LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110521\
Data File : VU045596.D
Acq On : 06 Nov 2021 06:20
Operator : SY/MD
Sample : M4472-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-JS

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_U\Method\82U110521W.M
Title : SW846 8260

Signal : TIC: VU045596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.292	1213	1229	1243	rBV2	119950	253604	8.94%	2.153%
2	5.378	1243	1256	1273	rVB	180494	368485	12.99%	3.128%
3	5.706	1343	1358	1380	rBV	136313	276165	9.73%	2.345%
4	5.912	1410	1422	1435	rBV	15651	30839	1.09%	0.262%
5	6.066	1448	1470	1472	rBV3	25673	90572	3.19%	0.769%
6	6.253	1516	1528	1542	rVB	295757	546390	19.26%	4.639%
7	6.931	1718	1739	1757	rVB3	12638	41226	1.45%	0.350%
8	7.041	1757	1773	1809	rBV	1136246	1980343	69.79%	16.813%
9	7.738	1976	1990	2001	rBV	155416	259516	9.15%	2.203%
10	7.899	2024	2040	2070	rBV	469703	822804	29.00%	6.985%
11	8.160	2109	2121	2137	rBV	16769	28699	1.01%	0.244%
12	8.465	2203	2216	2233	rBV	39244	66237	2.33%	0.562%
13	8.574	2234	2250	2261	rVV	108744	182407	6.43%	1.549%
14	8.729	2280	2298	2320	rVV	1839118	2837650	100.00%	24.091%
15	8.835	2321	2331	2354	rVB	195622	312520	11.01%	2.653%
16	9.211	2434	2448	2482	rBV	1055590	1606808	56.62%	13.642%
17	9.420	2501	2513	2535	rVB	438958	730060	25.73%	6.198%
18	10.073	2705	2716	2732	rBV	34003	52164	1.84%	0.443%
19	10.632	2879	2890	2910	rVB	346995	545540	19.23%	4.632%
20	11.812	3244	3257	3275	rBV	481686	746739	26.32%	6.340%

