LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100219\
Data File : VU034907.D
Acq On : 01 Oct 2019 22:51
Operator : JC/SP
Sample : K5028-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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	23	27	33	rBV	8134	6941	0.48%	0.042%
2	1.392	87	94	105	rVB	157813	162802	11.30%	0.985%
3	1.466	111	117	127	rVB	54701	57623	4.00%	0.349%
4	1.672	173	181	195	rVB	135927	171968	11.94%	1.040%
5	2.257	353	363	372	rBV	260142	394778	27.41%	2.389%
6	2.306	372	378	400	rVB	75868	123658	8.59%	0.748%
7	2.611	465	473	482	rBV	2706	4311	0.30%	0.026%
8	2.685	483	496	524	rBV	599517	1085684	75.38%	6.569%
9	3.055	607	611	614	rVB2	399	299	0.02%	0.002%
10	3.100	623	625	627	rVB	473	210	0.01%	0.001%
11	3.122	631	632	633	rBV	368	130	0.01%	0.001%
12	3.170	634	647	664	rVV3	8658	19727	1.37%	0.119%
13	3.341	697	700	703	rBV3	225	177	0.01%	0.001%
14	3.405	711	720	723	rBV5	1005	1281	0.09%	0.008%
15	3.463	736	738	743	rBV2	532	456	0.03%	0.003%
16	3.543	753	763	765	rBV3	1426	1793	0.12%	0.011%
17	3.614	776	785	795	rBV6	2483	6014	0.42%	0.036%
18	3.762	829	831	835	rVB3	564	341	0.02%	0.002%
19	3.785	835	838	841	rBV2	531	384	0.03%	0.002%
20	3.801	841	843	845	rVV2	317	177	0.01%	0.001%
21	3.826	849	851	854	rVB2	344	232	0.02%	0.001%
22	3.849	854	858	861	rVB	313	286	0.02%	0.002%
23	3.904	873	875	879	rBV	429	304	0.02%	0.002%
24	3.926	879	882	885	rBV3	261	220	0.02%	0.001%
25	3.942	885	887	889	rBV2	311	222	0.02%	0.001%
26	3.984	897	900	903	rBV3	352	261	0.02%	0.002%
27	4.022	910	912	914	rBV	321	145	0.01%	0.001%
28	4.042	916	918	920	rVB2	324	141	0.01%	0.001%
29	4.080	925	930	932	rBV3	428	359	0.02%	0.002%
30	4.100	932	936	937	rBV	410	346	0.02%	0.002%
31	4.151	940	952	975	rBV	156884	422141	29.31%	2.554%
32	4.508	1061	1063	1065	rBV	446	217	0.02%	0.001%
33	4.624	1082	1099	1125	rBV	232300	553712	38.44%	3.350%
34	4.810	1155	1157	1158	rBV	422	202	0.01%	0.001%

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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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	4.961	1199	1204	1207	rBV4	805	901	0.06%	0.005%
36	5.035	1221	1227	1230	rVB5	429	415	0.03%	0.003%
37	5.058	1230	1234	1235	rBV3	289	203	0.01%	0.001%
38	5.090	1240	1244	1248	rBV2	297	215	0.01%	0.001%
39	5.132	1254	1257	1262	rVB4	422	288	0.02%	0.002%
40	5.167	1265	1268	1270	rBV	222	132	0.01%	0.001%
41	5.222	1283	1285	1291	rVB2	322	264	0.02%	0.002%
42	5.315	1291	1314	1345	rBV2	464551	1440299	100.00%	8.714%
43	5.530	1370	1381	1404	rBV2	45376	101878	7.07%	0.616%
44	5.675	1423	1426	1428	rVB3	619	323	0.02%	0.002%
45	5.691	1428	1431	1437	rVB6	914	1100	0.08%	0.007%
46	5.720	1437	1440	1441	rBV2	733	428	0.03%	0.003%
47	5.749	1447	1449	1451	rBV3	443	266	0.02%	0.002%
48	5.865	1471	1485	1504	rBV	442616	905686	62.88%	5.480%
49	6.309	1609	1623	1643	rBV	329902	671102	46.59%	4.060%
50	6.685	1728	1740	1779	rBV	672920	1251371	86.88%	7.571%
51	7.206	1890	1902	1922	rBV	176633	326295	22.65%	1.974%
52	7.399	1952	1962	1975	rBV	139262	239950	16.66%	1.452%
53	7.543	1995	2007	2025	rBV	613851	1101062	76.45%	6.662%
54	7.829	2085	2096	2119	rBV2	136883	253028	17.57%	1.531%
55	8.135	2178	2191	2207	rBV	241155	403231	28.00%	2.440%
56	8.215	2208	2216	2217	rBV2	12903	14589	1.01%	0.088%
57	8.289	2230	2239	2262	rBV	588629	1020120	70.83%	6.172%
58	8.395	2263	2272	2296	rVB	331690	540136	37.50%	3.268%
59	8.813	2400	2402	2404	rBV2	402	243	0.02%	0.001%
60	8.884	2412	2424	2457	rBV	457076	750543	52.11%	4.541%
61	9.067	2463	2481	2521	rVB	651483	1135522	78.84%	6.870%
62	9.225	2526	2530	2531	rBV2	1421	977	0.07%	0.006%
63	9.353	2559	2570	2589	rBV	70528	119620	8.31%	0.724%
64	9.588	2633	2643	2663	rBV3	12315	25425	1.77%	0.154%
65	9.701	2675	2678	2682	rVB3	586	428	0.03%	0.003%
66	9.752	2683	2694	2713	rBV3	44820	88460	6.14%	0.535%
67	9.923	2739	2747	2756	rBV6	2703	5913	0.41%	0.036%
68	10.022	2775	2778	2781	rBV2	1096	752	0.05%	0.005%
69	10.144	2807	2816	2828	rVB	13470	23588	1.64%	0.143%
70	10.193	2828	2831	2833	rBV3	507	290	0.02%	0.002%
71	10.257	2848	2851	2855	rVB3	694	444	0.03%	0.003%

