LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045029.D
Acq On : 30 Sep 2021 06:12
Operator : SY/MD
Sample : M3971-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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: VU045029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% of max.	% of total
1	2.630	388	401	422	rBV	29824	52191	1.55%	0.332%
2	3.051	521	532	548	rBV2	20377	38463	1.14%	0.245%
3	5.295	1214	1230	1243	rBV	178657	379568	11.28%	2.414%
4	5.379	1243	1256	1273	rVB	308702	632912	18.81%	4.025%
5	5.707	1343	1358	1373	rBV	220027	442769	13.16%	2.815%
6	5.916	1410	1423	1439	rBV	22241	43886	1.30%	0.279%
7	6.163	1459	1500	1502	rBV3	15195	75796	2.25%	0.482%
8	6.253	1515	1528	1578	rVB	482542	975107	28.98%	6.200%
9	6.928	1729	1738	1755	rVB2	18912	50408	1.50%	0.321%
10	7.041	1759	1773	1803	rBV	1428798	2435721	72.39%	15.488%
11	7.742	1977	1991	2002	rBV	218090	356280	10.59%	2.266%
12	7.903	2025	2041	2062	rBV	735599	1275538	37.91%	8.111%
13	8.469	2204	2217	2231	rBV	55197	88681	2.64%	0.564%
14	8.578	2233	2251	2262	rBV	135654	230835	6.86%	1.468%
15	8.729	2279	2298	2316	rBV	2178472	3364630	100.00%	21.395%
16	8.835	2322	2331	2359	rVB	196935	325048	9.66%	2.067%
17	9.215	2433	2449	2485	rBV	1294162	1987552	59.07%	12.638%
18	9.420	2501	2513	2531	rVB	670365	1091516	32.44%	6.941%
19	10.076	2706	2717	2737	rVB	34149	54394	1.62%	0.346%
20	10.636	2878	2891	2915	rBV	513043	810619	24.09%	5.155%
21	11.816	3245	3258	3275	rBV	642596	1014362	30.15%	6.450%

Sum of corrected areas: 15726276

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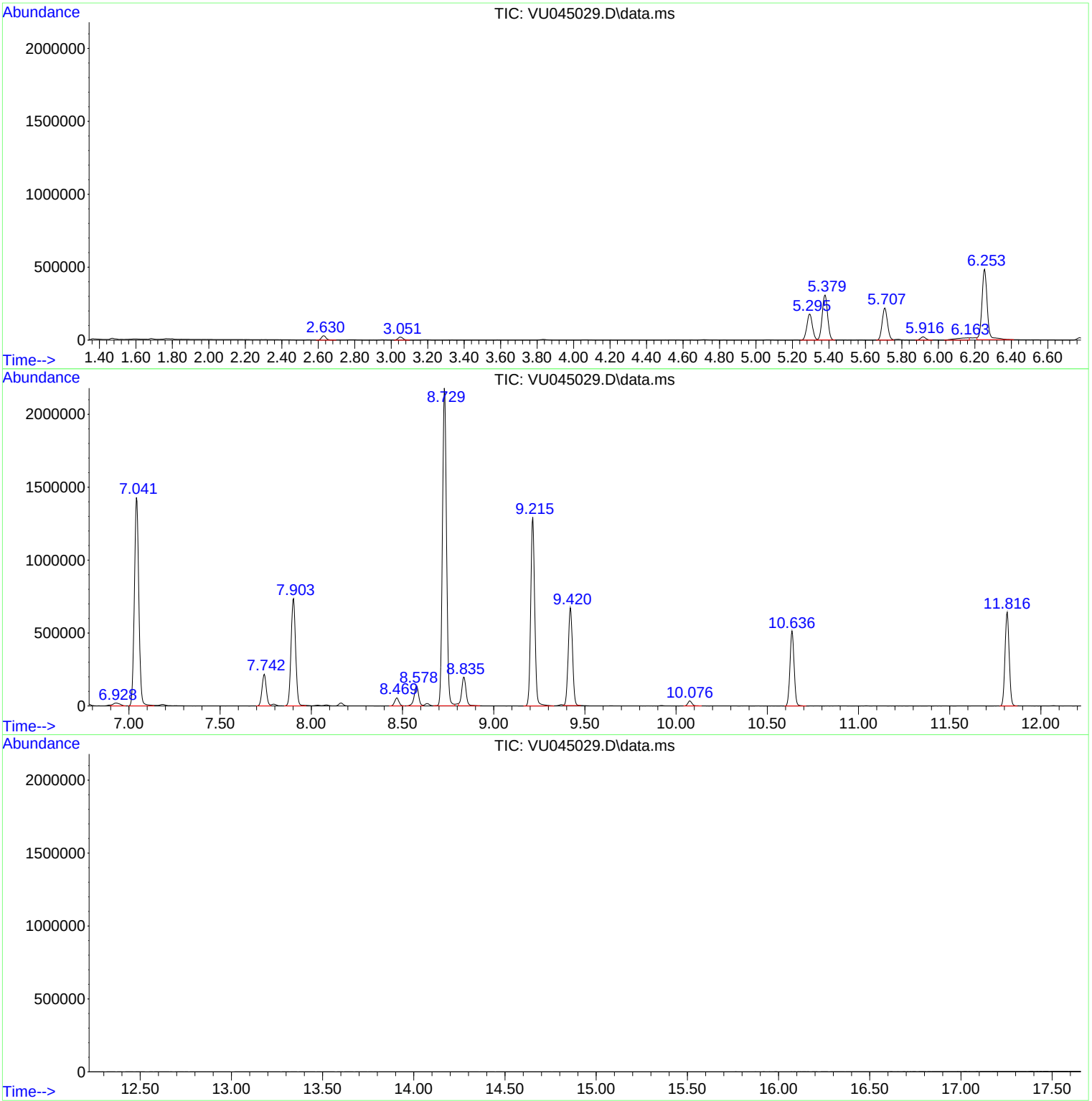
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
RO-COMP-1

