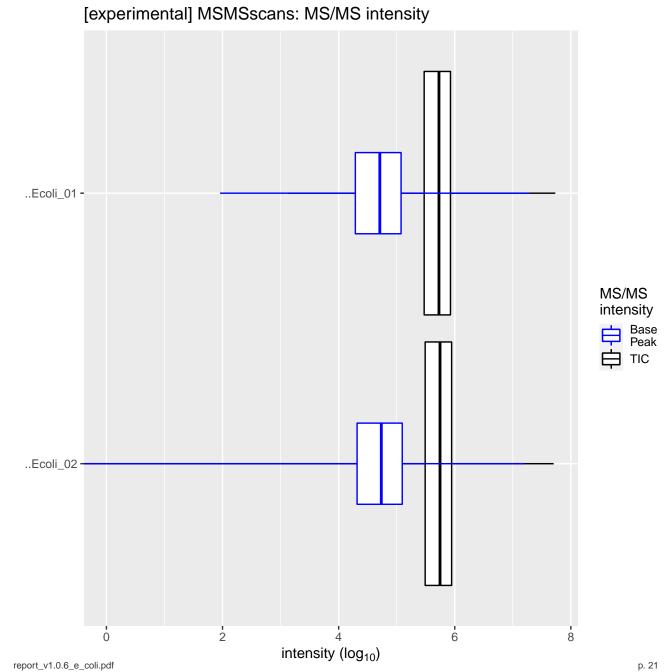


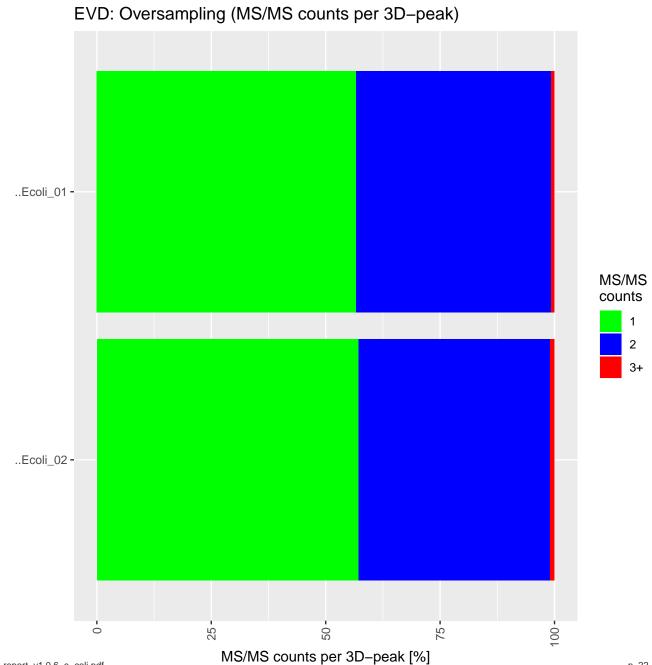
[experimental] EVD: Clustering Tree of Raw files

