LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045366.D
Acq On : 22 Oct 2021 15:48
Operator : SY/MD
Sample : M4315-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-S

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\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045366.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.684	91	107	130	rBV	58859	181144	3.65%	0.848%
2	3.041	517	529	551	rVB	33172	65959	1.33%	0.309%
3	5.292	1213	1229	1242	rBV	192444	414175	8.34%	1.939%
4	5.375	1242	1255	1277	rVB	328826	685094	13.79%	3.207%
5	5.703	1339	1357	1380	rBV	230253	479762	9.66%	2.246%
6	5.922	1410	1425	1450	rBV2	23827	62934	1.27%	0.295%
7	6.041	1450	1462	1485	rBV3	73945	295621	5.95%	1.384%
8	6.250	1516	1527	1582	rVB	581560	1479986	29.79%	6.928%
9	6.948	1722	1744	1761	rVV2	24745	76121	1.53%	0.356%
10	7.047	1761	1775	1808	rVV	1391784	3425056	68.94%	16.033%
11	7.748	1979	1993	2013	rBV	219804	502817	10.12%	2.354%
12	7.902	2026	2041	2063	rBV	777807	1390151	27.98%	6.507%
13	8.173	2114	2125	2145	rVB2	23100	51404	1.03%	0.241%
14	8.478	2207	2220	2230	rBV	73997	154503	3.11%	0.723%
15	8.587	2243	2254	2266	rVB2	178969	367452	7.40%	1.720%
16	8.742	2285	2302	2321	rBV	2640956	4967936	100.00%	23.255%
17	8.848	2323	2335	2358	rVB	283308	531070	10.69%	2.486%
18	9.224	2435	2452	2486	rBV	1715369	2907693	58.53%	13.611%
19	9.423	2490	2514	2538	rVB	697671	1236685	24.89%	5.789%
20	10.082	2707	2719	2731	rBV	64788	101634	2.05%	0.476%
21	10.639	2879	2892	2915	rVB	544460	889989	17.91%	4.166%
22	11.819	3246	3259	3277	rBV	704793	1095497	22.05%	5.128%

Sum of corrected areas: 21362683

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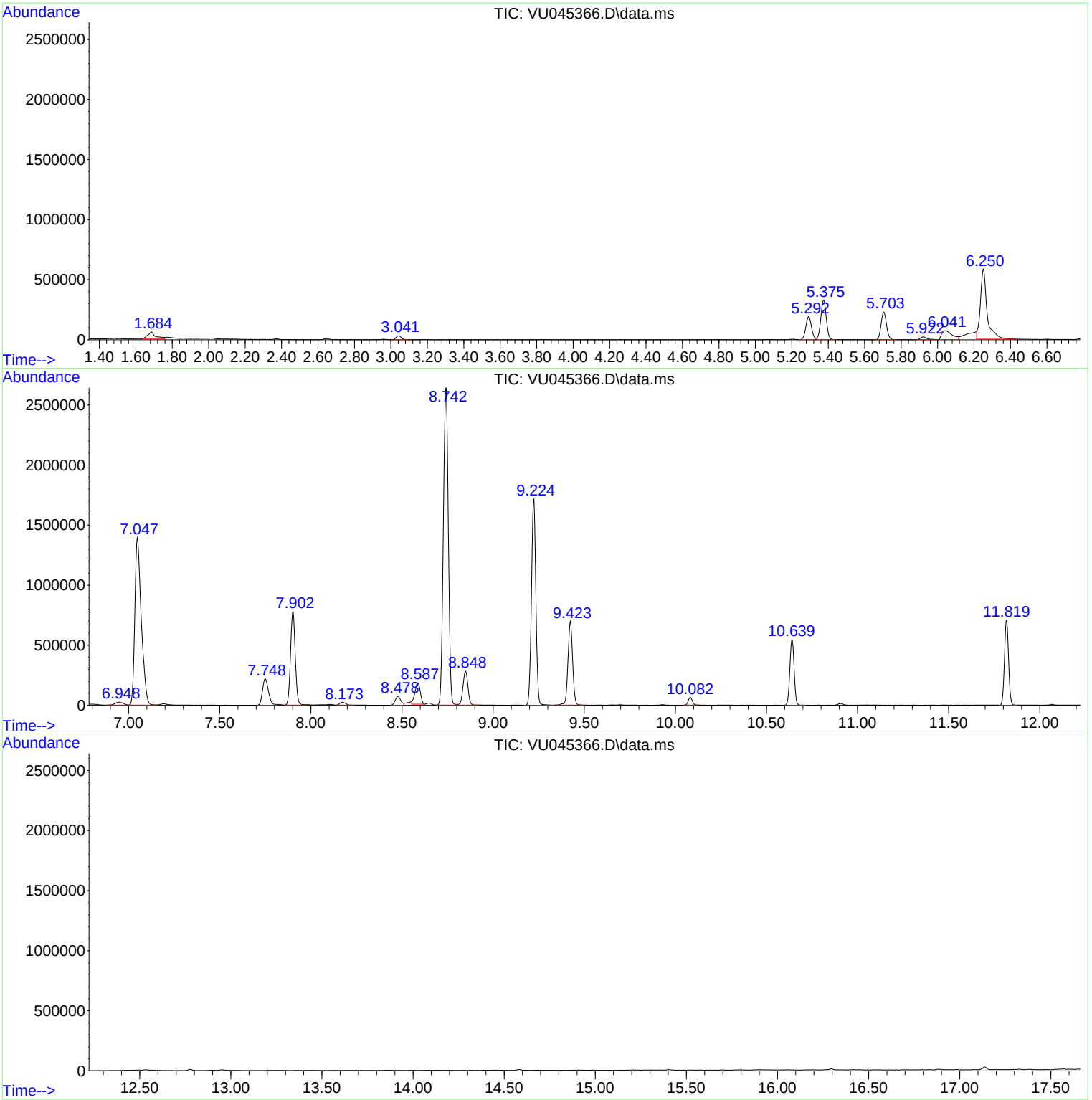
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-S

