LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032833.D
Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

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\SOMULM061719WMA.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	1.180	23	28	37	rBV	6895	6727	0.48%	0.063%
2	1.395	87	95	104	rBV	112503	114112	8.22%	1.061%
3	1.469	112	118	128	rBV	16091	17803	1.28%	0.166%
4	1.675	175	182	194	rVB	89299	109069	7.85%	1.014%
5	2.267	355	366	375	rBV	184075	279619	20.13%	2.600%
6	2.318	376	382	398	rVB	28095	44113	3.18%	0.410%
7	2.598	465	469	470	rBV	594	379	0.03%	0.004%
8	2.617	470	475	485	rVB4	1470	2509	0.18%	0.023%
9	2.694	490	499	511	rVB2	10372	17384	1.25%	0.162%
10	2.903	559	564	565	rBV2	304	252	0.02%	0.002%
11	2.939	572	575	577	rBV2	498	288	0.02%	0.003%
12	2.958	577	581	582	rBV	390	223	0.02%	0.002%
13	2.968	582	584	588	rVB3	332	236	0.02%	0.002%
14	3.042	603	607	609	rBV3	398	307	0.02%	0.003%
15	3.148	637	640	642	rBV2	435	289	0.02%	0.003%
16	3.180	642	650	660	rVV4	2282	4605	0.33%	0.043%
17	3.312	689	691	696	rVB3	351	271	0.02%	0.003%
18	3.360	703	706	709	rVB2	466	327	0.02%	0.003%
19	3.408	709	721	732	rBV2	7605	16748	1.21%	0.156%
20	3.492	746	747	752	rVB3	569	267	0.02%	0.002%
21	3.646	792	795	800	rBV3	574	488	0.04%	0.005%
22	3.669	800	802	807	rVB2	413	221	0.02%	0.002%
23	3.900	870	874	878	rVB2	256	224	0.02%	0.002%
24	4.051	918	921	924	rBV2	361	237	0.02%	0.002%
25	4.170	945	958	987	rBV	83675	243390	17.52%	2.263%
26	4.501	1057	1061	1063	rBV4	329	272	0.02%	0.003%
27	4.640	1087	1104	1132	rVV	147358	343338	24.72%	3.192%
28	4.797	1147	1153	1157	rBV3	375	366	0.03%	0.003%
29	4.829	1157	1163	1166	rBV3	257	217	0.02%	0.002%
30	4.855	1166	1171	1172	rBV2	265	212	0.02%	0.002%
31	4.865	1172	1174	1178	rVV4	570	390	0.03%	0.004%
32	4.884	1178	1180	1189	rVB2	689	718	0.05%	0.007%
33	4.923	1189	1192	1197	rVB2	500	361	0.03%	0.003%
34	5.058	1227	1234	1242	rVB3	389	615	0.04%	0.006%

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Sample : K3324-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

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\SOMULM061719WMA.M
Title : VOC Analysis

35	5.103	1242	1248	1252	rBV3	344	431	0.03%	0.004%
36	5.144	1258	1261	1264	rVB2	352	288	0.02%	0.003%
37	5.334	1293	1320	1345	rBV2	294358	859492	61.88%	7.992%
38	5.550	1376	1387	1401	rBV2	5971	13010	0.94%	0.121%
39	5.652	1417	1419	1426	rVB4	448	462	0.03%	0.004%
40	5.784	1454	1460	1463	rBV3	258	369	0.03%	0.003%
41	5.881	1476	1490	1509	rBV	289220	566579	40.79%	5.268%
42	6.042	1537	1540	1545	rBV3	431	516	0.04%	0.005%
43	6.177	1572	1582	1596	rVB10	3533	7312	0.53%	0.068%
44	6.251	1602	1605	1608	rVB4	400	255	0.02%	0.002%
45	6.324	1614	1628	1648	rBV	195651	391800	28.21%	3.643%
46	6.418	1650	1657	1680	rVB	8058	17299	1.25%	0.161%
47	6.534	1684	1693	1699	rBV2	3736	6561	0.47%	0.061%
48	6.572	1701	1705	1712	rBV	3557	5172	0.37%	0.048%
49	6.697	1731	1744	1774	rBV	780577	1389044	100.00%	12.916%
50	7.054	1852	1855	1858	rBV2	325	236	0.02%	0.002%
51	7.090	1863	1866	1870	rBV	381	346	0.02%	0.003%
52	7.222	1895	1907	1929	rBV	113817	204520	14.72%	1.902%
53	7.414	1955	1967	1993	rBV	147572	256795	18.49%	2.388%
54	7.559	1999	2012	2029	rBV	407627	703813	50.67%	6.544%
55	7.697	2048	2055	2061	rBV5	1580	2628	0.19%	0.024%
56	7.842	2089	2100	2124	rBV2	92767	164554	11.85%	1.530%
57	8.151	2184	2196	2210	rBV	84606	137690	9.91%	1.280%
58	8.257	2212	2229	2235	rBV3	33862	62990	4.53%	0.586%
59	8.305	2235	2244	2265	rVB	286255	476560	34.31%	4.431%
60	8.411	2266	2277	2293	rBV	589519	901469	64.90%	8.382%
61	8.521	2303	2311	2329	rVB	37831	64489	4.64%	0.600%
62	8.659	2351	2354	2357	rBV3	563	415	0.03%	0.004%
63	8.771	2386	2389	2392	rBV3	373	244	0.02%	0.002%
64	8.849	2406	2413	2416	rBV2	265	242	0.02%	0.002%
65	8.900	2416	2429	2457	rBV	411117	650427	46.83%	6.048%
66	9.025	2464	2468	2469	rBV2	468	315	0.02%	0.003%
67	9.083	2471	2486	2511	rVV	440488	736789	53.04%	6.851%
68	9.241	2533	2535	2541	rVB4	654	651	0.05%	0.006%
69	9.270	2541	2544	2547	rBV2	535	363	0.03%	0.003%
70	9.292	2547	2551	2554	rBV3	385	334	0.02%	0.003%
71	9.366	2567	2574	2576	rBV4	423	542	0.04%	0.005%

