

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053611.D
 Acq On : 10 Apr 2023 11:39
 Operator : JC/MD
 Sample : 02251-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMC6

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053611.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	96	rVB	122598	140050	0.05%	0.013%
2	1.713	114	116	118	rBV	922	472	0.00%	0.000%
3	1.909	169	177	195	rVB	96615	135546	0.05%	0.013%
4	2.247	279	282	285	rBV3	931	867	0.00%	0.000%
5	2.565	369	381	397	rBV3	209788	382872	0.15%	0.037%
6	2.748	430	438	446	rBV4	1366	2178	0.00%	0.000%
7	2.954	497	502	506	rBV2	417	436	0.00%	0.000%
8	3.041	519	529	543	rBV3	6538	12218	0.00%	0.001%
9	3.134	549	558	572	rVB3	5998	11464	0.00%	0.001%
10	3.356	620	627	631	rBV4	1250	1831	0.00%	0.000%
11	3.398	636	640	643	rBV2	283	240	0.00%	0.000%
12	3.436	650	652	657	rVB2	350	271	0.00%	0.000%
13	3.504	665	673	676	rBV2	351	353	0.00%	0.000%
14	3.552	682	688	690	rBV2	233	242	0.00%	0.000%
15	3.691	727	731	732	rBV	671	476	0.00%	0.000%
16	3.861	779	784	795	rBV3	662	1045	0.00%	0.000%
17	4.530	974	992	1007	rBV2	35204	87338	0.03%	0.008%
18	4.613	1007	1018	1045	rVV	67373	162664	0.06%	0.016%
19	5.080	1140	1163	1191	rBV	1698356	3999501	1.55%	0.385%
20	5.385	1245	1258	1274	rVB3	21368	48448	0.02%	0.005%
21	5.452	1276	1279	1287	rVB3	653	483	0.00%	0.000%
