

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041923\
 Data File : VN077383.D
 Acq On : 19 Apr 2023 18:22
 Operator : JC\MD
 Sample : PB152199ZHE#11
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB152199ZHE#11

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: VN077383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.843	144	154	160	rBV5	51728	154649	2.31%	0.330%
2	5.289	559	570	582	rBV2	44968	145820	2.18%	0.311%
3	7.572	949	958	967	rBV	63115	144259	2.16%	0.308%
4	8.172	1050	1060	1065	rBV	506063	1236205	18.49%	2.639%
5	8.230	1065	1070	1086	rVB	881188	1952527	29.20%	4.169%
6	8.583	1119	1130	1139	rBV	508983	1147754	17.16%	2.450%
7	8.695	1139	1149	1159	rBV	387876	970556	14.51%	2.072%
8	9.107	1210	1219	1236	rBV	1319111	2690496	40.23%	5.744%
9	9.672	1307	1315	1320	rBV2	176691	384358	5.75%	0.821%
10	9.742	1320	1327	1345	rVV	3607864	6686998	100.00%	14.276%
11	10.360	1424	1432	1442	rBV	911605	1550989	23.19%	3.311%
12	10.571	1459	1468	1479	rBV	2011391	3852746	57.62%	8.225%
13	10.730	1487	1495	1506	rVB	1089832	1912808	28.60%	4.084%
14	10.989	1530	1539	1547	rBV	1260827	2128652	31.83%	4.545%
15	11.083	1547	1555	1563	rVV3	239730	459137	6.87%	0.980%
16	11.207	1563	1576	1584	rVV2	1968043	3978692	59.50%	8.494%
17	11.289	1584	1590	1603	rVB	1195802	2030113	30.36%	4.334%
18	11.601	1635	1643	1660	rBV	3887010	6232837	93.21%	13.307%
19	11.765	1667	1671	1680	rVB3	54776	104075	1.56%	0.222%
20	11.865	1680	1688	1700	rVV	1828500	3371269	50.42%	7.197%
21	11.965	1700	1705	1714	rVB	56259	99130	1.48%	0.212%
22	12.213	1741	1747	1753	rBV3	48658	79094	1.18%	0.169%
23	12.307	1755	1763	1773	rBV	353500	589028	8.81%	1.258%
24	12.854	1847	1856	1866	rBV	1306626	2315553	34.63%	4.944%
25	13.795	2008	2016	2028	rBV	1496337	2622253	39.21%	5.598%

