LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069062.D
Acq On : 20 Oct 2021 15:21
Operator : JC/MD
Sample : M4259-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WC-1-AS

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: VN069062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.101	1137	1160	1191	rVB4	22180	75059	1.53%	0.319%
2	8.024	2228	2250	2262	rBV	240171	578432	11.81%	2.462%
3	8.088	2262	2274	2303	rVB	462818	1054427	21.54%	4.488%
4	8.440	2385	2405	2432	rBV	260244	607403	12.41%	2.585%
5	8.568	2436	2453	2459	rBV3	42813	92543	1.89%	0.394%
6	8.971	2584	2603	2631	rBV	670946	1409965	28.80%	6.001%
7	9.550	2802	2819	2830	rBV3	28728	66336	1.35%	0.282%
8	9.625	2830	2847	2888	rVV	1674929	3213215	65.63%	13.675%
9	10.245	3061	3078	3100	rBV	306909	544378	11.12%	2.317%
10	10.446	3134	3153	3181	rBV	1057925	2001063	40.87%	8.517%
11	10.617	3205	3217	3237	rVB	32379	61405	1.25%	0.261%
12	10.875	3297	3313	3331	rBV	86390	151023	3.08%	0.643%
13	10.969	3333	3348	3369	rVV	188895	331760	6.78%	1.412%
14	11.092	3371	3394	3416	rVV	2857368	4896010	100.00%	20.837%
15	11.181	3416	3427	3458	rVB	291010	523195	10.69%	2.227%
16	11.494	3526	3544	3577	rBV	1963130	3315015	67.71%	14.109%
17	11.747	3621	3638	3670	rVB	996521	1800887	36.78%	7.665%
