

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047955.D
 Acq On : 12 Apr 2022 15:03
 Operator : SY/MD
 Sample : N2345-01DL 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J73DL

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047955.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	98	rBV	185666	215451	12.17%	1.614%
2	1.916	172	179	202	rVB	143184	201444	11.38%	1.509%
3	2.572	370	383	398	rBV	307998	505219	28.54%	3.784%
4	3.362	627	629	634	rBV2	270	175	0.01%	0.001%
5	3.395	635	639	642	rVB2	527	421	0.02%	0.003%
6	3.411	642	644	645	rBV	169	85	0.00%	0.001%
7	3.469	658	662	664	rBV	346	257	0.01%	0.002%
8	3.549	684	687	688	rBV	222	113	0.01%	0.001%
9	3.655	718	720	727	rBV3	237	285	0.02%	0.002%
10	3.848	778	780	781	rVB3	241	91	0.01%	0.001%
11	3.874	786	788	792	rVB	241	150	0.01%	0.001%
12	3.896	792	795	797	rBV	213	167	0.01%	0.001%
13	3.928	802	805	810	rVB3	451	365	0.02%	0.003%
14	3.951	810	812	813	rBV3	156	69	0.00%	0.001%
15	4.025	831	835	839	rVV2	218	176	0.01%	0.001%
16	4.044	839	841	843	rVB	332	173	0.01%	0.001%
17	4.067	843	848	849	rBV	280	152	0.01%	0.001%
18	4.121	862	865	867	rVB	118	72	0.00%	0.001%
19	4.134	867	869	874	rVB	253	221	0.01%	0.002%
20	4.163	874	878	880	rBV	297	207	0.01%	0.002%
21	4.202	887	890	891	rBV	262	111	0.01%	0.001%
22	4.350	933	936	938	rBV2	235	159	0.01%	0.001%
23	4.424	954	959	961	rBV	387	337	0.02%	0.003%
24	4.475	973	975	978	rBV2	179	81	0.00%	0.001%
25	4.549	995	998	1002	rBV2	251	224	0.01%	0.002%
26	4.575	1002	1006	1007	rBV2	429	261	0.01%	0.002%
27	4.620	1007	1020	1052	rBV	140723	340834	19.25%	2.553%
28	5.067	1143	1159	1184	rBV	255692	558418	31.54%	4.183%
29	5.378	1255	1256	1260	rVB3	515	174	0.01%	0.001%
30	5.398	1260	1262	1265	rVB2	339	162	0.01%	0.001%
31	5.414	1265	1267	1272	rVB2	284	182	0.01%	0.001%
32	5.449	1272	1278	1281	rBV	274	357	0.02%	0.003%
33	5.485	1284	1289	1292	rVB2	355	267	0.02%	0.002%
34	5.526	1293	1302	1304	rBV4	1142	1357	0.08%	0.010%
35	5.594	1320	1323	1325	rBV	147	102	0.01%	0.001%
36	5.604	1325	1326	1331	rVB2	213	102	0.01%	0.001%

