LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032817.D
Acq On : 18 Jun 2019 12:28
Operator : JC/SP
Sample : K3363-18
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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	24	28	34	rVB2	6788	5665	0.45%	0.058%
2	1.392	88	94	107	rVB	93767	98516	7.79%	1.013%
3	1.675	175	182	195	rVB	81982	99350	7.85%	1.021%
4	2.267	355	366	376	rBV	162384	242697	19.18%	2.495%
5	2.415	408	412	413	rBV2	484	310	0.02%	0.003%
6	2.540	447	451	460	rBV3	630	570	0.05%	0.006%
7	2.611	471	473	477	rBV4	633	548	0.04%	0.006%
8	2.695	489	499	511	rVB2	7869	13056	1.03%	0.134%
9	2.830	534	541	546	rBV4	554	792	0.06%	0.008%
10	2.990	588	591	594	rBV2	306	249	0.02%	0.003%
11	3.142	635	638	644	rVB3	364	309	0.02%	0.003%
12	3.196	647	655	657	rBV4	350	370	0.03%	0.004%
13	3.254	669	673	678	rVB3	411	472	0.04%	0.005%
14	3.283	678	682	684	rBV2	352	334	0.03%	0.003%
15	3.379	707	712	715	rBV3	370	338	0.03%	0.003%
16	3.482	738	744	746	rBV3	287	295	0.02%	0.003%
17	3.653	793	797	801	rVB2	531	492	0.04%	0.005%
18	3.849	856	858	864	rVB	315	247	0.02%	0.003%
19	3.945	887	888	895	rVB2	305	291	0.02%	0.003%
20	3.978	895	898	900	rBV2	405	217	0.02%	0.002%
21	4.087	926	932	935	rBV3	337	410	0.03%	0.004%
22	4.167	943	957	986	rBV2	84532	223728	17.68%	2.300%
23	4.367	1017	1019	1023	rBV3	340	252	0.02%	0.003%
24	4.579	1082	1085	1088	rBV	356	313	0.02%	0.003%
25	4.640	1088	1104	1130	rVV	136012	321395	25.40%	3.304%
26	4.756	1136	1140	1142	rBV3	331	266	0.02%	0.003%
27	4.788	1146	1150	1155	rVB4	504	581	0.05%	0.006%
28	4.817	1155	1159	1165	rBV4	427	589	0.05%	0.006%
29	4.929	1189	1194	1199	rBV2	362	323	0.03%	0.003%
30	5.071	1234	1238	1241	rVB3	326	251	0.02%	0.003%
31	5.235	1284	1289	1291	rBV2	333	227	0.02%	0.002%
32	5.331	1291	1319	1346	rBV2	266787	797230	63.01%	8.196%
33	5.547	1376	1386	1402	rBV3	5655	12480	0.99%	0.128%
34	5.736	1442	1445	1451	rBV3	248	255	0.02%	0.003%

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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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	5.878	1476	1489	1513	rBV	277642	546121	43.16%	5.614%
36	6.180	1573	1583	1598	rVB3	14476	28140	2.22%	0.289%
37	6.325	1612	1628	1646	rBV	186689	371128	29.33%	3.815%
38	6.421	1650	1658	1673	rVB2	5404	10483	0.83%	0.108%
39	6.530	1686	1692	1698	rBV2	2651	4258	0.34%	0.044%
40	6.572	1699	1705	1712	rBV2	4941	7665	0.61%	0.079%
41	6.698	1731	1744	1774	rBV	716479	1265290	100.00%	13.008%
42	7.080	1858	1863	1868	rBV4	429	414	0.03%	0.004%
43	7.222	1895	1907	1923	rBV2	93756	167930	13.27%	1.726%
44	7.328	1938	1940	1944	rVB3	542	345	0.03%	0.004%
45	7.370	1944	1953	1954	rBV2	842	759	0.06%	0.008%
46	7.415	1955	1967	1989	rVV	134755	232909	18.41%	2.394%
47	7.559	1998	2012	2030	rBV	352890	623745	49.30%	6.412%
48	7.842	2088	2100	2122	rBV2	78249	137462	10.86%	1.413%
49	8.013	2150	2153	2157	rBV3	411	298	0.02%	0.003%
50	8.074	2169	2172	2179	rVB2	533	467	0.04%	0.005%
51	8.148	2184	2195	2209	rBV	72489	119565	9.45%	1.229%
52	8.225	2209	2219	2223	rBV3	20758	32485	2.57%	0.334%
53	8.305	2235	2244	2265	rVB	293385	485674	38.38%	4.993%
54	8.408	2266	2276	2301	rVV	482852	764681	60.44%	7.861%
55	8.521	2303	2311	2331	rVB	28410	50736	4.01%	0.522%
56	8.595	2331	2334	2335	rBV	339	216	0.02%	0.002%
57	8.685	2357	2362	2364	rBV	440	353	0.03%	0.004%
58	8.897	2415	2428	2458	rBV	338587	536355	42.39%	5.514%
59	9.083	2466	2486	2519	rBV	425975	710448	56.15%	7.304%
60	9.235	2530	2533	2537	rBV2	405	272	0.02%	0.003%
61	9.328	2558	2562	2565	rVB4	403	277	0.02%	0.003%
62	9.373	2572	2576	2583	rVB3	722	923	0.07%	0.009%
63	9.415	2583	2589	2595	rBV2	187	299	0.02%	0.003%
64	9.501	2614	2616	2620	rVB3	550	357	0.03%	0.004%
65	9.527	2620	2624	2626	rBV2	339	249	0.02%	0.003%
66	9.601	2637	2647	2658	rBV2	4824	8108	0.64%	0.083%
67	9.762	2688	2697	2708	rBV2	13749	22140	1.75%	0.228%
68	9.919	2741	2746	2748	rVV3	275	243	0.02%	0.002%
69	9.935	2748	2751	2754	rVV3	376	300	0.02%	0.003%
70	9.952	2754	2756	2761	rVB2	367	257	0.02%	0.003%
71	10.061	2782	2790	2793	rBV2	264	334	0.03%	0.003%

