

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072924\
 Data File : VX042707.D
 Acq On : 29 Jul 2024 21:38
 Operator : JC/MD
 Sample : P3388-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20S3

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042707.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	19	rVB2	9228	12298	2.43%	0.316%
2	1.264	23	29	35	rVV4	6997	9995	1.97%	0.257%
3	1.368	42	46	57	rBV	41752	53627	10.58%	1.378%
4	1.642	88	91	100	rVB	24048	34020	6.71%	0.874%
5	1.801	116	117	118	rBV	392	242	0.05%	0.006%
6	1.941	135	140	144	rVB2	2835	4058	0.80%	0.104%
7	2.118	166	169	170	rBV2	368	366	0.07%	0.009%
8	2.294	192	198	210	rBV	82035	132810	26.20%	3.413%
9	2.441	220	222	226	rVB2	385	292	0.06%	0.008%
10	2.502	229	232	235	rBV2	356	551	0.11%	0.014%
11	2.563	240	242	245	rVB	304	228	0.04%	0.006%
12	2.605	245	249	250	rBV	208	232	0.05%	0.006%
13	2.794	273	280	281	rBV3	882	1600	0.32%	0.041%
14	2.941	302	304	306	rVV2	820	912	0.18%	0.023%
15	3.093	323	329	334	rVV3	773	1372	0.27%	0.035%
16	3.441	383	386	392	rVB3	758	1266	0.25%	0.033%
17	3.739	433	435	438	rVB2	330	296	0.06%	0.008%
18	3.782	438	442	444	rBV	167	284	0.06%	0.007%
19	4.020	478	481	482	rBV	300	295	0.06%	0.008%
20	4.148	497	502	504	rBV2	270	511	0.10%	0.013%
