LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032692.D
Acq On : 13 Jun 2019 14:21
Operator : JC/SP
Sample : K3286-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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	39	rVB	5028	5311	0.49%	0.068%
2	1.396	88	95	103	rBV	68668	70140	6.49%	0.904%
3	1.470	114	118	130	rVB	6320	6960	0.64%	0.090%
4	1.675	175	182	194	rVB	59500	71359	6.60%	0.920%
5	2.267	356	366	376	rBV	119740	180911	16.74%	2.332%
6	2.318	376	382	396	rVB	15776	25648	2.37%	0.331%
7	2.437	416	419	428	rVB4	459	663	0.06%	0.009%
8	2.476	428	431	433	rBV4	395	238	0.02%	0.003%
9	2.527	444	447	450	rBV2	265	195	0.02%	0.003%
10	2.617	468	475	477	rBV3	706	688	0.06%	0.009%
11	2.698	490	500	511	rVB2	7433	12282	1.14%	0.158%
12	2.762	515	520	523	rBV	199	229	0.02%	0.003%
13	2.830	539	541	545	rVB2	331	209	0.02%	0.003%
14	2.855	545	549	558	rBV	234	315	0.03%	0.004%
15	3.138	633	637	641	rBV	312	216	0.02%	0.003%
16	3.177	641	649	651	rBV2	375	467	0.04%	0.006%
17	3.209	657	659	662	rVB	353	214	0.02%	0.003%
18	3.235	662	667	673	rVB3	290	351	0.03%	0.005%
19	3.286	677	683	686	rBV	298	225	0.02%	0.003%
20	3.360	702	706	712	rBV	154	179	0.02%	0.002%
21	3.415	712	723	739	rBV5	4748	11567	1.07%	0.149%
22	3.781	828	837	839	rBV2	139	190	0.02%	0.002%
23	3.994	900	903	913	rVB2	230	352	0.03%	0.005%
24	4.042	913	918	921	rBV	230	208	0.02%	0.003%
25	4.170	946	958	989	rBV	63227	175443	16.24%	2.261%
26	4.437	1038	1041	1044	rBV2	299	231	0.02%	0.003%
27	4.643	1089	1105	1132	rBV	98464	234592	21.71%	3.024%
28	4.810	1154	1157	1158	rBV	282	189	0.02%	0.002%
29	4.852	1168	1170	1176	rVB2	186	170	0.02%	0.002%
30	5.231	1282	1288	1292	rBV2	188	239	0.02%	0.003%
31	5.334	1297	1320	1347	rBV2	191748	568371	52.60%	7.326%
32	5.428	1347	1349	1355	rVB2	436	320	0.03%	0.004%
33	5.553	1378	1388	1402	rBV3	3497	7883	0.73%	0.102%
34	5.675	1422	1426	1430	rVB3	384	358	0.03%	0.005%

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Sample : K3286-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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	5.698	1430	1433	1439	rVB	323	231	0.02%	0.003%
36	5.727	1439	1442	1443	rBV2	348	195	0.02%	0.003%
37	5.881	1469	1490	1517	rBV	218522	462823	42.83%	5.966%
38	6.183	1576	1584	1601	rVB7	9277	18708	1.73%	0.241%
39	6.325	1614	1628	1649	rBV	135494	268533	24.85%	3.461%
40	6.428	1652	1660	1678	rVB3	5134	12041	1.11%	0.155%
41	6.534	1686	1693	1700	rBV2	1645	2688	0.25%	0.035%
42	6.582	1701	1708	1714	rBV2	3385	5754	0.53%	0.074%
43	6.698	1732	1744	1775	rBV	603428	1080587	100.00%	13.928%
44	7.026	1843	1846	1850	rVB3	400	268	0.02%	0.003%
45	7.225	1893	1908	1924	rBV	73923	134299	12.43%	1.731%
46	7.328	1937	1940	1945	rVB2	445	423	0.04%	0.005%
47	7.415	1953	1967	1995	rBV	107737	193084	17.87%	2.489%
48	7.559	1999	2012	2031	rBV	257109	450302	41.67%	5.804%
49	7.707	2054	2058	2069	rVB5	1234	1898	0.18%	0.024%
50	7.846	2090	2101	2128	rBV	59313	107079	9.91%	1.380%
51	8.045	2158	2163	2166	rBV3	245	201	0.02%	0.003%
52	8.151	2184	2196	2213	rVV	60801	101776	9.42%	1.312%
53	8.231	2213	2221	2222	rVV5	9110	10589	0.98%	0.136%
54	8.257	2224	2229	2235	rVV2	25958	38297	3.54%	0.494%
55	8.305	2235	2244	2265	rVV	223226	395760	36.62%	5.101%
56	8.411	2266	2277	2304	rVV	435144	709157	65.63%	9.141%
57	8.524	2304	2312	2331	rVB	27288	49057	4.54%	0.632%
58	8.685	2359	2362	2369	rVB2	211	182	0.02%	0.002%
59	8.900	2415	2429	2456	rBV	295702	477473	44.19%	6.154%
60	9.083	2472	2486	2515	rBV	314147	531741	49.21%	6.854%
61	9.270	2541	2544	2546	rVV3	400	214	0.02%	0.003%
62	9.296	2550	2552	2556	rBV2	330	261	0.02%	0.003%
63	9.447	2594	2599	2603	rVB2	284	222	0.02%	0.003%
64	9.511	2616	2619	2624	rVV	190	182	0.02%	0.002%
65	9.608	2639	2649	2666	rBV4	3277	6827	0.63%	0.088%
66	9.765	2689	2698	2719	rVV2	13274	23652	2.19%	0.305%
67	9.971	2758	2762	2765	rBV2	181	182	0.02%	0.002%
68	10.032	2776	2781	2783	rVB	291	237	0.02%	0.003%
69	10.051	2784	2787	2790	rBV2	256	205	0.02%	0.003%
70	10.096	2797	2801	2803	rBV	433	362	0.03%	0.005%
71	10.260	2850	2852	2858	rVB3	252	250	0.02%	0.003%