LSC Area Percent Report

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Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

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\SOMULM061719WMA.M
Title : VOC Analysis

72	9.395	2576	2583	2585	rBV4	469	418	0.03%	0.004%
73	9.511	2615	2619	2621	rBV2	242	213	0.02%	0.002%
74	9.537	2625	2627	2631	rBV2	270	227	0.02%	0.002%
75	9.601	2639	2647	2658	rBV2	5606	9971	0.72%	0.093%
76	9.707	2677	2680	2682	rBV2	347	234	0.02%	0.002%
77	9.762	2686	2697	2713	rVV	22745	36476	2.63%	0.339%
78	9.987	2765	2767	2770	rBV2	346	274	0.02%	0.003%
79	10.035	2777	2782	2784	rBV3	487	427	0.03%	0.004%
80	10.144	2814	2816	2820	rVB	348	234	0.02%	0.002%
81	10.283	2856	2859	2862	rVB2	385	223	0.02%	0.002%
82	10.427	2888	2904	2924	rBV	283277	463334	33.36%	4.308%
83	10.623	2961	2965	2967	rBV2	289	234	0.02%	0.002%
84	10.723	2991	2996	2999	rBV2	533	428	0.03%	0.004%
85	10.765	3005	3009	3010	rBV2	406	311	0.02%	0.003%
86	11.479	3219	3231	3256	rBV	461492	729759	52.54%	6.785%
87	11.855	3335	3348	3373	rBV	412953	674907	48.59%	6.275%
88	12.260	3470	3474	3475	rBV2	328	243	0.02%	0.002%
89	12.286	3480	3482	3488	rVB2	450	284	0.02%	0.003%
90	12.340	3495	3499	3501	rBV2	353	239	0.02%	0.002%
91	12.450	3530	3533	3539	rVB2	420	375	0.03%	0.003%
92	12.739	3617	3623	3631	rBV4	586	954	0.07%	0.009%
93	12.864	3658	3662	3665	rBV2	369	263	0.02%	0.002%
94	13.167	3753	3756	3759	rBV2	346	287	0.02%	0.003%
95	13.237	3774	3778	3779	rBV2	398	289	0.02%	0.003%
96	13.704	3918	3923	3926	rBV2	579	617	0.04%	0.006%
97	13.768	3939	3943	3947	rBV3	564	523	0.04%	0.005%
98	13.858	3968	3971	3973	rBV	611	299	0.02%	0.003%
99	14.080	4036	4040	4044	rBV3	575	518	0.04%	0.005%
100	14.893	4291	4293	4297	rBV3	787	577	0.04%	0.005%

