

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
 Data File : VN070592.D
 Acq On : 12 Jan 2022 17:42
 Operator : JC/MD
 Sample : N1097-16
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-3D

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2225	2249	2260	rBV	578219	1375017	8.19%	2.016%
2	8.086	2261	2273	2296	rVB	1013485	2287885	13.64%	3.354%
3	8.437	2382	2404	2433	rBV	723203	1661598	9.90%	2.436%
4	8.563	2435	2451	2463	rBV2	113609	274902	1.64%	0.403%
5	8.965	2583	2601	2639	rVB	1571114	3309503	19.72%	4.851%
6	9.545	2801	2817	2830	rBV3	107332	252202	1.50%	0.370%
7	9.622	2830	2846	2887	rVV	6607474	12464235	74.29%	18.270%
8	10.242	3060	3077	3098	rBV	995530	1774546	10.58%	2.601%
9	10.440	3134	3151	3178	rBV	2552846	4730172	28.19%	6.934%
10	10.615	3204	3216	3238	rVB2	113467	213037	1.27%	0.312%
11	10.872	3298	3312	3331	rBV	271495	466292	2.78%	0.683%
12	10.963	3331	3346	3368	rVV	630565	1109950	6.62%	1.627%
13	11.089	3369	3393	3414	rVV	9778171	16778865	100.00%	24.595%
14	11.178	3415	3426	3468	rVB	1028975	1940184	11.56%	2.844%
15	11.489	3523	3542	3578	rBV	5836403	9888934	58.94%	14.495%
16	11.744	3620	3637	3667	rVB	2099476	3788922	22.58%	5.554%
17	12.194	3792	3805	3826	rBV	154168	271321	1.62%	0.398%
18	12.731	3987	4005	4035	rBV	1686334	3026929	18.04%	4.437%
19	13.675	4340	4357	4381	rBV	1461279	2607265	15.54%	3.822%

