

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU051019\
 Data File : VU031898.D
 Acq On : 10 May 2019 19:08
 Operator : JC/SP
 Sample : K2741-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFHK4

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.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	rVB2	16952	16423	0.38%	0.051%
2	1.396	88	95	108	rBV	619959	630512	14.54%	1.943%
3	1.669	173	180	201	rVB	464156	611089	14.10%	1.884%
4	2.264	355	365	378	rVB	939594	1423158	32.83%	4.387%
5	2.437	415	419	421	rBV3	1668	1390	0.03%	0.004%
6	2.531	444	448	450	rBV4	1332	1043	0.02%	0.003%
7	2.547	451	453	458	rVB3	1447	1006	0.02%	0.003%
8	2.656	483	487	490	rVB4	1073	766	0.02%	0.002%
9	2.672	490	492	494	rBV2	1080	597	0.01%	0.002%
10	2.698	497	500	501	rBV2	1474	912	0.02%	0.003%
11	2.765	517	521	522	rBV3	1305	810	0.02%	0.002%
12	2.804	528	533	534	rBV4	1096	1012	0.02%	0.003%
13	2.833	535	542	555	rVB4	5972	12962	0.30%	0.040%
14	2.936	572	574	577	rVB	990	505	0.01%	0.002%
15	2.958	577	581	582	rBV3	764	499	0.01%	0.002%
16	3.064	611	614	617	rVB	929	501	0.01%	0.002%
17	3.109	626	628	633	rVB3	875	541	0.01%	0.002%
18	3.302	686	688	696	rVB5	1470	1599	0.04%	0.005%
19	3.389	711	715	717	rBV2	1147	826	0.02%	0.003%
20	3.441	729	731	738	rVB5	1001	866	0.02%	0.003%
21	3.479	738	743	748	rBV3	650	695	0.02%	0.002%
22	3.576	770	773	776	rBV2	891	557	0.01%	0.002%
23	3.646	792	795	800	rVV5	745	638	0.01%	0.002%
24	3.672	800	803	807	rVV2	874	624	0.01%	0.002%
25	3.714	813	816	818	rVV3	957	598	0.01%	0.002%
26	3.740	821	824	827	rVV2	1009	695	0.02%	0.002%
27	3.836	849	854	858	rVB3	862	842	0.02%	0.003%
28	3.923	878	881	889	rVB3	1319	1179	0.03%	0.004%
29	3.958	889	892	894	rBV3	894	603	0.01%	0.002%
30	3.987	897	901	905	rVB5	923	905	0.02%	0.003%
31	4.010	905	908	911	rBV2	751	591	0.01%	0.002%
32	4.058	921	923	927	rVB2	782	519	0.01%	0.002%
33	4.093	930	934	938	rVB3	1203	1029	0.02%	0.003%
34	4.170	942	958	994	rBV	411884	1117296	25.77%	3.444%

