LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045367.D
Acq On : 22 Oct 2021 16:11
Operator : SY/MD
Sample : M4315-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-D

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: VU045367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.642	84	94	106	rBV2	34718	91265	1.89%	0.443%
2	3.044	519	530	546	rVB	34802	65663	1.36%	0.318%
3	5.292	1213	1229	1242	rBV	193503	409447	8.46%	1.986%
4	5.375	1242	1255	1276	rVB	326229	666910	13.79%	3.234%
5	5.703	1339	1357	1376	rBV	227167	462783	9.57%	2.244%
6	5.919	1409	1424	1441	rBV2	26420	56734	1.17%	0.275%
7	6.031	1447	1459	1477	rBV2	72512	256695	5.31%	1.245%
8	6.250	1516	1527	1599	rVB	573859	1387572	28.68%	6.729%
9	6.941	1718	1742	1758	rBV3	25339	75075	1.55%	0.364%
10	7.044	1759	1774	1805	rBV	1722017	3299598	68.21%	16.001%
11	7.745	1977	1992	2005	rBV	266441	475769	9.84%	2.307%
12	7.899	2025	2040	2058	rBV	776969	1352711	27.96%	6.560%
13	8.166	2111	2123	2144	rBV	27438	50618	1.05%	0.245%
14	8.472	2205	2218	2228	rBV	78349	145082	3.00%	0.704%
15	8.581	2238	2252	2263	rVB2	200017	378197	7.82%	1.834%
16	8.735	2283	2300	2319	rBV	2955528	4837335	100.00%	23.457%
17	8.841	2321	2333	2359	rVB	308198	523107	10.81%	2.537%
18	9.218	2434	2450	2484	rBV	1799012	2853285	58.98%	13.836%
19	9.420	2502	2513	2536	rVB	694087	1168242	24.15%	5.665%
20	10.079	2706	2718	2732	rBV	61467	97408	2.01%	0.472%
21	10.635	2878	2891	2913	rBV	547354	874666	18.08%	4.241%
22	11.815	3245	3258	3280	rBV	704318	1093539	22.61%	5.303%

Sum of corrected areas: 20621701

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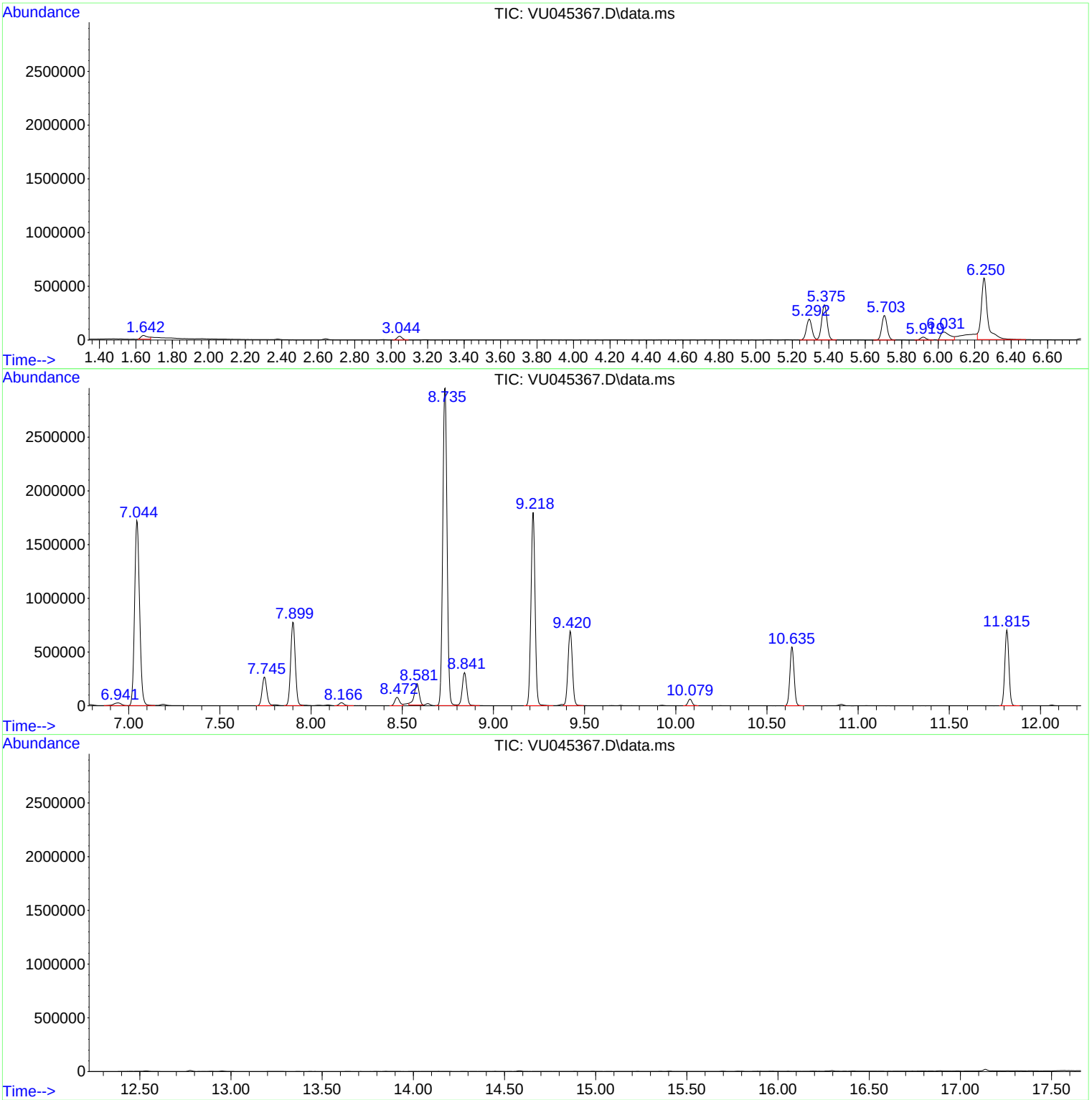
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-D

