

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
 Data File : VN070591.D
 Acq On : 12 Jan 2022 17:17
 Operator : JC/MD
 Sample : N1097-13
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-3S

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: VN070591.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	621390	1500317	8.84%	2.119%
2	8.083	2260	2272	2305	rVB	1096642	2507960	14.77%	3.542%
3	8.437	2382	2404	2434	rBV	780754	1808198	10.65%	2.554%
4	8.563	2435	2451	2464	rBV3	127946	321591	1.89%	0.454%
5	8.965	2583	2601	2639	rVB	1728351	3584641	21.11%	5.063%
6	9.545	2801	2817	2829	rBV3	114315	260368	1.53%	0.368%
7	9.622	2829	2846	2889	rVV	6788309	12563202	73.99%	17.745%
8	10.242	3059	3077	3099	rBV	1039131	1819011	10.71%	2.569%
9	10.440	3133	3151	3180	rBV	2706156	5058497	29.79%	7.145%
10	10.612	3204	3215	3237	rVB	111597	203824	1.20%	0.288%
11	10.872	3297	3312	3329	rBV	272286	475836	2.80%	0.672%
12	10.963	3331	3346	3367	rVV	653134	1138971	6.71%	1.609%
13	11.090	3369	3393	3413	rVV	9871820	16980649	100.00%	23.985%
14	11.178	3415	3426	3468	rVB	1033116	1897247	11.17%	2.680%
15	11.489	3524	3542	3577	rBV	5992979	10054977	59.21%	14.203%
16	11.744	3620	3637	3669	rVB	2276347	4120221	24.26%	5.820%
17	12.195	3788	3805	3825	rBV	162491	280392	1.65%	0.396%
18	12.731	3987	4005	4036	rBV	1847827	3306635	19.47%	4.671%
19	13.675	4339	4357	4381	rBV	1651146	2914299	17.16%	4.116%

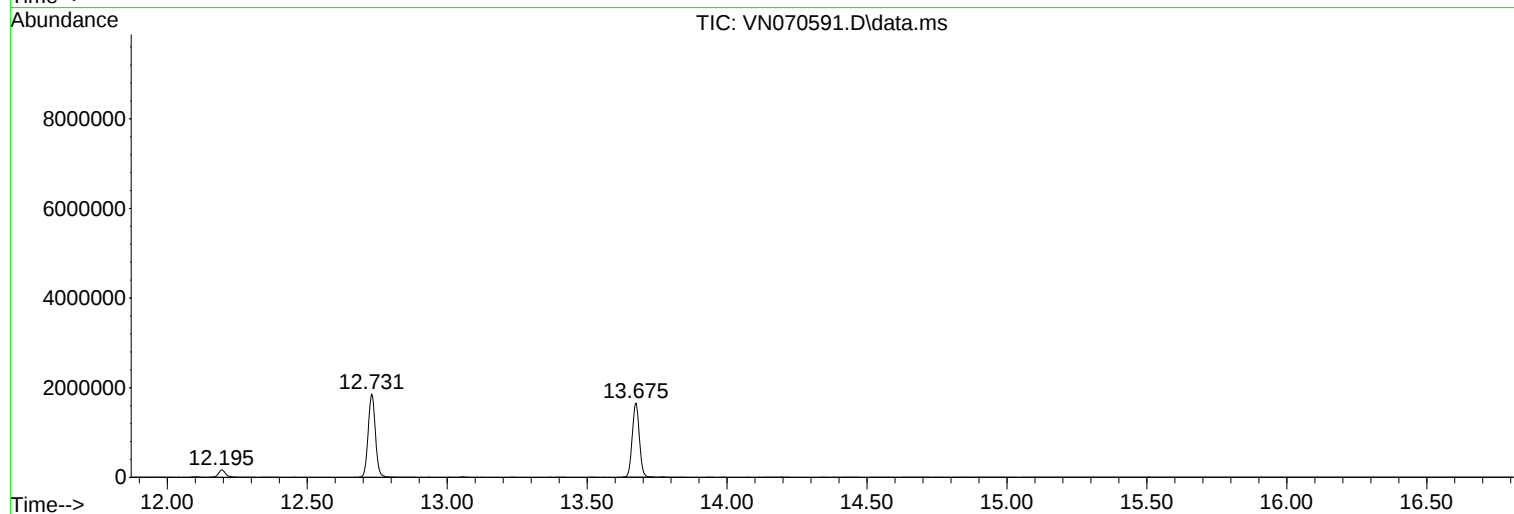
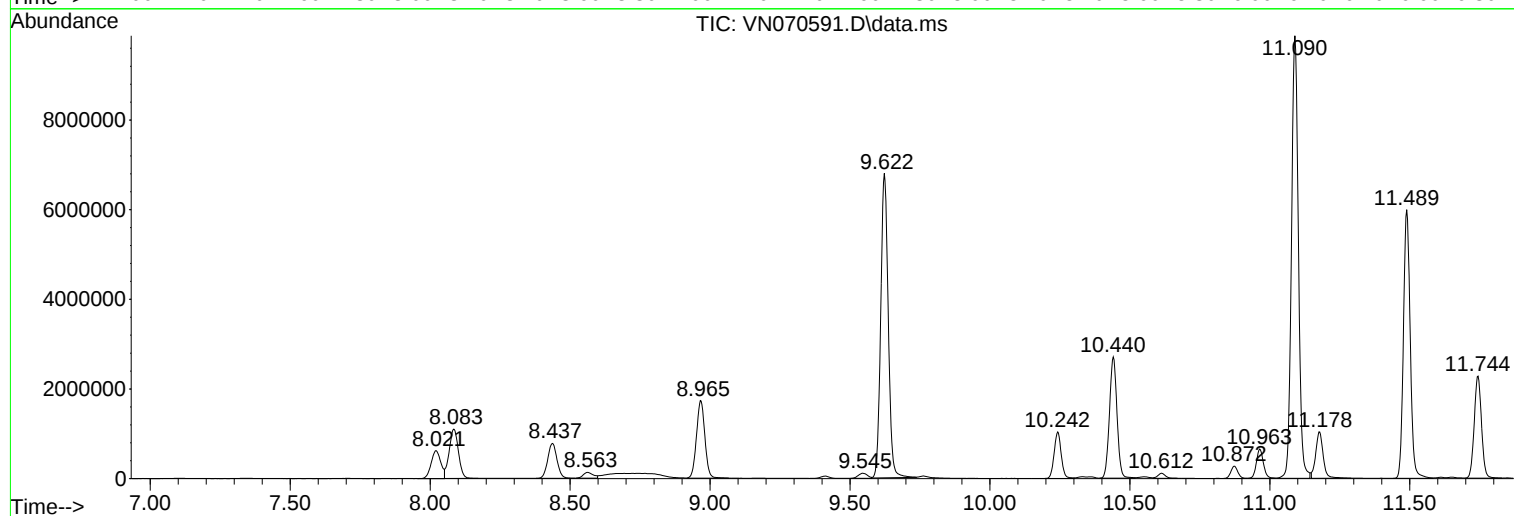
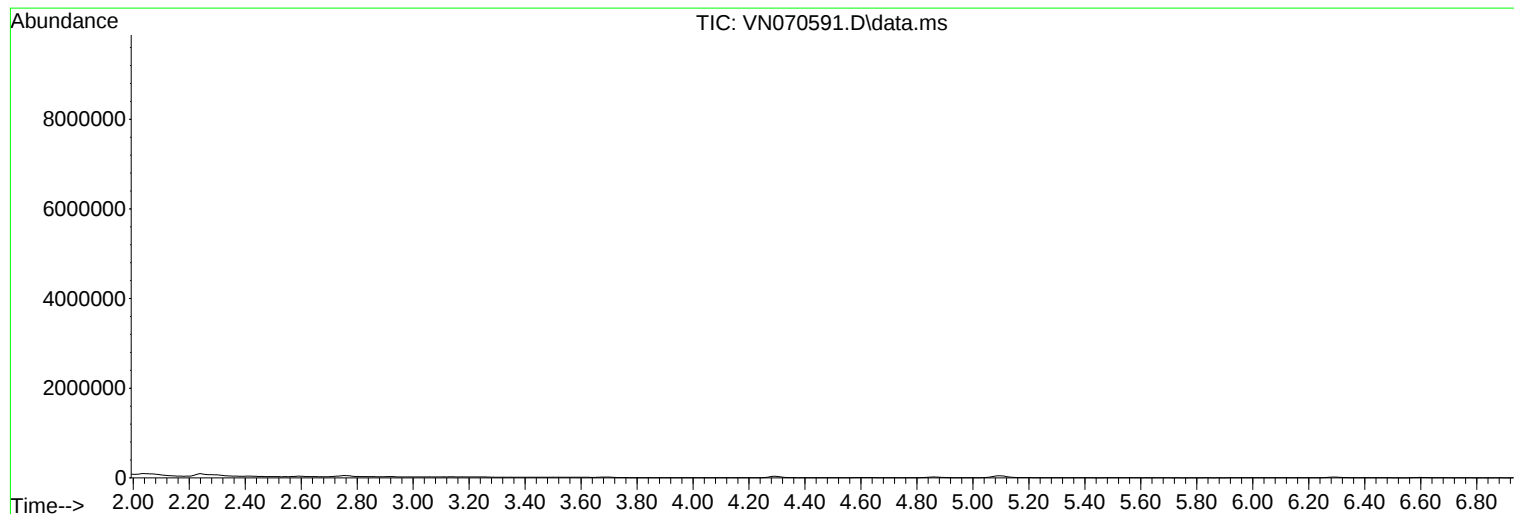
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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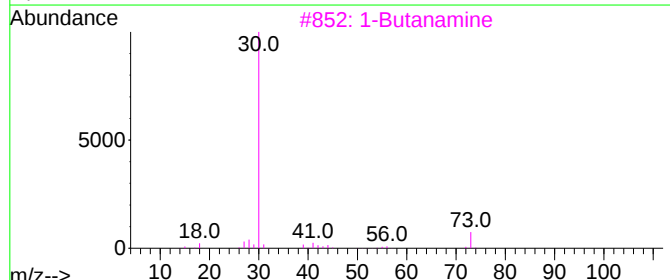
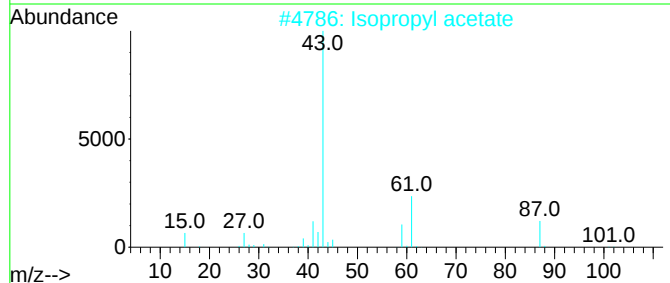
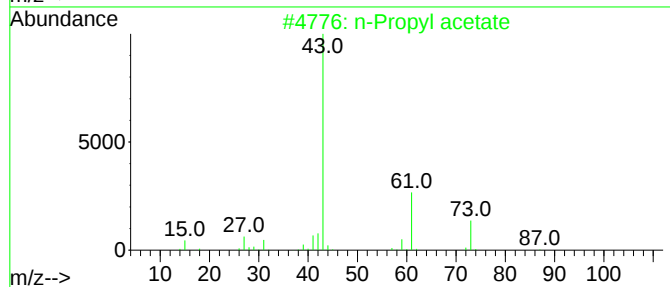
