LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045365.D
Acq On : 22 Oct 2021 15:24
Operator : SY/MD
Sample : M4315-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-D-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: VU045365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.700	89	112	130	rBV	61374	232408	4.89%	1.120%
2	3.041	517	529	549	rVB	33277	65937	1.39%	0.318%
3	5.292	1214	1229	1242	rBV	187911	409957	8.62%	1.976%
4	5.372	1242	1254	1275	rVB	329544	684384	14.39%	3.299%
5	5.703	1342	1357	1380	rBV	230527	474713	9.98%	2.288%
6	5.919	1411	1424	1438	rBV	23784	55593	1.17%	0.268%
7	6.044	1452	1463	1486	rBV	63624	254194	5.35%	1.225%
8	6.250	1515	1527	1579	rVB	572552	1362600	28.66%	6.568%
9	6.948	1725	1744	1760	rBV2	24022	71635	1.51%	0.345%
10	7.047	1760	1775	1806	rVV	1431576	3362984	70.73%	16.211%
11	7.748	1979	1993	2010	rBV	221850	482470	10.15%	2.326%
12	7.899	2026	2040	2062	rBV	783888	1383893	29.11%	6.671%
13	8.173	2114	2125	2140	rBV2	22707	48454	1.02%	0.234%
14	8.475	2206	2219	2230	rBV	74384	160015	3.37%	0.771%
15	8.584	2243	2253	2266	rVB2	181855	371350	7.81%	1.790%
16	8.739	2285	2301	2321	rBV	2565444	4754425	100.00%	22.919%
17	8.848	2323	2335	2366	rVB	274299	518622	10.91%	2.500%
18	9.221	2436	2451	2486	rBV	1628170	2791275	58.71%	13.455%
19	9.423	2486	2514	2534	rBV	680832	1207715	25.40%	5.822%
20	10.083	2706	2719	2736	rBV	58699	95465	2.01%	0.460%
21	10.639	2880	2892	2914	rVB	533831	863044	18.15%	4.160%
22	11.816	3246	3258	3278	rBV	656902	1037648	21.82%	5.002%
23	17.137	4905	4913	4923	rVB	38289	55830	1.17%	0.269%

Sum of corrected areas: 20744611

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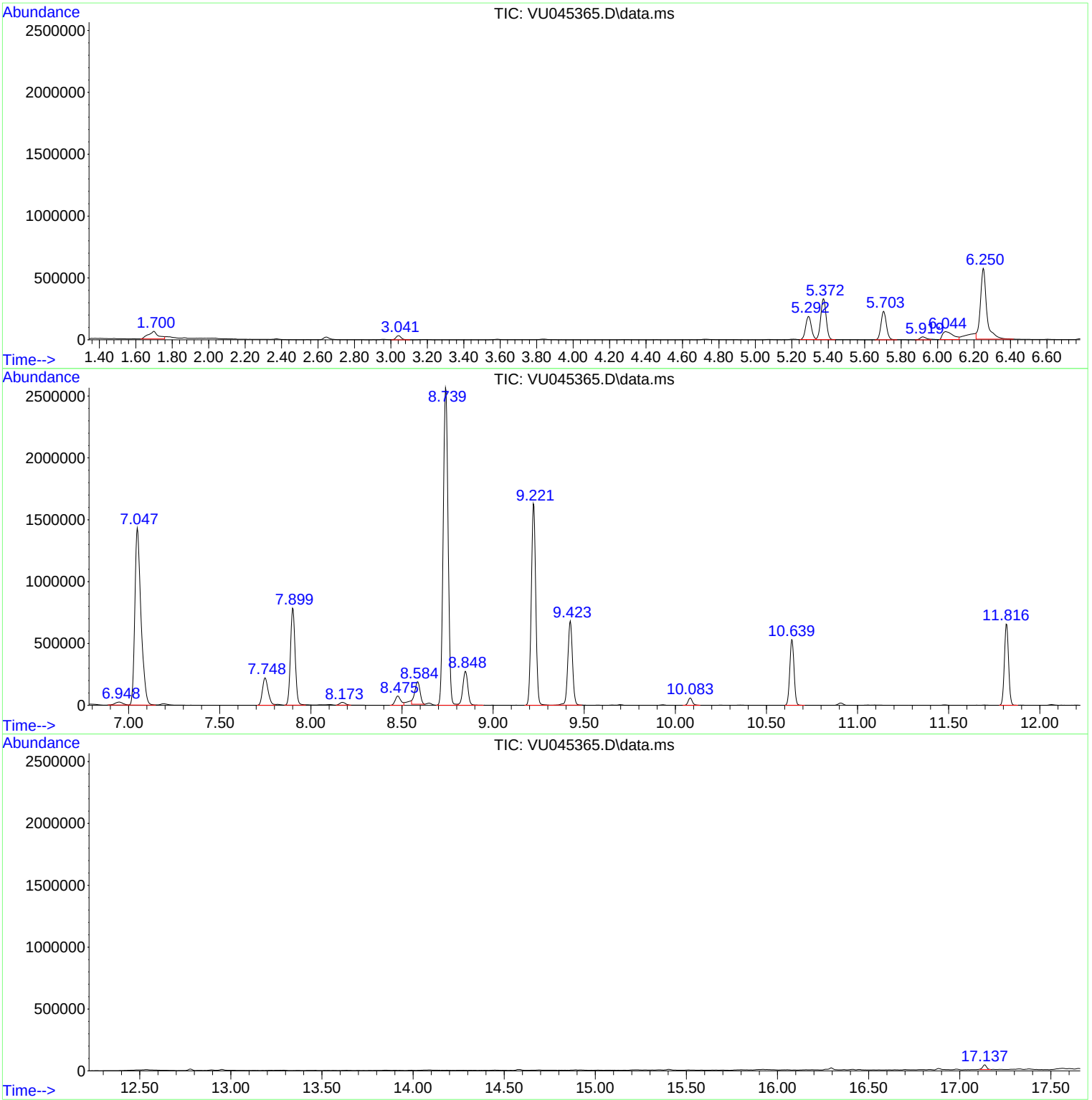
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-D-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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Quant Title : SW846 8260