LSC Area Percent Report

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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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

72	10.408	2886	2898	2923	rBV	461416	752376	52.24%	4.552%
73	10.569	2938	2948	2956	rBV	9713	16148	1.12%	0.098%
74	10.659	2971	2976	2979	rBV4	1703	1672	0.12%	0.010%
75	10.887	3042	3047	3048	rBV2	544	495	0.03%	0.003%
76	10.948	3057	3066	3076	rBV2	14423	22756	1.58%	0.138%
77	11.128	3113	3122	3139	rVB	24954	37860	2.63%	0.229%
78	11.196	3141	3143	3148	rBV3	570	425	0.03%	0.003%
79	11.299	3172	3175	3183	rVB5	4443	4743	0.33%	0.029%
80	11.459	3213	3225	3244	rBV	568116	958856	66.57%	5.801%
81	11.550	3248	3253	3261	rVB2	14875	20993	1.46%	0.127%
82	11.746	3305	3314	3325	rBV2	30314	49125	3.41%	0.297%
83	11.836	3330	3342	3368	rBV	583328	976404	67.79%	5.907%
84	12.231	3456	3465	3473	rBV2	12728	21549	1.50%	0.130%
85	12.334	3489	3497	3516	rVB5	8769	20570	1.43%	0.124%
86	12.527	3550	3557	3567	rBV7	2611	4426	0.31%	0.027%
87	12.598	3570	3579	3583	rBV5	5009	7829	0.54%	0.047%
88	12.630	3585	3589	3597	rVV2	10195	14012	0.97%	0.085%
89	12.685	3598	3606	3623	rVB3	10672	19440	1.35%	0.118%
90	12.948	3682	3688	3697	rBV5	5059	7113	0.49%	0.043%
91	13.103	3728	3736	3747	rVB4	23479	36972	2.57%	0.224%
92	13.276	3782	3790	3801	rBV4	5278	9953	0.69%	0.060%
93	13.376	3812	3821	3833	rVB7	8937	14567	1.01%	0.088%
94	13.585	3883	3886	3892	rBB5	2469	2347	0.16%	0.014%
95	13.730	3920	3931	3951	rBV2	19133	46083	3.20%	0.279%
96	13.919	3987	3990	3992	rBV2	1732	1218	0.08%	0.007%
97	14.138	4050	4058	4059	rBV7	1889	2168	0.15%	0.013%
98	14.424	4144	4147	4149	rBV3	779	514	0.04%	0.003%
99	14.967	4310	4316	4319	rBV4	1264	1418	0.10%	0.009%
100	15.045	4333	4340	4359	rVB2	17221	33203	2.31%	0.201%

