

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
 Data File : VV022512.D
 Acq On : 02 Oct 2021 15:43
 Operator : SY/MD
 Sample : M3996-18
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F4A37

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_V\Method\SFAMVLM100121WMA.M

Title : VOC Analysis

Signal : TIC: VV022512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	74	82	94	rVB	122785	136157	19.90%	2.497%
2	1.568	157	164	176	rBV	88239	100114	14.63%	1.836%
3	2.108	322	332	347	rBV	184858	273551	39.99%	5.017%
4	2.542	466	467	468	rBV	330	85	0.01%	0.002%
5	2.580	476	479	482	rBV3	423	294	0.04%	0.005%
6	2.606	483	487	488	rBV3	1168	836	0.12%	0.015%
7	2.770	526	538	552	rVB4	4746	10024	1.47%	0.184%
8	2.915	582	583	585	rBV	208	68	0.01%	0.001%
9	2.979	599	603	606	rBV	341	295	0.04%	0.005%
10	3.223	676	679	680	rBV	377	217	0.03%	0.004%
11	3.497	761	764	765	rBV2	235	95	0.01%	0.002%
12	3.664	814	816	817	rBV	309	121	0.02%	0.002%
13	3.719	831	833	835	rBV2	188	127	0.02%	0.002%
14	3.899	873	889	927	rBV3	56517	214617	31.37%	3.937%
15	4.301	1012	1014	1018	rBV3	405	296	0.04%	0.005%
16	4.375	1020	1037	1062	rVV	108831	275362	40.25%	5.051%
17	4.886	1194	1196	1198	rVB	364	145	0.02%	0.003%
18	4.902	1198	1201	1203	rBB	218	87	0.01%	0.002%
19	4.918	1203	1206	1207	rBV	162	73	0.01%	0.001%
20	4.931	1207	1210	1212	rBV	207	111	0.02%	0.002%
21	5.047	1229	1246	1267	rBV2	268884	684124	100.00%	12.548%
22	5.329	1333	1334	1338	rBV	277	195	0.03%	0.004%
23	5.387	1350	1352	1354	rBV2	350	149	0.02%	0.003%
24	5.458	1371	1374	1378	rBV2	198	203	0.03%	0.004%
25	5.510	1386	1390	1391	rBV	195	141	0.02%	0.003%
26	5.545	1395	1401	1404	rBV3	1227	1399	0.20%	0.026%
27	5.619	1413	1424	1452	rBV	120426	244060	35.67%	4.477%
28	5.860	1496	1499	1500	rBV	458	223	0.03%	0.004%
29	5.905	1500	1513	1539	rVV2	145111	335377	49.02%	6.151%
30	6.072	1552	1565	1590	rBV	151808	310066	45.32%	5.687%
31	6.259	1620	1623	1627	rBV4	526	506	0.07%	0.009%
32	6.365	1654	1656	1658	rBB	271	66	0.01%	0.001%
33	6.391	1661	1664	1667	rVV	235	154	0.02%	0.003%
34	6.429	1673	1676	1679	rBV2	326	239	0.03%	0.004%
35	6.471	1687	1689	1690	rVB	222	69	0.01%	0.001%
36	6.580	1719	1723	1726	rBV2	303	318	0.05%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
 Title : VOC Analysis

