LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069061.D
Acq On : 20 Oct 2021 14:56
Operator : JC/MD
Sample : M4259-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WC-1-BD

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: VN069061.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	1139	1162	1191	rBV5	22431	73273	1.50%	0.320%
2	8.024	2229	2250	2261	rBV2	223762	531114	10.84%	2.321%
3	8.088	2262	2274	2308	rVB	435140	988899	20.18%	4.322%
4	8.440	2386	2405	2429	rBV	246384	569543	11.63%	2.489%
5	8.566	2436	2452	2460	rBV4	34006	77136	1.57%	0.337%
6	8.971	2584	2603	2638	rBV	632779	1321014	26.96%	5.773%
7	9.547	2802	2818	2830	rBV3	30760	68244	1.39%	0.298%
8	9.625	2830	2847	2886	rVV	1661793	3209253	65.51%	14.025%
9	10.245	3061	3078	3099	rBV	306468	538605	10.99%	2.354%
10	10.446	3134	3153	3178	rBV	1008052	1879340	38.36%	8.213%
11	10.615	3205	3216	3232	rVB2	32103	58868	1.20%	0.257%
12	10.878	3299	3314	3330	rBV	87300	150865	3.08%	0.659%
13	10.969	3333	3348	3371	rVV	192374	341116	6.96%	1.491%
14	11.092	3371	3394	3416	rVV	2855593	4899234	100.00%	21.411%
15	11.181	3416	3427	3455	rVB	297001	529990	10.82%	2.316%