Sum of corrected areas: 16528264

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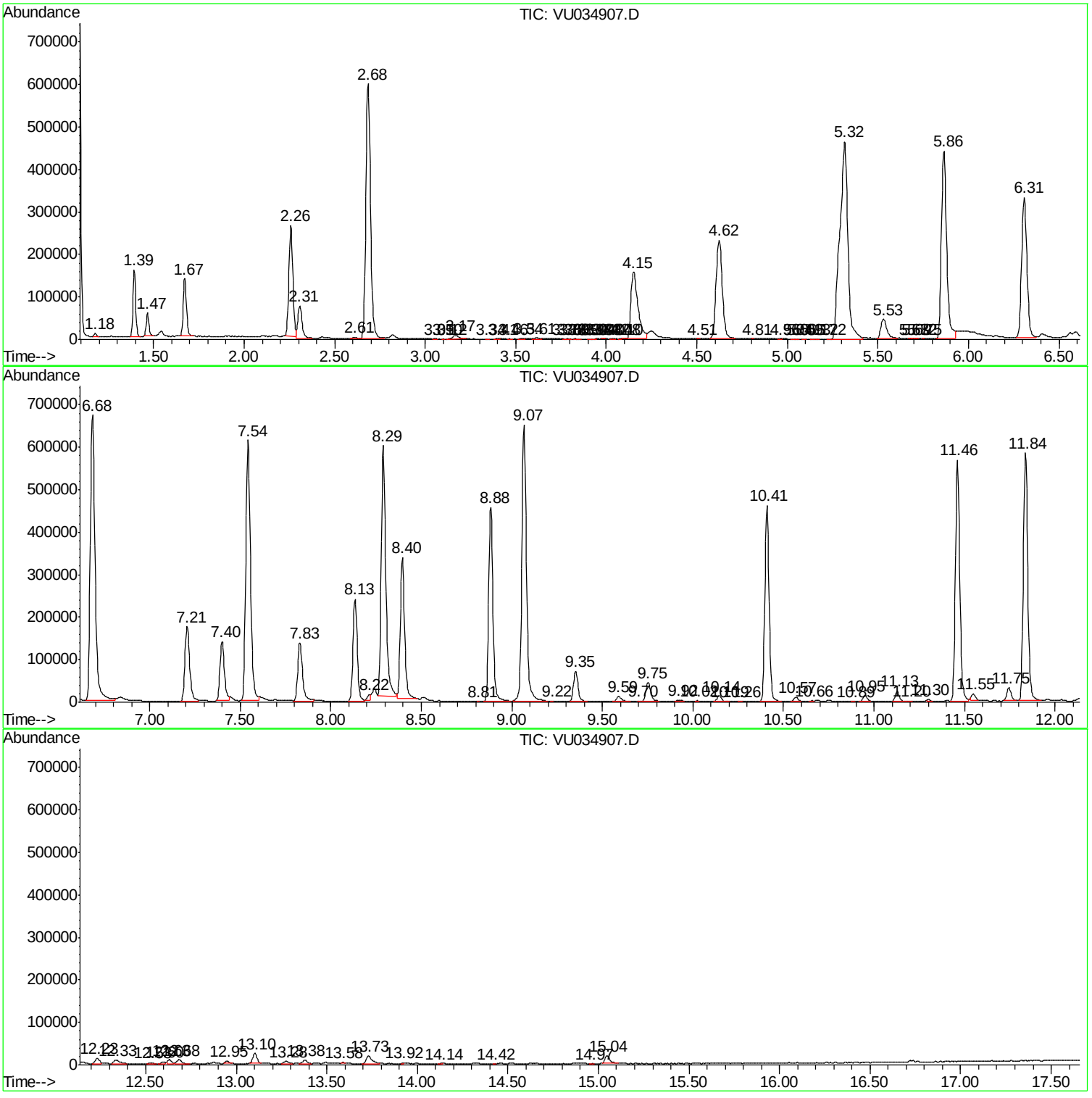
Sample : K5028-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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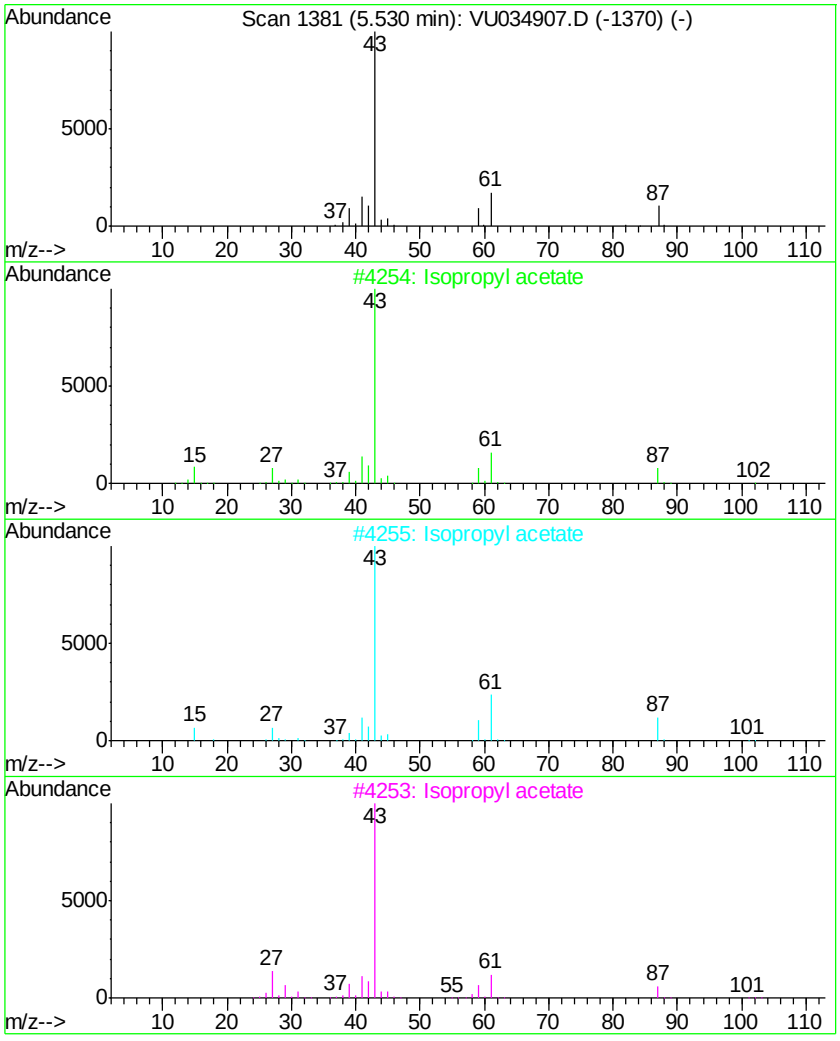
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

