LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032682.D
Acq On : 13 Jun 2019 10:32
Operator : JC/SP
Sample : K3286-15
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

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\SOMULM060619WMA.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	36	rVB	4571	3996	0.36%	0.052%
2	1.396	88	95	104	rBV	69731	71059	6.48%	0.921%
3	1.675	175	182	198	rVB	59268	73325	6.69%	0.950%
4	2.267	356	366	377	rBV	119943	182101	16.61%	2.360%
5	2.318	377	382	398	rVB	9475	15611	1.42%	0.202%
6	2.695	491	499	512	rVB	7481	12350	1.13%	0.160%
7	2.826	534	540	541	rBV	228	195	0.02%	0.003%
8	2.949	575	578	585	rBV2	157	188	0.02%	0.002%
9	3.209	654	659	662	rVB2	195	164	0.01%	0.002%
10	3.231	662	666	669	rBV2	192	146	0.01%	0.002%
11	3.254	670	673	678	rVB2	239	197	0.02%	0.003%
12	3.312	688	691	699	rVB2	295	354	0.03%	0.005%
13	3.354	699	704	709	rBV2	139	150	0.01%	0.002%
14	3.421	715	725	739	rVV3	1487	3556	0.32%	0.046%
15	3.502	748	750	755	rVB	382	241	0.02%	0.003%
16	3.527	755	758	761	rBV2	258	185	0.02%	0.002%
17	3.624	784	788	792	rBV2	199	173	0.02%	0.002%
18	4.026	906	913	918	rBV2	254	384	0.04%	0.005%
19	4.170	946	958	991	rBV	65608	173255	15.80%	2.246%
20	4.428	1036	1038	1042	rVB2	357	189	0.02%	0.002%
21	4.643	1089	1105	1133	rBV	101231	238550	21.75%	3.092%
22	4.772	1143	1145	1150	rVB	367	282	0.03%	0.004%
23	4.810	1154	1157	1161	rVB2	329	271	0.02%	0.004%
24	4.891	1176	1182	1189	rBV4	503	789	0.07%	0.010%
25	4.919	1189	1191	1197	rVB2	246	192	0.02%	0.002%
26	4.955	1197	1202	1203	rBV	244	202	0.02%	0.003%
27	5.334	1297	1320	1352	rBV2	195394	582313	53.10%	7.548%
28	5.553	1379	1388	1404	rBV2	4024	8888	0.81%	0.115%
29	5.614	1404	1407	1412	rVB2	475	306	0.03%	0.004%
30	5.730	1440	1443	1446	rVV2	276	180	0.02%	0.002%
31	5.881	1476	1490	1509	rBV	216463	433473	39.53%	5.618%
32	6.325	1615	1628	1648	rBV	137670	272982	24.89%	3.538%
33	6.424	1652	1659	1675	rVV2	5118	10418	0.95%	0.135%
34	6.537	1687	1694	1700	rBV2	1744	3074	0.28%	0.040%

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

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\SOMULM060619WMA.M
Title : VOC Analysis

35	6.579	1700	1707	1713	rBV2	3773	5987	0.55%	0.078%
36	6.698	1732	1744	1777	rBV	606557	1096552	100.00%	14.213%
37	7.054	1852	1855	1861	rVB3	371	278	0.03%	0.004%
38	7.083	1861	1864	1868	rBV3	280	181	0.02%	0.002%
39	7.225	1896	1908	1929	rBV	76946	138630	12.64%	1.797%
40	7.415	1955	1967	1994	rBV	108794	190783	17.40%	2.473%
41	7.559	2000	2012	2031	rBV	262800	459446	41.90%	5.955%
42	7.775	2076	2079	2082	rBV2	323	176	0.02%	0.002%
43	7.794	2082	2085	2089	rVV2	238	219	0.02%	0.003%
44	7.845	2090	2101	2126	rBV2	60802	109303	9.97%	1.417%
45	7.997	2144	2148	2150	rBV3	345	246	0.02%	0.003%
46	8.022	2153	2156	2159	rVB	350	193	0.02%	0.003%
47	8.061	2164	2168	2170	rBV2	175	142	0.01%	0.002%
48	8.151	2183	2196	2213	rBV	57764	98233	8.96%	1.273%
49	8.257	2214	2229	2235	rVV3	24785	45457	4.15%	0.589%
50	8.305	2235	2244	2266	rVV	222202	400733	36.54%	5.194%
51	8.411	2267	2277	2303	rVV	429519	694776	63.36%	9.005%
52	8.521	2304	2311	2326	rVB	26038	44292	4.04%	0.574%
53	8.656	2350	2353	2354	rBV2	241	167	0.02%	0.002%
54	8.730	2374	2376	2379	rVB2	349	206	0.02%	0.003%
55	8.765	2383	2387	2393	rVB2	334	350	0.03%	0.005%
56	8.807	2396	2400	2404	rBV2	207	209	0.02%	0.003%
57	8.900	2417	2429	2464	rBV	283137	457170	41.69%	5.926%
58	9.083	2474	2486	2510	rBV	318028	532813	48.59%	6.906%
59	9.447	2596	2599	2603	rBV2	192	174	0.02%	0.002%
60	9.485	2608	2611	2614	rVB2	256	201	0.02%	0.003%
61	9.524	2620	2623	2626	rBV3	205	180	0.02%	0.002%
62	9.543	2626	2629	2632	rVB2	287	169	0.02%	0.002%
63	9.559	2632	2634	2636	rBV	238	164	0.01%	0.002%
64	9.607	2640	2649	2662	rBV4	3248	5692	0.52%	0.074%
65	9.678	2669	2671	2675	rVB4	338	172	0.02%	0.002%
66	9.765	2688	2698	2716	rBV2	11941	20750	1.89%	0.269%
67	9.852	2723	2725	2728	rVB4	303	184	0.02%	0.002%
68	9.942	2751	2753	2756	rBV2	247	158	0.01%	0.002%
69	9.980	2761	2765	2768	rVV2	225	199	0.02%	0.003%
70	10.000	2768	2771	2774	rVB2	233	151	0.01%	0.002%
71	10.119	2802	2808	2810	rBV	213	174	0.02%	0.002%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

