

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110121\
 Data File : VN069326.D
 Acq On : 1 Nov 2021 17:49
 Operator : JC/MD
 Sample : M4411-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MH-HHD

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82N102821W.M
 Title : SW846 8260

Signal : TIC: VN069326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.296	837	860	882	rBV	22426	66360	1.47%	0.298%
2	8.024	2228	2250	2261	rBV	237250	562135	12.46%	2.525%
3	8.088	2262	2274	2302	rVB	436491	992066	21.98%	4.456%
4	8.440	2384	2405	2433	rBV	259887	609021	13.50%	2.736%
5	8.566	2437	2452	2460	rBV3	25212	54773	1.21%	0.246%
6	8.968	2585	2602	2628	rVB	663232	1388948	30.78%	6.239%
7	9.547	2802	2818	2830	rBV3	27495	63622	1.41%	0.286%
8	9.628	2831	2848	2888	rVV	1573617	2979530	66.03%	13.384%
9	10.245	3062	3078	3099	rBV	264052	467380	10.36%	2.100%
10	10.443	3134	3152	3176	rBV	1039894	1959419	43.42%	8.802%
11	10.617	3206	3217	3232	rVB	26519	45902	1.02%	0.206%
12	10.877	3297	3314	3331	rBV2	74173	130204	2.89%	0.585%
13	10.966	3333	3347	3369	rVV	175484	309289	6.85%	1.389%
14	11.092	3369	3394	3415	rVV	2660067	4512555	100.00%	20.271%
15	11.181	3416	3427	3466	rVB	274510	498617	11.05%	2.240%
16	11.492	3527	3543	3578	rBV	1781132	2948195	65.33%	13.244%
17	11.746	3621	3638	3671	rVB	1014525	1822991	40.40%	8.189%
18	12.197	3793	3806	3828	rBV	55038	91728	2.03%	0.412%
19	12.733	3989	4006	4037	rBV	750294	1313264	29.10%	5.899%
20	13.677	4341	4358	4380	rBV	833450	1445277	32.03%	6.492%

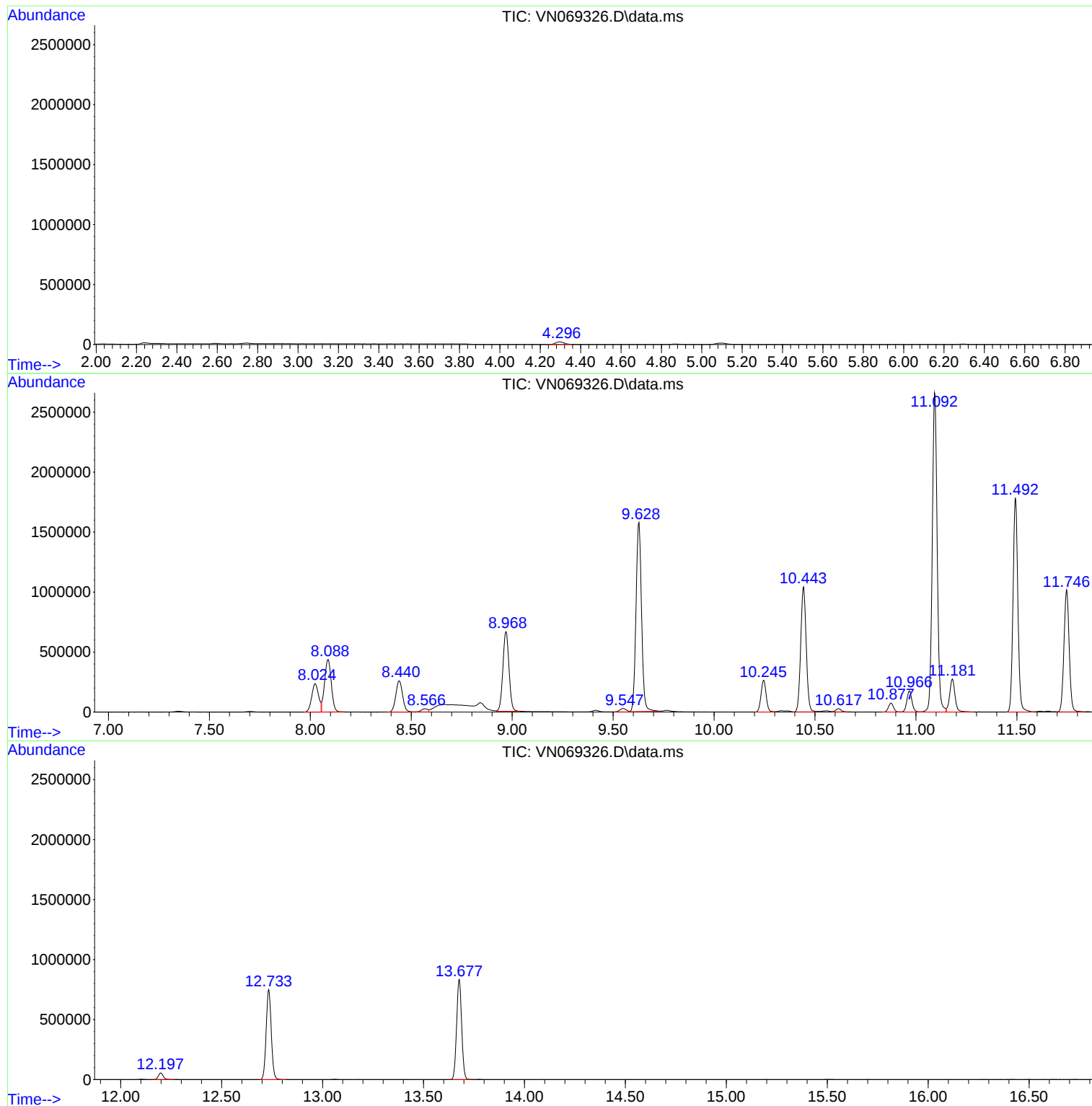
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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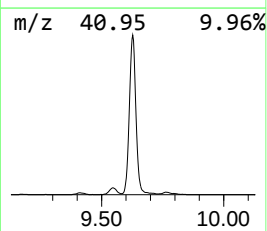