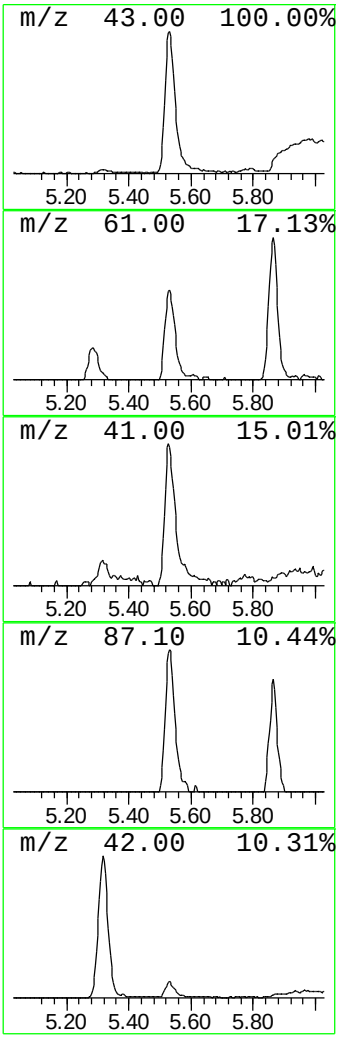
****

Peak Number 2 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	5.62 ug/L	101878	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate	102	C5H10O2	000108-21-4	78
2	Isopropyl acetate	102	C5H10O2	000108-21-4	74
3	Isopropyl acetate	102	C5H10O2	000108-21-4	64
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	1,1-Ethanediol, diacetate	146	C6H10O4	000542-10-9	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100219\
Data File : VU034907.D
Acq On : 01 Oct 2019 22:51
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Sample : K5028-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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

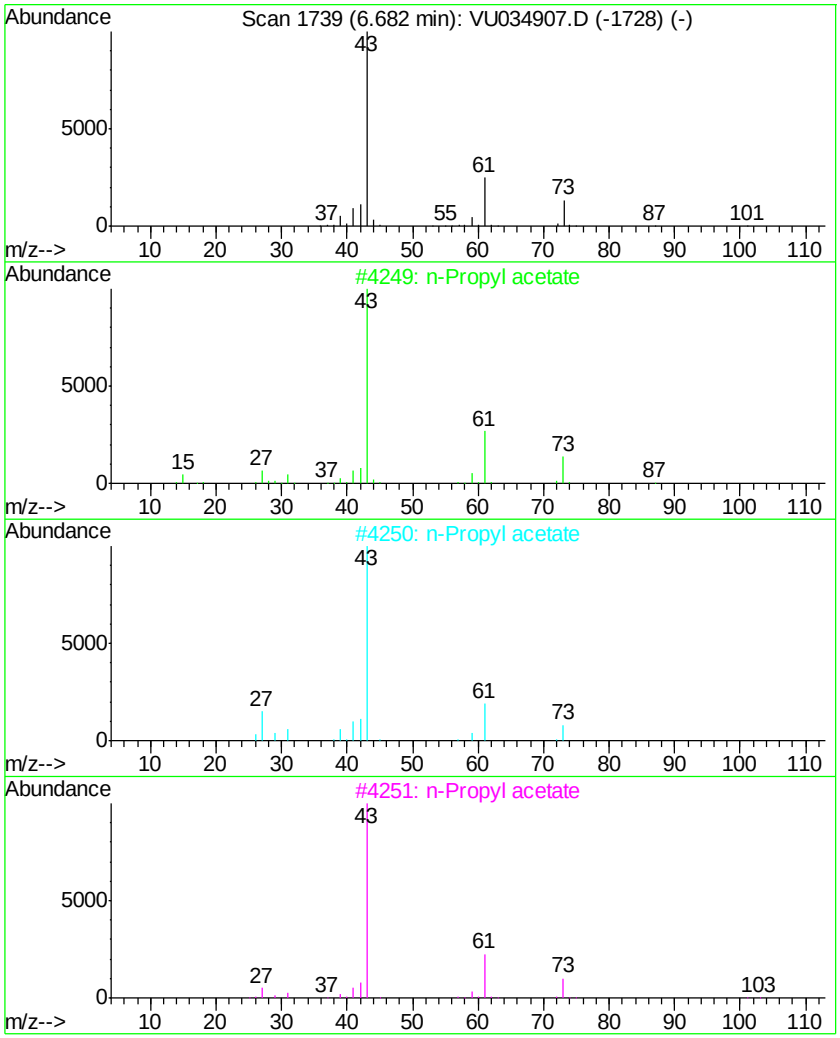
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

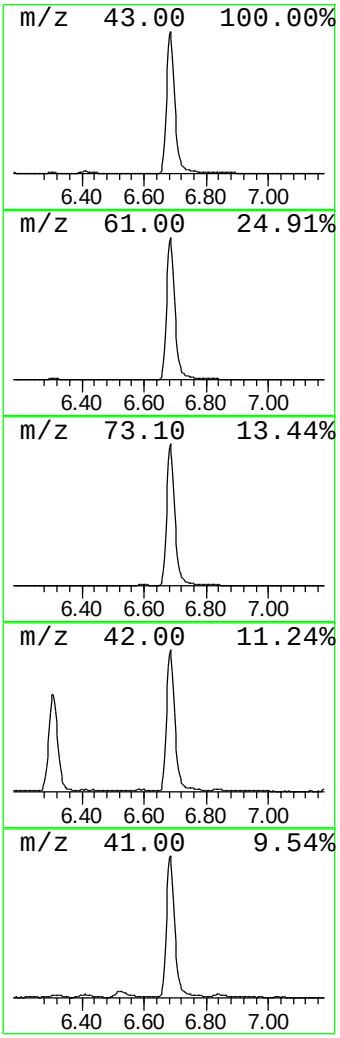
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	69.08 ug/L	1251370	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	38
5	1-Butanamine	73	C4H11N	000109-73-9	7