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\SOMULM060619WMA.M
Title : VOC Analysis

72	10.138	2810	2814	2818	rBV2	174	170	0.02%	0.002%
73	10.427	2892	2904	2926	rBV	207872	339222	30.94%	4.397%
74	10.723	2990	2996	2998	rBV2	180	210	0.02%	0.003%
75	10.913	3053	3055	3058	rVB	369	215	0.02%	0.003%
76	10.990	3077	3079	3087	rVB2	271	249	0.02%	0.003%
77	11.479	3219	3231	3255	rBV	314811	510481	46.55%	6.617%
78	11.855	3332	3348	3371	rBV	283109	464879	42.39%	6.025%
79	12.276	3476	3479	3484	rVB2	319	223	0.02%	0.003%
80	12.344	3496	3500	3505	rBV2	169	186	0.02%	0.002%
81	12.485	3540	3544	3547	rBV	261	189	0.02%	0.002%
82	12.530	3554	3558	3562	rVB2	287	219	0.02%	0.003%
83	12.617	3581	3585	3588	rBV2	240	213	0.02%	0.003%
84	12.771	3627	3633	3635	rBV2	215	221	0.02%	0.003%
85	13.028	3710	3713	3718	rVB2	259	213	0.02%	0.003%
86	13.057	3718	3722	3725	rBV2	182	189	0.02%	0.002%
87	13.144	3746	3749	3753	rBB	190	145	0.01%	0.002%
88	13.469	3847	3850	3854	rBV2	234	188	0.02%	0.002%
89	13.569	3878	3881	3883	rBV2	221	169	0.02%	0.002%
90	13.643	3899	3904	3906	rBV2	291	271	0.02%	0.004%
91	13.842	3963	3966	3973	rVB3	403	338	0.03%	0.004%
92	13.974	4004	4007	4010	rVB	262	164	0.01%	0.002%
93	14.102	4043	4047	4050	rBV2	280	302	0.03%	0.004%
94	14.212	4077	4081	4083	rBV2	296	222	0.02%	0.003%
95	14.273	4097	4100	4104	rVB3	265	217	0.02%	0.003%
96	14.302	4104	4109	4114	rBV2	229	289	0.03%	0.004%
97	14.340	4118	4121	4126	rVB3	249	233	0.02%	0.003%
98	14.369	4126	4130	4133	rVB	316	229	0.02%	0.003%
99	14.395	4133	4138	4142	rBV2	403	484	0.04%	0.006%
100	15.054	4340	4343	4345	rBV2	372	278	0.03%	0.004%

