LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042023\
Data File : VN077398.D
Acq On : 20 Apr 2023 14:21
Operator : JC\MD
Sample : 02389-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPB-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: VN077398.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	157	rBV5	35851	94286	1.88%	0.294%
2	4.443	418	426	435	rBV2	23022	68624	1.37%	0.214%
3	5.290	558	570	583	rBV2	43272	144581	2.89%	0.451%
4	7.572	950	958	967	rVB	59285	144419	2.88%	0.450%
5	8.172	1051	1060	1065	rBV	422287	1028217	20.53%	3.205%
6	8.231	1065	1070	1080	rVB	751482	1633736	32.62%	5.093%
7	8.584	1113	1130	1140	rBV2	412089	998114	19.93%	3.111%
8	8.695	1140	1149	1158	rBV	341897	741977	14.81%	2.313%
9	9.107	1207	1219	1234	rBV	1064809	2233431	44.59%	6.962%
10	9.678	1306	1316	1321	rBV	170393	380735	7.60%	1.187%
11	9.748	1321	1328	1339	rVB	2697446	5008906	100.00%	15.614%
12	10.360	1423	1432	1441	rBV	727923	1268038	25.32%	3.953%
13	10.572	1459	1468	1477	rBV	1678424	3109981	62.09%	9.695%
14	10.731	1488	1495	1502	rVB	283086	482917	9.64%	1.505%
15	10.989	1531	1539	1549	rBV	850570	1432808	28.61%	4.467%
16	11.083	1549	1555	1562	rVB3	161698	304932	6.09%	0.951%
17	11.207	1571	1576	1584	rVB	1113400	1959938	39.13%	6.110%
18	11.289	1584	1590	1601	rVB	276377	476836	9.52%	1.486%
19	11.601	1634	1643	1656	rBV	2279958	3652061	72.91%	11.385%
20	11.766	1666	1671	1680	rVB2	40313	76941	1.54%	0.240%
21	11.866	1680	1688	1700	rVV	1470561	2665752	53.22%	8.310%
22	12.213	1738	1747	1755	rBV3	31475	55996	1.12%	0.175%
23	12.307	1757	1763	1773	rVB	98430	166926	3.33%	0.520%
24	12.854	1847	1856	1868	rBV	1136453	1933225	38.60%	6.026%
25	13.795	2009	2016	2027	rBV	1179262	2015586	40.24%	6.283%

Sum of corrected areas: 32078963

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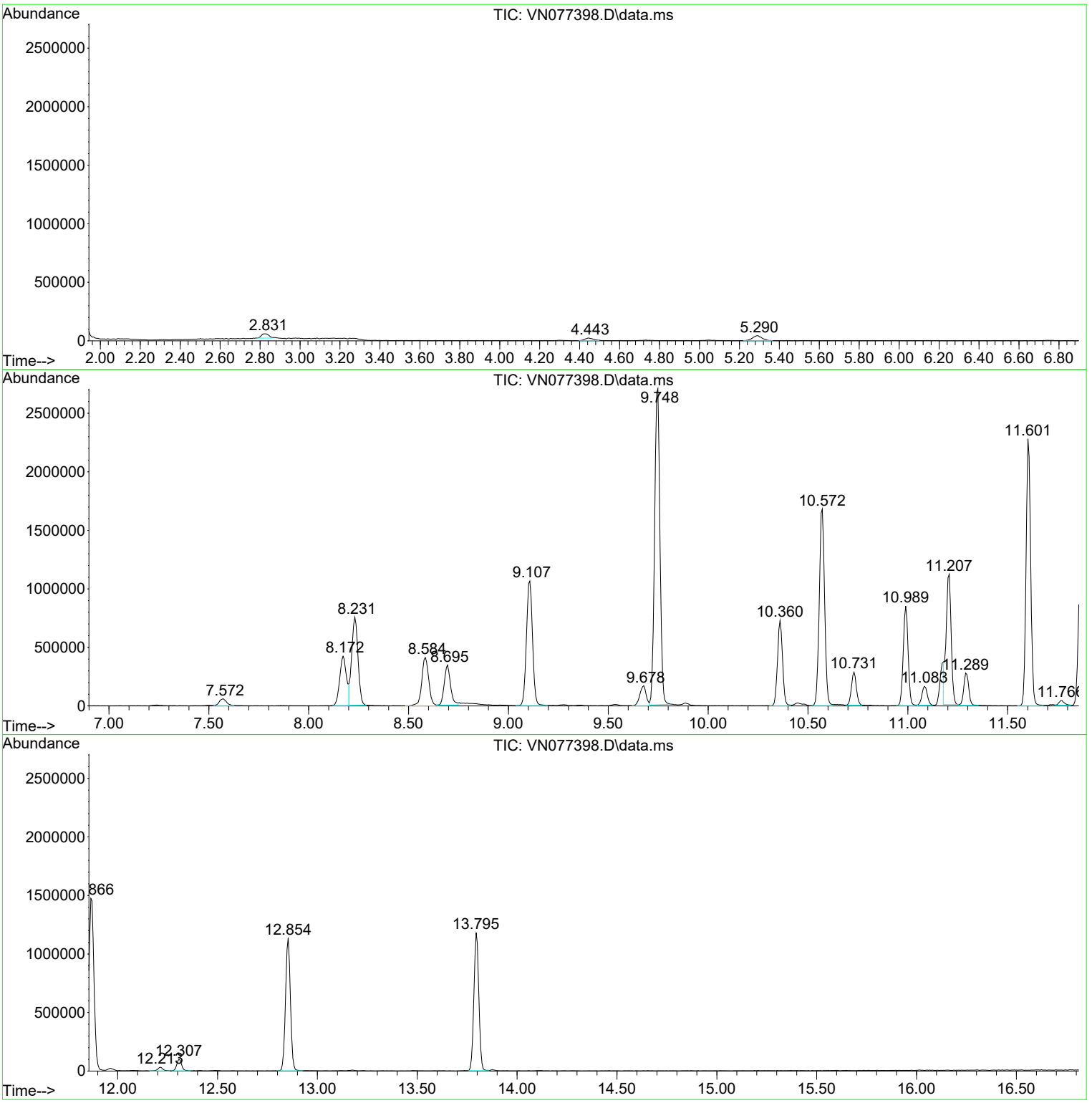
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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