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ClientSampleId : BFDL7

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

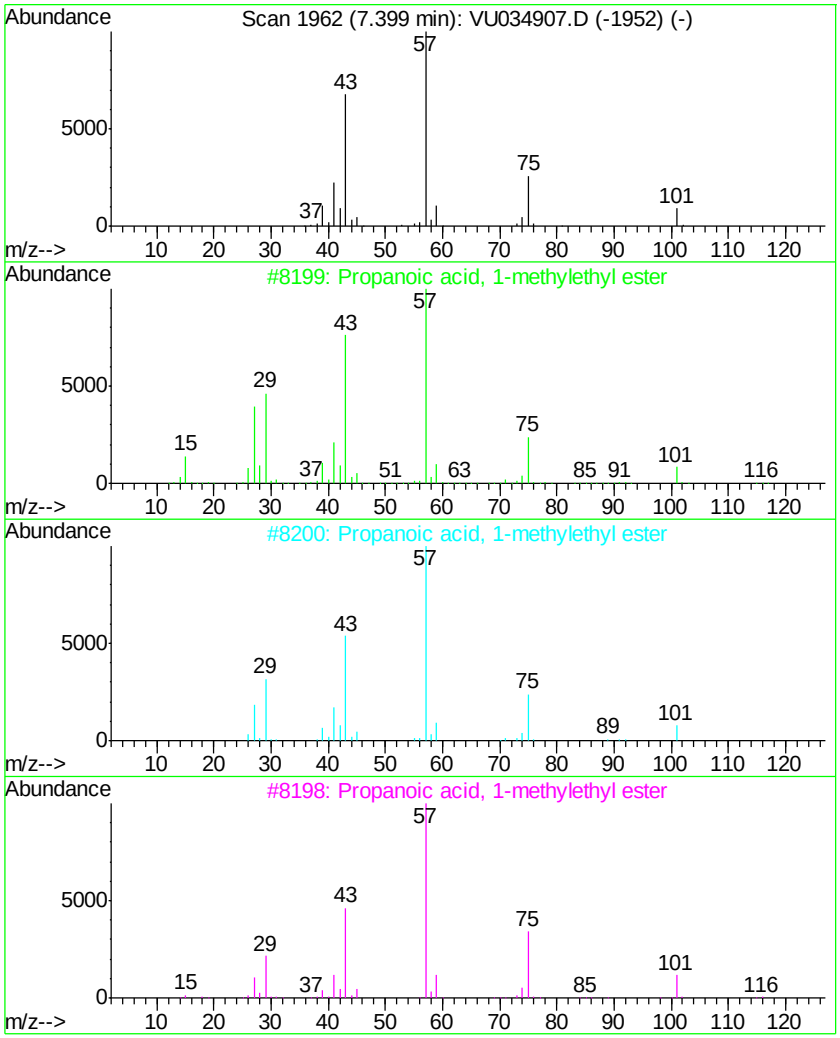
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

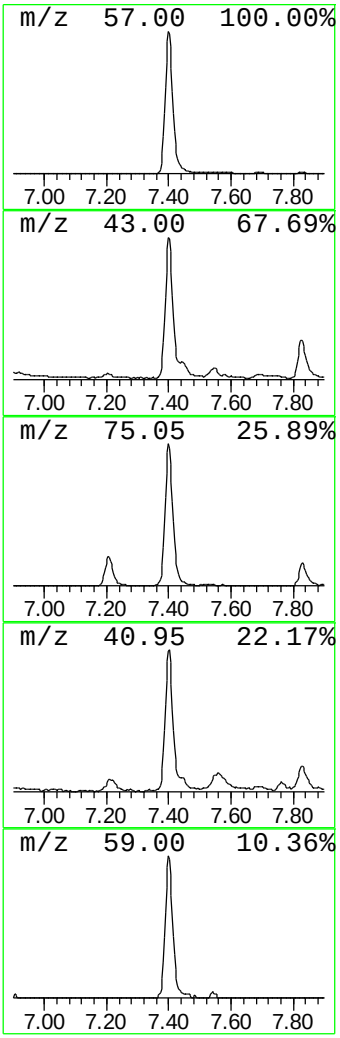
****

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	13.25 ug/L	239950	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	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50





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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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

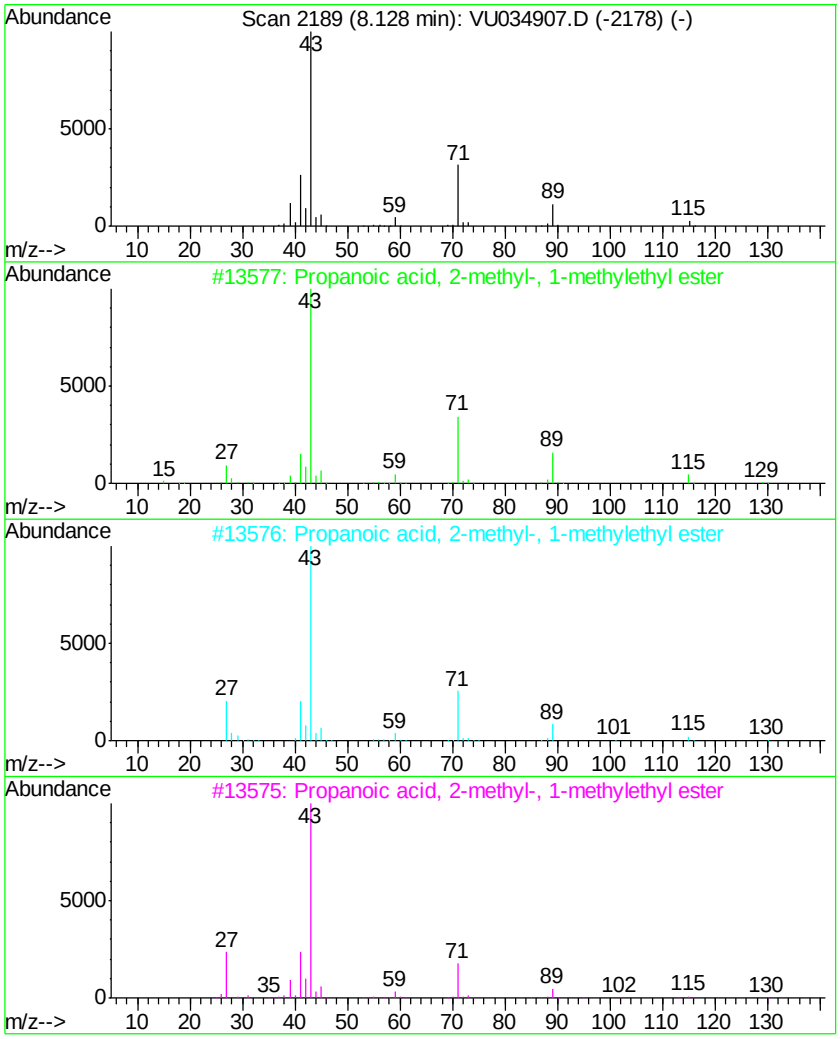
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