18	12.200	3793	3807	3825	rBV	59888	99754	2.04%	0.425%
19	12.733	3987	4006	4031	rBV	729823	1283528	26.22%	5.463%
20	13.678	4341	4358	4378	rBV	820495	1390868	28.41%	5.920%

Sum of corrected areas: 23496266

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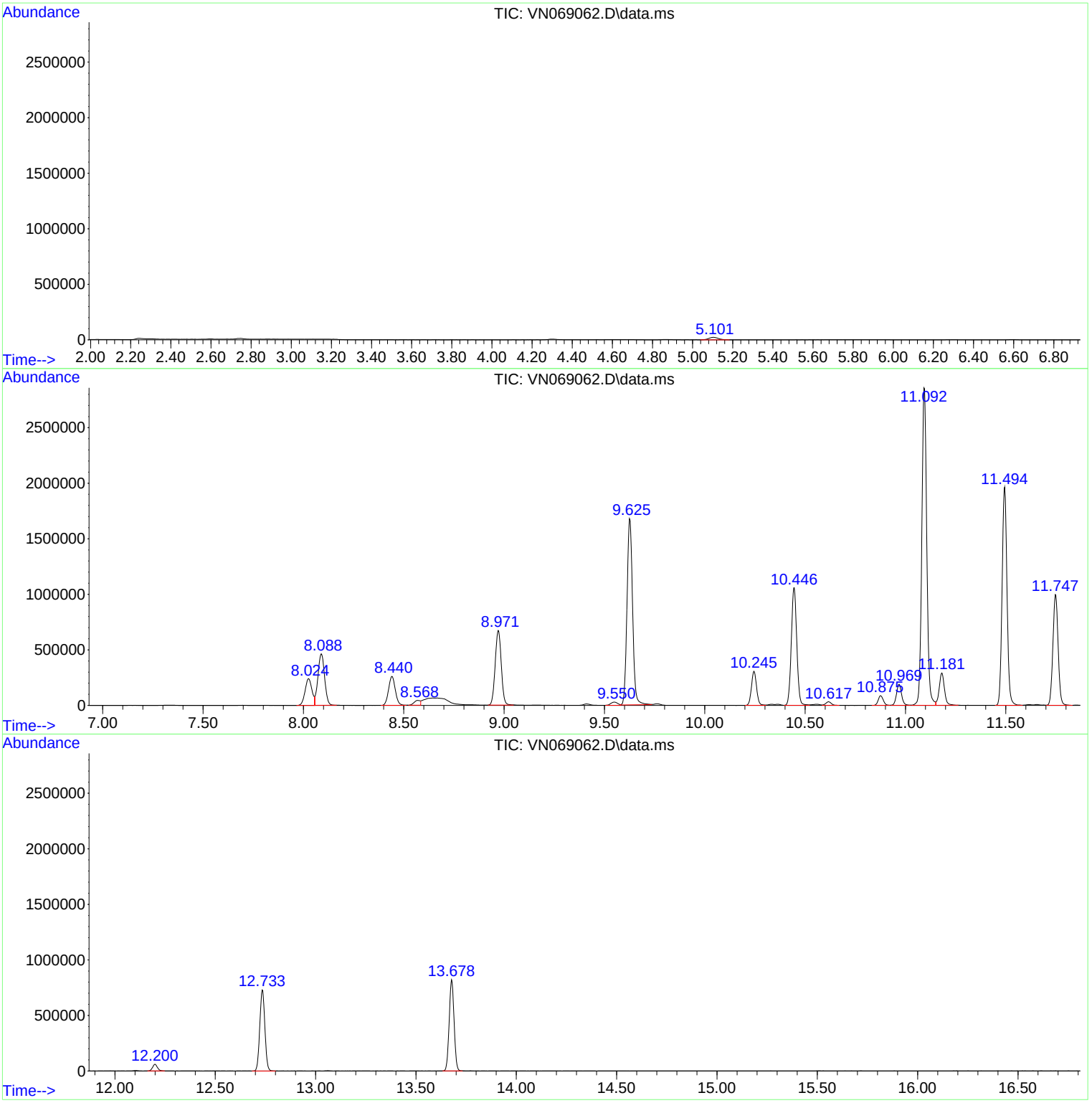
Instrument :
MSVOA_N
ClientSampleId :
WC-1-AS

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

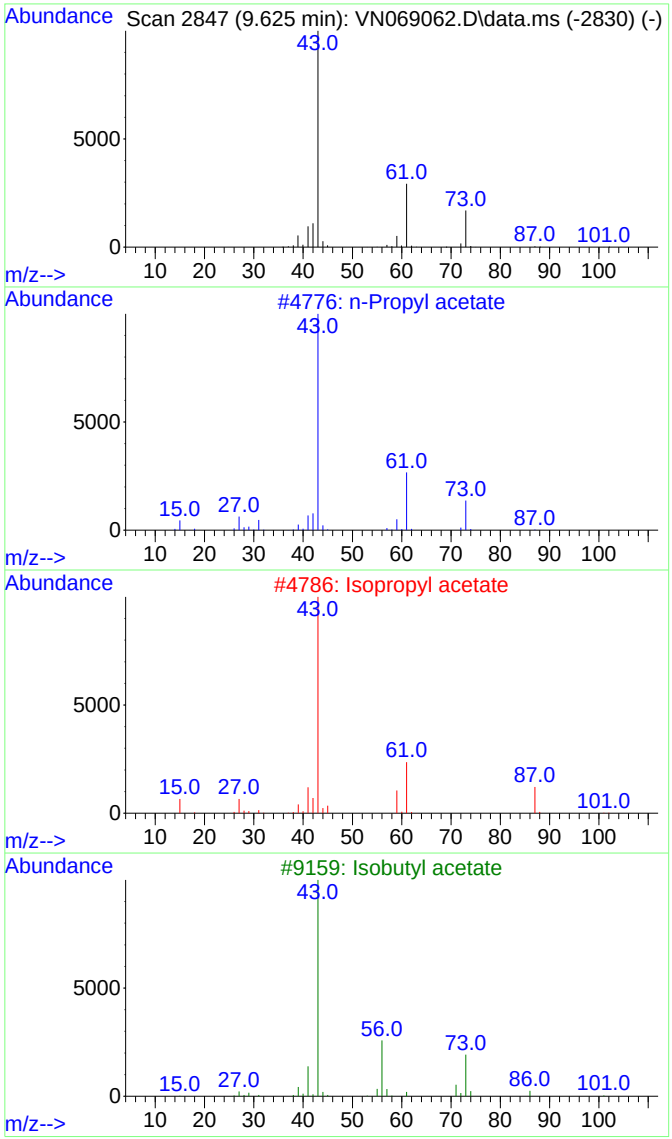
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

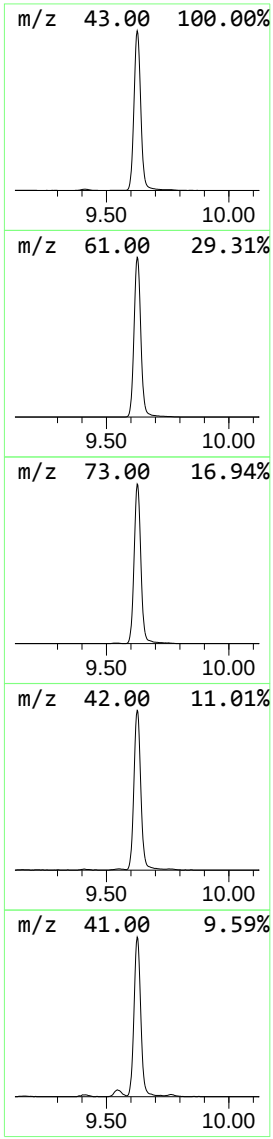
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.625	113.95 ug/l	3213220	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	36