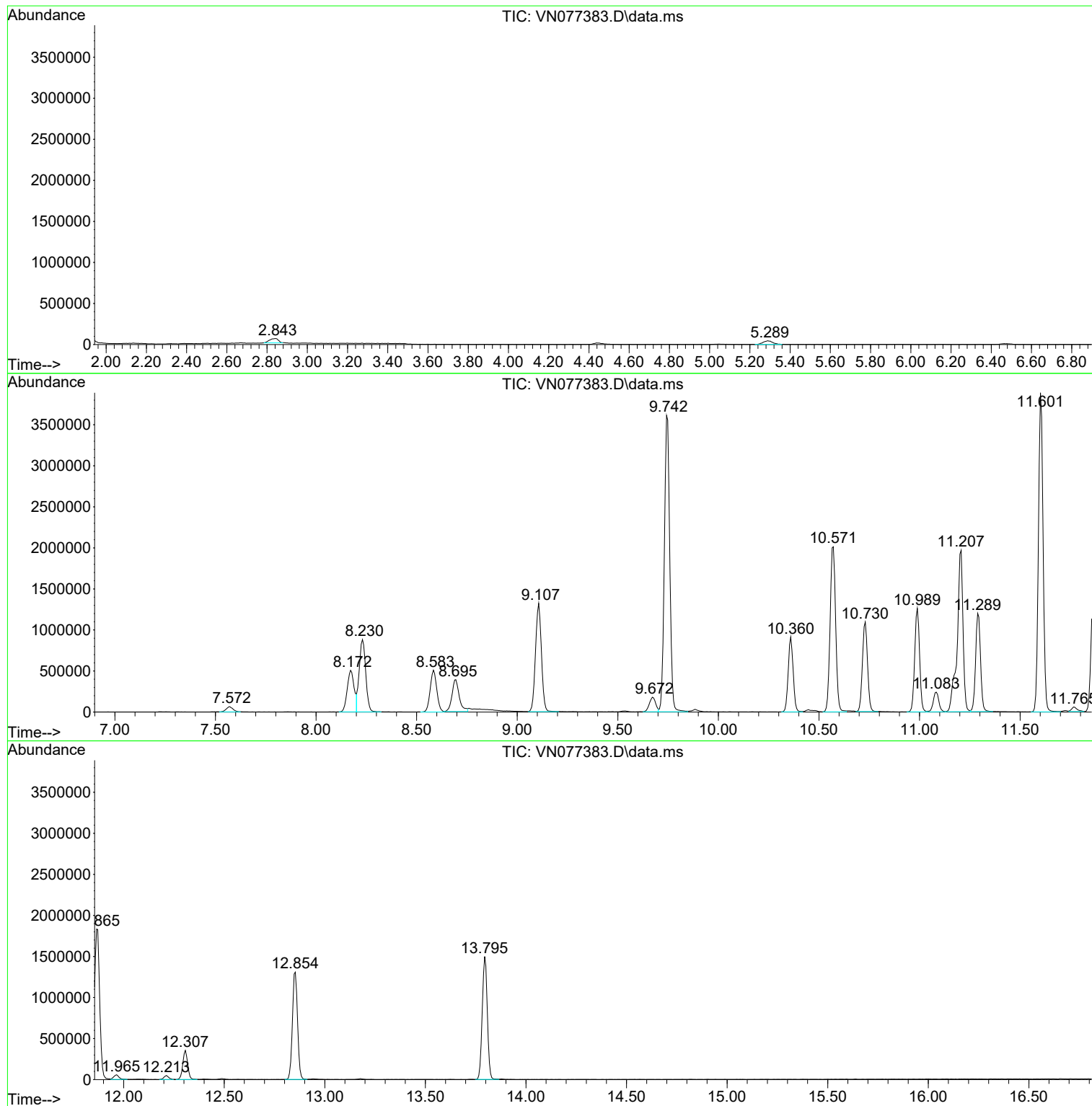
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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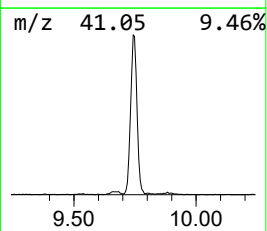
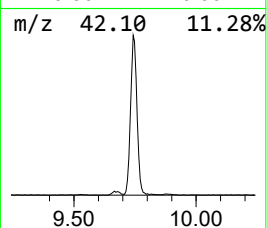
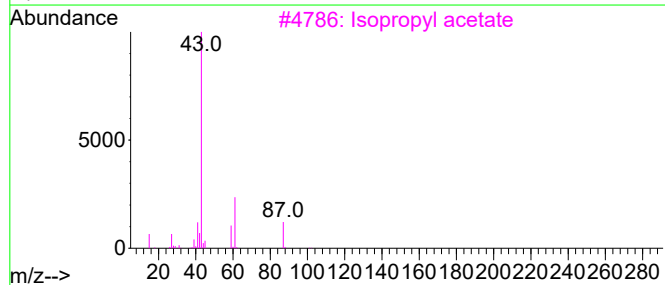
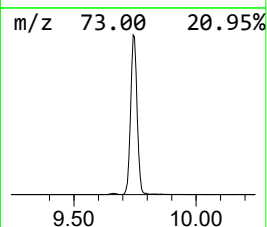
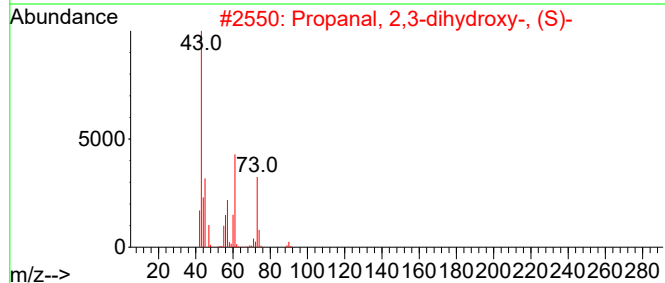
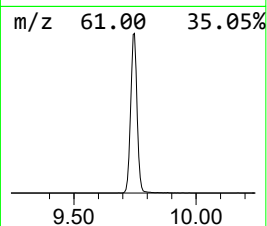
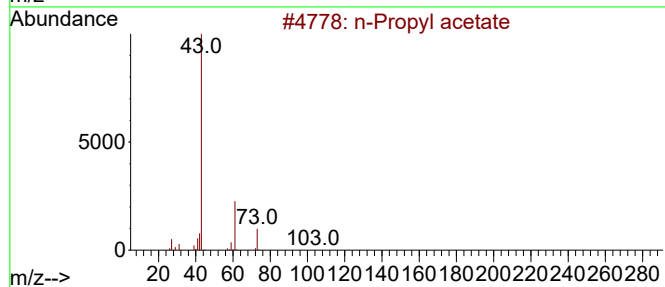
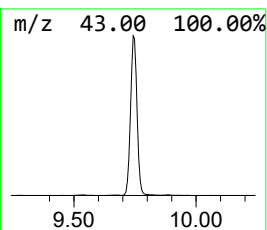
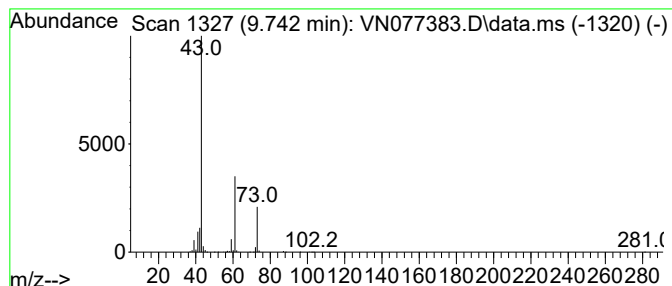
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Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.742	124.27 ug/l	6687000	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	33
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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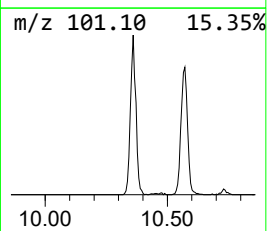
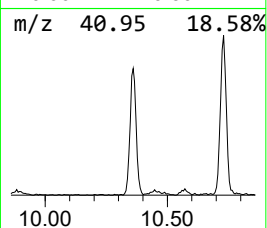
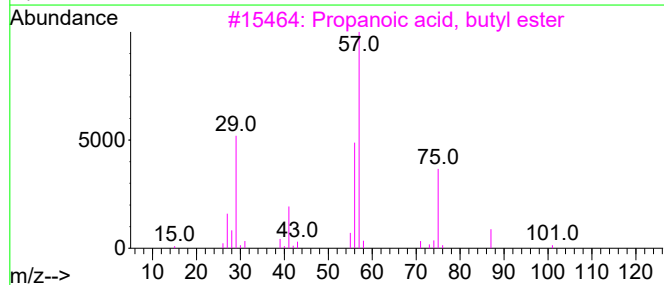
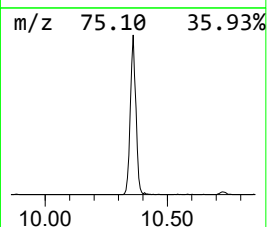
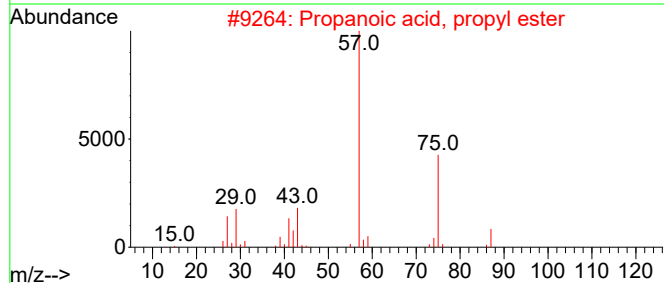
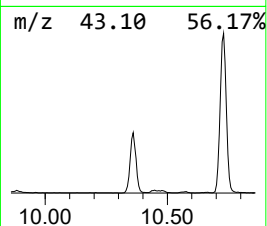
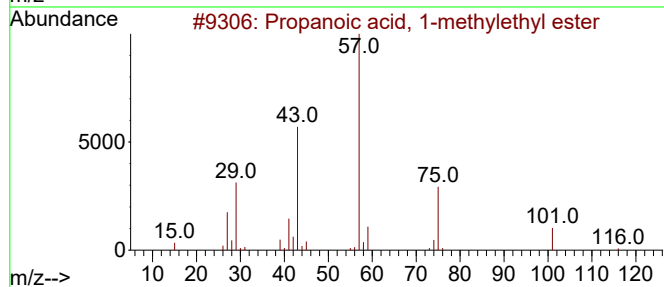
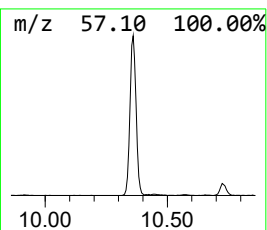
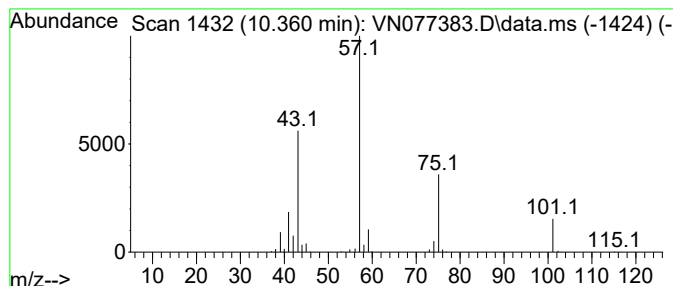
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Quant Title : SW846 8260

