LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032823.D
Acq On : 18 Jun 2019 14:46
Operator : JC/SP
Sample : K3363-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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	34	rBV2	6020	5618	0.39%	0.051%
2	1.396	88	95	106	rVB	127299	126392	8.71%	1.141%
3	1.675	174	182	195	rVB	99437	120839	8.32%	1.091%
4	2.267	355	366	377	rBV	205628	311853	21.48%	2.816%
5	2.318	377	382	393	rVB3	7095	11079	0.76%	0.100%
6	2.614	469	474	487	rVB2	2149	3575	0.25%	0.032%
7	2.694	490	499	510	rVB2	6299	9977	0.69%	0.090%
8	2.813	534	536	539	rVB3	463	239	0.02%	0.002%
9	2.833	539	542	547	rBV3	278	305	0.02%	0.003%
10	2.916	564	568	570	rBV2	339	289	0.02%	0.003%
11	3.180	648	650	653	rBV3	317	225	0.02%	0.002%
12	3.276	677	680	683	rBV3	426	317	0.02%	0.003%
13	3.312	689	691	694	rBV2	392	254	0.02%	0.002%
14	3.579	771	774	780	rBV3	352	425	0.03%	0.004%
15	3.637	788	792	793	rBV2	297	204	0.01%	0.002%
16	3.688	803	808	811	rBV	379	353	0.02%	0.003%
17	3.759	828	830	835	rVB2	333	279	0.02%	0.003%
18	3.791	835	840	844	rBV2	478	549	0.04%	0.005%
19	3.820	847	849	853	rVB	427	279	0.02%	0.003%
20	3.942	886	887	894	rBV3	165	184	0.01%	0.002%
21	4.010	905	908	912	rVB3	406	312	0.02%	0.003%
22	4.093	931	934	941	rVB2	275	283	0.02%	0.003%
23	4.167	945	957	987	rBV	88552	230727	15.89%	2.083%
24	4.366	1017	1019	1022	rVB	460	234	0.02%	0.002%
25	4.395	1024	1028	1032	rVV3	318	245	0.02%	0.002%
26	4.540	1070	1073	1077	rVB3	374	249	0.02%	0.002%
27	4.640	1086	1104	1132	rVV	155329	367953	25.34%	3.322%
28	4.762	1137	1142	1147	rVB3	492	513	0.04%	0.005%
29	4.868	1167	1175	1176	rBV4	533	470	0.03%	0.004%
30	4.971	1202	1207	1210	rBV2	504	376	0.03%	0.003%
31	4.993	1210	1214	1218	rBV3	552	404	0.03%	0.004%
32	5.141	1256	1260	1264	rVB4	265	233	0.02%	0.002%
33	5.161	1264	1266	1268	rBV2	322	175	0.01%	0.002%
34	5.222	1281	1285	1287	rBV	280	214	0.01%	0.002%

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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\SOMULM061719WMA.M
Title : VOC Analysis

35	5.331	1296	1319	1350	rBV2	311754	921819	63.49%	8.324%
36	5.546	1375	1386	1397	rBV3	5995	12861	0.89%	0.116%
37	5.736	1443	1445	1448	rBV2	323	239	0.02%	0.002%
38	5.881	1475	1490	1509	rBV	283255	552138	38.03%	4.986%
39	6.325	1614	1628	1646	rBV	210187	420277	28.95%	3.795%
40	6.424	1650	1659	1671	rBV2	6427	13035	0.90%	0.118%
41	6.530	1688	1692	1698	rBV4	1694	1968	0.14%	0.018%
42	6.575	1699	1706	1713	rBV2	4854	8105	0.56%	0.073%
43	6.698	1731	1744	1776	rBV	815215	1451909	100.00%	13.110%
44	7.042	1848	1851	1853	rBV2	271	190	0.01%	0.002%
45	7.222	1895	1907	1925	rBV	112192	197768	13.62%	1.786%
46	7.415	1950	1967	1990	rBV	153430	265128	18.26%	2.394%
47	7.559	1999	2012	2029	rBV	438306	757009	52.14%	6.835%
48	7.842	2090	2100	2116	rBV2	91913	159170	10.96%	1.437%
49	8.038	2158	2161	2166	rVB2	367	250	0.02%	0.002%
50	8.151	2184	2196	2211	rBV	88579	145994	10.06%	1.318%
51	8.257	2211	2229	2235	rVV3	33406	67307	4.64%	0.608%
52	8.305	2235	2244	2265	rVV	307800	527377	36.32%	4.762%
53	8.411	2266	2277	2301	rVV	604049	966003	66.53%	8.723%
54	8.521	2303	2311	2336	rVB	41296	71681	4.94%	0.647%
55	8.900	2416	2429	2457	rBV	425282	669550	46.12%	6.046%
56	9.083	2468	2486	2510	rBV	430183	714275	49.20%	6.450%
57	9.257	2534	2540	2542	rBV5	312	282	0.02%	0.003%
58	9.308	2553	2556	2560	rVB2	373	188	0.01%	0.002%
59	9.331	2560	2563	2569	rVB3	591	687	0.05%	0.006%
60	9.357	2569	2571	2574	rBV3	389	295	0.02%	0.003%
61	9.373	2574	2576	2581	rVB3	391	277	0.02%	0.003%
62	9.398	2581	2584	2586	rBV2	295	222	0.02%	0.002%
63	9.456	2598	2602	2603	rBV2	571	398	0.03%	0.004%
64	9.601	2638	2647	2659	rBV2	5801	10353	0.71%	0.093%
65	9.762	2688	2697	2712	rBV	22120	35275	2.43%	0.319%
66	9.887	2732	2736	2741	rBV3	262	259	0.02%	0.002%
67	10.035	2779	2782	2784	rVB2	305	183	0.01%	0.002%
68	10.048	2784	2786	2789	rBV2	350	250	0.02%	0.002%
69	10.096	2796	2801	2807	rBV3	478	555	0.04%	0.005%
70	10.205	2832	2835	2837	rBV2	294	197	0.01%	0.002%
71	10.292	2860	2862	2867	rVB4	430	254	0.02%	0.002%

