LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045369.D
Acq On : 22 Oct 2021 16:59
Operator : SY/MD
Sample : M4316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2A-ID

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: VU045369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.675	95	104	134	rBV	45686	137878	2.80%	0.651%
2	3.044	518	530	549	rVB	34185	66187	1.34%	0.313%
3	5.292	1213	1229	1242	rBV	197386	417130	8.46%	1.970%
4	5.375	1242	1255	1279	rVB	329208	682275	13.84%	3.222%
5	5.703	1341	1357	1374	rBV	234875	477337	9.69%	2.255%
6	5.919	1409	1424	1449	rBV2	25400	60458	1.23%	0.286%
7	6.035	1449	1460	1480	rBV2	79284	292765	5.94%	1.383%
8	6.250	1516	1527	1596	rVB	586378	1474144	29.91%	6.963%
9	6.945	1721	1743	1760	rVV2	26668	76710	1.56%	0.362%
10	7.047	1760	1775	1806	rVV	1590303	3437730	69.75%	16.237%
11	7.745	1978	1992	2007	rBV	245705	488556	9.91%	2.307%
12	7.899	2026	2040	2075	rBV	786781	1390381	28.21%	6.567%
13	8.170	2113	2124	2141	rBV	25681	51054	1.04%	0.241%
14	8.475	2205	2219	2230	rBV	74802	144783	2.94%	0.684%
15	8.584	2239	2253	2264	rVB	185634	355929	7.22%	1.681%
16	8.739	2284	2301	2321	rBV	2817046	4928383	100.00%	23.277%
17	8.845	2322	2334	2358	rVB	298285	531134	10.78%	2.509%
18	9.218	2435	2450	2481	rBV	1732138	2869139	58.22%	13.551%
19	9.420	2502	2513	2538	rVB	700671	1201693	24.38%	5.676%
20	10.079	2705	2718	2739	rBV	63830	101401	2.06%	0.479%
21	10.639	2879	2892	2913	rVB	563397	892907	18.12%	4.217%
22	11.816	3246	3258	3273	rBV	699765	1094594	22.21%	5.170%

Sum of corrected areas: 21172568

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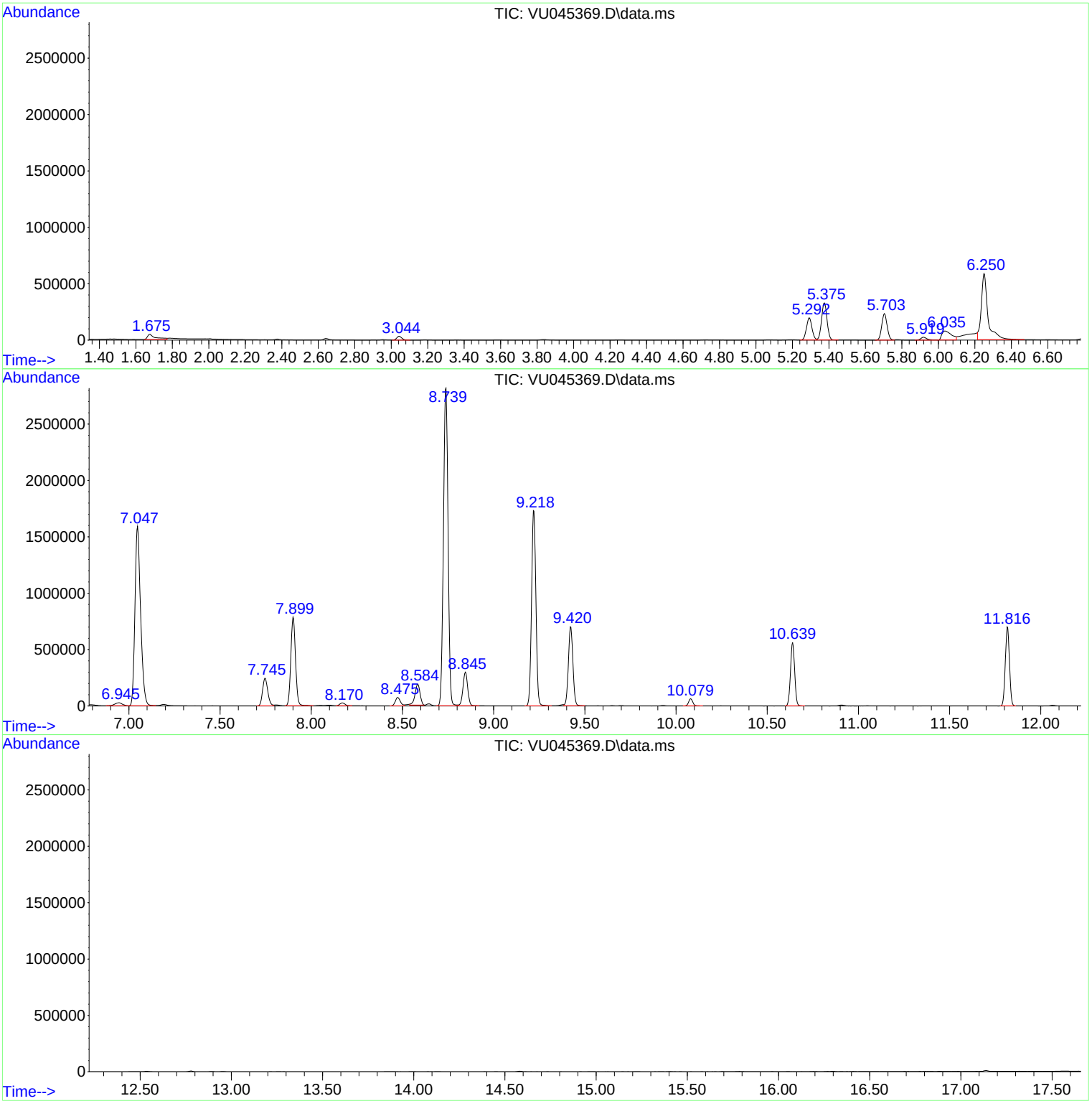
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2A-ID