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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Quant Title : SW846 8260

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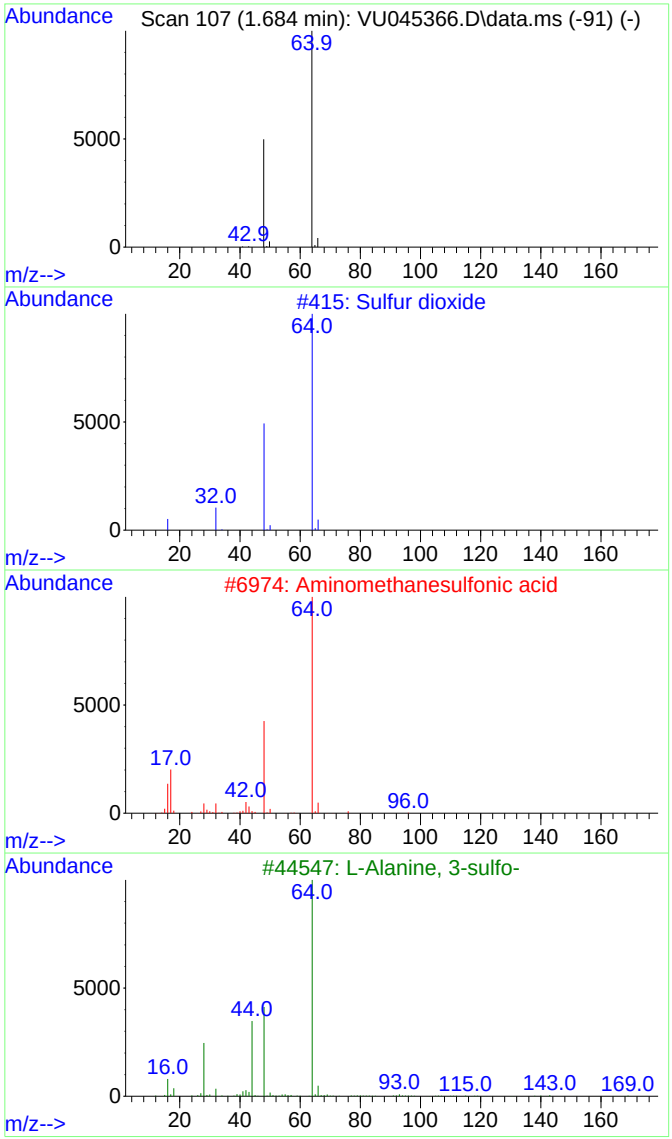
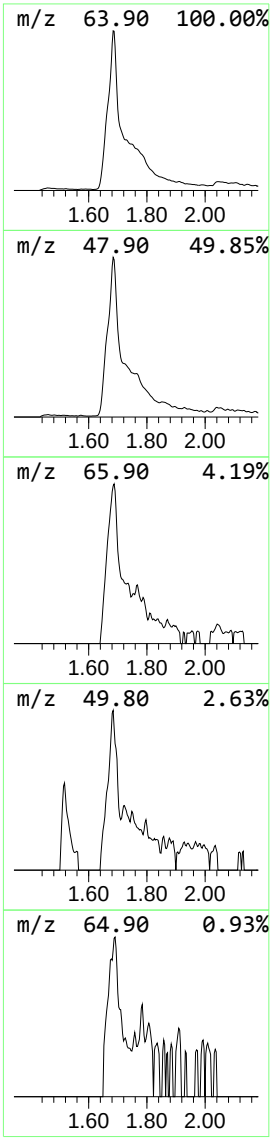
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	13.22 ug/l	181144	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument : MSVOA_U
ClientSampleId : MH-DD-S