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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	28.82 ug/l	1550990	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	78
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	9



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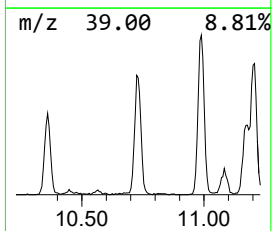
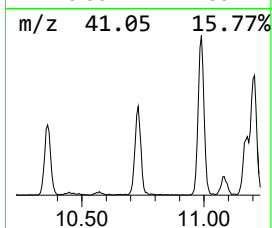
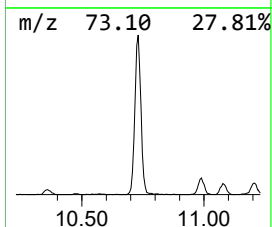
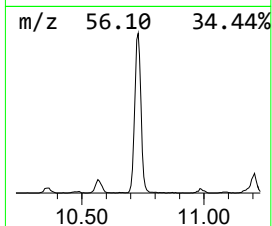
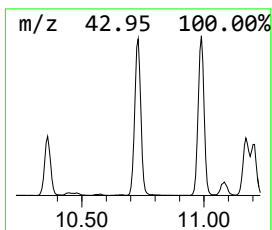
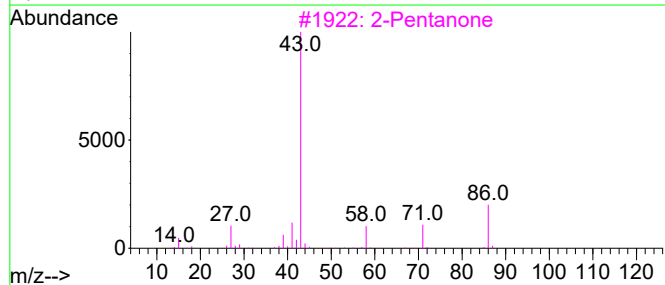
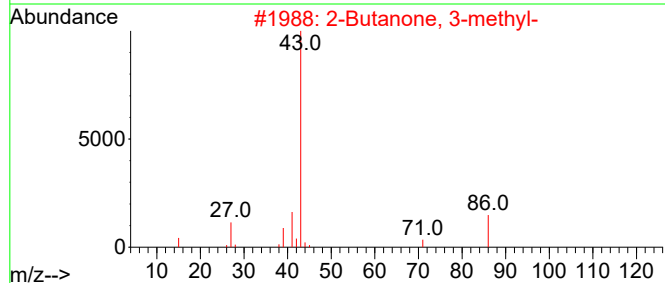
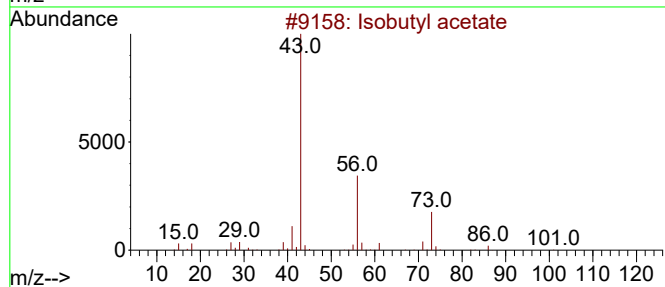
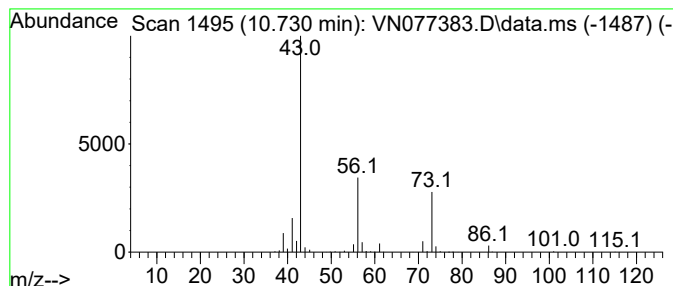
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Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	28.37 ug/l	1912810	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			2-Pentanone	86	C5H10O	000107-87-9	9
4			Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	9
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9



