LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122118\
Data File : VU028874.D
Acq On : 21 Dec 2018 15:23
Operator : MD/SY
Sample : J6468-21DL 20X
Misc : 6.27g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JH9DL

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\SOMULM122018WMA.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	63	69	82	rVB	85471	83537	4.39%	1.010%
2	1.659	145	151	169	rVB	63505	79995	4.20%	0.967%
3	2.263	328	339	354	rBV	126257	191502	10.06%	2.316%
4	2.469	399	403	404	rBV	228	175	0.01%	0.002%
5	2.627	444	452	455	rBV	304	471	0.02%	0.006%
6	2.698	467	474	480	rBV4	585	877	0.05%	0.011%
7	3.115	596	604	606	rBV	95	116	0.01%	0.001%
8	3.215	633	635	638	rBV	148	104	0.01%	0.001%
9	3.437	699	704	707	rBV2	517	530	0.03%	0.006%
10	3.659	770	773	778	rVB	117	109	0.01%	0.001%
11	4.058	892	897	901	rBV	113	117	0.01%	0.001%
12	4.177	921	934	964	rBV	66221	181481	9.54%	2.195%
13	4.488	1028	1031	1035	rVB2	187	129	0.01%	0.002%
14	4.514	1035	1039	1040	rBV2	221	117	0.01%	0.001%
15	4.556	1050	1052	1057	rBV	190	119	0.01%	0.001%
16	4.643	1064	1079	1104	rBV	97986	230362	12.11%	2.786%
17	4.742	1109	1110	1114	rBV2	236	125	0.01%	0.002%
18	4.871	1149	1150	1152	rBV	273	144	0.01%	0.002%
19	4.987	1183	1186	1189	rVV2	250	197	0.01%	0.002%
20	5.103	1215	1222	1228	rBV	115	187	0.01%	0.002%
21	5.337	1272	1295	1320	rBV2	212569	613598	32.25%	7.420%
22	5.562	1361	1365	1368	rVB2	233	186	0.01%	0.002%
23	5.723	1408	1415	1423	rBV2	323	634	0.03%	0.008%
24	5.813	1441	1443	1445	rVB	136	74	0.00%	0.001%
25	5.884	1450	1465	1494	rBV	214804	421809	22.17%	5.101%
26	6.160	1536	1551	1570	rVB3	22258	56167	2.95%	0.679%
27	6.238	1570	1575	1577	rBV	111	93	0.00%	0.001%
28	6.270	1583	1585	1587	rVB	146	79	0.00%	0.001%
29	6.328	1588	1603	1624	rBV	143499	285958	15.03%	3.458%
30	6.466	1635	1646	1659	rBV3	8692	17052	0.90%	0.206%
31	6.566	1673	1677	1679	rBV2	206	163	0.01%	0.002%
32	6.633	1695	1698	1701	rVV	171	122	0.01%	0.001%
33	6.765	1737	1739	1742	rBV	122	72	0.00%	0.001%
34	6.852	1763	1766	1769	rVB	131	75	0.00%	0.001%

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Sample : J6468-21DL 20X
Misc : 6.27g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JH9DL

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\SOMULM122018WMA.M
Title : VOC Analysis

