LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069068.D
Acq On : 20 Oct 2021 17:52
Operator : JC/MD
Sample : M4252-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TEST-BB-(1)

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\82N101221W.M
Title : SW846 8260

Signal : TIC: VN069068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.106	1137	1162	1194	rVB3	20781	68495	1.43%	0.310%
2	8.024	2228	2250	2261	rBV2	215176	508933	10.65%	2.301%
3	8.088	2262	2274	2300	rVB2	414490	934303	19.55%	4.224%
4	8.440	2385	2405	2427	rBV2	235496	545962	11.42%	2.468%
5	8.574	2435	2455	2456	rBV2	53829	91849	1.92%	0.415%
6	8.971	2583	2603	2632	rBV	594481	1255599	26.27%	5.676%
7	9.547	2802	2818	2830	rBV3	29252	67124	1.40%	0.303%
8	9.625	2830	2847	2888	rVV	1652031	3166857	66.26%	14.316%
9	10.245	3059	3078	3099	rBV	306110	541490	11.33%	2.448%
10	10.443	3134	3152	3181	rBV	955616	1793174	37.52%	8.106%
11	10.617	3205	3217	3233	rVB	29816	55445	1.16%	0.251%
12	10.877	3300	3314	3329	rBV	86361	148708	3.11%	0.672%
13	10.969	3334	3348	3369	rVV2	182437	323984	6.78%	1.465%
14	11.092	3369	3394	3416	rVV	2788612	4779259	100.00%	21.605%
15	11.181	3416	3427	3456	rVB	273155	489891	10.25%	2.215%
16	11.494	3525	3544	3570	rBV	1912652	3204339	67.05%	14.486%
17	11.746	3621	3638	3669	rVB	903463	1626099	34.02%	7.351%
18	12.200	3792	3807	3827	rBV	54133	92098	1.93%	0.416%
19	12.733	3990	4006	4035	rVB	668107	1159828	24.27%	5.243%
20	13.677	4341	4358	4381	rBV	748468	1267522	26.52%	5.730%