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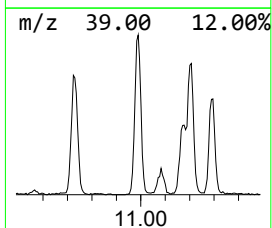
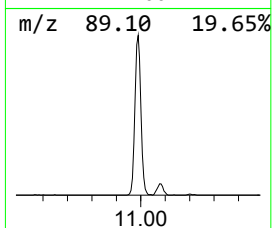
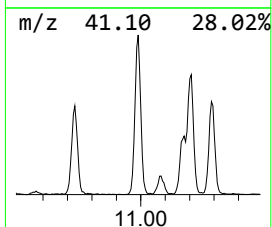
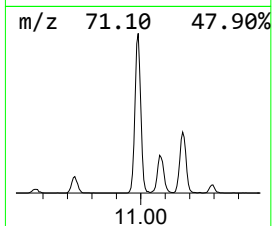
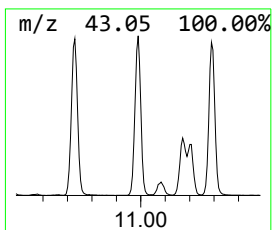
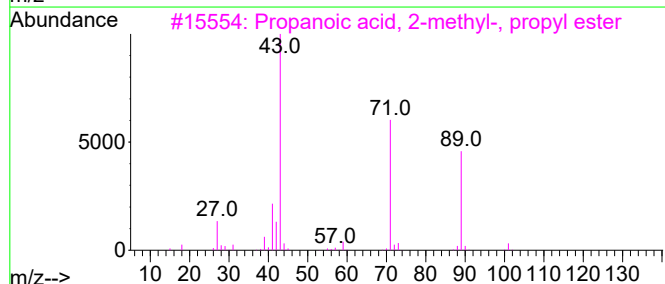
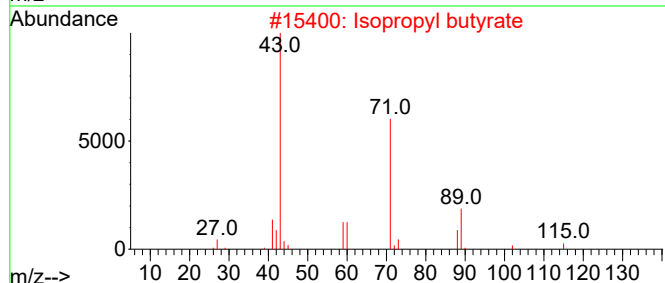
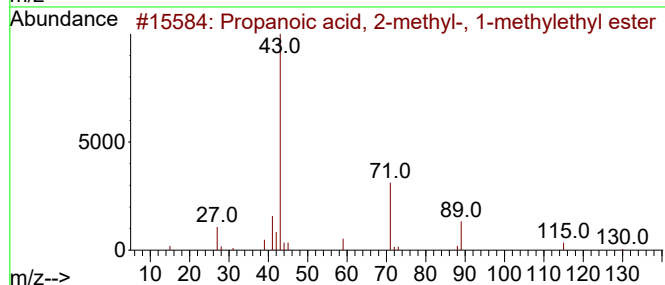
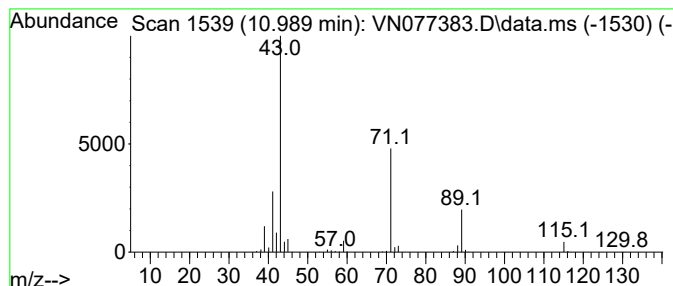
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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	31.57 ug/l	2128650	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	86
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50