35	6.939	1789	1793	1795	rBV	199	119	0.01%	0.001%
36	7.003	1809	1813	1818	rVB	103	103	0.01%	0.001%
37	7.106	1841	1845	1850	rBV	146	128	0.01%	0.002%
38	7.170	1861	1865	1867	rBV	204	170	0.01%	0.002%
39	7.228	1871	1883	1902	rBV	79610	140902	7.41%	1.704%
40	7.366	1922	1926	1929	rVB	240	159	0.01%	0.002%
41	7.402	1934	1937	1942	rBV	70	78	0.00%	0.001%
42	7.562	1974	1987	2003	rBV	271637	479003	25.17%	5.792%
43	7.791	2055	2058	2060	rBV2	185	134	0.01%	0.002%
44	7.848	2066	2076	2094	rBV	54890	92018	4.84%	1.113%
45	7.974	2111	2115	2118	rVV2	262	153	0.01%	0.002%
46	8.003	2121	2124	2127	rVB	172	117	0.01%	0.001%
47	8.025	2127	2131	2134	rBV	119	96	0.01%	0.001%
48	8.051	2136	2139	2143	rVB	236	130	0.01%	0.002%
49	8.083	2147	2149	2152	rVB	181	106	0.01%	0.001%
50	8.102	2153	2155	2157	rVB	170	71	0.00%	0.001%
51	8.119	2157	2160	2165	rVB2	253	170	0.01%	0.002%
52	8.144	2165	2168	2169	rBV2	159	72	0.00%	0.001%
53	8.225	2189	2193	2200	rBV3	908	1000	0.05%	0.012%
54	8.254	2200	2202	2208	rVB	112	89	0.00%	0.001%
55	8.311	2208	2220	2245	rBV	237491	399650	21.00%	4.833%
56	8.559	2295	2297	2300	rVB	312	122	0.01%	0.001%
57	8.585	2303	2305	2307	rVV	229	121	0.01%	0.001%
58	8.598	2307	2309	2310	rVV	244	99	0.01%	0.001%
59	8.620	2310	2316	2322	rVB3	651	1006	0.05%	0.012%
60	8.665	2327	2330	2333	rBV	103	81	0.00%	0.001%
61	8.697	2337	2340	2341	rBV	272	131	0.01%	0.002%
62	8.906	2400	2405	2415	rVB3	2189	2545	0.13%	0.031%
63	9.028	2438	2443	2449	rBV3	1648	1878	0.10%	0.023%
64	9.090	2449	2462	2488	rBV	307539	517180	27.18%	6.254%
65	9.247	2500	2511	2536	rBV	309740	498190	26.18%	6.024%
66	9.372	2537	2550	2567	rBV	1160536	1902780	100.00%	23.010%
67	9.546	2601	2604	2607	rVB2	330	185	0.01%	0.002%
68	9.717	2652	2657	2663	rVB2	877	999	0.05%	0.012%
69	9.778	2663	2676	2706	rBV	486067	773479	40.65%	9.353%
70	9.945	2724	2728	2736	rVB6	1388	1754	0.09%	0.021%
71	10.041	2751	2758	2766	rBV3	1400	1766	0.09%	0.021%

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Misc : 6.27g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JH9DL

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\SOMULM122018WMA.M
Title : VOC Analysis

72	10.080	2767	2770	2771	rBV2	354	195	0.01%	0.002%
73	10.167	2789	2797	2809	rVB2	6134	9272	0.49%	0.112%
74	10.241	2817	2820	2821	rBV2	150	81	0.00%	0.001%
75	10.253	2821	2824	2825	rBV2	422	204	0.01%	0.002%
76	10.299	2836	2838	2839	rBV2	239	79	0.00%	0.001%
77	10.430	2867	2879	2894	rBV	210169	334297	17.57%	4.043%
78	10.588	2921	2928	2939	rVB2	2816	4737	0.25%	0.057%
79	10.646	2943	2946	2947	rBV2	181	84	0.00%	0.001%
80	10.681	2950	2957	2963	rBV3	7498	11561	0.61%	0.140%
81	10.771	2980	2985	2991	rBV3	3117	3558	0.19%	0.043%
82	10.974	3039	3048	3056	rVB	2085	2896	0.15%	0.035%
83	11.064	3073	3076	3078	rBV2	309	190	0.01%	0.002%
84	11.109	3085	3090	3094	rBV3	1222	1345	0.07%	0.016%
85	11.147	3096	3102	3115	rVB2	11487	16547	0.87%	0.200%
86	11.257	3133	3136	3137	rBV2	158	77	0.00%	0.001%
87	11.289	3143	3146	3148	rBV2	178	126	0.01%	0.002%
88	11.356	3164	3167	3170	rBV2	157	102	0.01%	0.001%
89	11.401	3175	3181	3184	rVB2	603	644	0.03%	0.008%
90	11.430	3184	3190	3195	rBV3	423	562	0.03%	0.007%
91	11.482	3195	3206	3227	rBV	292591	463359	24.35%	5.603%
92	11.572	3229	3234	3242	rVB3	3890	5038	0.26%	0.061%
93	11.649	3256	3258	3261	rBV2	293	177	0.01%	0.002%
94	11.771	3292	3296	3302	rBV4	934	1074	0.06%	0.013%
95	11.858	3312	3323	3342	rBV	268027	428883	22.54%	5.186%
96	12.128	3404	3407	3409	rBV	241	130	0.01%	0.002%
97	12.151	3411	3414	3418	rVV	317	261	0.01%	0.003%
98	12.443	3503	3505	3508	rBV	243	116	0.01%	0.001%
99	12.700	3582	3585	3589	rBV3	307	289	0.02%	0.003%
100	13.009	3676	3681	3684	rBV2	341	284	0.01%	0.003%

