LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032832.D
Acq On : 18 Jun 2019 18:16
Operator : JC/SP
Sample : K3379-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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	25	28	34	rVB	4506	3642	0.30%	0.036%
2	1.395	88	95	108	rVB	120477	118730	9.85%	1.179%
3	1.675	175	182	199	rVB	95153	116008	9.62%	1.152%
4	2.267	355	366	377	rBV	195658	294079	24.39%	2.921%
5	2.444	412	421	427	rBV6	2161	3422	0.28%	0.034%
6	2.611	469	473	474	rBV3	1235	796	0.07%	0.008%
7	2.694	490	499	513	rVB2	7727	13179	1.09%	0.131%
8	2.862	549	551	556	rVB3	424	318	0.03%	0.003%
9	3.106	622	627	630	rBV3	367	347	0.03%	0.003%
10	3.241	667	669	674	rVV	393	313	0.03%	0.003%
11	3.280	679	681	685	rVB	316	215	0.02%	0.002%
12	3.325	691	695	699	rVB3	260	223	0.02%	0.002%
13	3.424	723	726	731	rVB4	345	281	0.02%	0.003%
14	3.460	734	737	740	rVV2	257	222	0.02%	0.002%
15	3.482	742	744	750	rVB	436	331	0.03%	0.003%
16	3.511	750	753	757	rBV4	401	370	0.03%	0.004%
17	3.627	785	789	790	rBV2	477	324	0.03%	0.003%
18	3.694	806	810	815	rBV3	290	288	0.02%	0.003%
19	3.807	841	845	847	rVB3	334	238	0.02%	0.002%
20	3.823	847	850	852	rVB2	426	239	0.02%	0.002%
21	3.849	852	858	860	rBV	412	356	0.03%	0.004%
22	3.923	877	881	884	rVB3	450	319	0.03%	0.003%
23	3.977	892	898	903	rBV3	451	603	0.05%	0.006%
24	4.019	907	911	914	rVB2	370	289	0.02%	0.003%
25	4.167	944	957	988	rBV	82773	220910	18.32%	2.194%
26	4.389	1023	1026	1030	rVB3	488	317	0.03%	0.003%
27	4.498	1058	1060	1067	rBV3	418	480	0.04%	0.005%
28	4.640	1088	1104	1130	rBV	150946	351455	29.15%	3.491%
29	4.884	1172	1180	1183	rBV3	527	732	0.06%	0.007%
30	4.913	1186	1189	1194	rVB3	379	327	0.03%	0.003%
31	4.942	1194	1198	1201	rBV2	368	256	0.02%	0.003%
32	4.987	1209	1212	1217	rBV2	304	336	0.03%	0.003%
33	5.334	1295	1320	1344	rBV2	302402	885914	73.48%	8.800%
34	5.550	1378	1387	1405	rVB2	5640	12008	1.00%	0.119%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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	5.656	1417	1420	1423	rVV2	342	288	0.02%	0.003%
36	5.743	1445	1447	1452	rVV3	299	243	0.02%	0.002%
37	5.881	1476	1490	1512	rBV	282584	556235	46.13%	5.526%
38	6.325	1614	1628	1646	rBV	202612	406996	33.76%	4.043%
39	6.418	1650	1657	1678	rVB	6717	16051	1.33%	0.159%
40	6.534	1688	1693	1697	rBV3	1748	2195	0.18%	0.022%
41	6.698	1731	1744	1780	rBV	676919	1205701	100.00%	11.977%
42	7.032	1845	1848	1850	rBV	390	293	0.02%	0.003%
43	7.173	1890	1892	1894	rBV	389	244	0.02%	0.002%
44	7.222	1895	1907	1922	rVV	102383	182378	15.13%	1.812%
45	7.334	1940	1942	1944	rBV3	406	223	0.02%	0.002%
46	7.415	1952	1967	1990	rBV	135932	235622	19.54%	2.341%
47	7.559	2000	2012	2029	rBV	417853	724665	60.10%	7.199%
48	7.688	2048	2052	2053	rBV3	937	638	0.05%	0.006%
49	7.845	2090	2101	2119	rBV2	82166	145214	12.04%	1.443%
