

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
 Data File : VN070589.D
 Acq On : 12 Jan 2022 16:26
 Operator : JC/MD
 Sample : N1097-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-2S

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: VN070589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.242	82	94	101	rBV3	70007	150190	1.03%	0.236%
2	8.021	2226	2249	2260	rBV	561181	1369178	9.43%	2.154%
3	8.086	2260	2273	2299	rVB2	1058285	2438086	16.80%	3.835%
4	8.437	2382	2404	2434	rBV	712933	1643598	11.32%	2.585%
5	8.563	2436	2451	2463	rBV2	110233	256666	1.77%	0.404%
6	8.965	2583	2601	2638	rVB	1626730	3448128	23.76%	5.424%
7	9.547	2800	2818	2830	rBV3	107918	249511	1.72%	0.392%
8	9.622	2830	2846	2888	rVV	5864824	11033499	76.01%	17.355%
9	10.242	3060	3077	3098	rBV	983033	1734144	11.95%	2.728%
10	10.440	3134	3151	3180	rBV	2476810	4643897	31.99%	7.305%
11	10.612	3205	3215	3236	rVB	87814	162653	1.12%	0.256%
12	10.872	3297	3312	3331	rBV	264462	458593	3.16%	0.721%
13	10.963	3332	3346	3367	rVV	559813	980058	6.75%	1.542%
14	11.089	3369	3393	3414	rVV	8412668	14515232	100.00%	22.832%
15	11.178	3415	3426	3449	rVB	746252	1358923	9.36%	2.138%
16	11.489	3525	3542	3577	rBV	5443453	9186294	63.29%	14.450%
17	11.741	3620	3636	3666	rBV	2150908	3940774	27.15%	6.199%
18	12.194	3792	3805	3823	rBV2	118969	205733	1.42%	0.324%
19	12.731	3987	4005	4034	rBV	1700074	3017618	20.79%	4.747%
20	13.675	4339	4357	4376	rBV	1595944	2780893	19.16%	4.374%

