

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN042220\
 Data File : VN061146.D
 Acq On : 22 Apr 2020 22:33
 Operator : JC/MD
 Sample : L2359-08
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-1B-D

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.548	598	609	629	rBV2	11267	28905	1.69%	0.294%
2	6.503	1509	1528	1545	rBV3	9541	30860	1.81%	0.314%
3	7.313	1763	1780	1793	rBV	104509	264062	15.45%	2.685%
4	7.400	1793	1807	1830	rVB	220898	524930	30.71%	5.337%
5	7.767	1905	1921	1940	rBV	138545	314905	18.42%	3.202%
6	7.918	1953	1968	1985	rBV	45713	99227	5.81%	1.009%
7	8.349	2087	2102	2127	rBV	348408	710797	41.58%	7.227%
8	8.969	2278	2295	2306	rBV	22526	43850	2.57%	0.446%
9	9.056	2306	2322	2347	rBV	965715	1709323	100.00%	17.380%
10	9.705	2510	2524	2537	rBV	132275	224518	13.13%	2.283%
11	9.882	2566	2579	2599	rVB	586268	1023075	59.85%	10.402%
12	10.085	2630	2642	2655	rVB	42993	71171	4.16%	0.724%
13	10.352	2712	2725	2739	rBV	251763	406211	23.76%	4.130%
14	10.445	2743	2754	2767	rVB	43502	67904	3.97%	0.690%
15	10.525	2767	2779	2785	rBV	64044	106446	6.23%	1.082%
16	10.574	2785	2794	2810	rVV	402444	623205	36.46%	6.337%
17	10.664	2812	2822	2831	rVB2	23487	37774	2.21%	0.384%
18	10.982	2906	2921	2937	rBV	558855	852515	49.87%	8.668%
19	11.210	2977	2992	3013	rVB	556563	918816	53.75%	9.342%
20	11.590	3099	3110	3122	rBV2	14010	21723	1.27%	0.221%
21	11.693	3132	3142	3156	rBV	76618	115698	6.77%	1.176%
22	12.213	3290	3304	3322	rBV	454983	718908	42.06%	7.310%
23	13.152	3584	3596	3614	rBV	596071	920223	53.84%	9.357%

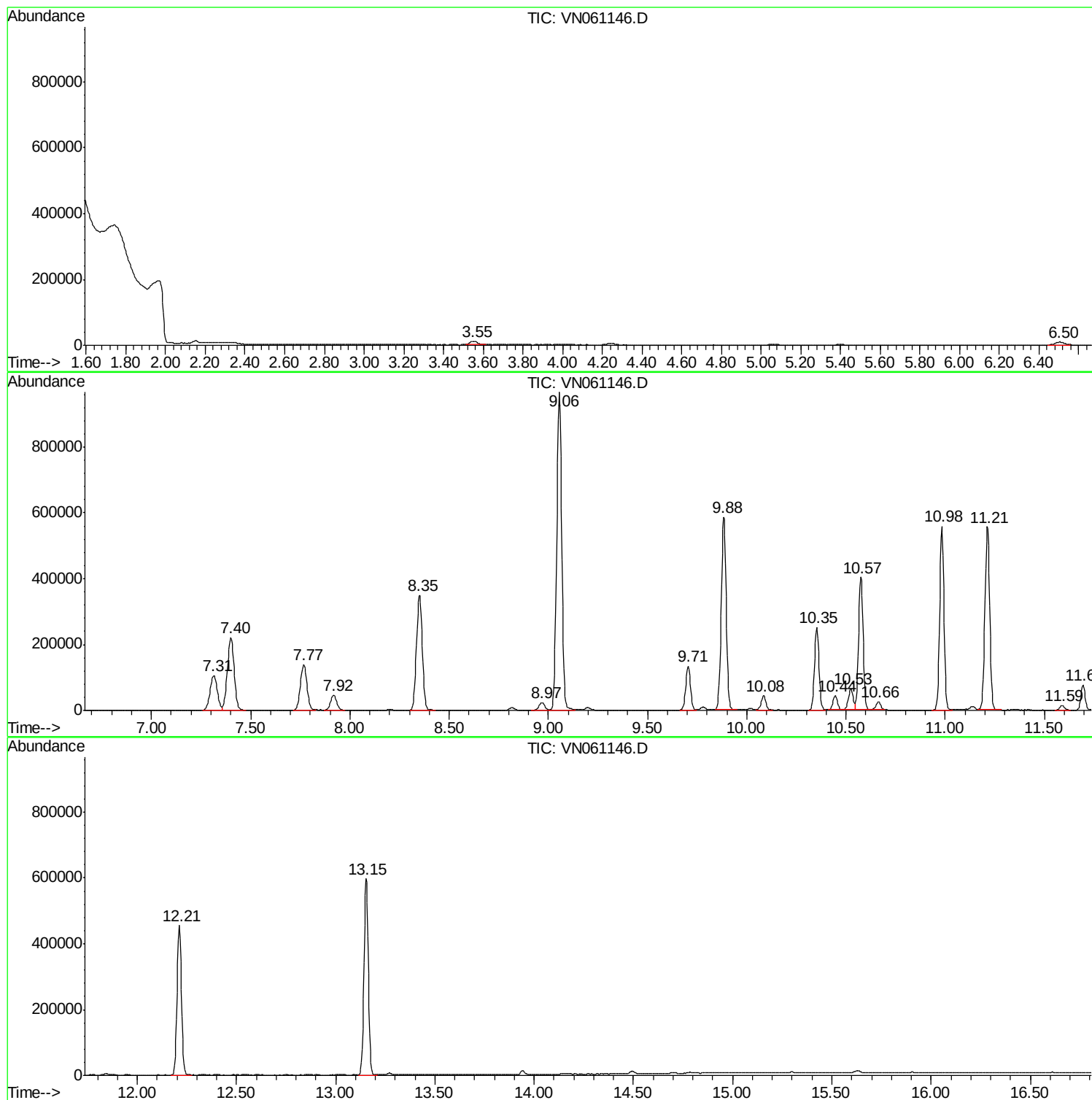
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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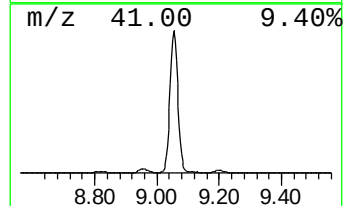
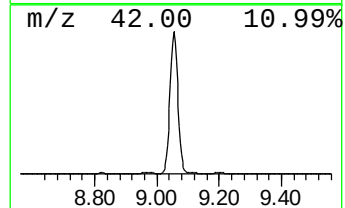
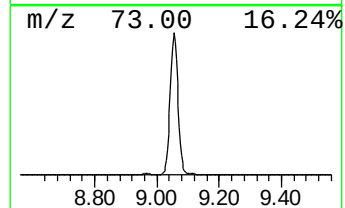
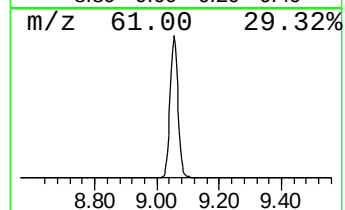
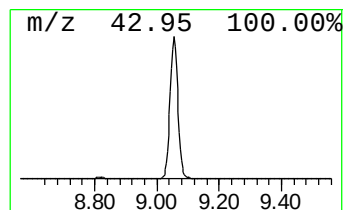
