LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011723\
Data File : VN076280.D
Acq On : 17 Jan 2023 15:12
Operator : JC\MD
Sample : 01159-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MH-6

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: VN076280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.442	398	406	423	rBV	16765	53117	2.23%	0.281%
2	5.283	540	549	550	rBV2	19569	34791	1.46%	0.184%
3	7.571	931	938	948	rVB2	19556	49253	2.07%	0.260%
4	8.171	1030	1040	1045	rBV	249570	611555	25.69%	3.232%
5	8.230	1045	1050	1067	rVB	478851	1057974	44.44%	5.591%
6	8.583	1095	1110	1117	rBV	252449	572641	24.06%	3.026%
7	8.695	1117	1129	1141	rBV2	179515	549803	23.10%	2.906%
8	9.106	1190	1199	1214	rVB	648666	1346178	56.55%	7.114%
9	9.671	1285	1295	1300	rBV2	71687	155526	6.53%	0.822%
10	9.747	1300	1308	1326	rVV	1278038	2380427	100.00%	12.580%
11	10.359	1404	1412	1422	rBV	346139	588149	24.71%	3.108%
12	10.447	1422	1427	1431	rBV2	14393	26024	1.09%	0.138%
13	10.571	1438	1448	1458	rBV	1008003	1834231	77.05%	9.693%
14	10.730	1468	1475	1486	rVB	320348	539564	22.67%	2.851%
15	10.989	1511	1519	1528	rBV	497199	814228	34.21%	4.303%
16	11.083	1528	1535	1543	rVB3	88788	154033	6.47%	0.814%
17	11.206	1551	1556	1564	rVB	639000	1100690	46.24%	5.817%
18	11.289	1564	1570	1583	rVB	328211	554450	23.29%	2.930%
19	11.600	1616	1623	1640	rBV	1372273	2210736	92.87%	11.683%
20	11.771	1646	1652	1661	rVB3	21513	40175	1.69%	0.212%
21	11.865	1661	1668	1679	rVV	886023	1577014	66.25%	8.334%
22	11.965	1679	1685	1693	rVB2	13800	26208	1.10%	0.138%
23	12.212	1721	1727	1736	rBV	17851	28699	1.21%	0.152%
24	12.306	1736	1743	1750	rBV	87199	138550	5.82%	0.732%
25	12.853	1826	1836	1843	rBV	669858	1135992	47.72%	6.003%
26	13.794	1987	1996	2006	rBV	800110	1342798	56.41%	7.096%

Sum of corrected areas: 18922806

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ALS Vial : 12 Sample Multiplier: 1

