LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032693.D
Acq On : 13 Jun 2019 14:44
Operator : JC/SP
Sample : K3286-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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	37	rVB	4062	3679	0.32%	0.047%
2	1.395	88	95	106	rBV	68254	70834	6.13%	0.897%
3	1.675	175	182	198	rBV	58072	71576	6.19%	0.906%
4	2.267	356	366	376	rBV	118068	177162	15.32%	2.242%
5	2.318	377	382	394	rVB	10304	15612	1.35%	0.198%
6	2.620	469	476	480	rBV2	941	1171	0.10%	0.015%
7	2.698	490	500	512	rVB2	7566	12718	1.10%	0.161%
8	2.833	536	542	545	rVB2	339	280	0.02%	0.004%
9	2.855	545	549	553	rBV	456	321	0.03%	0.004%
10	2.965	578	583	587	rVB2	191	206	0.02%	0.003%
11	2.990	587	591	597	rBV2	275	287	0.02%	0.004%
12	3.087	617	621	627	rBV	355	370	0.03%	0.005%
13	3.167	639	646	651	rBV2	132	201	0.02%	0.003%
14	3.411	713	722	739	rBV3	2969	7439	0.64%	0.094%
15	3.553	762	766	771	rVB2	238	218	0.02%	0.003%
16	3.836	849	854	858	rBV2	260	284	0.02%	0.004%
17	3.961	888	893	899	rVB2	162	202	0.02%	0.003%
18	4.096	929	935	944	rVB2	241	438	0.04%	0.006%
19	4.167	944	957	985	rBV	63782	168449	14.57%	2.132%
20	4.643	1089	1105	1125	rVV	99191	233071	20.16%	2.950%
21	4.804	1149	1155	1157	rVB3	266	228	0.02%	0.003%
22	4.842	1164	1167	1170	rVV	264	163	0.01%	0.002%
23	4.894	1177	1183	1188	rVB2	359	423	0.04%	0.005%
24	4.987	1207	1212	1216	rVV2	268	254	0.02%	0.003%
25	5.083	1237	1242	1249	rVB2	258	312	0.03%	0.004%
26	5.190	1272	1275	1281	rVB2	242	170	0.01%	0.002%
27	5.235	1286	1289	1294	rVB2	206	193	0.02%	0.002%
28	5.334	1294	1320	1347	rBV2	189750	567908	49.11%	7.188%
29	5.469	1359	1362	1368	rVB2	401	358	0.03%	0.005%
30	5.553	1380	1388	1400	rBV3	3768	7352	0.64%	0.093%
31	5.675	1424	1426	1429	rVB2	407	202	0.02%	0.003%
32	5.723	1435	1441	1442	rBV2	274	207	0.02%	0.003%
33	5.881	1467	1490	1512	rBV	218750	462719	40.02%	5.857%
34	6.325	1615	1628	1651	rBV	133144	266158	23.02%	3.369%

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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	6.424	1652	1659	1673	rVB2	5154	9598	0.83%	0.121%
36	6.579	1702	1707	1717	rBV2	2715	4268	0.37%	0.054%
37	6.698	1732	1744	1779	rBV	649073	1156324	100.00%	14.636%
38	7.225	1896	1908	1933	rVV2	72299	133237	11.52%	1.686%
39	7.415	1956	1967	1993	rBV	111713	196590	17.00%	2.488%
40	7.559	2000	2012	2033	rBV	251196	448453	38.78%	5.676%
41	7.697	2050	2055	2058	rBV5	699	725	0.06%	0.009%
42	7.794	2079	2085	2088	rBV4	750	819	0.07%	0.010%
43	7.845	2091	2101	2123	rVV2	60160	107733	9.32%	1.364%
44	7.980	2141	2143	2150	rVB4	472	365	0.03%	0.005%
45	8.151	2183	2196	2213	rBV	61509	104878	9.07%	1.327%
46	8.257	2213	2229	2235	rVV4	28687	55927	4.84%	0.708%
47	8.305	2235	2244	2266	rVV	222266	404351	34.97%	5.118%
48	8.411	2266	2277	2303	rVV	474821	770881	66.67%	9.757%
49	8.521	2304	2311	2335	rVB	31348	57938	5.01%	0.733%
50	8.701	2362	2367	2373	rVB3	493	486	0.04%	0.006%
51	8.900	2417	2429	2459	rBV	318742	506019	43.76%	6.405%
52	9.083	2474	2486	2517	rVB	319349	529577	45.80%	6.703%
53	9.347	2566	2568	2576	rVV3	197	241	0.02%	0.003%
54	9.389	2577	2581	2584	rVB3	357	260	0.02%	0.003%
55	9.418	2588	2590	2597	rVB3	244	252	0.02%	0.003%
56	9.498	2611	2615	2618	rBV2	202	163	0.01%	0.002%
57	9.521	2618	2622	2626	rBV3	197	165	0.01%	0.002%
58	9.607	2641	2649	2660	rBV2	3444	6130	0.53%	0.078%
59	9.726	2681	2686	2689	rBV	253	281	0.02%	0.004%
60	9.765	2689	2698	2716	rVV	16435	27885	2.41%	0.353%
61	10.029	2778	2780	2786	rVB2	272	235	0.02%	0.003%
62	10.106	2802	2804	2809	rVB	466	296	0.03%	0.004%
63	10.135	2809	2813	2815	rBV2	228	195	0.02%	0.002%
64	10.167	2820	2823	2826	rVV2	208	200	0.02%	0.003%
65	10.196	2829	2832	2840	rVB2	335	345	0.03%	0.004%
66	10.295	2858	2863	2869	rVB2	266	300	0.03%	0.004%
67	10.427	2891	2904	2923	rBV	207209	335979	29.06%	4.253%
68	10.765	3005	3009	3010	rBV	422	216	0.02%	0.003%
69	10.794	3015	3018	3021	rVV4	350	254	0.02%	0.003%
70	10.823	3024	3027	3028	rVV2	311	165	0.01%	0.002%
71	10.848	3032	3035	3043	rVV3	272	372	0.03%	0.005%