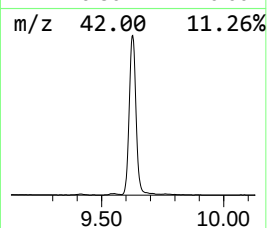
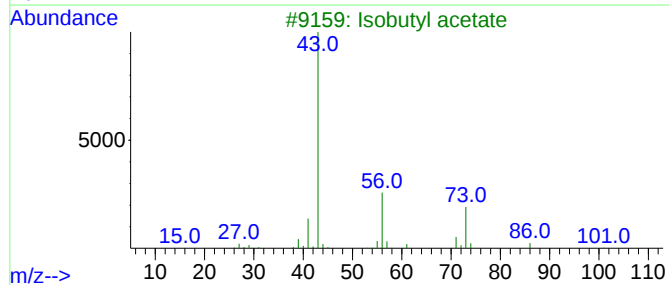
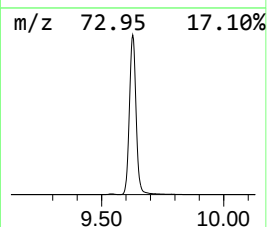
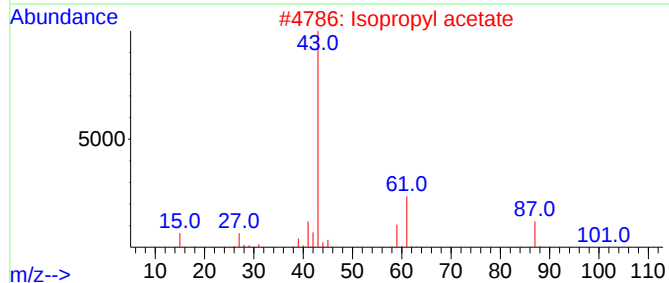
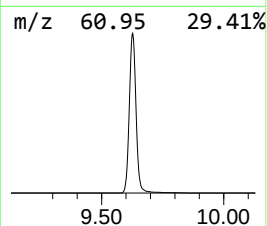
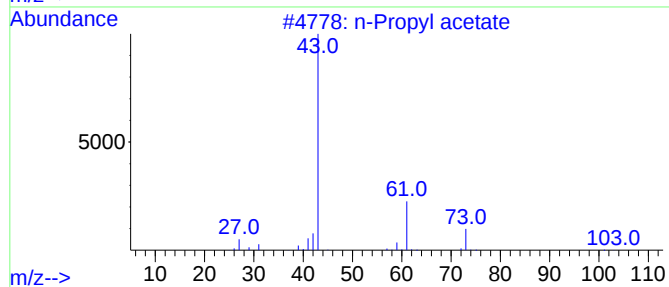
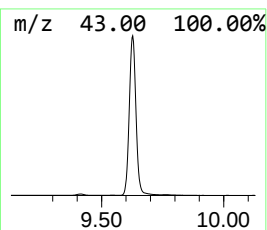
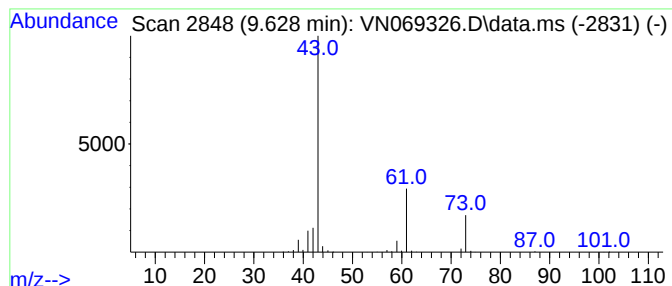
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.628	107.26 ug/l	2979530	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			Isobutyl acetate	116	C6H12O2	000110-19-0	9
4			1-Butanamine	73	C4H11N	000109-73-9	5
5			Isobutylamine	73	C4H11N	000078-81-9	4



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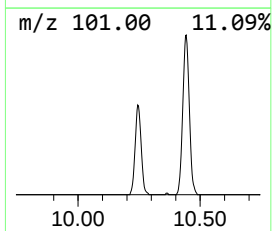
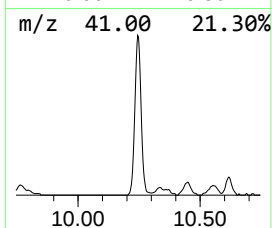
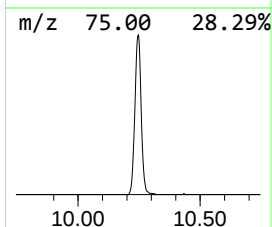
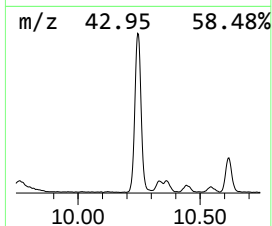
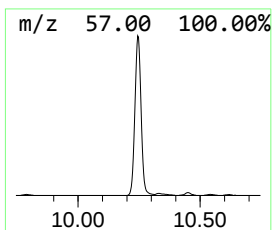