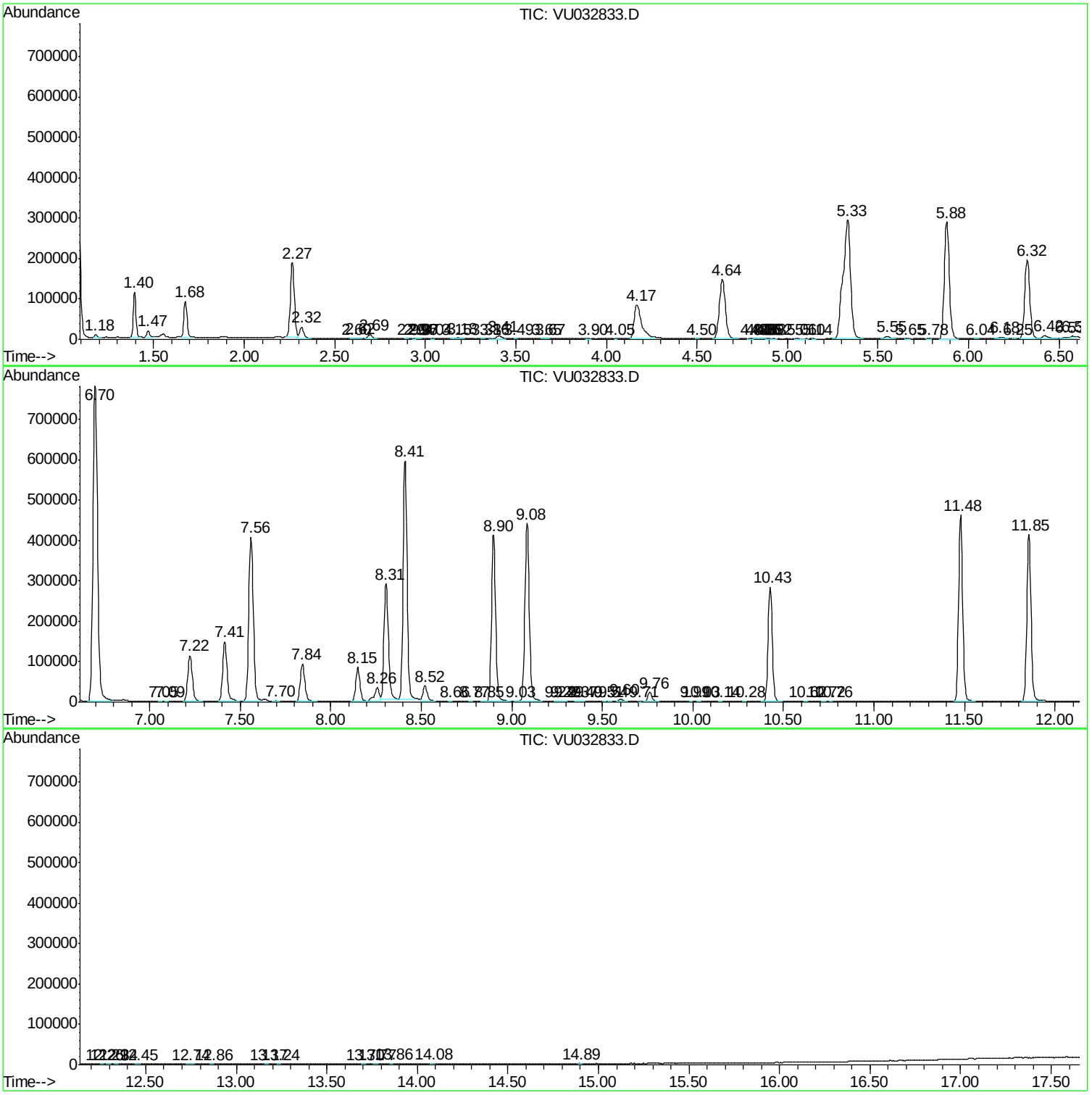
Sum of corrected areas: 10754717

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032833.D
Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
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Quant Title : VOC Analysis

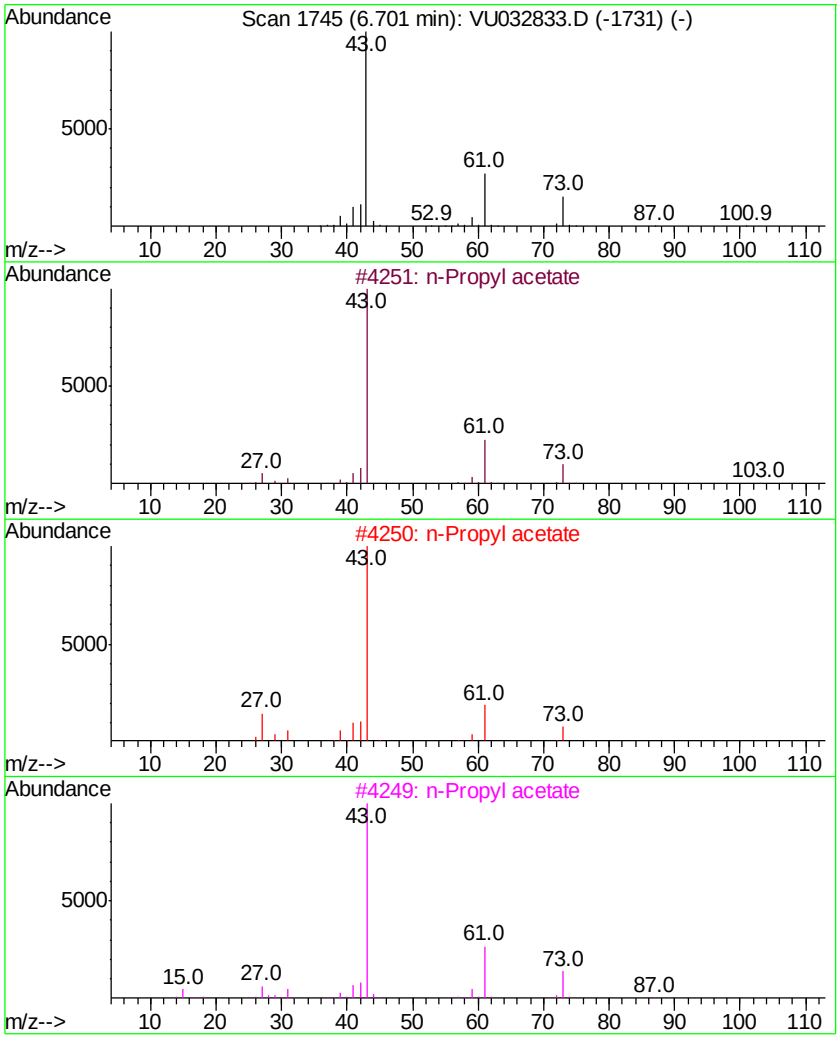
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

