LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078055.D
Acq On : 05 Jun 2023 19:33
Operator : JC\MD
Sample : 03018-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
72-11991

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\82N051523W.M
Title : SW846 8260

Signal : TIC: VN078055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.830	141	149	155	rVB3	29920	66180	1.62%	0.250%
2	5.289	554	567	577	rBV4	17207	56806	1.39%	0.214%
3	7.577	948	956	965	rBV3	38668	96260	2.35%	0.363%
4	8.177	1047	1058	1062	rBV	317389	752062	18.38%	2.839%
5	8.230	1062	1067	1080	rVB	530848	1199288	29.31%	4.527%
6	8.588	1117	1128	1137	rBV	328624	723712	17.69%	2.732%
7	8.694	1137	1146	1158	rBV	270217	711458	17.39%	2.686%
8	9.106	1208	1216	1233	rBV	770452	1637157	40.01%	6.180%
9	9.677	1302	1313	1318	rBV	105581	234960	5.74%	0.887%
10	9.747	1318	1325	1340	rVV	2233773	4092204	100.00%	15.447%
11	10.365	1422	1430	1439	rBV	535747	910147	22.24%	3.436%
12	10.571	1457	1465	1476	rBV	1228348	2314760	56.57%	8.737%
13	10.735	1486	1493	1505	rVB	602105	1064440	26.01%	4.018%
14	10.994	1529	1537	1544	rBV	716523	1201736	29.37%	4.536%
15	11.088	1547	1553	1561	rVV4	116708	228913	5.59%	0.864%
16	11.206	1561	1573	1582	rVV2	946676	2034084	49.71%	7.678%
17	11.294	1582	1588	1600	rVB	565598	935537	22.86%	3.531%
18	11.606	1633	1641	1652	rBV	1989032	3126670	76.41%	11.802%
19	11.771	1664	1669	1678	rVB2	28776	53322	1.30%	0.201%
20	11.871	1678	1686	1696	rVV	1102596	2009799	49.11%	7.586%
21	12.306	1753	1760	1769	rBV2	109306	195221	4.77%	0.737%
22	12.853	1845	1853	1862	rBV	850668	1481456	36.20%	5.592%
23	13.800	2004	2014	2024	rBV	785672	1366119	33.38%	5.157%

