

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
 Data File : VN077333.D
 Acq On : 13 Apr 2023 17:03
 Operator : JC\MD
 Sample : PB152070ZHE#05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB152070ZHE#05

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\82N040523W.M
 Title : SW846 8260

Signal : TIC: VN077333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.831	144	152	162	rBV5	50175	164424	2.33%	0.371%
2	3.972	336	346	356	rBV4	29466	84017	1.19%	0.190%
3	4.443	416	426	435	rBV	35684	111345	1.58%	0.251%
4	5.284	556	569	584	rBV3	119771	416439	5.91%	0.939%
5	6.472	760	771	784	rBV5	34177	108734	1.54%	0.245%
6	7.572	951	958	972	rVB2	62129	159773	2.27%	0.360%
7	8.172	1050	1060	1065	rBV	441953	1048643	14.88%	2.365%
8	8.231	1065	1070	1083	rVB	794944	1721995	24.43%	3.884%
9	8.584	1119	1130	1140	rBV	438747	1011942	14.35%	2.282%
10	8.695	1140	1149	1160	rBV	409131	1065406	15.11%	2.403%
11	9.107	1209	1219	1236	rBV	1156145	2361668	33.50%	5.327%
12	9.678	1307	1316	1321	rBV	188663	406246	5.76%	0.916%
13	9.748	1321	1328	1342	rVV	3920505	7049621	100.00%	15.900%
14	10.366	1423	1433	1442	rBV	826241	1460351	20.72%	3.294%
15	10.448	1442	1447	1459	rVB5	31526	89630	1.27%	0.202%
16	10.572	1459	1468	1478	rBV	1897856	3454057	49.00%	7.791%
17	10.730	1488	1495	1509	rVB	1079615	1831880	25.99%	4.132%
18	10.989	1531	1539	1549	rBV	1120528	1882875	26.71%	4.247%
19	11.083	1549	1555	1564	rVV3	238986	438071	6.21%	0.988%
20	11.207	1564	1576	1584	rVV2	1915698	3828371	54.31%	8.635%
21	11.295	1584	1591	1602	rVB	1222983	2031755	28.82%	4.583%
22	11.607	1634	1644	1655	rBV	3532272	5684869	80.64%	12.822%
23	11.772	1667	1672	1681	rVB4	57653	104642	1.48%	0.236%
24	11.872	1681	1689	1700	rVV	1655111	2946213	41.79%	6.645%
25	11.966	1700	1705	1713	rVB2	45269	85378	1.21%	0.193%
26	12.219	1741	1748	1755	rBV	47480	80175	1.14%	0.181%
27	12.307	1755	1763	1771	rBV	311334	509349	7.23%	1.149%
28	12.854	1847	1856	1867	rBV	1156608	1997183	28.33%	4.505%
29	13.795	2007	2016	2026	rBV	1252607	2200886	31.22%	4.964%

