

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

original	short	best
Ŭ	name	effort
10_DMSO_SDS_3	file 01	10_DMSO_SDS3
10_DMSO_SDS_3_5uL_20200612085223	file 02	10_DMSO_SDS_3_5uL20200612085223
10_insol_WT	file 03	10_insolWT
11_Cpt_wcl_3	file 04	11_Cpt_wcl3
11_WCL_ATM	file 05	11_WCLATM
12_Cpt_SDS_3	file 06	12_Cpt_SDS3
12_Cpt_SDS_3_5uL	file 07	12_Cpt_SDS_35uL
12_insol_ATM	file 08	12_insolATM
13_DMSO_wcl_4	file 09	13_DMSO_wcl4
13_WCL_WT	file 10	13_WCLWT
14_DMSO_SDS_4	file 11	14_DMSO_SDS4
14_DMSO_SDS_4_5uL	file 12	14_DMSO_SDS_45uL
15_Cpt_wcl_4	file 13	15_Cpt_wcl4
15_WCT_ATM	file 14	15_WCTATM
16_Cpt_SDS_4	file 15	16_Cpt_SDS4
16_Cpt_SDS_4_5uL	file 16	16_Cpt_SDS_45uL
1_DMSO_wcl_1	file 17	1_DMSO_wcl1

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

original	short	best	
ong.na.	name	effort	
1_WCL_WT	file 18	1_WCLWT	
2_DMSO_SDS_1	file 19	2_DMSO_SDS1	
2_DMSO_SDS_1_5uL	file 20	2_DMSO_SDS_15uL	
2_insol_WT	file 21	2_insolWT	
3_Cpt_wcl_1	file 22	3_Cpt_wcl1	
3_WCL_ATM	file 23	3_WCLATM	
4_cpt_SDS_1	file 24	4_cpt_SDS1	
4_cpt_SDS_1_5uL	file 25	4_cpt_SDS_15uL	
4_insol_ATM	file 26	4_insolATM	
5_DMSO_wcl_2	file 27	5_DMSO_wcl2	
5_WCL_WT_20200702083455	file 28	5_WCL_WT20200702083455	
6_DMSO_SDS_2	file 29	6_DMSO_SDS2	
6_DMSO_SDS_2_5uL	file 30	6_DMSO_SDS_25uL	
7_Cpt_wcl_2	file 31	7_Cpt_wcl2	
7_WCL_ATM	file 32	7_WCLATM	
8_Cpt_SDS_2	file 33	8_Cpt_SDS2	
8_Cpt_SDS_2_5uL	file 34	8_Cpt_SDS_25uL	

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

original	short name	best effort
	namo	onore
9_DMSO_wcl_3	file 35	9_DMSO_wcl3
9_WCL_WT	file 36	9_WCLWT
insol_ATM_1	file 37	insol_ATM1
insol_ATM_2	file 38	insol_ATM2
insol_ATM_3	file 39	insol_ATM3
insol_ATM_3_20200725191715	file 40	insol_ATM_320200725191715
insol_ATM_3_20200727092836	file 41	insol_ATM_320200727092836
insol_ATM_4	file 42	insol_ATM4
insol_ATM_4_20200729233315	file 43	insol_ATM_420200729233315
insol_WT_1_20200727152510	file 44	insol_WT_120200727152510
insol_WT_2	file 45	insol_WT2
insol_WT_2_20200727173305	file 46	insol_WT_220200727173305
insol_WT_3	file 47	insol_WT3
insol_WT_3_20200727194055	file 48	insol_WT_320200727194055
insol_WT_4	file 49	insol_WT4
insol_WT_4_20200727214846	file 50	insol_WT_420200727214846

PAR: parameters

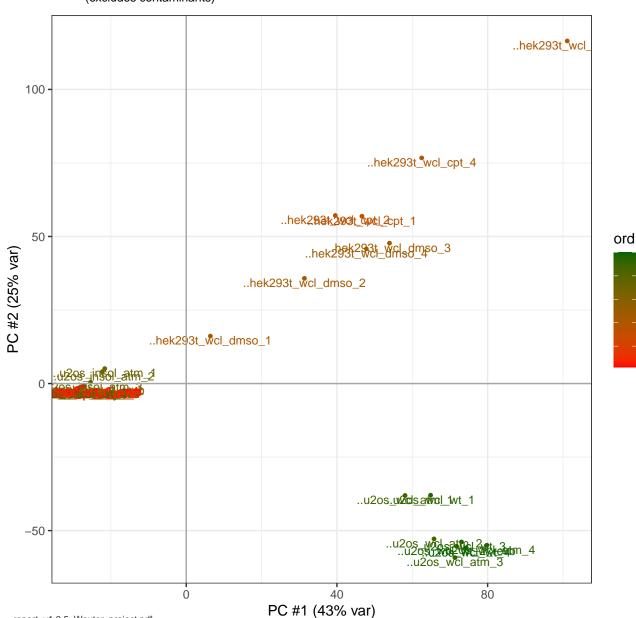
parameter	value	parameter	value
Advanced ratios	True	Min. score for modified pept	40
Calculate peak properties	False	Modifications included in pr	Oxidation (M) Acetyl (Protein N-term)
Combined folder location	C:\Users\lacav\Desktop\MQ\ Wouter_project	MS/MS deisotoping tolerance	ppm
Da interval. (FTMS)	100	MS/MS deisotoping tolerance	0.15
Date of writing	09/21/2020 12:23:37	MS/MS deisotoping tolerance	Da
Decoy mode	revert	MS/MS deisotoping tolerance	0.01
Fixed andromeda index folder	C:\Users\lacav\Desktop\MQ\ Andromeda	MS/MS tol. (FTMS)	20 ppm
Label min. ratio count	2	MS/MS tol. (ITMS)	0.5 Da
Machine name	DESKTOP-OMCDT80	MS/MS tol. (TOF)	40 ppm
Main search max. combination	200	Peptides used for protein qu	Razor
Max mods in site table	3	Site tables	Oxidation (M)Sites.txt Phospho (STY)Sites.txt
Max. peptide length for unsp	25	Temporary folder	C:\Users\lacav\Desktop\MQ\ Temp
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	lacav
Min. peptide Length	7	Variation mode	None
Min. peptide length for unsp	8	Version	1.6.7.0
Min. peptides	1	NA	NA

 $uniprot-proteome_up000005640+AND+reviewed_yes.fasta$

PG: PCA of 'raw intensity'

(excludes contaminants)

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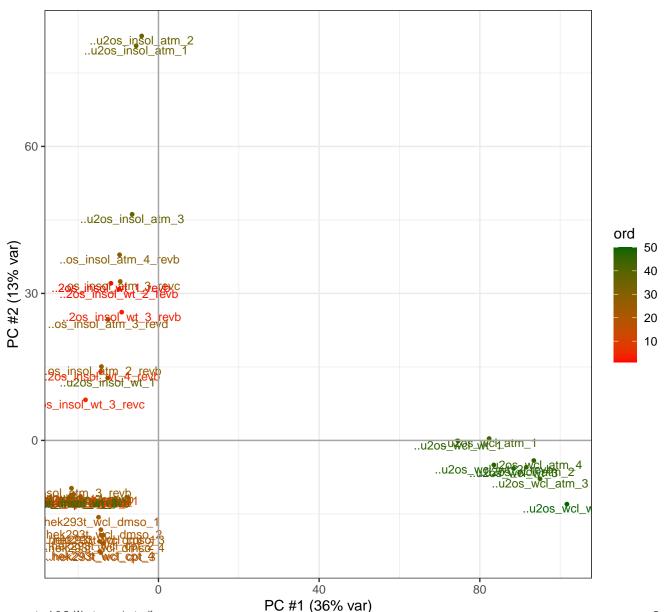
50 40

30 20

10

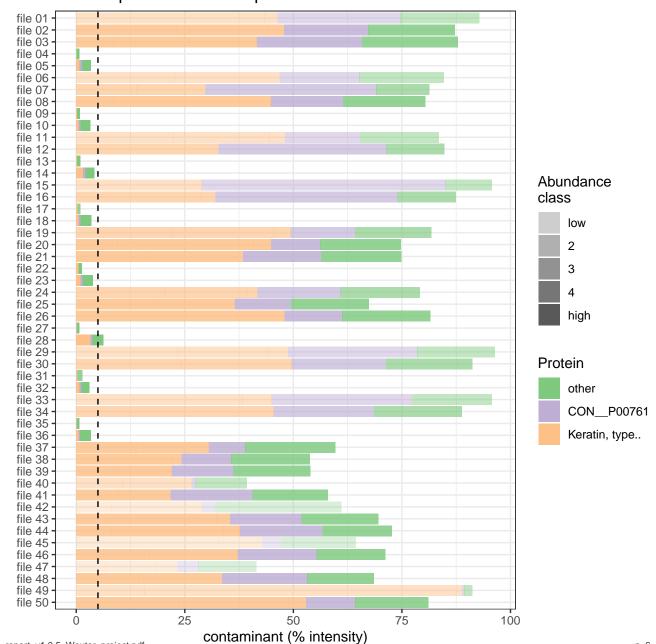
PG: PCA of 'Ifq intensity'

(excludes contaminants)



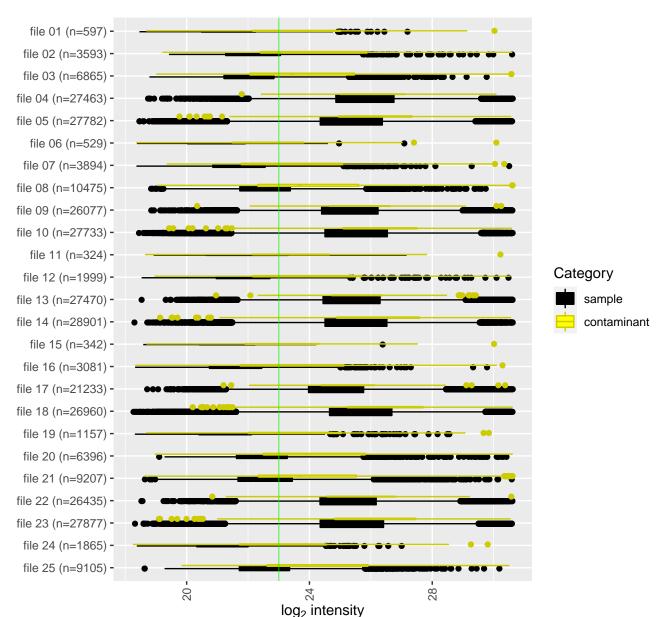
report_v1.0.5_Wouter_project.pdf

EVD: Top5 Contaminants per Raw file



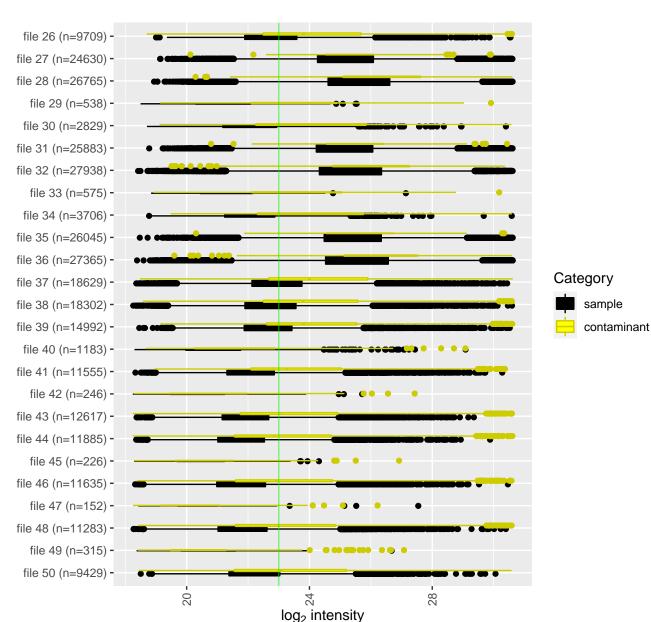
EVD: peptide intensity distribution

RSD 7.4% (expected < 5%)



EVD: peptide intensity distribution

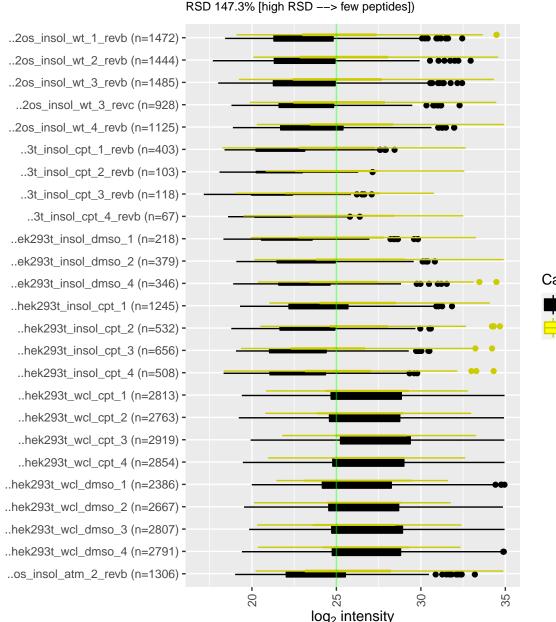
RSD 7.4% (expected < 5%)



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PG: intensity distribution

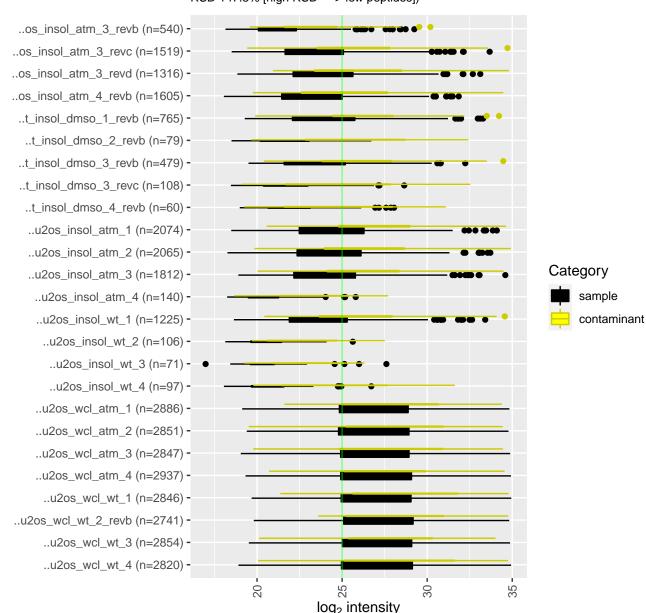
RSD 9.2% (w/o zero int.; expected < 5%) RSD 147.3% [high RSD --> few peptides])