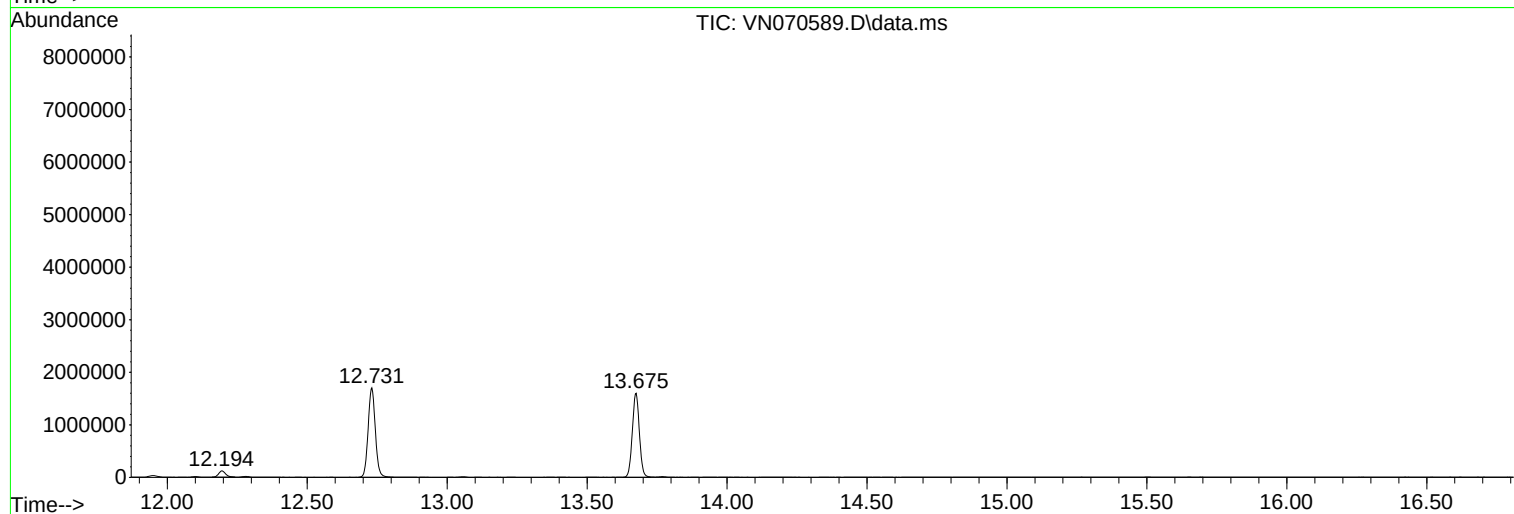
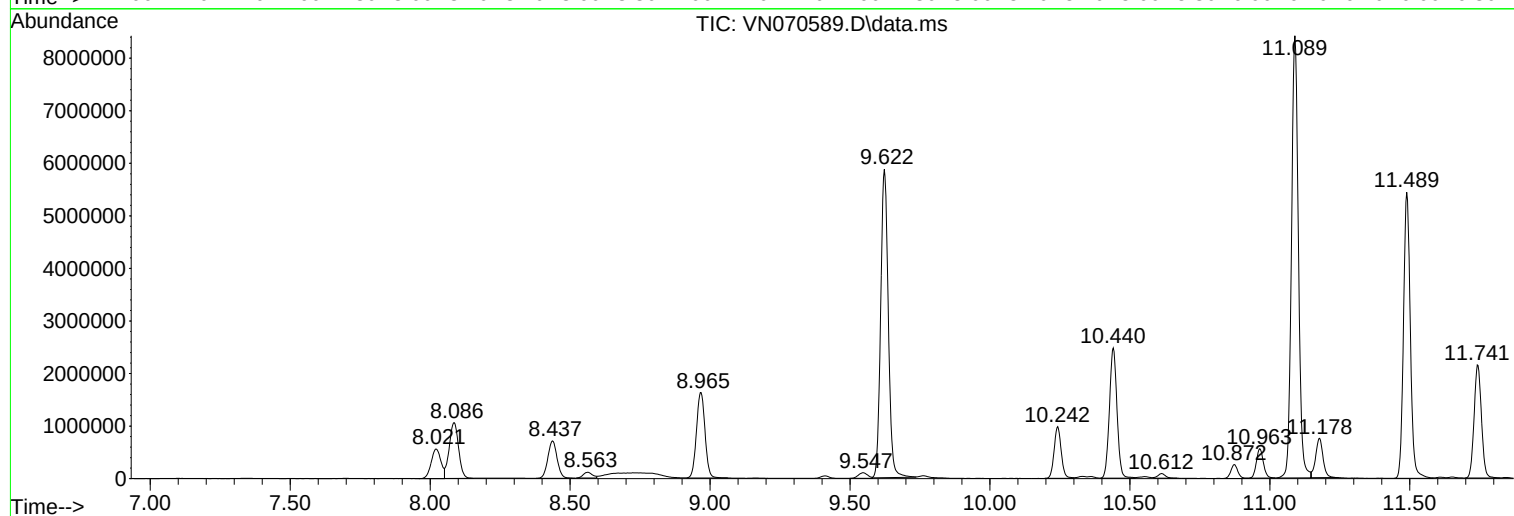
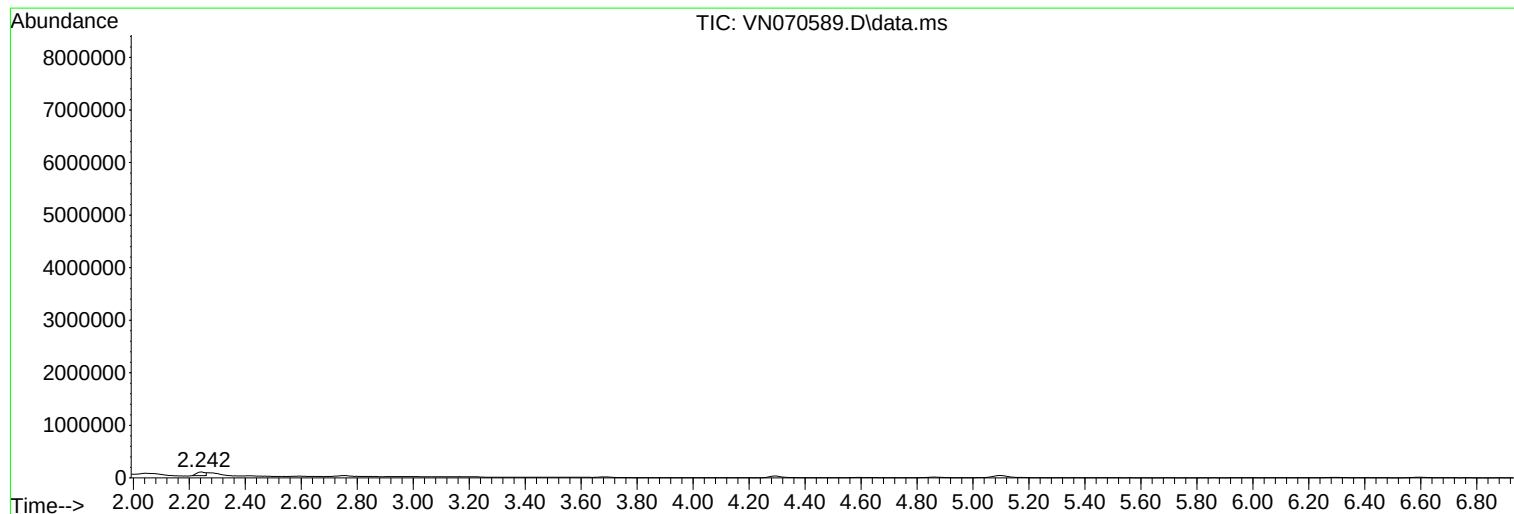
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Quant Title : SW846 8260

