

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
 Data File : VN065607.D
 Acq On : 26 Jan 2021 16:27
 Operator : JC/MD
 Sample : PB134336TB
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB134336TB

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: VN065607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.782	623	635	651	rVB	17652	43561	1.39%	0.299%
2	4.505	842	860	879	rVB2	14912	43486	1.39%	0.299%
3	5.698	1209	1231	1253	rBV3	14217	49094	1.57%	0.337%
4	7.550	1788	1807	1818	rBV	131276	328565	10.49%	2.256%
5	7.624	1818	1830	1854	rVB	260791	617504	19.72%	4.240%
6	7.987	1927	1943	1964	rBV	158806	376338	12.02%	2.584%
7	8.129	1973	1987	2005	rVB	17539	39290	1.25%	0.270%
8	8.547	2101	2117	2144	rBV	399896	842428	26.90%	5.784%
9	9.155	2293	2306	2317	rBV3	19689	42845	1.37%	0.294%
10	9.235	2317	2331	2359	rBV	1119062	2050175	65.46%	14.077%
11	9.872	2516	2529	2544	rBV	205400	356275	11.38%	2.446%
12	10.058	2573	2587	2602	rBV	638609	1170498	37.37%	8.037%
13	10.251	2637	2647	2659	rVB	21407	37823	1.21%	0.260%
14	10.515	2714	2729	2742	rBV	63258	108095	3.45%	0.742%
15	10.608	2746	2758	2773	rVV	132277	222354	7.10%	1.527%
16	10.733	2785	2797	2815	rVV	1930133	3131835	100.00%	21.504%
17	10.823	2815	2825	2846	rVB	208731	354866	11.33%	2.437%
18	11.138	2908	2923	2943	rBV	1379622	2166452	69.18%	14.876%
19	11.376	2982	2997	3020	rBV	540964	952403	30.41%	6.540%
20	11.849	3134	3144	3159	rBV	49087	79620	2.54%	0.547%
21	12.373	3295	3307	3335	rBV	390580	701478	22.40%	4.817%
22	13.315	3587	3600	3617	rBV	437230	749198	23.92%	5.144%
23	14.765	4038	4051	4068	rVB4	33281	99462	3.18%	0.683%