37	6.632	1737	1739	1741	rBV	202	140	0.02%	0.003%
38	6.751	1771	1776	1777	rBV2	491	326	0.05%	0.006%
39	6.783	1785	1786	1789	rVB	326	119	0.02%	0.002%
40	6.805	1789	1793	1794	rBV	223	167	0.02%	0.003%
41	6.989	1839	1850	1867	rBV	81251	145486	21.27%	2.669%
42	7.210	1917	1919	1921	rVB2	250	99	0.01%	0.002%
43	7.317	1938	1952	1970	rBV	318865	555635	81.22%	10.191%
44	7.622	2038	2047	2075	rVB	54115	96752	14.14%	1.775%
45	7.722	2075	2078	2083	rBV4	392	338	0.05%	0.006%
46	7.808	2103	2105	2108	rBV	380	243	0.04%	0.004%
47	7.873	2123	2125	2127	rBV2	341	137	0.02%	0.003%
48	7.892	2129	2131	2133	rVB2	367	108	0.02%	0.002%
49	7.924	2139	2141	2143	rVB2	377	157	0.02%	0.003%
50	7.976	2145	2157	2179	rBV	351025	587898	85.93%	10.783%
51	8.095	2184	2194	2219	rBV3	135654	284714	41.62%	5.222%
52	8.345	2270	2272	2273	rBV3	252	127	0.02%	0.002%
53	8.429	2296	2298	2299	rBV3	338	121	0.02%	0.002%
54	8.561	2337	2339	2340	rBV	132	71	0.01%	0.001%
55	8.619	2353	2357	2363	rBV2	424	438	0.06%	0.008%
56	8.853	2419	2430	2454	rBV	180173	297528	43.49%	5.457%
57	9.082	2500	2501	2504	rBV2	228	107	0.02%	0.002%
58	9.133	2515	2517	2518	rBV2	230	81	0.01%	0.001%
59	9.230	2543	2547	2549	rBV	218	151	0.02%	0.003%
60	9.255	2553	2555	2560	rVV3	304	279	0.04%	0.005%
61	9.342	2579	2582	2584	rBV2	214	166	0.02%	0.003%
62	9.448	2613	2615	2617	rBV	301	150	0.02%	0.003%
63	9.477	2622	2624	2626	rBV2	262	113	0.02%	0.002%
64	9.551	2644	2647	2650	rBV	440	451	0.07%	0.008%
65	9.603	2659	2663	2678	rVB2	4610	6791	0.99%	0.125%
66	9.718	2697	2699	2706	rVB4	600	547	0.08%	0.010%
67	9.792	2720	2722	2724	rVB	132	53	0.01%	0.001%
68	9.808	2724	2727	2731	rBV2	355	305	0.04%	0.006%
69	9.940	2763	2768	2770	rBV2	306	348	0.05%	0.006%
70	10.123	2822	2825	2834	rVB4	1834	2251	0.33%	0.041%
71	10.185	2843	2844	2848	rVB	278	105	0.02%	0.002%
72	10.255	2865	2866	2873	rVB2	508	341	0.05%	0.006%
73	10.516	2938	2947	2957	rBV2	2829	4760	0.70%	0.087%
74	10.619	2978	2979	2983	rVB2	238	140	0.02%	0.003%
75	10.670	2993	2995	2999	rBV2	303	186	0.03%	0.003%
76	10.795	3031	3034	3036	rBV2	219	174	0.03%	0.003%

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Sampling : 1

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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_V\Method\SFAMVLM100121WMA.M
 Title : VOC Analysis

77	10.834	3045	3046	3048	rVB	368	111	0.02%	0.002%
78	10.850	3048	3051	3052	rBV	283	141	0.02%	0.003%
79	10.914	3065	3071	3072	rBV2	1358	1121	0.16%	0.021%
80	11.046	3104	3112	3126	rBV2	4365	6752	0.99%	0.124%
81	11.152	3139	3145	3151	rVB3	1138	1257	0.18%	0.023%
82	11.201	3156	3160	3162	rBV	424	342	0.05%	0.006%
83	11.249	3165	3175	3191	rBV	177657	277803	40.61%	5.095%
84	11.377	3212	3215	3216	rBV2	850	372	0.05%	0.007%
85	11.529	3252	3262	3280	rBV	45900	79550	11.63%	1.459%
86	11.625	3281	3292	3311	rVB	324263	503795	73.64%	9.241%
87	11.866	3365	3367	3369	rBV2	386	155	0.02%	0.003%
88	11.911	3378	3381	3382	rBV	476	276	0.04%	0.005%
89	11.992	3403	3406	3408	rBV	317	196	0.03%	0.004%
90	12.146	3453	3454	3455	rBV	215	52	0.01%	0.001%
91	12.461	3549	3552	3555	rBV2	276	245	0.04%	0.004%
92	12.766	3646	3647	3648	rVB2	307	59	0.01%	0.001%
93	13.037	3730	3731	3733	rBV	204	76	0.01%	0.001%
94	13.207	3782	3784	3787	rBV2	271	154	0.02%	0.003%
95	13.303	3813	3814	3815	rBV2	245	52	0.01%	0.001%
96	13.438	3854	3856	3859	rBV2	261	146	0.02%	0.003%
97	13.782	3961	3963	3966	rVB	291	112	0.02%	0.002%
98	14.040	4042	4043	4047	rVB2	573	325	0.05%	0.006%
99	14.072	4048	4053	4055	rBV2	498	436	0.06%	0.008%
100	14.950	4323	4326	4331	rBV3	403	363	0.05%	0.007%

