LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069060.D
Acq On : 20 Oct 2021 14:30
Operator : JC/MD
Sample : M4259-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WC-1-BS

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: VN069060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.103	1138	1161	1195	rVB4	23975	78720	1.64%	0.342%
2	8.024	2227	2250	2261	rBV2	235410	561360	11.68%	2.436%
3	8.088	2262	2274	2301	rVB	447886	1029774	21.43%	4.468%
4	8.440	2384	2405	2433	rBV	261502	602897	12.55%	2.616%
5	8.563	2437	2451	2466	rBV	27802	61941	1.29%	0.269%
6	8.971	2582	2603	2632	rBV	671215	1379601	28.71%	5.986%
7	9.550	2800	2819	2830	rBV3	29406	67307	1.40%	0.292%
8	9.625	2830	2847	2888	rVV	1677586	3205837	66.72%	13.911%
9	10.245	3060	3078	3099	rBV	309172	551185	11.47%	2.392%
10	10.443	3134	3152	3181	rBV	1042101	1957623	40.74%	8.495%
11	10.617	3206	3217	3231	rVB3	31786	57089	1.19%	0.248%
12	10.875	3297	3313	3332	rBV	87957	152322	3.17%	0.661%
13	10.966	3332	3347	3369	rVV2	187191	334010	6.95%	1.449%
14	11.092	3371	3394	3415	rVV	2857556	4805046	100.00%	20.851%
15	11.181	3416	3427	3452	rVB	281431	503511	10.48%	2.185%
16	11.492	3526	3543	3577	rBV	1913853	3259278	67.83%	14.143%
17	11.747	3622	3638	3669	rVB	966461	1748902	36.40%	7.589%
18	12.200	3793	3807	3824	rBV2	56933	95636	1.99%	0.415%
19	12.734	3982	4006	4031	rBV	714089	1230567	25.61%	5.340%
20	13.678	4342	4358	4385	rVB	799633	1362618	28.36%	5.913%

Sum of corrected areas: 23045224

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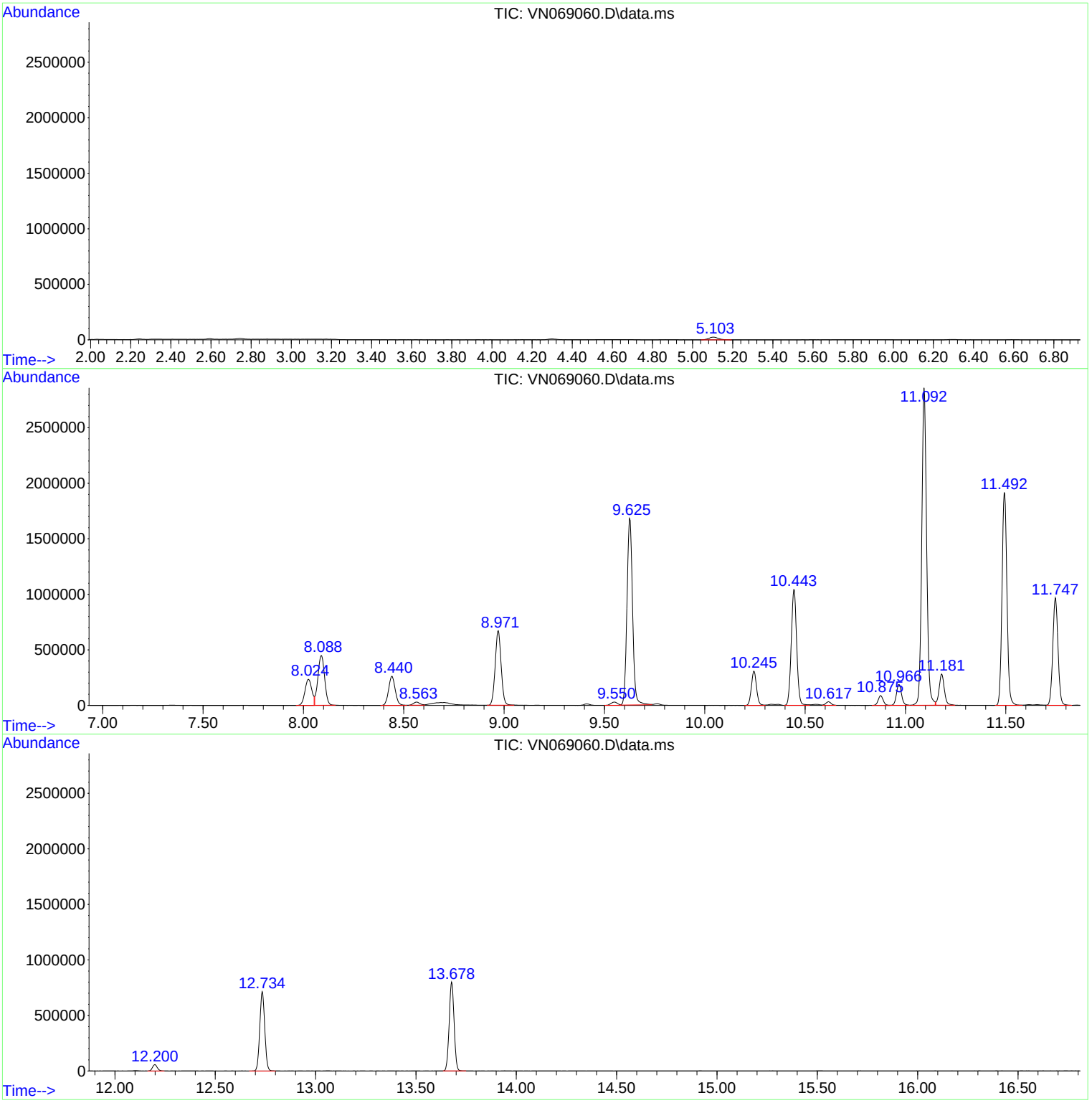
Instrument :
MSVOA_N
ClientSampleId :
WC-1-BS