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ClientSampleId : C0JQ9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Stop Thrs : 0 Peak Location: TOP

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

72	10.424	2888	2903	2927	rBV	280173	457164	36.13%	4.700%
73	10.688	2981	2985	2989	rVB3	473	438	0.03%	0.005%
74	10.714	2989	2993	2994	rBV	521	352	0.03%	0.004%
75	10.800	3016	3020	3022	rBV3	329	217	0.02%	0.002%
76	10.961	3064	3070	3074	rBV2	281	313	0.02%	0.003%
77	11.087	3105	3109	3111	rBV2	282	231	0.02%	0.002%
78	11.157	3128	3131	3133	rVV2	344	233	0.02%	0.002%
79	11.173	3133	3136	3140	rVV2	348	307	0.02%	0.003%
80	11.222	3148	3151	3157	rVB3	430	396	0.03%	0.004%
81	11.254	3157	3161	3162	rBV3	372	279	0.02%	0.003%
82	11.344	3185	3189	3192	rBV2	301	227	0.02%	0.002%
83	11.479	3217	3231	3250	rBV	433483	688051	54.38%	7.073%
84	11.855	3334	3348	3370	rBV	374051	618632	48.89%	6.360%
85	12.180	3444	3449	3452	rBV3	469	407	0.03%	0.004%
86	12.260	3471	3474	3478	rVB3	368	232	0.02%	0.002%
87	12.289	3478	3483	3485	rBV2	326	282	0.02%	0.003%
88	12.360	3501	3505	3507	rBV2	483	296	0.02%	0.003%
89	12.659	3595	3598	3601	rBV2	272	251	0.02%	0.003%
90	12.964	3685	3693	3694	rBV	489	439	0.03%	0.005%
91	12.993	3699	3702	3705	rVB3	457	290	0.02%	0.003%
92	13.160	3750	3754	3759	rVB3	359	345	0.03%	0.004%
93	13.199	3764	3766	3771	rVB	454	236	0.02%	0.002%
94	13.228	3771	3775	3782	rBV2	456	608	0.05%	0.006%
95	14.138	4056	4058	4062	rVB2	556	306	0.02%	0.003%
96	14.176	4068	4070	4073	rBV2	374	227	0.02%	0.002%
97	14.524	4175	4178	4183	rBV2	578	519	0.04%	0.005%
98	14.559	4187	4189	4191	rBV	468	252	0.02%	0.003%
99	14.890	4290	4292	4295	rBV2	579	237	0.02%	0.002%
100	15.096	4354	4356	4358	rBV2	813	481	0.04%	0.005%