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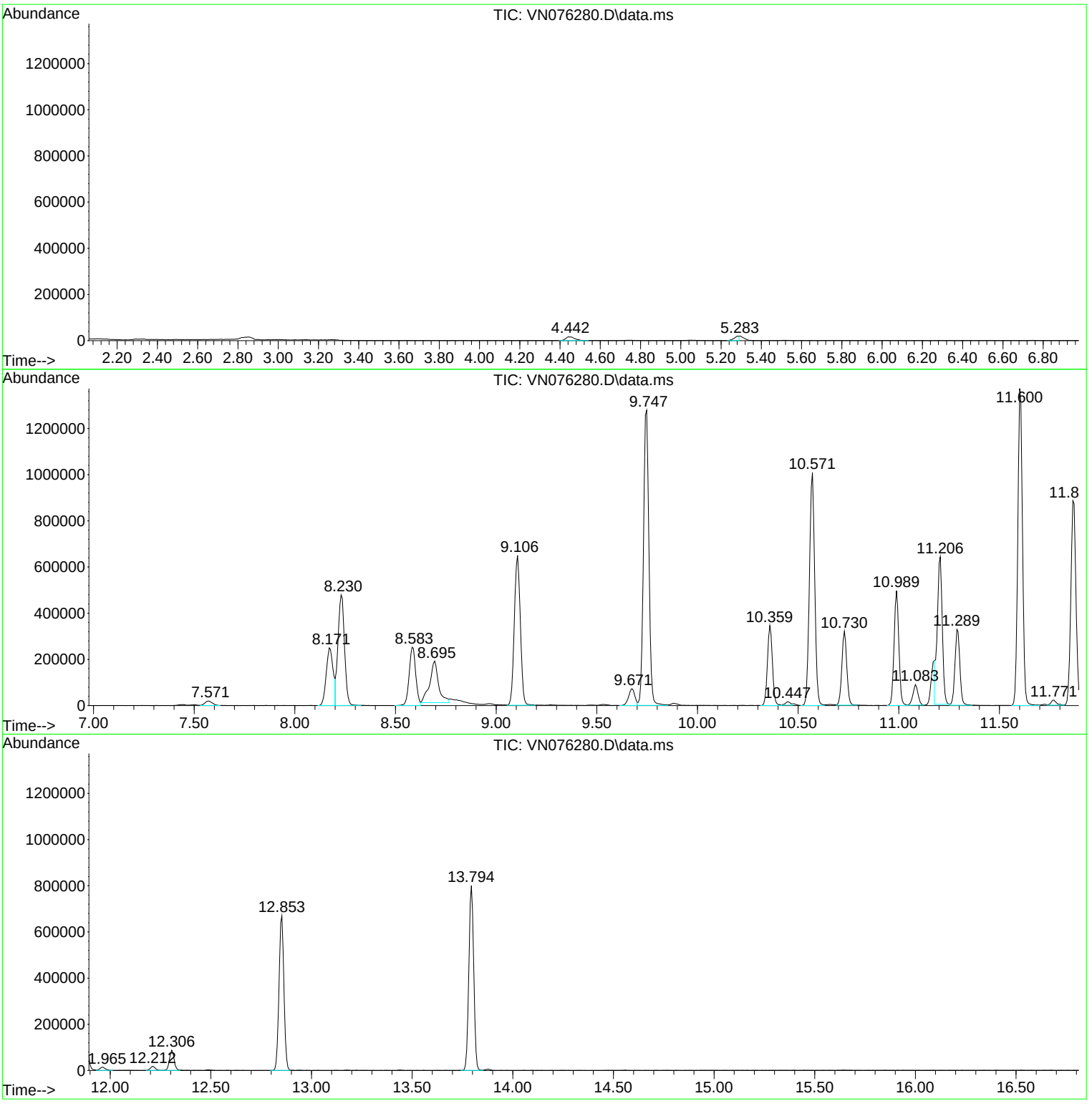
MSVOA_N
ClientSampleId :
MH-6

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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Data File : VN076280.D
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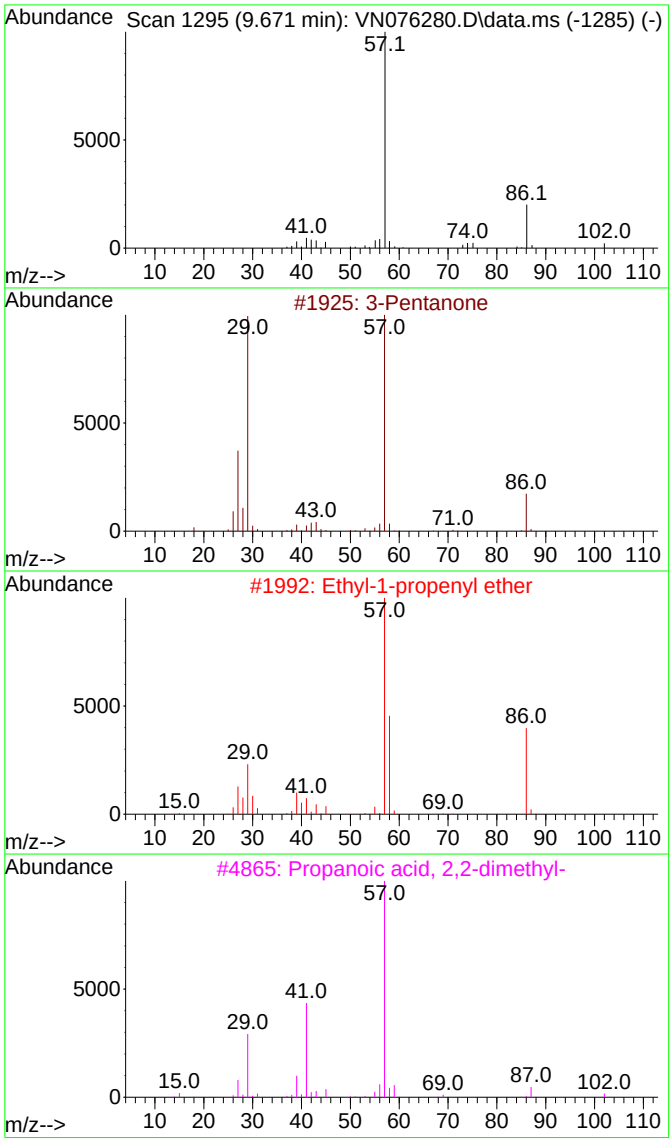
Quant Title : SW846 8260