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 Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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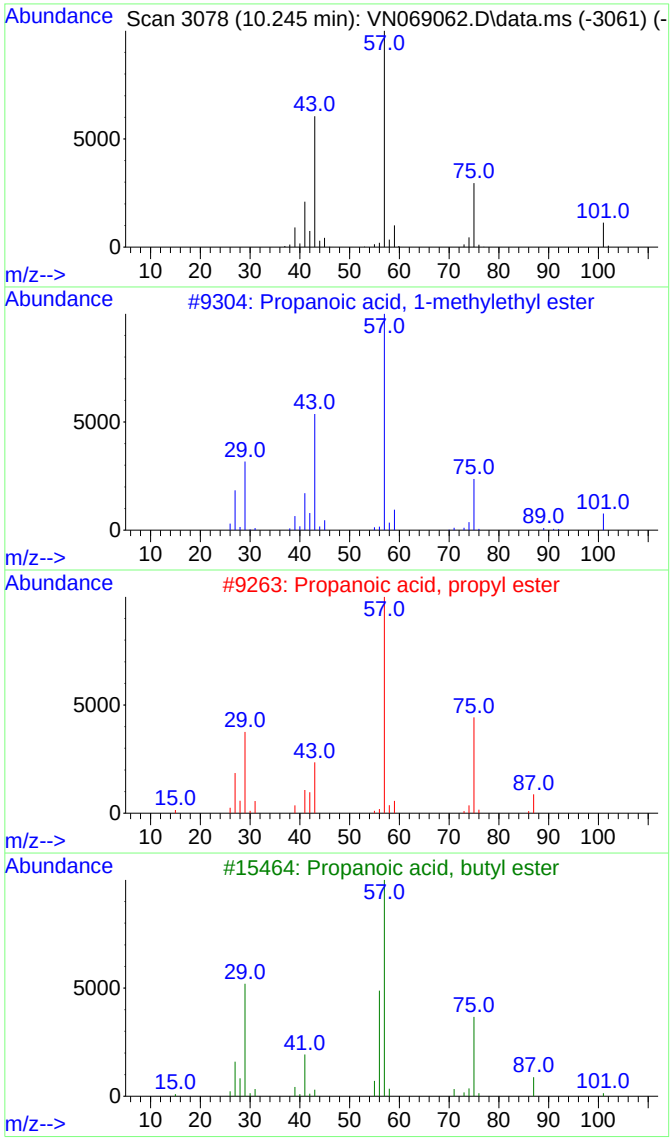
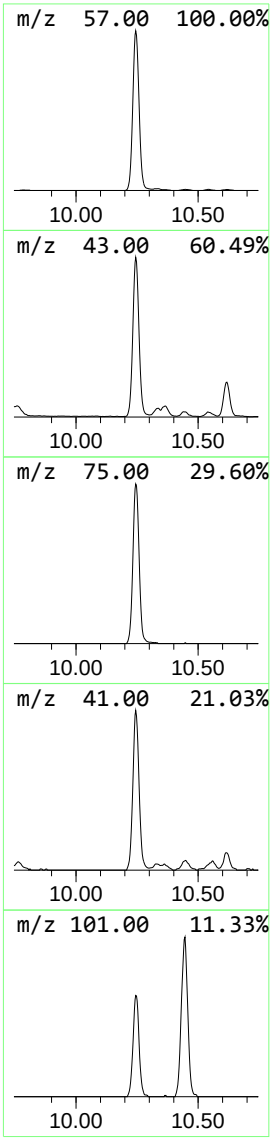
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	19.30 ug/l	544378	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	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





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

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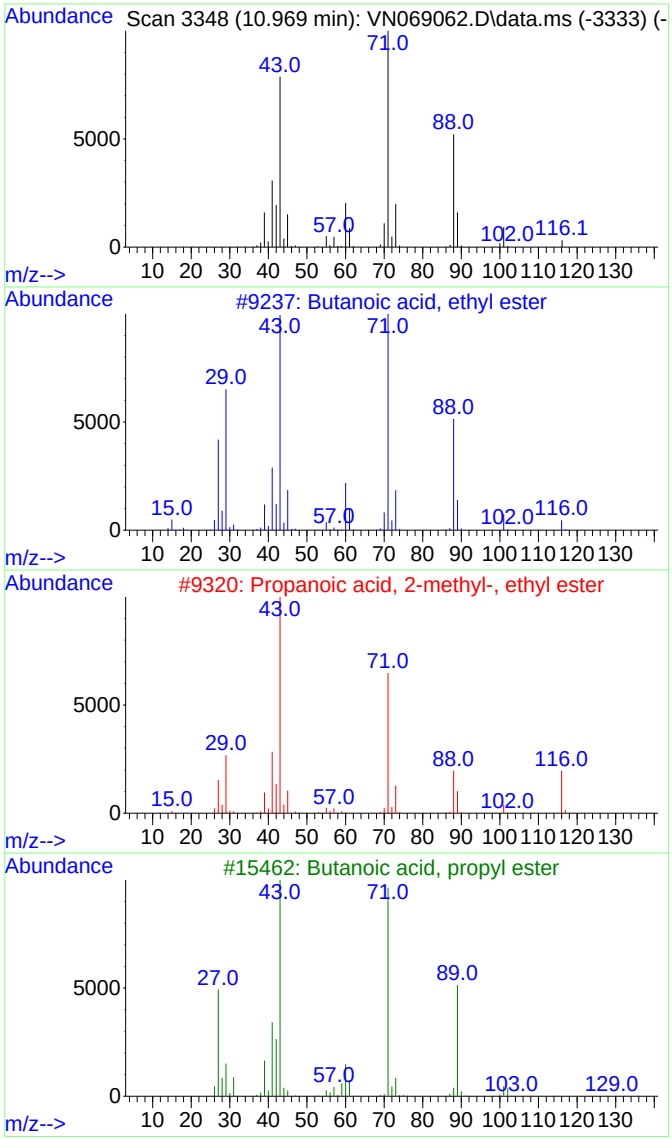
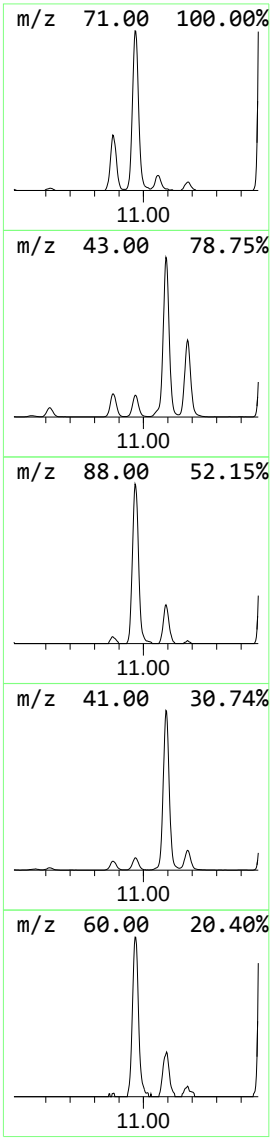