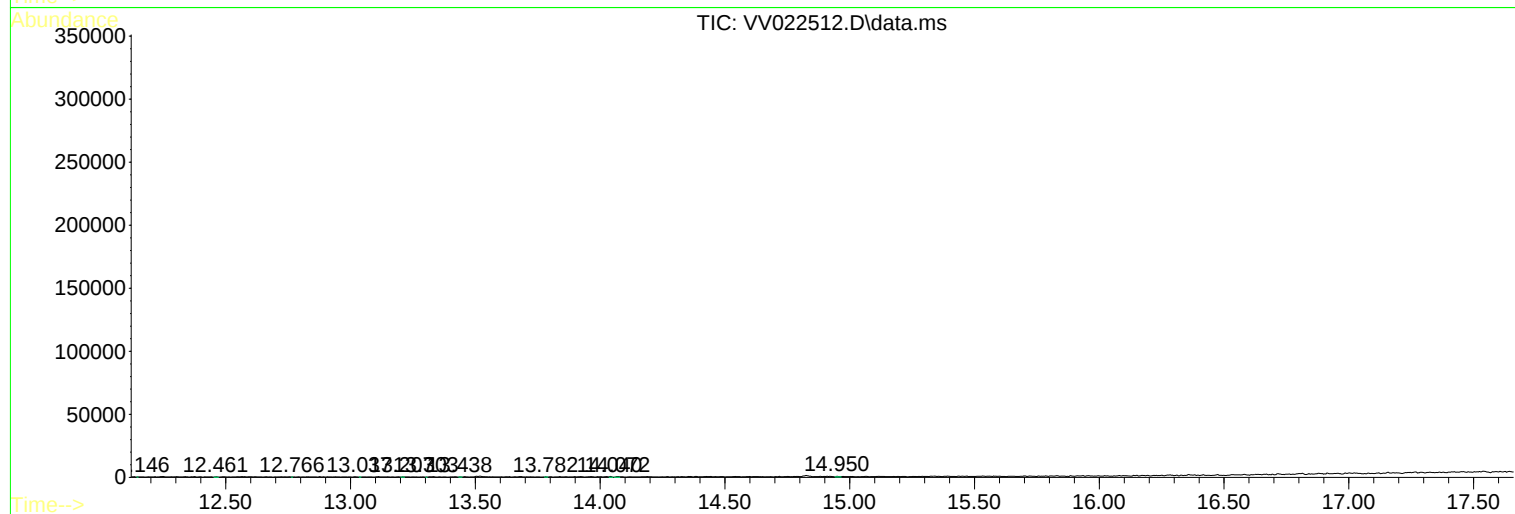
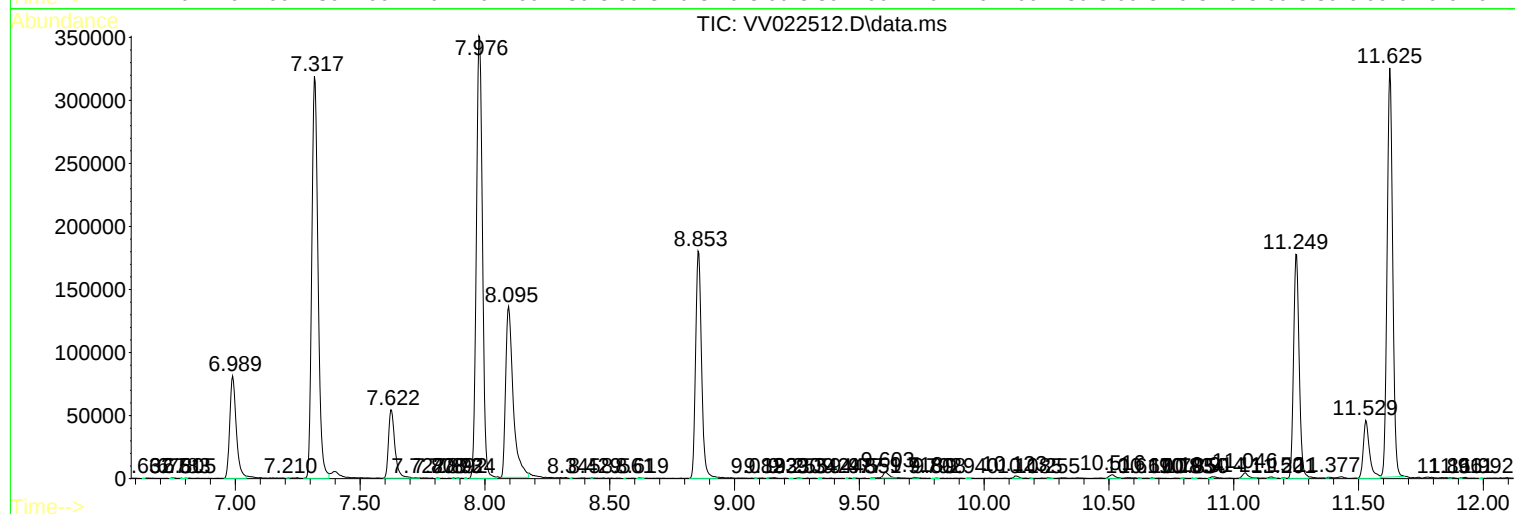