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 Title : VOC Analysis

37	5.632	1333	1335	1336	rBV	117	34	0.00%	0.000%
38	5.729	1342	1365	1373	rBV2	521541	1430527	80.80%	10.715%
39	6.147	1493	1495	1498	rVB2	305	140	0.01%	0.001%
40	6.250	1513	1527	1555	rBV	435841	820338	46.34%	6.145%
41	6.398	1570	1573	1578	rBV4	624	586	0.03%	0.004%
42	6.520	1607	1611	1614	rBV4	1306	1296	0.07%	0.010%
43	6.587	1631	1632	1633	rBV4	262	94	0.01%	0.001%
44	6.642	1647	1649	1650	rBV	111	42	0.00%	0.000%
45	6.690	1650	1664	1684	rBV	319673	629733	35.57%	4.717%
46	6.838	1708	1710	1712	rBV	360	161	0.01%	0.001%
47	6.935	1737	1740	1742	rBV2	385	290	0.02%	0.002%
48	6.973	1749	1752	1756	rVB3	385	237	0.01%	0.002%
49	7.034	1766	1771	1773	rBV2	387	394	0.02%	0.003%
50	7.131	1796	1801	1803	rBV	589	370	0.02%	0.003%
51	7.185	1809	1818	1830	rVB5	3833	7181	0.41%	0.054%
52	7.231	1830	1832	1833	rBV5	155	68	0.00%	0.001%
53	7.240	1833	1835	1837	rVB	144	45	0.00%	0.000%
54	7.282	1846	1848	1852	rVB2	259	152	0.01%	0.001%
55	7.340	1862	1866	1870	rBV2	295	299	0.02%	0.002%
56	7.366	1871	1874	1876	rBV2	231	141	0.01%	0.001%
57	7.459	1900	1903	1905	rBV	237	147	0.01%	0.001%
58	7.568	1924	1937	1958	rBV	169885	299786	16.93%	2.245%
59	7.767	1995	1999	2001	rBV	312	216	0.01%	0.002%
60	7.825	2011	2017	2019	rBV4	363	367	0.02%	0.003%
61	7.899	2026	2040	2055	rBV	651749	1135404	64.13%	8.504%
62	8.179	2115	2127	2145	rBV	123571	207868	11.74%	1.557%
63	8.632	2255	2268	2306	rBV	437025	806051	45.53%	6.038%
64	8.912	2352	2355	2359	rBV	342	282	0.02%	0.002%
65	9.015	2382	2387	2395	rVB4	1682	2640	0.15%	0.020%
66	9.279	2464	2469	2474	rBV2	345	491	0.03%	0.004%
67	9.362	2489	2495	2498	rBV5	1379	1470	0.08%	0.011%
68	9.420	2500	2513	2516	rBV	665726	1025141	57.91%	7.679%
69	9.738	2609	2612	2614	rBV2	261	194	0.01%	0.001%
70	9.857	2645	2649	2657	rVB4	402	422	0.02%	0.003%
71	9.944	2674	2676	2681	rBV2	222	130	0.01%	0.001%
72	10.282	2779	2781	2782	rBV	295	132	0.01%	0.001%
73	10.343	2798	2800	2806	rVB3	262	145	0.01%	0.001%
74	10.671	2894	2902	2907	rBV4	3155	4275	0.24%	0.032%
75	10.758	2917	2929	2950	rVB	478914	774600	43.75%	5.802%
76	11.459	3141	3147	3161	rVB9	2457	4282	0.24%	0.032%

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77	11.748	3227	3237	3245	rBV2	37086	56781	3.21%	0.425%
78	11.812	3245	3257	3282	rVB2	748281	1685925	95.23%	12.628%
79	12.195	3362	3376	3402	rBV3	772613	1770380	100.00%	13.261%
80	12.970	3608	3617	3628	rVB2	15395	27318	1.54%	0.205%
81	13.217	3688	3694	3695	rBV3	1297	1017	0.06%	0.008%
82	13.269	3706	3710	3711	rBV3	1018	714	0.04%	0.005%
83	13.330	3722	3729	3736	rBV3	9724	13982	0.79%	0.105%
84	13.375	3736	3743	3754	rVB3	29398	44315	2.50%	0.332%
85	13.841	3878	3888	3903	rVB2	43378	66918	3.78%	0.501%
86	14.333	4033	4041	4044	rBV3	13160	18647	1.05%	0.140%
87	15.545	4408	4418	4432	rVB2	127488	195744	11.06%	1.466%
88	16.388	4670	4680	4692	rBV	302709	484395	27.36%	3.628%