Sum of corrected areas: 26492291

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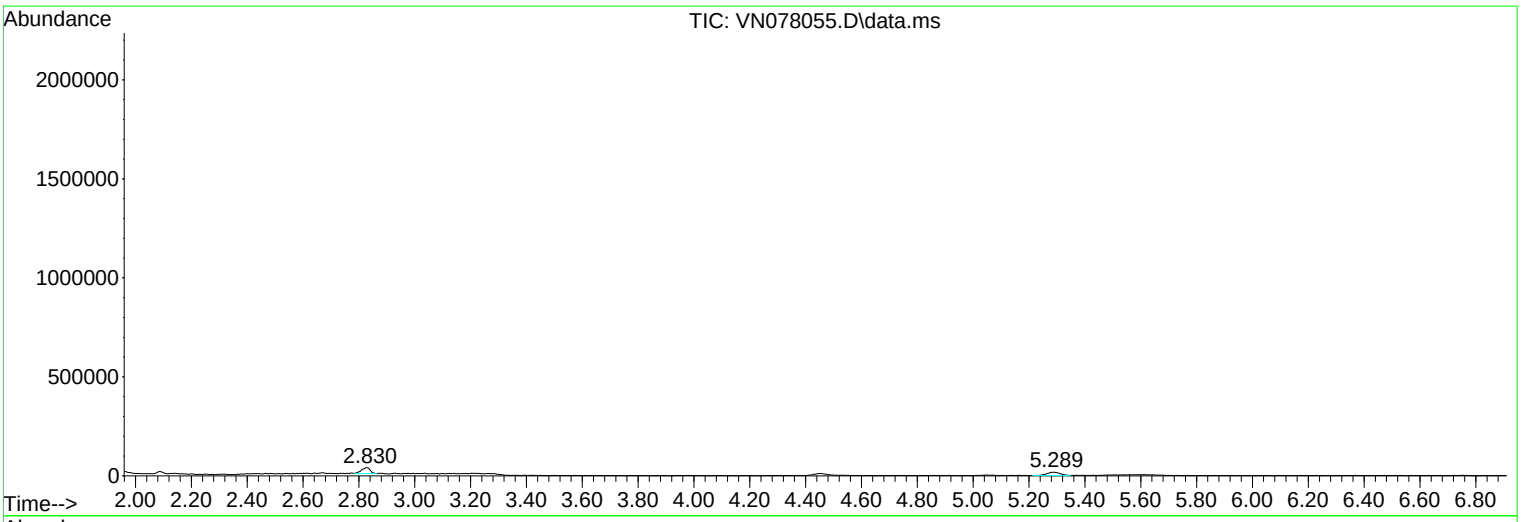
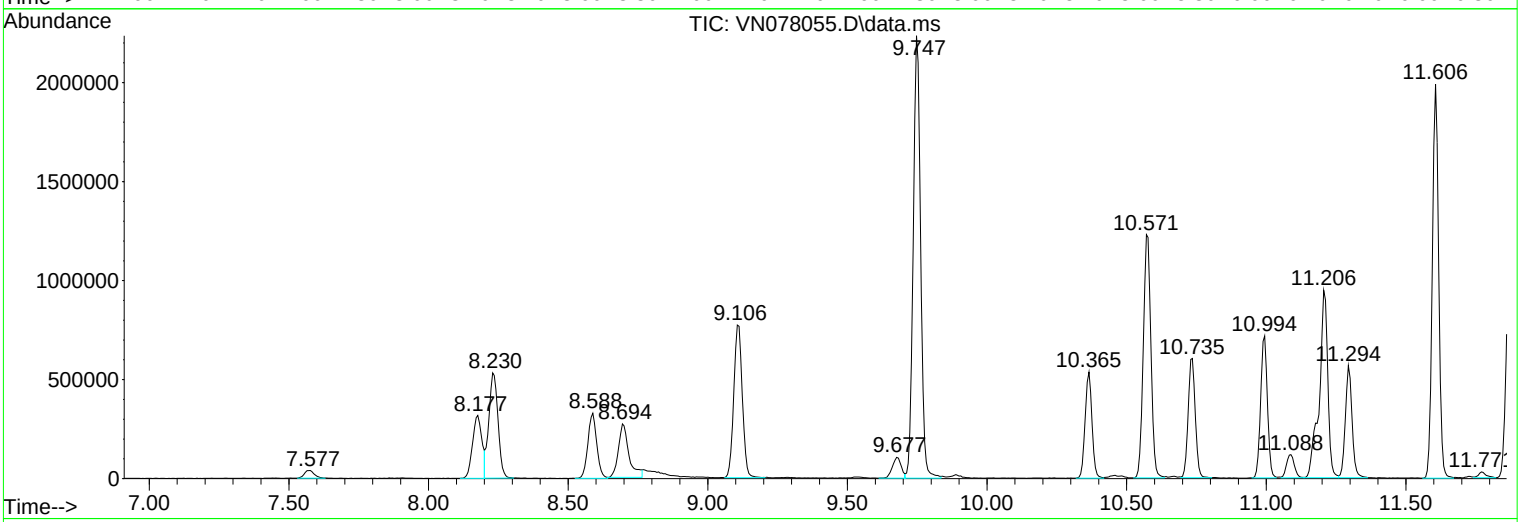
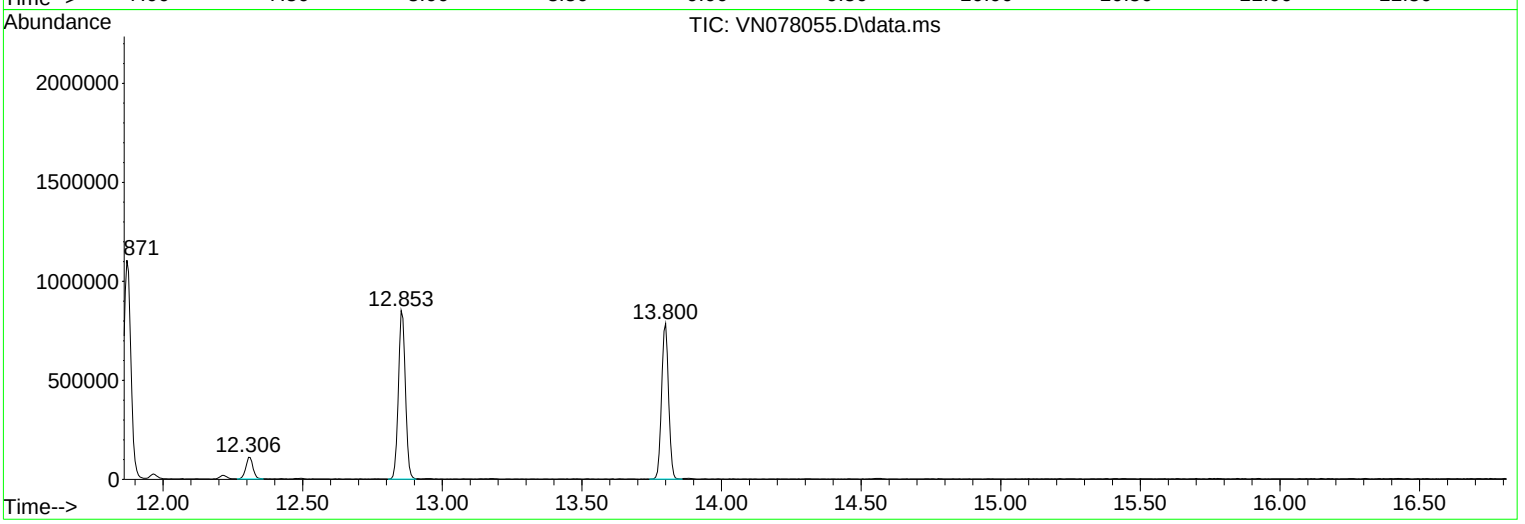
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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