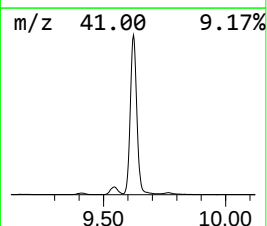
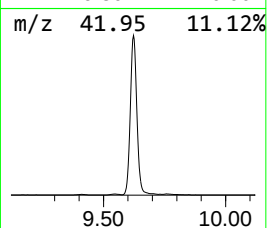
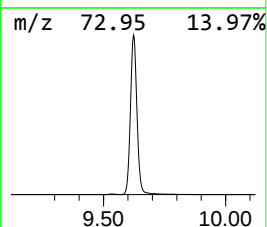
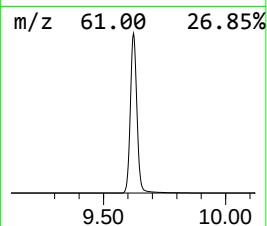
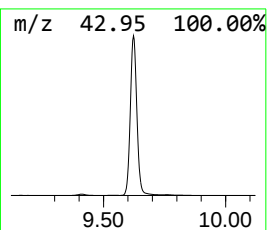
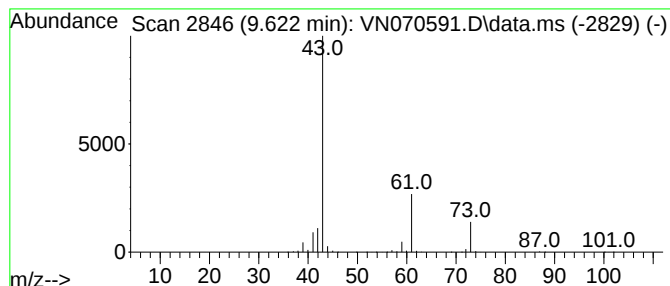
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Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	175.24 ug/l	12563200	1,4-Difluorobenzene	8.965

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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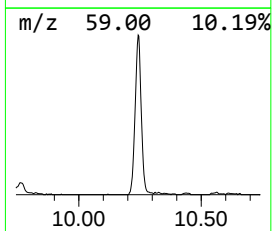
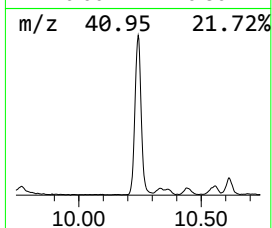
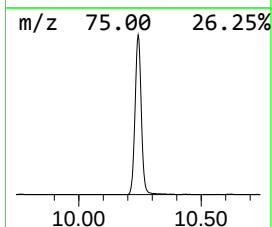
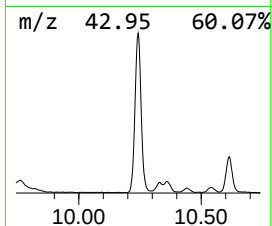
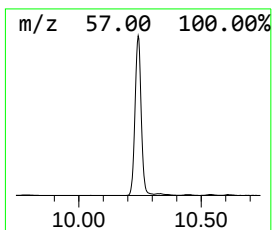
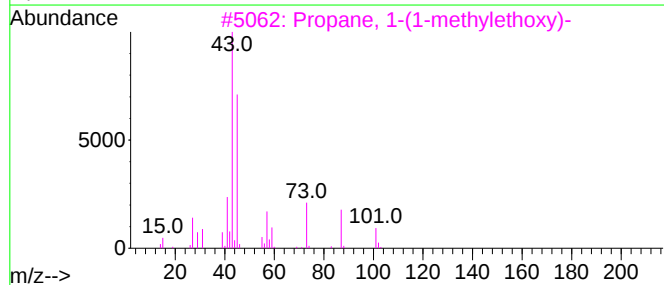
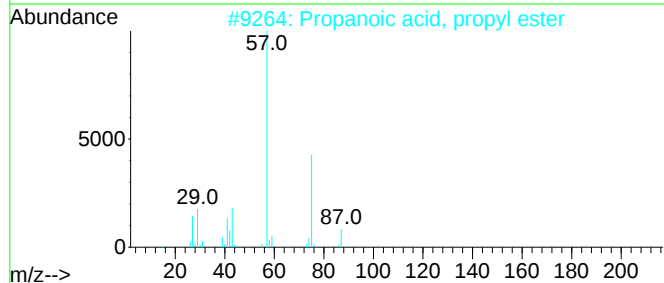
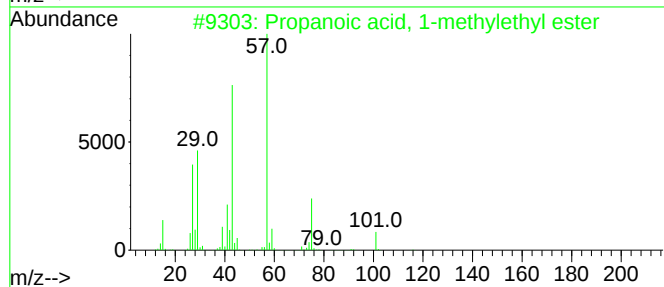