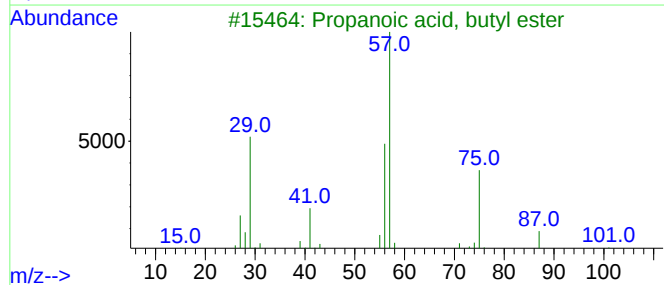
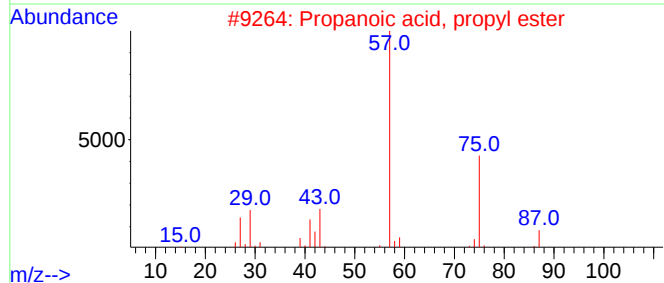
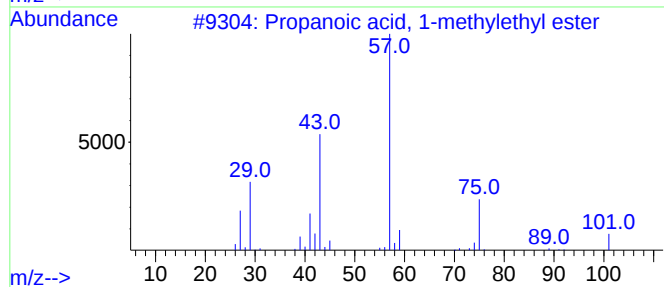
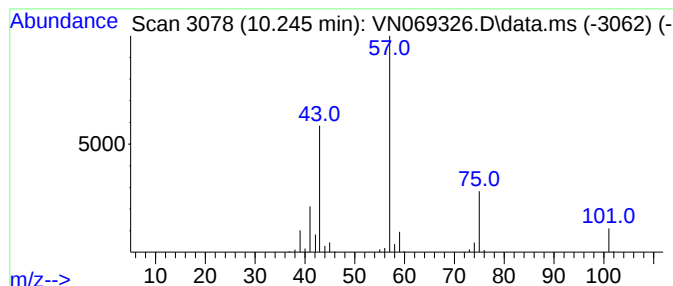
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	16.82 ug/l	467380	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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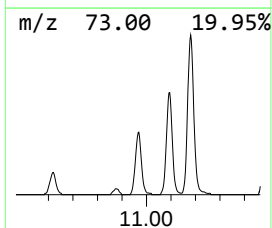
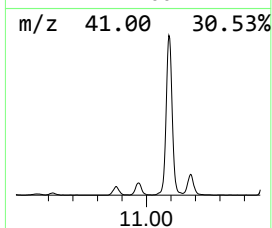
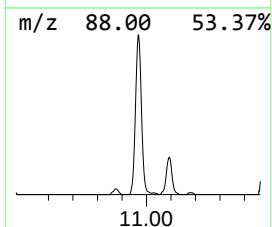
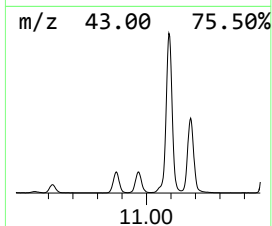
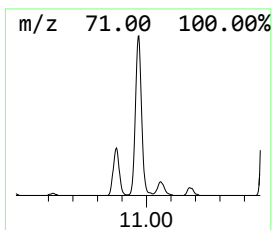
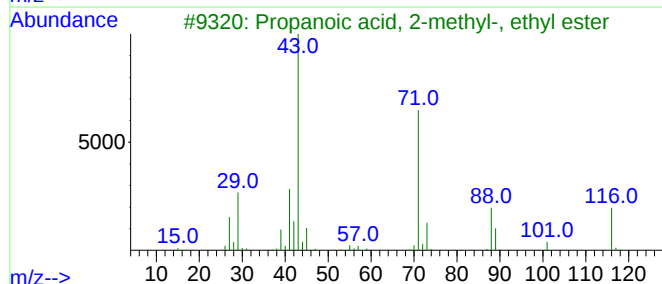
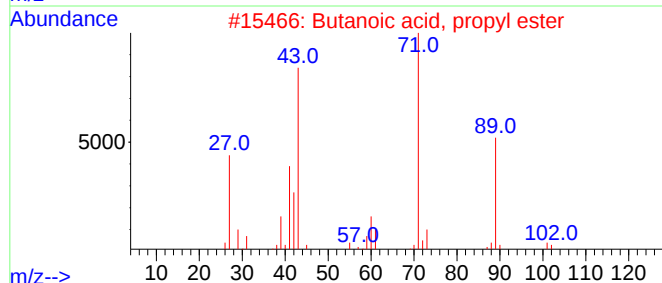
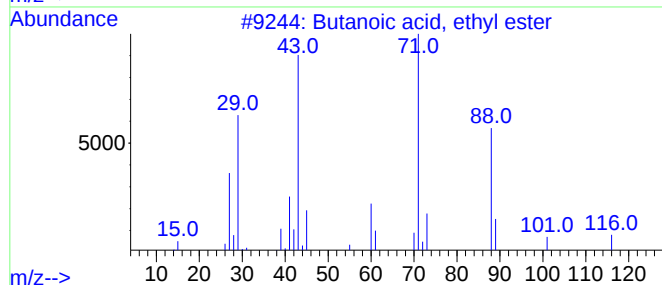
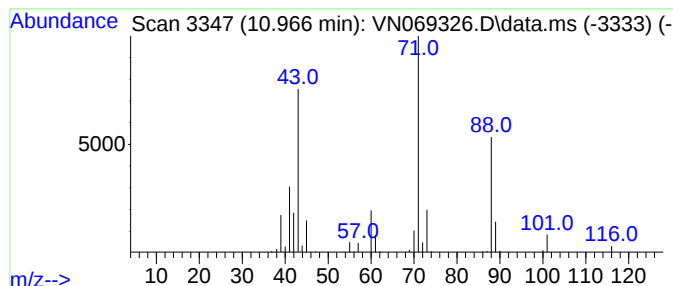