Sum of corrected areas: 11778768

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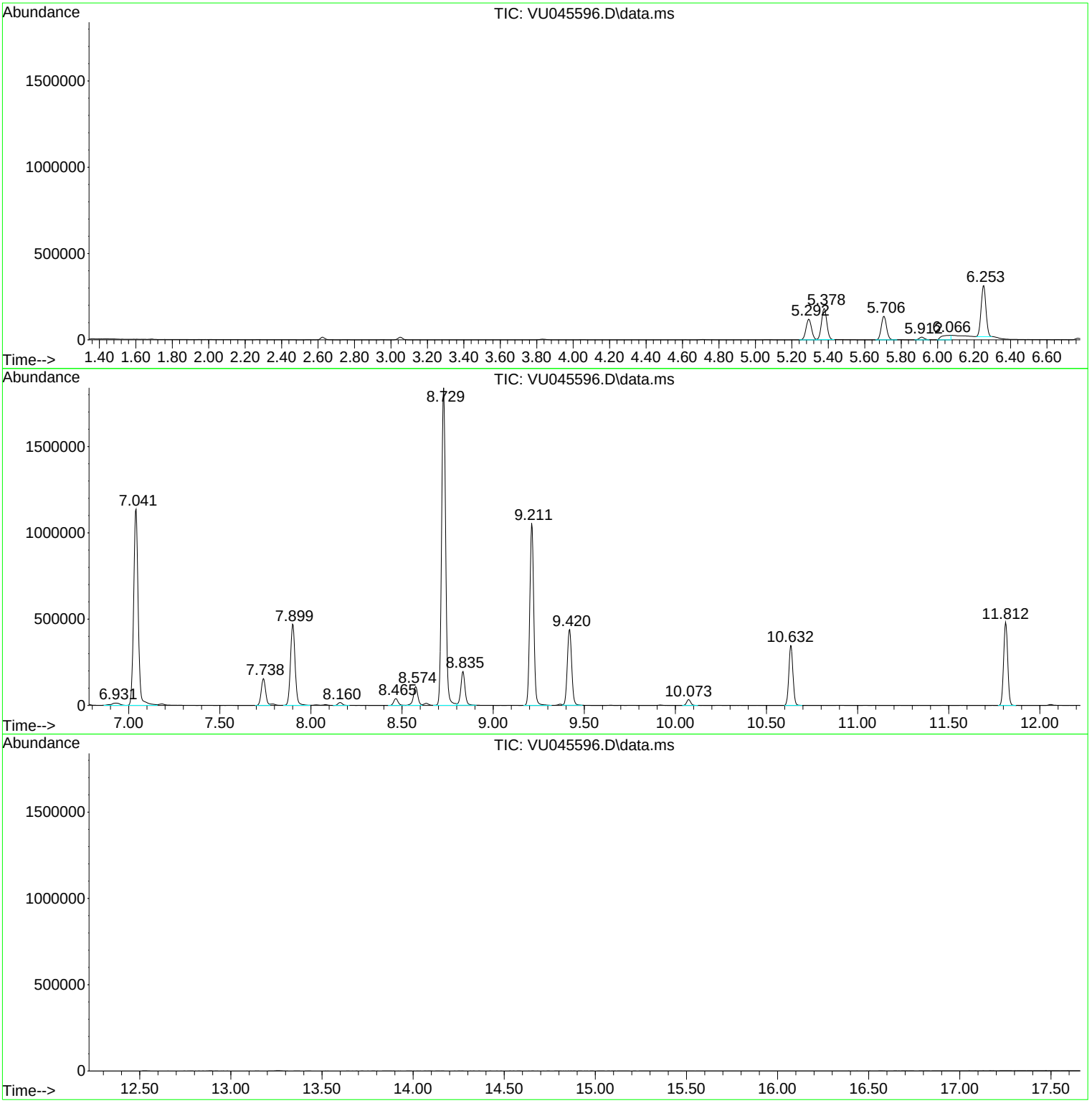
ClientSampleId :
WC-2-JS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

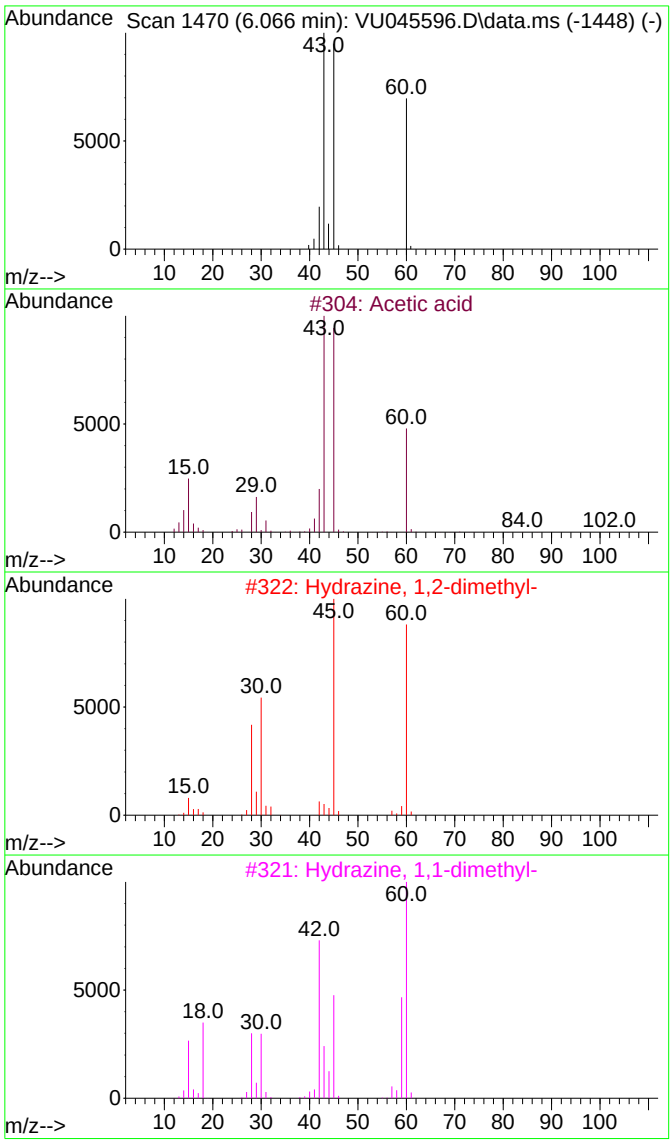
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

