LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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	24	28	36	rVB3	3991	3893	0.13%	0.034%
2	1.395	88	95	106	rVB2	124548	131707	4.46%	1.158%
3	1.675	174	182	194	rBV	89682	110428	3.74%	0.971%
4	2.267	355	366	379	rBV3	214933	357068	12.10%	3.139%
5	2.694	495	499	506	rVB4	1141	1367	0.05%	0.012%
6	2.833	530	542	555	rVB2	5125	11072	0.38%	0.097%
7	2.977	575	587	605	rBV	51050	96049	3.26%	0.844%
8	3.083	616	620	623	rBV3	424	375	0.01%	0.003%
9	3.167	643	646	648	rBV2	350	250	0.01%	0.002%
10	3.350	697	703	707	rBV2	446	578	0.02%	0.005%
11	3.383	711	713	718	rVB2	321	242	0.01%	0.002%
12	3.418	721	724	727	rBV	406	312	0.01%	0.003%
13	3.559	763	768	771	rVB3	424	313	0.01%	0.003%
14	3.691	803	809	812	rBV3	300	276	0.01%	0.002%
15	3.791	837	840	843	rVV	346	220	0.01%	0.002%
16	3.852	856	859	864	rBV2	365	277	0.01%	0.002%
17	3.916	876	879	883	rBV3	402	281	0.01%	0.002%
18	4.096	932	935	940	rBV3	433	408	0.01%	0.004%
19	4.215	945	972	1012	rBV2	1120597	2950414	100.00%	25.941%
20	4.563	1077	1080	1082	rBV2	459	294	0.01%	0.003%
21	4.575	1082	1084	1087	rVB3	475	249	0.01%	0.002%
22	4.640	1087	1104	1122	rBV2	149001	347400	11.77%	3.054%
23	4.752	1136	1139	1141	rBV4	326	218	0.01%	0.002%
24	4.813	1153	1158	1161	rBV4	490	467	0.02%	0.004%
25	4.887	1176	1181	1187	rVB4	893	817	0.03%	0.007%
26	4.936	1191	1196	1197	rBV2	370	328	0.01%	0.003%
27	4.997	1213	1215	1219	rVB	403	224	0.01%	0.002%
28	5.038	1224	1228	1235	rBV4	186	221	0.01%	0.002%
29	5.334	1296	1320	1340	rBV2	296657	871286	29.53%	7.661%
30	5.534	1380	1382	1384	rBV2	463	315	0.01%	0.003%
31	5.669	1420	1424	1428	rVB3	228	220	0.01%	0.002%
32	5.881	1474	1490	1519	rBV	277658	546468	18.52%	4.805%
33	6.090	1550	1555	1562	rBV6	707	900	0.03%	0.008%
34	6.125	1562	1566	1568	rBV2	563	522	0.02%	0.005%

