LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032796.D
Acq On : 17 Jun 2019 20:30
Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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	23	28	34	rBV2	6887	6730	0.46%	0.063%
2	1.396	88	95	111	rVB	101175	102135	7.01%	0.963%
3	1.675	174	182	195	rVB	83343	102634	7.05%	0.968%
4	2.267	356	366	376	rVB	168791	253234	17.38%	2.388%
5	2.614	465	474	487	rBV5	1850	3881	0.27%	0.037%
6	2.691	490	498	510	rVB	6066	10356	0.71%	0.098%
7	2.775	520	524	526	rBV2	690	538	0.04%	0.005%
8	2.920	566	569	572	rVB	415	261	0.02%	0.002%
9	3.158	638	643	646	rBV2	258	273	0.02%	0.003%
10	3.212	657	660	665	rVB4	443	359	0.02%	0.003%
11	3.286	680	683	685	rBV2	485	342	0.02%	0.003%
12	3.402	715	719	723	rVV2	311	255	0.02%	0.002%
13	3.476	738	742	748	rVB3	443	432	0.03%	0.004%
14	3.662	796	800	803	rBV3	342	322	0.02%	0.003%
15	3.707	811	814	819	rVB3	423	266	0.02%	0.003%
16	3.775	830	835	838	rBV2	357	332	0.02%	0.003%
17	3.916	875	879	883	rVB3	330	287	0.02%	0.003%
18	3.978	896	898	904	rVB3	314	278	0.02%	0.003%
19	4.167	944	957	991	rBV	88388	244461	16.78%	2.305%
20	4.527	1065	1069	1073	rBB3	337	251	0.02%	0.002%
21	4.640	1088	1104	1126	rBV	141251	330029	22.66%	3.112%
22	4.797	1150	1153	1155	rVB2	422	243	0.02%	0.002%
23	4.810	1155	1157	1163	rVB3	349	319	0.02%	0.003%
24	4.839	1163	1166	1168	rBV2	482	292	0.02%	0.003%
25	4.875	1172	1177	1179	rBV2	485	460	0.03%	0.004%
26	5.029	1221	1225	1228	rBV2	241	240	0.02%	0.002%
27	5.180	1267	1272	1275	rBV2	355	294	0.02%	0.003%
28	5.331	1294	1319	1344	rBV2	275021	815241	55.96%	7.688%
29	5.466	1357	1361	1364	rBV3	420	326	0.02%	0.003%
30	5.547	1375	1386	1402	rBV4	6474	14609	1.00%	0.138%
31	5.801	1462	1465	1468	rBV3	323	251	0.02%	0.002%
32	5.823	1468	1472	1475	rBV4	307	286	0.02%	0.003%
33	5.881	1475	1490	1510	rBV	282174	554516	38.07%	5.229%
34	6.180	1574	1583	1597	rVB2	16217	31347	2.15%	0.296%

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Sample : K3324-11
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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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	6.325	1614	1628	1648	rVB	190945	377461	25.91%	3.560%
36	6.418	1649	1657	1673	rBV2	6940	12969	0.89%	0.122%
37	6.530	1684	1692	1698	rBV2	3019	5334	0.37%	0.050%
38	6.572	1701	1705	1712	rVV2	3970	5623	0.39%	0.053%
39	6.698	1731	1744	1773	rBV	830514	1456725	100.00%	13.737%
40	7.103	1869	1870	1873	rVB2	610	252	0.02%	0.002%
41	7.119	1873	1875	1880	rBV3	362	400	0.03%	0.004%
42	7.164	1887	1889	1895	rVB4	518	430	0.03%	0.004%
43	7.222	1895	1907	1925	rBV	107655	194104	13.32%	1.830%
44	7.370	1948	1953	1955	rBV4	520	521	0.04%	0.005%
45	7.415	1955	1967	1990	rVV	148675	256066	17.58%	2.415%
46	7.559	1999	2012	2030	rBV	371437	645056	44.28%	6.083%
47	7.701	2051	2056	2066	rVB6	2156	3372	0.23%	0.032%
48	7.746	2066	2070	2071	rBV3	621	441	0.03%	0.004%
49	7.759	2071	2074	2075	rBV4	626	377	0.03%	0.004%
50	7.842	2086	2100	2123	rBV2	92967	161745	11.10%	1.525%
51	8.148	2185	2195	2211	rBV	86989	144247	9.90%	1.360%
52	8.228	2211	2220	2221	rBV2	8866	10448	0.72%	0.099%
53	8.254	2223	2228	2235	rVV2	31229	48151	3.31%	0.454%
54	8.305	2235	2244	2265	rVV	324305	543065	37.28%	5.121%
55	8.408	2266	2276	2296	rVB	609209	942431	64.70%	8.887%
56	8.521	2302	2311	2327	rVB	42545	70407	4.83%	0.664%
57	8.617	2338	2341	2344	rBV2	663	445	0.03%	0.004%
58	8.698	2363	2366	2368	rBV3	587	340	0.02%	0.003%
59	8.897	2414	2428	2451	rBV	423566	663565	45.55%	6.258%
60	9.083	2468	2486	2509	rBV	433472	712357	48.90%	6.718%
61	9.334	2561	2564	2567	rBV4	535	346	0.02%	0.003%
62	9.373	2572	2576	2581	rVB3	292	277	0.02%	0.003%
63	9.431	2590	2594	2595	rBV2	433	280	0.02%	0.003%
64	9.508	2616	2618	2622	rBV3	288	247	0.02%	0.002%
65	9.562	2631	2635	2638	rBV3	569	422	0.03%	0.004%
66	9.598	2638	2646	2664	rVV3	5994	11198	0.77%	0.106%
67	9.691	2671	2675	2682	rVB4	586	610	0.04%	0.006%
68	9.762	2687	2697	2712	rBV2	23262	36723	2.52%	0.346%
69	9.923	2741	2747	2748	rBV3	448	385	0.03%	0.004%
70	10.042	2778	2784	2786	rBV4	442	446	0.03%	0.004%
71	10.112	2803	2806	2807	rBV2	444	242	0.02%	0.002%