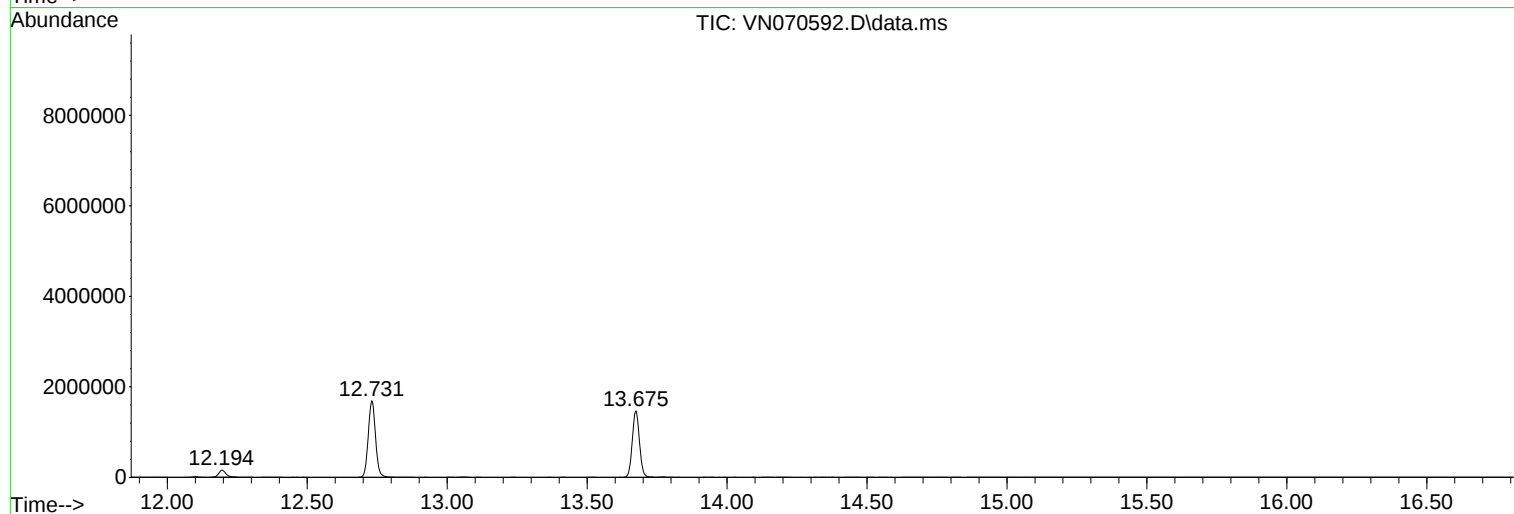
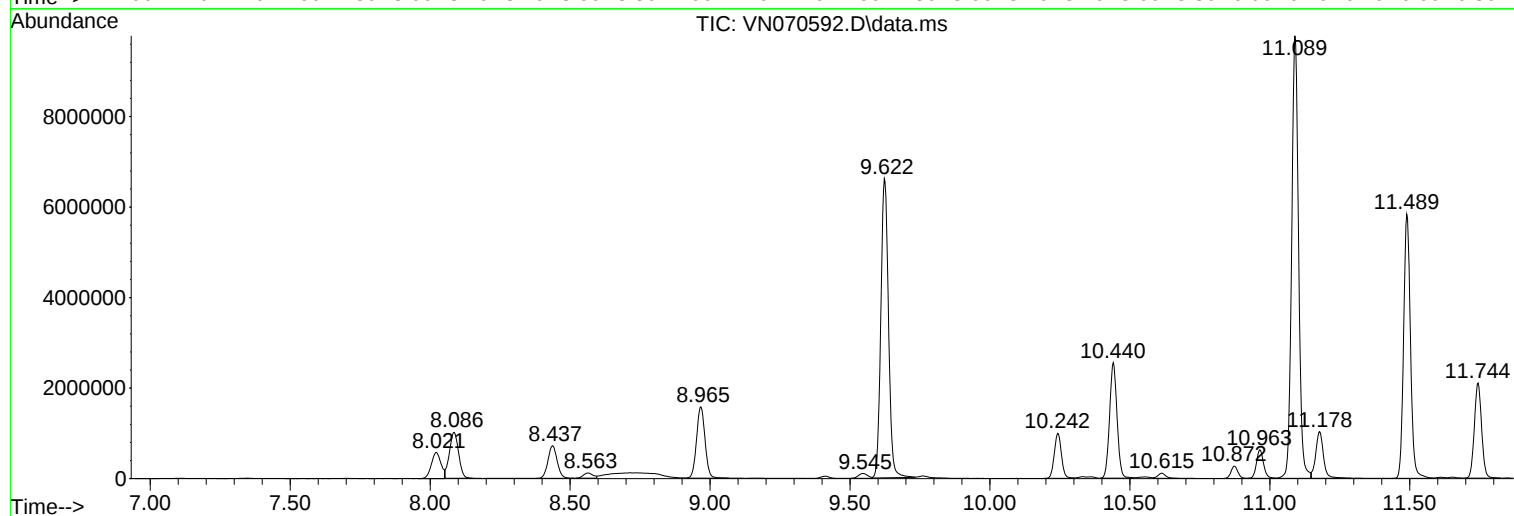
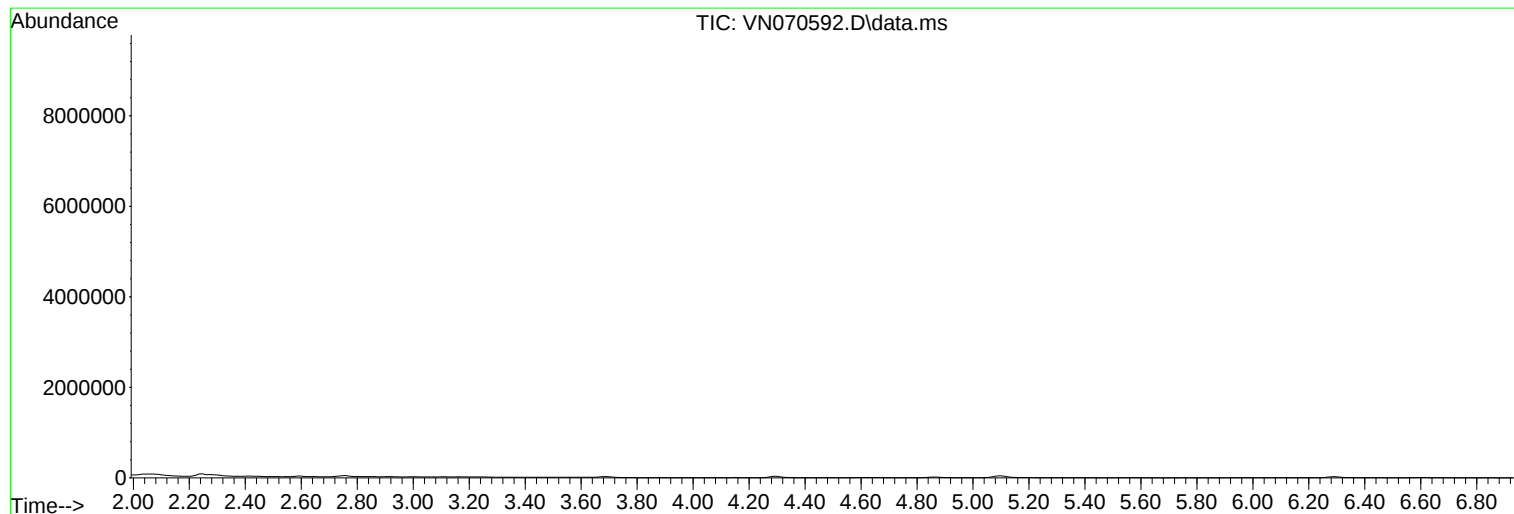
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Quant Title : SW846 8260

