

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
 Data File : VN070590.D
 Acq On : 12 Jan 2022 16:51
 Operator : JC/MD
 Sample : N1097-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-2D

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: VN070590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	81	93	101	rBV3	78926	169479	1.05%	0.251%
2	8.021	2222	2249	2260	rBV	580594	1389620	8.57%	2.061%
3	8.083	2260	2272	2300	rVB	1020853	2341716	14.45%	3.473%
4	8.437	2383	2404	2431	rBV	721063	1665684	10.28%	2.470%
5	8.563	2435	2451	2462	rBV2	116749	281129	1.73%	0.417%
6	8.965	2583	2601	2628	rVB	1588270	3327218	20.53%	4.934%
7	9.547	2796	2818	2829	rBV3	107867	255364	1.58%	0.379%
8	9.622	2829	2846	2888	rVV	6559255	12254557	75.61%	18.174%
9	10.242	3060	3077	3098	rBV	1002264	1776658	10.96%	2.635%
10	10.440	3133	3151	3171	rBV	2533910	4690747	28.94%	6.956%
11	10.612	3205	3215	3235	rVB2	103052	191971	1.18%	0.285%
12	10.872	3298	3312	3330	rBV	269462	464325	2.86%	0.689%
13	10.963	3330	3346	3367	rVV	594895	1055095	6.51%	1.565%
14	11.089	3369	3393	3413	rVV	9306459	16206976	100.00%	24.035%
15	11.178	3415	3426	3467	rVB	976604	1817559	11.21%	2.695%
16	11.489	3524	3542	3577	rBV	5738278	9683824	59.75%	14.361%
17	11.744	3620	3637	3669	rVB	2114606	3828412	23.62%	5.678%
18	12.194	3792	3805	3821	rBV	140571	244221	1.51%	0.362%
19	12.731	3987	4005	4032	rBV	1708218	3071062	18.95%	4.554%
20	13.675	4340	4357	4378	rBV	1529054	2715129	16.75%	4.027%

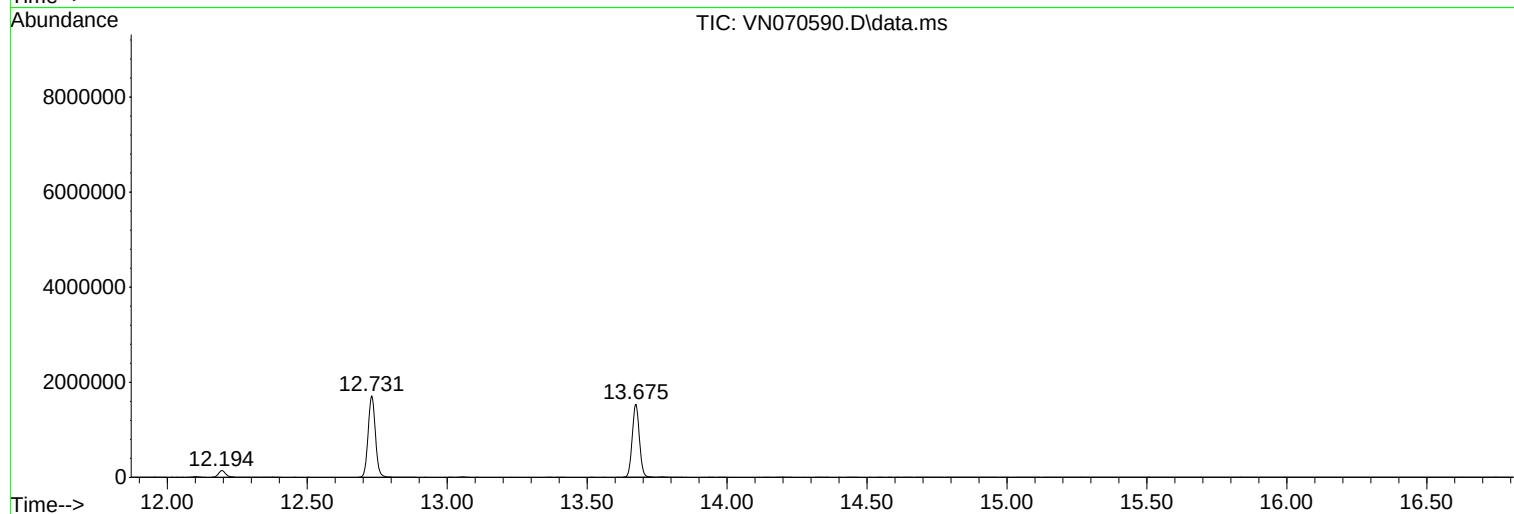
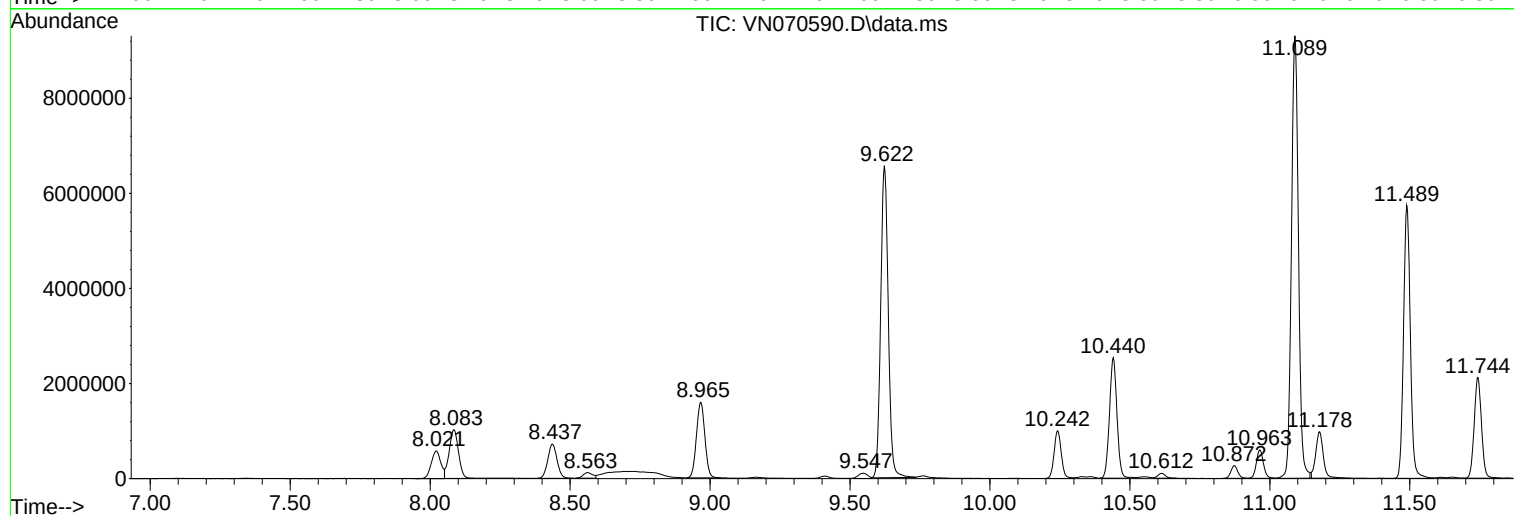
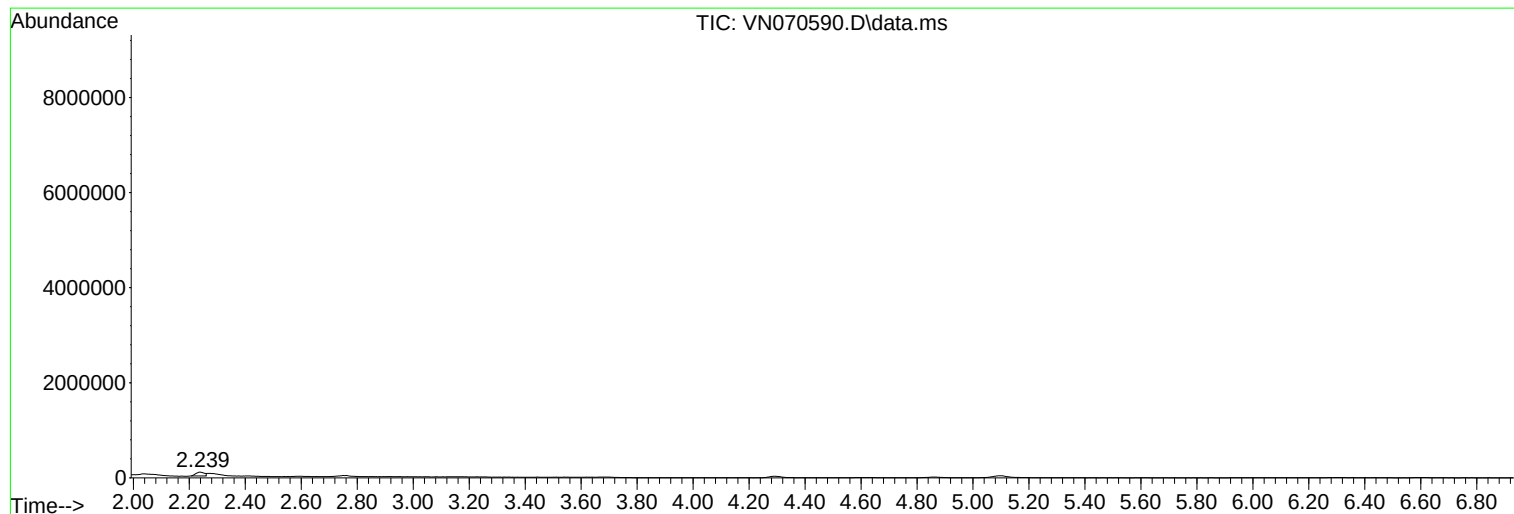
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Quant Title : SW846 8260

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



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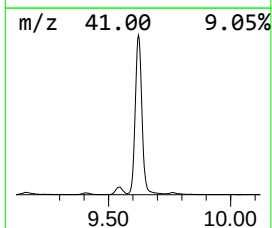
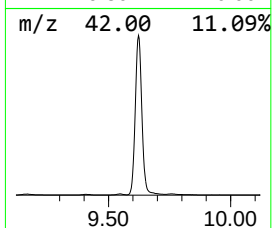