22	5.526	1291	1302	1311	rVB4	2397	5030	0.00%	0.000%
23	5.594	1319	1323	1327	rVB4	873	665	0.00%	0.000%
24	5.623	1327	1332	1334	rBV5	753	718	0.00%	0.000%
25	5.790	1342	1384	1412	rBV3	58053887	150748547	58.36%	14.496%
26	6.243	1514	1525	1545	rVB	327340	611781	0.24%	0.059%
27	6.536	1602	1616	1632	rVB6	35246	76587	0.03%	0.007%
28	6.687	1649	1663	1678	rBV	206722	407484	0.16%	0.039%
29	6.980	1743	1754	1763	rBV6	3226	5918	0.00%	0.001%
30	7.102	1781	1792	1804	rVV3	11998	21180	0.01%	0.002%
31	7.186	1813	1818	1828	rVB4	1488	2295	0.00%	0.000%
32	7.327	1854	1862	1867	rBV3	461	715	0.00%	0.000%
33	7.404	1879	1886	1895	rVB6	2715	4393	0.00%	0.000%
34	7.440	1895	1897	1901	rBV2	322	229	0.00%	0.000%
35	7.497	1912	1915	1921	rVB3	367	330	0.00%	0.000%
36	7.562	1922	1935	1953	rBV	122967	213353	0.08%	0.021%

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 Title : VOC Analysis

37	7.687	1969	1974	1981	rVV5	893	994	0.00%	0.000%
38	7.716	1981	1983	1991	rVB3	567	361	0.00%	0.000%
39	7.896	2025	2039	2053	rVV	434320	760435	0.29%	0.073%
40	7.964	2055	2060	2076	rVV4	16868	30336	0.01%	0.003%
41	8.022	2076	2078	2082	rVV2	664	542	0.00%	0.000%
42	8.047	2082	2086	2087	rVV3	588	504	0.00%	0.000%
43	8.073	2091	2094	2098	rVV3	373	321	0.00%	0.000%
44	8.095	2098	2101	2103	rVB2	384	229	0.00%	0.000%
45	8.176	2114	2126	2150	rBV2	85136	143746	0.06%	0.014%