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



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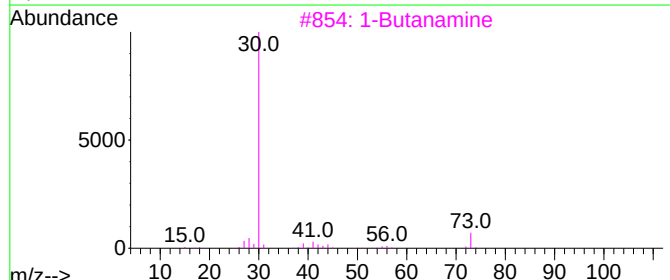
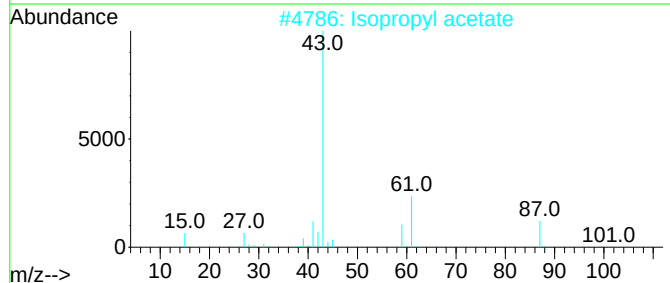
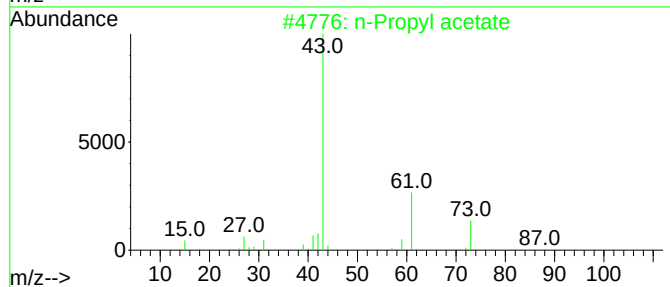
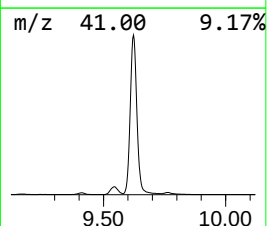
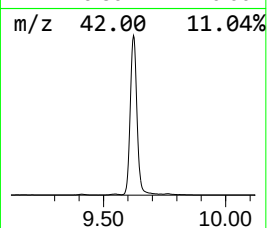
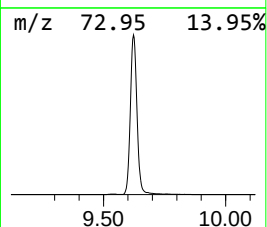
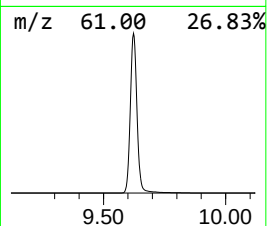
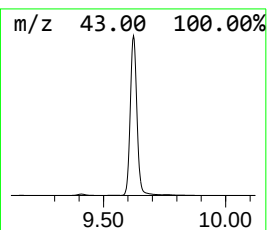
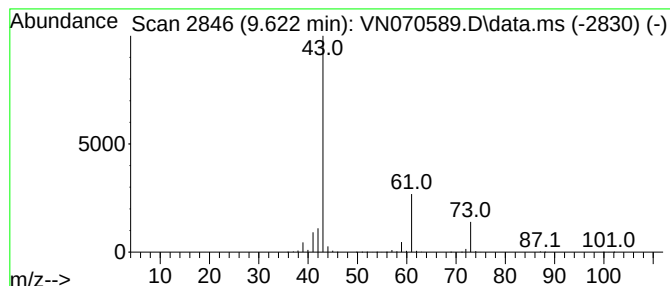
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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	159.99 ug/l	11033500	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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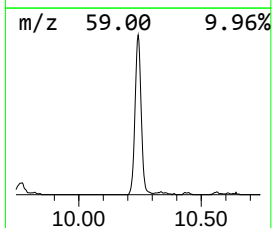
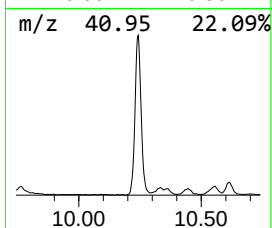
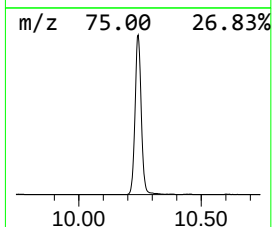
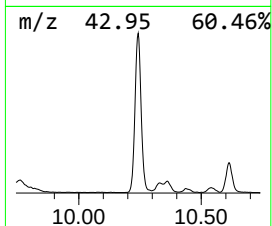
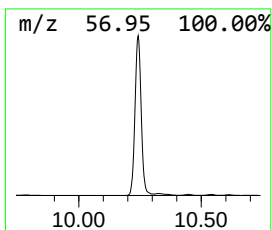
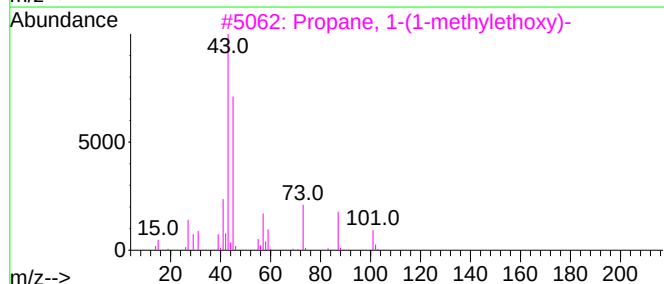
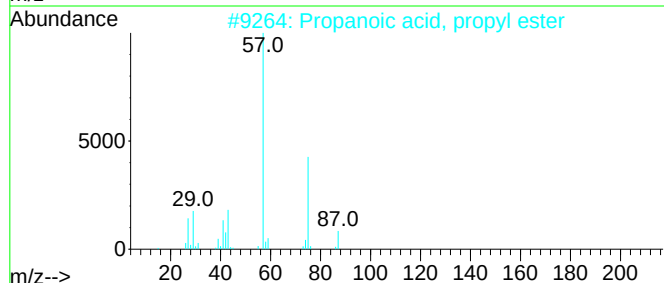
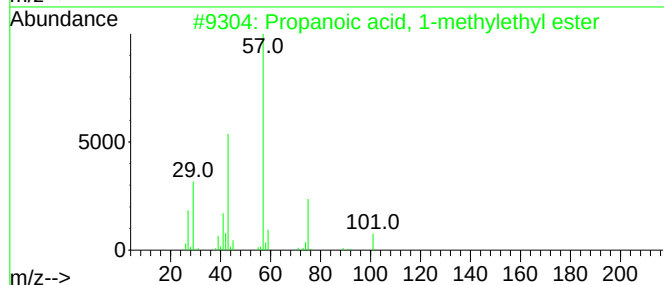
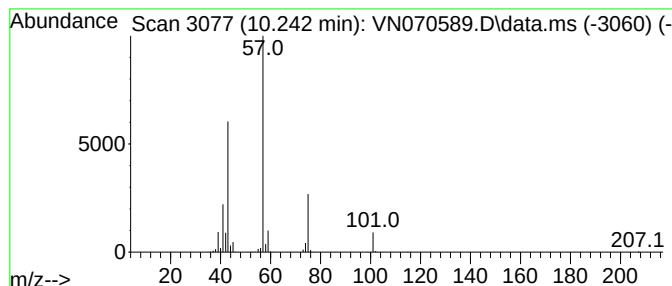
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Quant Title : SW846 8260