LSC Area Percent Report

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Operator : JC/SP
Sample : K3286-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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	10.919	3053	3057	3059	rVV3	325	277	0.02%	0.004%
73	10.938	3059	3063	3065	rVV2	282	275	0.02%	0.003%
74	10.951	3065	3067	3070	rVV3	339	211	0.02%	0.003%
75	11.170	3129	3135	3138	rBV2	285	299	0.03%	0.004%
76	11.350	3187	3191	3195	rBV2	180	179	0.02%	0.002%
77	11.405	3205	3208	3213	rVB3	255	205	0.02%	0.003%
78	11.479	3219	3231	3257	rBV	313714	508910	44.01%	6.441%
79	11.736	3306	3311	3314	rVB3	584	620	0.05%	0.008%
80	11.765	3314	3320	3322	rBV3	308	234	0.02%	0.003%
81	11.855	3334	3348	3372	rBV	270237	451714	39.06%	5.717%
82	12.209	3454	3458	3460	rBV2	312	238	0.02%	0.003%
83	12.411	3518	3521	3527	rBV2	238	209	0.02%	0.003%
84	12.501	3545	3549	3554	rBV2	290	318	0.03%	0.004%
85	12.620	3583	3586	3590	rVB2	235	165	0.01%	0.002%
86	12.739	3618	3623	3625	rBV2	196	203	0.02%	0.003%
87	12.906	3672	3675	3679	rBV	336	239	0.02%	0.003%
88	13.073	3724	3727	3732	rBV2	298	372	0.03%	0.005%
89	13.157	3747	3753	3756	rBV	245	263	0.02%	0.003%
90	13.363	3813	3817	3819	rVV	204	202	0.02%	0.003%
91	13.395	3823	3827	3829	rBV	222	201	0.02%	0.003%
92	13.662	3906	3910	3912	rBV	281	198	0.02%	0.003%
93	13.967	4001	4005	4011	rVB3	245	255	0.02%	0.003%
94	14.286	4100	4104	4106	rBV3	226	202	0.02%	0.003%
95	14.321	4109	4115	4117	rVB3	308	277	0.02%	0.004%
96	14.382	4131	4134	4137	rVB	326	206	0.02%	0.003%
97	14.421	4143	4146	4149	rBV2	278	189	0.02%	0.002%
98	14.598	4197	4201	4205	rBV3	333	282	0.02%	0.004%
99	15.826	4580	4583	4586	rBV2	396	291	0.03%	0.004%
100	15.871	4594	4597	4599	rBV2	353	204	0.02%	0.003%

Sum of corrected areas: 7900706

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032693.D
Acq On : 13 Jun 2019 14:44
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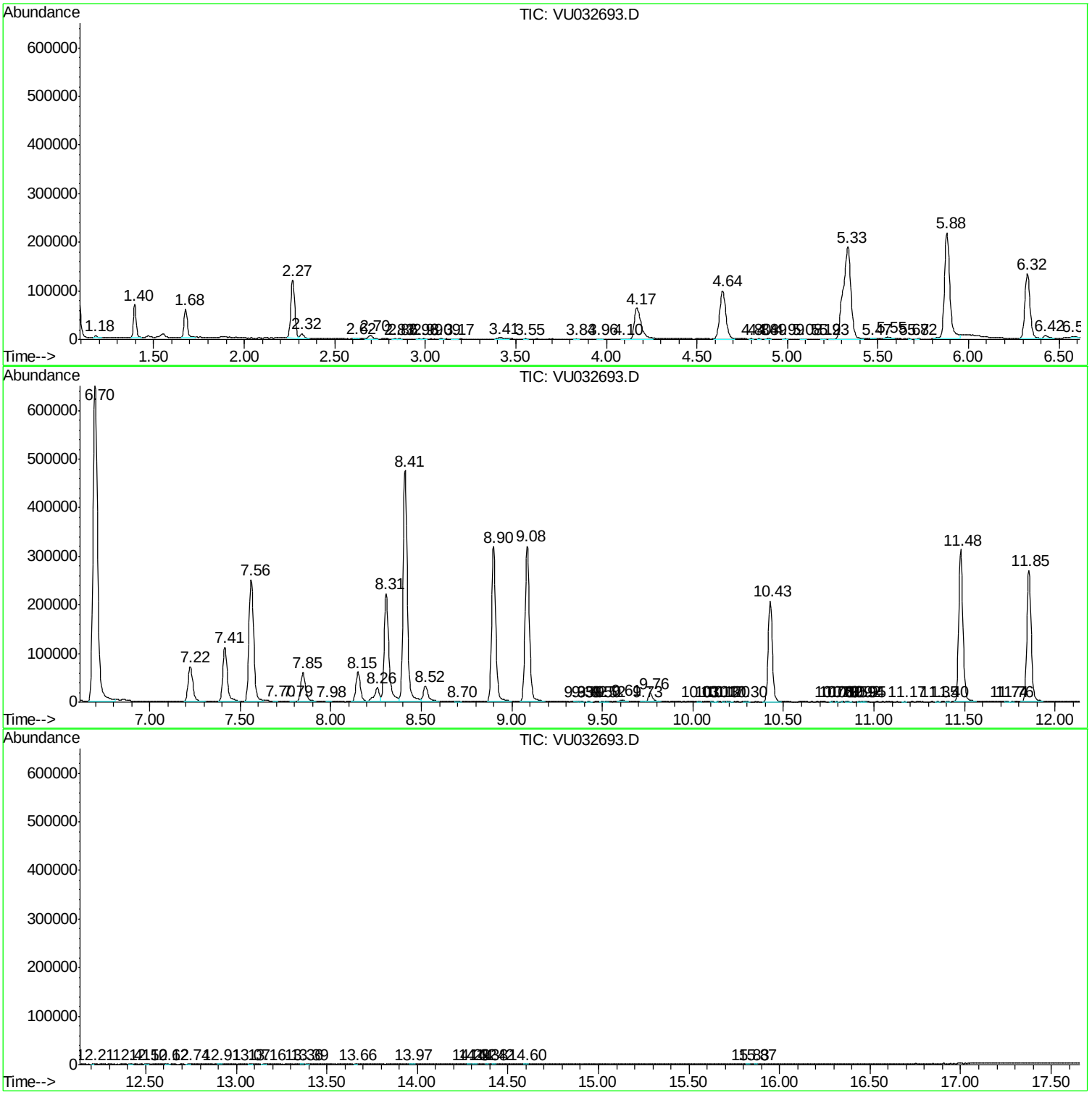
Sample : K3286-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