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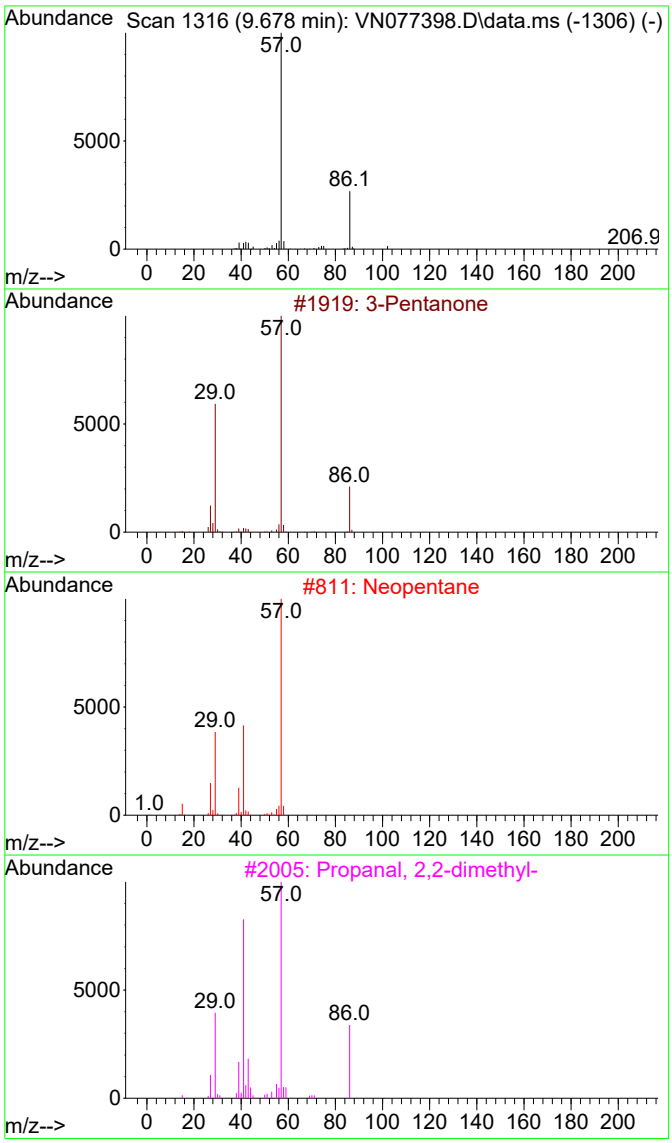
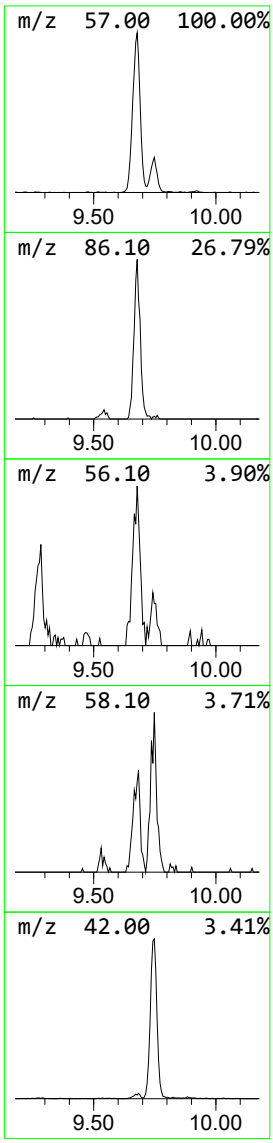
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.678	8.52 ug/l	380735	1,4-Difluorobenzene	9.107

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Neopentane	72	C5H12	000463-82-1	23
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
5	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9





