LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM091919WMA.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	24	27	31	rVB2	6305	4463	0.11%	0.016%
2	1.392	87	94	105	rBV	354842	377477	9.09%	1.364%
3	1.672	174	181	194	rVB	279394	352105	8.48%	1.272%
4	2.257	354	363	375	rVB	499062	756444	18.21%	2.734%
5	2.640	480	482	485	rVB4	1615	924	0.02%	0.003%
6	2.656	485	487	489	rVV3	1634	980	0.02%	0.004%
7	2.685	491	496	508	rVB5	10463	17217	0.41%	0.062%
8	2.897	560	562	566	rBV5	1396	1207	0.03%	0.004%
9	2.920	566	569	574	rVB7	1755	1571	0.04%	0.006%
10	2.965	577	583	586	rBV7	5902	7020	0.17%	0.025%
11	3.116	623	630	632	rBV5	2046	1866	0.04%	0.007%
12	3.129	632	634	637	rVV2	1782	1079	0.03%	0.004%
13	3.148	637	640	643	rVV4	2091	1312	0.03%	0.005%
14	3.174	643	648	653	rVB7	2186	2229	0.05%	0.008%
15	3.328	692	696	700	rBV4	1368	1257	0.03%	0.005%
16	3.360	703	706	708	rBV4	1547	886	0.02%	0.003%
17	3.421	720	725	727	rBV4	1966	1649	0.04%	0.006%
18	3.566	767	770	773	rVB3	1271	878	0.02%	0.003%
19	3.621	785	787	795	rVB7	1829	2385	0.06%	0.009%
20	3.662	795	800	803	rBV6	1715	1531	0.04%	0.006%
21	3.682	803	806	807	rBV2	1301	901	0.02%	0.003%
22	3.765	829	832	836	rVB5	1473	1249	0.03%	0.005%
23	3.862	856	862	865	rBV5	1509	1210	0.03%	0.004%
24	3.881	865	868	870	rVV3	1700	1114	0.03%	0.004%
25	3.923	879	881	885	rVB4	1592	974	0.02%	0.004%
26	4.026	910	913	915	rBV4	1381	891	0.02%	0.003%
27	4.103	933	937	940	rBV3	1104	885	0.02%	0.003%
28	4.151	940	952	981	rBV2	216387	588892	14.18%	2.128%
29	4.621	1081	1098	1120	rBV	370584	886433	21.34%	3.203%
30	5.045	1227	1230	1236	rBV7	1752	1969	0.05%	0.007%
31	5.106	1246	1249	1254	rBV6	2153	2202	0.05%	0.008%
32	5.315	1289	1314	1352	rBV2	770645	2332218	56.15%	8.428%
33	5.527	1370	1380	1401	rBV	98685	211091	5.08%	0.763%
34	5.788	1460	1461	1465	rVB4	1578	832	0.02%	0.003%

LSC Area Percent Report

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Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM091919WMA.M
Title : VOC Analysis

35	5.862	1471	1484	1502	rBV	629126	1279378	30.80%	4.623%
36	6.309	1610	1623	1644	rBV	529506	1070135	25.76%	3.867%
37	6.563	1695	1702	1705	rBV	14208	20792	0.50%	0.075%
38	6.682	1727	1739	1775	rBV	2248519	4153773	100.00%	15.011%
39	7.206	1888	1902	1930	rBV	319865	610047	14.69%	2.205%
40	7.399	1951	1962	1973	rBV	281569	484661	11.67%	1.751%
41	7.543	1993	2007	2031	rBV	1033521	1903886	45.84%	6.880%
42	7.826	2084	2095	2123	rBV2	300132	562723	13.55%	2.034%
43	8.132	2179	2190	2206	rBV	572812	963368	23.19%	3.481%
44	8.212	2209	2215	2217	rBV3	20745	23467	0.56%	0.085%
45	8.289	2230	2239	2262	rBV	809422	1438160	34.62%	5.197%
46	8.395	2262	2272	2299	rVB	835579	1378445	33.19%	4.981%
47	8.508	2301	2307	2319	rVB2	41159	66580	1.60%	0.241%
48	8.755	2378	2384	2385	rBV4	2095	1957	0.05%	0.007%
49	8.884	2411	2424	2460	rBV	1147063	1918771	46.19%	6.934%
50	9.067	2464	2481	2523	rVV	966146	1723152	41.48%	6.227%
51	9.228	2527	2531	2544	rVB5	9208	15812	0.38%	0.057%
52	9.318	2552	2559	2563	rBV7	6094	7856	0.19%	0.028%
53	9.450	2596	2600	2603	rVB4	1775	1403	0.03%	0.005%
54	9.588	2634	2643	2652	rBV3	21400	40219	0.97%	0.145%
55	9.746	2681	2692	2721	rBV	144613	279544	6.73%	1.010%
56	9.993	2767	2769	2775	rVB7	2163	1583	0.04%	0.006%
57	10.045	2781	2785	2787	rBV4	2118	1882	0.05%	0.007%
58	10.148	2809	2817	2827	rBV4	7288	11483	0.28%	0.041%
59	10.238	2842	2845	2851	rBV6	1499	1367	0.03%	0.005%
60	10.292	2858	2862	2864	rBV4	1242	979	0.02%	0.004%
61	10.305	2864	2866	2872	rVB5	1622	1291	0.03%	0.005%
62	10.350	2877	2880	2885	rVB6	1885	1697	0.04%	0.006%
63	10.408	2885	2898	2915	rBV	656465	1096497	26.40%	3.962%
64	10.546	2933	2941	2944	rBV7	2683	3877	0.09%	0.014%
65	10.749	2996	3004	3015	rBV	31926	49606	1.19%	0.179%
66	10.865	3035	3040	3042	rBV4	1302	1367	0.03%	0.005%
67	11.032	3091	3092	3096	rBV2	1591	879	0.02%	0.003%
68	11.058	3096	3100	3101	rBV3	1515	902	0.02%	0.003%
69	11.083	3106	3108	3110	rBV3	1866	974	0.02%	0.004%
70	11.128	3114	3122	3131	rBV6	9074	16266	0.39%	0.059%
71	11.228	3150	3153	3155	rBV3	1351	851	0.02%	0.003%