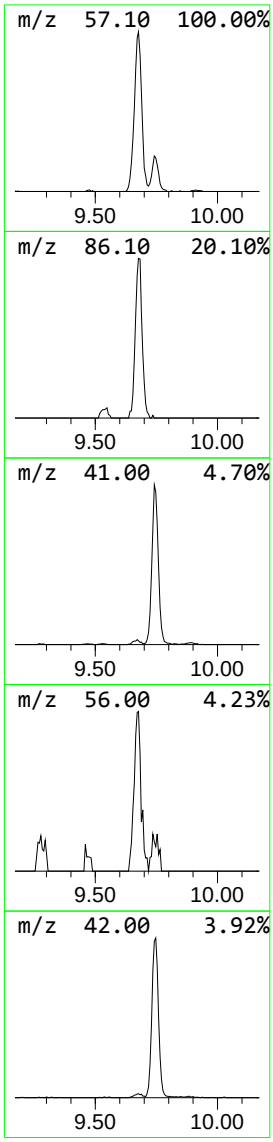
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	5.78 ug/l	155526	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	53
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
5	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MH-6

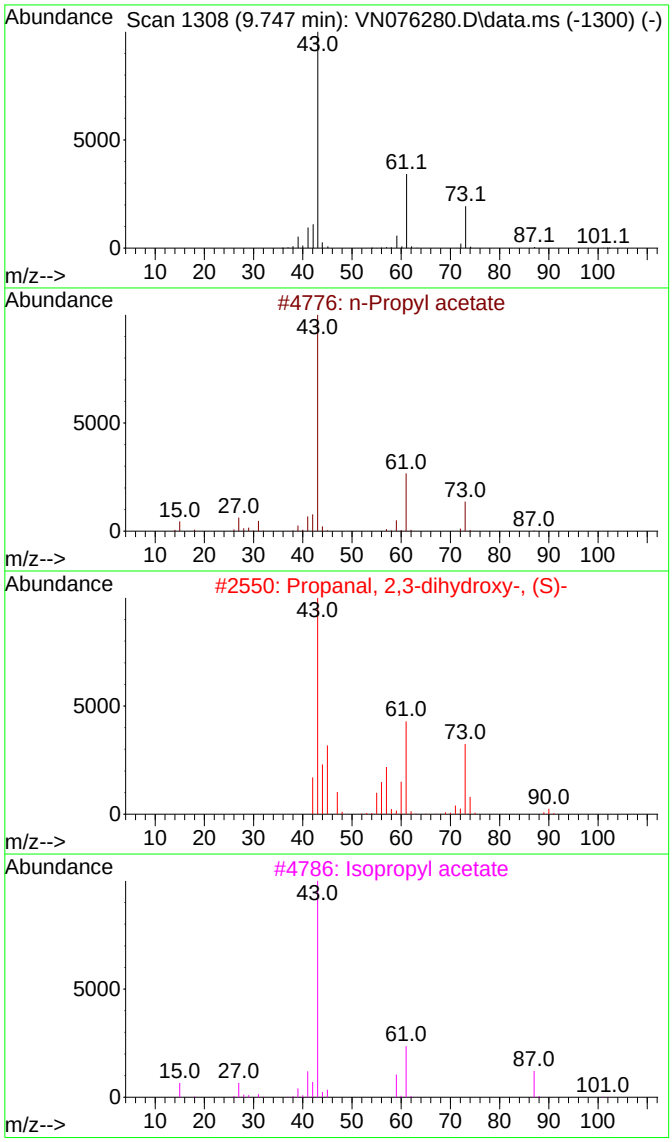
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

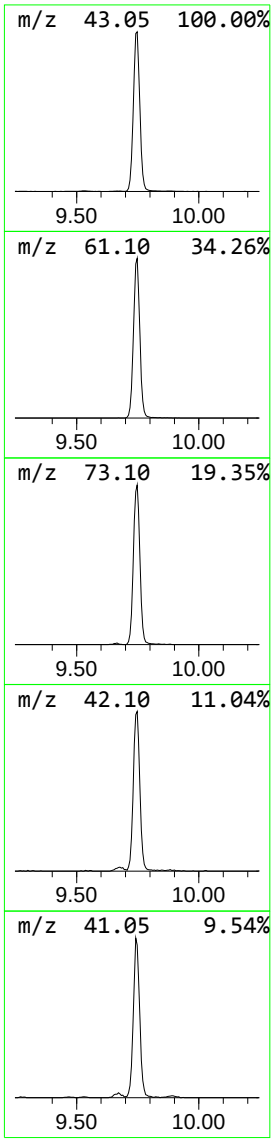
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	88.41 ug/l	2380430	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	Isobutylamine	73	C4H11N	000078-81-9	9
5	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MH-6

