

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051171.D
 Acq On : 06 Oct 2022 14:58
 Operator : JC/MD
 Sample : N4893-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5J48

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\SFAMULM092922WMA.M
 Title : VOC Analysis

Signal : TIC: VU051171.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.598	74	80	101	rVB	239715	278829	18.12%	2.316%
2	1.900	167	174	195	rVB	181169	246179	16.00%	2.045%
3	2.562	368	380	398	rBV	312973	514207	33.42%	4.272%
4	3.038	521	528	536	rBV5	1575	2475	0.16%	0.021%
5	3.096	543	546	549	rBV	378	247	0.02%	0.002%
6	3.189	563	575	588	rVB2	7063	15812	1.03%	0.131%
7	3.244	589	592	595	rBV2	421	329	0.02%	0.003%
8	3.360	625	628	629	rBV2	253	135	0.01%	0.001%
9	3.421	643	647	650	rBV2	364	267	0.02%	0.002%
10	3.446	650	655	658	rVB2	331	265	0.02%	0.002%
11	3.572	691	694	698	rVB	302	228	0.01%	0.002%
12	3.594	698	701	705	rBV2	427	325	0.02%	0.003%
13	3.707	734	736	738	rBV	334	157	0.01%	0.001%
14	3.720	738	740	744	rVV2	350	223	0.01%	0.002%
15	3.778	755	758	760	rBV	305	209	0.01%	0.002%
16	3.842	773	778	782	rBV2	263	329	0.02%	0.003%
17	3.980	818	821	824	rBV2	314	246	0.02%	0.002%
18	4.025	830	835	840	rBV	329	347	0.02%	0.003%
19	4.099	855	858	861	rBV2	298	195	0.01%	0.002%
