

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
 Data File : VN069067.D
 Acq On : 20 Oct 2021 17:27
 Operator : JC/MD
 Sample : M4252-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TEST-BA-(1)

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\82N101221W.M

Title : SW846 8260

Signal : TIC: VN069067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.101	1137	1160	1191	rBV4	21027	69296	1.44%	0.303%
2	8.027	2229	2251	2261	rBV3	230705	549420	11.45%	2.402%
3	8.088	2262	2274	2302	rVB	444891	1009859	21.05%	4.415%
4	8.440	2384	2405	2436	rBV	259744	598229	12.47%	2.615%
5	8.577	2436	2456	2458	rBV3	57621	113327	2.36%	0.495%
6	8.971	2584	2603	2633	rBV	657509	1361196	28.37%	5.951%
7	9.547	2801	2818	2831	rBV3	28989	67099	1.40%	0.293%
8	9.625	2831	2847	2889	rVV	1687891	3177404	66.23%	13.891%
9	10.245	3059	3078	3101	rBV	304021	548956	11.44%	2.400%
10	10.443	3134	3152	3179	rBV	1040225	1926387	40.15%	8.422%
11	10.615	3205	3216	3234	rVB	31103	56391	1.18%	0.247%
12	10.878	3298	3314	3329	rBV	86935	151881	3.17%	0.664%
13	10.966	3333	3347	3369	rVV	189123	329193	6.86%	1.439%
14	11.092	3369	3394	3416	rVV	2771756	4797807	100.00%	20.975%
15	11.181	3416	3427	3455	rVB	274001	491804	10.25%	2.150%
16	11.495	3526	3544	3578	rBV	1926139	3259339	67.93%	14.249%
17	11.747	3621	3638	3668	rVB	951713	1720334	35.86%	7.521%
18	12.200	3791	3807	3828	rBV	54629	93912	1.96%	0.411%
19	12.734	3987	4006	4030	rBV	686036	1204737	25.11%	5.267%
20	13.678	4341	4358	4384	rBV	780596	1347165	28.08%	5.890%

