LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032797.D
Acq On : 17 Jun 2019 20:53
Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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	1.395	88	95	105	rVB	101070	101253	8.13%	1.020%
2	1.675	175	182	195	rVB	84769	101316	8.14%	1.021%
3	2.267	355	366	377	rBV	165463	249095	20.00%	2.510%
4	2.444	416	421	425	rBV4	748	850	0.07%	0.009%
5	2.514	441	443	449	rVB	428	297	0.02%	0.003%
6	2.540	449	451	456	rBV3	433	333	0.03%	0.003%
7	2.569	456	460	462	rBV4	480	401	0.03%	0.004%
8	2.694	491	499	511	rVB	5336	9457	0.76%	0.095%
9	2.874	553	555	559	rVB3	554	389	0.03%	0.004%
10	2.971	581	585	587	rBV2	399	293	0.02%	0.003%
11	3.106	623	627	630	rBV	377	260	0.02%	0.003%
12	3.199	652	656	658	rBV2	395	267	0.02%	0.003%
13	3.222	659	663	667	rVB4	391	415	0.03%	0.004%
14	3.254	667	673	677	rBV2	395	523	0.04%	0.005%
15	3.276	677	680	686	rVB3	256	299	0.02%	0.003%
16	3.344	699	701	706	rVB3	301	278	0.02%	0.003%
17	3.450	731	734	736	rBV2	435	336	0.03%	0.003%
18	3.759	825	830	835	rBV3	272	396	0.03%	0.004%
19	3.971	892	896	902	rVB3	371	315	0.03%	0.003%
20	4.032	909	915	918	rBV4	357	346	0.03%	0.003%
21	4.067	918	926	929	rBV4	247	288	0.02%	0.003%
22	4.170	943	958	990	rBV	84848	243222	19.53%	2.451%
23	4.328	1005	1007	1013	rBV5	424	389	0.03%	0.004%
24	4.357	1013	1016	1021	rVB3	542	412	0.03%	0.004%
25	4.640	1087	1104	1128	rVV	140834	324481	26.06%	3.269%
26	4.868	1170	1175	1177	rBV4	330	303	0.02%	0.003%
27	4.971	1202	1207	1211	rBV4	582	547	0.04%	0.006%
28	5.334	1296	1320	1342	rBV2	270766	803510	64.53%	8.096%
29	5.476	1360	1364	1369	rVB3	546	439	0.04%	0.004%
30	5.550	1374	1387	1402	rBV3	5851	13260	1.06%	0.134%
31	5.707	1433	1436	1439	rBV2	321	275	0.02%	0.003%
32	5.746	1445	1448	1453	rVB3	373	326	0.03%	0.003%
33	5.826	1470	1473	1476	rBV	386	282	0.02%	0.003%
34	5.881	1476	1490	1508	rBV	276457	541063	43.45%	5.451%

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Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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	6.180	1573	1583	1598	rVB6	11601	23920	1.92%	0.241%
36	6.324	1612	1628	1647	rBV2	188856	372730	29.93%	3.755%
37	6.418	1650	1657	1669	rBV2	5146	10280	0.83%	0.104%
38	6.530	1683	1692	1695	rBV3	2408	3845	0.31%	0.039%
39	6.575	1699	1706	1713	rBV	4439	7810	0.63%	0.079%
40	6.697	1731	1744	1776	rBV	702741	1245226	100.00%	12.546%
41	6.939	1816	1819	1824	rBV5	487	430	0.03%	0.004%
42	6.990	1833	1835	1838	rVB3	550	283	0.02%	0.003%
43	7.051	1852	1854	1859	rVV3	450	321	0.03%	0.003%
44	7.138	1877	1881	1883	rBV2	544	427	0.03%	0.004%
45	7.221	1893	1907	1924	rBV	105922	189640	15.23%	1.911%
46	7.366	1948	1952	1953	rBV3	553	339	0.03%	0.003%
47	7.414	1955	1967	1989	rVB	140361	238232	19.13%	2.400%
48	7.559	1998	2012	2031	rBV	363884	632131	50.76%	6.369%
49	7.746	2068	2070	2073	rBV2	512	276	0.02%	0.003%
50	7.842	2090	2100	2117	rBV2	86401	150987	12.13%	1.521%
51	7.919	2121	2124	2127	rBV3	618	344	0.03%	0.003%
52	8.148	2182	2195	2210	rBV	81081	134589	10.81%	1.356%
53	8.228	2211	2220	2221	rVV4	8424	10620	0.85%	0.107%
54	8.254	2223	2228	2235	rVV2	28851	45841	3.68%	0.462%
55	8.305	2235	2244	2265	rVV	303494	519846	41.75%	5.238%
56	8.408	2266	2276	2302	rVV	494700	790582	63.49%	7.965%
57	8.517	2302	2310	2329	rVB	29189	51610	4.14%	0.520%
58	8.742	2377	2380	2386	rVB2	368	273	0.02%	0.003%
59	8.794	2392	2396	2398	rVB3	369	266	0.02%	0.003%
60	8.858	2412	2416	2417	rBV2	463	353	0.03%	0.004%
61	8.897	2417	2428	2451	rBV	366922	578435	46.45%	5.828%
62	9.083	2469	2486	2508	rVV	418810	697248	55.99%	7.025%
63	9.247	2534	2537	2540	rVB4	647	467	0.04%	0.005%
64	9.289	2545	2550	2552	rVB2	330	287	0.02%	0.003%
65	9.331	2559	2563	2565	rBV3	345	308	0.02%	0.003%
66	9.379	2572	2578	2580	rBV3	414	382	0.03%	0.004%
67	9.466	2602	2605	2608	rBV2	460	347	0.03%	0.003%
68	9.601	2640	2647	2655	rBV3	4576	7311	0.59%	0.074%
69	9.762	2685	2697	2708	rBV2	17384	27468	2.21%	0.277%
70	9.926	2745	2748	2751	rVB3	345	260	0.02%	0.003%
71	9.945	2751	2754	2757	rBV4	478	462	0.04%	0.005%