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 : VU045369.D
Acq On : 22 Oct 2021 16:59
Operator : SY/MD
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Instrument :
MSVOA_U
ClientSampleId :
WC-2A-ID

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

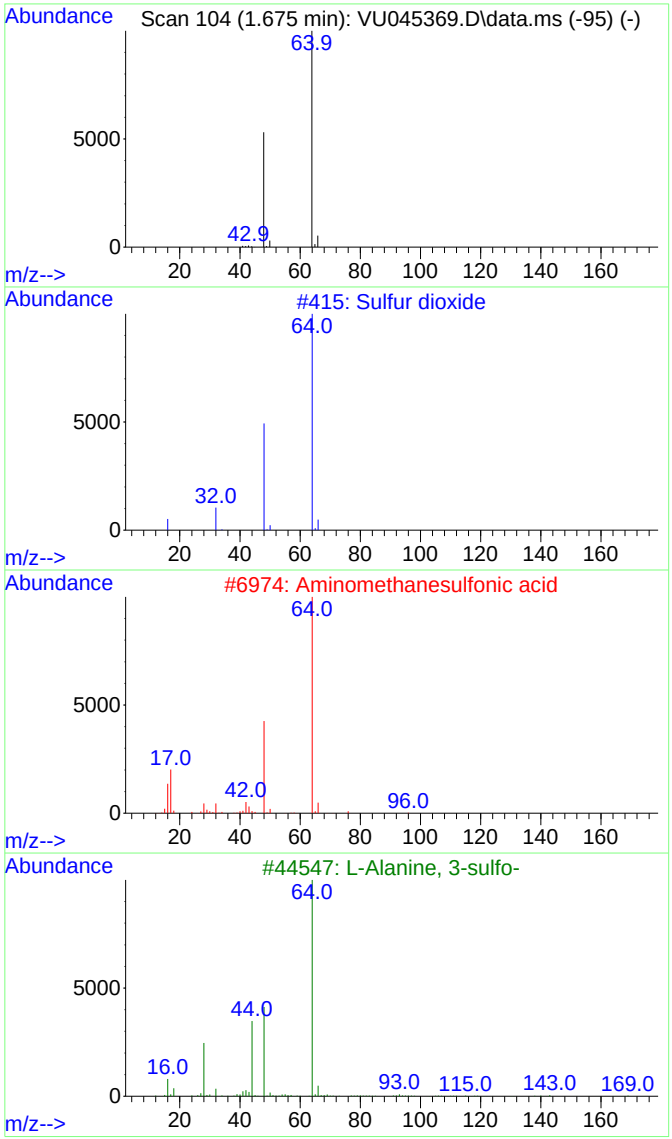
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

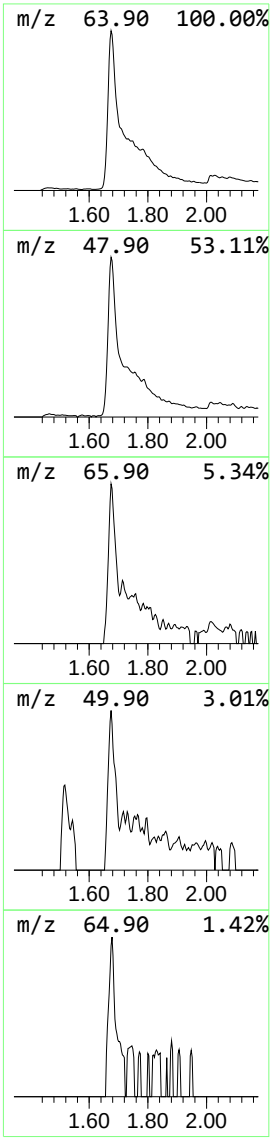
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.675	10.10 ug/l	137878	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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Data File : VU045369.D
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Operator : SY/MD
Sample : M4316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2A-ID

