

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065581.D
 Acq On : 25 Jan 2021 16:57
 Operator : JC/MD
 Sample : PB134285ZHE#01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB134285ZHE#01

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M

Title : SW846 8260

Signal : TIC: VN065581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.499	842	858	882	rVB3	16493	51234	1.92%	0.403%
2	7.550	1785	1807	1817	rBV	124194	309630	11.58%	2.433%
3	7.624	1818	1830	1856	rVB	243999	581562	21.76%	4.569%
4	7.987	1925	1943	1965	rBV	153359	354642	13.27%	2.786%
5	8.129	1976	1987	2003	rVB	14916	32349	1.21%	0.254%
6	8.547	2101	2117	2137	rBV	376712	795971	29.78%	6.253%
7	9.151	2292	2305	2317	rBV3	17667	37440	1.40%	0.294%
8	9.235	2317	2331	2361	rVV	966493	1794419	67.13%	14.098%
9	9.872	2516	2529	2545	rBV	175261	306146	11.45%	2.405%
10	10.058	2573	2587	2607	rBV	601479	1102432	41.24%	8.661%
11	10.248	2637	2646	2657	rVB	17898	30555	1.14%	0.240%
12	10.515	2716	2729	2740	rBV	53789	90317	3.38%	0.710%
13	10.608	2746	2758	2774	rBV	111524	186684	6.98%	1.467%
14	10.733	2785	2797	2814	rVV	1657877	2673039	100.00%	21.000%
15	10.823	2815	2825	2843	rVB	170437	283470	10.60%	2.227%
16	11.138	2907	2923	2947	rBV	1159529	1842839	68.94%	14.478%
17	11.376	2983	2997	3018	rVB	511123	892776	33.40%	7.014%
18	11.849	3134	3144	3159	rBV	38575	63794	2.39%	0.501%
19	12.373	3294	3307	3331	rBV	364988	621863	23.26%	4.886%
20	13.315	3587	3600	3621	rBV	400962	677376	25.34%	5.322%

