LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045020.D
Acq On : 30 Sep 2021 02:40
Operator : SY/MD
Sample : PB139450ZHE#03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB139450ZHE#03

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_U\Method\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.629	390	401	420	rBV	42945	75151	1.62%	0.400%
2	3.047	519	531	549	rVB	26388	52054	1.12%	0.277%
3	5.292	1212	1229	1242	rBV	168833	355576	7.68%	1.890%
4	5.375	1242	1255	1276	rVB	299178	614035	13.26%	3.264%
5	5.703	1339	1357	1377	rBV	206485	421450	9.10%	2.240%
6	5.916	1407	1423	1437	rBV	23952	47704	1.03%	0.254%
7	6.250	1515	1527	1575	rVB	473534	989413	21.36%	5.260%
8	6.935	1719	1740	1756	rVB3	23682	68886	1.49%	0.366%
9	7.044	1756	1774	1805	rBV	1728001	3004687	64.86%	15.973%
10	7.742	1970	1991	2002	rBV	254163	422185	9.11%	2.244%
11	7.899	2026	2040	2070	rBV	714780	1245821	26.89%	6.623%
12	8.163	2111	2122	2136	rBV	27798	47384	1.02%	0.252%
13	8.468	2206	2217	2233	rBV	68505	112321	2.42%	0.597%
14	8.578	2233	2251	2262	rVV	185297	312482	6.75%	1.661%
15	8.732	2282	2299	2318	rVV	2974405	4632419	100.00%	24.627%
16	8.838	2321	2332	2368	rVB	322467	522104	11.27%	2.776%
17	9.214	2435	2449	2483	rBV	1746834	2696351	58.21%	14.334%
18	9.420	2502	2513	2533	rVB	696301	1134264	24.49%	6.030%
19	10.076	2705	2717	2745	rBV	61808	100273	2.16%	0.533%
20	10.636	2878	2891	2913	rBV	561300	874677	18.88%	4.650%
21	11.816	3245	3258	3280	rBV	687313	1081392	23.34%	5.749%

Sum of corrected areas: 18810629

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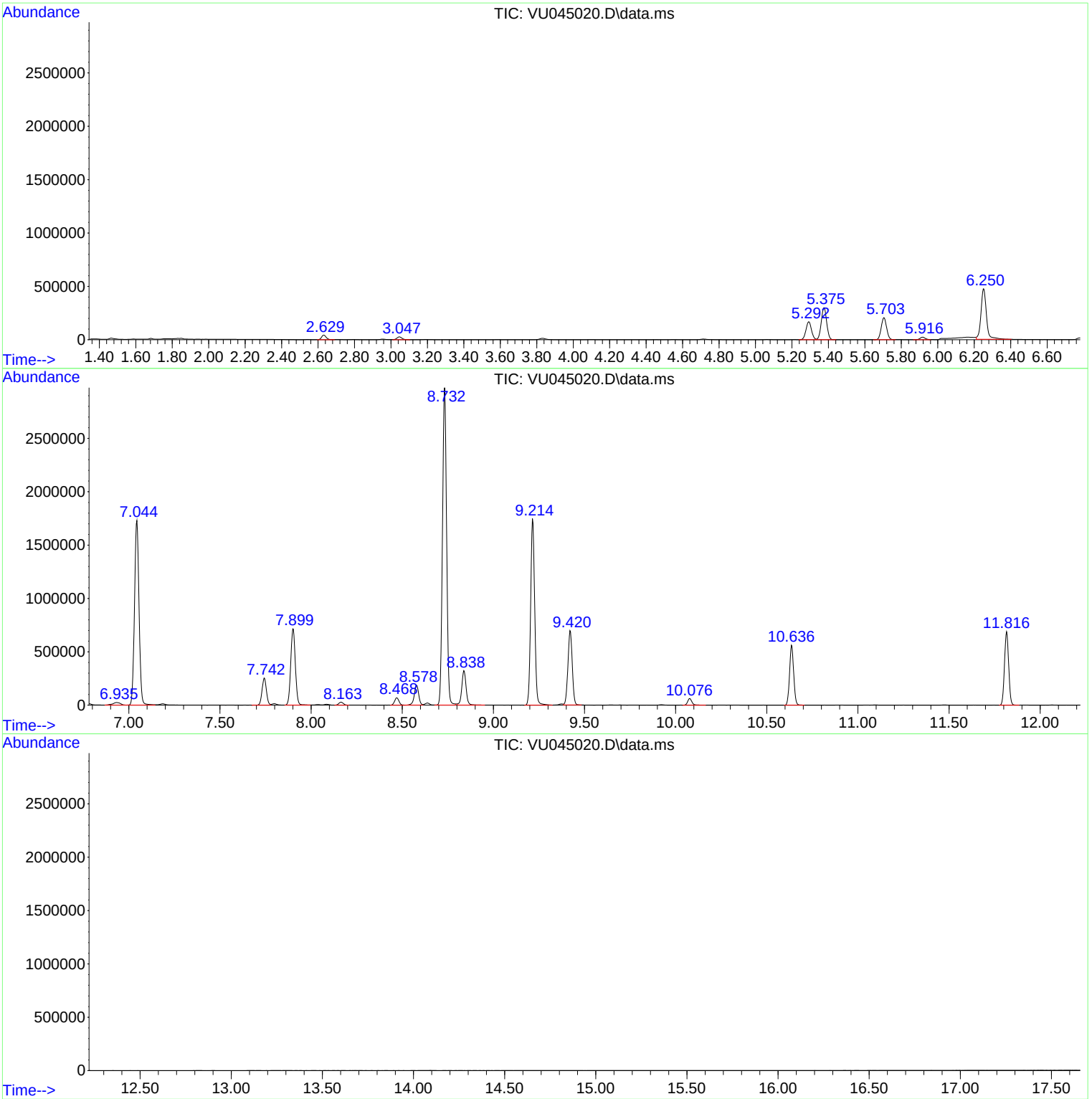
ClientSampleId :
PB139450ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