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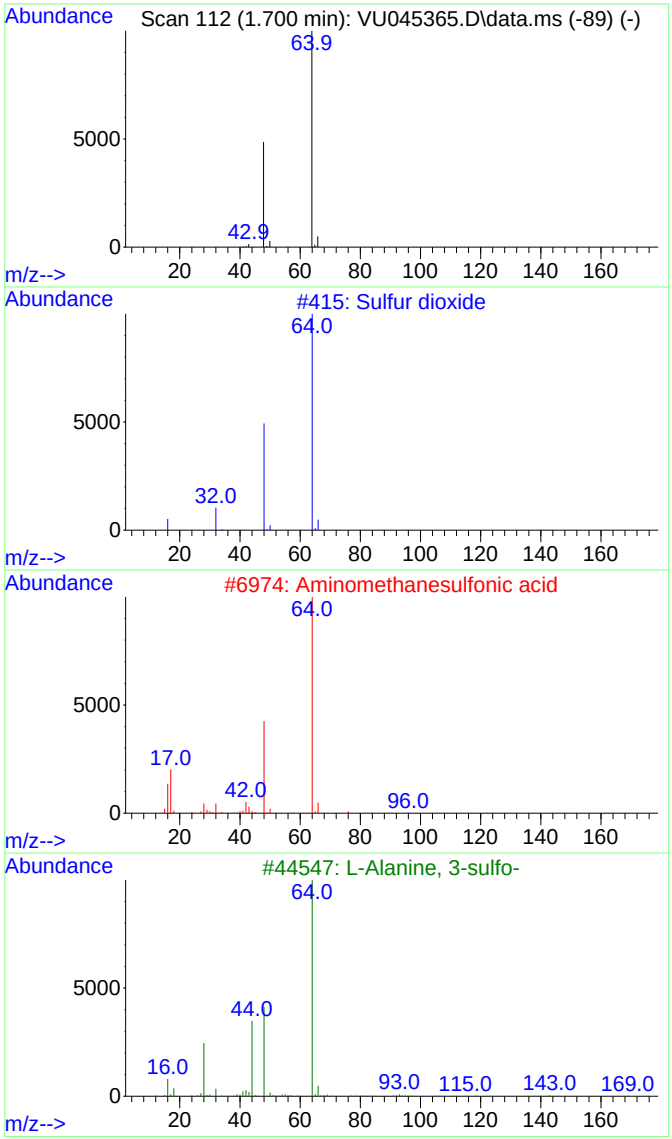
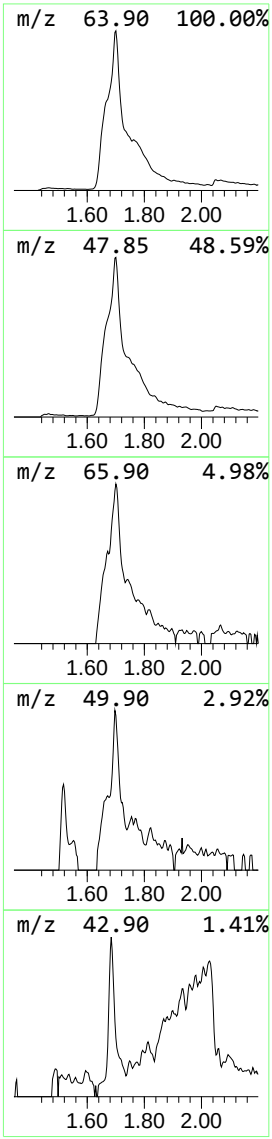
****

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.700	16.98 ug/l	232408	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	5
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4