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

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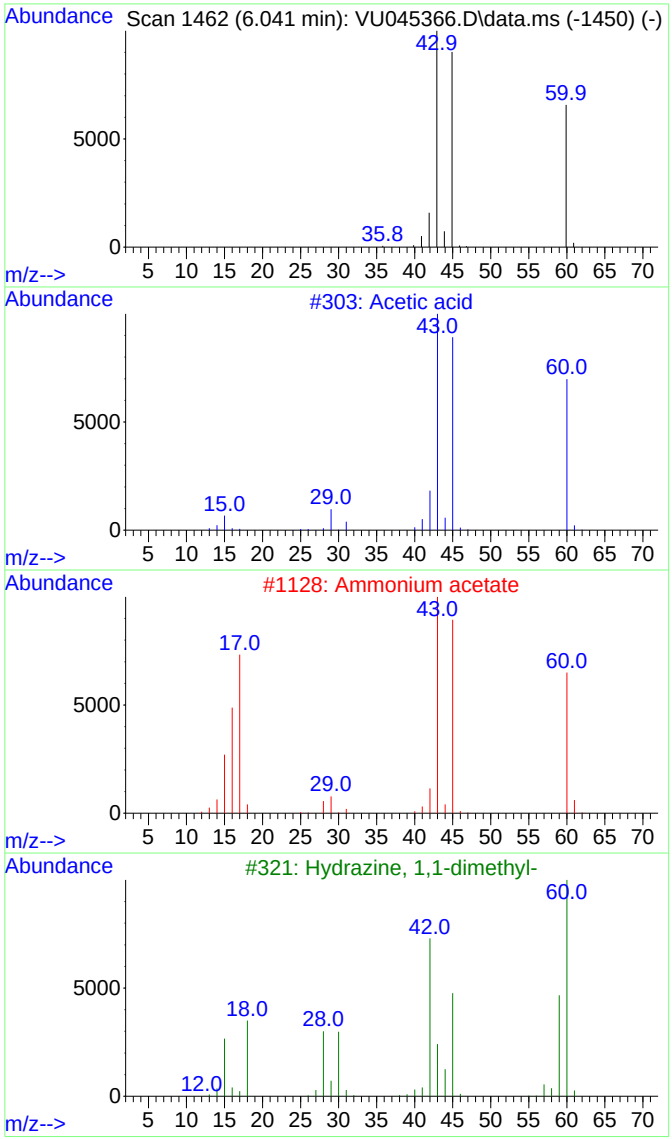
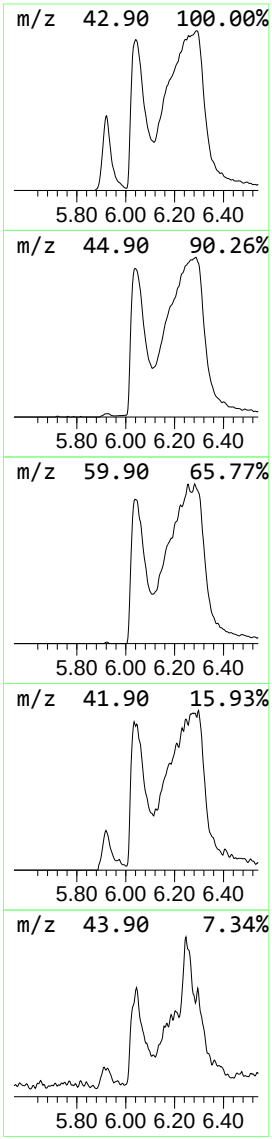
****

Peak Number 2 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.041	9.99 ug/l	295621	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	16
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Thiirane	60	C2H4S	000420-12-2	5





