

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051976.D
 Acq On : 20 Nov 2022 16:04
 Operator : JC/MD
 Sample : N5679-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KZ1

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\SFAMULM111522WMA.M

Title : VOC Analysis

Signal : TIC: VU051976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	94	rBV	110539	128635	10.11%	1.194%
2	1.906	168	176	199	rVB	107388	162901	12.80%	1.511%
3	2.565	369	381	392	rBV	177154	287154	22.57%	2.664%
4	2.623	393	399	419	rVB	21336	38775	3.05%	0.360%
5	2.826	459	462	464	rVB2	394	194	0.02%	0.002%
6	2.842	464	467	470	rBV2	174	119	0.01%	0.001%
7	2.896	478	484	485	rBV	623	571	0.04%	0.005%
8	2.951	490	501	515	rBV2	4463	9150	0.72%	0.085%
9	3.131	554	557	561	rBV2	346	304	0.02%	0.003%
10	3.176	562	571	573	rBV4	1800	2388	0.19%	0.022%
11	3.295	606	608	612	rVB	299	146	0.01%	0.001%
12	3.385	633	636	640	rVB2	385	260	0.02%	0.002%
13	3.414	640	645	648	rBV2	270	289	0.02%	0.003%
14	3.436	648	652	654	rBV2	247	162	0.01%	0.002%
15	3.543	682	685	688	rVB	262	141	0.01%	0.001%
16	3.562	688	691	695	rBV3	472	359	0.03%	0.003%
17	3.588	696	699	702	rBV2	293	203	0.02%	0.002%
18	3.780	755	759	760	rBV2	174	110	0.01%	0.001%
19	3.813	766	769	773	rBV2	255	209	0.02%	0.002%
20	3.903	788	797	804	rBV2	235	397	0.03%	0.004%
21	3.941	804	809	813	rVB	489	403	0.03%	0.004%
22	3.973	813	819	823	rBV2	190	212	0.02%	0.002%
23	3.993	823	825	829	rVB	202	114	0.01%	0.001%
24	4.015	829	832	836	rBV2	220	187	0.01%	0.002%
25	4.070	846	849	854	rBV	185	203	0.02%	0.002%
26	4.131	864	868	871	rBV	260	174	0.01%	0.002%
27	4.285	913	916	918	rBV	125	85	0.01%	0.001%
28	4.317	923	926	930	rBV2	158	129	0.01%	0.001%
29	4.375	938	944	946	rBV2	353	333	0.03%	0.003%
30	4.433	959	962	963	rBV2	404	281	0.02%	0.003%
31	4.562	1000	1002	1005	rVB	196	92	0.01%	0.001%
32	4.616	1005	1019	1041	rBV	164516	408269	32.09%	3.788%
33	5.060	1141	1157	1177	rBV	264978	585393	46.01%	5.432%
34	5.285	1220	1227	1240	rBV5	1144	2558	0.20%	0.024%
35	5.337	1240	1243	1247	rBV2	199	139	0.01%	0.001%
36	5.372	1250	1254	1260	rVB3	409	478	0.04%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
 Title : VOC Analysis

