

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046422.D
 Acq On : 16 Dec 2021 15:39
 Operator : SY/MD
 Sample : M5038-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C00Z6

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	101	rBV	73962	90866	16.04%	2.045%
2	1.845	154	157	161	rBV	338	208	0.04%	0.005%
3	1.919	171	180	209	rBV	51223	75113	13.26%	1.691%
4	2.391	325	327	331	rVB	280	118	0.02%	0.003%
5	2.571	371	383	398	rBV	122857	203648	35.96%	4.584%
6	2.655	400	409	433	rVB2	5840	15556	2.75%	0.350%
7	2.790	448	451	456	rBV	159	201	0.04%	0.005%
8	2.874	475	477	482	rBV	124	151	0.03%	0.003%
9	2.957	499	503	508	rBV2	173	179	0.03%	0.004%
10	3.022	520	523	527	rBV	139	178	0.03%	0.004%
11	3.115	549	552	556	rBB	163	157	0.03%	0.004%
12	3.137	556	559	561	rBV	143	119	0.02%	0.003%
13	3.150	561	563	567	rVB	149	122	0.02%	0.003%
14	3.173	568	570	572	rBV	391	238	0.04%	0.005%
15	3.195	573	577	584	rVB2	504	626	0.11%	0.014%
16	3.462	657	660	662	rBV	146	119	0.02%	0.003%
17	3.591	697	700	703	rBV	157	148	0.03%	0.003%
18	3.880	787	790	792	rBV	137	116	0.02%	0.003%
19	4.636	1010	1025	1045	rBV	46244	122905	21.70%	2.767%
20	4.806	1075	1078	1083	rVV2	191	208	0.04%	0.005%
21	4.832	1084	1086	1094	rVB3	496	643	0.11%	0.014%