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-S

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

TIC Library : C:\Database\NIST20.L
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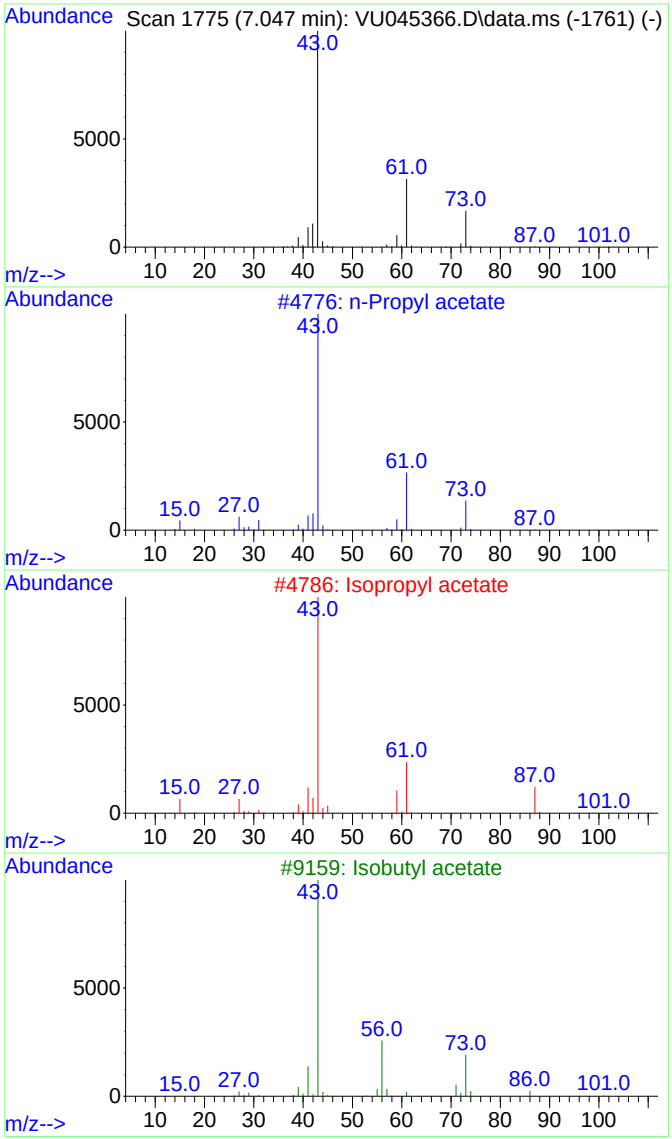
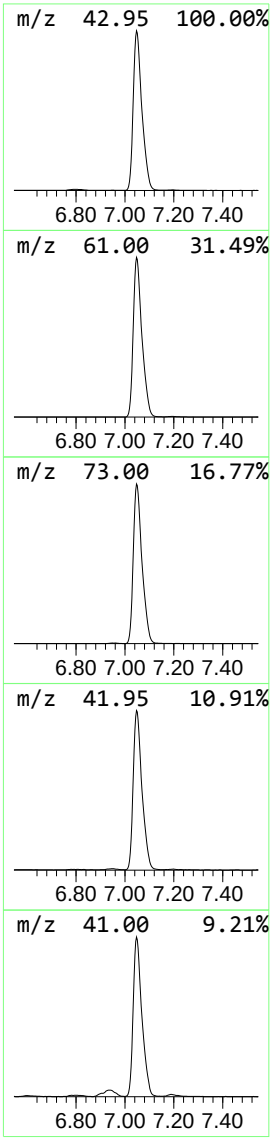
****
Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.047	115.71 ug/l	3425060	1,4-Difluorobenzene	6.250

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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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-S

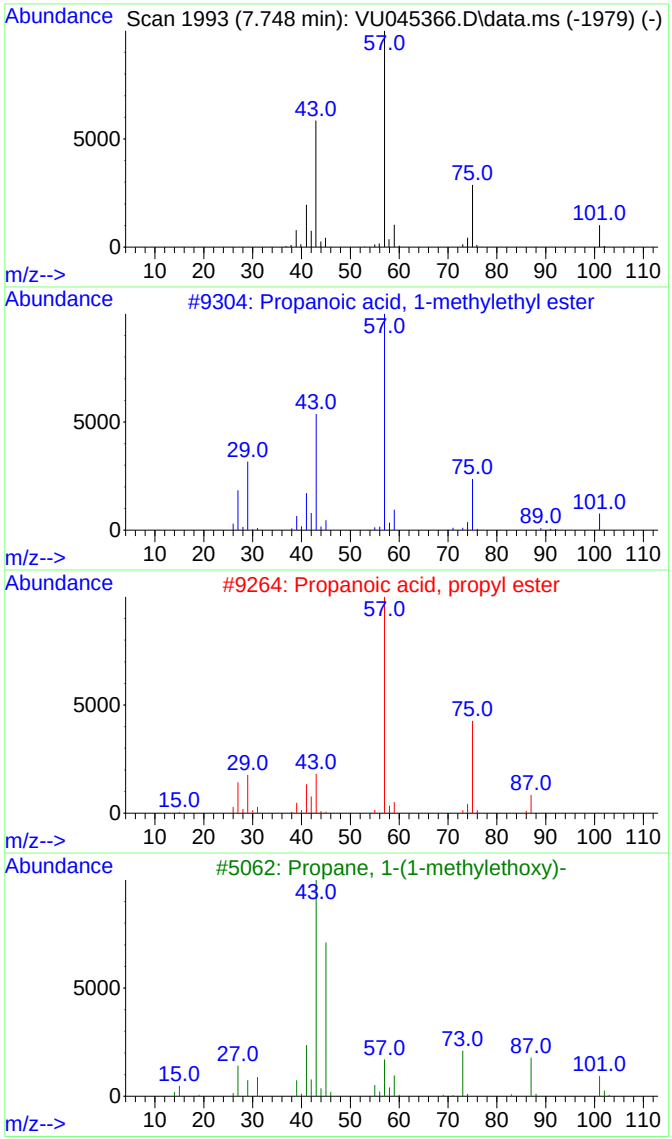
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

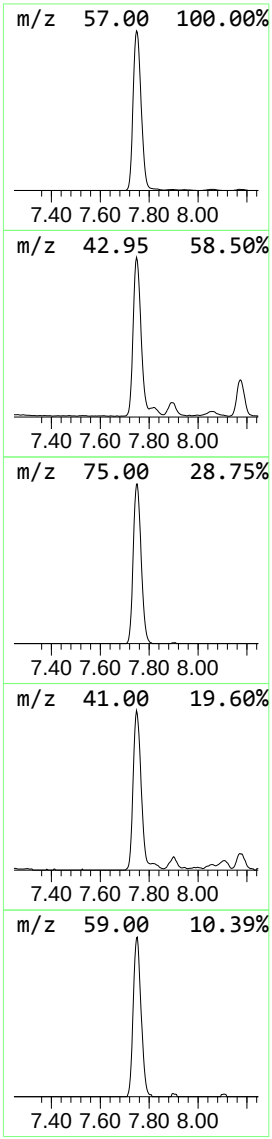
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.748	16.99 ug/l	502817	1,4-Difluorobenzene	6.250