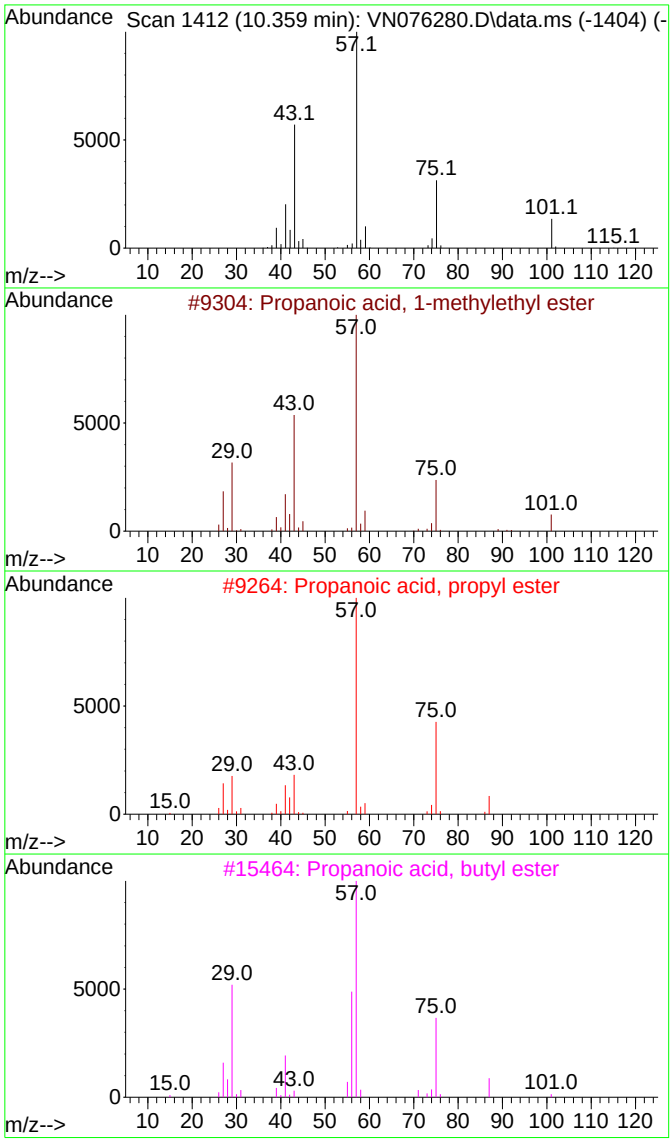
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

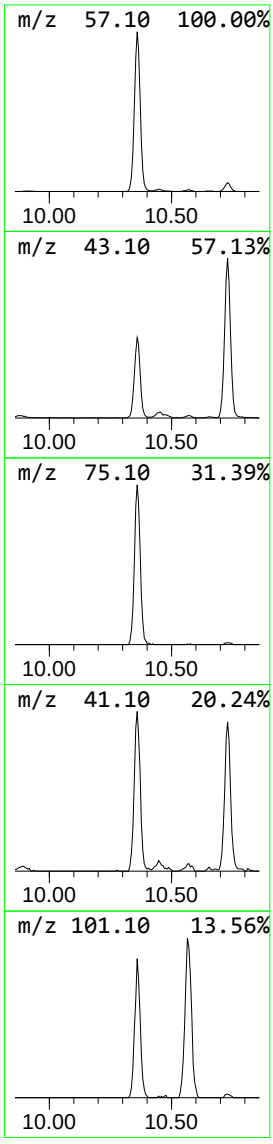
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	21.85 ug/l	588149	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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	10
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MH-6

