

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060823\
 Data File : VX036076.D
 Acq On : 08 Jun 2023 17:28
 Operator : JC/MD
 Sample : 03097-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EZES1

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_X\Method\SFAMXML060623WMA.M
 Title : VOC Analysis

Signal : TIC: VX036076.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	15	rVB	9626	9079	0.67%	0.090%
2	1.264	26	29	32	rBV3	1938	2041	0.15%	0.020%
3	1.368	42	46	59	rVB	136891	166384	12.19%	1.654%
4	1.673	91	96	112	rBV	105285	163978	12.01%	1.630%
5	2.307	194	200	210	rBV	293190	456618	33.45%	4.540%
6	2.672	258	260	262	rBV	191	219	0.02%	0.002%
7	2.788	274	279	283	rBV5	979	2006	0.15%	0.020%
8	2.892	294	296	297	rBV	254	165	0.01%	0.002%
9	2.977	308	310	311	rBV2	297	265	0.02%	0.003%
10	3.044	319	321	322	rBV2	678	371	0.03%	0.004%
11	3.331	365	368	371	rBV2	223	288	0.02%	0.003%
12	3.428	381	384	386	rBV	344	340	0.02%	0.003%
13	3.593	407	411	413	rBV2	323	503	0.04%	0.005%
14	3.611	413	414	415	rVV	305	149	0.01%	0.001%
15	3.630	415	417	420	rVV2	339	335	0.02%	0.003%
16	3.660	420	422	423	rVV	188	150	0.01%	0.001%
17	3.709	427	430	431	rVV	232	171	0.01%	0.002%
18	4.331	531	532	535	rVB	228	129	0.01%	0.001%
19	4.477	545	556	586	rBV2	75224	278348	20.39%	2.767%
20	5.056	637	651	668	rBV	179561	549683	40.27%	5.465%
21	5.208	674	676	677	rBV2	413	263	0.02%	0.003%
22	5.379	702	704	705	rBV	376	223	0.02%	0.002%
23	5.550	725	732	733	rBV2	1323	1852	0.14%	0.018%
24	5.617	741	743	746	rVB2	215	155	0.01%	0.002%
25	5.641	746	747	752	rBV	232	211	0.02%	0.002%
26	5.745	762	764	766	rVB	236	163	0.01%	0.002%
27	5.971	789	801	816	rBV2	452705	1364960	100.00%	13.571%
28	6.233	843	844	850	rBV2	252	341	0.02%	0.003%
29	6.367	864	866	869	rBV	214	143	0.01%	0.001%
30	6.464	878	882	887	rVB2	296	436	0.03%	0.004%
31	6.513	887	890	891	rBV	192	132	0.01%	0.001%
32	6.641	909	911	912	rBV	353	332	0.02%	0.003%
33	6.757	921	930	948	rBV	330207	803552	58.87%	7.989%
34	7.105	982	987	996	rVB5	1678	4638	0.34%	0.046%
35	7.178	996	999	1000	rBV	365	434	0.03%	0.004%
36	7.306	1011	1020	1035	rBV	284972	625459	45.82%	6.218%