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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Data File : VU045367.D
Acq On : 22 Oct 2021 16:11
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Instrument : MSVOA_U
ClientSampleId : MH-DD-D

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

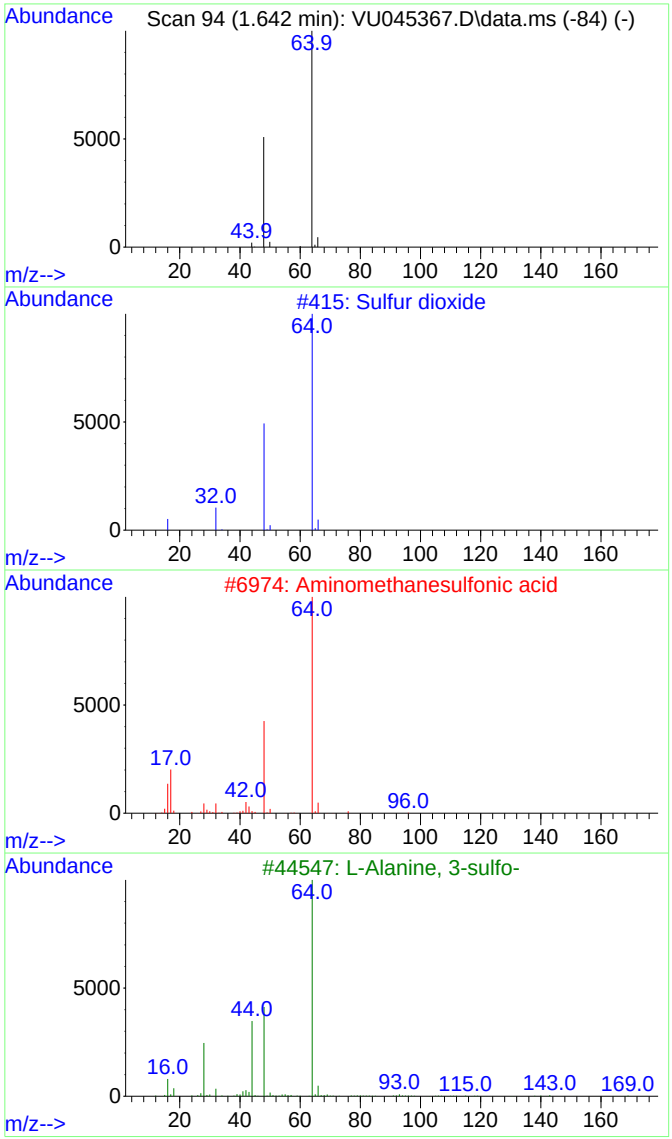
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

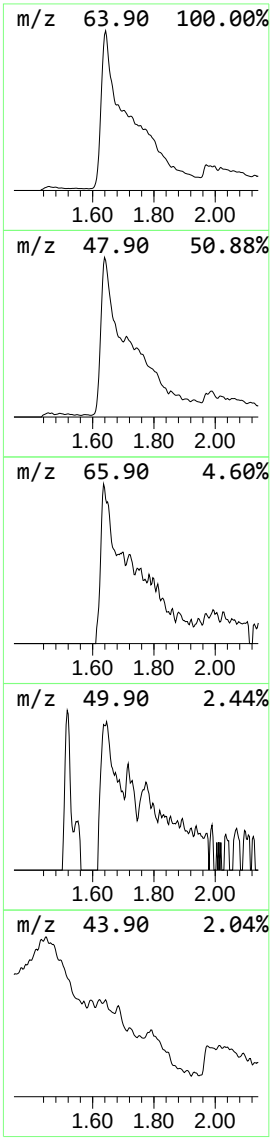
****

Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.642	6.84 ug/l	91265	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
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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ALS Vial : 14 Sample Multiplier: 1