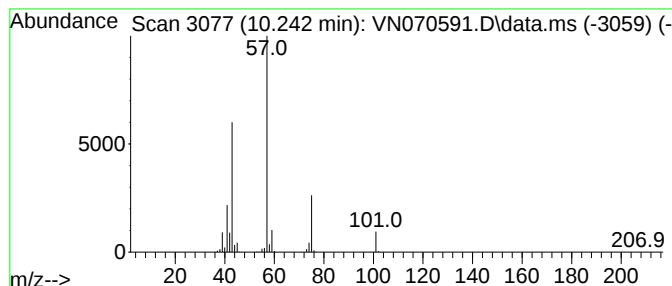
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.242	25.37 ug/l	1819010	1,4-Difluorobenzene	8.965

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			Azetidine	57	C3H7N	000503-29-7	12
5			o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9



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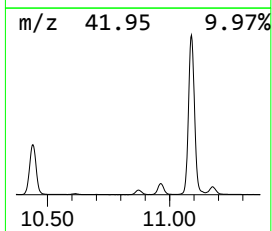
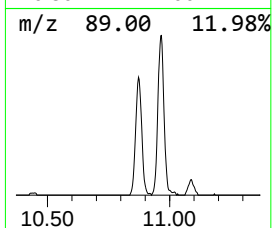
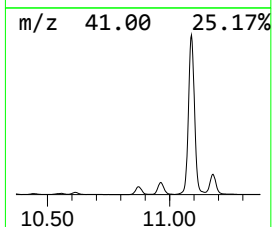
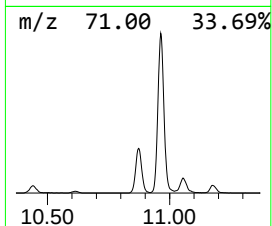
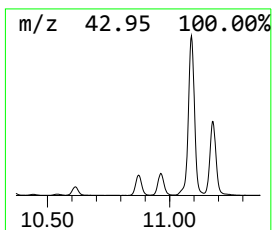
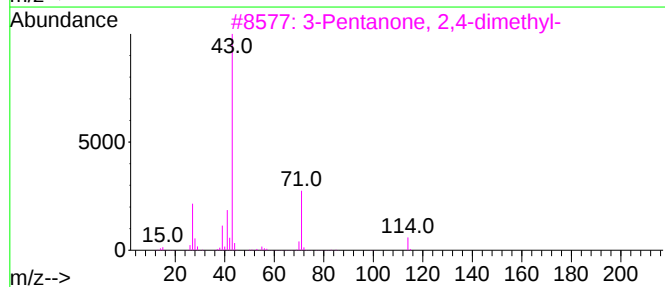
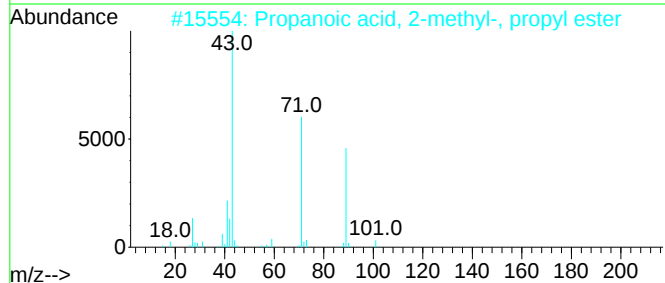
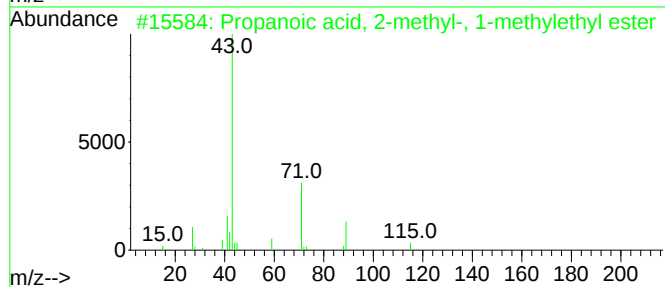
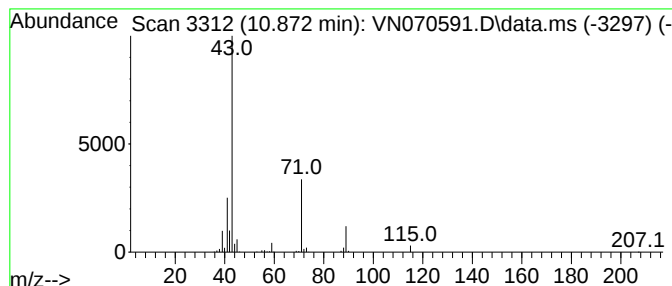
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.872	5.77 ug/l	475836	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			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38