LSC Area Percent Report

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Operator : JC/SP
Sample : K3363-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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	10.331	2871	2874	2877	rVB3	547	387	0.03%	0.003%
73	10.353	2877	2881	2885	rBV4	420	286	0.02%	0.003%
74	10.424	2890	2903	2925	rBV	303916	487921	33.61%	4.406%
75	10.527	2931	2935	2938	rBV3	257	247	0.02%	0.002%
76	10.652	2971	2974	2979	rVV3	315	307	0.02%	0.003%
77	10.736	2997	3000	3001	rBV2	522	320	0.02%	0.003%
78	10.823	3024	3027	3031	rVB2	218	172	0.01%	0.002%
79	10.868	3037	3041	3043	rBV3	318	244	0.02%	0.002%
80	10.961	3067	3070	3073	rBV2	256	193	0.01%	0.002%
81	11.093	3107	3111	3114	rBV4	326	254	0.02%	0.002%
82	11.337	3185	3187	3191	rVB	455	229	0.02%	0.002%
83	11.427	3212	3215	3218	rVB2	335	188	0.01%	0.002%
84	11.479	3218	3231	3251	rBV	439134	700968	48.28%	6.329%
85	11.855	3332	3348	3366	rBV	428864	710041	48.90%	6.411%
86	12.183	3448	3450	3456	rVB4	325	221	0.02%	0.002%
87	12.337	3496	3498	3500	rBV2	357	195	0.01%	0.002%
88	12.366	3505	3507	3512	rVB3	415	271	0.02%	0.002%
89	12.398	3514	3517	3521	rBV2	269	247	0.02%	0.002%
90	12.440	3528	3530	3534	rBV3	324	174	0.01%	0.002%
91	12.614	3580	3584	3587	rVB4	279	217	0.01%	0.002%
92	12.713	3612	3615	3618	rBV2	352	213	0.01%	0.002%
93	12.794	3638	3640	3643	rVB2	463	229	0.02%	0.002%
94	12.839	3652	3654	3656	rBV2	355	186	0.01%	0.002%
95	13.038	3713	3716	3718	rBV2	278	186	0.01%	0.002%
96	13.080	3726	3729	3732	rBV2	415	202	0.01%	0.002%
97	13.247	3778	3781	3784	rBV	381	258	0.02%	0.002%
98	13.479	3850	3853	3858	rBV4	446	389	0.03%	0.004%
99	13.729	3927	3931	3934	rVB2	520	381	0.03%	0.003%
100	14.215	4080	4082	4084	rBV2	432	245	0.02%	0.002%