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

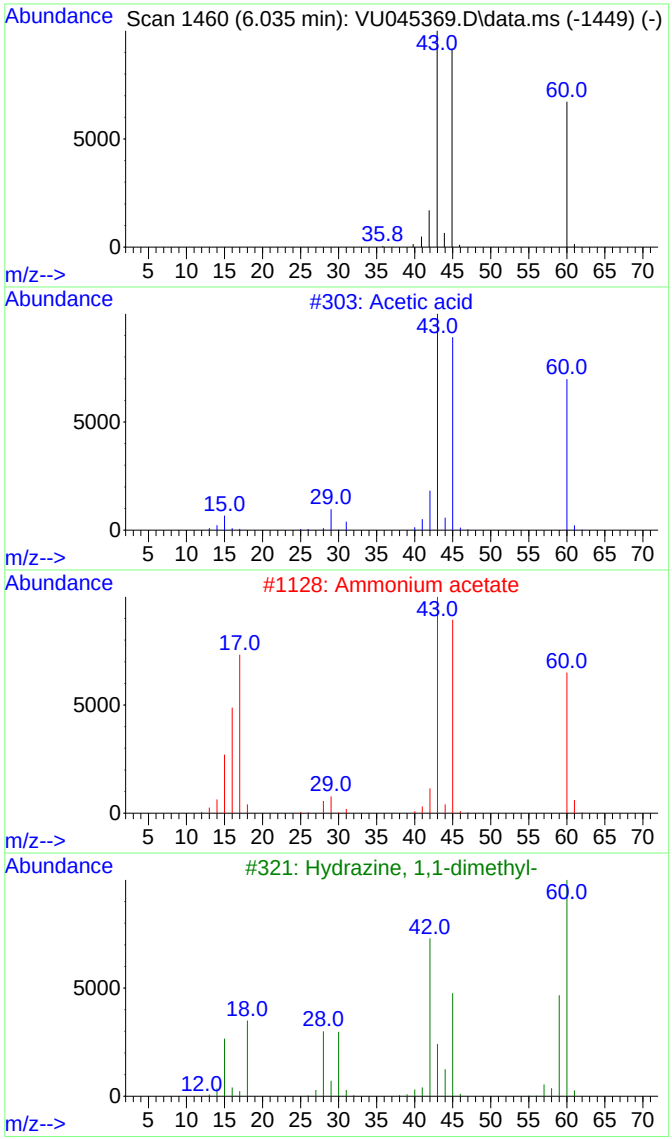
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

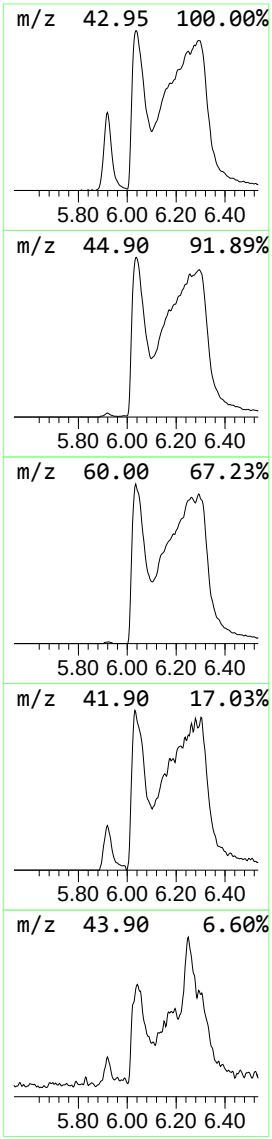
****

Peak Number 2 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.035	9.93 ug/l	292765	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, 1,1-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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Data File : VU045369.D
Acq On : 22 Oct 2021 16:59
Operator : SY/MD
Sample : M4316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2A-ID

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

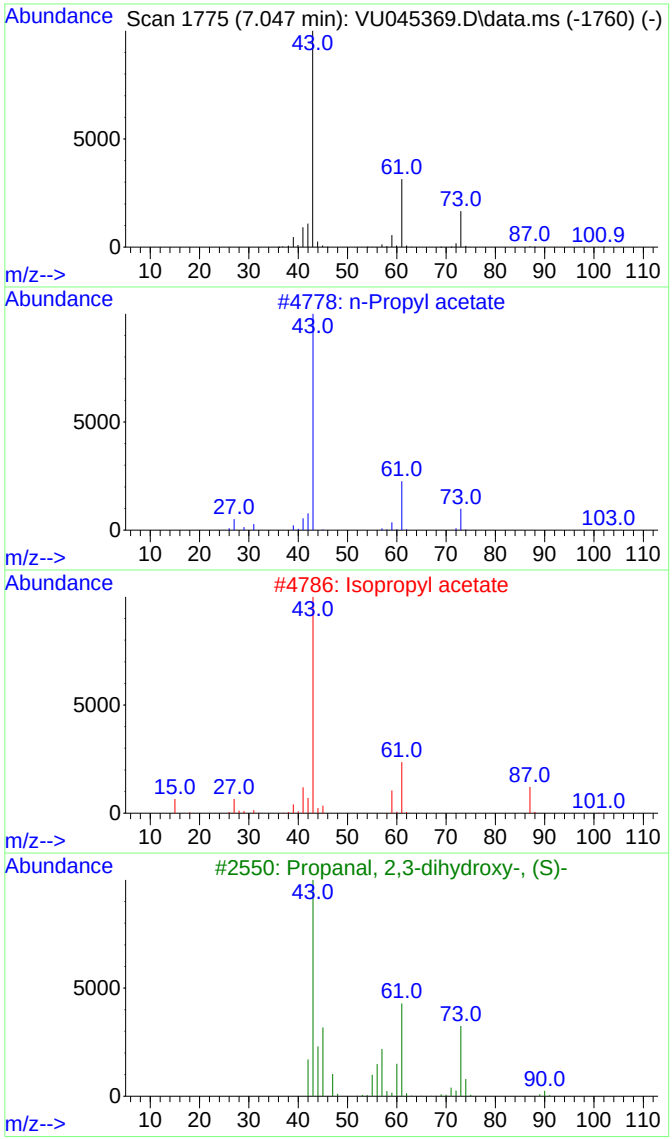
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