LSC Area Percent Report

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Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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	6.180	1568	1583	1609	rVV	494248	948343	32.14%	8.338%
36	6.325	1614	1628	1651	rVB	200483	401367	13.60%	3.529%
37	6.534	1691	1693	1695	rVV2	393	215	0.01%	0.002%
38	6.582	1701	1708	1713	rBV4	916	1297	0.04%	0.011%
39	6.640	1724	1726	1732	rVB2	472	360	0.01%	0.003%
40	6.701	1732	1745	1772	rBV	116761	213846	7.25%	1.880%
41	6.823	1782	1783	1785	rBV2	562	287	0.01%	0.003%
42	6.961	1823	1826	1829	rBV	343	253	0.01%	0.002%
43	7.087	1860	1865	1868	rBV3	576	537	0.02%	0.005%
44	7.132	1876	1879	1884	rBV3	341	364	0.01%	0.003%
45	7.160	1884	1888	1893	rVV4	228	254	0.01%	0.002%
46	7.222	1895	1907	1930	rBV	116060	206255	6.99%	1.813%
47	7.415	1956	1967	1978	rBV	25847	42638	1.45%	0.375%
48	7.559	1999	2012	2028	rBV	405207	699109	23.70%	6.147%
49	7.771	2075	2078	2083	rVB3	473	459	0.02%	0.004%
50	7.845	2089	2101	2124	rBV	84057	147672	5.01%	1.298%
51	7.951	2131	2134	2137	rVB4	460	292	0.01%	0.003%
52	8.019	2152	2155	2160	rVB3	388	335	0.01%	0.003%
53	8.048	2160	2164	2168	rBV2	299	268	0.01%	0.002%
54	8.151	2184	2196	2208	rBV2	13945	23749	0.80%	0.209%
55	8.257	2215	2229	2234	rBV4	4935	9204	0.31%	0.081%
56	8.305	2234	2244	2266	rVV	252048	442983	15.01%	3.895%
57	8.411	2268	2277	2294	rVB	85907	138746	4.70%	1.220%
58	8.527	2306	2313	2321	rVB3	3697	5424	0.18%	0.048%
59	8.614	2336	2340	2350	rVB7	1272	1937	0.07%	0.017%
60	8.733	2374	2377	2384	rVB3	273	234	0.01%	0.002%
61	8.823	2401	2405	2410	rVB4	308	268	0.01%	0.002%
62	8.900	2415	2429	2448	rBV	61884	101242	3.43%	0.890%
63	8.987	2454	2456	2460	rVB2	513	353	0.01%	0.003%
64	9.083	2471	2486	2509	rBV	424107	698466	23.67%	6.141%
65	9.504	2614	2617	2620	rVB	493	319	0.01%	0.003%
66	9.556	2629	2633	2637	rVB2	379	311	0.01%	0.003%
67	9.607	2642	2649	2655	rBV4	873	1206	0.04%	0.011%
68	9.668	2664	2668	2671	rVB4	348	289	0.01%	0.003%
69	9.694	2671	2676	2680	rBV3	369	377	0.01%	0.003%
70	9.765	2689	2698	2706	rBV5	2652	4435	0.15%	0.039%
71	9.987	2764	2767	2773	rVV4	286	307	0.01%	0.003%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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	10.016	2773	2776	2780	rVB2	284	264	0.01%	0.002%
73	10.041	2780	2784	2790	rBV2	348	376	0.01%	0.003%
74	10.083	2795	2797	2800	rVB2	394	238	0.01%	0.002%
75	10.119	2800	2808	2810	rBV3	561	694	0.02%	0.006%
76	10.157	2814	2820	2822	rBV2	214	228	0.01%	0.002%
77	10.221	2835	2840	2841	rBV2	373	284	0.01%	0.002%
78	10.283	2854	2859	2863	rBV2	288	332	0.01%	0.003%
79	10.347	2873	2879	2882	rBV2	387	500	0.02%	0.004%
80	10.427	2892	2904	2922	rBV	284463	462220	15.67%	4.064%
81	10.492	2922	2924	2934	rVB4	669	709	0.02%	0.006%
82	10.771	3009	3011	3017	rVB3	504	469	0.02%	0.004%
83	10.874	3036	3043	3046	rVB2	345	459	0.02%	0.004%
84	10.932	3058	3061	3065	rVB2	287	240	0.01%	0.002%
85	10.977	3065	3075	3079	rBV2	411	643	0.02%	0.006%
86	11.135	3119	3124	3127	rBV2	316	226	0.01%	0.002%
87	11.180	3134	3138	3144	rBV3	276	395	0.01%	0.003%
88	11.479	3219	3231	3254	rBV	439848	697283	23.63%	6.131%
89	11.787	3324	3327	3329	rBV3	364	215	0.01%	0.002%
90	11.855	3336	3348	3373	rBV	403759	674686	22.87%	5.932%
91	12.350	3499	3502	3506	rBV2	389	325	0.01%	0.003%
92	12.421	3521	3524	3530	rVV2	501	400	0.01%	0.004%
93	12.450	3530	3533	3541	rVB3	465	490	0.02%	0.004%
94	12.710	3610	3614	3618	rVB3	388	321	0.01%	0.003%
95	12.945	3684	3687	3689	rBV	358	254	0.01%	0.002%
96	13.138	3744	3747	3749	rBV2	423	276	0.01%	0.002%
97	13.173	3754	3758	3760	rBV3	311	263	0.01%	0.002%
98	13.790	3947	3950	3957	rVB3	569	486	0.02%	0.004%
99	13.861	3968	3972	3975	rBV4	529	487	0.02%	0.004%
100	14.913	4296	4299	4300	rBV2	535	266	0.01%	0.002%