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 : VU045029.D
Acq On : 30 Sep 2021 06:12
Operator : SY/MD
Sample : M3971-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

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

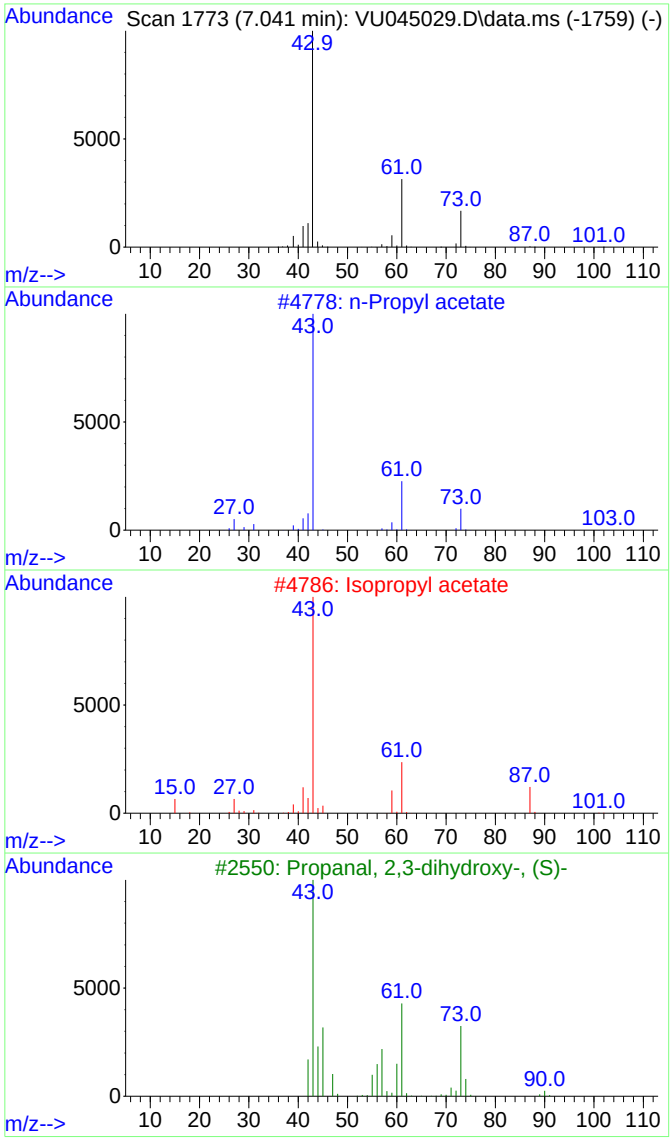
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