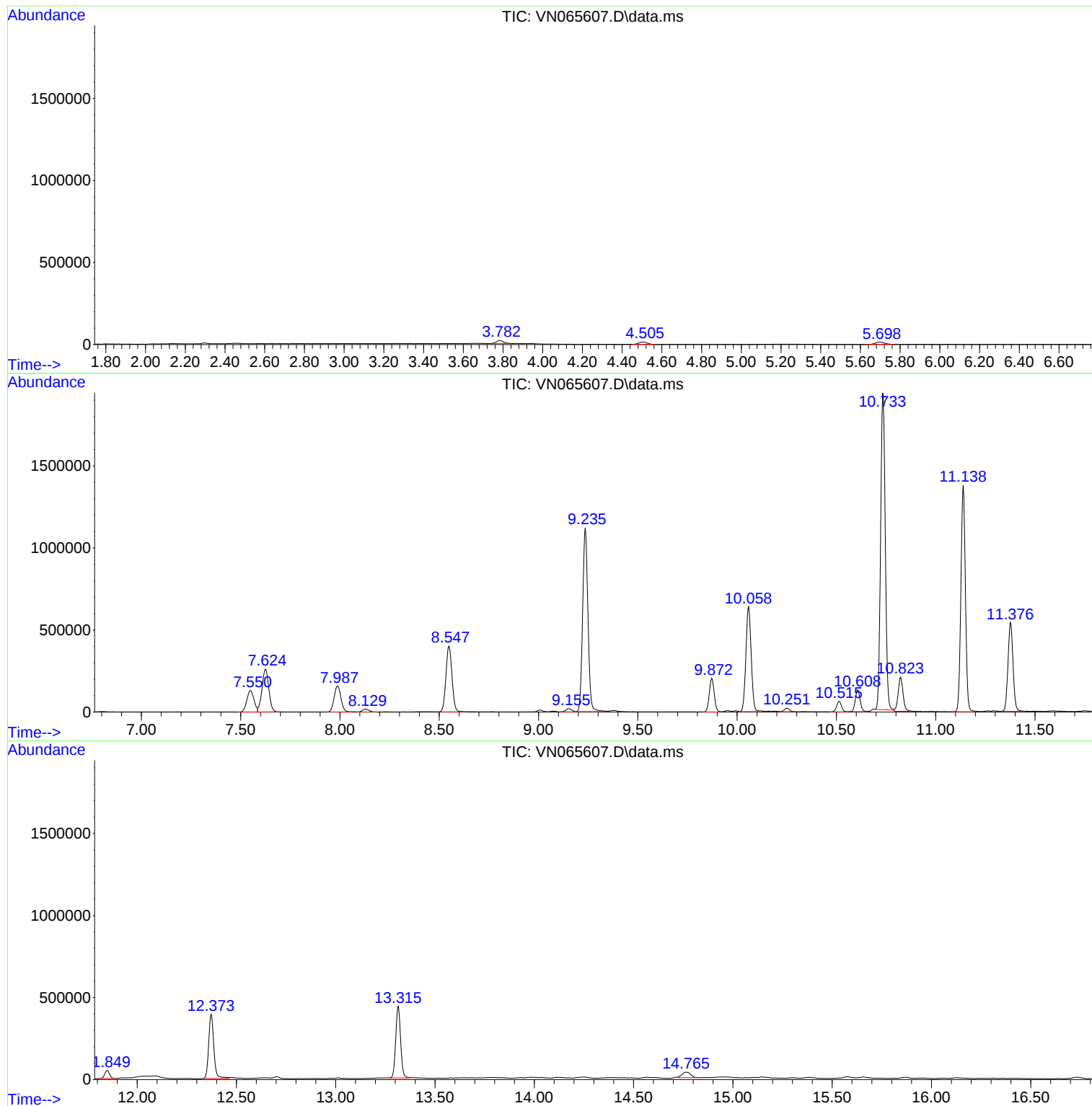
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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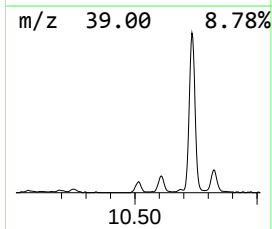
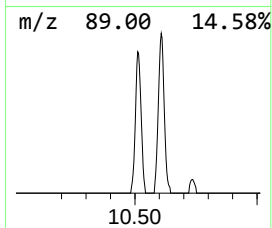
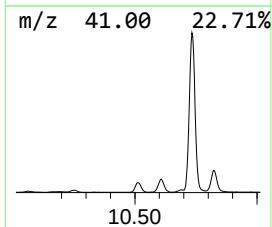
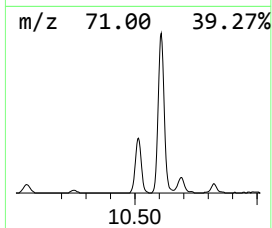
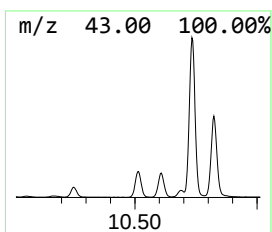
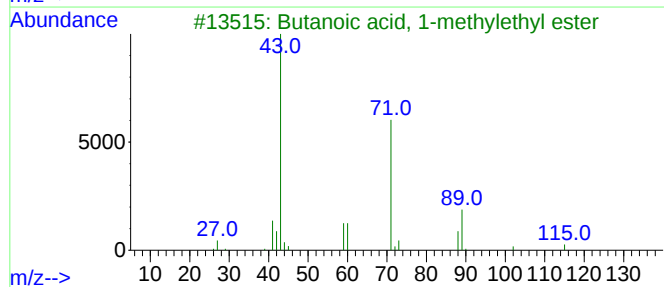
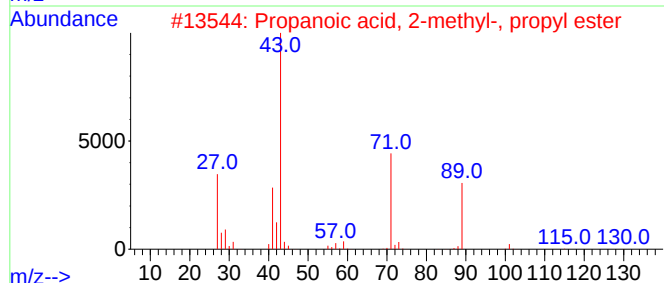
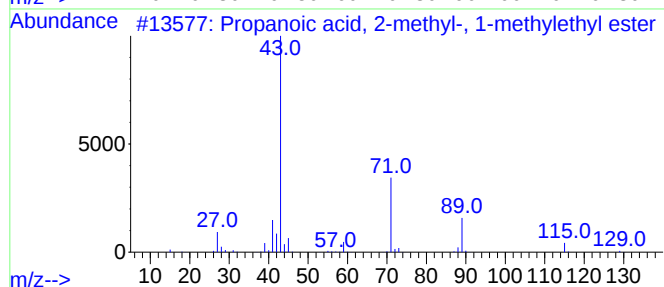
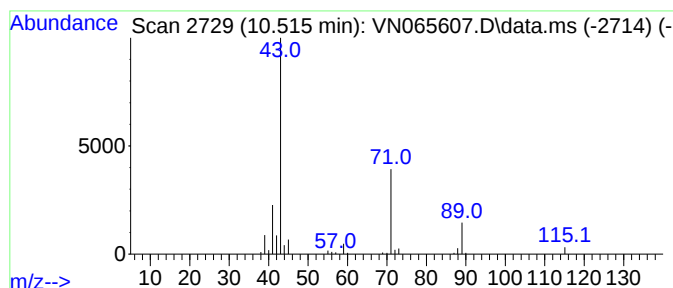
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.515	5.67 ug/l	108095	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	78
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	50
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
5	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	39