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



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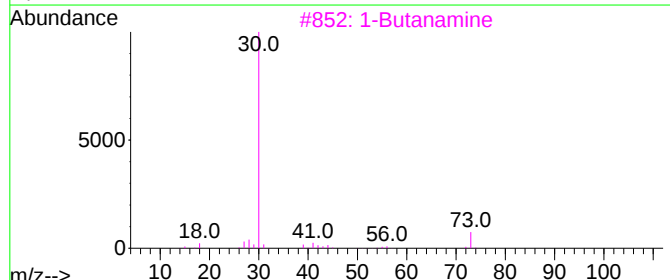
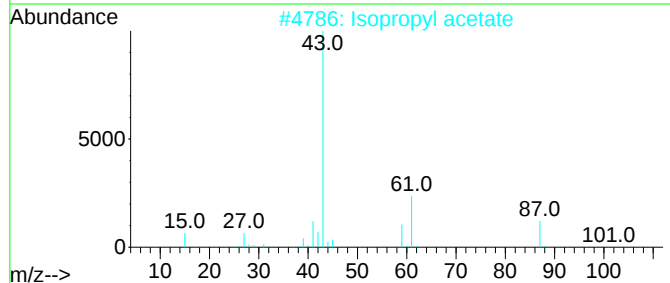
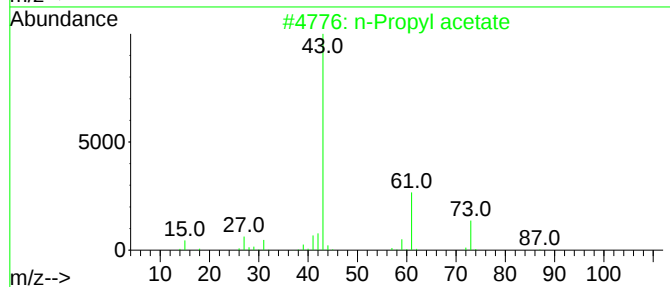
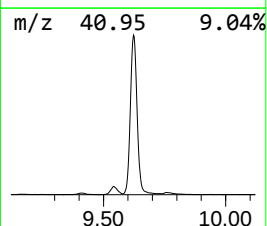
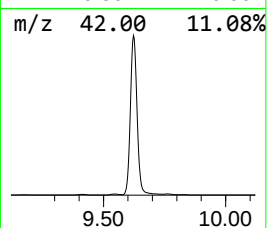
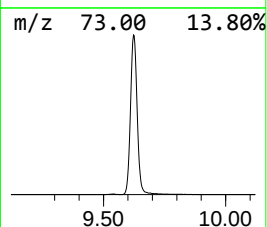
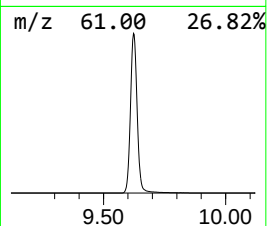
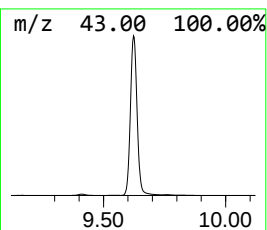
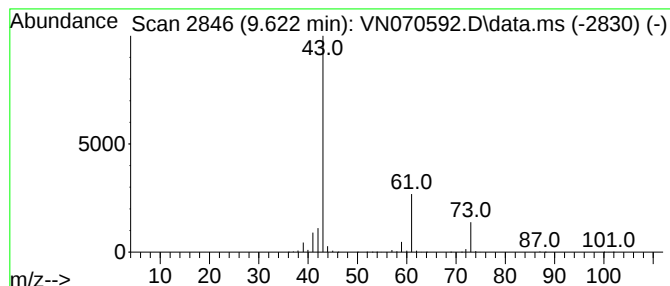
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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.
9.622	188.31 ug/l	12464200	1,4-Difluorobenzene	8.968

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	38
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	4