21	4.190	507	509	513	rVB2	178	243	0.05%	0.006%
22	4.306	521	528	531	rVB3	716	1454	0.29%	0.037%
23	4.373	538	539	543	rVB2	219	275	0.05%	0.007%
24	4.465	543	554	573	rBV	44519	135558	26.74%	3.484%
25	4.898	624	625	629	rVV2	180	228	0.04%	0.006%
26	5.056	640	651	669	rVV	70793	213905	42.20%	5.498%
27	5.343	696	698	703	rBV2	239	310	0.06%	0.008%
28	5.404	706	708	711	rBV	301	334	0.07%	0.009%
29	5.477	714	720	723	rVB3	660	1096	0.22%	0.028%
30	5.721	758	760	764	rBV2	202	236	0.05%	0.006%
31	5.873	784	785	788	rVB	275	222	0.04%	0.006%
32	5.964	788	800	816	rBV2	167222	506888	100.00%	13.028%
33	6.135	826	828	831	rBV	395	286	0.06%	0.007%
34	6.342	859	862	864	rBV	305	358	0.07%	0.009%
35	6.367	864	866	868	rVB	285	232	0.05%	0.006%
36	6.446	878	879	882	rBV	266	241	0.05%	0.006%

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37	6.653	912	913	916	rVB	340	279	0.06%	0.007%
38	6.690	916	919	920	rBV	256	255	0.05%	0.007%
39	6.763	922	931	950	rBV	155393	375276	74.04%	9.645%
40	7.129	984	991	998	rBV5	7751	17879	3.53%	0.460%
41	7.226	1004	1007	1009	rBV2	472	416	0.08%	0.011%
42	7.306	1012	1020	1030	rBV	104159	233452	46.06%	6.000%
43	7.489	1048	1050	1054	rVB2	376	420	0.08%	0.011%
44	7.531	1054	1057	1060	rBV	346	461	0.09%	0.012%
45	7.611	1068	1070	1074	rBV	253	300	0.06%	0.008%