by Correlation of Corrected Retention Times

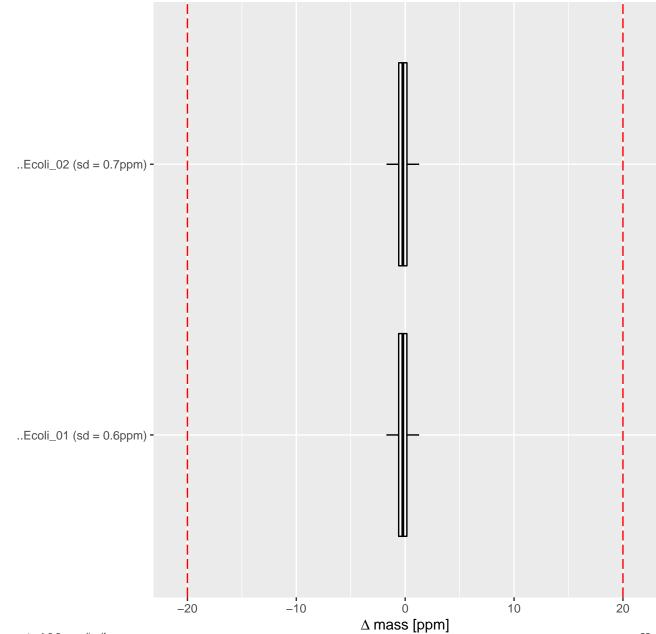






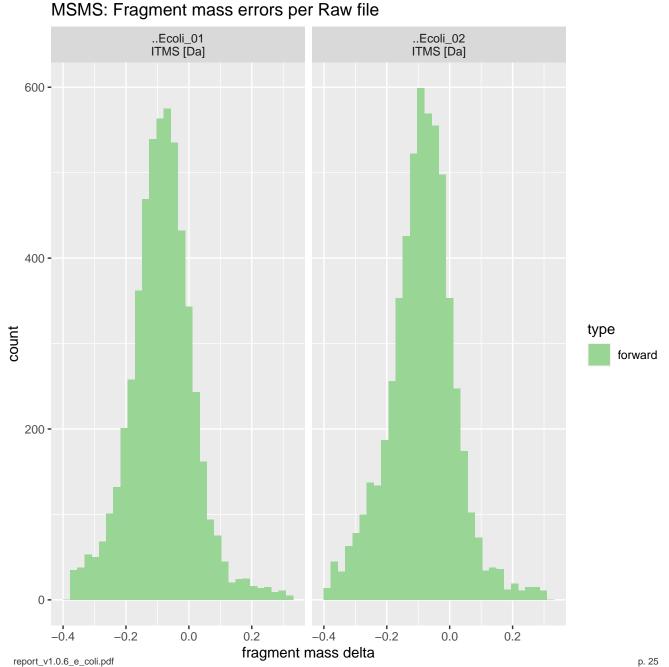


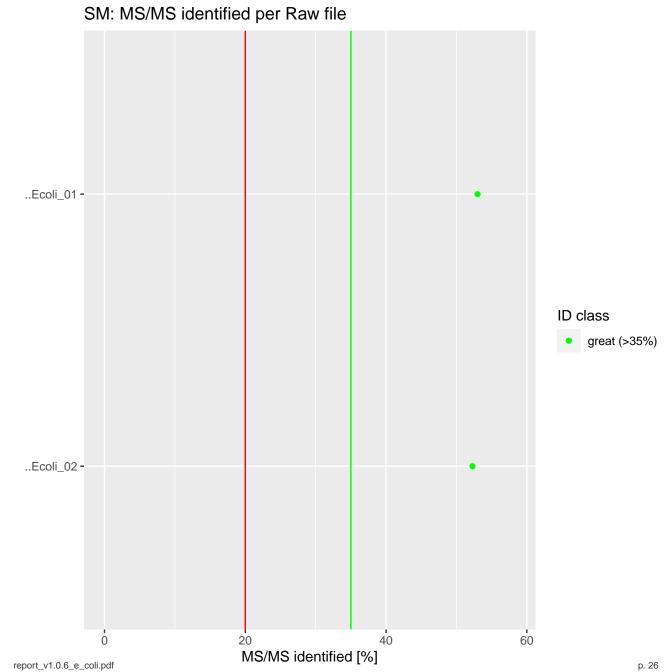


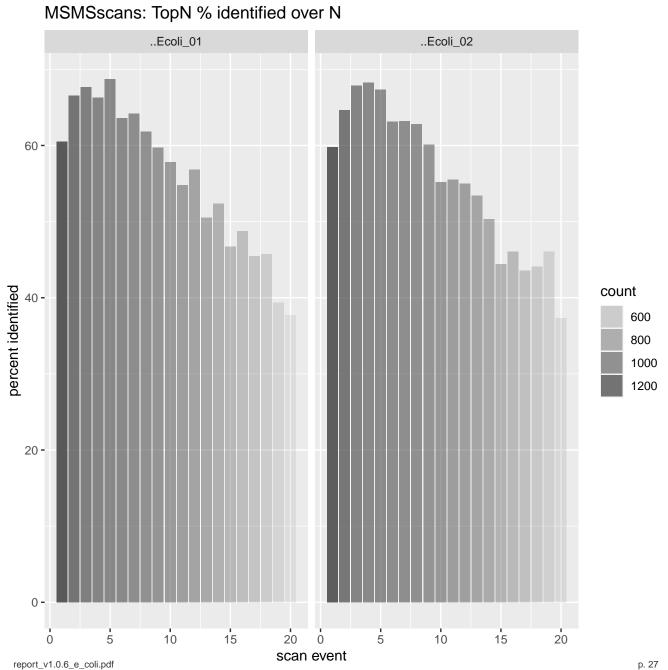


EVD: Calibrated mass error ..Ecoli_01 -..Ecoli_02 -5.0 0.0 2.5 -2.5 -5.0 Δ mass [ppm]

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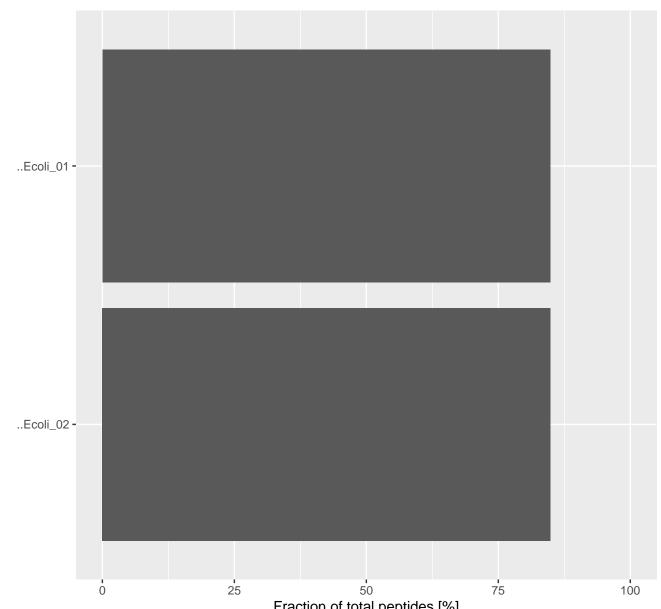