LSC Area Percent Report

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Acq On : 13 Jun 2019 14:21
Operator : JC/SP
Sample : K3286-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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	10.318	2869	2870	2878	rVB3	297	318	0.03%	0.004%
73	10.360	2878	2883	2888	rBV2	302	409	0.04%	0.005%
74	10.427	2892	2904	2924	rBV	200997	333971	30.91%	4.305%
75	10.585	2949	2953	2957	rBV3	248	224	0.02%	0.003%
76	10.768	3007	3010	3014	rBV2	365	218	0.02%	0.003%
77	10.858	3035	3038	3046	rVB	219	224	0.02%	0.003%
78	11.206	3139	3146	3151	rBV2	223	339	0.03%	0.004%
79	11.350	3189	3191	3197	rVB2	194	177	0.02%	0.002%
80	11.389	3197	3203	3205	rBV2	259	233	0.02%	0.003%
81	11.479	3219	3231	3258	rBV	316633	506213	46.85%	6.525%
82	11.855	3336	3348	3369	rBV	272500	448214	41.48%	5.777%
83	12.119	3426	3430	3435	rVB4	536	408	0.04%	0.005%
84	12.167	3440	3445	3448	rBV2	318	308	0.03%	0.004%
85	12.196	3448	3454	3458	rBV3	370	341	0.03%	0.004%
86	12.270	3473	3477	3481	rBV2	236	291	0.03%	0.004%
87	12.437	3524	3529	3535	rBV2	266	352	0.03%	0.005%
88	12.720	3613	3617	3621	rBV2	228	216	0.02%	0.003%
89	13.299	3793	3797	3802	rBV	206	199	0.02%	0.003%
90	13.469	3846	3850	3855	rBV2	278	273	0.03%	0.004%
91	13.575	3880	3883	3887	rBV	220	182	0.02%	0.002%
92	13.659	3907	3909	3915	rVB	259	191	0.02%	0.002%
93	14.016	4018	4020	4026	rVB3	319	251	0.02%	0.003%
94	14.048	4027	4030	4034	rVB	277	211	0.02%	0.003%
95	14.090	4040	4043	4051	rBV2	226	332	0.03%	0.004%
96	14.221	4080	4084	4087	rBV2	360	277	0.03%	0.004%
97	14.292	4102	4106	4110	rBV2	378	306	0.03%	0.004%
98	14.315	4110	4113	4116	rBV2	233	188	0.02%	0.002%
99	14.553	4180	4187	4191	rBV3	282	447	0.04%	0.006%
100	14.768	4251	4254	4256	rBV	249	217	0.02%	0.003%