LSC Area Percent Report

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Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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	10.196	2830	2832	2835	rVB	526	278	0.02%	0.003%
73	10.283	2857	2859	2866	rVB4	396	393	0.03%	0.004%
74	10.424	2890	2903	2925	rBV	293633	465598	31.96%	4.391%
75	10.575	2944	2950	2951	rBV3	474	366	0.03%	0.003%
76	10.601	2953	2958	2962	rVV4	560	605	0.04%	0.006%
77	10.726	2992	2997	3000	rBV3	576	498	0.03%	0.005%
78	10.765	3004	3009	3018	rVB4	754	972	0.07%	0.009%
79	10.868	3037	3041	3044	rBV2	446	302	0.02%	0.003%
80	10.926	3054	3059	3060	rBV2	484	288	0.02%	0.003%
81	10.993	3078	3080	3084	rVB2	456	304	0.02%	0.003%
82	11.025	3085	3090	3092	rBV2	333	271	0.02%	0.003%
83	11.074	3101	3105	3111	rVB3	393	443	0.03%	0.004%
84	11.161	3124	3132	3135	rBV3	423	628	0.04%	0.006%
85	11.215	3146	3149	3151	rBV4	327	244	0.02%	0.002%
86	11.347	3185	3190	3193	rBV3	469	482	0.03%	0.005%
87	11.424	3209	3214	3218	rVB3	466	349	0.02%	0.003%
88	11.479	3218	3231	3250	rBV	431805	699842	48.04%	6.600%
89	11.672	3288	3291	3296	rVB3	539	335	0.02%	0.003%
90	11.855	3328	3348	3366	rBV	389297	643805	44.20%	6.071%
91	12.408	3518	3520	3523	rBV3	467	327	0.02%	0.003%
92	12.453	3530	3534	3536	rBV3	374	272	0.02%	0.003%
93	12.527	3554	3557	3563	rVB3	542	588	0.04%	0.006%
94	12.742	3622	3624	3630	rVB3	379	317	0.02%	0.003%
95	12.906	3671	3675	3677	rBV	566	446	0.03%	0.004%
96	12.990	3697	3701	3707	rBV3	630	619	0.04%	0.006%
97	13.302	3794	3798	3802	rVB3	498	474	0.03%	0.004%
98	13.459	3844	3847	3850	rBV3	482	293	0.02%	0.003%
99	14.395	4136	4138	4141	rVB2	452	242	0.02%	0.002%
100	14.501	4165	4171	4174	rBV4	913	991	0.07%	0.009%

