LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011723\
Data File : VN076279.D
Acq On : 17 Jan 2023 14:48
Operator : JC\MD
Sample : 01159-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-E

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\82N011623W.M
Title : SW846 8260

Signal : TIC: VN076279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.448	399	407	419	rBV	16283	48727	2.19%	0.272%
2	5.289	538	550	562	rBV3	18269	59064	2.65%	0.329%
3	7.571	931	938	946	rVB3	18586	42706	1.92%	0.238%
4	8.171	1031	1040	1045	rBV	229770	578312	25.96%	3.226%
5	8.230	1045	1050	1065	rVB	460243	1003311	45.04%	5.597%
6	8.583	1097	1110	1118	rBV	238700	533808	23.96%	2.978%
7	8.695	1118	1129	1139	rBV	156532	448556	20.14%	2.502%
8	9.106	1191	1199	1214	rVB	621185	1268445	56.94%	7.076%
9	9.677	1287	1296	1301	rBV	72923	154616	6.94%	0.863%
10	9.747	1301	1308	1320	rVB	1207165	2227697	100.00%	12.427%
11	10.359	1403	1412	1421	rBV	314256	545905	24.51%	3.045%
12	10.447	1421	1427	1437	rVB4	15134	35392	1.59%	0.197%
13	10.571	1439	1448	1458	rBV	920012	1723587	77.37%	9.615%
14	10.730	1468	1475	1495	rVB	299719	510730	22.93%	2.849%
15	10.989	1511	1519	1529	rBV	467411	776892	34.87%	4.334%
16	11.083	1529	1535	1543	rVV3	77046	143531	6.44%	0.801%
17	11.206	1543	1556	1564	rVV2	595628	1291501	57.97%	7.205%
18	11.289	1564	1570	1582	rVB	292026	486838	21.85%	2.716%
19	11.600	1615	1623	1639	rBV	1302435	2084567	93.57%	11.629%
20	11.771	1647	1652	1660	rVB4	18396	37123	1.67%	0.207%
21	11.865	1660	1668	1679	rVV	837809	1482340	66.54%	8.269%
22	12.212	1721	1727	1734	rBV2	16306	26417	1.19%	0.147%
23	12.306	1736	1743	1751	rBV	72884	119205	5.35%	0.665%
24	12.853	1828	1836	1844	rBV	626593	1066813	47.89%	5.951%
25	13.794	1989	1996	2006	rBV	737829	1229796	55.20%	6.860%