50	7.948	2130	2133	2140	rVB5	497	386	0.03%	0.004%
51	7.990	2145	2146	2151	rVB2	572	312	0.03%	0.003%
52	8.022	2153	2156	2161	rBV3	396	338	0.03%	0.003%
53	8.151	2182	2196	2211	rBV	73226	121156	10.05%	1.204%
54	8.225	2211	2219	2222	rVV5	8940	12161	1.01%	0.121%
55	8.257	2224	2229	2235	rVV2	23216	34309	2.85%	0.341%
56	8.305	2235	2244	2266	rVV	284606	491847	40.79%	4.886%
57	8.411	2266	2277	2302	rVV	460092	735998	61.04%	7.311%
58	8.521	2303	2311	2327	rVB	26018	45005	3.73%	0.447%
59	8.617	2339	2341	2346	rVB3	544	376	0.03%	0.004%
60	8.900	2416	2429	2461	rBV	323468	512189	42.48%	5.088%
61	9.035	2468	2471	2472	rBV3	611	365	0.03%	0.004%
62	9.083	2472	2486	2512	rVV	428603	711269	58.99%	7.066%
63	9.456	2597	2602	2605	rBV3	492	521	0.04%	0.005%
64	9.492	2610	2613	2617	rVV3	254	213	0.02%	0.002%
65	9.537	2624	2627	2632	rBV3	455	463	0.04%	0.005%
66	9.601	2638	2647	2662	rVV2	5673	10344	0.86%	0.103%
67	9.726	2680	2686	2689	rBV2	474	419	0.03%	0.004%
68	9.762	2689	2697	2716	rVB2	11709	18994	1.58%	0.189%
69	10.035	2779	2782	2789	rVB4	515	434	0.04%	0.004%
70	10.074	2789	2794	2795	rBV3	394	335	0.03%	0.003%
71	10.209	2833	2836	2839	rBV2	270	229	0.02%	0.002%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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	10.286	2856	2860	2863	rBV3	289	257	0.02%	0.003%
73	10.427	2892	2904	2922	rVV	291253	471492	39.11%	4.684%
74	10.537	2934	2938	2942	rBV2	273	297	0.02%	0.003%
75	10.588	2951	2954	2956	rBV2	404	240	0.02%	0.002%
76	10.607	2956	2960	2964	rVB2	631	534	0.04%	0.005%
77	10.685	2979	2984	2990	rBV2	551	719	0.06%	0.007%
78	10.762	3004	3008	3012	rBV3	499	509	0.04%	0.005%
79	10.881	3041	3045	3049	rBV3	498	538	0.04%	0.005%
80	10.961	3066	3070	3076	rVB3	464	508	0.04%	0.005%
81	11.064	3098	3102	3109	rVB4	381	413	0.03%	0.004%
82	11.479	3219	3231	3255	rBV	439782	705011	58.47%	7.003%
83	11.659	3285	3287	3291	rBV3	431	359	0.03%	0.004%
84	11.855	3336	3348	3368	rBV	412133	678271	56.26%	6.738%
85	12.238	3465	3467	3472	rVB3	542	278	0.02%	0.003%
86	12.337	3496	3498	3501	rVB2	418	219	0.02%	0.002%
87	12.434	3524	3528	3530	rVV3	371	222	0.02%	0.002%
88	12.575	3569	3572	3577	rVB3	475	405	0.03%	0.004%
89	12.601	3577	3580	3582	rBV2	513	269	0.02%	0.003%
90	12.723	3615	3618	3620	rBV	301	246	0.02%	0.002%
91	13.141	3745	3748	3750	rBV	330	245	0.02%	0.002%
92	13.189	3760	3763	3765	rBV2	339	229	0.02%	0.002%
93	13.344	3808	3811	3815	rBV2	356	343	0.03%	0.003%
94	13.508	3860	3862	3865	rBV	342	231	0.02%	0.002%
95	13.572	3880	3882	3885	rBV	483	274	0.02%	0.003%
96	13.787	3944	3949	3955	rBV3	550	771	0.06%	0.008%
97	13.938	3993	3996	3997	rBV	399	247	0.02%	0.002%
98	14.202	4075	4078	4079	rBV2	425	230	0.02%	0.002%
99	14.417	4143	4145	4148	rBV2	635	274	0.02%	0.003%
100	14.482	4162	4165	4168	rBV3	688	530	0.04%	0.005%