Sum of corrected areas: 22120959

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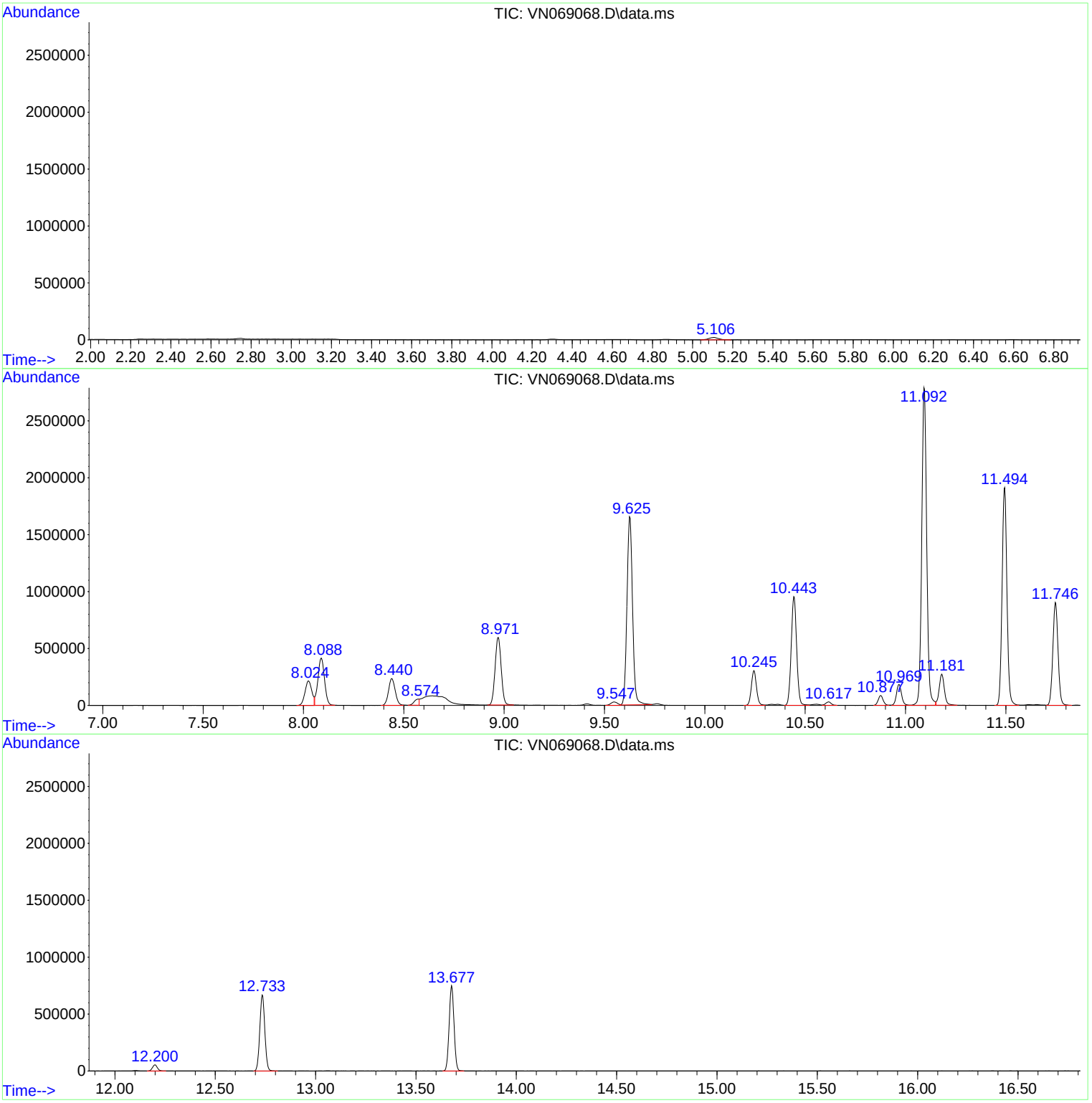
Instrument :
MSVOA_N
ClientSampleId :
TEST-BB-(1)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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Data File : VN069068.D
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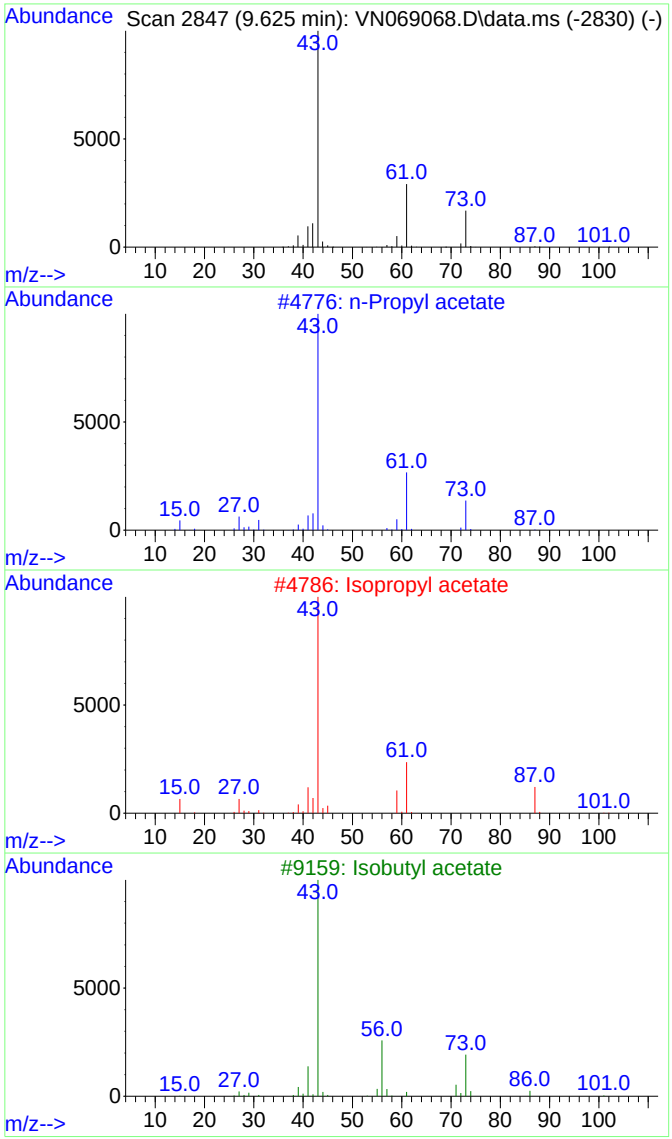
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