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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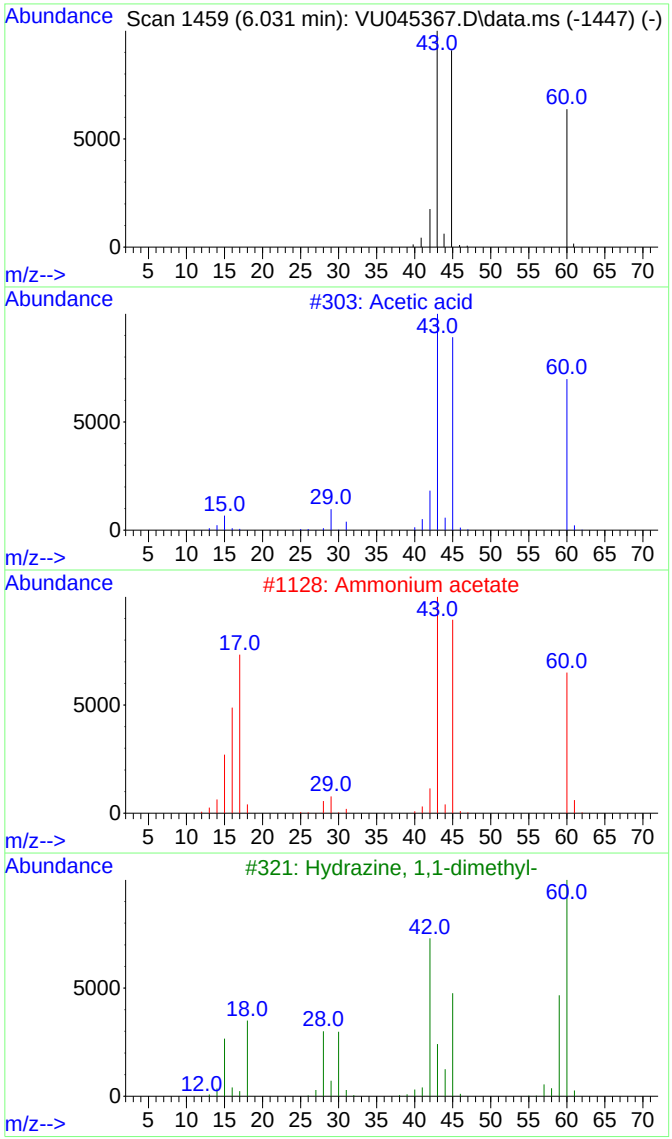
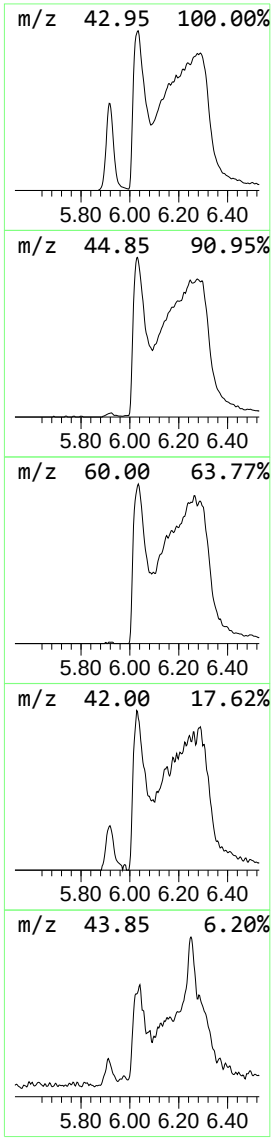
****

Peak Number 2 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.031	9.25 ug/l	256695	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	91
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	5
5	Thiirane	60	C2H4S	000420-12-2	5





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Acq On : 22 Oct 2021 16:11
Operator : SY/MD
Sample : M4315-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-D