Sum of corrected areas: 11074722

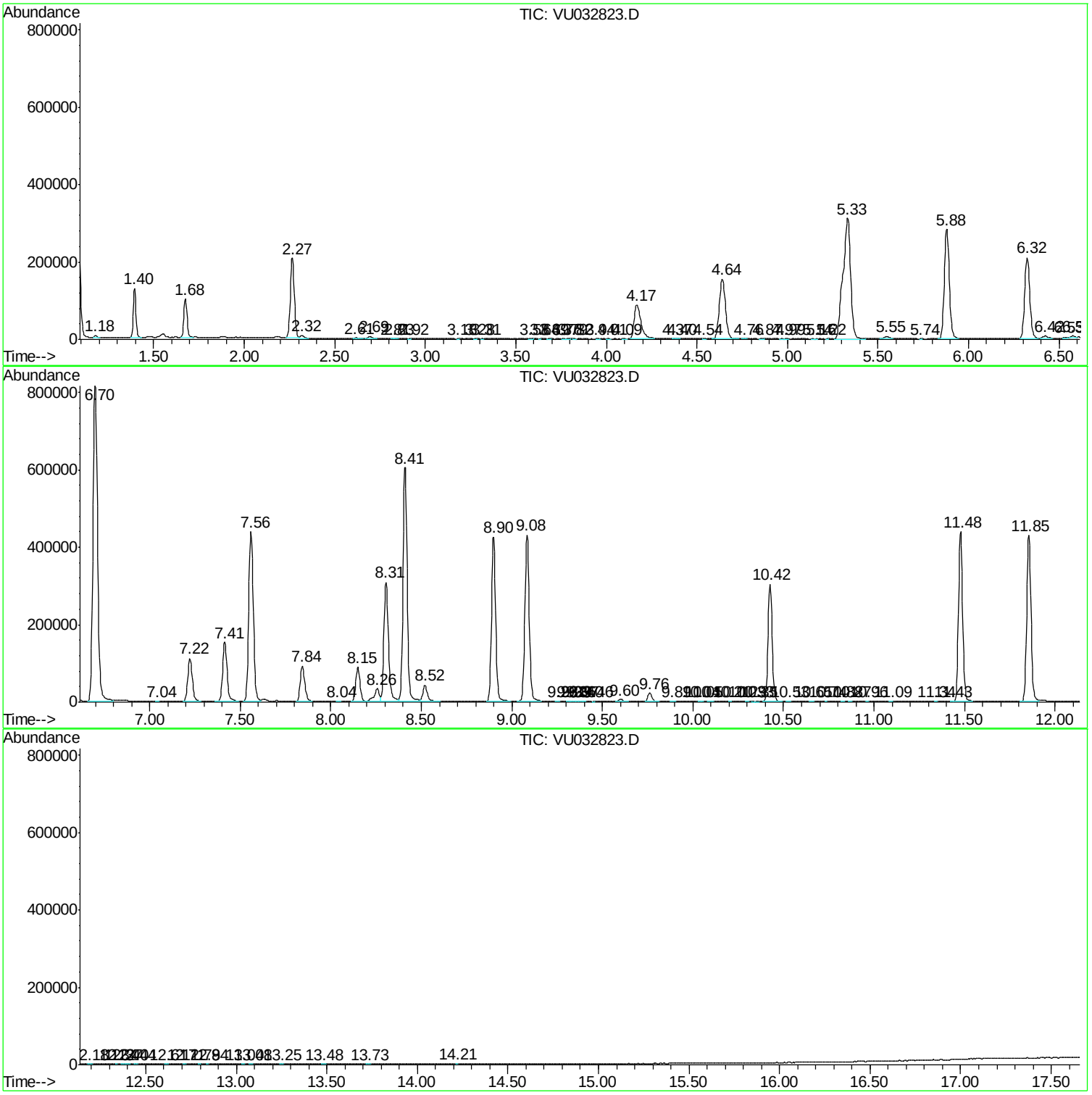
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032823.D
Acq On : 18 Jun 2019 14:46
Operator : JC/SP
Sample : K3363-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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



Library Search Compound Report

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

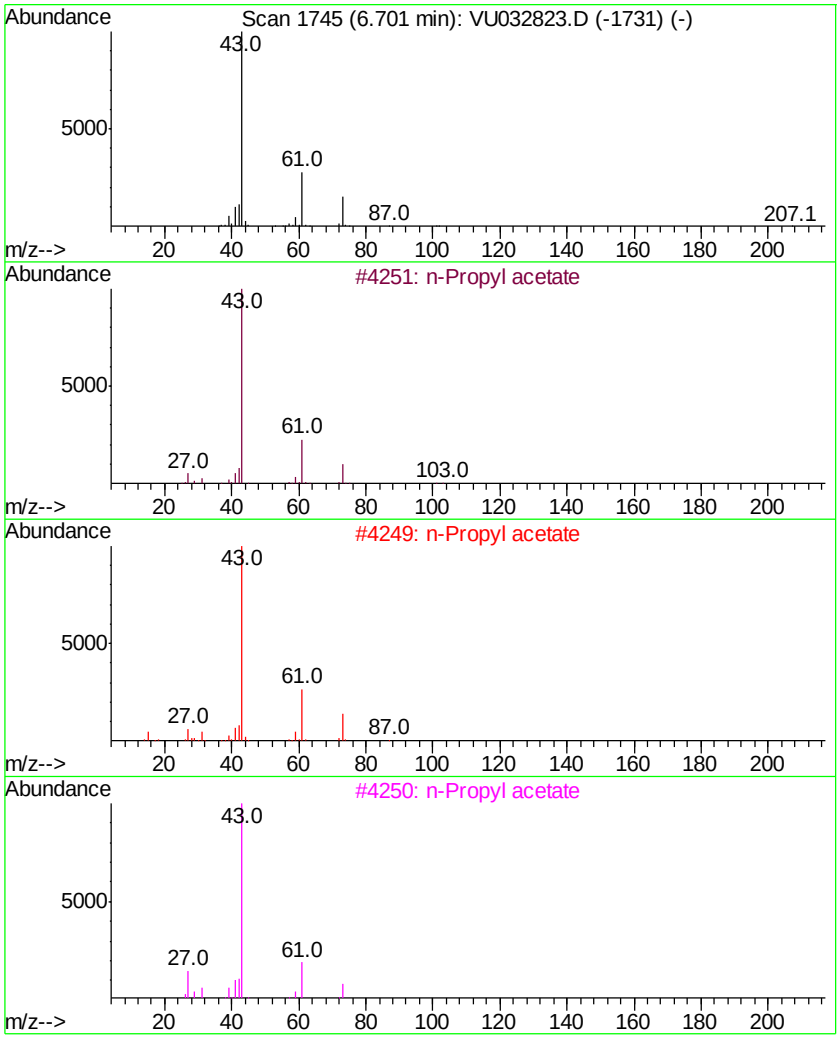
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