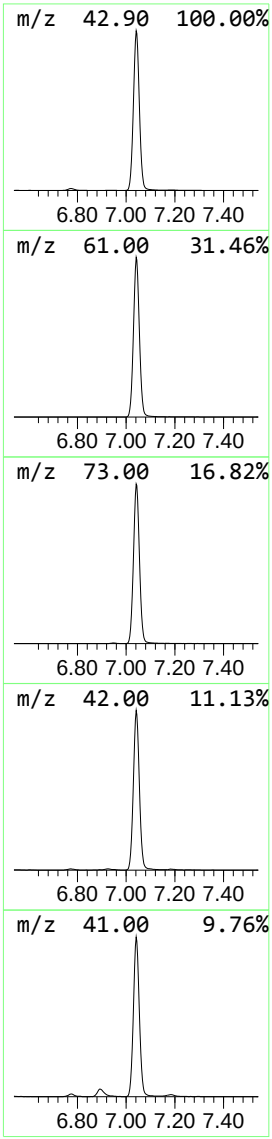
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	124.90 ug/l	2435720	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	Isobutylamine	73	C4H11N	000078-81-9	5





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Acq On : 30 Sep 2021 06:12
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ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

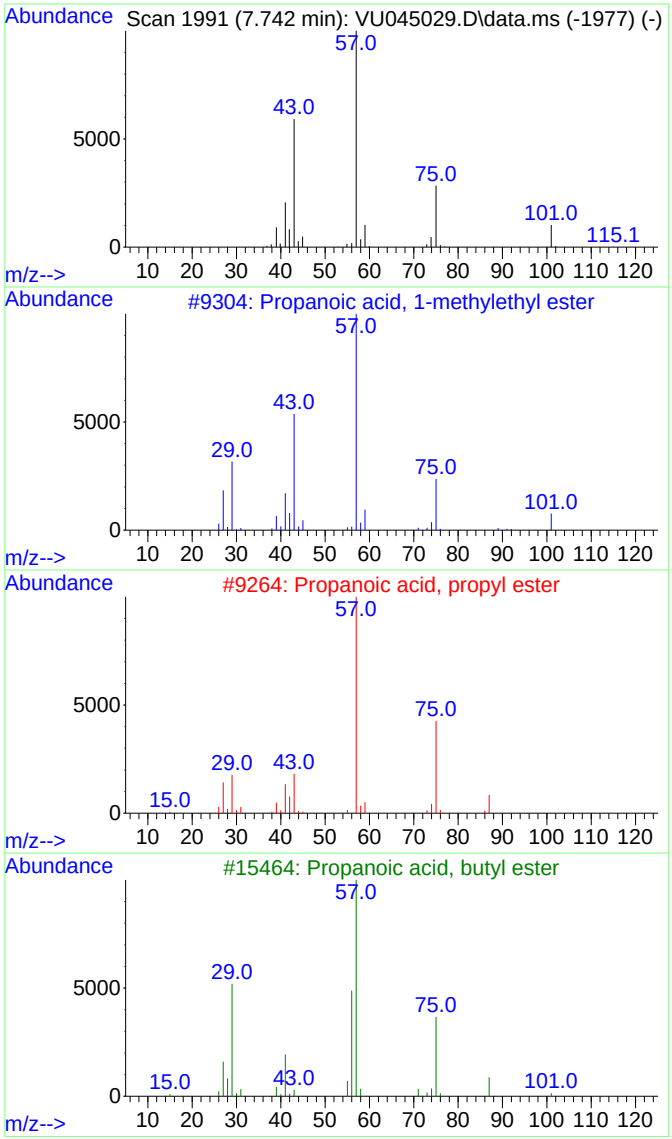
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