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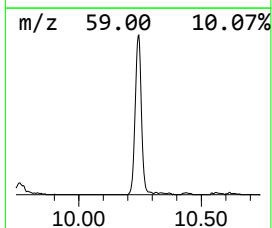
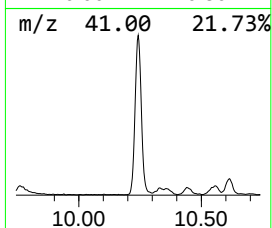
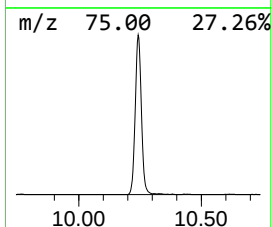
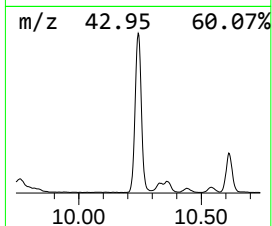
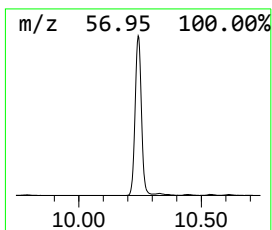
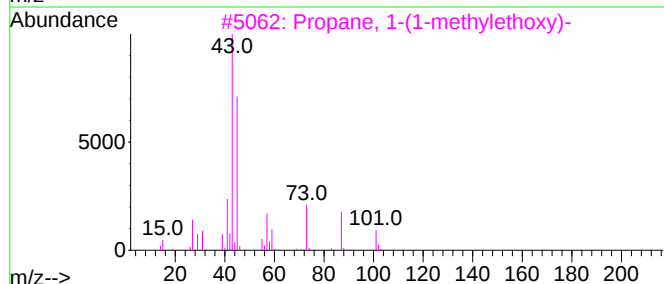
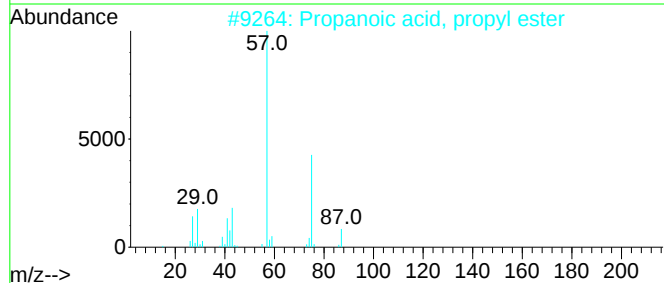
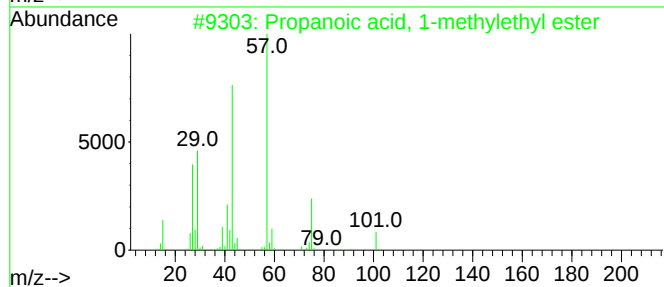
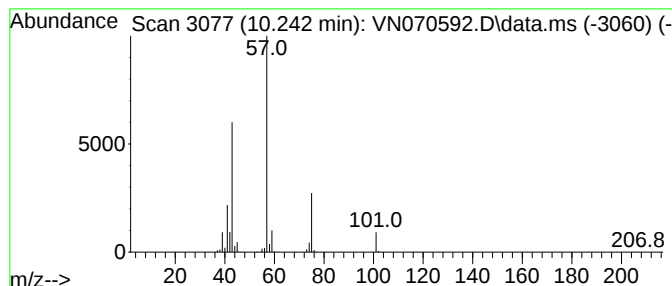
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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.242	26.81 ug/l	1774550	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	22