Sum of corrected areas: 17925879

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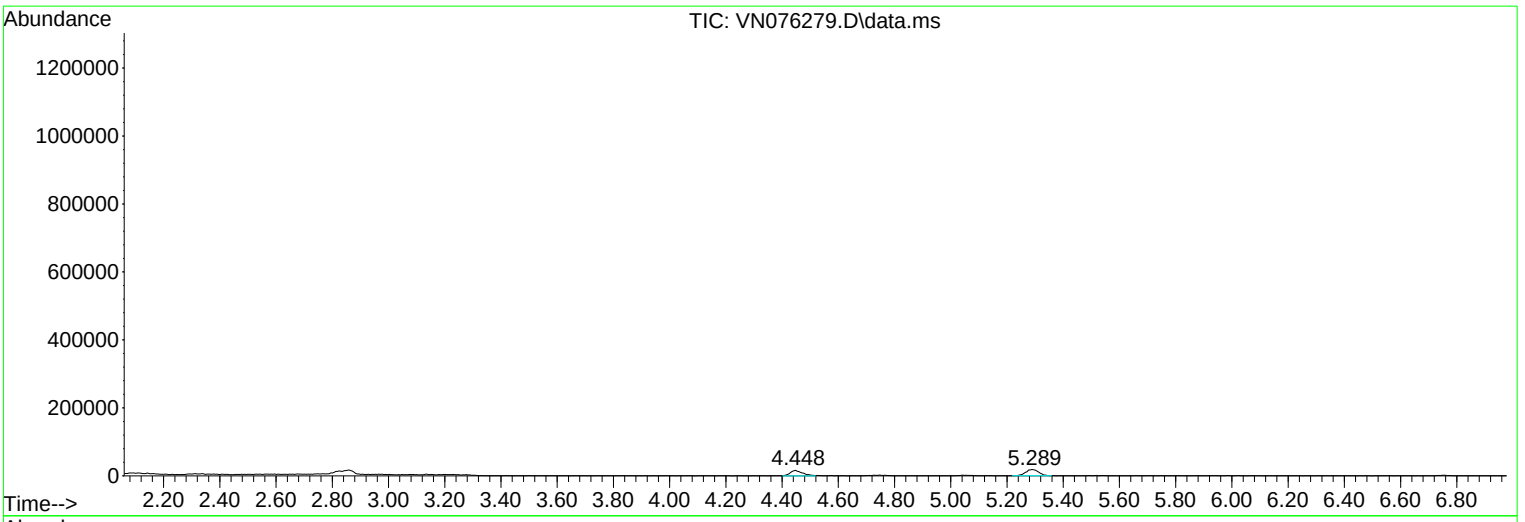
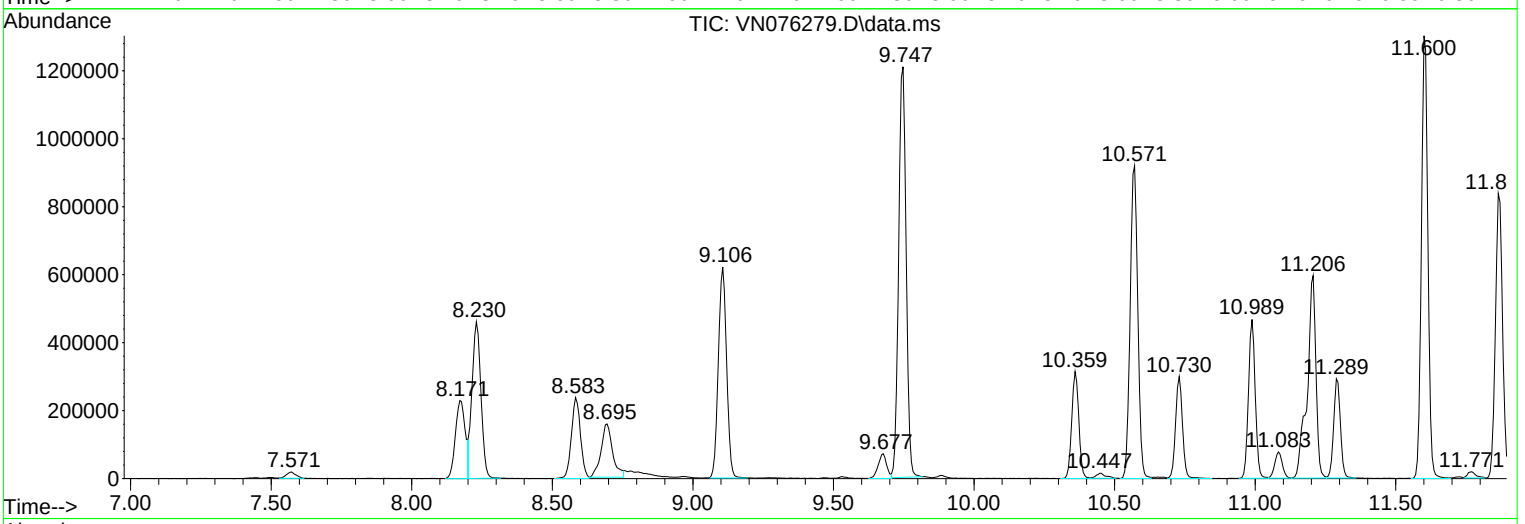
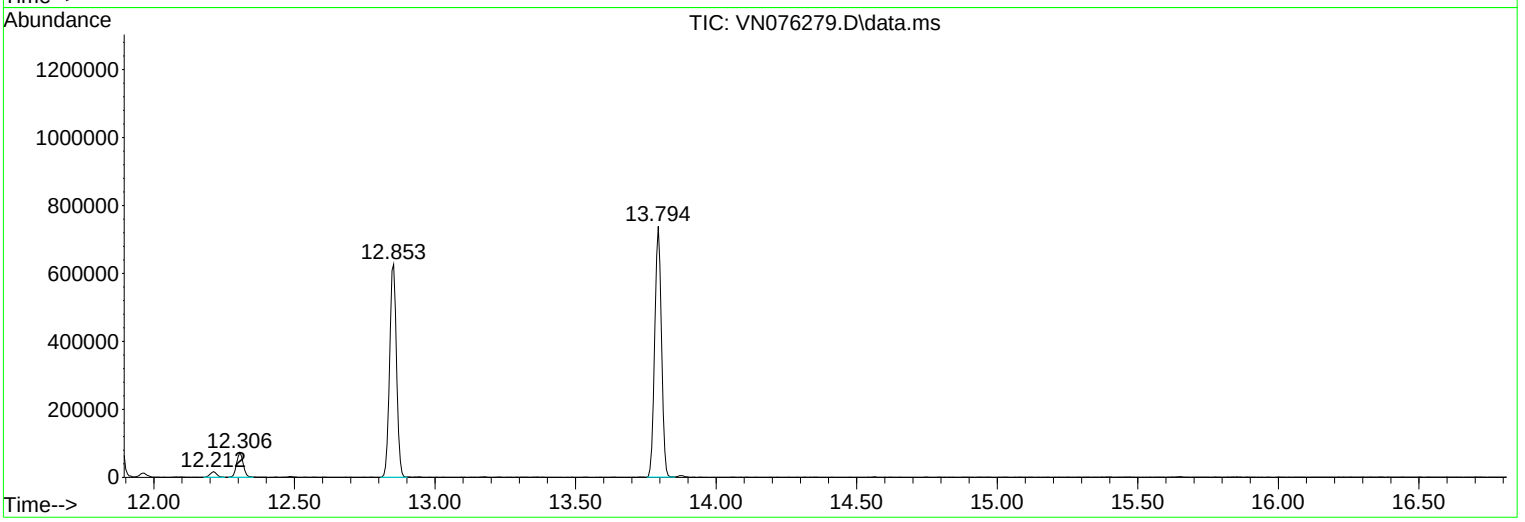
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