22	4.996	1134	1137	1140	rBV	131	138	0.02%	0.003%
23	5.067	1144	1159	1186	rBV	103262	227873	40.24%	5.129%
24	5.160	1186	1188	1191	rVV2	366	230	0.04%	0.005%
25	5.182	1191	1195	1197	rVV	262	121	0.02%	0.003%
26	5.391	1256	1260	1264	rBB	141	144	0.03%	0.003%
27	5.729	1343	1365	1390	rBV2	208964	566323	100.00%	12.748%
28	5.848	1400	1402	1407	rVB	287	232	0.04%	0.005%
29	6.105	1479	1482	1485	rBB	144	118	0.02%	0.003%
30	6.253	1514	1528	1552	rBV	174319	325525	57.48%	7.327%
31	6.571	1626	1627	1631	rVV	229	172	0.03%	0.004%
32	6.693	1651	1665	1682	rBV	130961	251028	44.33%	5.650%
33	6.787	1689	1694	1698	rVB	329	313	0.06%	0.007%
34	6.812	1698	1702	1707	rBB	245	266	0.05%	0.006%
35	6.886	1721	1725	1728	rBV	144	172	0.03%	0.004%
36	6.915	1731	1734	1741	rBV	131	203	0.04%	0.005%

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 Title : VOC Analysis

37	7.021	1764	1767	1769	rBV	144	119	0.02%	0.003%
38	7.176	1812	1815	1816	rBV	266	171	0.03%	0.004%
39	7.568	1925	1937	1958	rBV	69542	121143	21.39%	2.727%
40	7.693	1973	1976	1978	rVV	265	171	0.03%	0.004%
41	7.706	1978	1980	1984	rVB	156	130	0.02%	0.003%
42	7.800	2005	2009	2011	rBV2	243	186	0.03%	0.004%
43	7.899	2027	2040	2057	rVV	257845	442526	78.14%	9.961%
44	7.973	2057	2063	2073	rVB	4002	6334	1.12%	0.143%