LSC Area Percent Report

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Sample : K3324-12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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	10.353	2874	2881	2886	rBV3	318	379	0.03%	0.004%
73	10.424	2891	2903	2923	rBV	284327	456844	36.69%	4.603%
74	10.582	2947	2952	2953	rBV2	329	278	0.02%	0.003%
75	10.614	2958	2962	2967	rVB4	436	358	0.03%	0.004%
76	10.890	3044	3048	3051	rBV2	478	358	0.03%	0.004%
77	10.948	3063	3066	3072	rVB2	470	424	0.03%	0.004%
78	10.996	3076	3081	3084	rVB4	332	271	0.02%	0.003%
79	11.035	3089	3093	3096	rBV2	434	331	0.03%	0.003%
80	11.186	3134	3140	3144	rBV4	325	422	0.03%	0.004%
81	11.247	3153	3159	3160	rBV2	477	489	0.04%	0.005%
82	11.479	3218	3231	3253	rBV	431735	687587	55.22%	6.928%
83	11.639	3279	3281	3287	rVB5	717	637	0.05%	0.006%
84	11.733	3308	3310	3315	rVB3	410	273	0.02%	0.003%
85	11.774	3317	3323	3326	rBV3	290	269	0.02%	0.003%
86	11.797	3326	3330	3334	rVB2	583	495	0.04%	0.005%
87	11.855	3334	3348	3376	rBV	378524	631323	50.70%	6.361%
88	12.347	3498	3501	3504	rBV	351	280	0.02%	0.003%
89	12.376	3506	3510	3513	rVB	394	298	0.02%	0.003%
90	12.430	3522	3527	3532	rVB4	387	405	0.03%	0.004%
91	12.504	3548	3550	3554	rVB	474	284	0.02%	0.003%
92	13.260	3782	3785	3788	rVB2	438	269	0.02%	0.003%
93	13.276	3788	3790	3795	rBV2	373	328	0.03%	0.003%
94	13.855	3968	3970	3975	rVB3	730	427	0.03%	0.004%
95	14.041	4026	4028	4035	rVB4	603	471	0.04%	0.005%
96	14.186	4070	4073	4077	rVB3	409	284	0.02%	0.003%
97	14.623	4206	4209	4210	rBV2	624	356	0.03%	0.004%
98	14.697	4230	4232	4235	rVB3	640	277	0.02%	0.003%
99	14.752	4247	4249	4251	rBV	554	278	0.02%	0.003%
100	15.269	4408	4410	4412	rBV3	686	455	0.04%	0.005%

Sum of corrected areas: 9925242

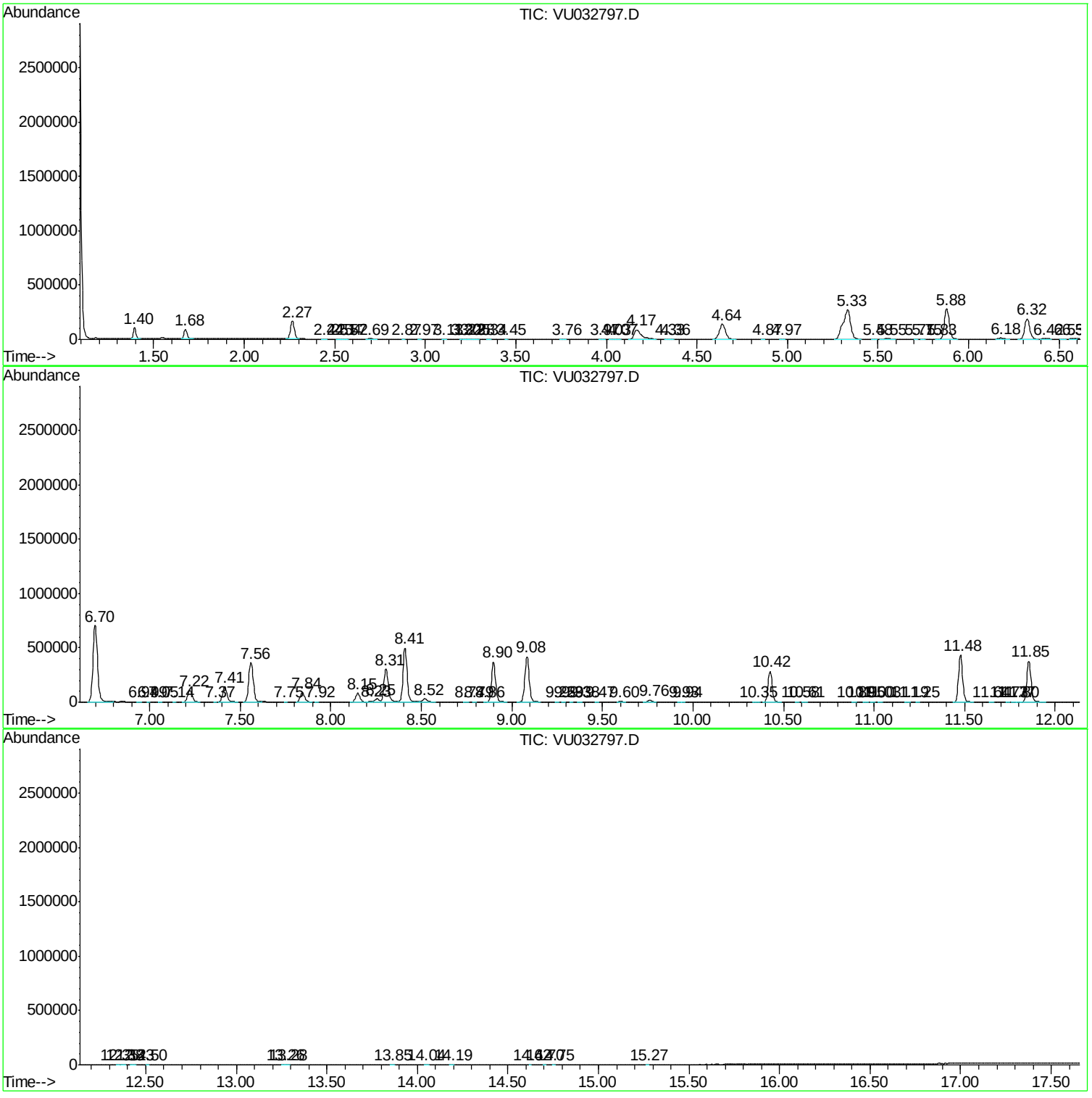
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032797.D
Acq On : 17 Jun 2019 20:53
Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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\VU061719\
Data File : VU032797.D
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Instrument : MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