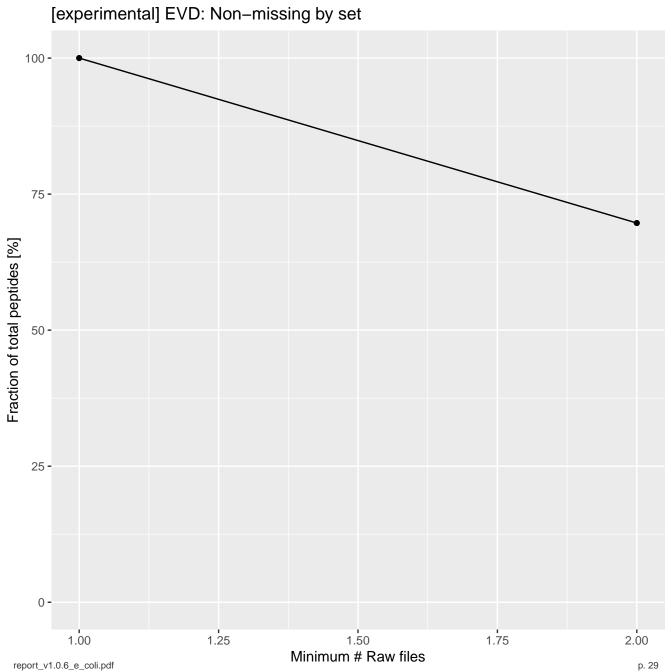
[experimental] EVD: Non–Missing Peptides

compared to all peptides seen in experiment

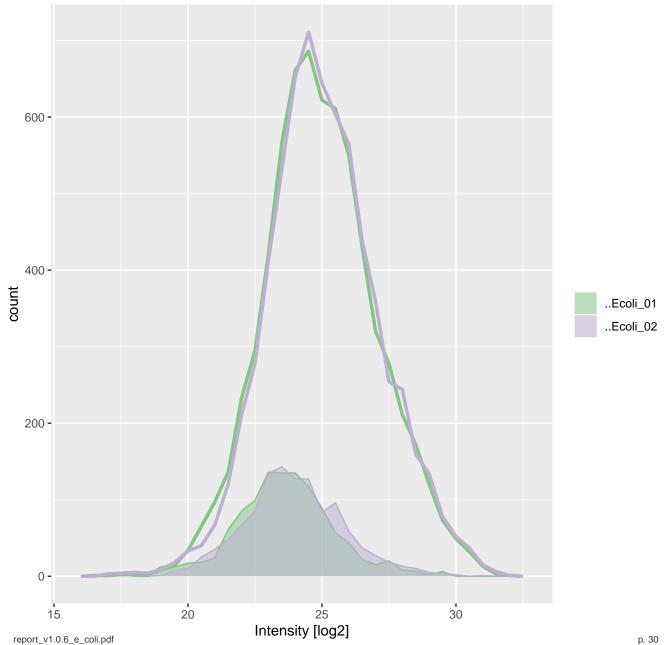


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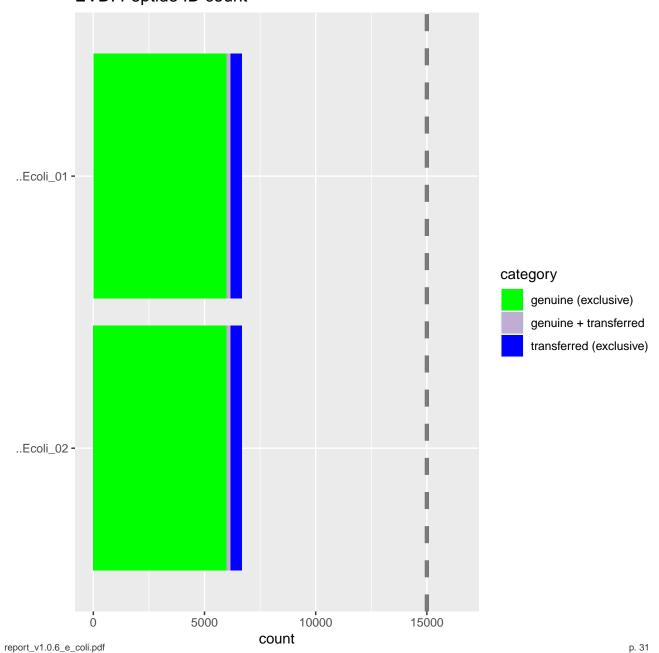
Fraction of total peptides [%]



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



EVD: Peptide ID count



EVD: ProteinGroups count

MBR gain: +2%