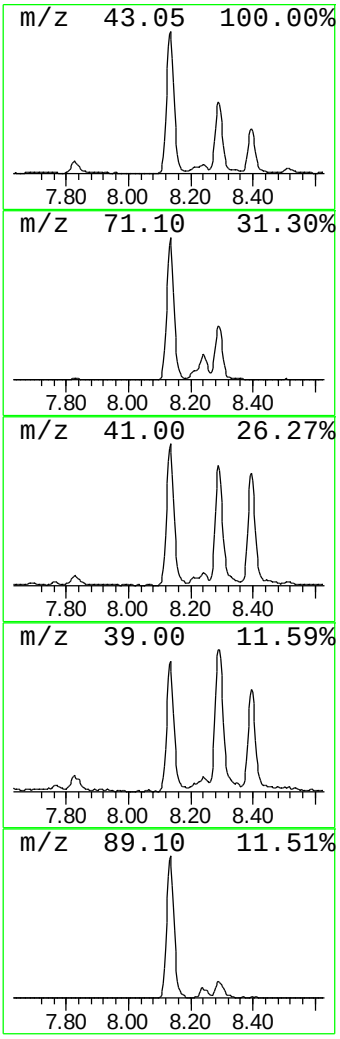
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	17.76 ug/L	403231	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-, 1-met...	130	C7H14O2	000617-50-5	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	42





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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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

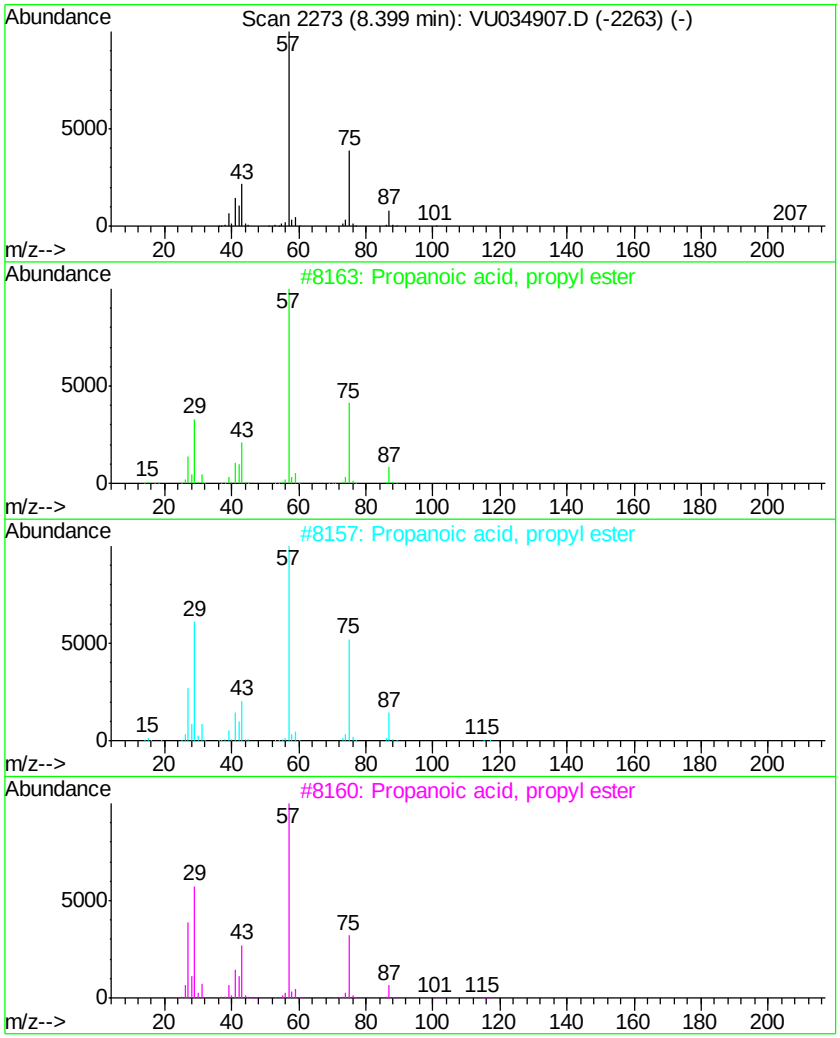
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