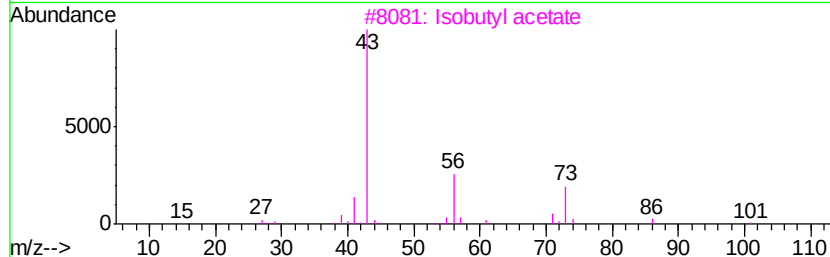
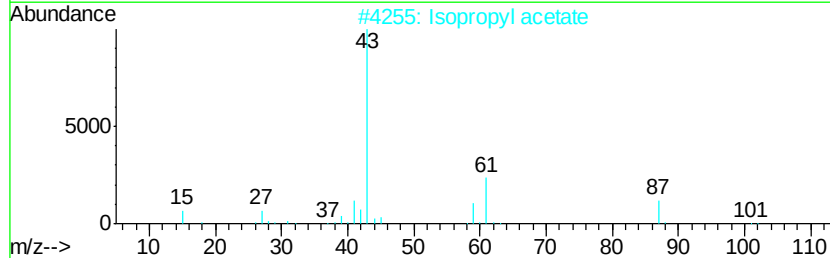
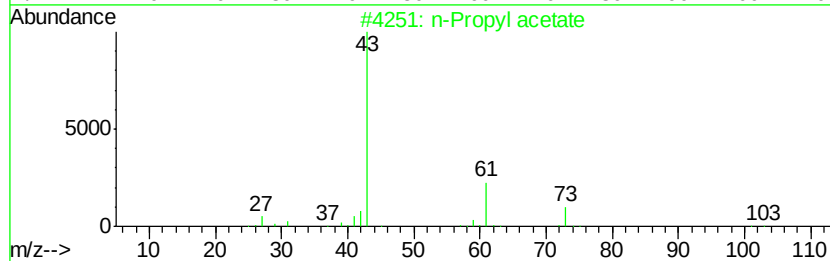
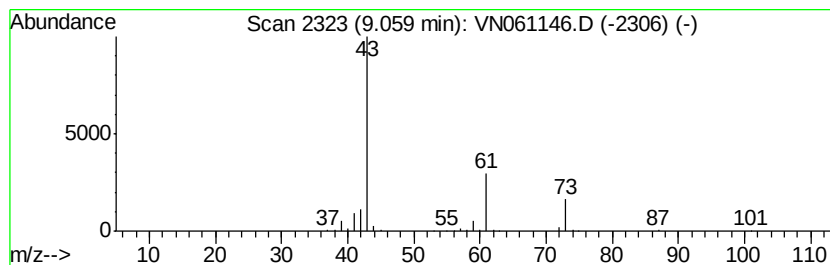
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	120.24 ug/l	1709320	1,4-Difluorobenzene	8.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Butane, 2-methyl-	72	C5H12	000078-78-4	4



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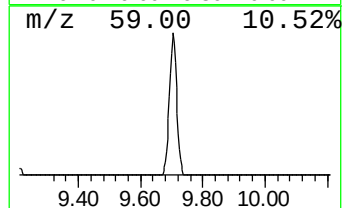
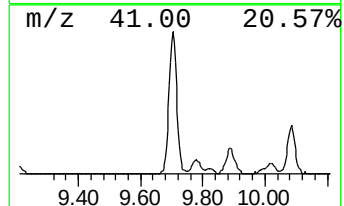
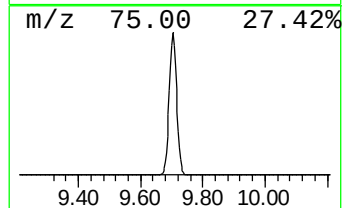
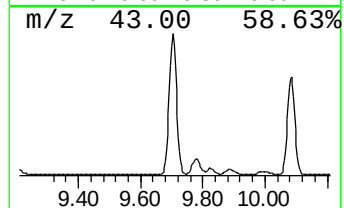
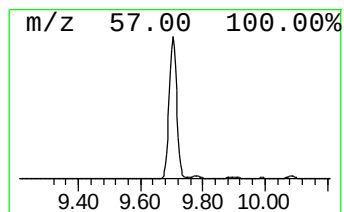
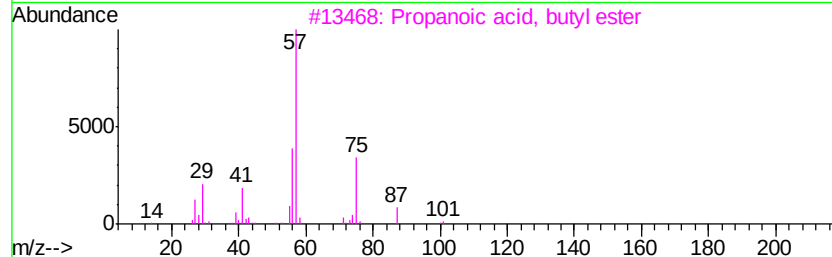
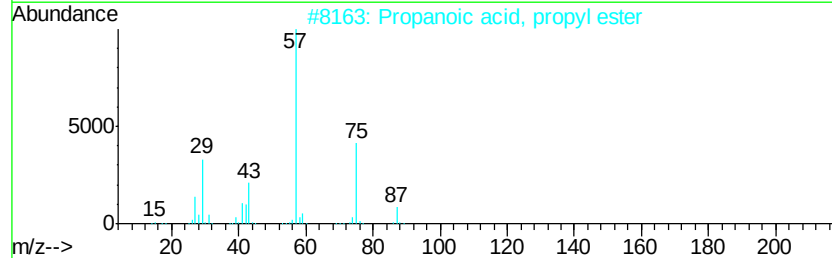
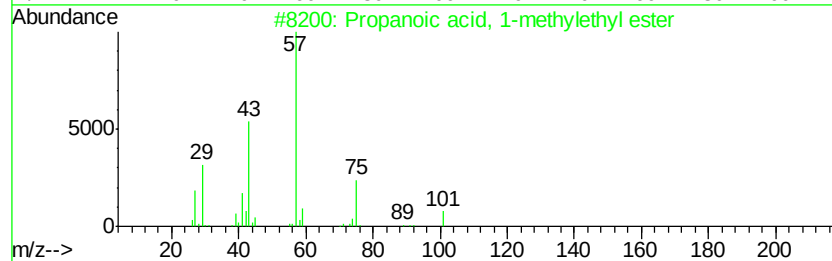
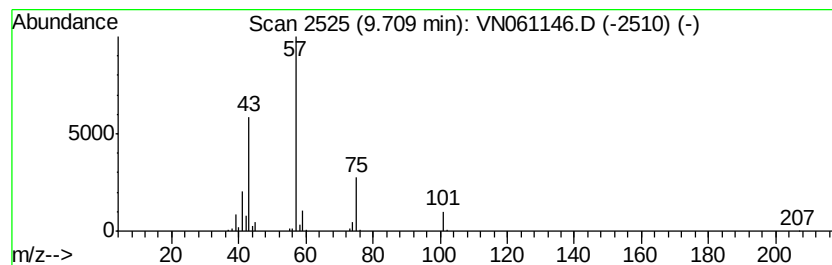
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.71	15.79 ug/l	224518	1,4-Difluorobenzene	8.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40