16	11.494	3523	3544	3569	rBV	1945380	3307629	67.51%	14.455%
17	11.747	3621	3638	3666	rVB	933024	1702410	34.75%	7.440%
18	12.200	3794	3807	3826	rVB	62548	103471	2.11%	0.452%
19	12.733	3990	4006	4032	rBV	693374	1209019	24.68%	5.284%
20	13.678	4341	4358	4387	rBV2	767522	1323032	27.00%	5.782%

Sum of corrected areas: 22882055

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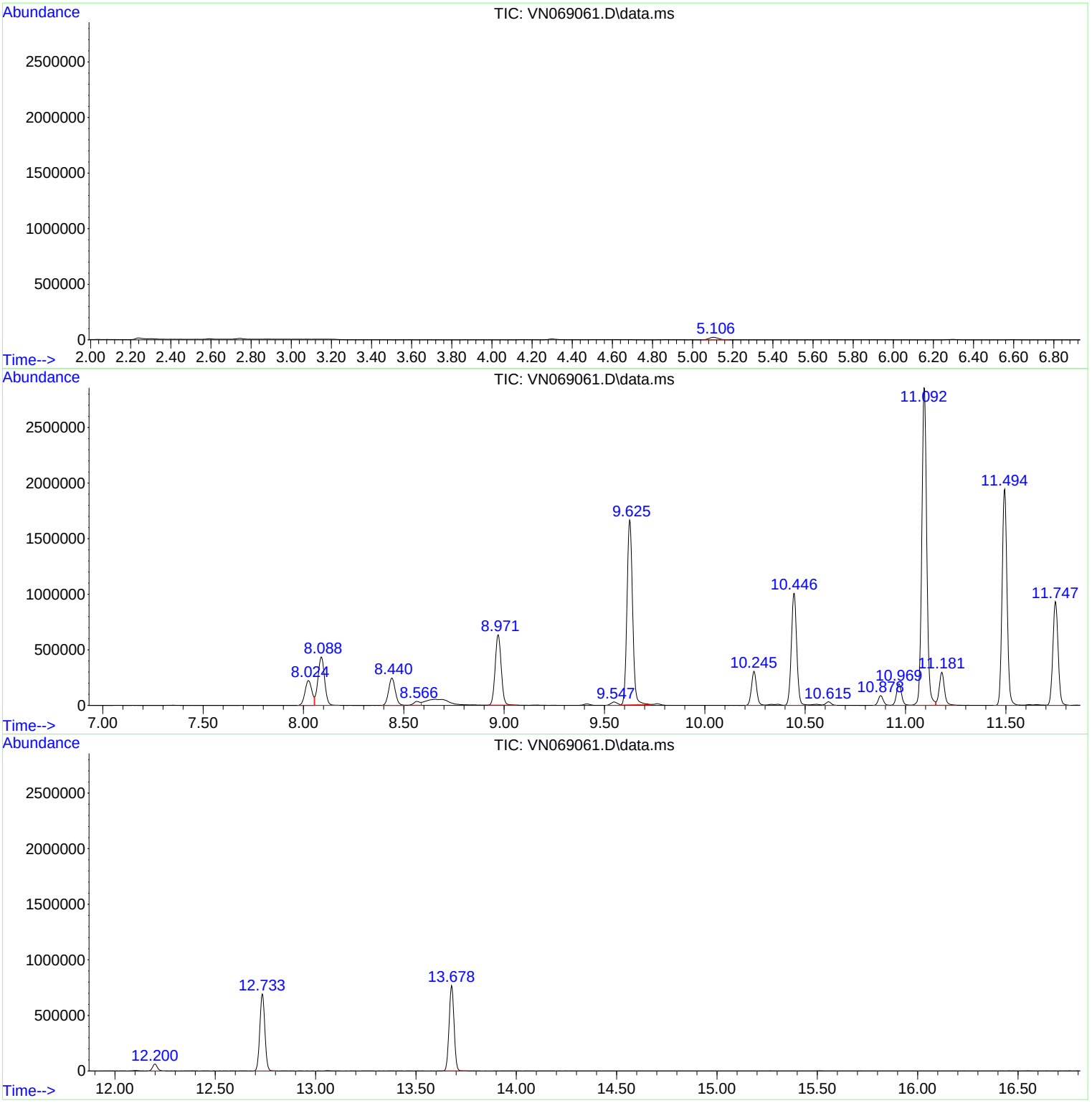
MSVOA_N
ClientSampleId :
WC-1-BD

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

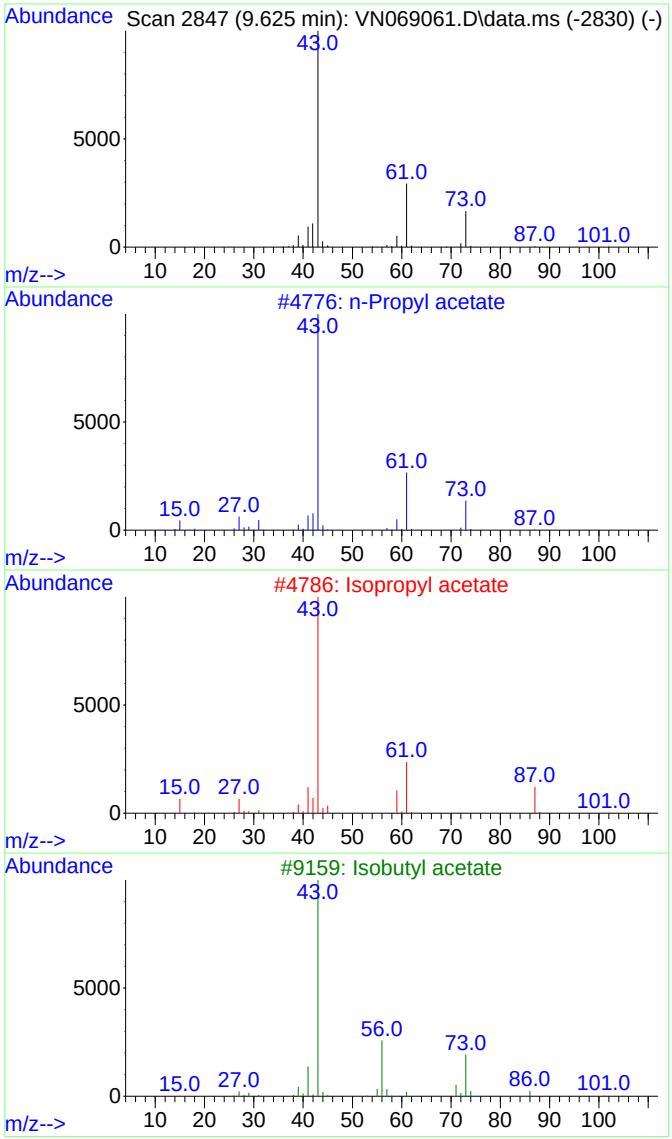
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