20	4.115	861	863	865	rVV	170	114	0.01%	0.001%
21	4.141	868	871	874	rVB	339	211	0.01%	0.002%
22	4.228	896	898	901	rBV2	179	102	0.01%	0.001%
23	4.282	912	915	922	rVB2	303	288	0.02%	0.002%
24	4.321	922	927	930	rBV2	343	255	0.02%	0.002%
25	4.340	930	933	935	rBV	310	212	0.01%	0.002%
26	4.372	941	943	946	rVB2	261	113	0.01%	0.001%
27	4.398	948	951	953	rBV2	271	167	0.01%	0.001%
28	4.417	953	957	959	rBV2	272	213	0.01%	0.002%
29	4.482	974	977	980	rVB	267	185	0.01%	0.002%
30	4.501	980	983	987	rBV2	216	198	0.01%	0.002%
31	4.620	1007	1020	1052	rBV	142705	360777	23.45%	2.997%
32	5.060	1141	1157	1182	rBV	287483	632860	41.13%	5.258%
33	5.482	1283	1288	1290	rBV	335	265	0.02%	0.002%
34	5.594	1321	1323	1327	rVB2	187	112	0.01%	0.001%
35	5.623	1327	1332	1335	rBV3	255	238	0.02%	0.002%
36	5.649	1335	1340	1342	rBV2	317	269	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
 Title : VOC Analysis

37	5.723	1342	1363	1385	rBV2	571099	1538722	100.00%	12.784%
38	6.015	1452	1454	1458	rBV2	293	181	0.01%	0.002%
39	6.035	1458	1460	1463	rBV2	408	289	0.02%	0.002%
40	6.109	1481	1483	1486	rBV2	262	162	0.01%	0.001%
41	6.186	1503	1507	1511	rBV2	415	316	0.02%	0.003%
42	6.247	1511	1526	1546	rBV	485761	926000	60.18%	7.693%
43	6.523	1603	1612	1614	rBV4	2956	3239	0.21%	0.027%