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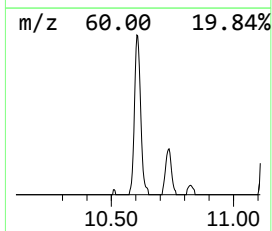
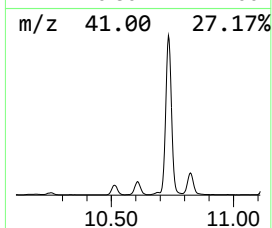
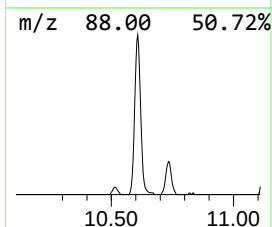
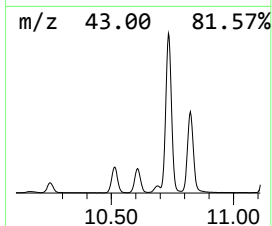
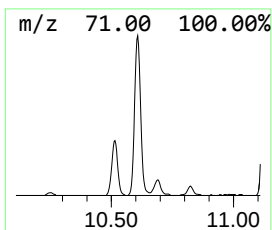
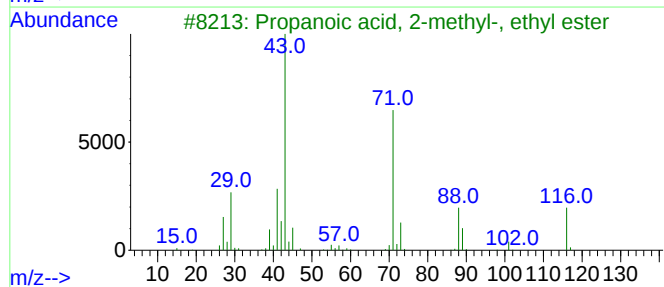
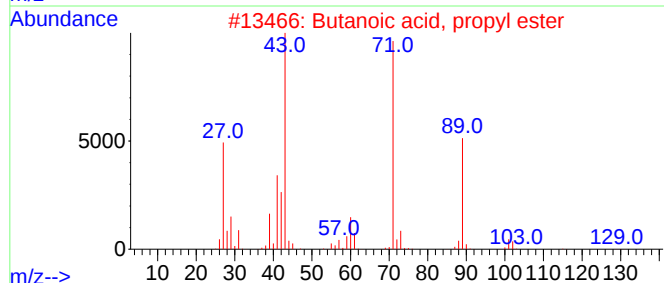
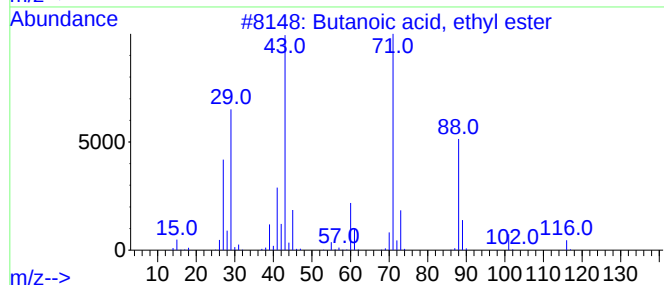
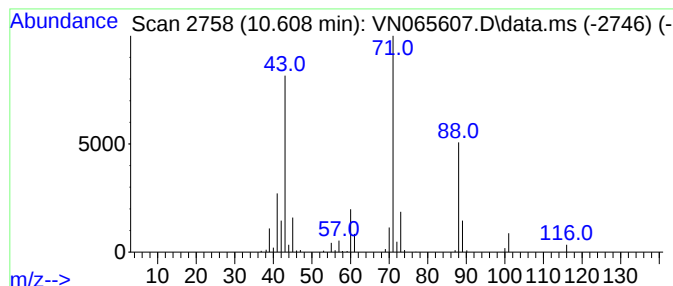
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Quant Title : SW846 8260