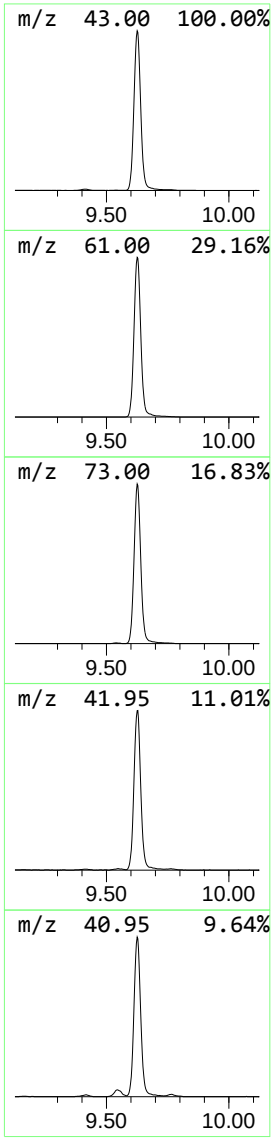
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.625	126.11 ug/l	3166860	1,4-Difluorobenzene	8.971

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	5
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Instrument :
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ClientSampleId :
TEST-BB-(1)

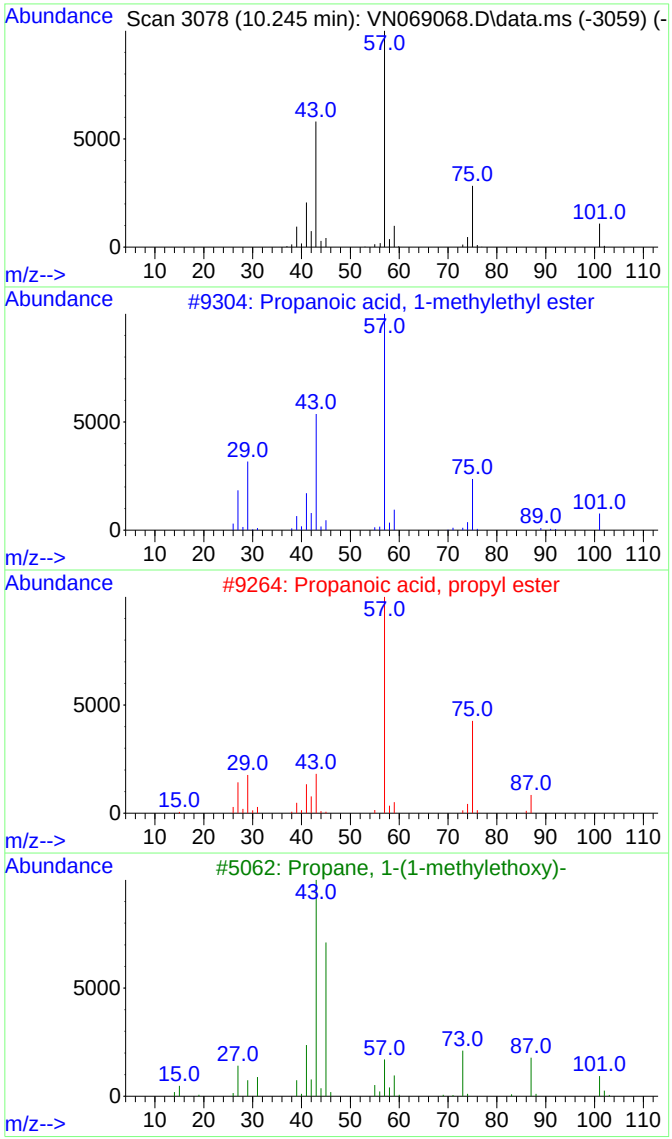
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