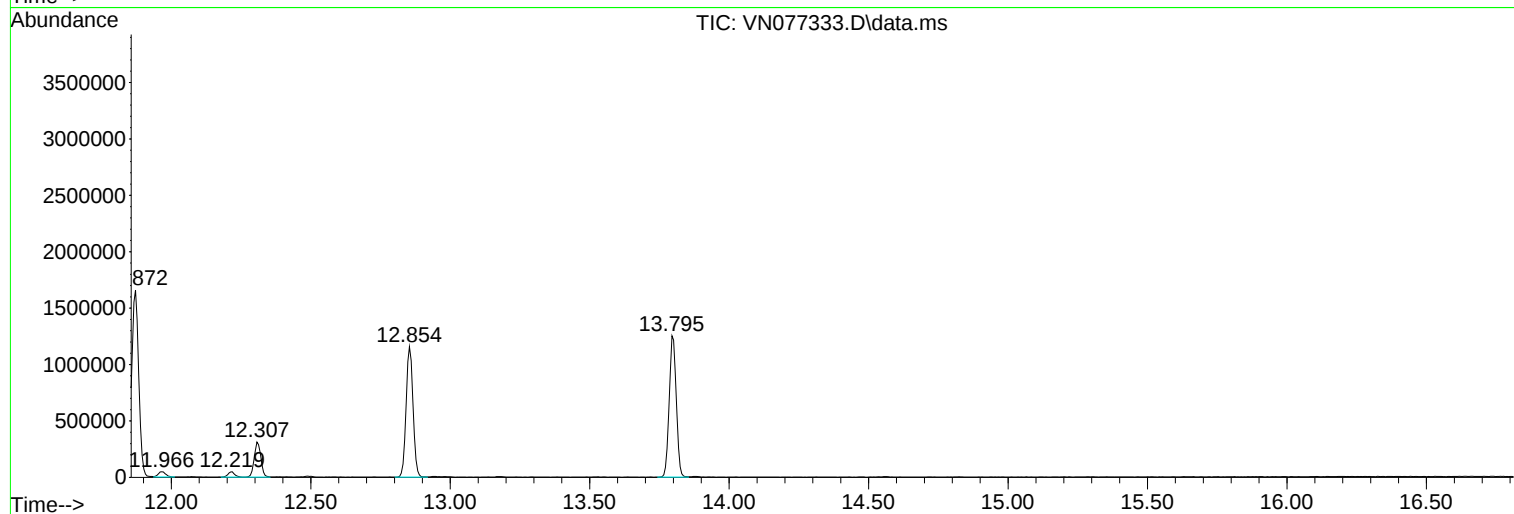
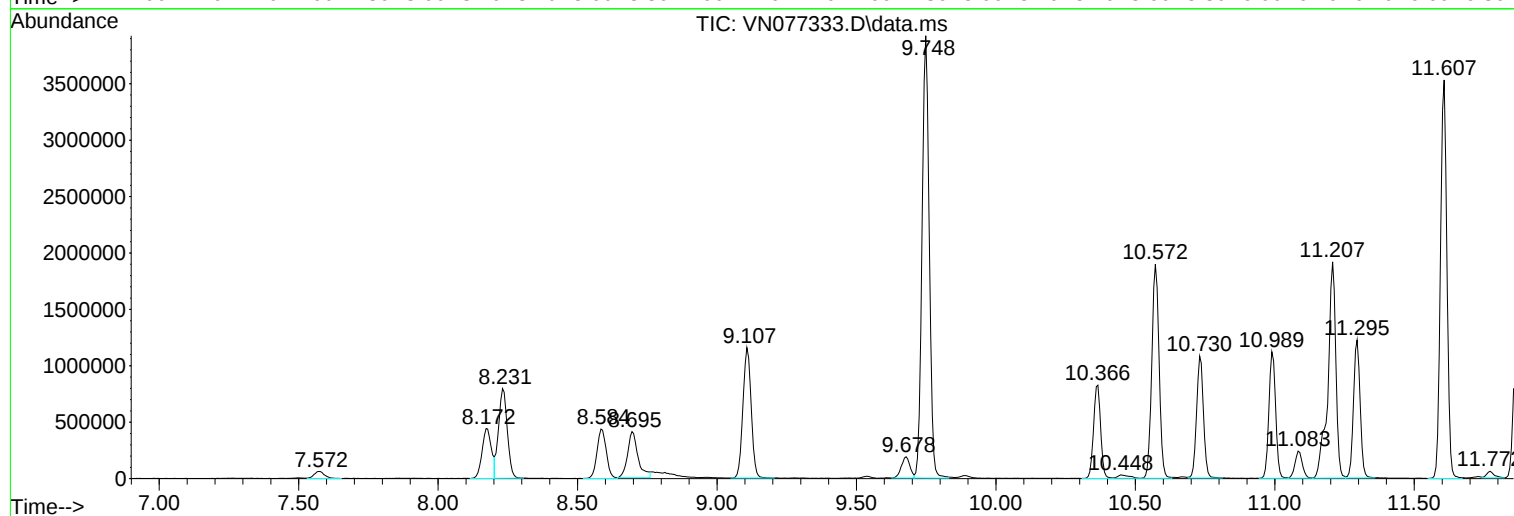
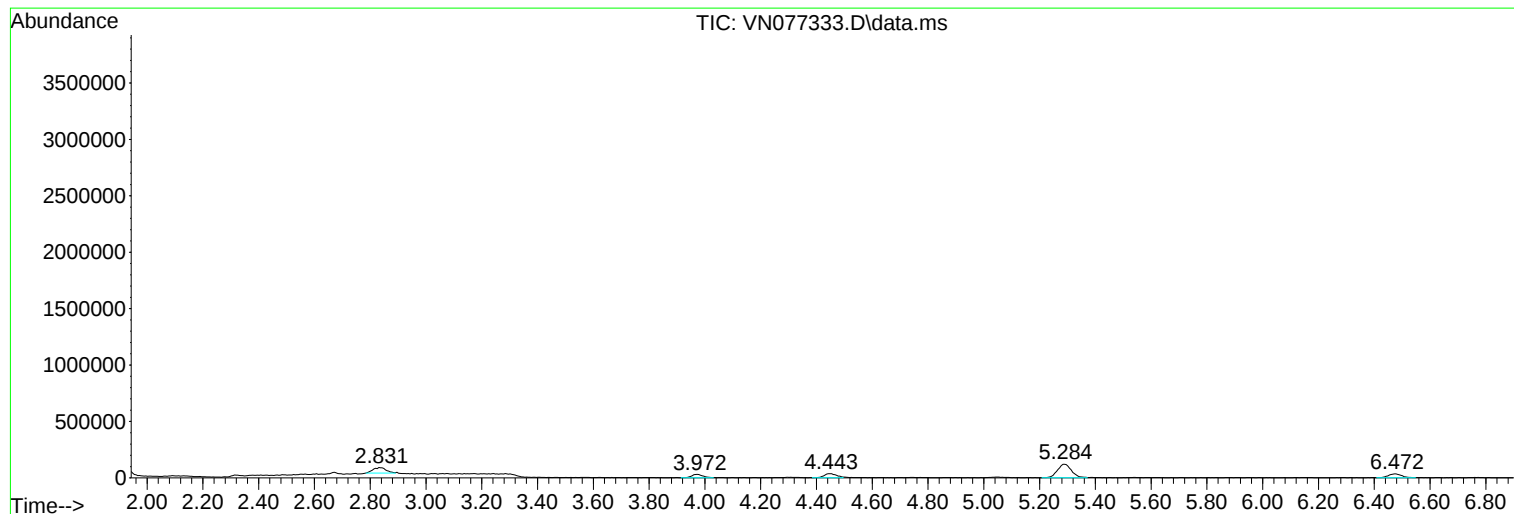
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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
PB152070ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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



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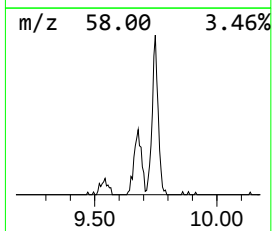
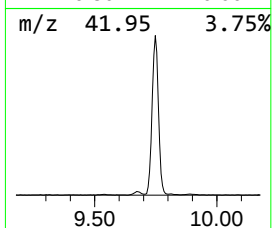
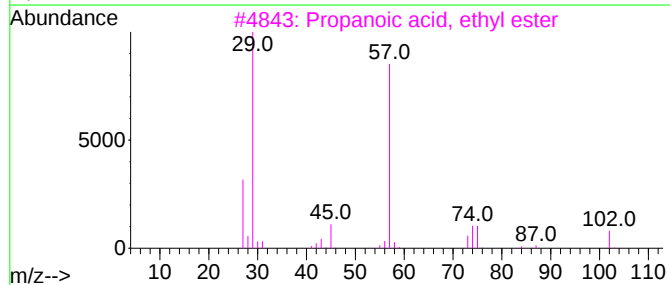
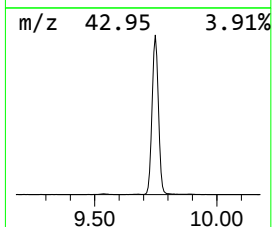
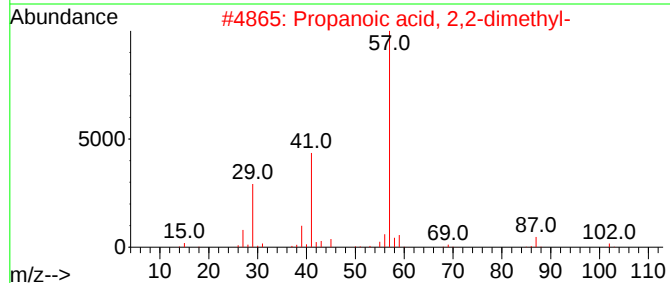
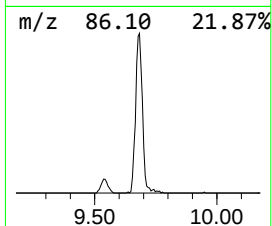
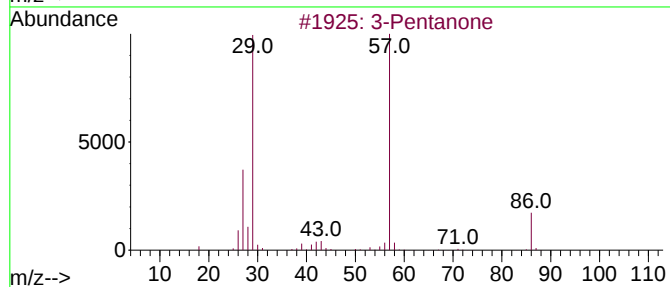
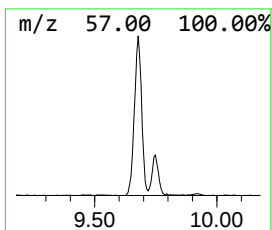
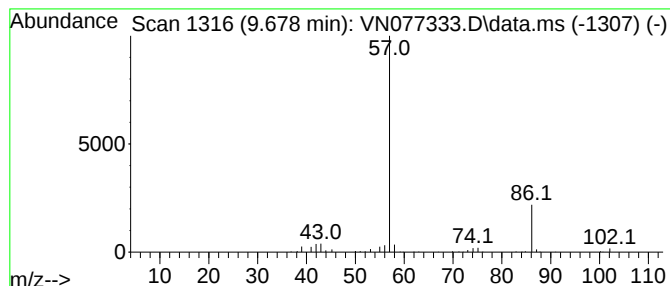
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.678	8.60 ug/l	406246	1,4-Difluorobenzene	9.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	80
2			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
3			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	9
4			Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	9
5			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	9