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	25.15 ug/l	1734140	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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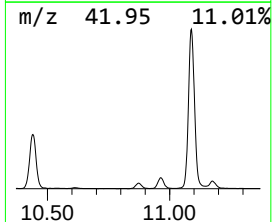
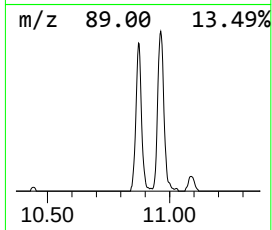
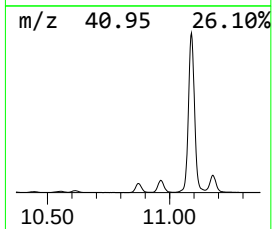
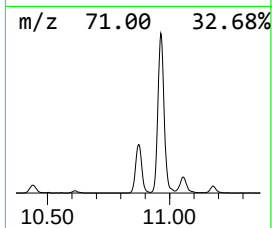
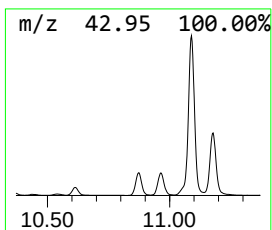
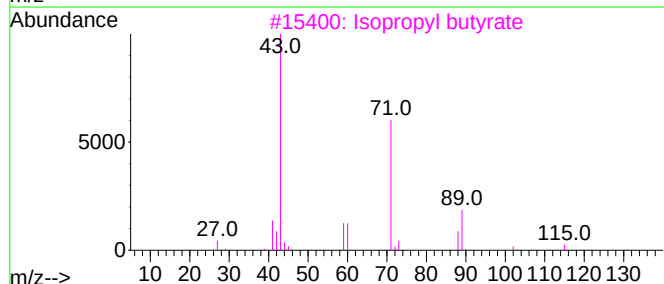
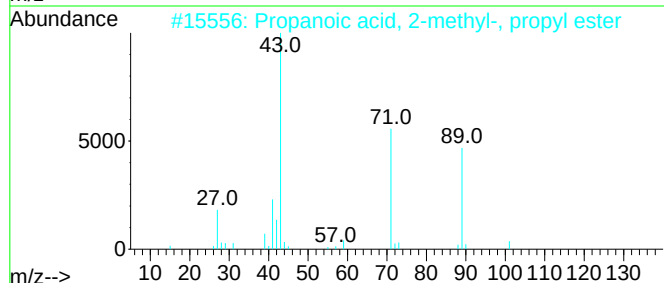
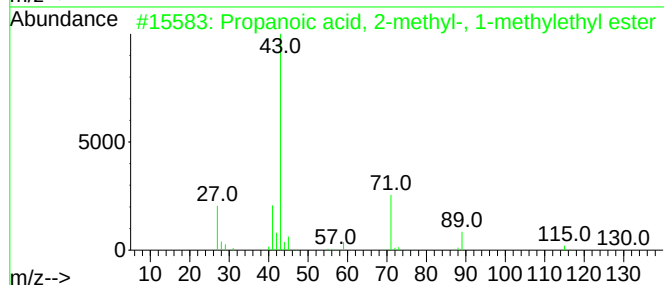
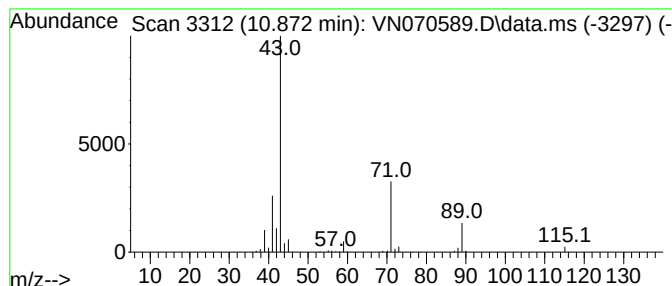
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.872	5.82 ug/l	458593	Chlorobenzene-d5	11.741