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Instrument : MSVOA_U
ClientSampleId : MH-D-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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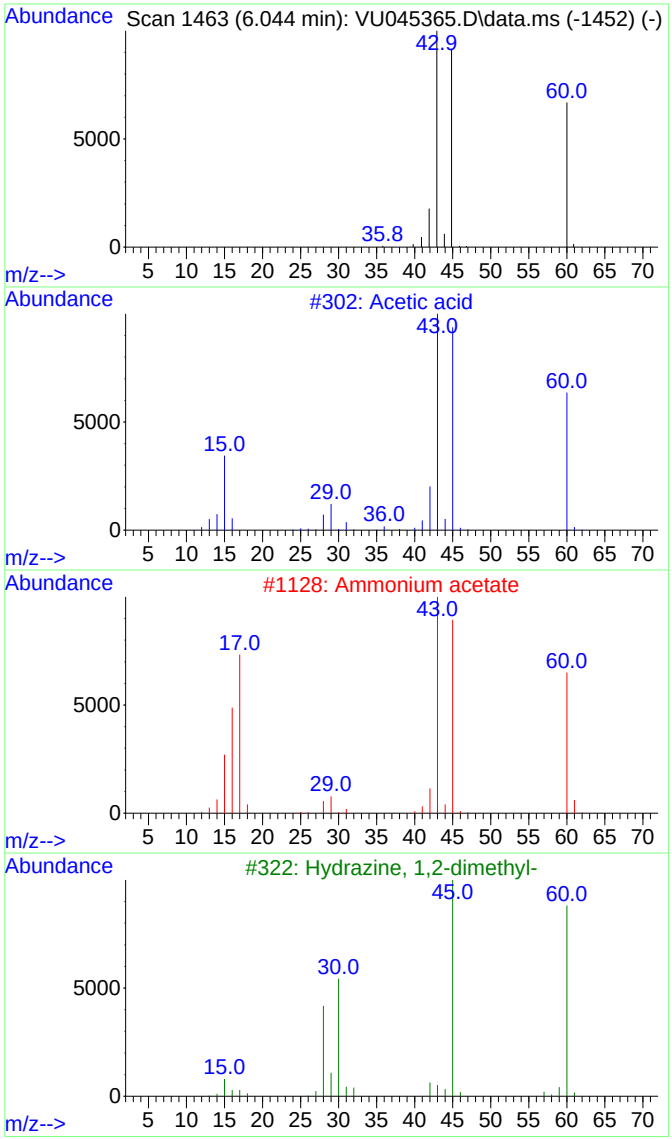
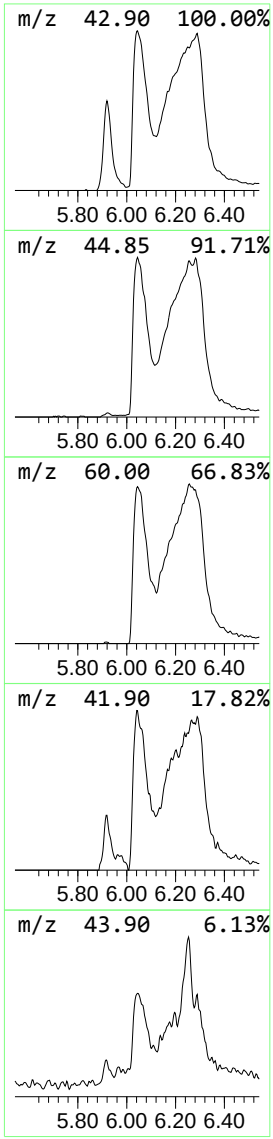
****

Peak Number 2 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.044	9.33 ug/l	254194	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	64
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Formamidoxime	60	CH4N2O	000624-82-8	5
5	Thiirane	60	C2H4S	000420-12-2	5