3		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5		Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10



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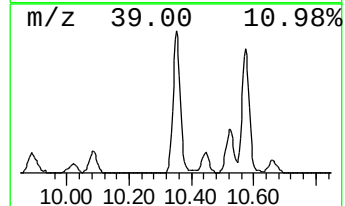
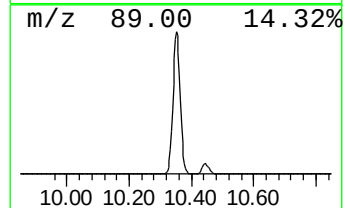
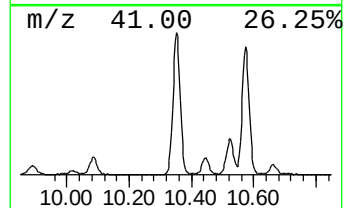
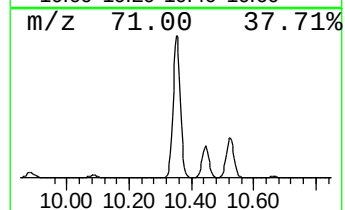
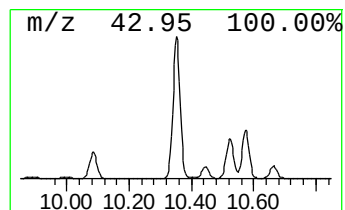
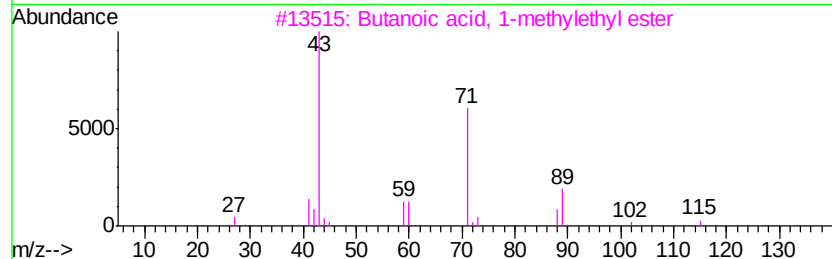
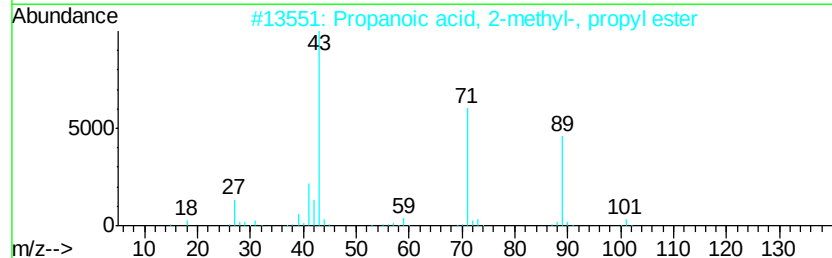
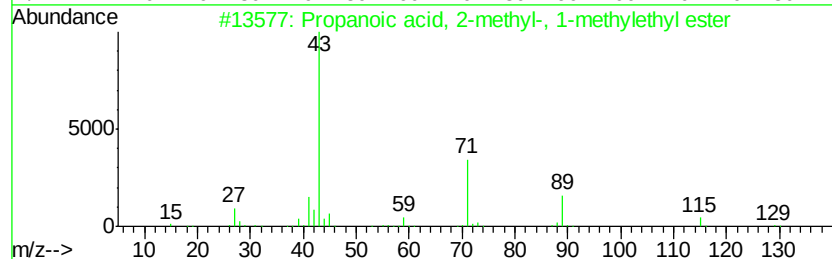
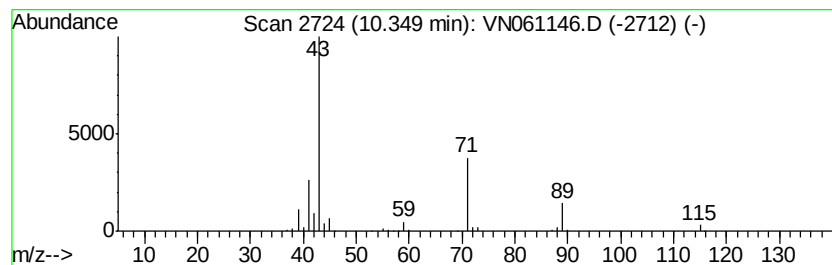
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ClientSampled :
TP-1B-D

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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.35	22.11 ug/l	406211	Chlorobenzene-d5	11.21		
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		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
4		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38