Category
sample
contaminant

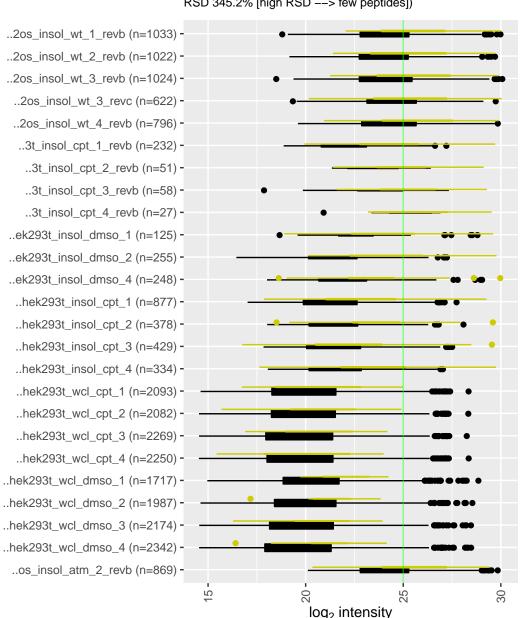
PG: intensity distribution

RSD 9.2% (w/o zero int.; expected < 5%) RSD 147.3% [high RSD --> few peptides])



PG: LFQ intensity distribution

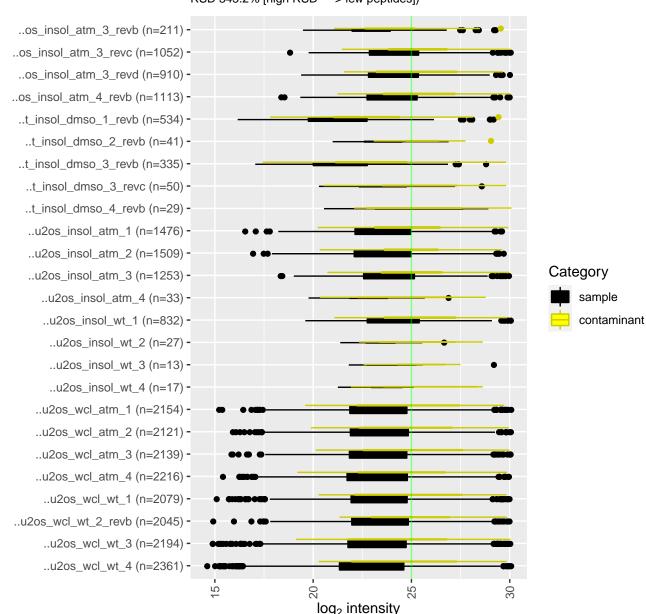
RSD 7.7% (w/o zero int.; expected < 5%)
RSD 345.2% [high RSD --> few peptides])



Category
sample
contaminant

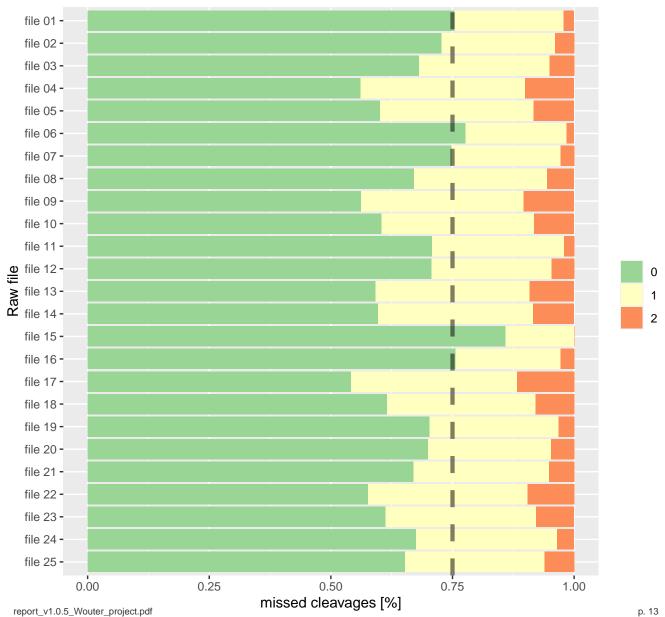
PG: LFQ intensity distribution

RSD 7.7% (w/o zero int.; expected < 5%) RSD 345.2% [high RSD ---> few peptides])



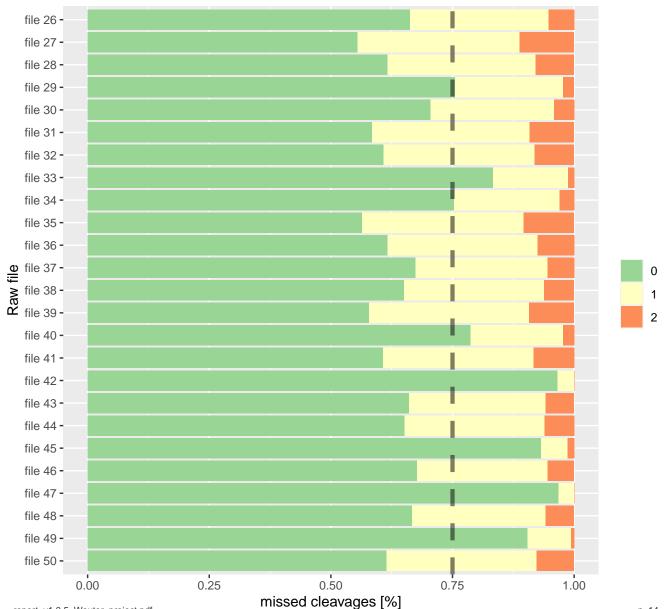
MSMS: Missed cleavages per Raw file

(excludes contaminants)

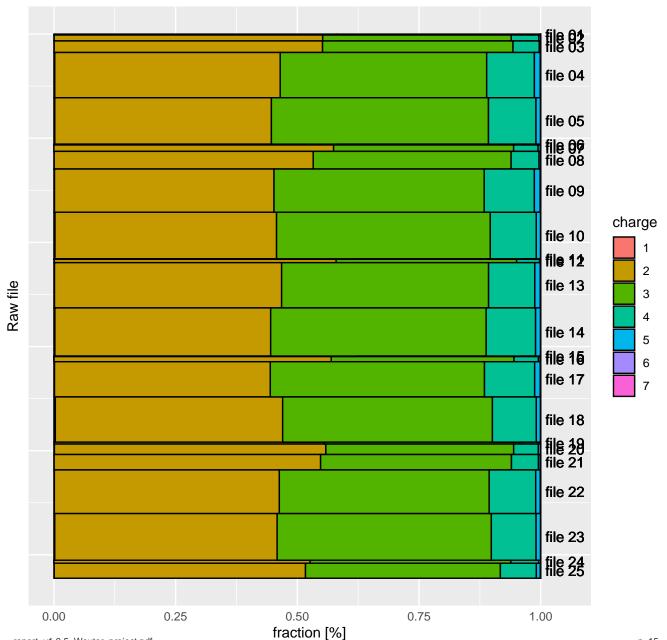


MSMS: Missed cleavages per Raw file

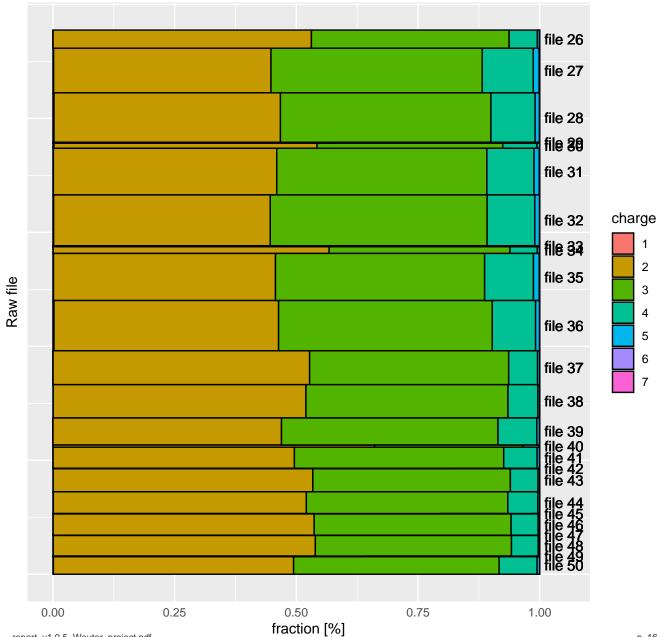
(excludes contaminants)