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

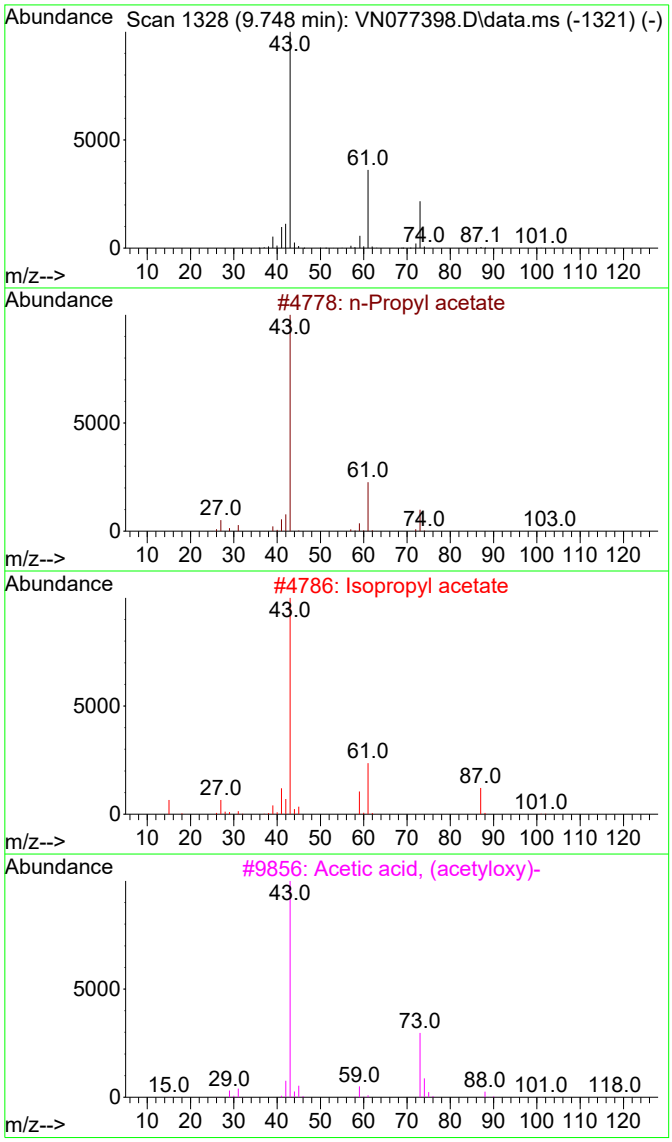
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

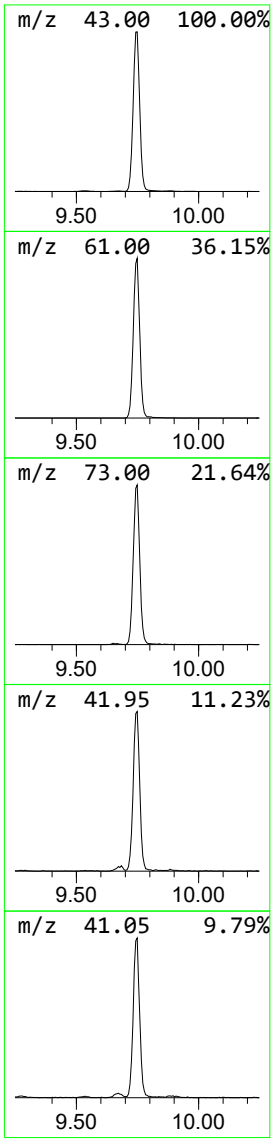
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.748	112.14 ug/l	5008910	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	Isopropyl acetate	102	C5H10O2	000108-21-4	9
3	Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9
4	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
5	Methyl glyoxal	72	C3H4O2	000078-98-8	7