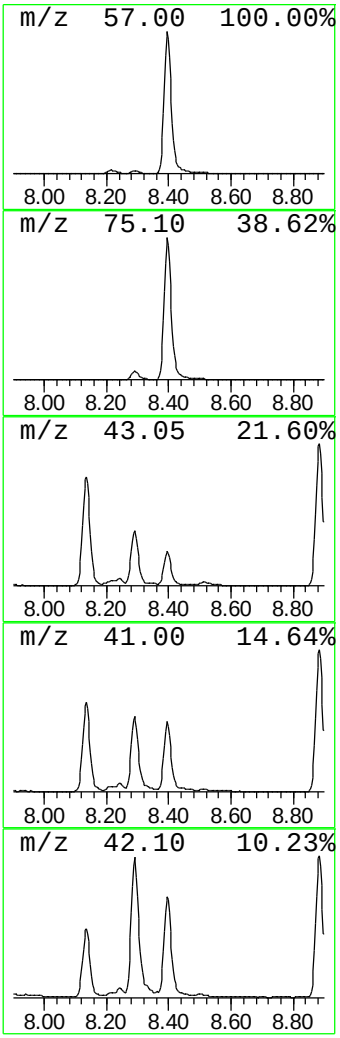
****

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	23.78 ug/L	540136	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	78
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38





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Data File : VU034907.D
Acq On : 01 Oct 2019 22:51
Operator : JC/SP
Sample : K5028-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

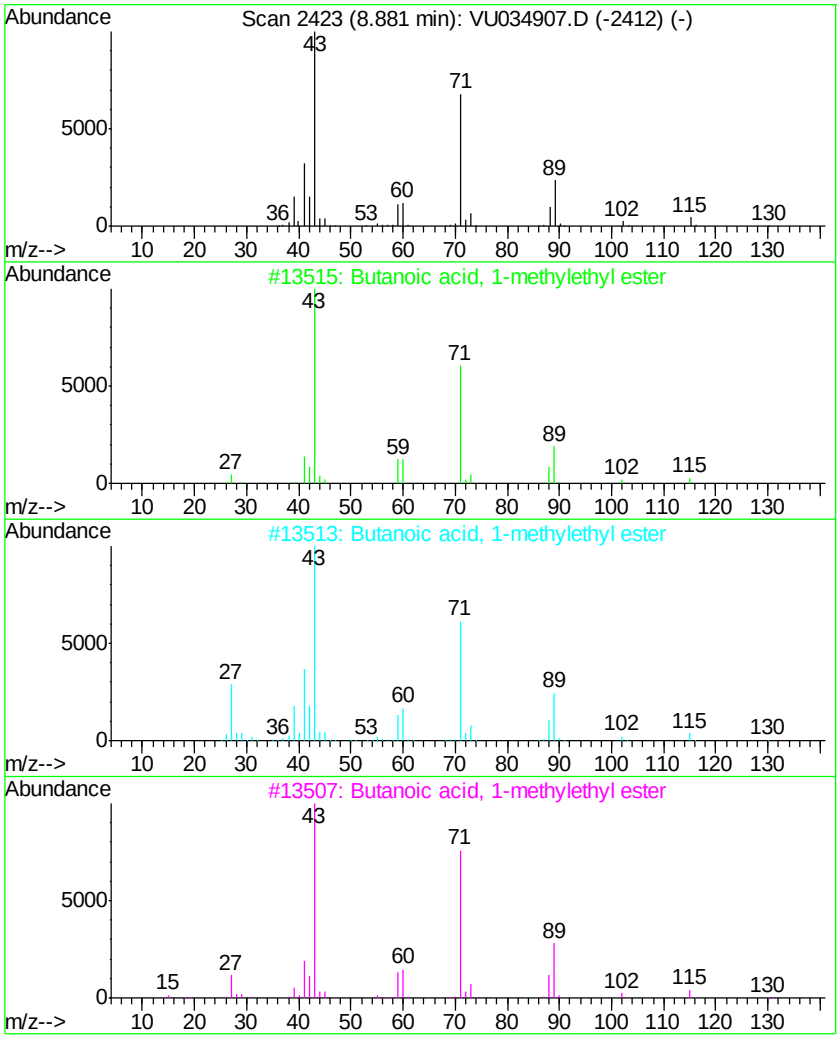
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100119WMA.M
Quant Title : VOC Analysis

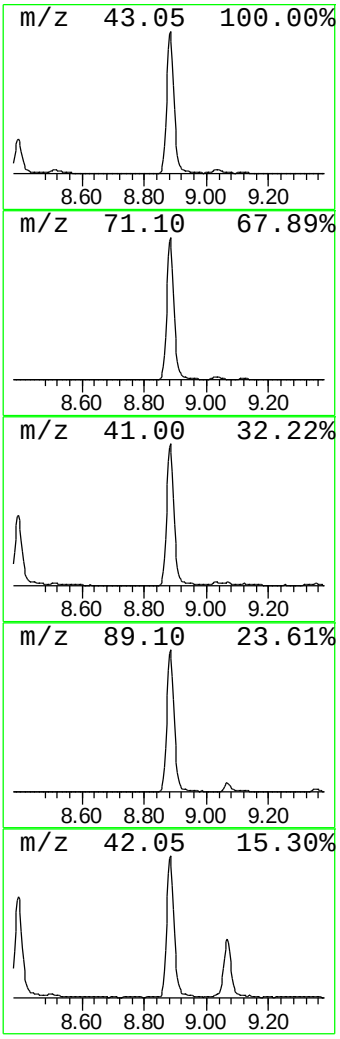
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	33.05 ug/L	750543	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	87
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	86
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100219\
Data File : VU034907.D
Acq On : 01 Oct 2019 22:51
Operator : JC/SP
Sample : K5028-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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