46	7.812	1102	1103	1106	rBV	277	373	0.07%	0.010%
47	7.952	1125	1126	1128	rBV	318	253	0.05%	0.007%
48	8.007	1132	1135	1136	rBV	397	423	0.08%	0.011%
49	8.324	1182	1187	1200	rVV	56716	94800	18.70%	2.437%
50	8.488	1211	1214	1216	rVB	249	224	0.04%	0.006%
51	8.519	1216	1219	1220	rBV	595	456	0.09%	0.012%
52	8.586	1227	1230	1231	rBV	313	341	0.07%	0.009%
53	8.647	1234	1240	1249	rBV	222208	353229	69.69%	9.079%
54	8.909	1281	1283	1285	rBV	188	227	0.04%	0.006%
55	8.952	1285	1290	1303	rBV	38884	62684	12.37%	1.611%
56	9.098	1312	1314	1318	rVB2	358	238	0.05%	0.006%
57	9.208	1329	1332	1334	rVB	291	307	0.06%	0.008%
58	9.232	1334	1336	1340	rBV	253	436	0.09%	0.011%
59	9.281	1340	1344	1345	rBV2	344	368	0.07%	0.009%
60	9.385	1356	1361	1382	rBV	181596	277644	54.77%	7.136%
61	9.763	1420	1423	1426	rVB3	268	307	0.06%	0.008%
62	9.897	1442	1445	1448	rVB2	187	237	0.05%	0.006%
63	9.945	1451	1453	1456	rBV	184	251	0.05%	0.006%
64	10.055	1465	1471	1486	rVV	308302	424593	83.76%	10.913%
65	10.159	1486	1488	1492	rVV3	633	849	0.17%	0.022%
66	10.195	1492	1494	1501	rVV3	1225	2140	0.42%	0.055%
67	10.305	1507	1512	1522	rVV2	1483	3018	0.60%	0.078%
68	10.470	1536	1539	1544	rBV2	208	390	0.08%	0.010%
69	10.640	1565	1567	1574	rVB3	733	885	0.17%	0.023%
70	10.829	1593	1598	1601	rBV2	171	326	0.06%	0.008%