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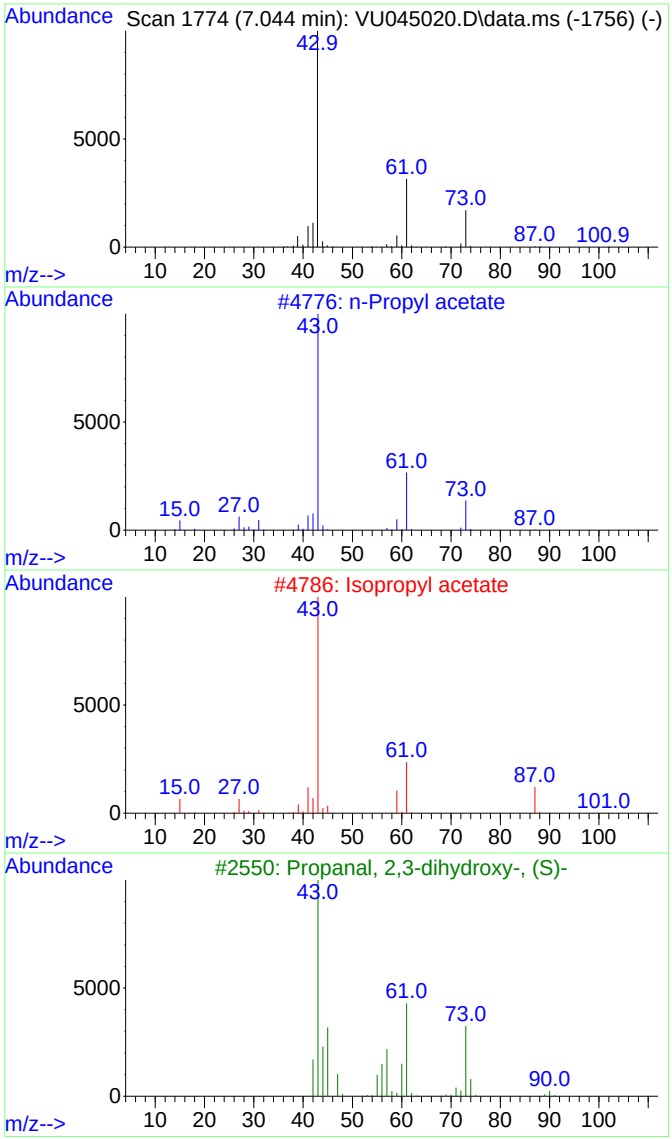
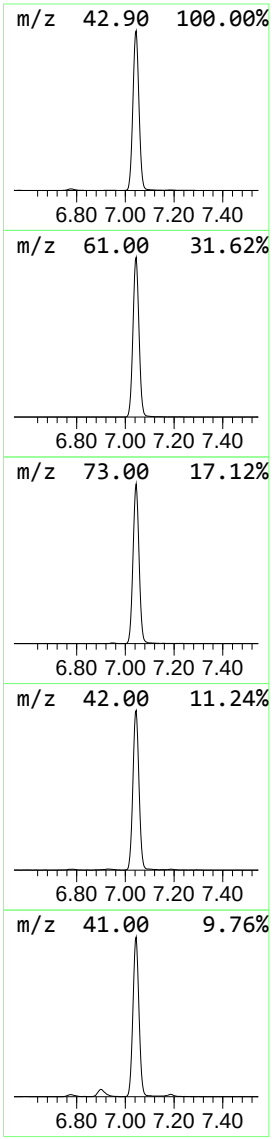
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	151.84 ug/l	3004690	1,4-Difluorobenzene	6.253