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

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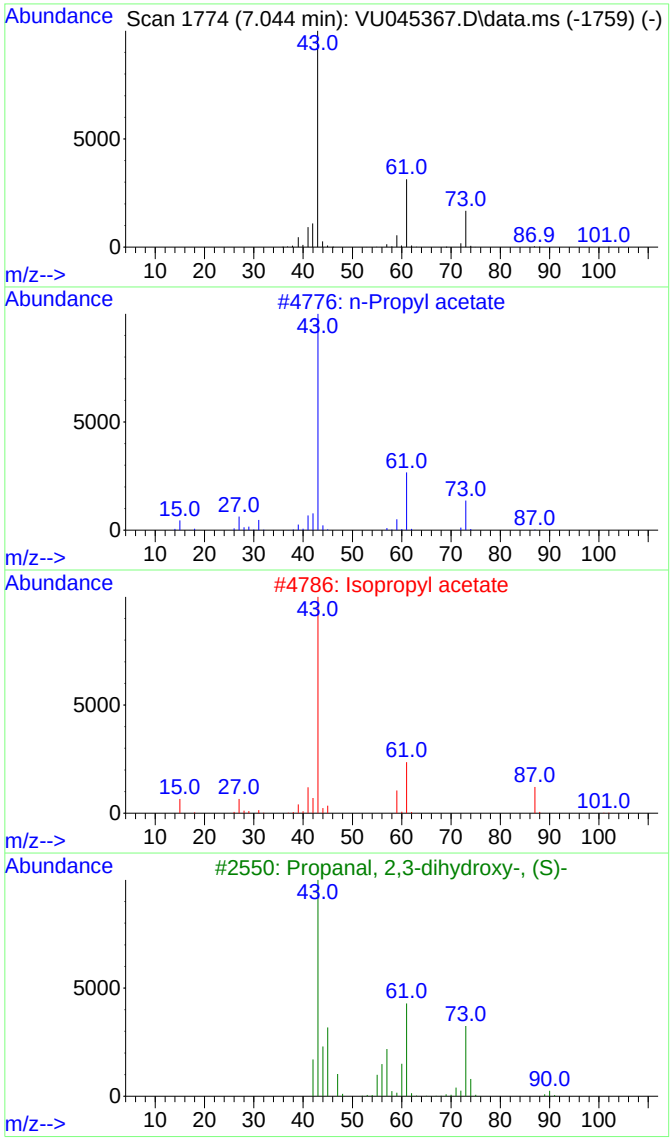
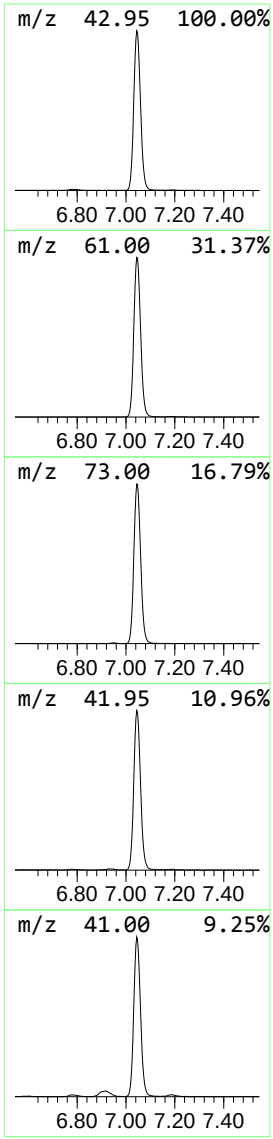
****
Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	118.90 ug/l	3299600	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	7





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Operator : SY/MD
Sample : M4315-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-D

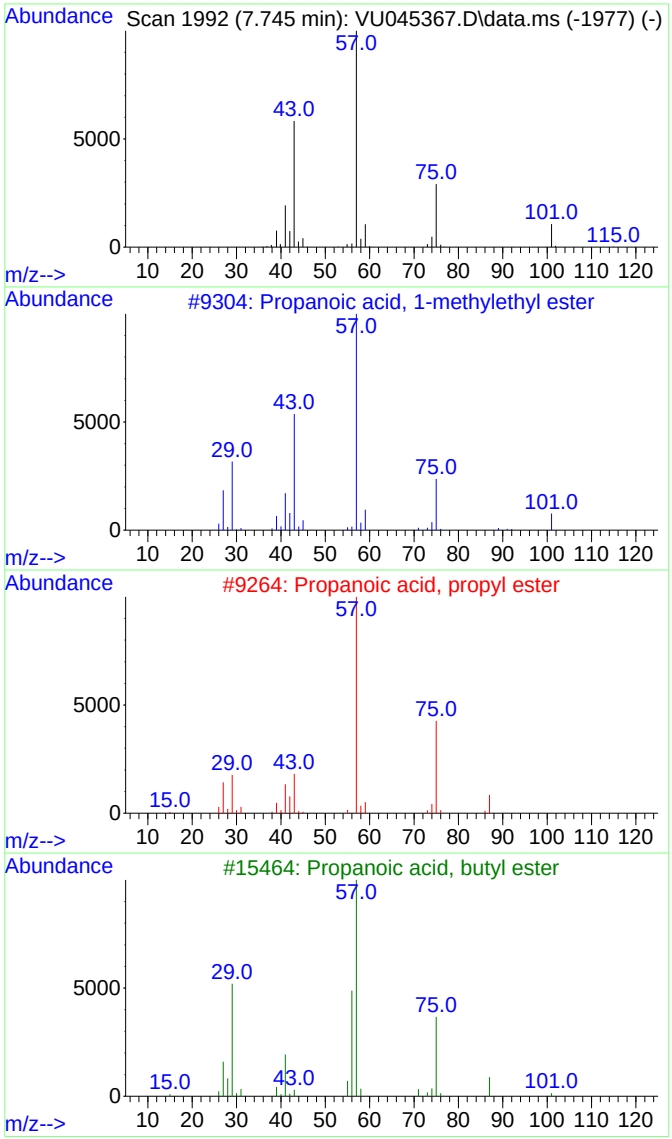
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