LSC Area Percent Report

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Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM091919WMA.M
Title : VOC Analysis

72	11.257	3159	3162	3167	rVV6	1410	1125	0.03%	0.004%
73	11.286	3168	3171	3175	rVB6	1444	953	0.02%	0.003%
74	11.398	3195	3206	3214	rBV6	11039	19098	0.46%	0.069%
75	11.460	3214	3225	3251	rVV	844973	1430990	34.45%	5.171%
76	11.681	3292	3294	3297	rBV4	1798	1102	0.03%	0.004%
77	11.697	3297	3299	3303	rVV5	2061	1426	0.03%	0.005%
78	11.765	3318	3320	3322	rBV3	1789	1210	0.03%	0.004%
79	11.784	3322	3326	3329	rVV6	2387	2239	0.05%	0.008%
80	11.836	3330	3342	3367	rVV	861919	1472651	35.45%	5.322%
81	12.389	3511	3514	3518	rVB5	2152	1470	0.04%	0.005%
82	12.450	3529	3533	3535	rBV3	1523	1065	0.03%	0.004%
83	12.517	3552	3554	3559	rVB6	2348	1431	0.03%	0.005%
84	12.546	3559	3563	3566	rBV5	1310	1043	0.03%	0.004%
85	12.585	3570	3575	3577	rBV5	1674	1822	0.04%	0.007%
86	12.665	3598	3600	3606	rVB6	2182	1513	0.04%	0.005%
87	12.871	3656	3664	3666	rBV8	6429	7041	0.17%	0.025%
88	12.984	3696	3699	3702	rVB4	1444	956	0.02%	0.003%
89	13.176	3755	3759	3762	rVB5	1341	1167	0.03%	0.004%
90	13.270	3785	3788	3791	rBV4	2207	1170	0.03%	0.004%
91	13.366	3816	3818	3820	rBV3	2023	1161	0.03%	0.004%
92	13.588	3885	3887	3890	rBV3	1504	915	0.02%	0.003%
93	13.990	4001	4012	4017	rBV3	4966	9206	0.22%	0.033%
94	14.337	4117	4120	4122	rBV3	1794	1408	0.03%	0.005%
95	14.395	4136	4138	4141	rBV2	1498	768	0.02%	0.003%
96	14.575	4191	4194	4197	rBV3	1939	1565	0.04%	0.006%
97	14.665	4218	4222	4224	rBV3	2500	2130	0.05%	0.008%
98	14.717	4236	4238	4242	rBV3	1707	1446	0.03%	0.005%
99	15.096	4353	4356	4361	rVV7	2154	1939	0.05%	0.007%
100	15.324	4424	4427	4429	rBV3	1800	1012	0.02%	0.004%