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Instrument : MSVOA_U
ClientSampleId : MH-D-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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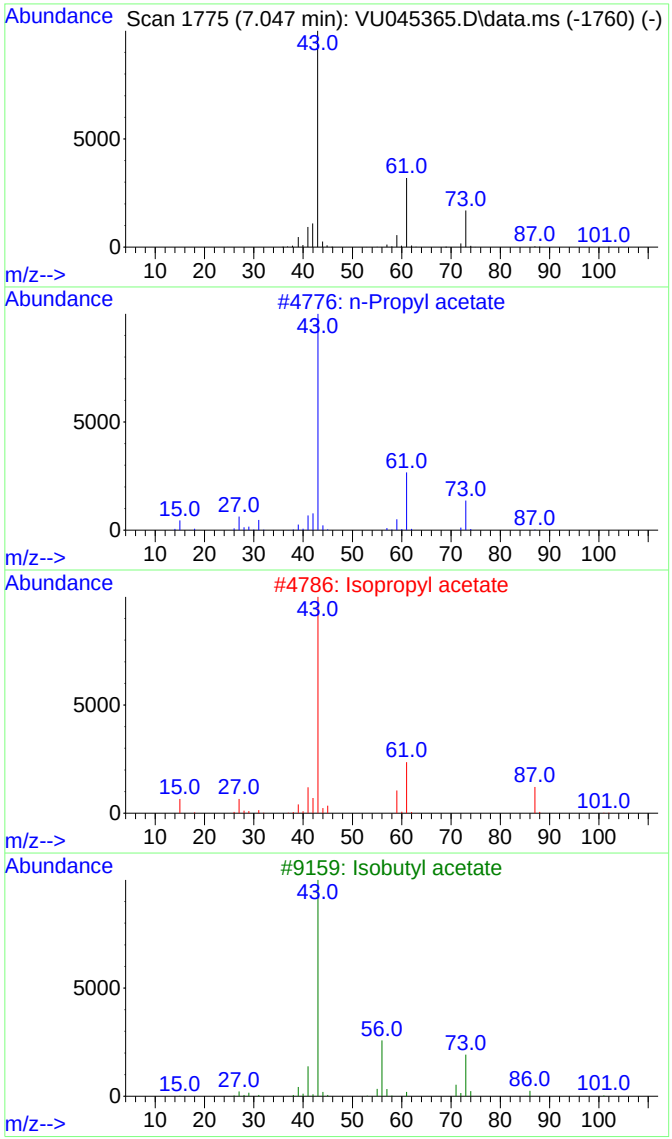
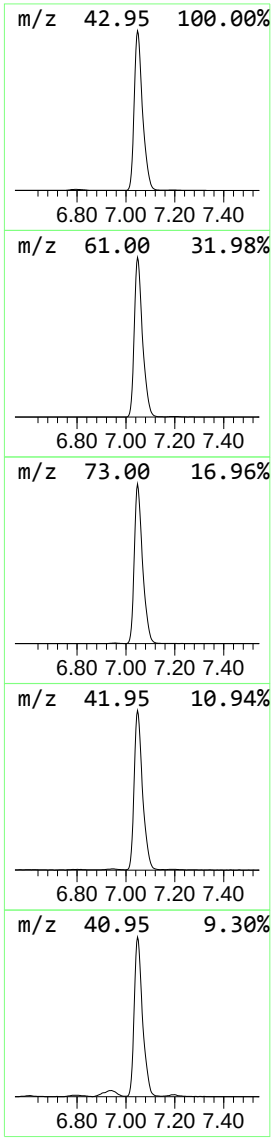
****