Sum of corrected areas: 7715257

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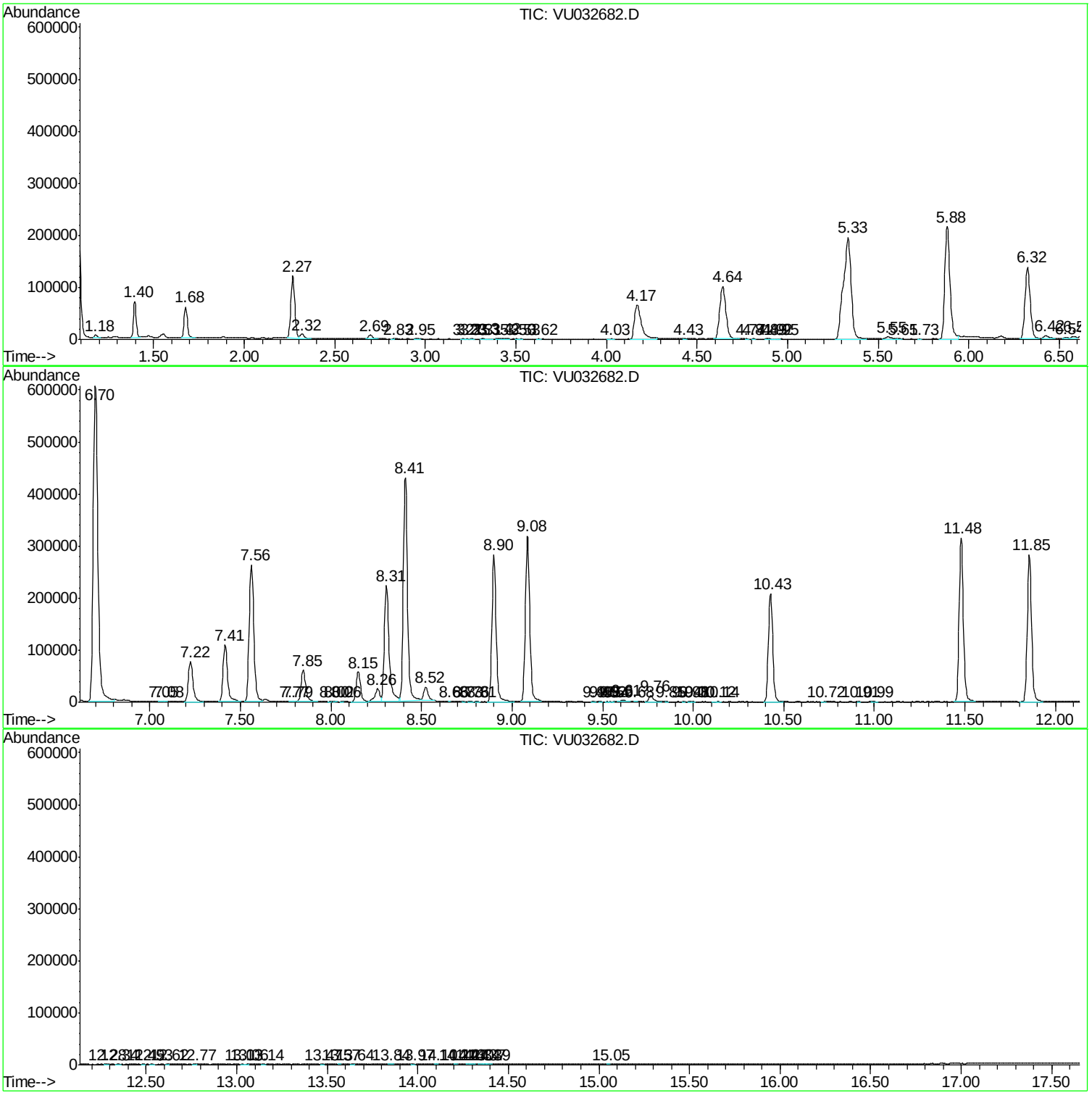
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

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Data File : VU032682.D
Acq On : 13 Jun 2019 10:32
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Quant Title : VOC Analysis

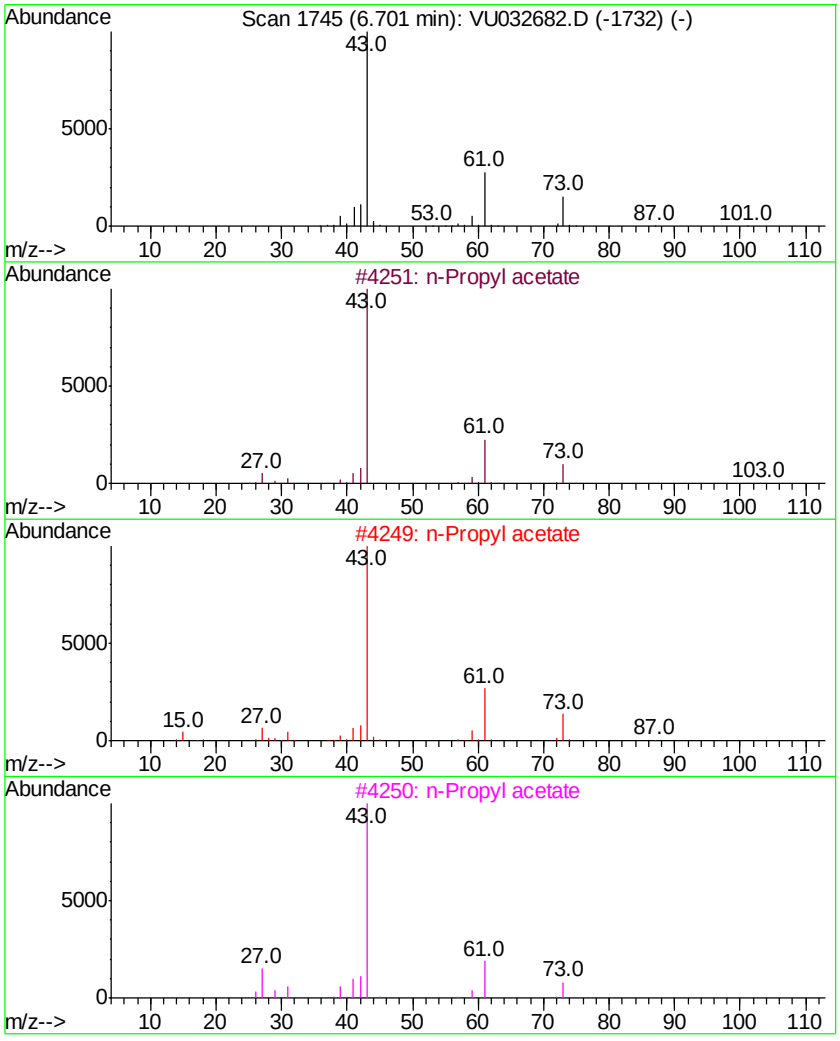
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