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-S

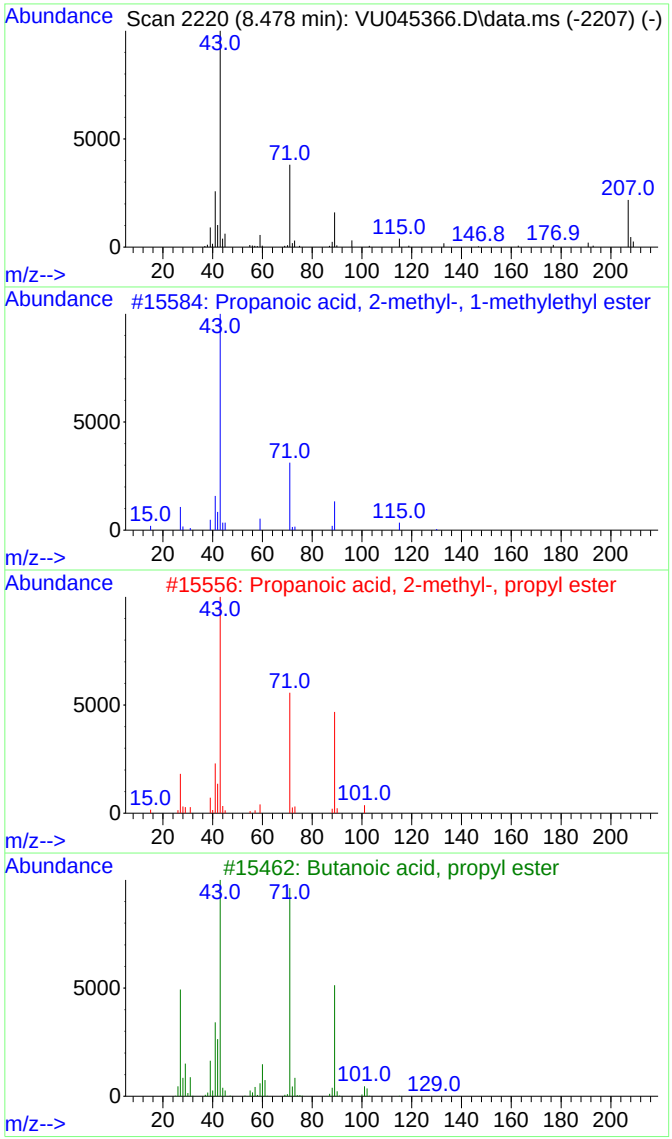
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

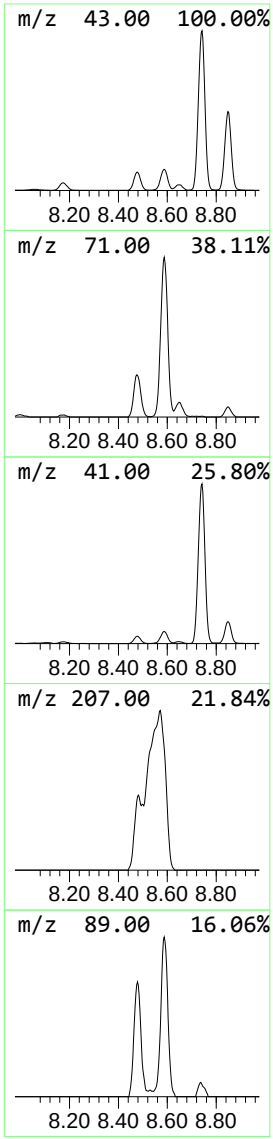
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.478	6.25 ug/l	154503	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	40
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	38