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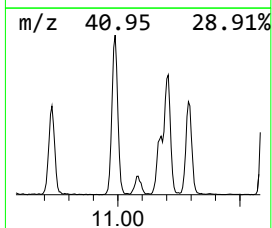
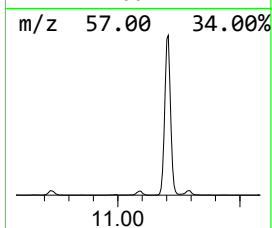
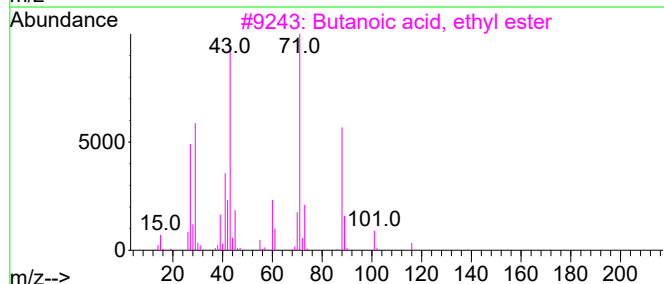
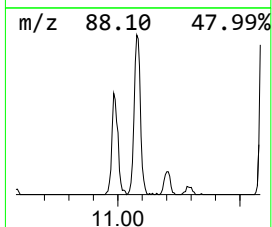
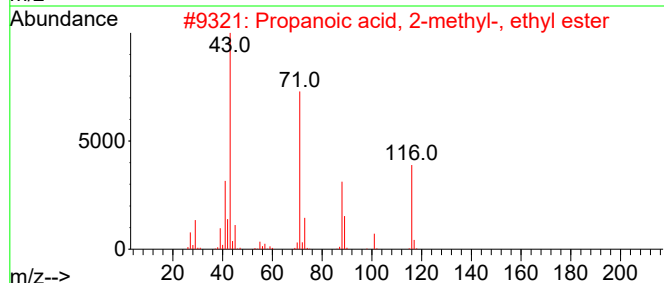
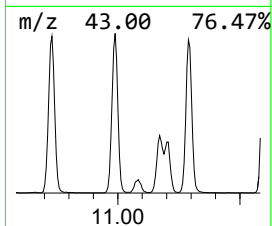
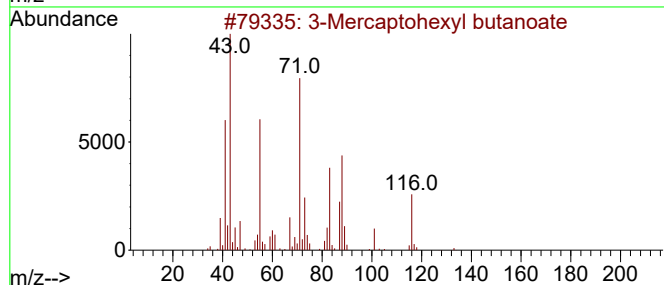
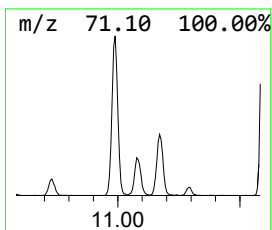
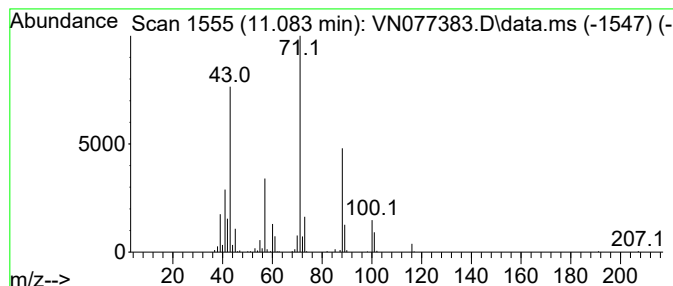
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TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Mercaptohexyl butanoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.083	6.81 ug/l	459137	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	64
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	64
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	58
4			Butanoic acid, 2,2-dimethyl-	116	C6H12O2	000595-37-9	50
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43