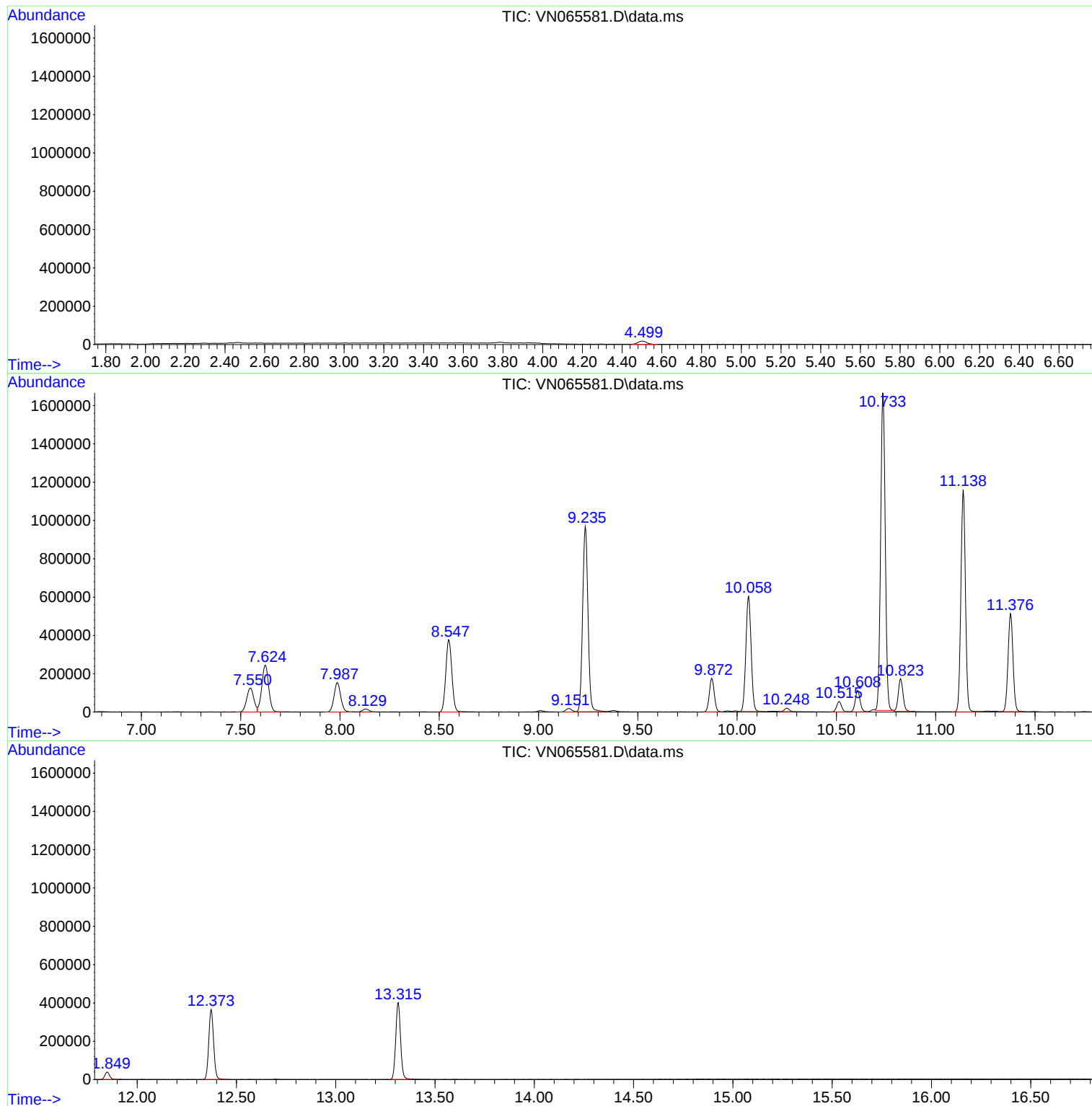
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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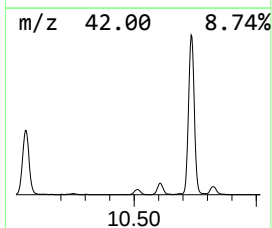
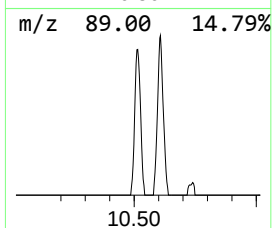
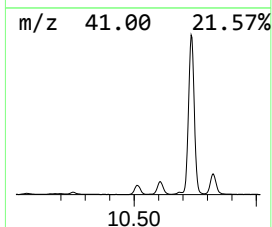
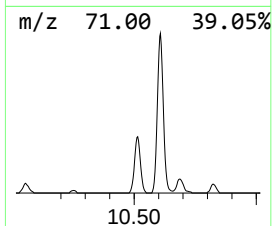
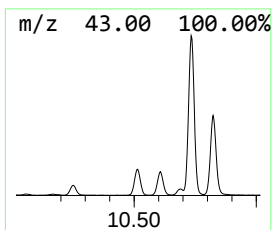
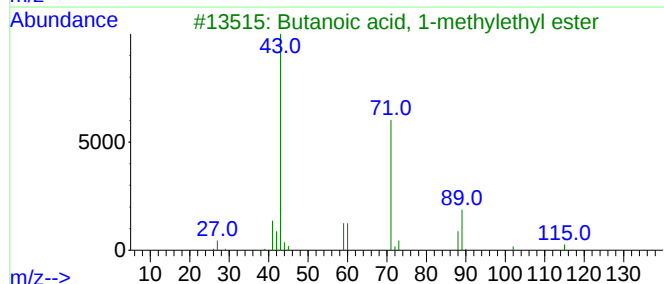
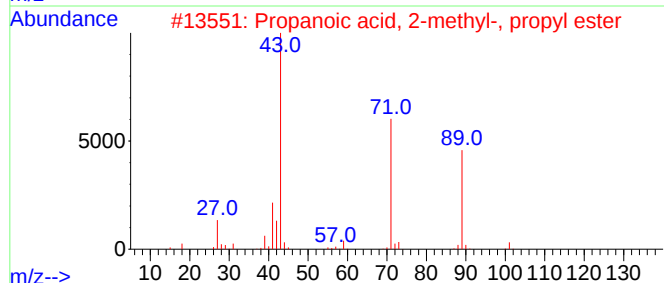
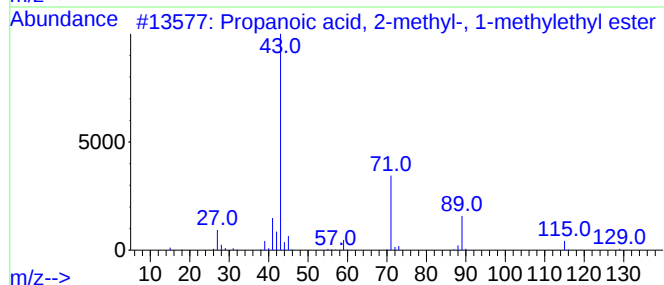
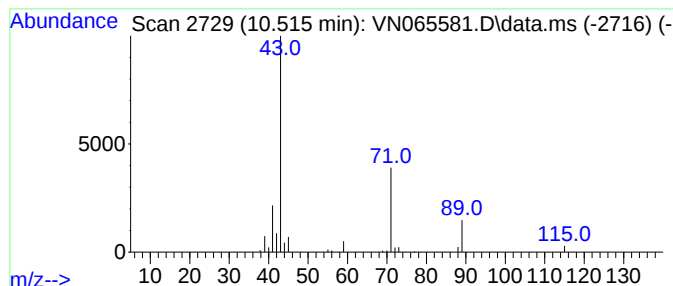
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.515	5.06 ug/l	90317	Chlorobenzene-d5	11.376	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	40
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	39
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38