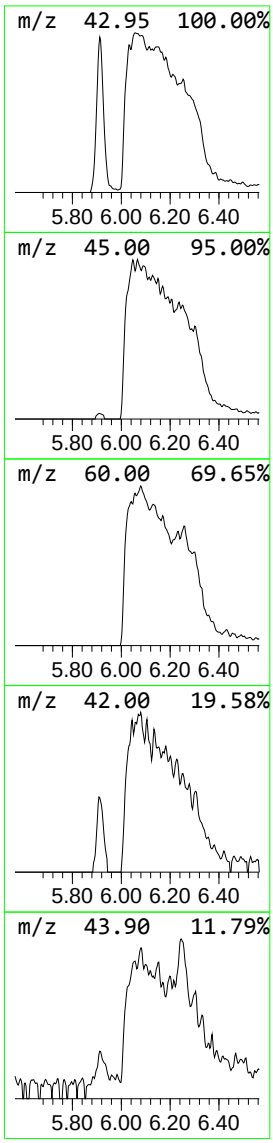
****

Peak Number 1 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.066	8.29 ug/l	90572	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	59
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Ammonium acetate	77	C2H7NO2	000631-61-8	9
5	Thiirane	60	C2H4S	000420-12-2	5





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ALS Vial : 51 Sample Multiplier: 1

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MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

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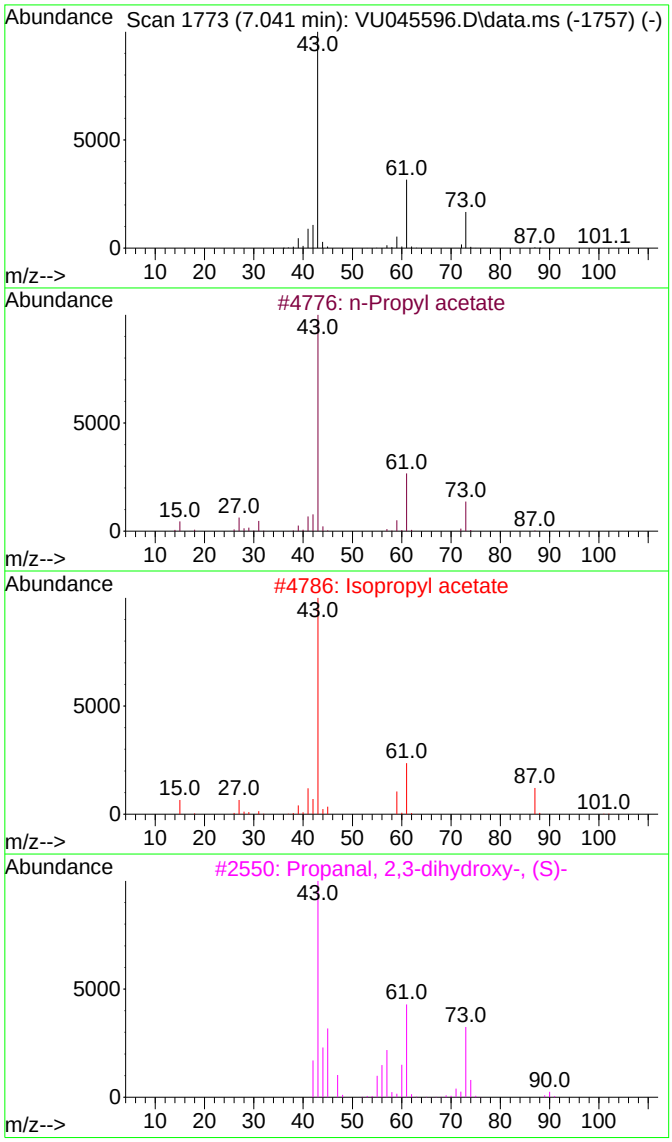
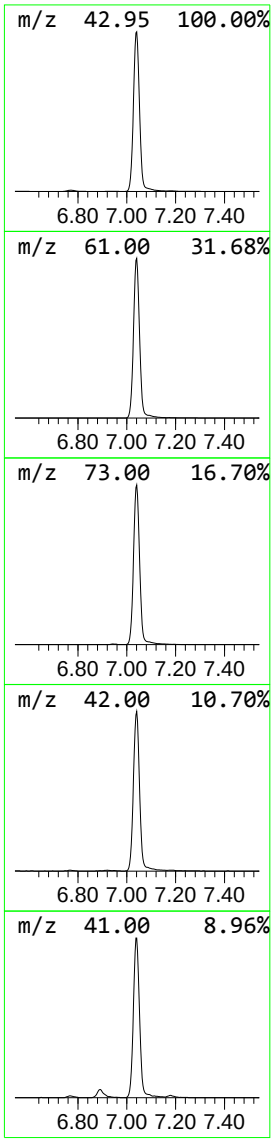
****