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 Title : VOC Analysis

35	4.556	1073	1078	1086	rVB8	1456	2141	0.05%	0.007%
36	4.643	1086	1105	1130	rBV	700887	1676316	38.67%	5.167%
37	5.113	1245	1251	1256	rVB6	1373	1878	0.04%	0.006%
38	5.161	1263	1266	1271	rBV5	893	962	0.02%	0.003%
39	5.206	1277	1280	1284	rVB5	831	653	0.02%	0.002%
40	5.334	1297	1320	1356	rBV2	1446621	4335044	100.00%	13.362%
41	5.662	1420	1422	1425	rBV4	1758	1173	0.03%	0.004%
42	5.813	1466	1469	1475	rBV6	1223	1093	0.03%	0.003%
43	5.881	1475	1490	1514	rBV	1221797	2492241	57.49%	7.682%
44	6.174	1575	1581	1595	rVB6	17483	31772	0.73%	0.098%
45	6.325	1614	1628	1655	rBV	966505	1967946	45.40%	6.066%
46	6.659	1728	1732	1735	rBV4	1567	1091	0.03%	0.003%
47	6.749	1757	1760	1763	rBV2	1422	908	0.02%	0.003%
48	6.910	1808	1810	1814	rVB3	1321	747	0.02%	0.002%
49	6.942	1815	1820	1821	rBV4	1190	922	0.02%	0.003%
50	6.993	1835	1836	1842	rVB4	1074	612	0.01%	0.002%
51	7.103	1867	1870	1871	rBV2	956	576	0.01%	0.002%
52	7.122	1871	1876	1884	rBV2	2135	2358	0.05%	0.007%
53	7.154	1884	1886	1887	rBV2	1224	577	0.01%	0.002%
54	7.225	1894	1908	1932	rBV	482926	902111	20.81%	2.781%
55	7.563	1998	2013	2062	rBV	1739855	3300366	76.13%	10.173%
56	7.846	2091	2101	2128	rBV	330654	587462	13.55%	1.811%
57	8.077	2171	2173	2178	rVB4	1991	1714	0.04%	0.005%
58	8.103	2178	2181	2184	rBV3	1262	986	0.02%	0.003%
59	8.177	2198	2204	2214	rVB5	5502	9768	0.23%	0.030%
60	8.235	2217	2222	2233	rVB9	1650	2794	0.06%	0.009%
61	8.309	2233	2245	2285	rBV	1311385	2551306	58.85%	7.864%
62	8.466	2286	2294	2317	rVB2	83159	165963	3.83%	0.512%
63	8.768	2384	2388	2393	rBV8	1406	1386	0.03%	0.004%
64	8.807	2397	2400	2403	rVB5	1307	886	0.02%	0.003%
65	8.878	2417	2422	2425	rBV6	920	965	0.02%	0.003%
66	8.913	2431	2433	2437	rBV3	1079	656	0.02%	0.002%
67	9.016	2462	2465	2468	rBV3	1016	767	0.02%	0.002%
68	9.038	2469	2472	2474	rVV3	1013	603	0.01%	0.002%
69	9.087	2474	2487	2530	rVV	1805171	3215354	74.17%	9.911%
70	9.286	2547	2549	2555	rBV7	1155	918	0.02%	0.003%
71	9.476	2606	2608	2612	rVB3	1275	771	0.02%	0.002%

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 Title : VOC Analysis

72	9.624	2651	2654	2656	rBV3	1334	861	0.02%	0.003%
73	9.723	2682	2685	2693	rVB7	1609	1579	0.04%	0.005%
74	9.759	2693	2696	2699	rVB3	1284	706	0.02%	0.002%
75	9.788	2699	2705	2707	rBV4	2618	2781	0.06%	0.009%
76	9.836	2718	2720	2723	rVB3	1468	816	0.02%	0.003%
77	9.929	2747	2749	2750	rBV2	1300	694	0.02%	0.002%
78	9.952	2751	2756	2762	rVB7	2872	4090	0.09%	0.013%
79	10.038	2776	2783	2792	rBV10	4152	7761	0.18%	0.024%
80	10.154	2817	2819	2822	rBV	885	594	0.01%	0.002%
81	10.189	2827	2830	2834	rVB4	990	795	0.02%	0.002%
82	10.238	2842	2845	2847	rBV3	1132	679	0.02%	0.002%
83	10.427	2889	2904	2927	rBV	1308993	2136053	49.27%	6.584%
84	10.598	2949	2957	2966	rBV9	4770	8719	0.20%	0.027%
85	10.714	2990	2993	2996	rVB3	1001	790	0.02%	0.002%
86	11.029	3088	3091	3097	rVB3	1454	1198	0.03%	0.004%
87	11.058	3097	3100	3102	rBV3	986	561	0.01%	0.002%
88	11.083	3105	3108	3115	rVB5	2016	2279	0.05%	0.007%
89	11.341	3185	3188	3190	rBV3	1180	764	0.02%	0.002%
90	11.479	3218	3231	3257	rBV	1531304	2506036	57.81%	7.724%
91	11.855	3336	3348	3380	rBV	1598456	2656729	61.28%	8.189%
92	12.472	3537	3540	3543	rBV4	2029	1519	0.04%	0.005%
93	12.739	3620	3623	3628	rVB5	1612	1182	0.03%	0.004%
94	12.958	3688	3691	3693	rBV3	1279	603	0.01%	0.002%
95	13.173	3754	3758	3760	rBV3	1323	1193	0.03%	0.004%
96	13.279	3789	3791	3797	rBV5	1866	1870	0.04%	0.006%
97	13.418	3830	3834	3836	rBV4	1500	1152	0.03%	0.004%
98	13.553	3873	3876	3880	rBV3	1431	1213	0.03%	0.004%
99	14.016	4017	4020	4023	rBV4	1640	1136	0.03%	0.004%
100	14.443	4149	4153	4155	rBV3	1407	1171	0.03%	0.004%