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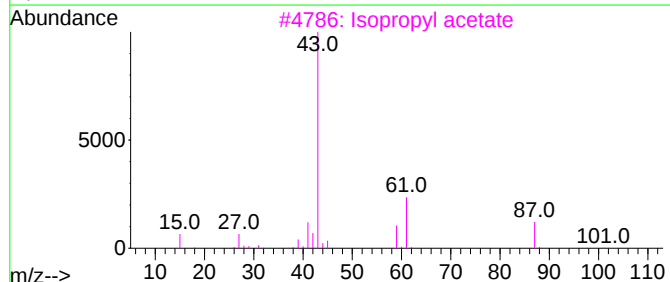
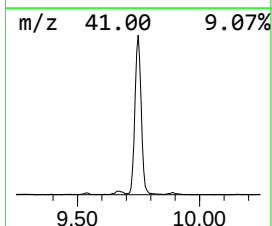
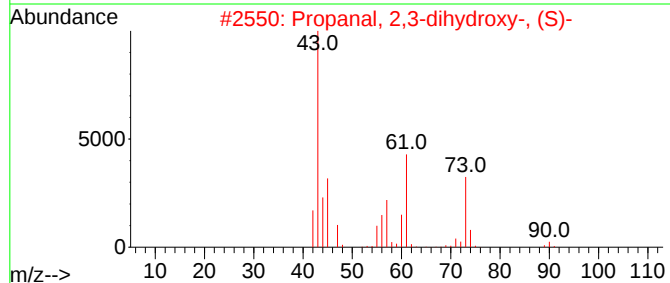
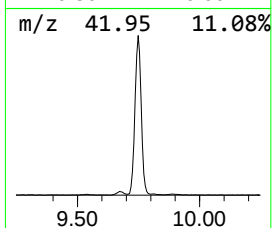
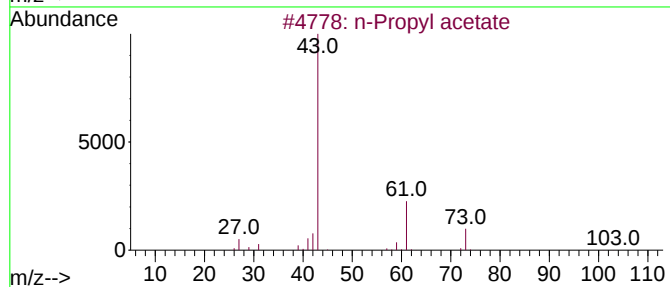
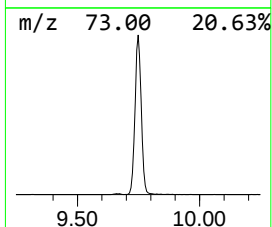
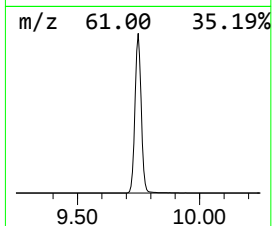
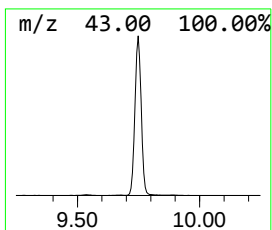
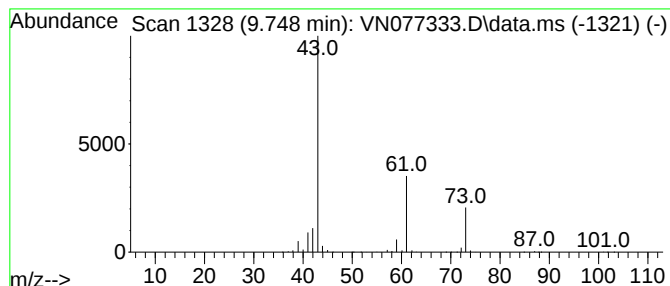
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.748	149.25 ug/l	7049620	1,4-Difluorobenzene	9.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3			Isopropyl acetate	102	C5H10O2	000108-21-4	28
4			Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
5			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9