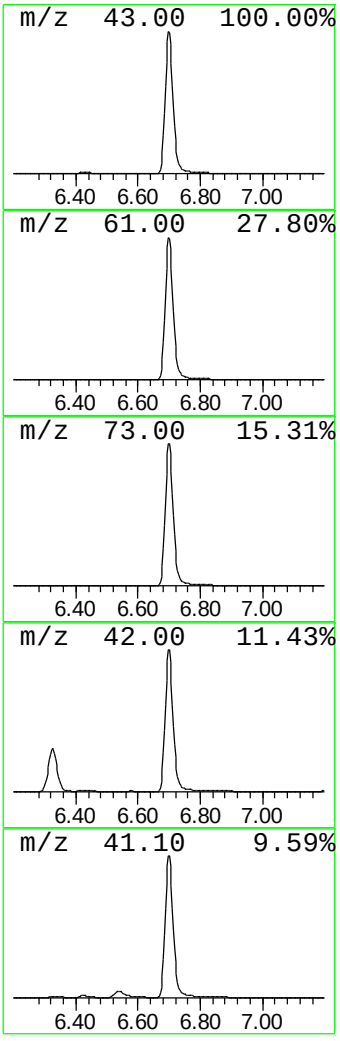
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	126.48 ug/L	1096550	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	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

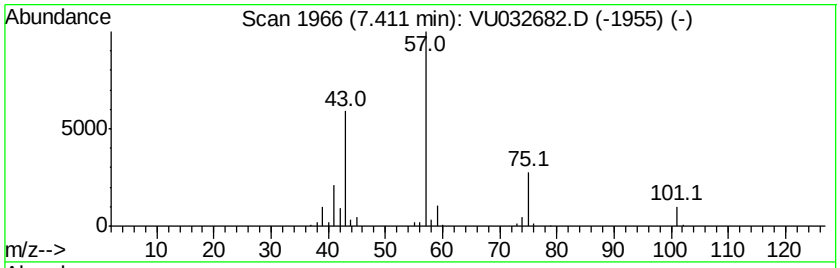
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

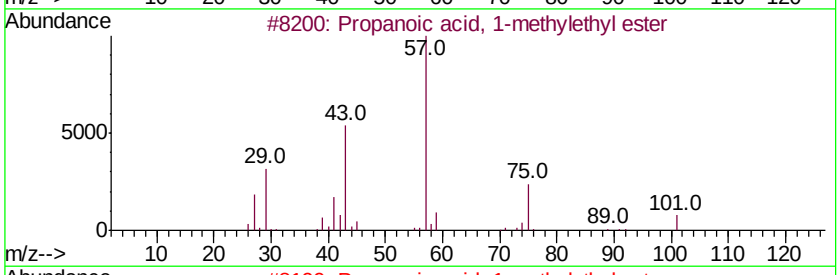
****

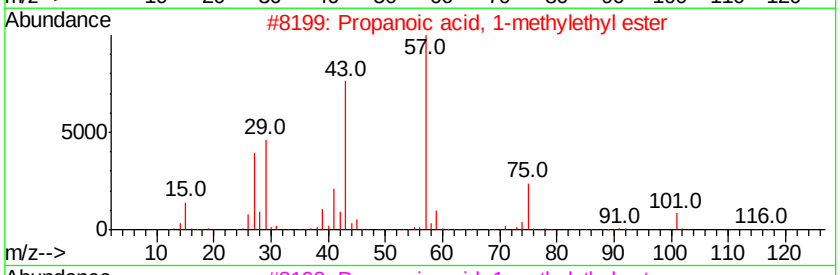
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