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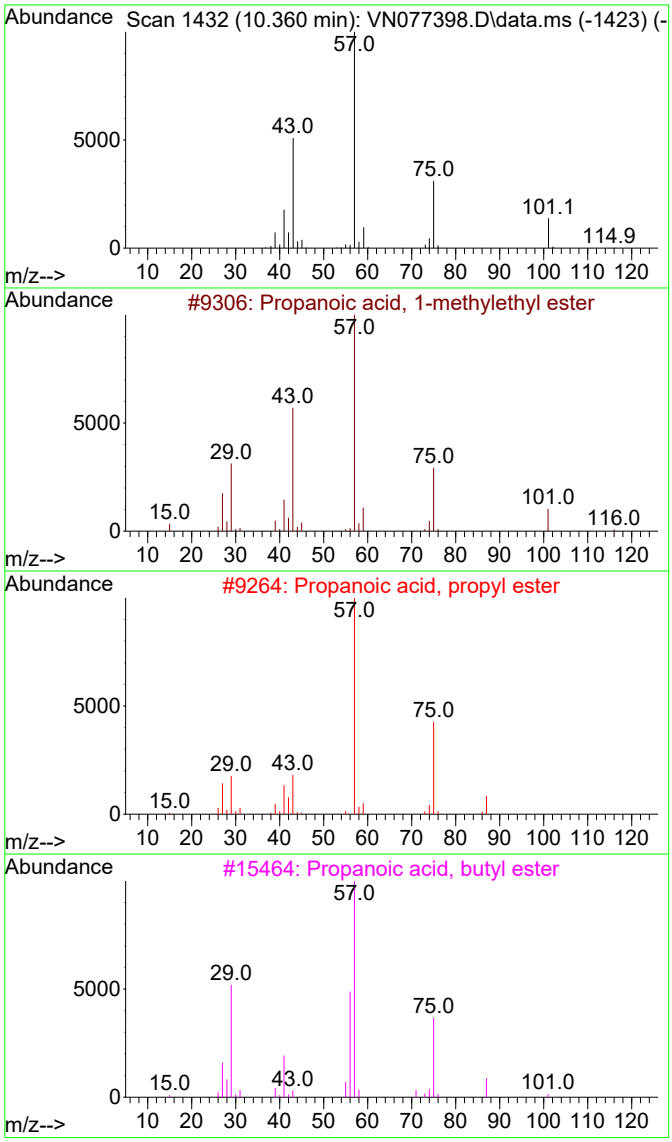
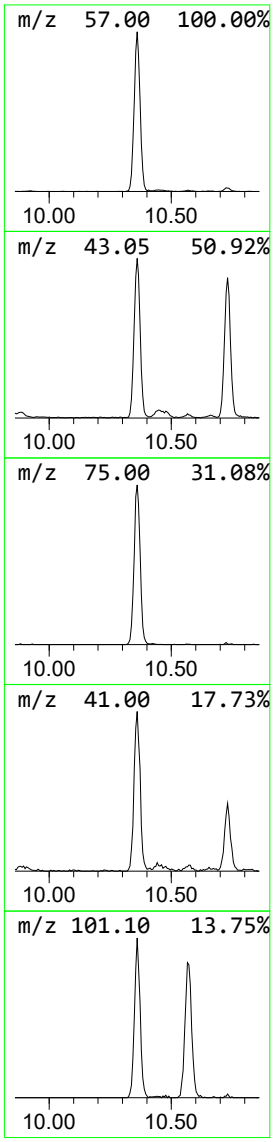
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	28.39 ug/l	1268040	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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10





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ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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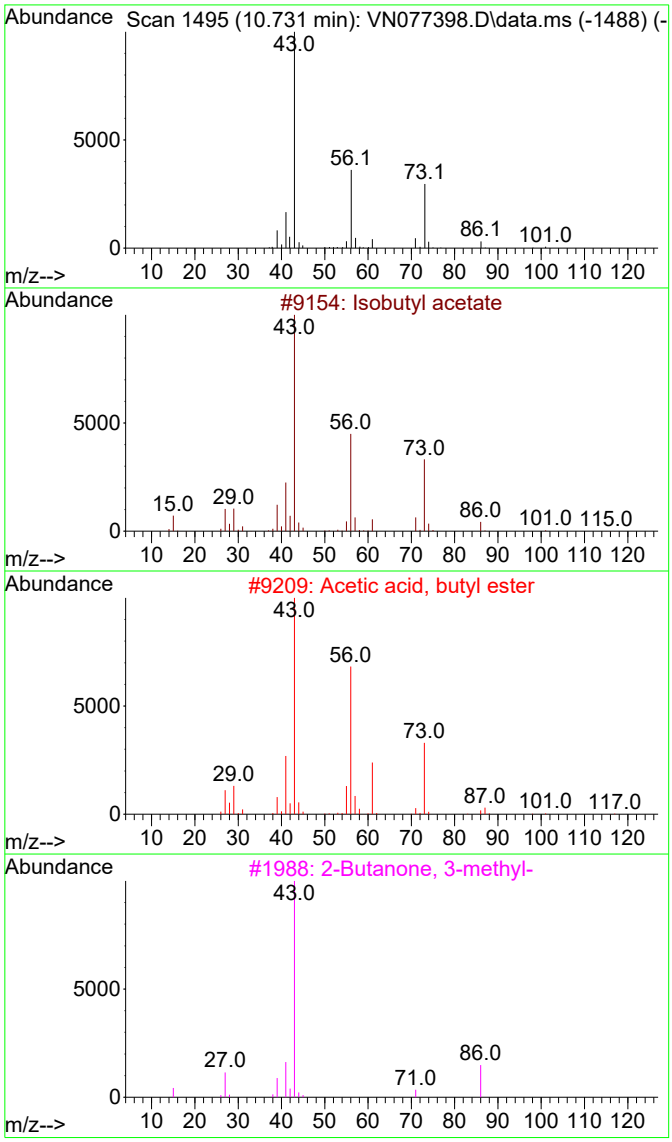
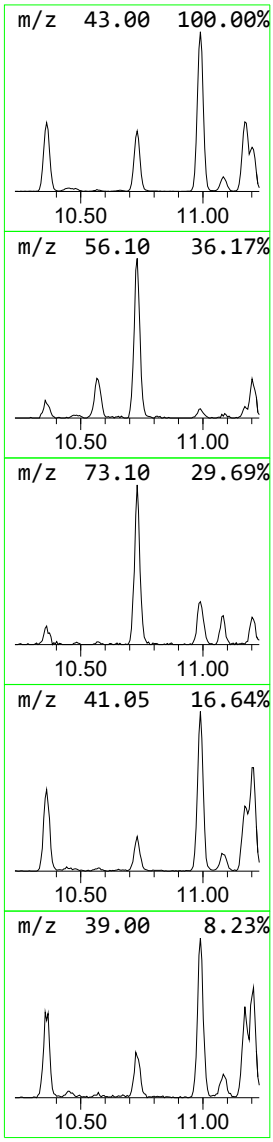
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	9.06 ug/l	482917	Chlorobenzene-d5	11.872