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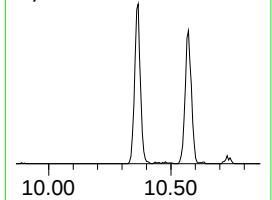
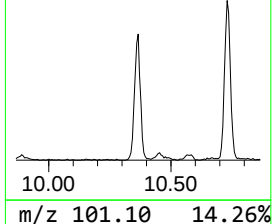
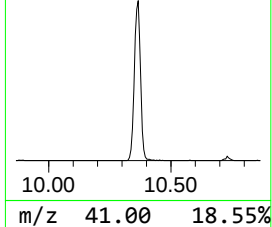
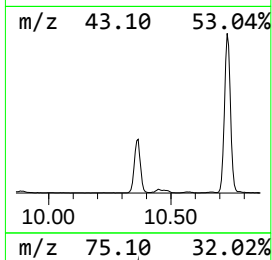
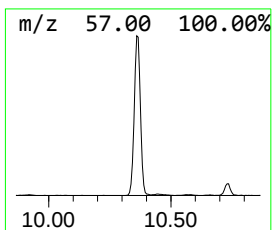
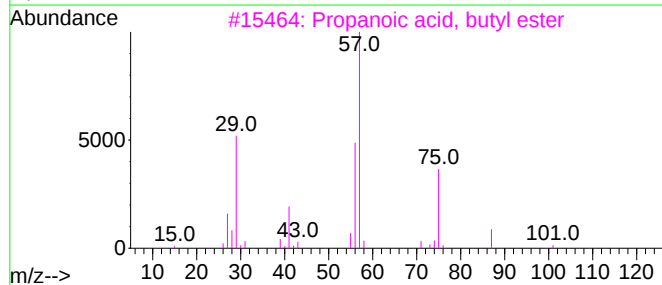
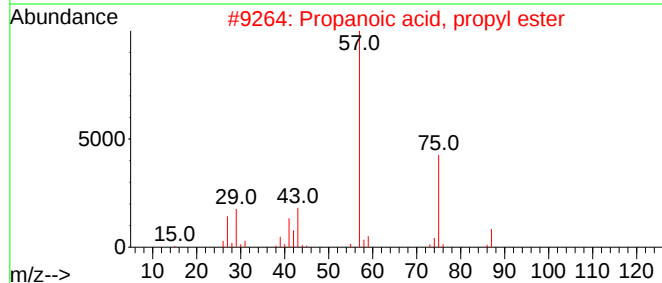
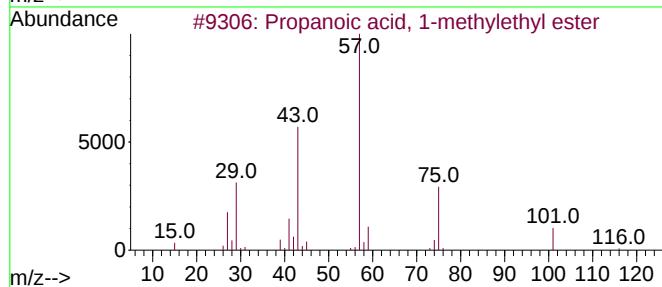
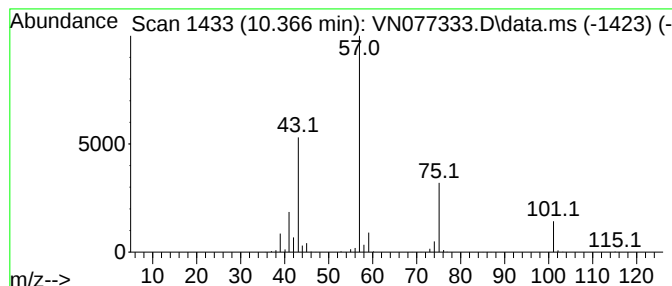
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.366	30.92 ug/l	1460350	1,4-Difluorobenzene	9.107	
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	53
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9



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Instrument :
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ClientSampleId :
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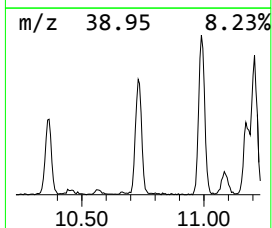
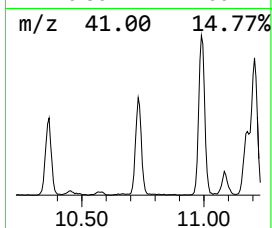
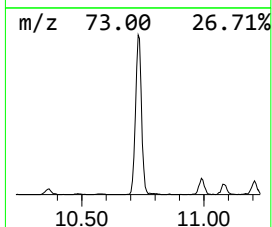
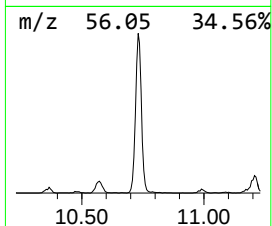
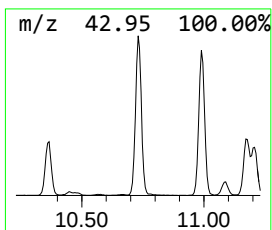
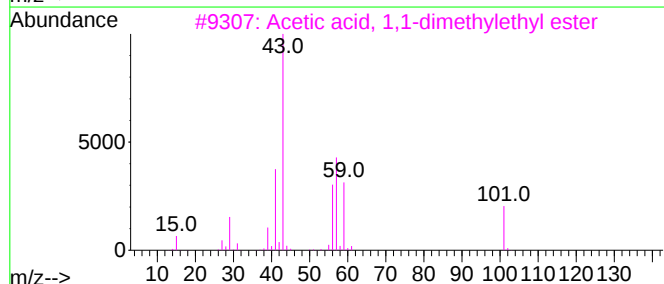
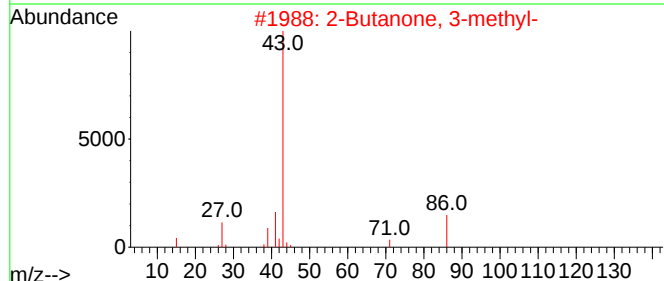
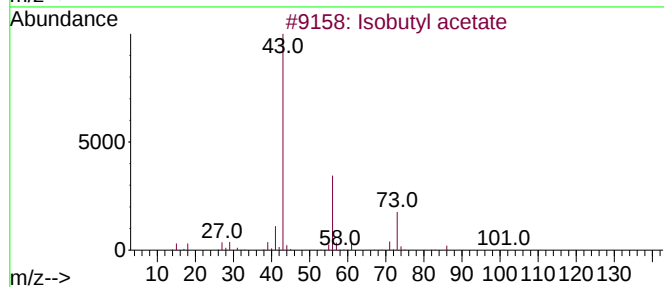
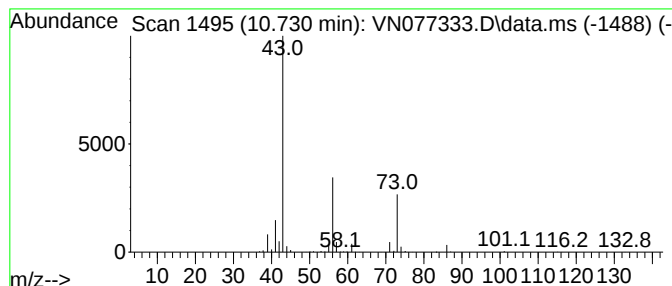
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	31.09 ug/l	1831880	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5			2-Pentanone	86	C5H10O	000107-87-9	9



