LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100219\
Data File : VU034894.D
Acq On : 01 Oct 2019 17:46
Operator : JC/SP
Sample : K5028-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SOMULM100119WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.177	22	27	39	rBV2	8040	13885	0.57%	0.082%
2	1.396	87	95	109	rBV	165373	172908	7.04%	1.019%
3	1.466	112	117	126	rVV	20777	22051	0.90%	0.130%
4	1.672	174	181	198	rVB	138558	171737	6.99%	1.012%
5	2.257	354	363	373	rBV	266166	398785	16.23%	2.350%
6	2.309	374	379	395	rVB	31543	48752	1.98%	0.287%
7	2.550	452	454	457	rVB2	623	329	0.01%	0.002%
8	2.569	458	460	463	rVB2	830	425	0.02%	0.003%
9	2.608	463	472	475	rBV2	2757	3625	0.15%	0.021%
10	2.685	485	496	516	rVB	79654	145310	5.91%	0.856%
11	2.817	529	537	548	rVB4	3204	6313	0.26%	0.037%
12	2.894	558	561	565	rBV2	462	408	0.02%	0.002%
13	2.942	574	576	578	rVB	375	152	0.01%	0.001%
14	2.971	582	585	587	rBV2	225	146	0.01%	0.001%
15	2.984	587	589	590	rBV2	401	175	0.01%	0.001%
16	3.029	600	603	604	rBV2	249	145	0.01%	0.001%
17	3.055	609	611	613	rVV3	378	186	0.01%	0.001%
18	3.170	635	647	661	rBV5	4864	11755	0.48%	0.069%
19	3.379	706	712	713	rBV3	361	272	0.01%	0.002%
20	3.392	713	716	718	rVV2	443	327	0.01%	0.002%
21	3.405	718	720	723	rVV3	426	317	0.01%	0.002%
22	3.431	726	728	733	rVV3	317	238	0.01%	0.001%
23	3.469	737	740	744	rBV2	205	198	0.01%	0.001%
24	3.508	749	752	757	rBV2	159	149	0.01%	0.001%
25	3.598	778	780	787	rVB3	418	331	0.01%	0.002%
26	3.640	787	793	798	rBV2	650	616	0.03%	0.004%
27	3.685	804	807	810	rVV2	153	137	0.01%	0.001%
28	3.717	815	817	818	rBV	462	207	0.01%	0.001%
29	3.762	828	831	834	rBV2	192	147	0.01%	0.001%
30	3.826	848	851	854	rBV2	313	183	0.01%	0.001%
31	3.842	854	856	861	rVB2	199	149	0.01%	0.001%
32	3.874	861	866	869	rBV2	206	230	0.01%	0.001%
33	3.984	891	900	901	rBV3	431	477	0.02%	0.003%
34	4.042	915	918	922	rVB3	316	215	0.01%	0.001%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SOMULM100119WMA.M
Title : VOC Analysis

35	4.067	924	926	930	rBV2	471	357	0.01%	0.002%
36	4.151	940	952	975	rBV	138099	374087	15.22%	2.205%
37	4.469	1048	1051	1053	rVB2	483	248	0.01%	0.001%
38	4.505	1059	1062	1067	rBV3	370	403	0.02%	0.002%
39	4.550	1073	1076	1079	rBV	348	254	0.01%	0.001%
40	4.624	1081	1099	1131	rBV2	227300	549968	22.38%	3.241%
41	4.965	1200	1205	1207	rBV4	602	470	0.02%	0.003%
42	4.974	1207	1208	1213	rVB3	830	472	0.02%	0.003%
43	5.000	1213	1216	1220	rBV3	319	227	0.01%	0.001%
44	5.042	1224	1229	1235	rBV3	410	478	0.02%	0.003%
45	5.071	1235	1238	1243	rVB2	548	368	0.01%	0.002%
46	5.231	1283	1288	1291	rBV2	547	359	0.01%	0.002%
47	5.318	1291	1315	1342	rBV2	464332	1406502	57.24%	8.289%
48	5.530	1370	1381	1405	rVB	61121	131227	5.34%	0.773%
49	5.865	1466	1485	1503	rBV	463296	1018079	41.43%	6.000%
50	6.308	1610	1623	1645	rVB	331651	666121	27.11%	3.926%
51	6.563	1696	1702	1704	rBV2	8348	10181	0.41%	0.060%
52	6.685	1727	1740	1779	rBV	1333327	2457265	100.00%	14.482%
53	7.206	1891	1902	1922	rBV	182394	334638	13.62%	1.972%
54	7.398	1951	1962	1988	rBV	170218	308055	12.54%	1.816%
55	7.543	1994	2007	2045	rBV	633060	1162015	47.29%	6.849%
56	7.829	2085	2096	2124	rBV	164919	311508	12.68%	1.836%
57	8.135	2178	2191	2206	rBV	319365	530471	21.59%	3.126%
58	8.289	2230	2239	2262	rBV	531615	943301	38.39%	5.560%
59	8.395	2262	2272	2299	rVV	476954	790152	32.16%	4.657%
60	8.511	2302	2308	2319	rVB2	20967	34414	1.40%	0.203%
61	8.778	2389	2391	2394	rVB2	589	254	0.01%	0.001%
62	8.794	2394	2396	2400	rBV3	471	394	0.02%	0.002%
63	8.884	2411	2424	2460	rBV	648581	1050440	42.75%	6.191%
64	9.067	2464	2481	2510	rVV	656102	1123459	45.72%	6.621%
65	9.308	2553	2556	2557	rBV3	834	441	0.02%	0.003%
66	9.543	2626	2629	2635	rBV5	666	646	0.03%	0.004%
67	9.588	2635	2643	2661	rBV3	12093	24594	1.00%	0.145%
68	9.749	2681	2693	2717	rBV	67325	121688	4.95%	0.717%
69	9.922	2740	2747	2750	rBV6	1964	2693	0.11%	0.016%
70	10.177	2823	2826	2828	rBV	281	198	0.01%	0.001%
71	10.244	2845	2847	2849	rBV3	455	286	0.01%	0.002%