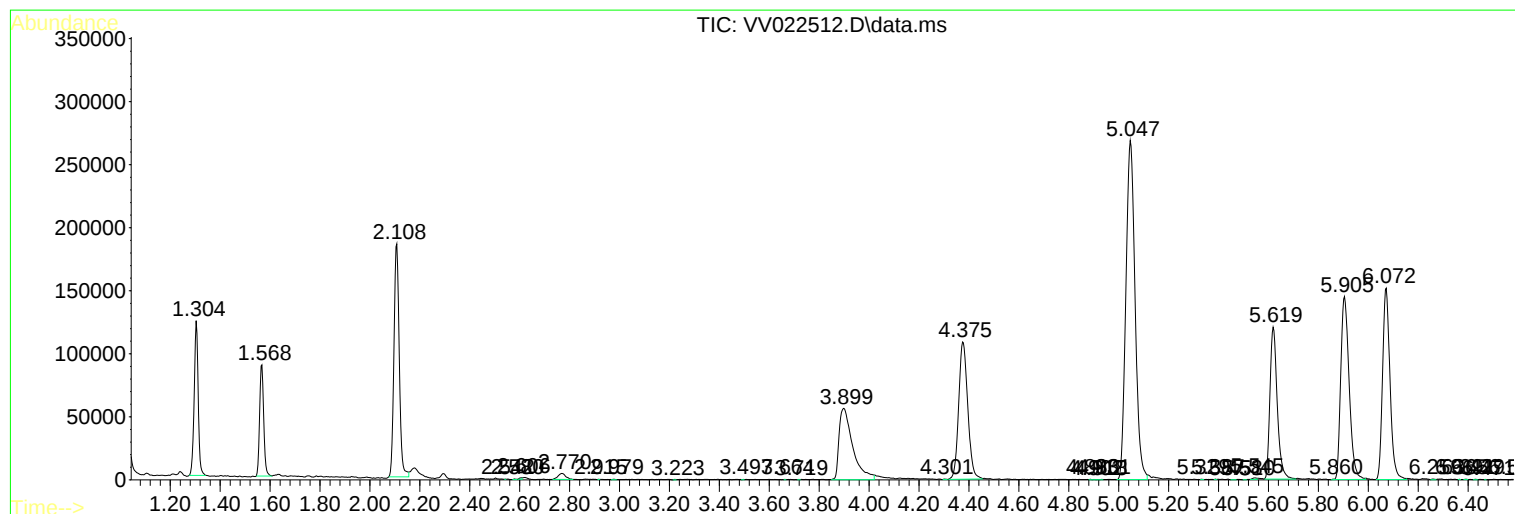
Sum of corrected areas: 5451958