46	8.301	2163	2165	2169	rVB2	314	248	0.00%	0.000%
47	8.324	2169	2172	2174	rBV2	448	289	0.00%	0.000%
48	8.459	2209	2214	2216	rBV	902	683	0.00%	0.000%
49	8.549	2233	2242	2254	rBV3	23739	39311	0.02%	0.004%
50	8.629	2254	2267	2297	rBV	221125	408609	0.16%	0.039%
51	8.767	2307	2310	2312	rBV2	353	264	0.00%	0.000%
52	8.803	2312	2321	2332	rVB3	5679	9557	0.00%	0.001%
53	9.160	2429	2432	2440	rBV3	460	558	0.00%	0.000%
54	9.472	2499	2529	2579	rBV4	80279545	214413314	83.01%	20.619%
55	10.105	2720	2726	2735	rVB7	2169	3656	0.00%	0.000%
56	10.211	2757	2759	2763	rBV3	516	411	0.00%	0.000%
57	10.288	2774	2783	2794	rVV2	14365	24347	0.01%	0.002%
58	10.337	2794	2798	2801	rVB4	653	499	0.00%	0.000%
59	10.407	2818	2820	2823	rBV2	351	228	0.00%	0.000%
60	10.481	2835	2843	2853	rBV8	1463	2672	0.00%	0.000%
61	10.591	2873	2877	2879	rBV2	427	281	0.00%	0.000%
62	10.629	2885	2889	2898	rVB7	1329	1794	0.00%	0.000%
63	10.665	2898	2900	2903	rBV2	490	299	0.00%	0.000%
64	10.751	2915	2927	2933	rBV	307520	550193	0.21%	0.053%
65	10.883	2966	2968	2970	rVV	732	465	0.00%	0.000%
66	10.909	2974	2976	2980	rVB4	734	461	0.00%	0.000%
67	10.941	2980	2986	2988	rBV4	508	446	0.00%	0.000%
68	10.983	2989	2999	3010	rBV	60103	98129	0.04%	0.009%
69	11.050	3016	3020	3025	rBV6	1713	1483	0.00%	0.000%
70	11.099	3025	3035	3050	rVB2	31607	52184	0.02%	0.005%