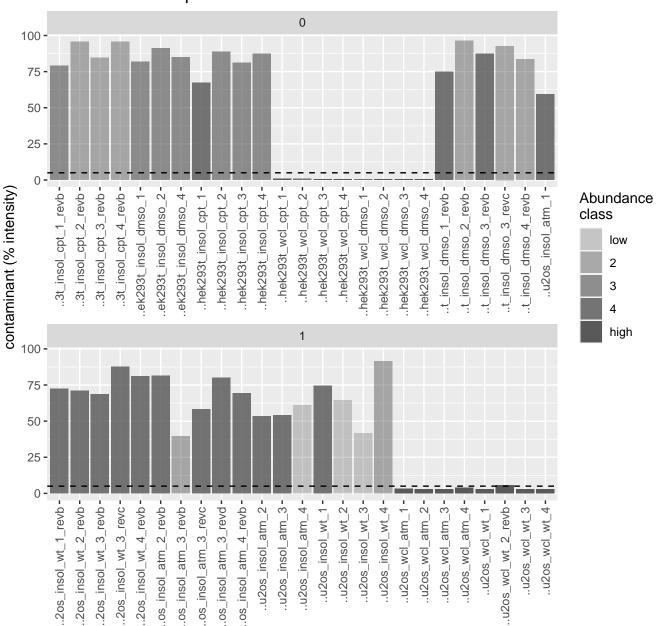
EVD: charge distribution

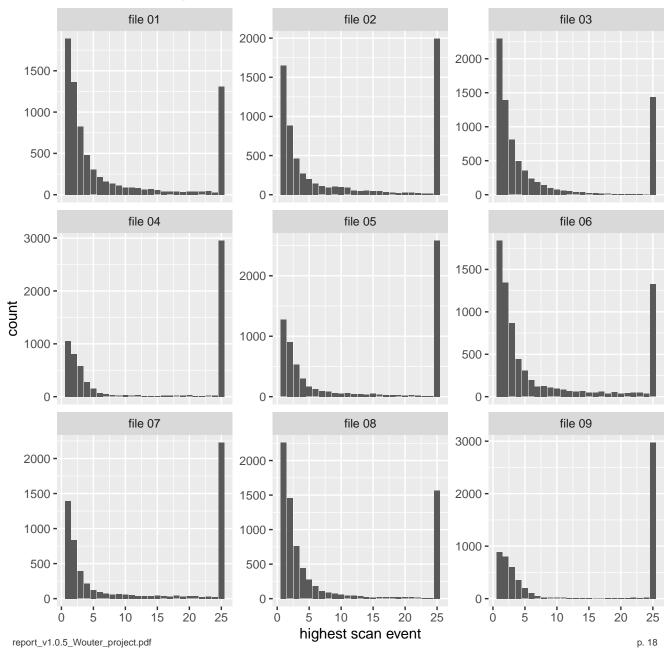


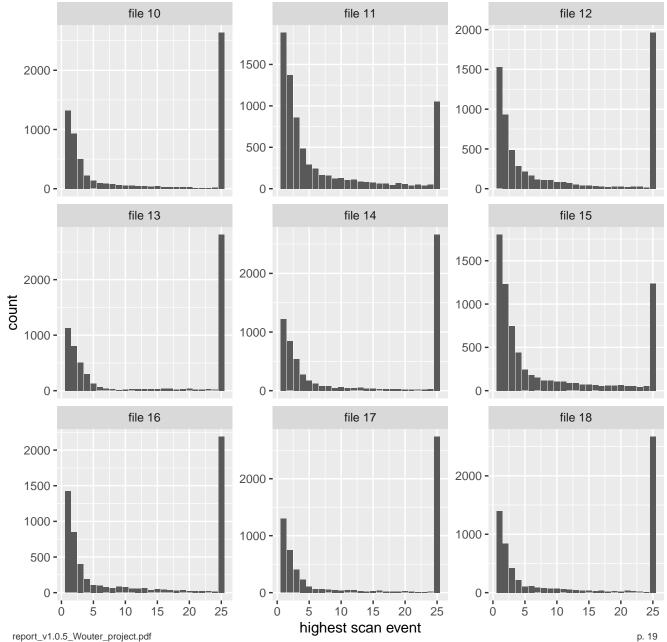
EVD: charge distribution

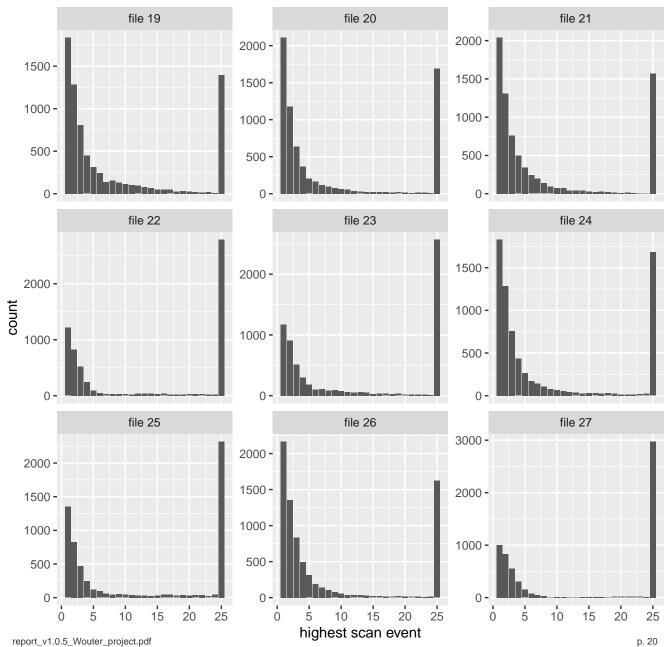


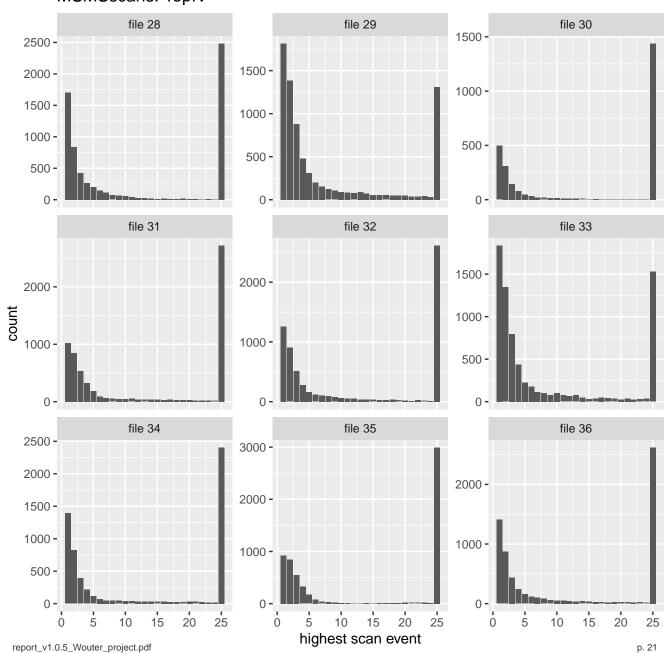
PG: Contaminant per condition

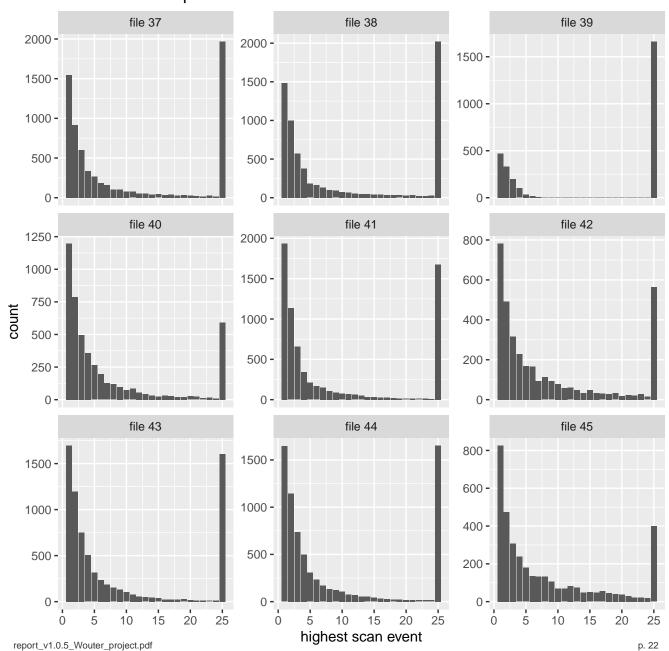


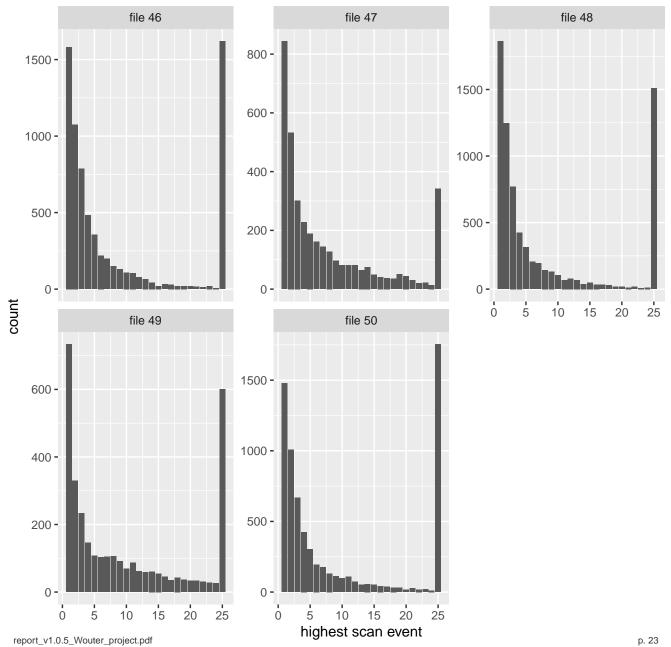


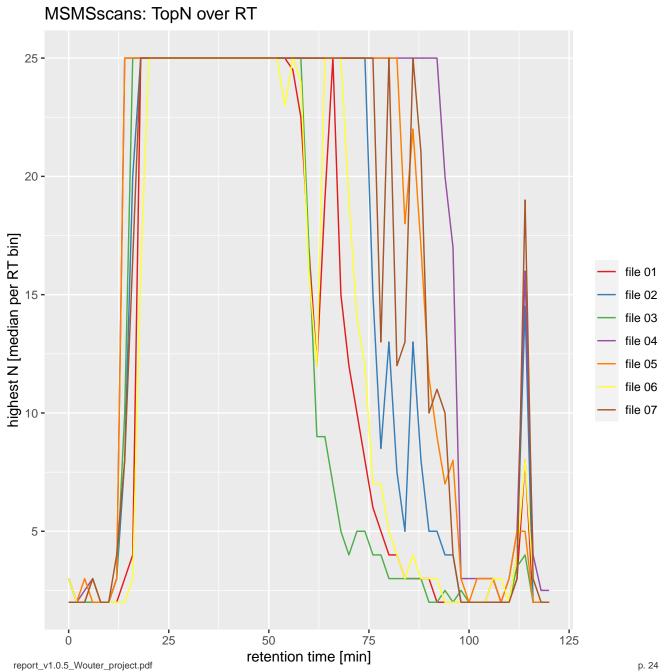


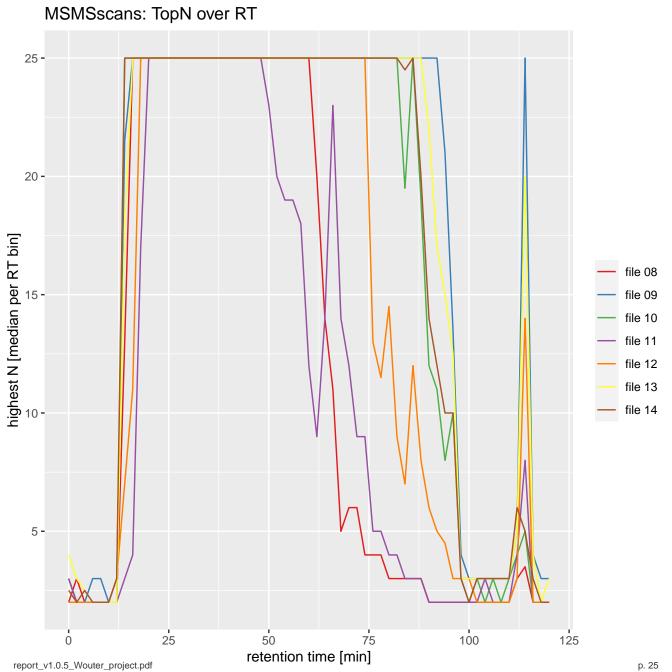


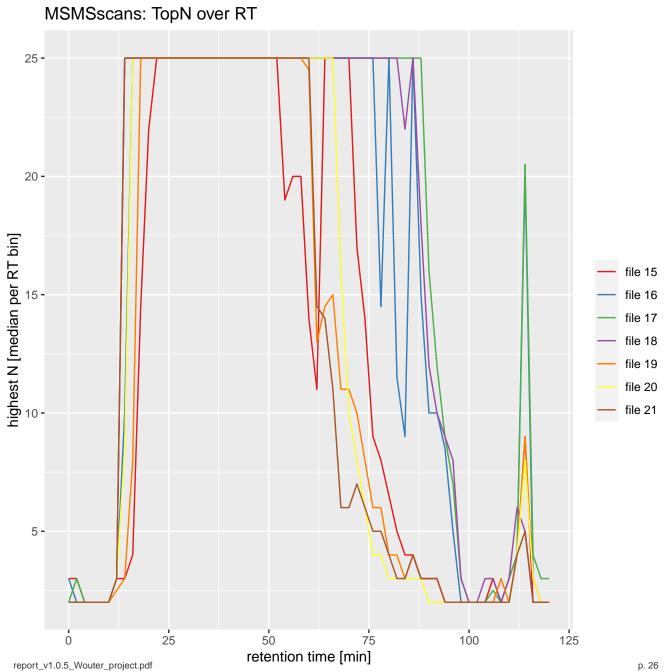


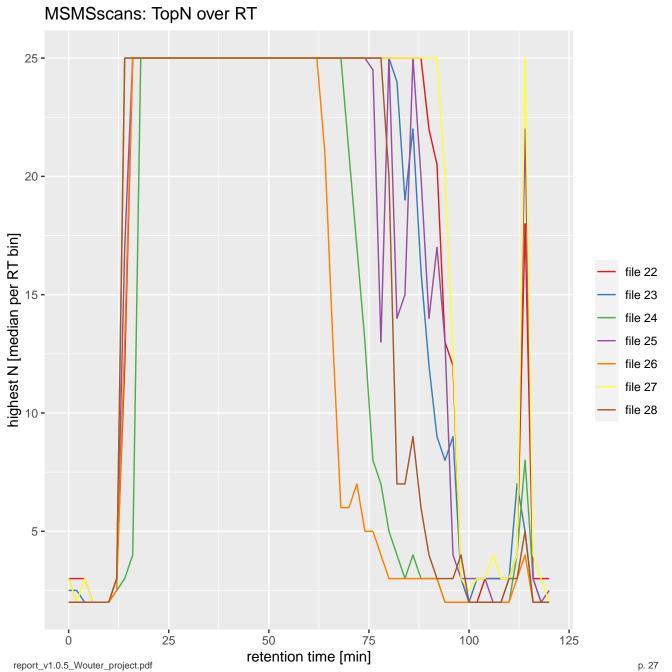


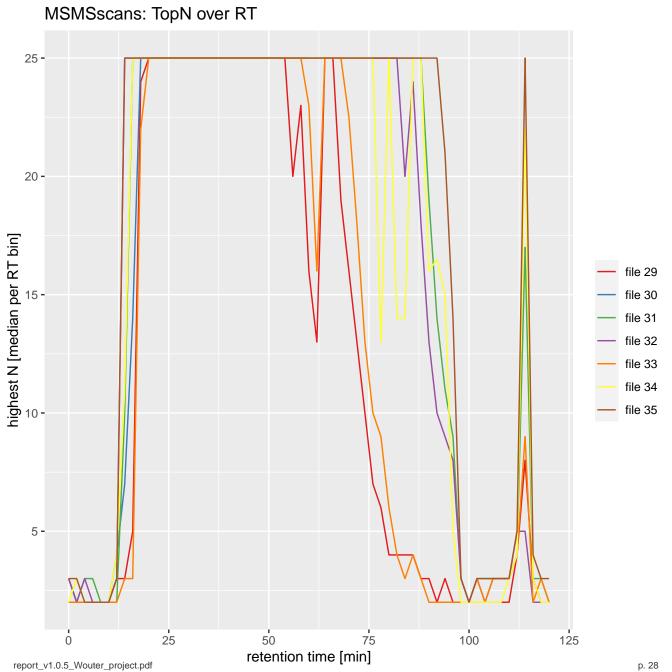


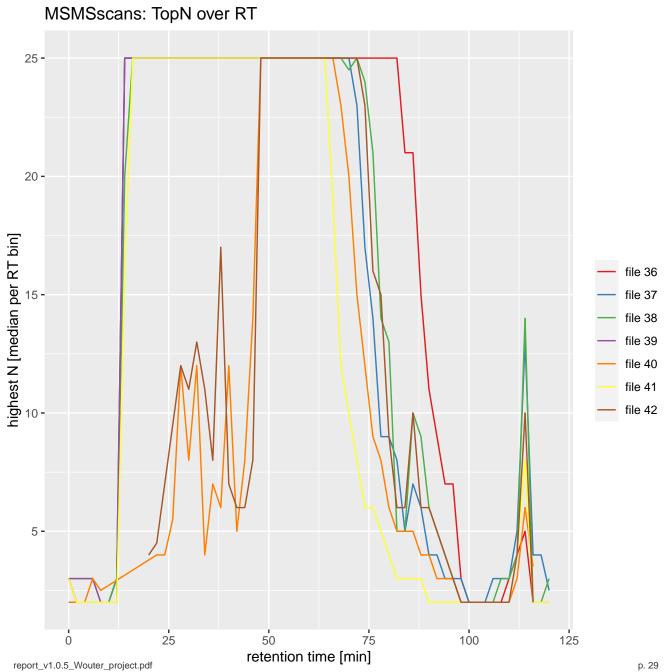




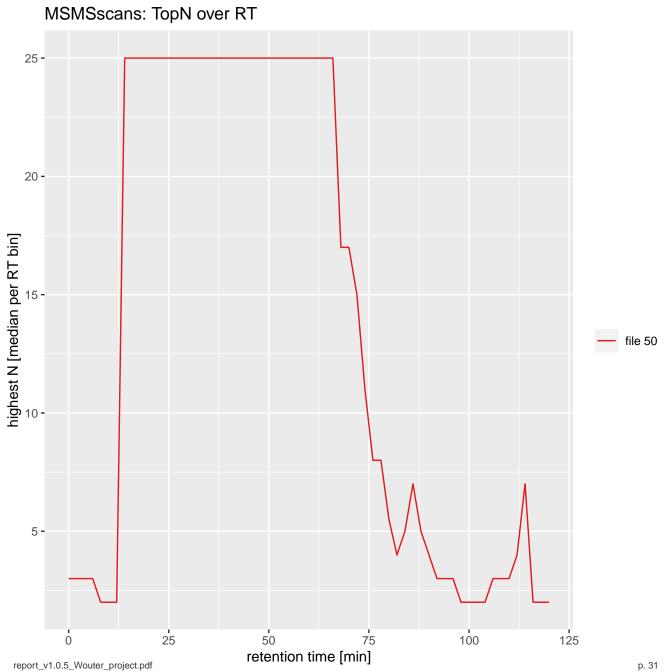








MSMSscans: TopN over RT 25 **-**20 highest N [median per RT bin] file 43 file 44 file 45 file 46 file 47 file 48 file 49 5 -Ó 25 50 75 100 125 retention time [min] report_v1.0.5_Wouter_project.pdf p. 30