Sum of corrected areas: 27671993

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Acq On : 19 Sep 2019 19:52
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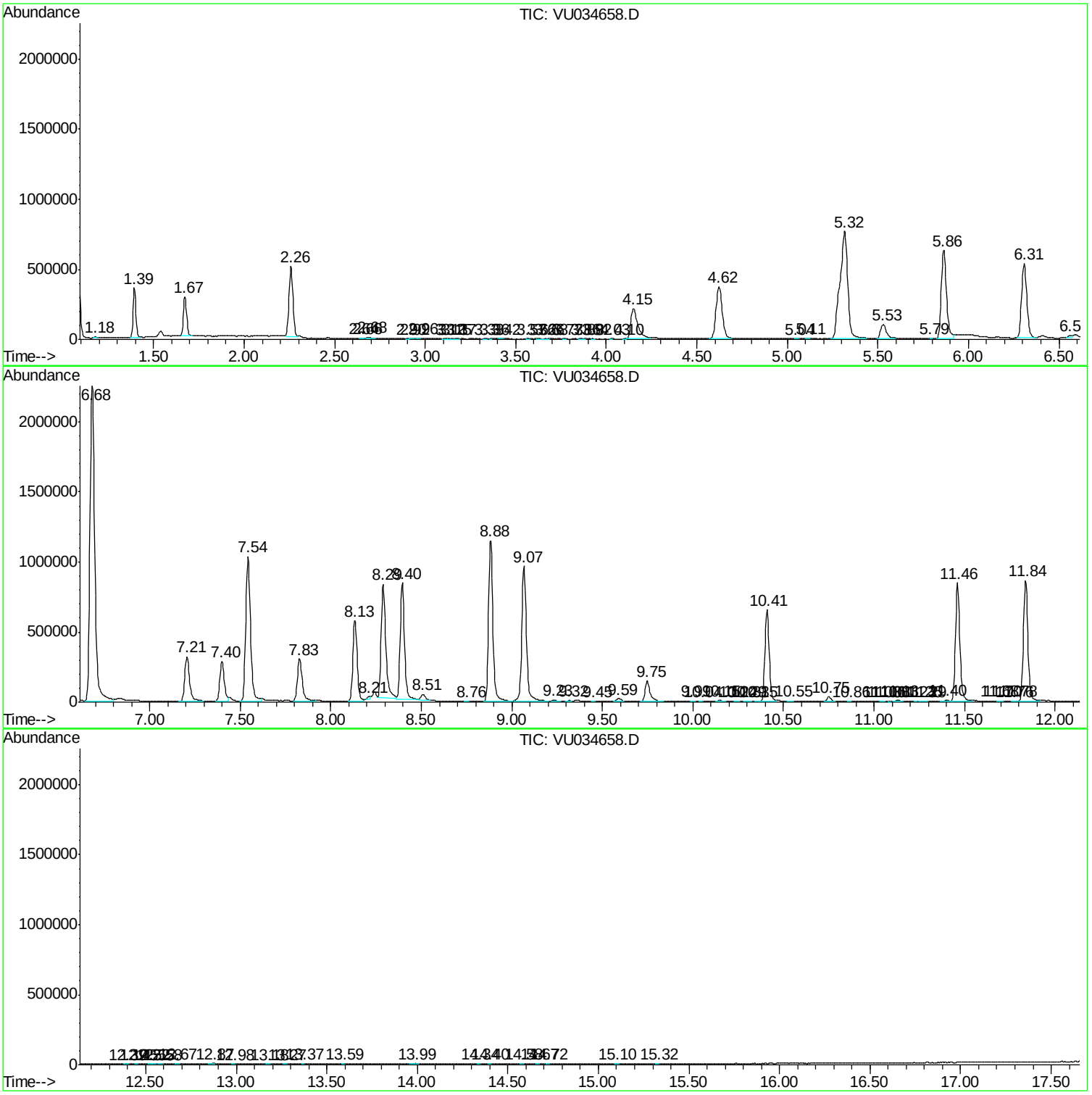
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

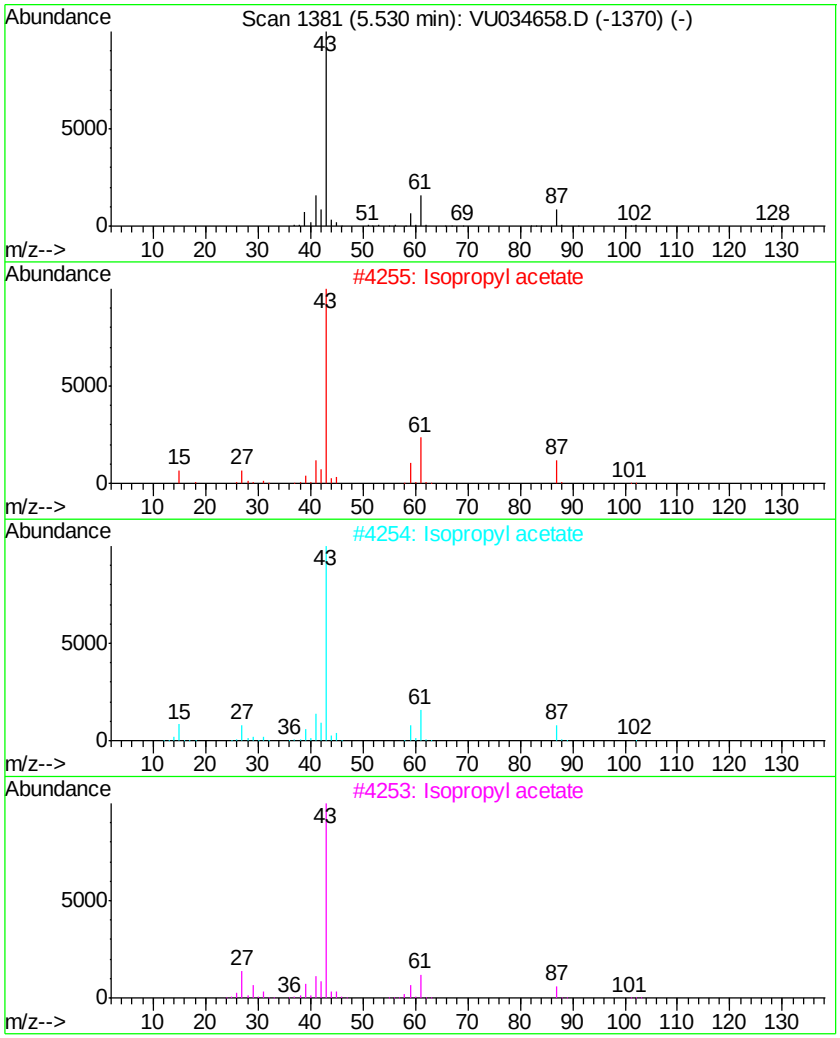
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