Sum of corrected areas: 10066677

LSC Report - Integrated Chromatogram

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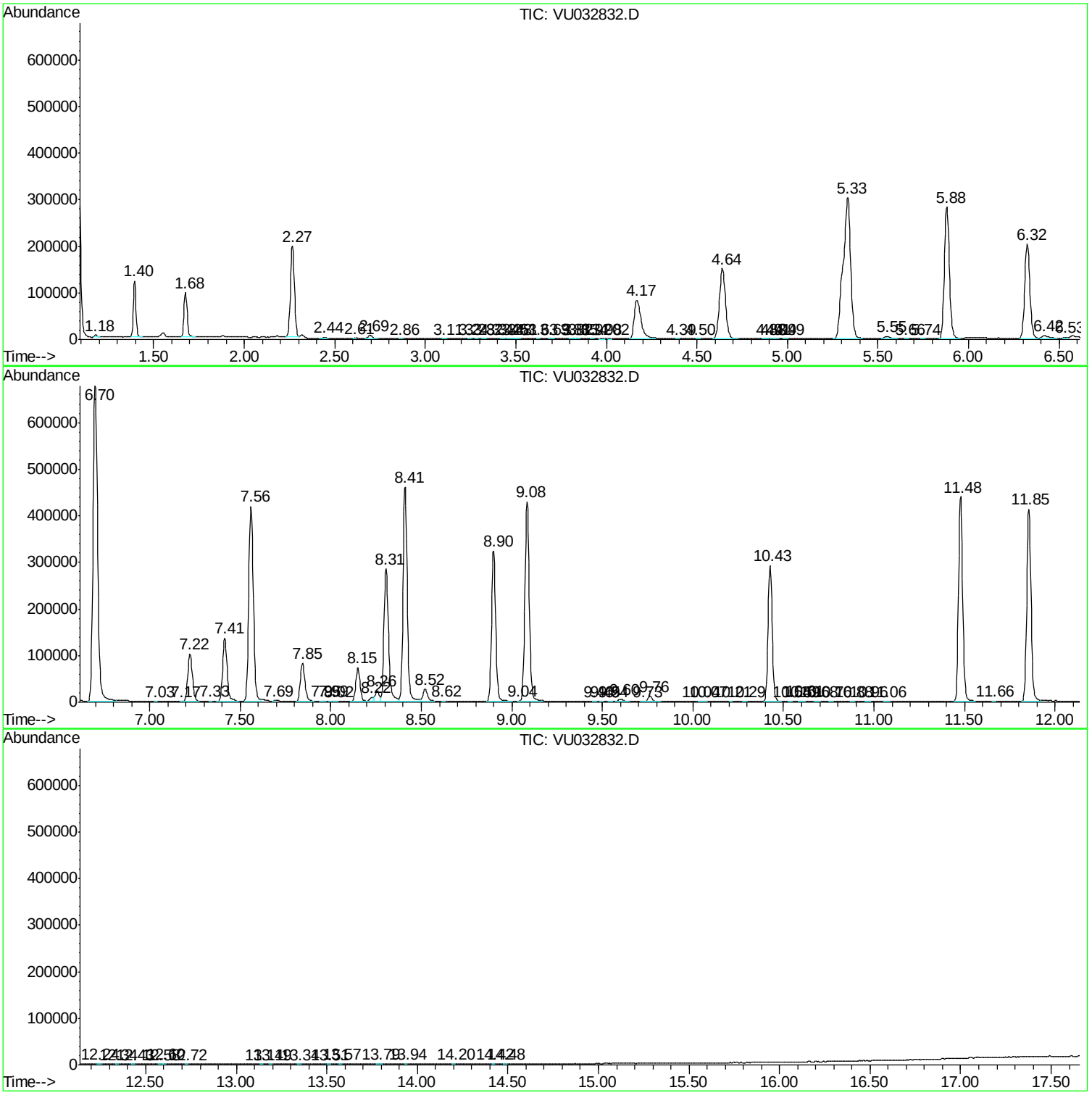
Sample : K3379-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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

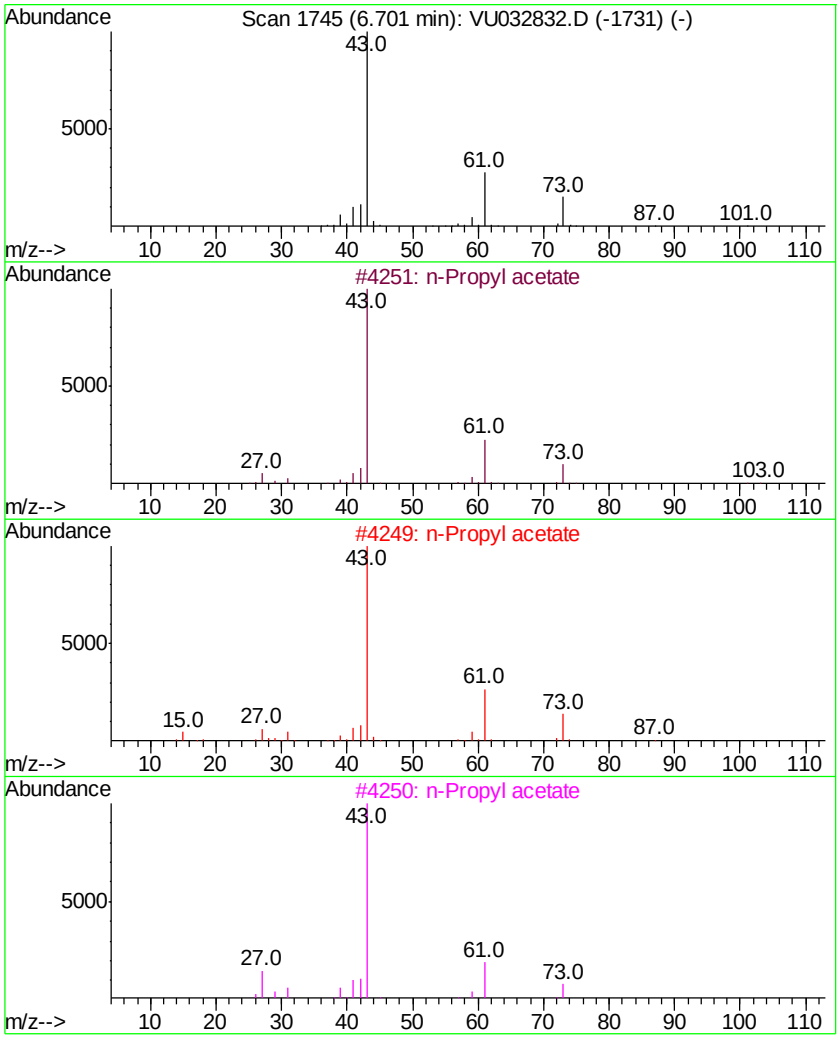
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