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 Title : VOC Analysis

37	7.409	1035	1037	1041	rVB2	364	333	0.02%	0.003%
38	7.482	1046	1049	1053	rVB3	509	903	0.07%	0.009%
39	7.653	1075	1077	1079	rBV2	231	226	0.02%	0.002%
40	7.732	1089	1090	1092	rVB	440	181	0.01%	0.002%
41	7.799	1099	1101	1106	rBV2	244	351	0.03%	0.003%
42	8.324	1180	1187	1195	rBV	176830	286892	21.02%	2.852%
43	8.549	1223	1224	1225	rBV	261	126	0.01%	0.001%
44	8.647	1233	1240	1249	rBV	698816	1081202	79.21%	10.749%
45	8.818	1267	1268	1269	rBV	246	131	0.01%	0.001%
46	8.854	1273	1274	1276	rVB	410	169	0.01%	0.002%
47	8.952	1284	1290	1299	rBV	124658	189956	13.92%	1.889%
48	9.129	1316	1319	1320	rVB2	443	377	0.03%	0.004%
49	9.147	1320	1322	1323	rBV	304	233	0.02%	0.002%
50	9.196	1326	1330	1331	rVV2	186	205	0.02%	0.002%
51	9.232	1335	1336	1340	rBV3	202	212	0.02%	0.002%
52	9.275	1340	1343	1346	rVV	931	1026	0.08%	0.010%
53	9.385	1355	1361	1375	rBV	423707	608555	44.58%	6.050%
54	9.622	1397	1400	1403	rBV2	315	389	0.03%	0.004%
55	9.750	1419	1421	1422	rVB	319	167	0.01%	0.002%
56	9.872	1440	1441	1444	rVB2	248	183	0.01%	0.002%
57	9.915	1446	1448	1449	rVV	220	126	0.01%	0.001%
58	9.958	1453	1455	1457	rVB2	273	161	0.01%	0.002%
59	10.055	1465	1471	1479	rBV	692281	941407	68.97%	9.360%
60	10.195	1491	1494	1496	rBV3	550	611	0.04%	0.006%
61	10.299	1508	1511	1516	rVB2	1582	1761	0.13%	0.018%
62	10.543	1550	1551	1555	rBV2	210	243	0.02%	0.002%
63	10.640	1565	1567	1572	rBV4	615	859	0.06%	0.009%
64	10.957	1615	1619	1621	rVB2	273	287	0.02%	0.003%
65	10.976	1621	1622	1623	rBV	222	122	0.01%	0.001%
66	11.085	1637	1640	1644	rBV2	449	617	0.05%	0.006%
67	11.189	1652	1657	1669	rVB	484835	610104	44.70%	6.066%
68	11.317	1675	1678	1683	rVB2	687	880	0.06%	0.009%
69	11.360	1683	1685	1688	rBV2	209	188	0.01%	0.002%
70	11.421	1691	1695	1701	rBV2	979	1656	0.12%	0.016%
71	11.506	1708	1709	1712	rVB	220	159	0.01%	0.002%
72	11.592	1722	1723	1726	rVB2	172	134	0.01%	0.001%
73	11.744	1746	1748	1749	rBV	249	189	0.01%	0.002%
74	11.835	1762	1763	1766	rBV2	212	245	0.02%	0.002%
75	11.982	1786	1787	1788	rBV	197	137	0.01%	0.001%
76	12.018	1788	1793	1805	rVV	687703	863915	63.29%	8.589%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
 Title : VOC Analysis

77	12.219	1820	1826	1837	rBV	71891	123158	9.02%	1.224%
78	12.317	1837	1842	1852	rVB	717690	895402	65.60%	8.902%
79	12.817	1922	1924	1926	rBV2	415	457	0.03%	0.005%
80	13.158	1978	1980	1983	rVB	341	307	0.02%	0.003%
81	13.378	2013	2016	2018	rBV	325	367	0.03%	0.004%
82	13.427	2022	2024	2025	rVV	503	329	0.02%	0.003%
83	13.481	2029	2033	2036	rBV2	528	657	0.05%	0.007%
84	13.628	2055	2057	2059	rVB	516	356	0.03%	0.004%
85	13.664	2061	2063	2065	rBV2	427	442	0.03%	0.004%
86	13.774	2079	2081	2086	rVB2	711	1057	0.08%	0.011%
87	13.896	2099	2101	2102	rBV2	352	290	0.02%	0.003%
88	13.981	2113	2115	2116	rBV	415	297	0.02%	0.003%
89	14.122	2135	2138	2141	rVB3	903	1173	0.09%	0.012%
90	14.353	2174	2176	2179	rBV	300	249	0.02%	0.002%
91	14.384	2179	2181	2184	rBV2	264	304	0.02%	0.003%
92	14.597	2214	2216	2218	rBV2	247	144	0.01%	0.001%
93	14.689	2229	2231	2234	rBV2	433	555	0.04%	0.006%
94	15.432	2351	2353	2354	rBV2	361	171	0.01%	0.002%
95	15.451	2354	2356	2359	rVB2	408	262	0.02%	0.003%
96	15.749	2403	2405	2408	rVB2	764	445	0.03%	0.004%
97	15.792	2410	2412	2415	rBV3	444	527	0.04%	0.005%
98	16.048	2452	2454	2456	rBV3	475	553	0.04%	0.005%
99	16.243	2484	2486	2487	rBV	435	207	0.02%	0.002%
100	16.456	2519	2521	2522	rBV2	521	379	0.03%	0.004%