Sum of corrected areas: 10604160

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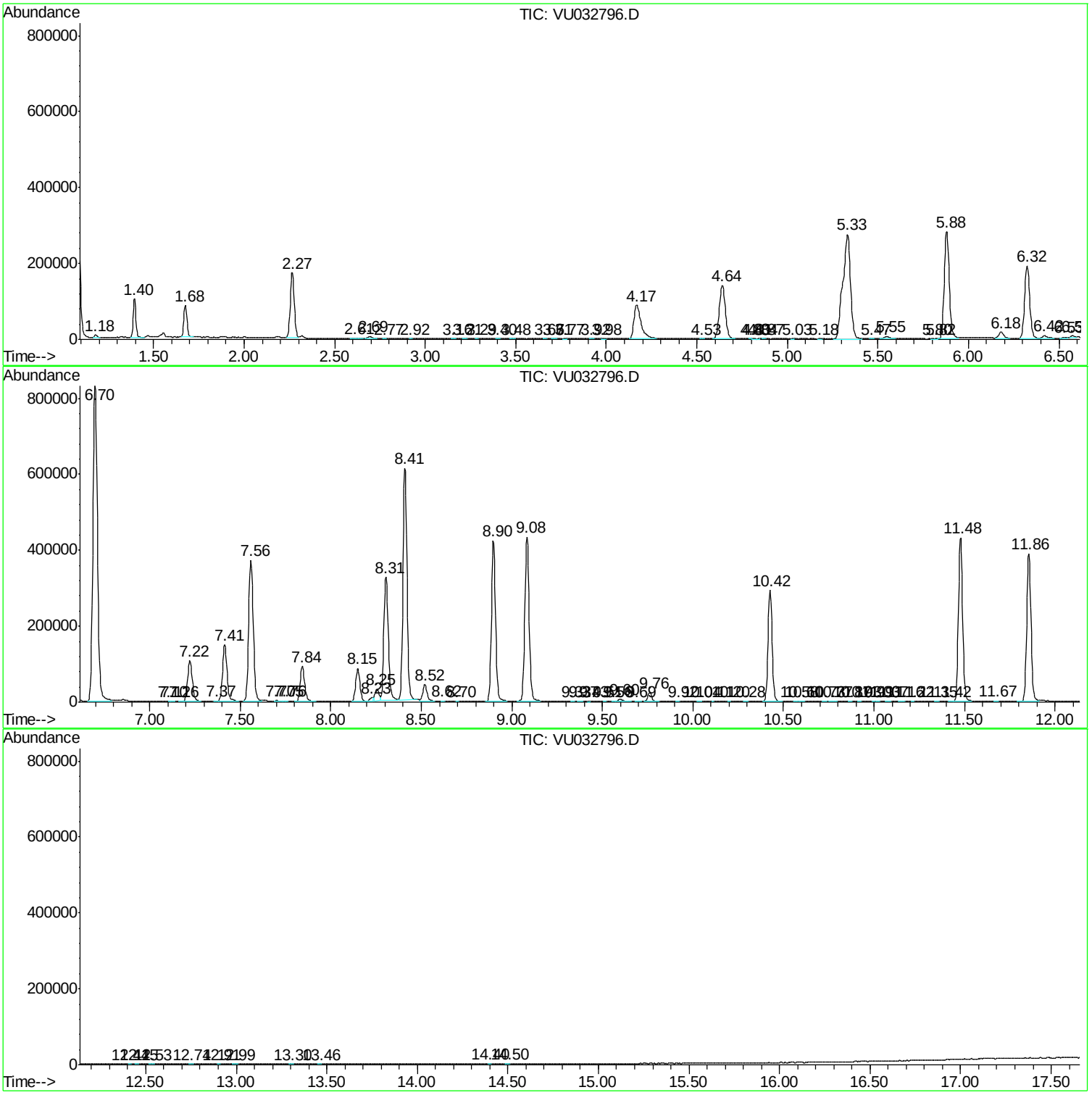
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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 : VU032796.D
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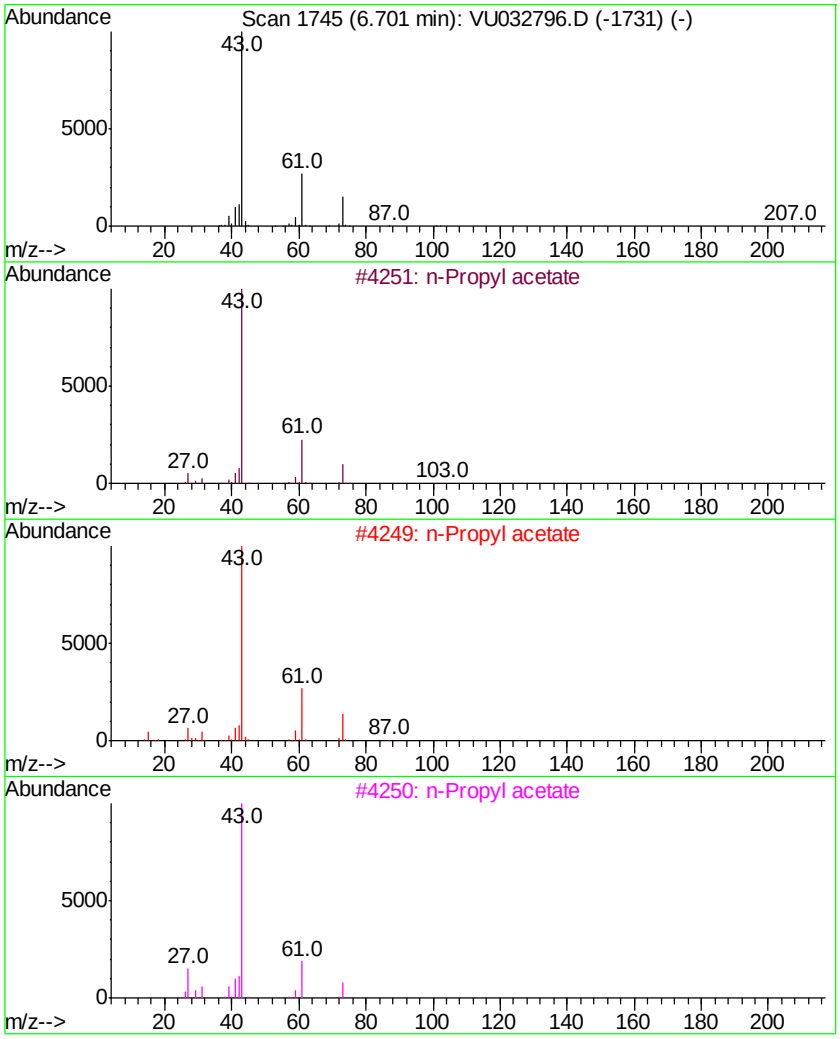
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

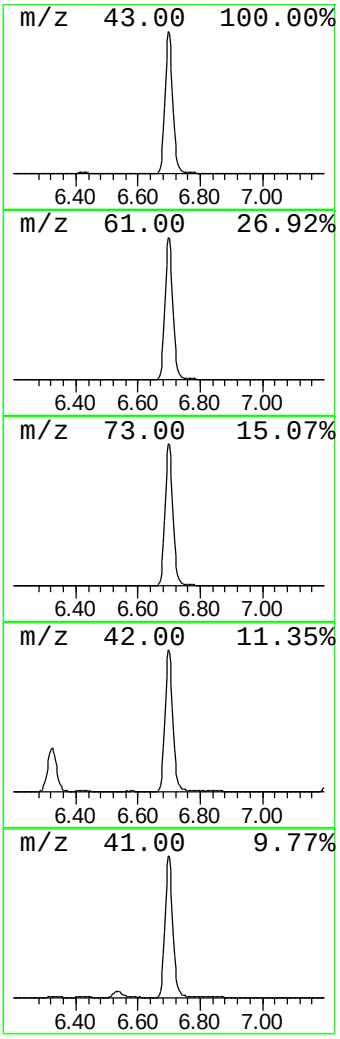
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	131.35 ug/L	1456730	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





Library Search Compound Report

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Acq On : 17 Jun 2019 20:30
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Sample : K3324-11
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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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