Sum of corrected areas: 7758183

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032692.D
Acq On : 13 Jun 2019 14:21
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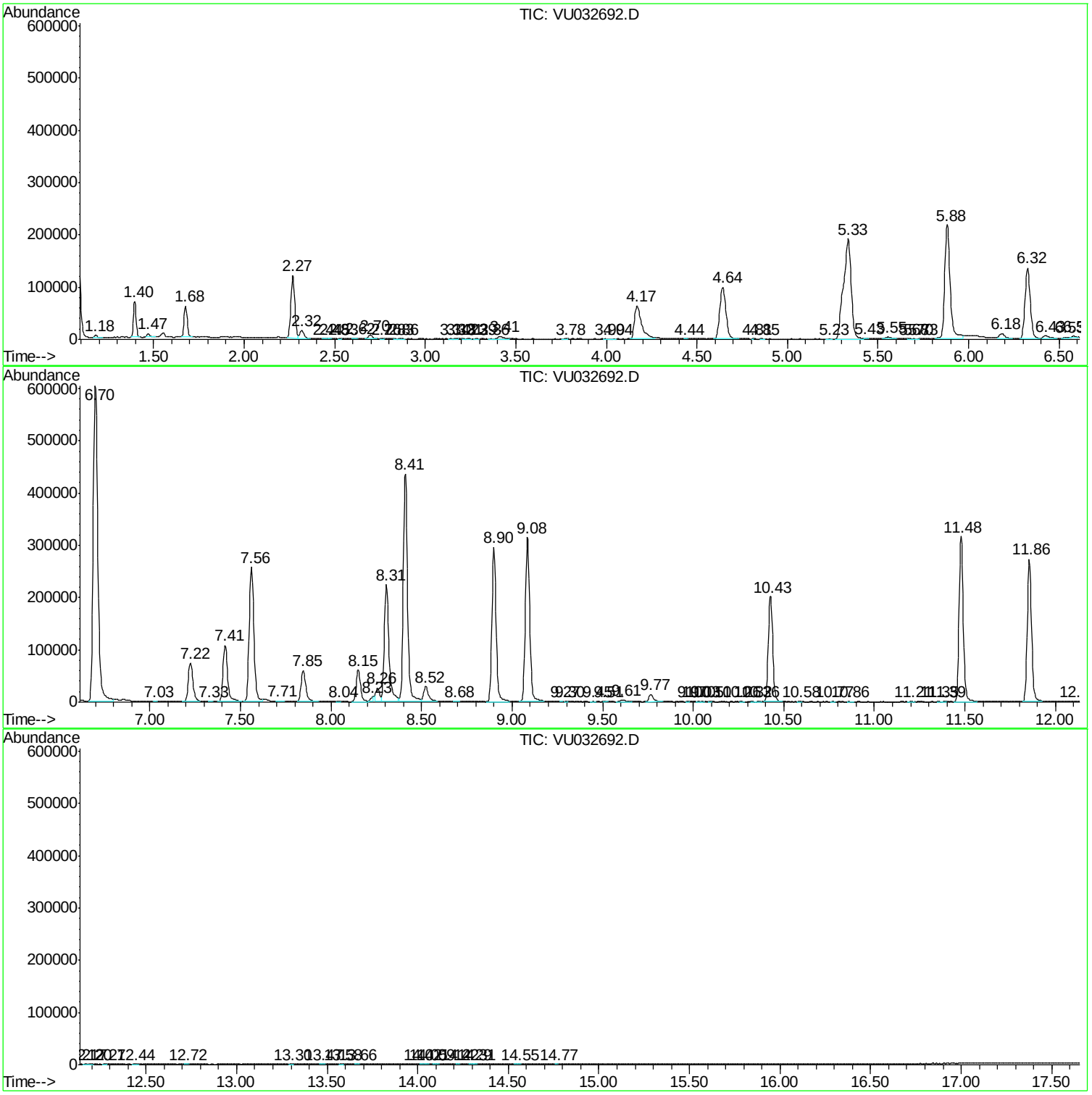
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
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Quant Title : VOC Analysis

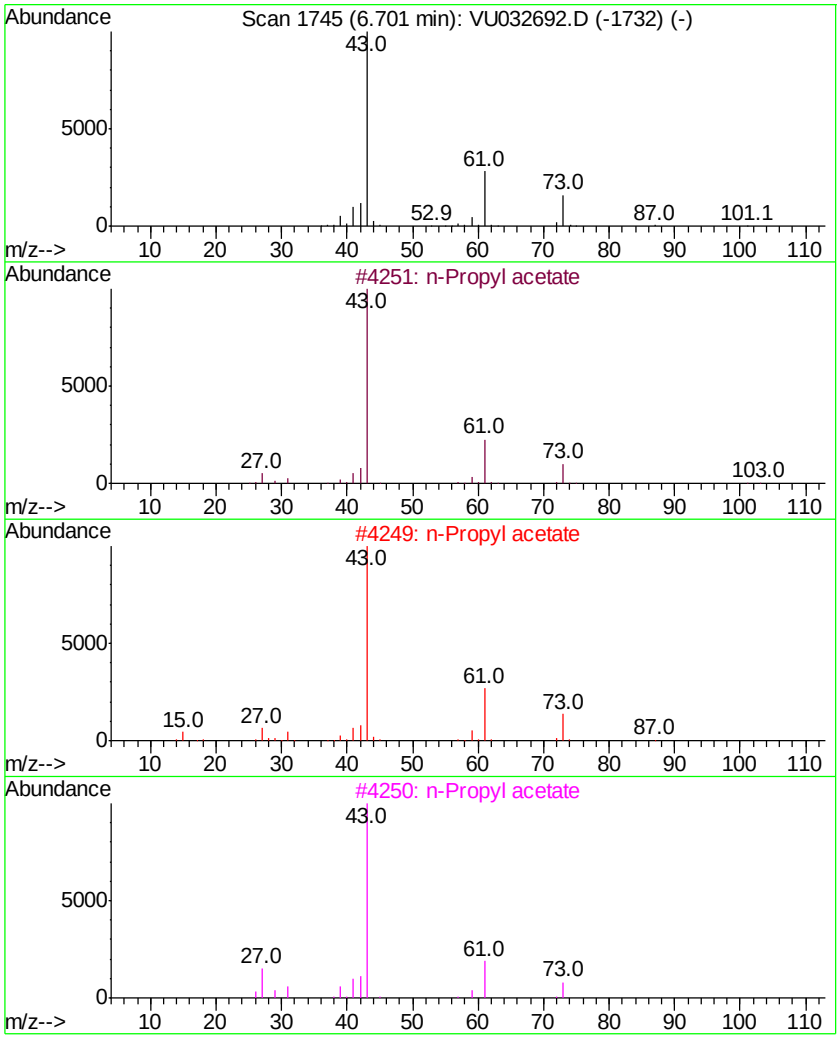
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