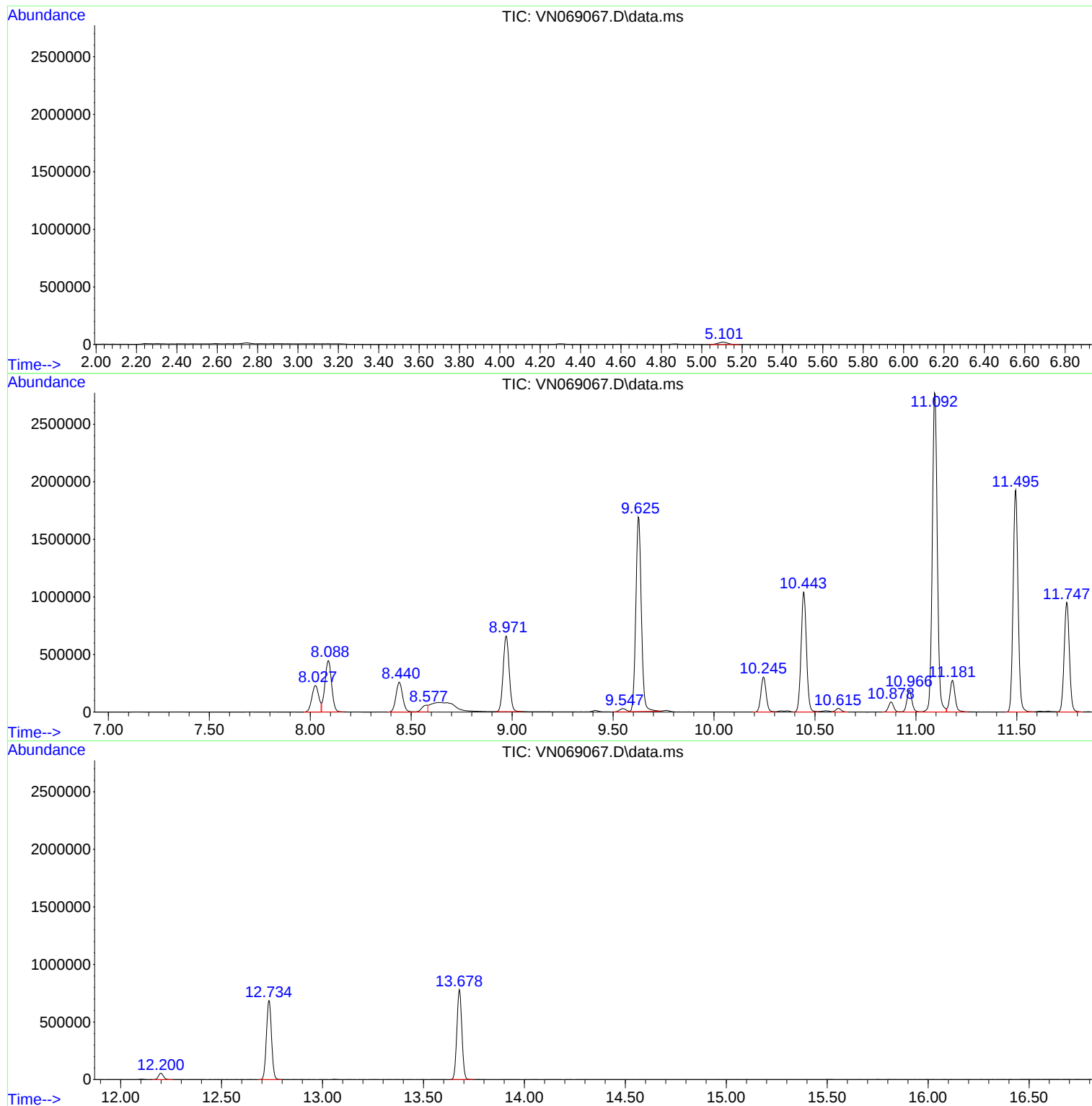
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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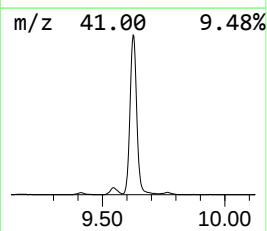
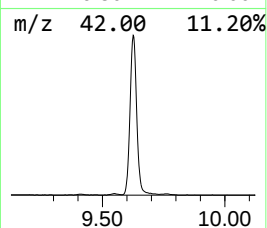
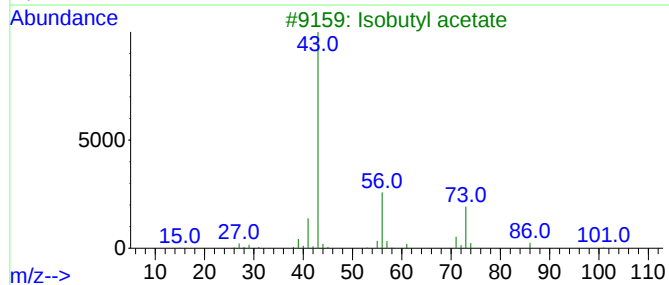
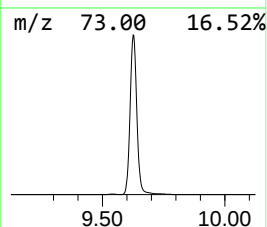
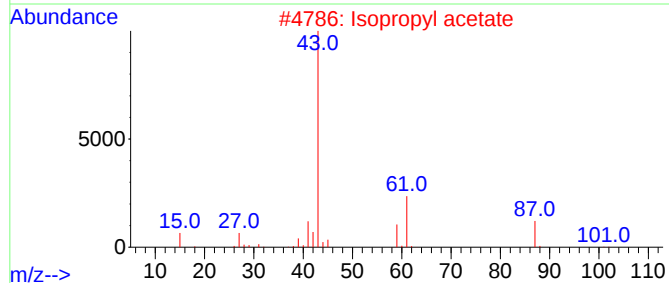
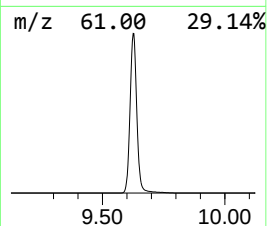
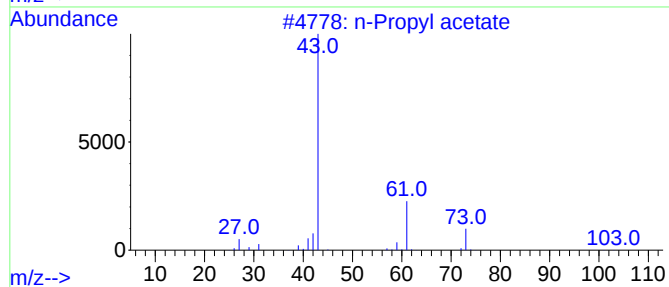
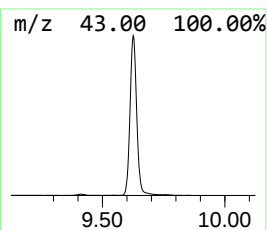
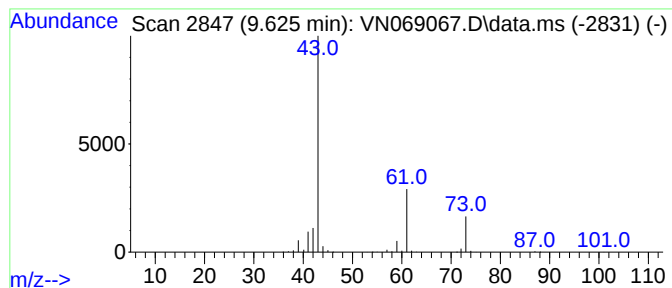
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.625	116.71 ug/l	3177400	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	7
5		Isobutylamine	73	C4H11N	000078-81-9	4