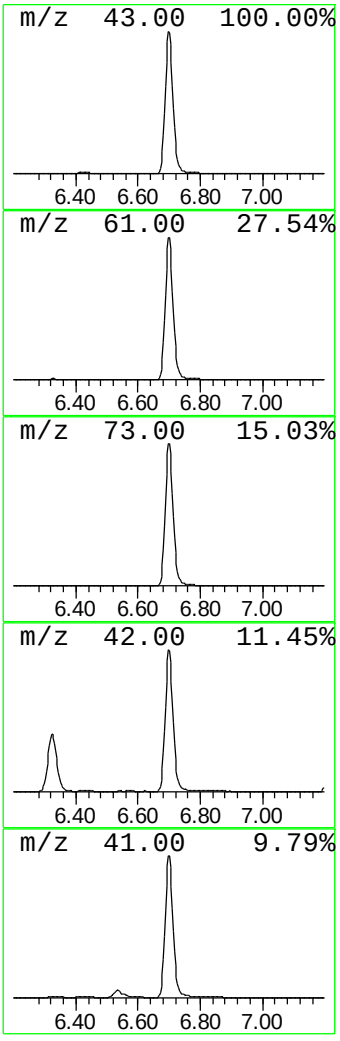
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	108.38 ug/L	1205700	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





Library Search Compound Report

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ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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

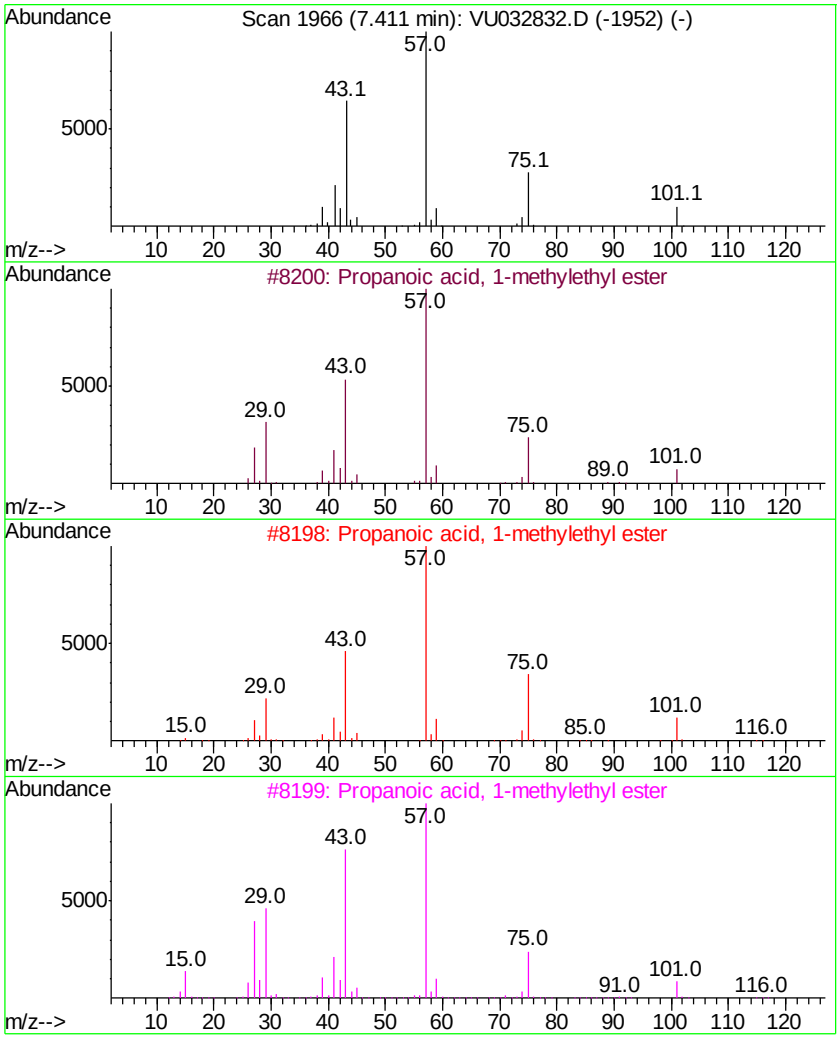
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