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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId : BFDN0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Title : VOC Analysis

72	10.295	2859	2863	2864	rBV2	460	363	0.01%	0.002%
73	10.408	2886	2898	2919	rBV	444240	719693	29.29%	4.242%
74	10.578	2949	2951	2953	rBV2	524	282	0.01%	0.002%
75	10.697	2985	2988	2990	rBV2	410	293	0.01%	0.002%
76	10.739	2997	3001	3003	rBV3	1023	828	0.03%	0.005%
77	11.135	3117	3124	3131	rBV7	1427	2015	0.08%	0.012%
78	11.199	3141	3144	3145	rBV	454	262	0.01%	0.002%
79	11.363	3192	3195	3199	rVB2	763	484	0.02%	0.003%
80	11.459	3213	3225	3248	rBV	561541	931046	37.89%	5.487%
81	11.720	3303	3306	3309	rBV3	712	542	0.02%	0.003%
82	11.836	3329	3342	3368	rBV	554617	941887	38.33%	5.551%
83	12.183	3449	3450	3453	rBV	482	229	0.01%	0.001%
84	12.215	3457	3460	3463	rBV3	551	301	0.01%	0.002%
85	12.234	3463	3466	3467	rBV2	669	352	0.01%	0.002%
86	12.283	3478	3481	3486	rBV2	474	364	0.01%	0.002%
87	12.311	3488	3490	3493	rBV4	521	340	0.01%	0.002%
88	12.450	3531	3533	3536	rBV	455	227	0.01%	0.001%
89	12.482	3539	3543	3548	rBV6	507	532	0.02%	0.003%
90	12.501	3548	3549	3554	rVB4	457	160	0.01%	0.001%
91	12.572	3569	3571	3573	rBV	399	190	0.01%	0.001%
92	12.758	3623	3629	3632	rBV4	691	906	0.04%	0.005%
93	13.041	3713	3717	3720	rBV3	612	617	0.03%	0.004%
94	13.061	3721	3723	3726	rVB2	558	299	0.01%	0.002%
95	13.183	3757	3761	3764	rBV3	726	656	0.03%	0.004%
96	13.250	3780	3782	3787	rBV3	449	465	0.02%	0.003%
97	13.356	3813	3815	3817	rBV2	513	267	0.01%	0.002%
98	13.659	3905	3909	3914	rBV5	782	978	0.04%	0.006%
99	13.749	3931	3937	3941	rBV5	3090	4156	0.17%	0.024%
100	14.305	4107	4110	4115	rBV4	801	638	0.03%	0.004%