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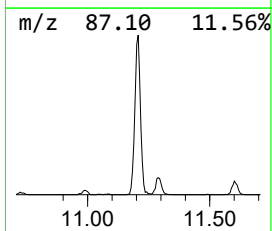
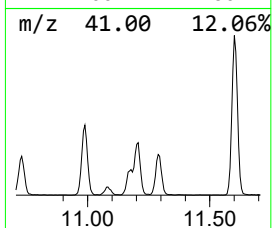
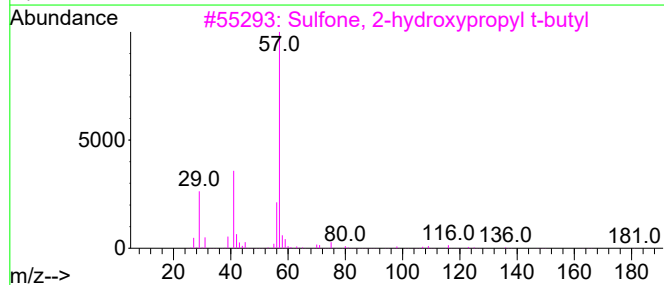
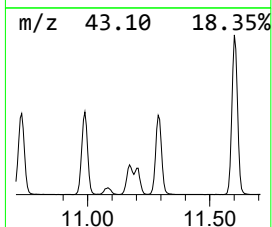
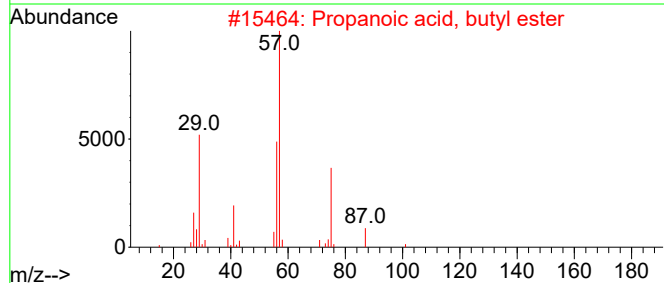
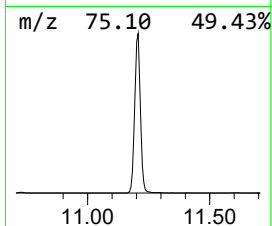
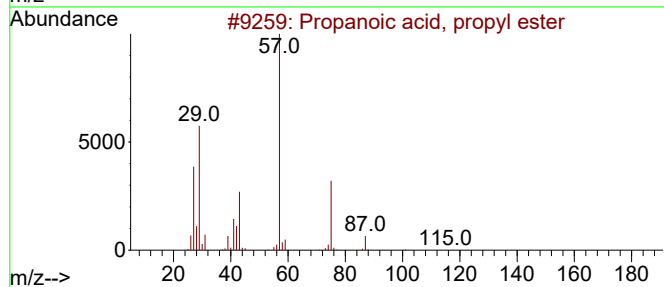
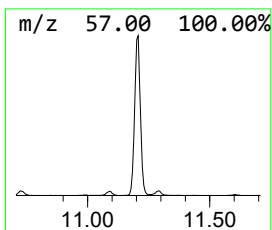
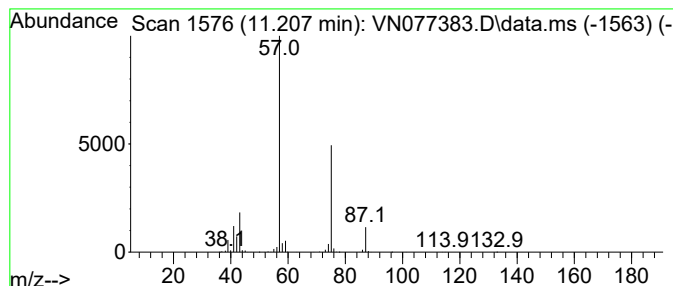
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Quant Title : SW846 8260

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	59.01 ug/l	3978690	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			Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041923\
Data File : VN077383.D
Acq On : 19 Apr 2023 18:22
Operator : JC\MD
Sample : PB152199ZHE#11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152199ZHE#11

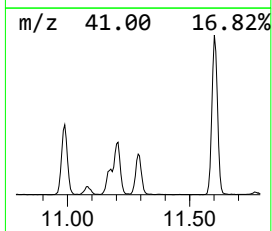
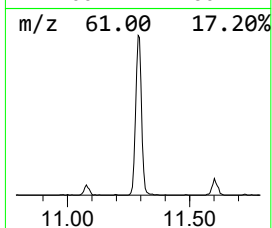
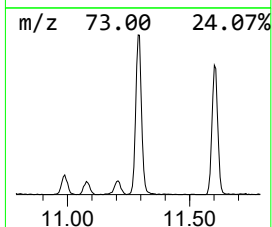
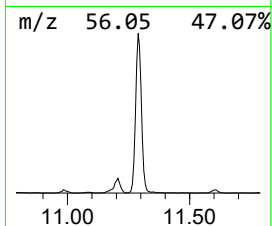
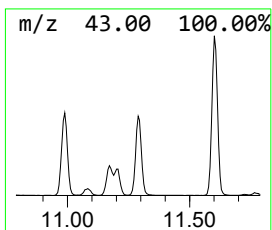
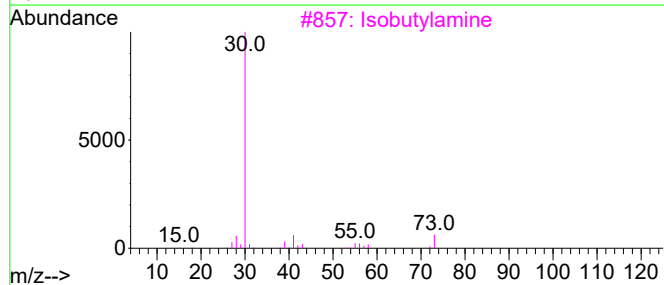
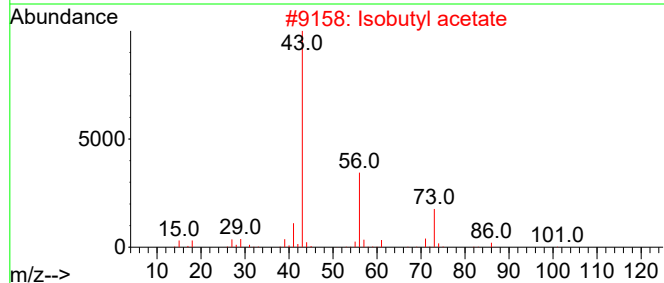
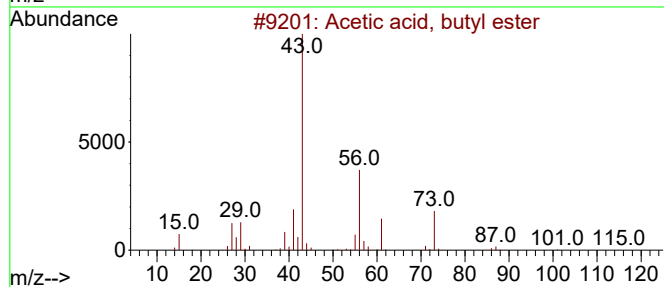
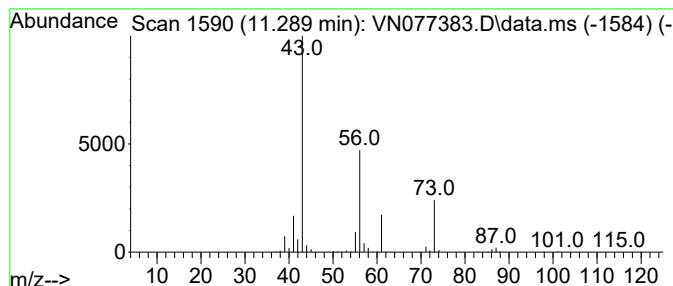
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Quant Title : SW846 8260