37	5.446	1272	1277	1282	rBV2	132	192	0.02%	0.002%
38	5.472	1283	1285	1286	rBV	193	70	0.01%	0.001%
39	5.555	1309	1311	1315	rVB2	256	117	0.01%	0.001%
40	5.587	1315	1321	1322	rBV2	240	228	0.02%	0.002%
41	5.723	1342	1363	1397	rBV2	445762	1272319	100.00%	11.805%
42	6.038	1459	1461	1462	rBV2	160	79	0.01%	0.001%
43	6.179	1503	1505	1508	rBV2	150	81	0.01%	0.001%
44	6.247	1512	1526	1549	rBV	519244	979583	76.99%	9.089%
45	6.465	1592	1594	1597	rBV	549	337	0.03%	0.003%
46	6.517	1606	1610	1612	rBV4	777	706	0.06%	0.007%
47	6.687	1649	1663	1683	rBV	328771	645191	50.71%	5.986%
48	6.931	1736	1739	1741	rBV	227	114	0.01%	0.001%
49	7.038	1766	1772	1776	rBV	243	247	0.02%	0.002%
50	7.070	1776	1782	1785	rVB2	332	306	0.02%	0.003%
51	7.086	1785	1787	1790	rBV	117	71	0.01%	0.001%
52	7.102	1790	1792	1794	rBV	440	189	0.01%	0.002%
53	7.186	1809	1818	1832	rVB2	6141	9647	0.76%	0.090%
54	7.266	1838	1843	1846	rBV	344	238	0.02%	0.002%
55	7.324	1857	1861	1863	rBV2	242	170	0.01%	0.002%
56	7.430	1891	1894	1897	rBV2	312	208	0.02%	0.002%
57	7.497	1913	1915	1921	rVB	193	109	0.01%	0.001%
58	7.565	1922	1936	1952	rBV	131052	233458	18.35%	2.166%
59	7.690	1971	1975	1989	rVB4	3100	4831	0.38%	0.045%
60	7.800	2001	2009	2011	rBV2	732	895	0.07%	0.008%
61	7.896	2025	2039	2063	rBV	444475	778358	61.18%	7.222%
62	8.124	2108	2110	2114	rVB	278	167	0.01%	0.002%
63	8.176	2114	2126	2150	rBV	98233	167148	13.14%	1.551%
64	8.510	2228	2230	2232	rBV	241	128	0.01%	0.001%
65	8.555	2239	2244	2249	rVB3	538	502	0.04%	0.005%
66	8.629	2256	2267	2307	rBV2	467632	912107	71.69%	8.463%
67	8.941	2362	2364	2367	rBV2	323	173	0.01%	0.002%
68	8.986	2375	2378	2381	rVV2	283	159	0.01%	0.001%
69	9.002	2381	2383	2388	rVB2	235	140	0.01%	0.001%
70	9.169	2433	2435	2438	rVV2	219	125	0.01%	0.001%
71	9.266	2461	2465	2470	rBV	569	432	0.03%	0.004%
72	9.414	2498	2511	2544	rBV	752695	1241367	97.57%	11.518%
73	9.623	2574	2576	2577	rBV	306	142	0.01%	0.001%
74	9.687	2593	2596	2600	rBV2	405	414	0.03%	0.004%
75	9.751	2614	2616	2620	rVB	189	100	0.01%	0.001%
76	9.771	2620	2622	2625	rVB	302	159	0.01%	0.001%

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 Title : VOC Analysis

77	9.793	2625	2629	2633	rBV3	365	279	0.02%	0.003%
78	9.812	2633	2635	2639	rBV	277	211	0.02%	0.002%
79	9.935	2668	2673	2680	rVB2	305	392	0.03%	0.004%
80	9.967	2680	2683	2685	rBV	166	114	0.01%	0.001%
81	10.057	2708	2711	2712	rBV2	254	108	0.01%	0.001%
82	10.073	2712	2716	2717	rBV	235	152	0.01%	0.001%
83	10.124	2727	2732	2733	rBV	577	412	0.03%	0.004%
84	10.523	2853	2856	2860	rBV2	202	187	0.01%	0.002%
85	10.754	2914	2928	2949	rBV	605919	970734	76.30%	9.007%
86	10.893	2964	2971	2975	rBV4	1094	1502	0.12%	0.014%
87	10.922	2978	2980	2984	rBV3	861	612	0.05%	0.006%
88	11.025	3009	3012	3015	rVB	221	133	0.01%	0.001%
89	11.044	3016	3018	3021	rBV2	271	213	0.02%	0.002%
90	11.353	3111	3114	3117	rBV	256	230	0.02%	0.002%
91	11.484	3148	3155	3158	rBV3	927	1316	0.10%	0.012%
92	11.809	3243	3256	3276	rBV	565727	907021	71.29%	8.416%
93	12.057	3324	3333	3357	rBV	45265	88735	6.97%	0.823%
94	12.189	3362	3374	3399	rVV	552801	915719	71.97%	8.497%
95	12.401	3437	3440	3443	rBV3	414	305	0.02%	0.003%
96	12.533	3476	3481	3486	rBV5	1199	1438	0.11%	0.013%
97	12.777	3550	3557	3567	rBV7	1076	1924	0.15%	0.018%
98	13.018	3629	3632	3644	rBV3	614	831	0.07%	0.008%
99	13.455	3765	3768	3772	rBV3	499	418	0.03%	0.004%
100	13.851	3887	3891	3901	rVB3	1808	2089	0.16%	0.019%