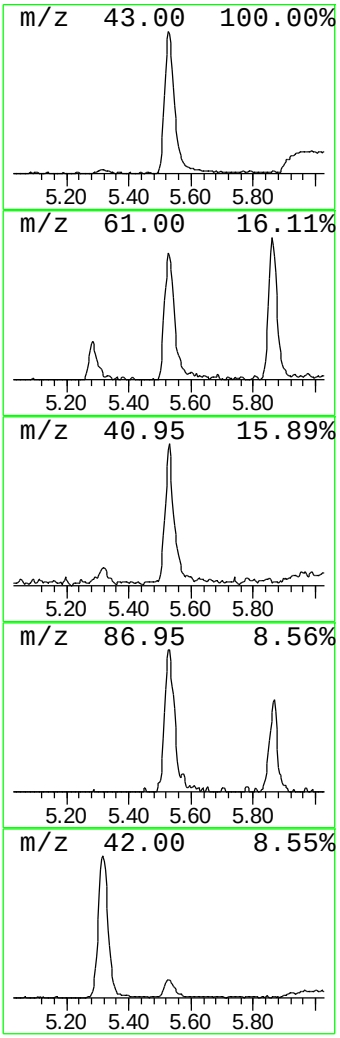
****

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	8.25 ug/L	211091	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	78
3	Isopropyl acetate	102	C5H10O2	000108-21-4	40
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\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

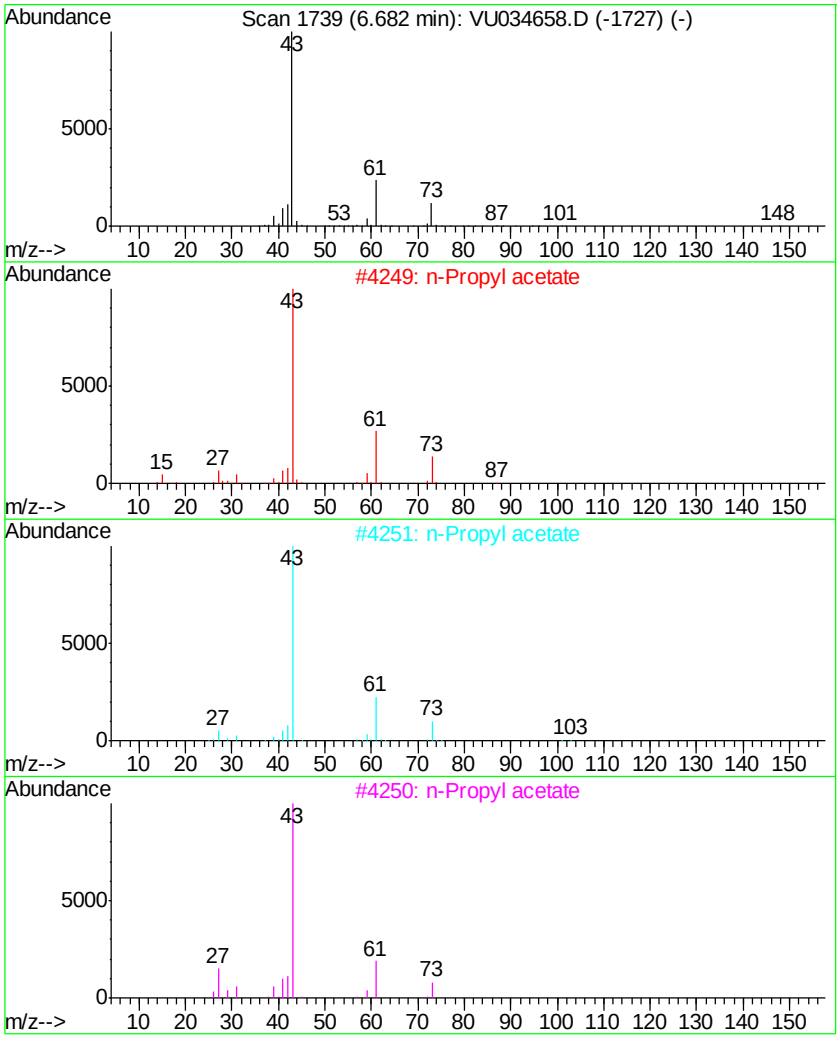
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

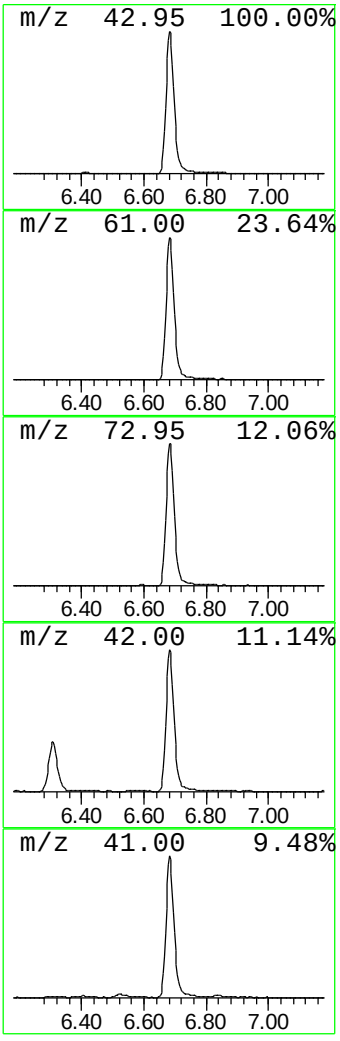
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	162.34 ug/L	4153770	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	45
4	Isopropyl acetate	102	C5H10O2	000108-21-4	38
5	Isobutylamine	73	C4H11N	000078-81-9	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