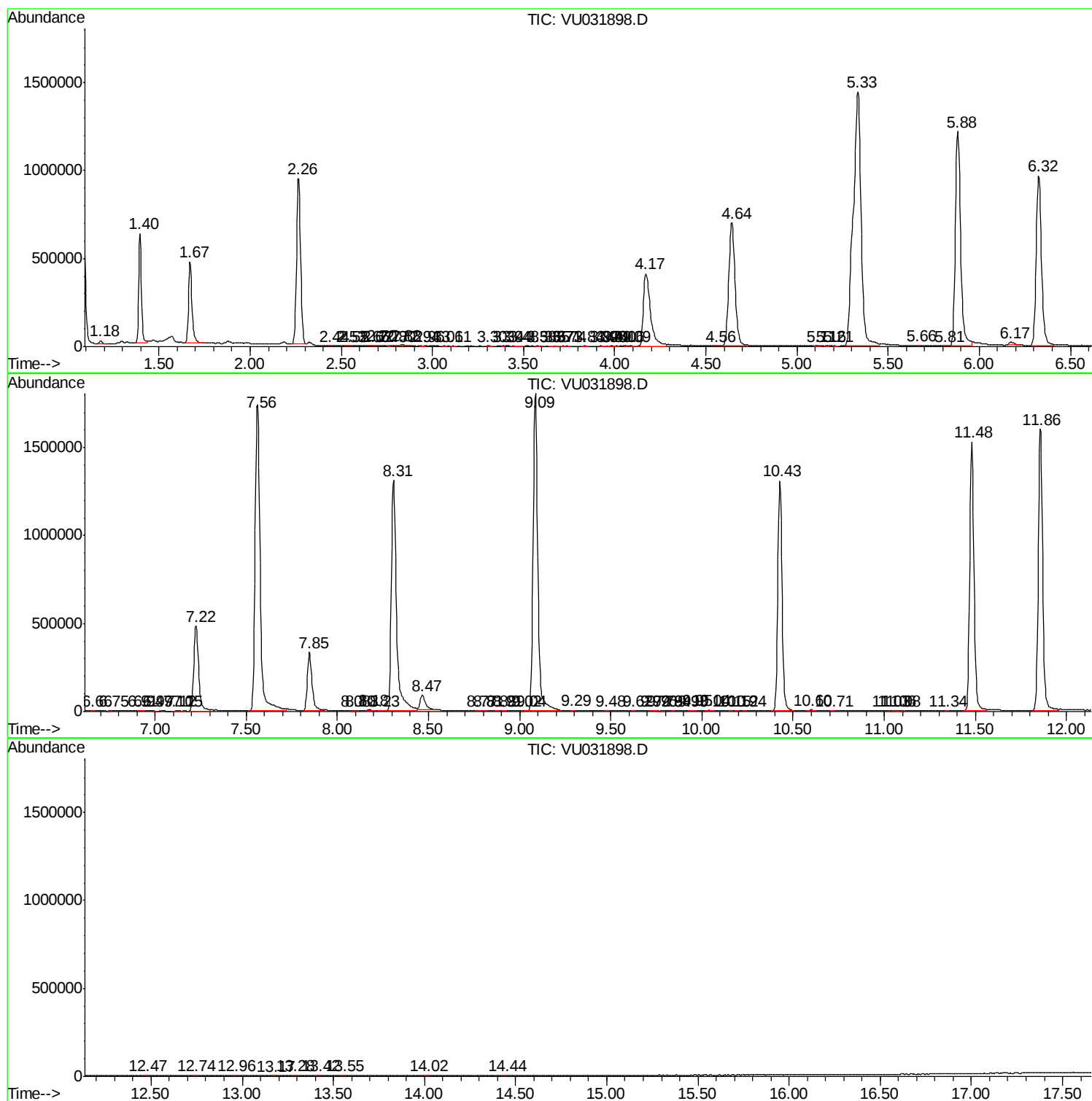
Sum of corrected areas: 32443098

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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