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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.966	8.48 ug/l	309289	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4			4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	40
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38



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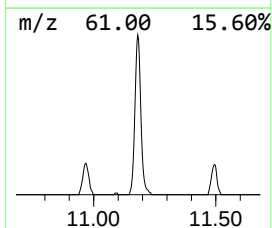
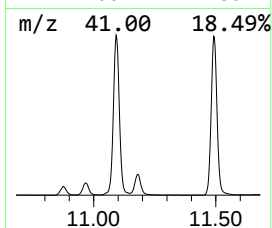
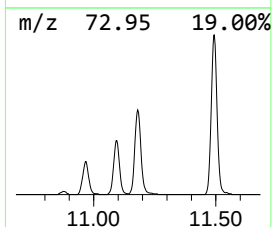
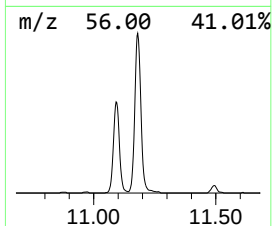
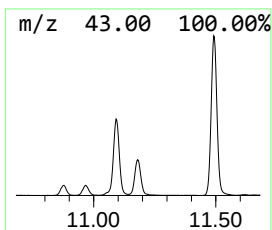
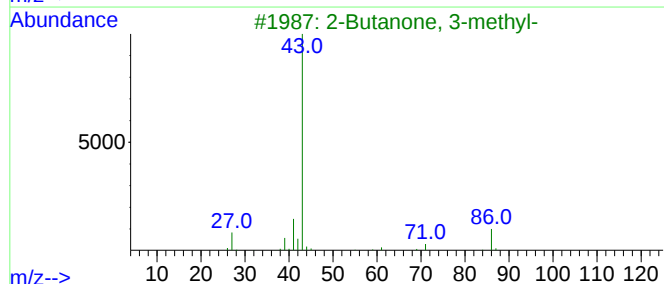
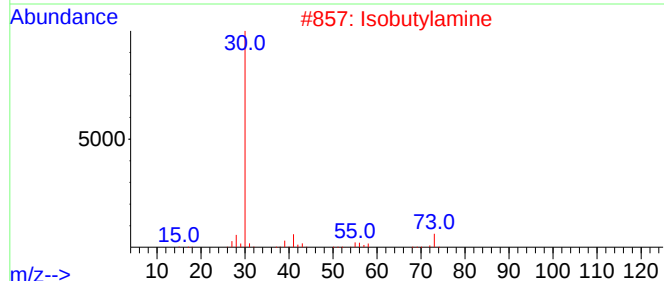
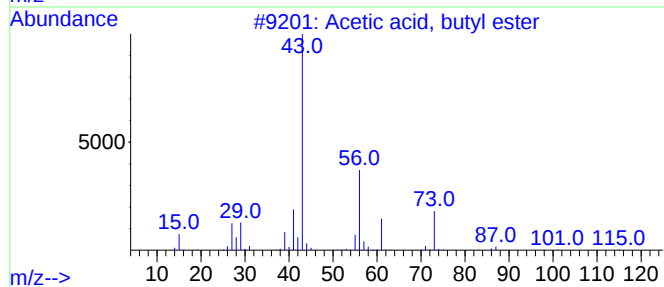
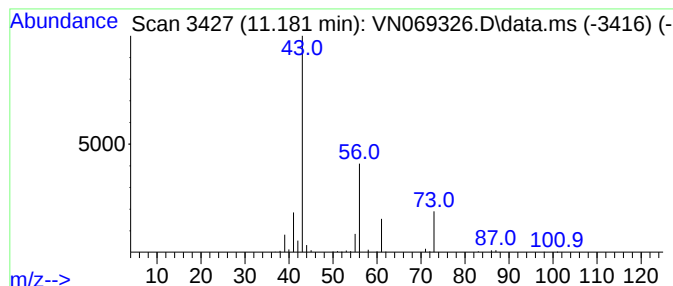
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	13.68 ug/l	498617	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutylamine	73	C4H11N	000078-81-9	9
3			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9