Sum of corrected areas: 11373489

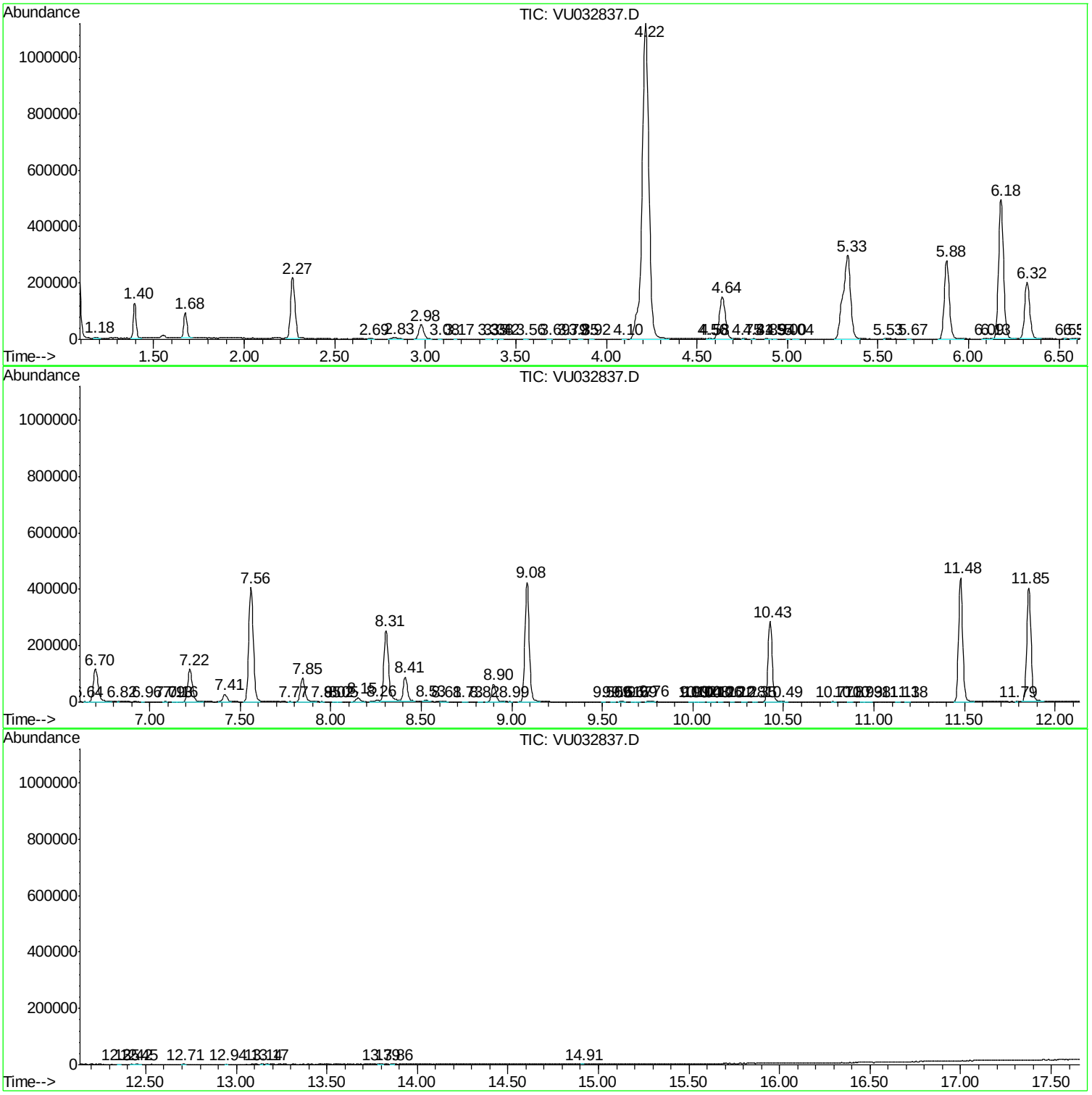
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032837.D
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Operator : JC/SP
Sample : K3363-02DL 5X
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ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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