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







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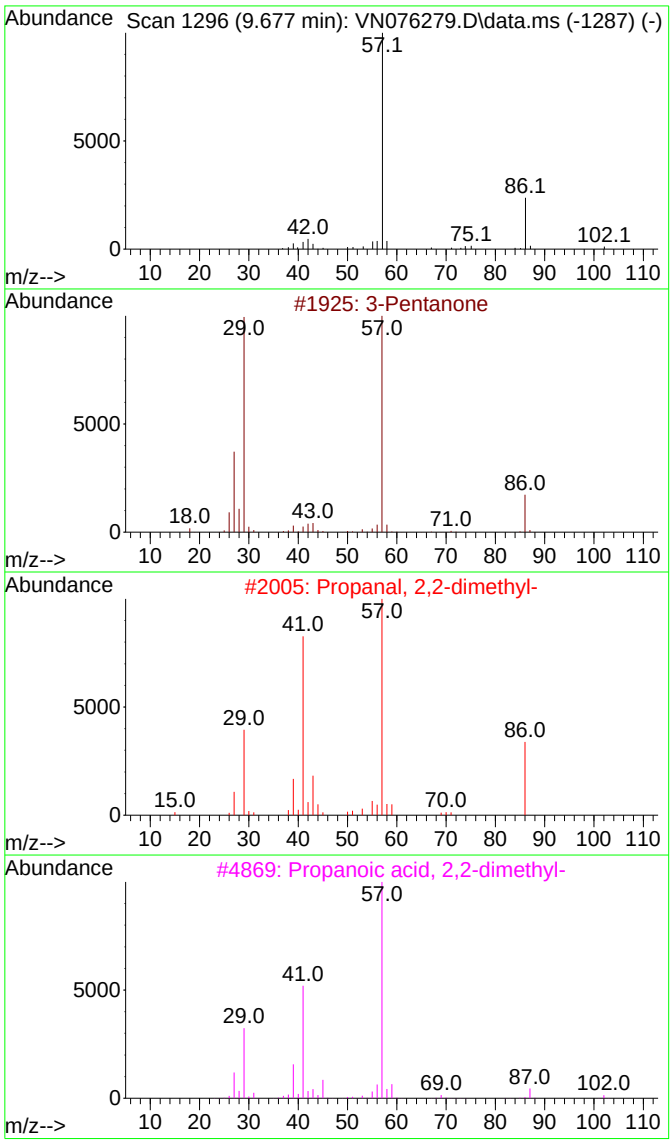
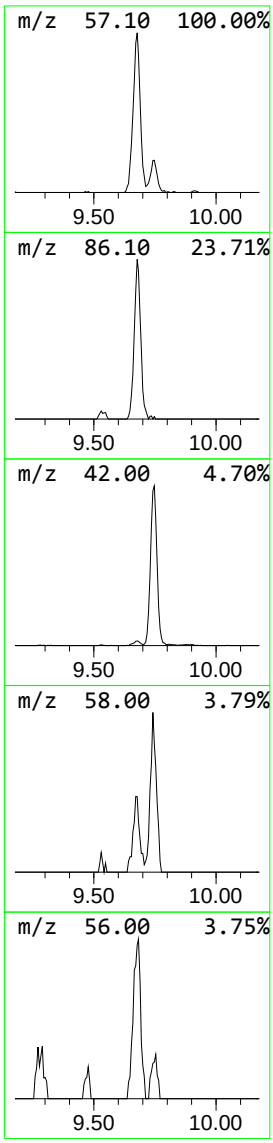
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	6.09 ug/l	154616	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	86
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	42
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4	Neopentane	72	C5H12	000463-82-1	9
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9