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.047	123.40 ug/l	3362980	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-D-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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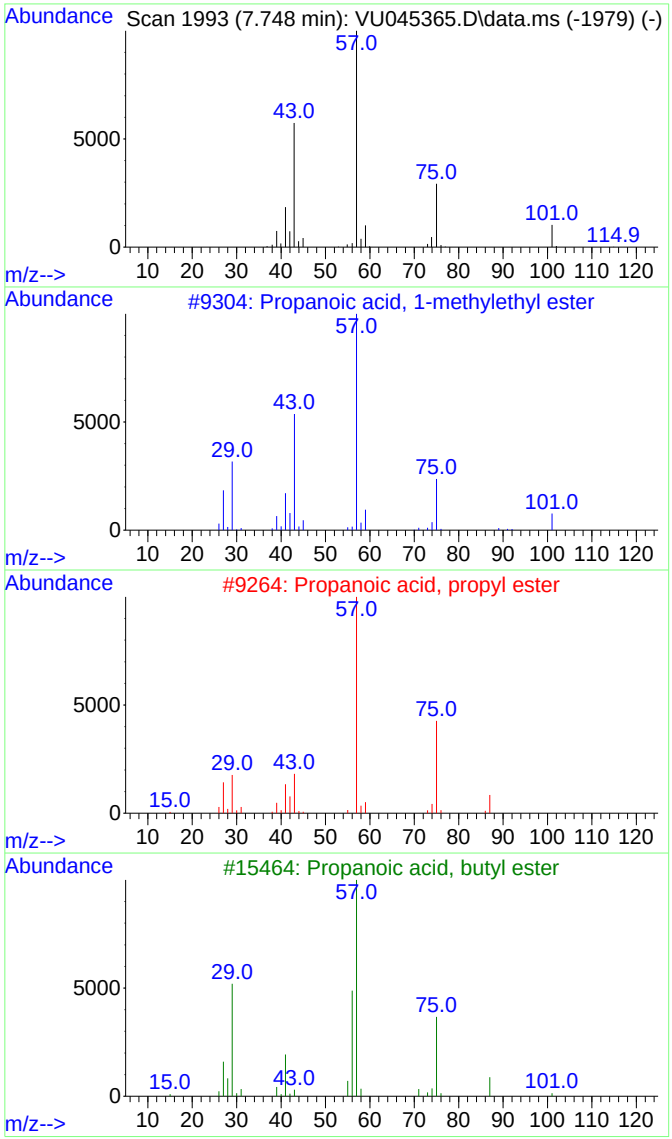
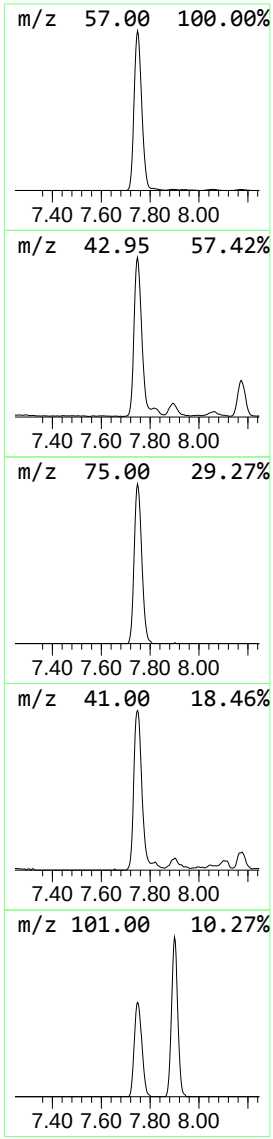
****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.748	17.70 ug/l	482470	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	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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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-D-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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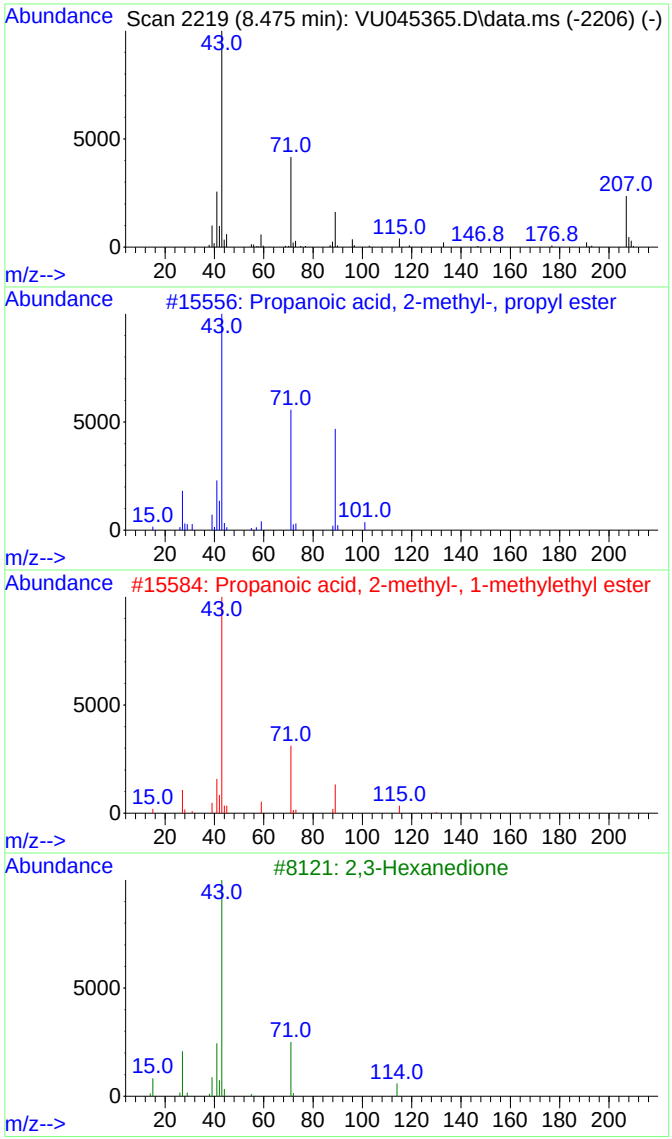
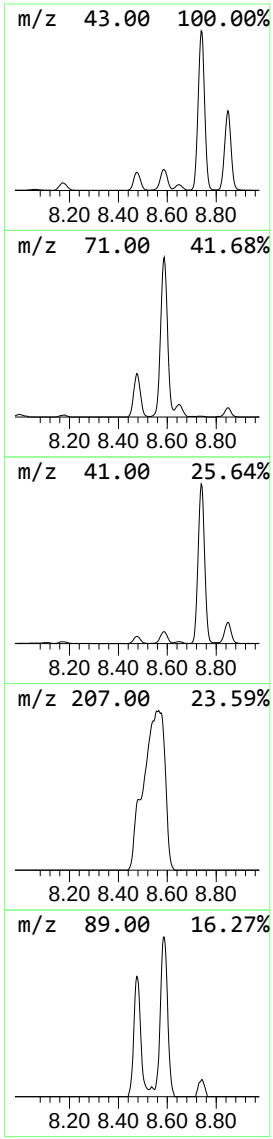
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	6.62 ug/l	160015	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	53
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	43
4	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	40