71	11.195	3061	3065	3069	rBV	327	312	0.00%	0.000%
72	11.250	3077	3082	3085	rBV2	338	286	0.00%	0.000%
73	11.455	3142	3146	3147	rVV2	1035	606	0.00%	0.000%
74	11.475	3148	3152	3160	rVB3	2039	2415	0.00%	0.000%
75	11.642	3201	3204	3207	rVV2	450	326	0.00%	0.000%
76	11.751	3220	3238	3252	rBV2	37513958	64908269	25.13%	6.242%

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 Title : VOC Analysis

77	11.864	3252	3273	3316	rVB5	91391593	239990582	92.91%	23.078%
78	12.246	3365	3392	3432	rBV5	94237904	258311868	100.00%	24.840%
79	12.684	3522	3528	3538	rVB3	7124	10862	0.00%	0.001%
80	12.899	3588	3595	3604	rVV3	8215	13082	0.01%	0.001%
81	12.967	3605	3616	3629	rVB	251389	387680	0.15%	0.037%
82	13.144	3660	3671	3678	rBV2	62787	131842	0.05%	0.013%
83	13.201	3679	3689	3716	rVV	2572681	3948800	1.53%	0.380%
84	13.324	3718	3727	3740	rVB	163543	265425	0.10%	0.026%
85	13.568	3796	3803	3817	rVB4	13006	23951	0.01%	0.002%
86	13.848	3872	3890	3920	rBV	43721068	70652493	27.35%	6.794%
87	14.086	3956	3964	3975	rVB	18011	28988	0.01%	0.003%
88	14.330	4024	4040	4062	rBV	16367202	25336880	9.81%	2.436%
89	14.555	4108	4110	4117	rBV5	1418	1891	0.00%	0.000%
90	14.722	4150	4162	4182	rBV	348152	584346	0.23%	0.056%
91	14.835	4190	4197	4205	rBV4	19151	29287	0.01%	0.003%
92	15.041	4252	4261	4271	rBV4	21115	36218	0.01%	0.003%
93	15.201	4305	4311	4312	rBV4	2080	2058	0.00%	0.000%