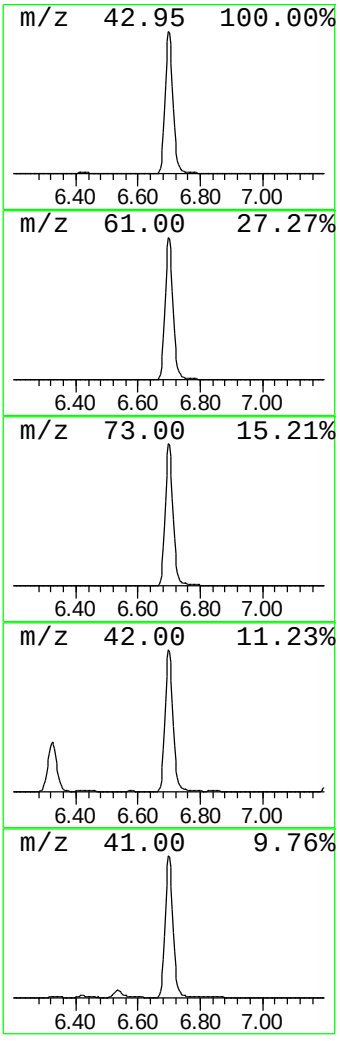
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	122.58 ug/L	1389040	1,4-Difluorobenzene	5.88

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	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

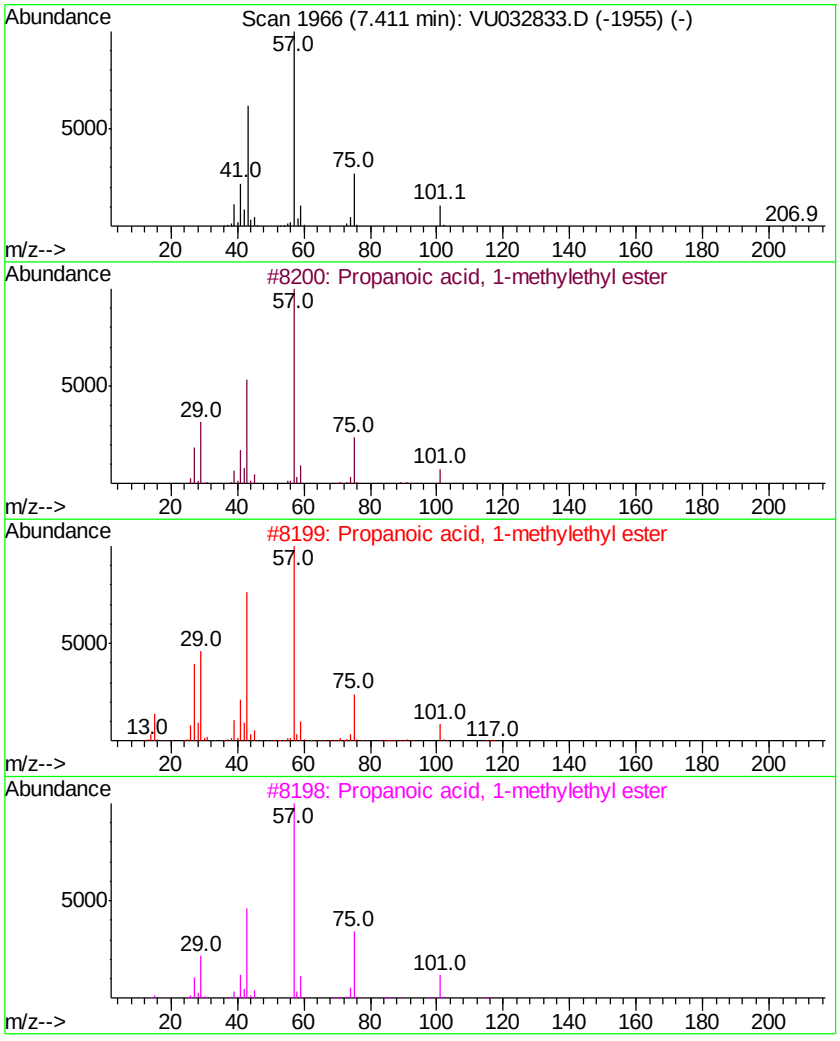
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