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.969	9.21 ug/l	331760	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	87
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	59
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38





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ClientSampleId : WC-1-AS

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Quant Title : SW846 8260

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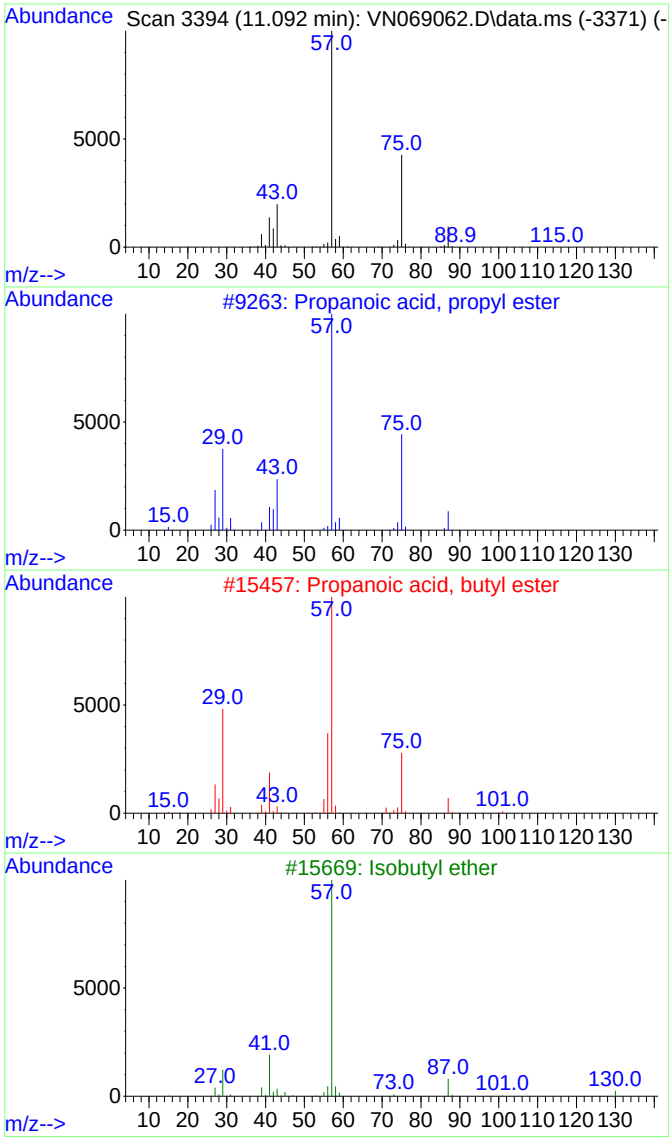
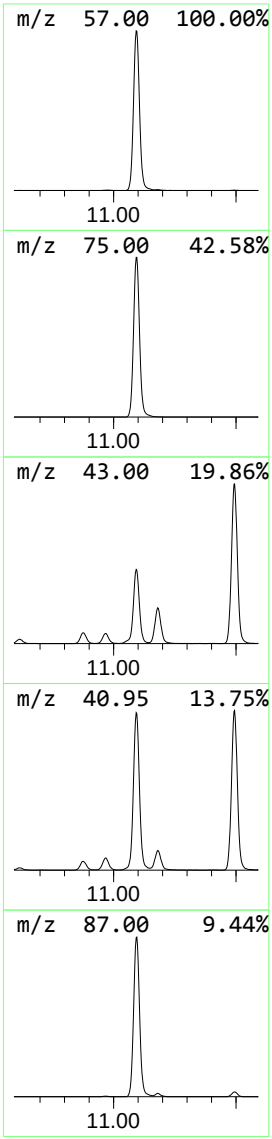