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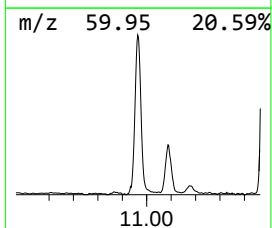
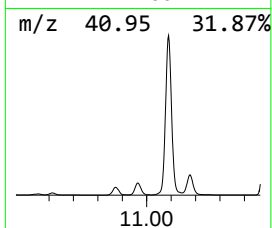
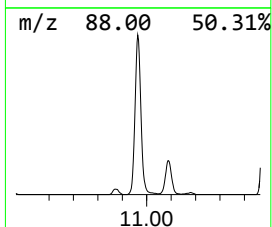
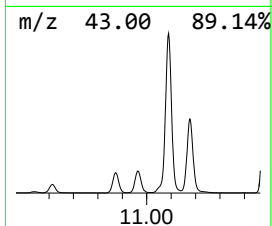
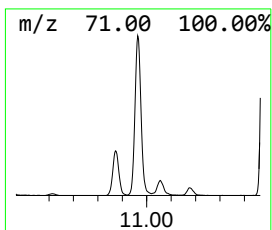
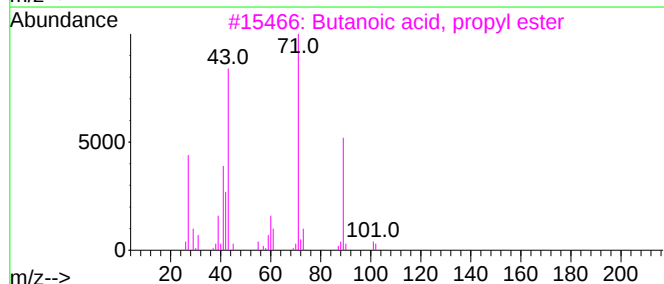
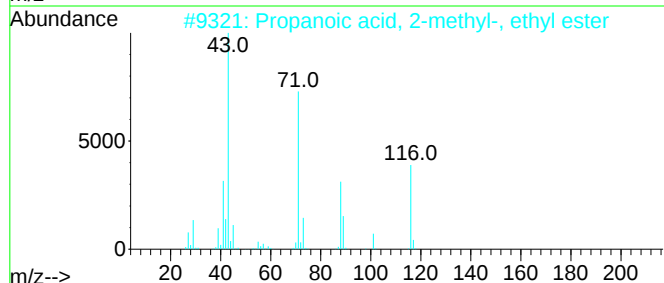
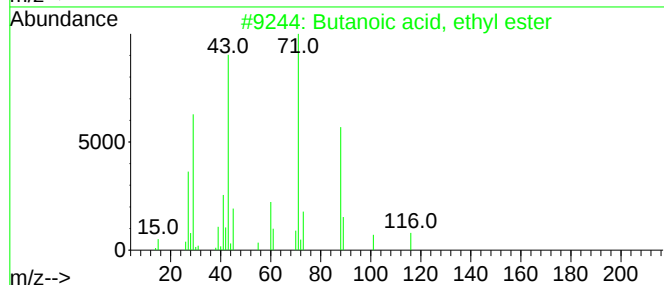
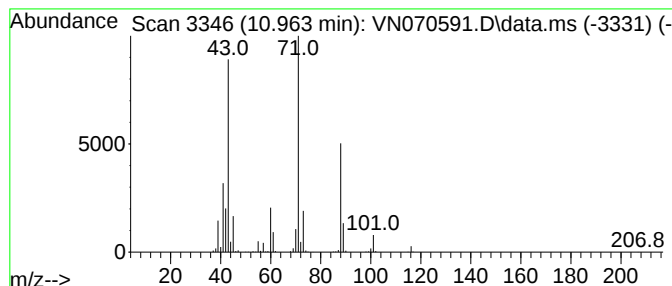
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.964	13.82 ug/l	1138970	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			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	58
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38



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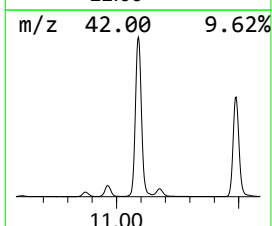
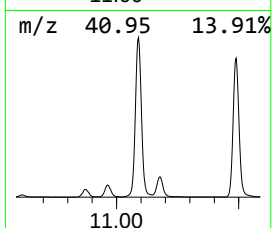