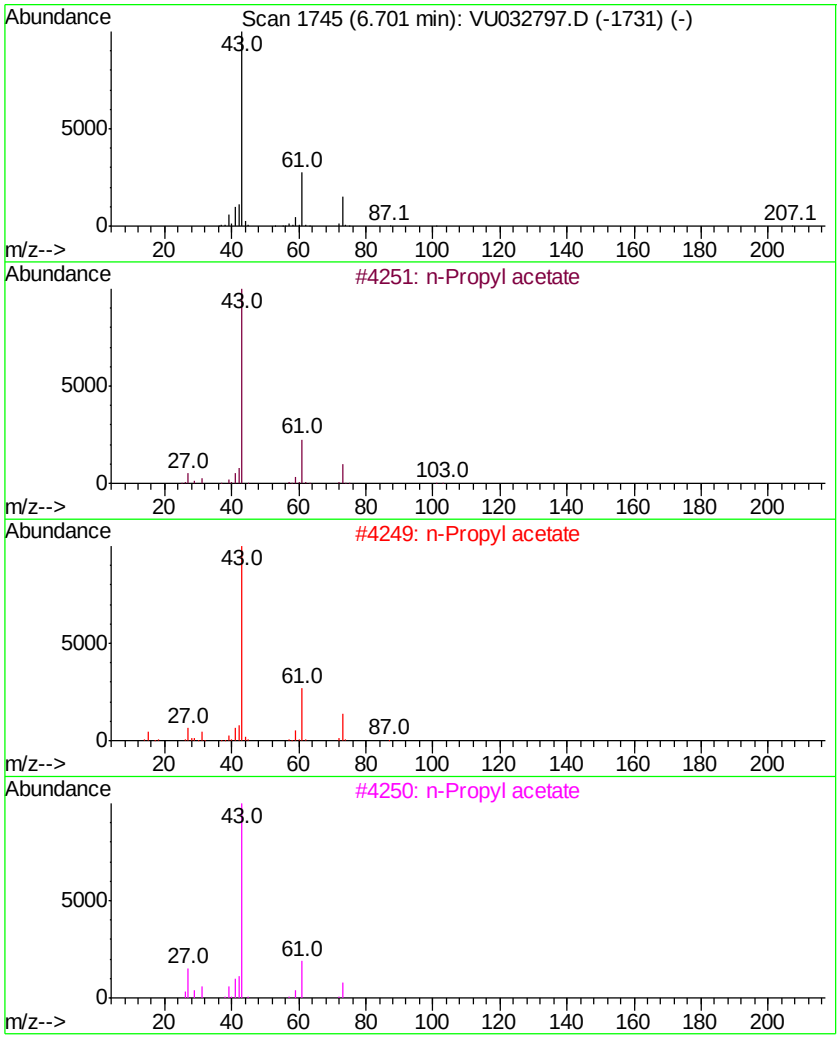
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