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Quant Title : SW846 8260

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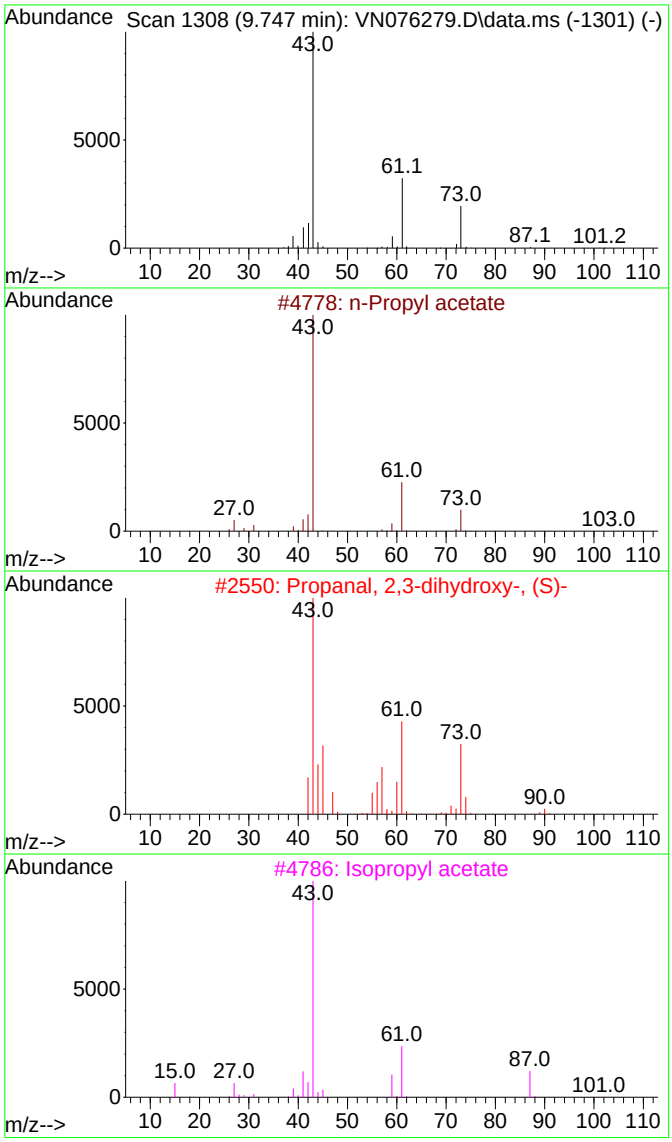
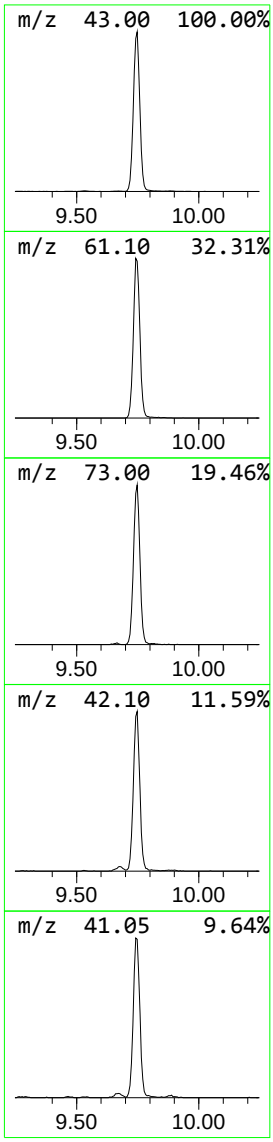
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	87.81 ug/l	2227700	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3	Isopropyl acetate	102	C5H10O2	000108-21-4	33
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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TIC Library : C:\Database\NIST20.L
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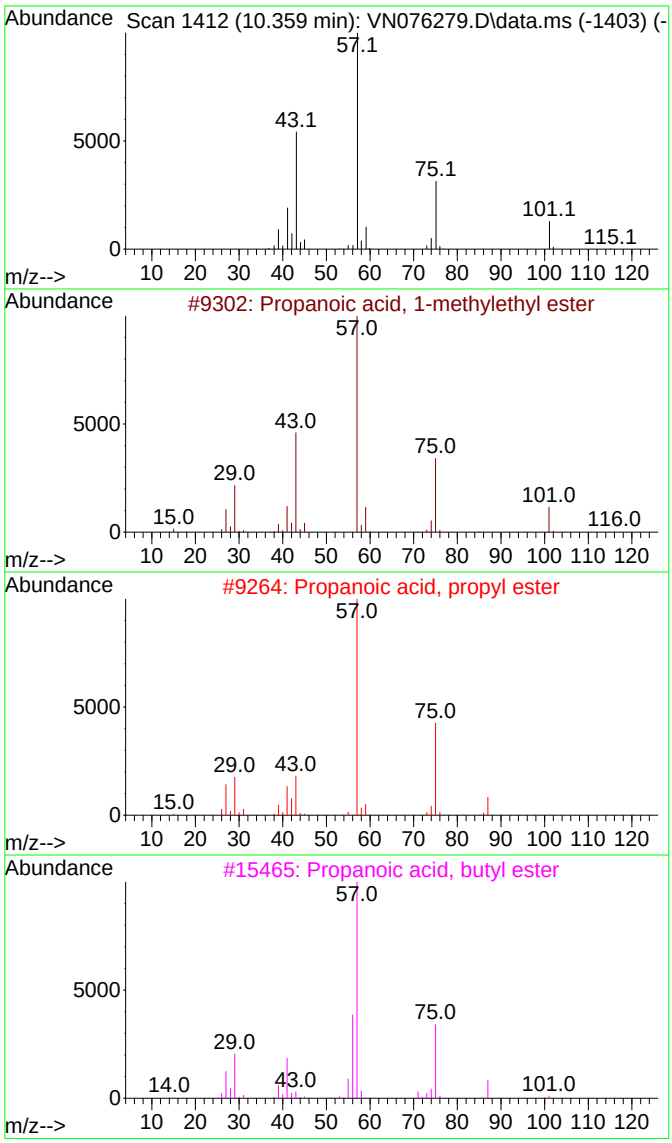
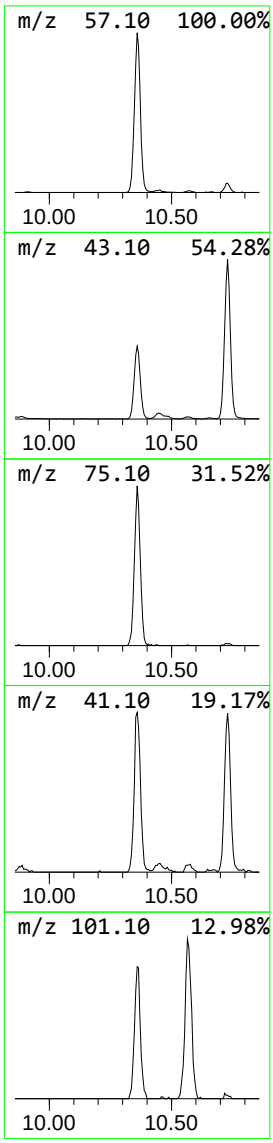
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	21.52 ug/l	545905	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	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
4	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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Instrument :
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Quant Title : SW846 8260