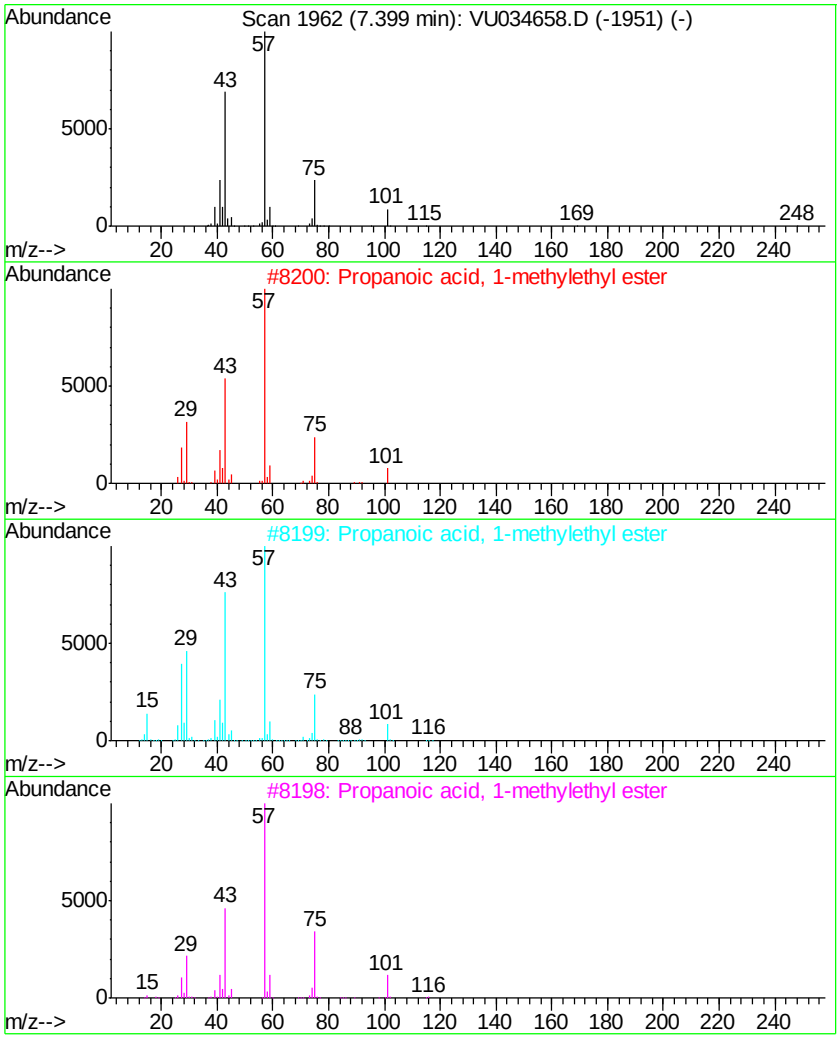
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

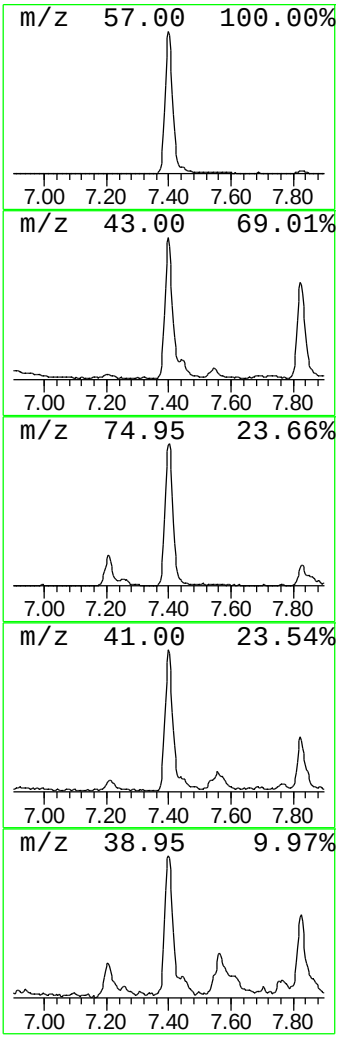
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	18.94 ug/L	484661	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	72
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	28





Library Search Compound Report

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Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