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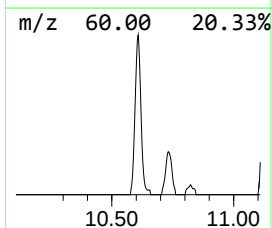
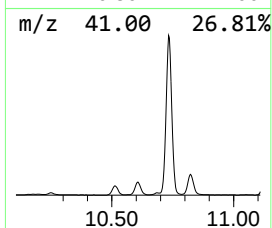
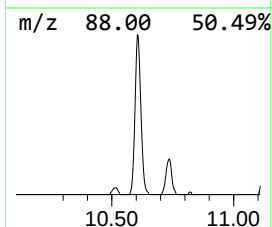
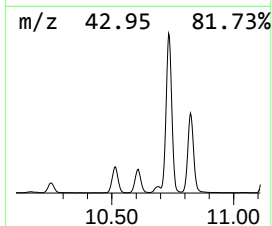
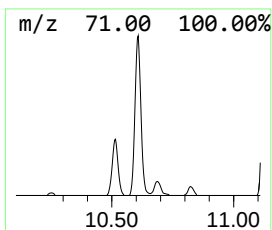
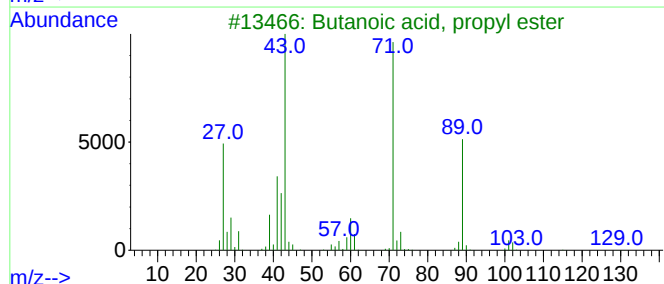
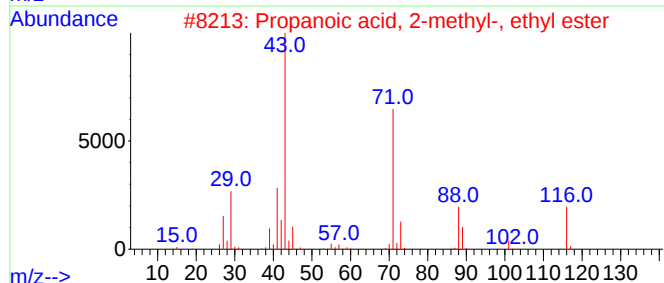
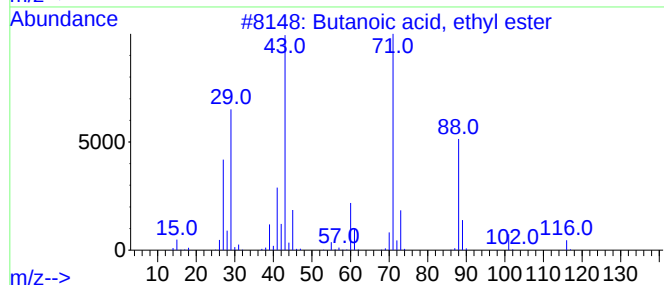
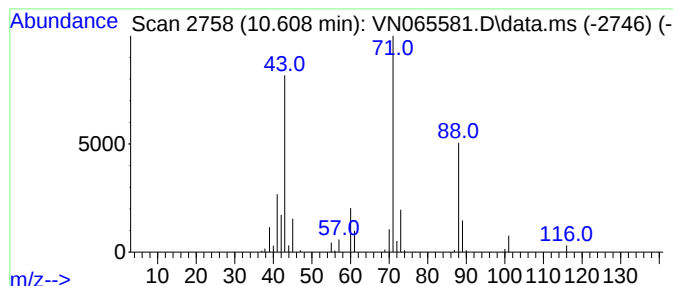
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Quant Title : SW846 8260