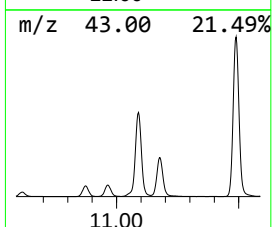
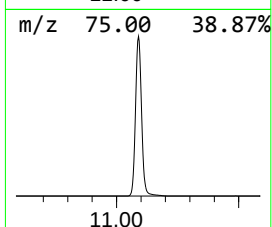
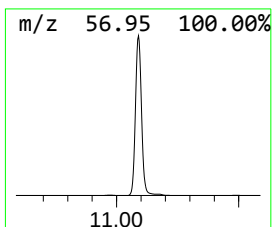
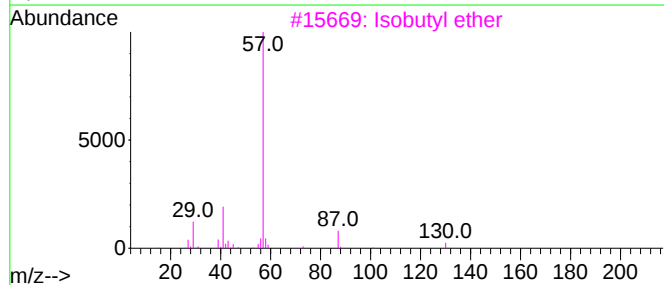
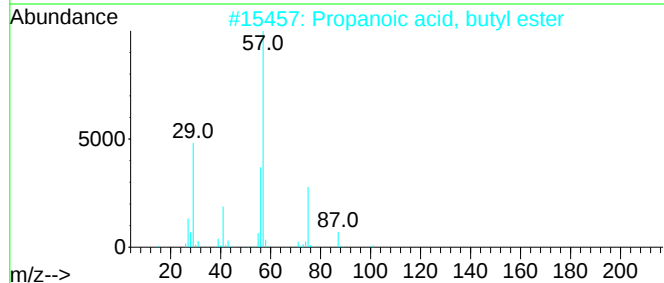
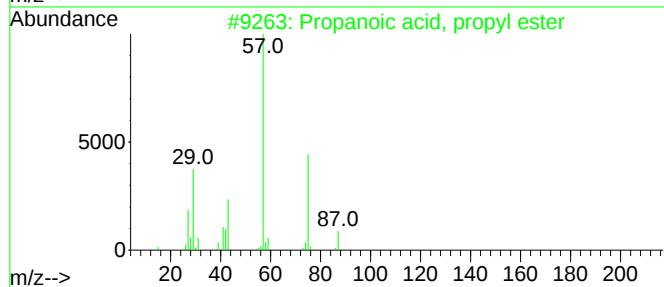
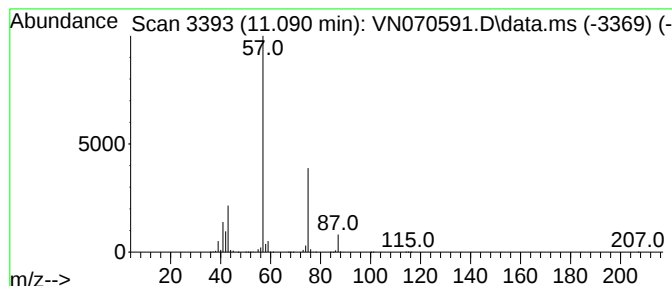
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.089	206.07 ug/l	16980600	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			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5			Azetidine	57	C3H7N	000503-29-7	4



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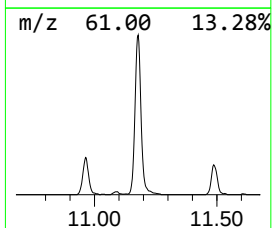
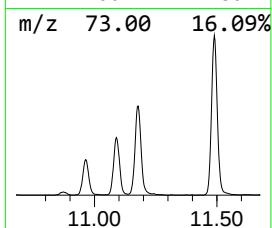
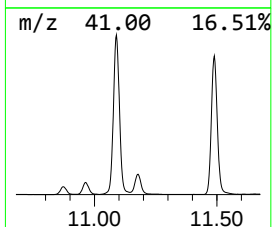
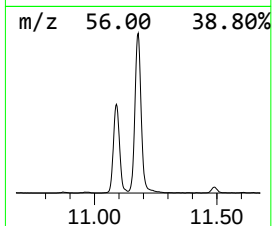
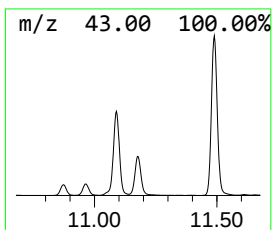
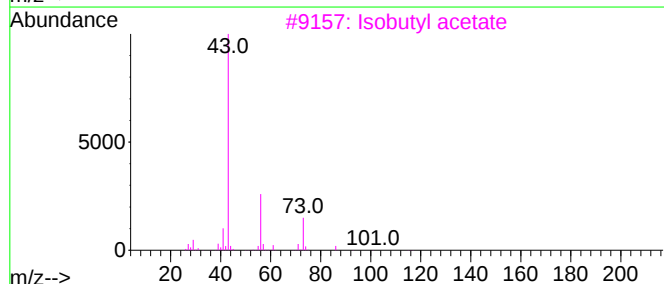
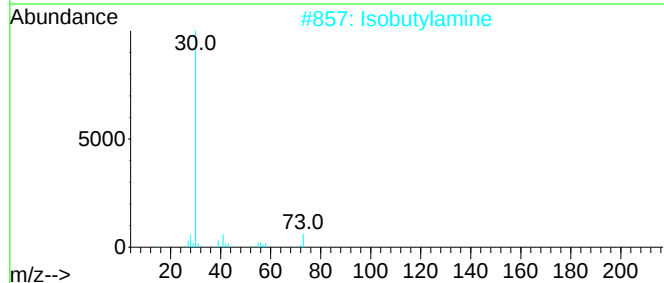
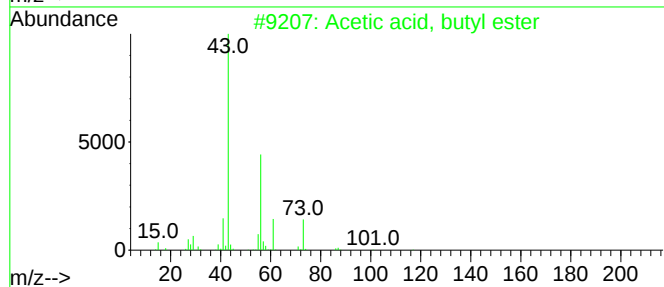