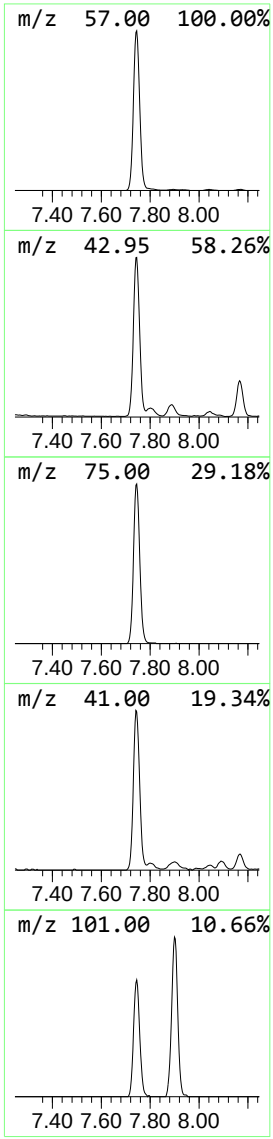
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.745	17.14 ug/l	475769	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	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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Operator : SY/MD
Sample : M4315-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-D

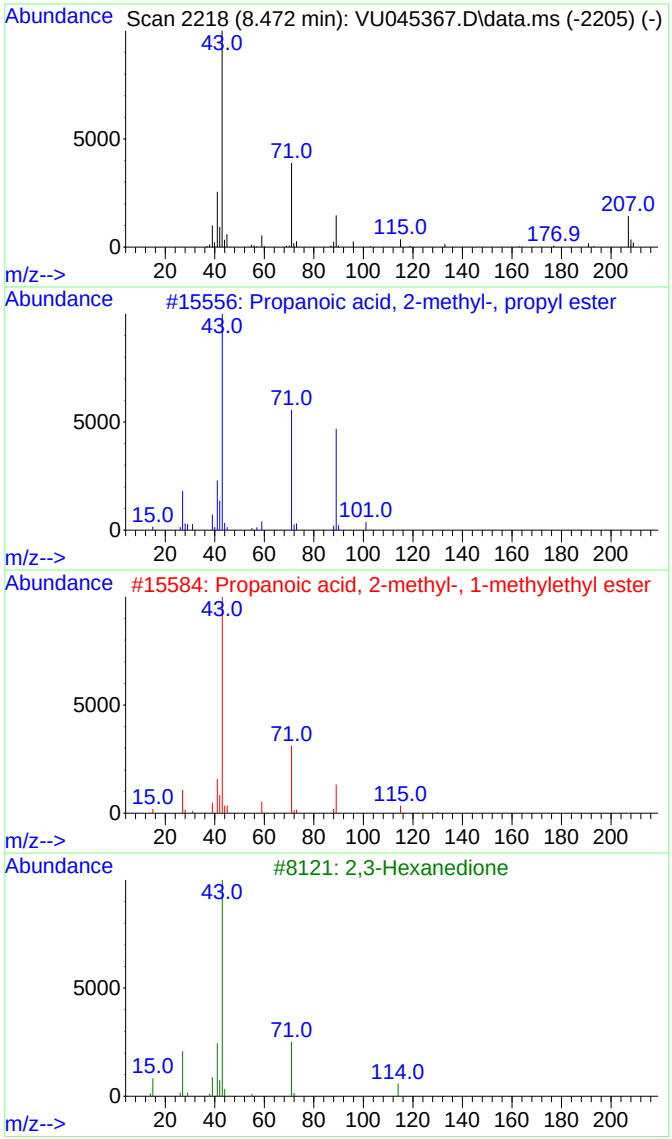
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

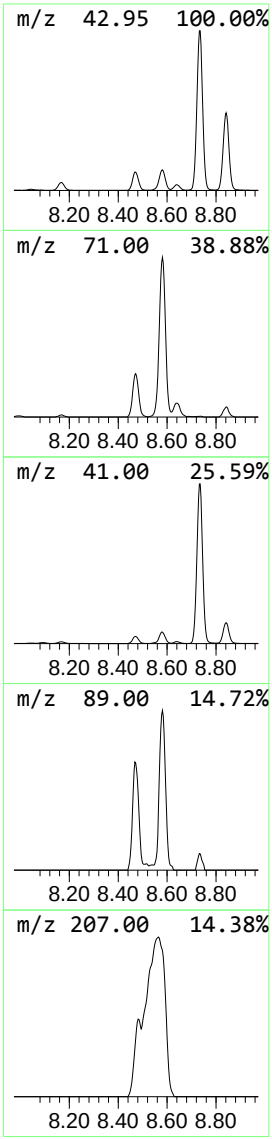
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.472	6.21 ug/l	145082	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	40
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	40