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	181.22 ug/l	1980340	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	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Operator : SY/MD
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ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-JS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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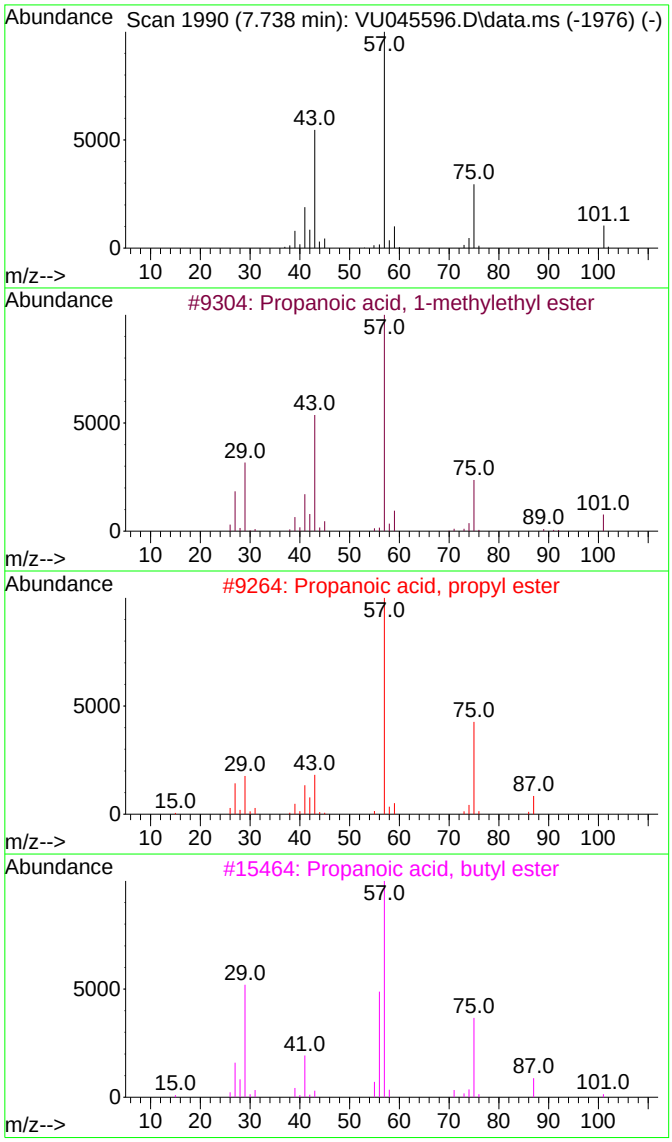
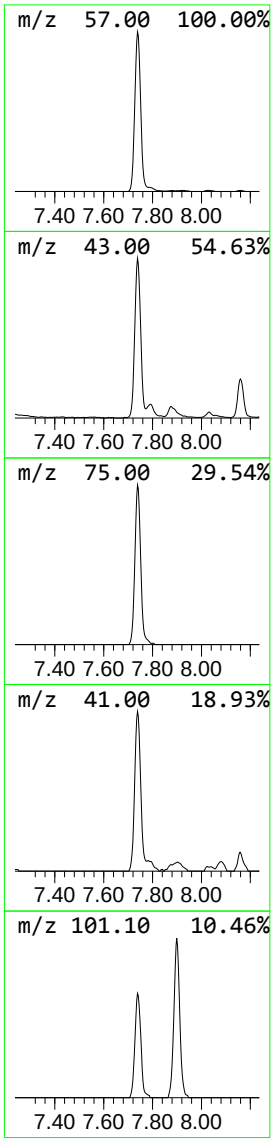
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	23.75 ug/l	259516	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	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument :
MSVOA_U
ClientSampleId :
WC-2-JS