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-S

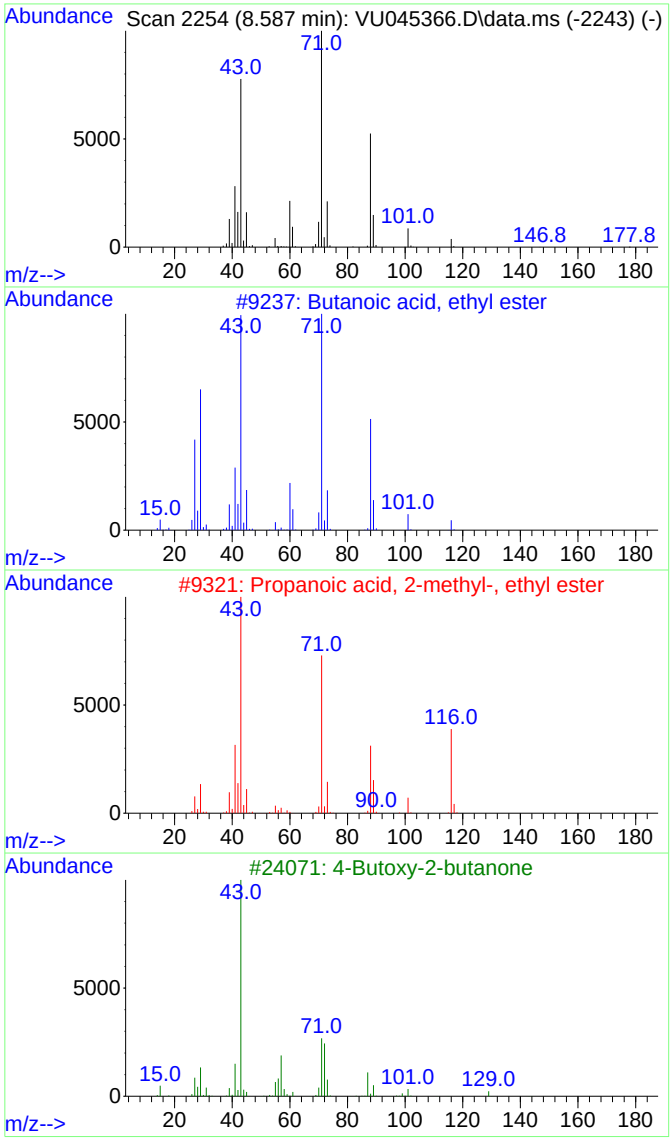
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

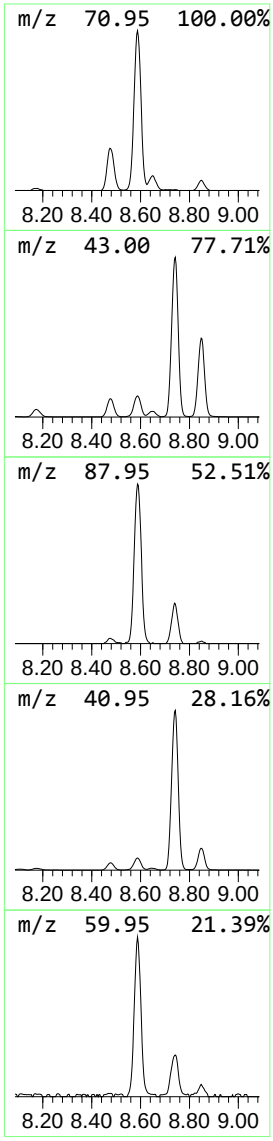
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.587	14.86 ug/l	367452	Chlorobenzene-d5	9.423

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	62
3	4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	50
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45





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

TIC Library : C:\Database\NIST20.L
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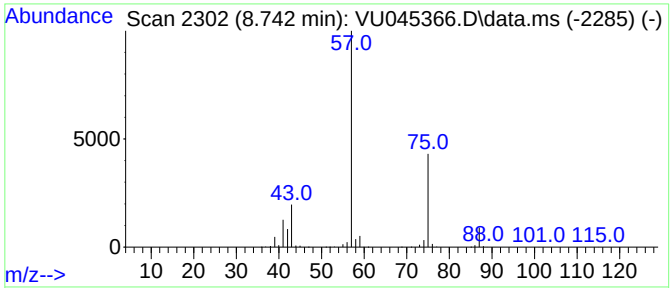
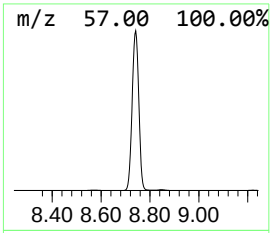
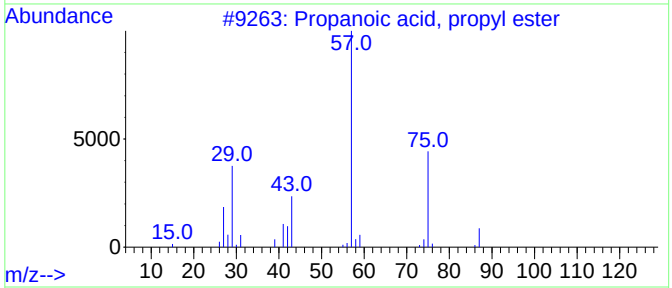
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 1

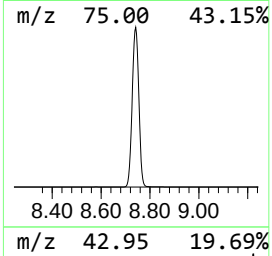
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.742	200.86 ug/l	4967940	Chlorobenzene-d5	9.423