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	90
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	9
5	2-Butoxyethyl acetate	160	C8H16O3	000112-07-2	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
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TIC Library : C:\Database\NIST20.L
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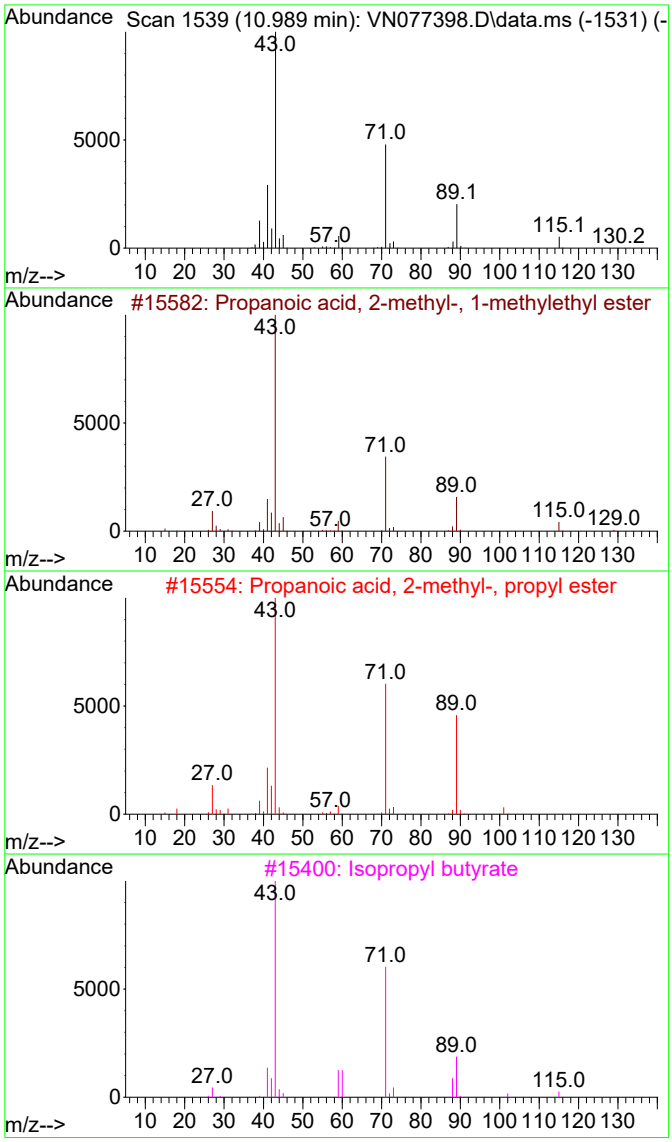
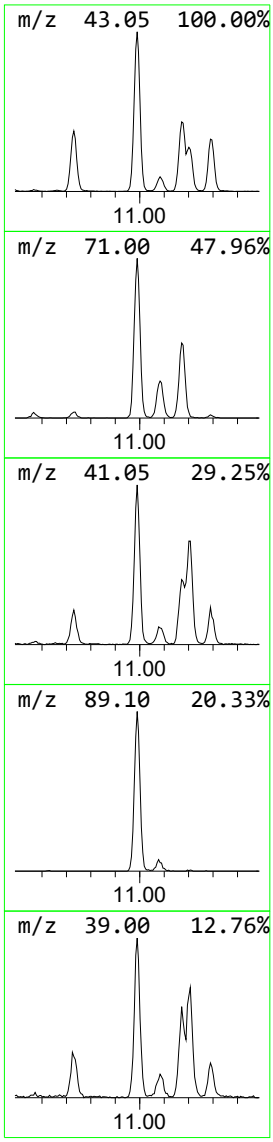
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	26.87 ug/l	1432810	Chlorobenzene-d5	11.872

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	72
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	50