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

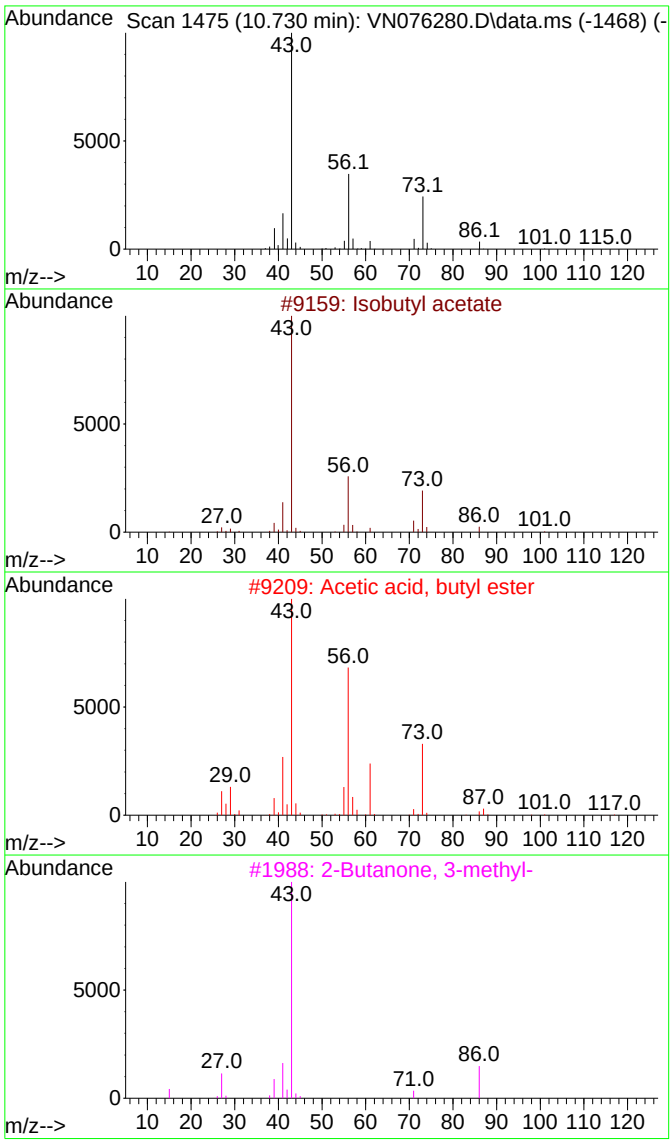
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

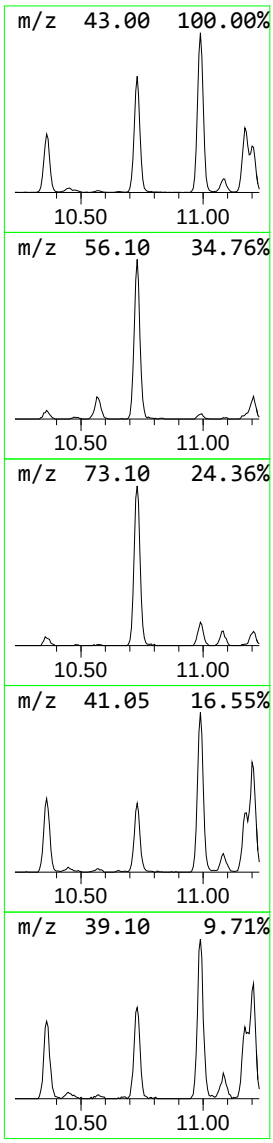
****

Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	17.11 ug/l	539564	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	33
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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Instrument :
MSVOA_N
ClientSampleId :
MH-6

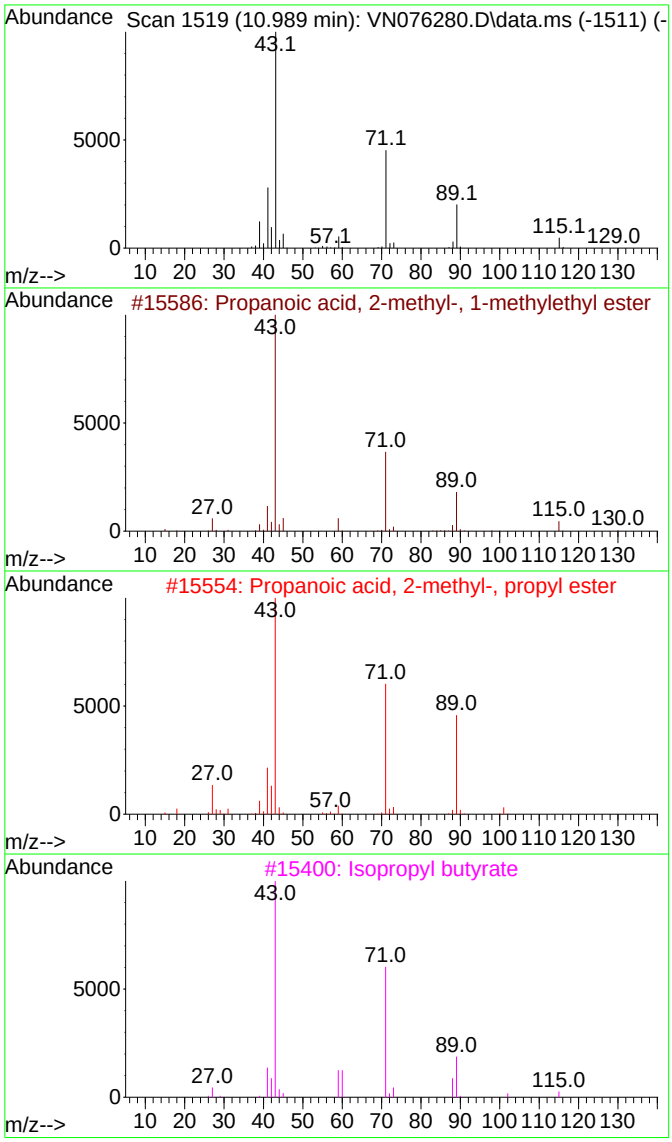
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