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			Isopropyl butyrate	130	C7H14O2	000638-11-9	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5			2,3-Hexanedione	114	C6H10O2	003848-24-6	42



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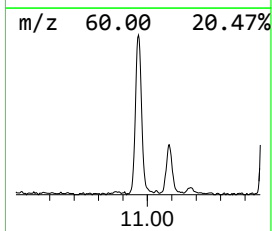
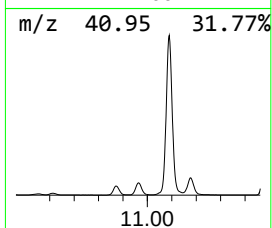
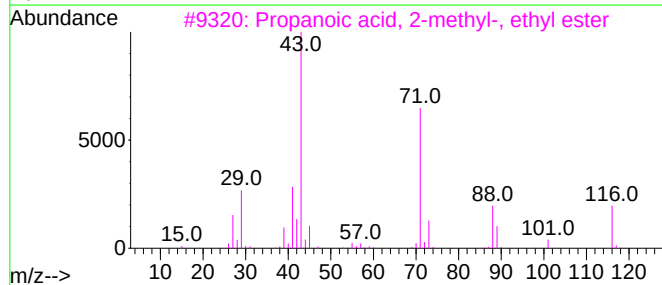
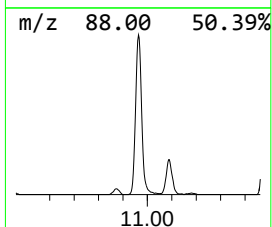
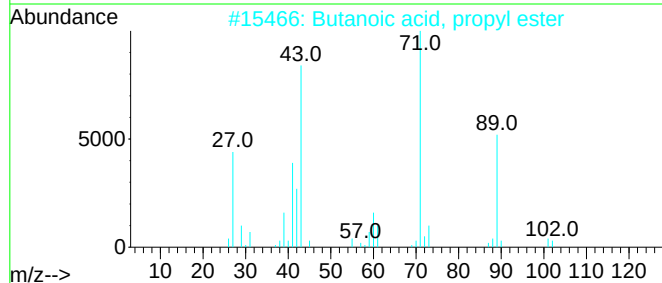
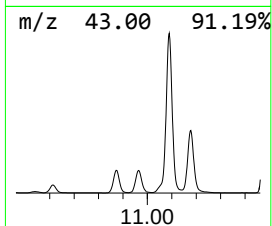
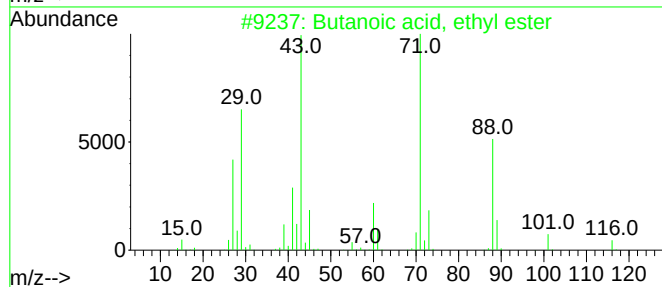
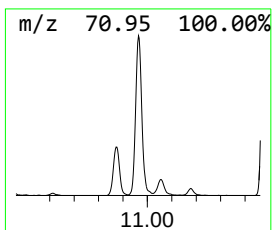
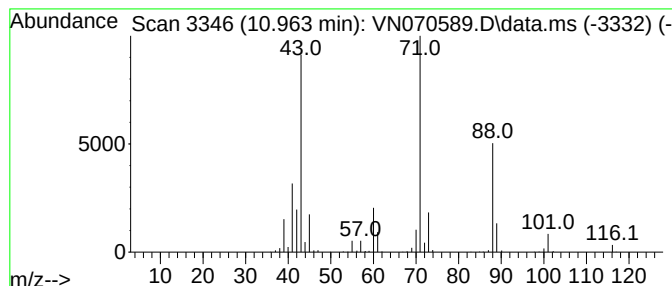
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Quant Title : SW846 8260