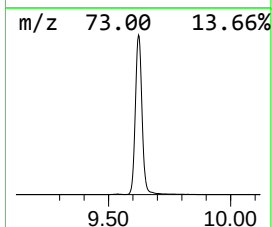
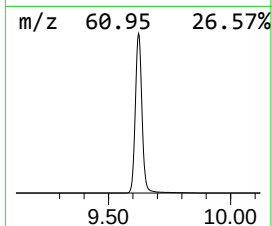
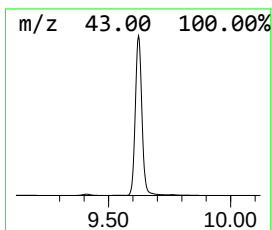
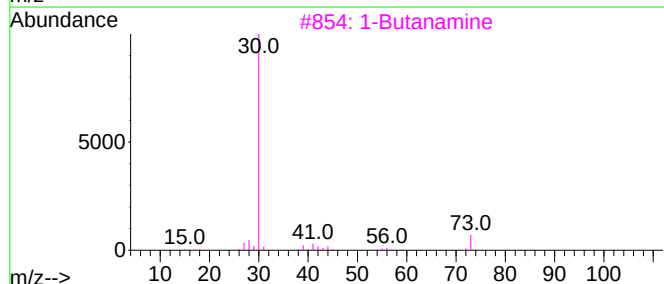
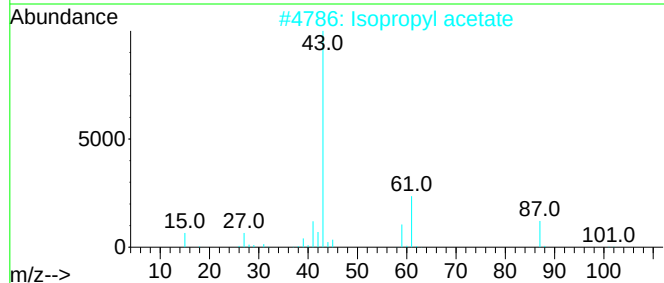
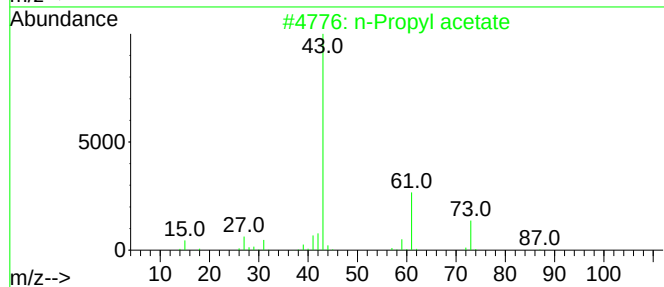
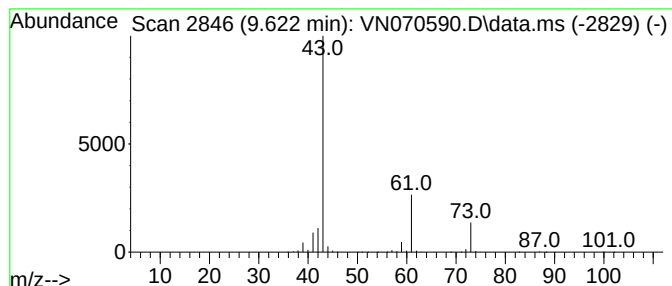
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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	184.16 ug/l	12254600	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			(3S)-3-Pyrrolidinol	87	C4H9NO	100243-39-8	4



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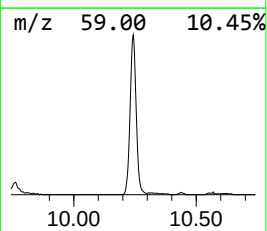
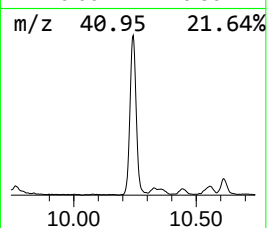
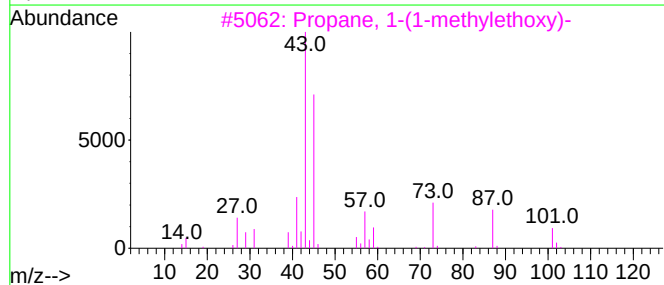
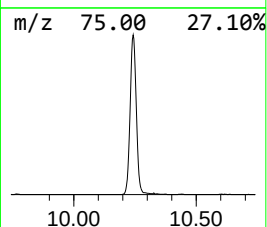
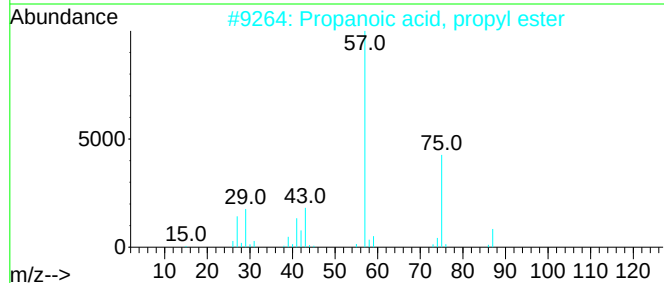
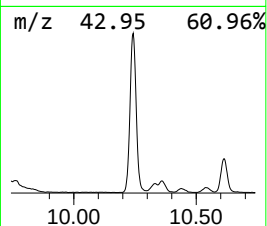
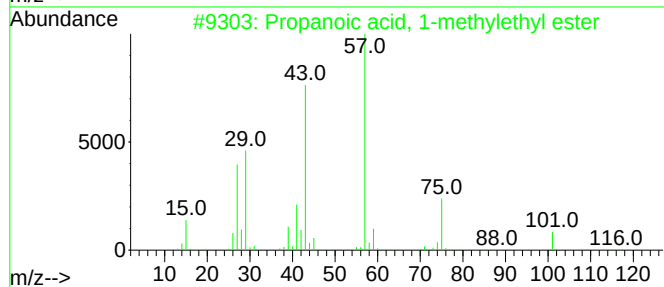
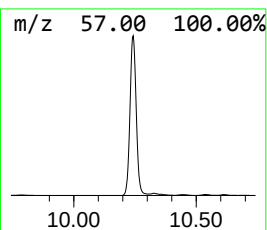
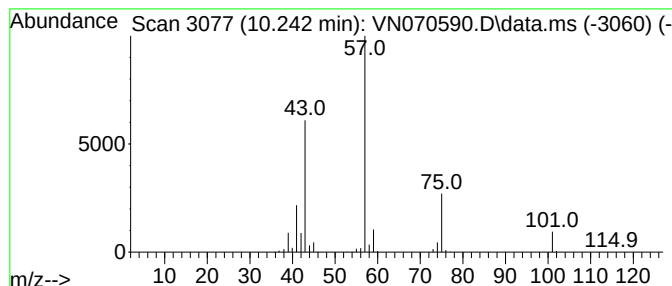