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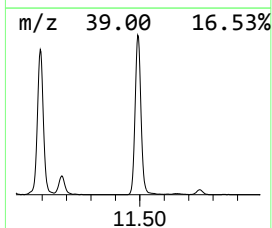
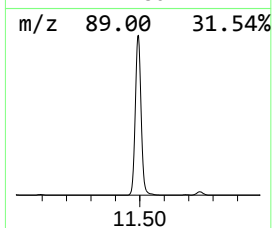
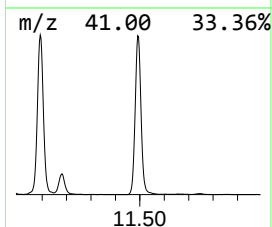
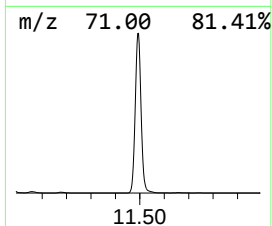
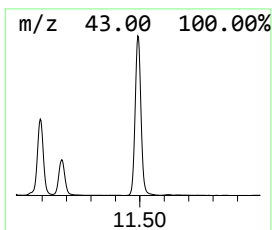
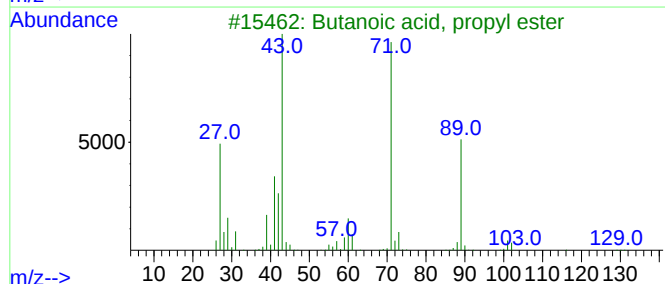
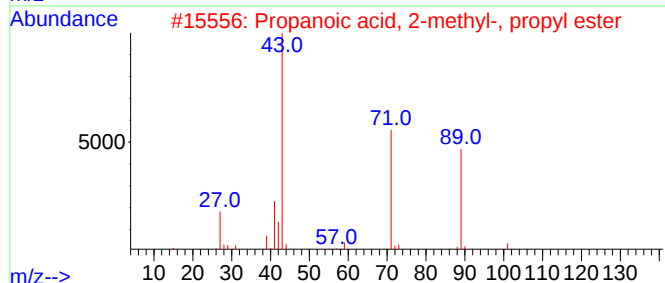
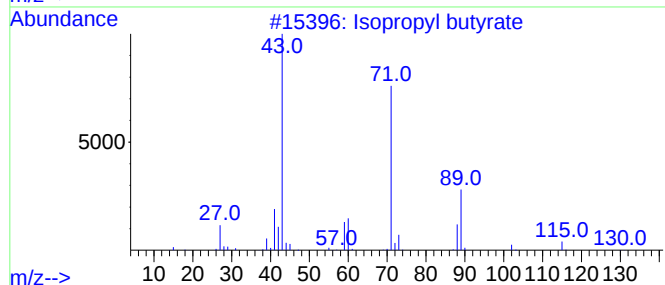
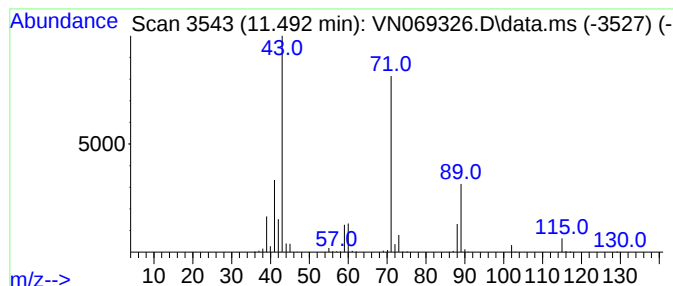
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.492	80.86 ug/l	2948200	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.628	107.3	ug/l	2979530	2	8.971	1388950	50.0
Propanoic acid,...	10.245	16.8	ug/l	467380	2	8.971	1388950	50.0
Butanoic acid, ...	10.966	8.5	ug/l	309289	3	11.746	1822990	50.0
Acetic acid, bu...	11.181	13.7	ug/l	498617	3	11.746	1822990	50.0
Isopropyl butyrate	11.492	80.9	ug/l	2948200	3	11.746	1822990	50.0