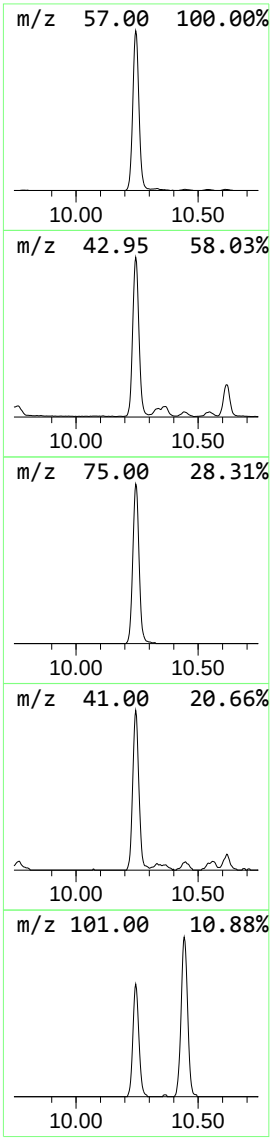
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	21.56 ug/l	541490	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9





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Instrument : MSVOA_N
ClientSampleId : TEST-BB-(1)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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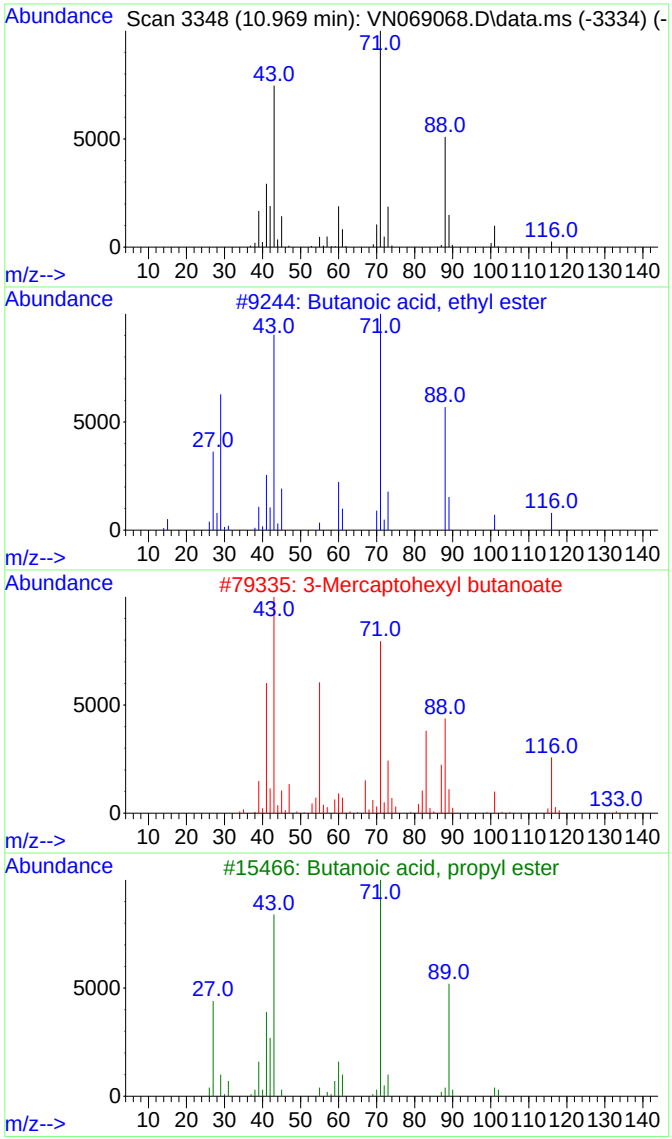
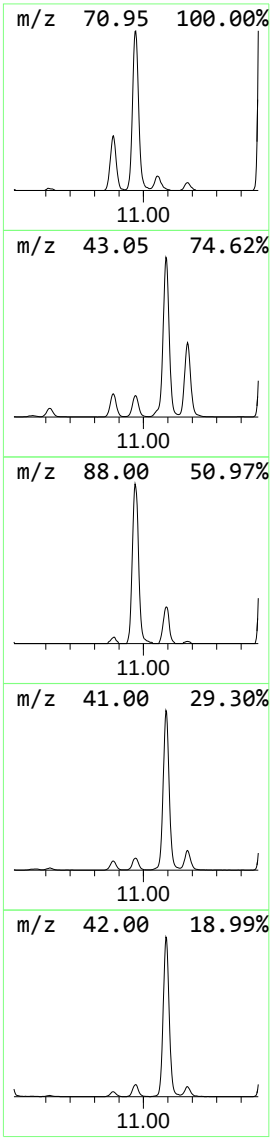
****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.969	9.96 ug/l	323984	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
2	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	56
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	47
5	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	45