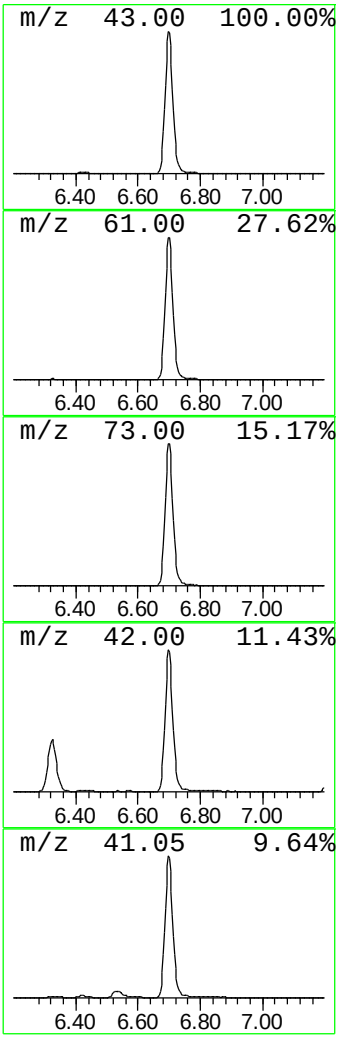
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	115.07 ug/L	1245230	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 : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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

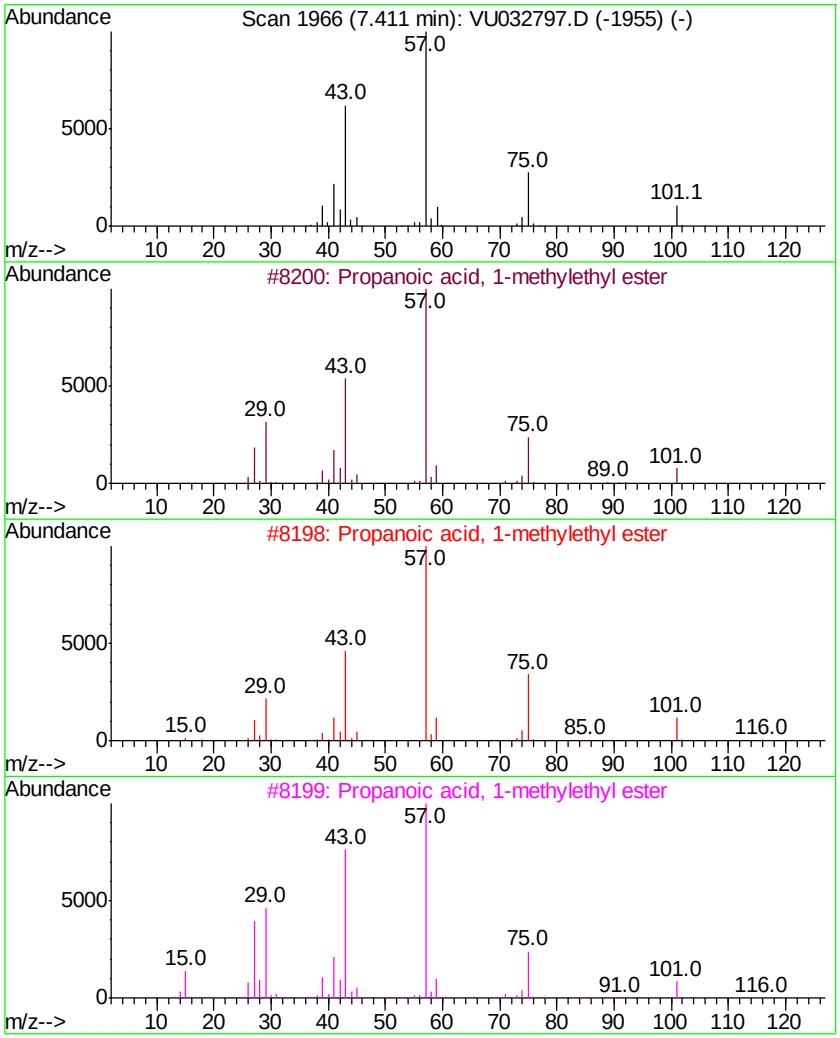
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

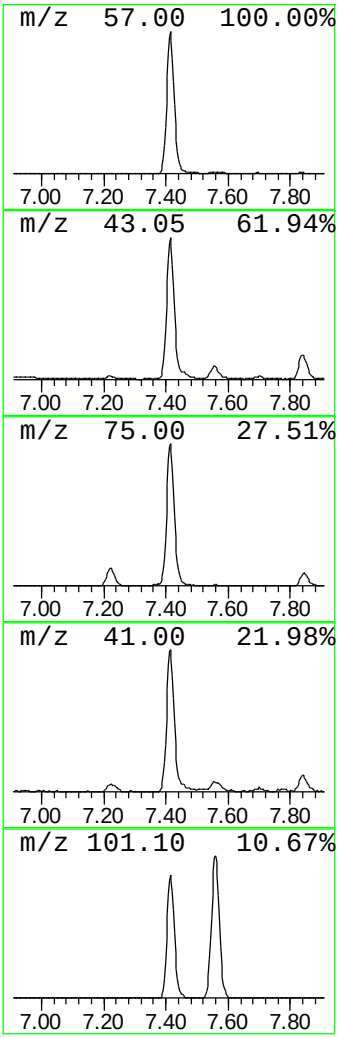
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	22.02 ug/L	238232	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	86
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	53
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45