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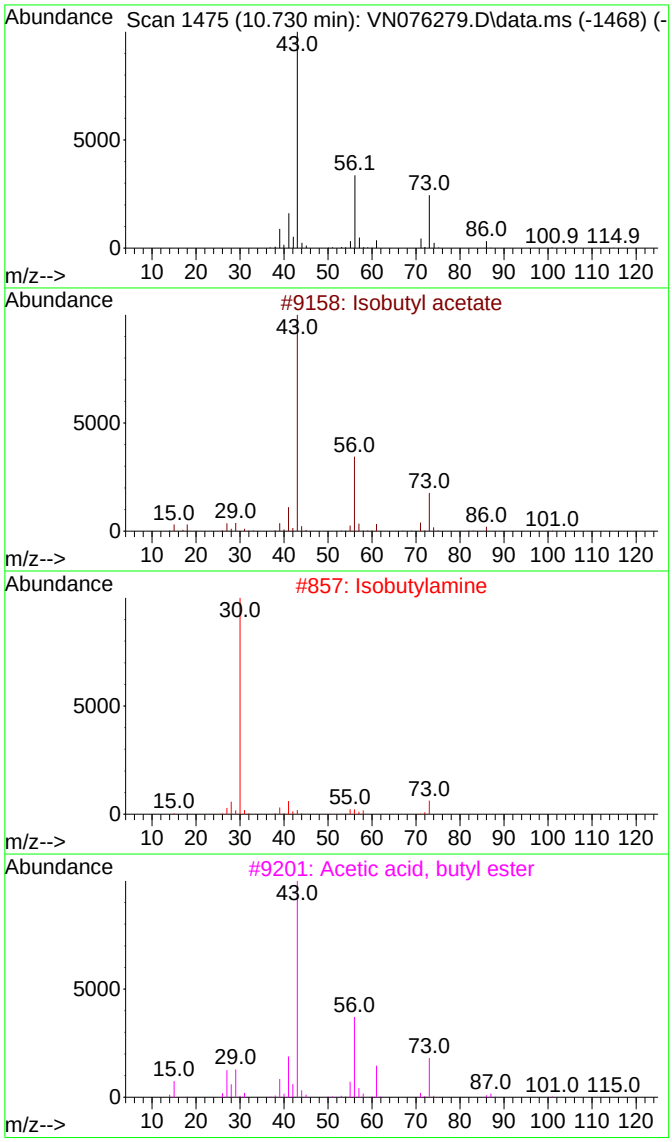
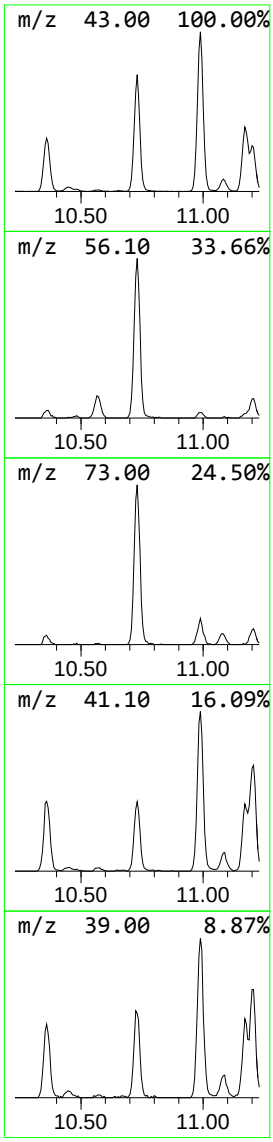
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	17.23 ug/l	510730	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Ethane, diazo-	56	C2H4N2	001117-96-0	7