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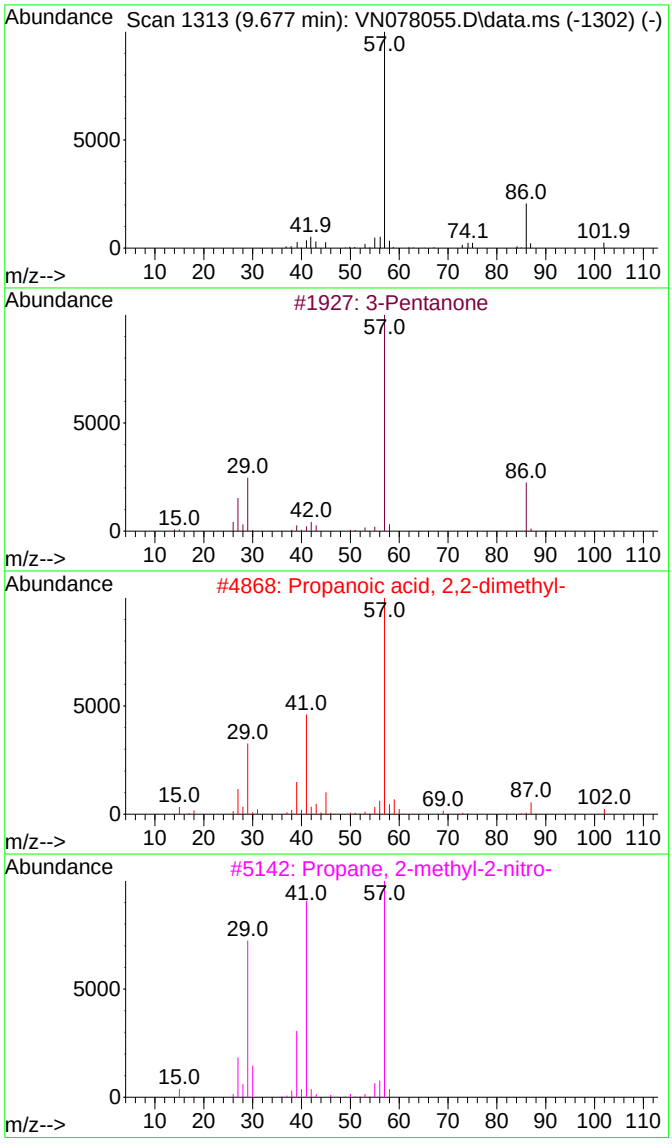
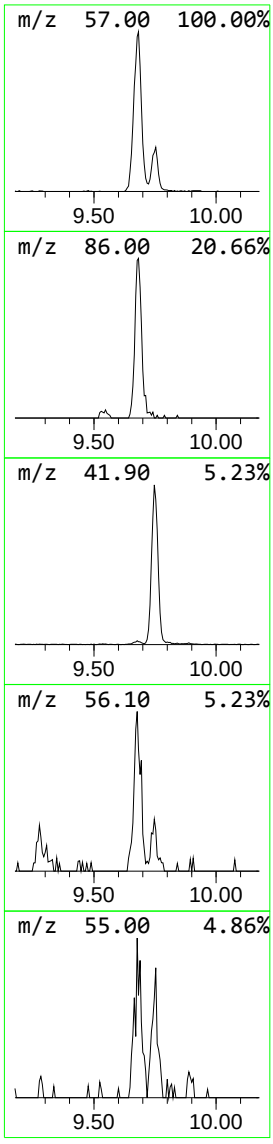
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	7.18 ug/l	234960	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	25
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	25
5	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	23





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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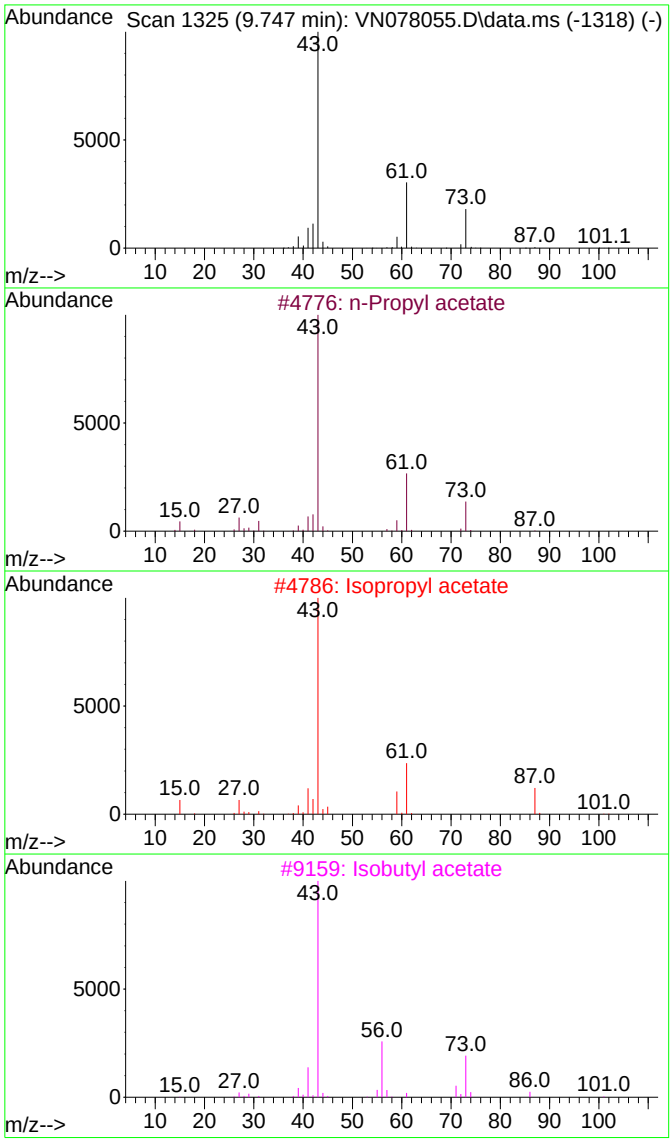
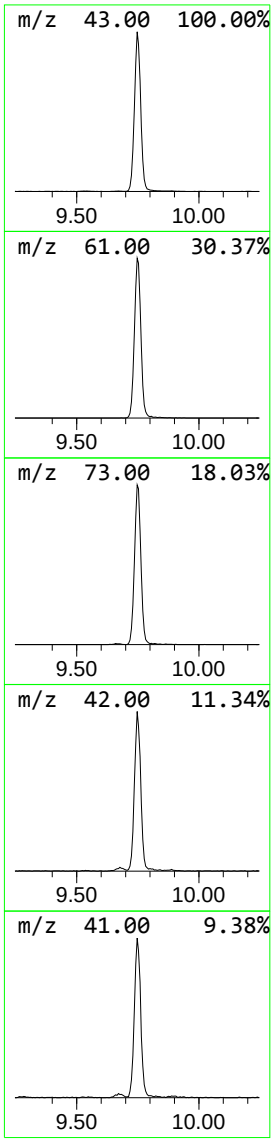
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	124.98 ug/l	4092200	1,4-Difluorobenzene	9.106