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.242	26.70 ug/l	1776660	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	42
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
5			Azetidine	57	C3H7N	000503-29-7	12



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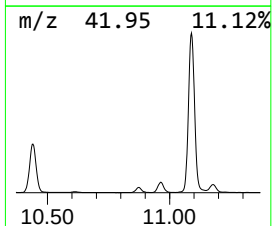
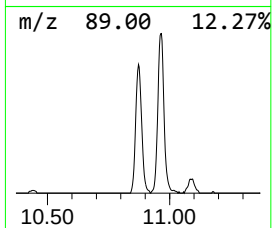
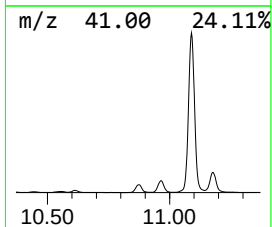
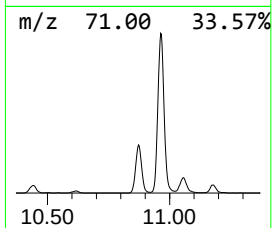
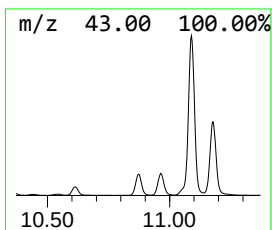
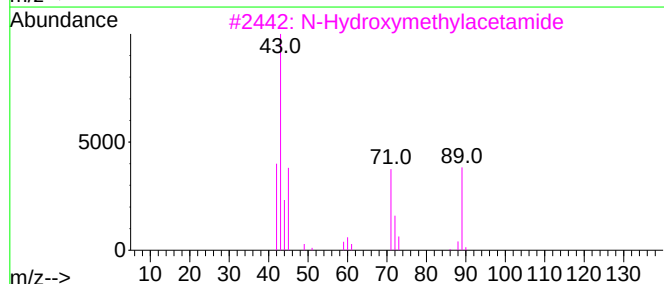
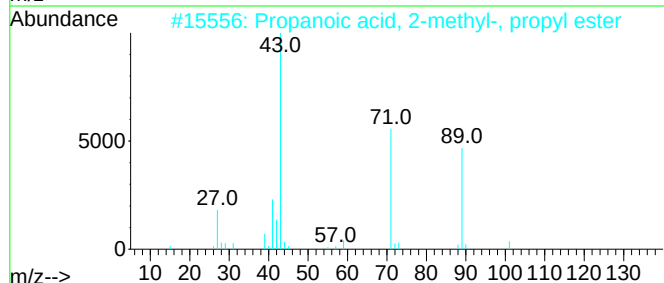
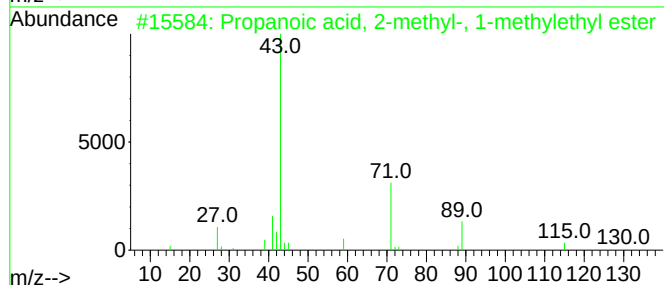
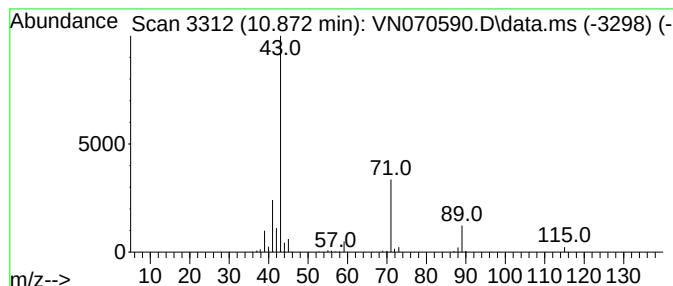
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Quant Title : SW846 8260

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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	6.06 ug/l	464325	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	64