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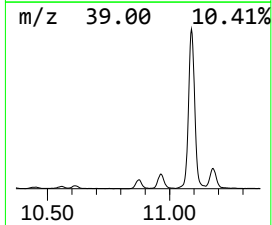
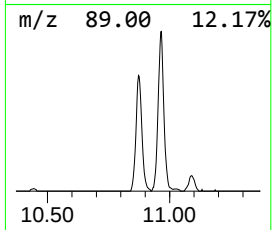
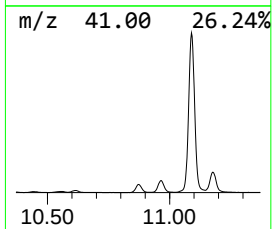
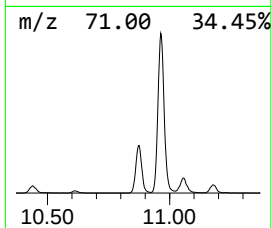
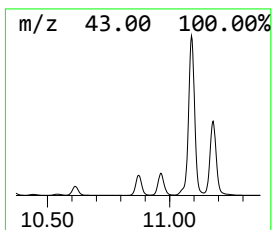
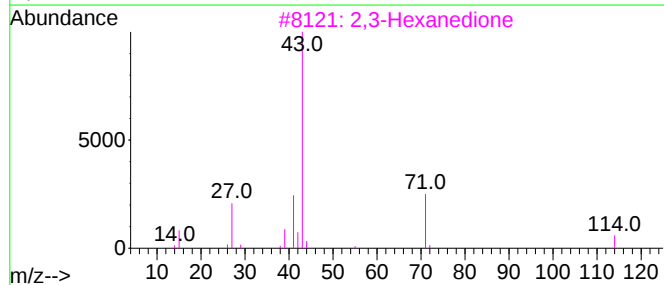
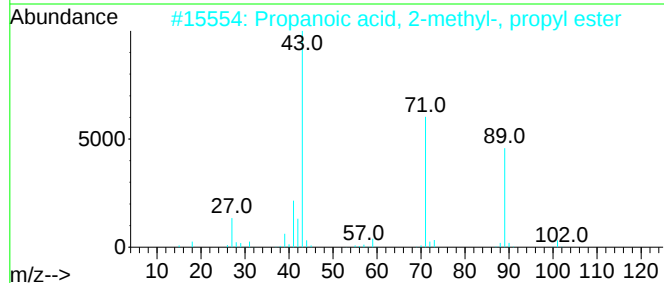
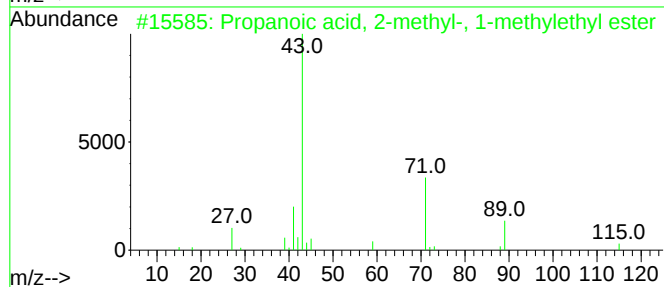
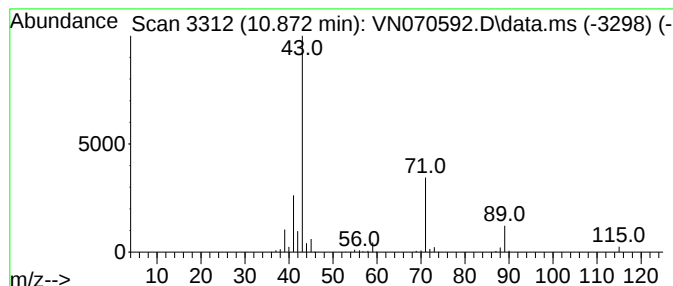
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.872	6.15 ug/l	466292	Chlorobenzene-d5	11.744	
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	2,3-Hexanedione	114	C6H10O2	003848-24-6	42
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	40



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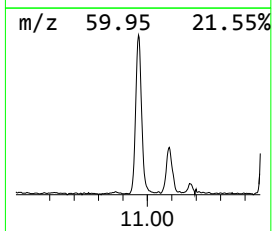
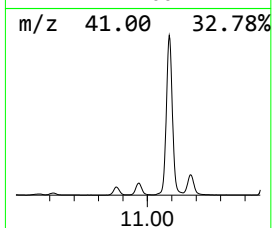
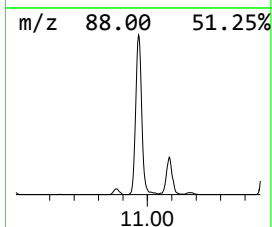
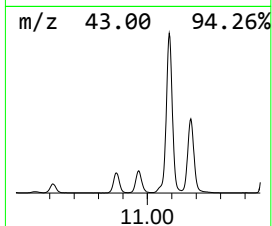
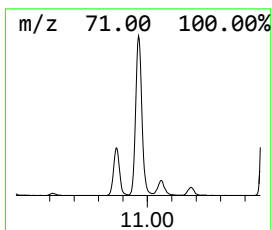
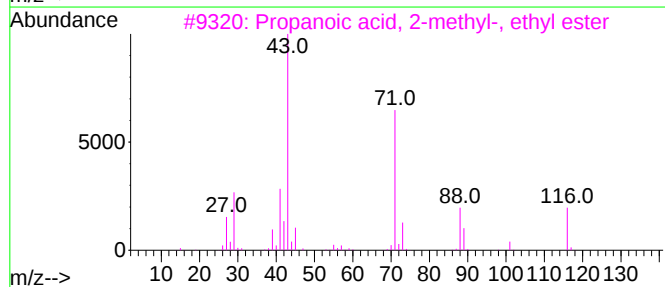
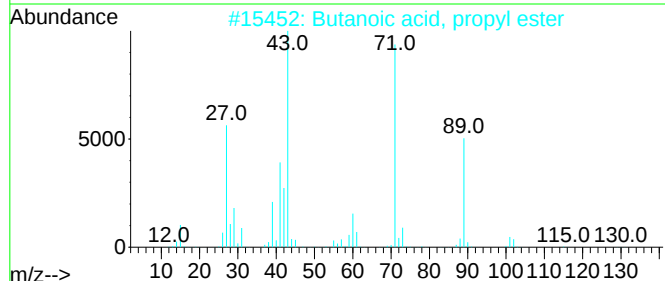
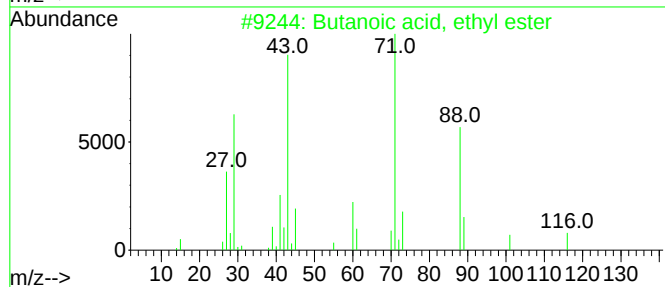
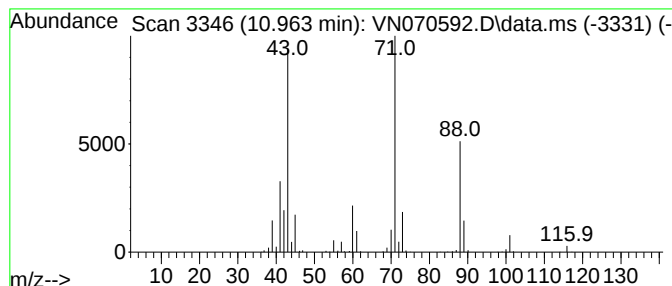
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.963	14.65 ug/l	1109950	Chlorobenzene-d5	11.744