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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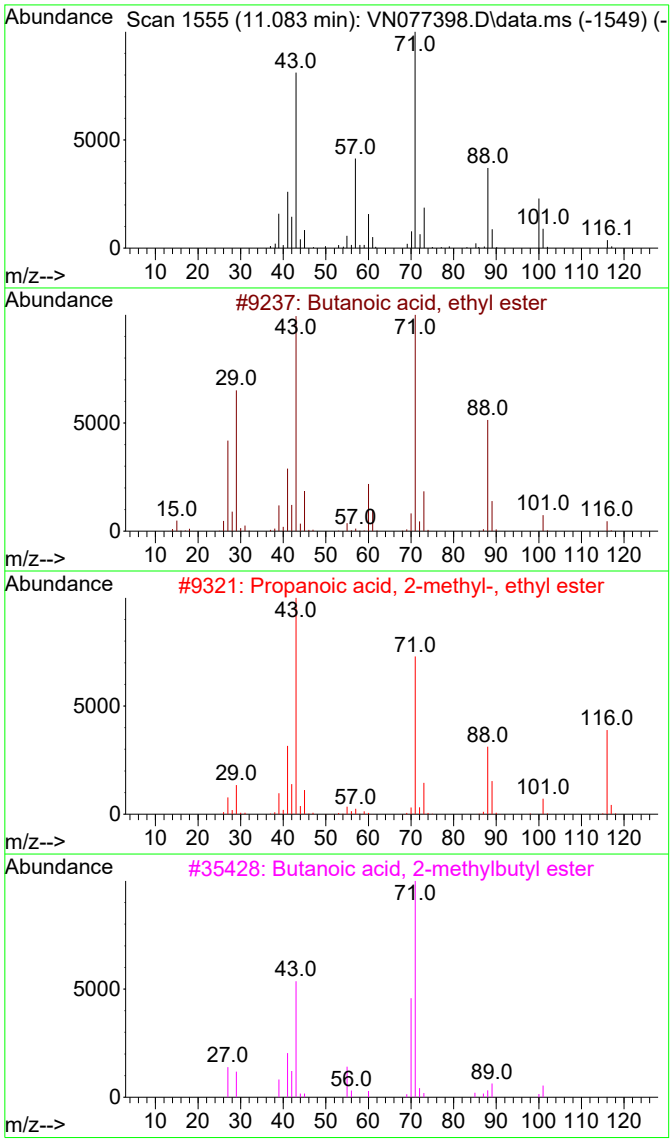
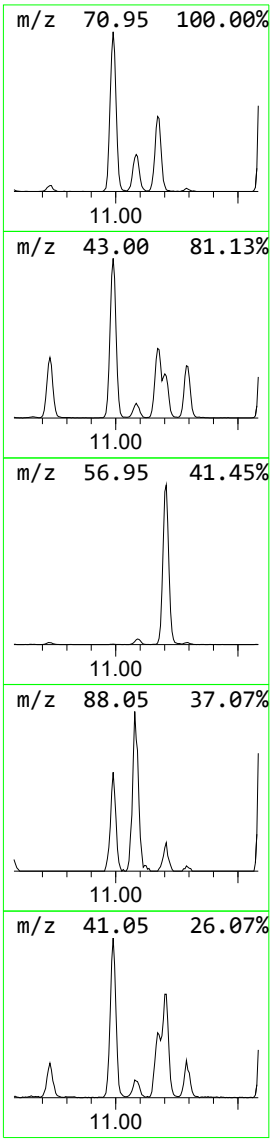
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.083	5.72 ug/l	304932	Chlorobenzene-d5	11.872

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	74
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	68
3	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	47
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	47
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	43





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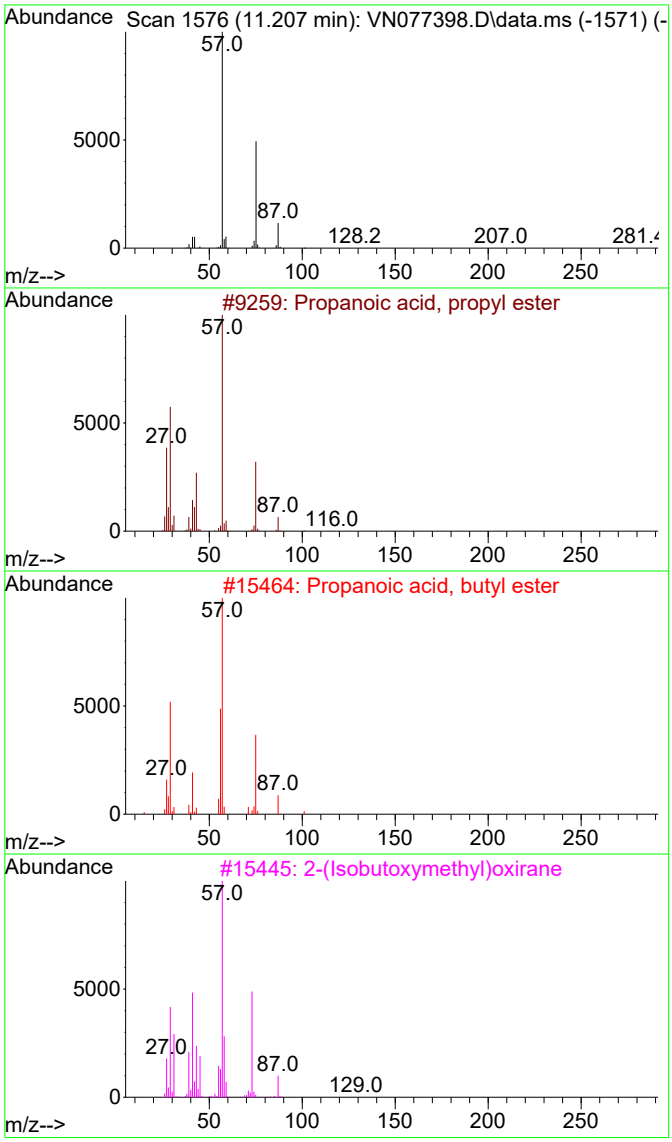
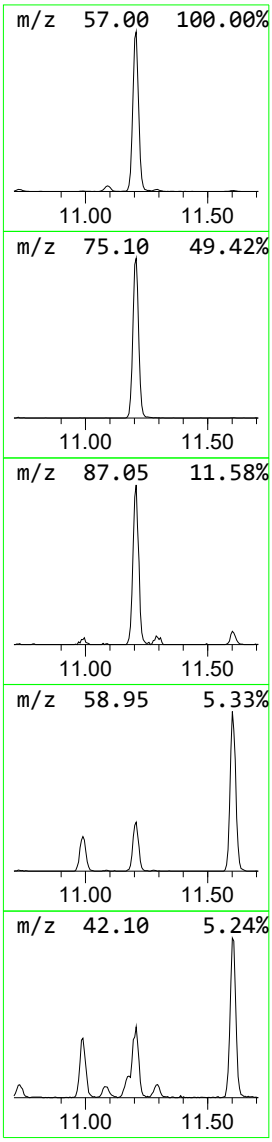
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.207	36.76 ug/l	1959940	Chlorobenzene-d5	11.872