44	6.687	1648	1663	1683	rBV	366989	717668	46.64%	5.962%
45	6.890	1723	1726	1729	rBV2	314	209	0.01%	0.002%
46	7.009	1757	1763	1766	rBV2	454	368	0.02%	0.003%
47	7.102	1786	1792	1806	rVB3	4235	7114	0.46%	0.059%
48	7.337	1861	1865	1868	rBV	304	267	0.02%	0.002%
49	7.395	1880	1883	1888	rVB	340	273	0.02%	0.002%
50	7.424	1888	1892	1896	rBV2	253	231	0.02%	0.002%
51	7.446	1896	1899	1901	rBV2	295	132	0.01%	0.001%
52	7.465	1901	1905	1912	rVB2	299	292	0.02%	0.002%
53	7.565	1922	1936	1958	rBV	174212	307377	19.98%	2.554%
54	7.761	1994	1997	1998	rBV2	228	148	0.01%	0.001%
55	7.896	2023	2039	2054	rBV	625502	1079033	70.13%	8.965%
56	8.070	2091	2093	2097	rVB3	649	481	0.03%	0.004%
57	8.176	2115	2126	2143	rBV	121335	204831	13.31%	1.702%
58	8.552	2231	2243	2256	rBV2	77823	130018	8.45%	1.080%
59	8.633	2257	2268	2302	rBV3	333283	759887	49.38%	6.313%
60	8.883	2344	2346	2348	rBV3	332	188	0.01%	0.002%
61	8.951	2364	2367	2371	rVB3	519	300	0.02%	0.002%
62	9.012	2383	2386	2395	rBV3	515	667	0.04%	0.006%
63	9.083	2406	2408	2409	rBV	283	122	0.01%	0.001%
64	9.102	2409	2414	2418	rVV	367	393	0.03%	0.003%
65	9.144	2424	2427	2429	rBV	264	201	0.01%	0.002%
66	9.160	2430	2432	2437	rVB4	499	371	0.02%	0.003%
67	9.269	2463	2466	2472	rVB2	498	499	0.03%	0.004%
68	9.298	2472	2475	2477	rBV	292	179	0.01%	0.001%