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

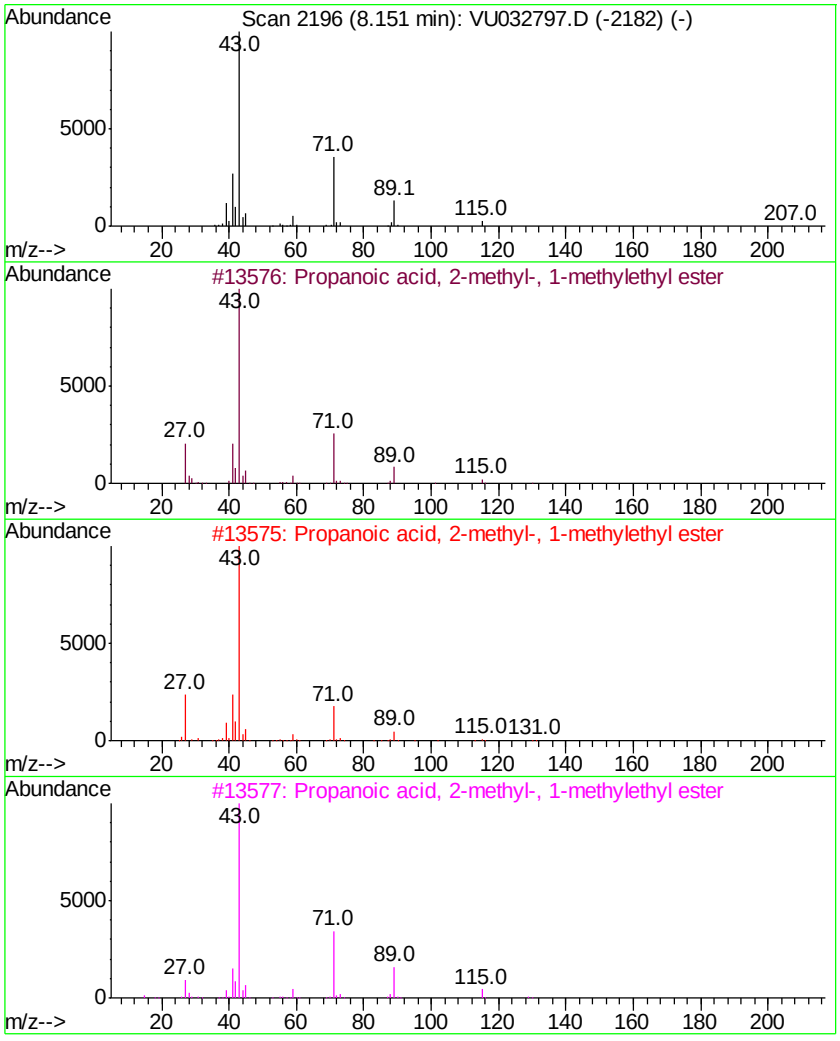
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

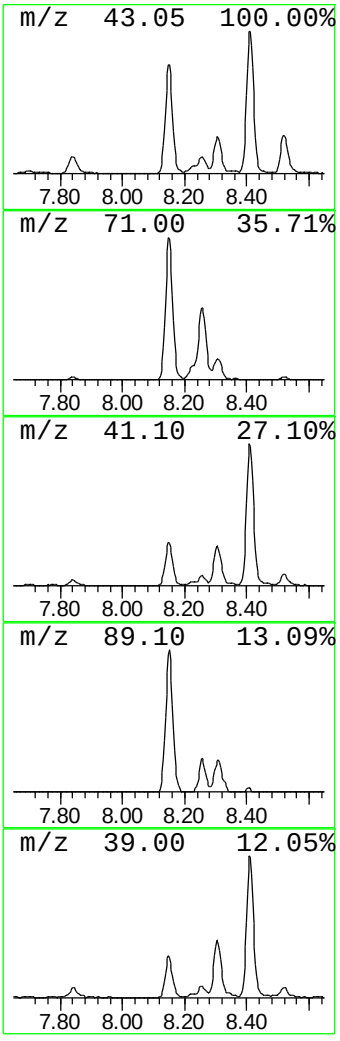
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.65 ug/L	134589	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42





Library Search Compound Report

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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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

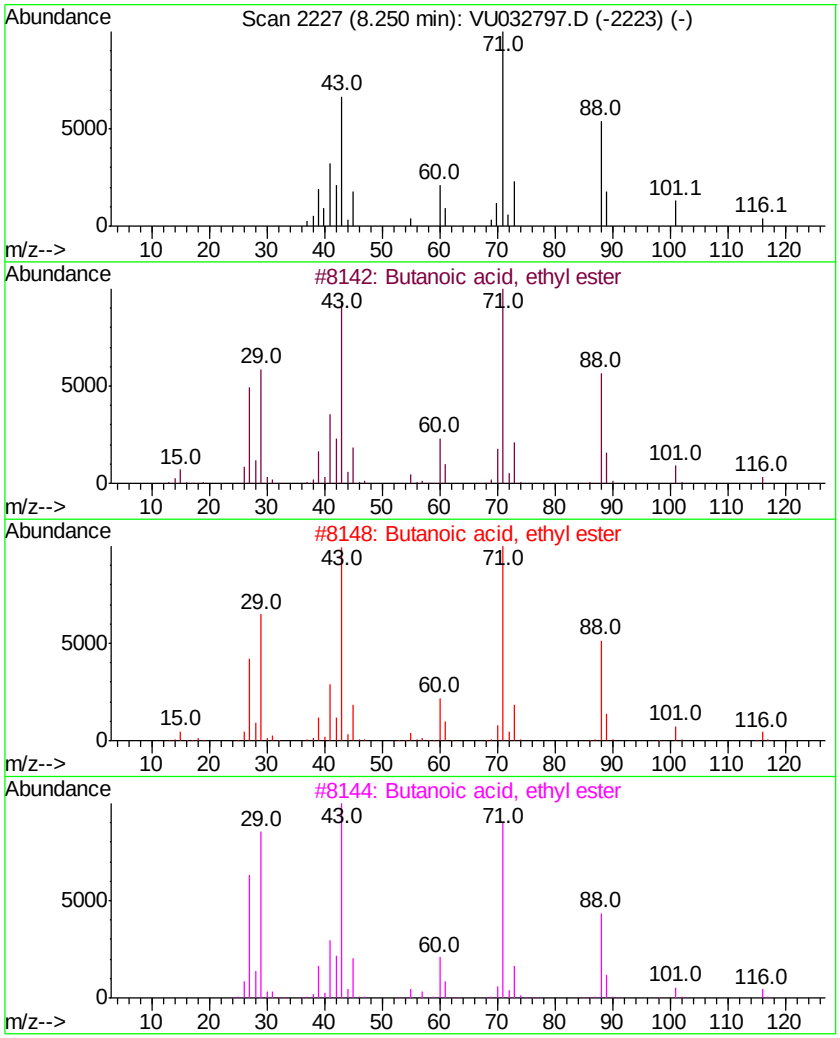
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