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-DD-D

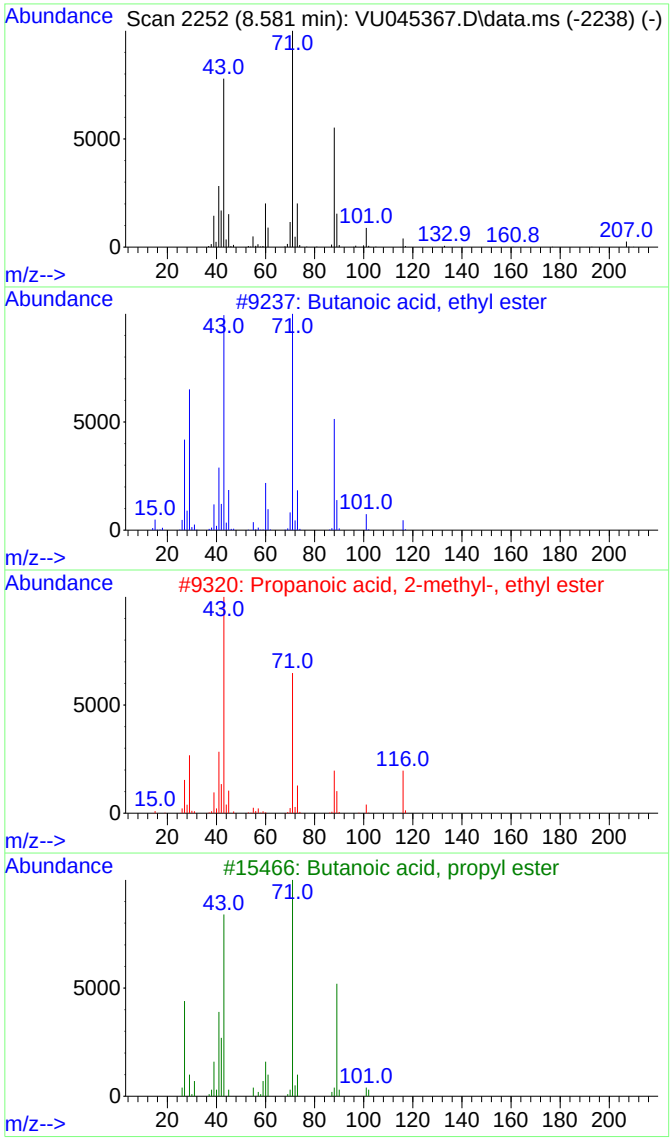
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

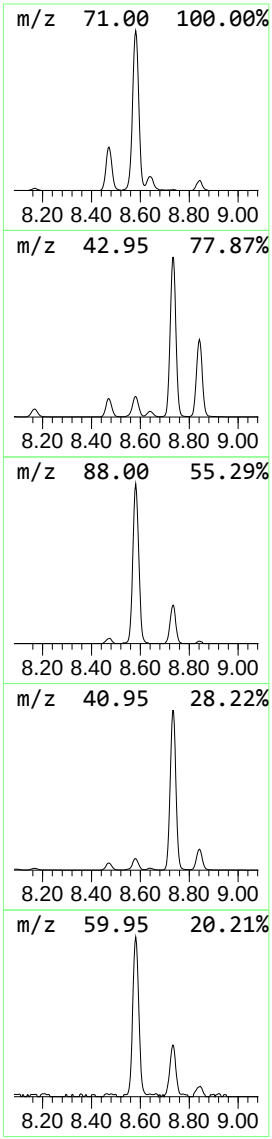
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	16.19 ug/l	378197	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	62
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-D

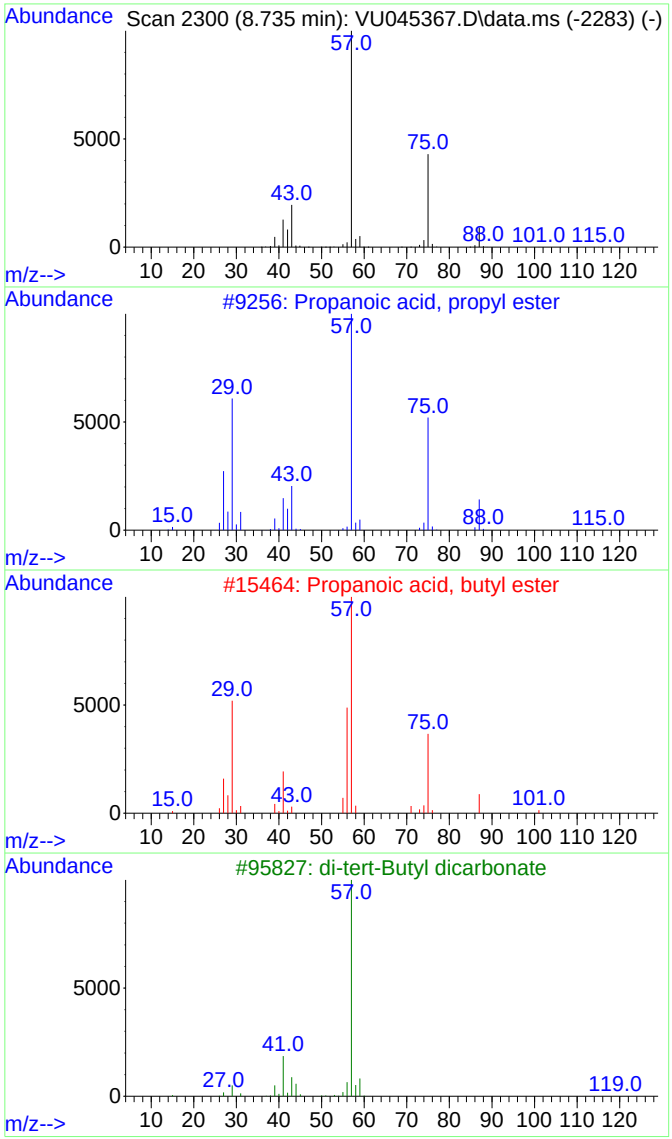
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