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	53
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	47
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	43



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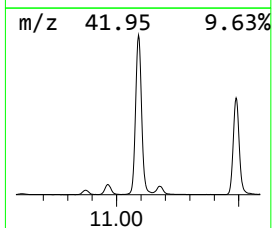
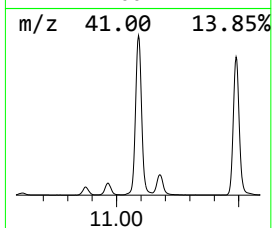
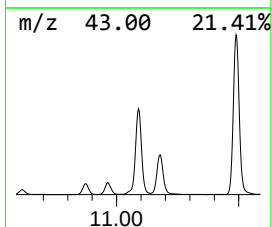
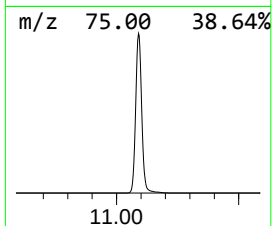
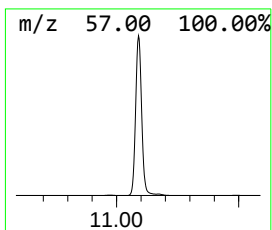
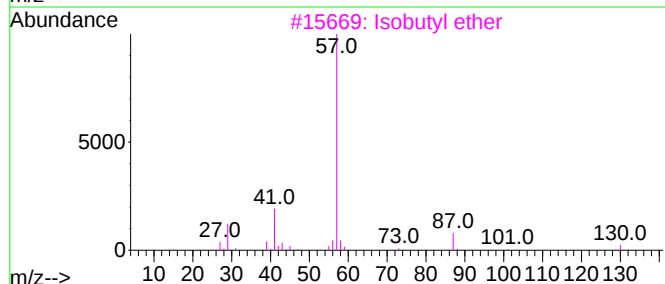
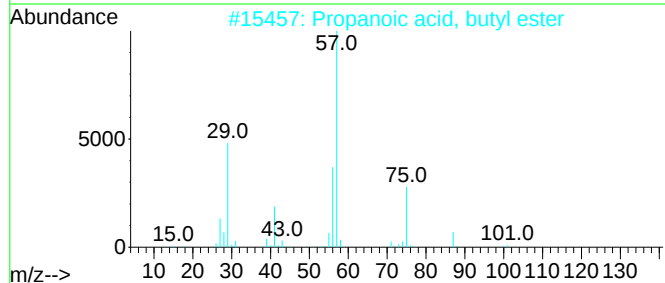
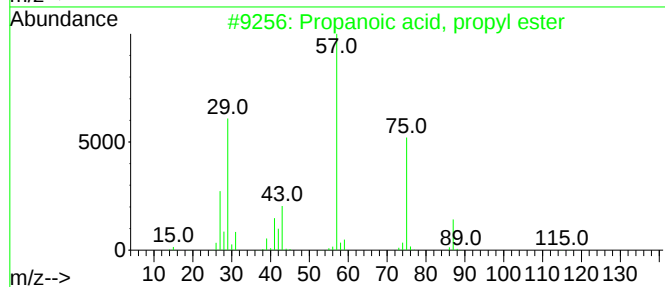
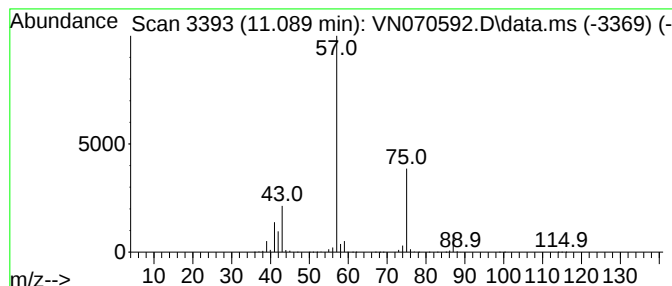
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Quant Title : SW846 8260