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

Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.289	30.11 ug/l	2030110	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			Isobutylamine	73	C4H11N	000078-81-9	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			Isopropyl acetate	102	C5H10O2	000108-21-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041923\
Data File : VN077383.D
Acq On : 19 Apr 2023 18:22
Operator : JC\MD
Sample : PB152199ZHE#11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152199ZHE#11

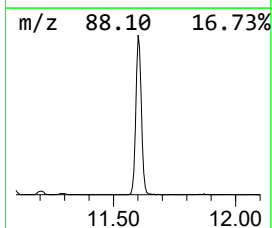
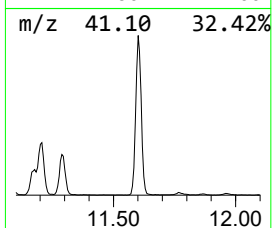
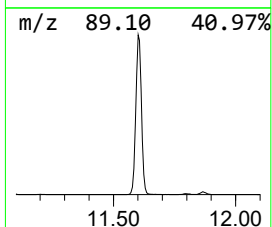
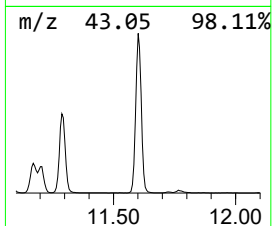
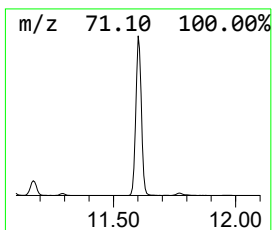
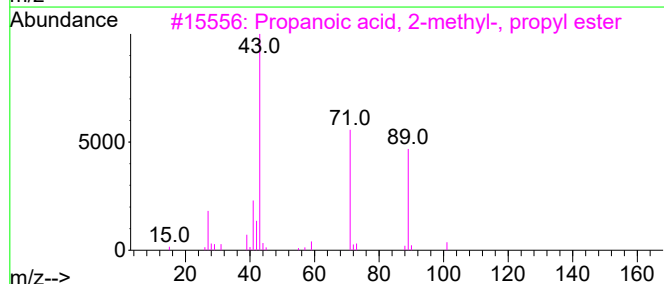
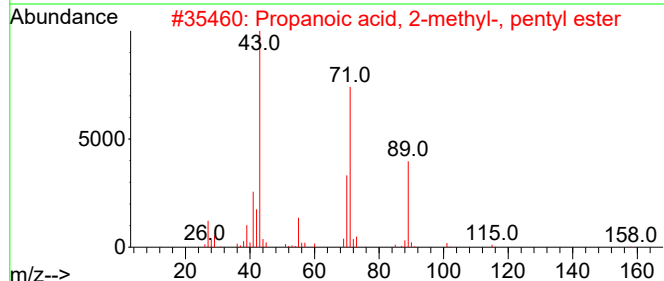
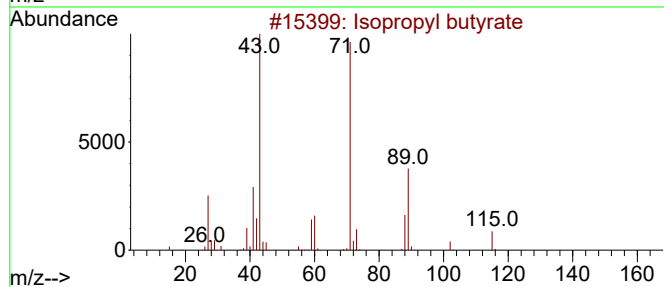
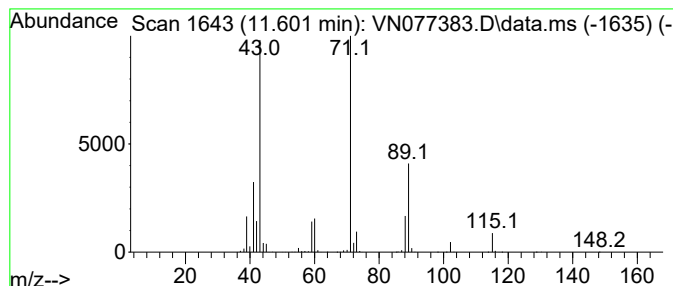
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Quant Title : SW846 8260