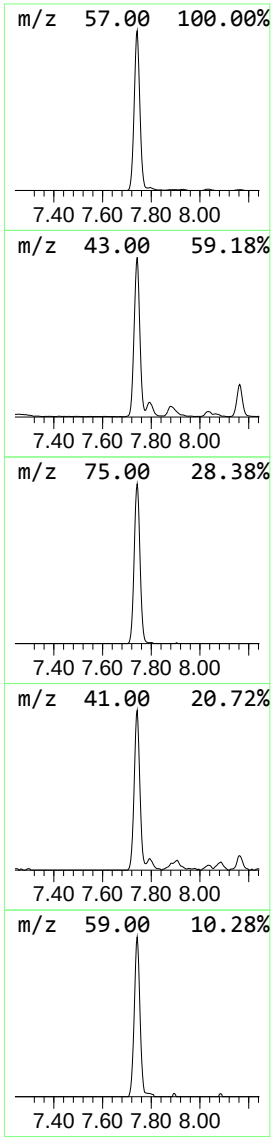
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	18.27 ug/l	356280	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	42
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : VU045029.D
Acq On : 30 Sep 2021 06:12
Operator : SY/MD
Sample : M3971-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

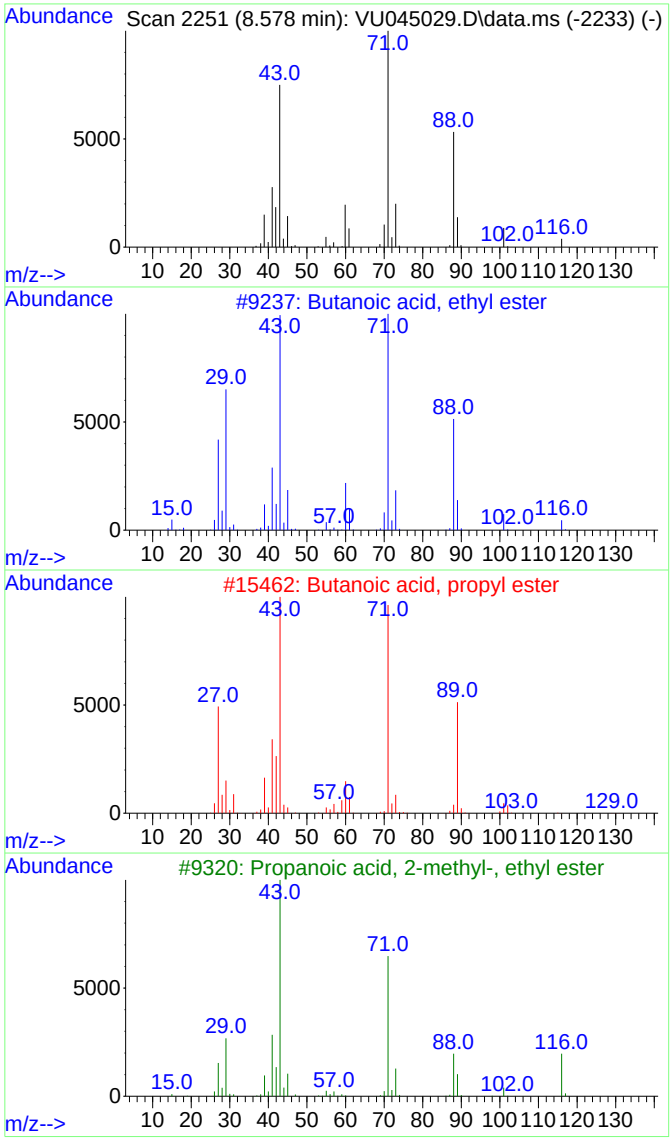
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

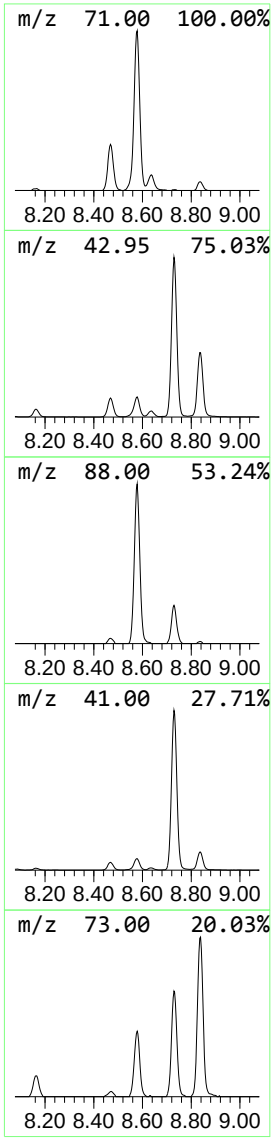
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.578	10.57 ug/l	230835	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	47
3	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4	3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	42
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37