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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Quant Title : SW846 8260

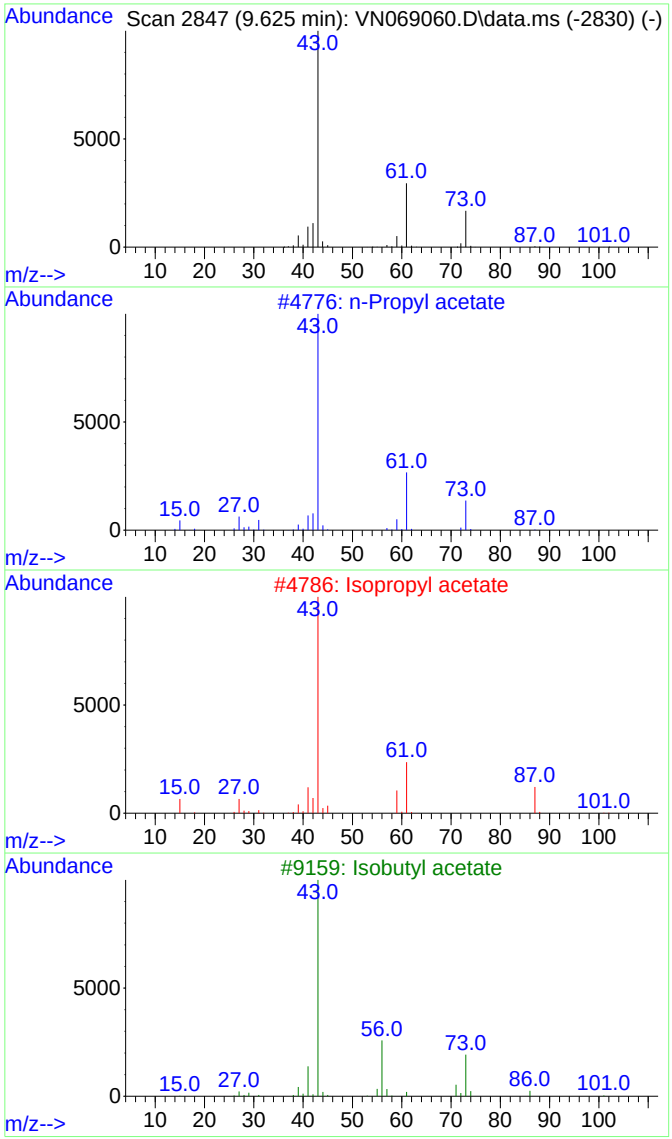
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