EVD: IDs over RT 2000 -1500 **-**Raw file file 01 file 02 1000 file 03 file 04 file 05 file 06 file 07 500 -0 -60 30 90 RT [min] p. 32 report_v1.0.5_Wouter_project.pdf

EVD: IDs over RT 2000 -1500 **-**Raw file file 08 file 09 ID count file 10 1000 file 11 file 12 file 13 file 14 500 -0 -60 30 90 RT [min] p. 33 report_v1.0.5_Wouter_project.pdf

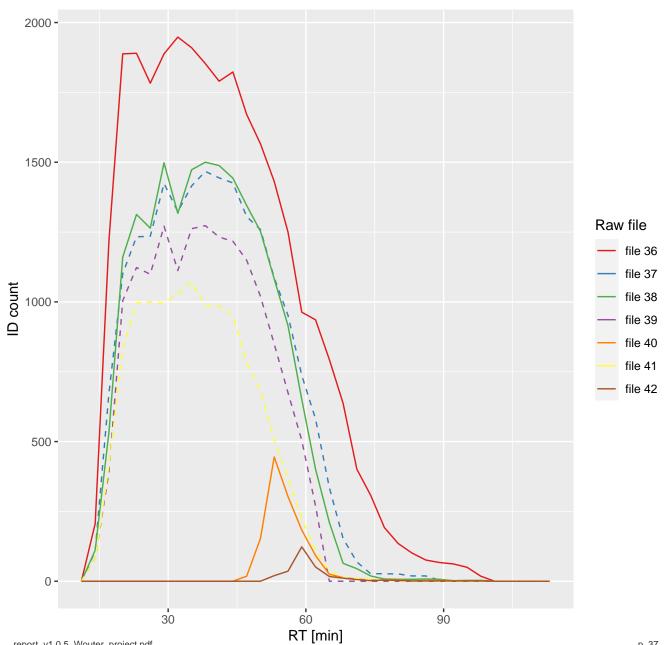
EVD: IDs over RT 1500 -Raw file file 15 file 16 1000 file 17 file 18 file 19 file 20 file 21 500 -0 -60 90 30 RT [min]

EVD: IDs over RT 2000 -1500 **-**Raw file file 22 file 23 1000 - Ont file 24 file 25 file 26 file 27 file 28 500 -0 -60 30 90 RT [min]

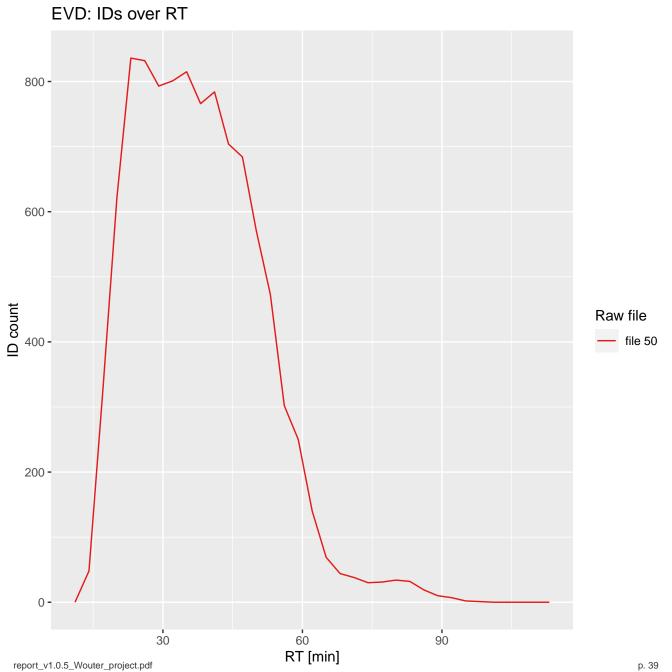
EVD: IDs over RT 2000 -1500 **-**Raw file file 29 file 30 00 nut file 31 file 32 file 33 file 34 file 35 500 -0 -60 90 30

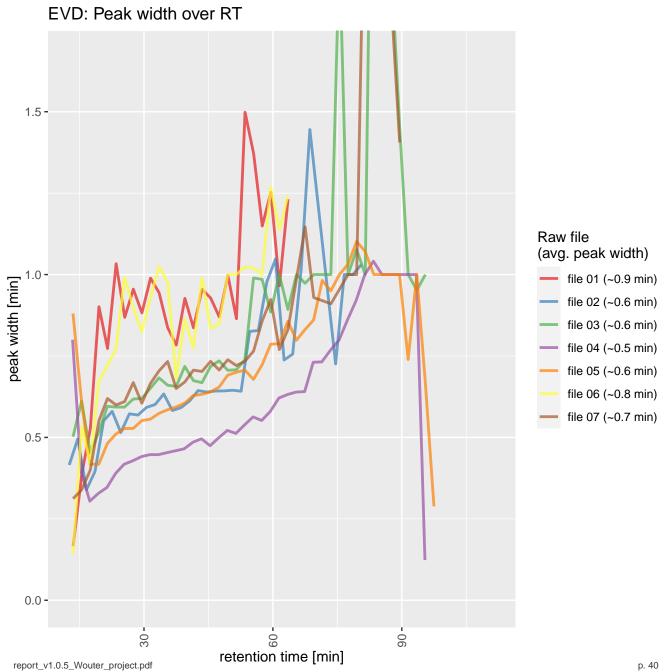
RT [min]

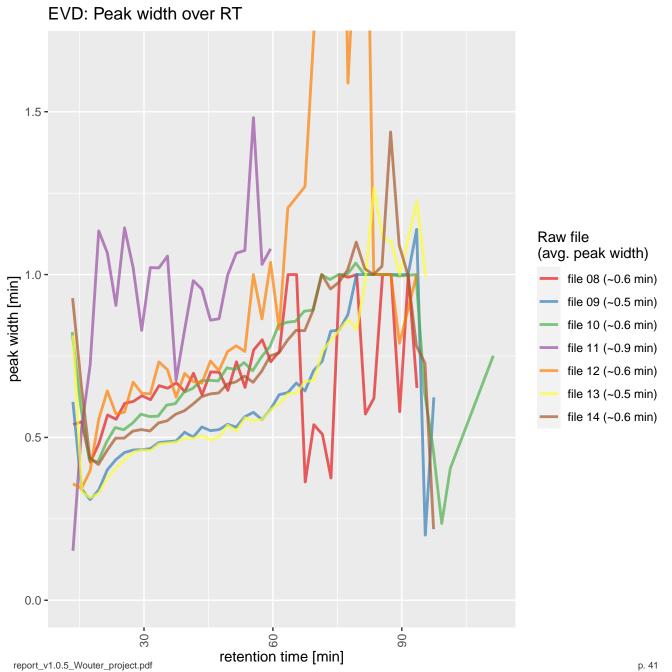
EVD: IDs over RT

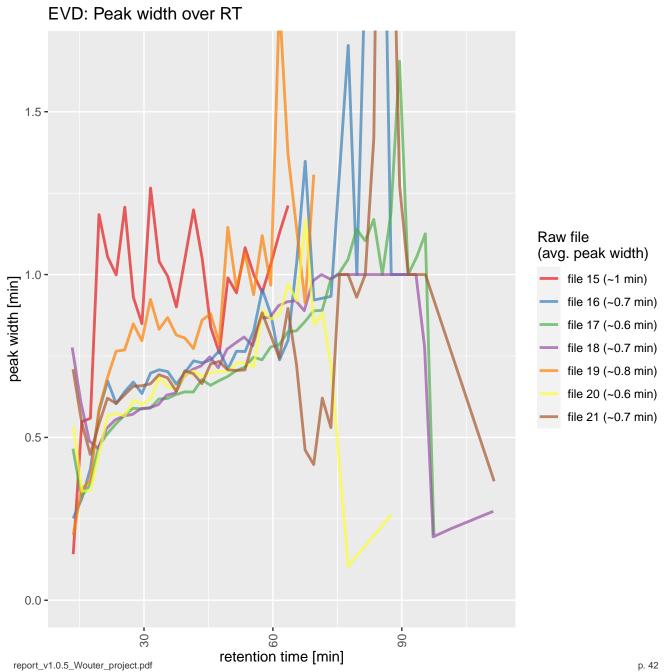


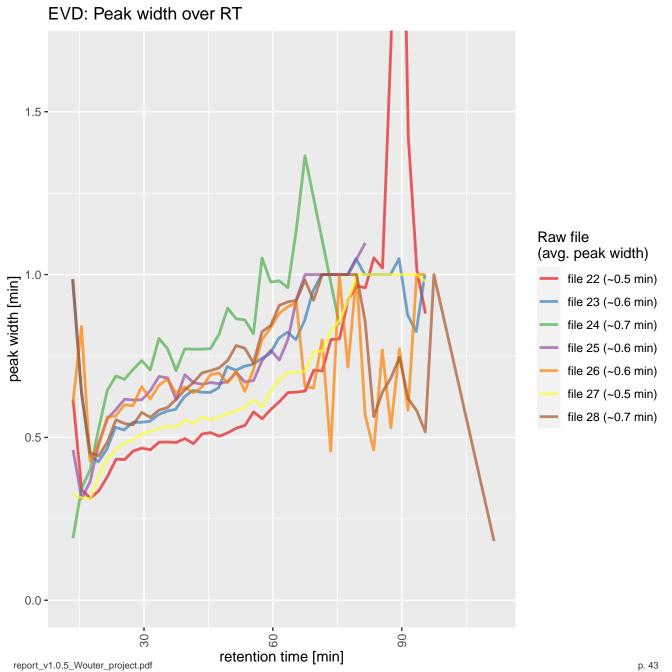
EVD: IDs over RT 1250 **-**1000 -Raw file 750 file 43 file 44 ID count file 45 file 46 file 47 500 file 48 file 49 250 **-**0 -60 90 30 RT [min] p. 38 report_v1.0.5_Wouter_project.pdf