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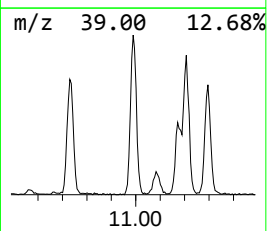
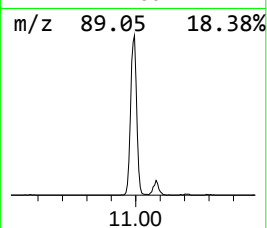
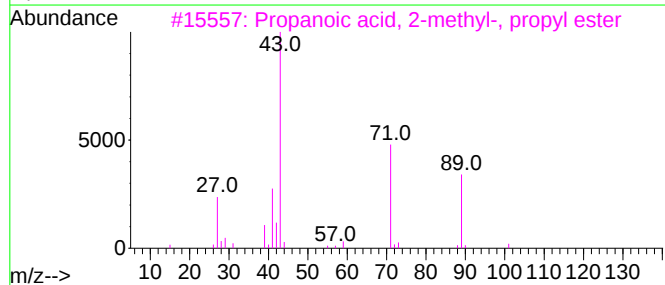
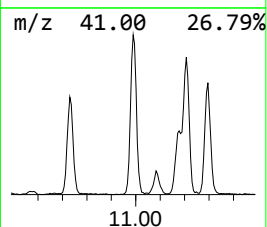
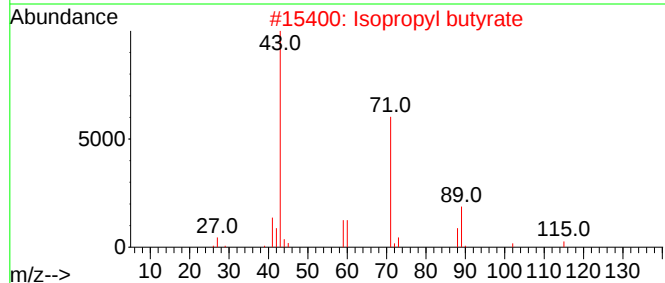
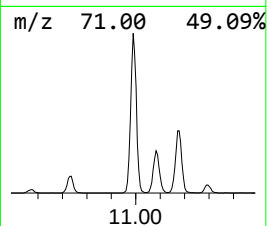
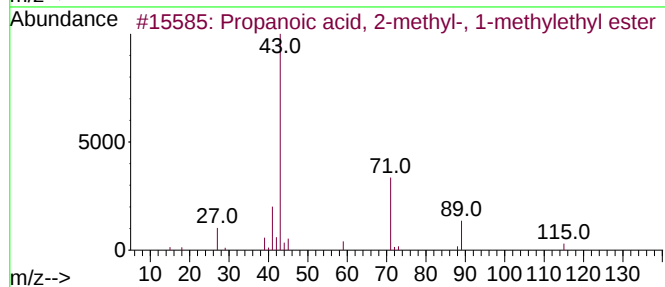
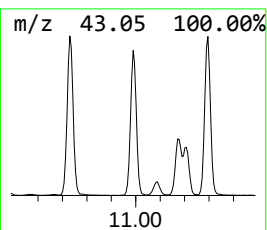
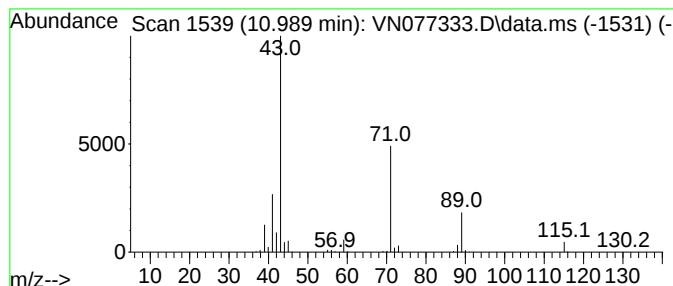
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Quant Title : SW846 8260

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	31.95 ug/l	1882880	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	72
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42