45	8.111	2104	2106	2111	rBV	146	174	0.03%	0.004%
46	8.182	2115	2128	2144	rBV	48510	81679	14.42%	1.839%
47	8.311	2165	2168	2172	rVB2	200	189	0.03%	0.004%
48	8.475	2207	2219	2230	rBV3	8136	15097	2.67%	0.340%
49	8.636	2257	2269	2286	rBV	160642	271815	48.00%	6.118%
50	8.783	2310	2315	2317	rBV	1568	1289	0.23%	0.029%
51	9.021	2386	2389	2393	rVB	197	182	0.03%	0.004%
52	9.044	2394	2396	2399	rBV	180	149	0.03%	0.003%
53	9.076	2403	2406	2411	rBB	164	183	0.03%	0.004%
54	9.211	2444	2448	2450	rBV	158	157	0.03%	0.004%
55	9.291	2469	2473	2477	rBB	161	182	0.03%	0.004%
56	9.356	2487	2493	2495	rBV	170	231	0.04%	0.005%
57	9.420	2500	2513	2534	rBV	263120	436573	77.09%	9.827%
58	9.632	2575	2579	2584	rBV	171	236	0.04%	0.005%
59	9.693	2593	2598	2608	rVB	574	728	0.13%	0.016%
60	9.861	2646	2650	2652	rBV	123	134	0.02%	0.003%
61	10.025	2696	2701	2704	rBV	136	191	0.03%	0.004%
62	10.221	2759	2762	2764	rBV	174	152	0.03%	0.003%
63	10.240	2766	2768	2774	rVB3	283	217	0.04%	0.005%
64	10.507	2848	2851	2856	rVB	194	181	0.03%	0.004%
65	10.536	2857	2860	2862	rBV	144	129	0.02%	0.003%
66	10.581	2868	2874	2881	rBV2	383	508	0.09%	0.011%
67	10.639	2890	2892	2896	rBV	174	163	0.03%	0.004%
68	10.677	2896	2904	2910	rVV3	1252	1573	0.28%	0.035%
69	10.758	2916	2929	2947	rBV	180508	287082	50.69%	6.462%