Sum of corrected areas: 16967365

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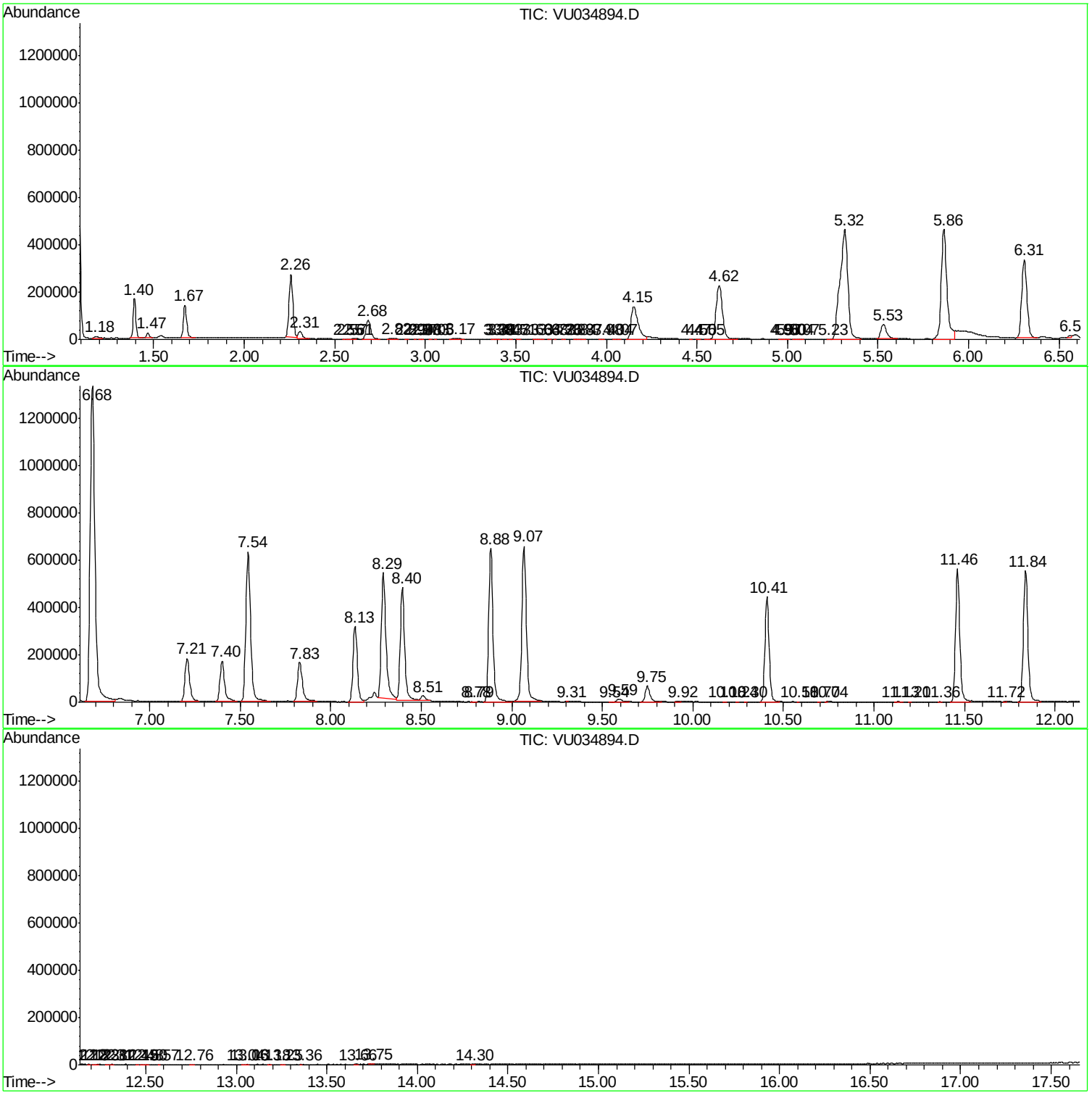
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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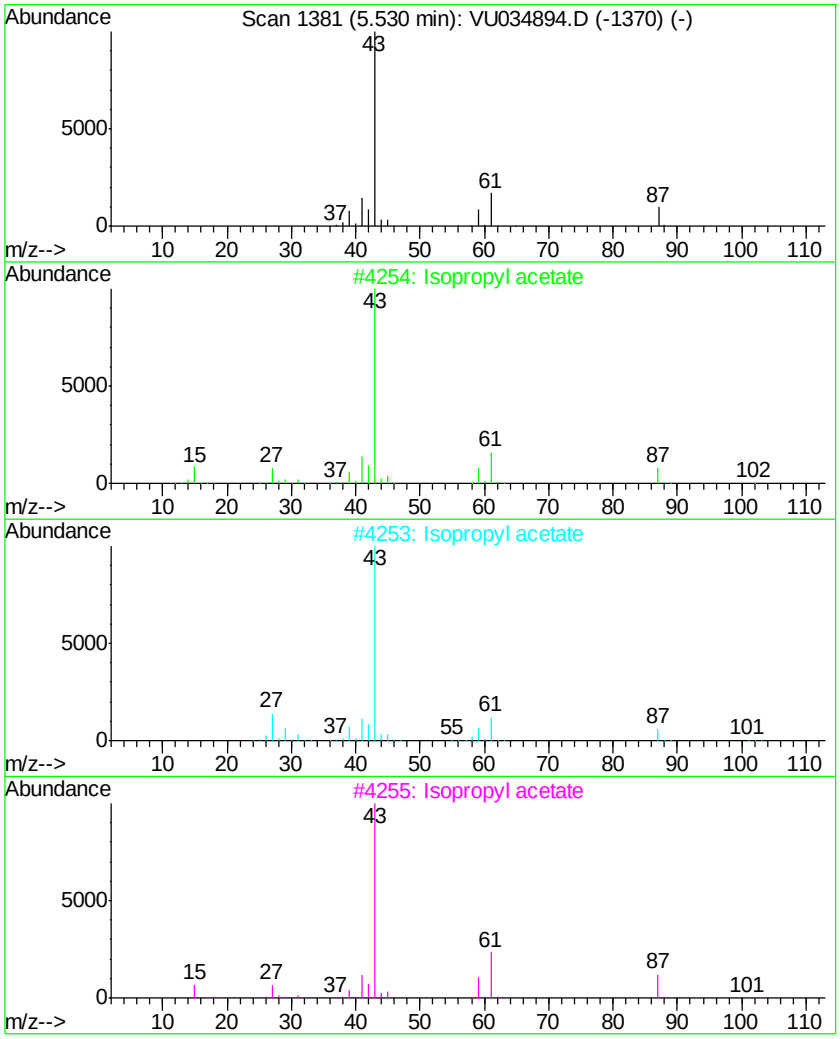
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