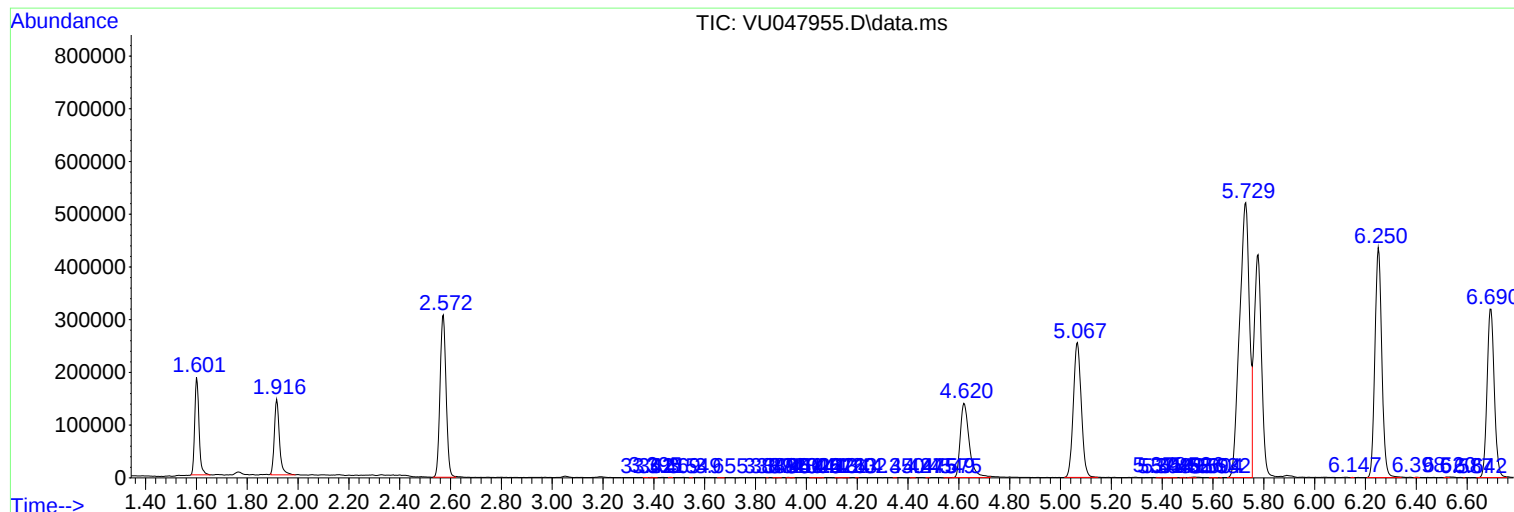
Sum of corrected areas: 13350728

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J73DL

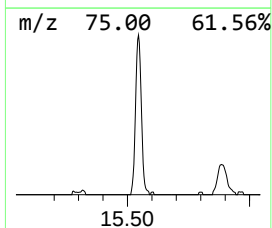
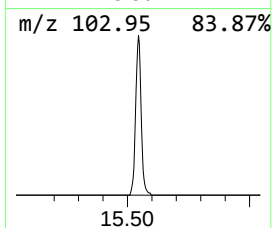
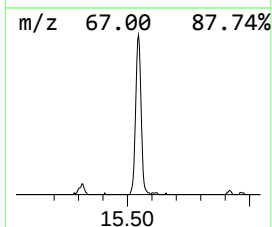
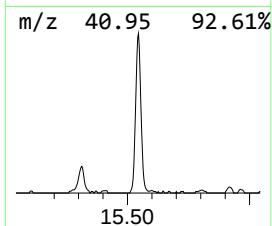
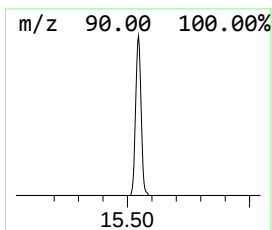
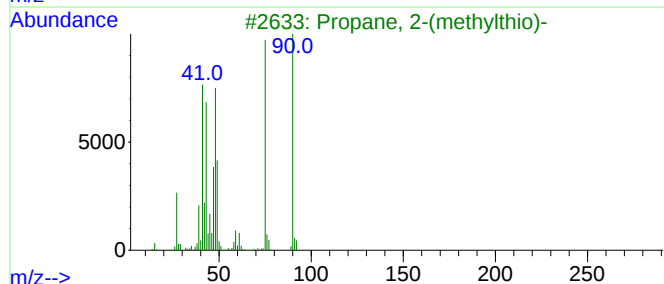
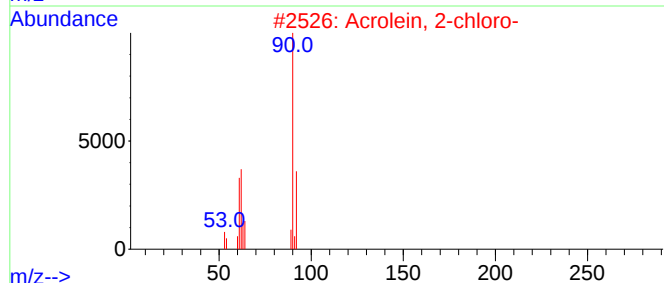
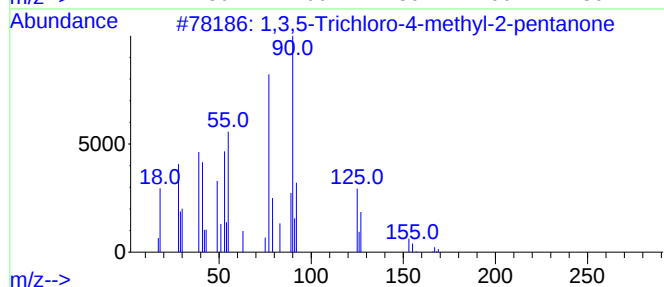
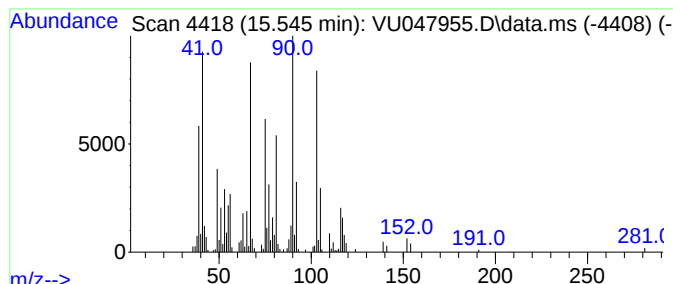
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	5.81 ug/L	195744	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	33
2			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	25
3			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	17
4			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	17
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	17