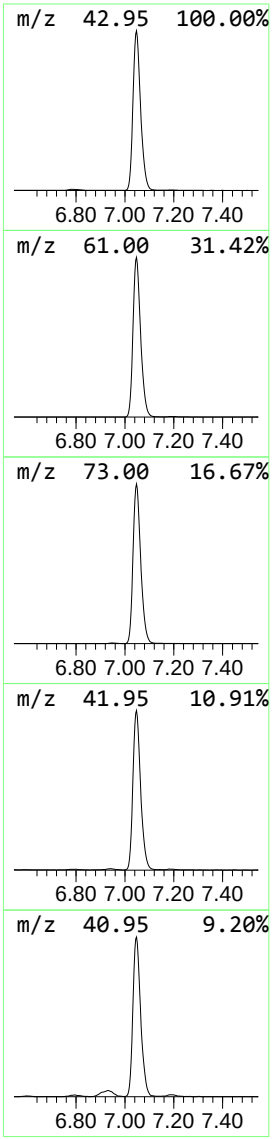
****

Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.047	116.60 ug/l	3437730	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	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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Sample : M4316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2A-ID

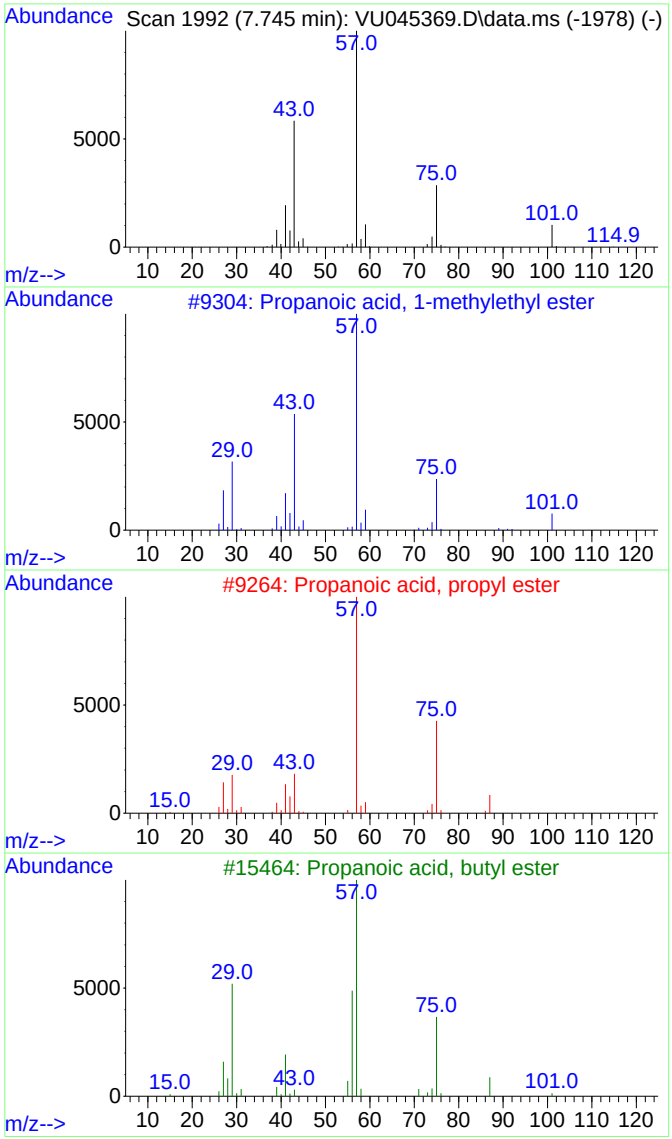
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

