

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
 Data File : VN077405.D
 Acq On : 20 Apr 2023 17:11
 Operator : JC\MD
 Sample : 02390-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SPC-2WC-23-04-17

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: VN077405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.825	144	151	159	rBV4	39969	102091	2.81%	0.340%
2	4.443	416	426	438	rBV2	23954	77679	2.14%	0.259%
3	5.296	557	571	581	rBV3	44509	148409	4.09%	0.494%
4	7.572	950	958	968	rVB2	43125	107330	2.96%	0.357%
5	8.172	1047	1060	1064	rBV	427442	975888	26.89%	3.250%
6	8.231	1064	1070	1082	rVB	755202	1708919	47.10%	5.692%
7	8.584	1114	1130	1140	rBV	432799	982373	27.07%	3.272%
8	8.695	1140	1149	1158	rBV	308081	768768	21.19%	2.560%
9	9.107	1209	1219	1234	rBV	1086010	2225584	61.34%	7.412%
10	9.672	1305	1315	1321	rBV	160692	362794	10.00%	1.208%
11	9.748	1321	1328	1345	rVV	1712002	3235511	89.17%	10.776%
12	10.360	1423	1432	1439	rBV	686767	1178276	32.47%	3.924%
13	10.448	1442	1447	1452	rBV	20565	41187	1.14%	0.137%
14	10.572	1457	1468	1478	rBV	1676737	3111710	85.76%	10.364%
15	10.731	1487	1495	1503	rVB	325749	549805	15.15%	1.831%
16	10.989	1532	1539	1547	rBV	813906	1360614	37.50%	4.532%
17	11.083	1549	1555	1563	rVB3	164048	305283	8.41%	1.017%
18	11.207	1571	1576	1584	rVB	988355	1764066	48.62%	5.875%
19	11.295	1584	1591	1600	rVB	271580	469000	12.93%	1.562%
20	11.601	1635	1643	1656	rBV	2201757	3628564	100.00%	12.085%
21	11.766	1667	1671	1678	rVB2	43474	77460	2.13%	0.258%
22	11.866	1681	1688	1699	rBV	1491839	2663564	73.41%	8.871%
23	12.213	1741	1747	1755	rVB2	36399	60146	1.66%	0.200%
24	12.307	1755	1763	1773	rBV3	67059	122310	3.37%	0.407%
25	12.854	1848	1856	1868	rBV	1110908	1943029	53.55%	6.471%
26	13.795	2009	2016	2027	rBV	1174102	2054556	56.62%	6.843%