5		Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	36



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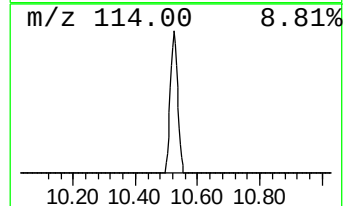
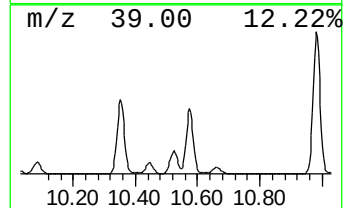
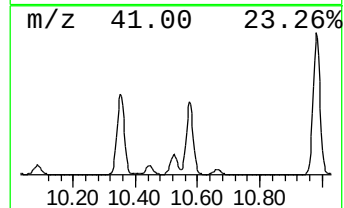
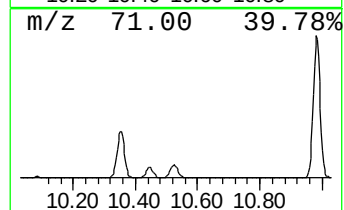
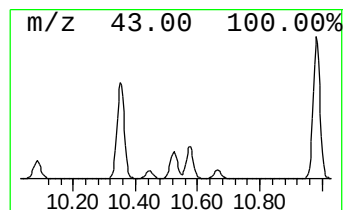
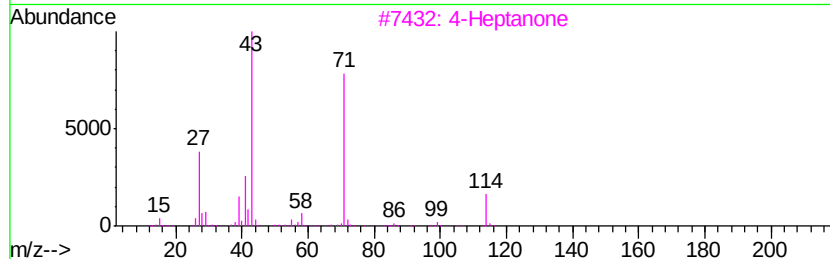
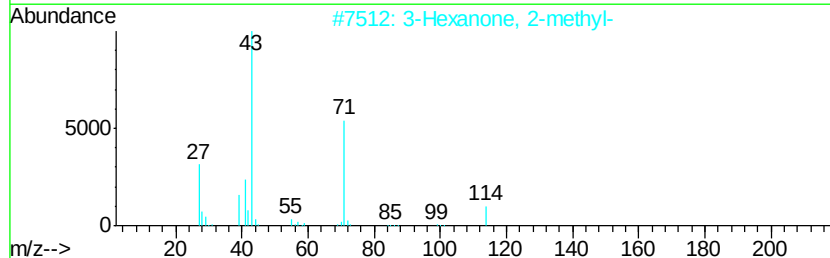
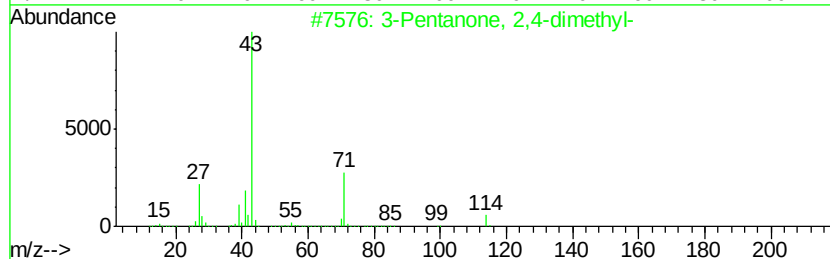
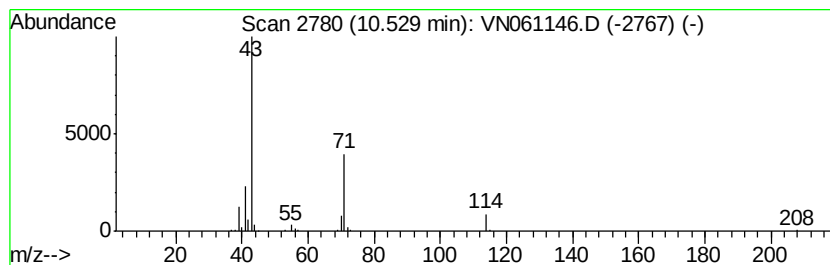
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Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	5.79 ug/l	106446	Chlorobenzene-d5	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
3		4-Heptanone	114	C7H14O	000123-19-3	59
4		2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5		Pyrrolidine	71	C4H9N	000123-75-1	45



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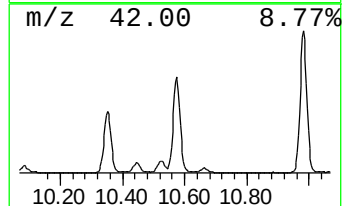
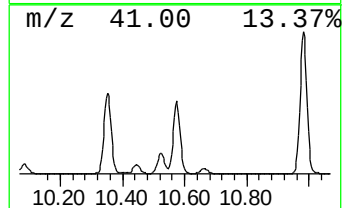