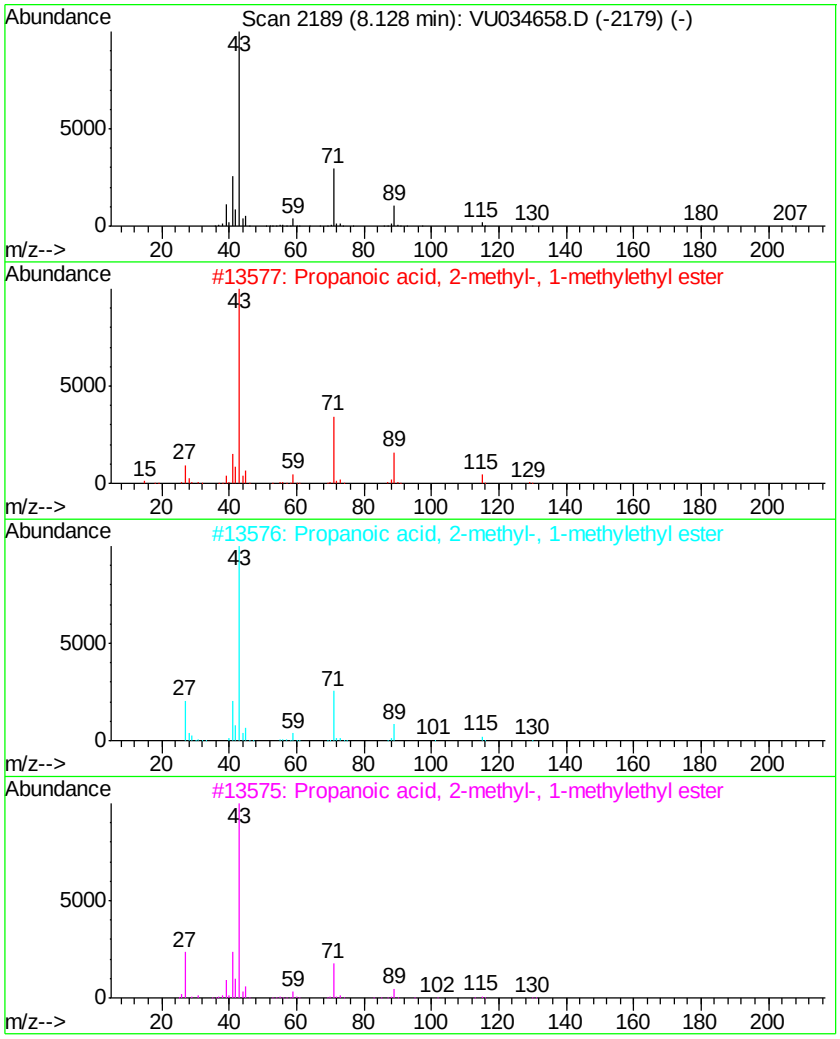
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

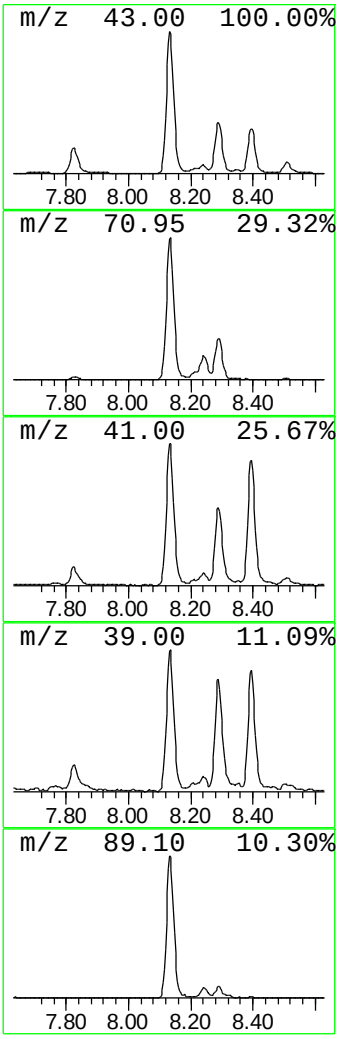
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	27.95 ug/L	963368	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	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	38
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	37





Library Search Compound Report

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Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

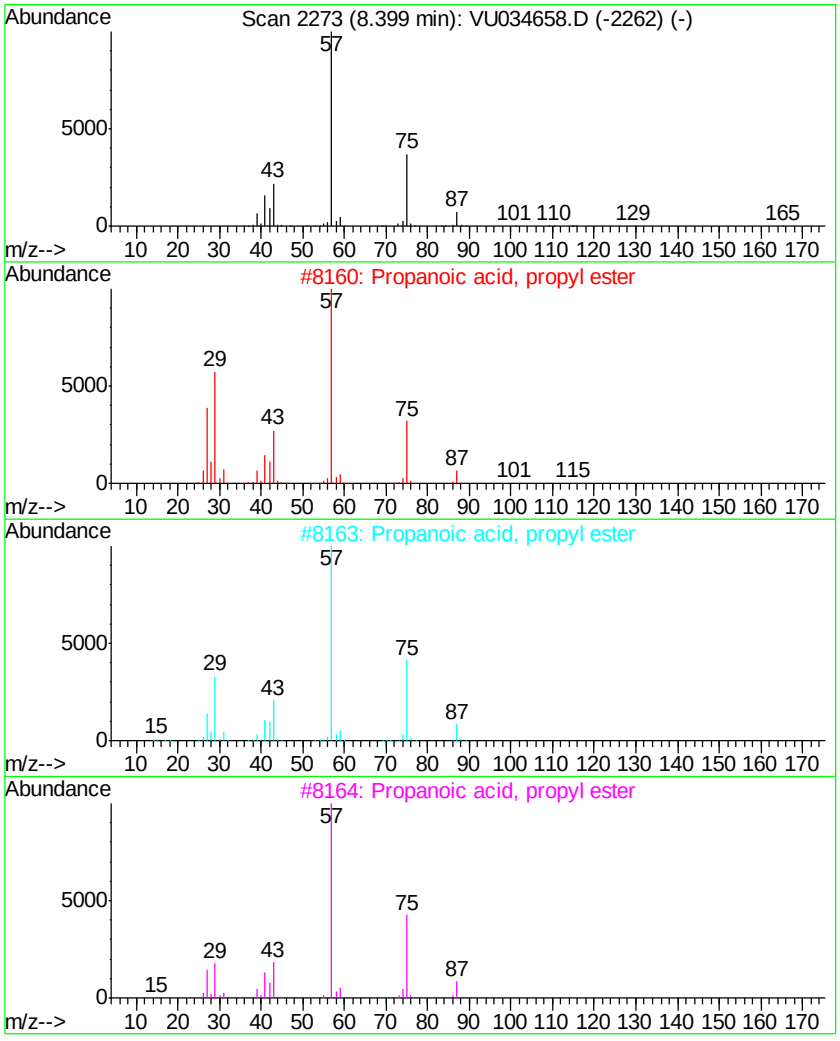
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