71	11.189	1652	1657	1668	rVB	216342	282204	55.67%	7.253%
72	11.274	1669	1671	1674	rBV2	477	358	0.07%	0.009%
73	11.396	1687	1691	1693	rBV	396	464	0.09%	0.012%
74	11.531	1709	1713	1715	rBV	224	279	0.06%	0.007%
75	11.750	1747	1749	1750	rBV2	599	421	0.08%	0.011%
76	11.976	1784	1786	1788	rBV	418	563	0.11%	0.014%

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Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
 Title : VOC Analysis

77	12.018	1788	1793	1801	rVV	234607	314756	62.10%	8.090%
78	12.219	1821	1826	1836	rBV	15005	21668	4.27%	0.557%
79	12.317	1837	1842	1854	rVV	219454	292744	57.75%	7.524%
80	12.396	1854	1855	1859	rVB2	533	380	0.07%	0.010%
81	12.518	1870	1875	1877	rBV	281	371	0.07%	0.010%
82	12.561	1880	1882	1884	rBV	285	294	0.06%	0.008%
83	12.658	1895	1898	1901	rBV2	178	264	0.05%	0.007%
84	12.921	1938	1941	1943	rVV	239	222	0.04%	0.006%
85	12.957	1943	1947	1948	rVB2	280	260	0.05%	0.007%
86	13.164	1979	1981	1984	rBV	371	417	0.08%	0.011%
87	13.780	2080	2082	2086	rVB	534	480	0.09%	0.012%
88	14.262	2159	2161	2163	rBV	262	270	0.05%	0.007%
89	14.353	2173	2176	2178	rBV	219	237	0.05%	0.006%
90	14.378	2178	2180	2182	rBV	327	232	0.05%	0.006%
91	14.603	2215	2217	2218	rBV	269	228	0.04%	0.006%
92	14.780	2244	2246	2250	rVB	359	387	0.08%	0.010%