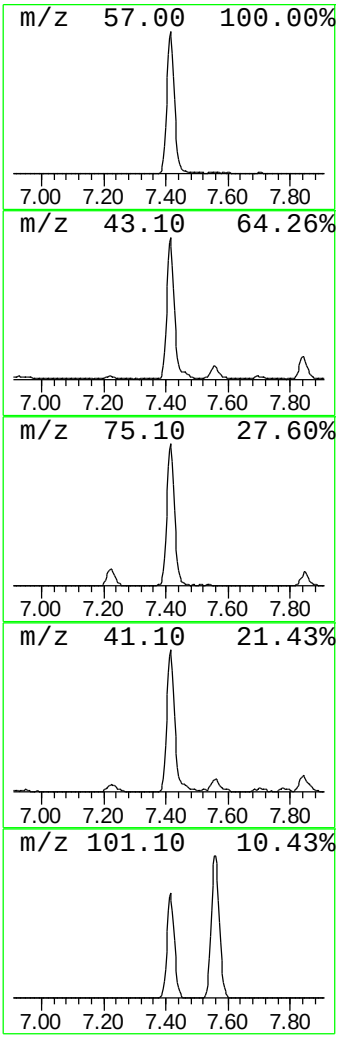
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	21.18 ug/L	235622	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	64
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
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

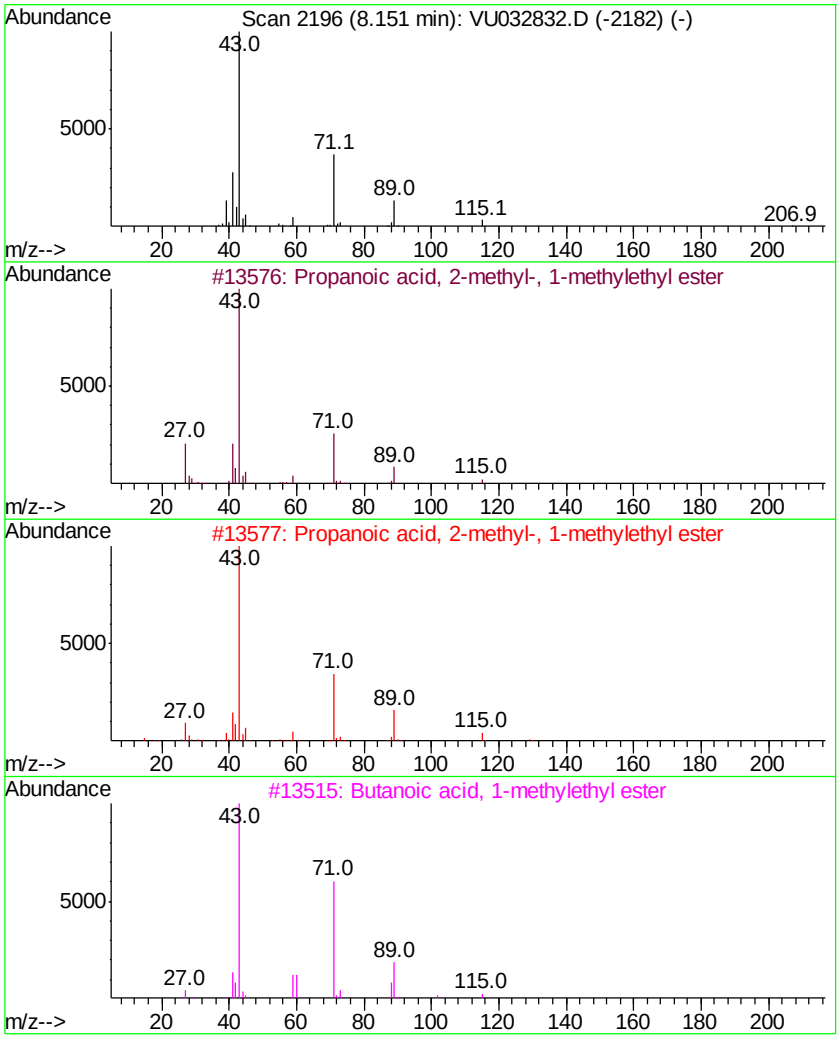
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