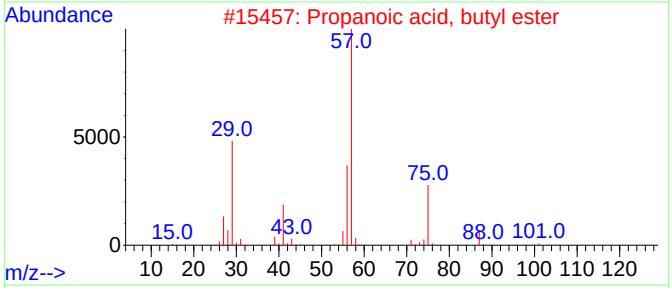
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7

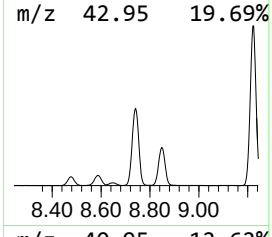


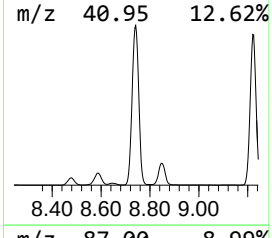


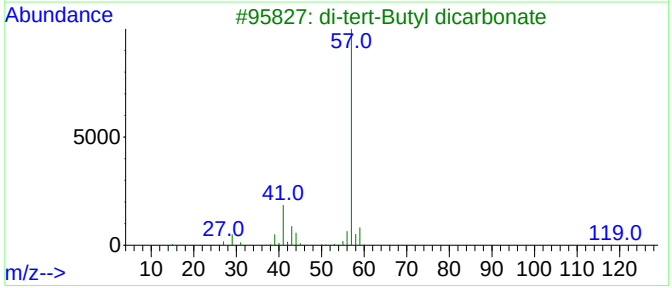


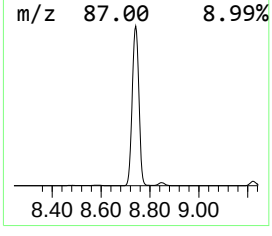












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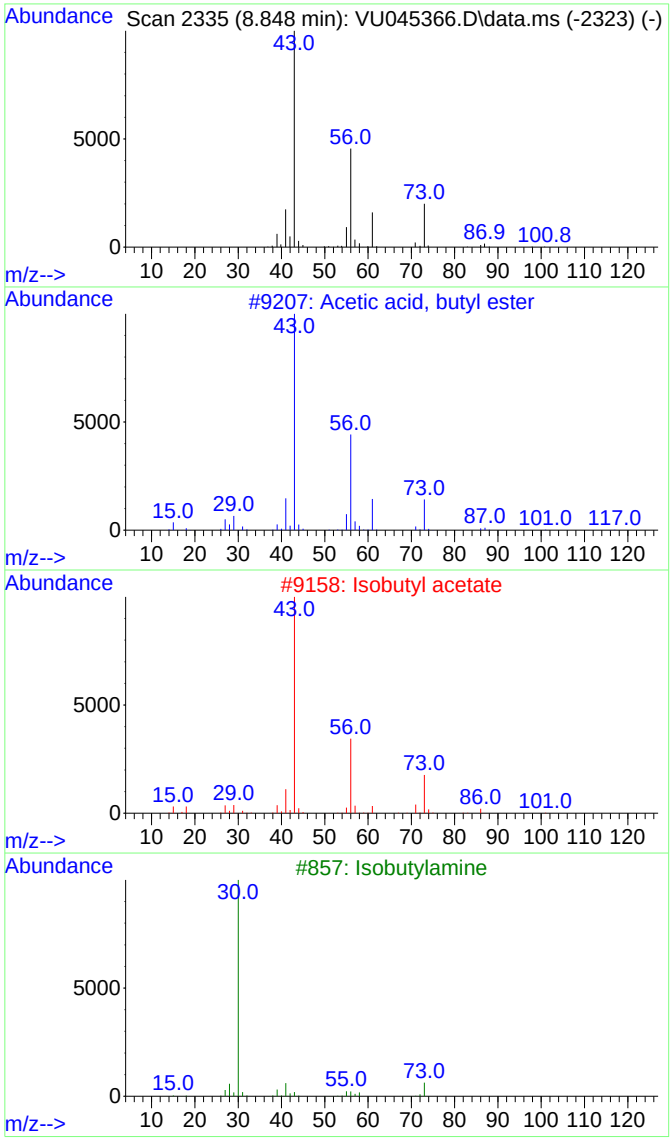
Quant Title : SW846 8260

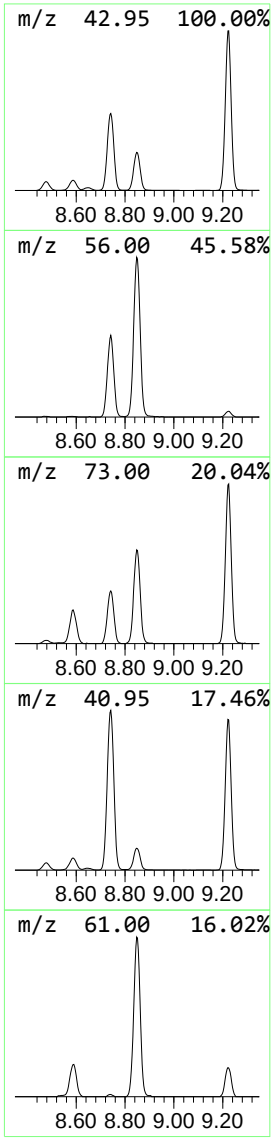
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.848	21.47 ug/l	531070	Chlorobenzene-d5	9.423