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

Peak Number 2 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.608	11.67 ug/l	222354	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	96
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	35
5			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	35



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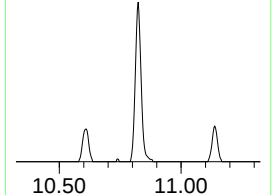
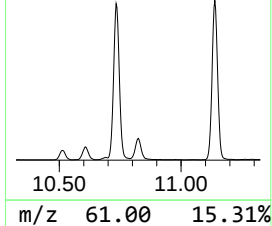
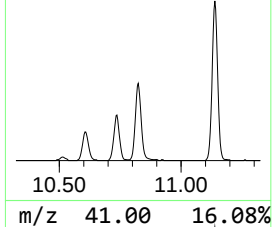
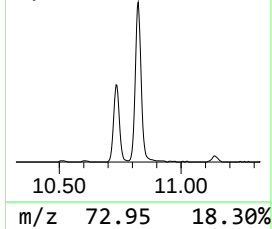
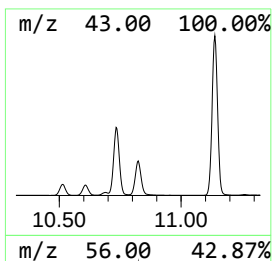
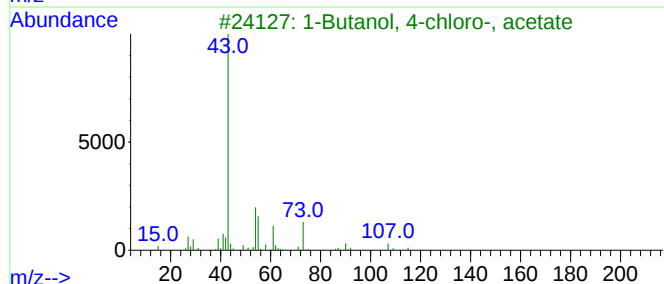
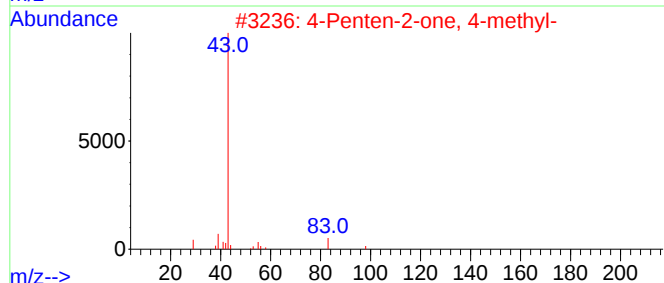
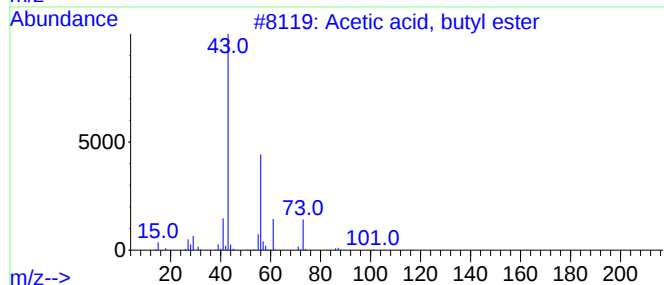
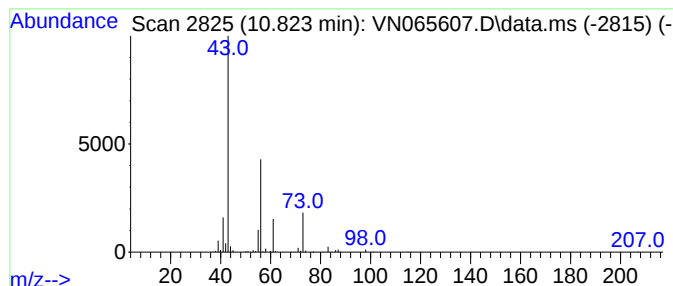
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Quant Title : SW846 8260