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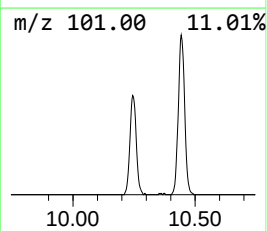
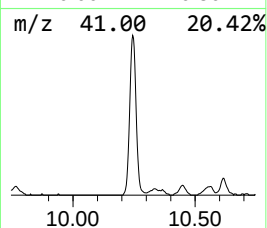
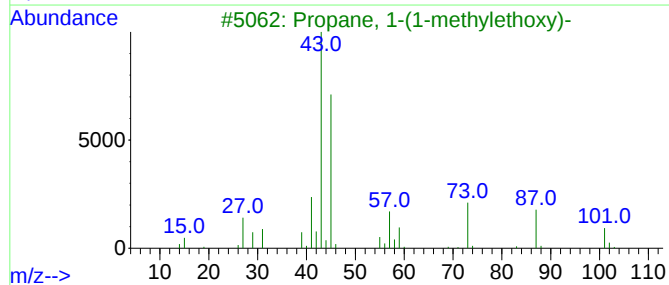
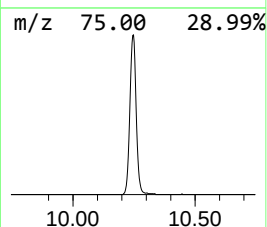
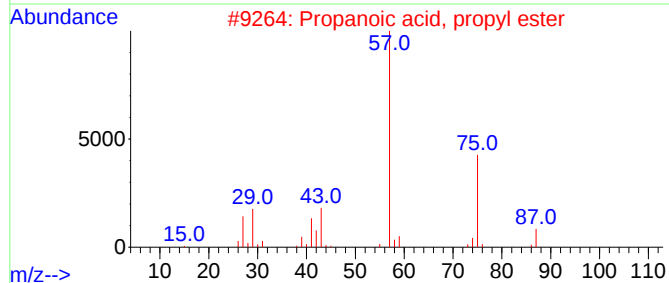
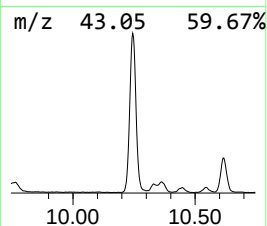
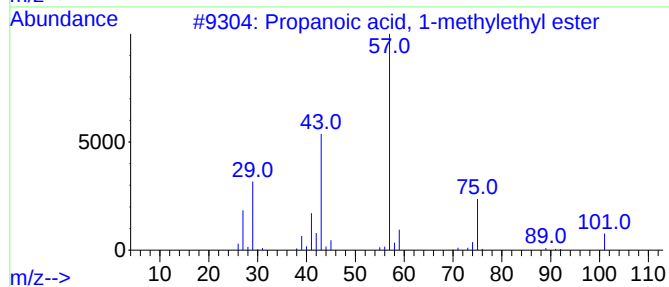
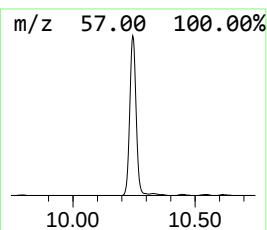
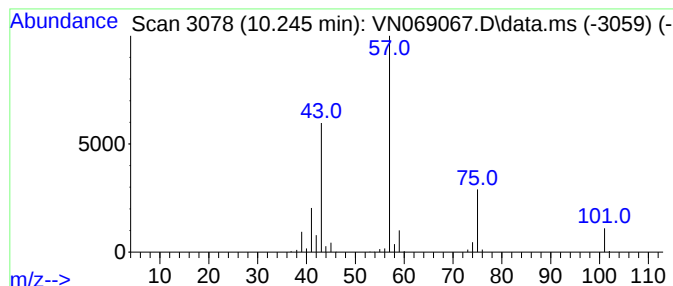
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	20.16 ug/l	548956	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	50
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
4			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	9
5			o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9