3			N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38



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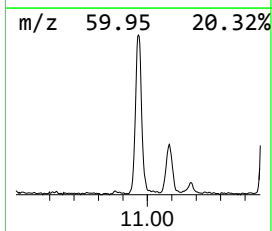
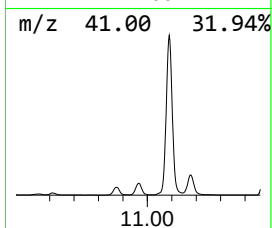
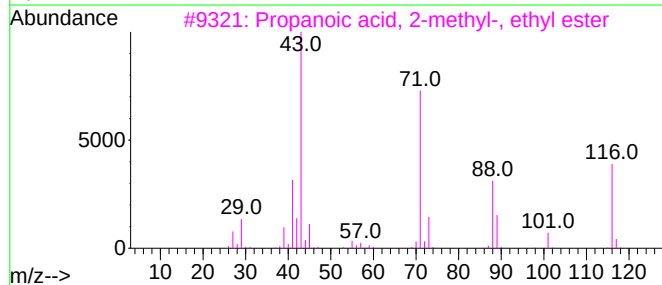
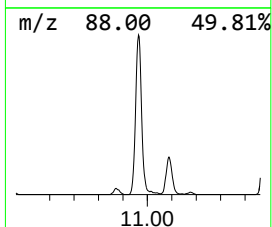
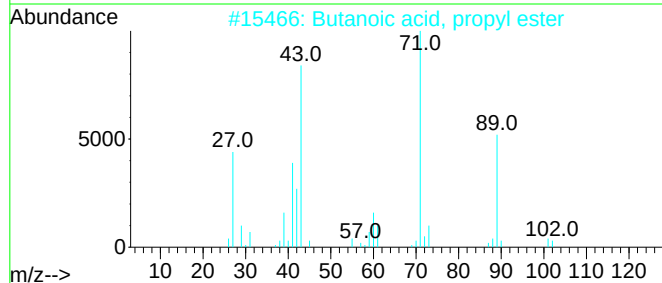
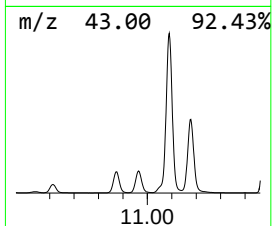
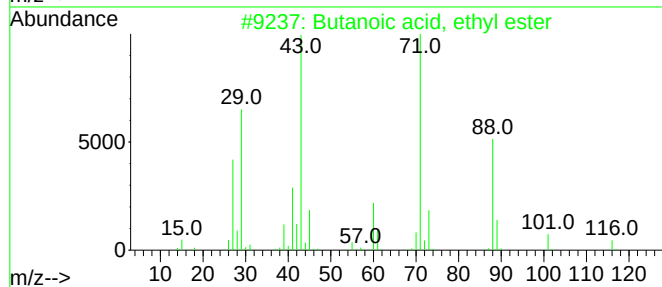
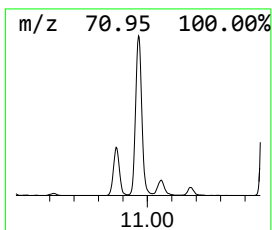
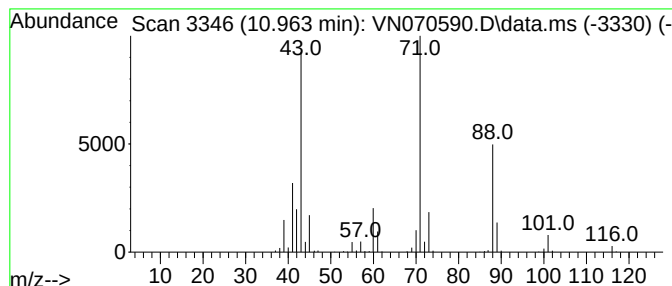
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.963	13.78 ug/l	1055100	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	52
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	47
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	42



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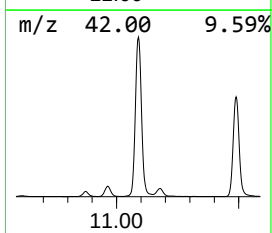
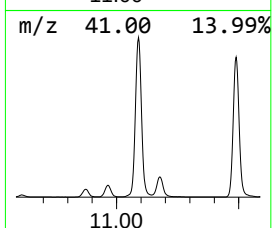
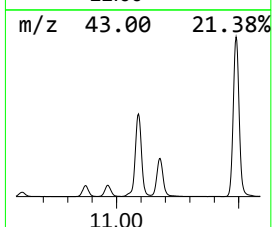