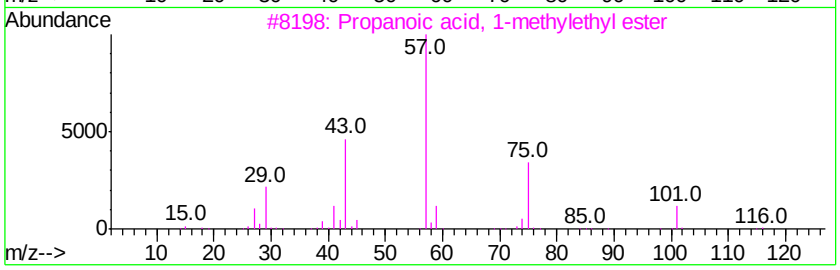
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	22.01 ug/L	190783	1,4-Difluorobenzene	5.88

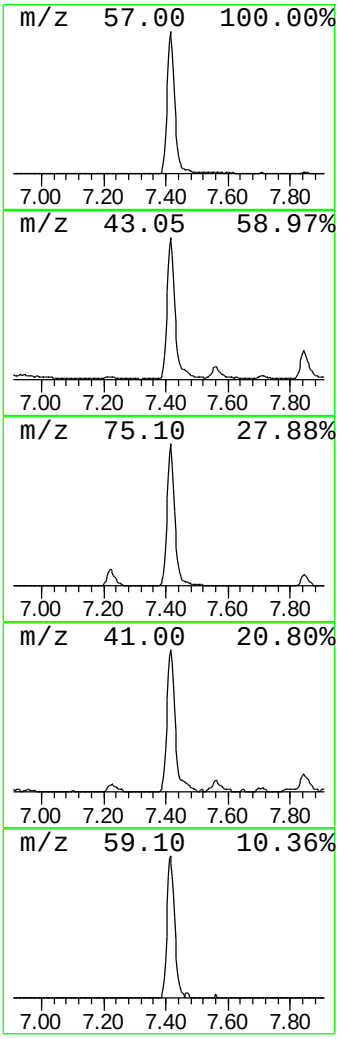
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50











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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

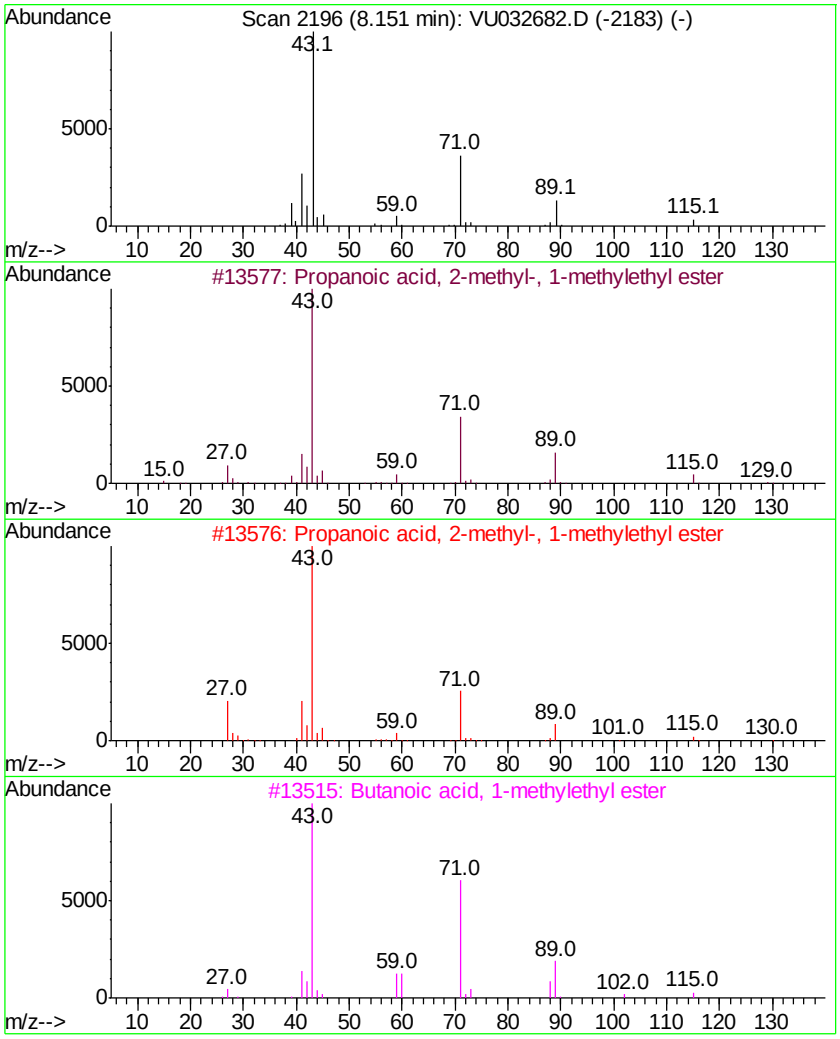
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