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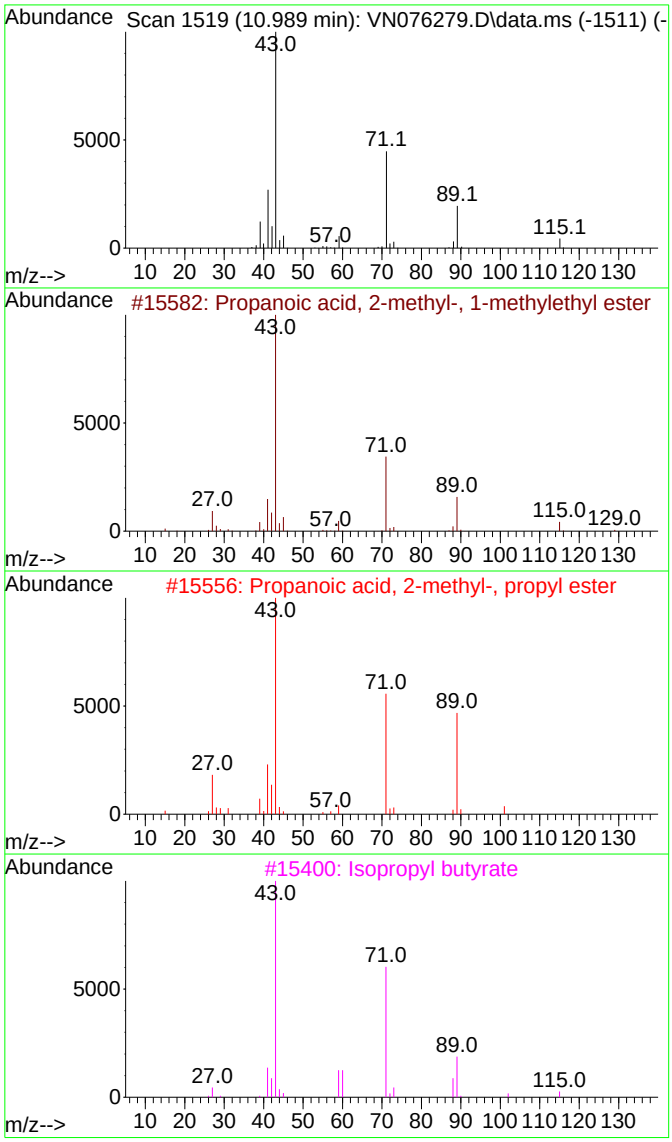
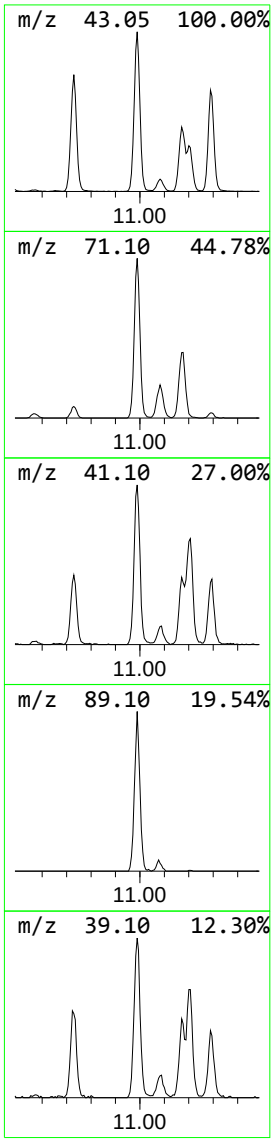
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	26.20 ug/l	776892	Chlorobenzene-d5	11.865

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	64
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	40
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	40