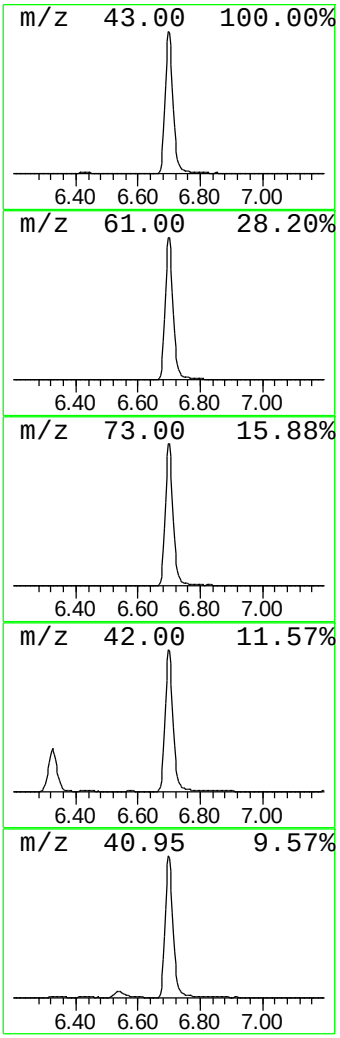
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	116.74 ug/L	1080590	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	Isobutylamine	73	C4H11N	000078-81-9	9





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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

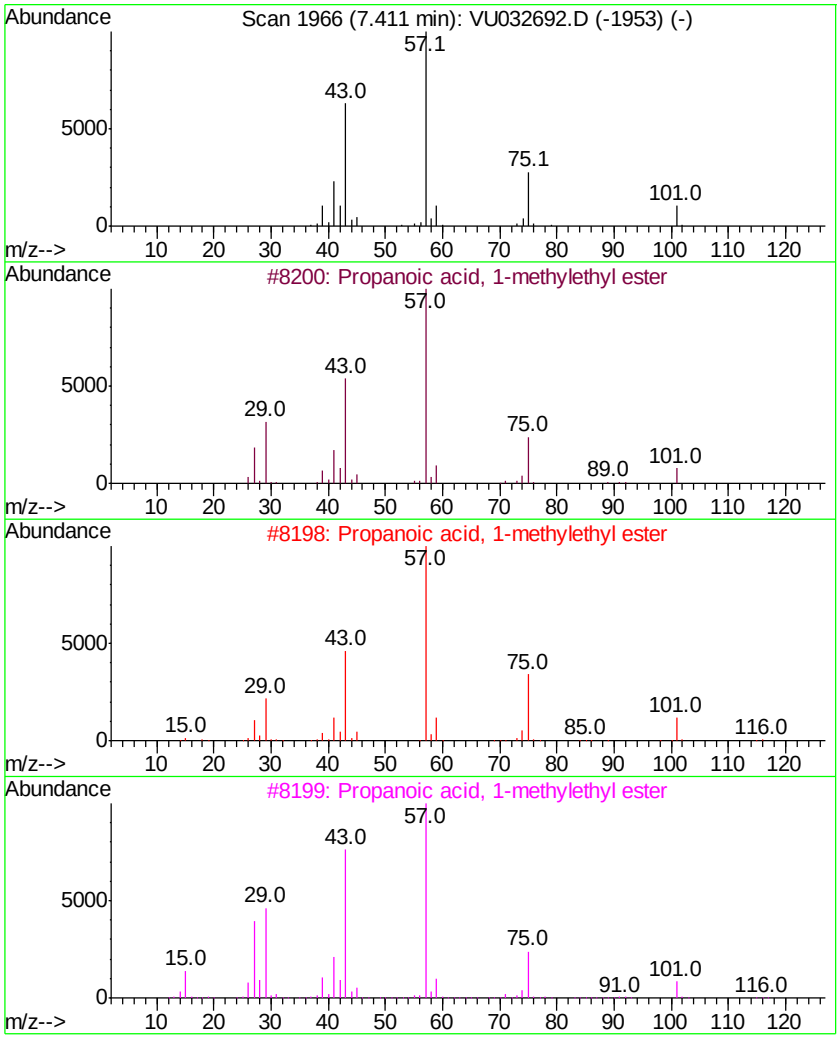
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