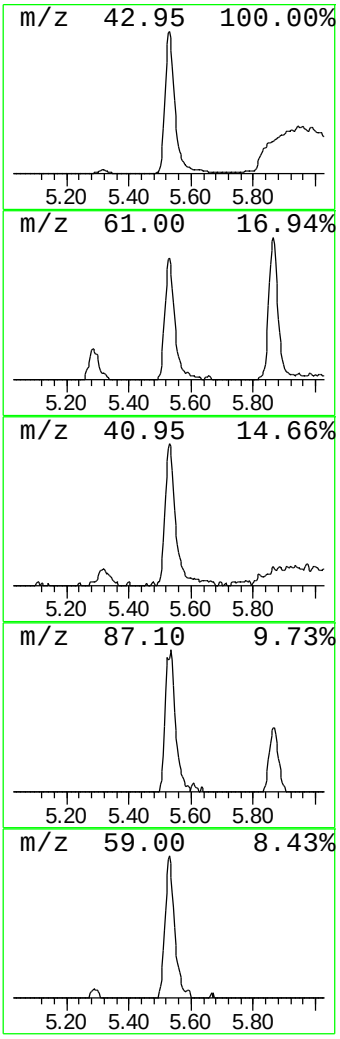
****

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	6.44 ug/L	131227	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate	102	C5H10O2	000108-21-4	72
2	Isopropyl acetate	102	C5H10O2	000108-21-4	72
3	Isopropyl acetate	102	C5H10O2	000108-21-4	64
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
5	1,1-Ethanediol, diacetate	146	C6H10O4	000542-10-9	9





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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

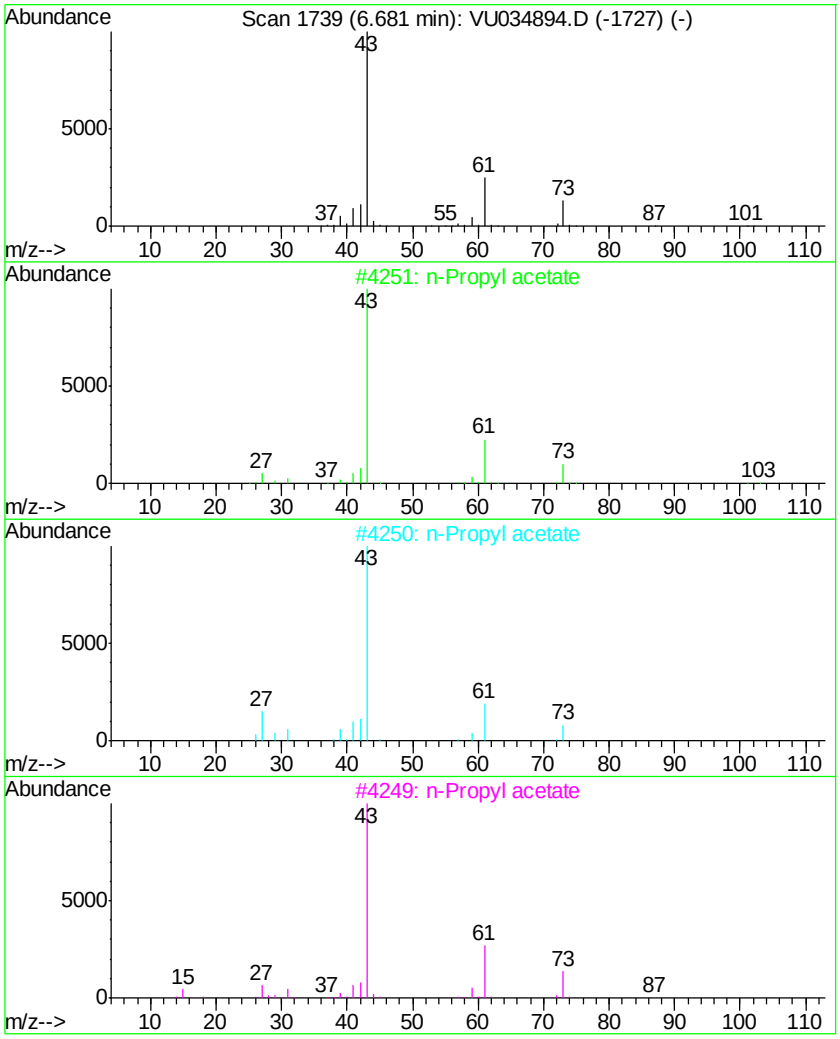
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

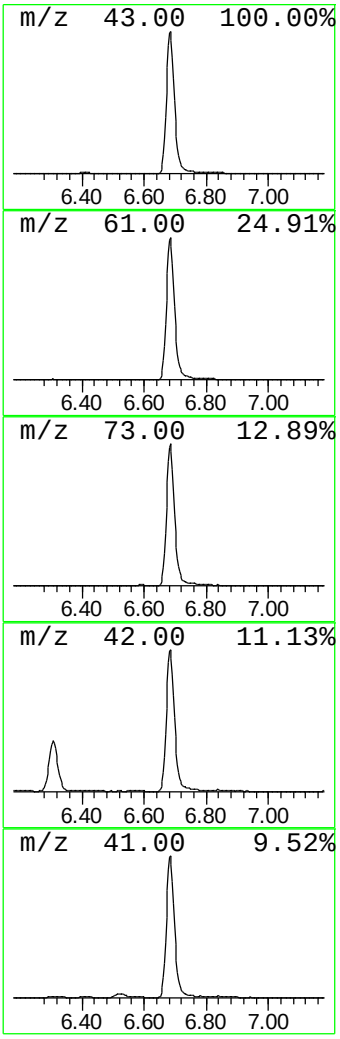
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	120.68 ug/L	2457270	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	n-Propyl acetate	102	C5H10O2	000109-60-4	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





Library Search Compound Report

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ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