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	38
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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ClientSampleId :
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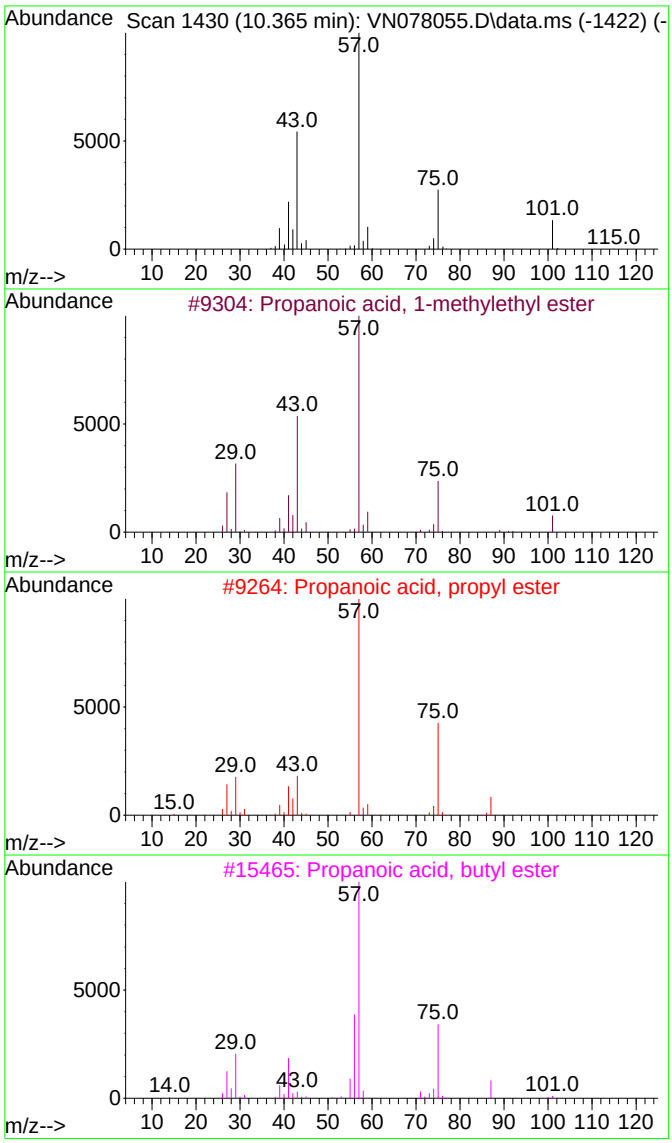
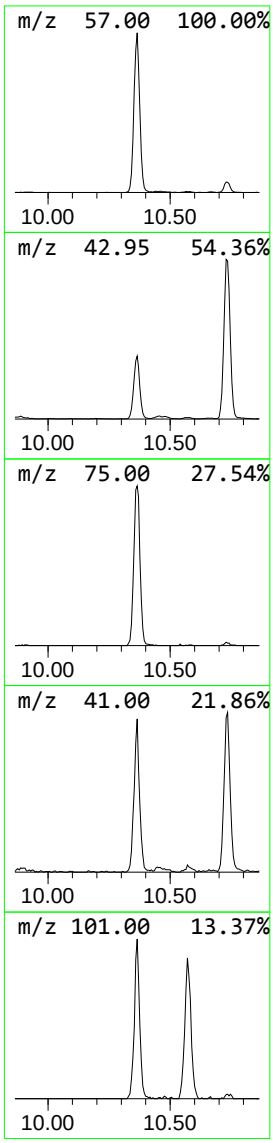
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	27.80 ug/l	910147	1,4-Difluorobenzene	9.106