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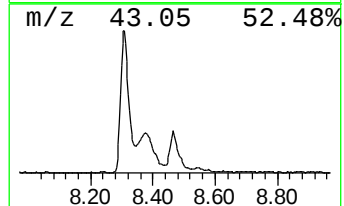
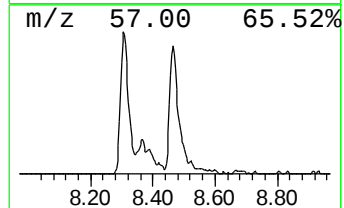
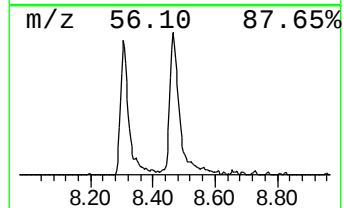
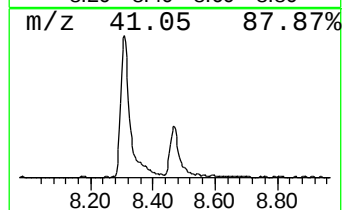
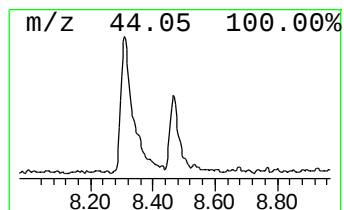
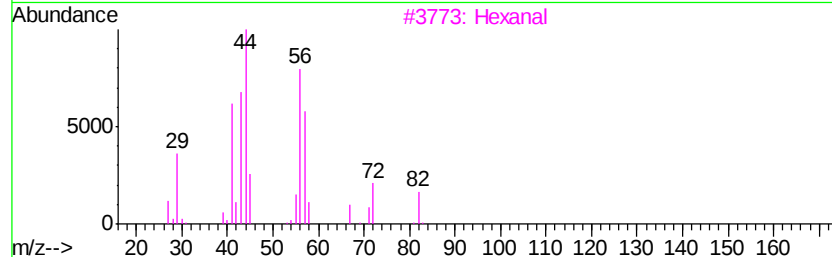
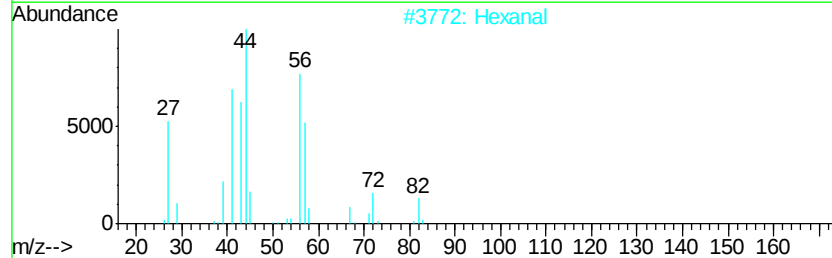
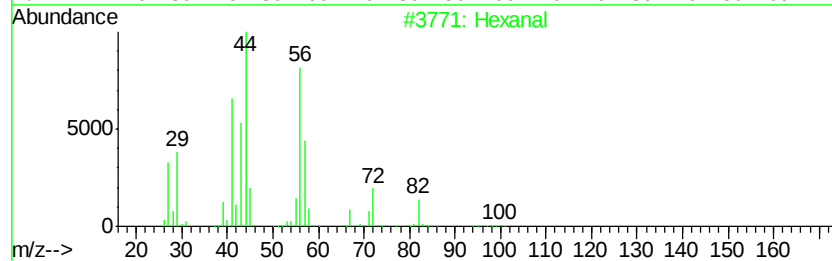
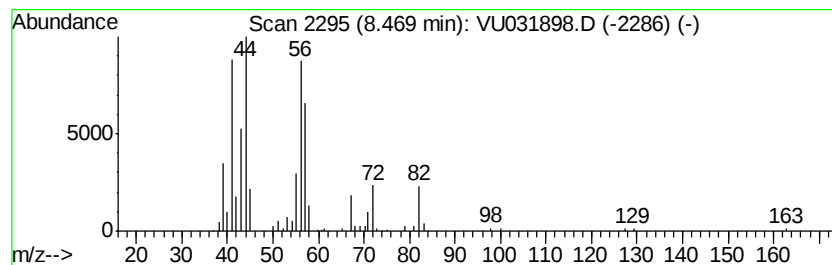
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	2.58 ug/L	165963	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	86
2		Hexanal	100	C6H12O	000066-25-1	86
3		Hexanal	100	C6H12O	000066-25-1	78
4		Hexanal	100	C6H12O	000066-25-1	78
5		Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.47	2.6	ug/L	165963	2	9.09	3215350	50.0