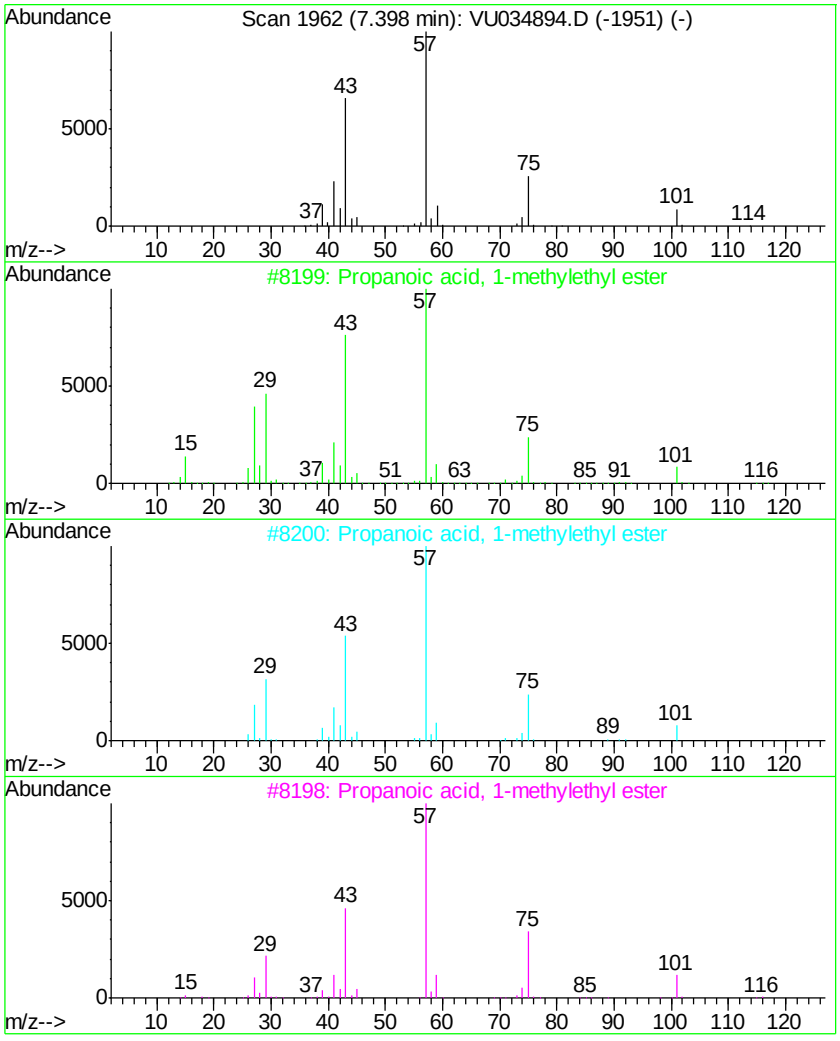
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

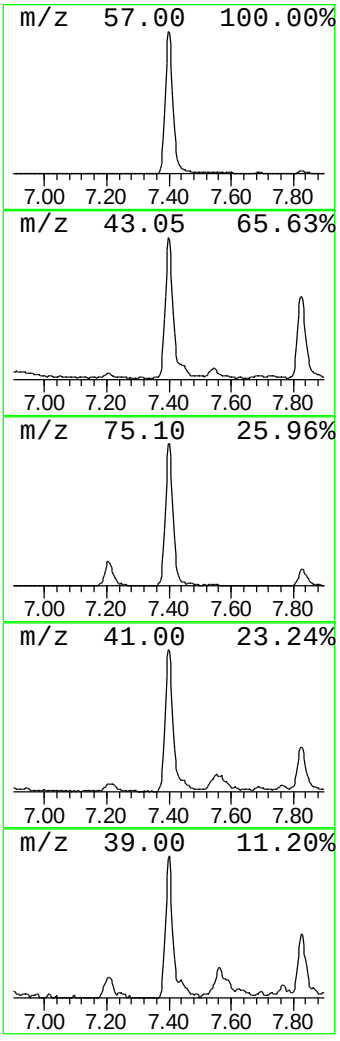
****

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	15.13 ug/L	308055	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42





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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

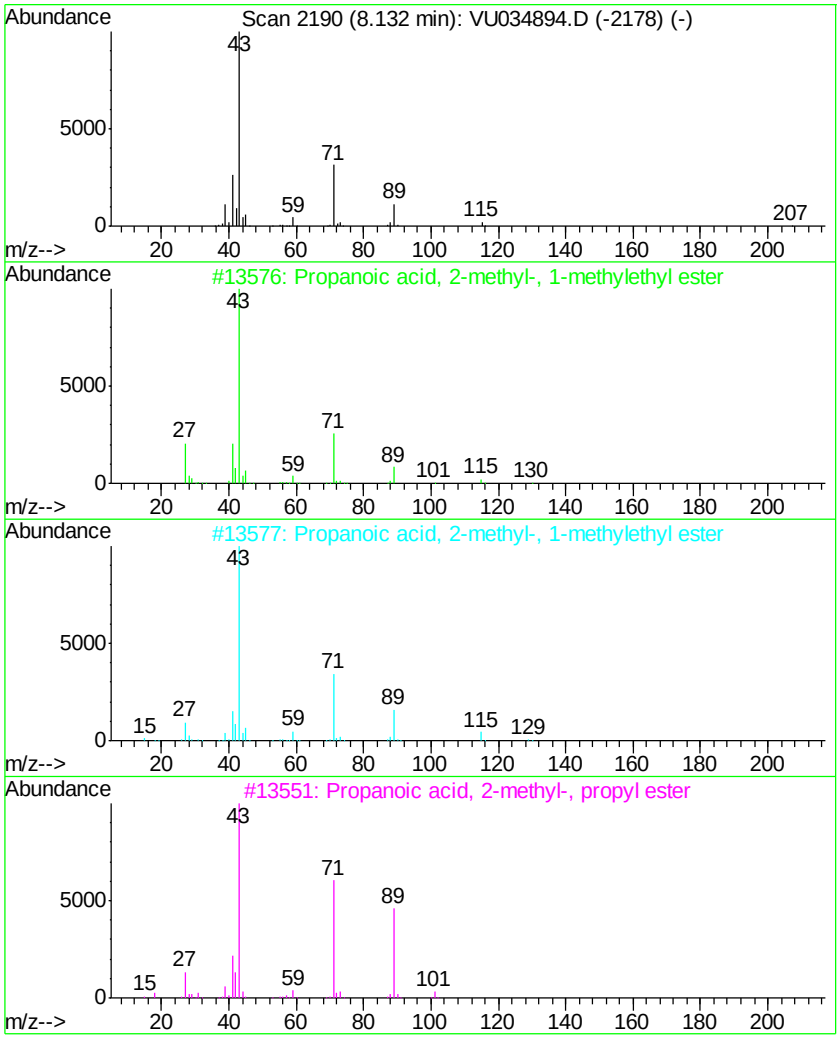
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