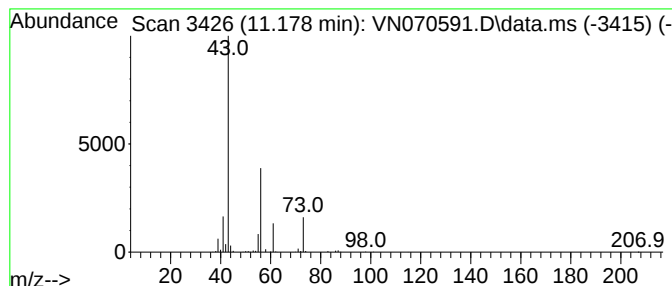
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Quant Title : SW846 8260

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.178	23.02 ug/l	1897250	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			2-Pentanone	86	C5H10O	000107-87-9	9
5			1-Butanamine	73	C4H11N	000109-73-9	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070591.D
Acq On : 12 Jan 2022 17:17
Operator : JC/MD
Sample : N1097-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3S

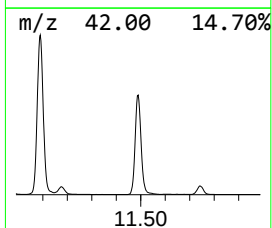
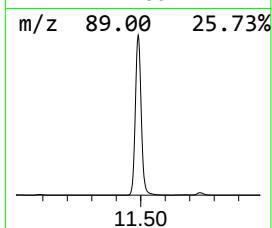
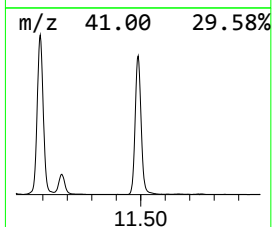
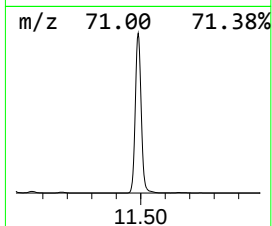
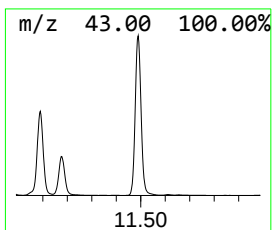
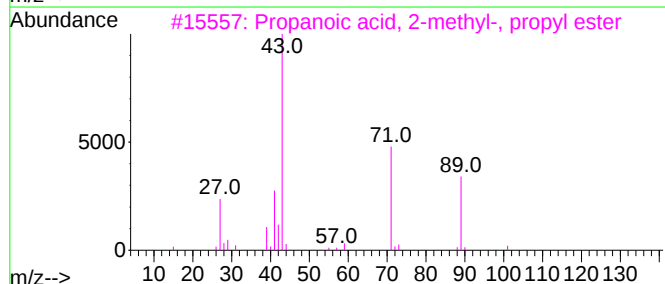
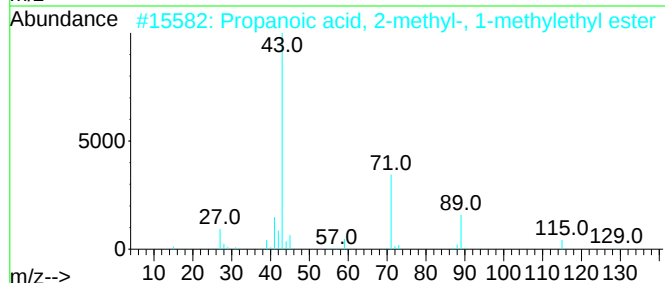
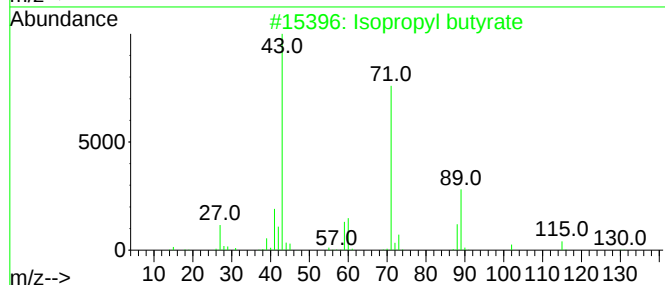