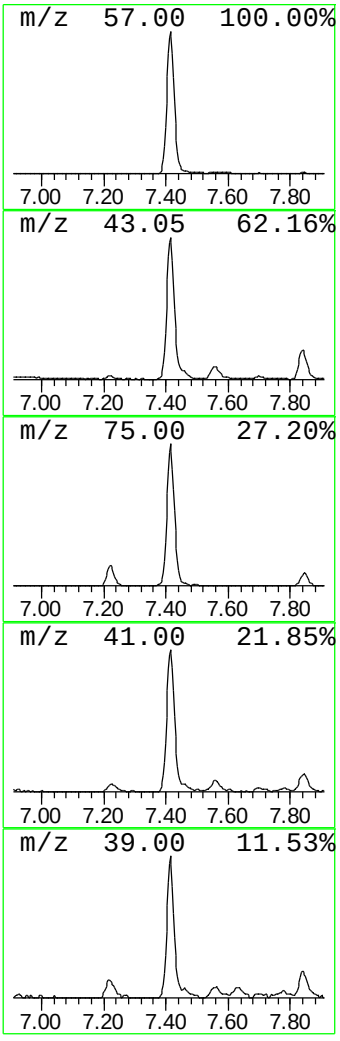
****

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	22.66 ug/L	256795	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

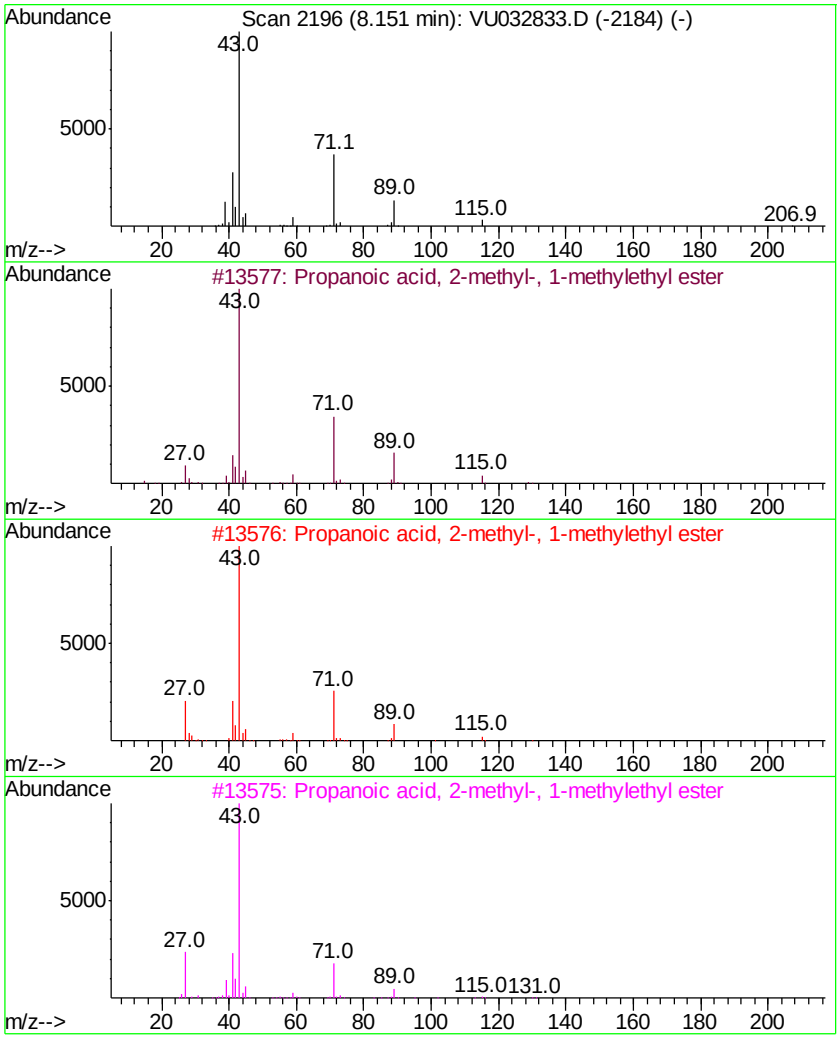
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