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Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.963	12.43 ug/l	980058	Chlorobenzene-d5	11.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
4			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	42



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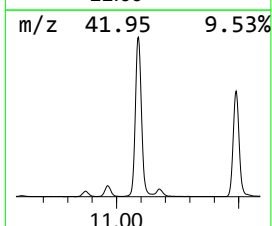
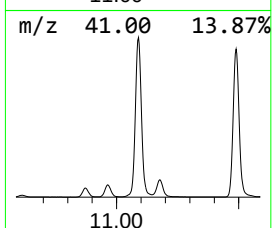
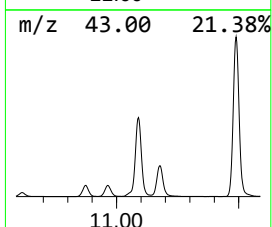
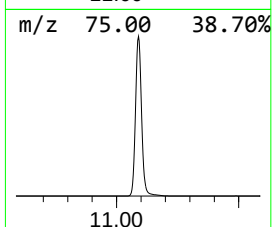
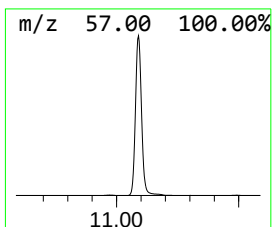
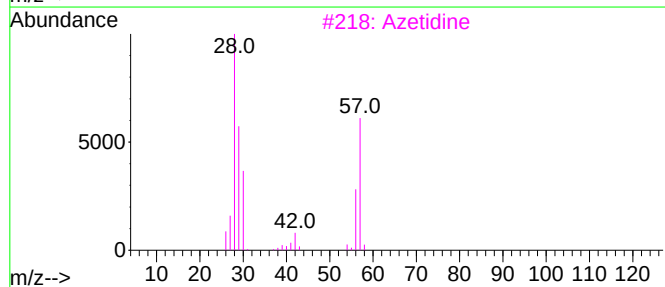
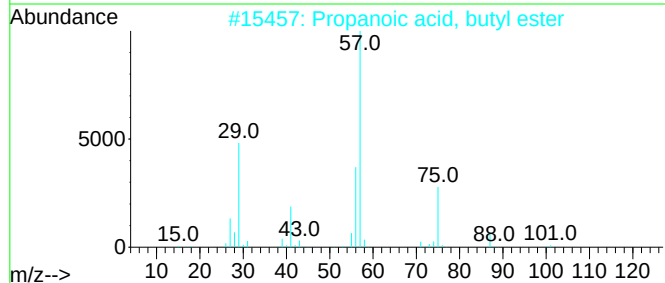
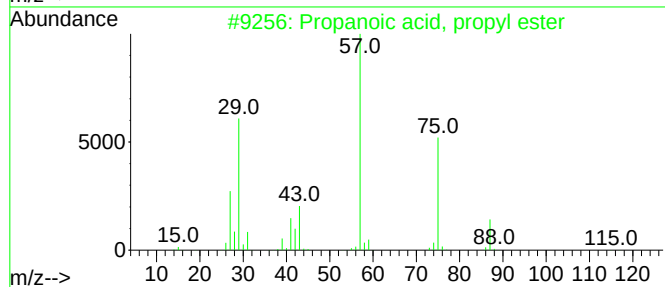
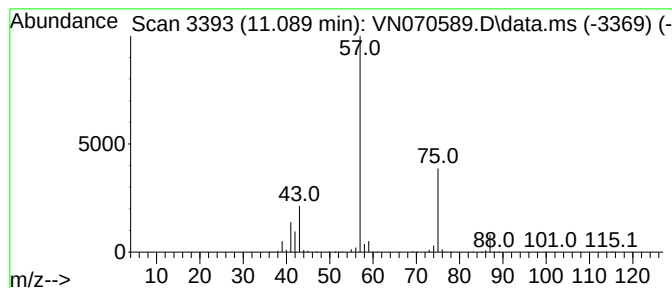
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.089	184.17 ug/l	14515200	Chlorobenzene-d5	11.741	
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	Azetidine	57	C3H7N	000503-29-7	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9