70	10.893	2962	2971	2983	rVB3	9362	15920	2.81%	0.358%
71	11.015	3006	3009	3012	rBV	199	192	0.03%	0.004%
72	11.436	3133	3140	3141	rBV2	177	203	0.04%	0.005%
73	11.449	3142	3144	3145	rBV2	362	146	0.03%	0.003%
74	11.574	3179	3183	3186	rVB2	214	158	0.03%	0.004%
75	11.687	3214	3218	3219	rBV2	241	171	0.03%	0.004%
76	11.812	3245	3257	3274	rBV	271471	421243	74.38%	9.482%

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 Title : VOC Analysis

77	11.934	3286	3295	3301	rBV2	321	508	0.09%	0.011%
78	11.973	3301	3307	3316	rVB3	692	852	0.15%	0.019%
79	12.060	3324	3334	3349	rBV3	15878	27115	4.79%	0.610%
80	12.137	3356	3358	3360	rBV2	293	160	0.03%	0.004%
81	12.147	3360	3361	3364	rVV	403	264	0.05%	0.006%
82	12.195	3364	3376	3392	rVB	253726	409823	72.37%	9.225%
83	12.327	3415	3417	3419	rBV	246	152	0.03%	0.003%
84	12.536	3476	3482	3487	rBV2	806	819	0.14%	0.018%
85	12.639	3511	3514	3519	rBV	189	173	0.03%	0.004%
86	12.774	3547	3556	3566	rVB2	3479	5227	0.92%	0.118%
87	12.825	3570	3572	3577	rVB2	274	170	0.03%	0.004%
88	12.886	3586	3591	3595	rBV3	885	913	0.16%	0.021%
89	12.970	3613	3617	3626	rVB2	752	845	0.15%	0.019%
90	13.883	3898	3901	3908	rBV	132	124	0.02%	0.003%
91	14.024	3940	3945	3948	rBV	133	131	0.02%	0.003%