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Peak Number 2 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.608	10.46 ug/l	186684	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4			3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	45
5			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37



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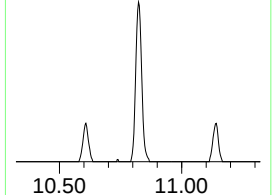
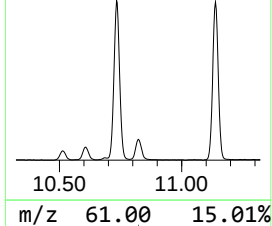
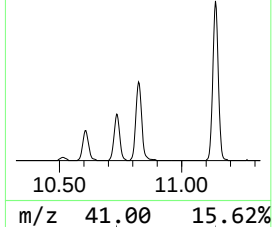
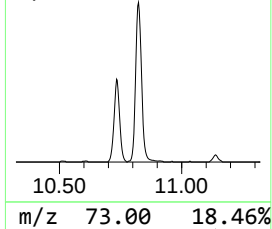
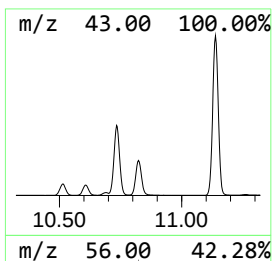
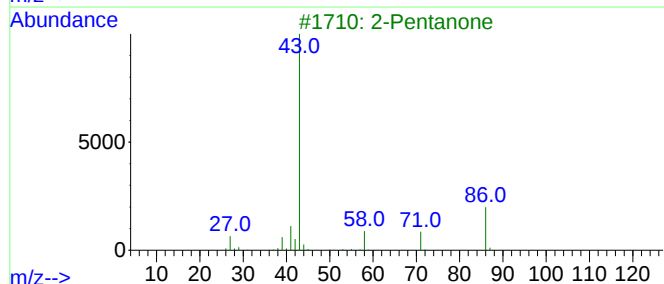
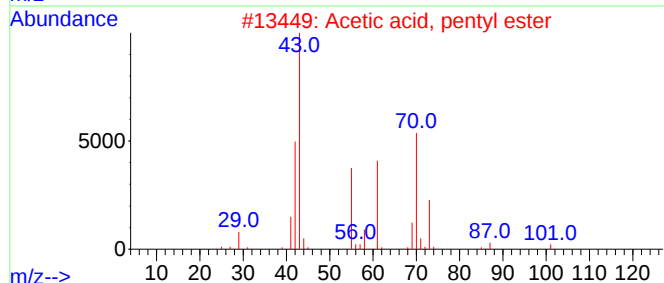
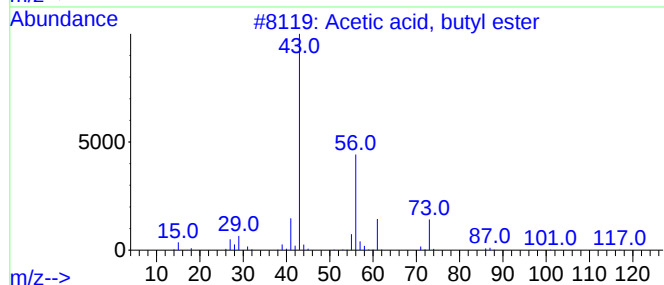
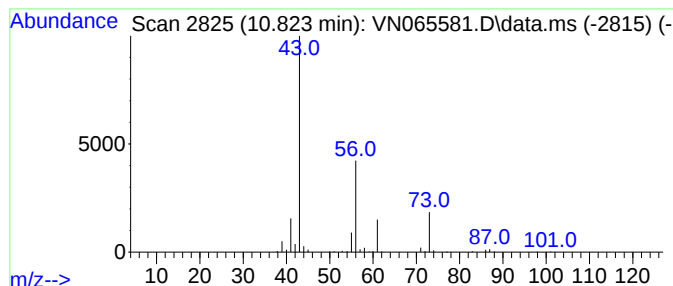
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Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	15.88 ug/l	283470	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
3			2-Pentanone	86	C5H10O	000107-87-9	9
4			n-Propyl acetate	102	C5H10O2	000109-60-4	9
5			1-Propanol, 3-chloro-, acetate	136	C5H9ClO2	000628-09-1	9