93	14.835	2253	2255	2257	rBV	319	315	0.06%	0.008%
94	15.073	2292	2294	2295	rBV	382	343	0.07%	0.009%
95	15.115	2299	2301	2304	rVB2	340	307	0.06%	0.008%
96	15.579	2376	2377	2380	rBV3	239	241	0.05%	0.006%
97	15.615	2380	2383	2385	rBV3	231	305	0.06%	0.008%
98	15.902	2429	2430	2432	rVV	359	232	0.05%	0.006%
99	16.597	2543	2544	2546	rBV2	270	223	0.04%	0.006%
100	16.774	2570	2573	2574	rBV2	403	496	0.10%	0.013%

Sum of corrected areas: 3890819

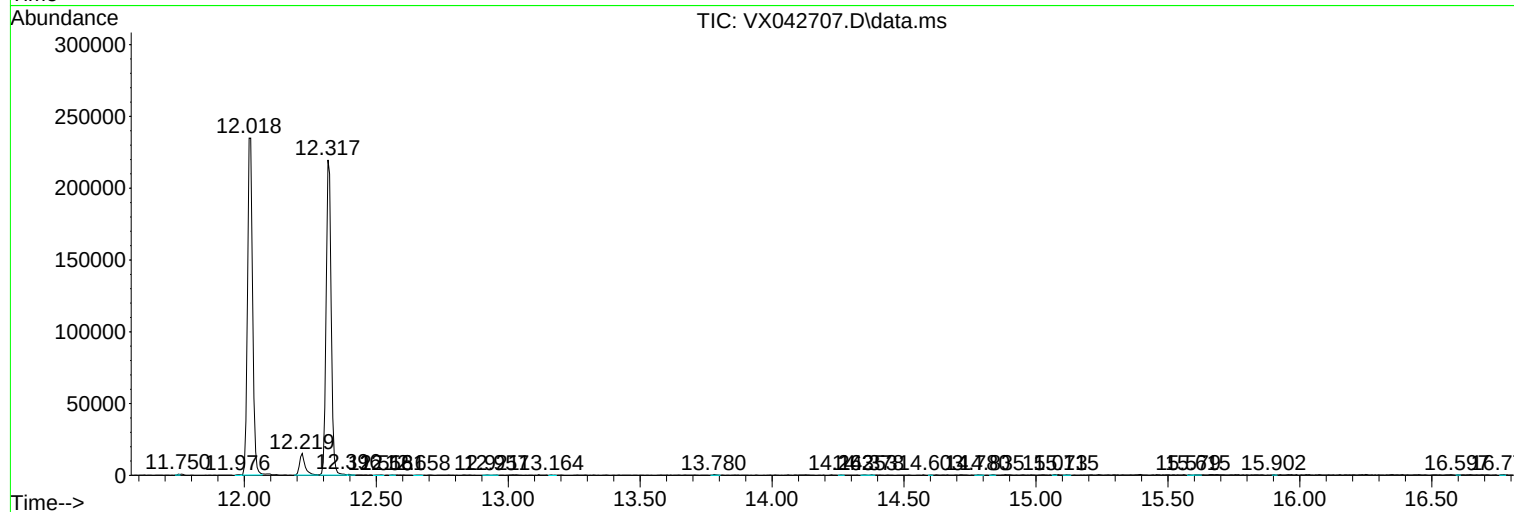
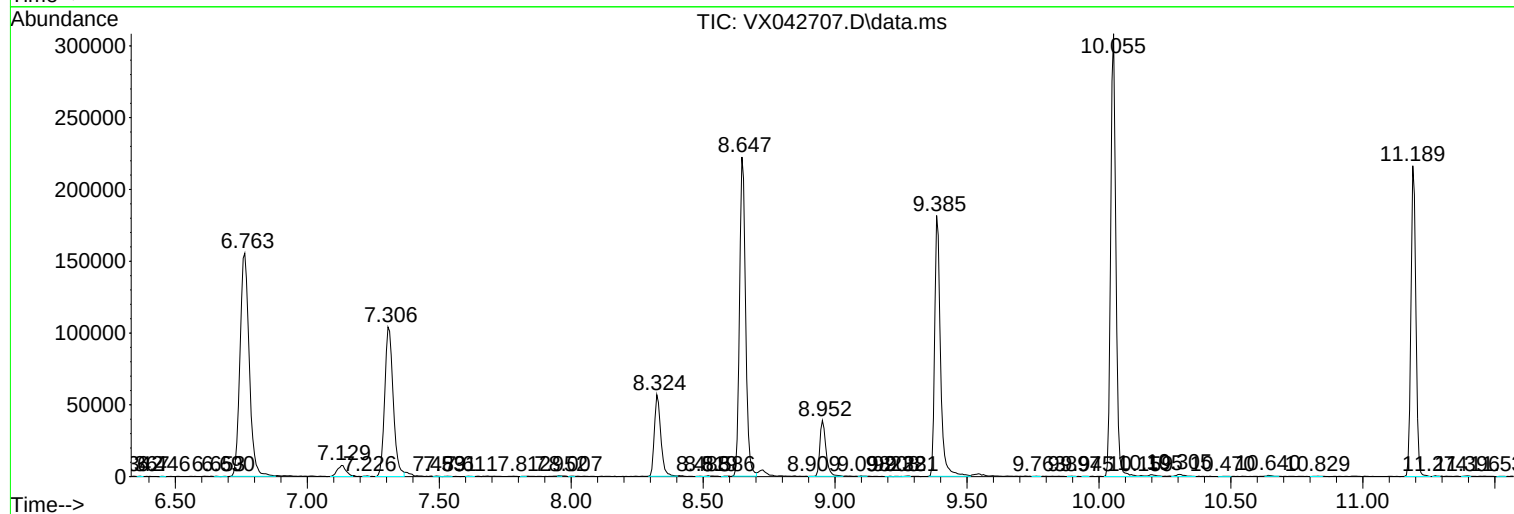
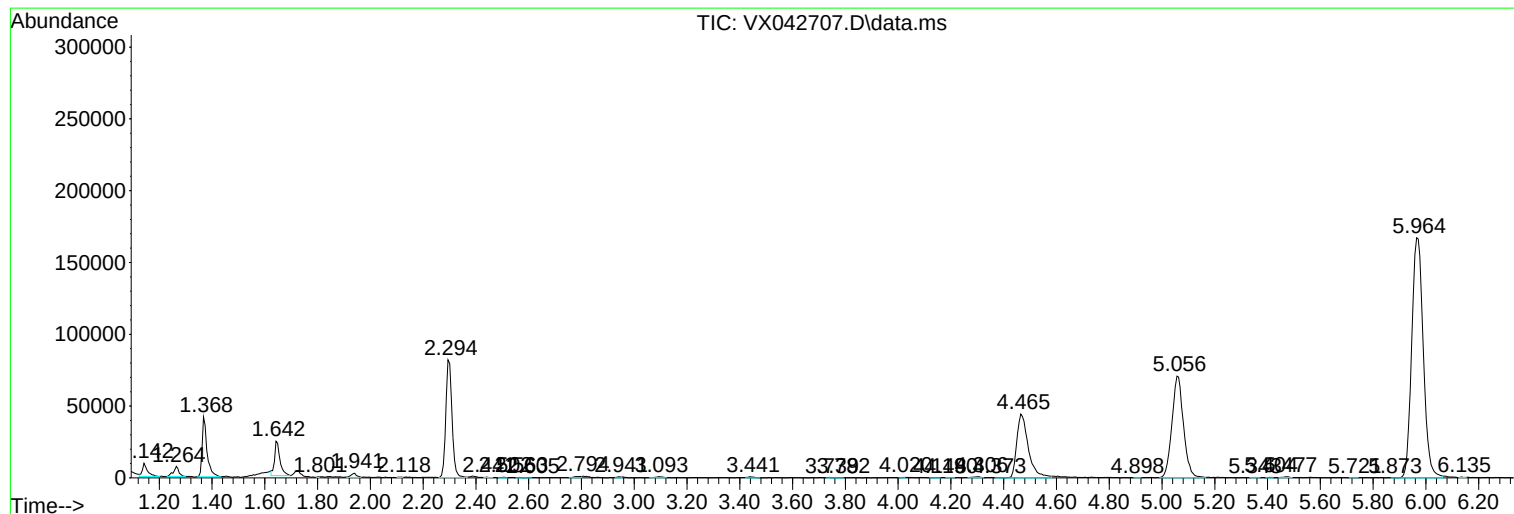
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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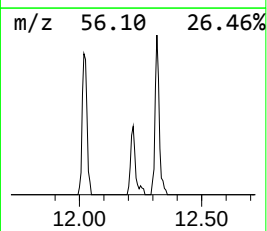
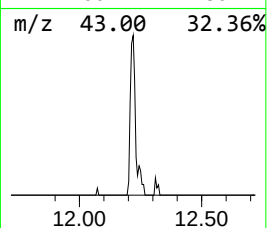
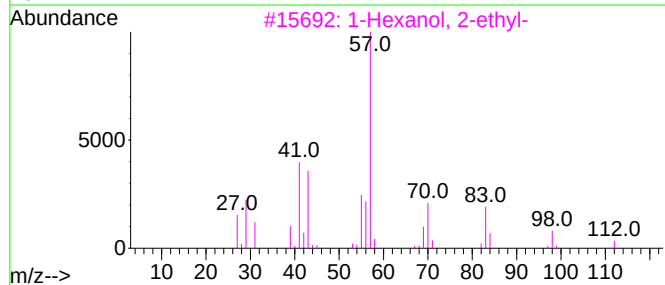
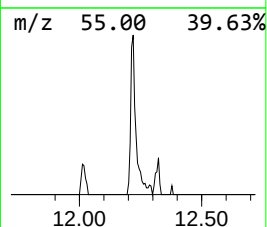
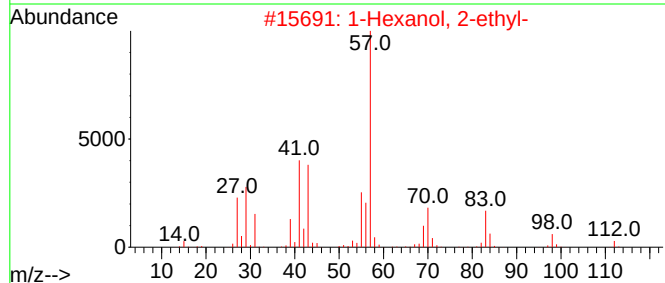
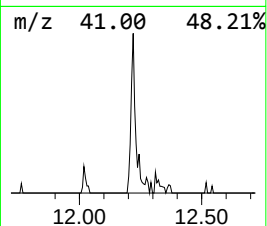
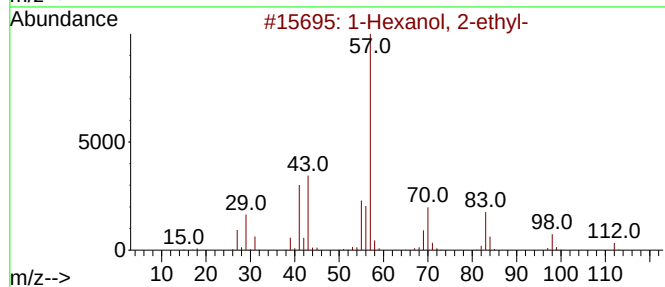
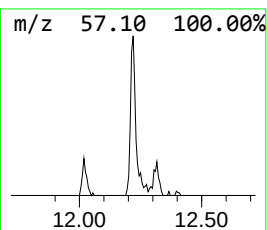
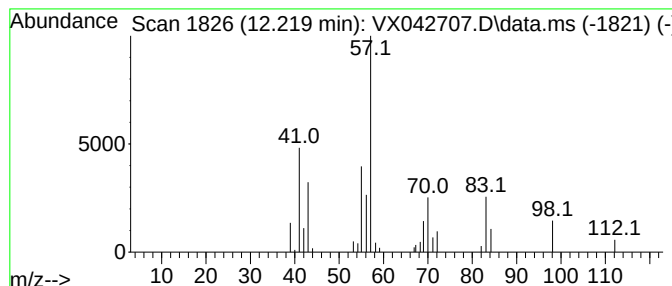
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
12.220	3.44 ug/L	21668	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	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.220	3.4	ug/L	21668	3	12.024	314756	50.0