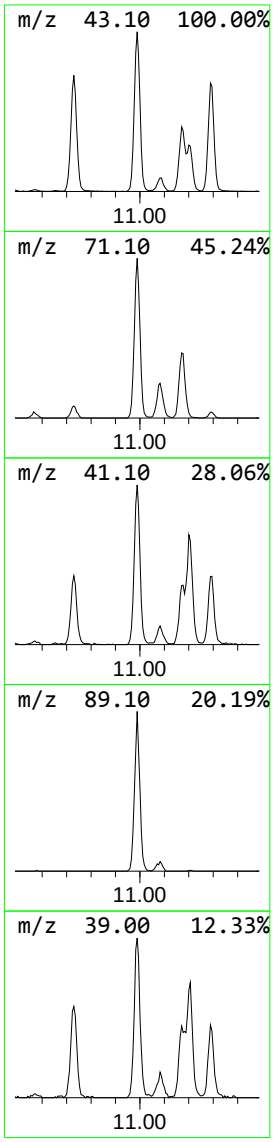
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	25.82 ug/l	814228	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	40
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40





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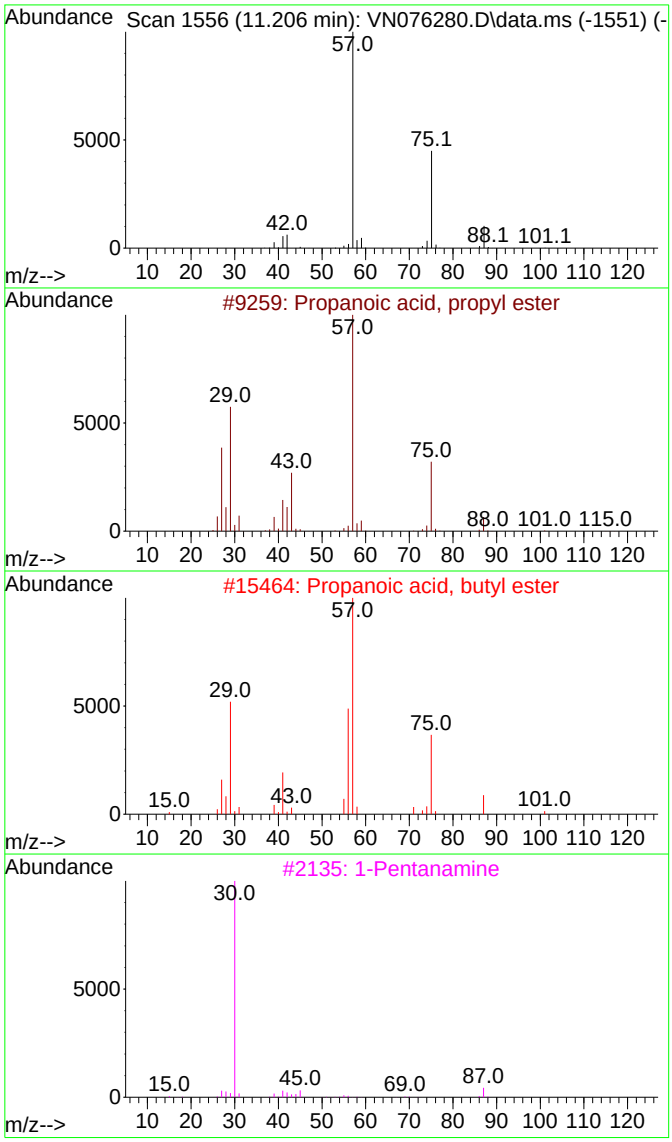
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