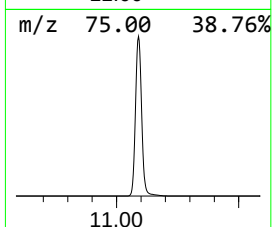
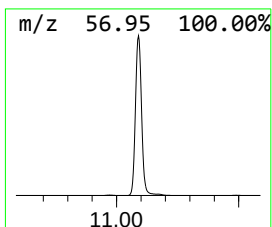
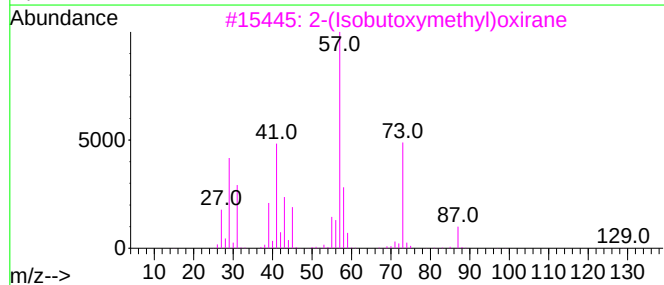
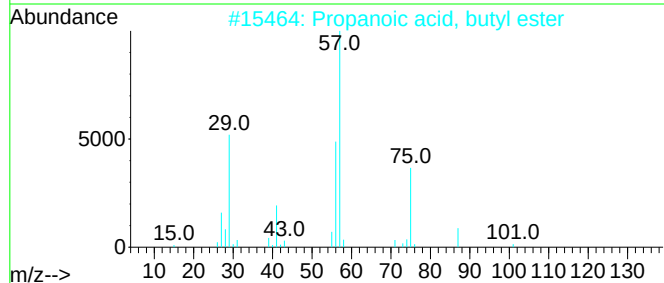
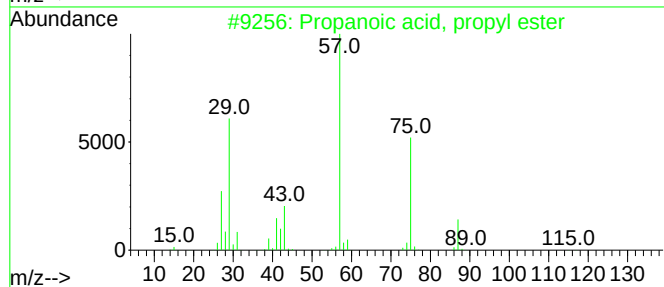
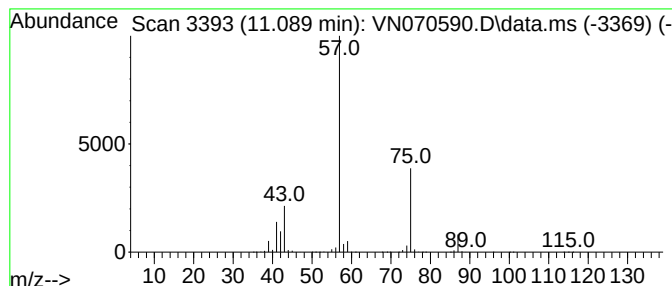
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.089	211.67 ug/l	16207000	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	39
3			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4			Isobutyl ether	130	C8H18O	000628-55-7	9
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



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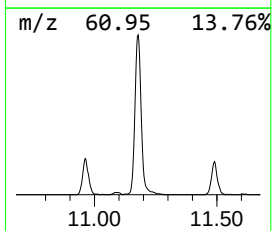
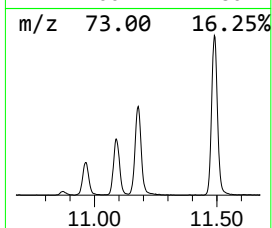
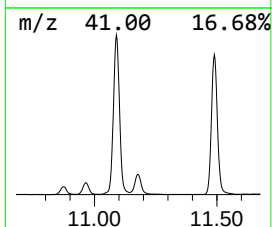
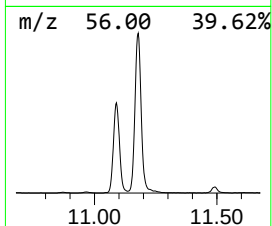
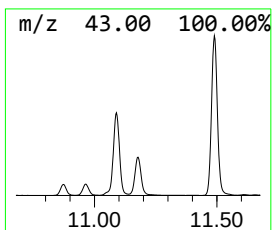
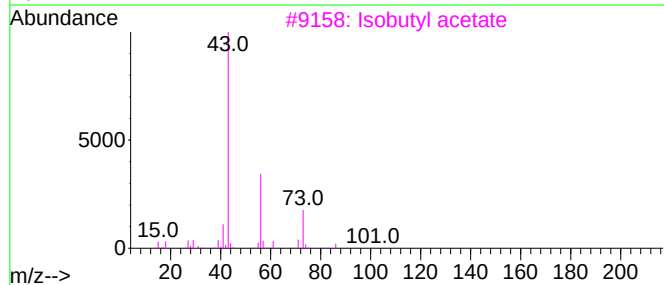
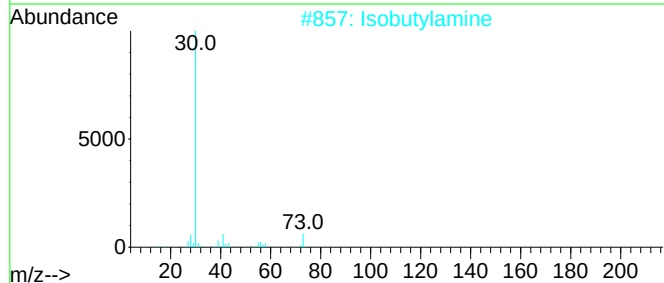
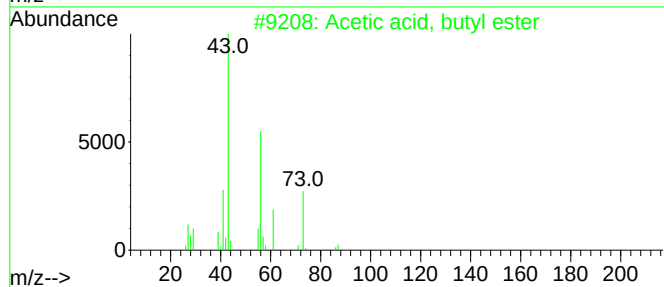
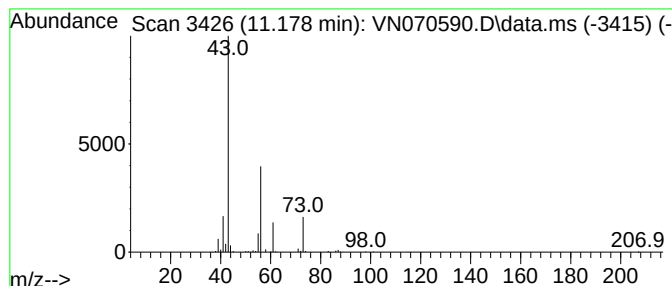