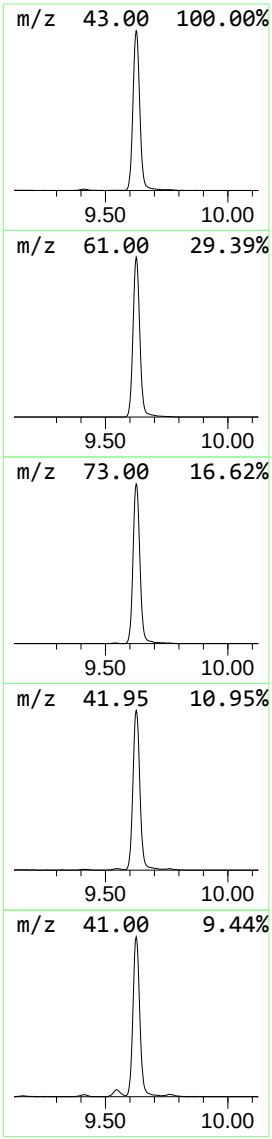
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.625	121.47 ug/l	3209250	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

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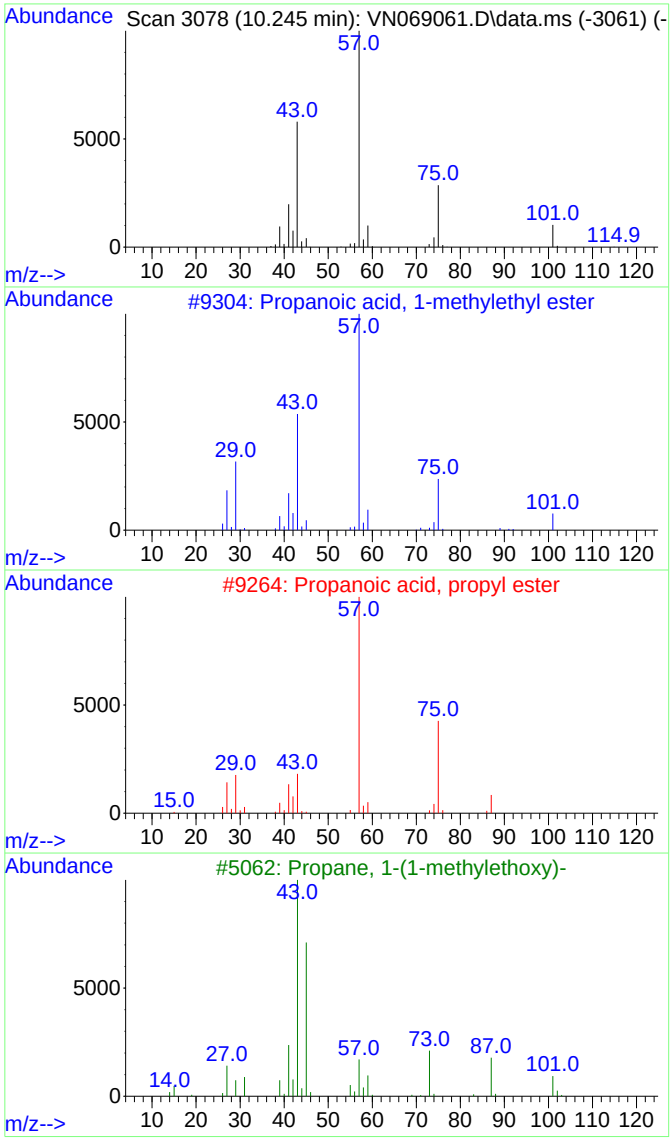
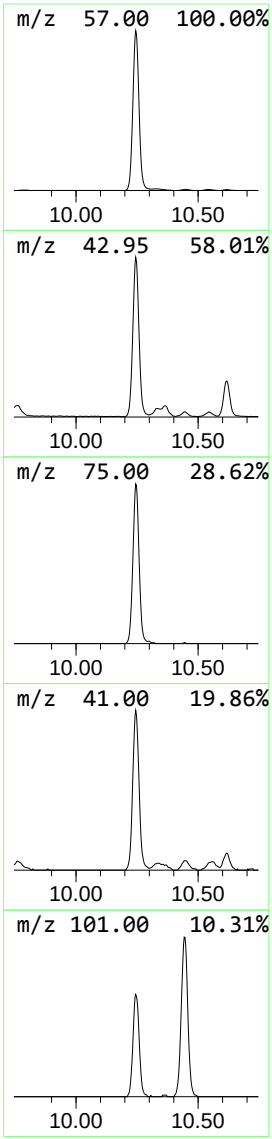
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	20.39 ug/l	538605	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	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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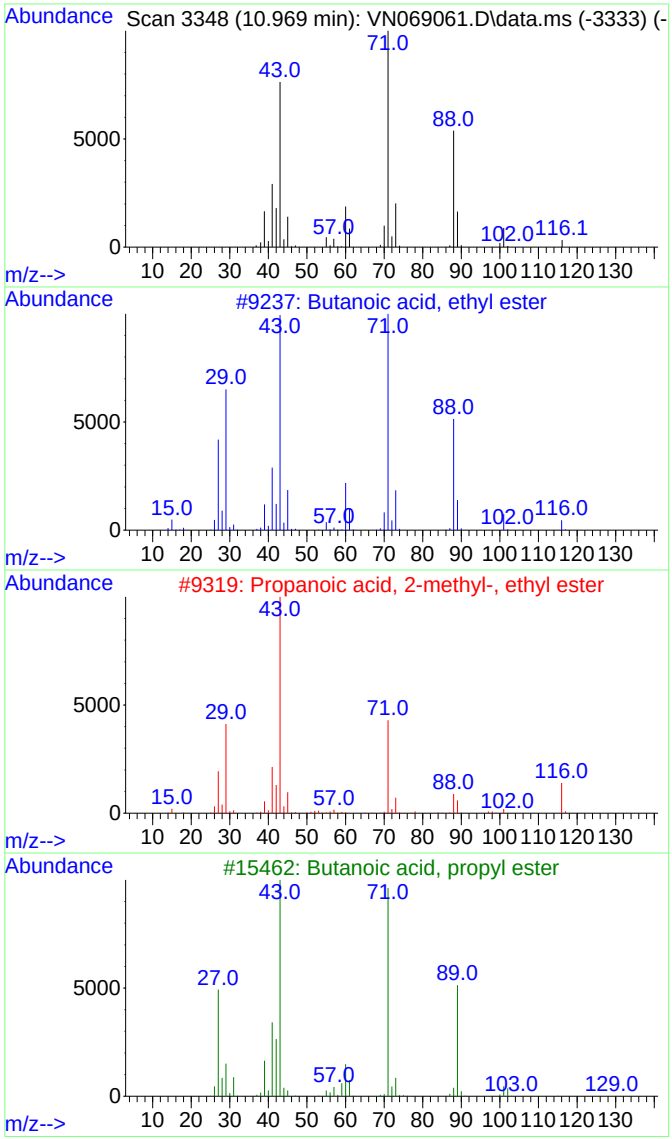