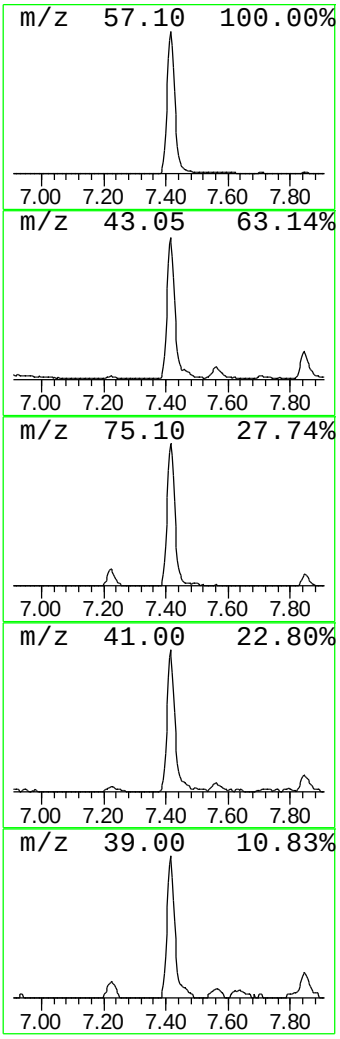
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	20.86 ug/L	193084	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	59
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50





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Instrument : MSVOA_U
ClientSampleId : C0JQ8

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

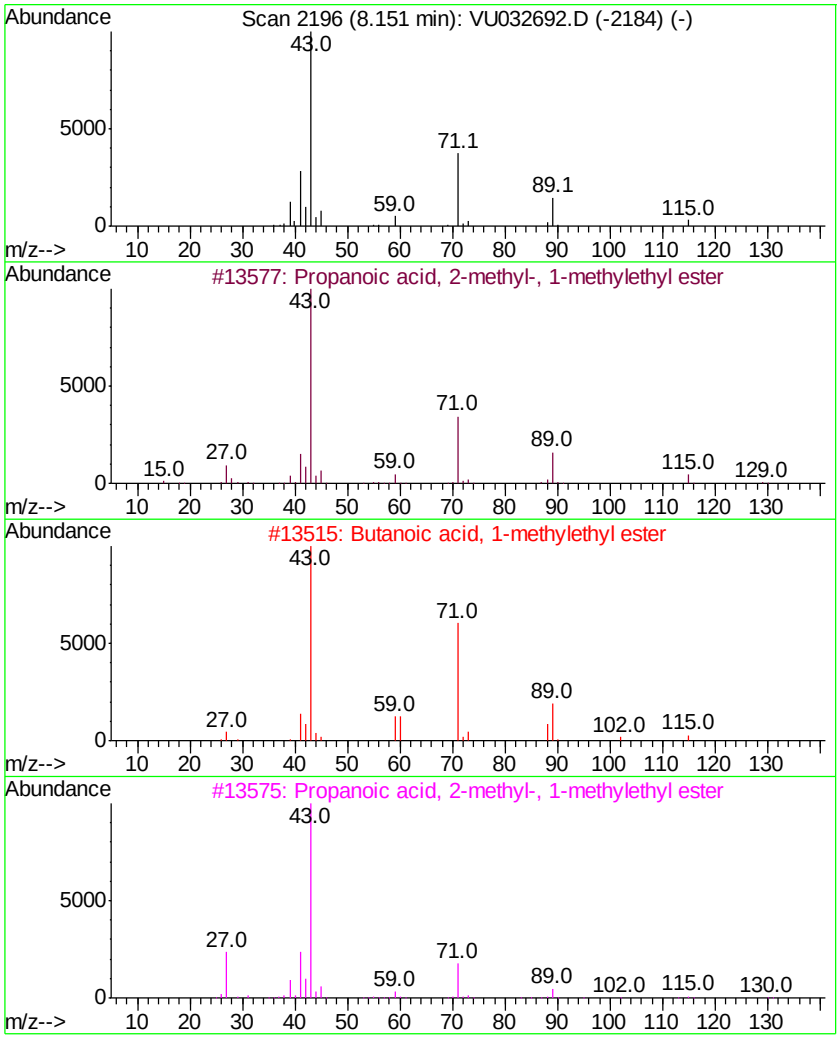
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