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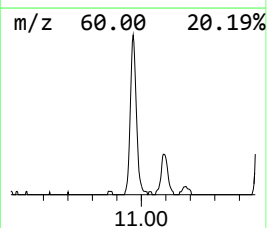
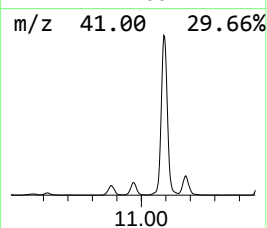
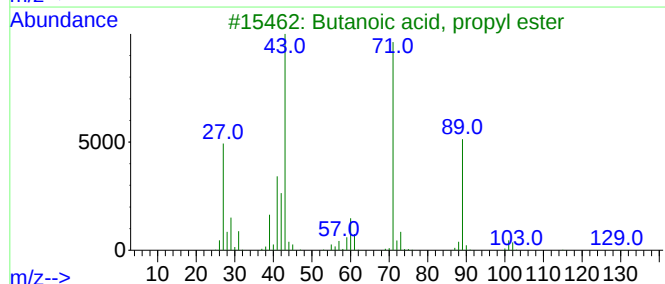
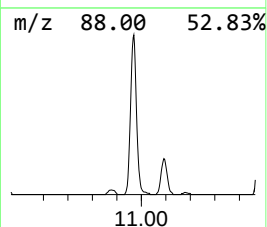
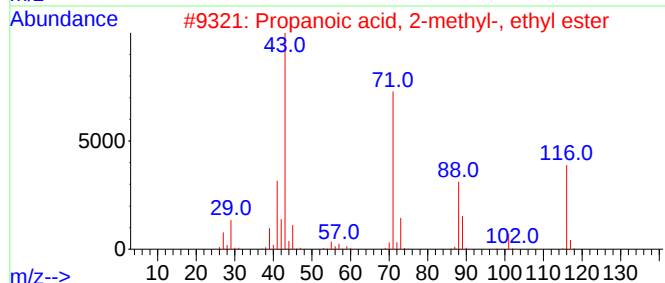
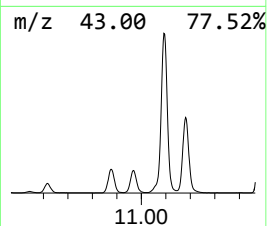
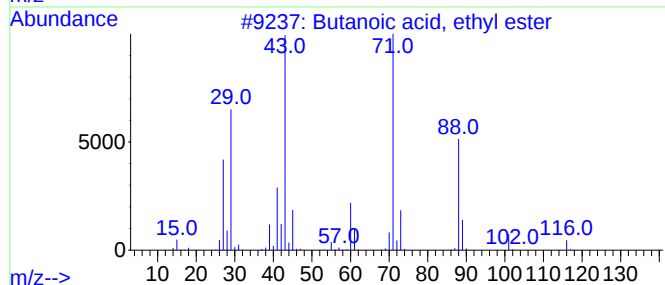
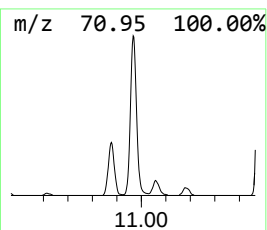
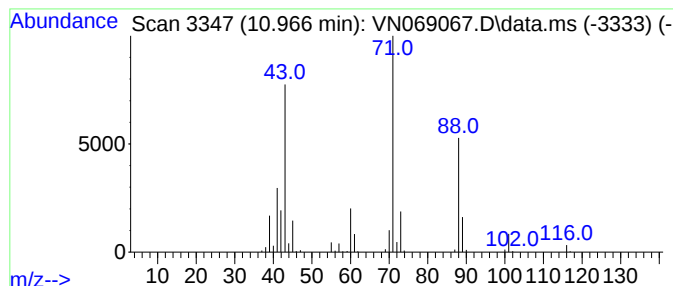
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Quant Title : SW846 8260