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	64
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Azetidine	57	C3H7N	000503-29-7	12
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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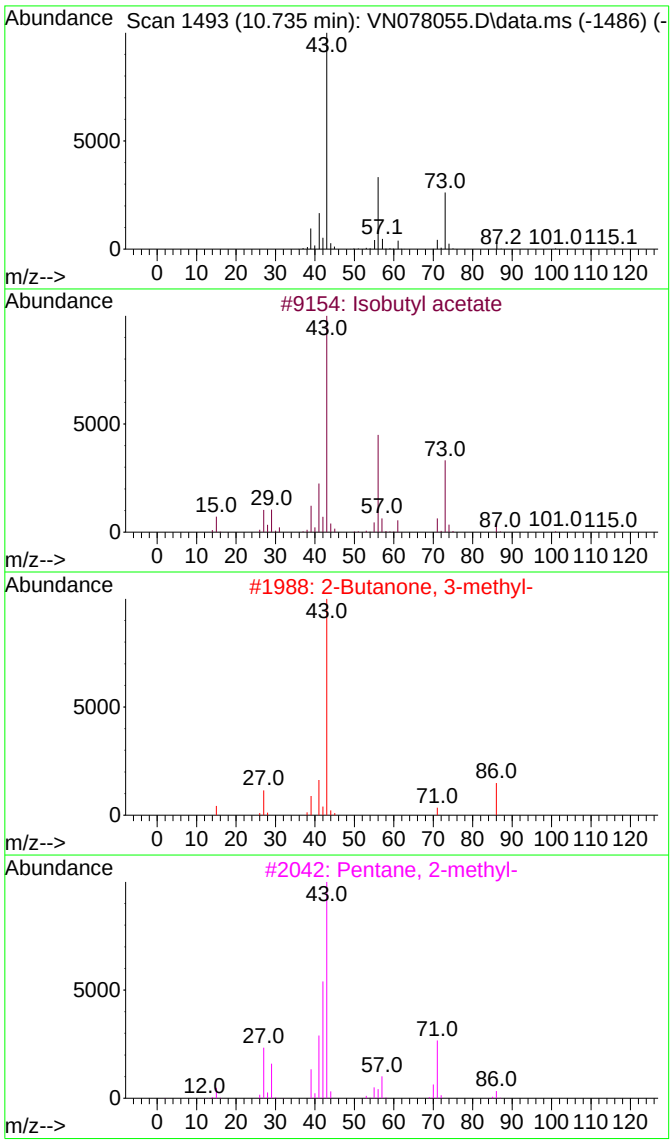
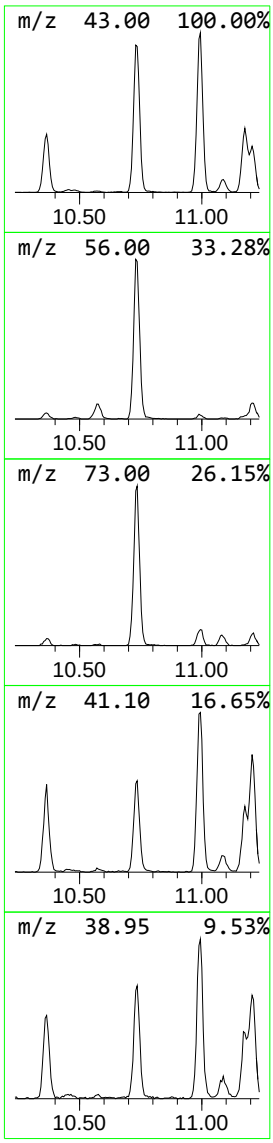
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	26.48 ug/l	1064440	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	90
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	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





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TIC Library : C:\Database\NIST20.L
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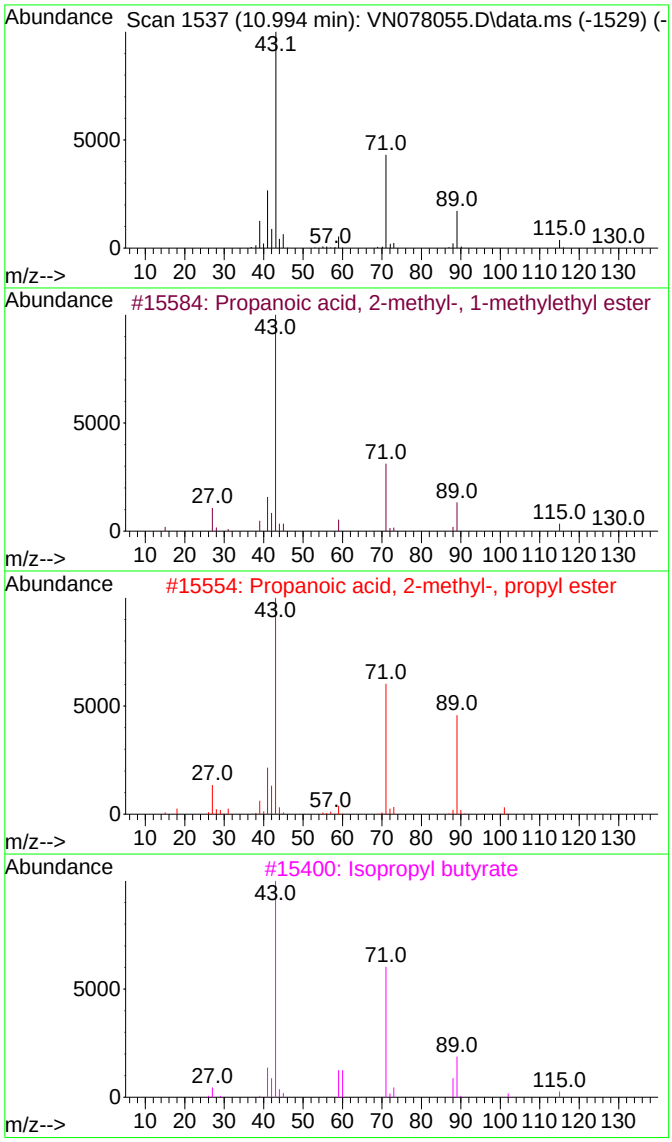
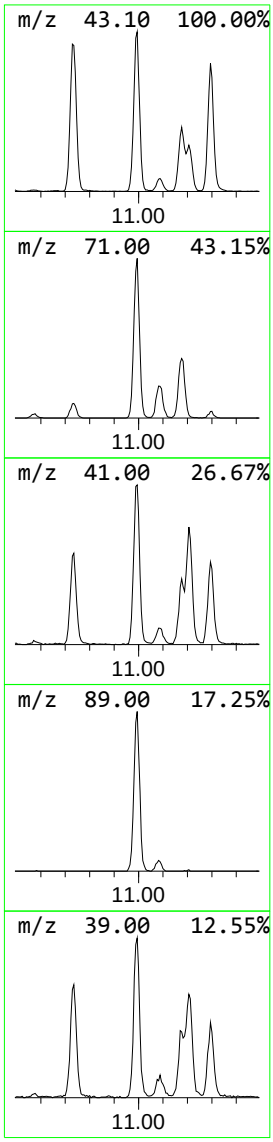
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	29.90 ug/l	1201740	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	50
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