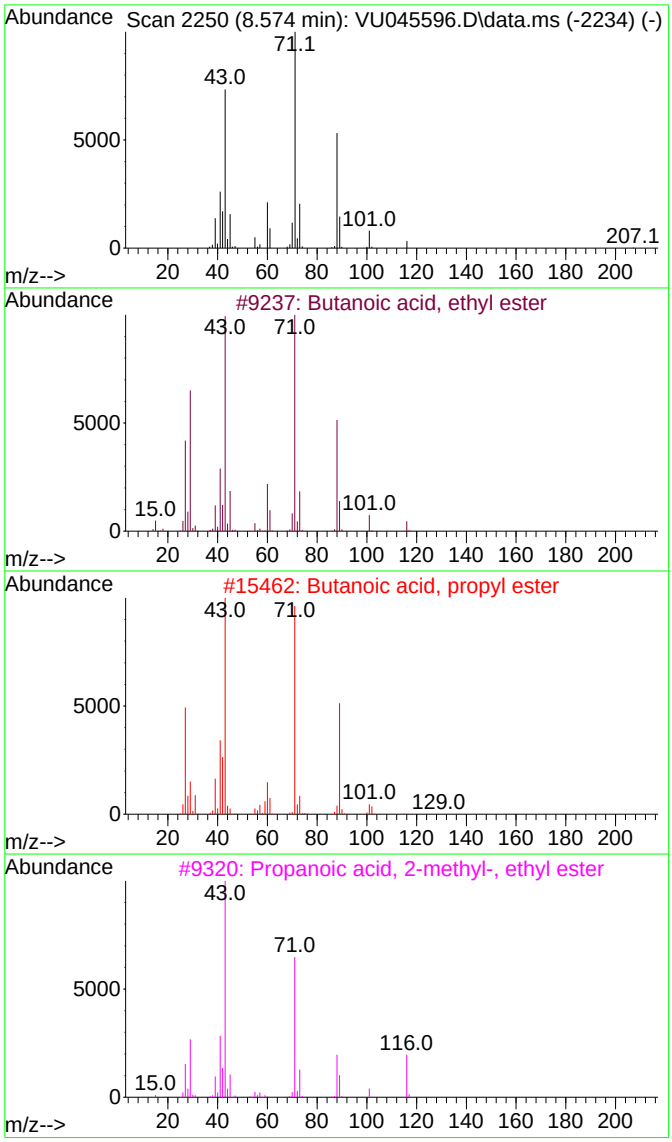
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

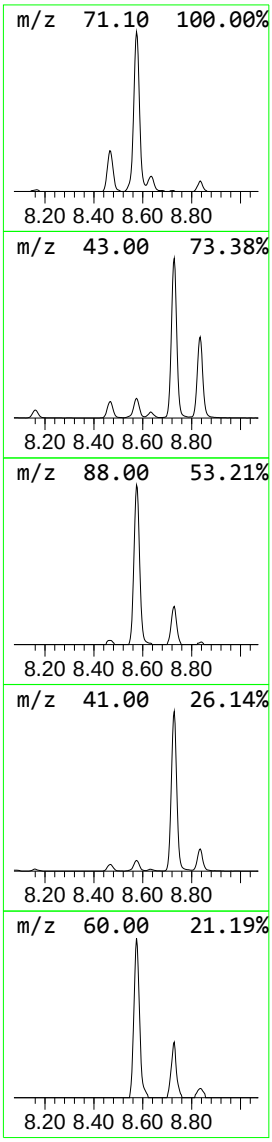
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	12.49 ug/l	182407	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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
3	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5	Ethyl hydrogen suberate	202	C10H18O4	1000342-39-2	38