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Instrument :
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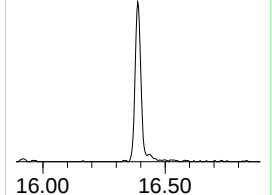
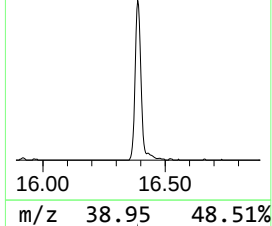
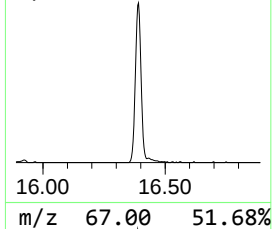
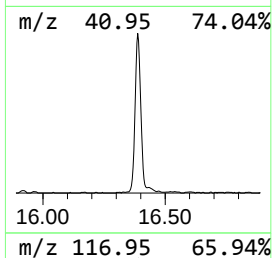
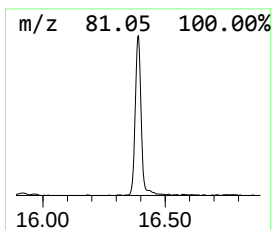
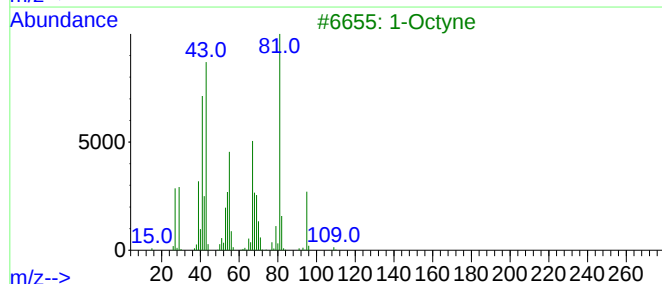
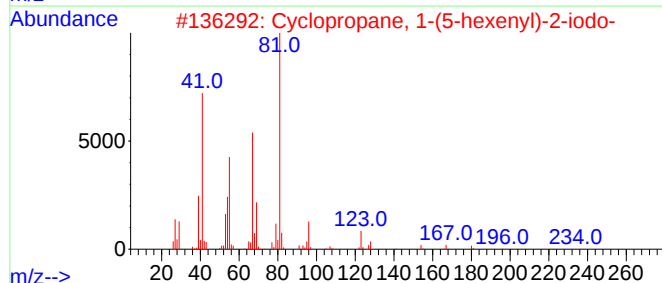
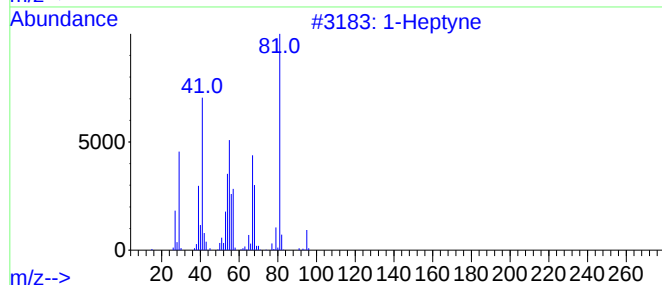
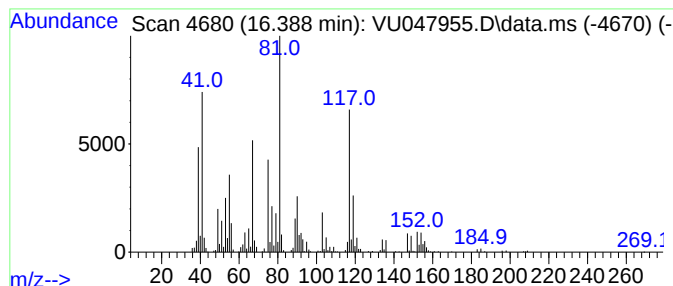
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	14.37 ug/L	484395	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptyne	96	C7H12	000628-71-7	22
2			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
3			1-Octyne	110	C8H14	000629-05-0	12
4			2,4-Dimethyl 1,4-pentadiene	96	C7H12	004161-65-3	11
5			Cyclohexene 3-(tert-butyl)peroxide	170	C10H18O2	051437-25-3	10



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	15.545	5.8	ug/L	195744	3	11.812	1685930	50.0
unknown-02	16.388	14.4	ug/L	484395	3	11.812	1685930	50.0