Instrument :
MSVOA_N
ClientSampleId :
TP-2D

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 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.178	23.74 ug/l	1817560	Chlorobenzene-d5		11.744	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	50
2	Isobutylamine		73	C4H11N	000078-81-9	9
3	Isobutyl acetate		116	C6H12O2	000110-19-0	9
4	1-Butanol, 4-chloro-, acetate		150	C6H11ClO2	006962-92-1	9
5	1-Butanamine		73	C4H11N	000109-73-9	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070590.D
Acq On : 12 Jan 2022 16:51
Operator : JC/MD
Sample : N1097-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2D

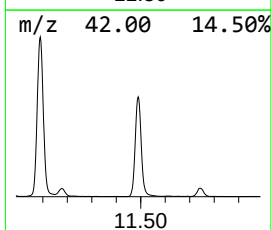
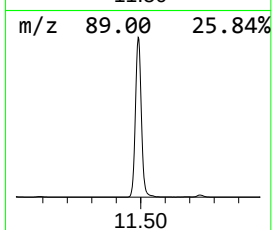
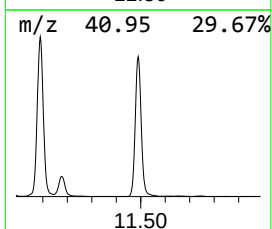
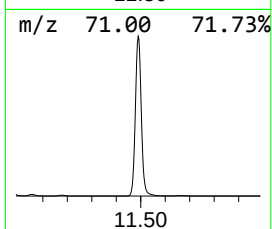
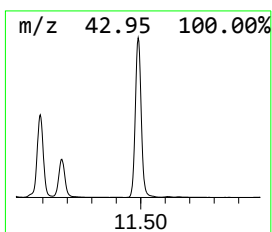
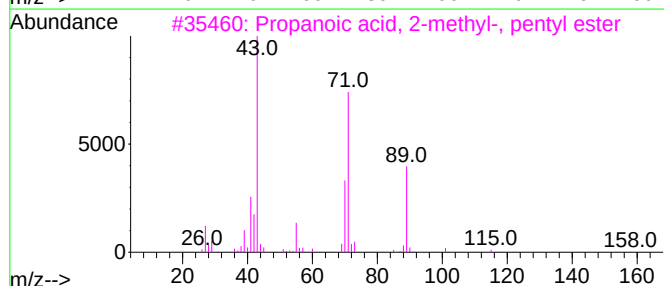
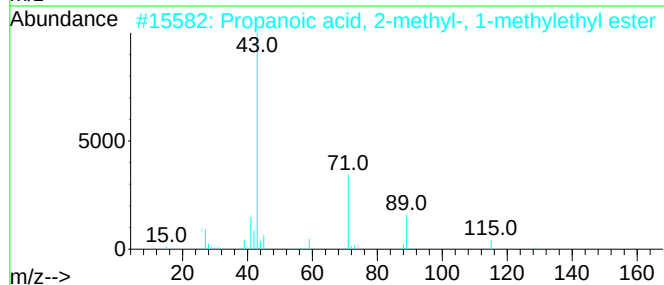