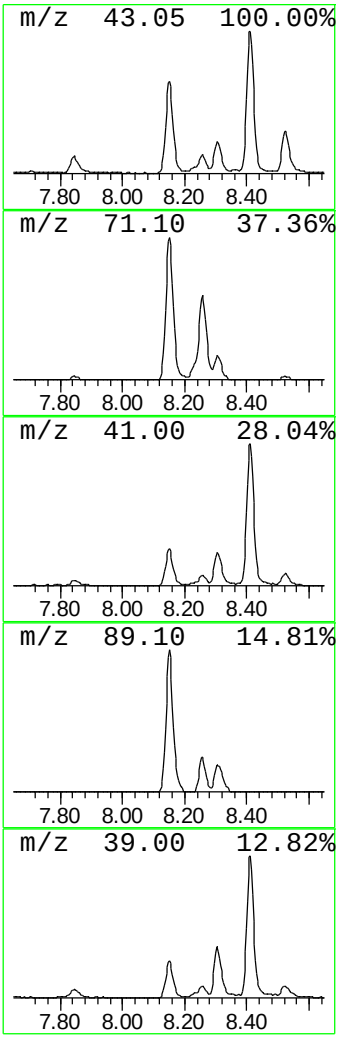
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.57 ug/L	101776	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	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56





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Operator : JC/SP
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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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

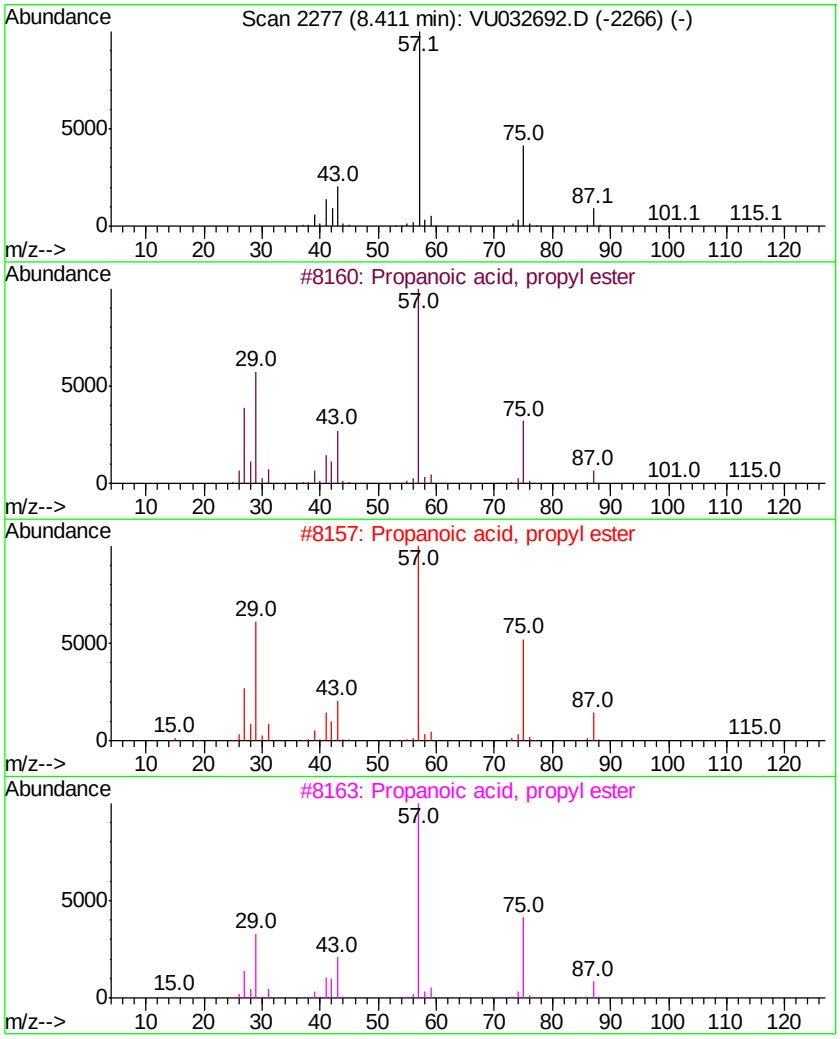
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

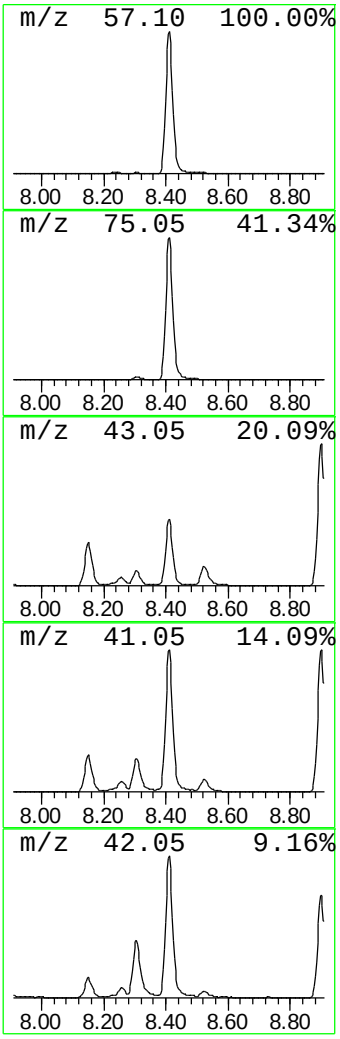
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	66.68 ug/L	709157	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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Data File : VU032692.D
Acq On : 13 Jun 2019 14:21
Operator : JC/SP
Sample : K3286-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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