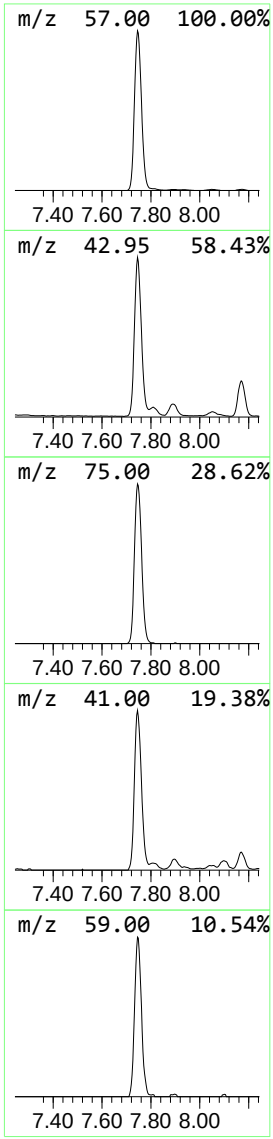
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.745	16.57 ug/l	488556	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	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : SY/MD
Sample : M4316-04
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2A-ID

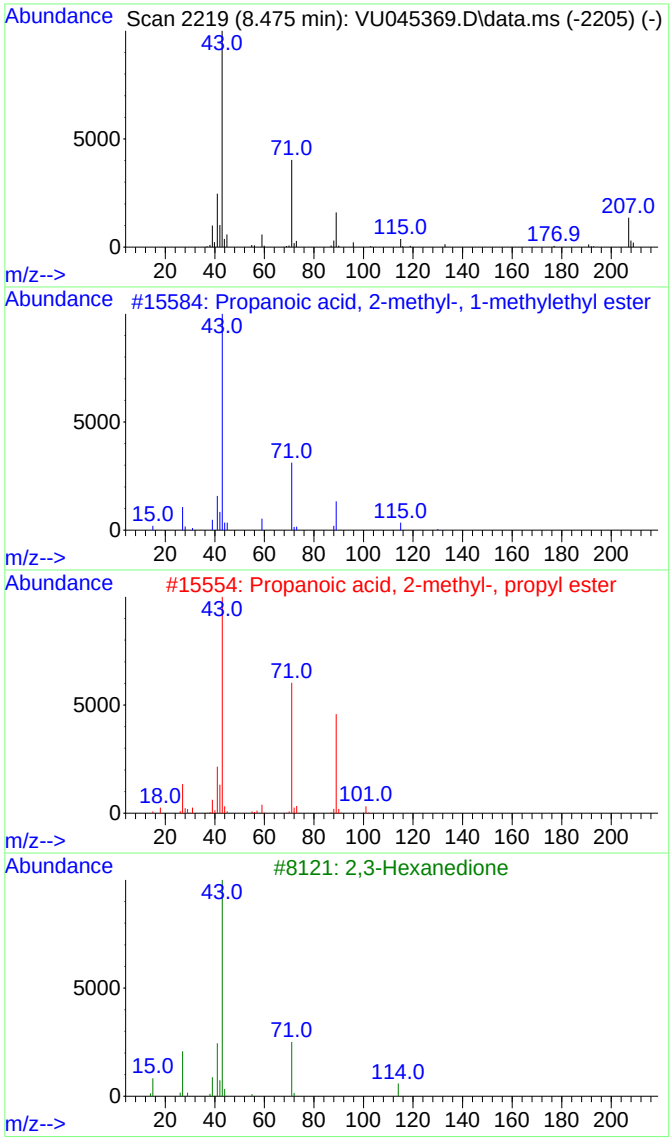
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

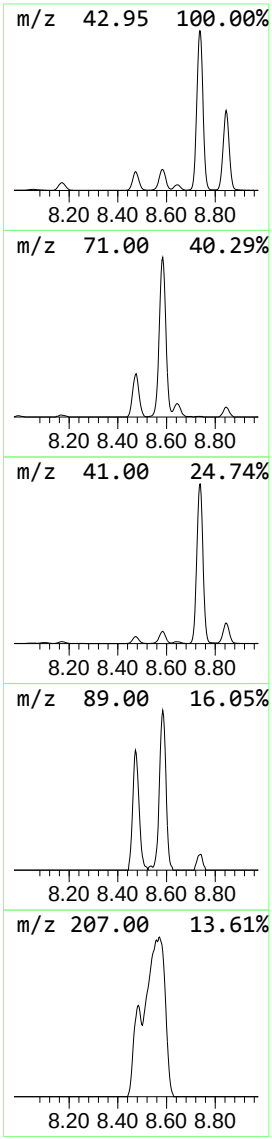
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	6.02 ug/l	144783	Chlorobenzene-d5	9.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	40
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	33