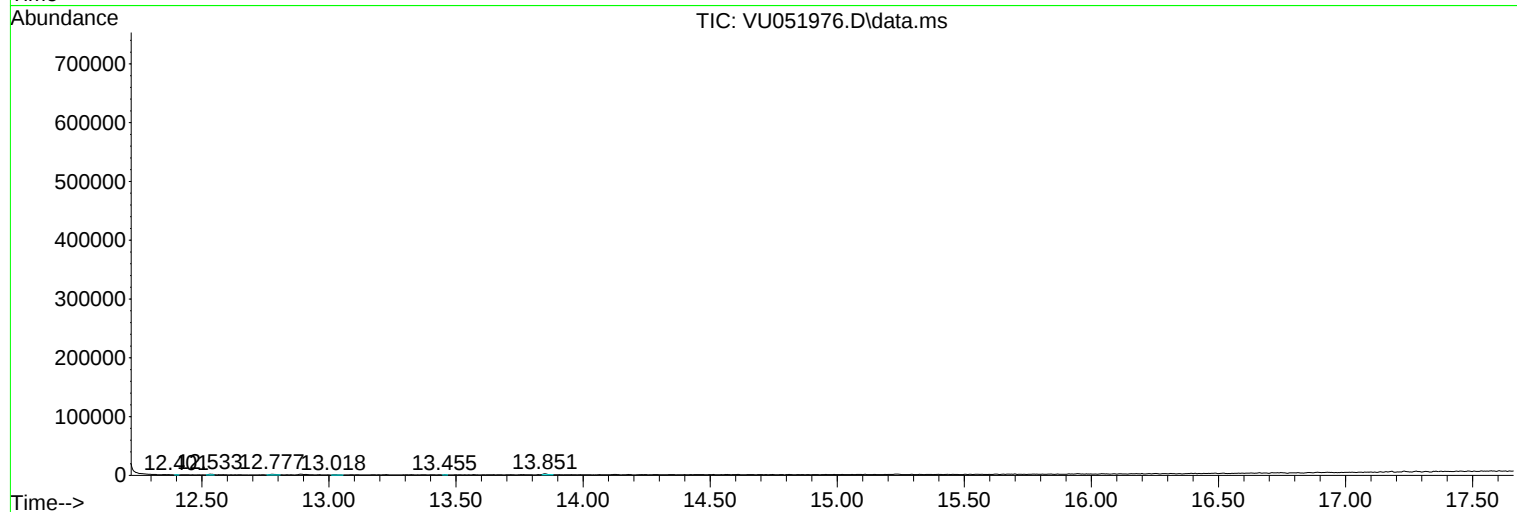
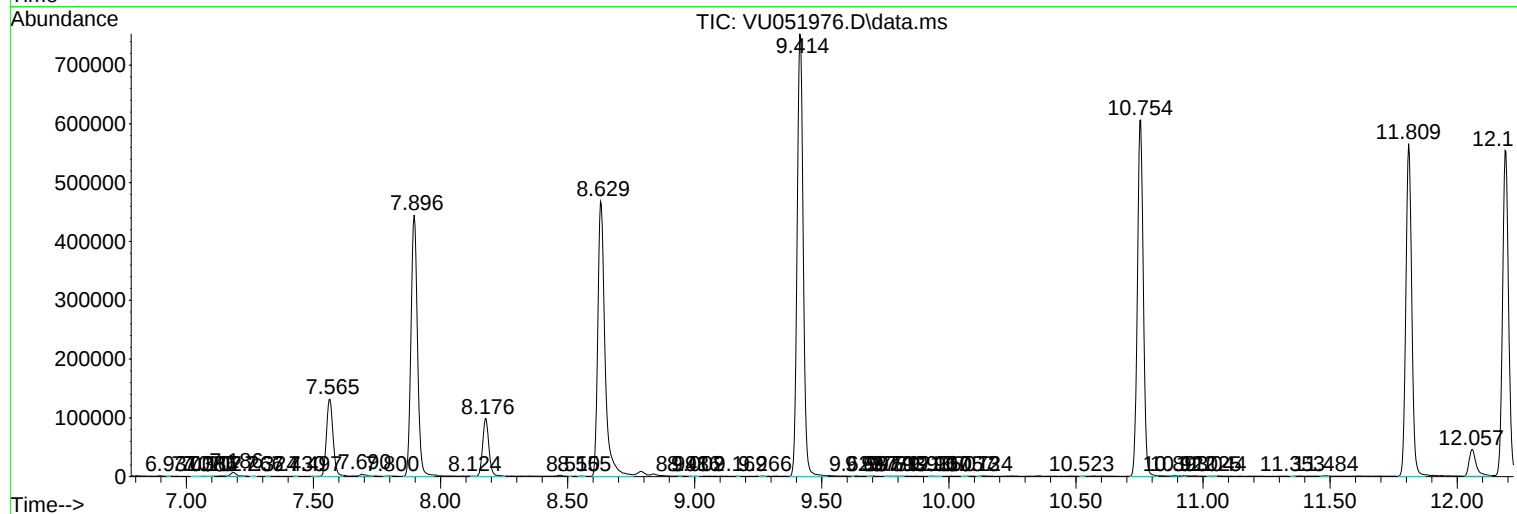