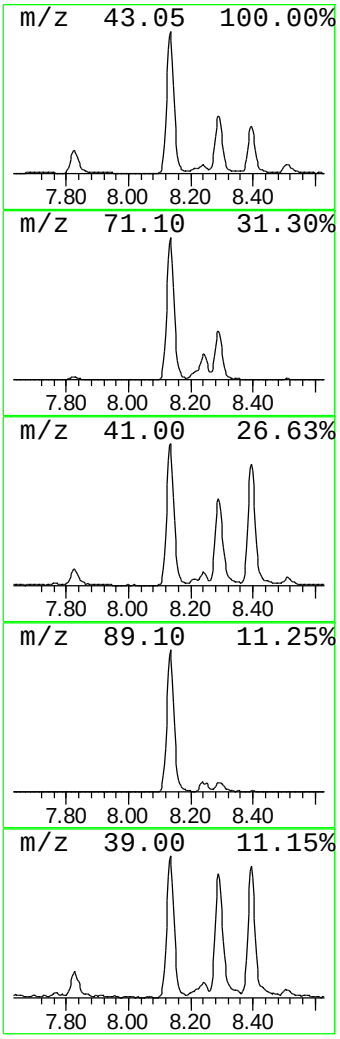
****

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	23.61 ug/L	530471	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53





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Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

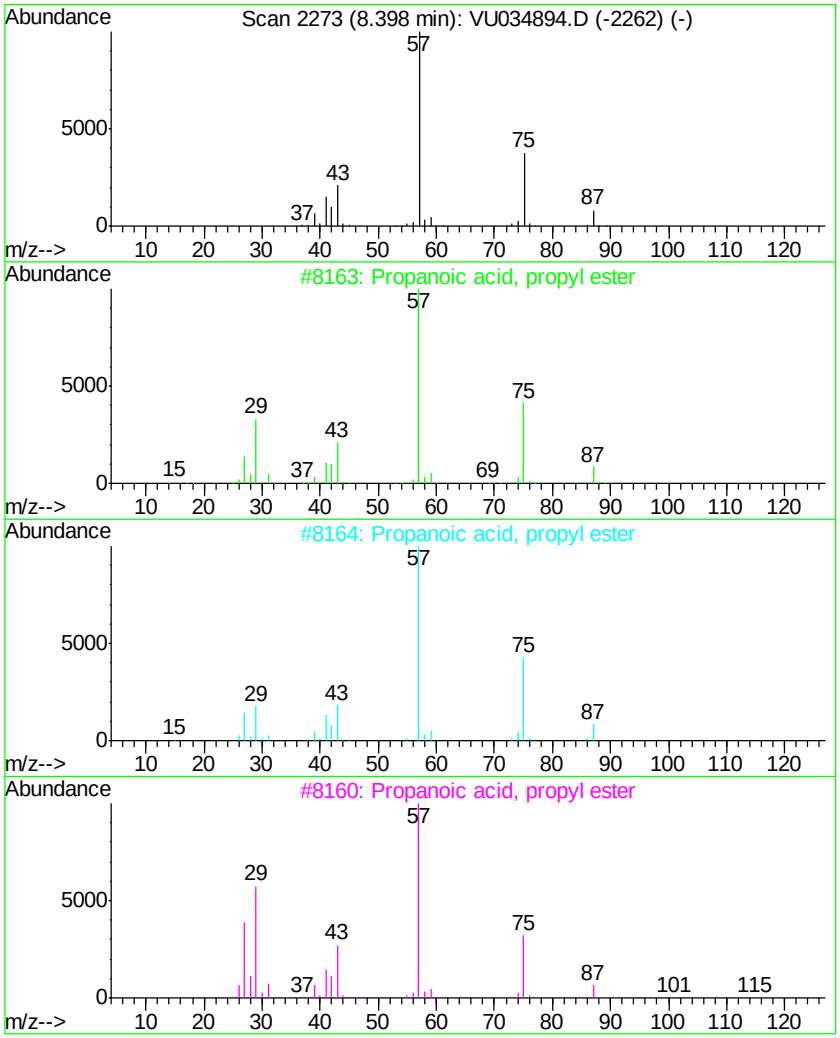
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