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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	5





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ClientSampleId :
PB139450ZHE#03

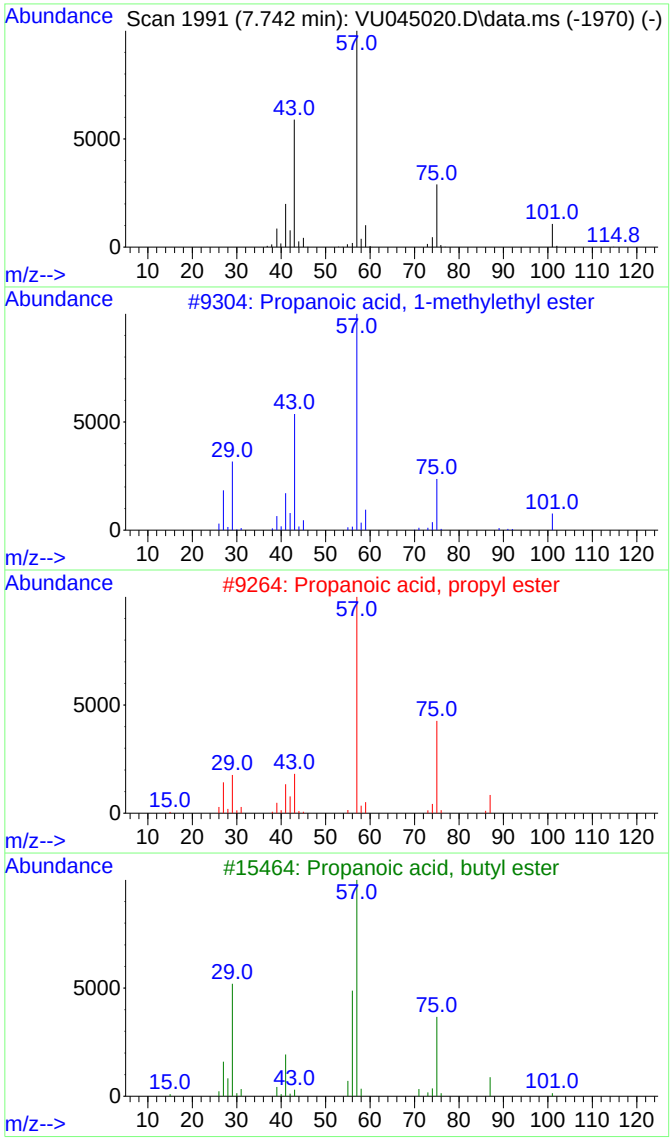
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