69	9.346	2489	2490	2494	rBV2	241	101	0.01%	0.001%
70	9.414	2498	2511	2550	rBV	705347	1182579	76.85%	9.825%
71	9.642	2580	2582	2584	rBV	298	148	0.01%	0.001%
72	9.665	2586	2589	2590	rVV	486	280	0.02%	0.002%
73	9.690	2590	2597	2605	rVV2	4461	6553	0.43%	0.054%
74	9.735	2609	2611	2614	rBV2	230	157	0.01%	0.001%
75	9.790	2625	2628	2631	rBV	297	195	0.01%	0.002%
76	9.845	2641	2645	2646	rBV2	213	152	0.01%	0.001%

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 Title : VOC Analysis

77	9.964	2679	2682	2685	rBV	277	147	0.01%	0.001%
78	9.980	2685	2687	2690	rBV	308	195	0.01%	0.002%
79	10.047	2704	2708	2709	rBV	237	134	0.01%	0.001%
80	10.260	2768	2774	2777	rBV3	578	655	0.04%	0.005%
81	10.350	2799	2802	2807	rBV2	225	183	0.01%	0.002%
82	10.401	2816	2818	2821	rVB	324	180	0.01%	0.001%
83	10.475	2838	2841	2844	rBV	625	534	0.03%	0.004%
84	10.543	2858	2862	2868	rBV2	362	364	0.02%	0.003%
85	10.591	2874	2877	2881	rVB3	548	418	0.03%	0.003%
86	10.623	2881	2887	2892	rBV3	555	696	0.05%	0.006%
87	10.658	2892	2898	2902	rBV3	399	422	0.03%	0.004%
88	10.681	2902	2905	2909	rBV	498	336	0.02%	0.003%
89	10.755	2913	2928	2949	rBV	524686	846959	55.04%	7.036%
90	11.044	3010	3018	3035	rBV3	14607	24410	1.59%	0.203%
91	11.243	3072	3080	3082	rBV3	510	625	0.04%	0.005%