Sum of corrected areas: 9727352

LSC Report - Integrated Chromatogram

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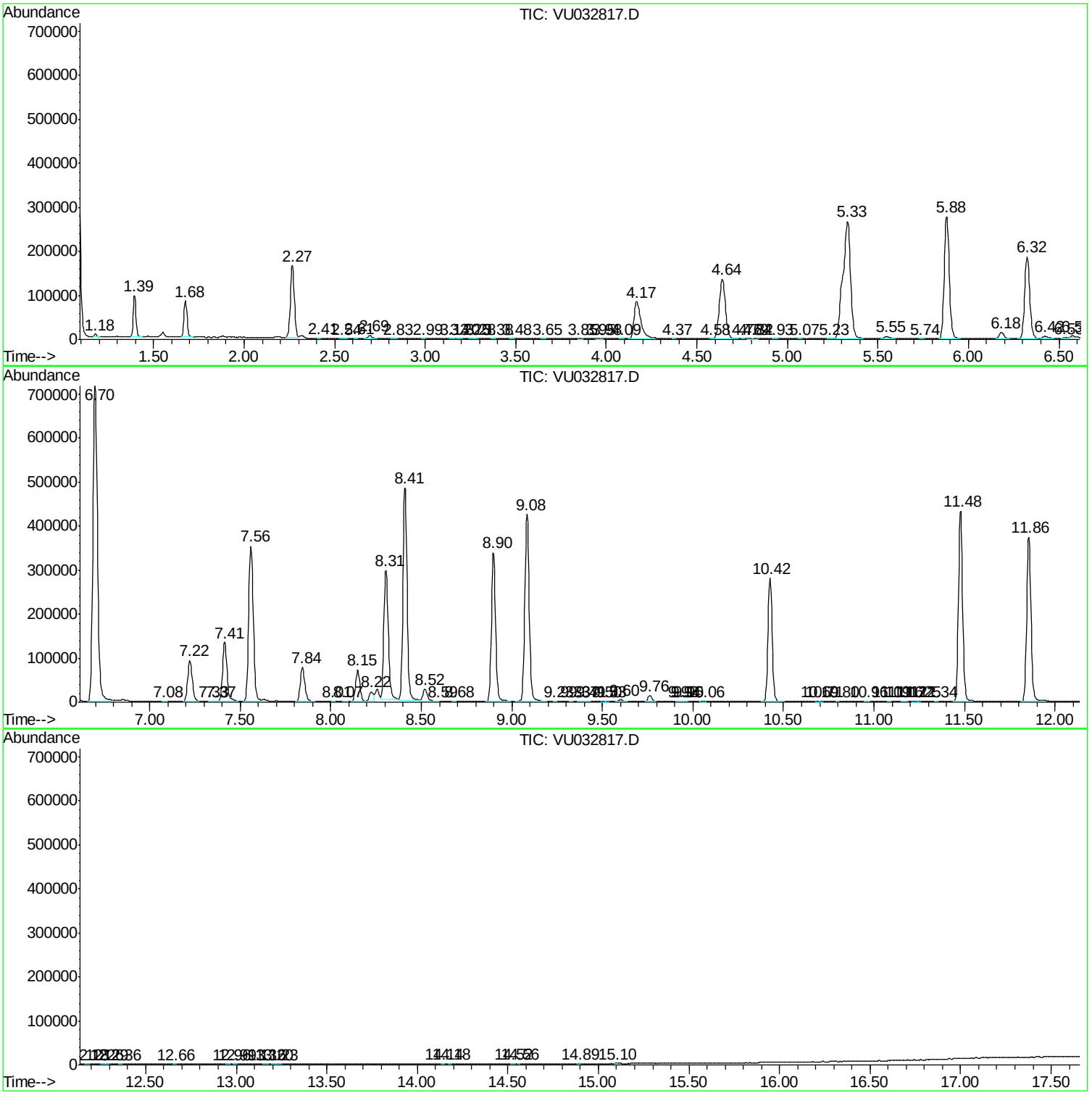
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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

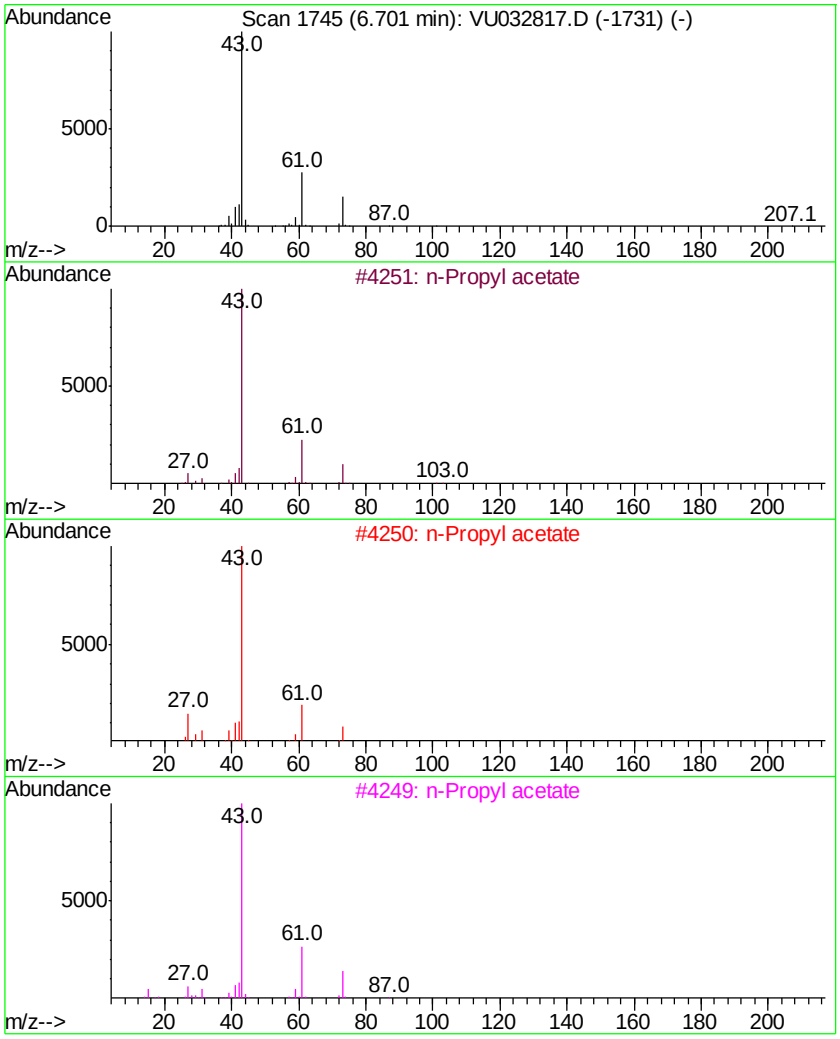
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