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	18.63 ug/l	354866	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
4			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5			Isobutyl acetate	116	C6H12O2	000110-19-0	9



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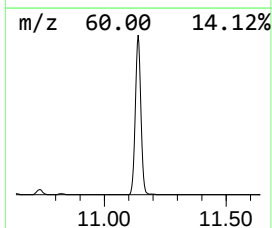
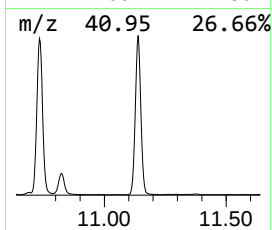
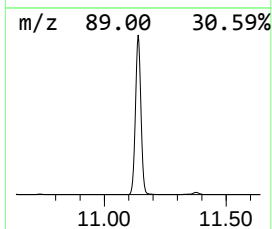
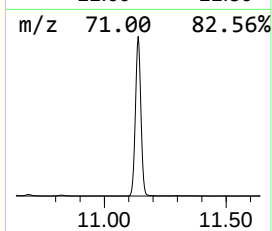
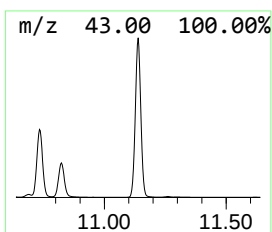
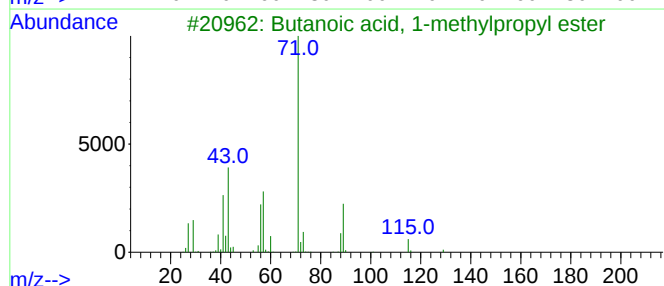
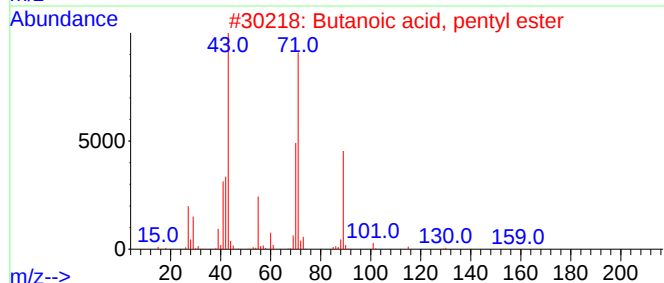
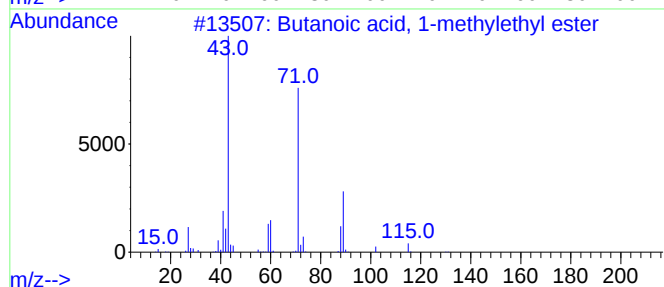
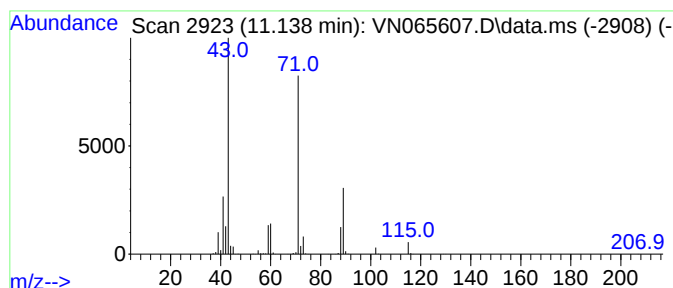
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.138	113.74 ug/l	2166450	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, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45