Sum of corrected areas: 10058222

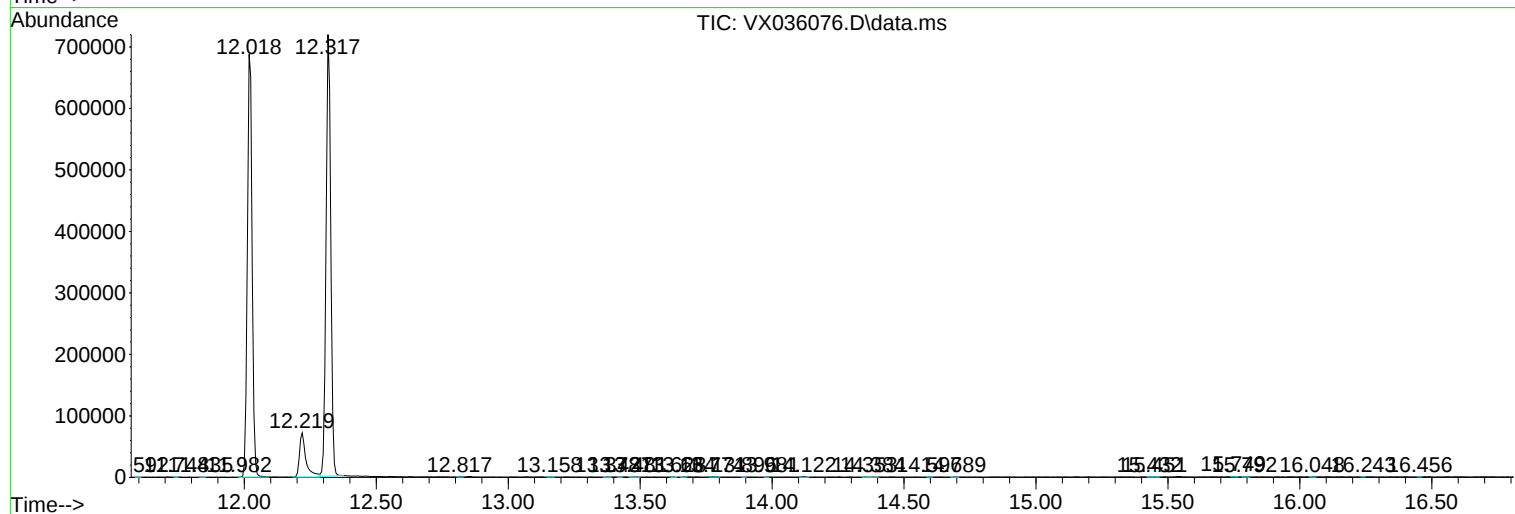
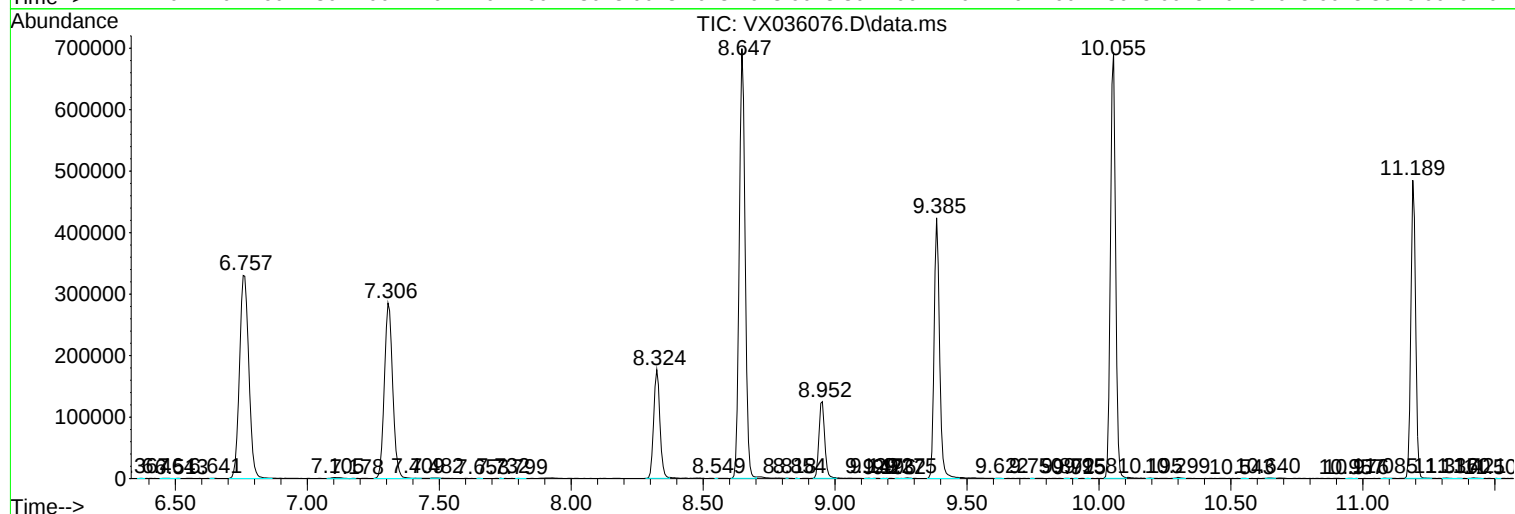
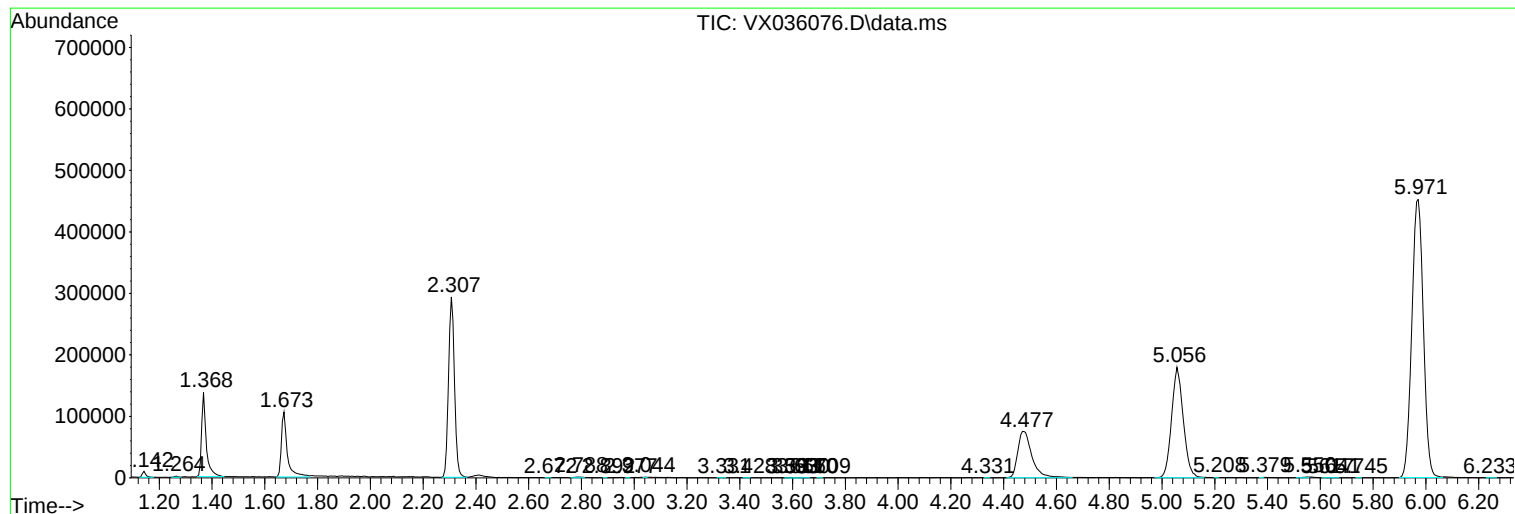
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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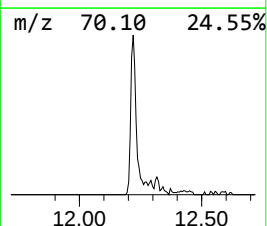