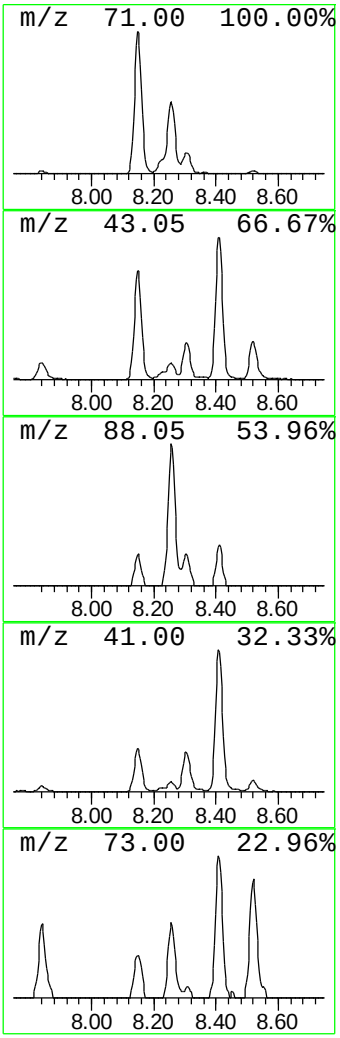
****

Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	3.29 ug/L	45841	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
3	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
4	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47





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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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

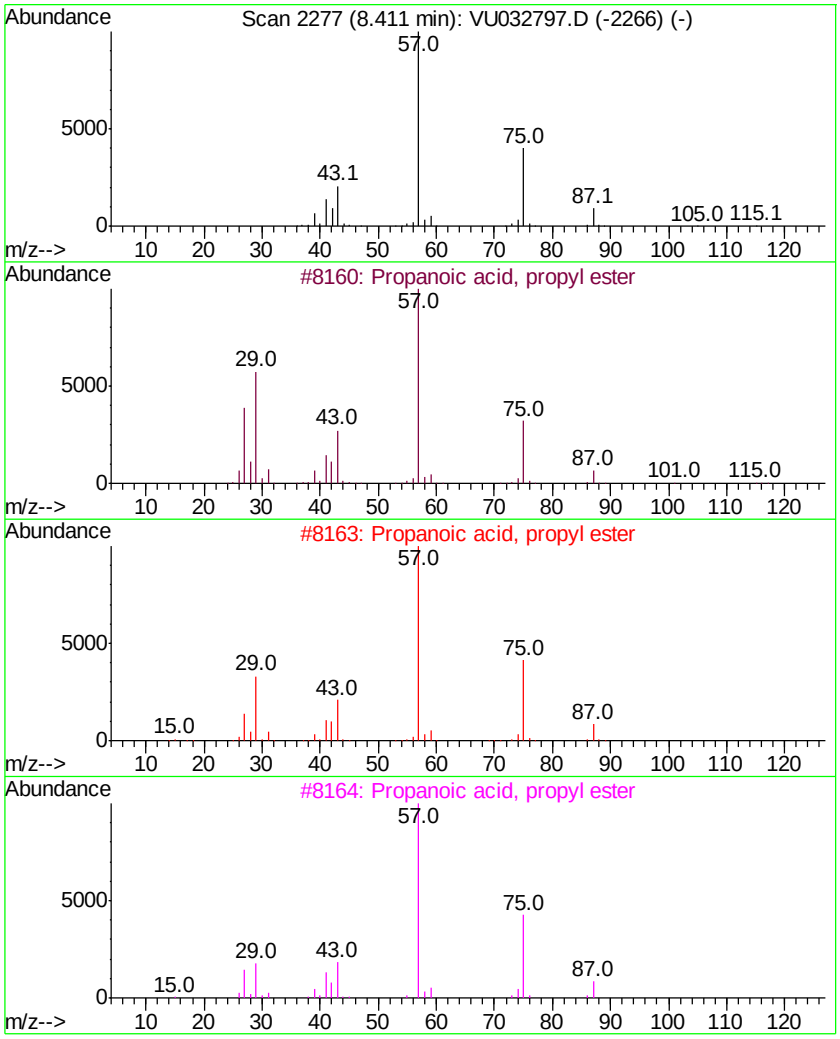
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