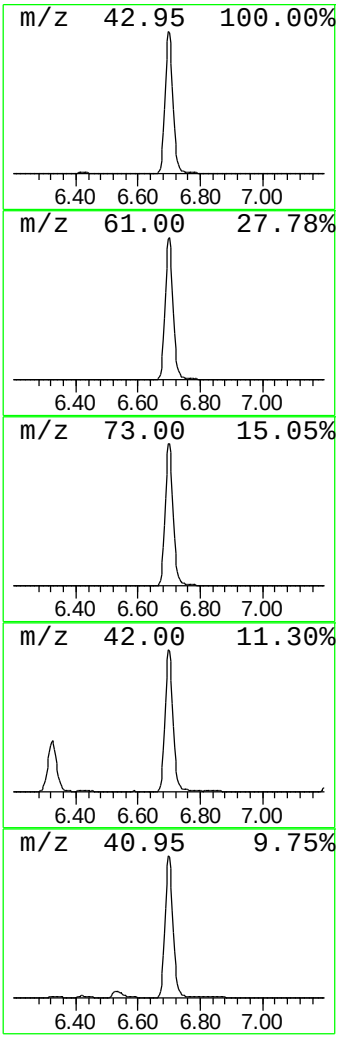
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	131.48 ug/L	1451910	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	64
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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

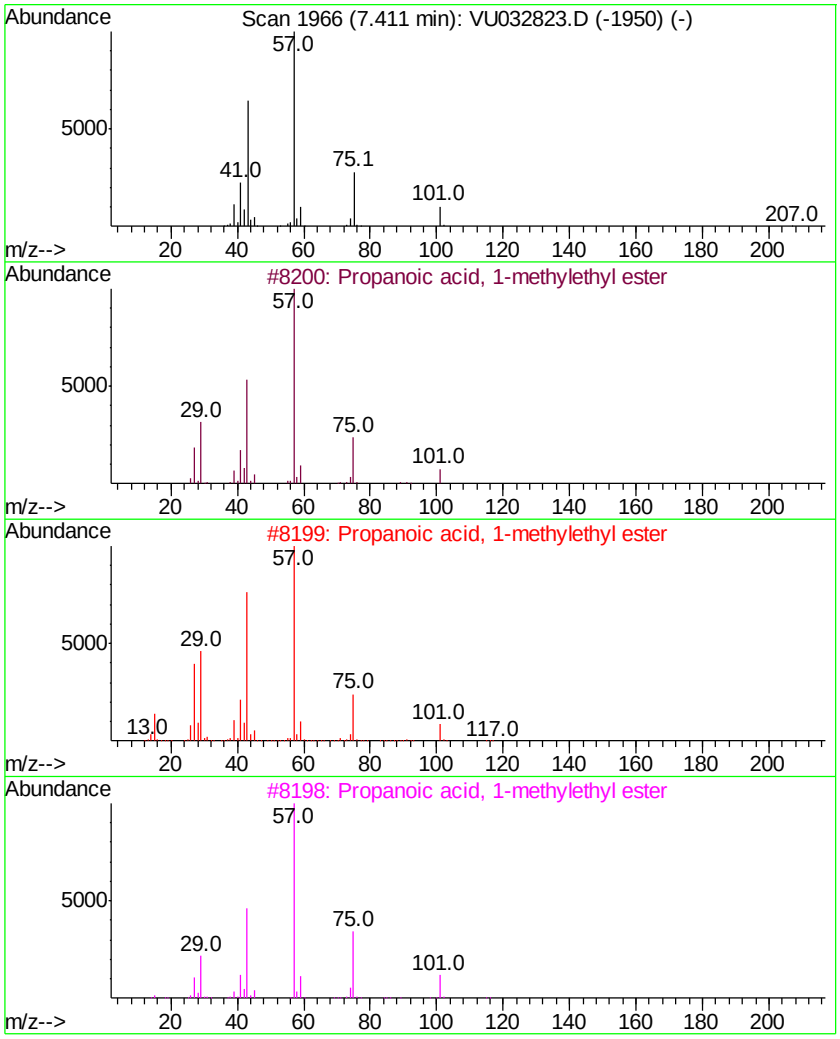
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