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-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	1-Penten-3-ol	86	C5H10O	000616-25-1	7
5	Morpholine	87	C4H9NO	000110-91-8	4





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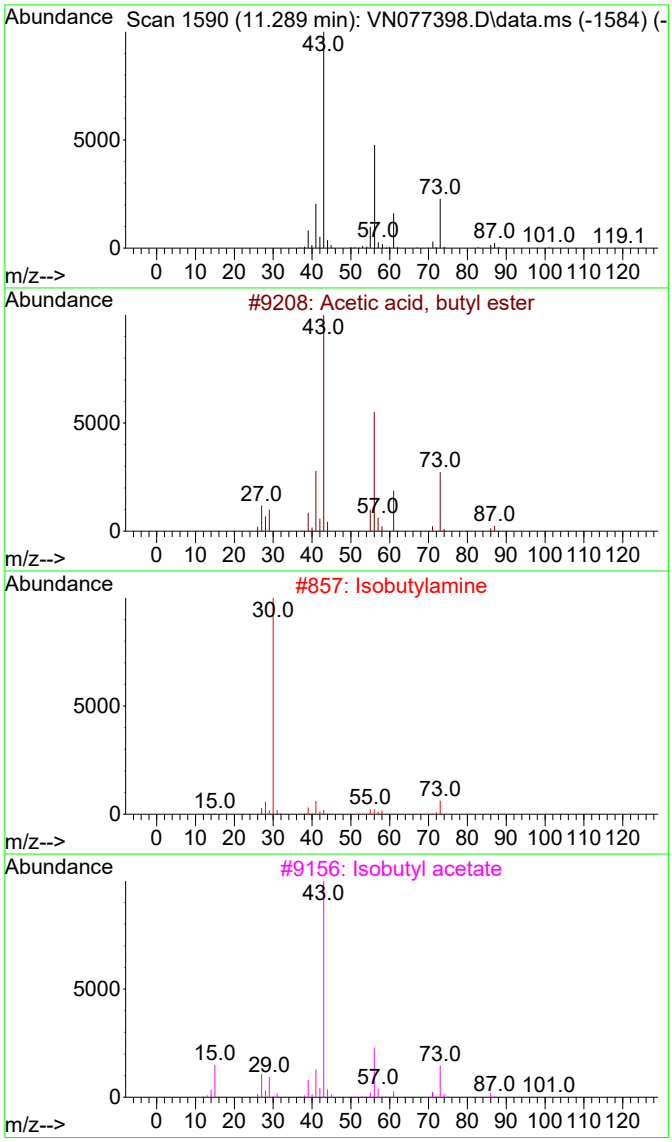
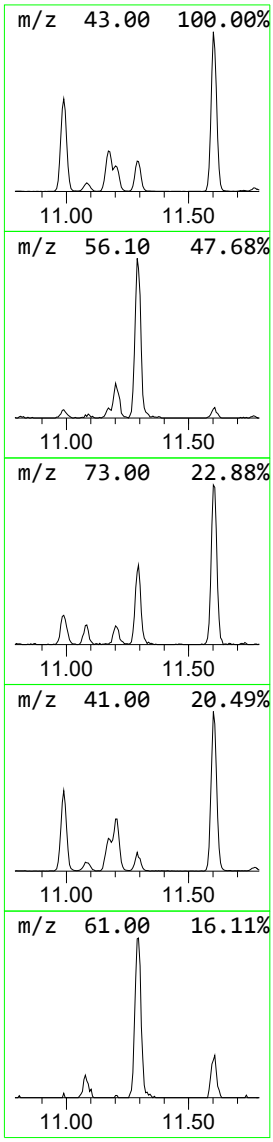
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.289	8.94 ug/l	476836	Chlorobenzene-d5	11.872