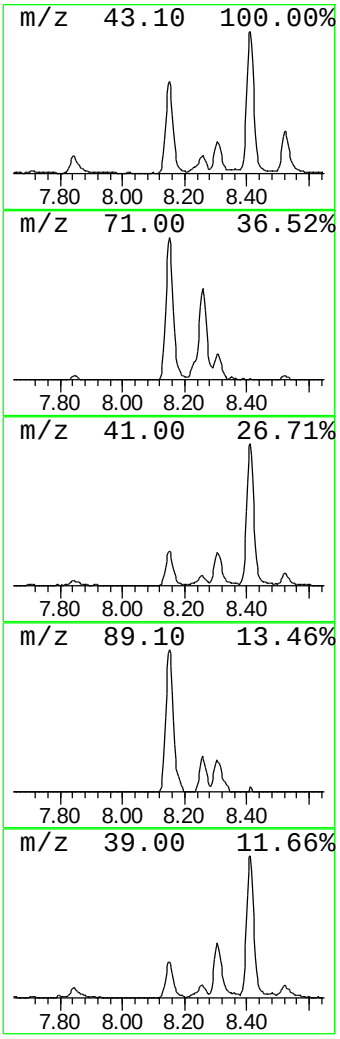
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.22 ug/L	98233	Chlorobenzene-d5	9.09

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	72
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59





Library Search Compound Report

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

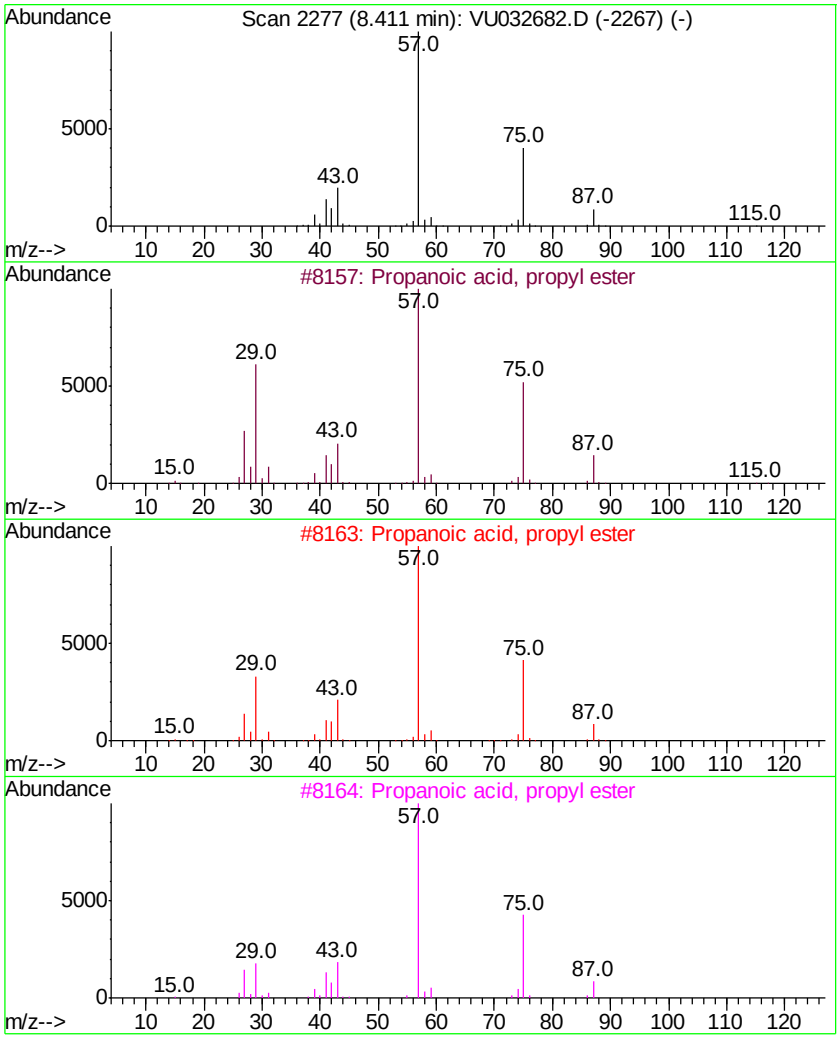
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

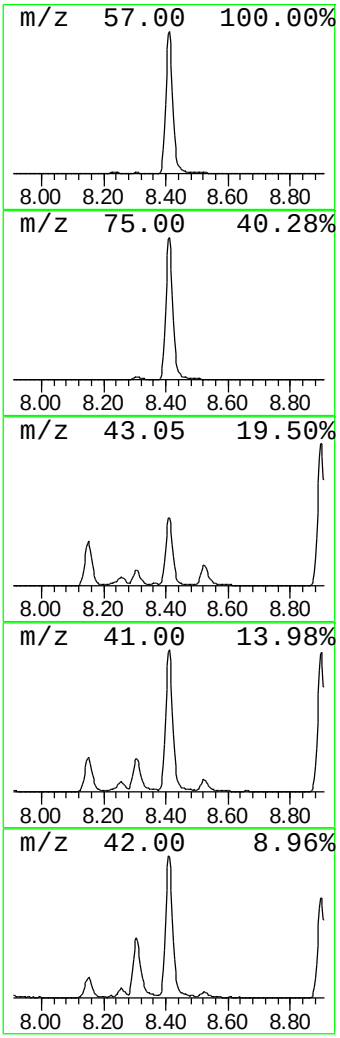
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	65.20 ug/L	694776	Chlorobenzene-d5	9.09