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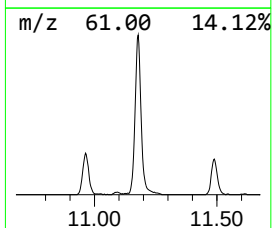
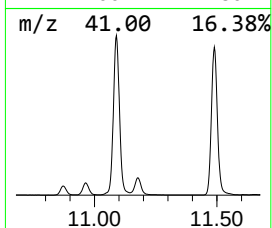
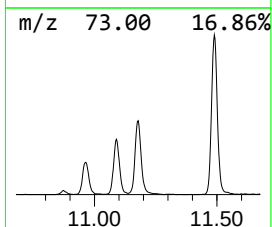
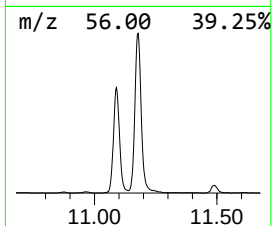
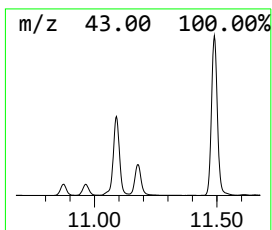
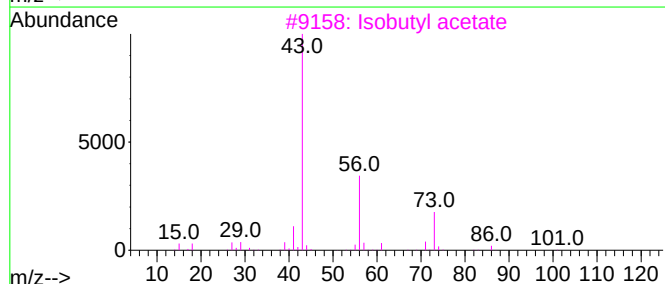
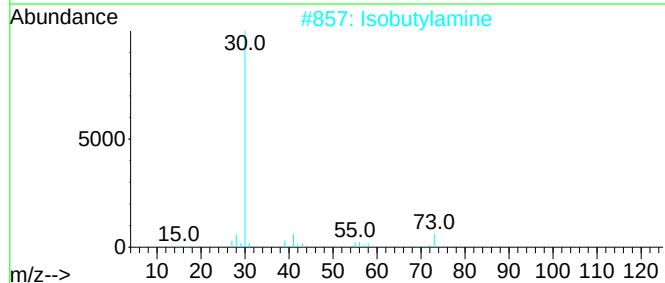
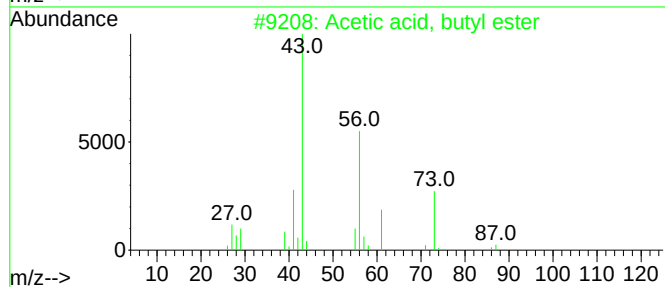
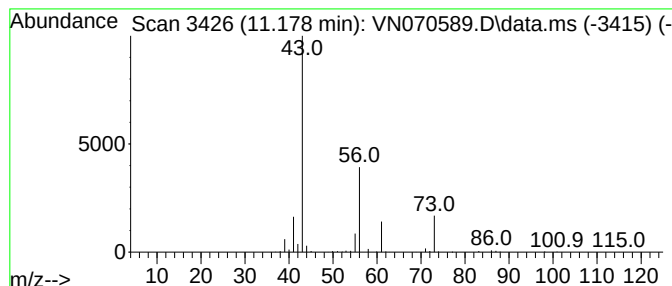
Instrument :
MSVOA_N
ClientSampleId :
TP-2S

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	17.24 ug/l	1358920	Chlorobenzene-d5		11.741	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	64
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	1-Butanol		74	C4H10O	000071-36-3	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070589.D
Acq On : 12 Jan 2022 16:26
Operator : JC/MD
Sample : N1097-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2S