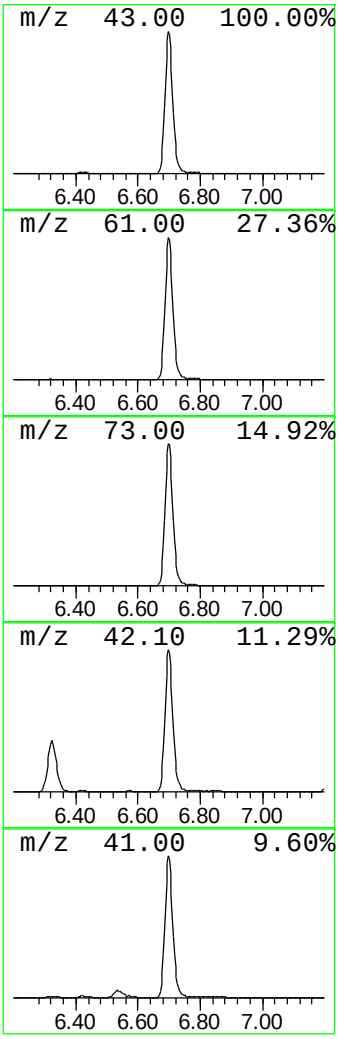
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	115.84 ug/L	1265290	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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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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

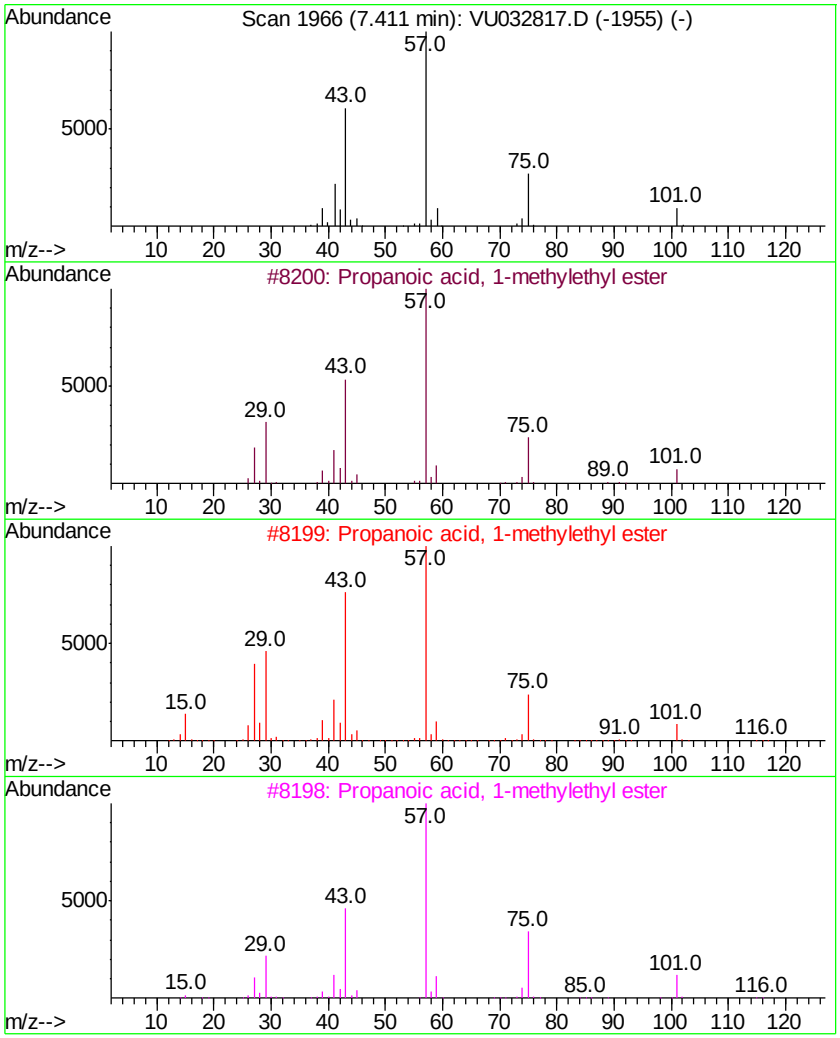
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