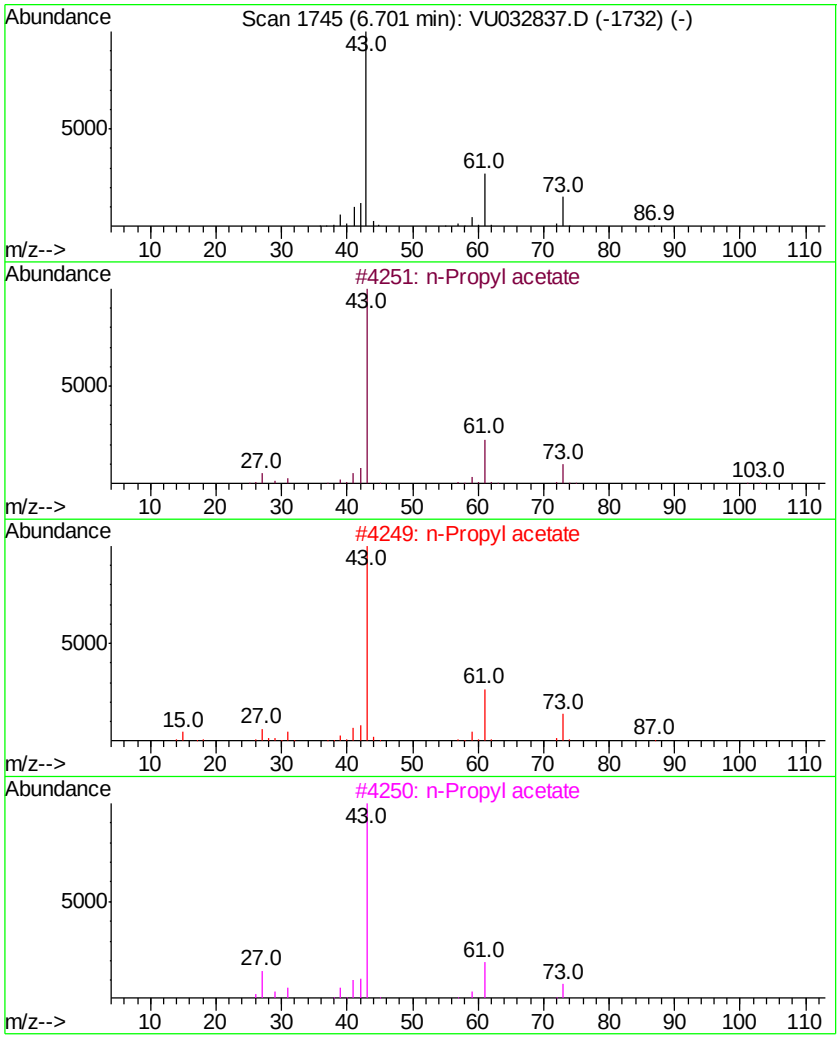
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

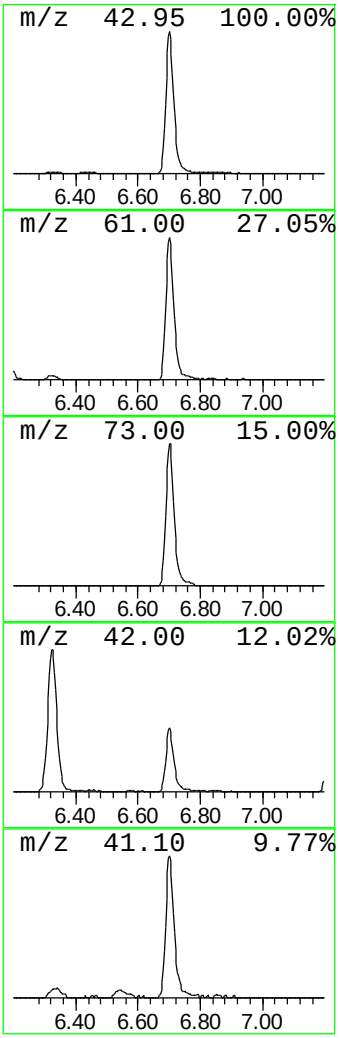
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	19.57 ug/L	213846	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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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