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TEST-BB-(1)

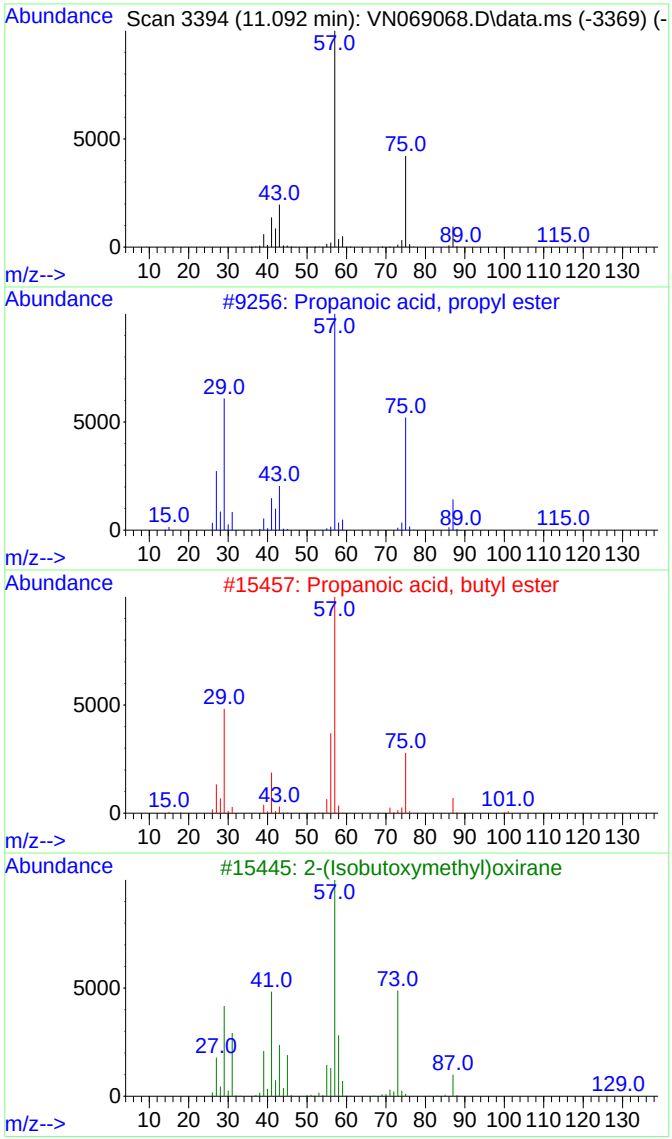
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

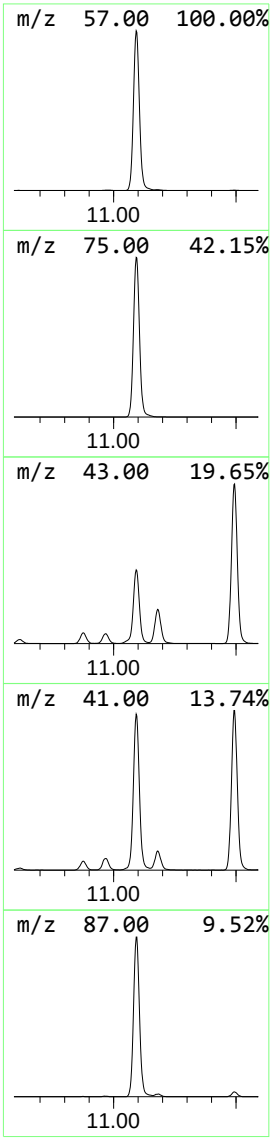
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.092	146.96 ug/l	4779260	Chlorobenzene-d5	11.746