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-D-D

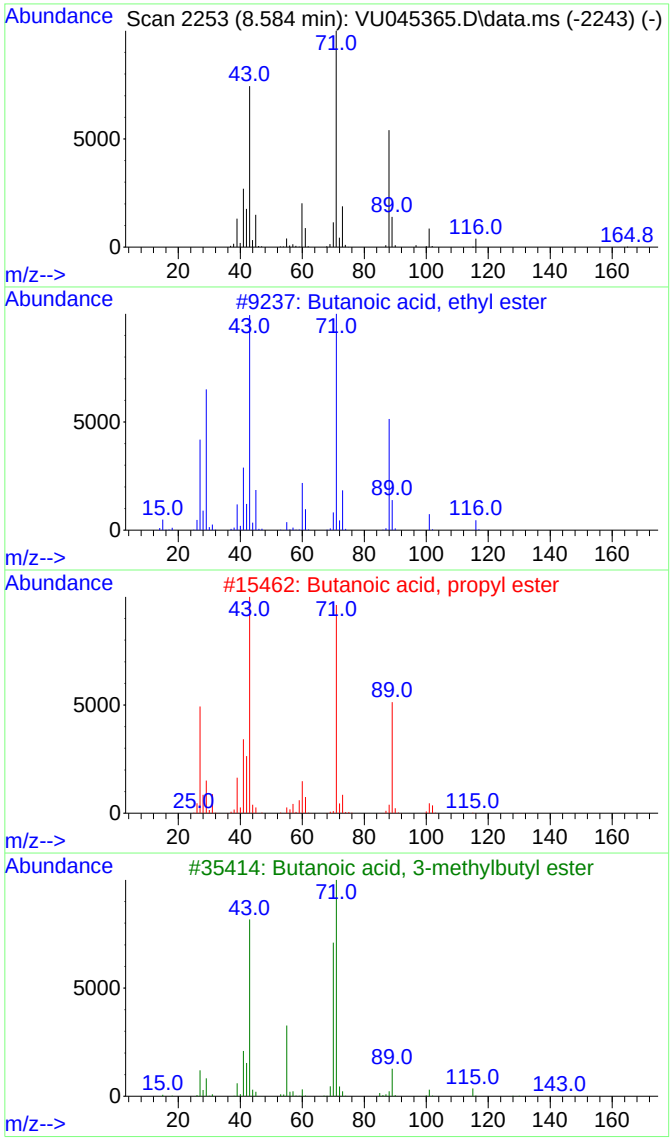
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

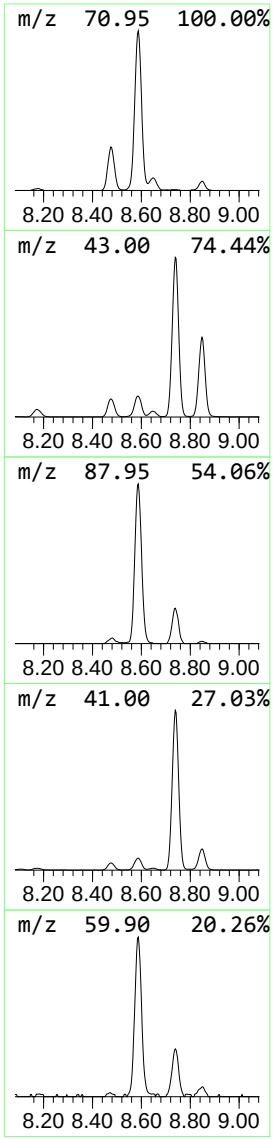
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.584	15.37 ug/l	371350	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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	40
5	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	37





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Quant Title : SW846 8260

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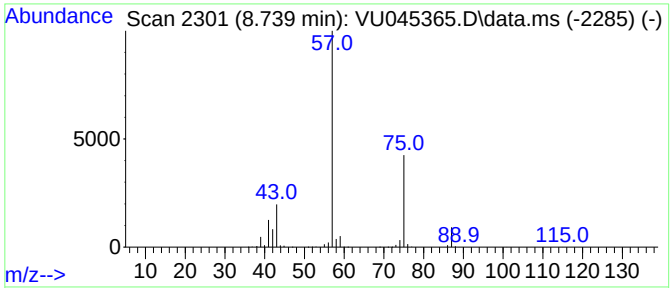
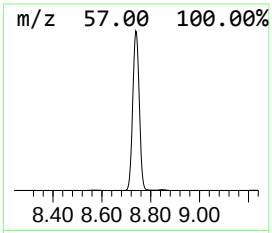
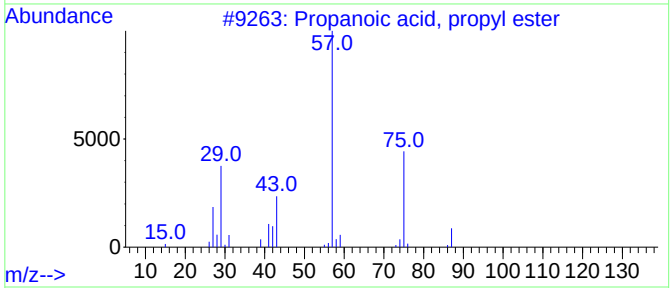
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 1

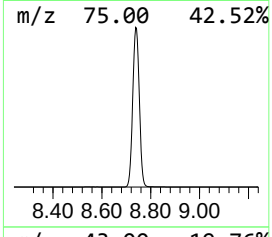
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.739	196.84 ug/l	4754430	Chlorobenzene-d5	9.423