Sum of corrected areas: 8269428

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Instrument :
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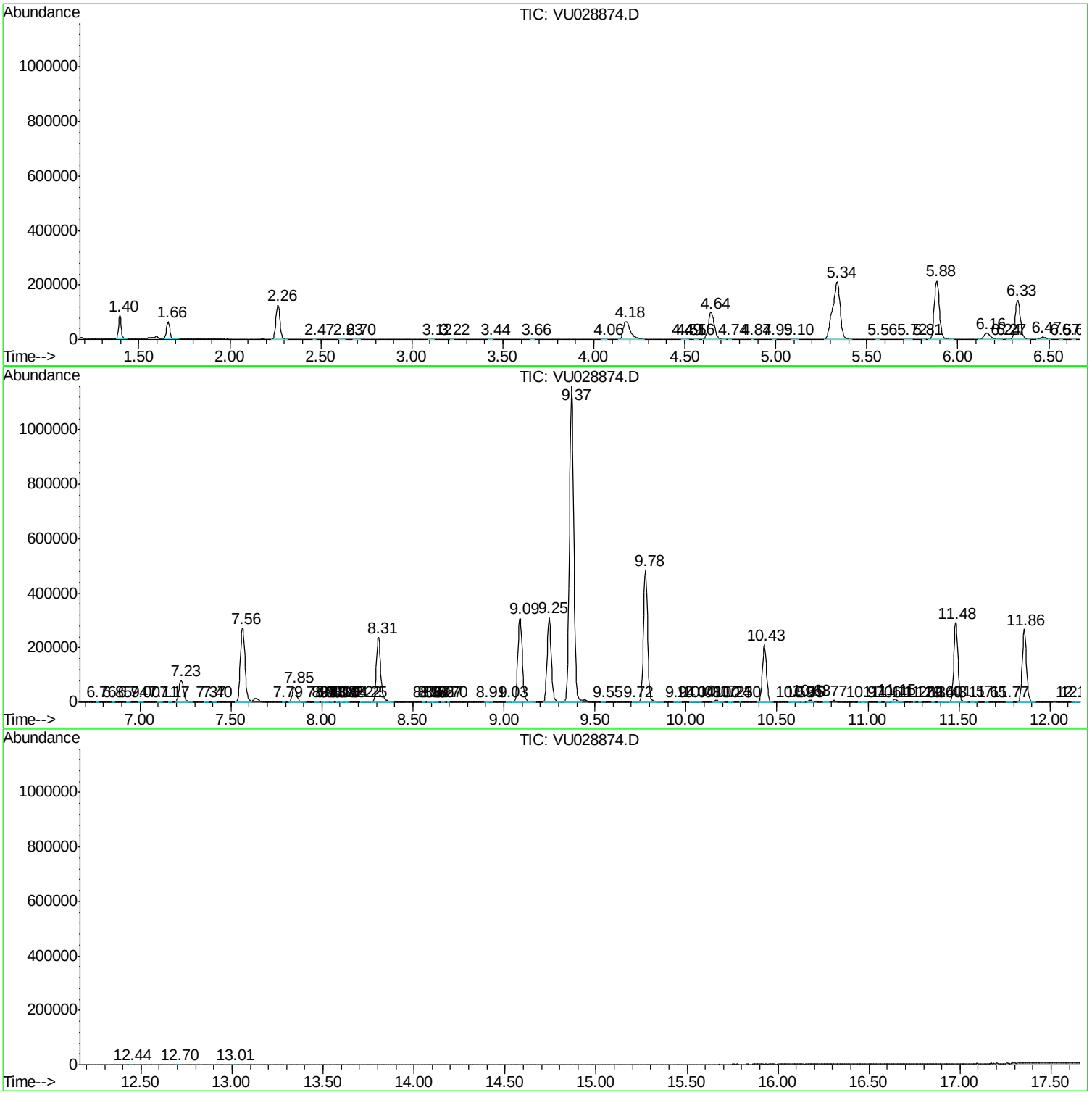
ClientSampleId :
C0JH9DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.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\VU122118\
Data File : VU028874.D
Acq On : 21 Dec 2018 15:23
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Instrument : MSVOA_U
ClientSampleId : C0JH9DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