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Data File : VU045029.D
Acq On : 30 Sep 2021 06:12
Operator : SY/MD
Sample : M3971-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

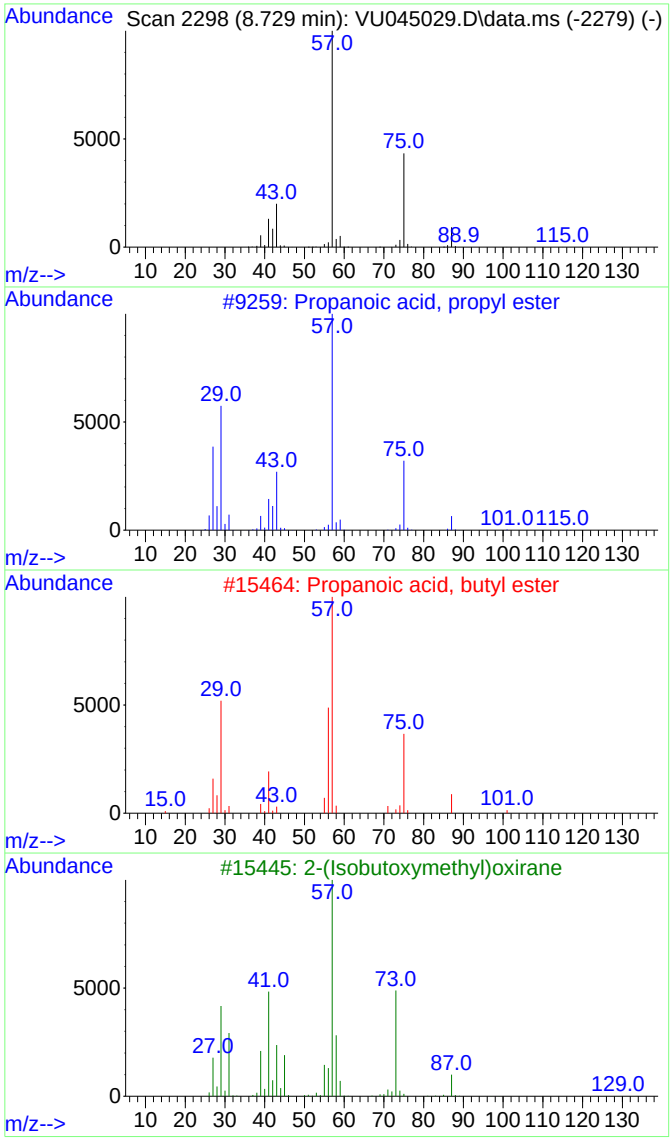
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

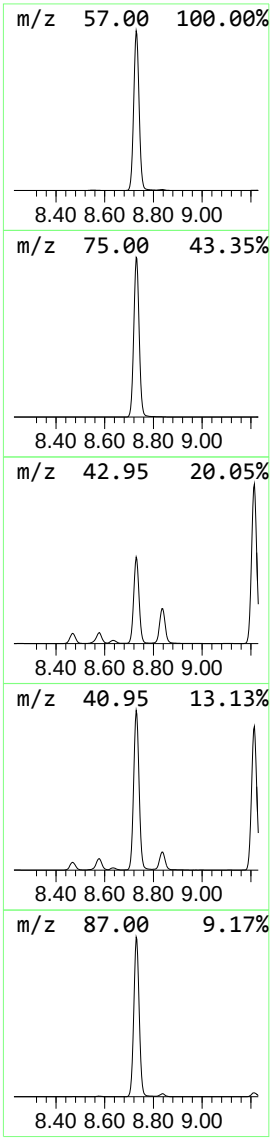
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	154.13 ug/l	3364630	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	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Data File : VU045029.D
Acq On : 30 Sep 2021 06:12
Operator : SY/MD
Sample : M3971-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
RO-COMP-1