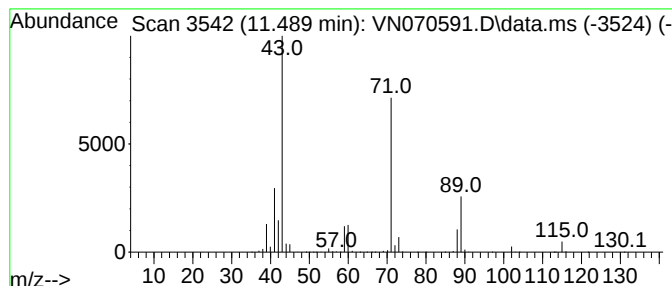
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Quant Title : SW846 8260

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	122.02 ug/l	10055000	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 : VN070591.D
Acq On : 12 Jan 2022 17:17
Operator : JC/MD
Sample : N1097-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3S

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	175.2	ug/l	12563200	2	8.965	3584640	50.0
Propanoic acid,...	10.242	25.4	ug/l	1819010	2	8.965	3584640	50.0
Propanoic acid,...	10.872	5.8	ug/l	475836	3	11.744	4120220	50.0
Butanoic acid, ...	10.964	13.8	ug/l	1138970	3	11.744	4120220	50.0
Propanoic acid,...	11.089	206.1	ug/l	16980600	3	11.744	4120220	50.0
Acetic acid, bu...	11.178	23.0	ug/l	1897250	3	11.744	4120220	50.0
Isopropyl butyrate	11.489	122.0	ug/l	10055000	3	11.744	4120220	50.0