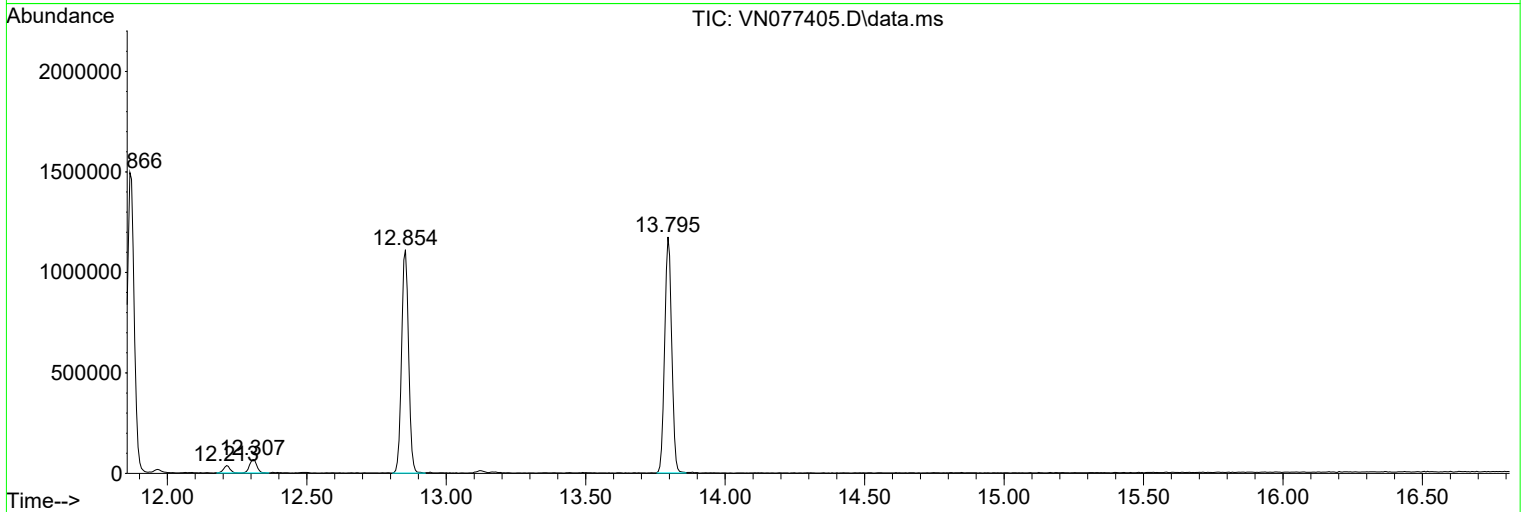
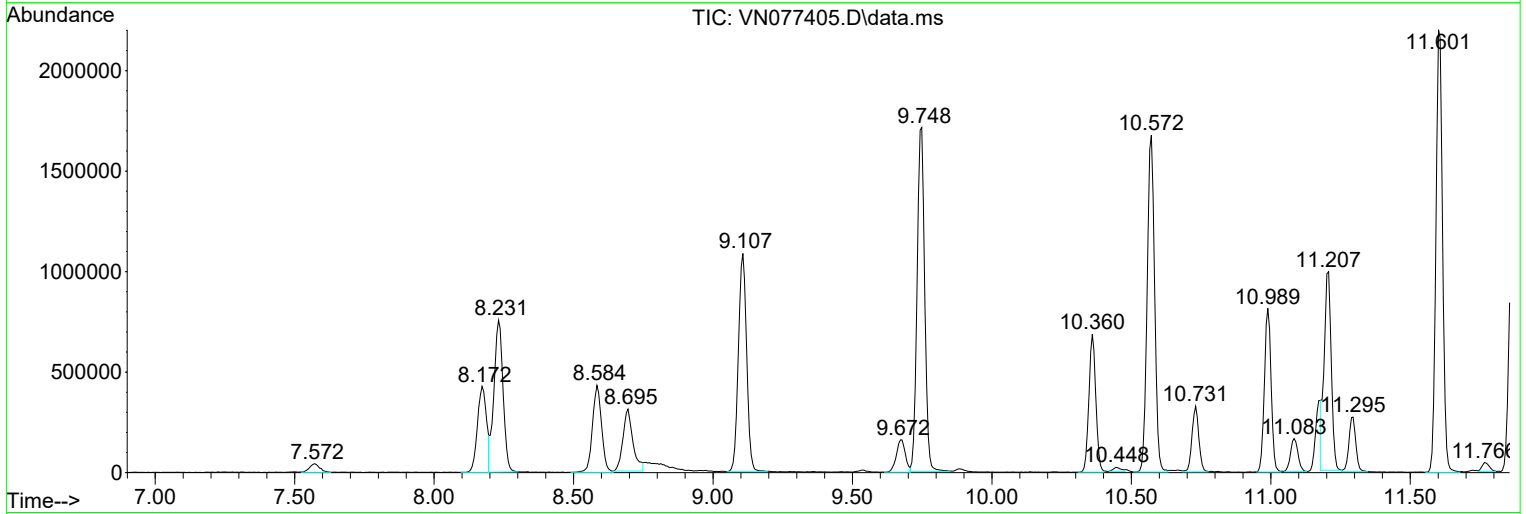
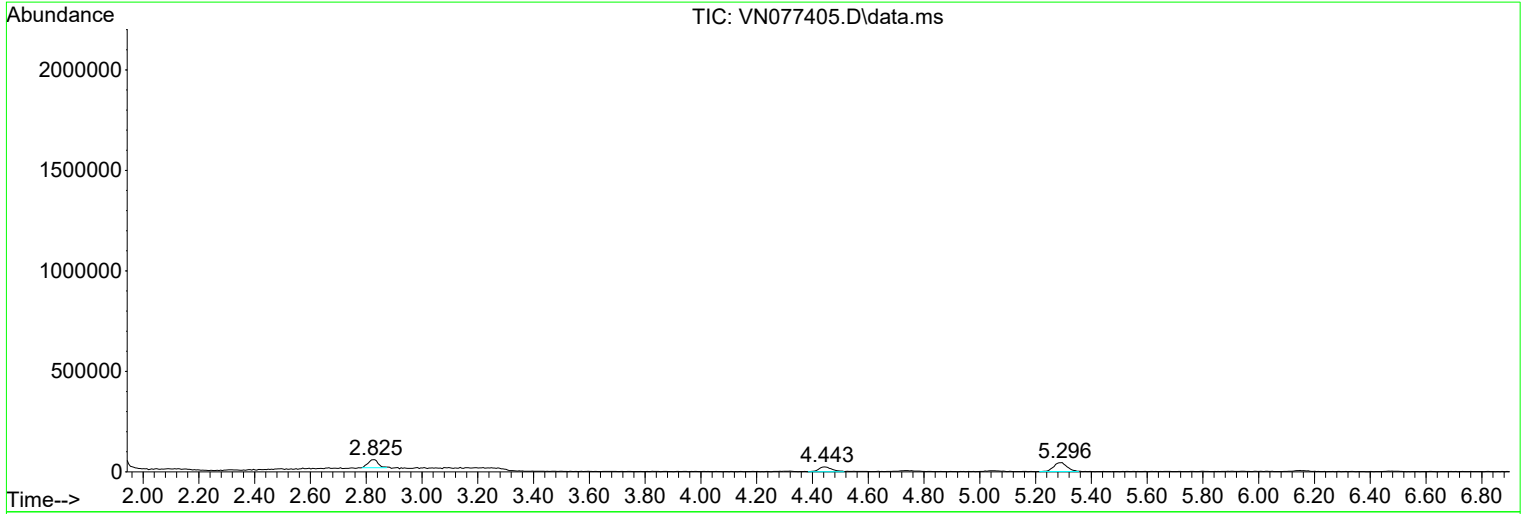
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
 Quant Title : SW846 8260