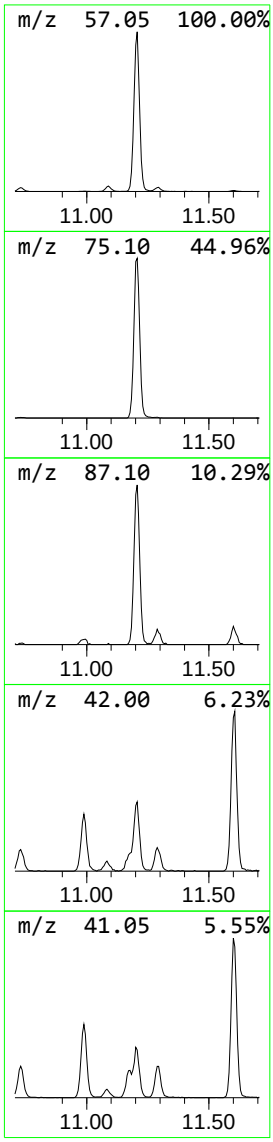
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	34.90 ug/l	1100690	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-Pentanamine	87	C5H13N	000110-58-7	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





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Instrument :
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ClientSampleId :
MH-6

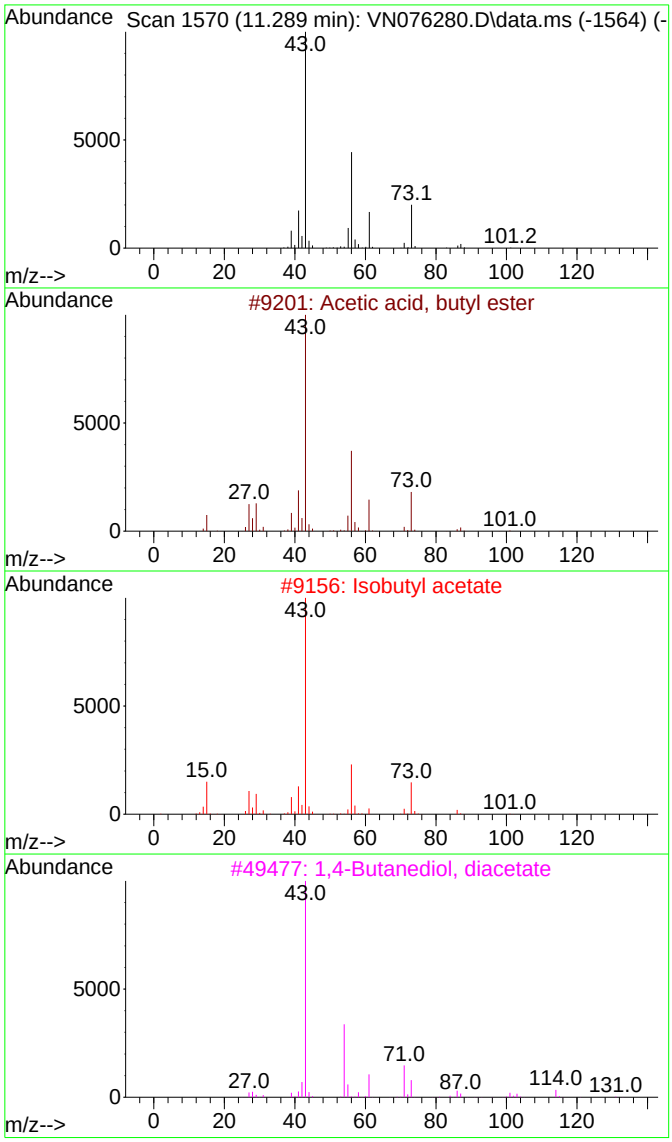
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

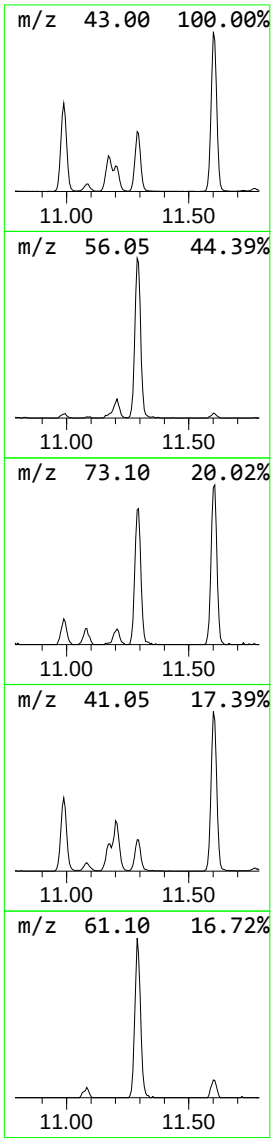
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.289	17.58 ug/l	554450	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	33
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isopropyl acetate	102	C5H10O2	000108-21-4	10
5	Isobutylamine	73	C4H11N	000078-81-9	9