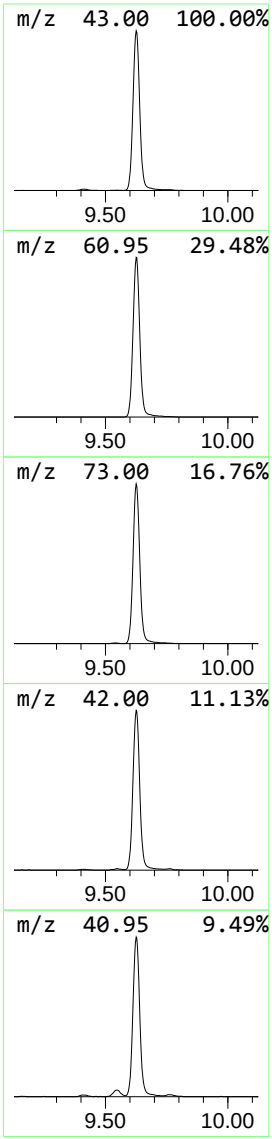
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.625	116.19 ug/l	3205840	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	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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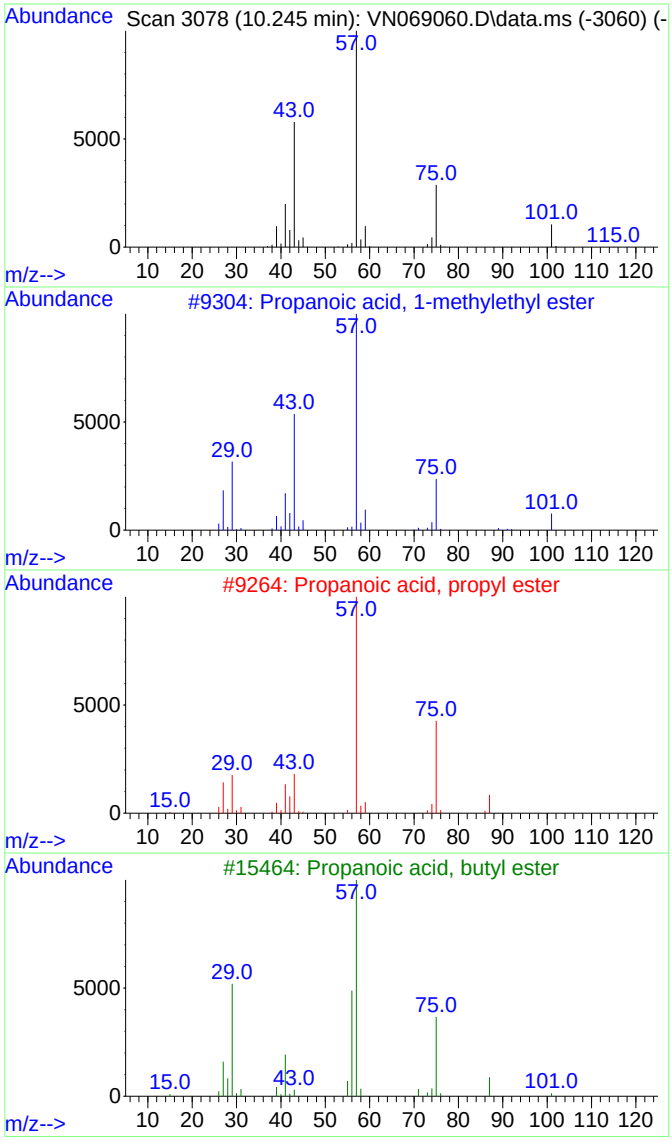
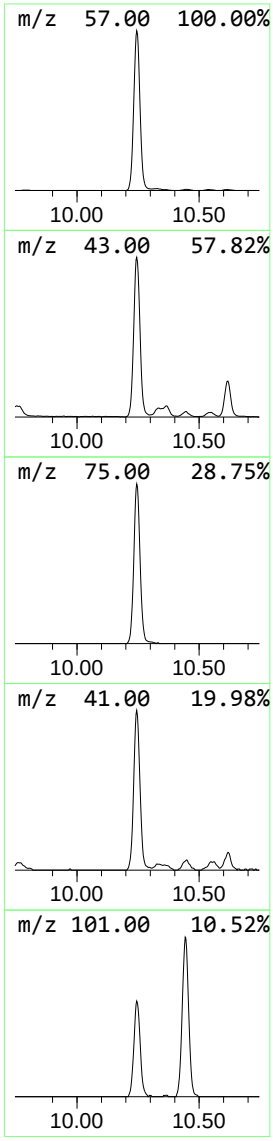
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	19.98 ug/l	551185	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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : MSVOA_N
ClientSampleId : WC-1-BS