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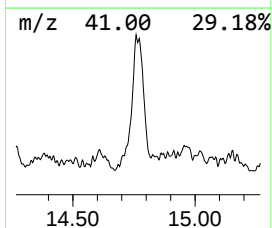
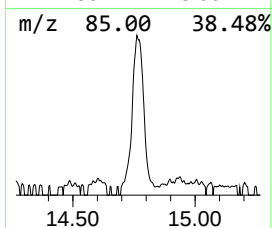
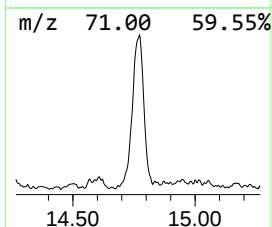
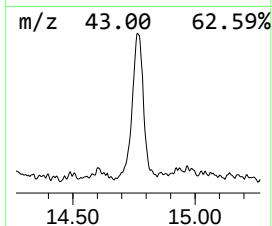
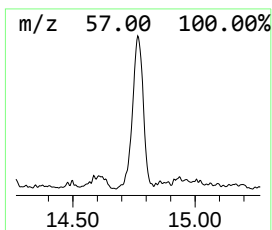
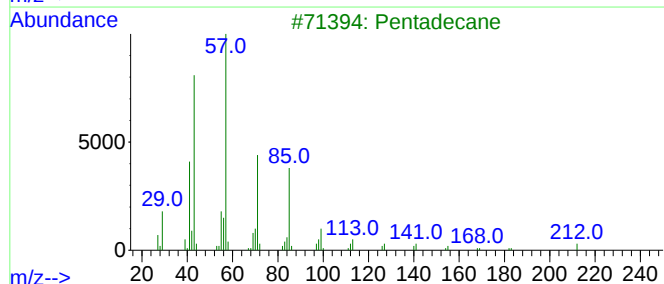
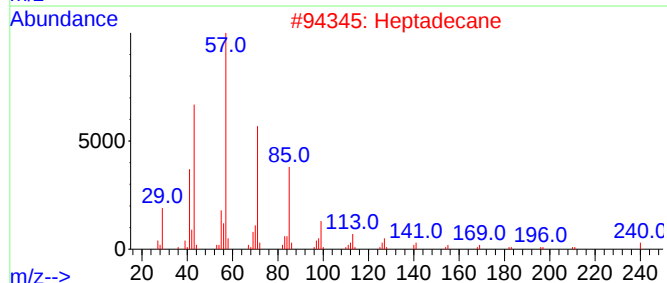
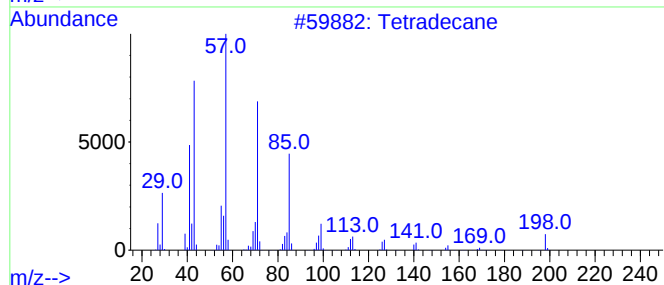
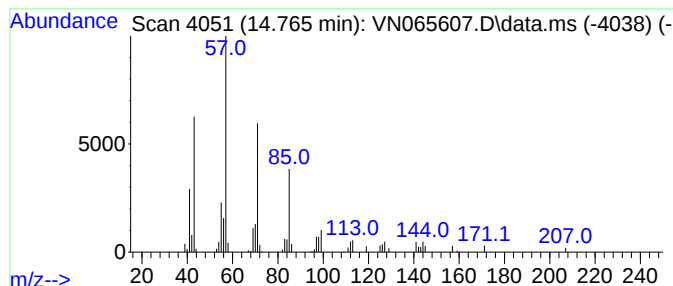
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.765	6.64 ug/l	99462	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	91
2			Heptadecane	240	C17H36	000629-78-7	90
3			Pentadecane	212	C15H32	000629-62-9	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	86



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	10.515	5.7	ug/l	108095	3	11.376	952403	50.0
Butanoic acid, ...	10.608	11.7	ug/l	222354	3	11.376	952403	50.0
Acetic acid, bu...	10.823	18.6	ug/l	354866	3	11.376	952403	50.0
Butanoic acid, ...	11.138	113.7	ug/l	2166450	3	11.376	952403	50.0
Tetradecane	14.765	6.6	ug/l	99462	4	13.315	749198	50.0