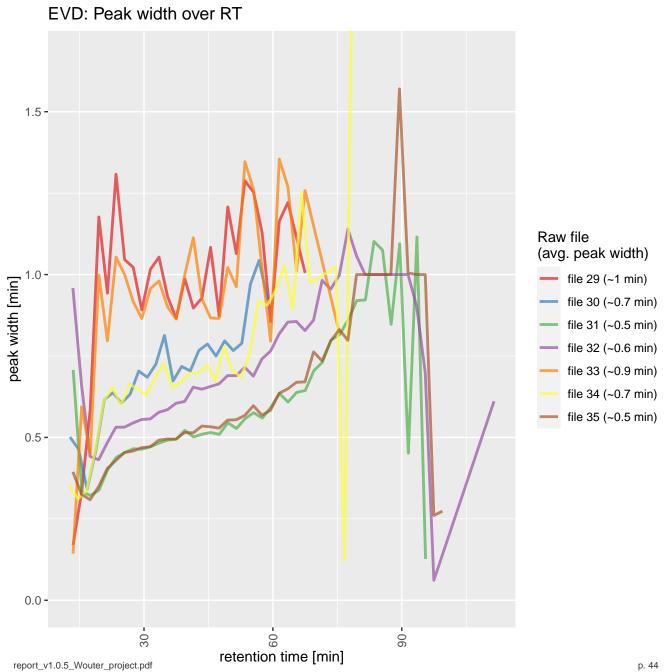


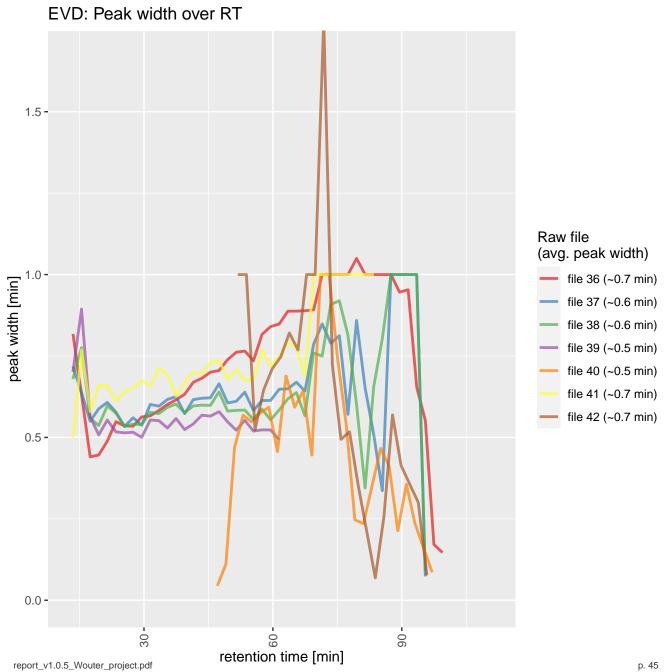


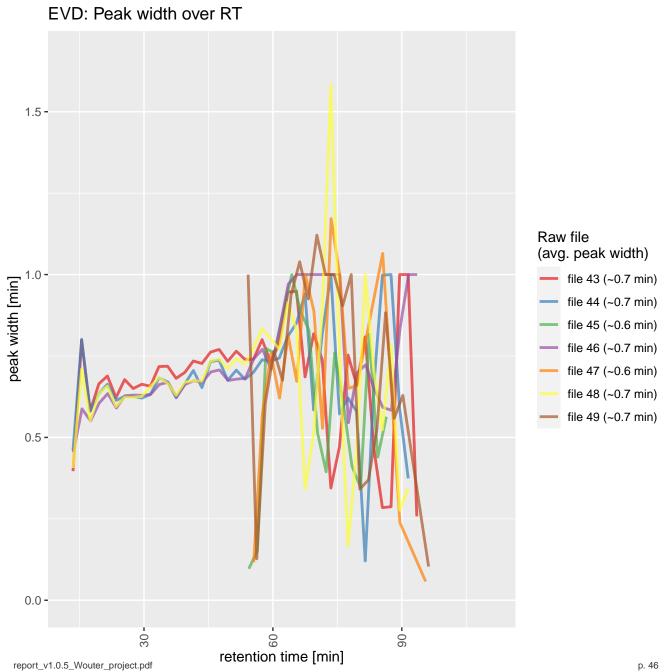


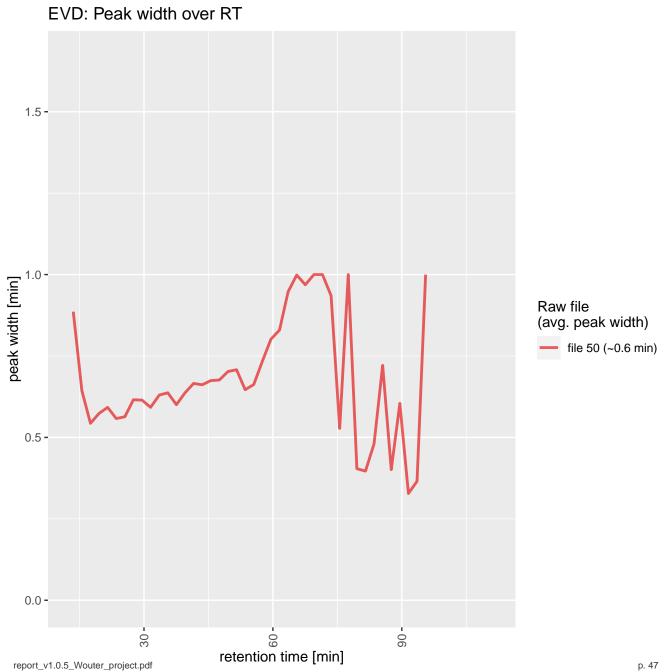


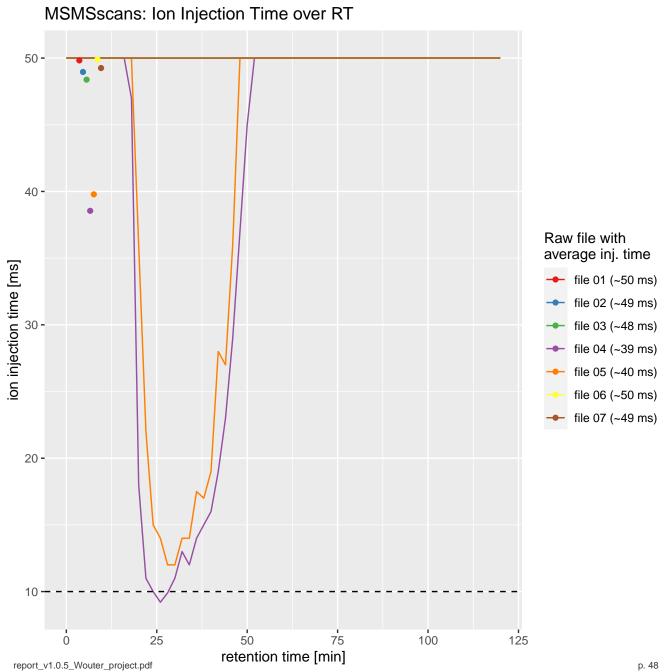


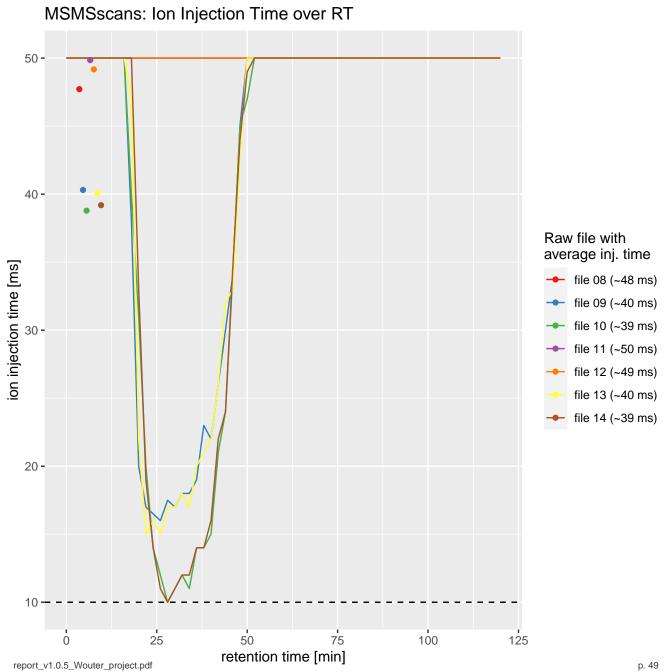


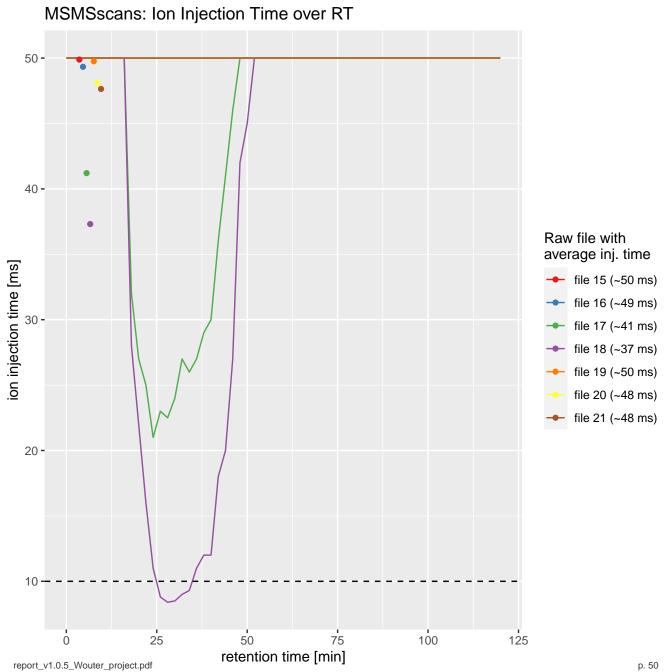


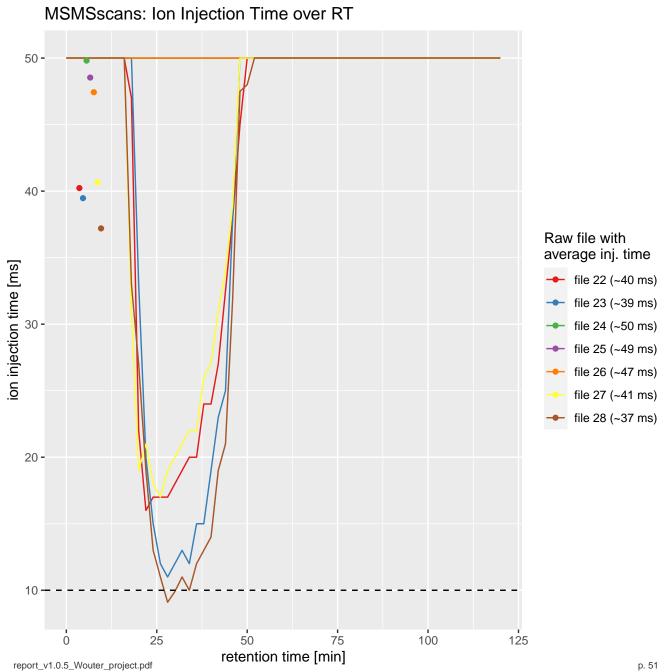


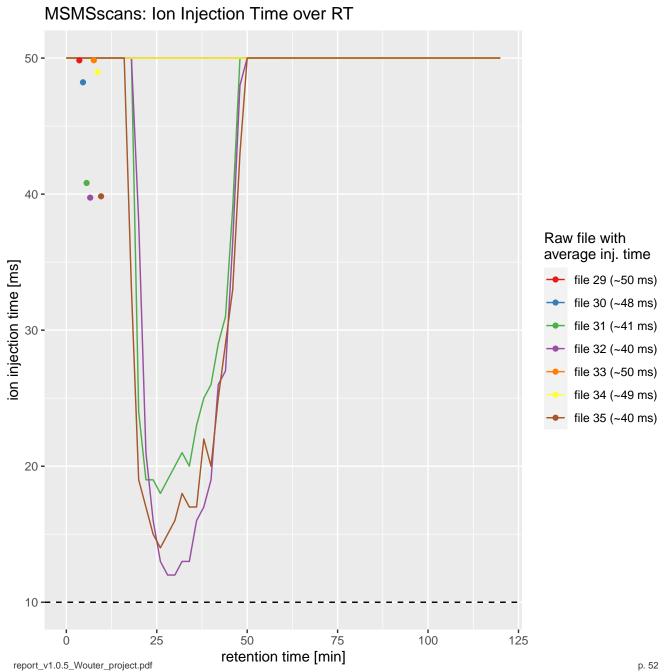


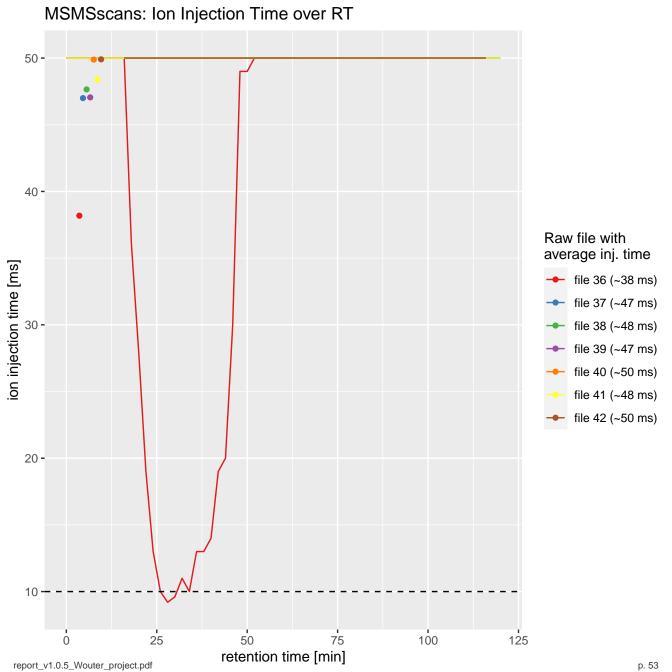


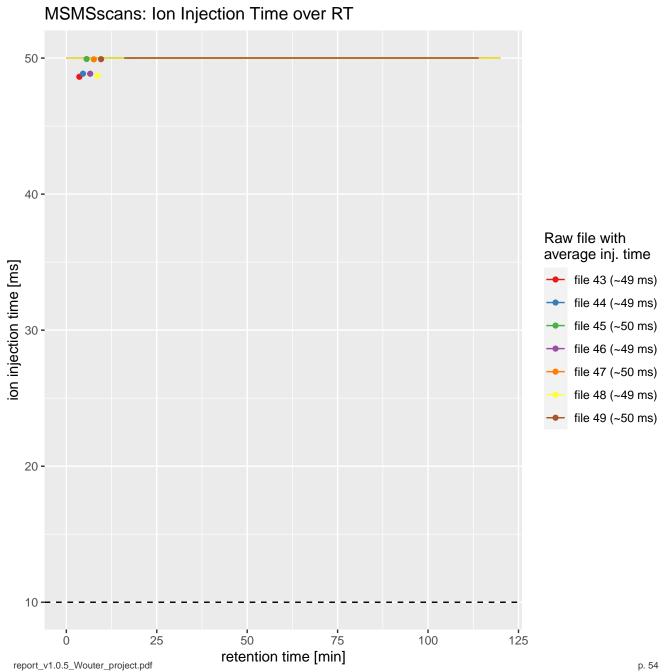


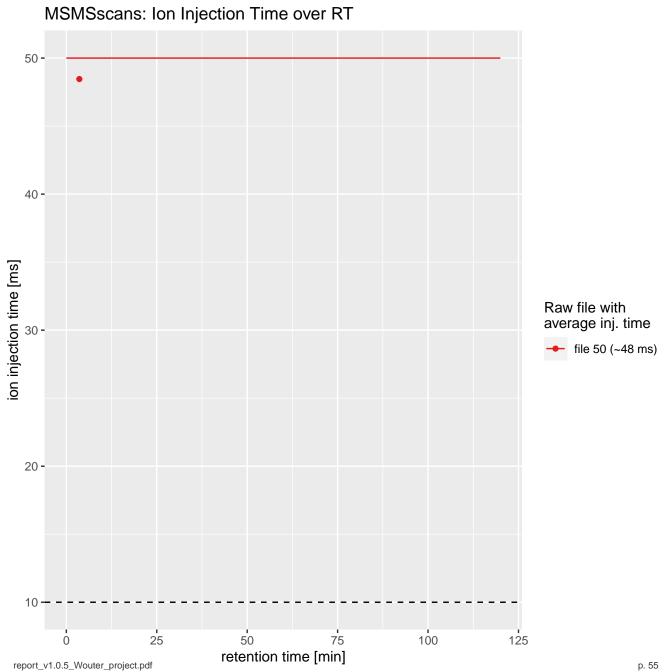








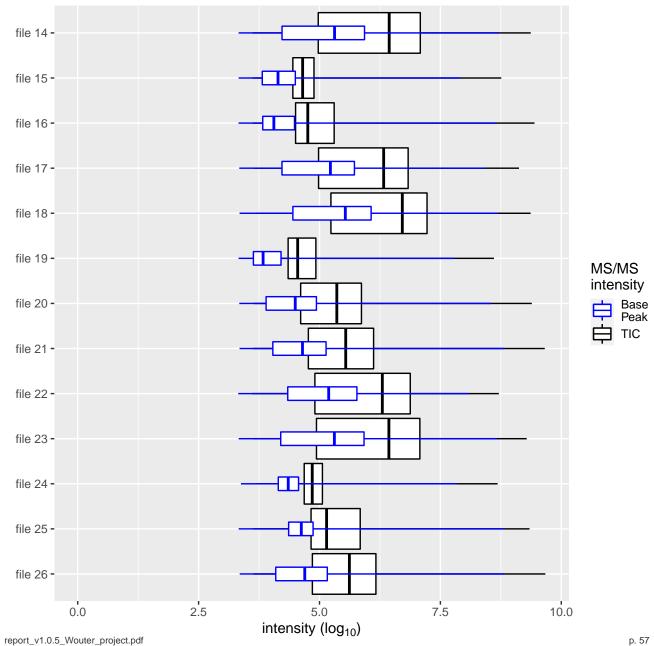




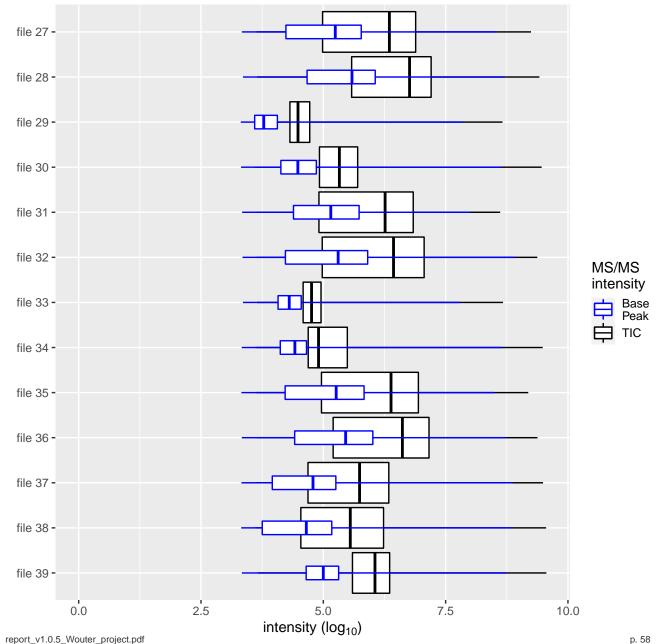
[experimental] MSMSscans: MS/MS intensity file 01 file 02 file 03 file 04 file 05 file 06 -MS/MS intensity Base Peak file 07 -TIC file 08 file 09 file 10 file 11 file 12 file 13 -2.5 5.0 7.5 0.0 10.0

intensity (log₁₀)