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Quant Title : SW846 8260

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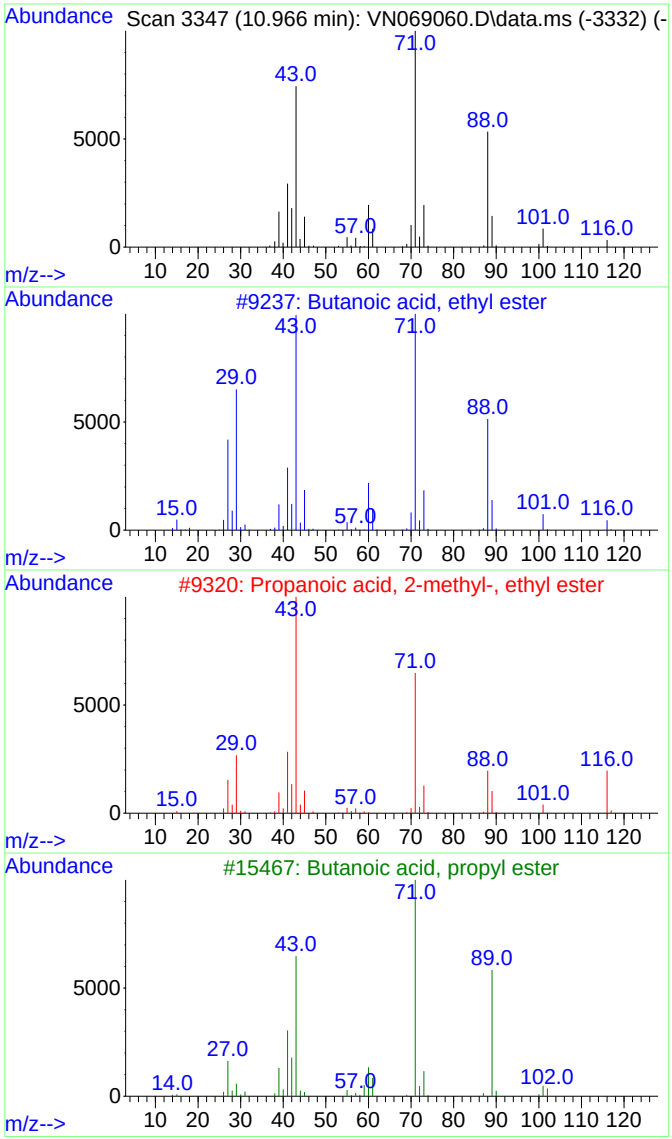
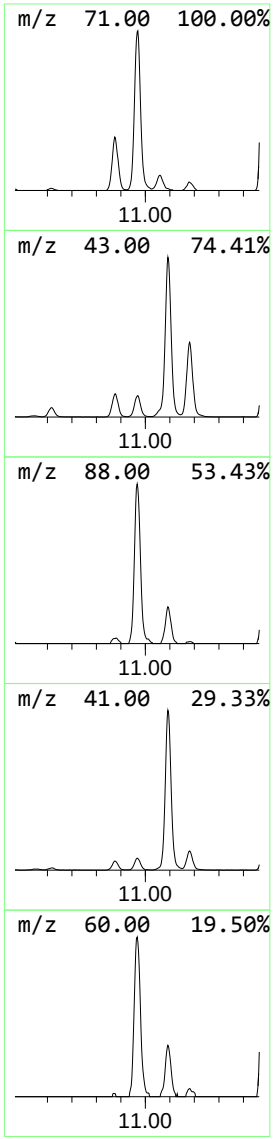
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.966	9.55 ug/l	334010	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	96
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	38
4	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	37