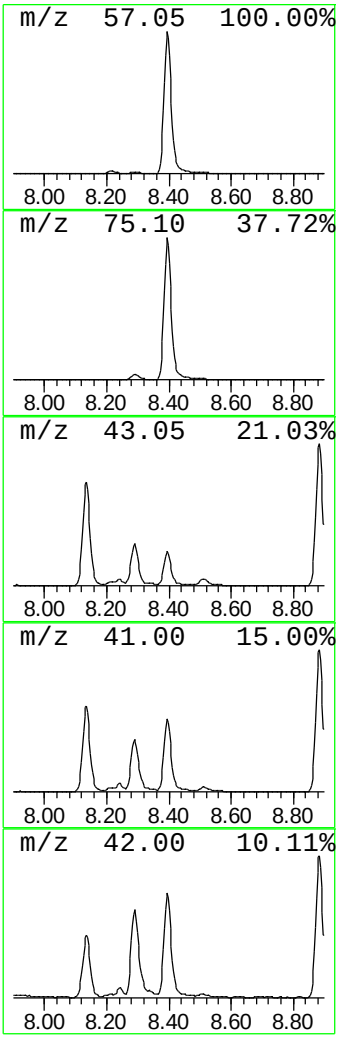
****

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	35.17 ug/L	790152	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36





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Sample : K5028-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

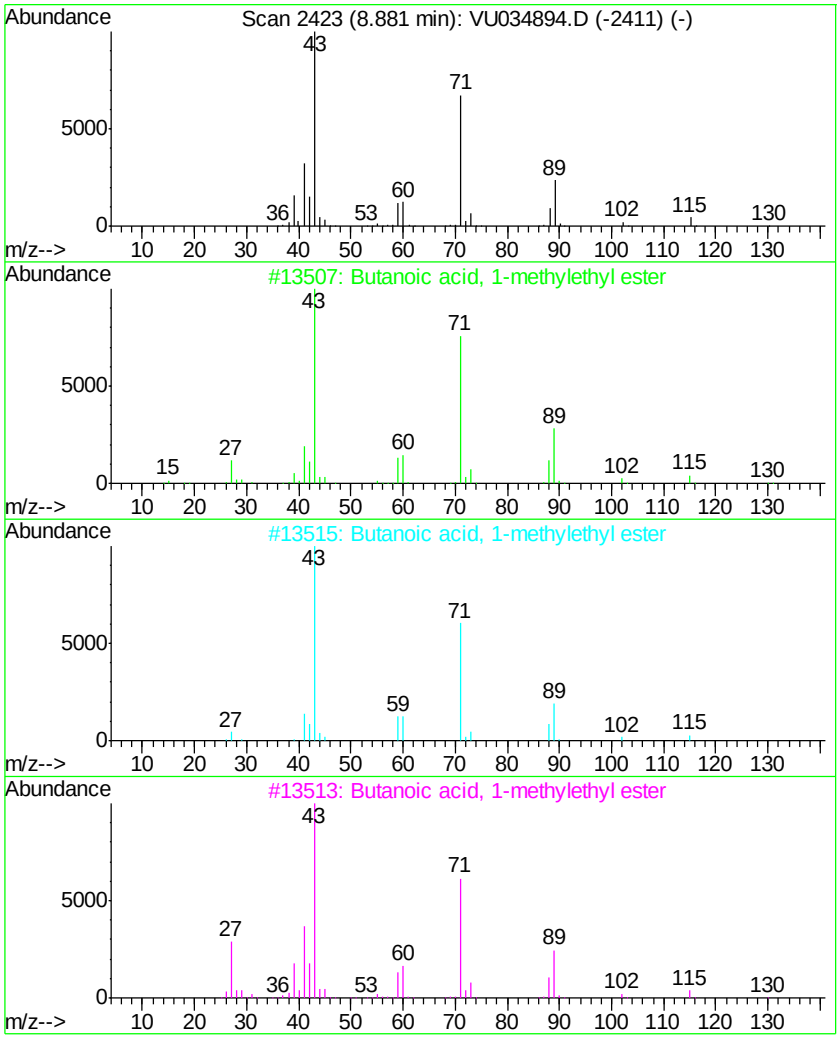
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

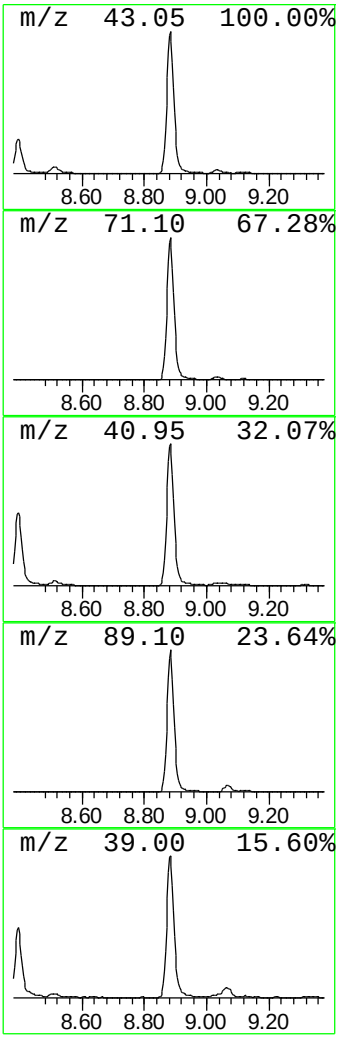
****

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	46.75 ug/L	1050440	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	86
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100219\
Data File : VU034894.D
Acq On : 01 Oct 2019 17:46
Operator : JC/SP
Sample : K5028-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