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	92.44 ug/l	6232840	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-, penty...	158	C9H18O2	002445-72-9	72
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041923\
Data File : VN077383.D
Acq On : 19 Apr 2023 18:22
Operator : JC\MD
Sample : PB152199ZHE#11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152199ZHE#11

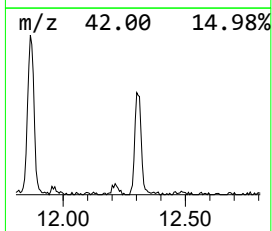
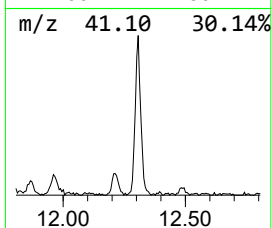
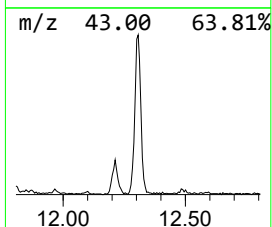
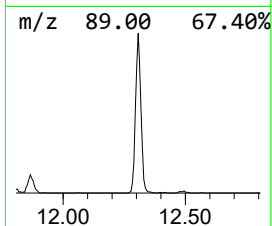
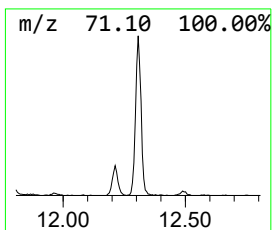
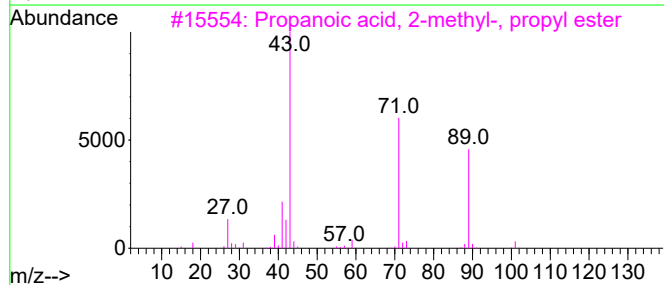
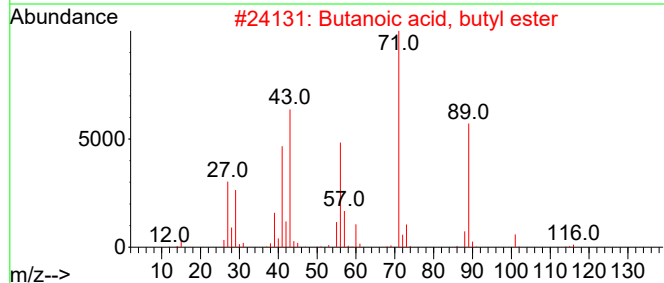
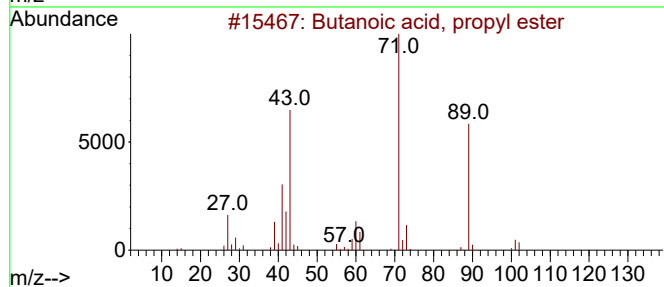
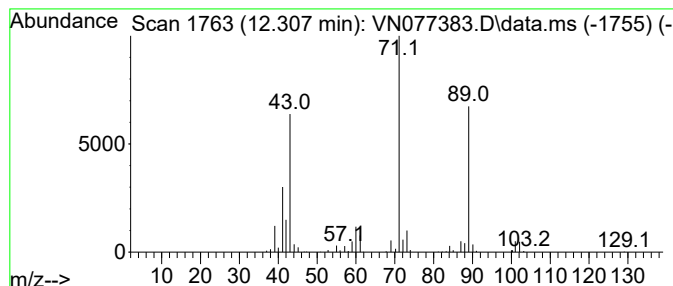
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Quant Title : SW846 8260

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	8.74 ug/l	589028	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041923\
Data File : VN077383.D
Acq On : 19 Apr 2023 18:22
Operator : JC\MD
Sample : PB152199ZHE#11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB152199ZHE#11

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
n-Propyl acetate	9.742	124.3	ug/l	6687000	2	9.107	2690500	50.0
Propanoic acid,...	10.360	28.8	ug/l	1550990	2	9.107	2690500	50.0
Isobutyl acetate	10.730	28.4	ug/l	1912810	3	11.871	3371270	50.0
Propanoic acid,...	10.989	31.6	ug/l	2128650	3	11.871	3371270	50.0
3-Mercaptohexyl...	11.083	6.8	ug/l	459137	3	11.871	3371270	50.0
Propanoic acid,...	11.207	59.0	ug/l	3978690	3	11.871	3371270	50.0
Acetic acid, bu...	11.289	30.1	ug/l	2030110	3	11.871	3371270	50.0
Isopropyl butyrate	11.601	92.4	ug/l	6232840	3	11.871	3371270	50.0
Butanoic acid, ...	12.307	8.7	ug/l	589028	3	11.871	3371270	50.0