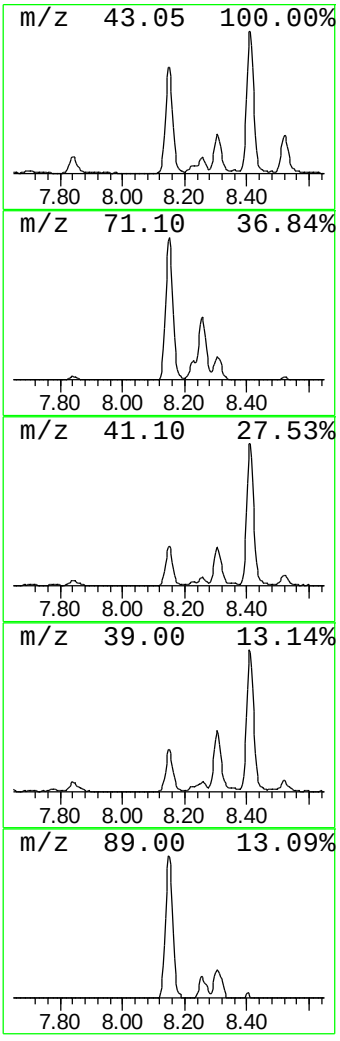
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	8.52 ug/L	121156	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	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50





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ClientSampleId : C0JW0

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

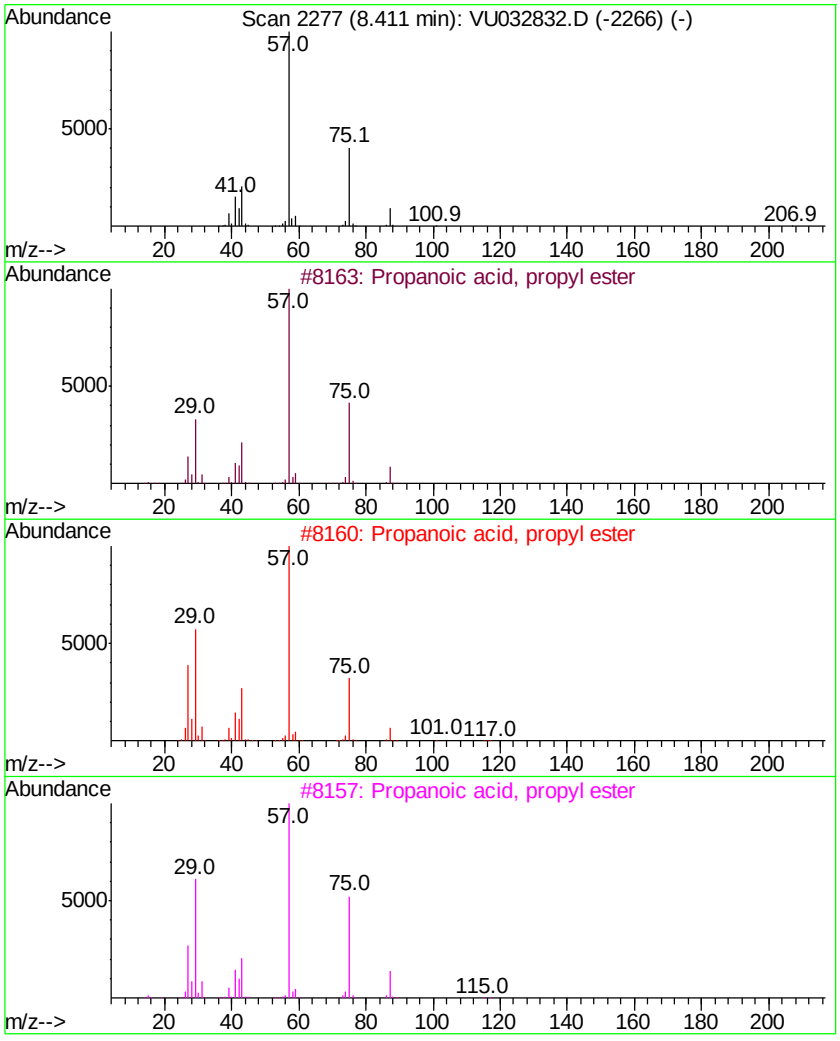
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

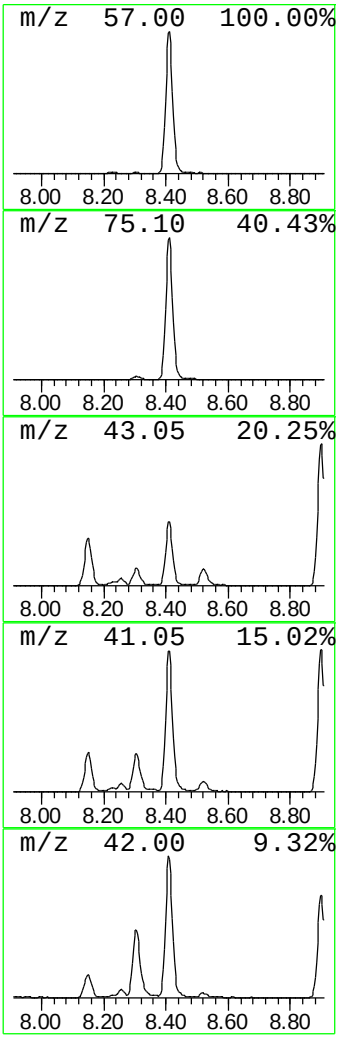
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	51.74 ug/L	735998	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