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



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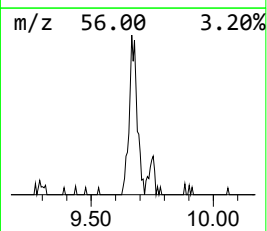
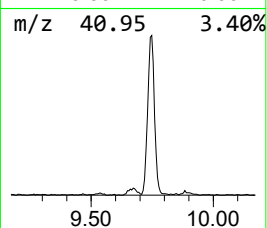
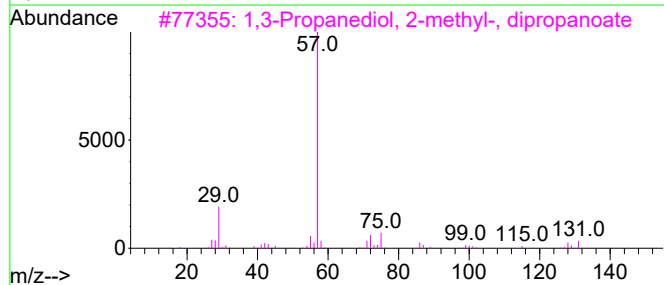
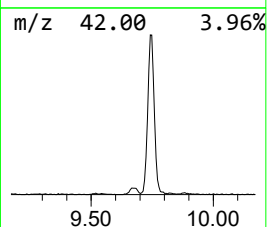
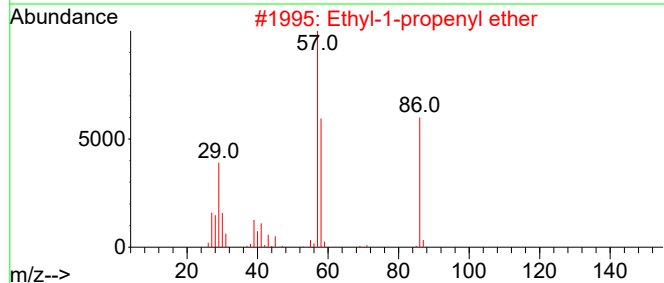
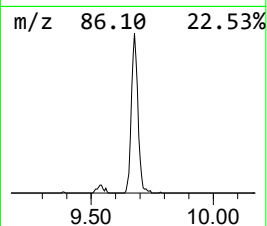
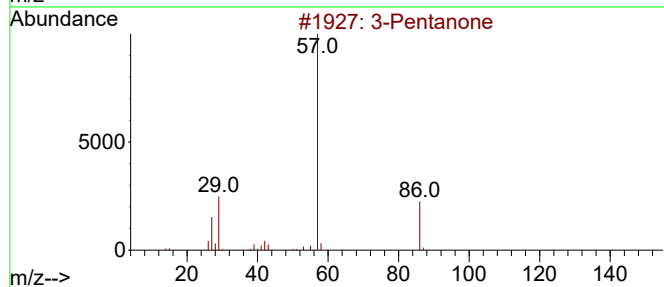
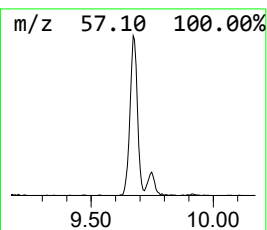
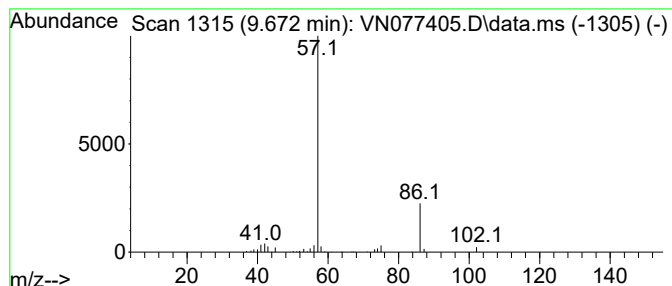
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 Quant Title : SW846 8260

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

 Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.672	8.15 ug/l	362794	1,4-Difluorobenzene	9.107

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pentanone	86	C5H10O	000096-22-0	64
2		Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
3		1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	9
4		Propanoic acid, anhydride	130	C6H10O3	000123-62-6	9
5		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9



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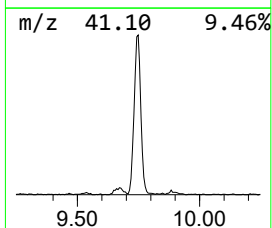
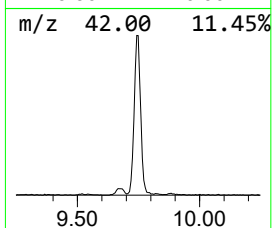
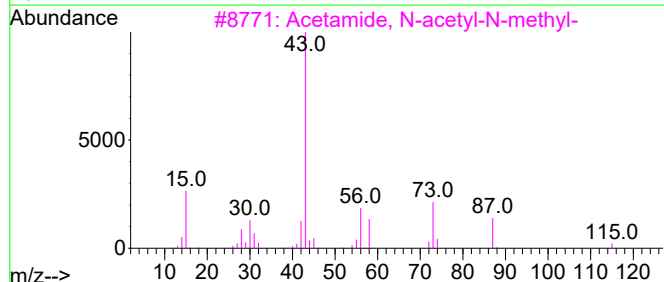
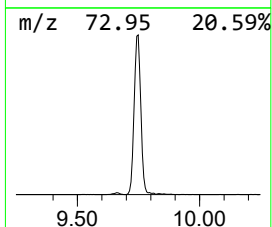
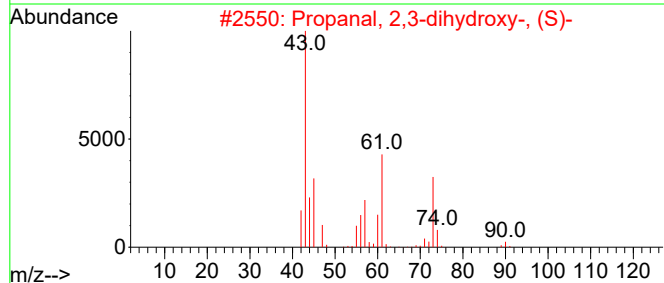
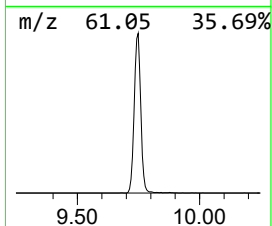
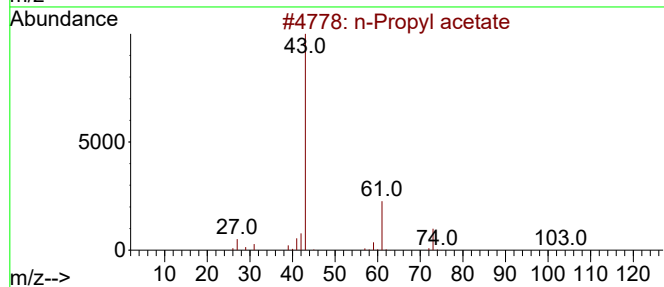
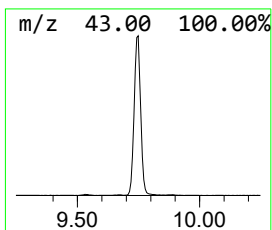
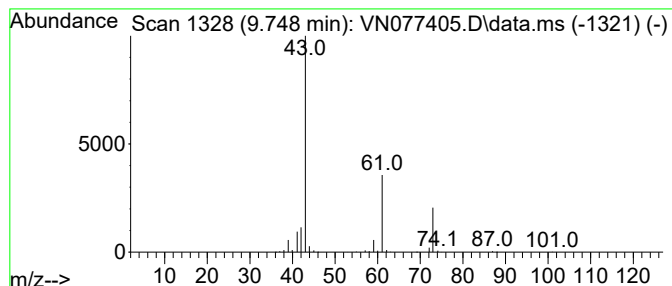
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 TIC Integration Parameters: LSCINT.P

 Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.748	72.69 ug/l	3235510	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		Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
4		Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9
5		1-Butanamine	73	C4H11N	000109-73-9	5



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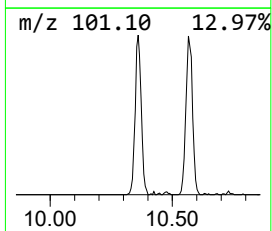
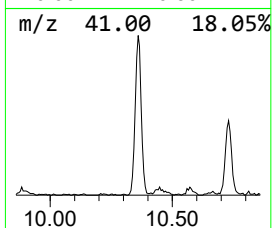
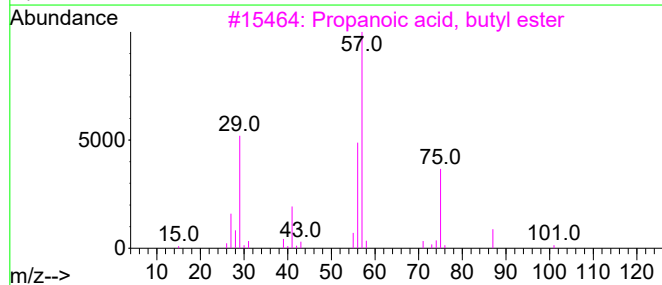
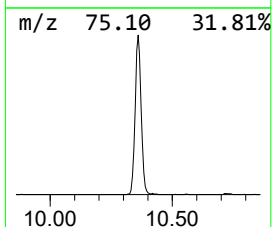
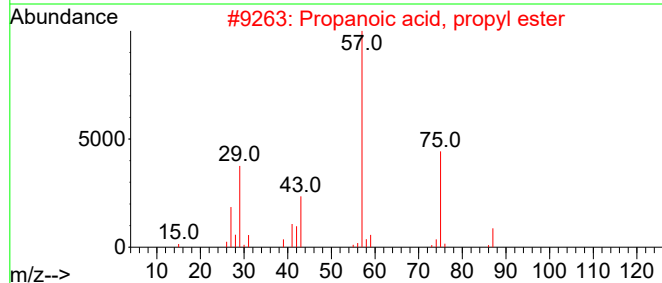
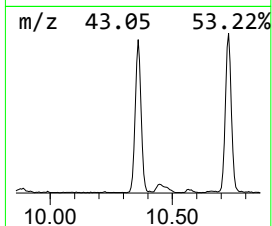
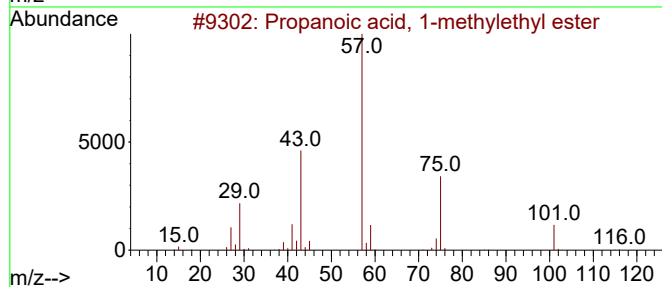
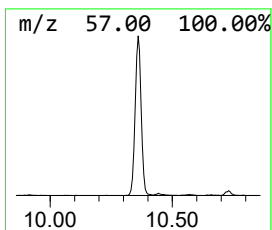
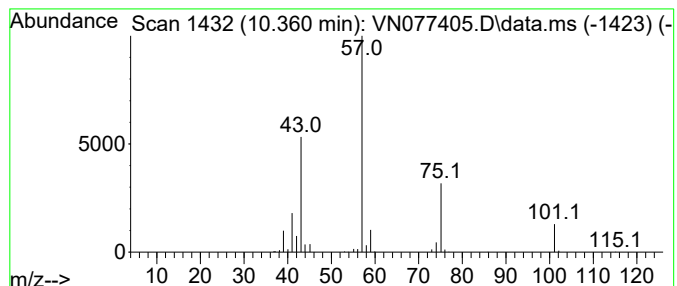
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 Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	26.47 ug/l	1178280	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	47
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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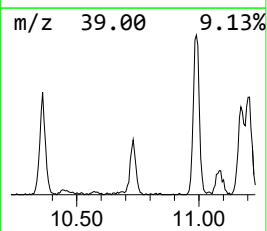
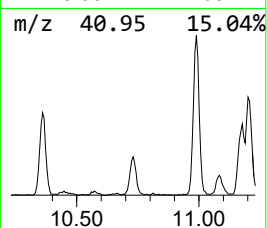
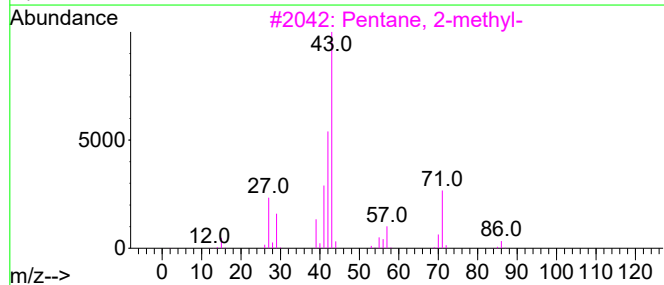
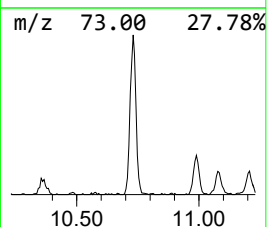
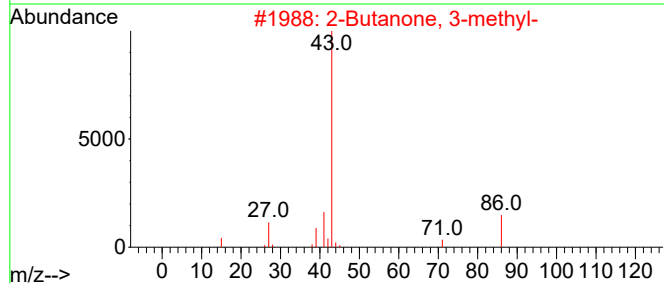
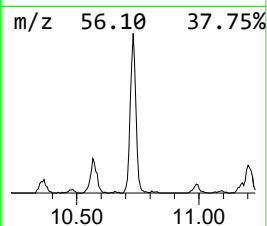
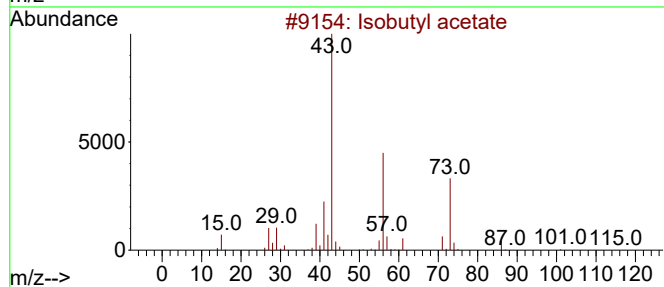
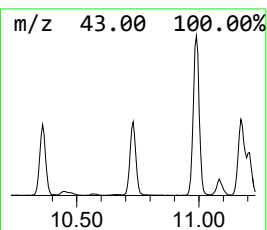
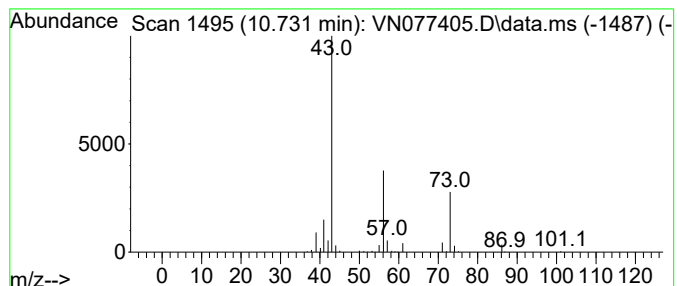
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 Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	10.32 ug/l	549805	Chlorobenzene-d5	11.866