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	83
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032682.D
Acq On : 13 Jun 2019 10:32
Operator : JC/SP
Sample : K3286-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

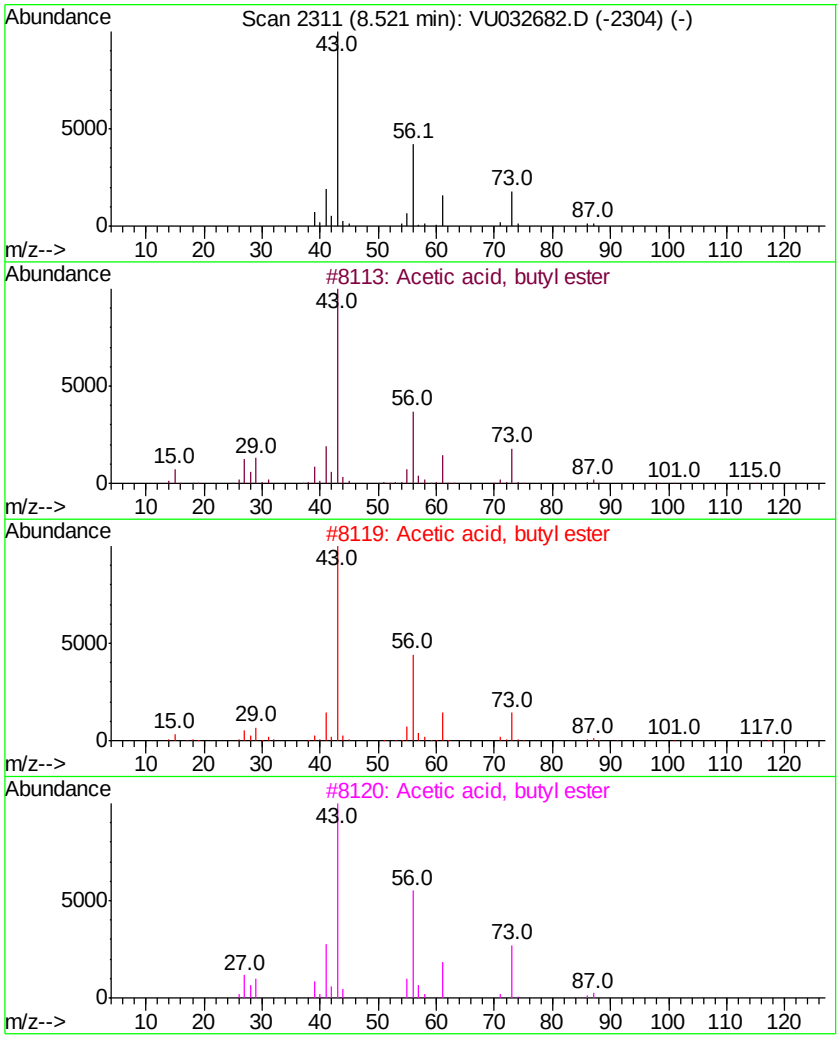
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

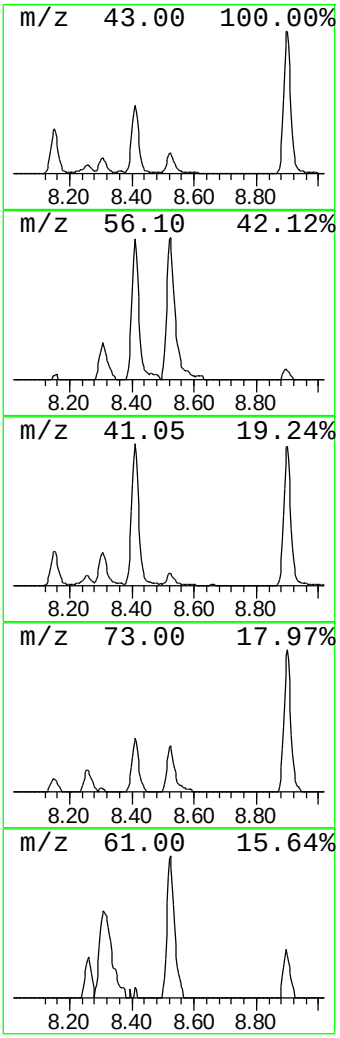
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.16 ug/L	44292	Chlorobenzene-d5	9.09

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	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032682.D
Acq On : 13 Jun 2019 10:32
Operator : JC/SP
Sample : K3286-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