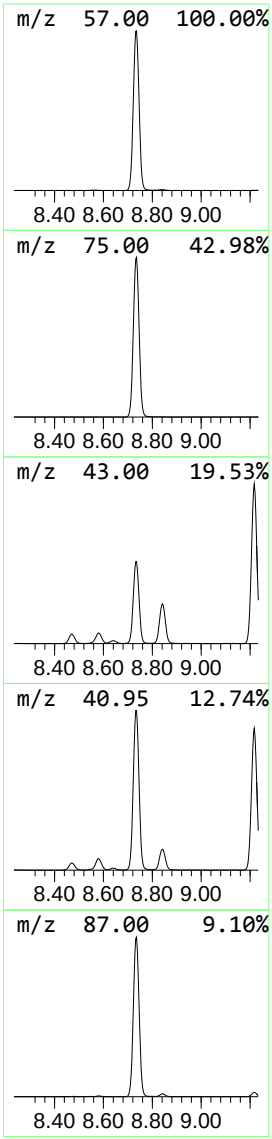
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.735	207.04 ug/l	4837340	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	40
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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Instrument : MSVOA_U
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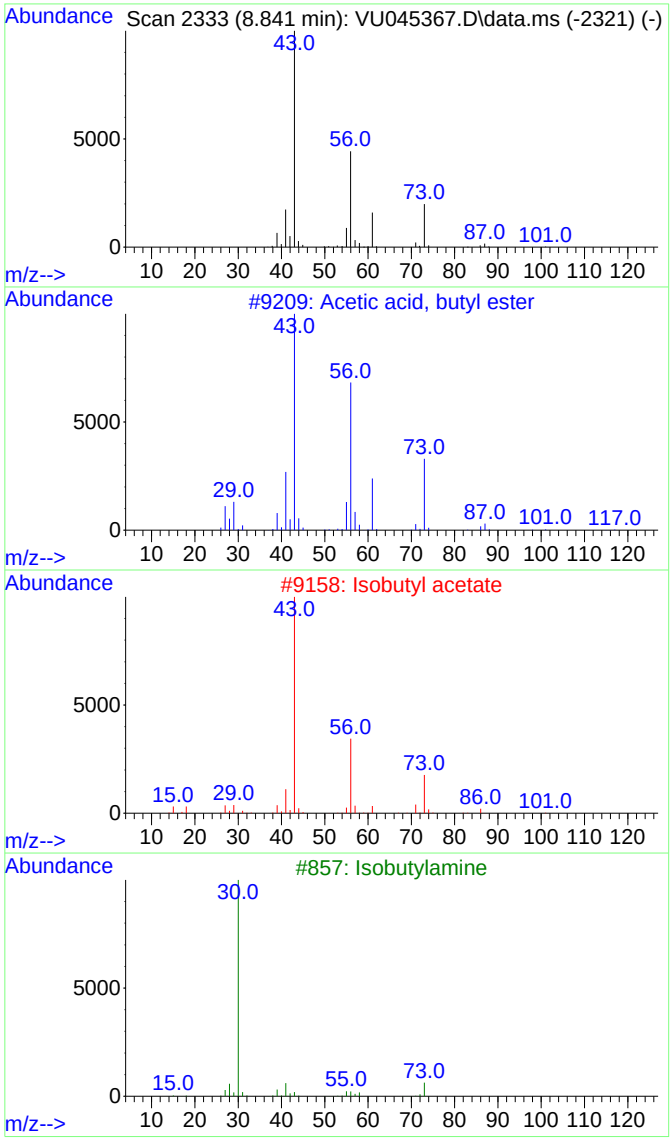
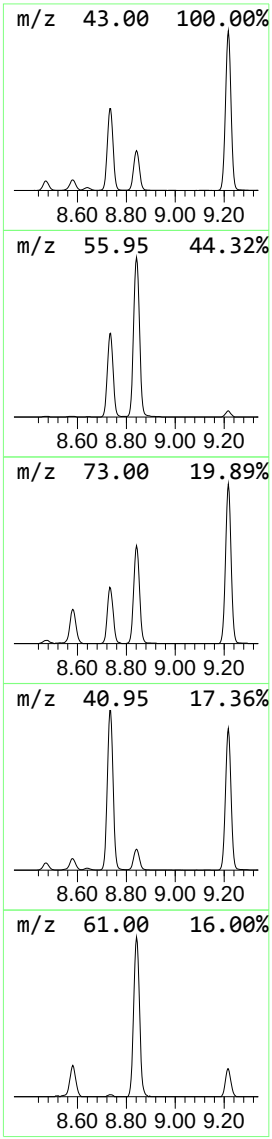
****

Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.841	22.39 ug/l	523107	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Isobutylamine	73	C4H11N	000078-81-9	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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Quant Title : SW846 8260