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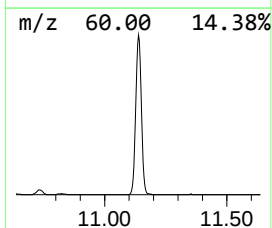
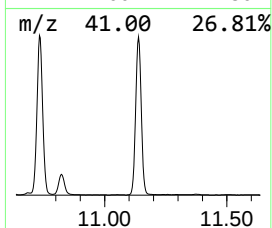
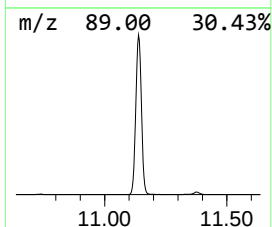
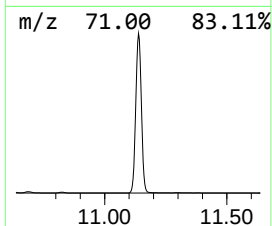
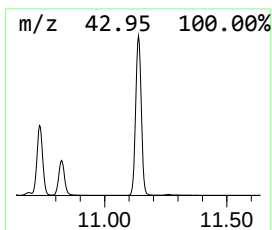
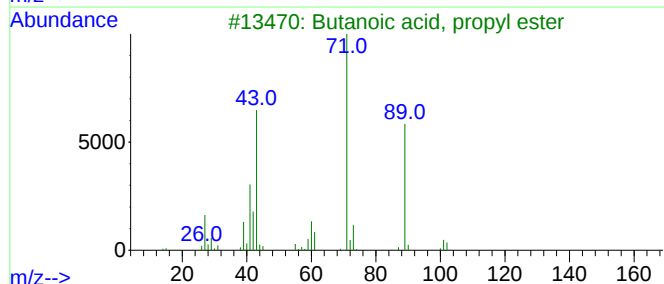
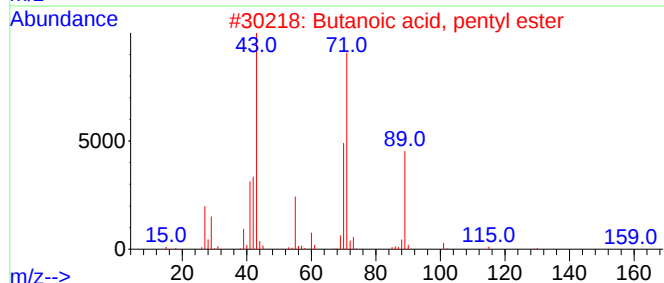
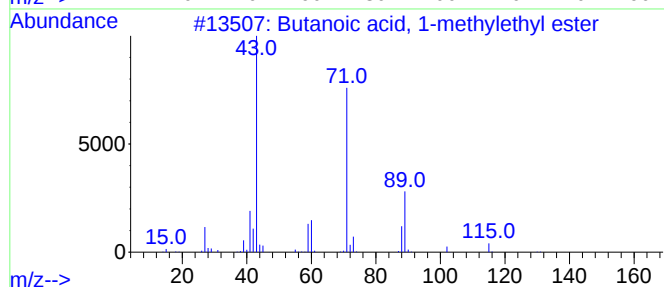
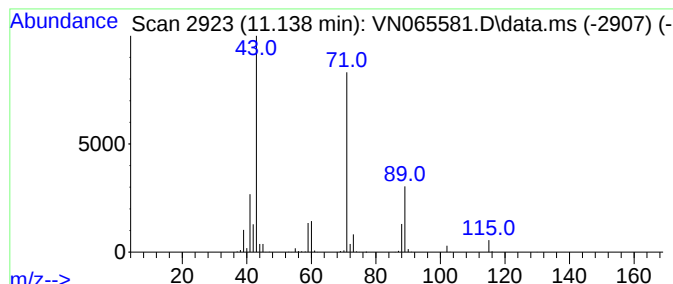
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Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.138	103.21 ug/l	1842840	Chlorobenzene-d5	11.376

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
4		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	10.515	5.1	ug/l	90317	3	11.376	892776	50.0
Butanoic acid, ...	10.608	10.5	ug/l	186684	3	11.376	892776	50.0
Acetic acid, bu...	10.823	15.9	ug/l	283470	3	11.376	892776	50.0
Butanoic acid, ...	11.138	103.2	ug/l	1842840	3	11.376	892776	50.0