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	Isobutylamine	73	C4H11N	000078-81-9	9
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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Quant Title : SW846 8260

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

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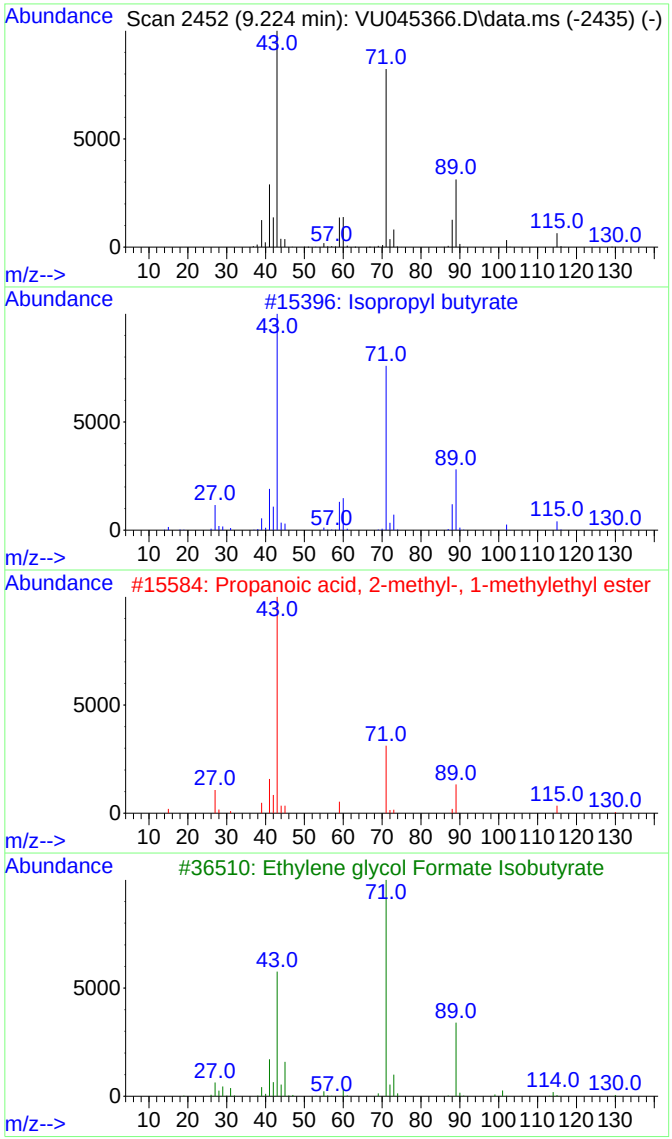
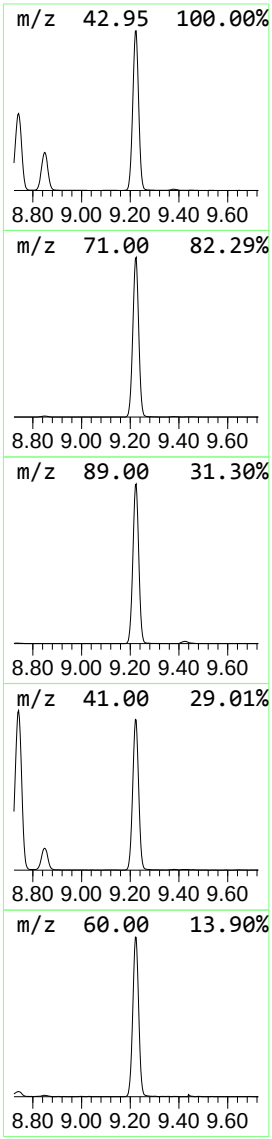
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.224	117.56 ug/l	2907690	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045366.D
Acq On : 22 Oct 2021 15:48
Operator : SY/MD
Sample : M4315-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-S

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.684	13.2	ug/l	181144	1	5.375	685094	50.0
Acetic acid	6.041	10.0	ug/l	295621	2	6.250	1479990	50.0
n-Propyl acetate	7.047	115.7	ug/l	3425060	2	6.250	1479990	50.0
Propanoic acid,...	7.748	17.0	ug/l	502817	2	6.250	1479990	50.0
Propanoic acid,...	8.478	6.3	ug/l	154503	3	9.423	1236690	50.0
Butanoic acid, ...	8.587	14.9	ug/l	367452	3	9.423	1236690	50.0
Propanoic acid,...	8.742	200.9	ug/l	4967940	3	9.423	1236690	50.0
Acetic acid, bu...	8.848	21.5	ug/l	531070	3	9.423	1236690	50.0
Isopropyl butyrate	9.224	117.6	ug/l	2907690	3	9.423	1236690	50.0