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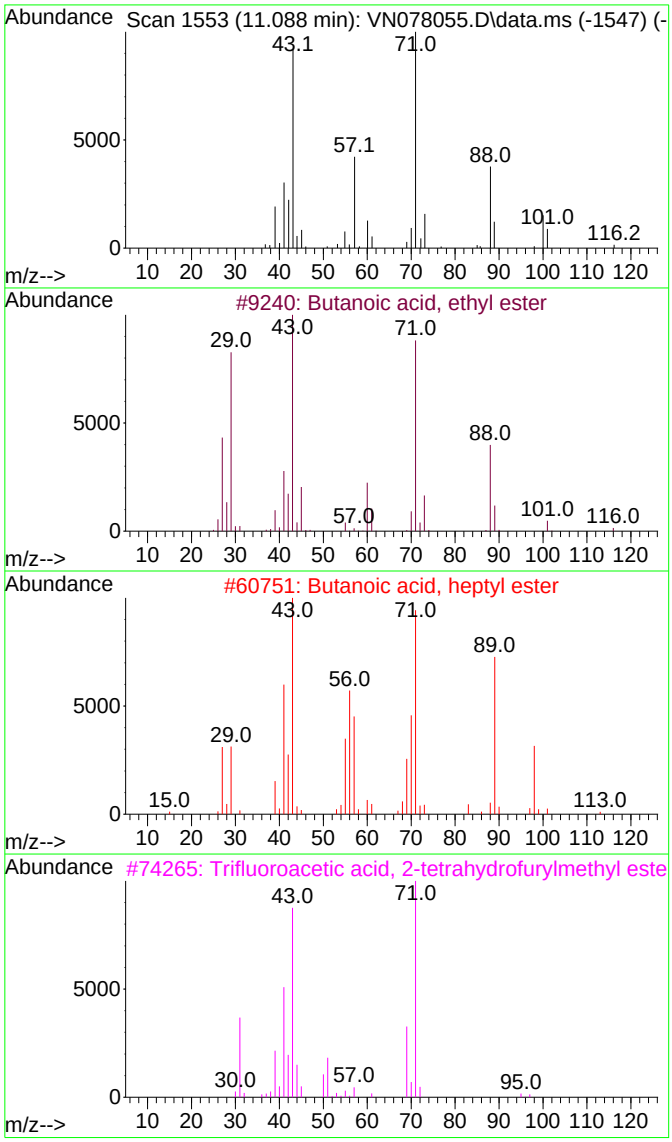
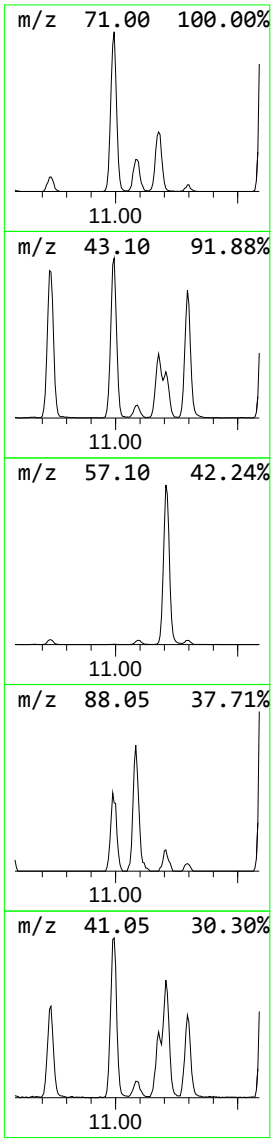
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	5.69 ug/l	228913	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	80
2	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	50
3	Trifluoroacetic acid, 2-tetrahyd...	198	C7H9F3O3	071239-15-1	47
4	Pentane, 1-bromo-	150	C5H11Br	000110-53-2	47
5	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	45