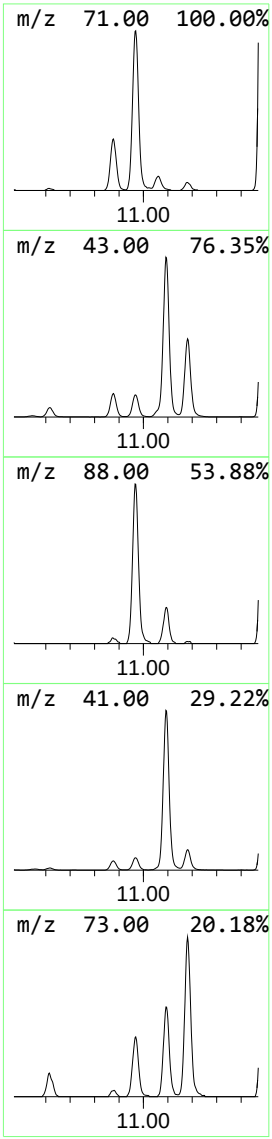
****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.969	10.02 ug/l	341116	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	59
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	43
5	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38





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Quant Title : SW846 8260

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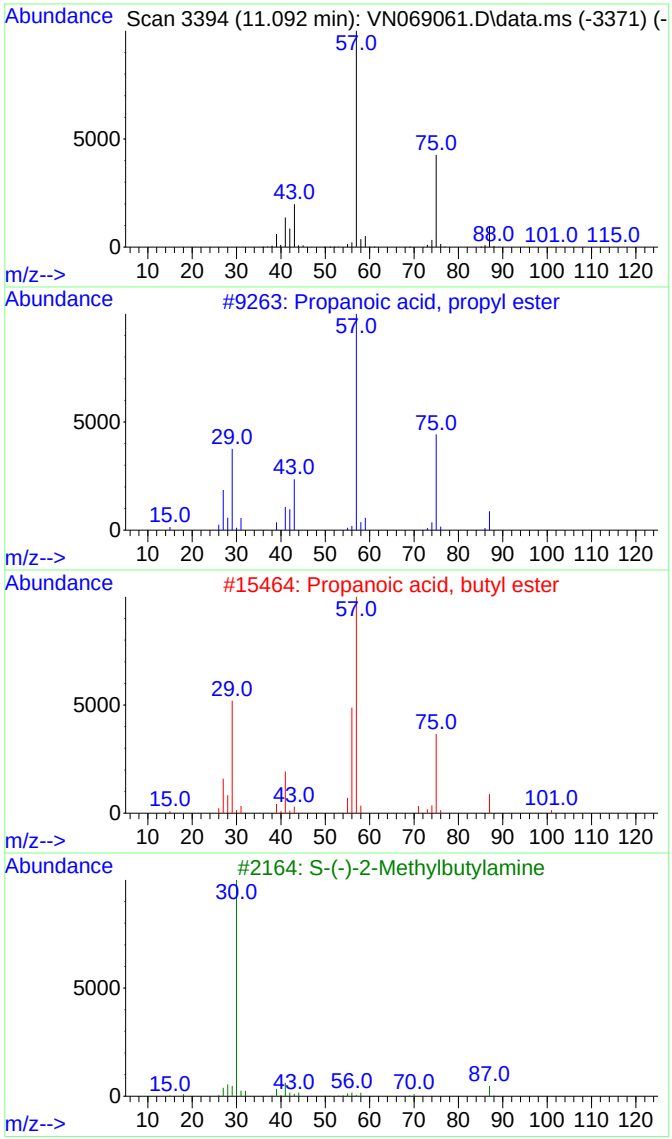
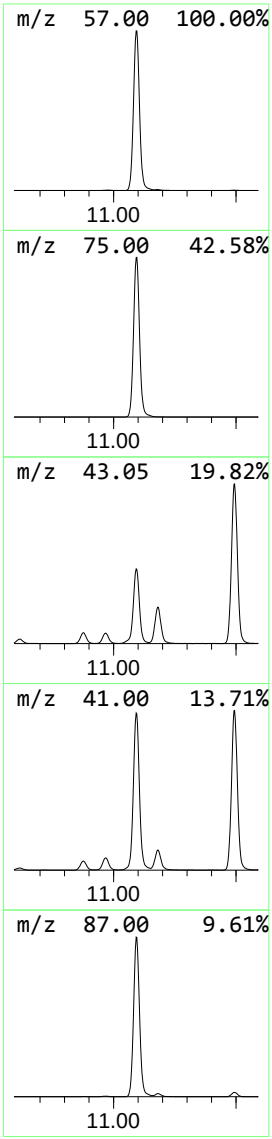