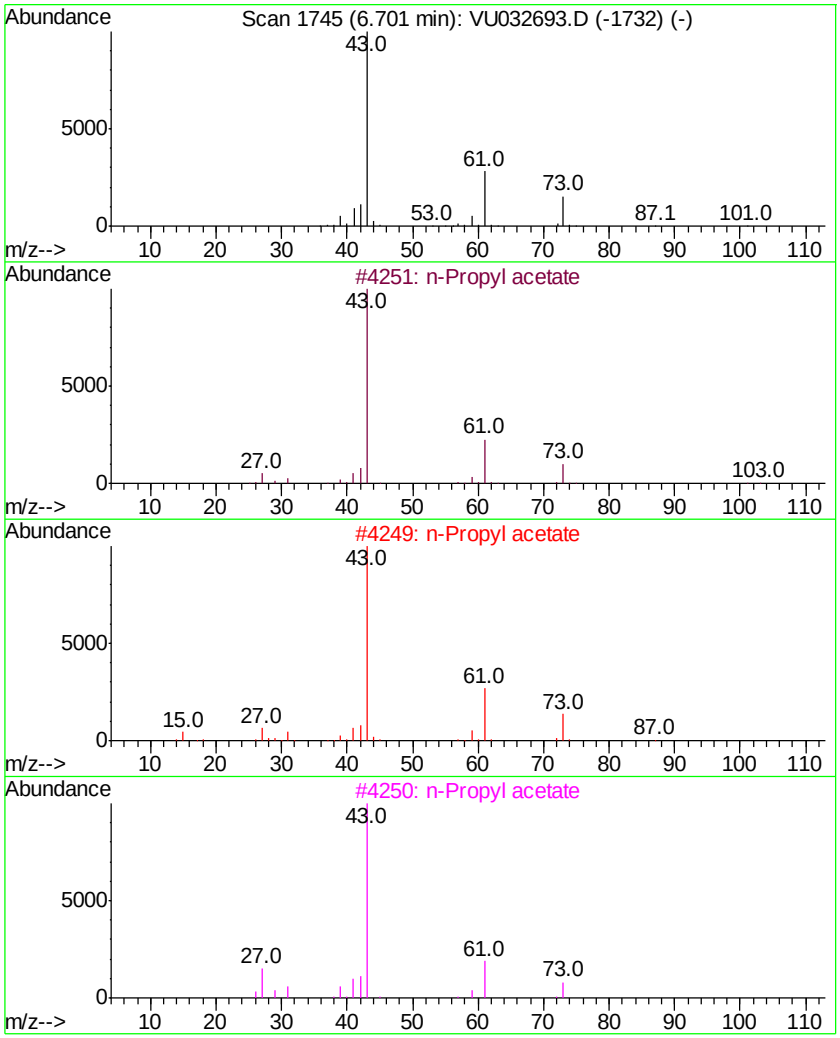
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