92	11.472	3146	3151	3154	rBV	901	755	0.05%	0.006%
93	11.809	3244	3256	3277	rBV	535247	863765	56.14%	7.176%
94	12.057	3322	3333	3359	rBV	216451	409403	26.61%	3.401%
95	12.192	3364	3375	3402	rVB	575453	957024	62.20%	7.951%
96	12.726	3539	3541	3544	rBV2	350	119	0.01%	0.001%
97	12.745	3544	3547	3548	rBV2	653	335	0.02%	0.003%
98	12.874	3585	3587	3589	rBV	440	131	0.01%	0.001%
99	13.095	3652	3656	3660	rBV3	536	515	0.03%	0.004%
100	15.243	4322	4324	4328	rBV2	777	512	0.03%	0.004%

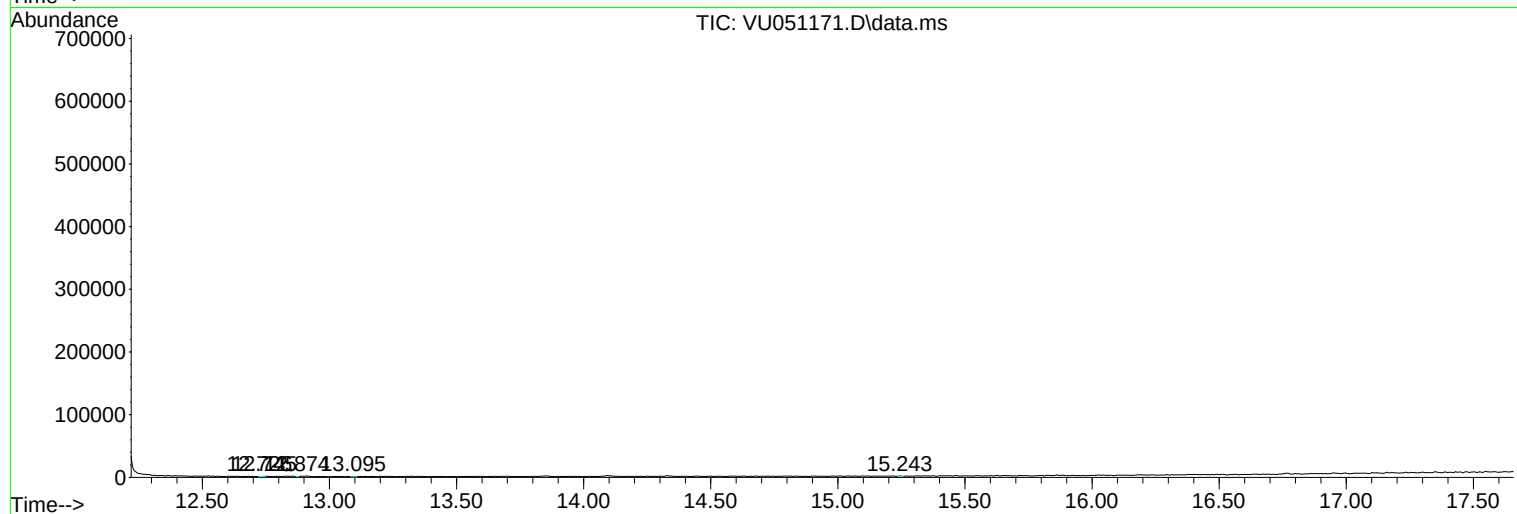
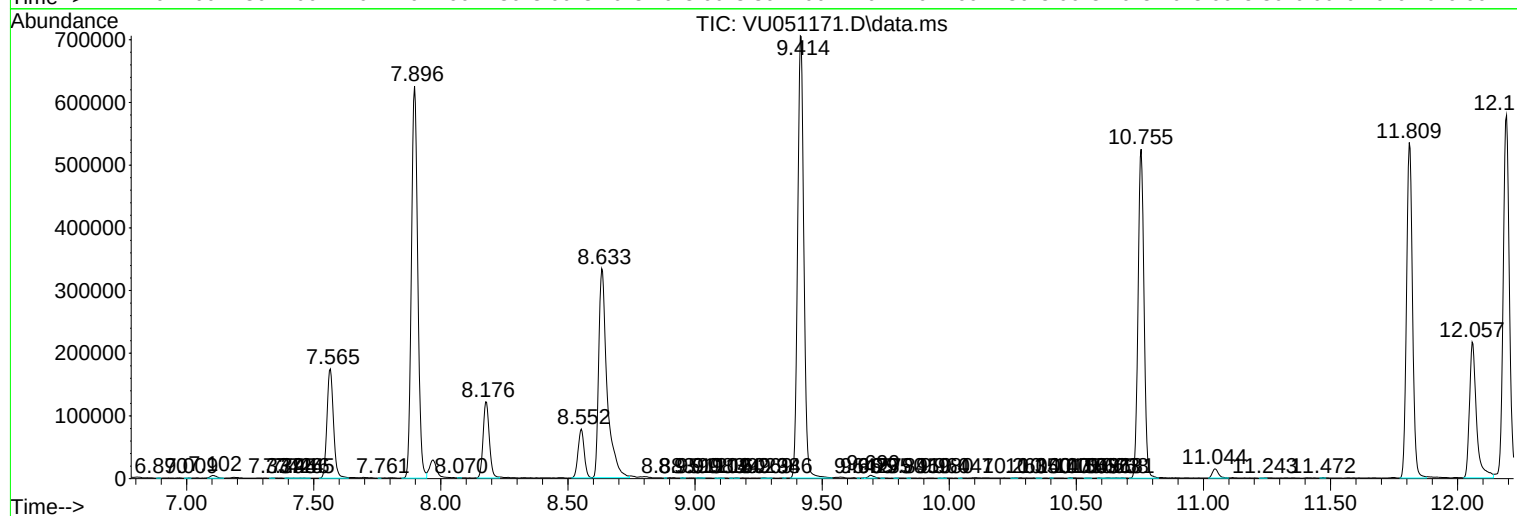
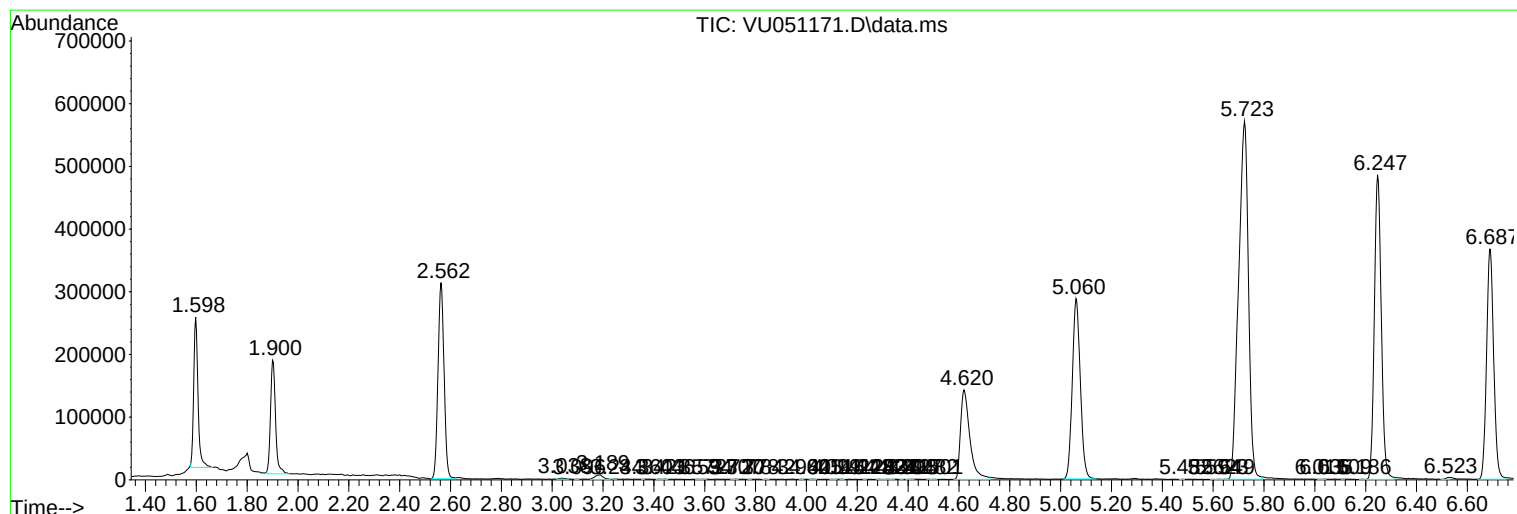
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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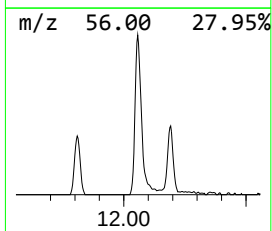
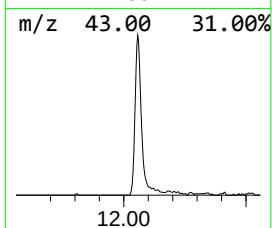
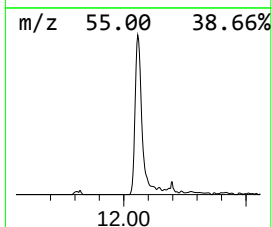
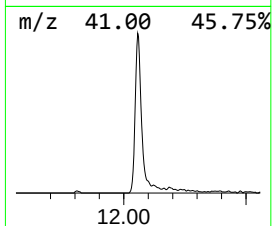
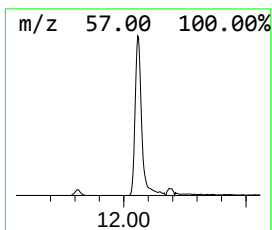
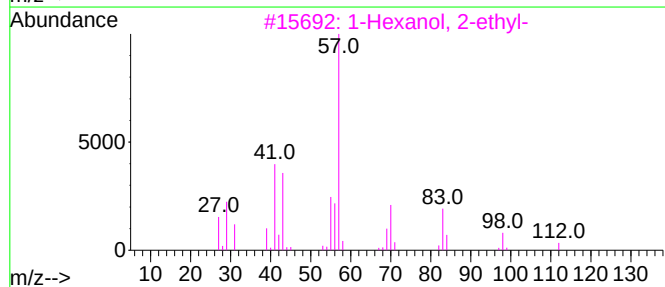
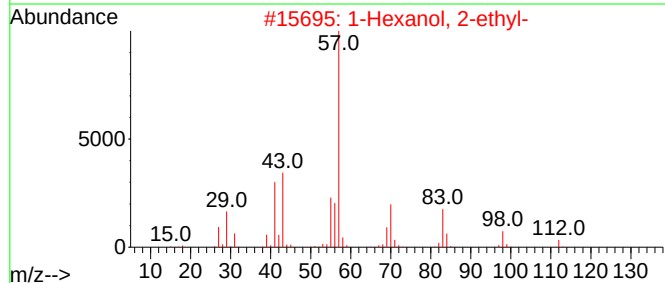
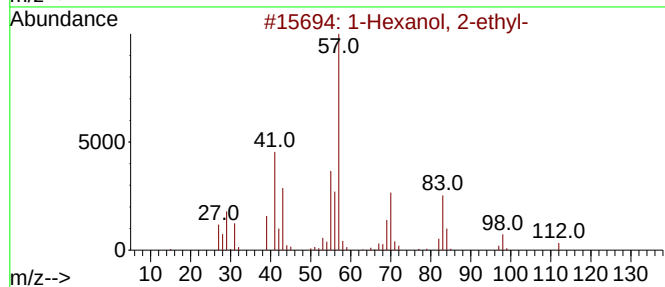
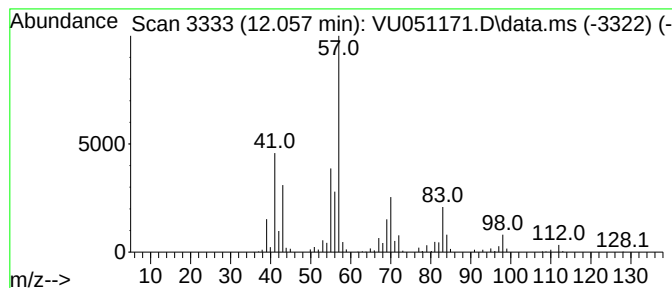
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	23.70 ug/L	409403	1,4-Dichlorobenzene-d4	11.813

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.057	23.7	ug/L	409403	3	11.813	863765	50.0