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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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

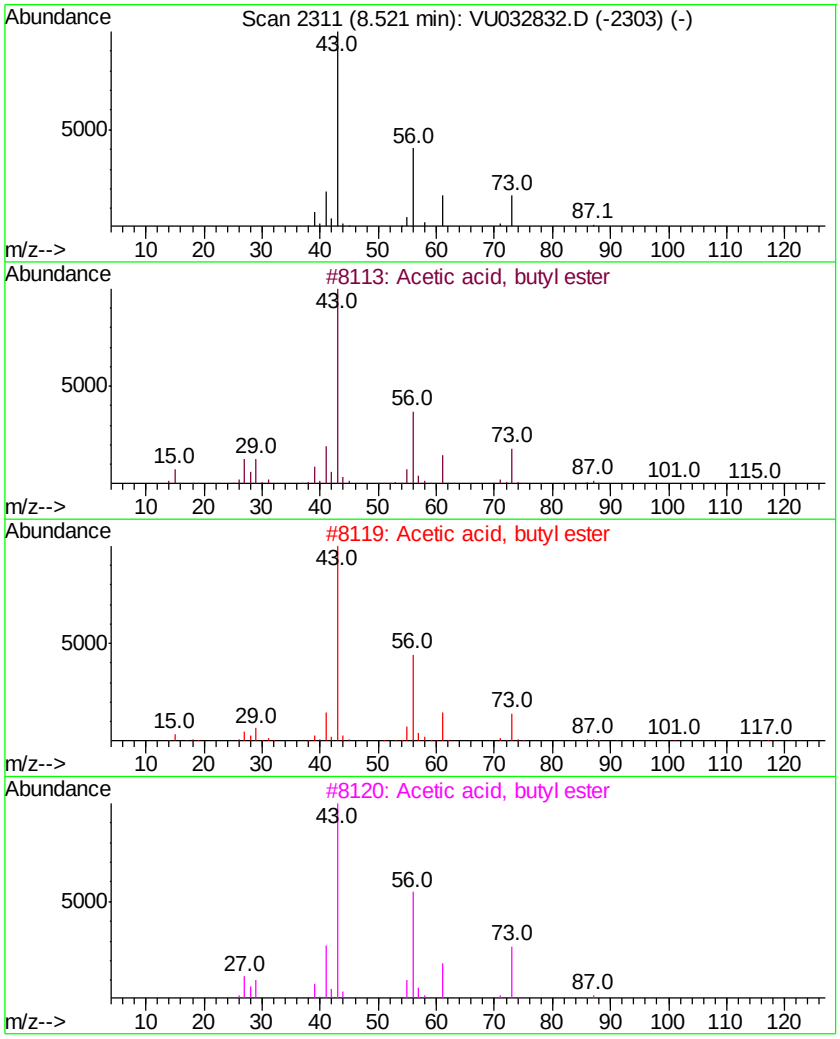
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

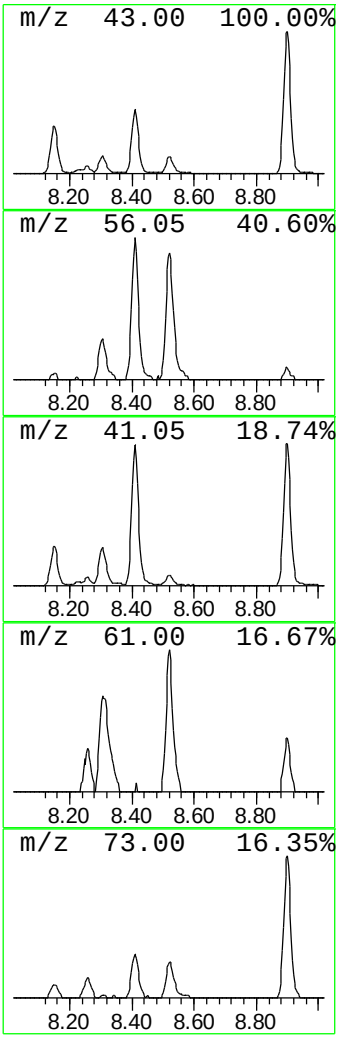
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	3.16 ug/L	45005	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	74
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	39
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032832.D
Acq On : 18 Jun 2019 18:16
Operator : JC/SP
Sample : K3379-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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