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	22
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9



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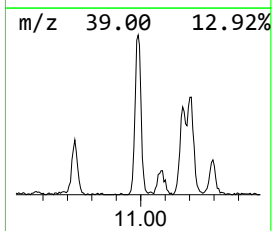
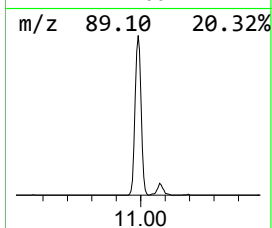
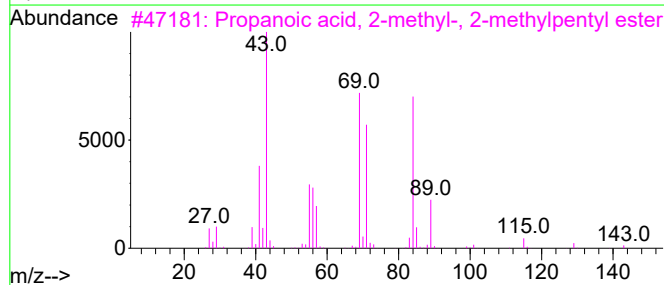
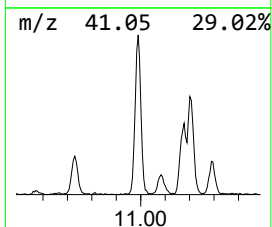
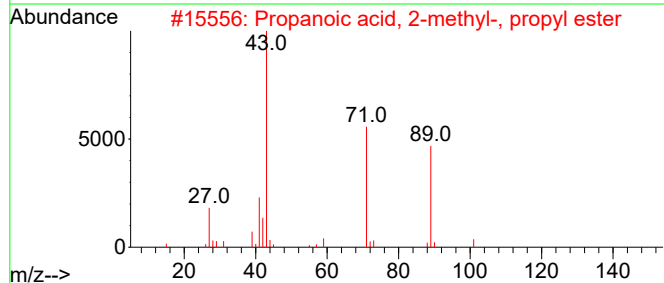
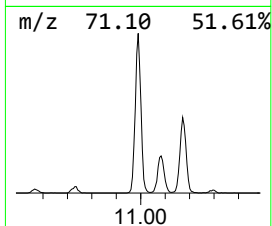
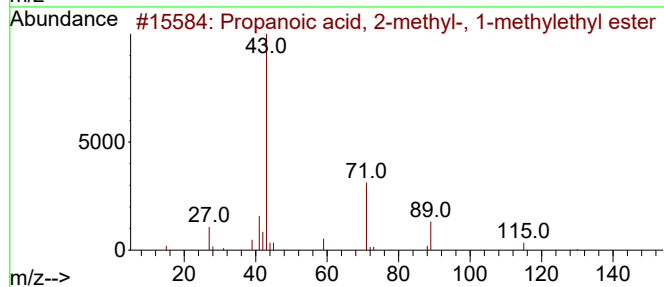
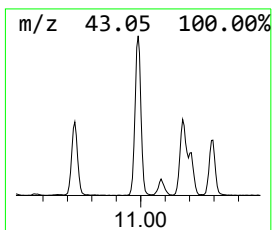
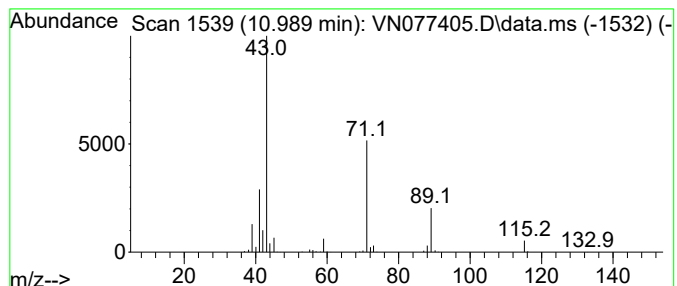
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 Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	25.54 ug/l	1360610	Chlorobenzene-d5	11.866