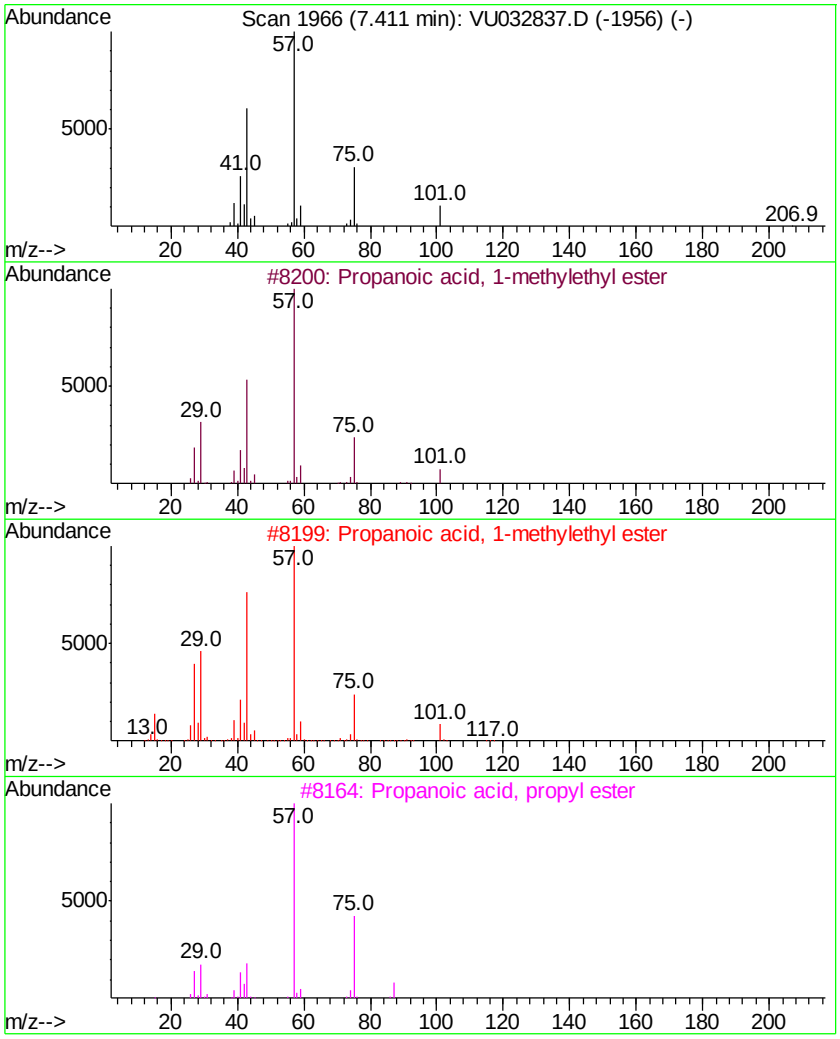
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

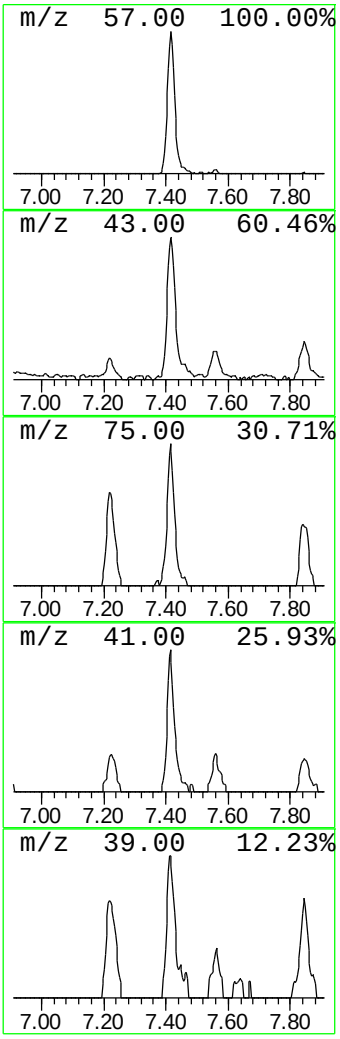
****

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	3.90 ug/L	42638	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, propyl ester	116	C6H12O2	000106-36-5	59
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45