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2A-ID

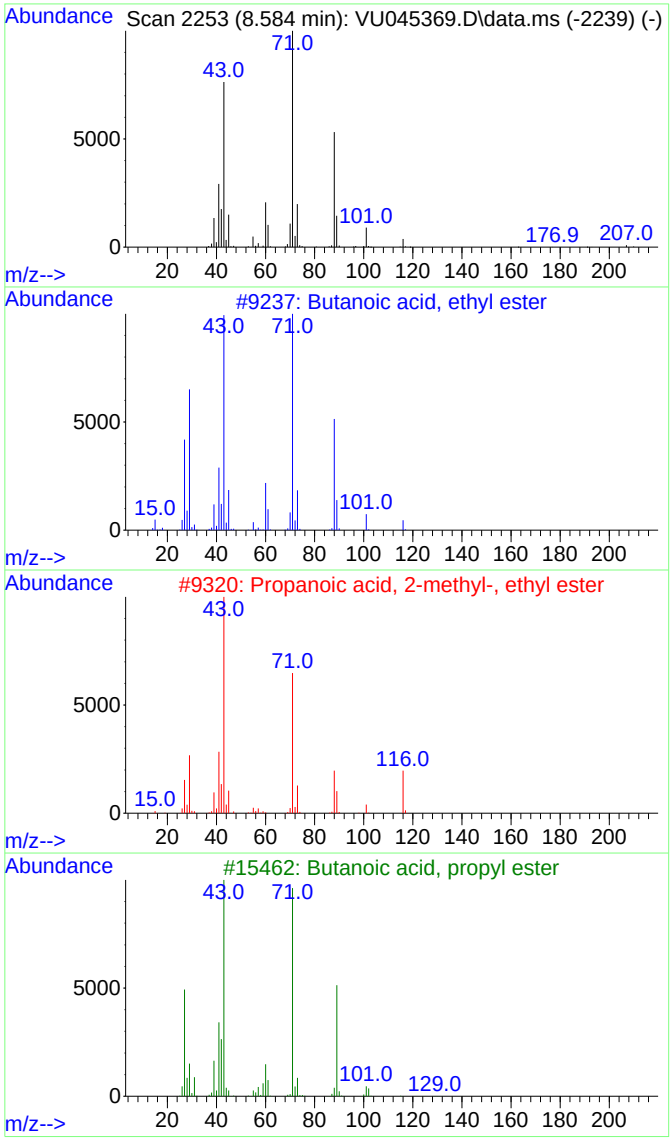
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

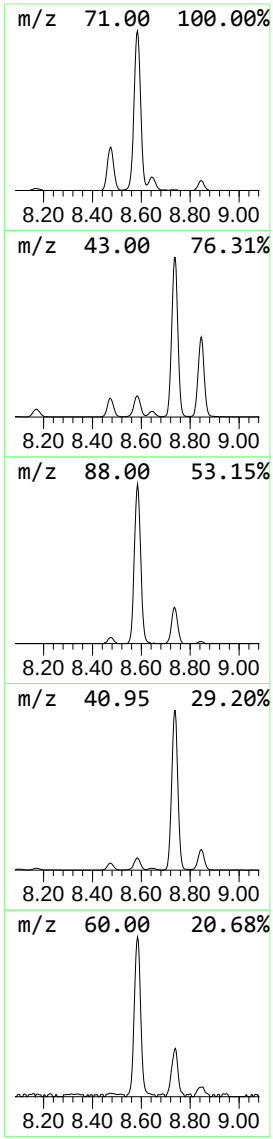
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.584	14.81 ug/l	355929	Chlorobenzene-d5	9.424

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	50
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
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 : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2A-ID

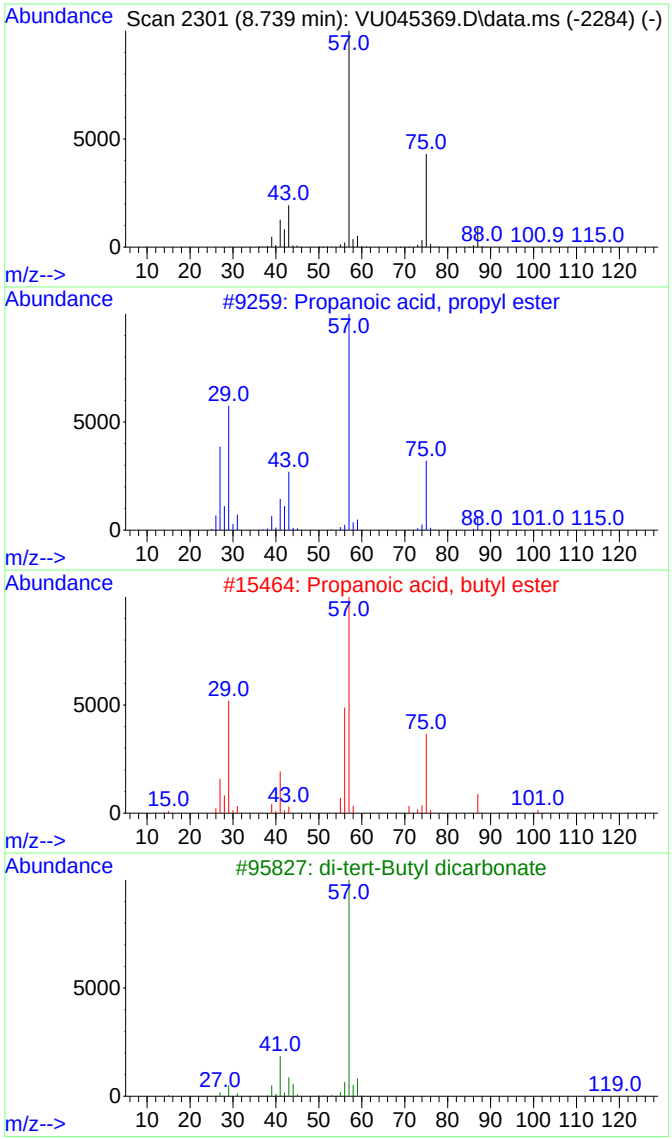
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