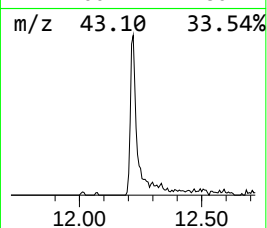
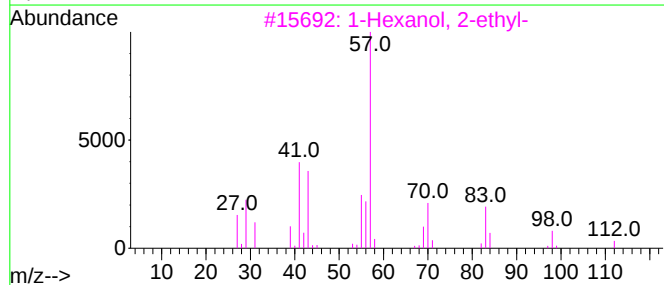
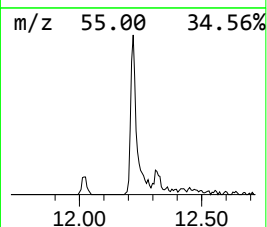
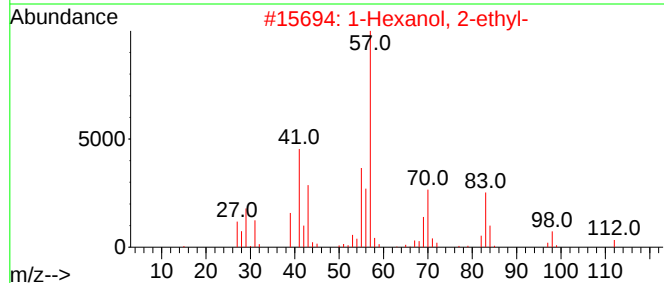
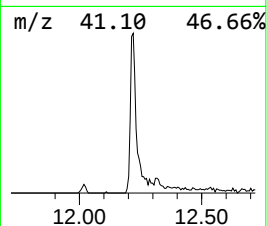
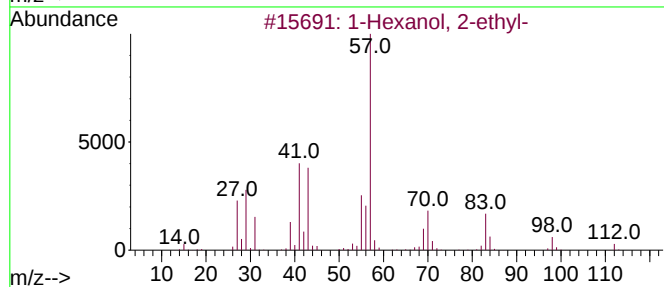
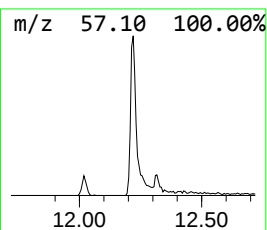
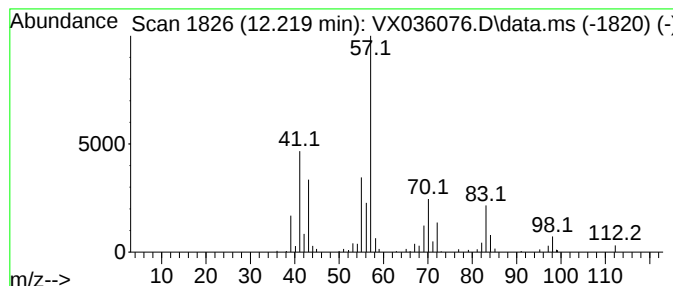
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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.
12.219	7.13 ug/L	123158	1,4-Dichlorobenzene-d4	12.024

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	86
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.219	7.1	ug/L	123158	3	12.024	863915	50.0