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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



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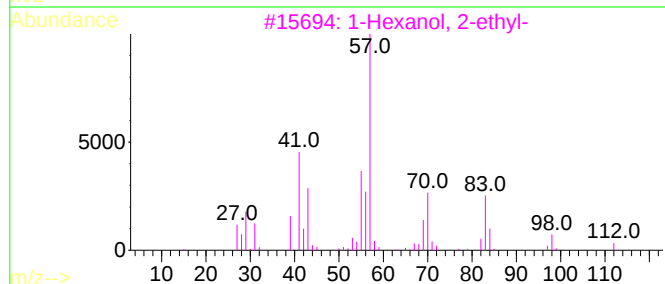
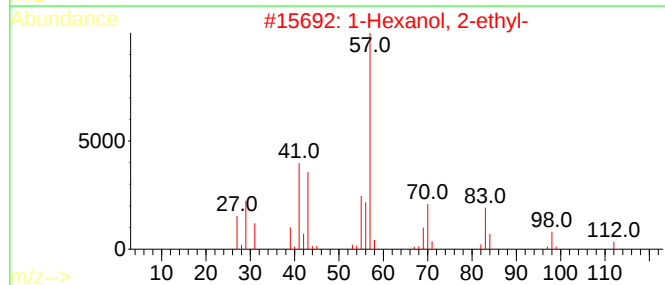
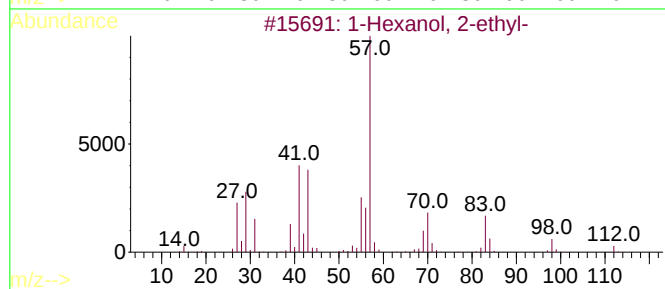
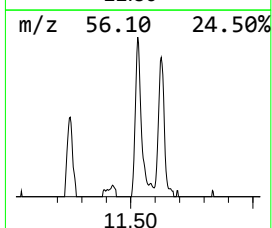
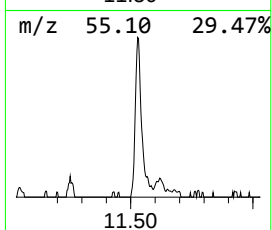
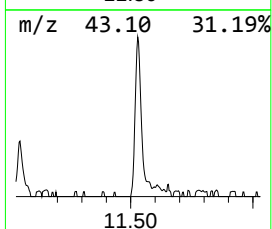
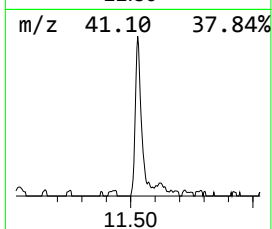
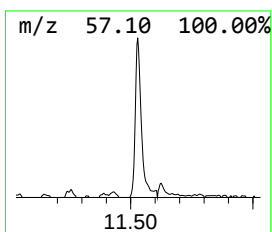
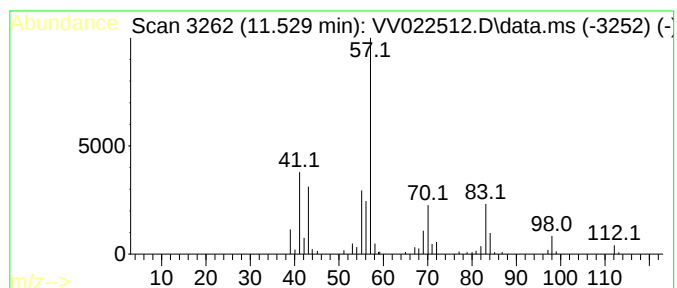
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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.
11.529	14.32 ug/L	79550	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	11.529	14.3	ug/L	79550	3	11.252	277803	50.0