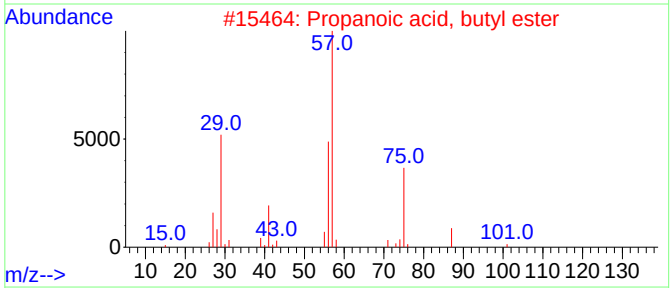
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	7

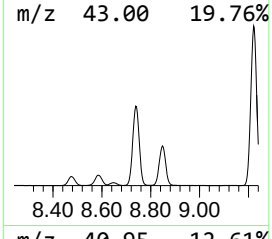


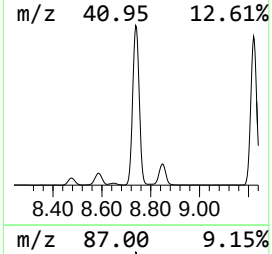


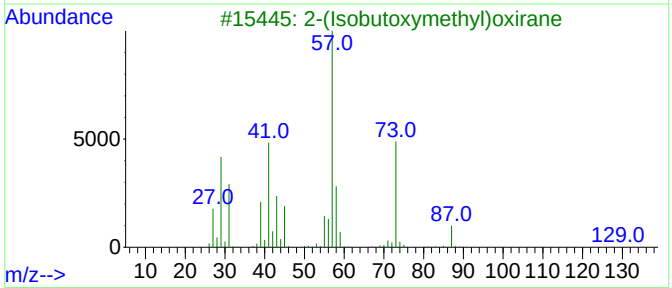


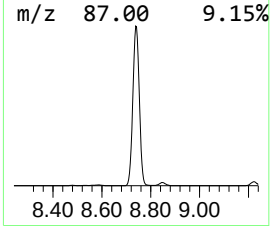












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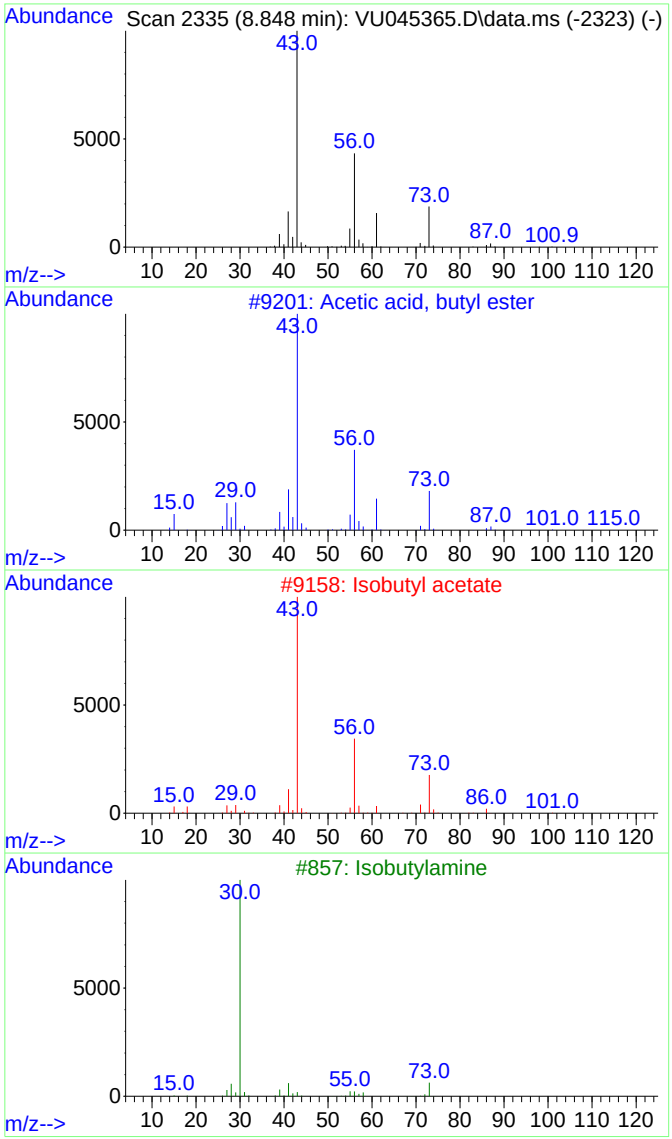
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