Library Search Compound Report

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

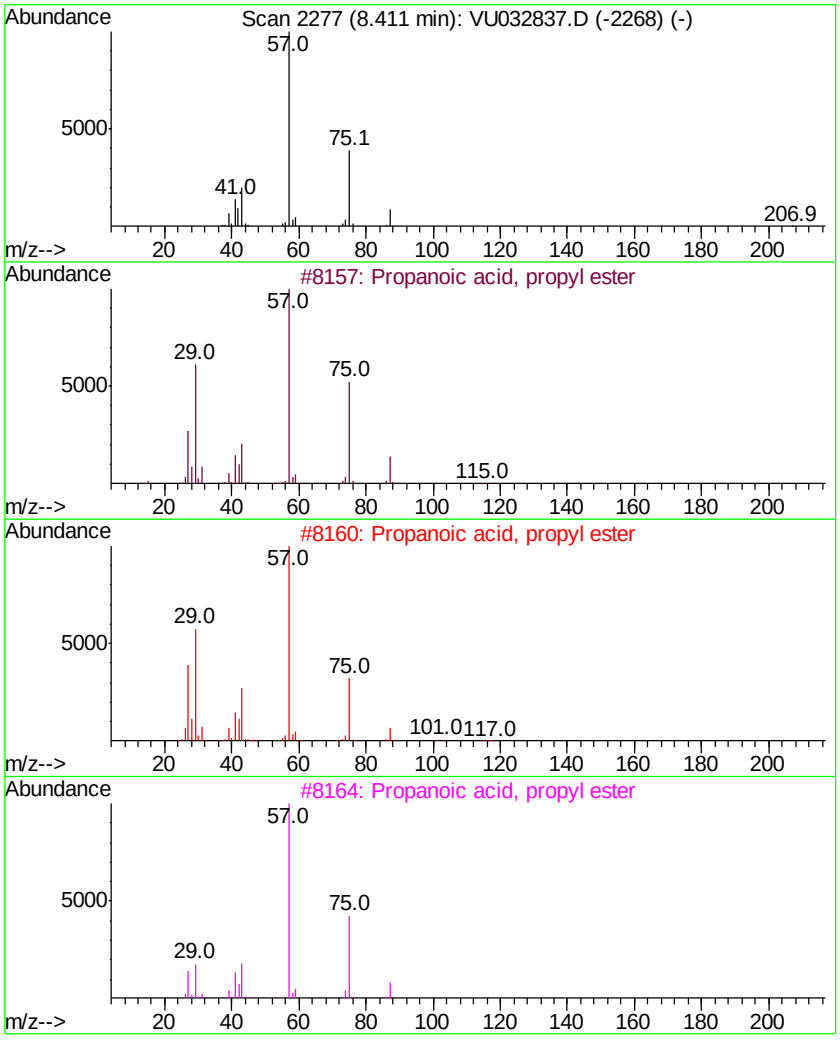
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

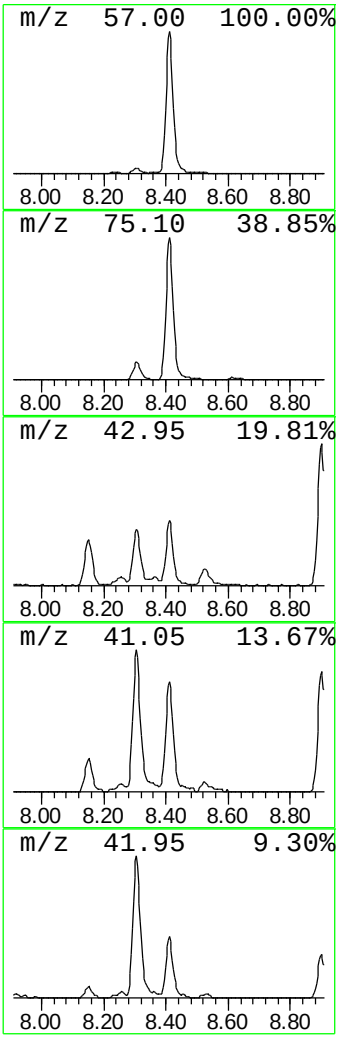
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	9.93 ug/L	138746	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	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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

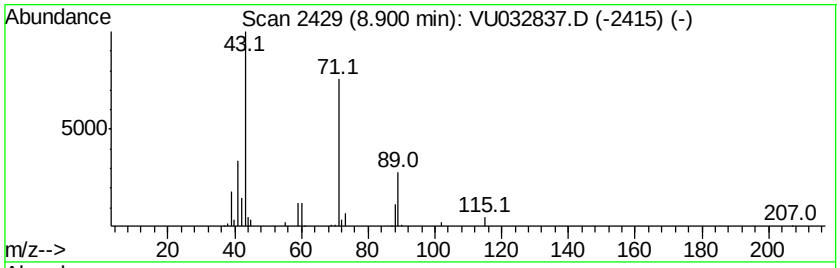
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