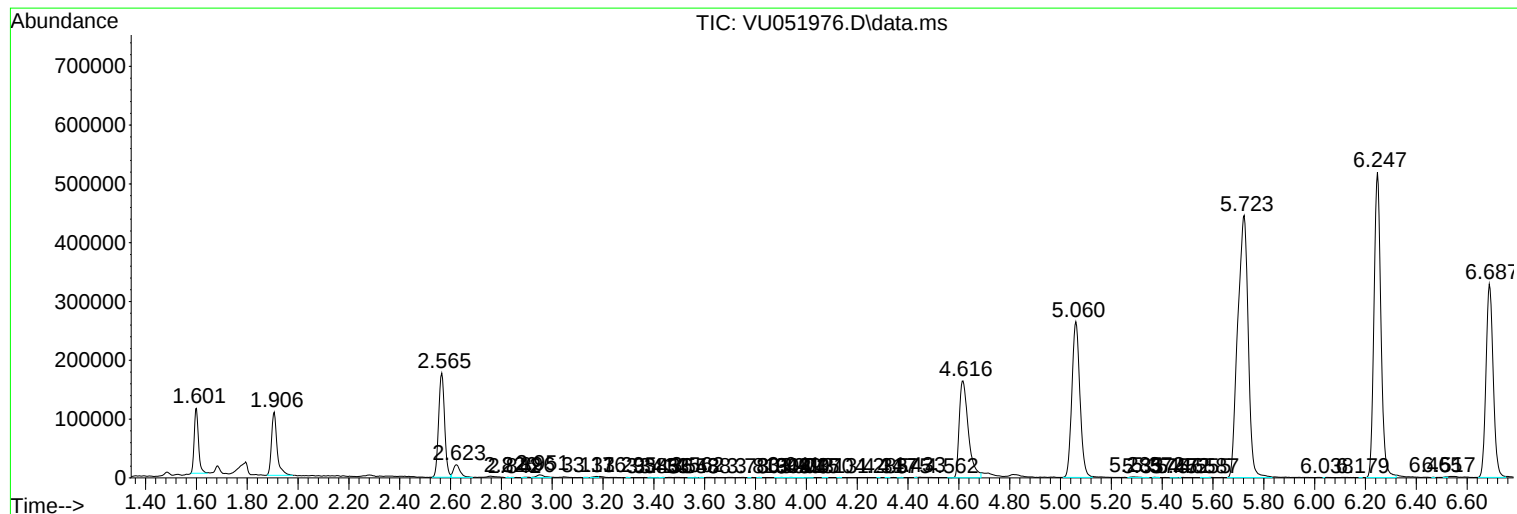
Sum of corrected areas: 10777599