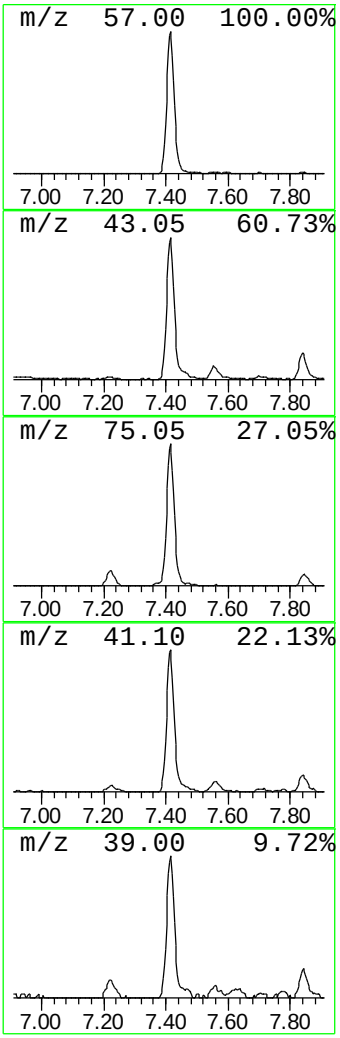
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	21.32 ug/L	232909	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	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

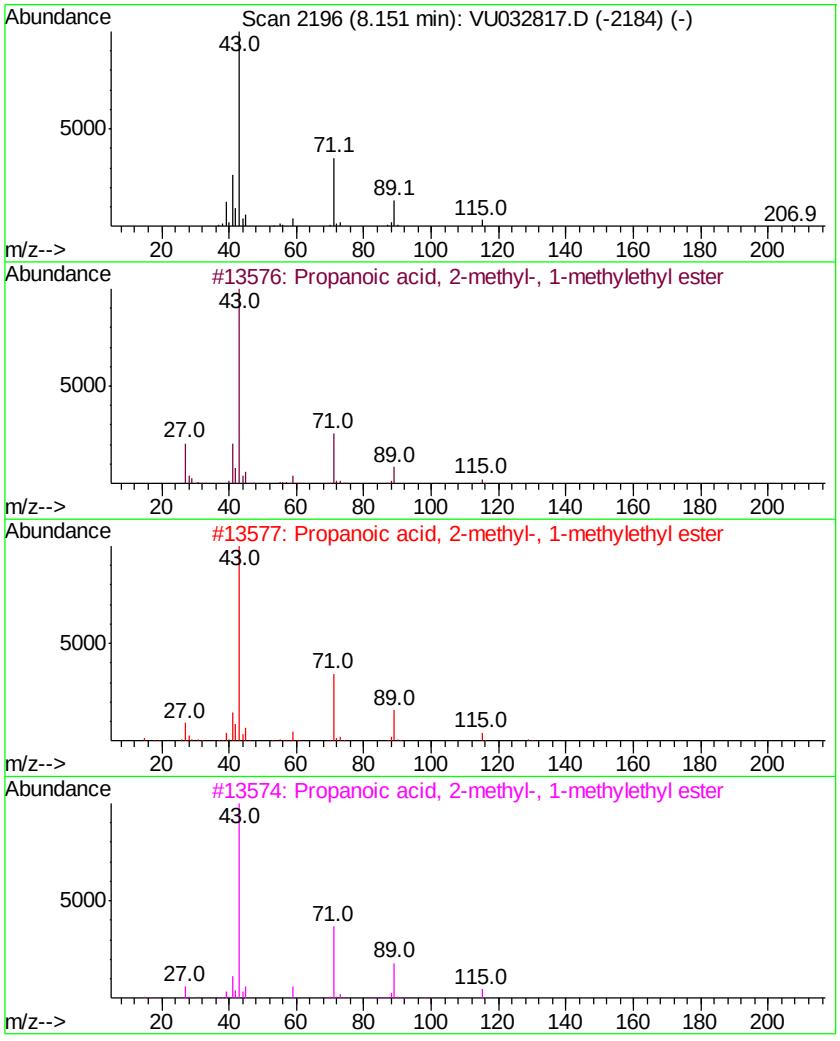
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