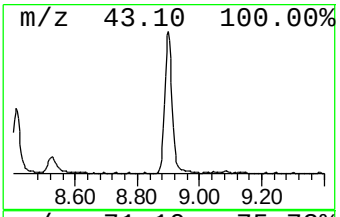
****

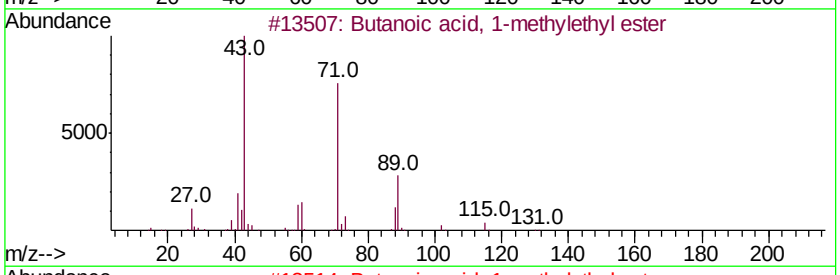
Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 4

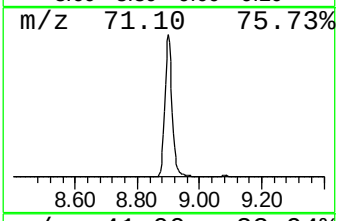
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	7.25 ug/L	101242	Chlorobenzene-d5	9.08

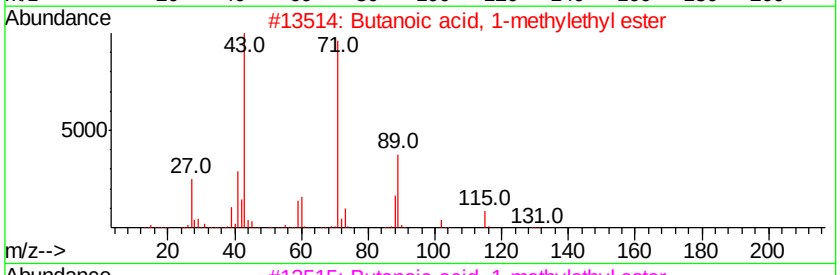
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64

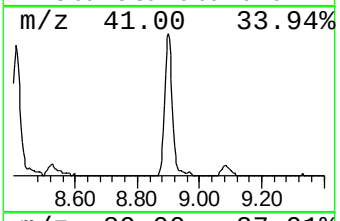


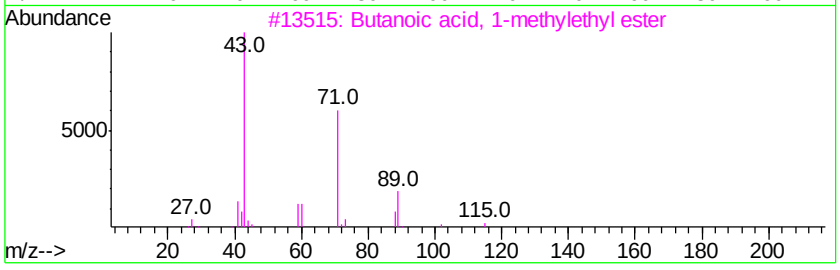


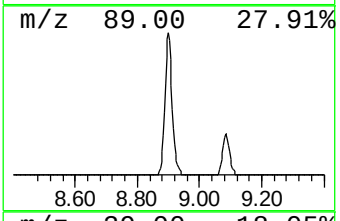


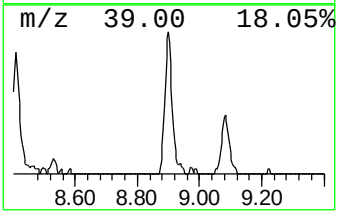












Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032837.D
Acq On : 18 Jun 2019 20:33
Operator : JC/SP
Sample : K3363-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT6DL

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	19.6	ug/L	213846	1	5.88	546468	50.0
Propanoic acid, 1...	7.41	3.9	ug/L	42638	1	5.88	546468	50.0
Propanoic acid, p...	8.41	9.9	ug/L	138746	2	9.08	698466	50.0
Butanoic acid, 1-...	8.90	7.3	ug/L	101242	2	9.08	698466	50.0