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9





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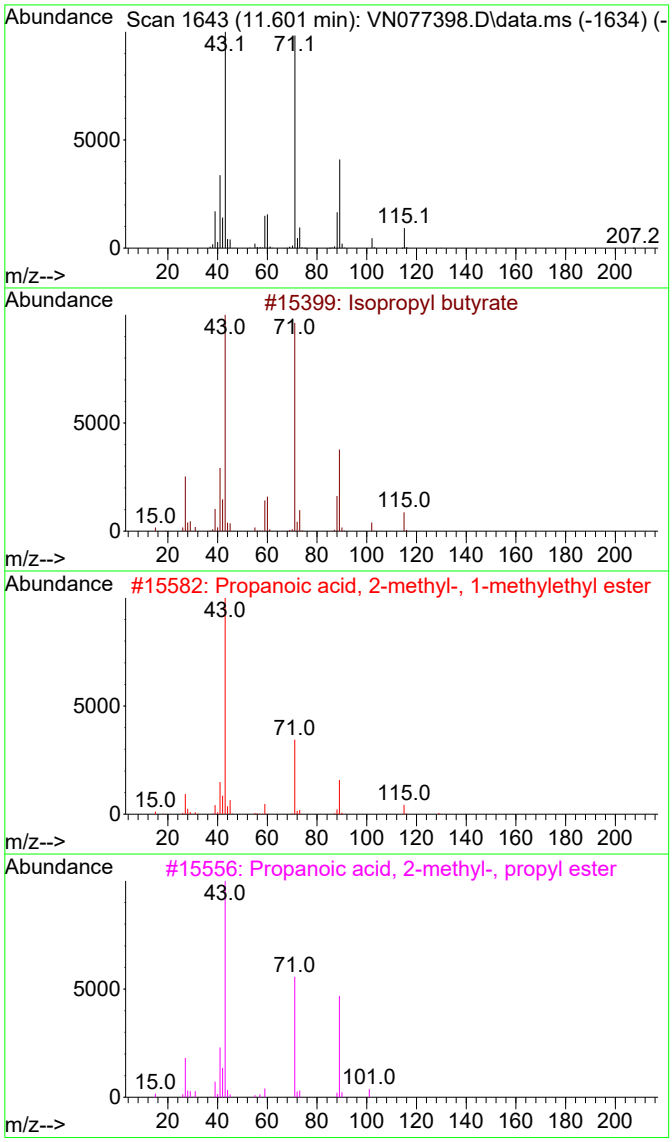
Quant Title : SW846 8260

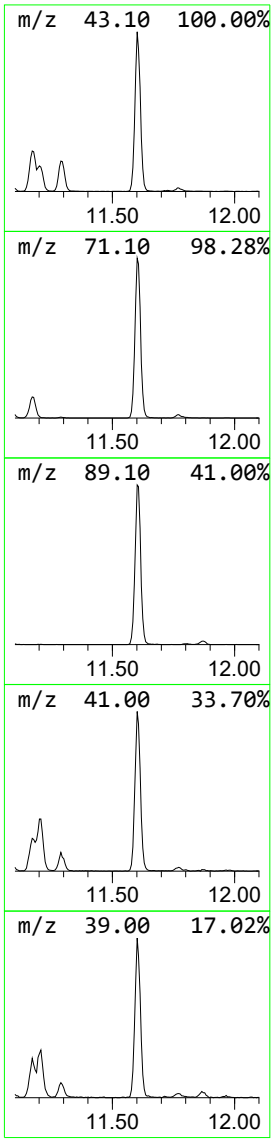
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.601	68.50 ug/l	3652060	Chlorobenzene-d5	11.872

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	59





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Pentanone	9.678	8.5	ug/l	380735	2	9.107	2233430	50.0
n-Propyl acetate	9.748	112.1	ug/l	5008910	2	9.107	2233430	50.0
Propanoic acid,...	10.360	28.4	ug/l	1268040	2	9.107	2233430	50.0
Isobutyl acetate	10.730	9.1	ug/l	482917	3	11.872	2665750	50.0
Propanoic acid,...	10.989	26.9	ug/l	1432810	3	11.872	2665750	50.0
Butanoic acid, ...	11.083	5.7	ug/l	304932	3	11.872	2665750	50.0
Propanoic acid,...	11.207	36.8	ug/l	1959940	3	11.872	2665750	50.0
Acetic acid, bu...	11.289	8.9	ug/l	476836	3	11.872	2665750	50.0
Isopropyl butyrate	11.601	68.5	ug/l	3652060	3	11.872	2665750	50.0