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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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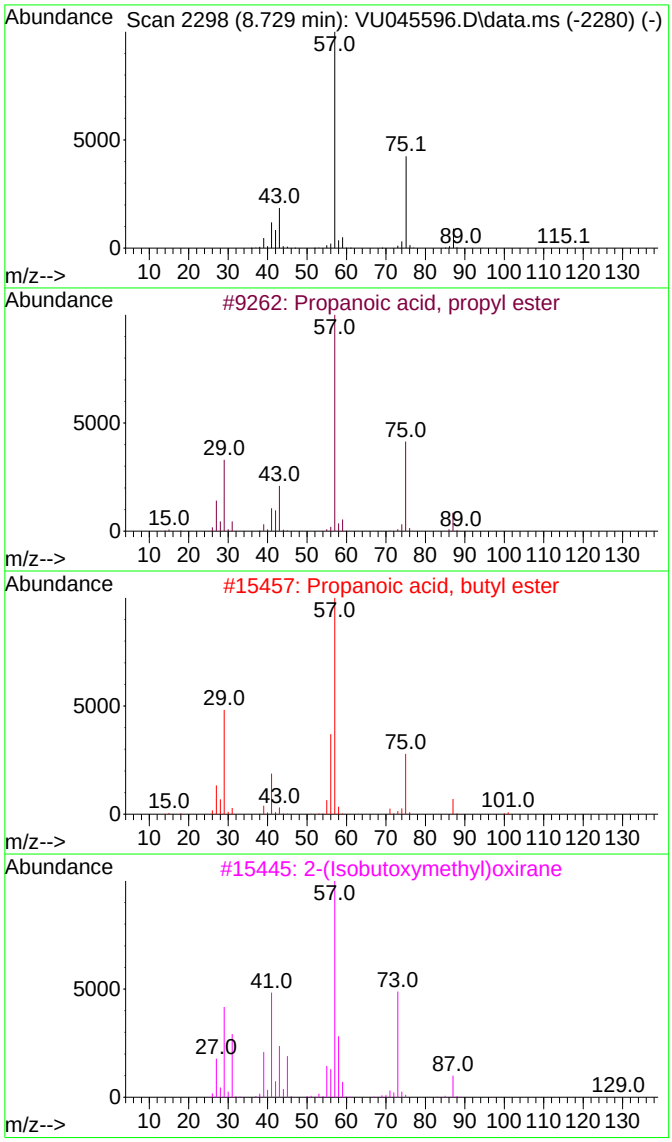
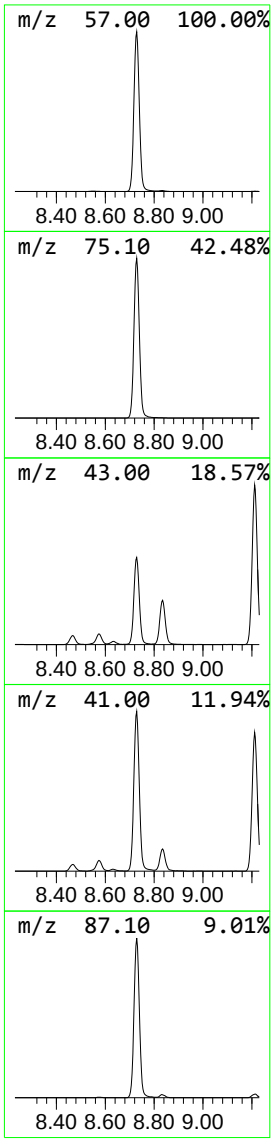
****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	194.34 ug/l	2837650	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	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	7