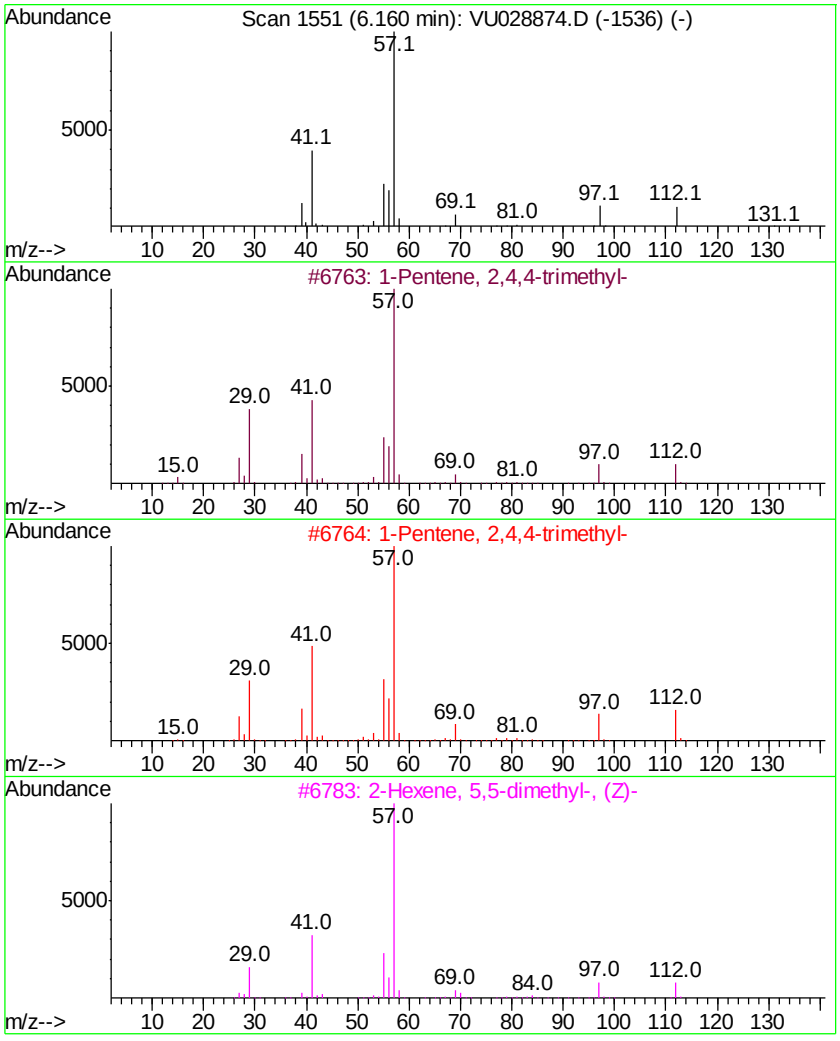
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

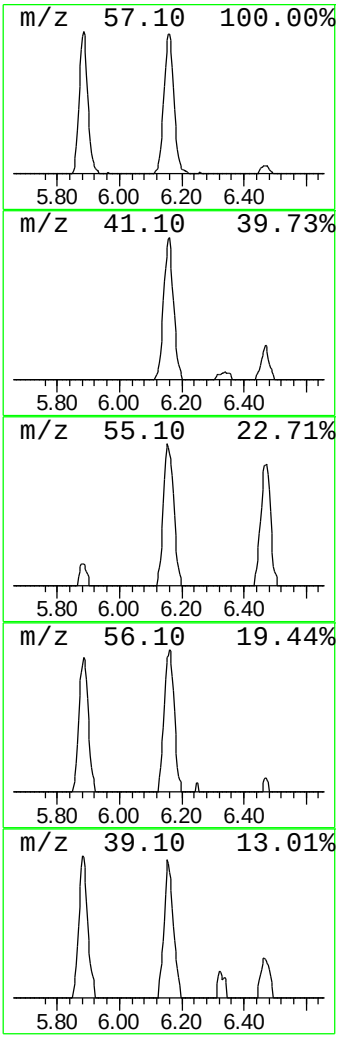
****

Peak Number 1 1-Pentene, 2,4,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	6.66 ug/L	56167	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	90
2	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	90
3	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	72
4	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	62
5	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	47





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.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
1-Pentene, 2,4,4-...	6.16	6.7	ug/L	56167	1	5.88	421809	50.0