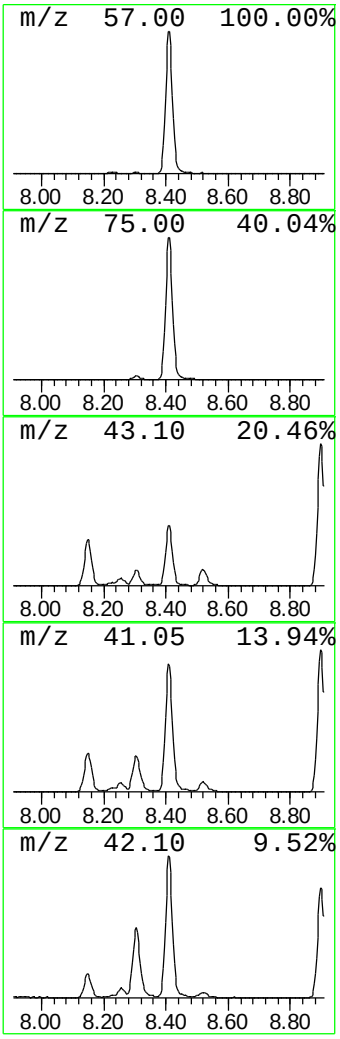
****

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	56.69 ug/L	790582	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	83
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032797.D
Acq On : 17 Jun 2019 20:53
Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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

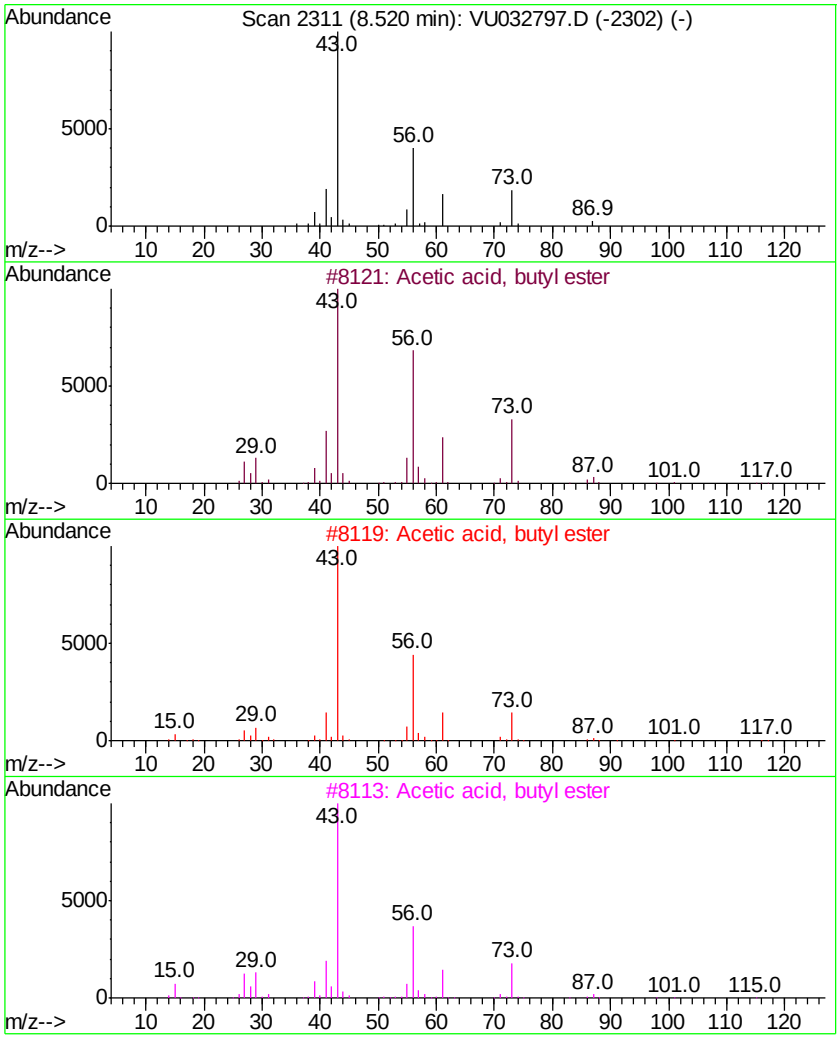
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

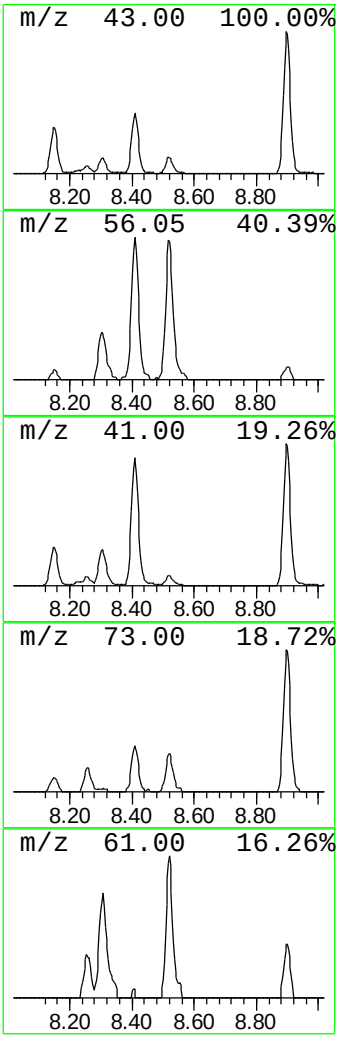
****

Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	3.70 ug/L	51610	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	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5	Isobutylamine	73	C4H11N	000078-81-9	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032797.D
Acq On : 17 Jun 2019 20:53
Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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