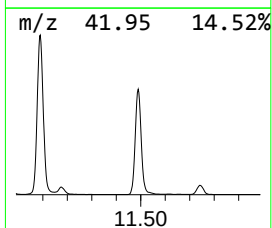
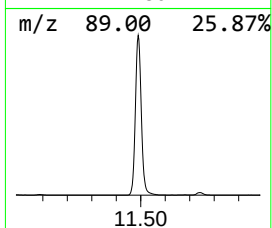
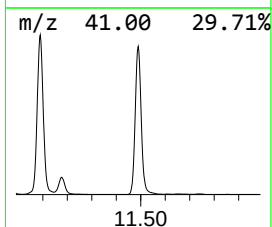
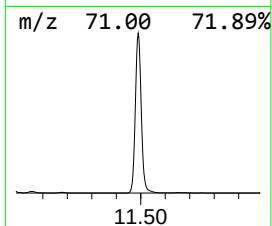
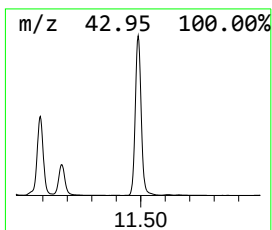
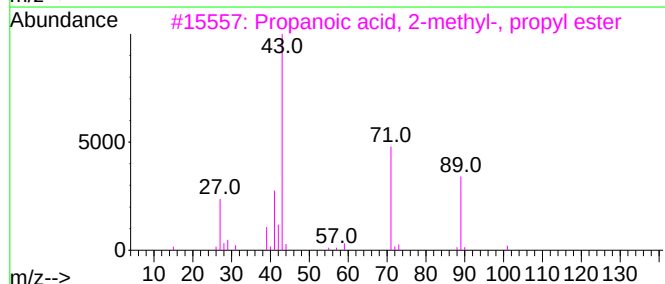
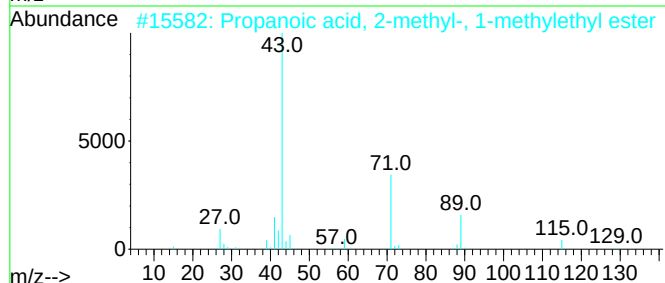
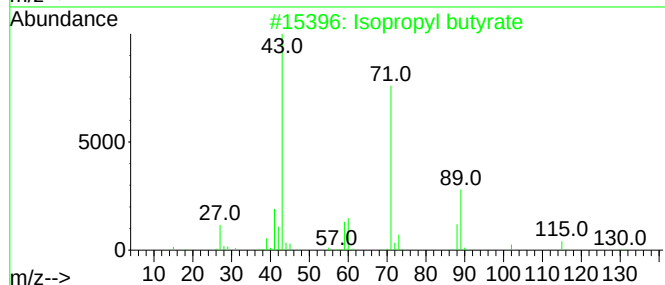
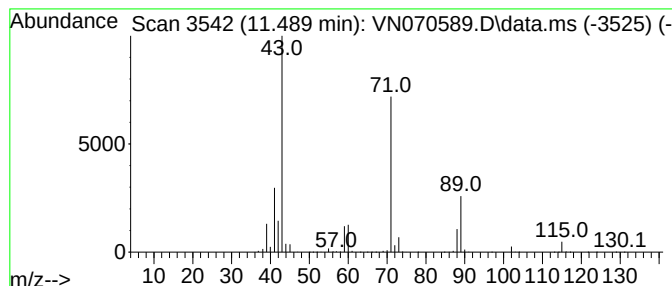
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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	116.55 ug/l	9186290	Chlorobenzene-d5	11.741

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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070589.D
Acq On : 12 Jan 2022 16:26
Operator : JC/MD
Sample : N1097-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2S

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	160.0	ug/l	11033500	2	8.968	3448130	50.0
Propanoic acid,...	10.242	25.1	ug/l	1734140	2	8.968	3448130	50.0
Propanoic acid,...	10.872	5.8	ug/l	458593	3	11.741	3940770	50.0
Butanoic acid, ...	10.963	12.4	ug/l	980058	3	11.741	3940770	50.0
Propanoic acid,...	11.089	184.2	ug/l	14515200	3	11.741	3940770	50.0
Acetic acid, bu...	11.178	17.2	ug/l	1358920	3	11.741	3940770	50.0
Isopropyl butyrate	11.489	116.6	ug/l	9186290	3	11.741	3940770	50.0