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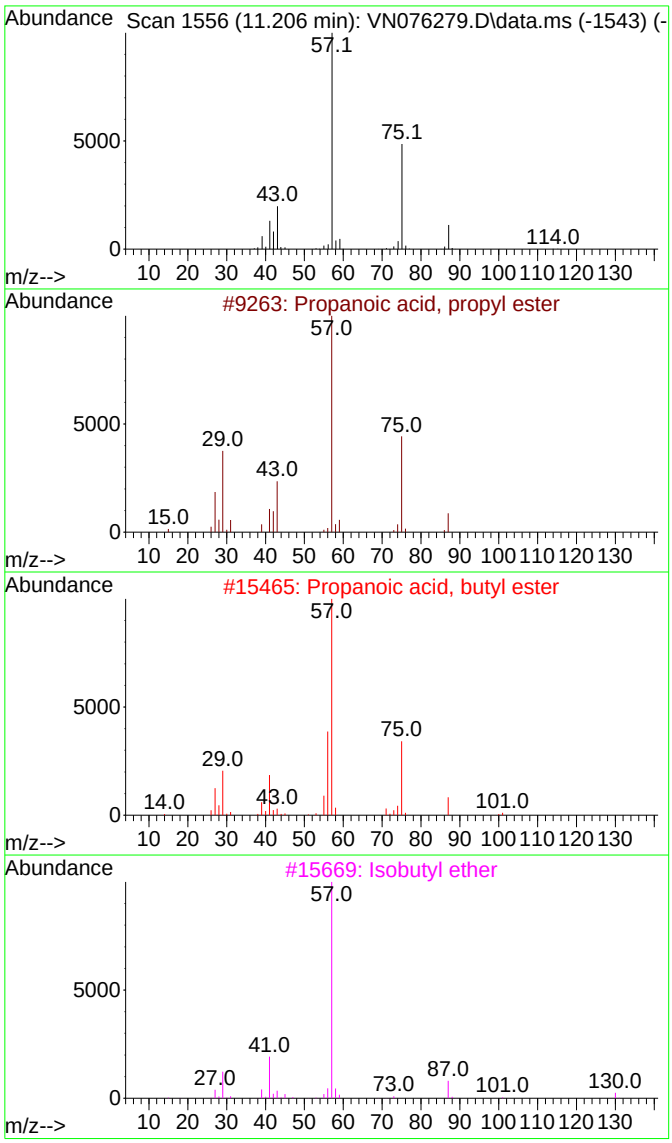
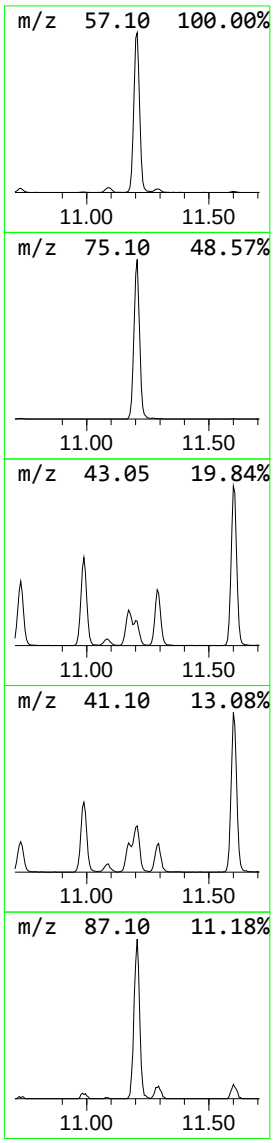
****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	43.56 ug/l	1291500	Chlorobenzene-d5	11.865

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	39
3	Isobutyl ether	130	C8H18O	000628-55-7	12
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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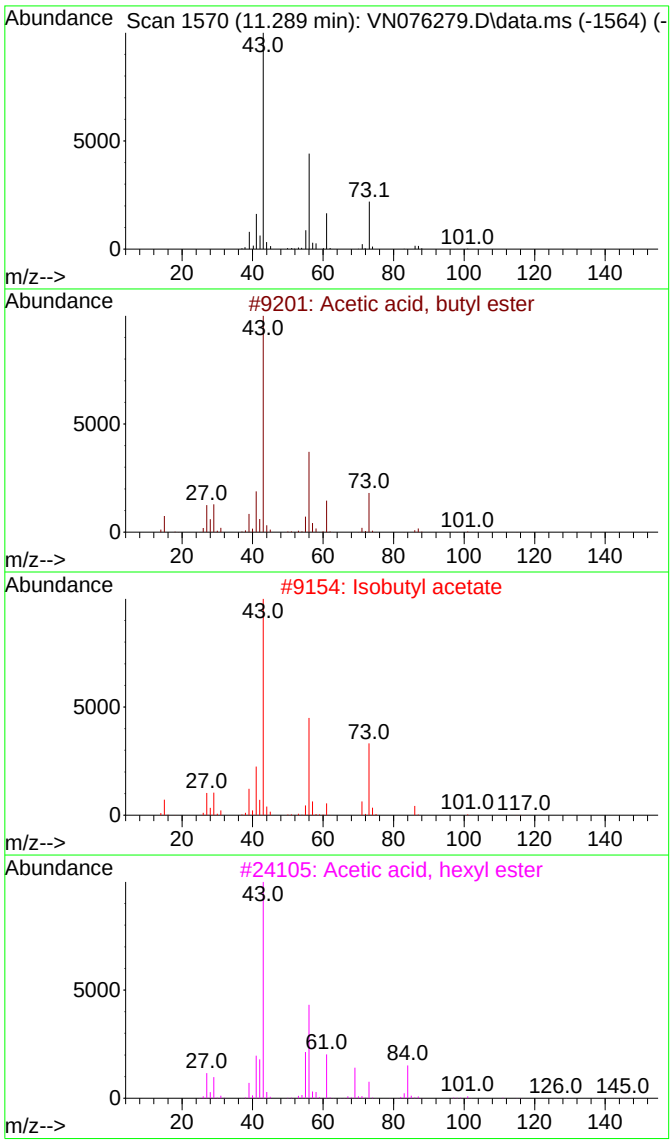
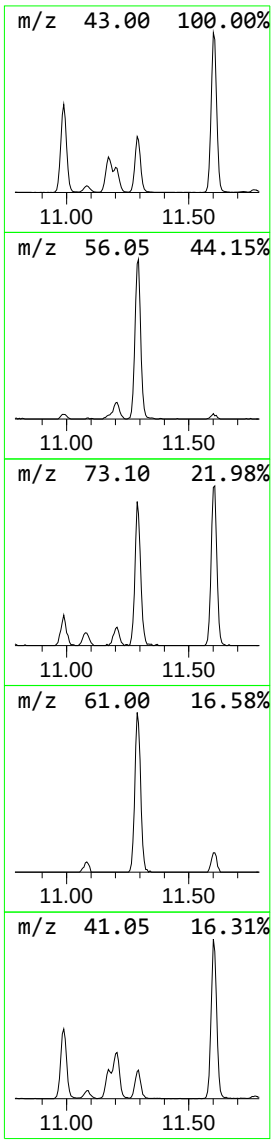
****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.289	16.42 ug/l	486838	Chlorobenzene-d5	11.865