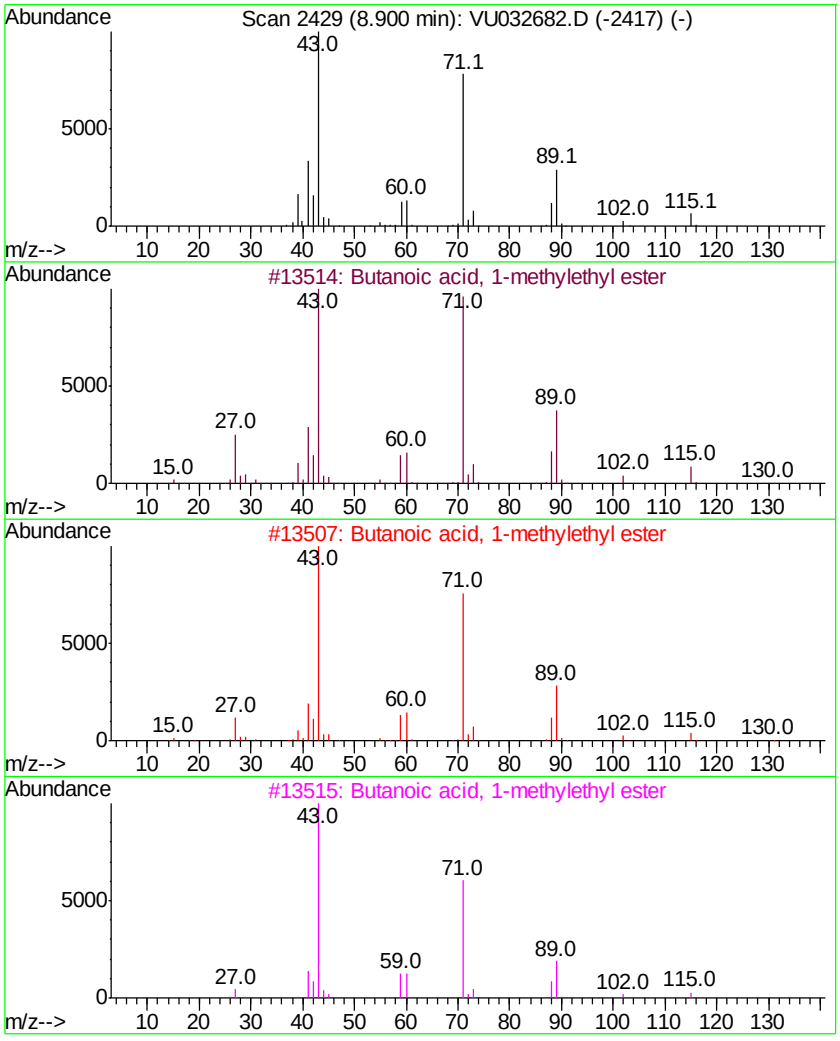
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

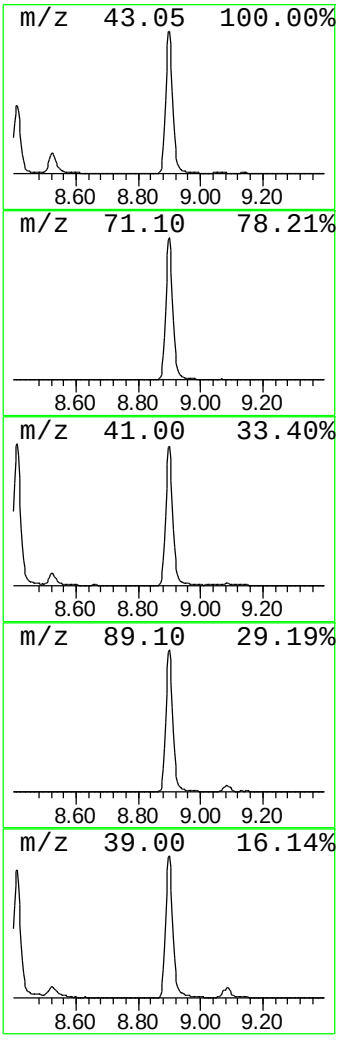
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	42.90 ug/L	457170	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
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-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032682.D
Acq On : 13 Jun 2019 10:32
Operator : JC/SP
Sample : K3286-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	126.5	ug/L	1096550	1	5.88	433473	50.0
Propanoic acid, 1...	7.41	22.0	ug/L	190783	1	5.88	433473	50.0
Propanoic acid, 2...	8.15	9.2	ug/L	98233	2	9.09	532813	50.0
Propanoic acid, p...	8.41	65.2	ug/L	694776	2	9.09	532813	50.0
Acetic acid, buty...	8.52	4.2	ug/L	44292	2	9.09	532813	50.0
Butanoic acid, 1-...	8.90	42.9	ug/L	457170	2	9.09	532813	50.0