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.089	221.42 ug/l	16778900	Chlorobenzene-d5	11.744

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	25
3			Isobutyl ether	130	C8H18O	000628-55-7	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



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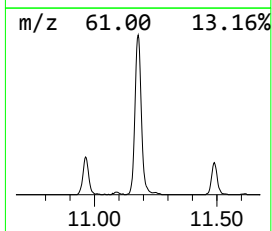
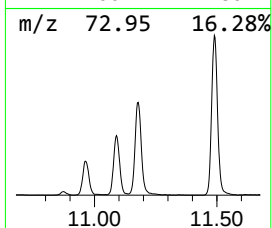
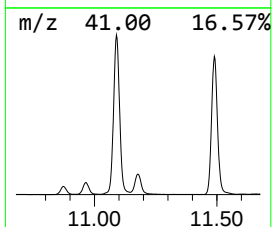
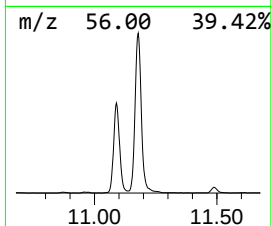
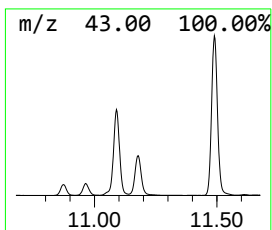
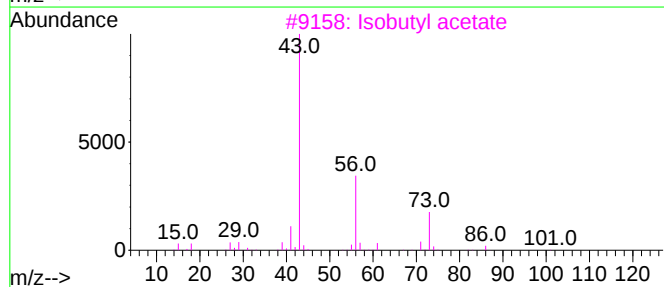
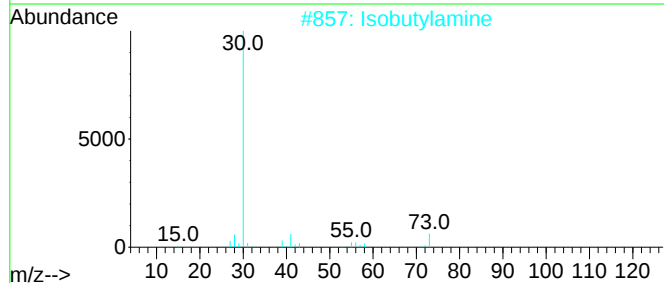
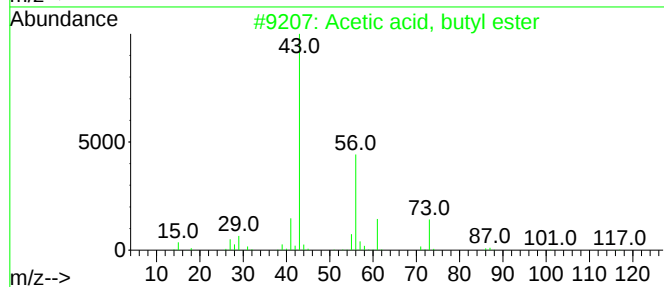
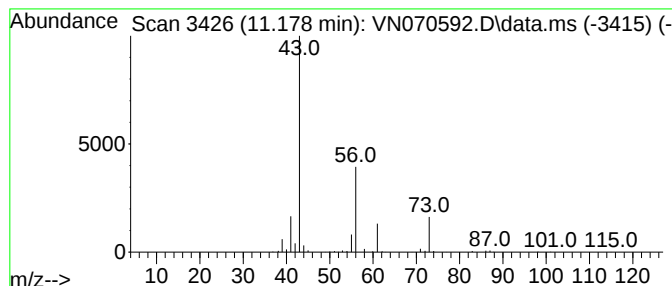
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Quant Title : SW846 8260

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.178	25.60 ug/l	1940180	Chlorobenzene-d5	11.744

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			Isobutyl acetate	116	C6H12O2	000110-19-0	9
4			1-Butanamine	73	C4H11N	000109-73-9	5
5			Ethane, diazo-	56	C2H4N2	001117-96-0	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070592.D
Acq On : 12 Jan 2022 17:42
Operator : JC/MD
Sample : N1097-16
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3D