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	28
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Instrument :
MSVOA_N
ClientSampleId :
TEST-BB-(1)

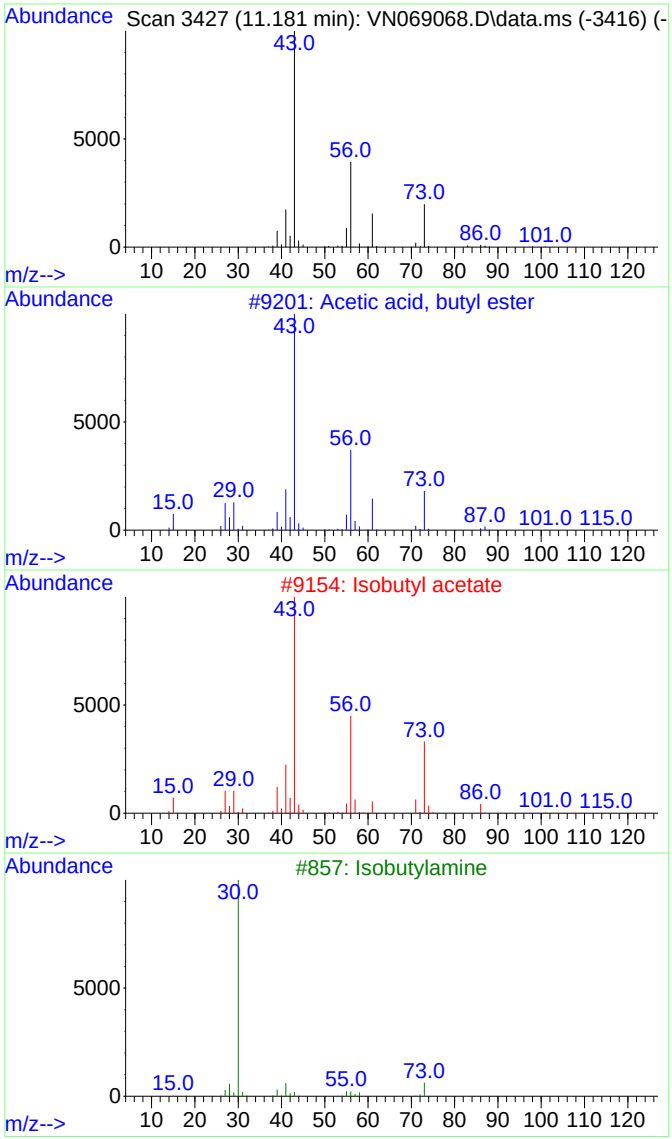
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

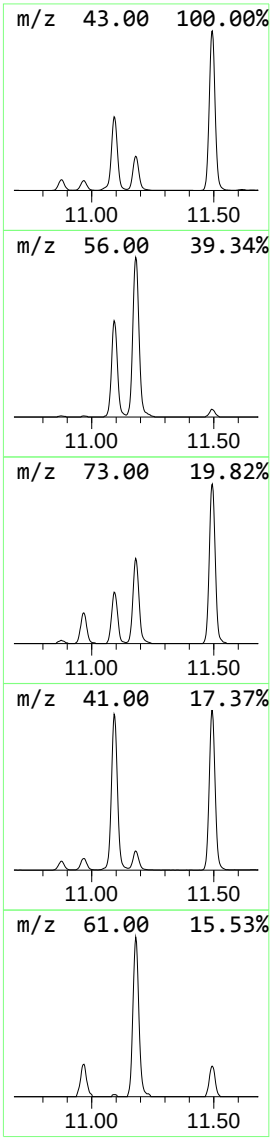
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	15.06 ug/l	489891	Chlorobenzene-d5	11.746

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	36
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	9
5	Isopropyl pyruvate	130	C6H10O3	1000431-41-9	9