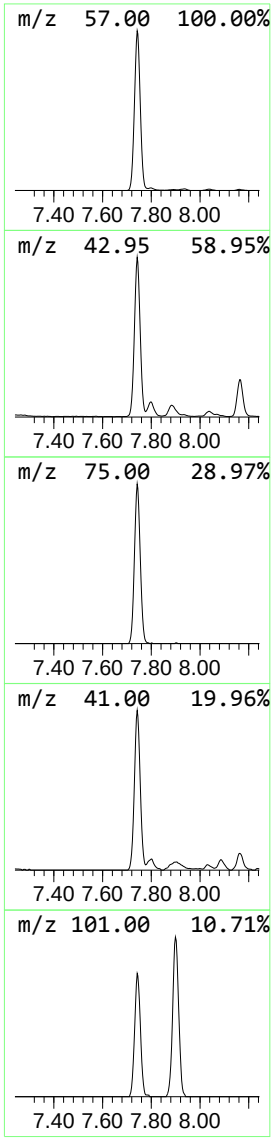
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	21.34 ug/l	422185	1,4-Difluorobenzene	6.253

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	25
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





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Instrument :
MSVOA_U
ClientSampleId :
PB139450ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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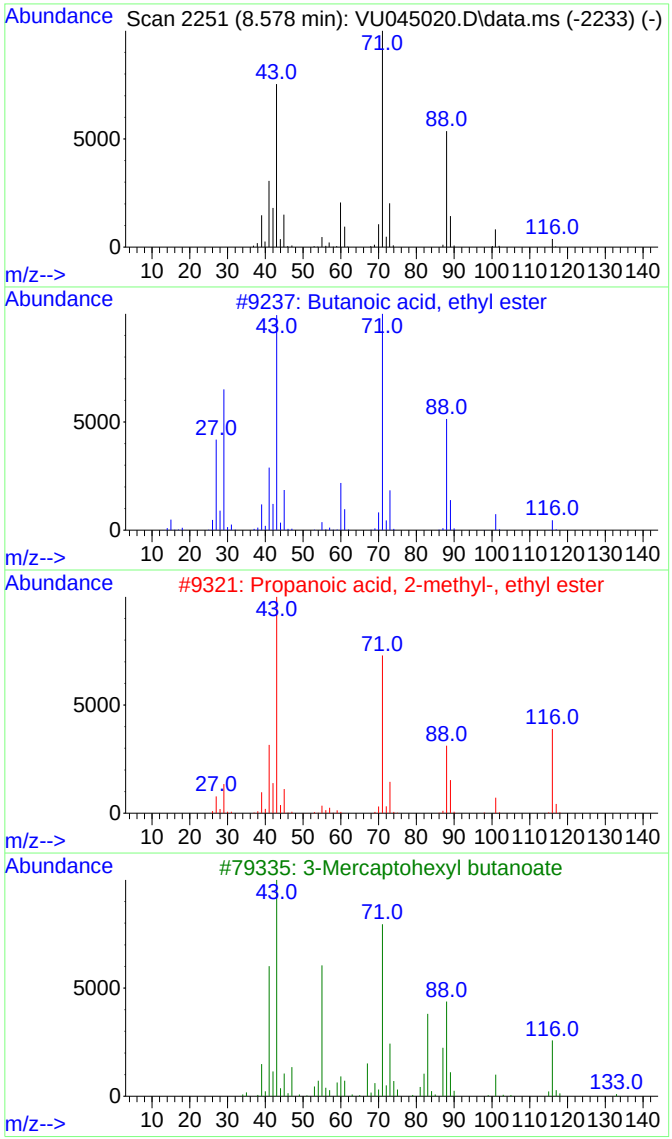
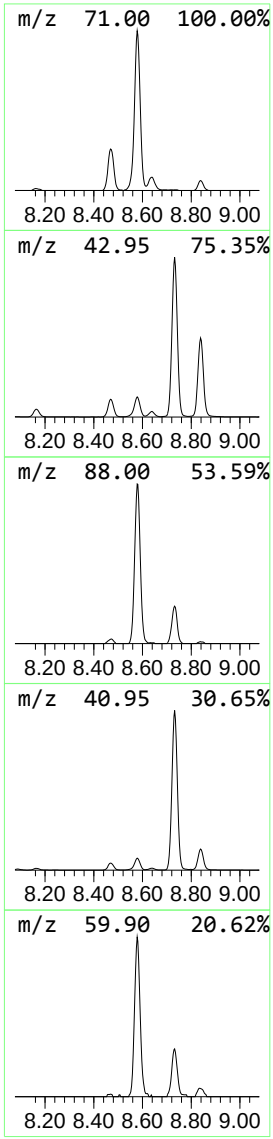
****