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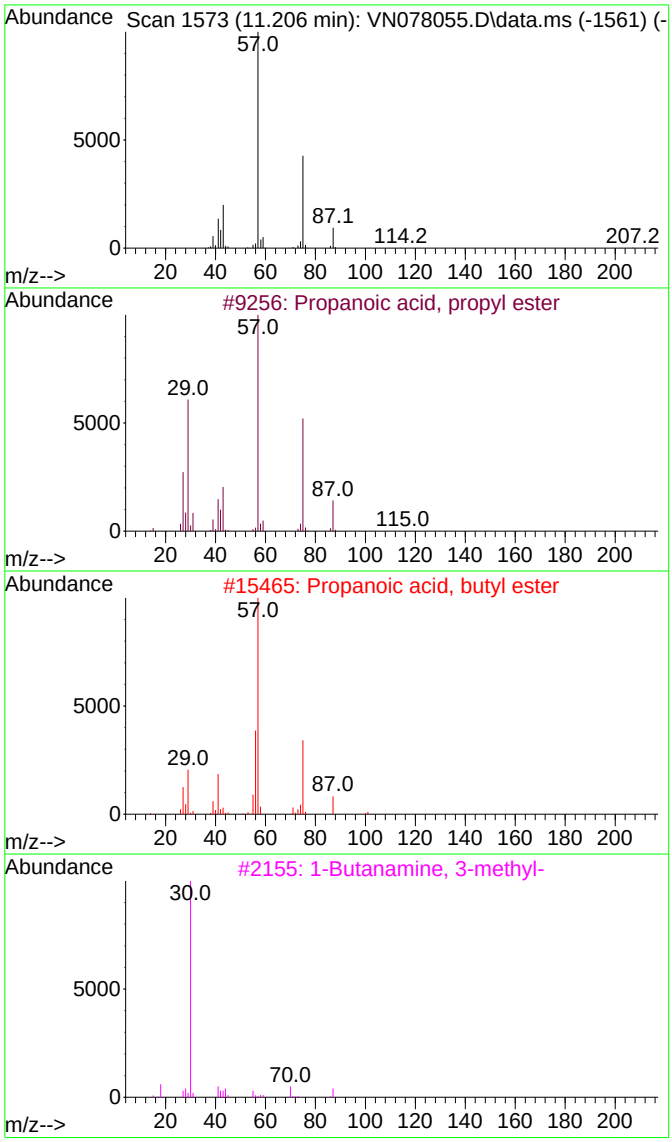
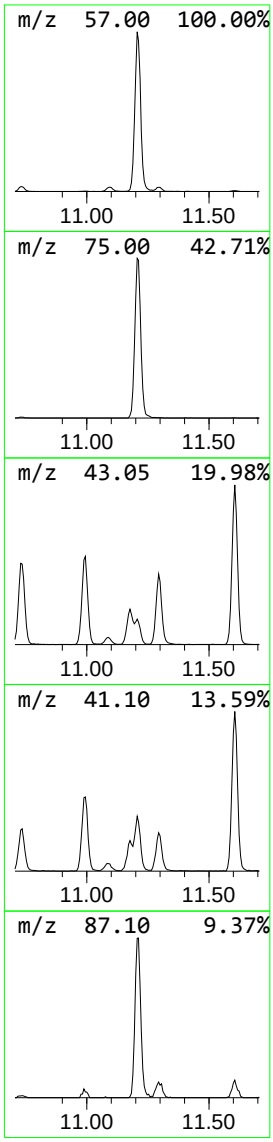
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	50.60 ug/l	2034080	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-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





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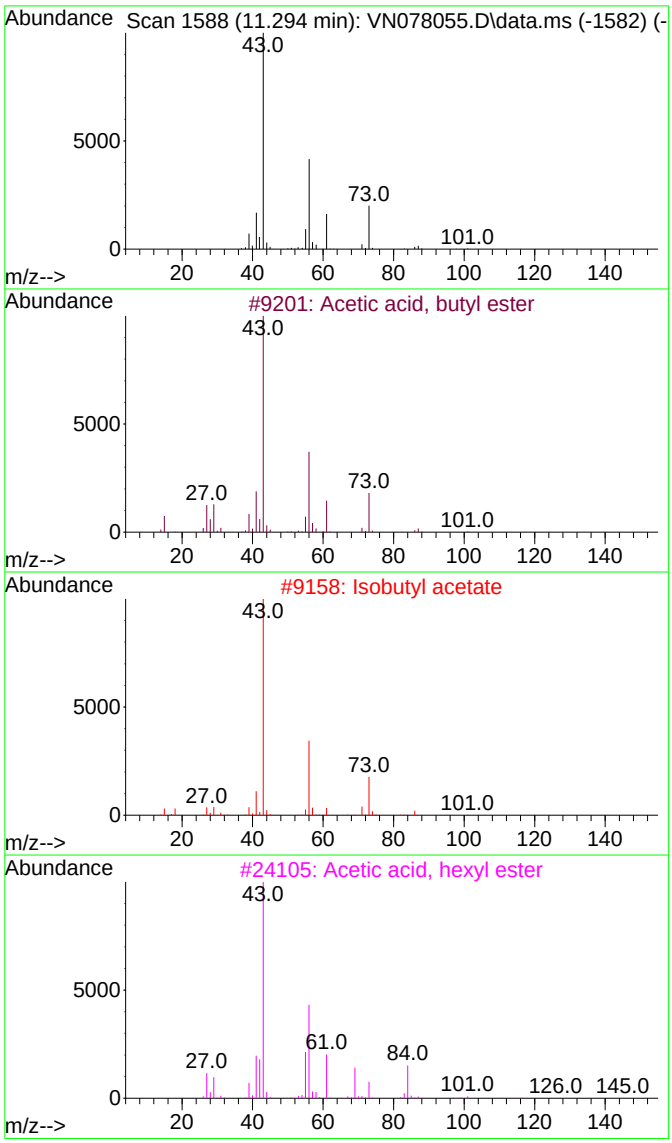
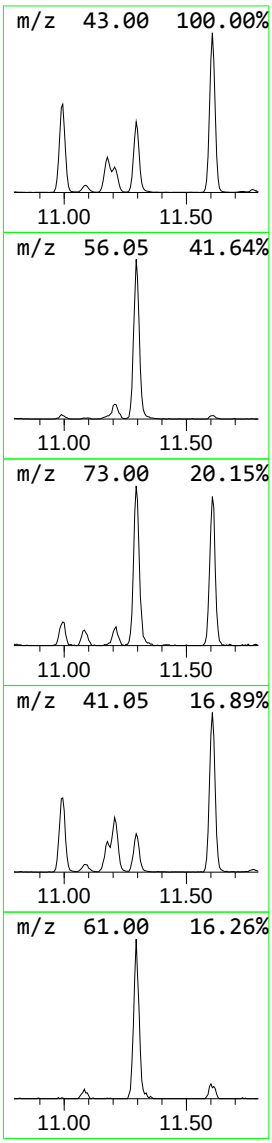
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	23.27 ug/l	935537	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
5	Isobutylamine	73	C4H11N	000078-81-9	9