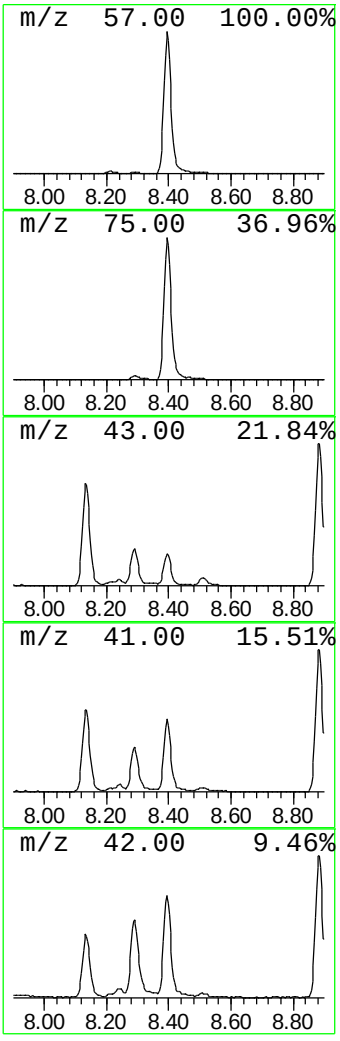
****

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	40.00 ug/L	1378450	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	78
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

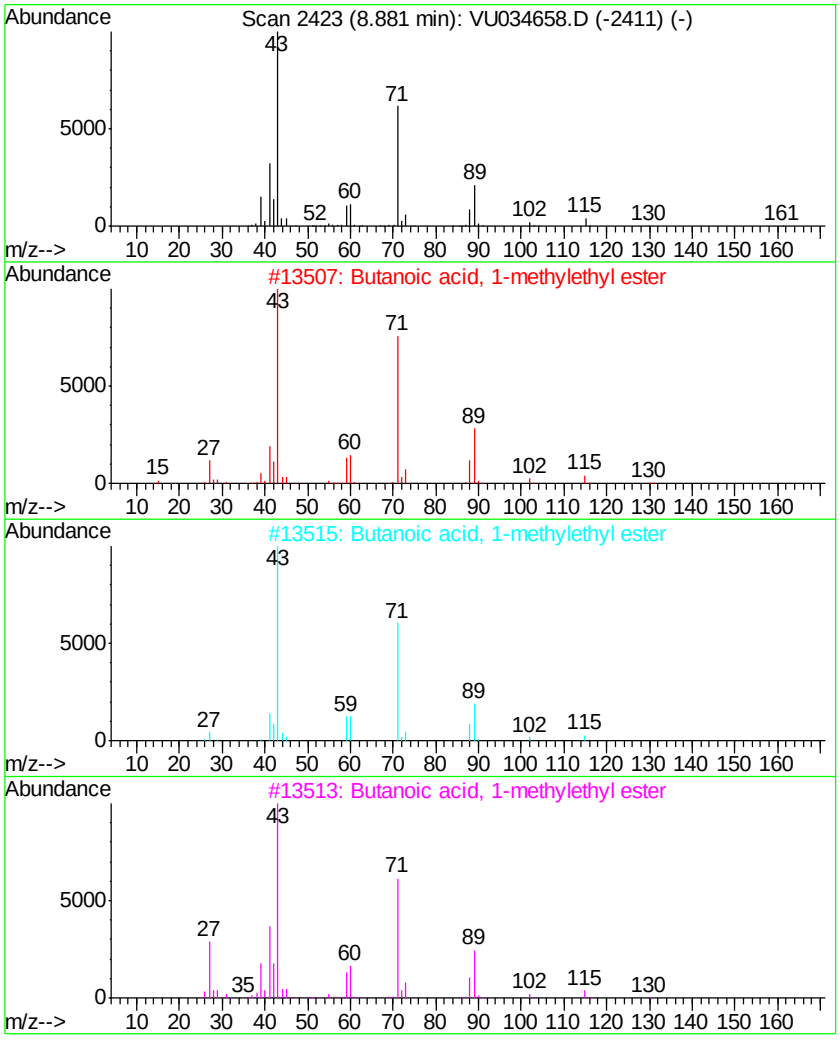
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

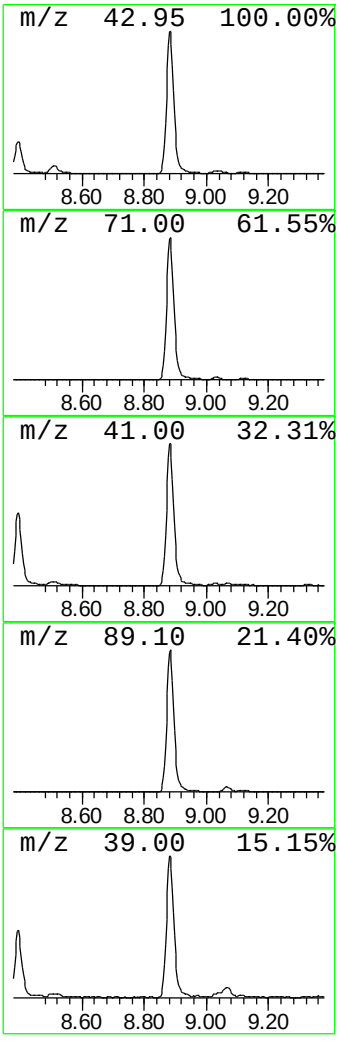
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	55.68 ug/L	1918770	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	90
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