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.578	13.77 ug/l	312482	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	52
3	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40
5	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38





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ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB139450ZHE#03

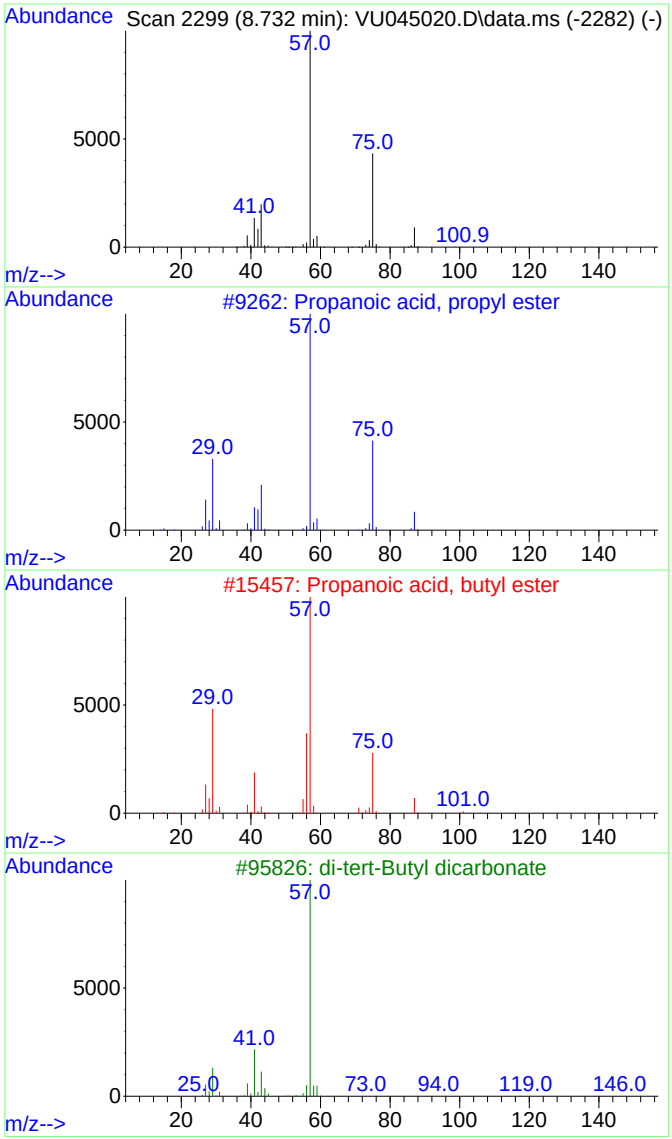
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

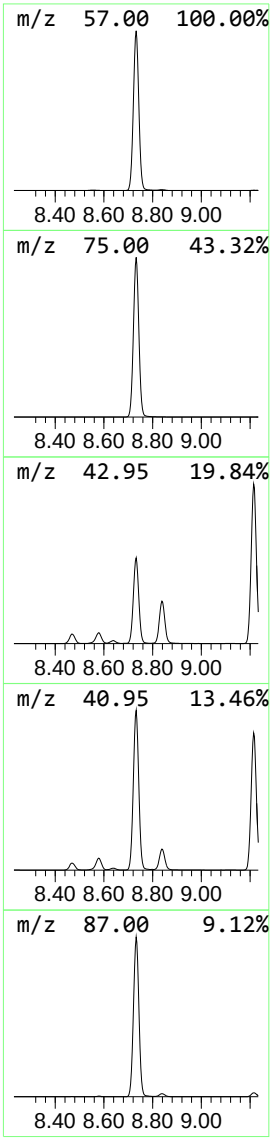
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	204.20 ug/l	4632420	Chlorobenzene-d5	9.420