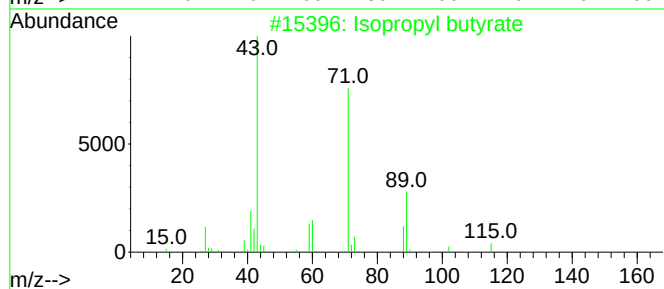
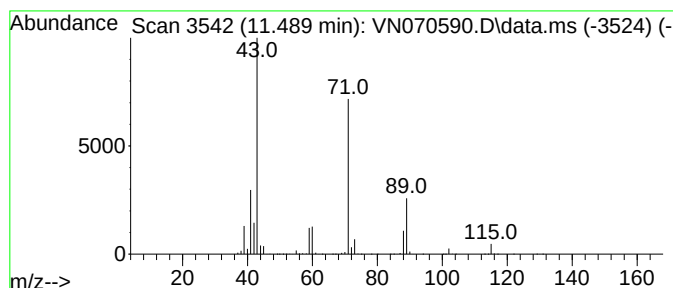
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.489	126.47 ug/l	9683820	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-, penty...	158	C9H18O2	002445-72-9	59
4			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070590.D
Acq On : 12 Jan 2022 16:51
Operator : JC/MD
Sample : N1097-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2D

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	184.2	ug/l	12254600	2	8.968	3327220	50.0
Propanoic acid,...	10.242	26.7	ug/l	1776660	2	8.968	3327220	50.0
Propanoic acid,...	10.872	6.1	ug/l	464325	3	11.744	3828410	50.0
Butanoic acid, ...	10.963	13.8	ug/l	1055100	3	11.744	3828410	50.0
Propanoic acid,...	11.089	211.7	ug/l	16207000	3	11.744	3828410	50.0
Acetic acid, bu...	11.178	23.7	ug/l	1817560	3	11.744	3828410	50.0
Isopropyl butyrate	11.489	126.5	ug/l	9683820	3	11.744	3828410	50.0