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	33
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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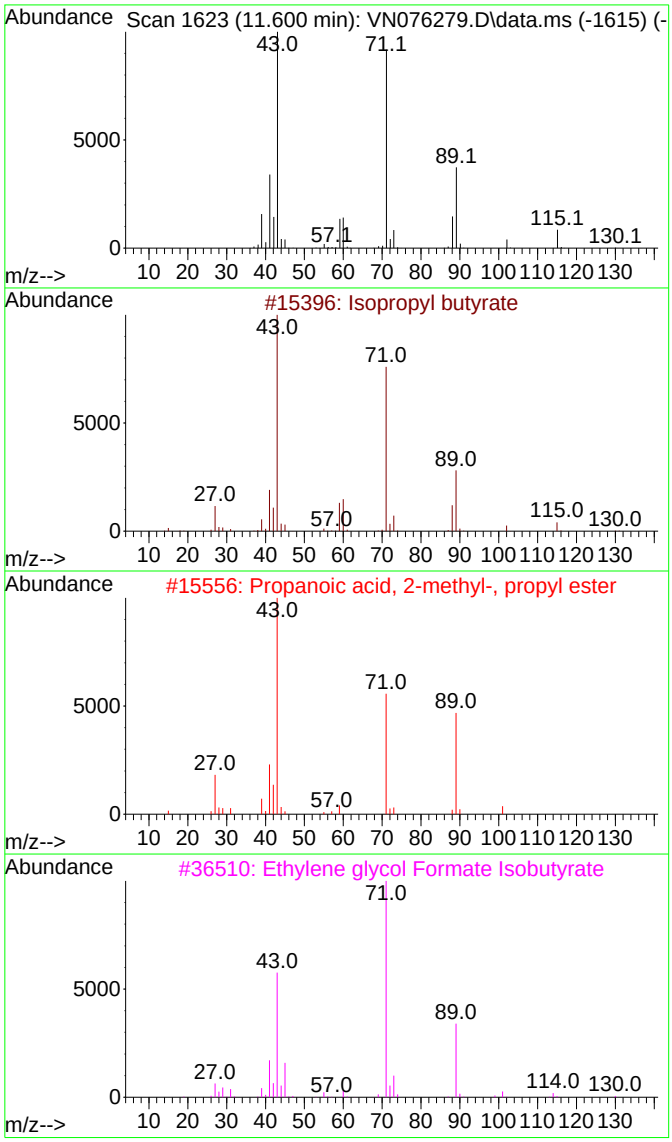
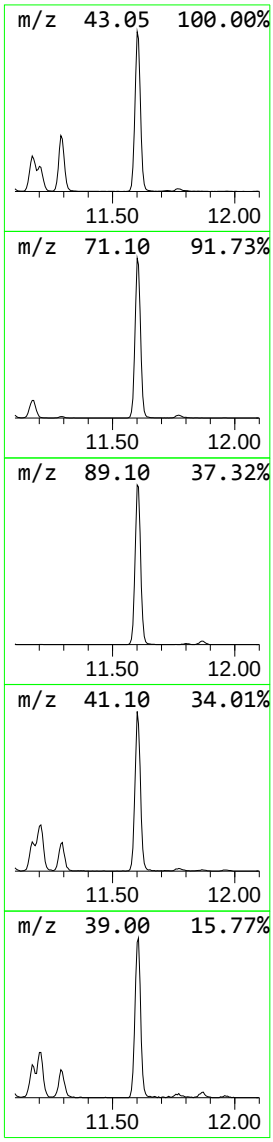
****
Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	70.31 ug/l	2084570	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





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	9.677	6.1	ug/l	154616	2	9.106	1268450	50.0
n-Propyl acetate	9.747	87.8	ug/l	2227700	2	9.106	1268450	50.0
Propanoic acid,...	10.359	21.5	ug/l	545905	2	9.106	1268450	50.0
Isobutyl acetate	10.730	17.2	ug/l	510730	3	11.865	1482340	50.0
Propanoic acid,...	10.989	26.2	ug/l	776892	3	11.865	1482340	50.0
Propanoic acid,...	11.206	43.6	ug/l	1291500	3	11.865	1482340	50.0
Acetic acid, bu...	11.289	16.4	ug/l	486838	3	11.865	1482340	50.0
Isopropyl butyrate	11.600	70.3	ug/l	2084570	3	11.865	1482340	50.0