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Instrument :
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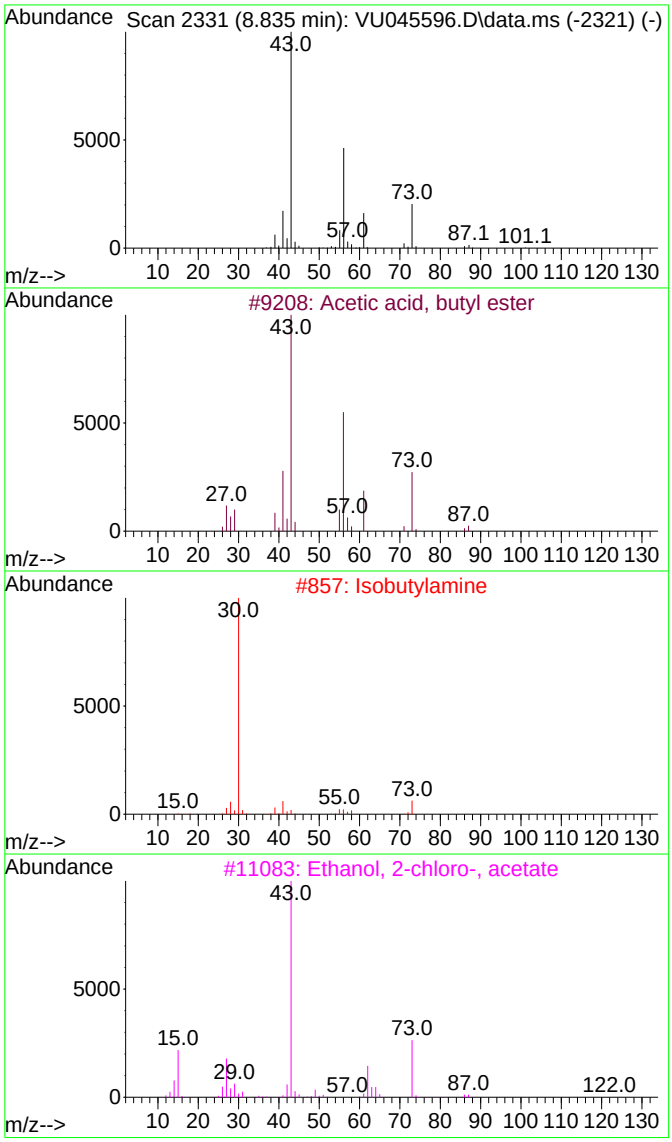
Quant Title : SW846 8260

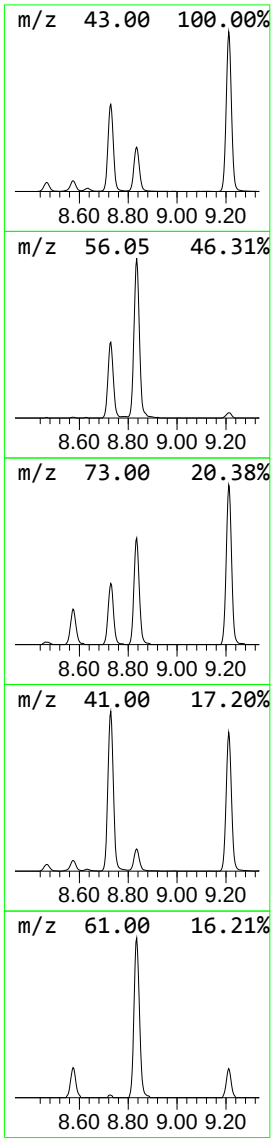
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	21.40 ug/l	312520	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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Quant Title : SW846 8260