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			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	56
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45



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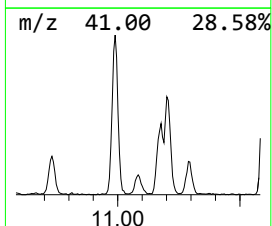
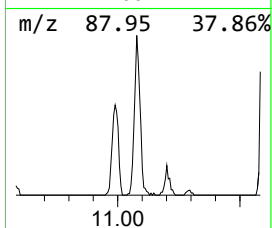
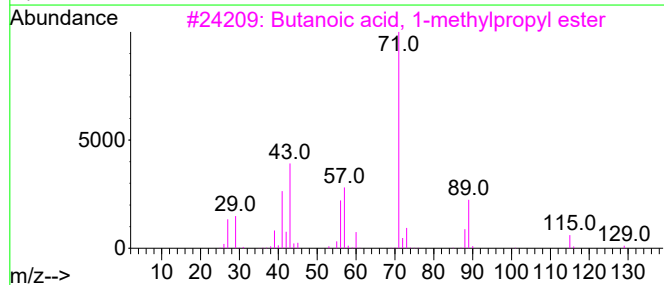
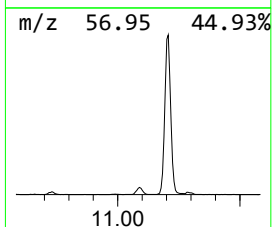
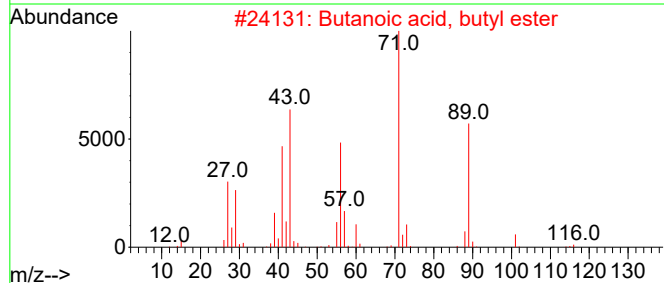
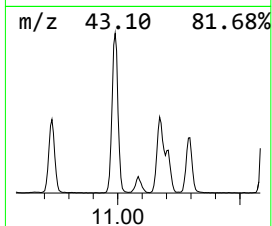
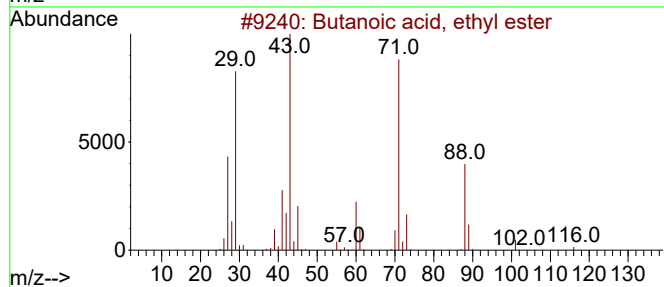
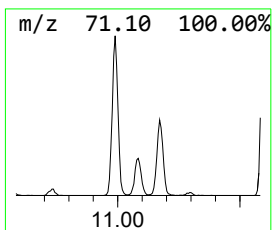
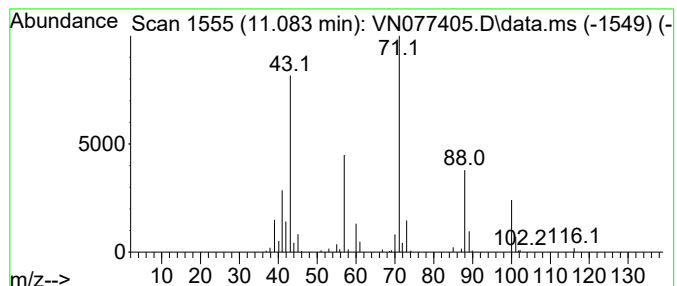
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 Quant Title : SW846 8260