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

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.966	9.57 ug/l	329193	Chlorobenzene-d5	11.747

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	50
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	43
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	43



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

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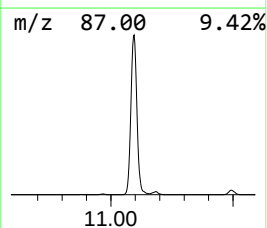
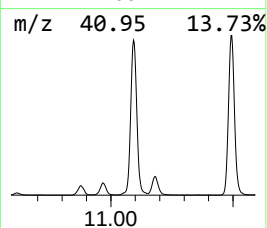
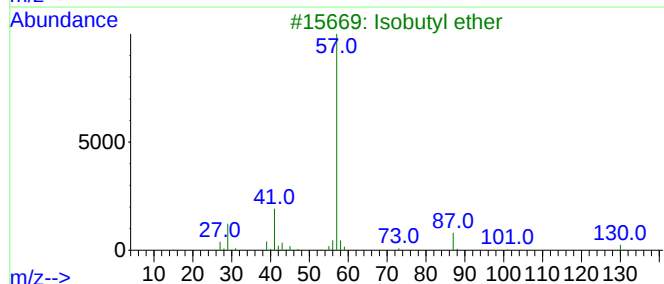
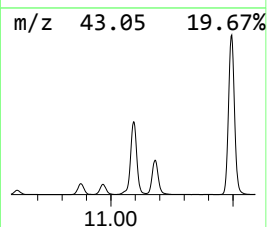
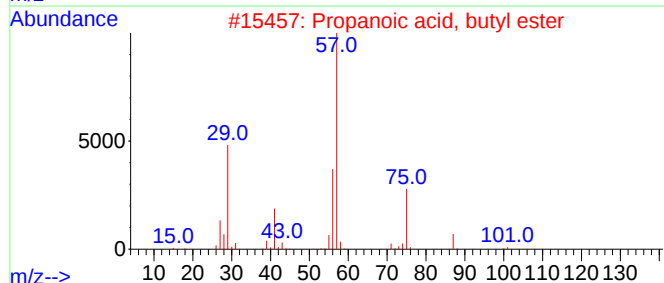
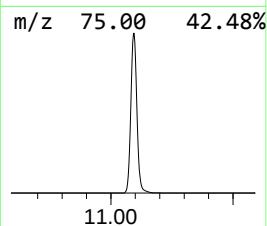
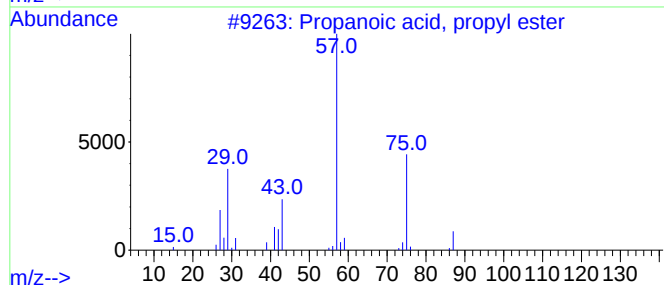
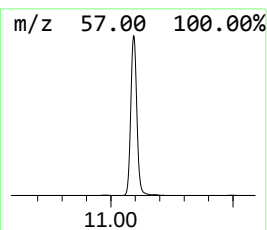
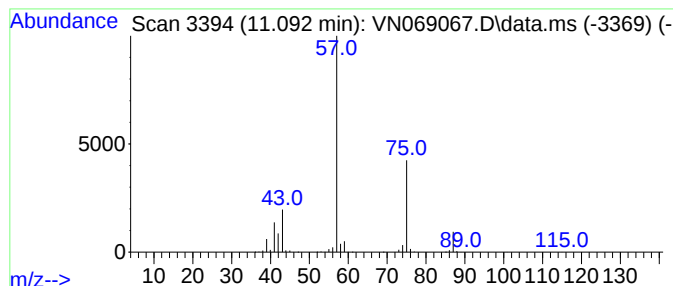
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.092	139.44 ug/l	4797810	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3			Isobutyl ether	130	C8H18O	000628-55-7	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9