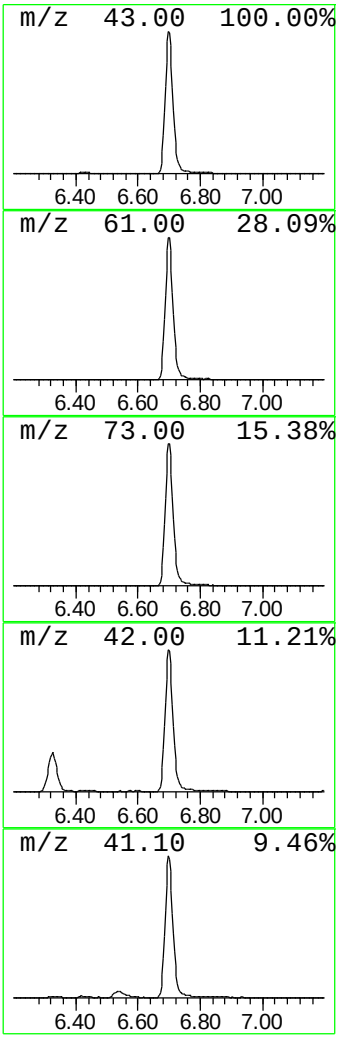
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	124.95 ug/L	1156320	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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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

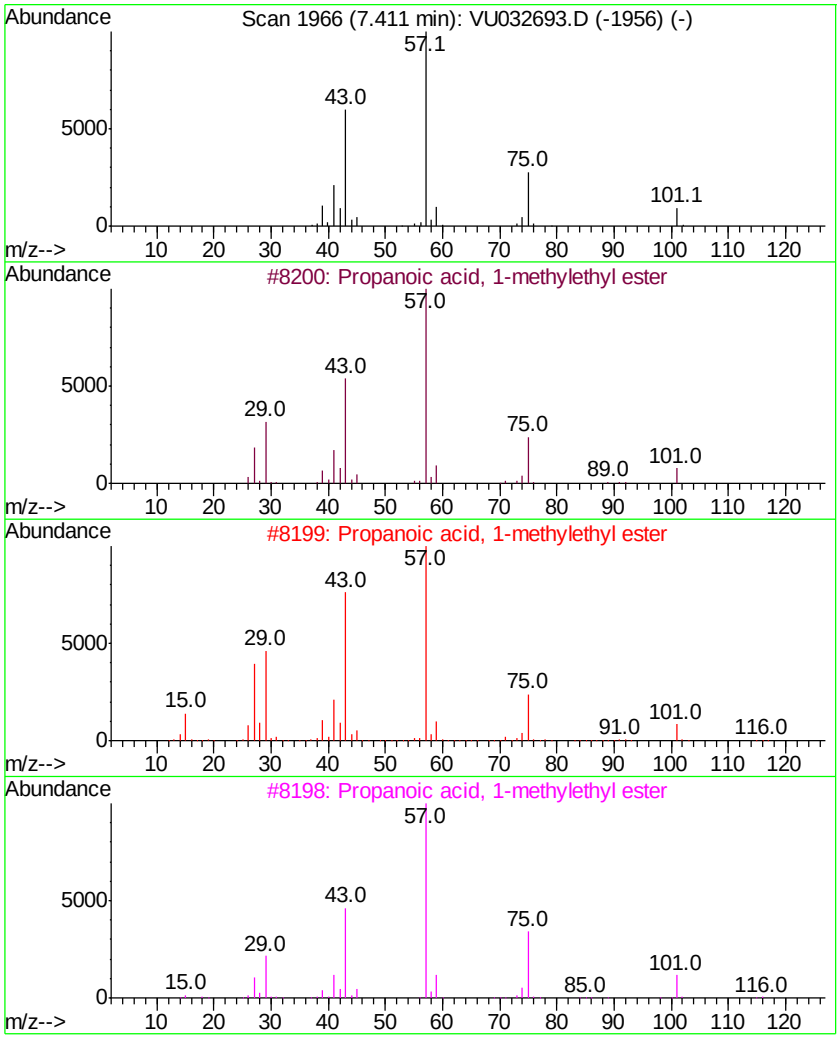
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

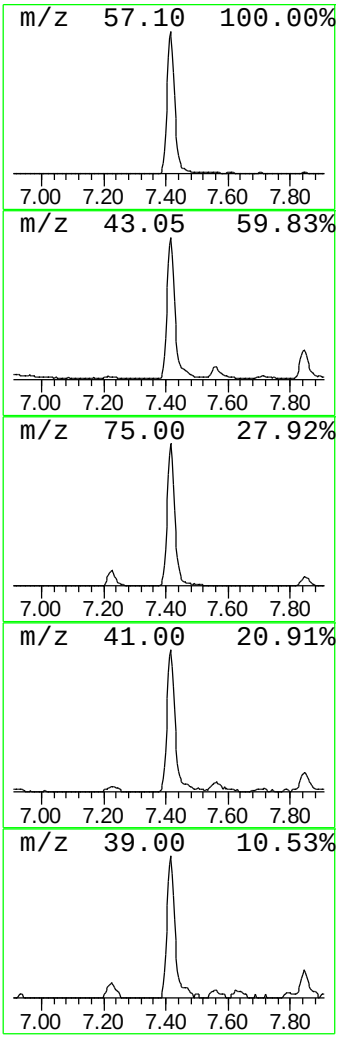
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	21.24 ug/L	196590	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	64
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\SOMULM060619WMA.M
Quant Title : VOC Analysis