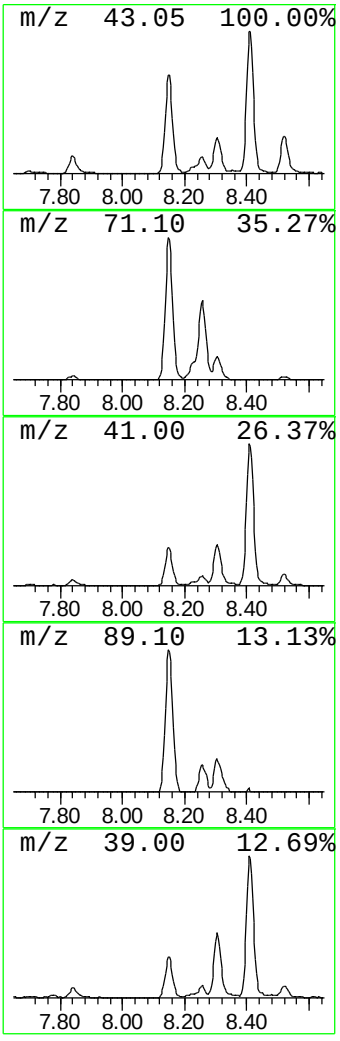
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	8.41 ug/L	119565	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	72
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59





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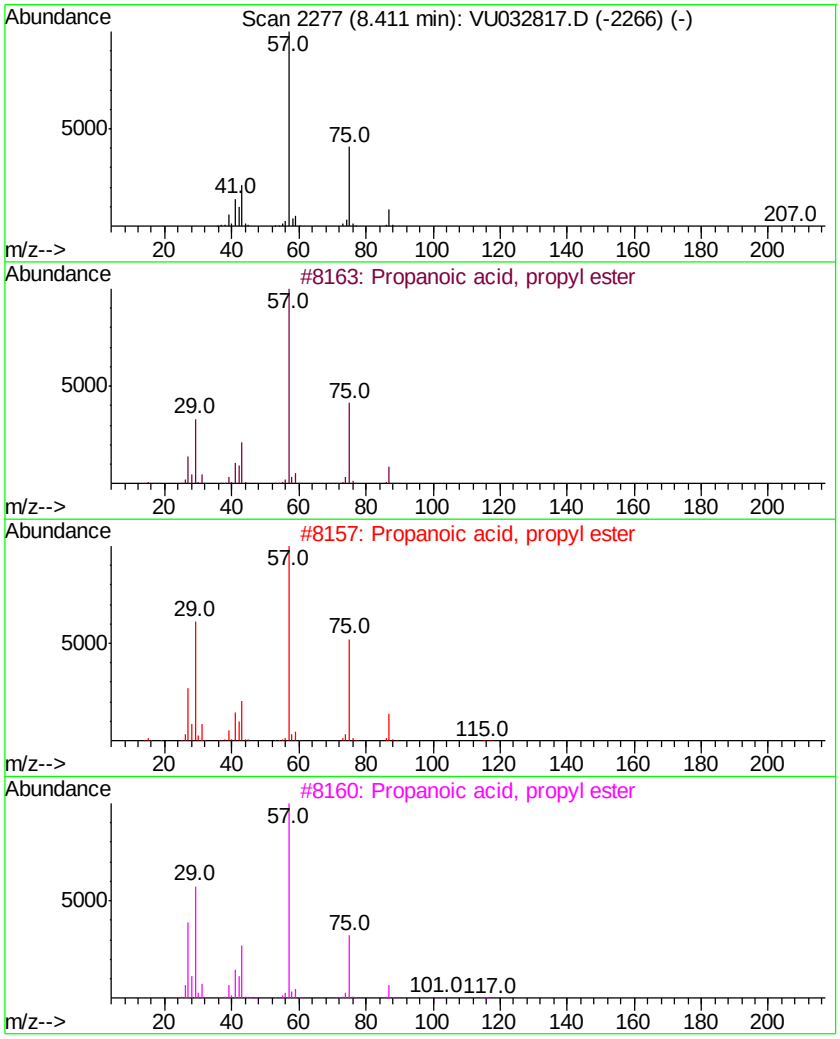
Quant Title : VOC Analysis

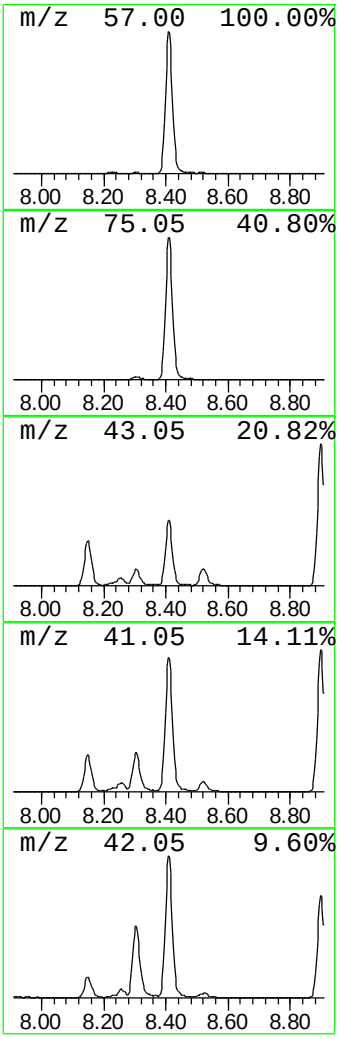
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	53.82 ug/L	764681	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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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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