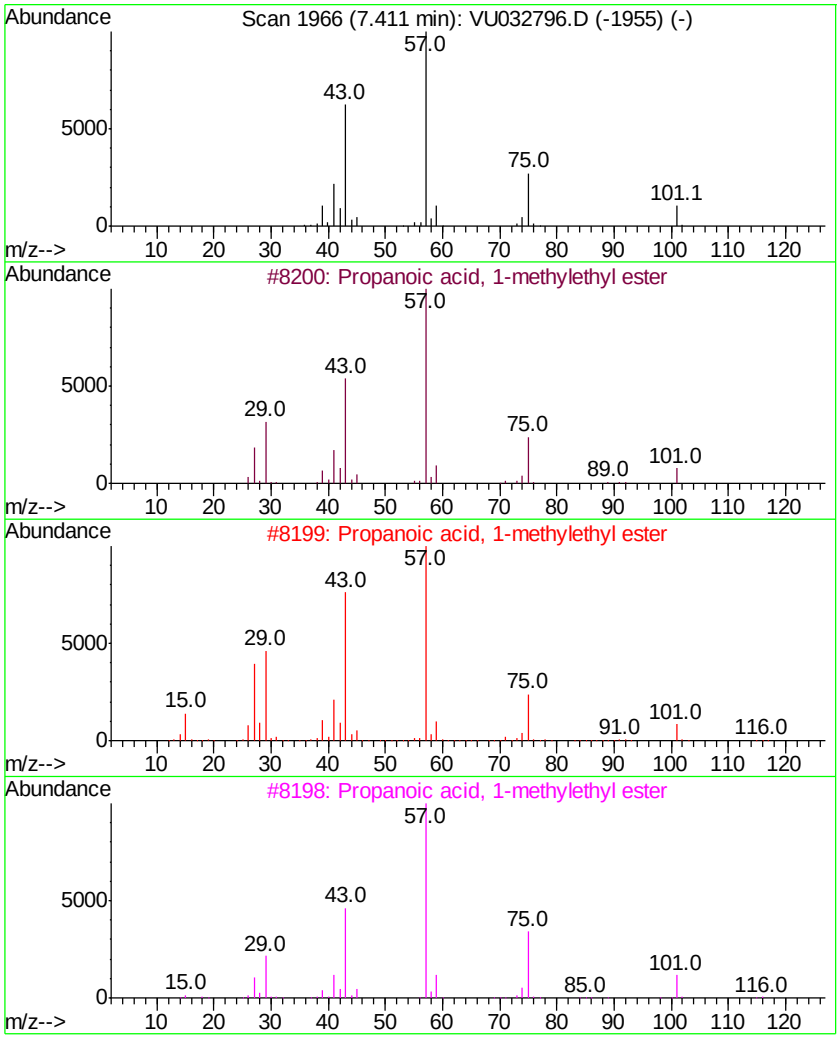
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

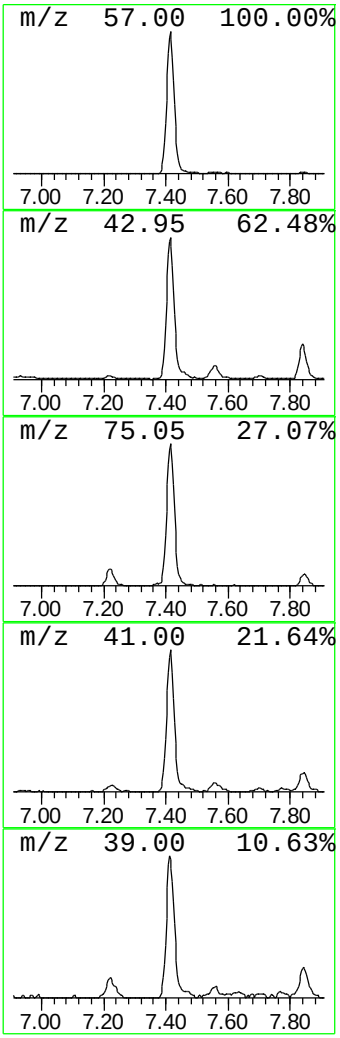
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	23.09 ug/L	256066	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	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
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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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

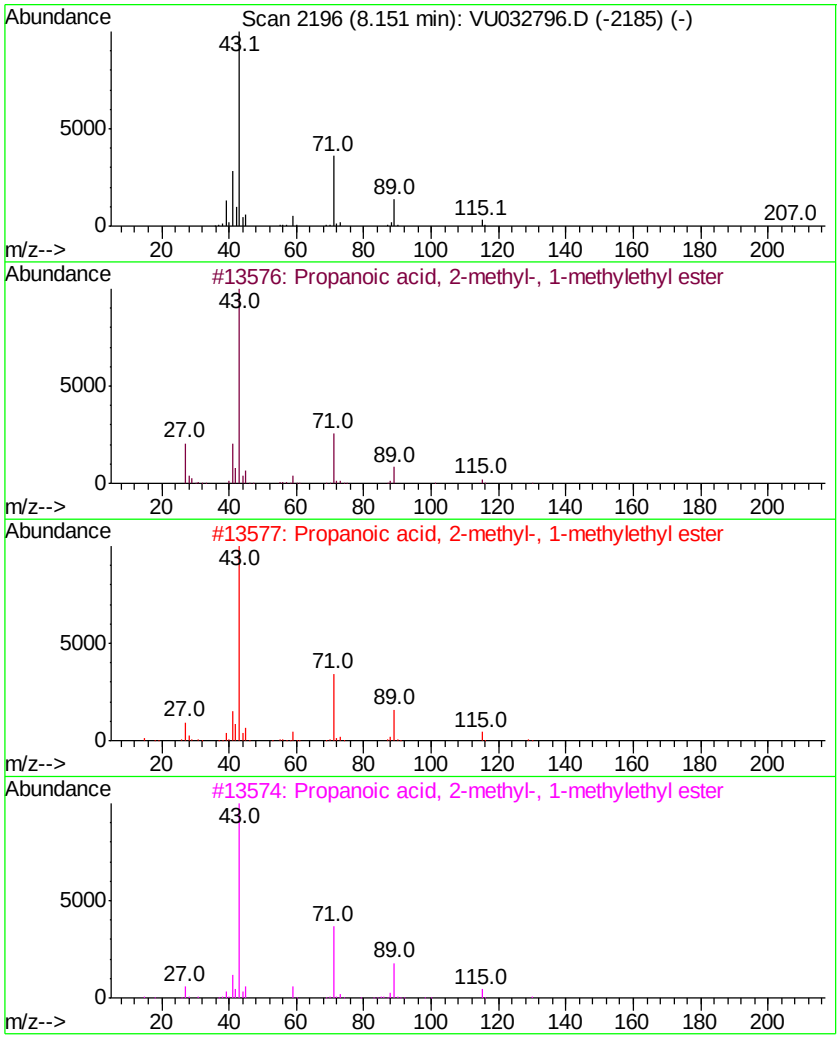
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