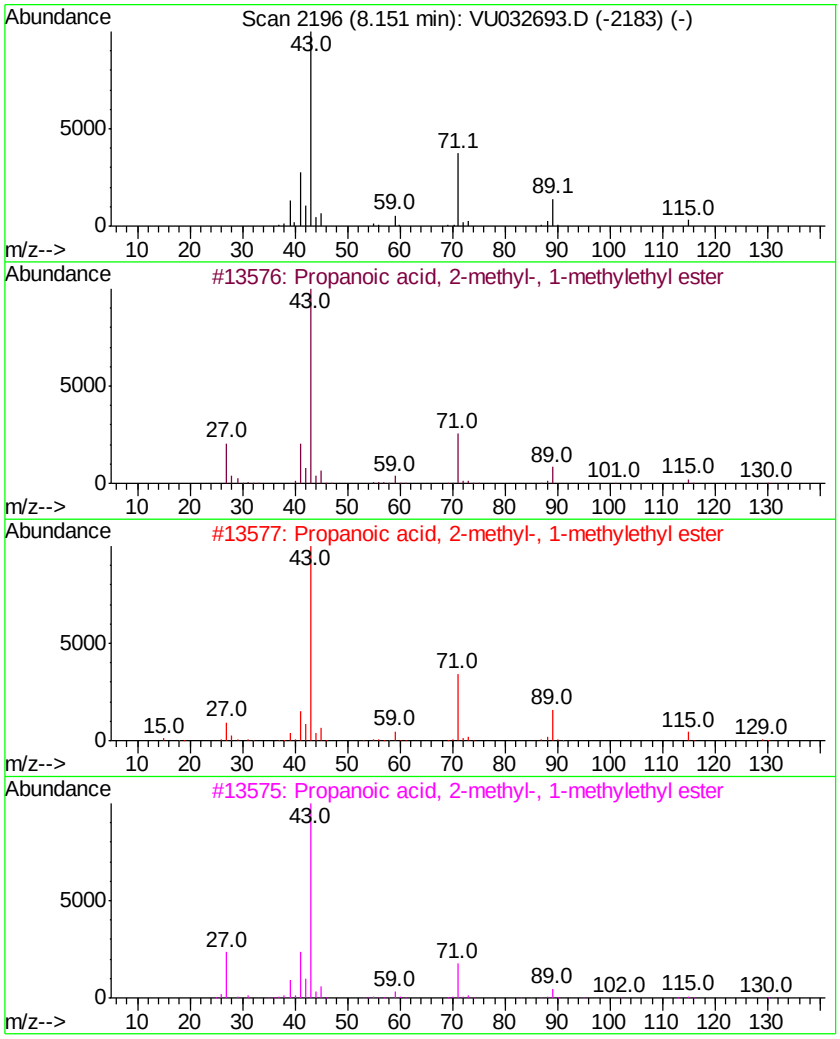
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

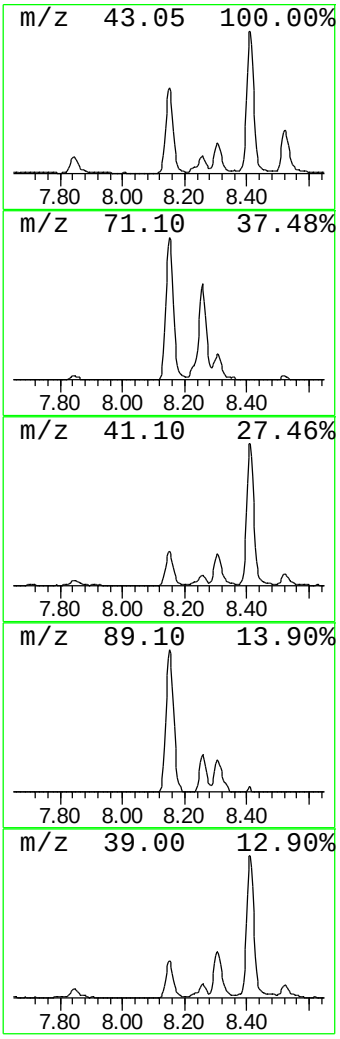
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.90 ug/L	104878	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





Library Search Compound Report

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Data File : VU032693.D
Acq On : 13 Jun 2019 14:44
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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

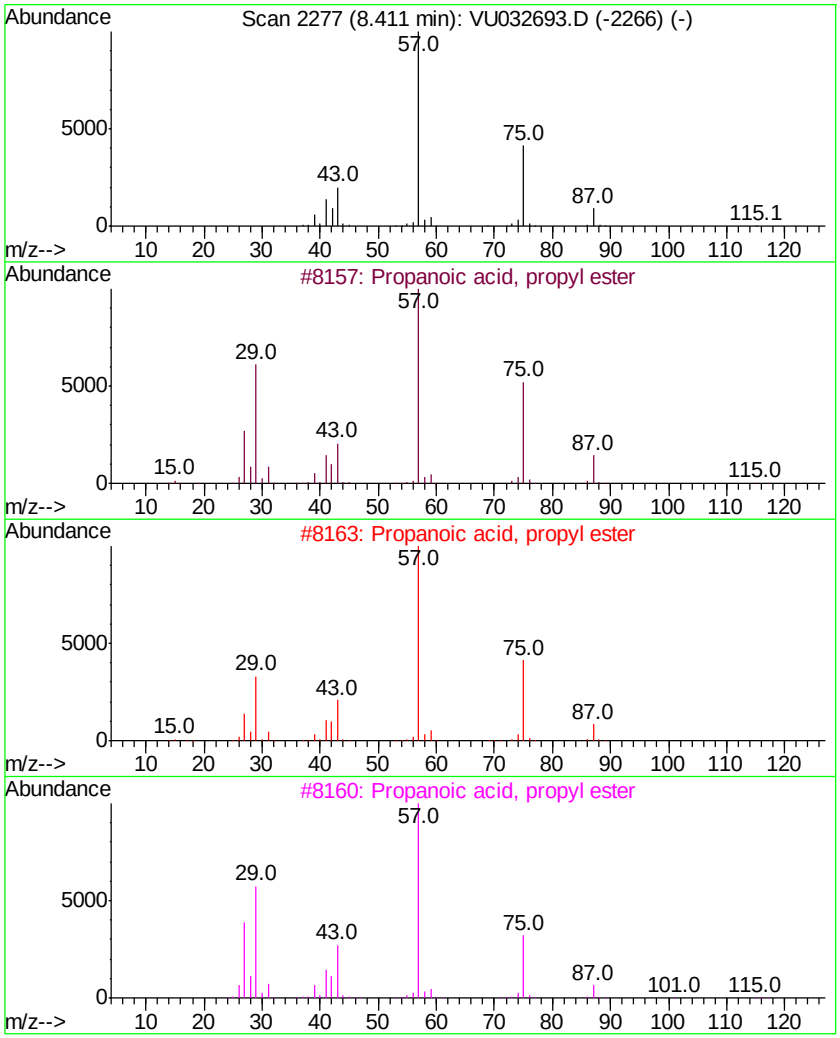
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