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

 Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.084	5.73 ug/l	305283	Chlorobenzene-d5	11.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	53
3			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	53
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
 Data File : VN077405.D
 Acq On : 20 Apr 2023 17:11
 Operator : JC\MD
 Sample : 02390-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
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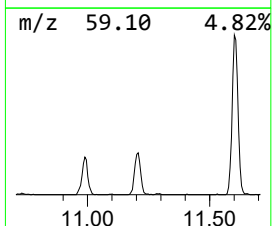
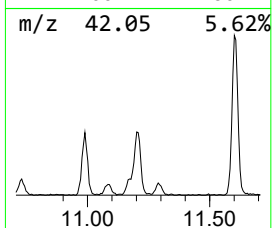
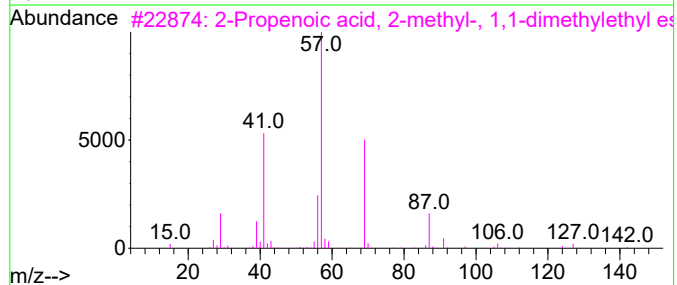
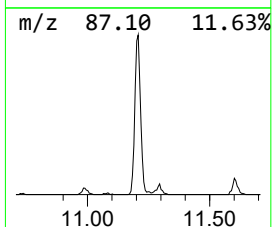
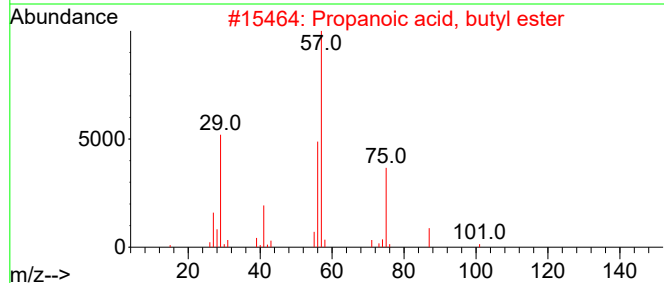
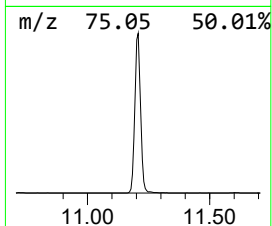
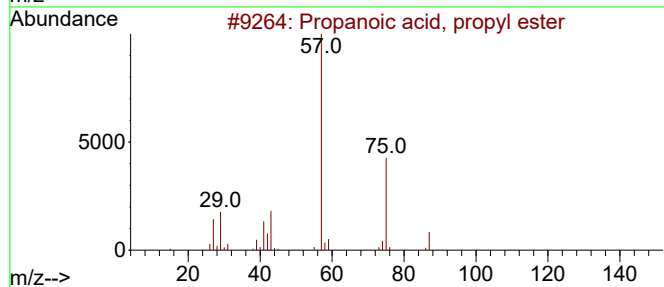
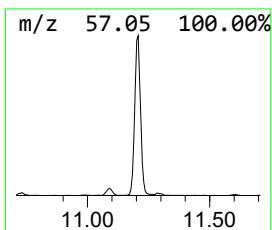
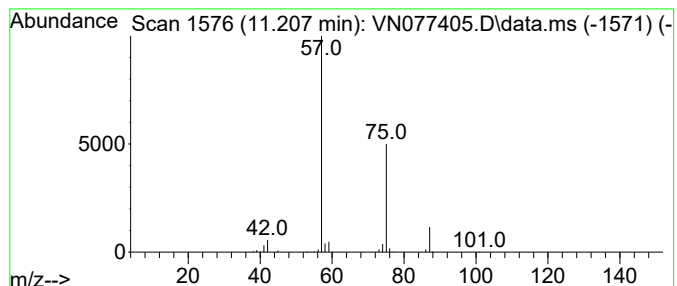
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 Quant Title : SW846 8260

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

 Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.207	33.11 ug/l	1764070	Chlorobenzene-d5	11.866

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			2-Propenoic acid, 2-methyl-, 1,1...	142	C8H14O2	000585-07-9	9
4			1-Penten-3-ol	86	C5H10O	000616-25-1	7
5			Neopentylamine	87	C5H13N	005813-64-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
 Data File : VN077405.D
 Acq On : 20 Apr 2023 17:11
 Operator : JC\MD
 Sample : 02390-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SPC-2WC-23-04-17

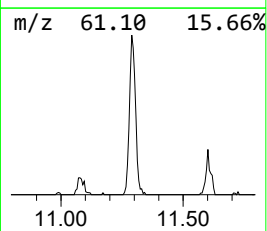
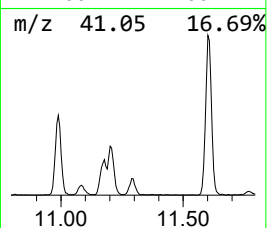
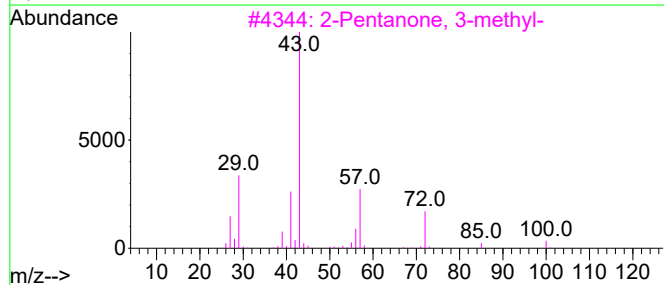
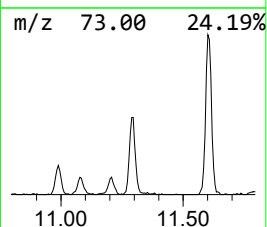
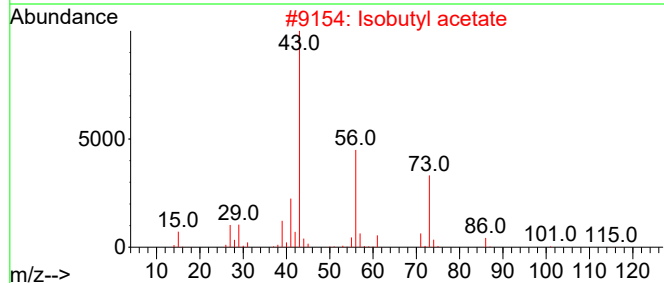
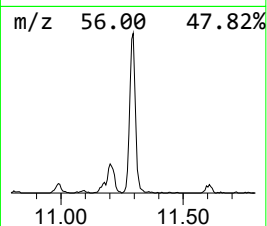
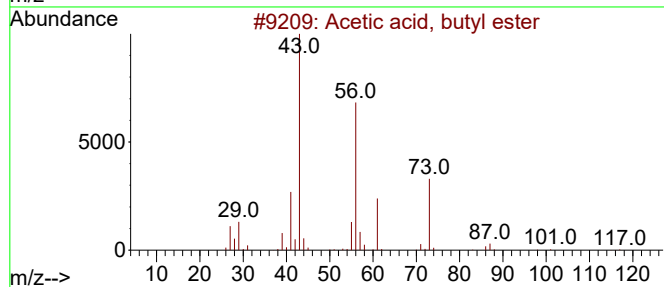
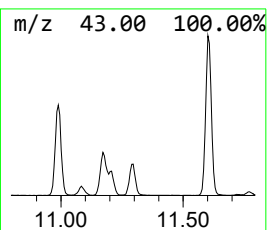
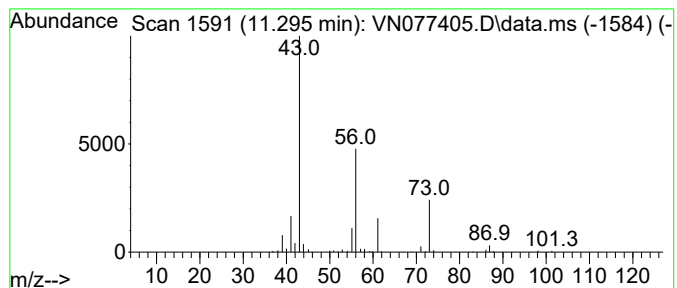
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 Quant Title : SW846 8260