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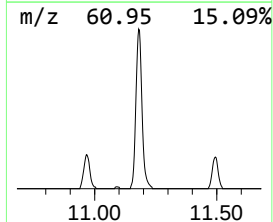
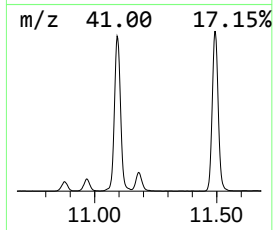
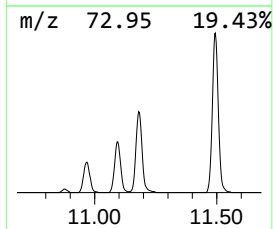
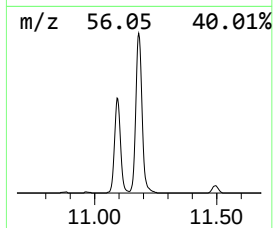
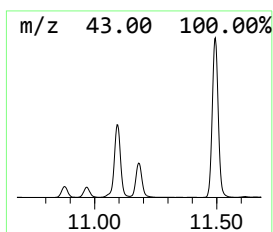
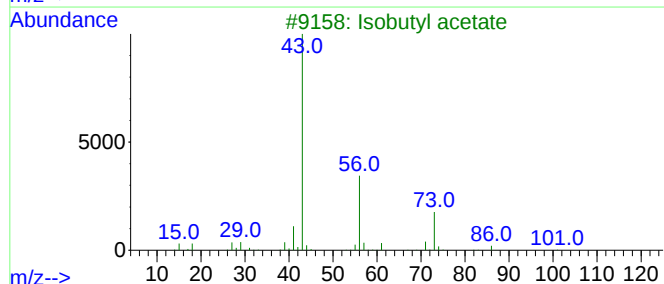
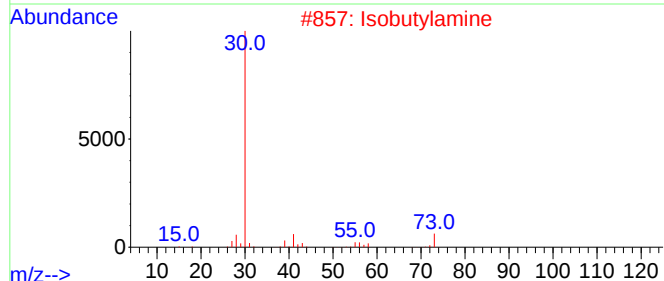
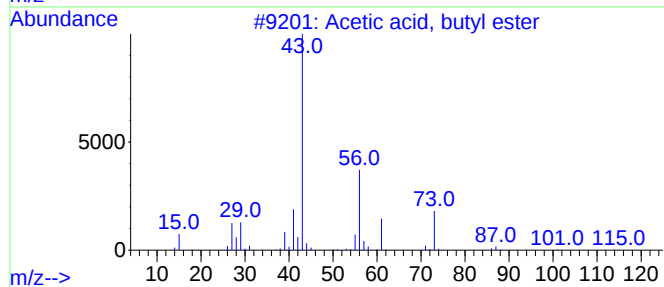
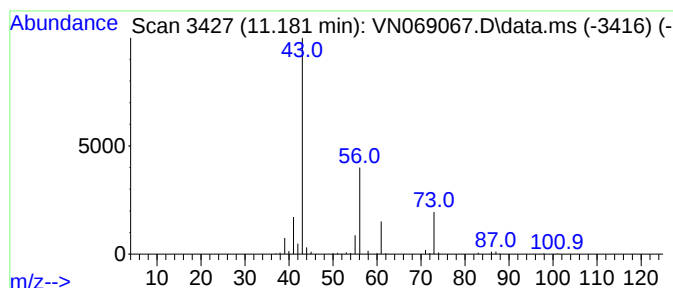
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.181	14.29 ug/l	491804	Chlorobenzene-d5	11.747	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9