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PB152070ZHE#05

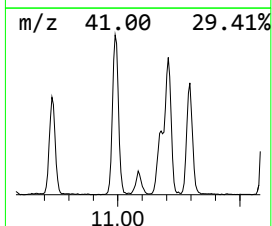
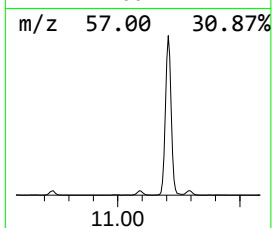
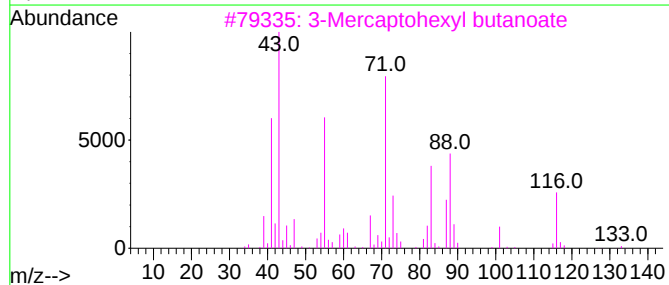
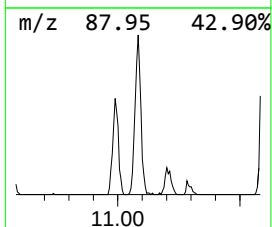
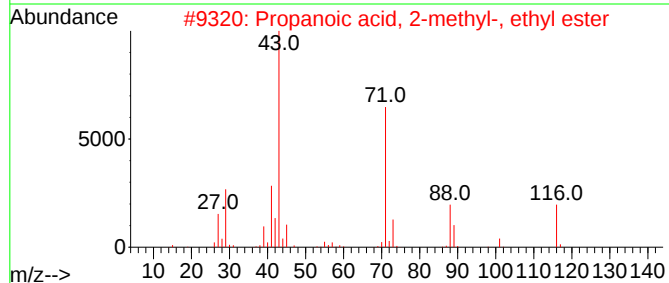
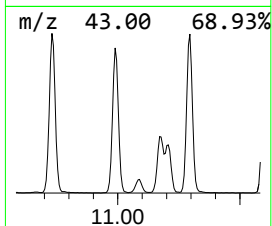
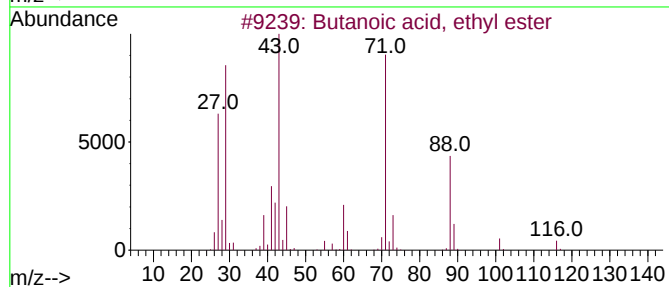
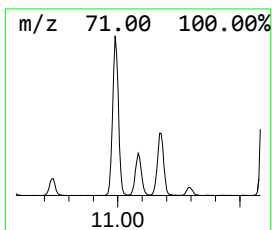
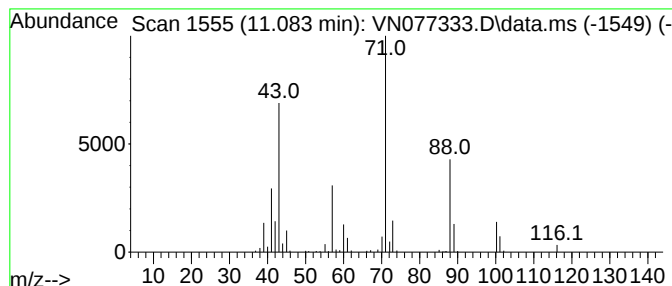
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.083	7.43 ug/l	438071	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	50
4			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	50
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077333.D
Acq On : 13 Apr 2023 17:03
Operator : JC\MD
Sample : PB152070ZHE#05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152070ZHE#05

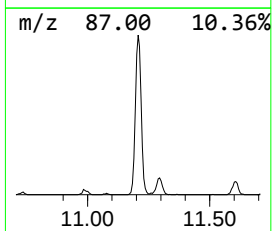
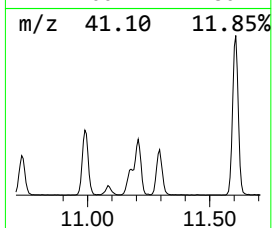
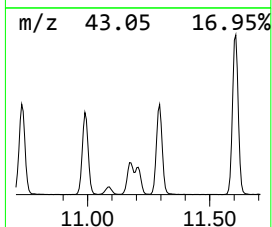
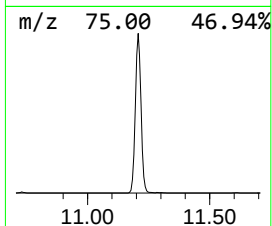
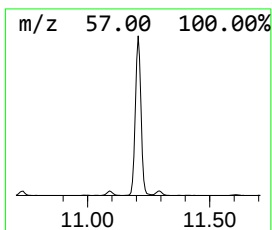
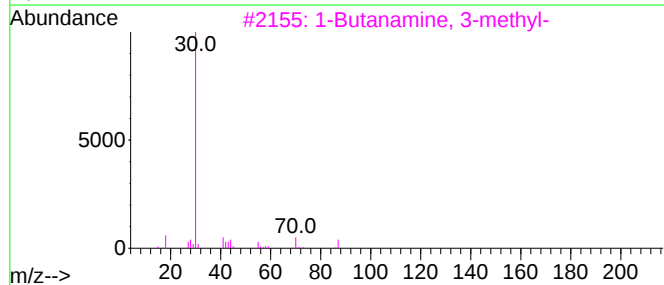
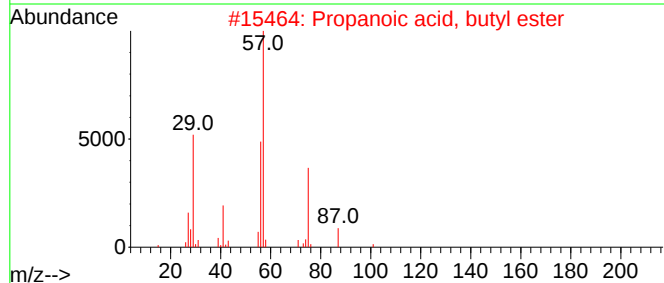
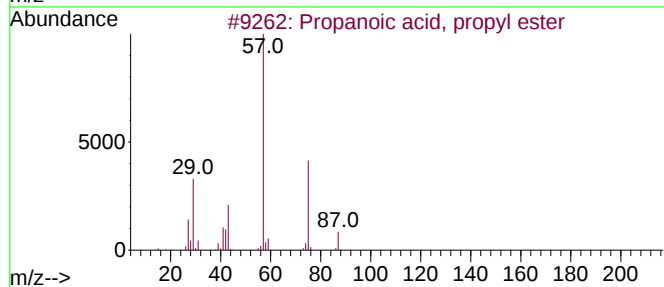
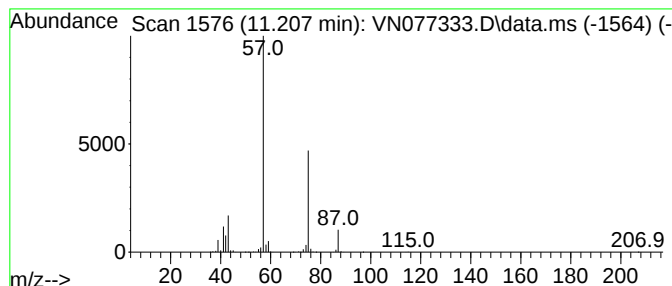
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Quant Title : SW846 8260

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.207	64.97 ug/l	3828370	Chlorobenzene-d5	11.871