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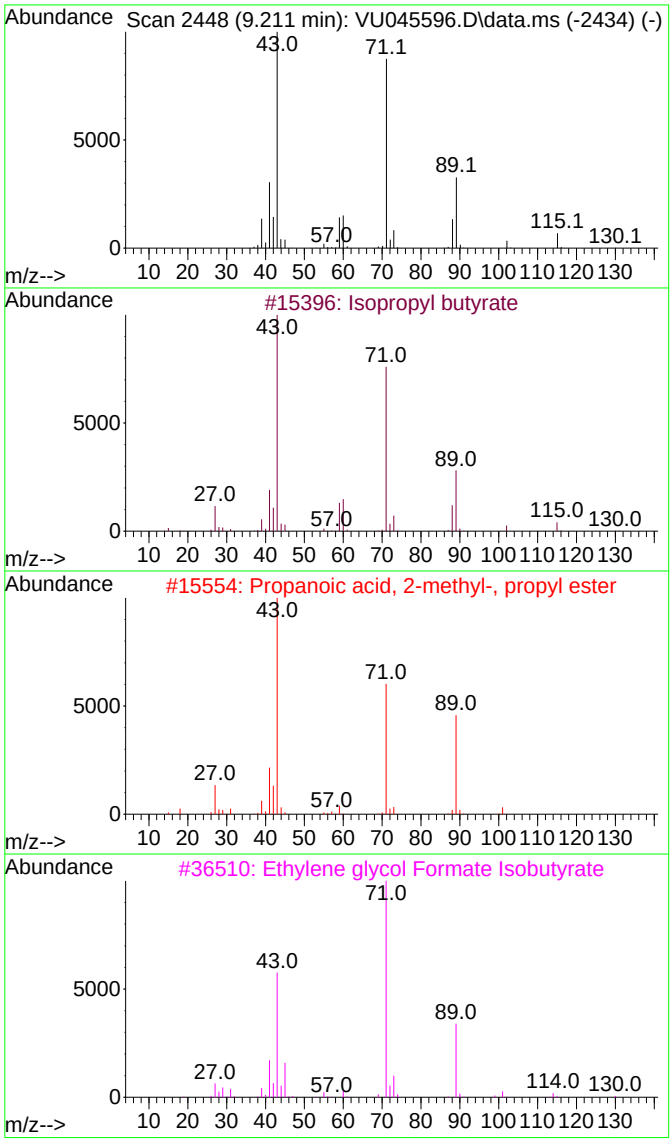
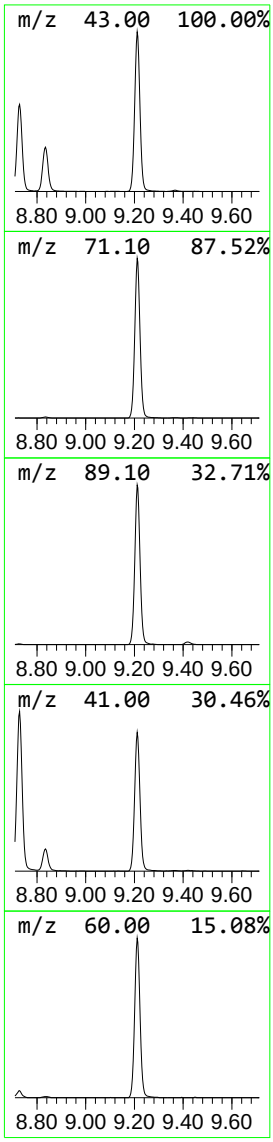
Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	110.05 ug/l	1606810	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-, propy...	130	C7H14O2	000644-49-5	72
3	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	59
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	50





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
Acetic acid	6.066	8.3	ug/l	90572	2	6.253	546390	50.0
n-Propyl acetate	7.041	181.2	ug/l	1980340	2	6.253	546390	50.0
Propanoic acid,...	7.738	23.8	ug/l	259516	2	6.253	546390	50.0
Butanoic acid, ...	8.574	12.5	ug/l	182407	3	9.420	730060	50.0
Propanoic acid,...	8.729	194.3	ug/l	2837650	3	9.420	730060	50.0
Acetic acid, bu...	8.835	21.4	ug/l	312520	3	9.420	730060	50.0
Isopropyl butyrate	9.211	110.1	ug/l	1606810	3	9.420	730060	50.0