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Instrument : MSVOA_N
ClientSampleId : WC-1-BS

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

TIC Library : C:\Database\NIST20.L
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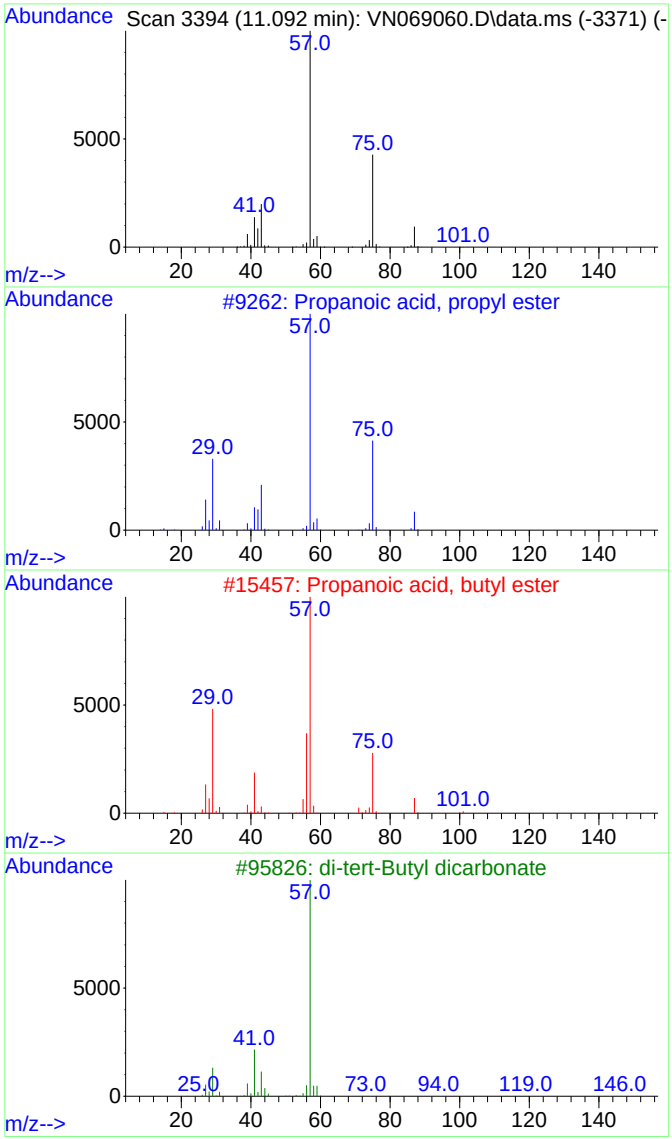
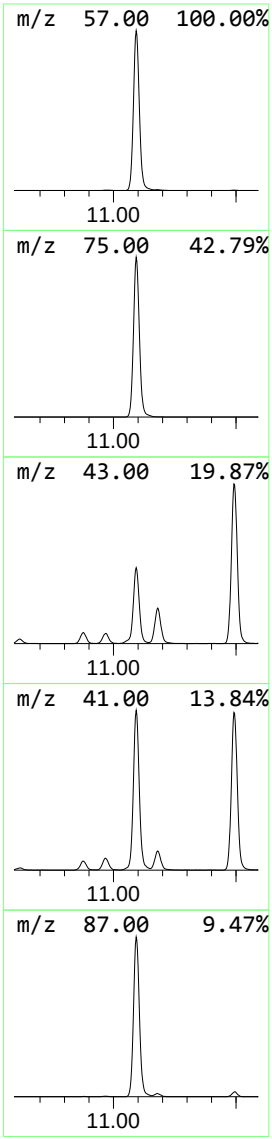
****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.092	137.37 ug/l	4805050	Chlorobenzene-d5	11.747