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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



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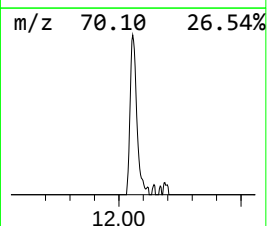
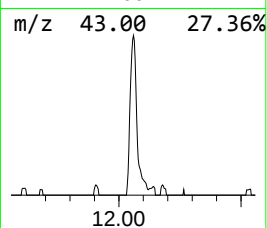
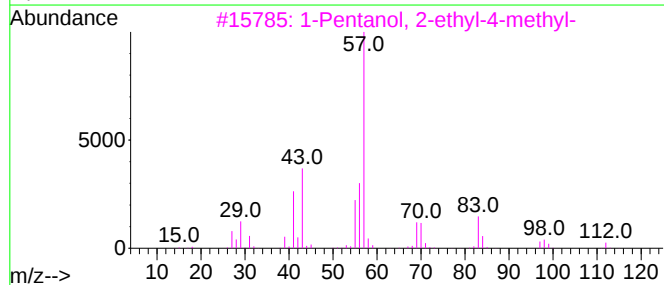
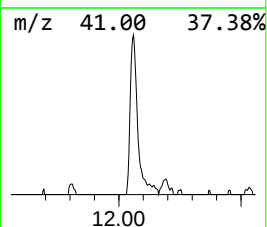
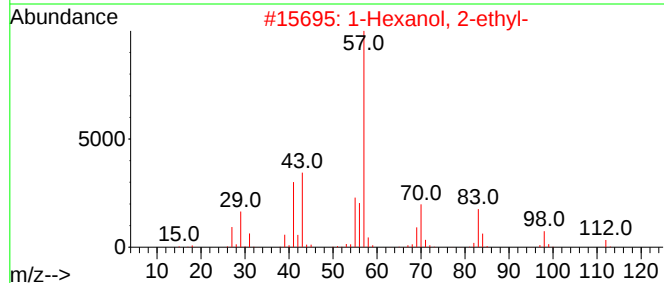
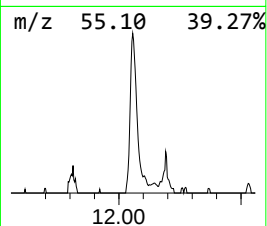
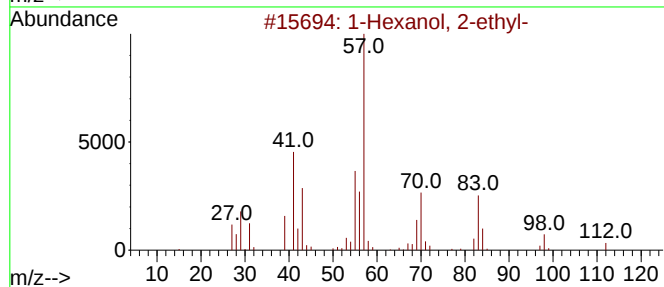
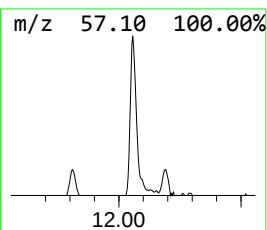
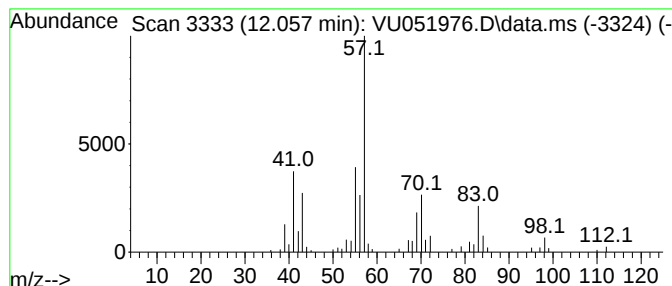
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	4.89 ug/L	88735	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59
3	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	53
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.057	4.9	ug/L	88735	3	11.809	907021	50.0