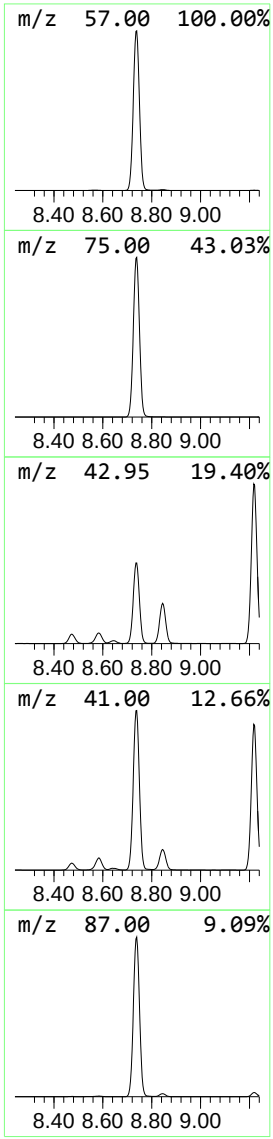
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.739	205.06 ug/l	4928380	Chlorobenzene-d5	9.424

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
ClientSampleId :
WC-2A-ID

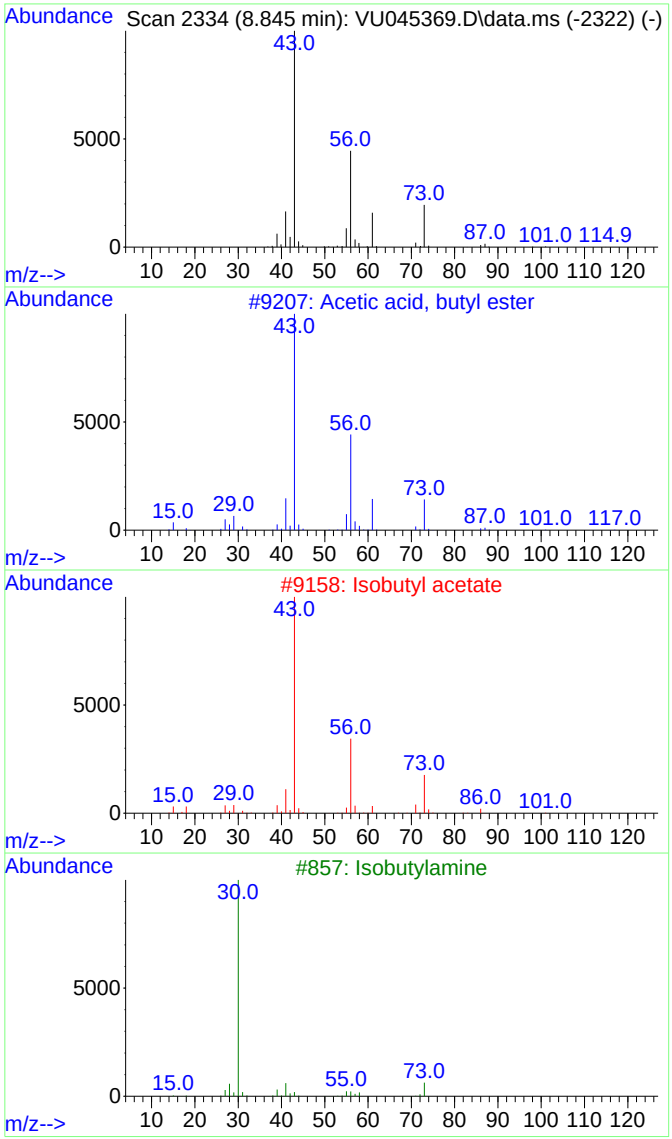
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

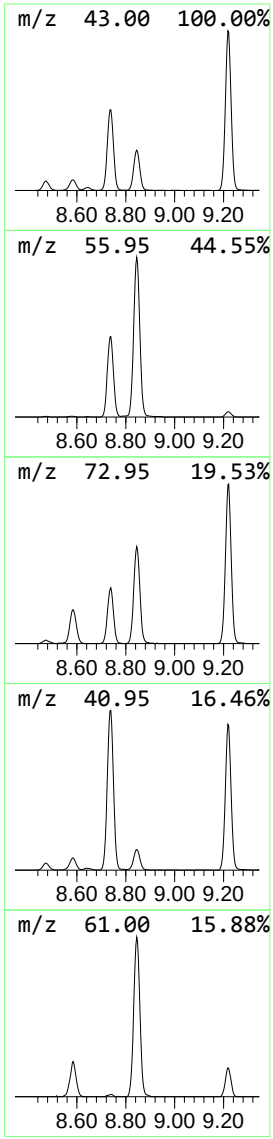
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.845	22.10 ug/l	531134	Chlorobenzene-d5	9.424