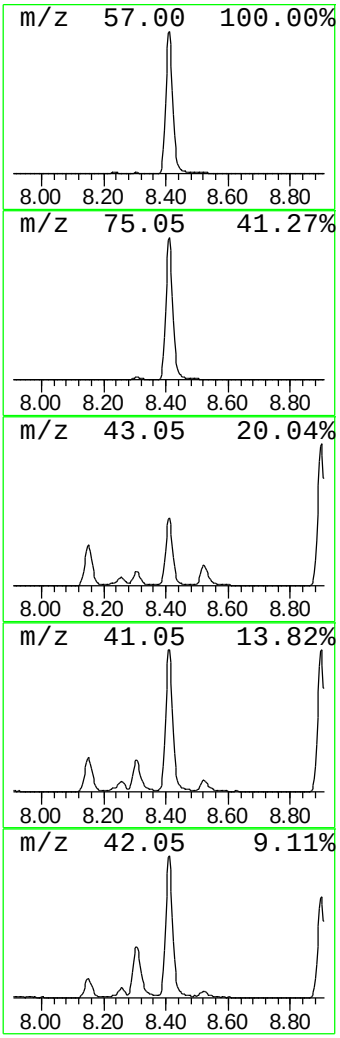
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	72.78 ug/L	770881	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	78
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39





Library Search Compound Report

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Acq On : 13 Jun 2019 14:44
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Sample : K3286-20
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

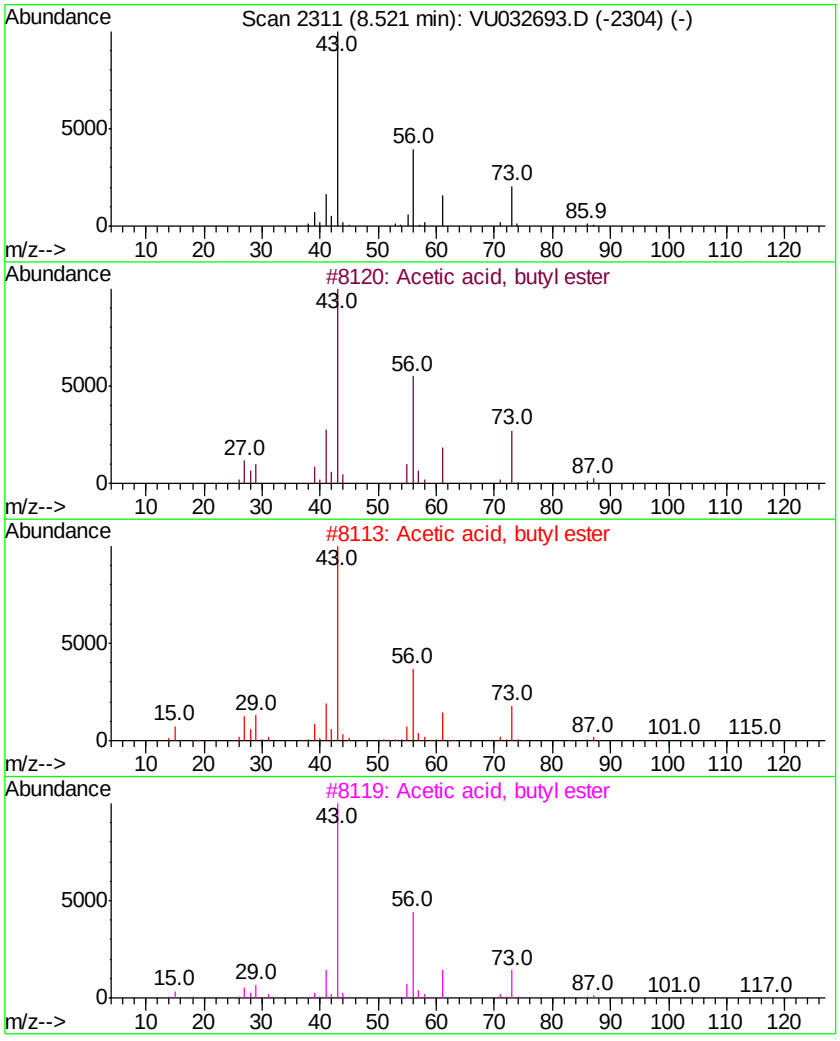
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