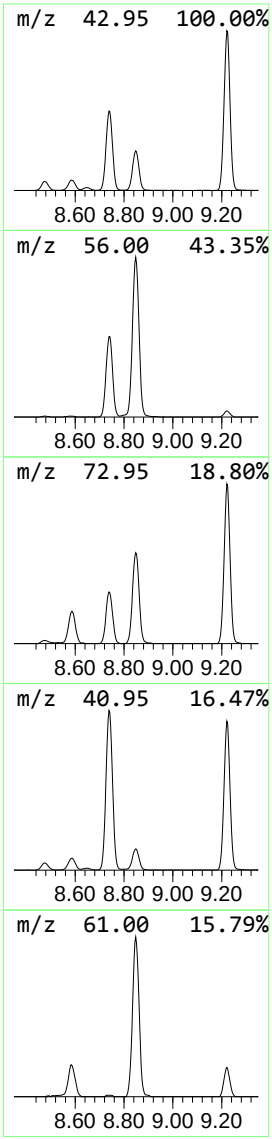
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.848	21.47 ug/l	518622	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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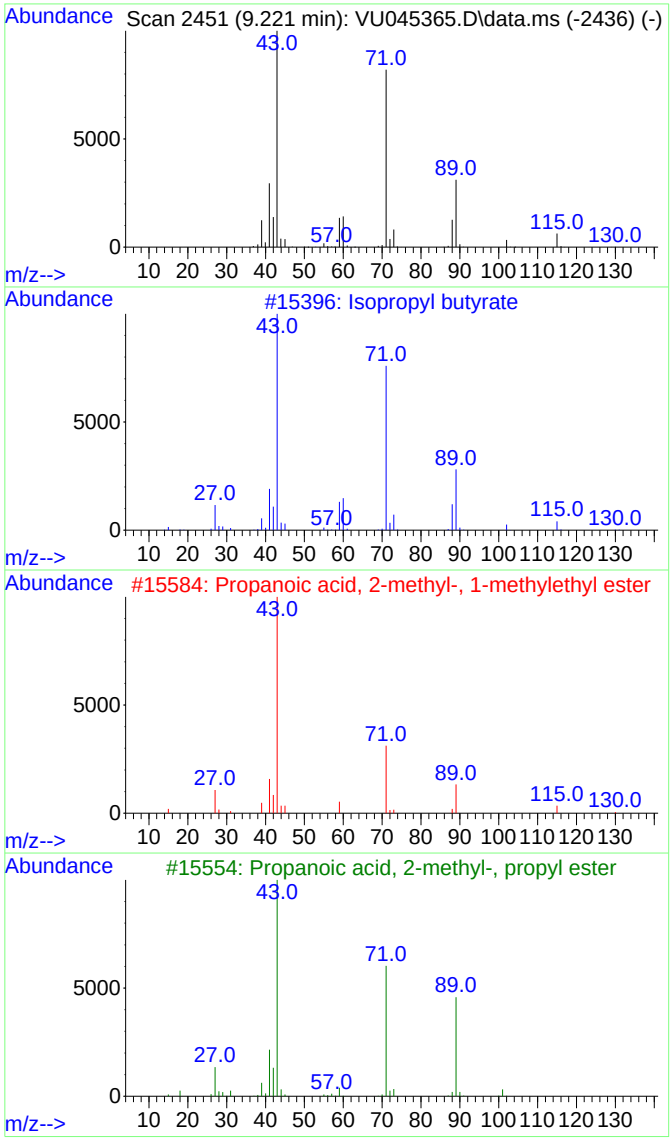
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

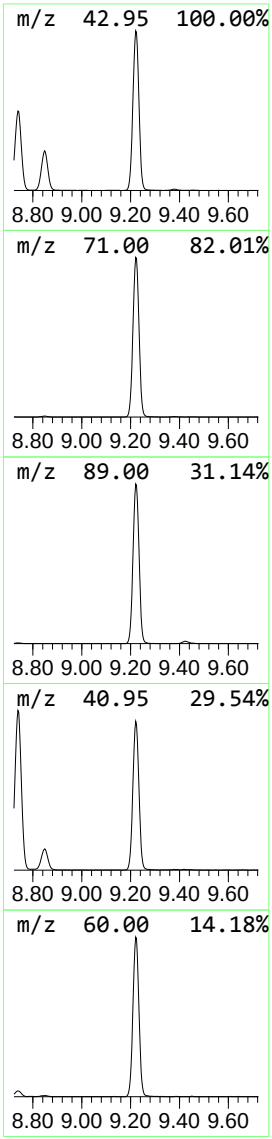
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.221	115.56 ug/l	2791280	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045365.D
Acq On : 22 Oct 2021 15:24
Operator : SY/MD
Sample : M4315-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-D-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	1.700	17.0	ug/l	232408	1	5.375	684384	50.0
Acetic acid	6.044	9.3	ug/l	254194	2	6.250	1362600	50.0
n-Propyl acetate	7.047	123.4	ug/l	3362980	2	6.250	1362600	50.0
Propanoic acid,...	7.748	17.7	ug/l	482470	2	6.250	1362600	50.0
Propanoic acid,...	8.475	6.6	ug/l	160015	3	9.423	1207720	50.0
Butanoic acid, ...	8.584	15.4	ug/l	371350	3	9.423	1207720	50.0
Propanoic acid,...	8.739	196.8	ug/l	4754430	3	9.423	1207720	50.0
Acetic acid, bu...	8.848	21.5	ug/l	518622	3	9.423	1207720	50.0
Isopropyl butyrate	9.221	115.6	ug/l	2791280	3	9.423	1207720	50.0