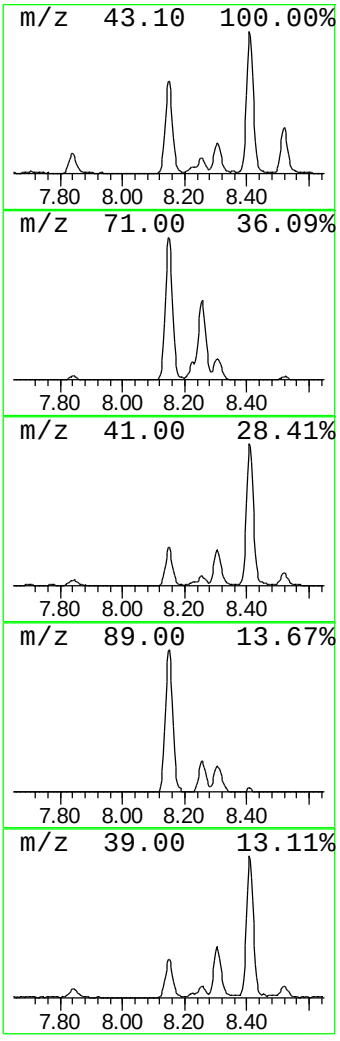
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.12 ug/L	144247	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	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59





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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

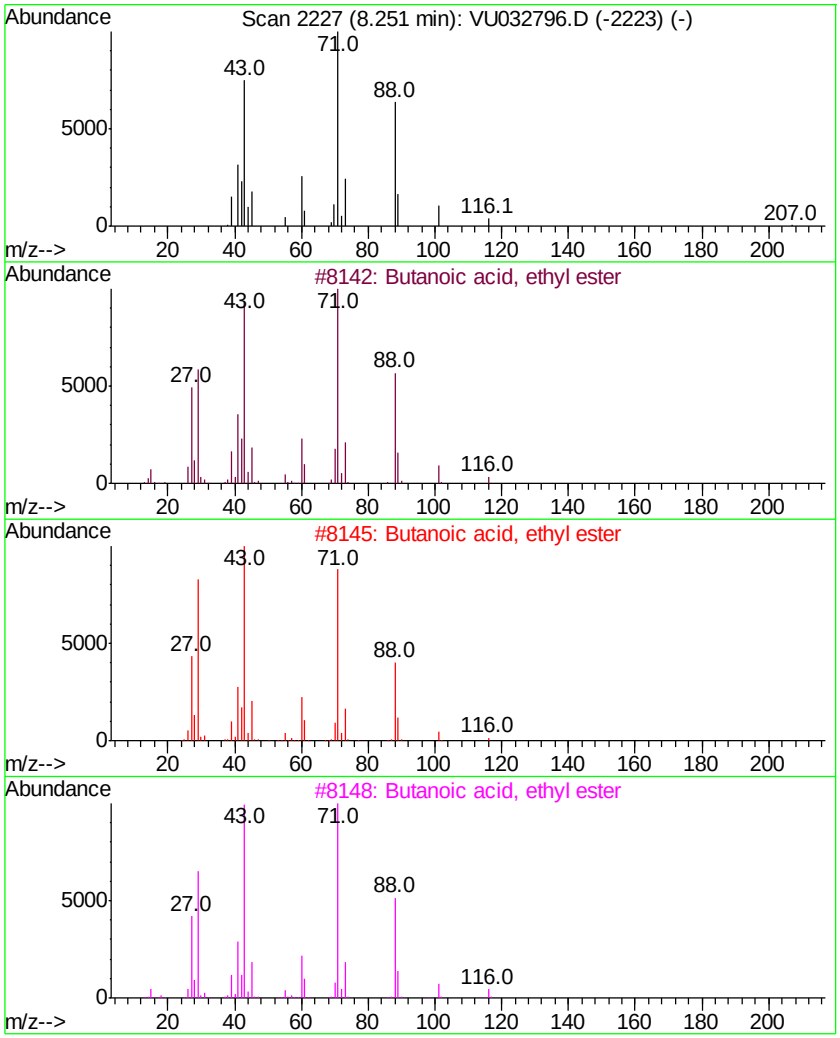
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

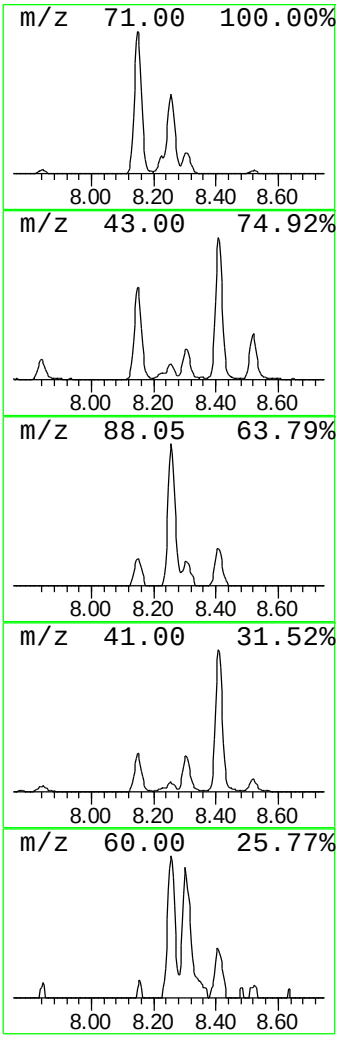
****

Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	3.38 ug/L	48151	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	96
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
3	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
4	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	53





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Acq On : 17 Jun 2019 20:30
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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