[experimental] MSMSscans: MS/MS intensity



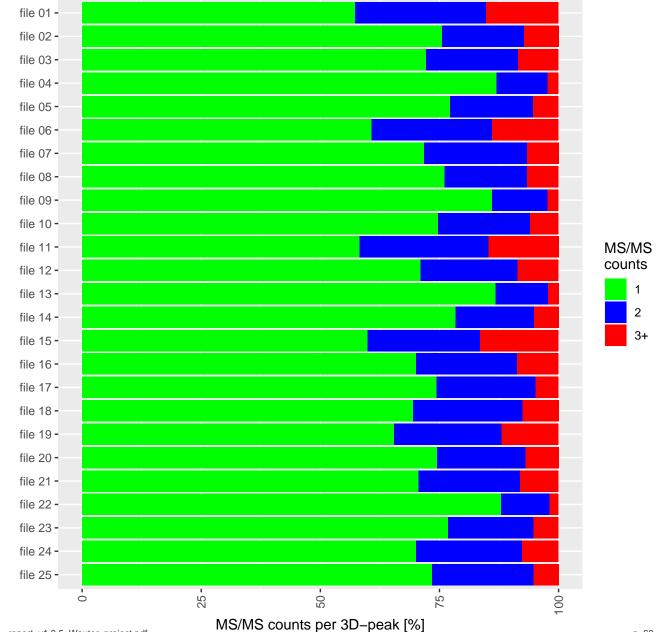
[experimental] MSMSscans: MS/MS intensity



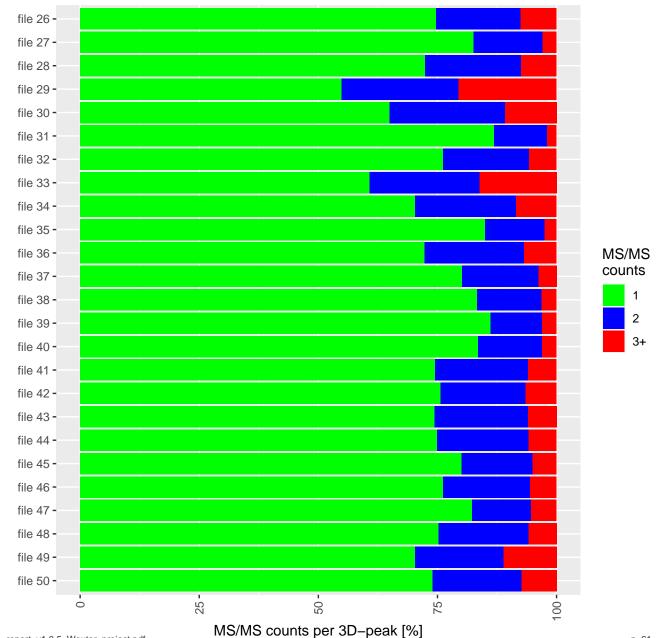
[experimental] MSMSscans: MS/MS intensity file 40 file 41 file 42 file 43 file 44 -MS/MS intensity file 45 -Base Peak TIC file 46 file 47 file 48 file 49 file 50 -5.0 7.5 0.0 2.5 intensity (log₁₀)

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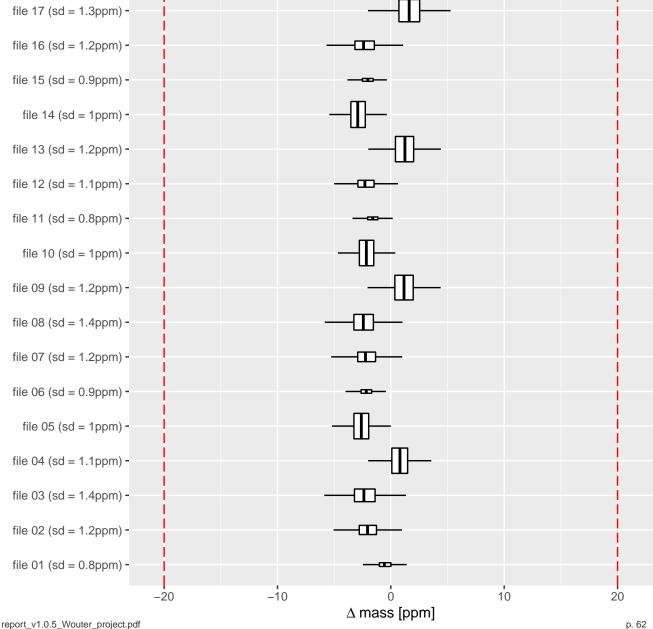
EVD: Oversampling (MS/MS counts per 3D-peak)



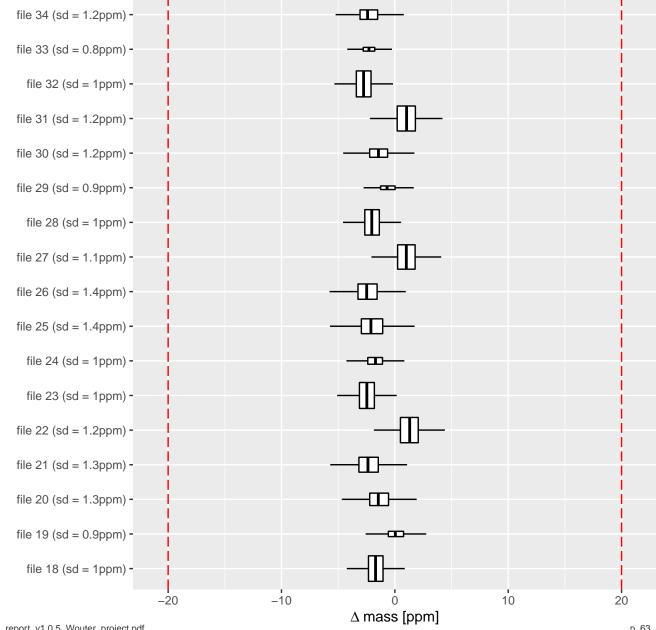
EVD: Oversampling (MS/MS counts per 3D-peak)