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	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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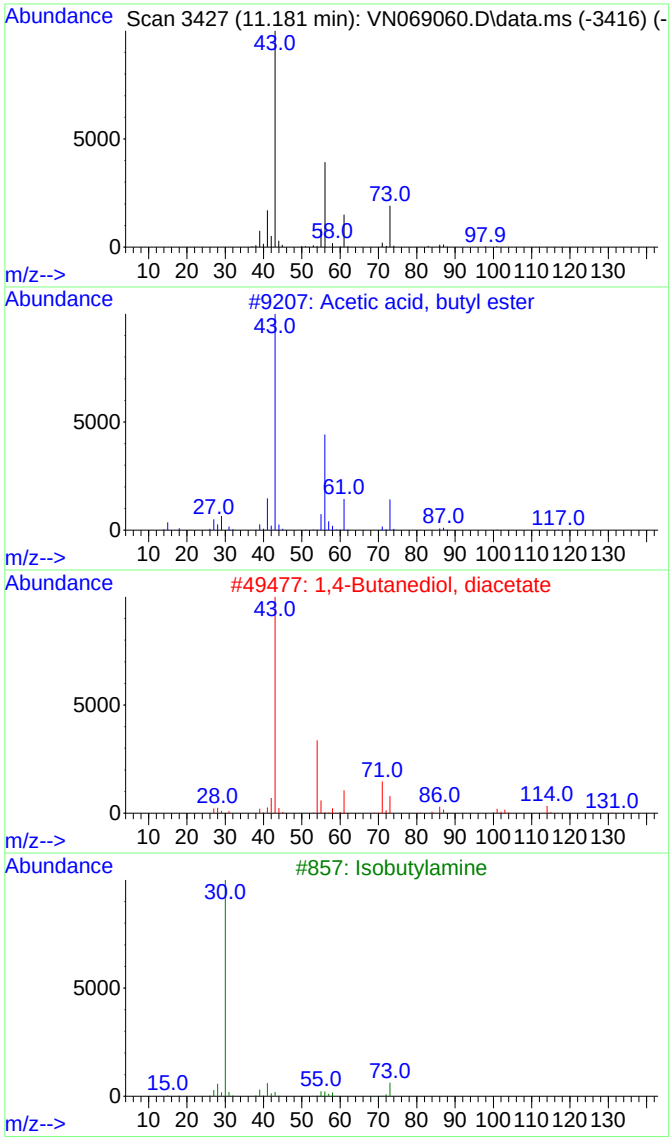
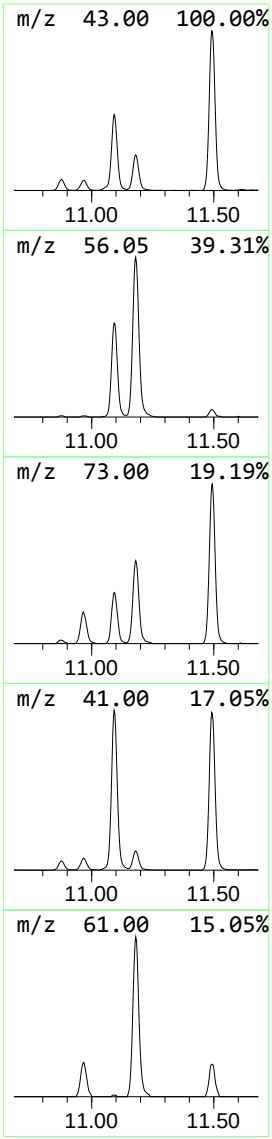
****

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	14.40 ug/l	503511	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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Instrument :
MSVOA_N
ClientSampleId :
WC-1-BS