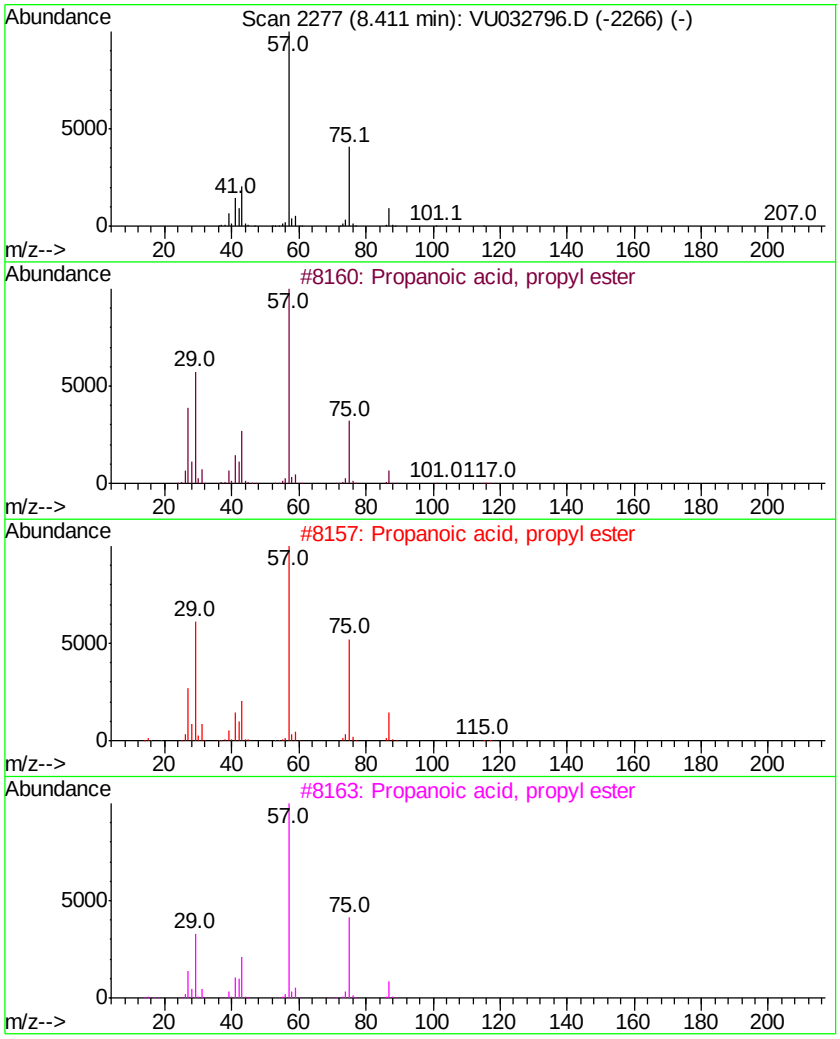
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

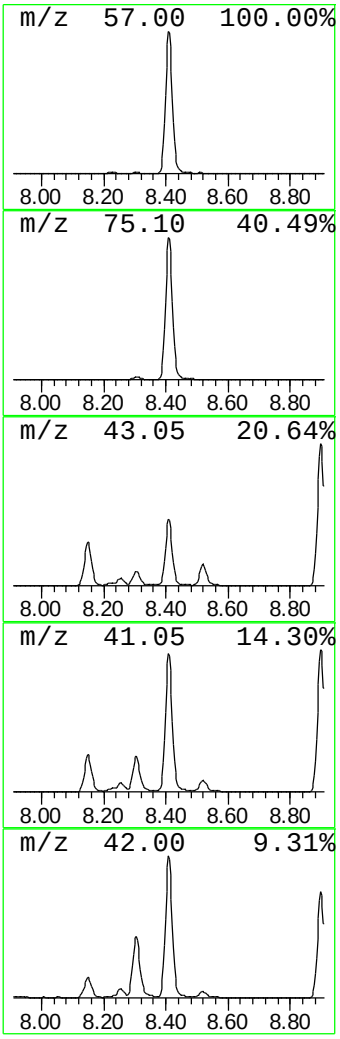
****

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	66.15 ug/L	942431	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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032796.D
Acq On : 17 Jun 2019 20:30
Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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

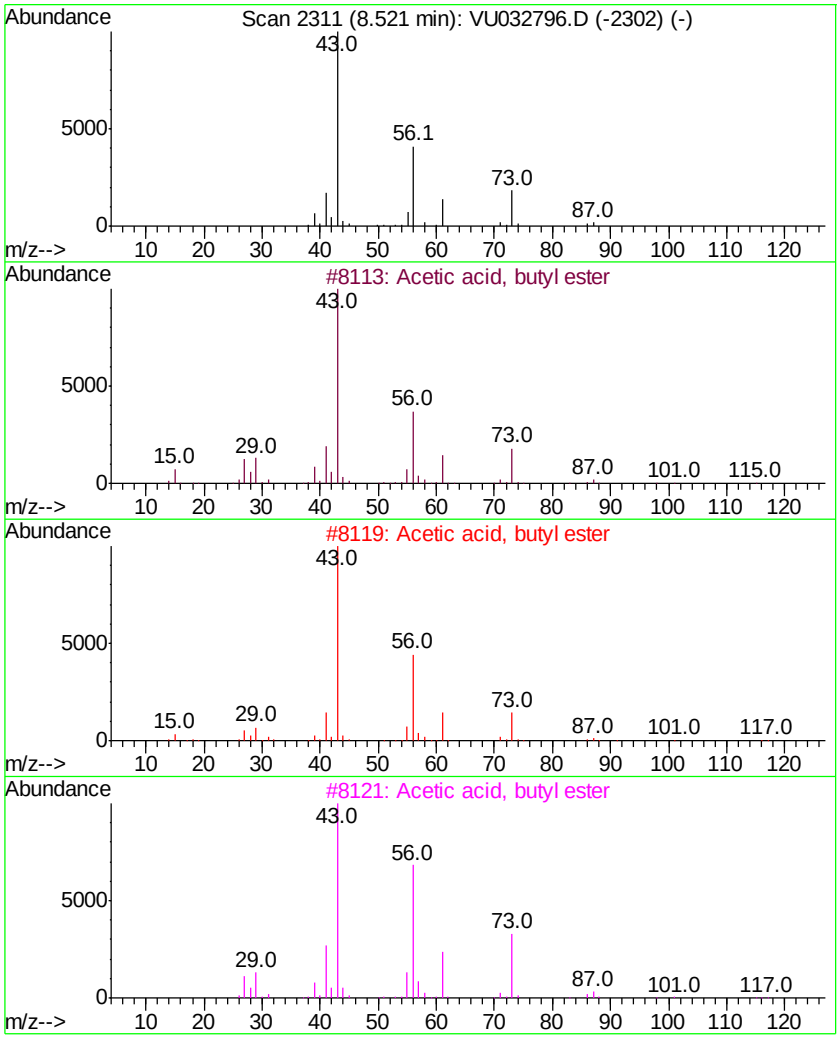
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