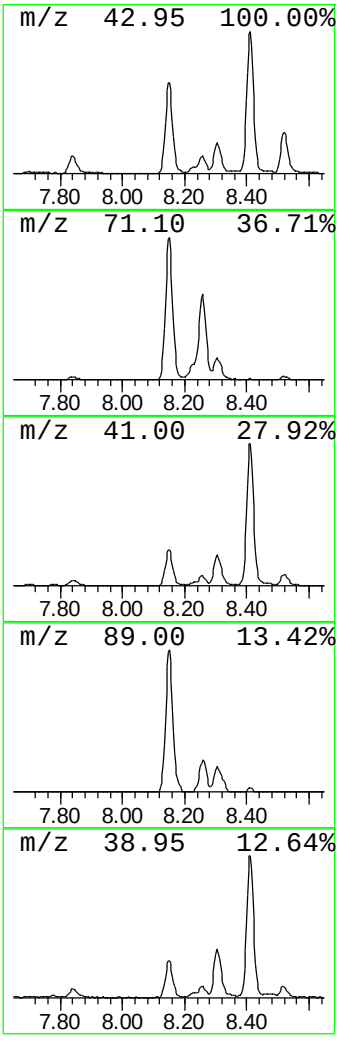
****

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.34 ug/L	137690	Chlorobenzene-d5	9.08

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-, 1-met...	130	C7H14O2	000617-50-5	56
5	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	43





Library Search Compound Report

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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

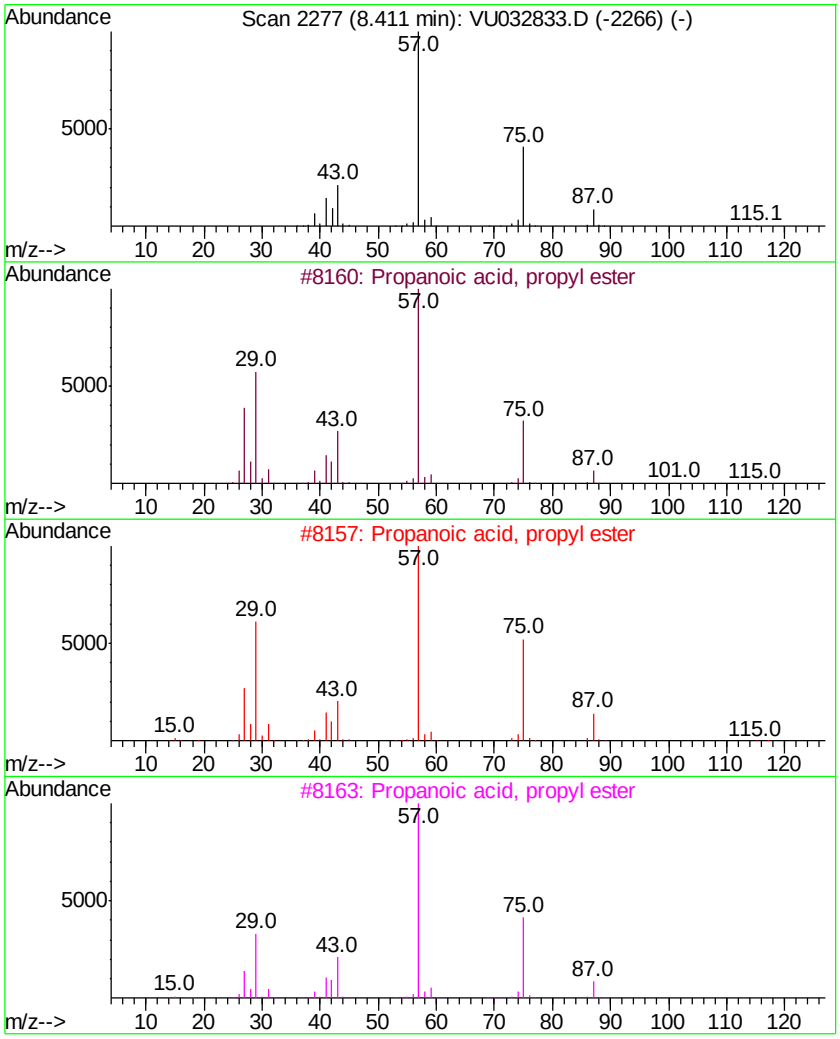
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

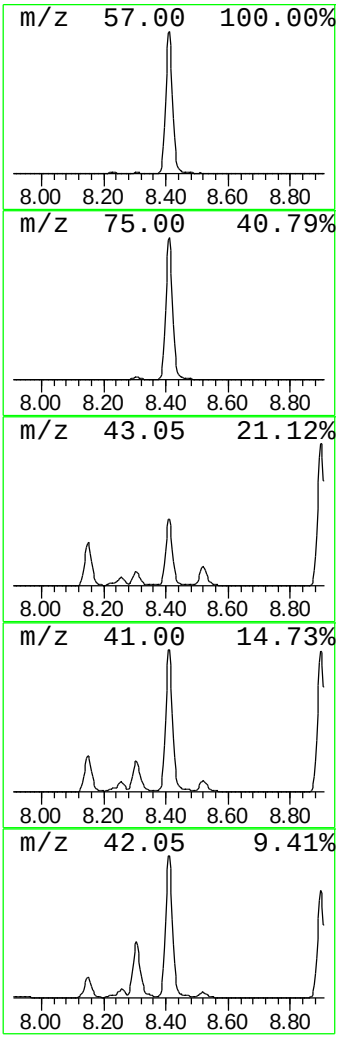
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	61.18 ug/L	901469	Chlorobenzene-d5	9.08