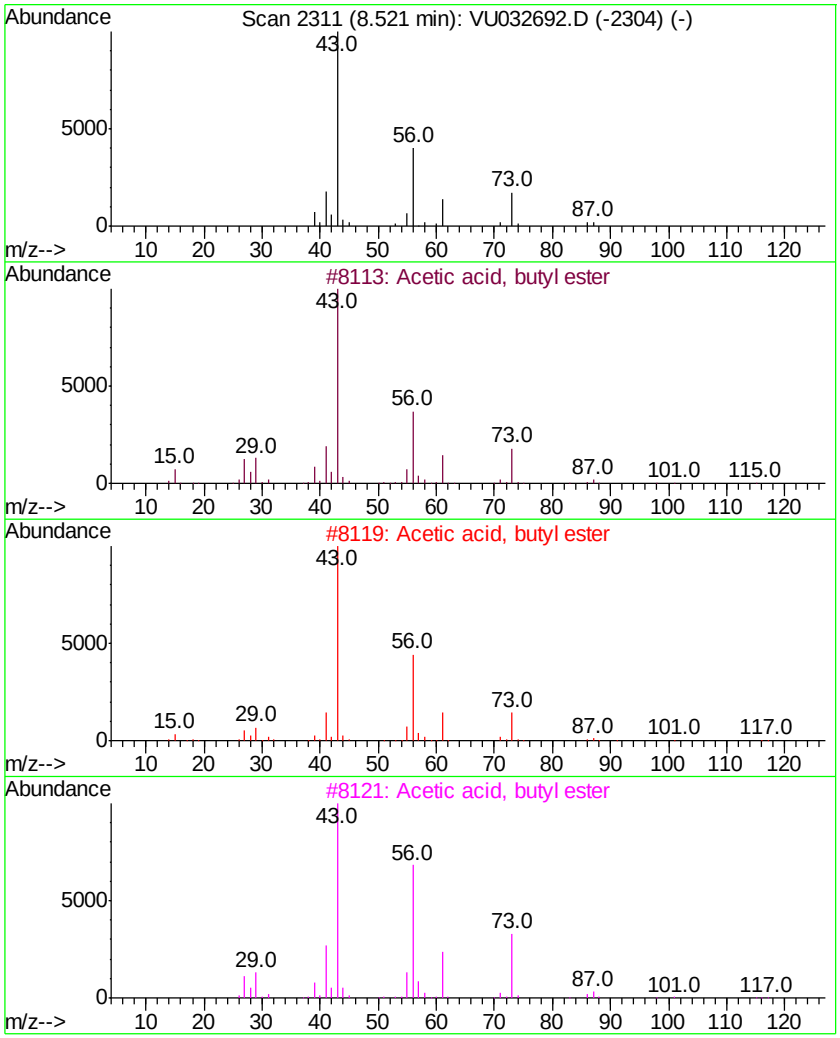
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

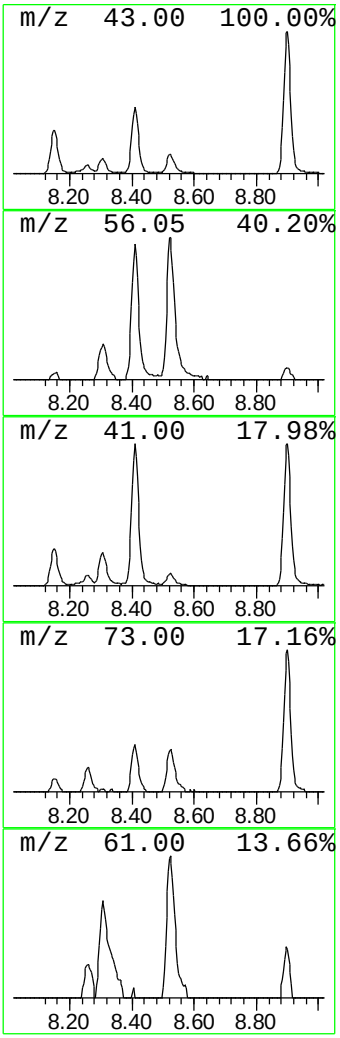
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.61 ug/L	49057	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	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032692.D
Acq On : 13 Jun 2019 14:21
Operator : JC/SP
Sample : K3286-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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