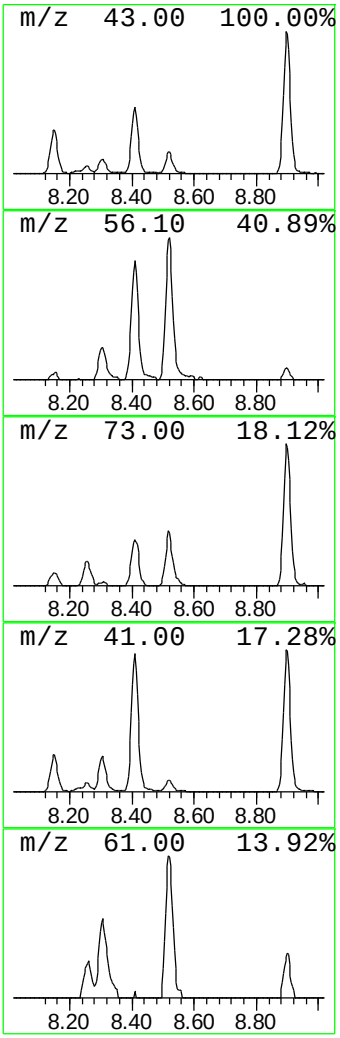
****

Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.94 ug/L	70407	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\VU061719\
Data File : VU032796.D
Acq On : 17 Jun 2019 20:30
Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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

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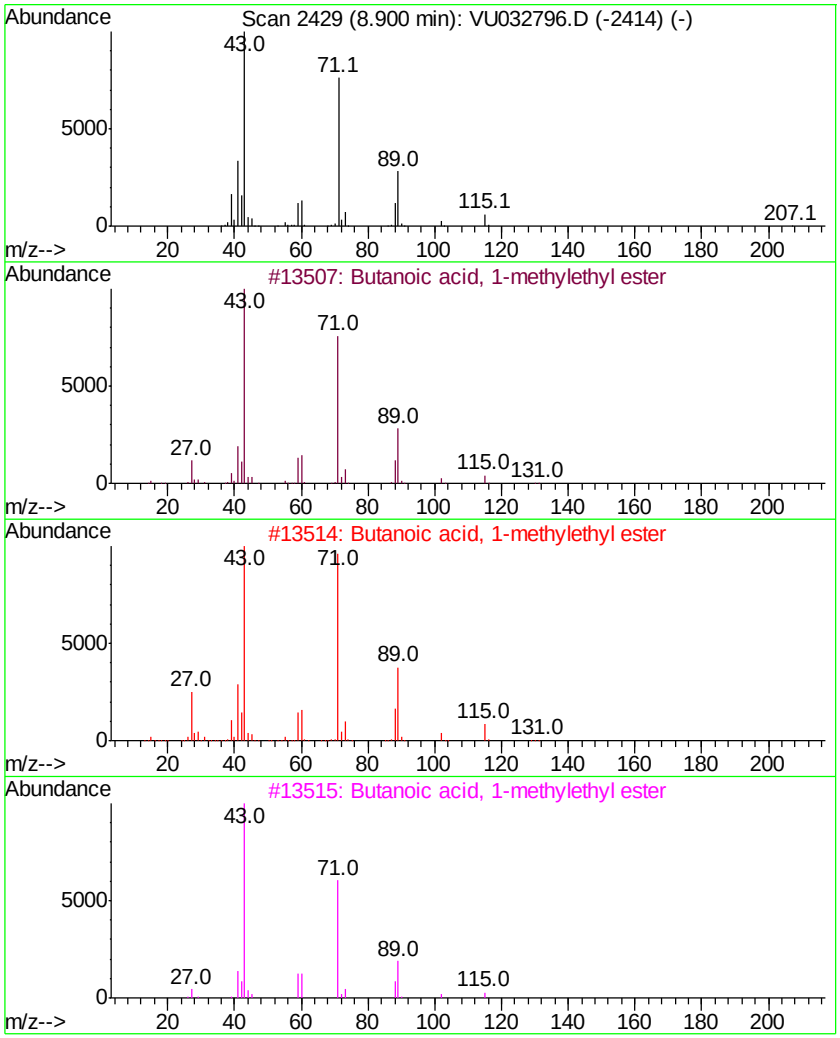
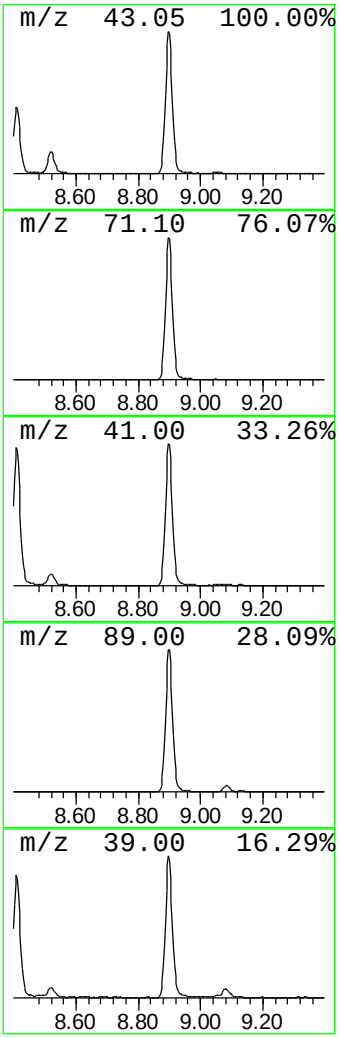
Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	46.58 ug/L	663565	Chlorobenzene-d5	9.08