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.092	135.93 ug/l	4896010	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	Isobutyl ether	130	C8H18O	000628-55-7	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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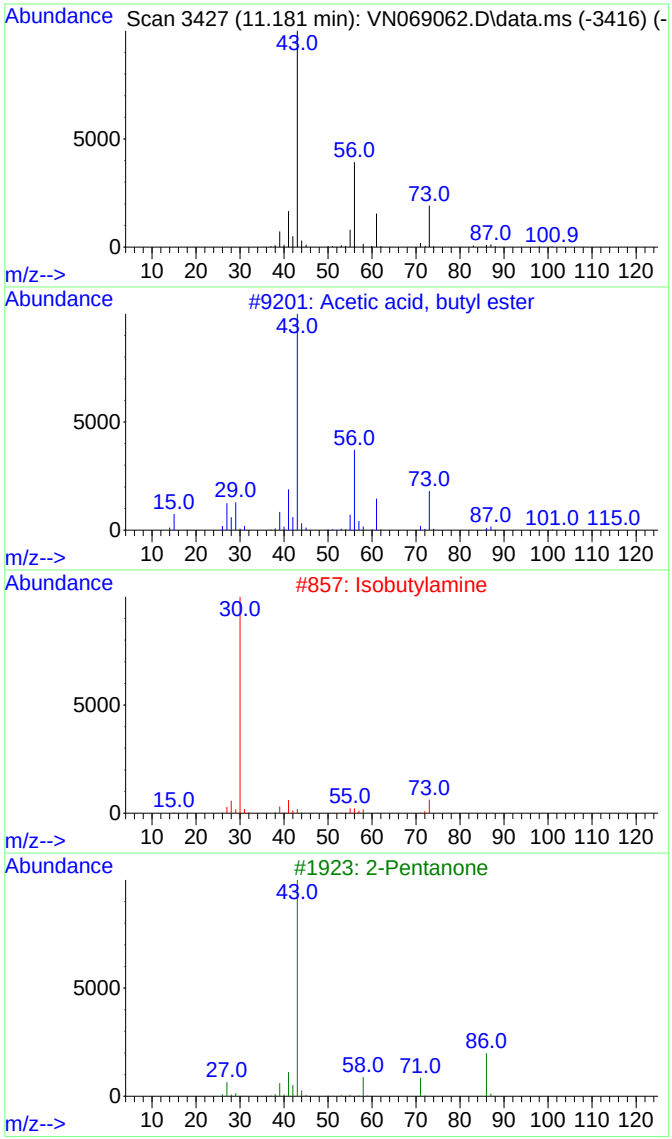
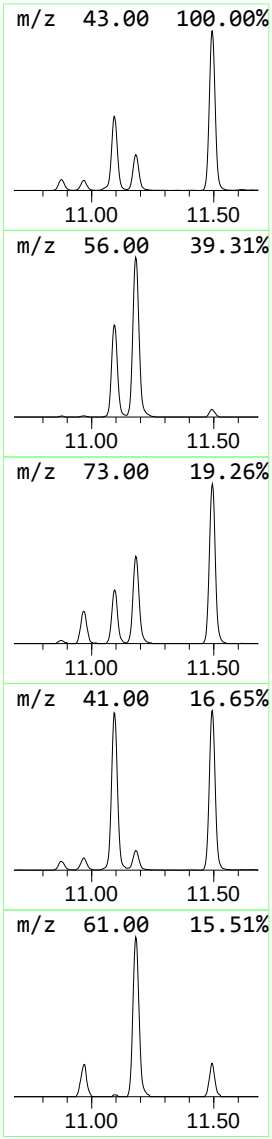
****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	14.53 ug/l	523195	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	Isobutylamine	73	C4H11N	000078-81-9	9
3	2-Pentanone	86	C5H10O	000107-87-9	9
4	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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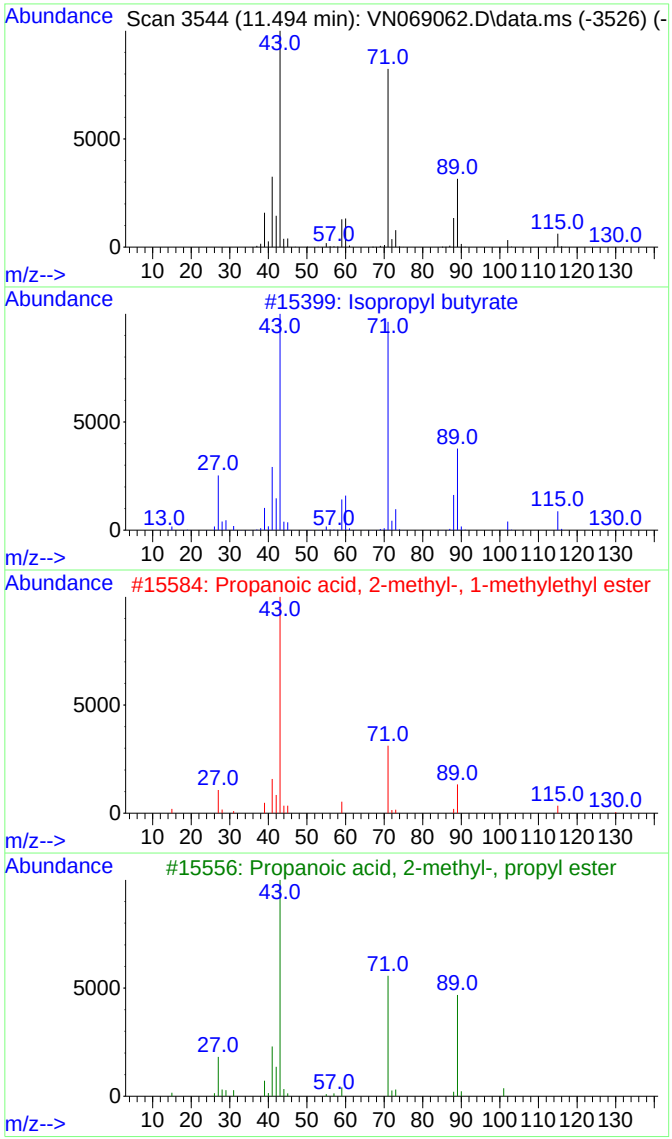