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





Library Search Compound Report

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Data File : VU032833.D
Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

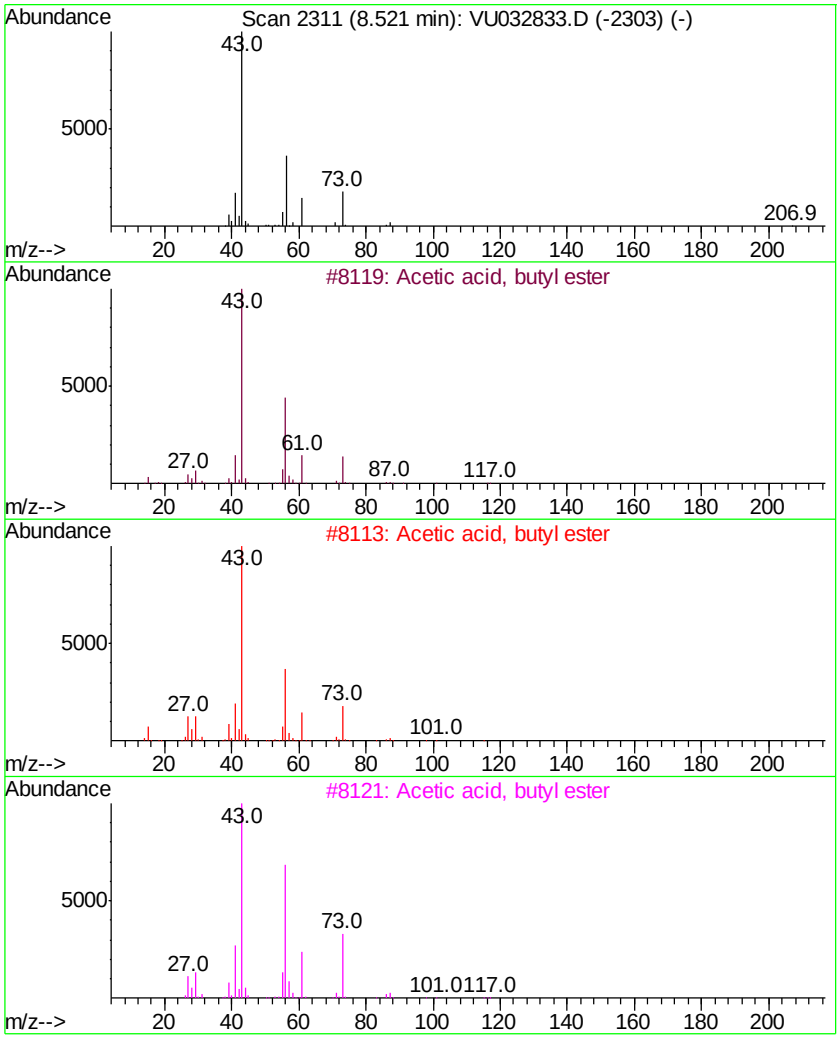
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

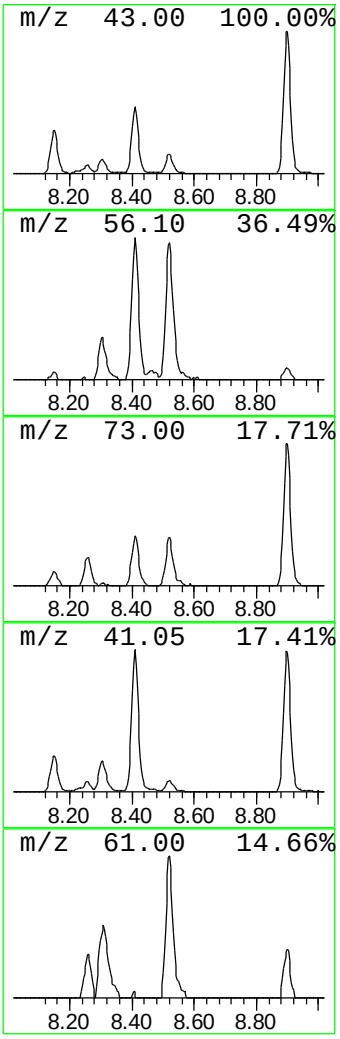
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.38 ug/L	64489	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032833.D
Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