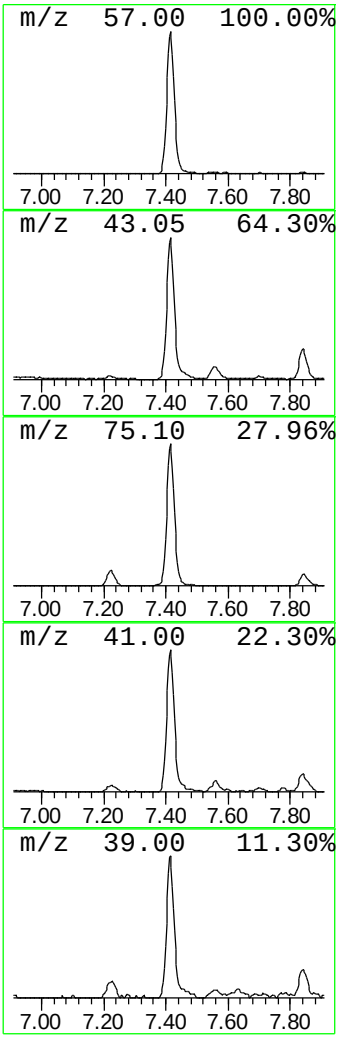
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	24.01 ug/L	265128	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	74
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42
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

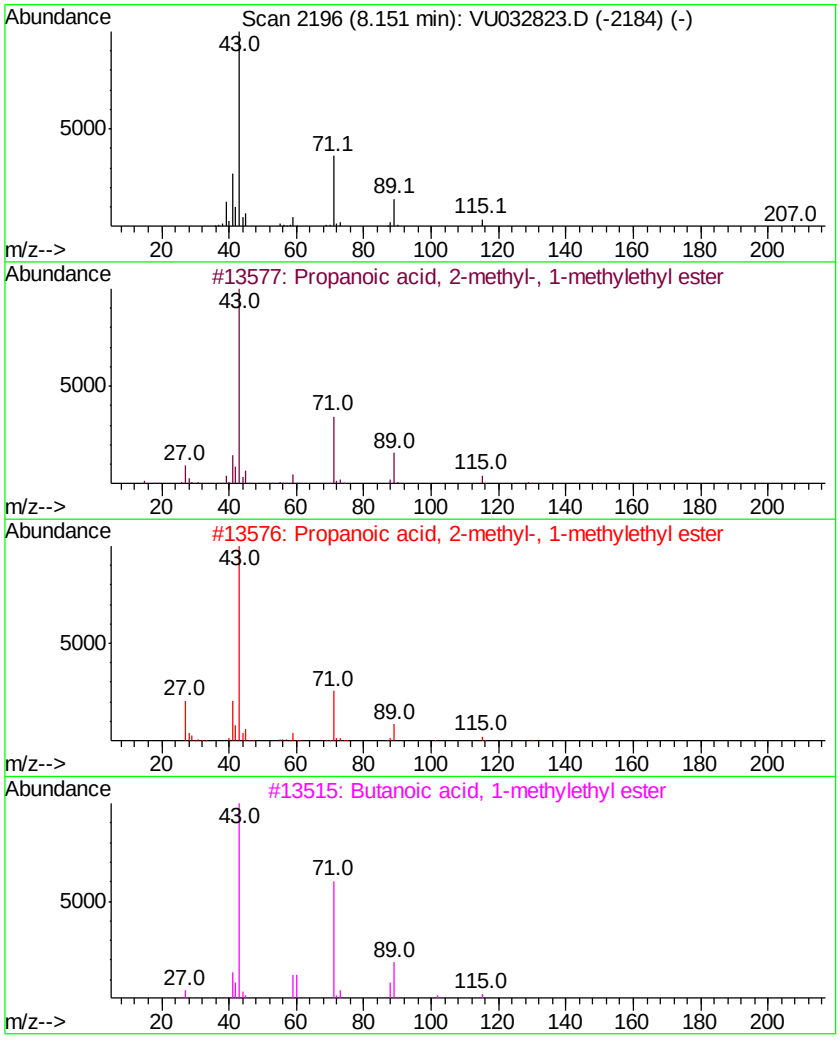
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