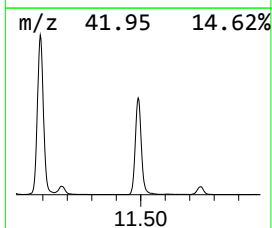
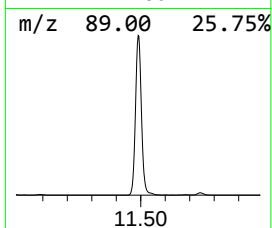
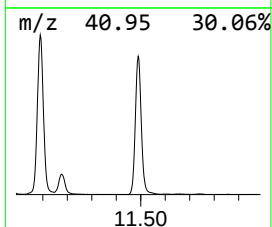
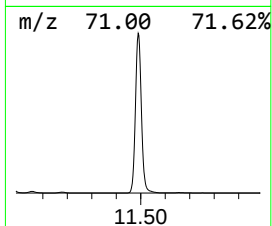
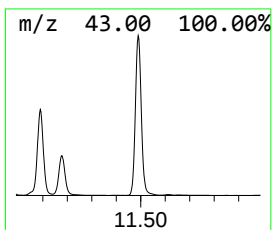
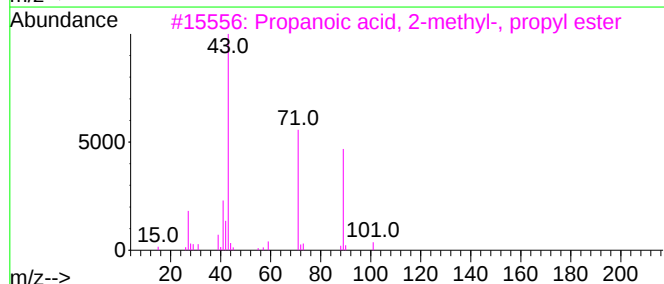
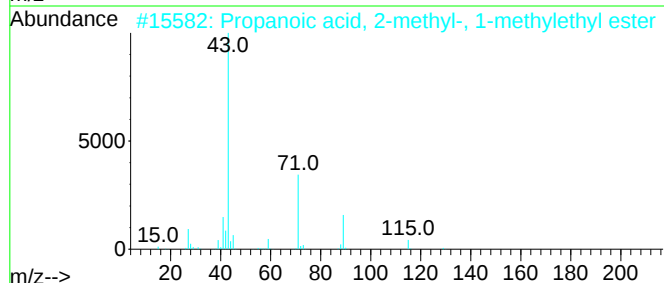
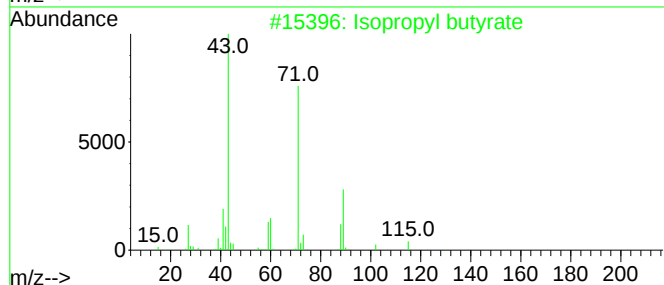
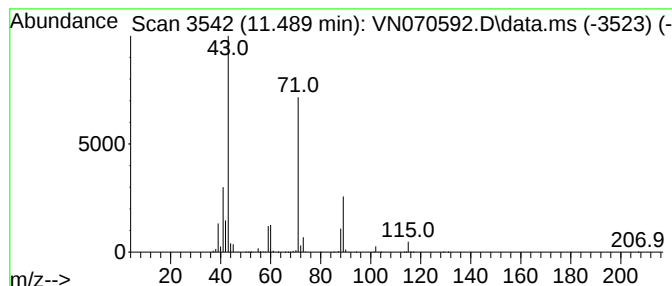
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Quant Title : SW846 8260

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.489	130.50 ug/l	9888930	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
4			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	59
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070592.D
Acq On : 12 Jan 2022 17:42
Operator : JC/MD
Sample : N1097-16
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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	9.622	188.3	ug/l	12464200	2	8.968	3309500	50.0
Propanoic acid,...	10.242	26.8	ug/l	1774550	2	8.968	3309500	50.0
Propanoic acid,...	10.872	6.2	ug/l	466292	3	11.744	3788920	50.0
Butanoic acid, ...	10.963	14.7	ug/l	1109950	3	11.744	3788920	50.0
Propanoic acid,...	11.089	221.4	ug/l	16778900	3	11.744	3788920	50.0
Acetic acid, bu...	11.178	25.6	ug/l	1940180	3	11.744	3788920	50.0
Isopropyl butyrate	11.489	130.5	ug/l	9888930	3	11.744	3788920	50.0