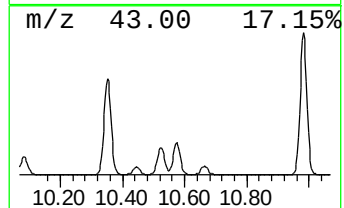
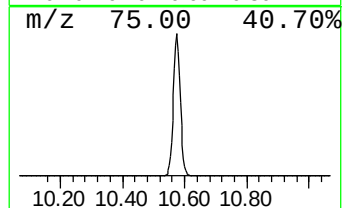
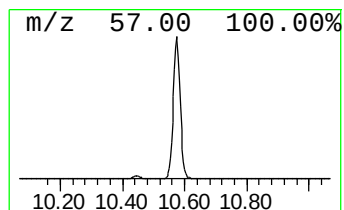
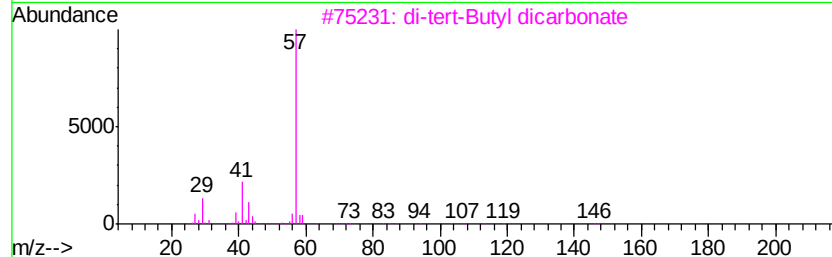
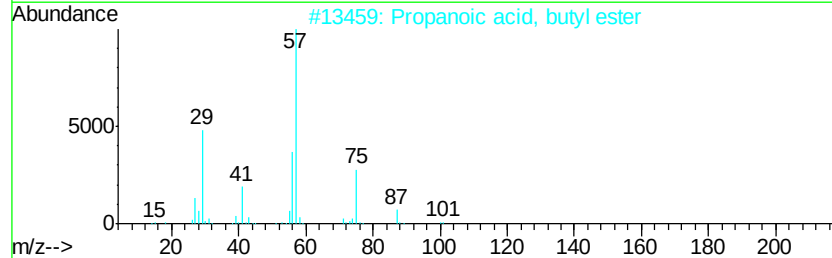
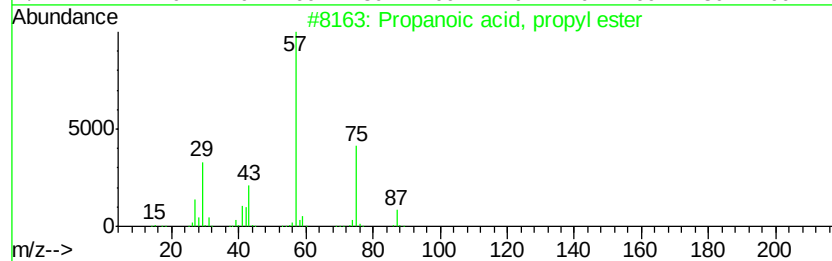
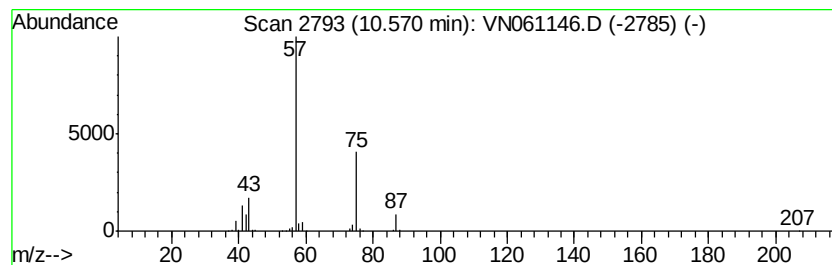
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	33.91 ug/l	623205	Chlorobenzene-d5	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
4		1-Penten-3-ol	86	C5H10O	000616-25-1	7
5		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



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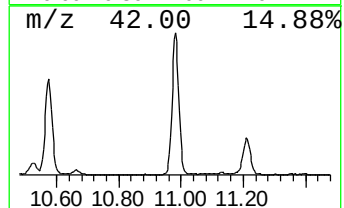
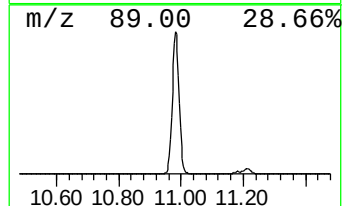
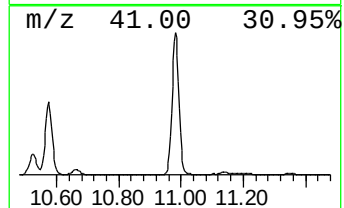
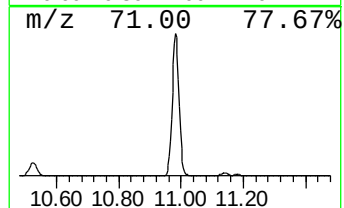
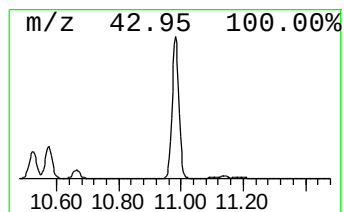
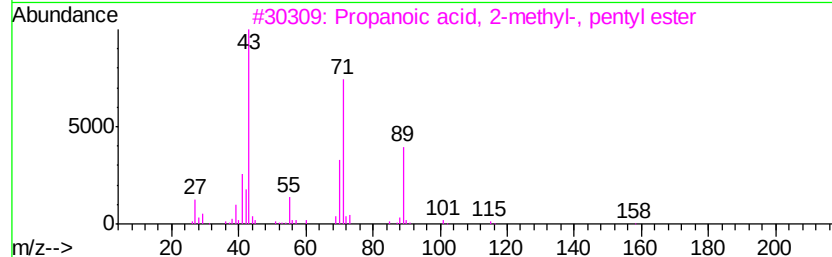
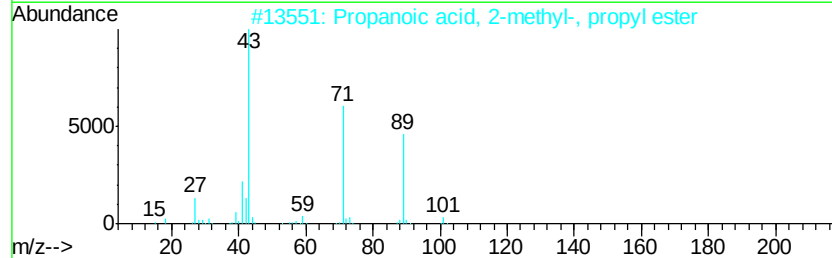
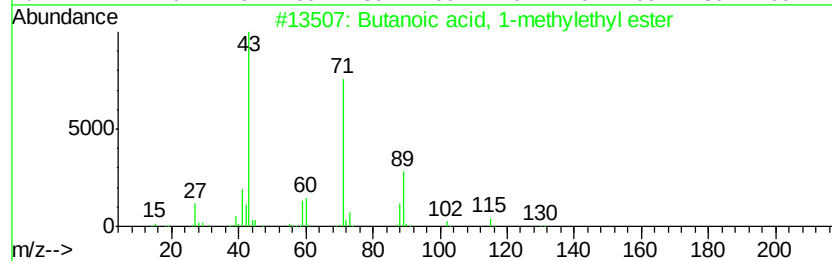
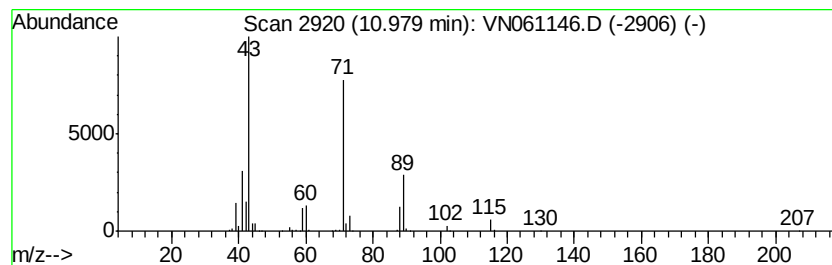