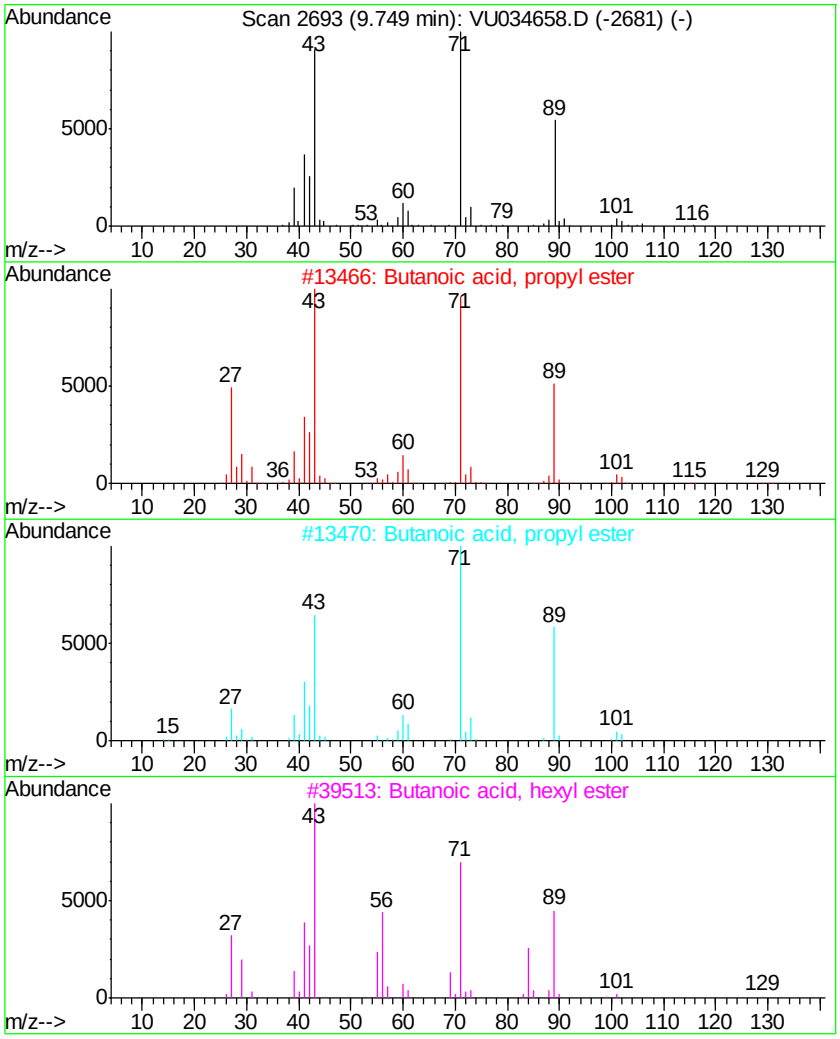
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

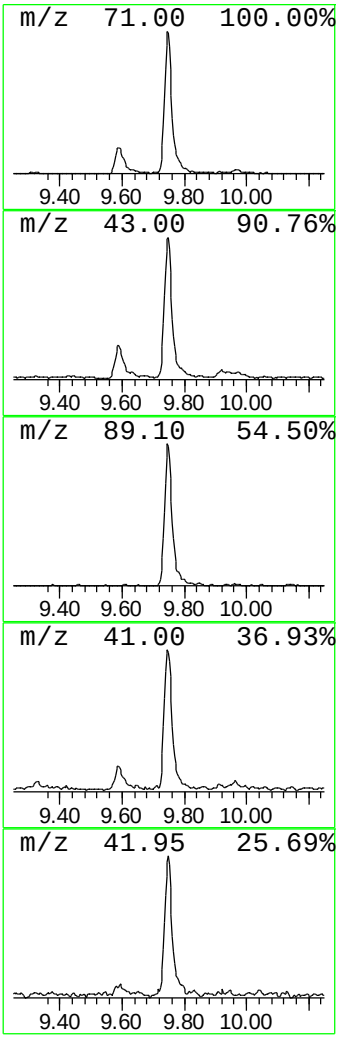
****

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	8.11 ug/L	279544	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, hexyl ester	172	C10H20O2	002639-63-6	74
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
5	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091919\
Data File : VU034658.D
Acq On : 19 Sep 2019 19:52
Operator : JC/SP
Sample : PB123216TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.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	8.3	ug/L	211091	1	5.86	1279380	50.0
n-Propyl acetate	6.68	162.3	ug/L	4153770	1	5.86	1279380	50.0
Propanoic acid, 1...	7.40	18.9	ug/L	484661	1	5.86	1279380	50.0
Propanoic acid, 2...	8.13	27.9	ug/L	963368	2	9.07	1723150	50.0
Propanoic acid, p...	8.40	40.0	ug/L	1378450	2	9.07	1723150	50.0
Butanoic acid, 1-...	8.88	55.7	ug/L	1918770	2	9.07	1723150	50.0
Butanoic acid, pr...	9.75	8.1	ug/L	279544	2	9.07	1723150	50.0