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	40
3			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			1-Penten-3-ol	86	C5H10O	000616-25-1	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077333.D
Acq On : 13 Apr 2023 17:03
Operator : JC\MD
Sample : PB152070ZHE#05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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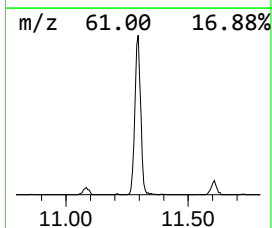
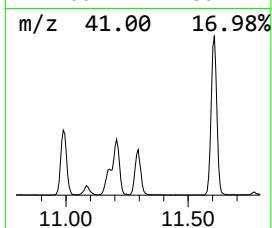
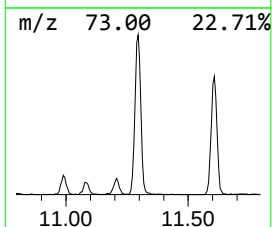
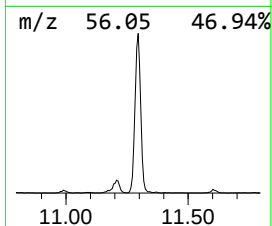
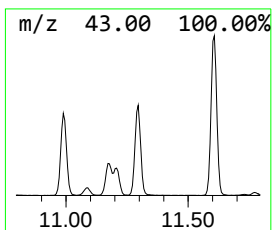
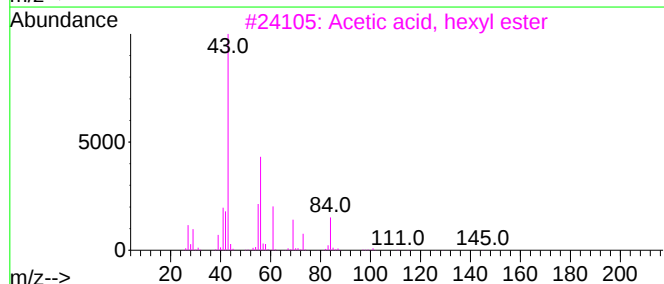
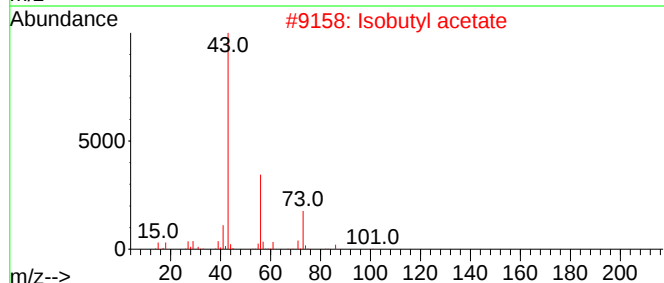
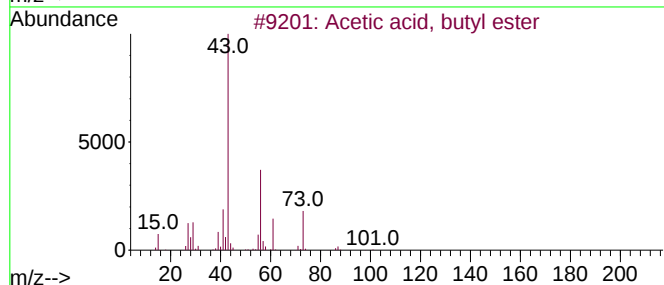
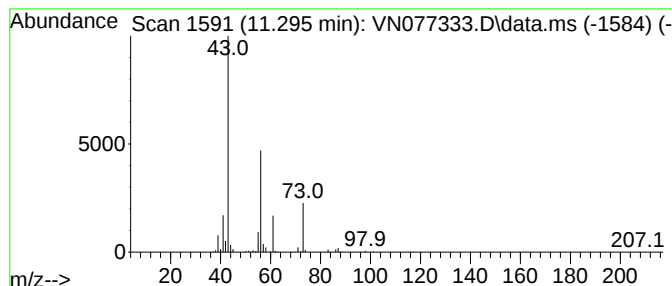
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Quant Title : SW846 8260

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

Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.295	34.48 ug/l	2031760	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	10
5			Isobutylamine	73	C4H11N	000078-81-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077333.D
Acq On : 13 Apr 2023 17:03
Operator : JC\MD
Sample : PB152070ZHE#05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152070ZHE#05

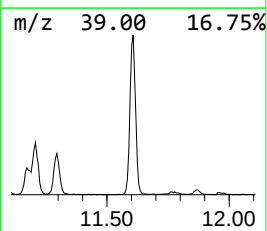
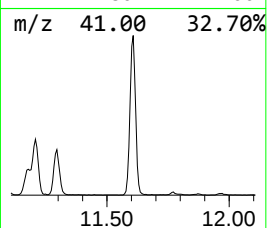
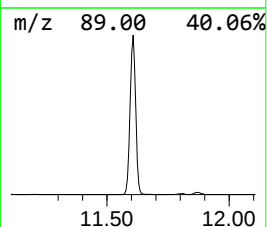
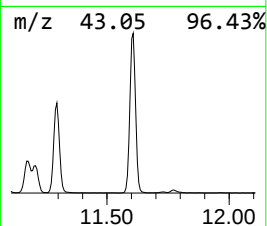
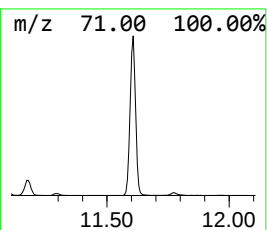
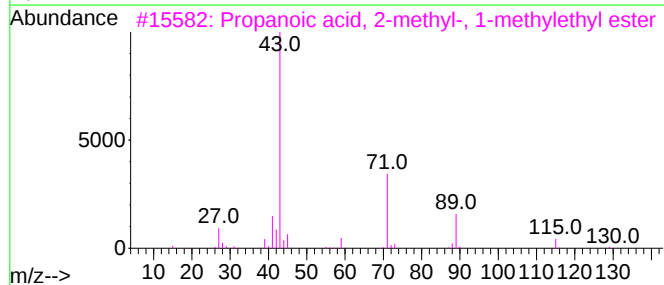
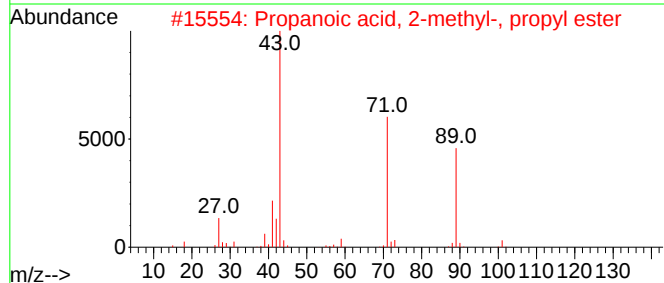
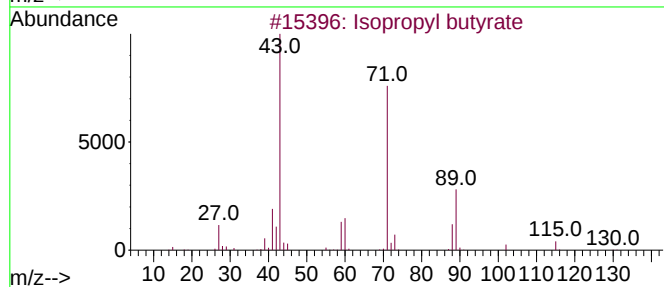
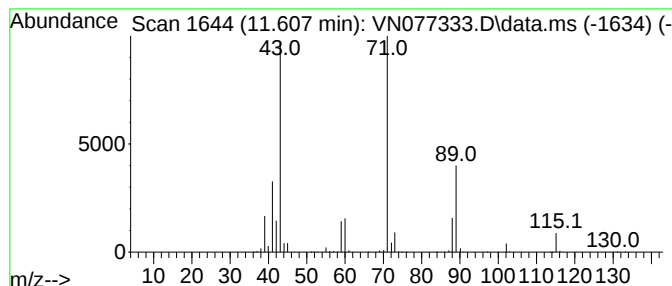
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Quant Title : SW846 8260