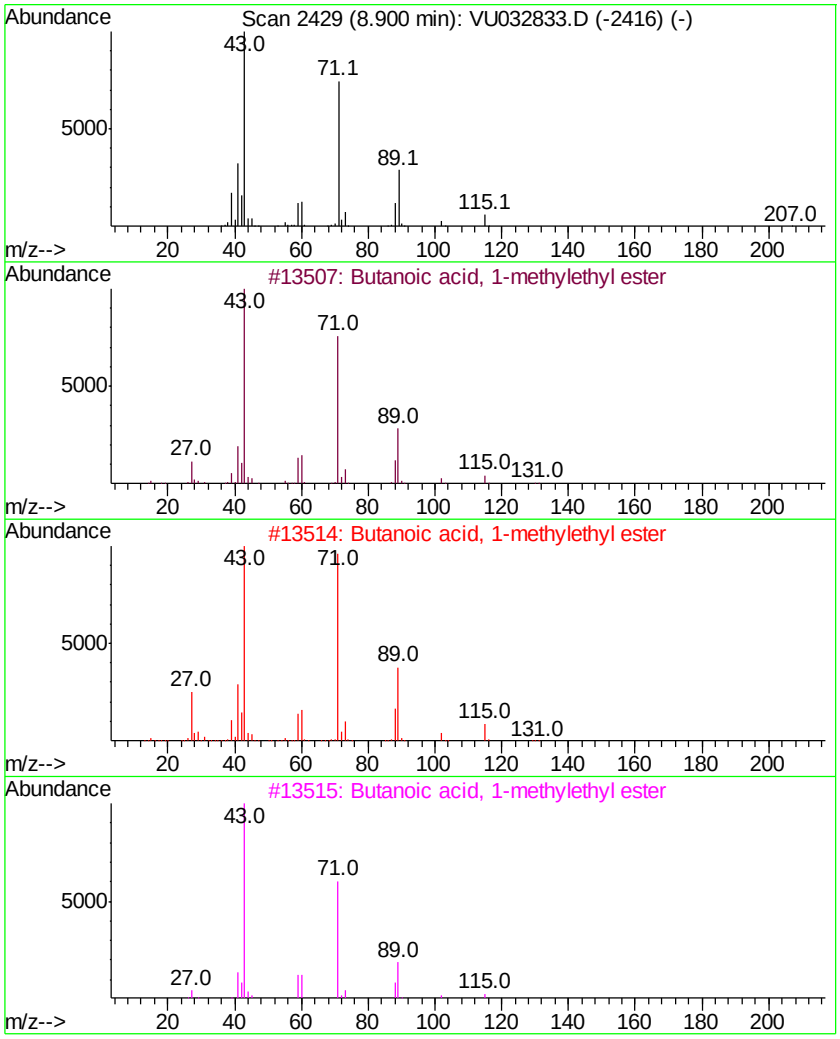
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

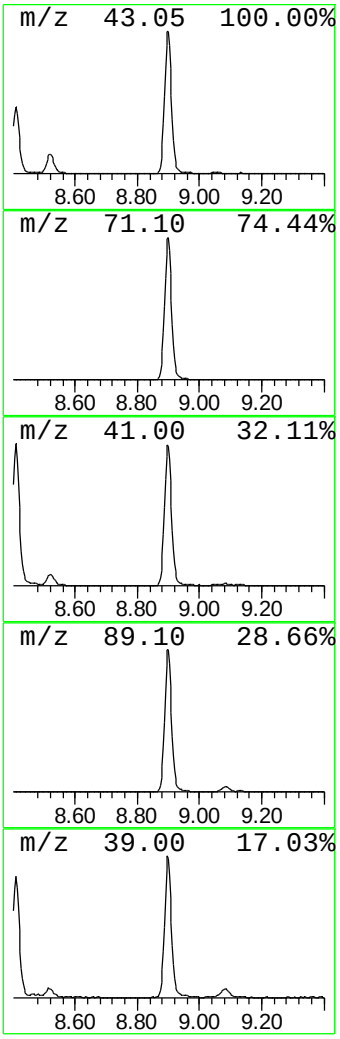
****

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	44.14 ug/L	650427	Chlorobenzene-d5	9.08

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	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032833.D
Acq On : 18 Jun 2019 19:02
Operator : JC/SP
Sample : K3324-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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
n-Propyl acetate	6.70	122.6	ug/L	1389040	1	5.88	566579	50.0
Propanoic acid, 1...	7.41	22.7	ug/L	256795	1	5.88	566579	50.0
Propanoic acid, 2...	8.15	9.3	ug/L	137690	2	9.08	736789	50.0
Propanoic acid, p...	8.41	61.2	ug/L	901469	2	9.08	736789	50.0
Acetic acid, buty...	8.52	4.4	ug/L	64489	2	9.08	736789	50.0
Butanoic acid, 1-...	8.90	44.1	ug/L	650427	2	9.08	736789	50.0