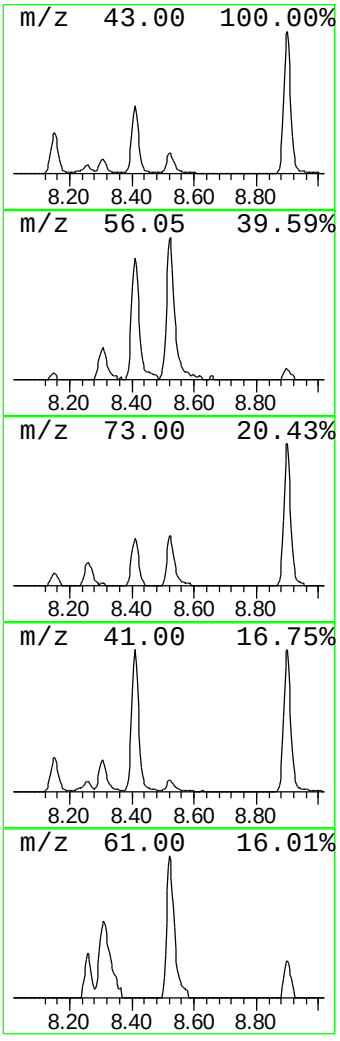
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	5.47 ug/L	57938	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	17
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032693.D
Acq On : 13 Jun 2019 14:44
Operator : JC/SP
Sample : K3286-20
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

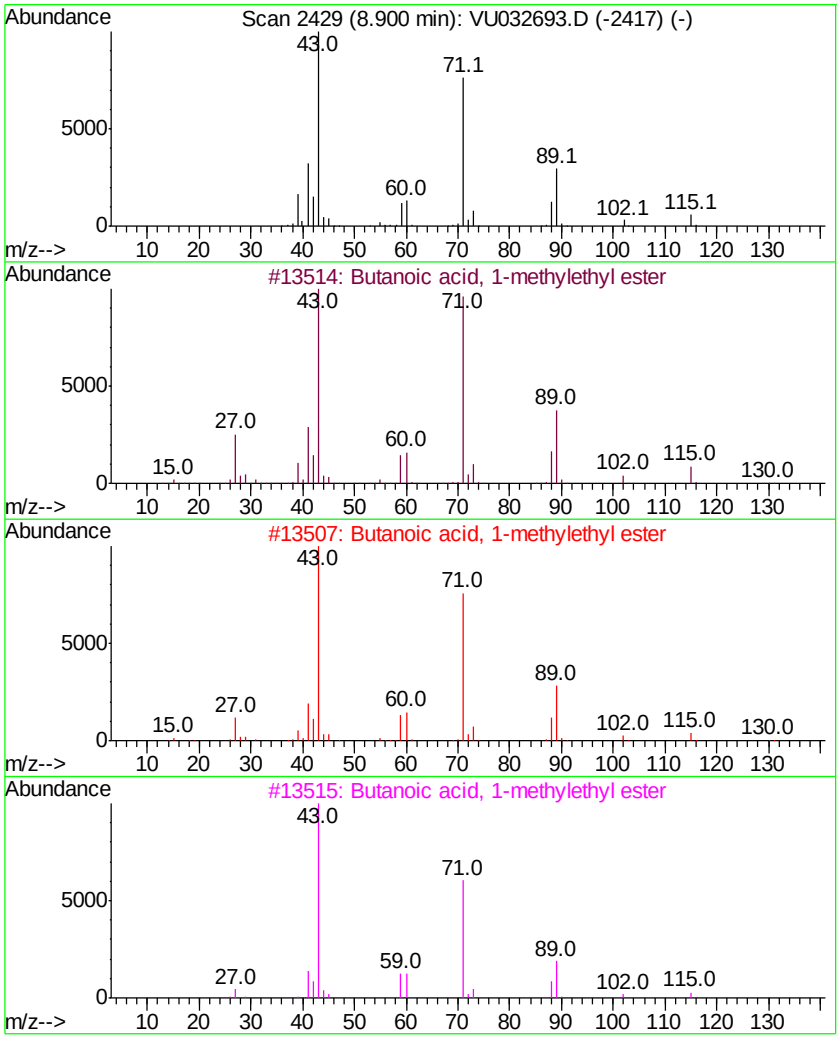
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

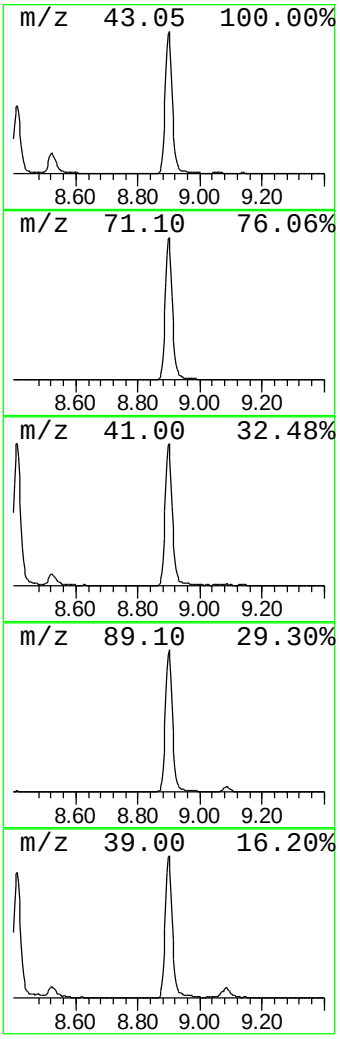
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	47.78 ug/L	506019	Chlorobenzene-d5	9.09