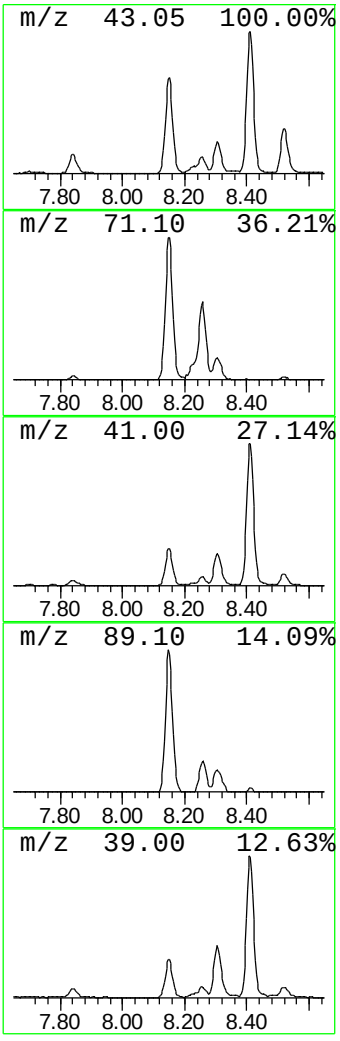
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.22 ug/L	145994	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	78
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : C0JT9

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

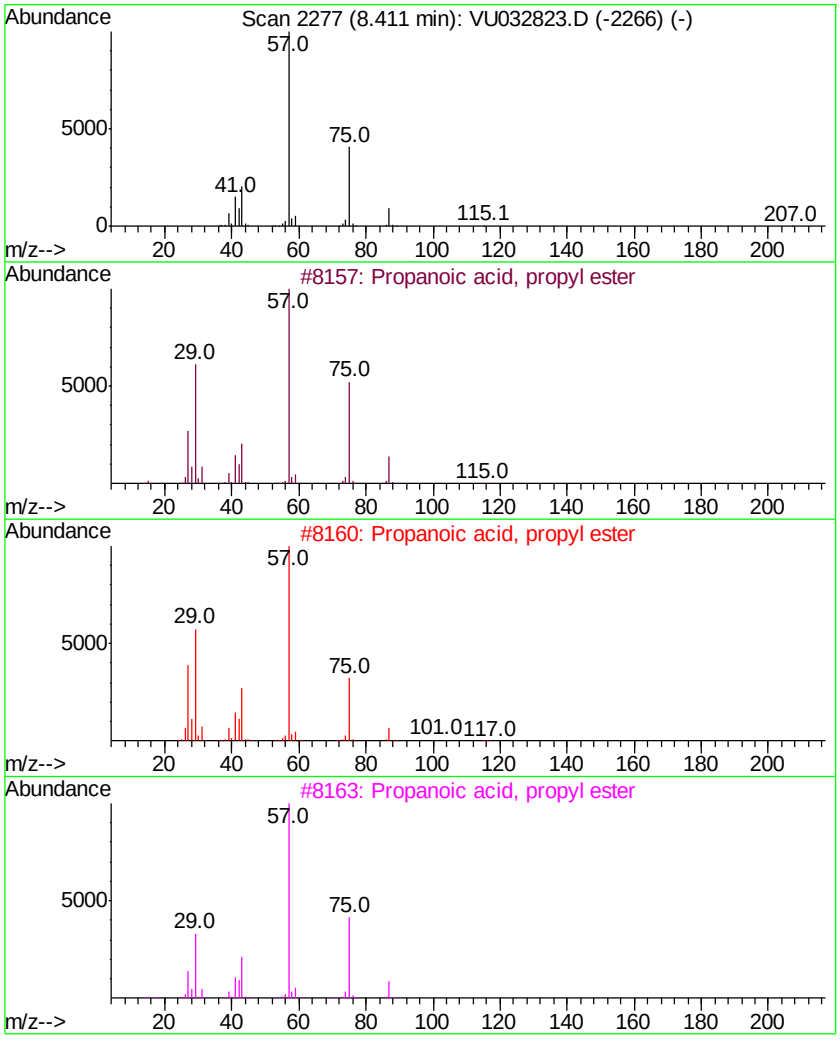
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

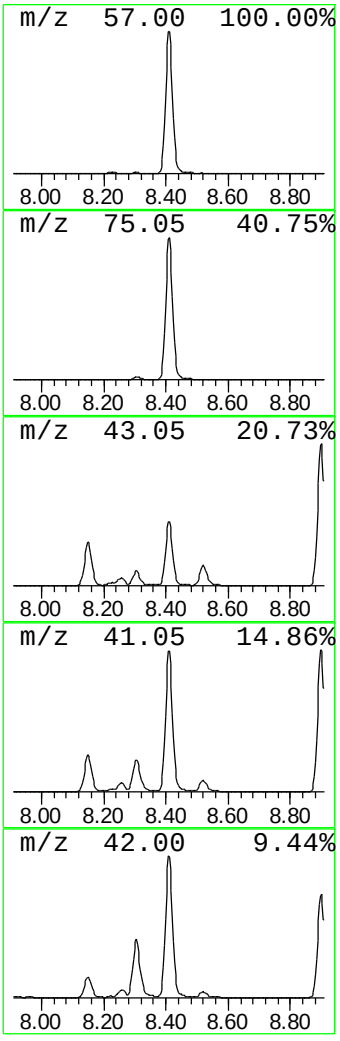
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	67.62 ug/L	966003	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	39