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

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.607	96.48 ug/l	5684870	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077333.D
Acq On : 13 Apr 2023 17:03
Operator : JC\MD
Sample : PB152070ZHE#05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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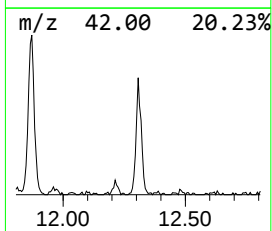
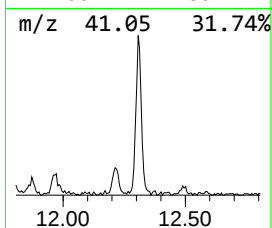
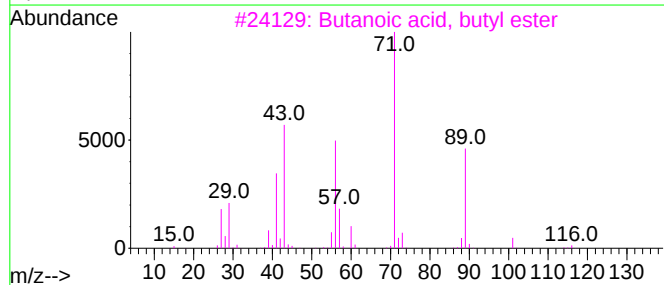
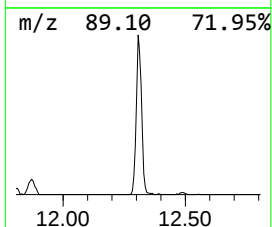
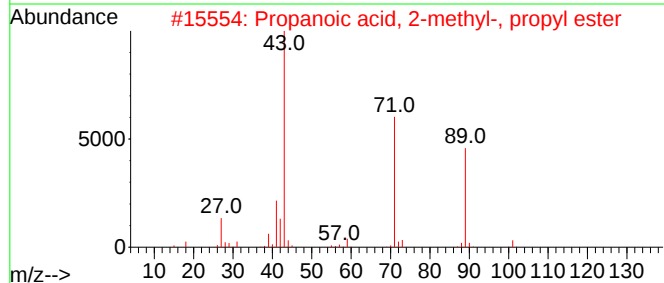
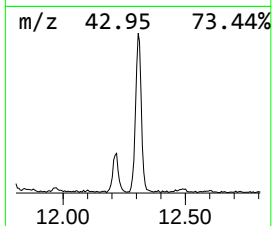
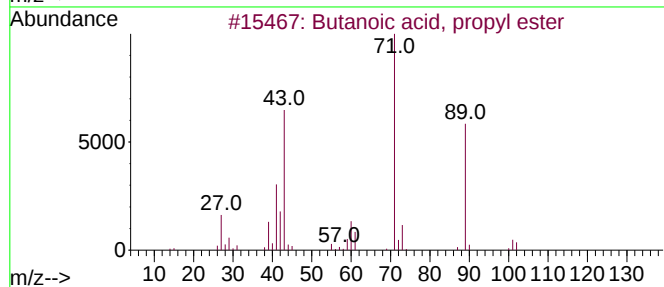
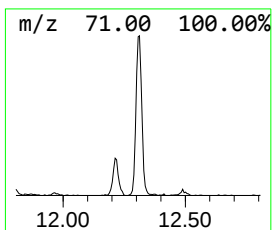
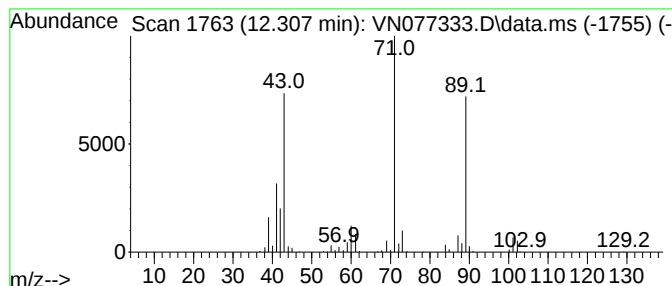
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Quant Title : SW846 8260

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

Peak Number 10 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.307	8.64 ug/l	509349	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
2			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	64
3			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	50
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077333.D
Acq On : 13 Apr 2023 17:03
Operator : JC\MD
Sample : PB152070ZHE#05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152070ZHE#05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.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
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n-Propyl acetate	9.748	149.3	ug/l	7049620	2	9.107	2361670	50.0
Propanoic acid,...	10.366	30.9	ug/l	1460350	2	9.107	2361670	50.0
Isobutyl acetate	10.730	31.1	ug/l	1831880	3	11.871	2946210	50.0
Propanoic acid,...	10.989	32.0	ug/l	1882880	3	11.871	2946210	50.0
Butanoic acid, ...	11.083	7.4	ug/l	438071	3	11.871	2946210	50.0
Propanoic acid,...	11.207	65.0	ug/l	3828370	3	11.871	2946210	50.0
Acetic acid, bu...	11.295	34.5	ug/l	2031760	3	11.871	2946210	50.0
Isopropyl butyrate	11.607	96.5	ug/l	5684870	3	11.871	2946210	50.0
Butanoic acid, ...	12.307	8.6	ug/l	509349	3	11.871	2946210	50.0