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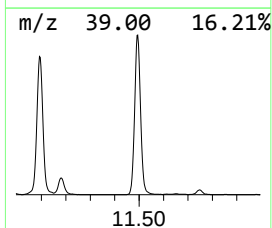
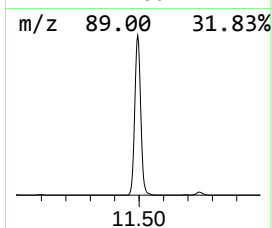
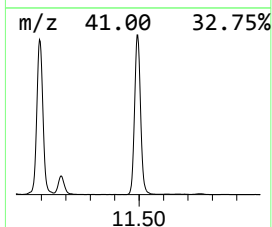
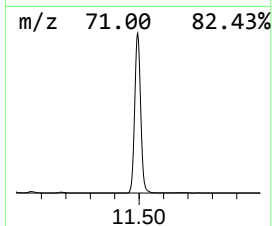
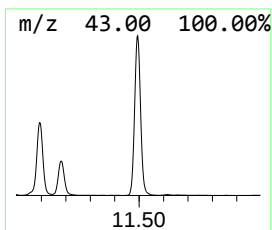
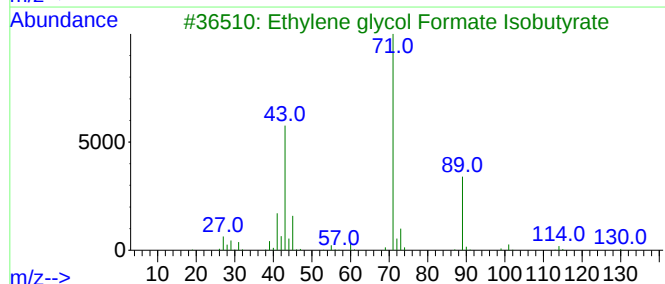
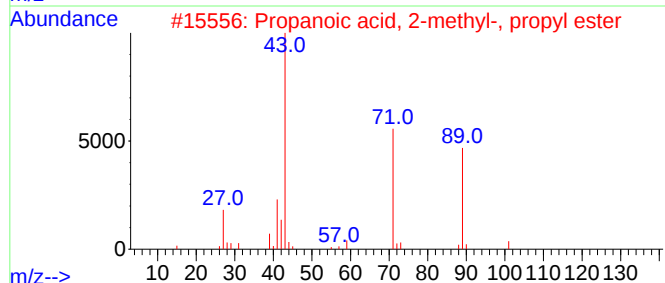
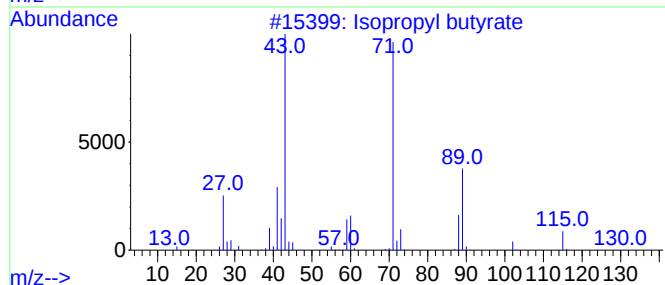
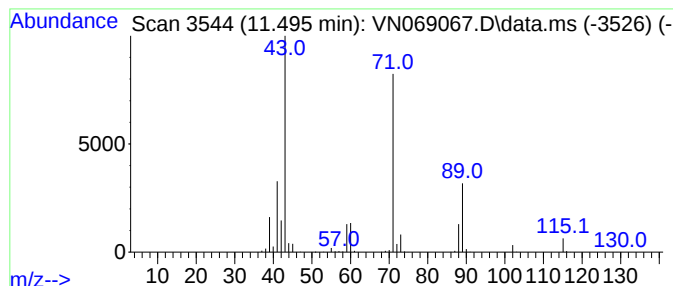
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.495	94.73 ug/l	3259340	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069067.D
Acq On : 20 Oct 2021 17:27
Operator : JC/MD
Sample : M4252-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TEST-BA-(1)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.625	116.7	ug/l	3177400	2	8.971	1361200	50.0
Propanoic acid,...	10.245	20.2	ug/l	548956	2	8.971	1361200	50.0
Butanoic acid, ...	10.966	9.6	ug/l	329193	3	11.747	1720330	50.0
Propanoic acid,...	11.092	139.4	ug/l	4797810	3	11.747	1720330	50.0
Acetic acid, bu...	11.181	14.3	ug/l	491804	3	11.747	1720330	50.0
Isopropyl butyrate	11.495	94.7	ug/l	3259340	3	11.747	1720330	50.0