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MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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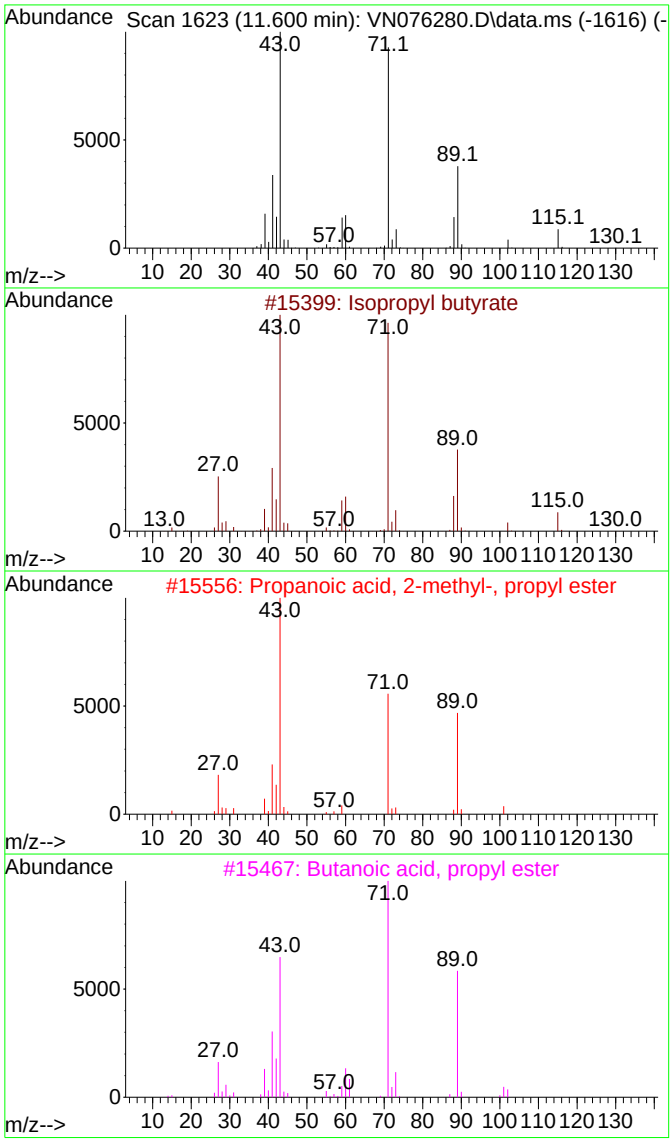
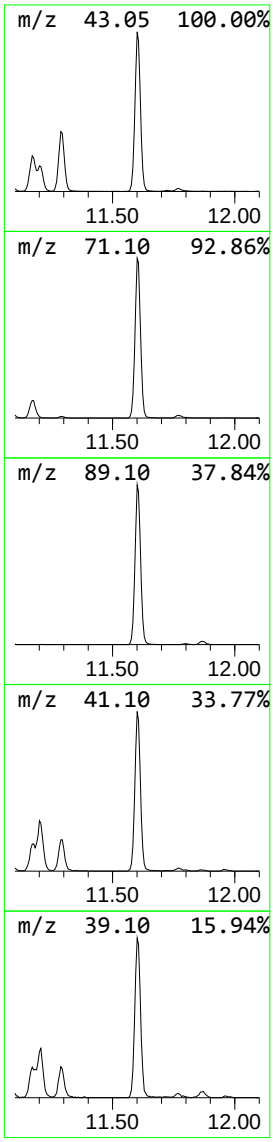
****
Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	70.09 ug/l	2210740	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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	50





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	9.671	5.8	ug/l	155526	2	9.106	1346180	50.0
n-Propyl acetate	9.747	88.4	ug/l	2380430	2	9.106	1346180	50.0
Propanoic acid,...	10.359	21.9	ug/l	588149	2	9.106	1346180	50.0
Isobutyl acetate	10.730	17.1	ug/l	539564	3	11.871	1577010	50.0
Propanoic acid,...	10.989	25.8	ug/l	814228	3	11.871	1577010	50.0
Propanoic acid,...	11.206	34.9	ug/l	1100690	3	11.871	1577010	50.0
Acetic acid, bu...	11.289	17.6	ug/l	554450	3	11.871	1577010	50.0
Isopropyl butyrate	11.600	70.1	ug/l	2210740	3	11.871	1577010	50.0