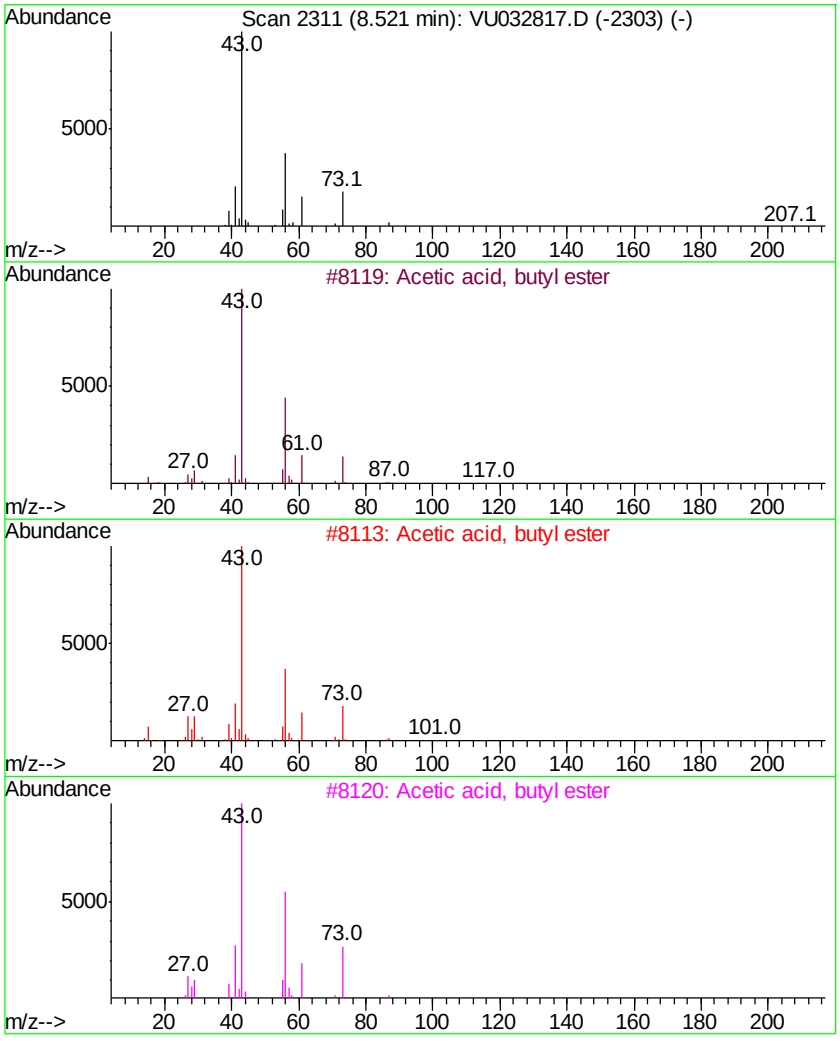
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

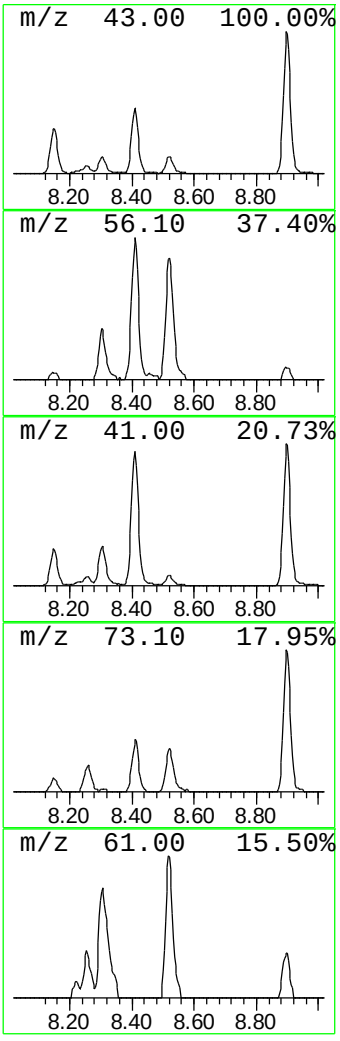
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	3.57 ug/L	50736	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36





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Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032817.D
Acq On : 18 Jun 2019 12:28
Operator : JC/SP
Sample : K3363-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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