92	14.089	3961	3965	3971	rVB2	328	413	0.07%	0.009%
93	14.584	4110	4119	4124	rBV	534	770	0.14%	0.017%
94	15.606	4433	4437	4442	rBV	316	417	0.07%	0.009%
95	15.645	4446	4449	4451	rBV	201	155	0.03%	0.003%
96	15.735	4474	4477	4480	rBV	169	158	0.03%	0.004%
97	15.822	4500	4504	4506	rBV2	240	207	0.04%	0.005%
98	15.925	4531	4536	4541	rBV2	267	382	0.07%	0.009%
99	15.992	4555	4557	4559	rBV2	213	147	0.03%	0.003%
100	16.622	4751	4753	4755	rBV2	332	174	0.03%	0.004%

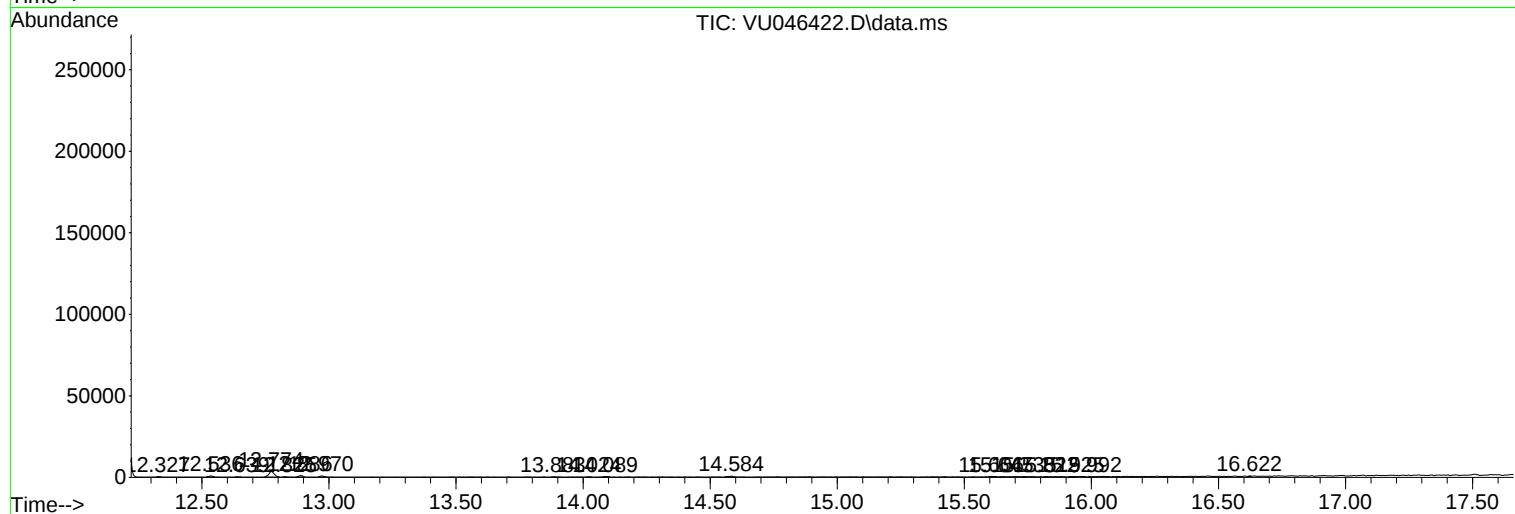
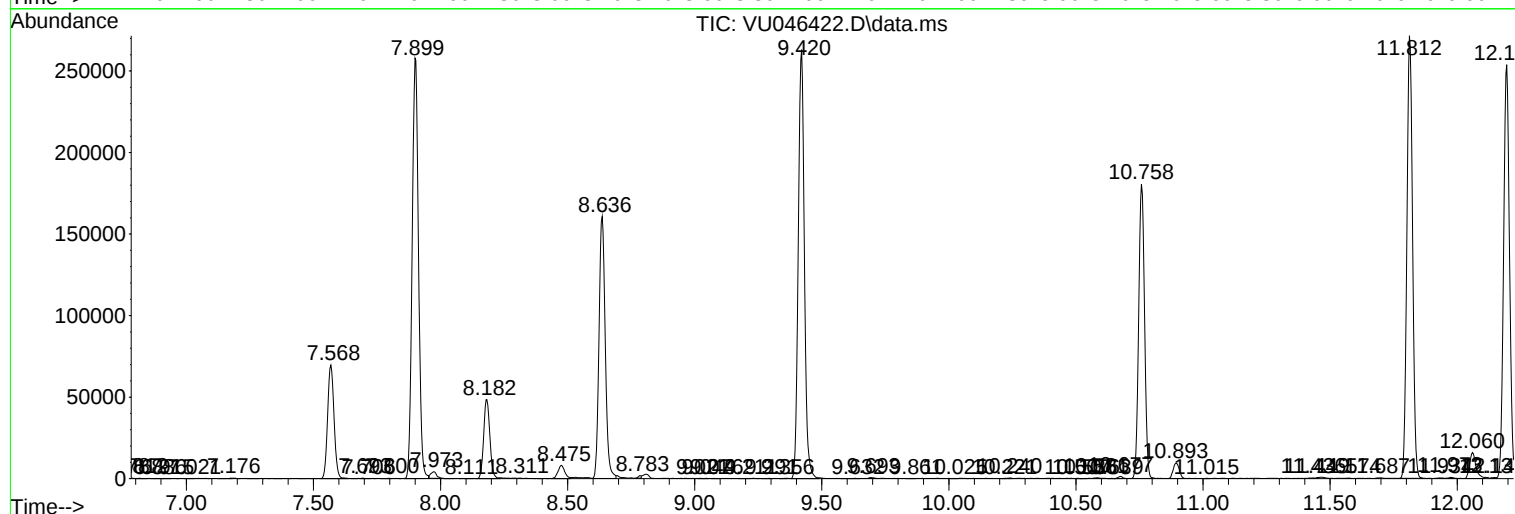
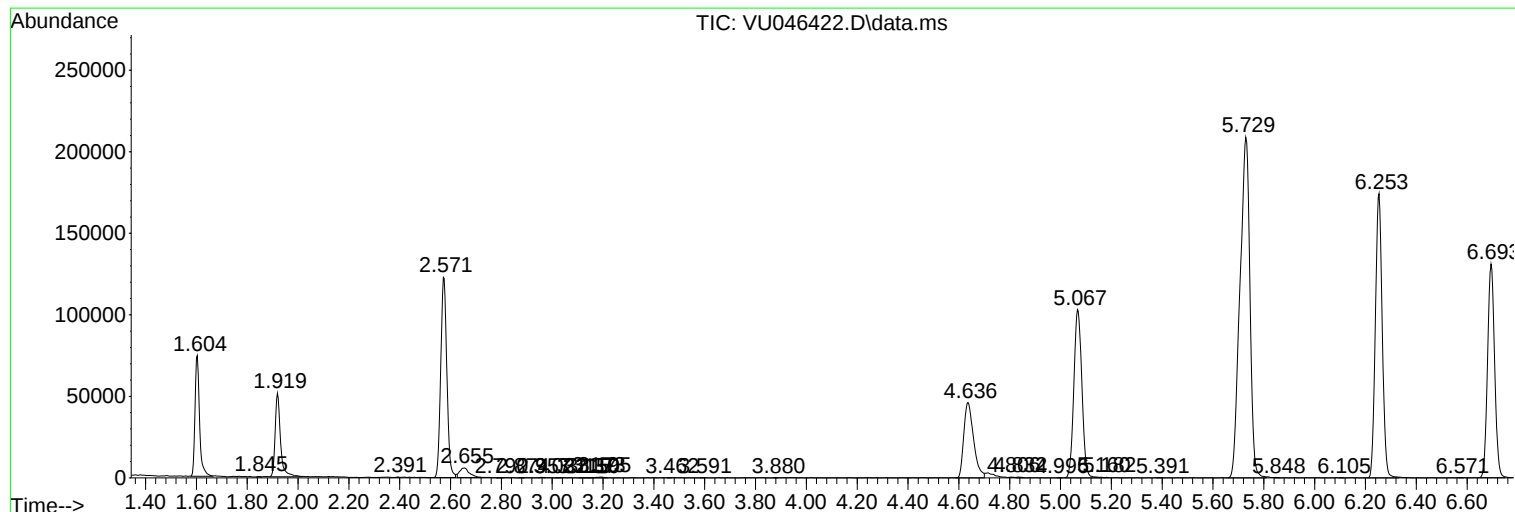
Sum of corrected areas: 4442583

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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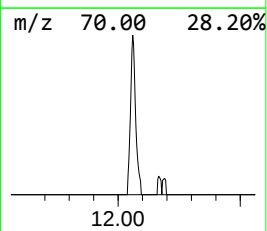
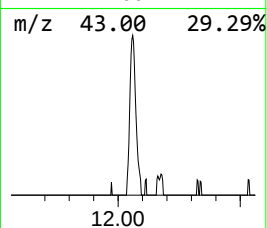
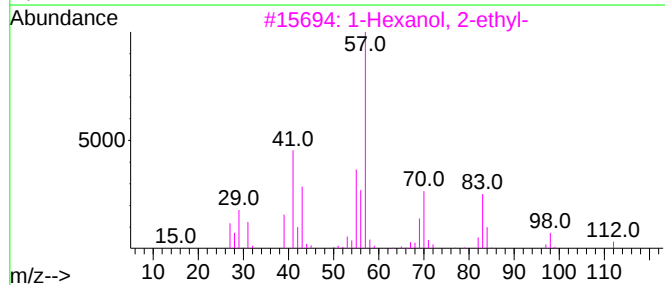
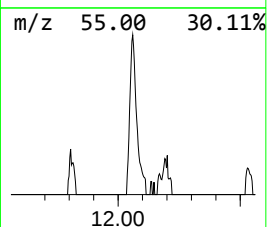
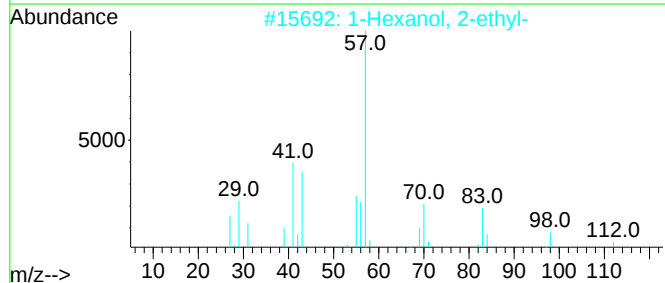
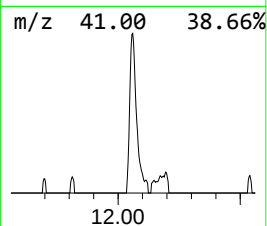
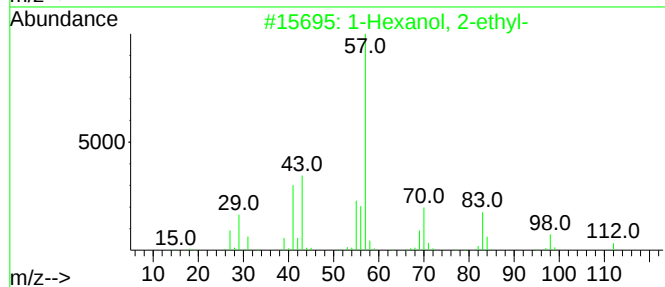
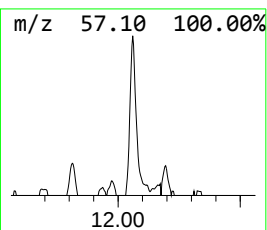
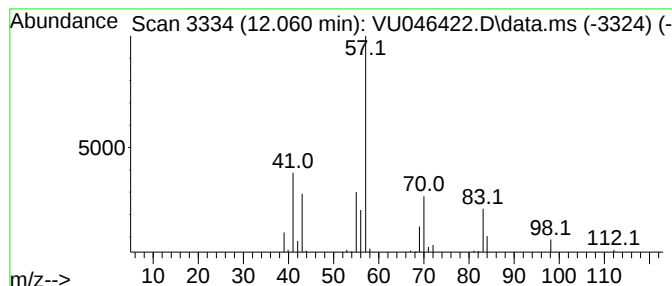
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
12.060	3.22 ug/L	27115	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.060	3.2	ug/L	27115	3	11.812	421243	50.0