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MSVOA_N
ClientSampleId :
TP-1B-D

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.98	46.39 ug/l	852515	Chlorobenzene-d5	11.21		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
3		Propanoic acid, 2-methyl-, pentyl ester	158	C9H18O2	002445-72-9	64
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN042220\
Data File : VN061146.D
Acq On : 22 Apr 2020 22:33
Operator : JC/MD
Sample : L2359-08
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1B-D

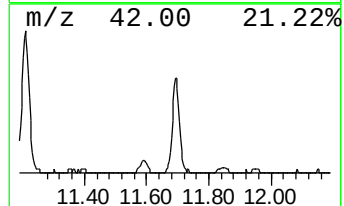
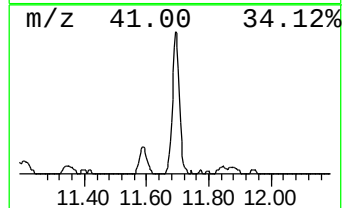
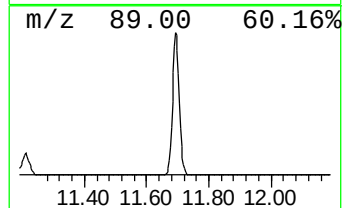
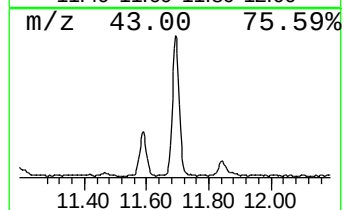
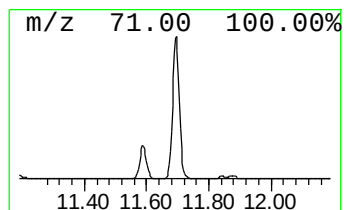
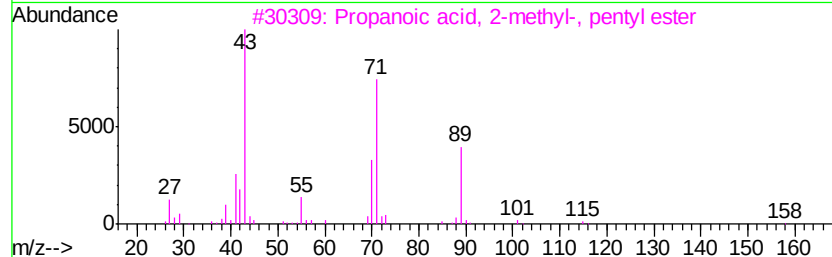
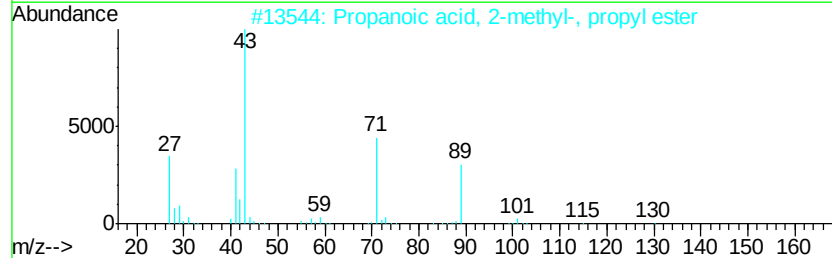
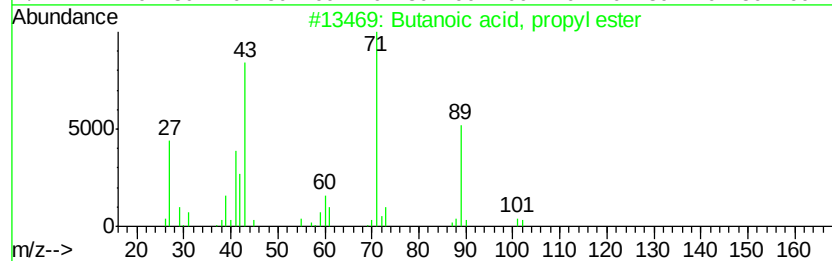
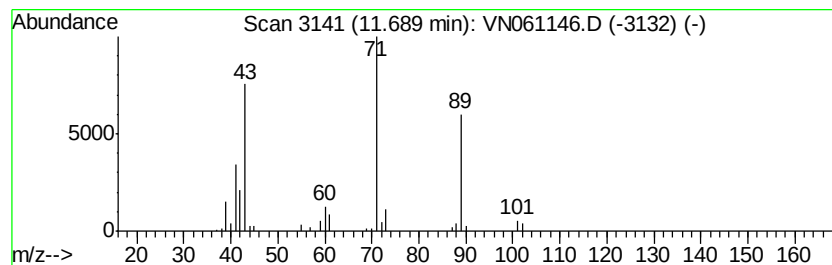
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Butanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	6.30 ug/l	115698	Chlorobenzene-d5	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	91
2		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	78
3		Propanoic acid, 2-methyl-, pentyl ester	158	C9H18O2	002445-72-9	64
4		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061146.D
Acq On : 22 Apr 2020 22:33
Operator : JC/MD
Sample : L2359-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1B-D

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.06	120.2	ug/l	1709320	2	8.35	710797	50.0
Propanoic acid, 1...	9.71	15.8	ug/l	224518	2	8.35	710797	50.0
Propanoic acid, 2...	10.35	22.1	ug/l	406211	3	11.21	918816	50.0
3-Pentanone, 2,4-...	10.53	5.8	ug/l	106446	3	11.21	918816	50.0
Propanoic acid, p...	10.57	33.9	ug/l	623205	3	11.21	918816	50.0
Butanoic acid, 1-...	10.98	46.4	ug/l	852515	3	11.21	918816	50.0
Butanoic acid, pr...	11.69	6.3	ug/l	115698	3	11.21	918816	50.0