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	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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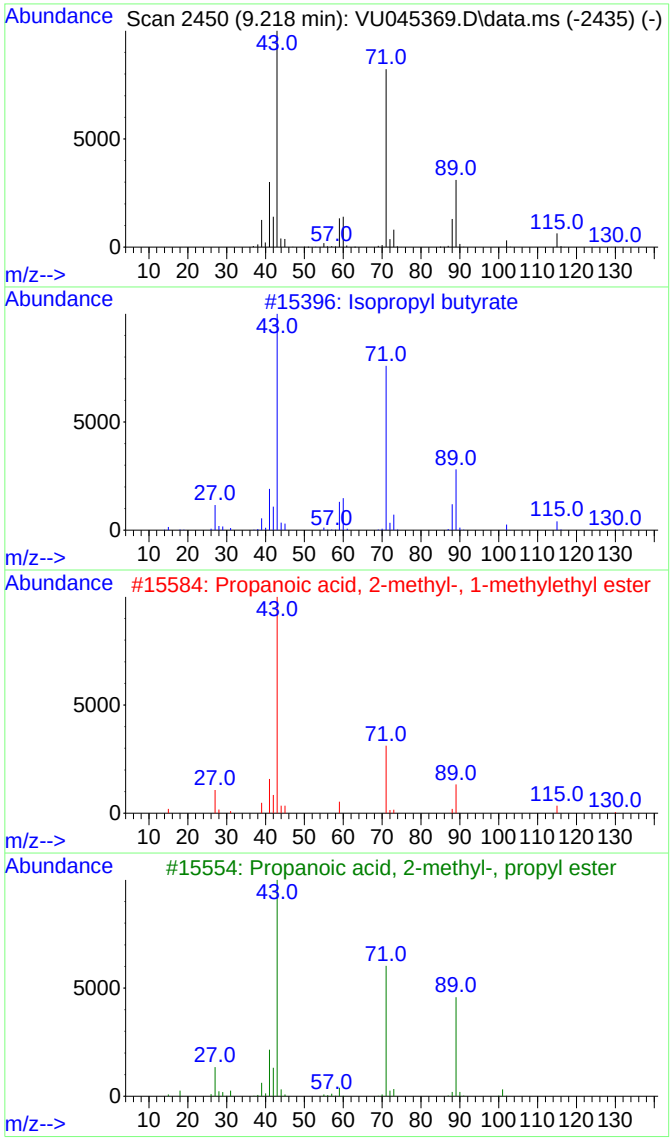
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

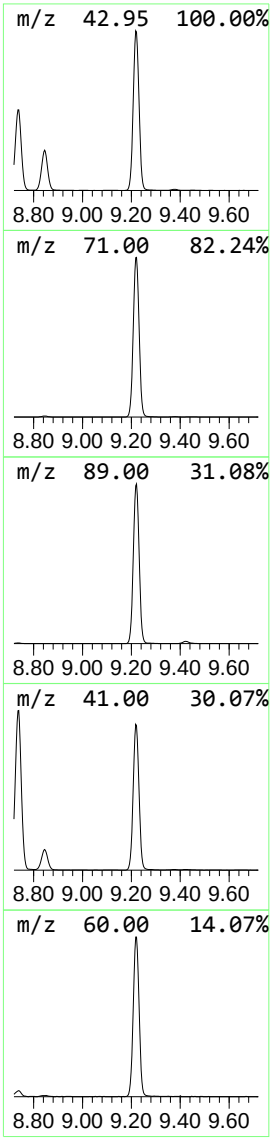
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.218	119.38 ug/l	2869140	Chlorobenzene-d5	9.424

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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2A-ID

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	1.675	10.1	ug/l	137878	1	5.375	682275	50.0
Acetic acid	6.035	9.9	ug/l	292765	2	6.250	1474140	50.0
n-Propyl acetate	7.047	116.6	ug/l	3437730	2	6.250	1474140	50.0
Propanoic acid,...	7.745	16.6	ug/l	488556	2	6.250	1474140	50.0
Propanoic acid,...	8.475	6.0	ug/l	144783	3	9.424	1201690	50.0
Butanoic acid, ...	8.584	14.8	ug/l	355929	3	9.424	1201690	50.0
Propanoic acid,...	8.739	205.1	ug/l	4928380	3	9.424	1201690	50.0
Acetic acid, bu...	8.845	22.1	ug/l	531134	3	9.424	1201690	50.0
Isopropyl butyrate	9.218	119.4	ug/l	2869140	3	9.424	1201690	50.0