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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ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
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TIC Library : C:\Database\NIST20.L
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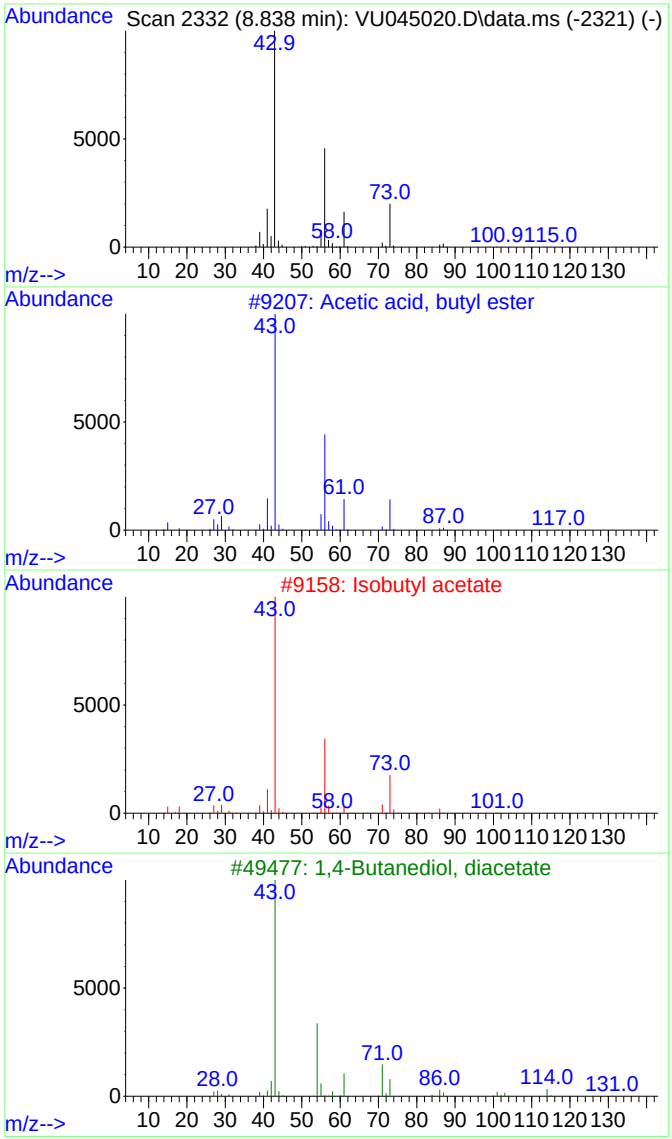
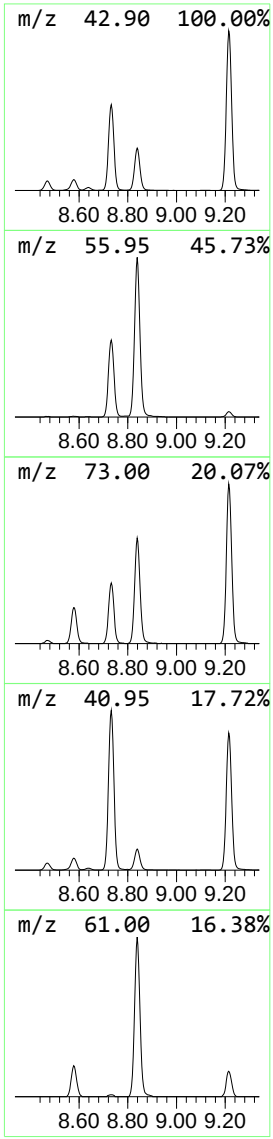
****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.838	23.02 ug/l	522104	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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ClientSampleId :
PB139450ZHE#03