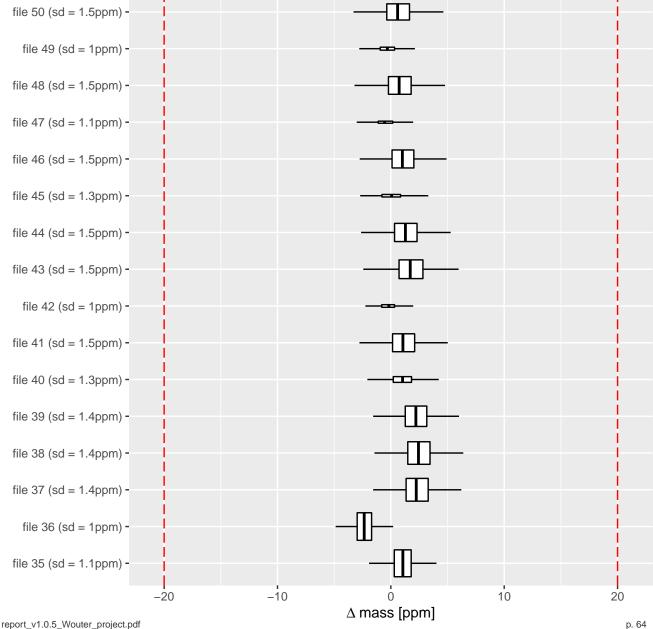
EVD: Uncalibrated mass error



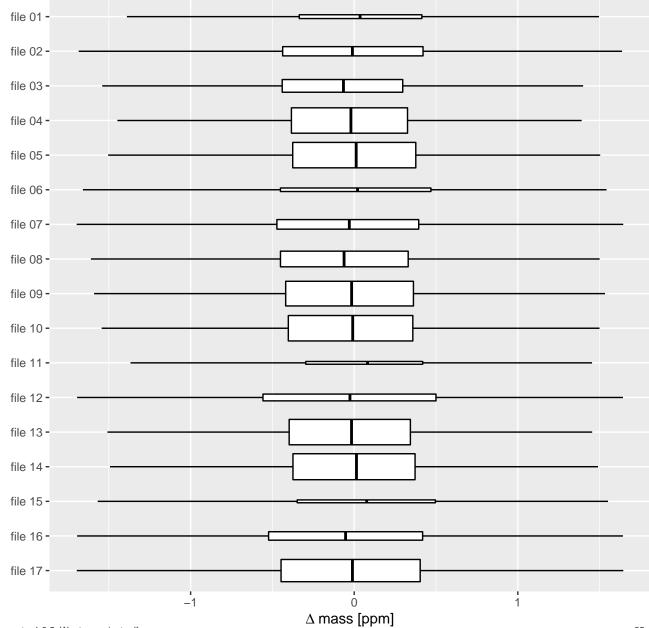
EVD: Uncalibrated mass error



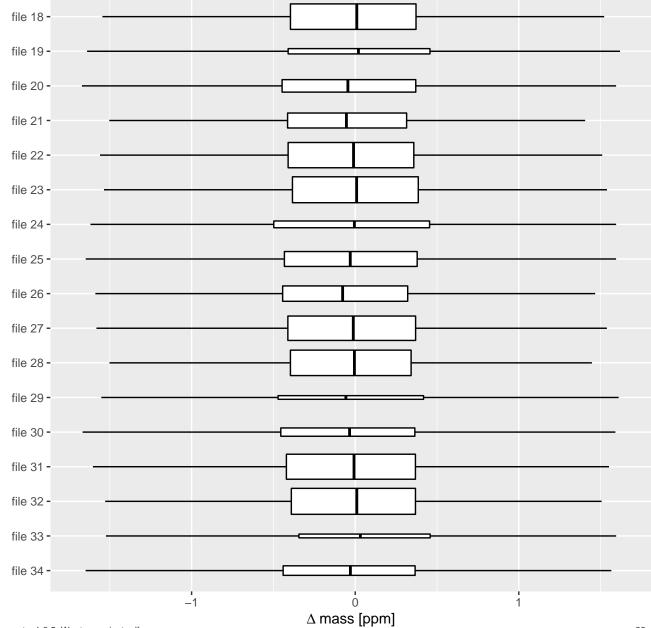
EVD: Uncalibrated mass error



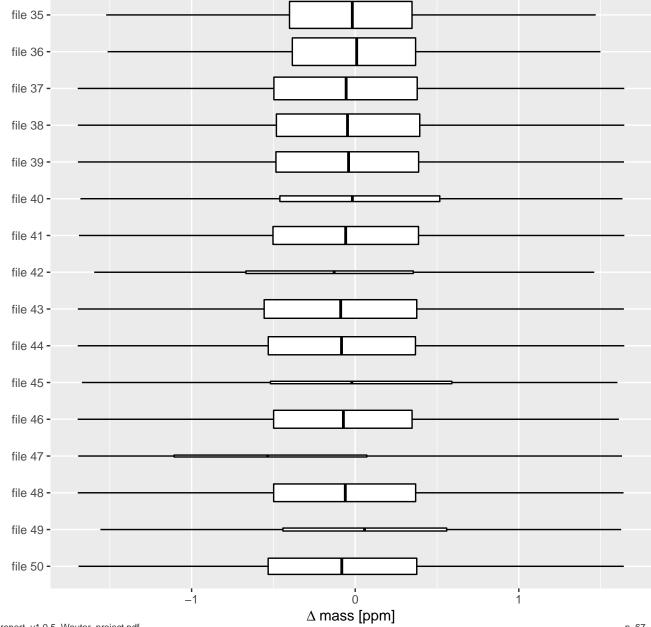
EVD: Calibrated mass error



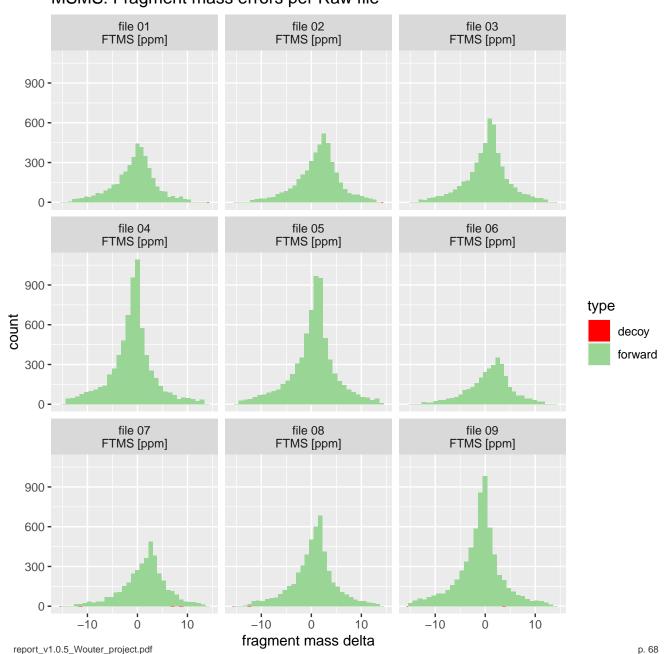
EVD: Calibrated mass error



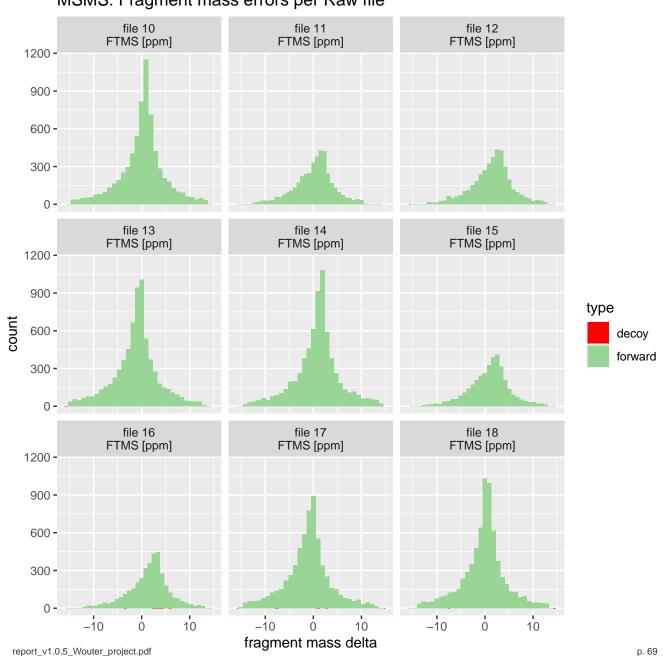
EVD: Calibrated mass error



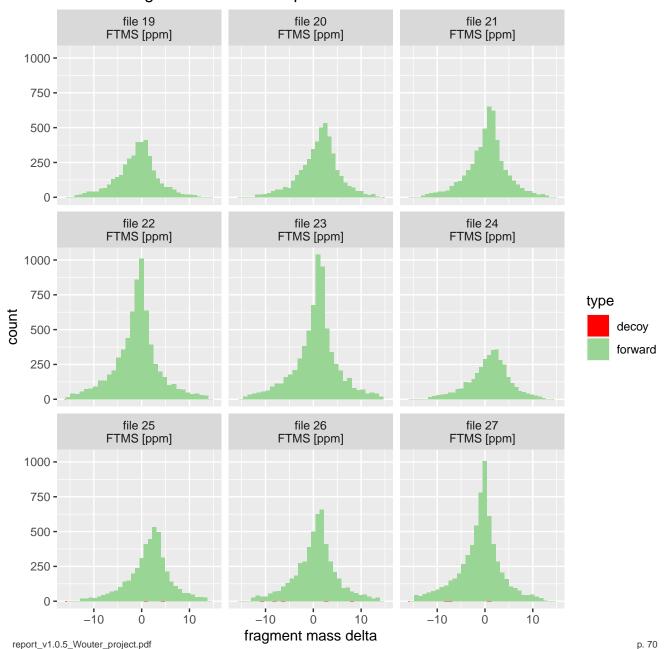
MSMS: Fragment mass errors per Raw file



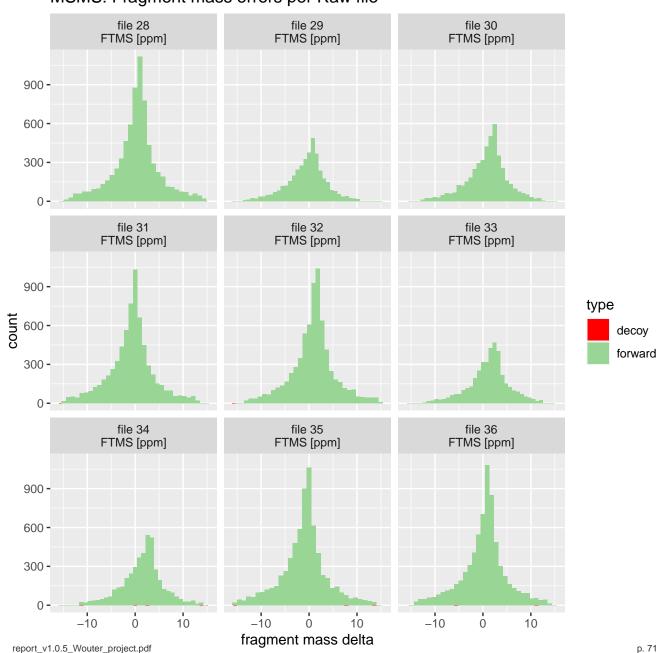
MSMS: Fragment mass errors per Raw file



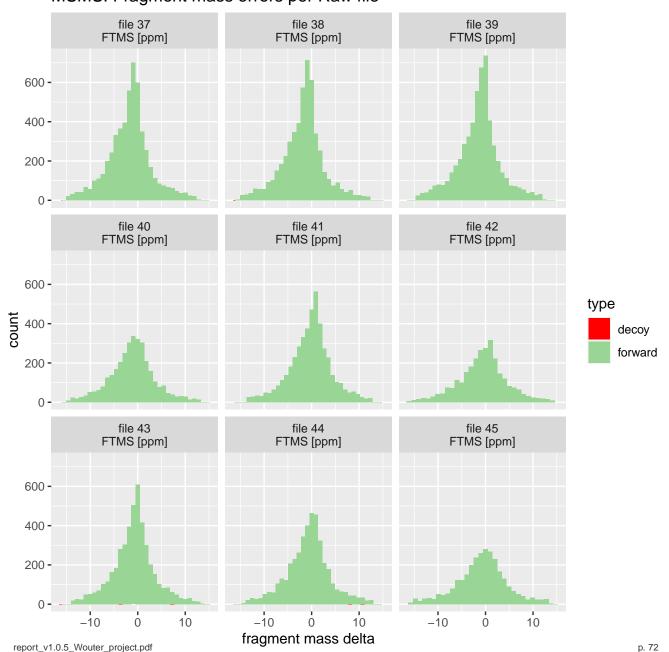
MSMS: Fragment mass errors per Raw file



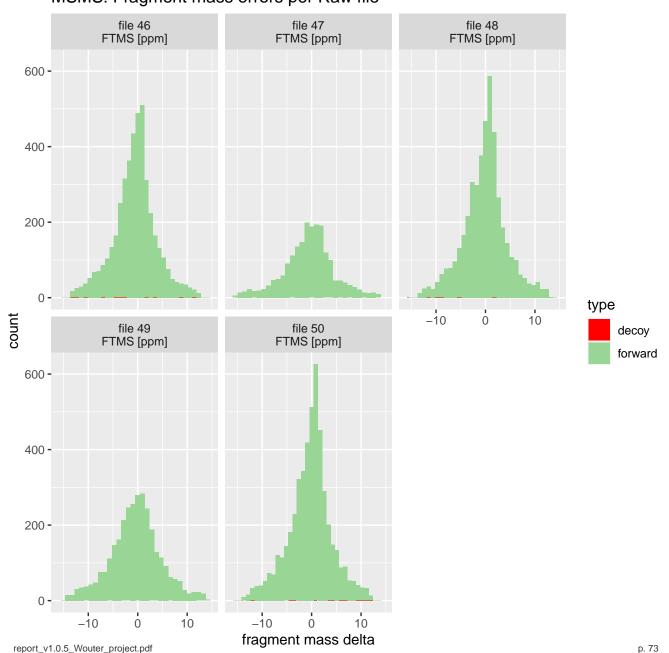
MSMS: Fragment mass errors per Raw file



MSMS: Fragment mass errors per Raw file



MSMS: Fragment mass errors per Raw file

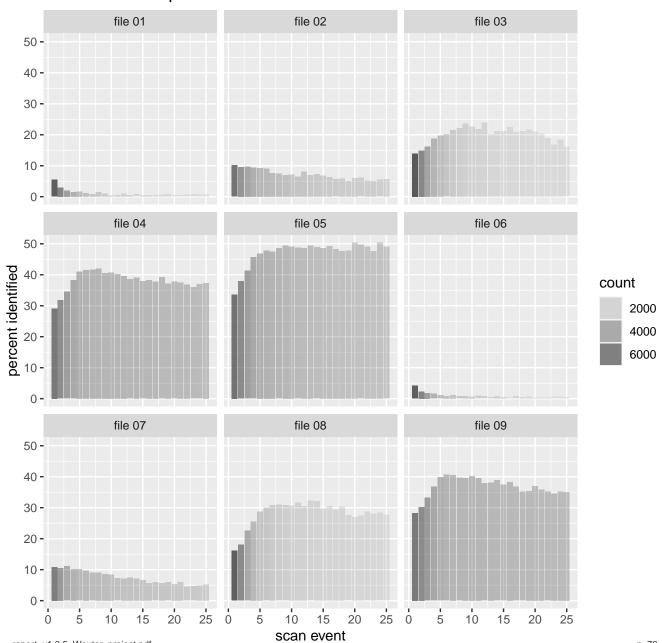


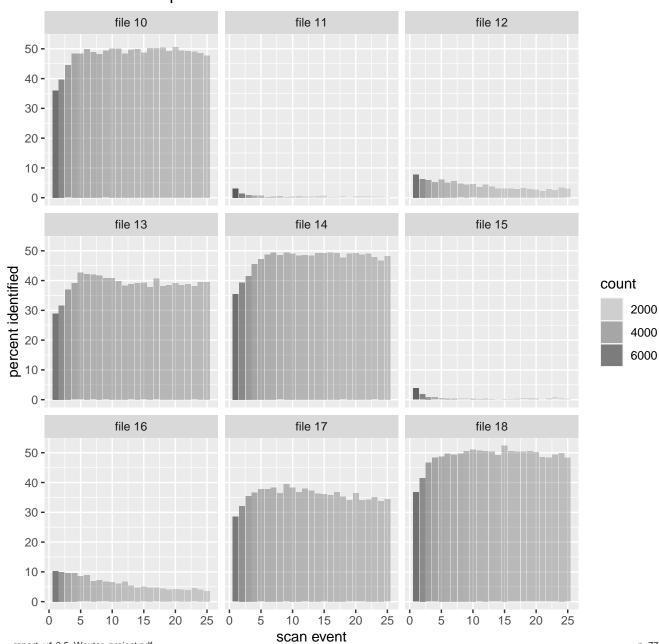
SM: MS/MS identified per Raw file file 01 file 04 file 07 file 09 file 12 file 14 file 17 file 20 file 22 -ID class bad (<20%) file 25 ok (20-35%) file 27 great (>35%) file 30 file 32 file 35 file 38 file 40 file 43 file 45 file 48 file 50 -10 30 40 0 20 MS/MS identified [%] report_v1.0.5_Wouter_project.pdf

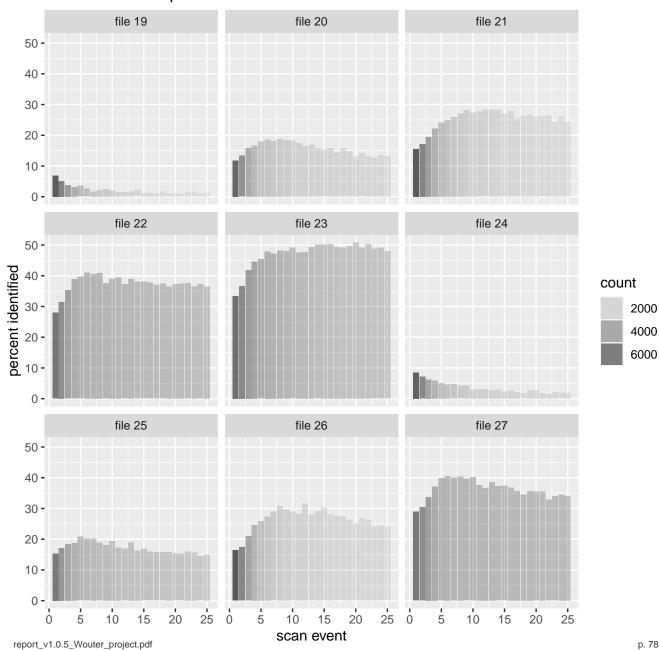
SM: Files with 'red' ID rate

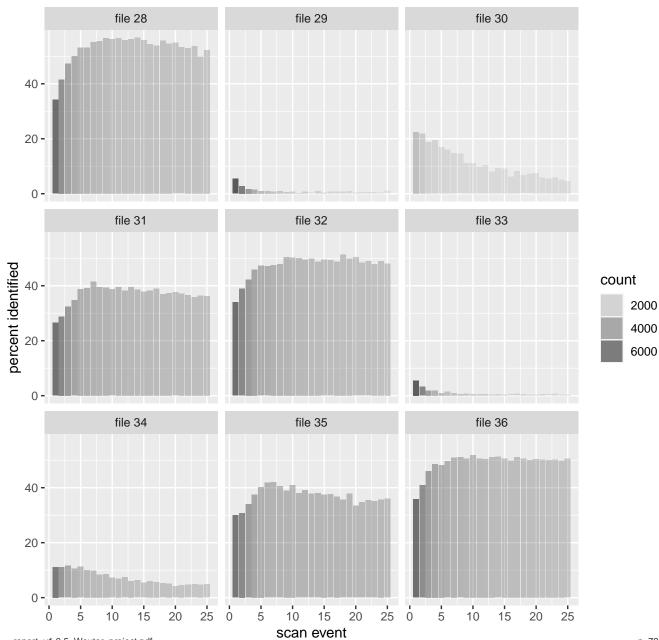
Raw file	% identified
10_DMSO_SDS_3	1.12
10_DMSO_SDS_3_5uL_20200612085223	5.22
10_insol_WT	13.29
12_Cpt_SDS_3	0.88
12_Cpt_SDS_3_5uL	5.32
12_insol_ATM	19.14
14_DMSO_SDS_4	0.58
14_DMSO_SDS_4_5uL	3.10
16_Cpt_SDS_4	0.60
16_Cpt_SDS_4_5uL	4.49
2_DMSO_SDS_1	1.98
2_DMSO_SDS_1_5uL	11.49
2_insol_WT	16.81
4_cpt_SDS_1	2.97
4_cpt_SDS_1_5uL	12.05
4_insol_ATM	17.93
6_DMSO_SDS_2	1.02
6_DMSO_SDS_2_5uL	9.69
8_Cpt_SDS_2	1.04
8_Cpt_SDS_2_5uL	5.22
insol_ATM_3_20200725191715	2.85
insol_ATM_4	0.74
insol_WT_1_20200727152510	19.33
insol_WT_2	0.61
insol_WT_2_20200727173305	18.72
insol_WT_3	0.42
insol_WT_3_20200727194055	19.23
insol_WT_4	1.00
insol_WT_4_20200727214846	15.67