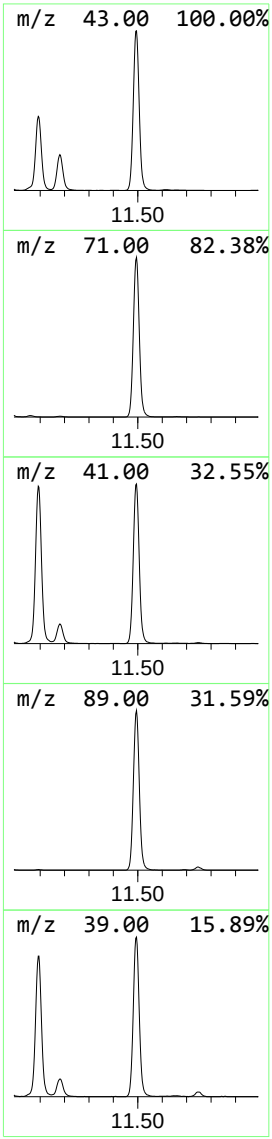
Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.494	92.04 ug/l	3315020	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
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	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	114.0	ug/l	3213220	2	8.971	1409970	50.0
Propanoic acid,...	10.245	19.3	ug/l	544378	2	8.971	1409970	50.0
Butanoic acid, ...	10.969	9.2	ug/l	331760	3	11.746	1800890	50.0
Propanoic acid,...	11.092	135.9	ug/l	4896010	3	11.746	1800890	50.0
Acetic acid, bu...	11.181	14.5	ug/l	523195	3	11.746	1800890	50.0
Isopropyl butyrate	11.494	92.0	ug/l	3315020	3	11.746	1800890	50.0