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Quant Title : SW846 8260

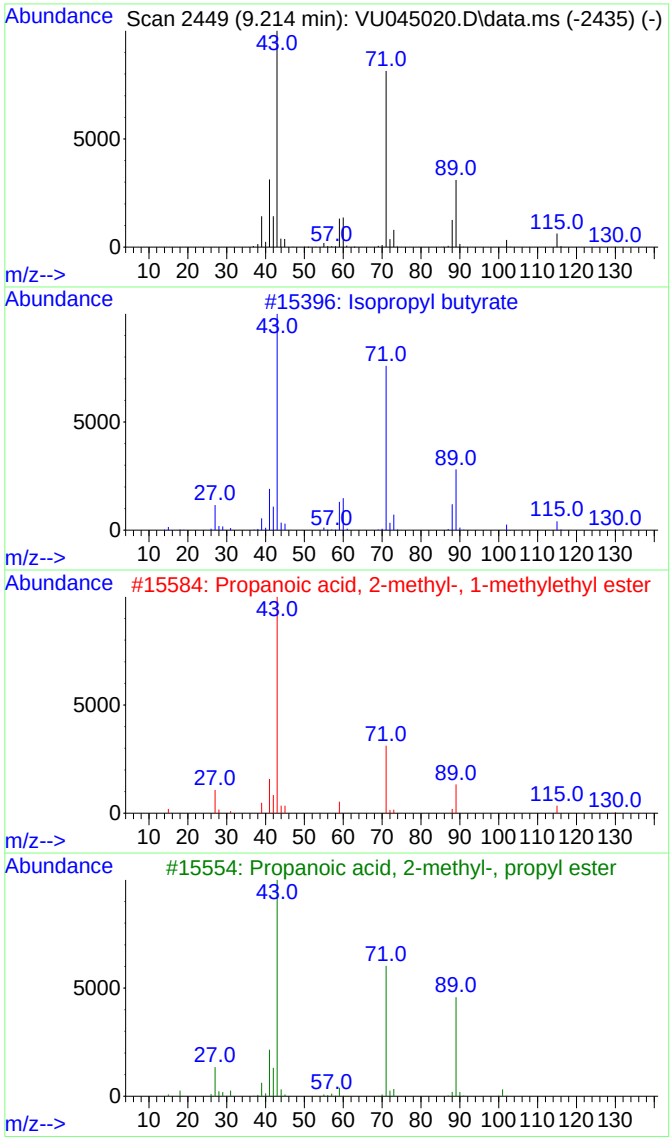
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

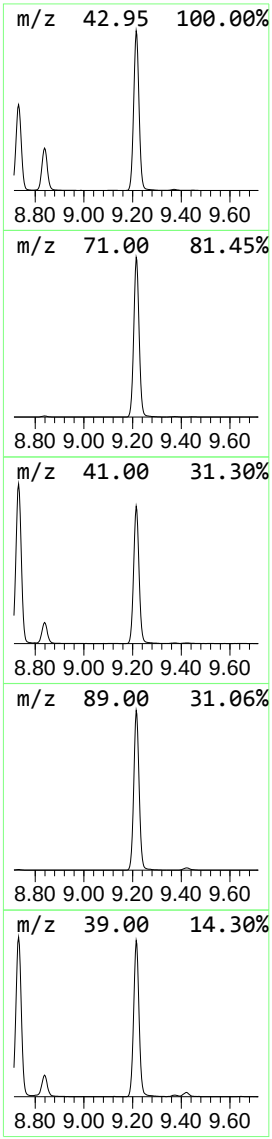
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.214	118.86 ug/l	2696350	Chlorobenzene-d5	9.420

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	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	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	7.044	151.8	ug/l	3004690	2	6.253	989413	50.0
Propanoic acid,...	7.742	21.3	ug/l	422185	2	6.253	989413	50.0
Butanoic acid, ...	8.578	13.8	ug/l	312482	3	9.420	1134260	50.0
Propanoic acid,...	8.732	204.2	ug/l	4632420	3	9.420	1134260	50.0
Acetic acid, bu...	8.838	23.0	ug/l	522104	3	9.420	1134260	50.0
Isopropyl butyrate	9.214	118.9	ug/l	2696350	3	9.420	1134260	50.0