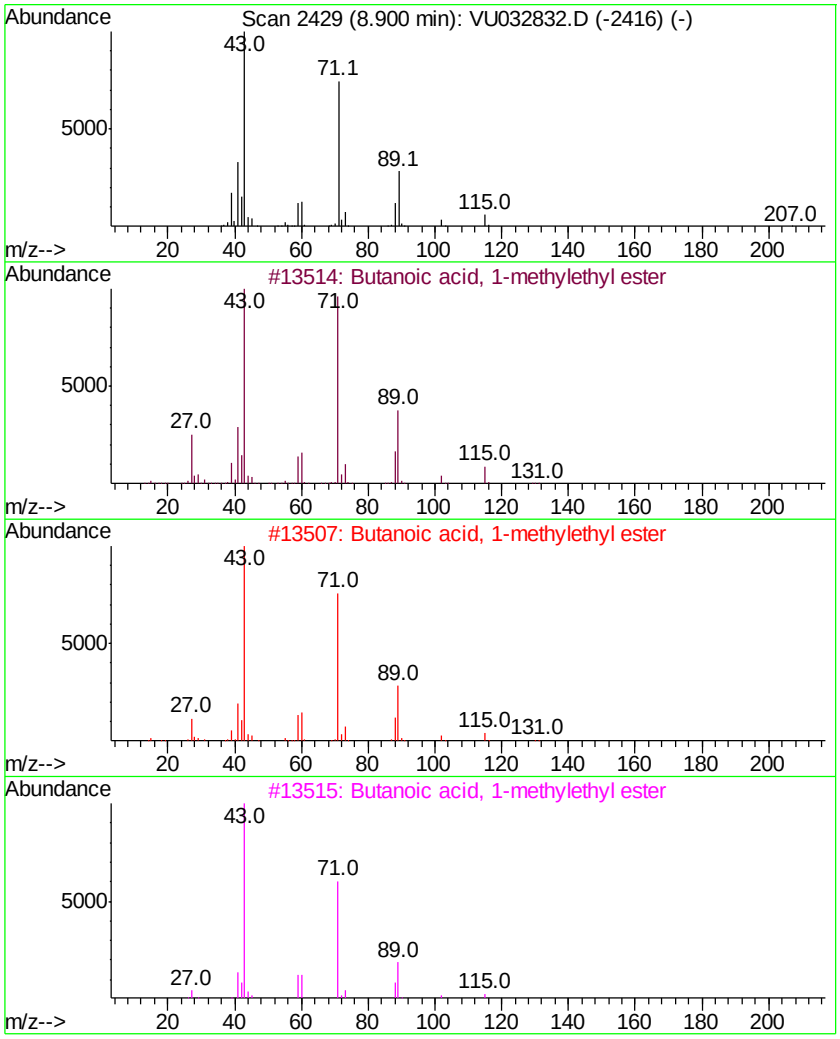
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

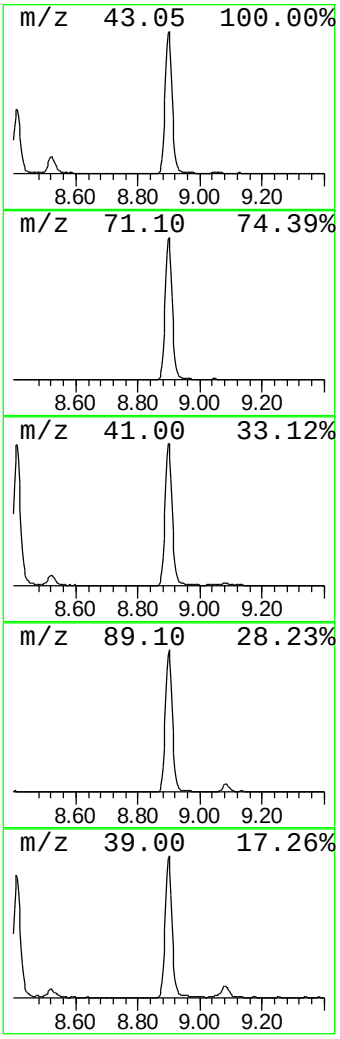
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	36.01 ug/L	512189	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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032832.D
Acq On : 18 Jun 2019 18:16
Operator : JC/SP
Sample : K3379-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JW0

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	108.4	ug/L	1205700	1	5.88	556235	50.0
Propanoic acid, 1...	7.41	21.2	ug/L	235622	1	5.88	556235	50.0
Propanoic acid, 2...	8.15	8.5	ug/L	121156	2	9.08	711269	50.0
Propanoic acid, p...	8.41	51.7	ug/L	735998	2	9.08	711269	50.0
Acetic acid, buty...	8.52	3.2	ug/L	45005	2	9.08	711269	50.0
Butanoic acid, 1-...	8.90	36.0	ug/L	512189	2	9.08	711269	50.0