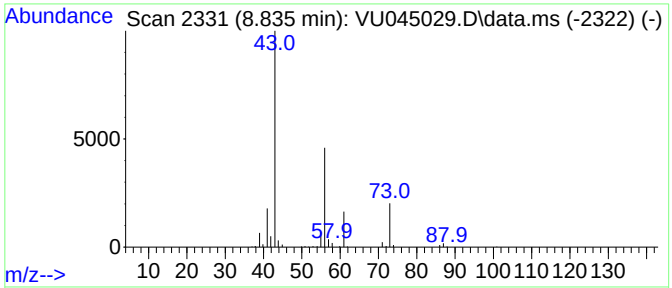
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

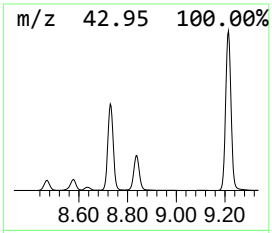
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

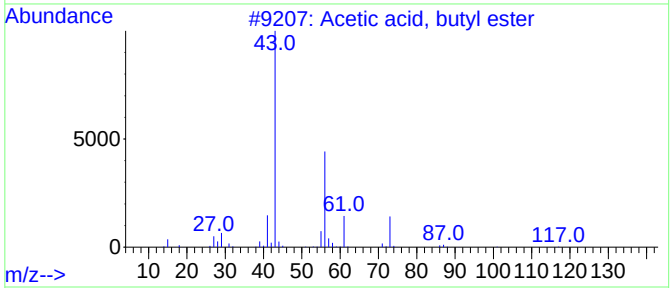
****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

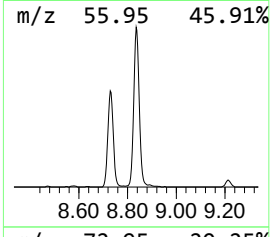
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	14.89 ug/l	325048	Chlorobenzene-d5	9.420

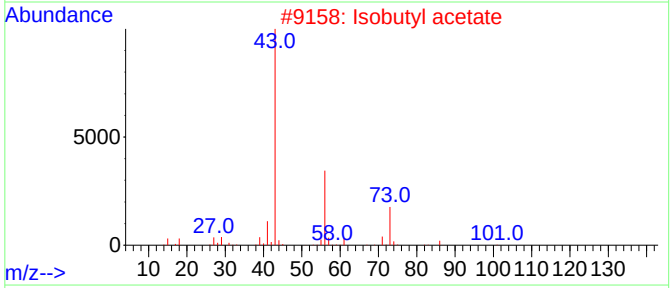
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9