94	15.285	4333	4337	4341	rBV5	888	789	0.00%	0.000%
95	15.349	4354	4357	4358	rBV2	2028	1075	0.00%	0.000%
96	15.410	4359	4376	4392	rVB	320885	580314	0.22%	0.056%
97	15.597	4429	4434	4438	rBV6	1586	1583	0.00%	0.000%
98	15.635	4444	4446	4448	rBV2	761	468	0.00%	0.000%
99	15.722	4471	4473	4480	rBV3	754	878	0.00%	0.000%
100	15.992	4541	4557	4572	rBV	633561	1008940	0.39%	0.097%

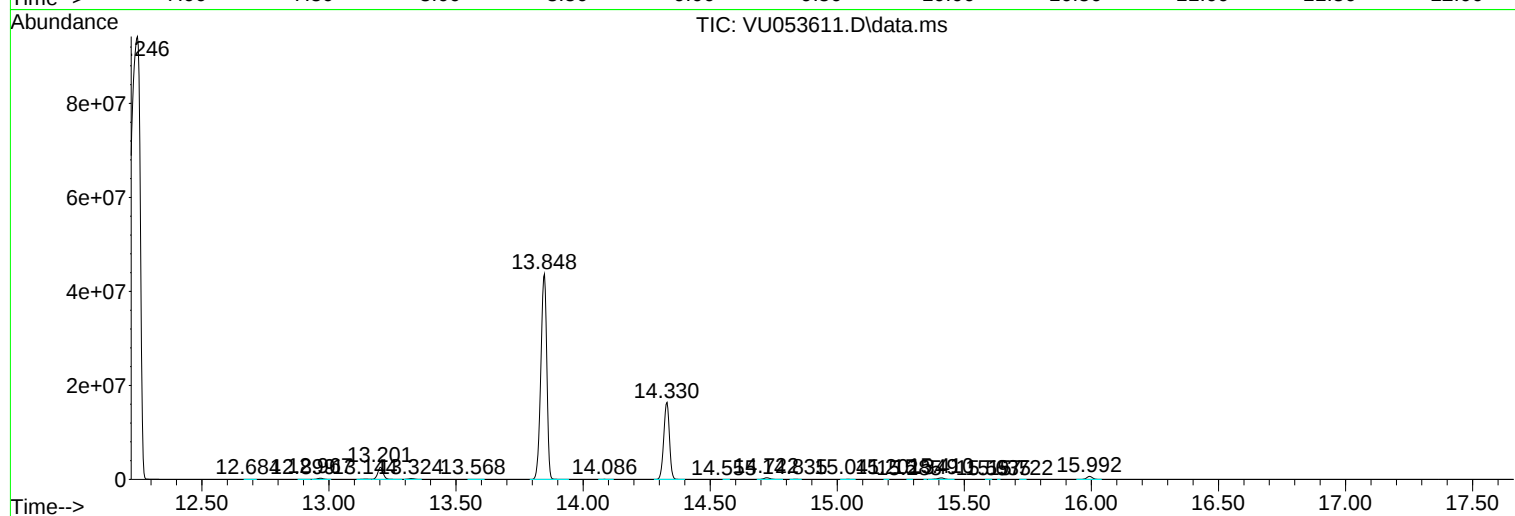
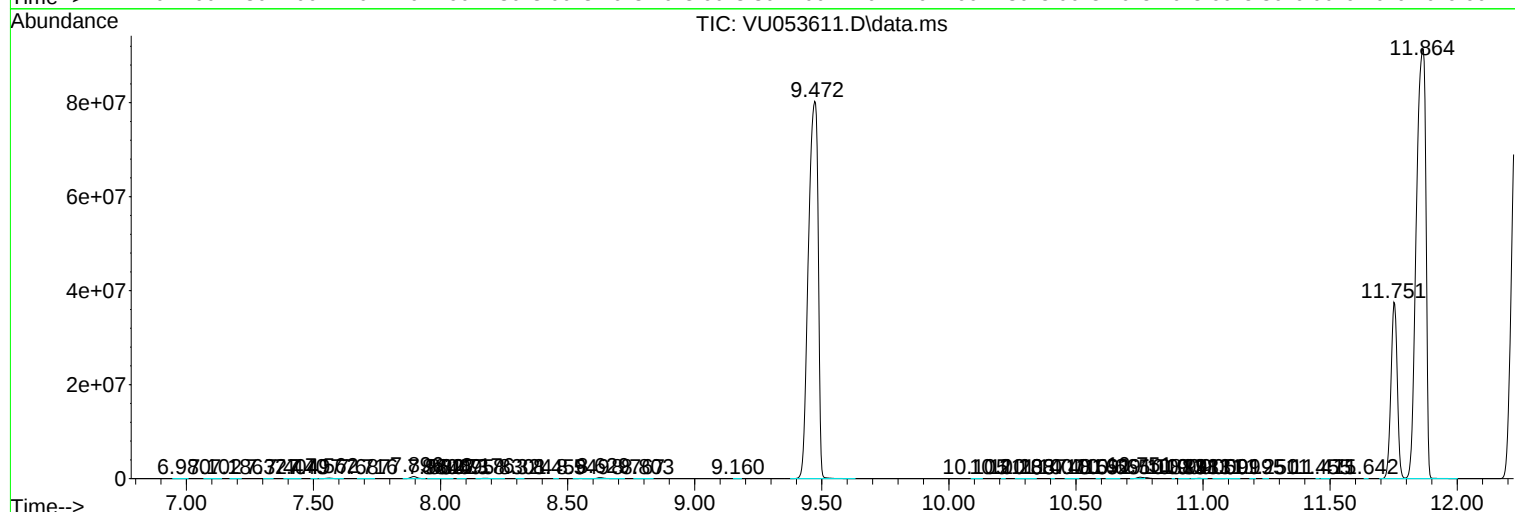
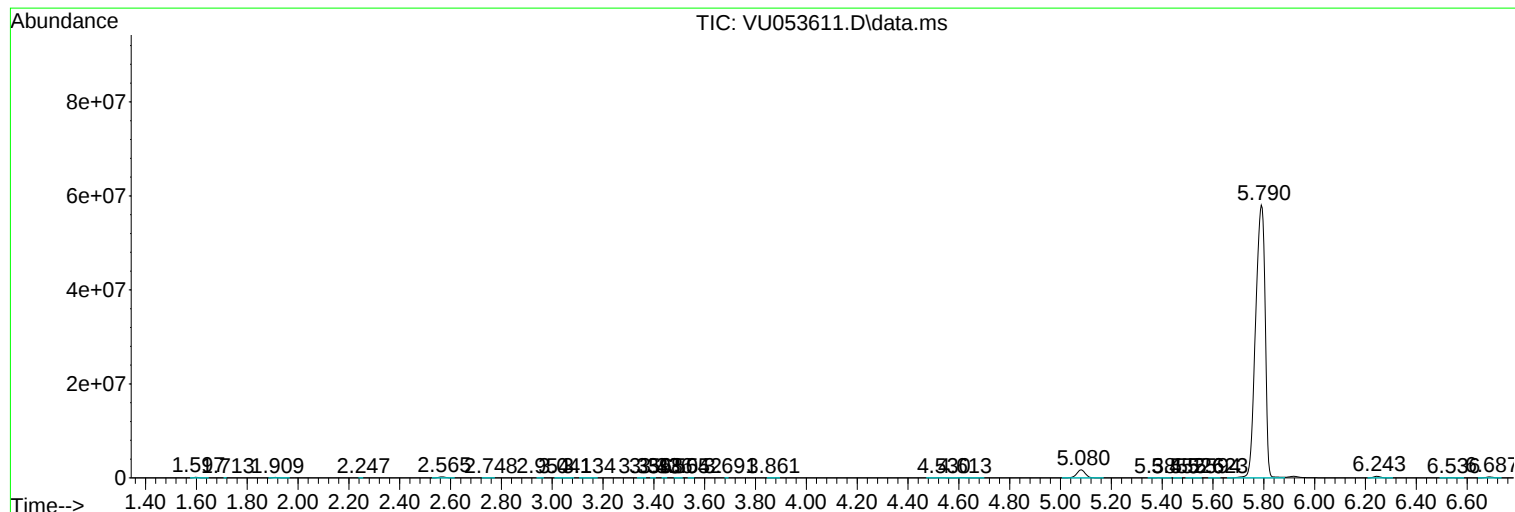
Sum of corrected areas: 1039898583

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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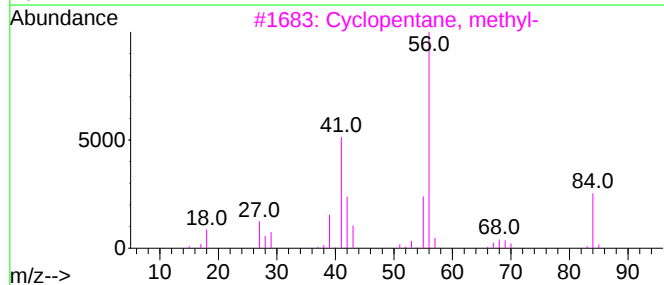
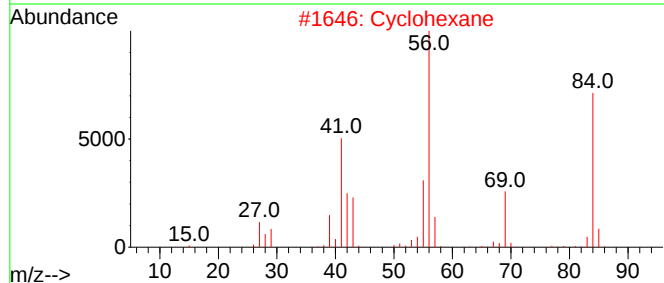
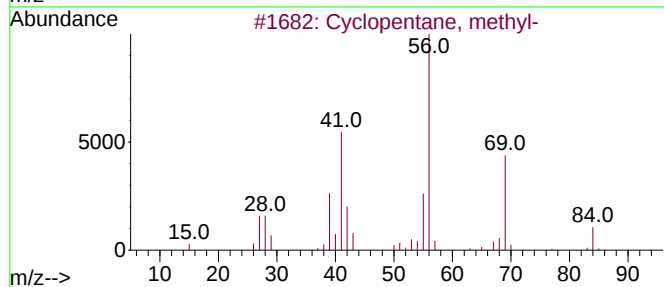
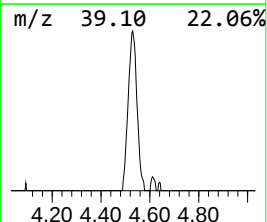
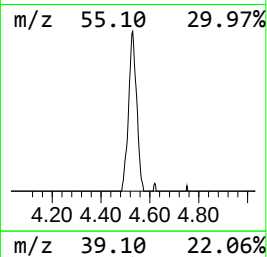
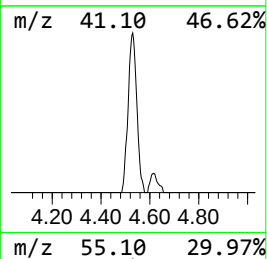
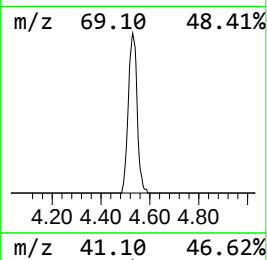
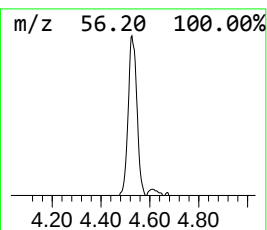
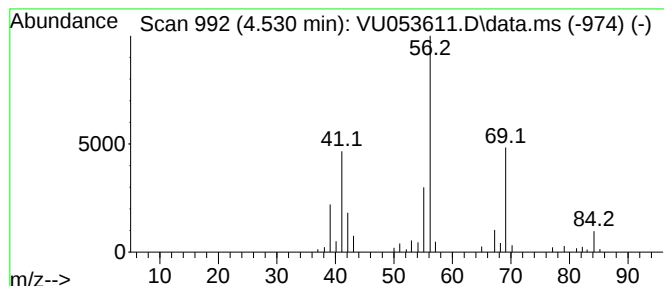
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.530 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.530	7.14 ug/L	87338	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclohexane	84	C6H12	000110-82-7	78
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	4.530	7.1	ug/L	87338	1	6.243	611781	50.0