****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.092	143.89 ug/l	4899230	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	40
3	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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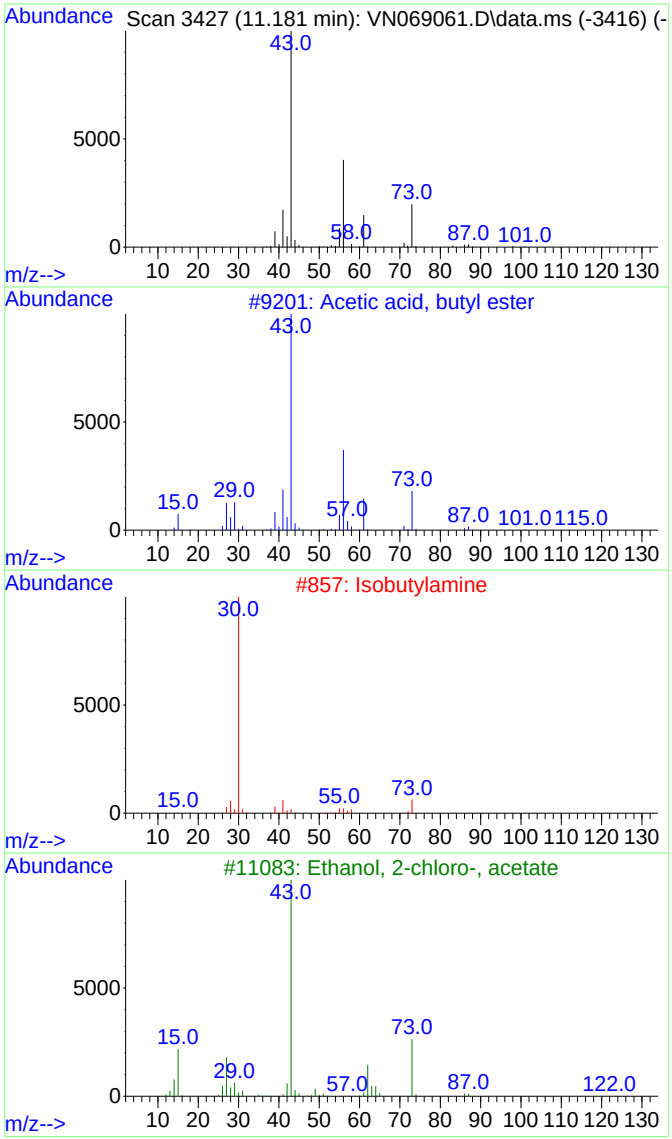
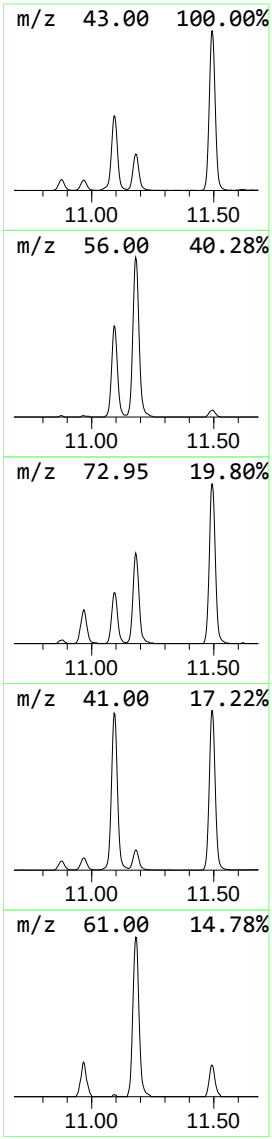
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	15.57 ug/l	529990	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





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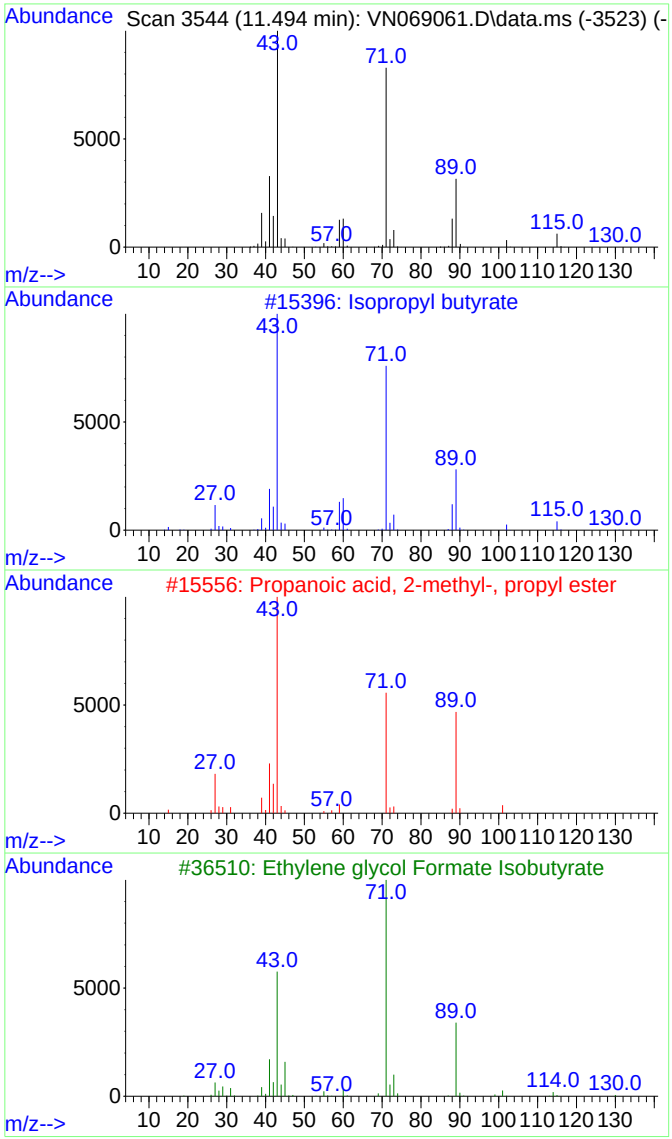
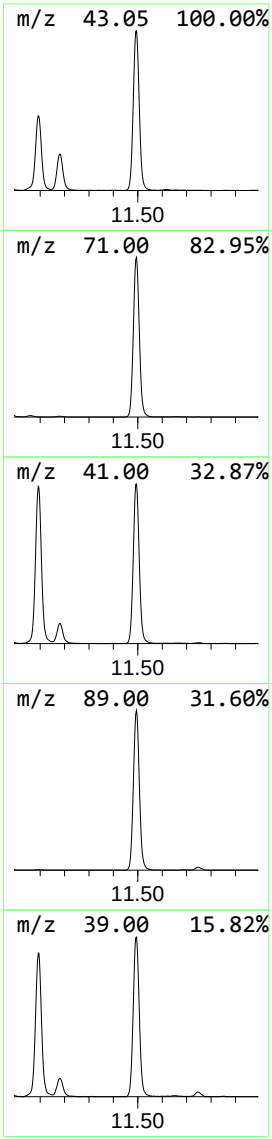
Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.494	97.15 ug/l	3307630	Chlorobenzene-d5	11.746

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

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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	121.5	ug/l	3209250	2	8.971	1321010	50.0
Propanoic acid,...	10.245	20.4	ug/l	538605	2	8.971	1321010	50.0
Butanoic acid, ...	10.969	10.0	ug/l	341116	3	11.746	1702410	50.0
Propanoic acid,...	11.092	143.9	ug/l	4899230	3	11.746	1702410	50.0
Acetic acid, bu...	11.181	15.6	ug/l	529990	3	11.746	1702410	50.0
Isopropyl butyrate	11.494	97.2	ug/l	3307630	3	11.746	1702410	50.0