Library Search Compound Report

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Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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

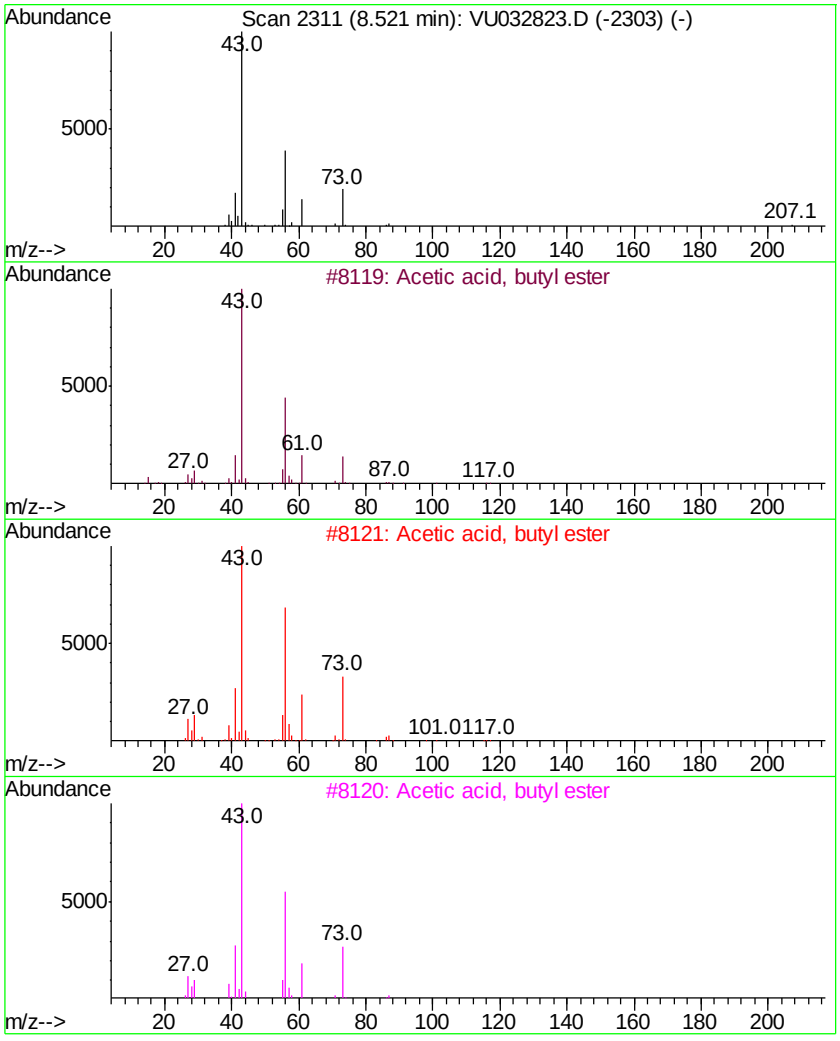
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

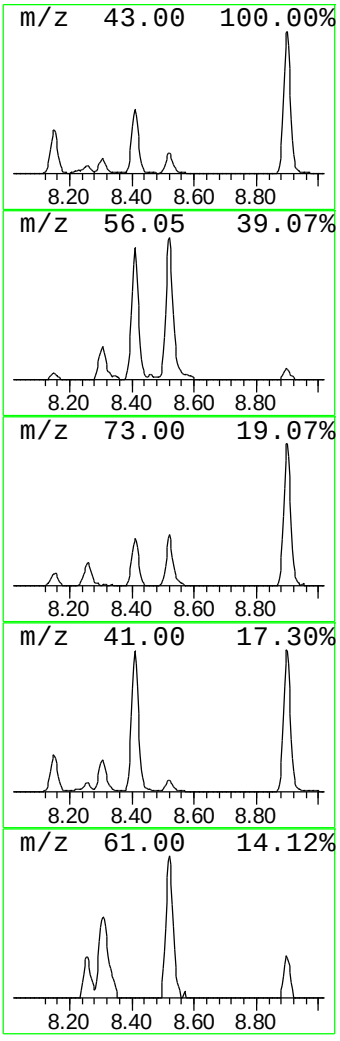
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	5.02 ug/L	71681	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032823.D
Acq On : 18 Jun 2019 14:46
Operator : JC/SP
Sample : K3363-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT9