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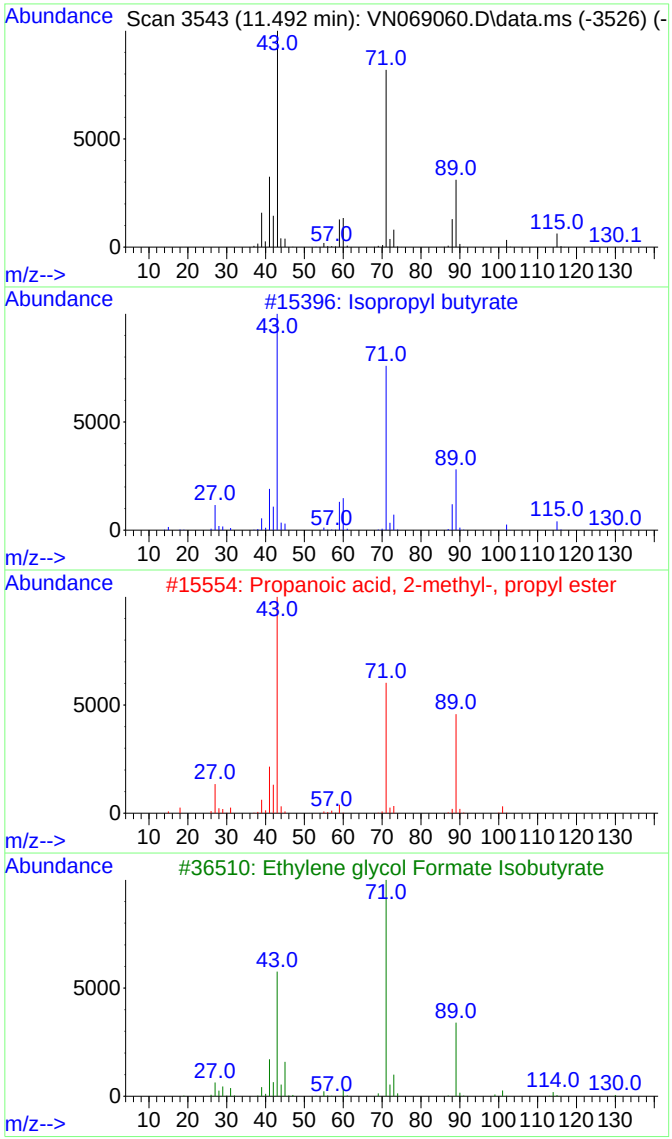
Quant Title : SW846 8260

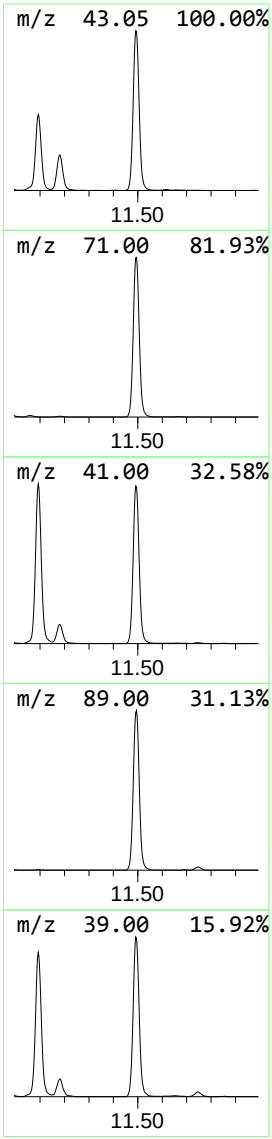
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.492	93.18 ug/l	3259280	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
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

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	9.625	116.2	ug/l	3205840	2	8.971	1379600	50.0
Propanoic acid,...	10.245	20.0	ug/l	551185	2	8.971	1379600	50.0
Butanoic acid, ...	10.966	9.6	ug/l	334010	3	11.747	1748900	50.0
Propanoic acid,...	11.092	137.4	ug/l	4805050	3	11.747	1748900	50.0
Acetic acid, bu...	11.181	14.4	ug/l	503511	3	11.747	1748900	50.0
Isopropyl butyrate	11.492	93.2	ug/l	3259280	3	11.747	1748900	50.0