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

 Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.295	8.80 ug/l	469000	Chlorobenzene-d5	11.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2			Isobutyl acetate	116	C6H12O2	000110-19-0	39
3			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
4			n-Propyl acetate	102	C5H10O2	000109-60-4	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
 Data File : VN077405.D
 Acq On : 20 Apr 2023 17:11
 Operator : JC\MD
 Sample : 02390-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 SPC-2WC-23-04-17

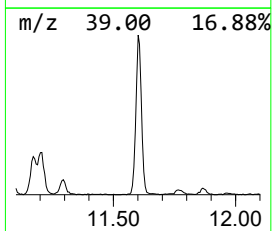
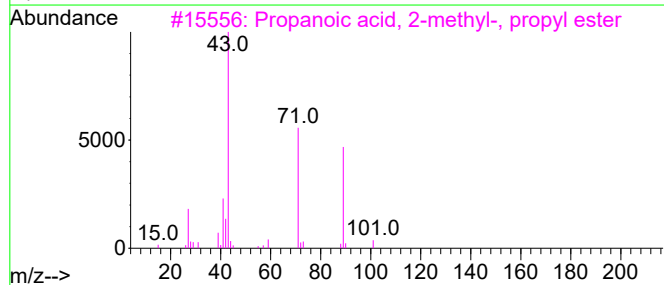
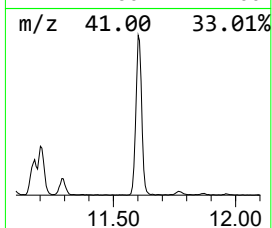
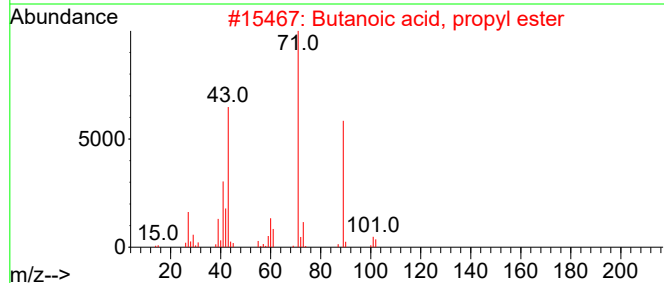
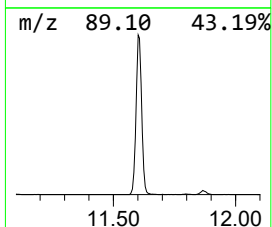
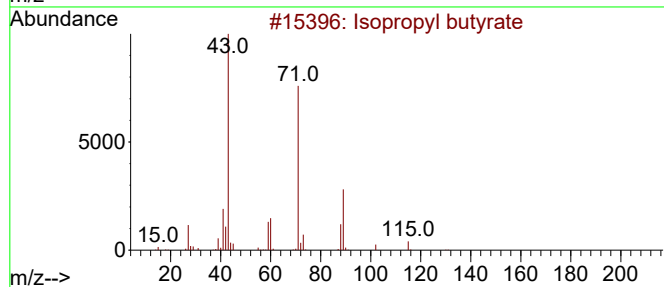
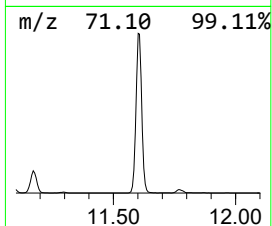
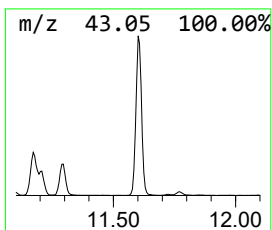
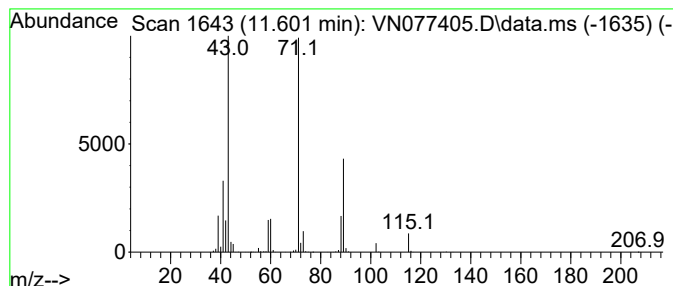
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 Quant Title : SW846 8260

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.
11.601	68.11 ug/l	3628560	Chlorobenzene-d5	11.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	93
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	56
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
Data File : VN077405.D
Acq On : 20 Apr 2023 17:11
Operator : JC\MD
Sample : 02390-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPC-2WC-23-04-17

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone	9.672	8.2	ug/l	362794	2	9.107	2225580	50.0
n-Propyl acetate	9.748	72.7	ug/l	3235510	2	9.107	2225580	50.0
Propanoic acid,...	10.360	26.5	ug/l	1178280	2	9.107	2225580	50.0
Isobutyl acetate	10.730	10.3	ug/l	549805	3	11.866	2663560	50.0
Propanoic acid,...	10.989	25.5	ug/l	1360610	3	11.866	2663560	50.0
Butanoic acid, ...	11.084	5.7	ug/l	305283	3	11.866	2663560	50.0
Propanoic acid,...	11.207	33.1	ug/l	1764070	3	11.866	2663560	50.0
Acetic acid, bu...	11.295	8.8	ug/l	469000	3	11.866	2663560	50.0
Isopropyl butyrate	11.601	68.1	ug/l	3628560	3	11.866	2663560	50.0