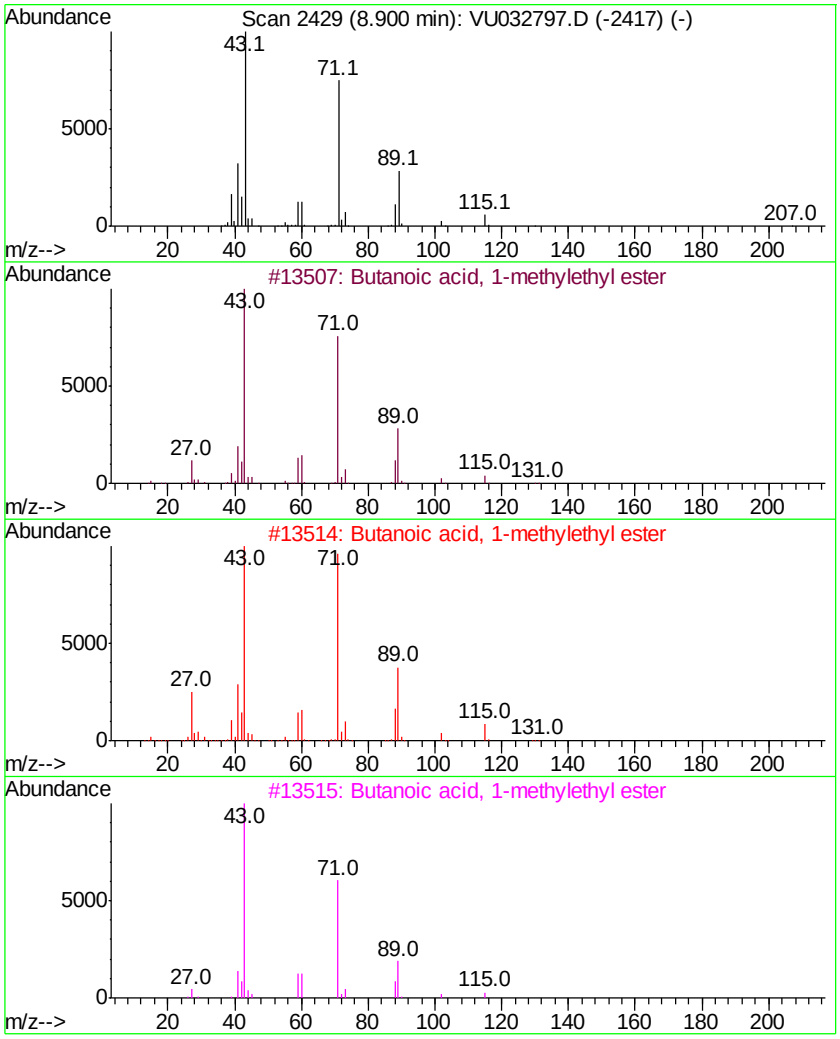
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

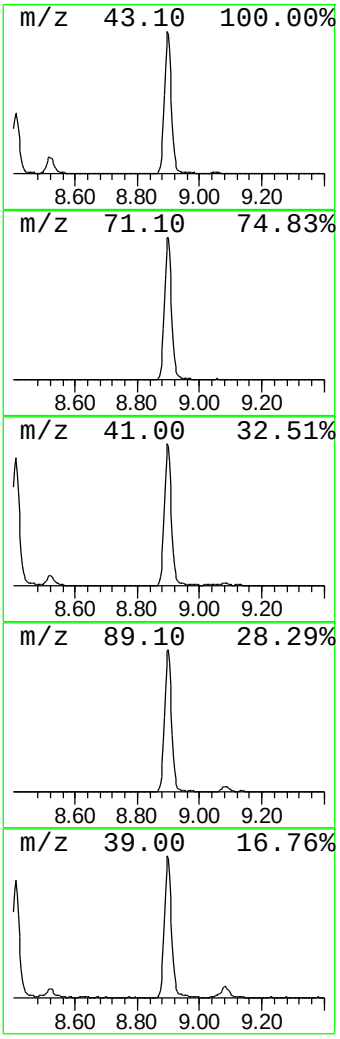
****

Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	41.48 ug/L	578435	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	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032797.D
Acq On : 17 Jun 2019 20:53
Operator : JC/SP
Sample : K3324-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR8

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	115.1	ug/L	1245230	1	5.88	541063	50.0
Propanoic acid, 1...	7.41	22.0	ug/L	238232	1	5.88	541063	50.0
Propanoic acid, 2...	8.15	9.7	ug/L	134589	2	9.08	697248	50.0
Butanoic acid, et...	8.25	3.3	ug/L	45841	2	9.08	697248	50.0
Propanoic acid, p...	8.41	56.7	ug/L	790582	2	9.08	697248	50.0
Acetic acid, buty...	8.52	3.7	ug/L	51610	2	9.08	697248	50.0
Butanoic acid, 1-...	8.90	41.5	ug/L	578435	2	9.08	697248	50.0