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Instrument :
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ClientSampleId :
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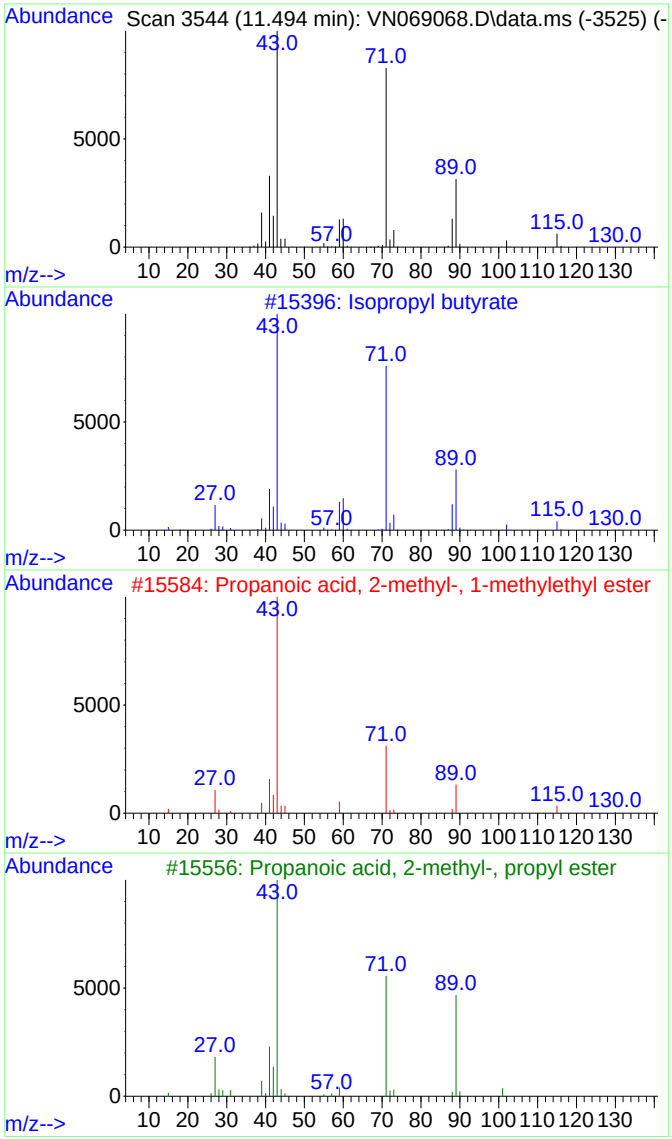
Quant Title : SW846 8260

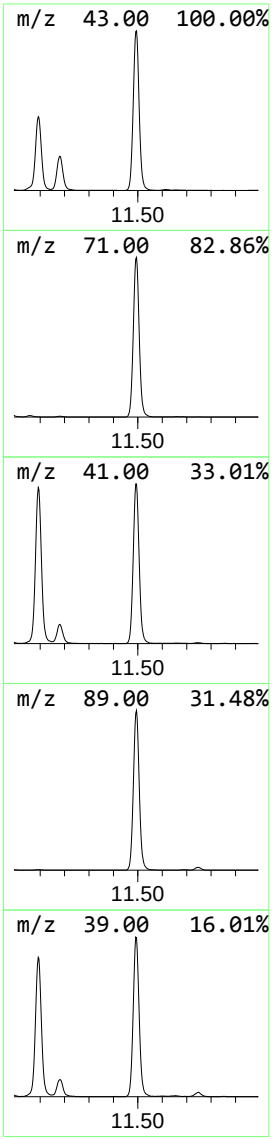
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.494	98.53 ug/l	3204340	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	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
n-Propyl acetate	9.625	126.1	ug/l	3166860	2	8.971	1255600	50.0
Propanoic acid,...	10.245	21.6	ug/l	541490	2	8.971	1255600	50.0
Butanoic acid, ...	10.969	10.0	ug/l	323984	3	11.746	1626100	50.0
Propanoic acid,...	11.092	147.0	ug/l	4779260	3	11.746	1626100	50.0
Acetic acid, bu...	11.181	15.1	ug/l	489891	3	11.746	1626100	50.0
Isopropyl butyrate	11.494	98.5	ug/l	3204340	3	11.746	1626100	50.0