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

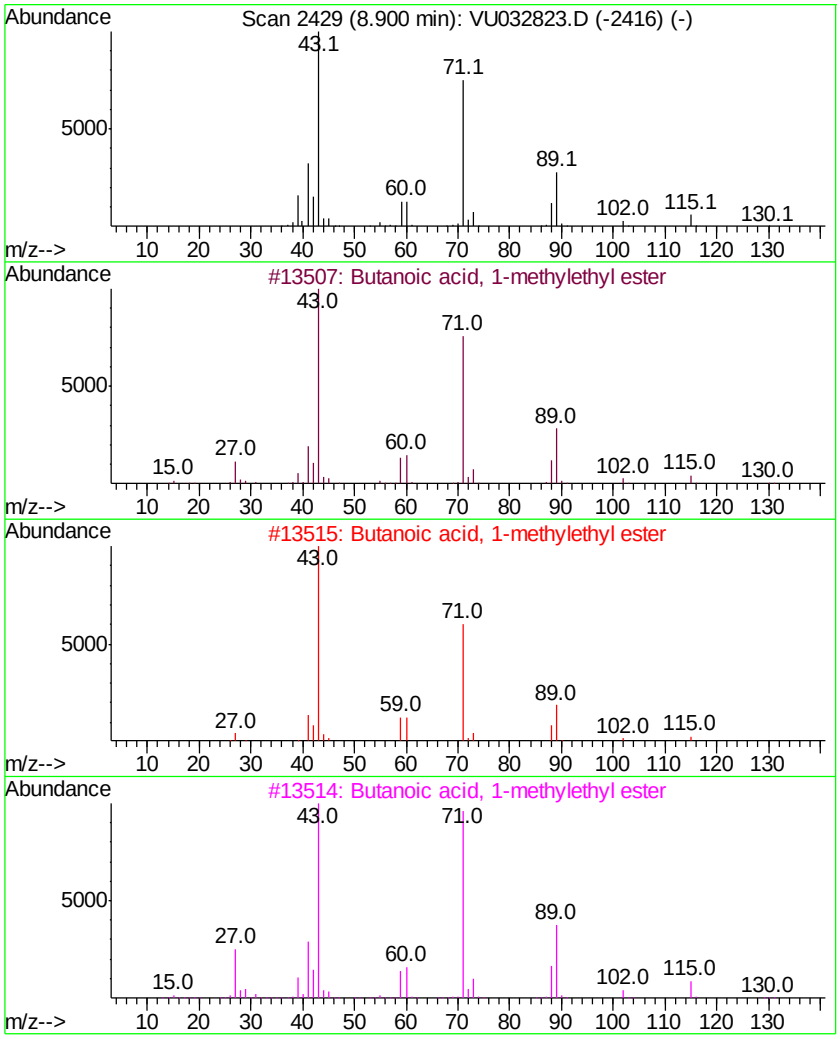
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

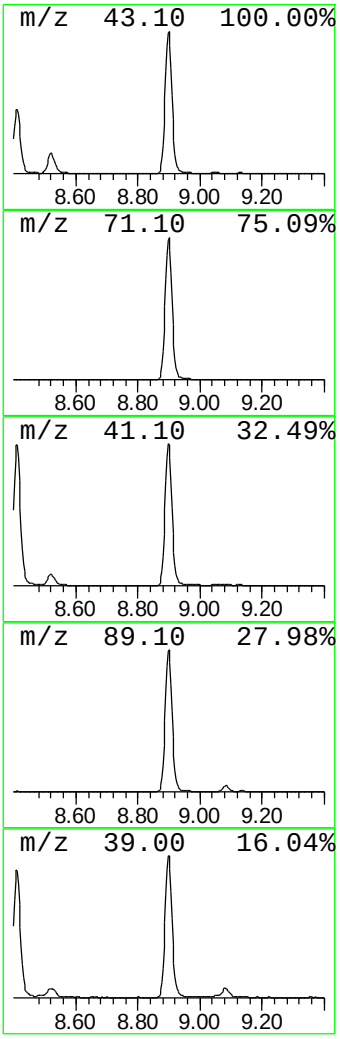
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	46.87 ug/L	669550	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

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ClientSampleId : C0JT9

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	131.5	ug/L	1451910	1	5.88	552138	50.0
Propanoic acid, 1...	7.41	24.0	ug/L	265128	1	5.88	552138	50.0
Propanoic acid, 2...	8.15	10.2	ug/L	145994	2	9.08	714275	50.0
Propanoic acid, p...	8.41	67.6	ug/L	966003	2	9.08	714275	50.0
Acetic acid, buty...	8.52	5.0	ug/L	71681	2	9.08	714275	50.0
Butanoic acid, 1-...	8.90	46.9	ug/L	669550	2	9.08	714275	50.0