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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032693.D
Acq On : 13 Jun 2019 14:44
Operator : JC/SP
Sample : K3286-20
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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

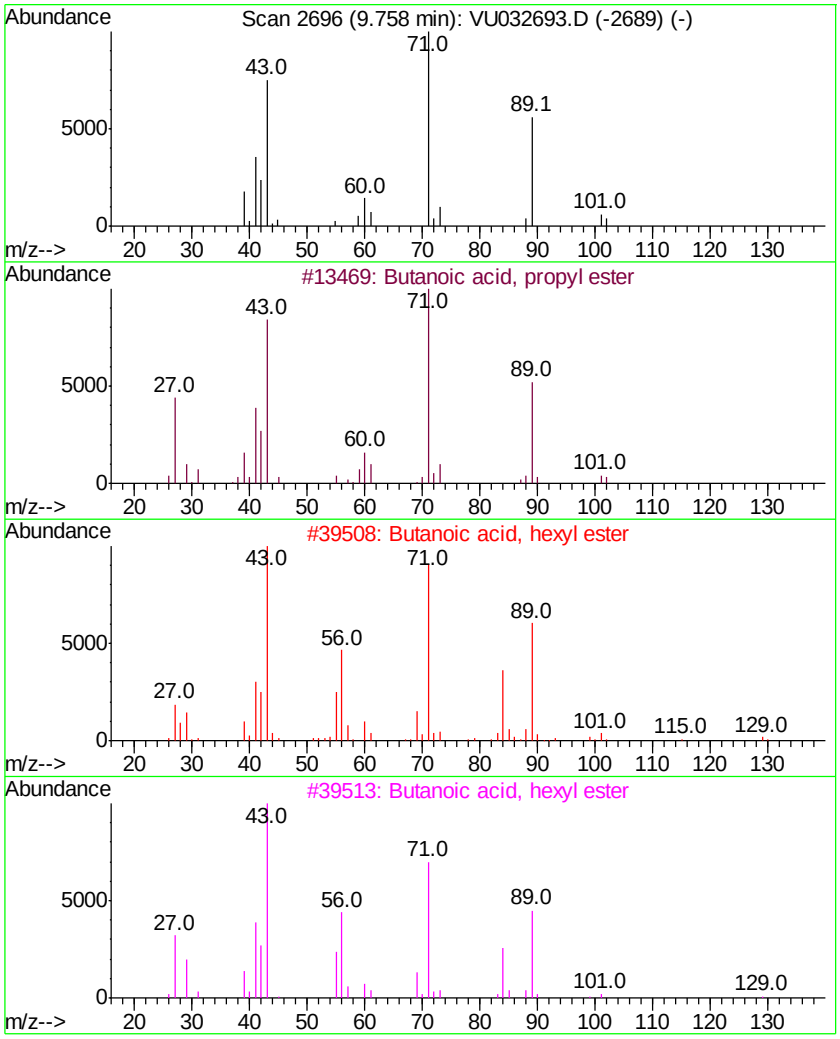
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

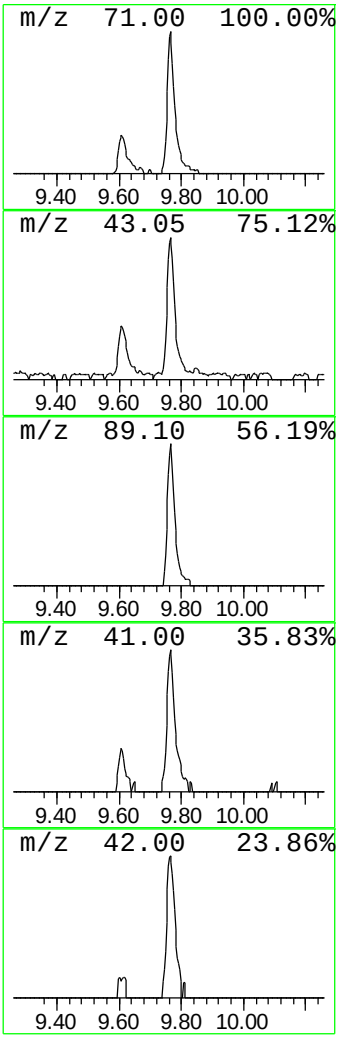
****

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.63 ug/L	27885	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
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 : VU032693.D
Acq On : 13 Jun 2019 14:44
Operator : JC/SP
Sample : K3286-20
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JS7

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	125.0	ug/L	1156320	1	5.88	462719	50.0
Propanoic acid, 1...	7.41	21.2	ug/L	196590	1	5.88	462719	50.0
Propanoic acid, 2...	8.15	9.9	ug/L	104878	2	9.09	529577	50.0
Propanoic acid, p...	8.41	72.8	ug/L	770881	2	9.09	529577	50.0
Acetic acid, buty...	8.52	5.5	ug/L	57938	2	9.09	529577	50.0
Butanoic acid, 1-...	8.90	47.8	ug/L	506019	2	9.09	529577	50.0
Butanoic acid, pr...	9.76	2.6	ug/L	27885	2	9.09	529577	50.0