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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032796.D
Acq On : 17 Jun 2019 20:30
Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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

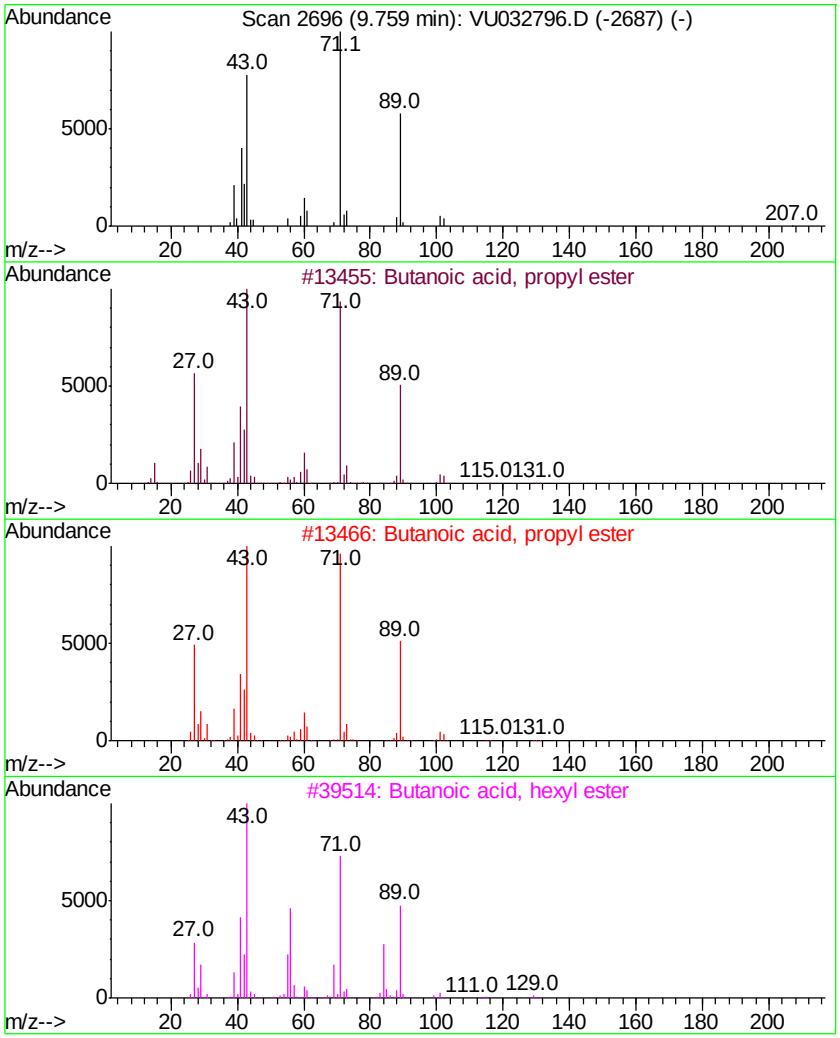
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

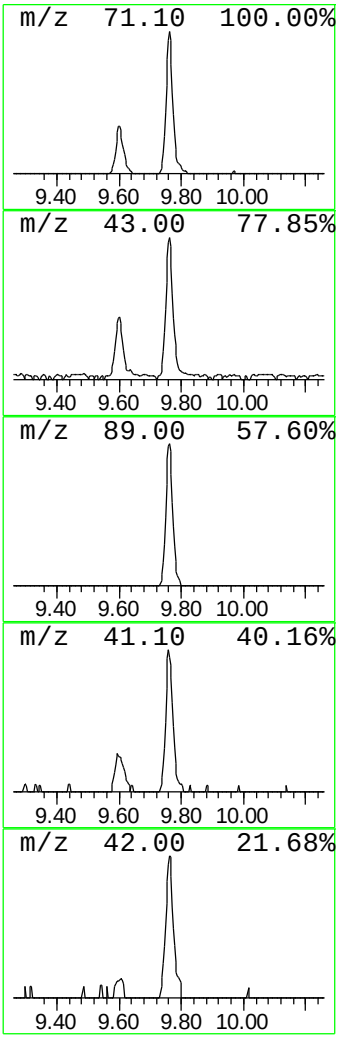
****

Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.58 ug/L	36723	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032796.D
Acq On : 17 Jun 2019 20:30
Operator : JC/SP
Sample : K3324-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JR7

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	131.3	ug/L	1456730	1	5.88	554516	50.0
Propanoic acid, 1...	7.41	23.1	ug/L	256066	1	5.88	554516	50.0
Propanoic acid, 2...	8.15	10.1	ug/L	144247	2	9.08	712357	50.0
Butanoic acid, et...	8.25	3.4	ug/L	48151	2	9.08	712357	50.0
Propanoic acid, p...	8.41	66.2	ug/L	942431	2	9.08	712357	50.0
Acetic acid, buty...	8.52	4.9	ug/L	70407	2	9.08	712357	50.0
Butanoic acid, 1-...	8.90	46.6	ug/L	663565	2	9.08	712357	50.0
Butanoic acid, pr...	9.76	2.6	ug/L	36723	2	9.08	712357	50.0