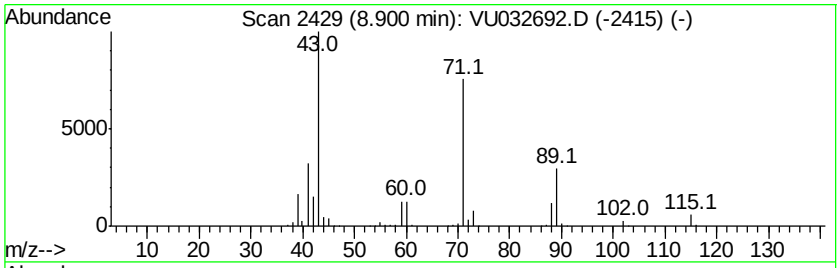
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

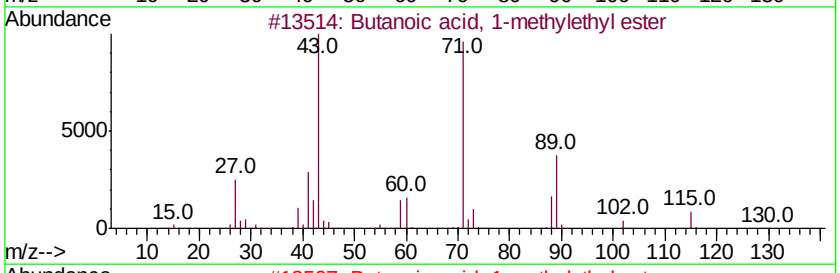
****

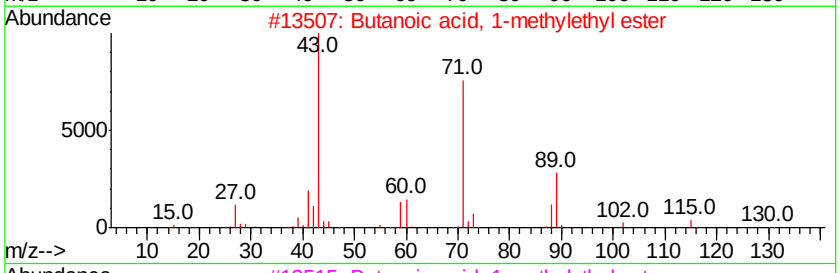
Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

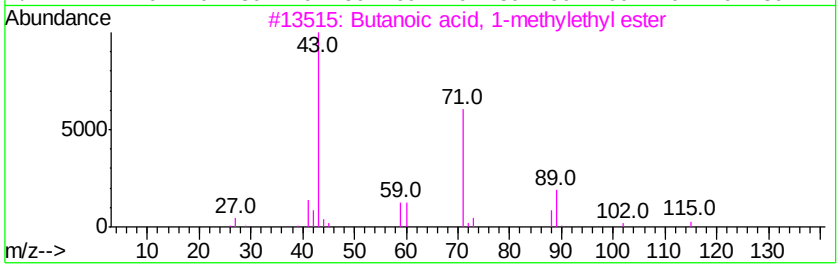
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	44.90 ug/L	477473	Chlorobenzene-d5	9.08

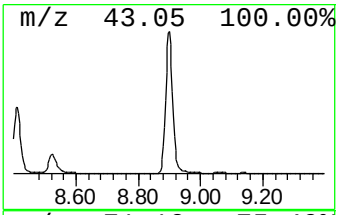
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64

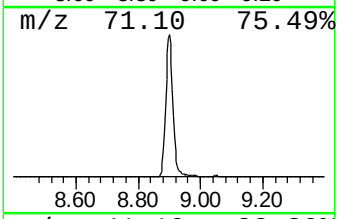


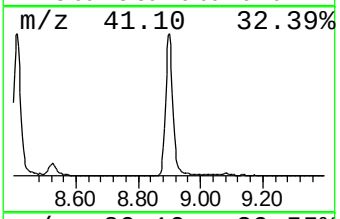


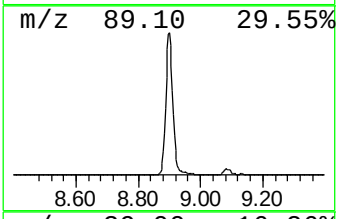


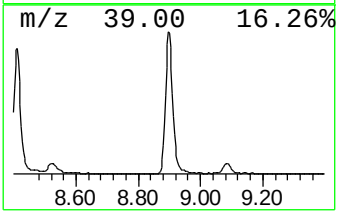












Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032692.D
Acq On : 13 Jun 2019 14:21
Operator : JC/SP
Sample : K3286-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JQ8

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	116.7	ug/L	1080590	1	5.88	462823	50.0
Propanoic acid, 1...	7.41	20.9	ug/L	193084	1	5.88	462823	50.0
Propanoic acid, 2...	8.15	9.6	ug/L	101776	2	9.08	531741	50.0
Propanoic acid, p...	8.41	66.7	ug/L	709157	2	9.08	531741	50.0
Acetic acid, buty...	8.52	4.6	ug/L	49057	2	9.08	531741	50.0
Butanoic acid, 1-...	8.90	44.9	ug/L	477473	2	9.08	531741	50.0