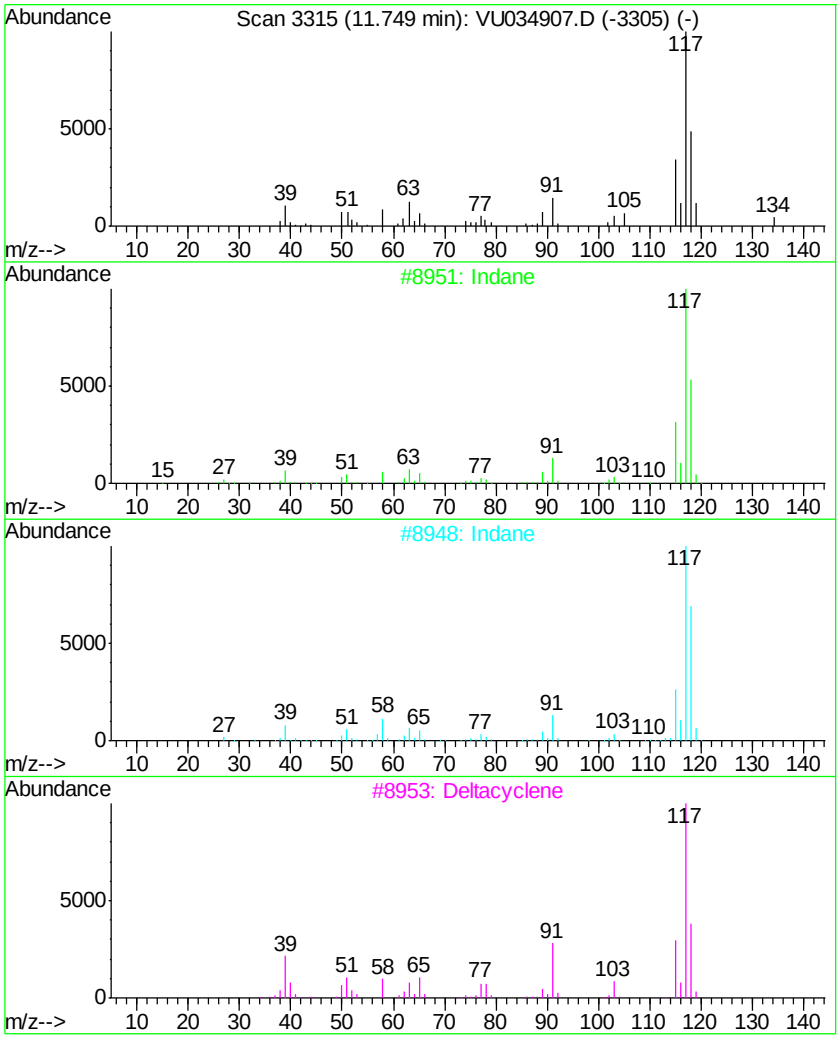
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

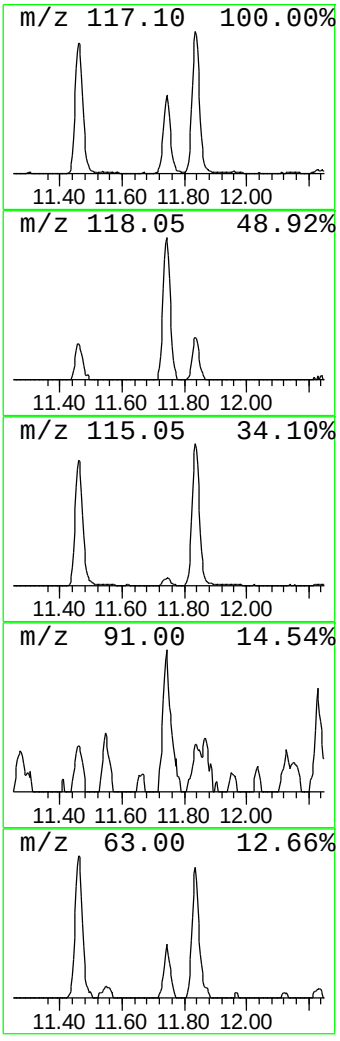
****

Peak Number 9 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.56 ug/L	49125	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Indane	118	C9H10	000496-11-7	81
3	Deltacyclene	118	C9H10	007785-10-6	76
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5	Indane	118	C9H10	000496-11-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100219\
Data File : VU034907.D
Acq On : 01 Oct 2019 22:51
Operator : JC/SP
Sample : K5028-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDL7

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	5.6	ug/L	101878	1	5.86	905686	50.0
n-Propyl acetate	6.68	69.1	ug/L	1251370	1	5.86	905686	50.0
Propanoic acid, 1...	7.40	13.3	ug/L	239950	1	5.86	905686	50.0
Propanoic acid, 2...	8.13	17.8	ug/L	403231	2	9.07	1135520	50.0
Propanoic acid, p...	8.40	23.8	ug/L	540136	2	9.07	1135520	50.0
Butanoic acid, 1-...	8.88	33.0	ug/L	750543	2	9.07	1135520	50.0
Indane	11.75	2.6	ug/L	49125	3	11.46	958856	50.0