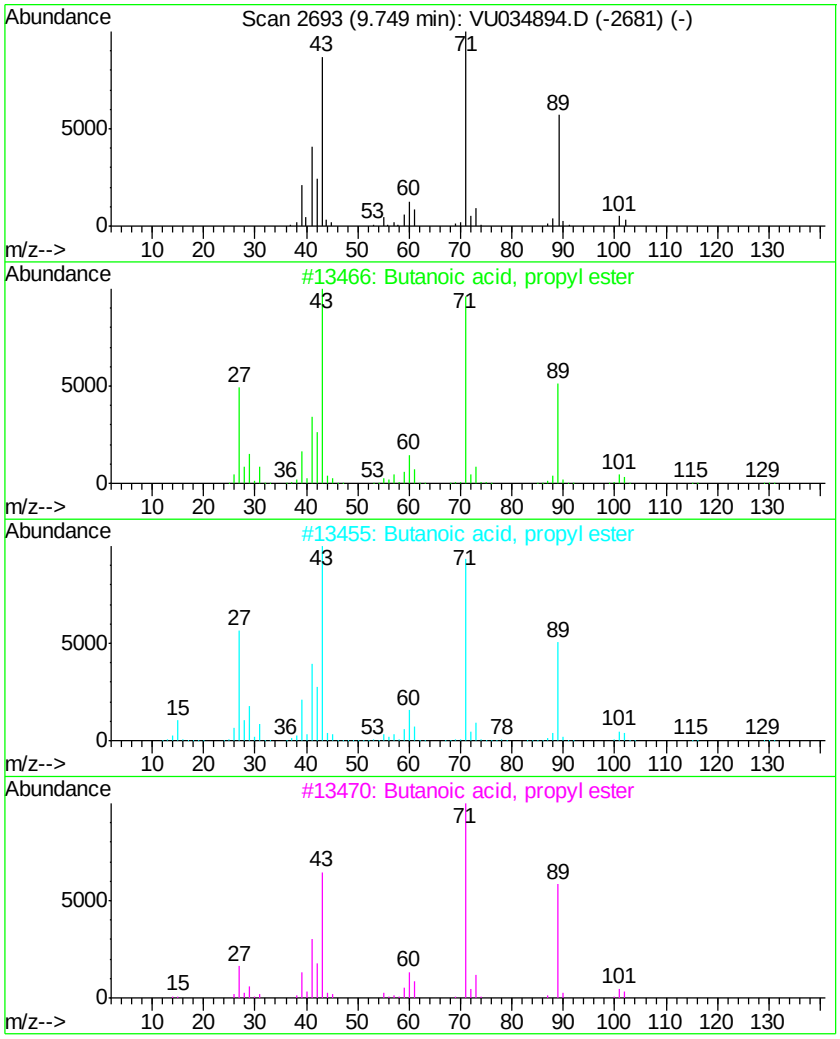
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

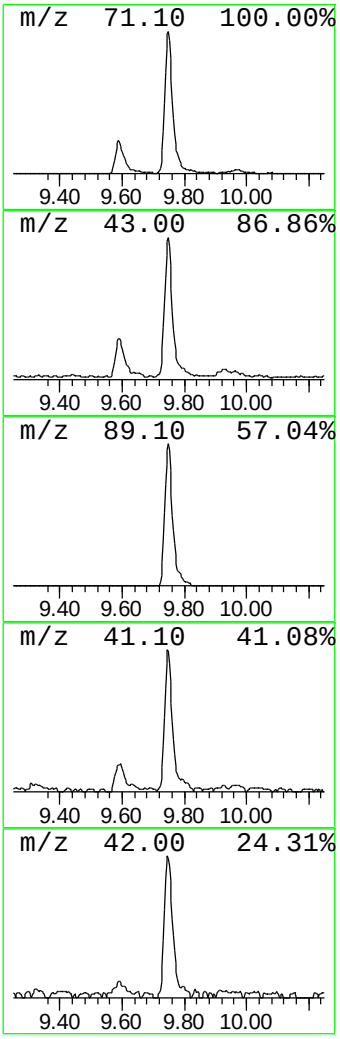
****

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	5.42 ug/L	121688	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100219\
Data File : VU034894.D
Acq On : 01 Oct 2019 17:46
Operator : JC/SP
Sample : K5028-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDN0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl acetate	5.53	6.4	ug/L	131227	1	5.86	1018080	50.0
n-Propyl acetate	6.68	120.7	ug/L	2457270	1	5.86	1018080	50.0
Propanoic acid, 1...	7.40	15.1	ug/L	308055	1	5.86	1018080	50.0
Propanoic acid, 2...	8.13	23.6	ug/L	530471	2	9.07	1123460	50.0
Propanoic acid, p...	8.40	35.2	ug/L	790152	2	9.07	1123460	50.0
Butanoic acid, 1-...	8.88	46.8	ug/L	1050440	2	9.07	1123460	50.0
Butanoic acid, pr...	9.75	5.4	ug/L	121688	2	9.07	1123460	50.0