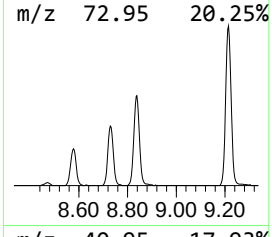


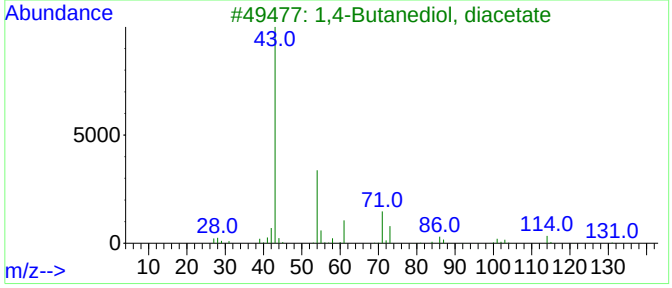


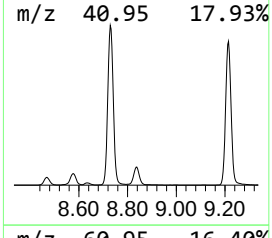


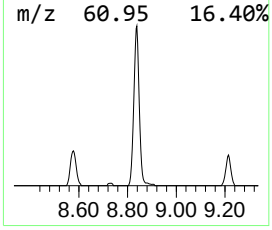












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ClientSampleId : RO-COMP-1

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

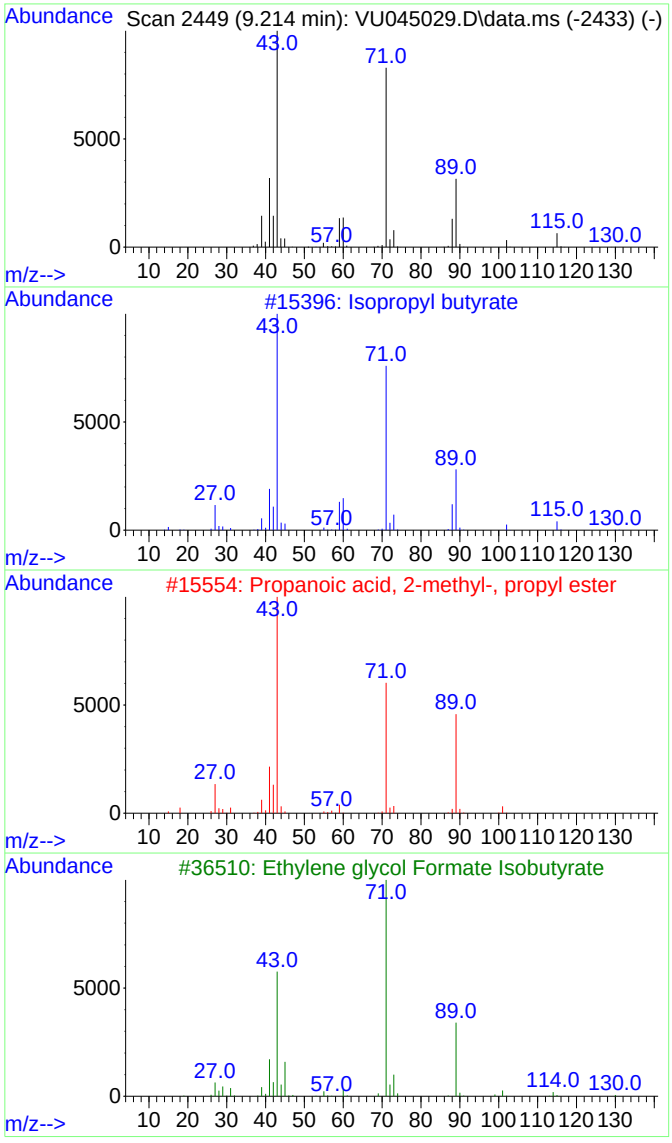
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

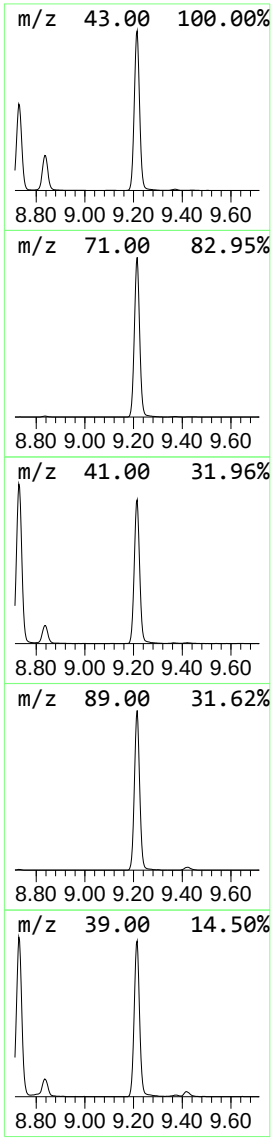
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.214	91.05 ug/l	1987550	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_U
ClientSampleId : RO-COMP-1

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
n-Propyl acetate	7.041	124.9	ug/l	2435720	2	6.253	975107	50.0
Propanoic acid,...	7.742	18.3	ug/l	356280	2	6.253	975107	50.0
Butanoic acid, ...	8.578	10.6	ug/l	230835	3	9.420	1091520	50.0
Propanoic acid,...	8.729	154.1	ug/l	3364630	3	9.420	1091520	50.0
Acetic acid, bu...	8.835	14.9	ug/l	325048	3	9.420	1091520	50.0
Isopropyl butyrate	9.214	91.0	ug/l	1987550	3	9.420	1091520	50.0