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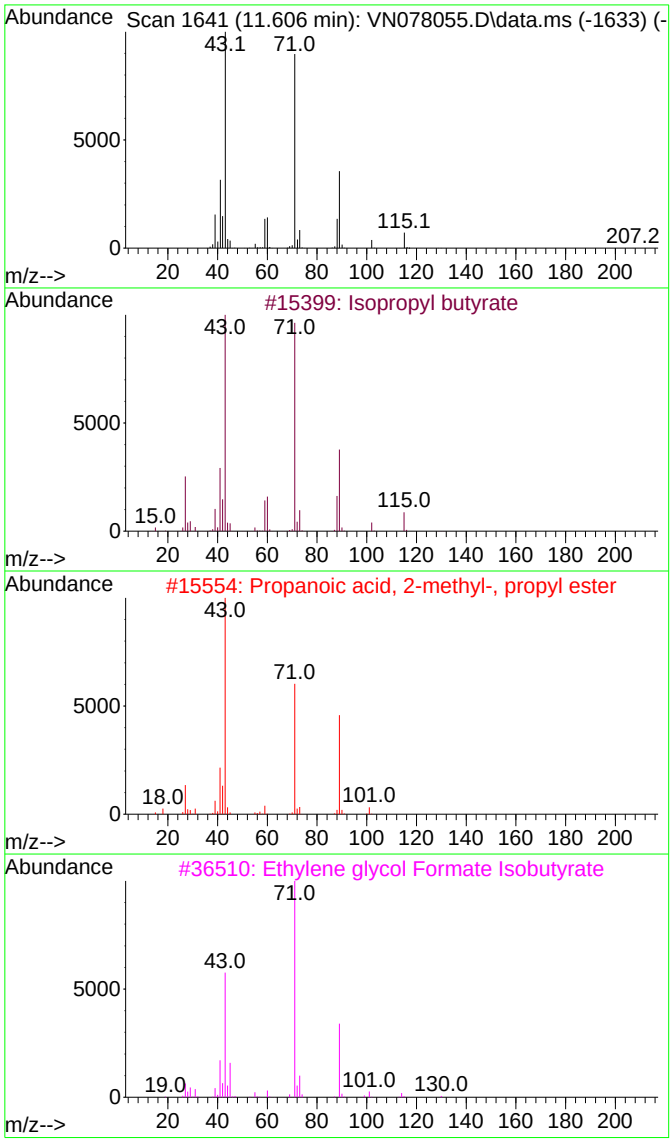
Quant Title : SW846 8260

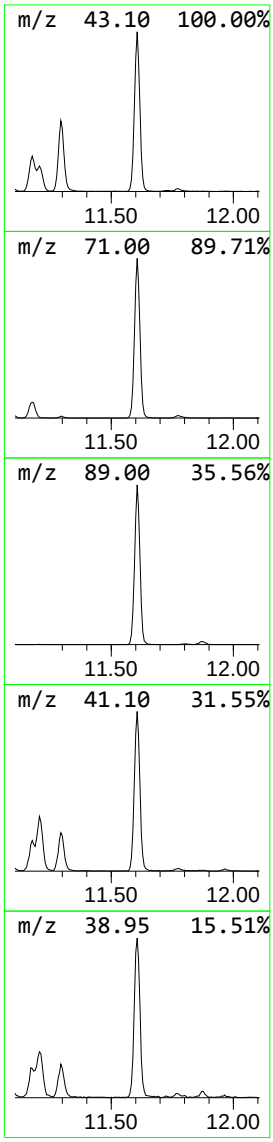
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	77.79 ug/l	3126670	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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56





Tentatively Identified Compound (LSC) summary

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Data File : VN078055.D
Acq On : 05 Jun 2023 19:33
Operator : JC\MD
Sample : 03018-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
72-11991

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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	9.677	7.2	ug/l	234960	2	9.106	1637160	50.0
n-Propyl acetate	9.747	125.0	ug/l	4092200	2	9.106	1637160	50.0
Propanoic acid,...	10.365	27.8	ug/l	910147	2	9.106	1637160	50.0
Isobutyl acetate	10.735	26.5	ug/l	1064440	3	11.871	2009800	50.0
Propanoic acid,...	10.994	29.9	ug/l	1201740	3	11.871	2009800	50.0
Butanoic acid, ...	11.088	5.7	ug/l	228913	3	11.871	2009800	50.0
Propanoic acid,...	11.206	50.6	ug/l	2034080	3	11.871	2009800	50.0
Acetic acid, bu...	11.294	23.3	ug/l	935537	3	11.871	2009800	50.0
Isopropyl butyrate	11.606	77.8	ug/l	3126670	3	11.871	2009800	50.0