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

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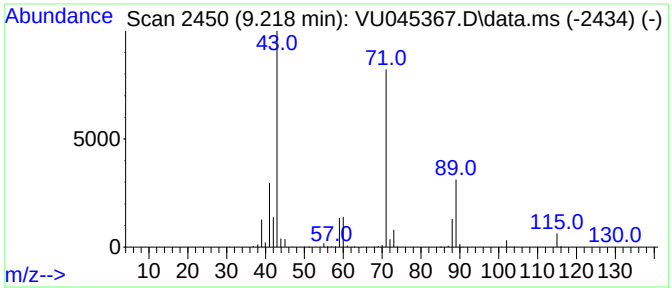
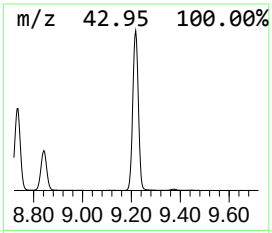
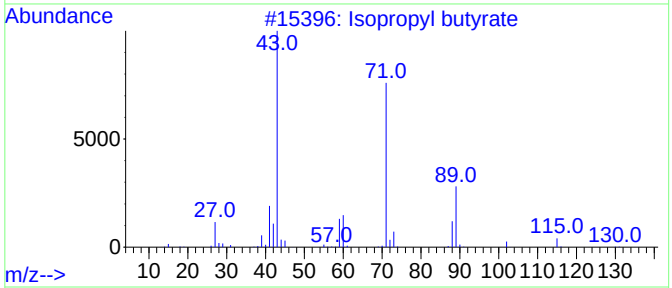
Peak Number 9 Isopropyl butyrate Concentration Rank 2

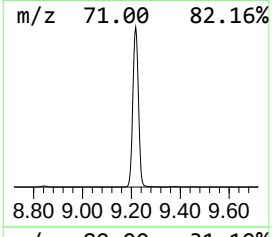
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.218	122.12 ug/l	2853290	Chlorobenzene-d5	9.420

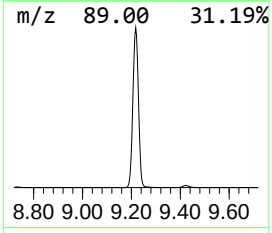
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64

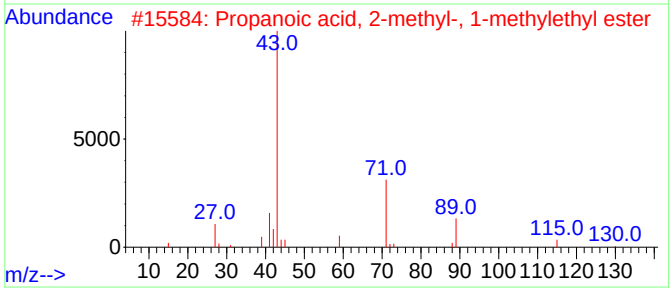


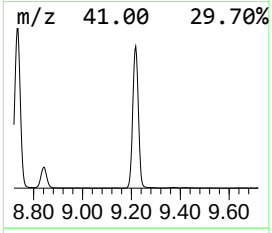


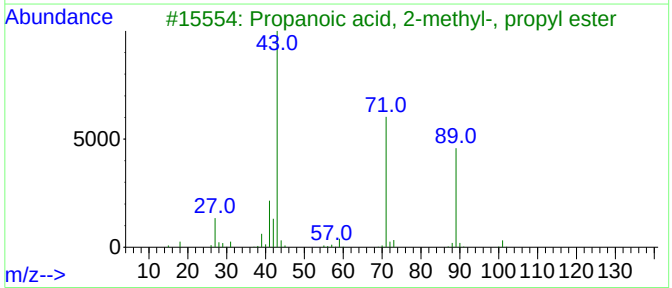


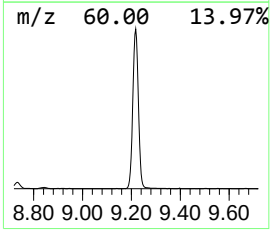












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045367.D
Acq On : 22 Oct 2021 16:11
Operator : SY/MD
Sample : M4315-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-DD-D

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	1.642	6.8	ug/l	91265	1	5.375	666910	50.0
Acetic acid	6.031	9.3	ug/l	256695	2	6.253	1387570	50.0
n-Propyl acetate	7.044	118.9	ug/l	3299600	2	6.253	1387570	50.0
Propanoic acid,...	7.745	17.1	ug/l	475769	2	6.253	1387570	50.0
Propanoic acid,...	8.472	6.2	ug/l	145082	3	9.420	1168240	50.0
Butanoic acid, ...	8.581	16.2	ug/l	378197	3	9.420	1168240	50.0
Propanoic acid,...	8.735	207.0	ug/l	4837340	3	9.420	1168240	50.0
Acetic acid, bu...	8.841	22.4	ug/l	523107	3	9.420	1168240	50.0
Isopropyl butyrate	9.218	122.1	ug/l	2853290	3	9.420	1168240	50.0