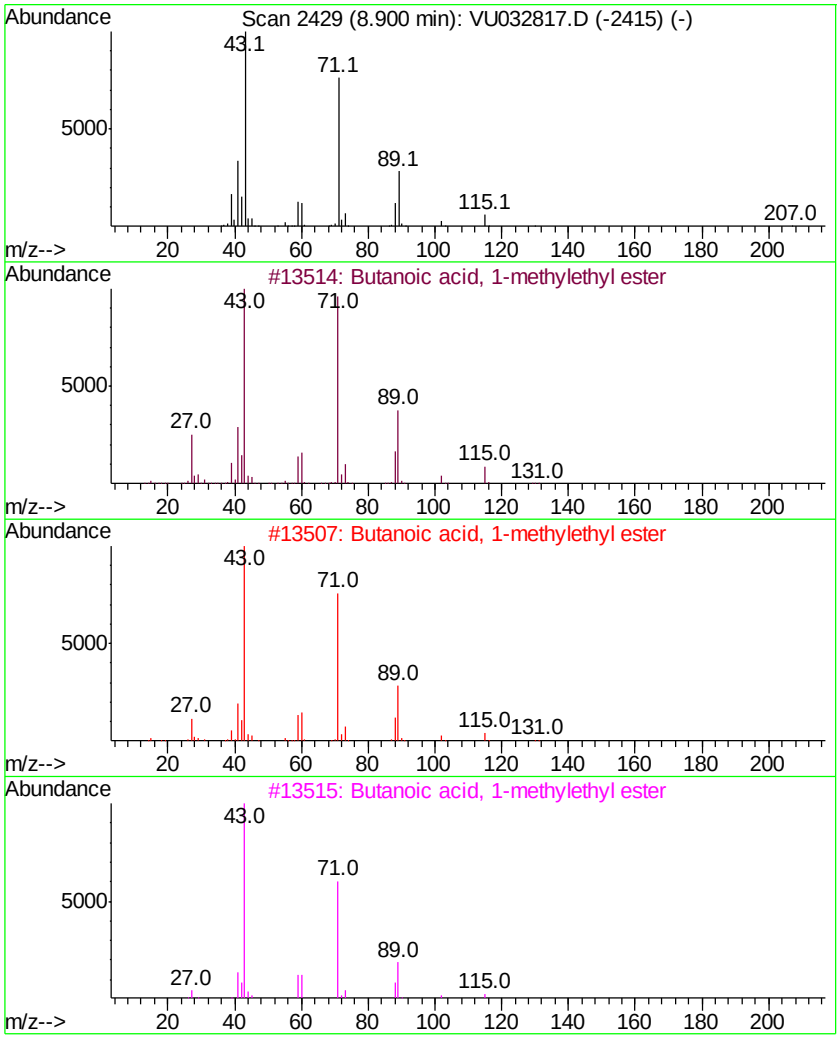
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

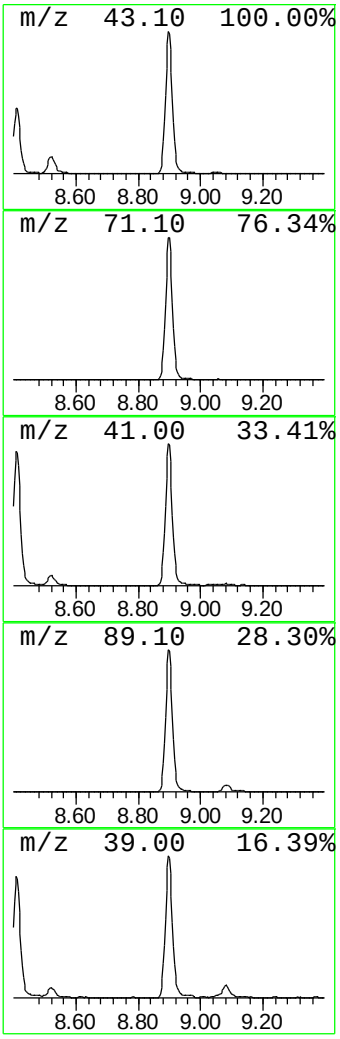
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	37.75 ug/L	536355	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032817.D
Acq On : 18 Jun 2019 12:28
Operator : JC/SP
Sample : K3363-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ9

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	115.8	ug/L	1265290	1	5.88	546121	50.0
Propanoic acid, 1...	7.41	21.3	ug/L	232909	1	5.88	546121	50.0
Propanoic acid, 2...	8.15	8.4	ug/L	119565	2	9.08	710448	50.0
Propanoic acid, p...	8.41	53.8	ug/L	764681	2	9.08	710448	50.0
Acetic acid, buty...	8.52	3.6	ug/L	50736	2	9.08	710448	50.0
Butanoic acid, 1-...	8.90	37.8	ug/L	536355	2	9.08	710448	50.0