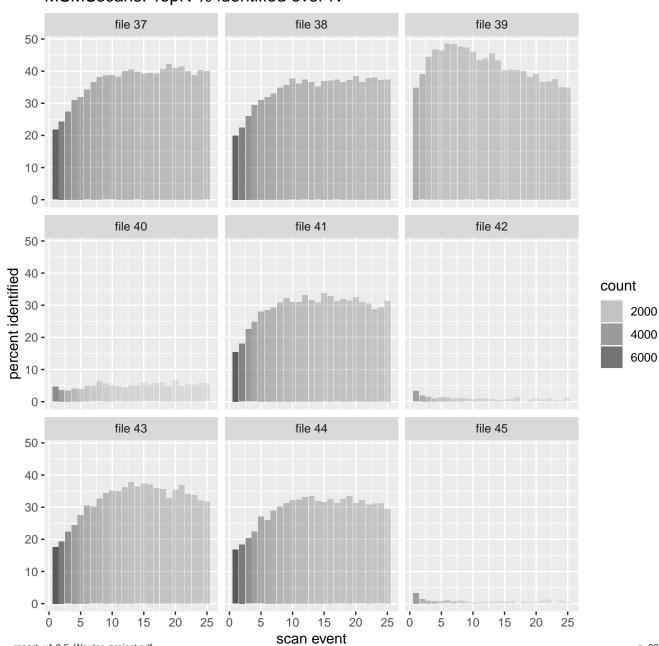
58% of samples)

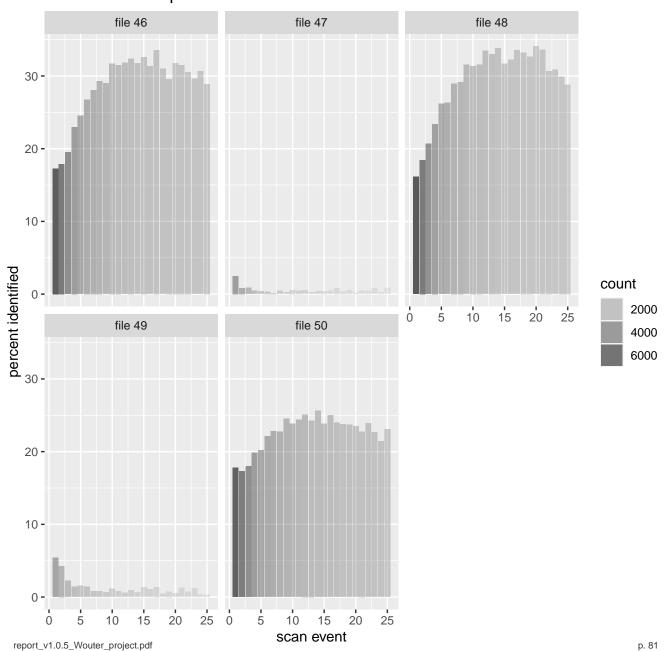






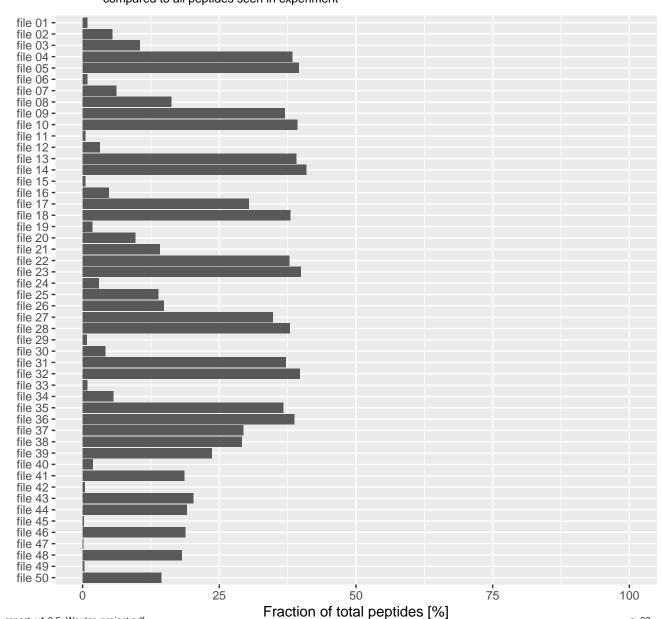






[experimental] EVD: Non-Missing Peptides

compared to all peptides seen in experiment

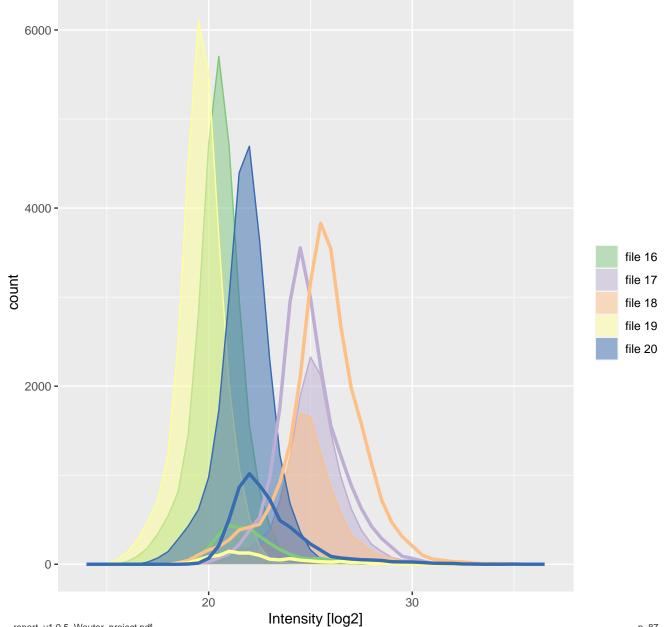


[experimental] EVD: Non-missing by set 100 -75 **-**Fraction of total peptides [%] 50 **-**25 **-**0 -10 20 30 40 50 0 Minimum # Raw files p. 83 report_v1.0.5_Wouter_project.pdf

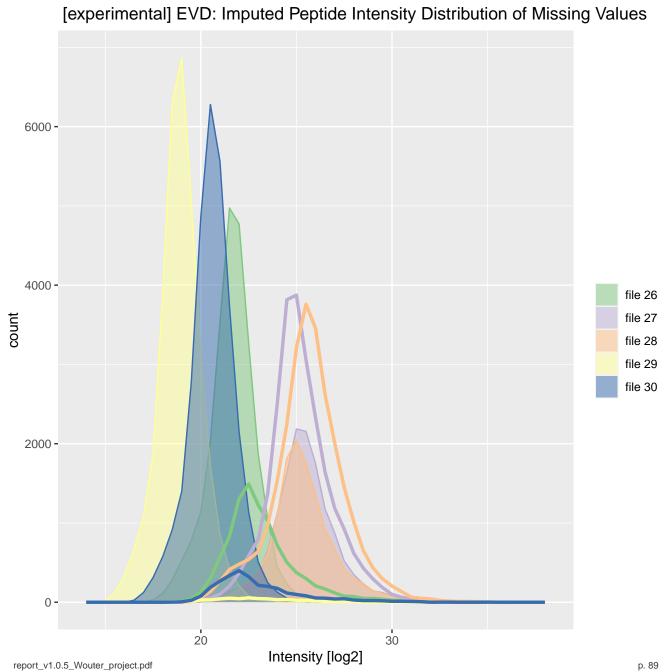
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 5000 -4000 -3000 file 01 count file 02 file 03 file 04 file 05 2000 -1000 -0 -20 30 Intensity [log2] p. 84 report_v1.0.5_Wouter_project.pdf

[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 6000 -4000 file 06 file 07 file 08 file 09 file 10 2000 -0 -20 30 Intensity [log2] p. 85 report_v1.0.5_Wouter_project.pdf

[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 6000 -4000 file 11 file 12 file 13 file 14 file 15 2000 -0 -20 25 30 15 35 Intensity [log2] report_v1.0.5_Wouter_project.pdf p. 86 [experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values



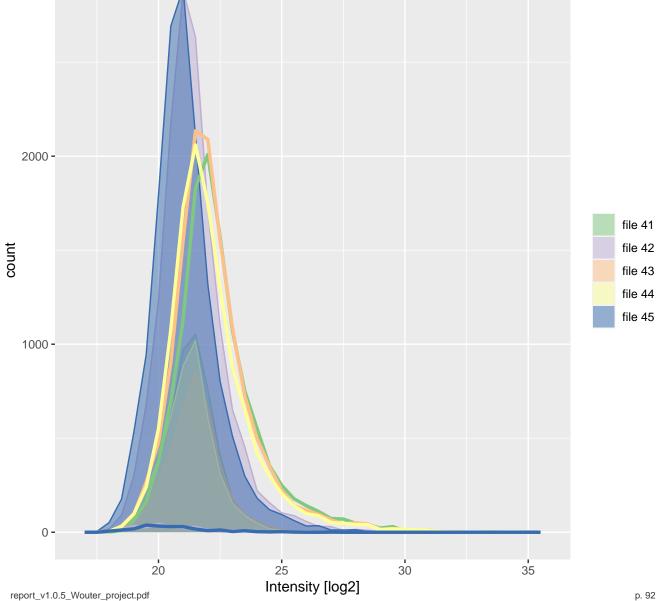
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 6000 file 21 4000 file 22 file 23 file 24 file 25 2000 -0 -20 30 Intensity [log2] p. 88 report_v1.0.5_Wouter_project.pdf



[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 6000 -4000 file 31 file 32 file 33 file 34 file 35 2000 -0 -20 25 35 15 30 Intensity [log2] p. 90 report_v1.0.5_Wouter_project.pdf

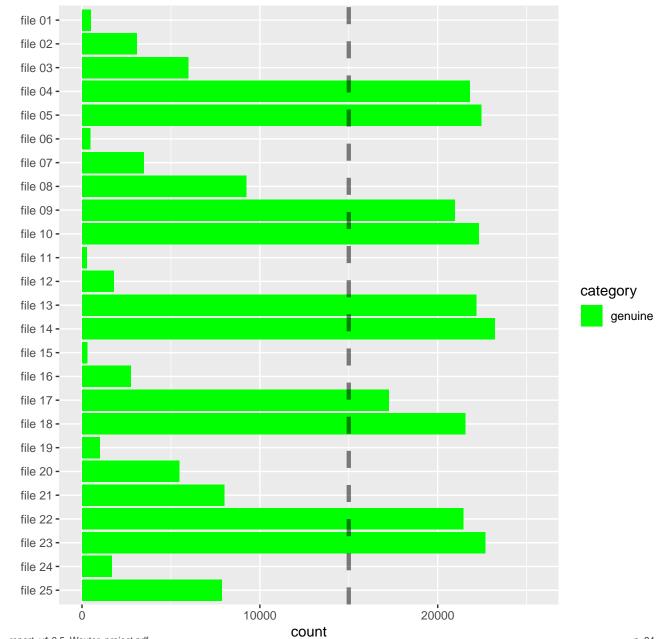
[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 6000 -4000 file 36 file 37 file 38 file 39 file 40 2000 -0 -20 40 30 Intensity [log2] report_v1.0.5_Wouter_project.pdf p. 91

[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 3000 -

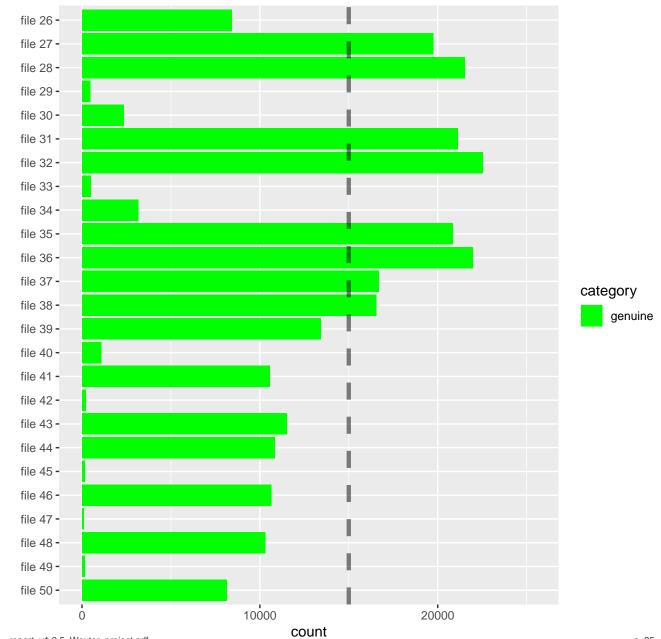


[experimental] EVD: Imputed Peptide Intensity Distribution of Missing Values 2000 file 46 file 47 file 48 file 49 file 50 1000 -0 -20 25 35 30 Intensity [log2] p. 93 report_v1.0.5_Wouter_project.pdf

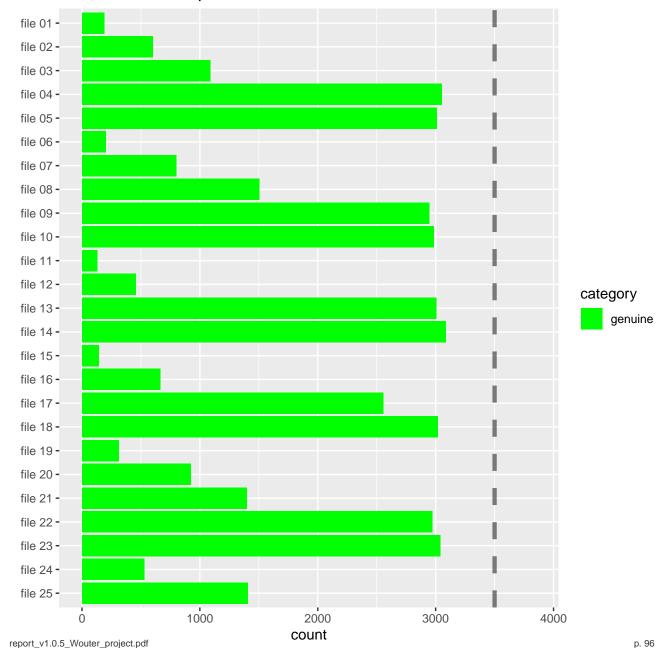
EVD: Peptide ID count



EVD: Peptide ID count



EVD: ProteinGroups count



EVD: ProteinGroups count

