

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035199.D
 Acq On : 20 Apr 2023 03:02
 Operator : JC/MD
 Sample : 02378-17
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMLO

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035199.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	33	rBV2	2554	3531	0.00%	0.001%
2	1.367	42	46	57	rVB	171844	189070	0.12%	0.037%
3	1.502	64	68	75	rVB	5304	7485	0.00%	0.001%
4	1.672	91	96	107	rBV	132554	174989	0.11%	0.034%
5	2.038	155	156	157	rBV	1035	436	0.00%	0.000%
6	2.306	194	200	210	rVV	331572	526677	0.34%	0.104%
7	2.386	210	213	221	rVV2	3287	7184	0.00%	0.001%
8	2.514	230	234	238	rBB2	885	1061	0.00%	0.000%
9	2.788	272	279	283	rVV7	2093	4912	0.00%	0.001%
10	2.867	283	292	296	rVV2	11779	26629	0.02%	0.005%
11	2.940	296	304	320	rVV	137902	324140	0.21%	0.064%
12	3.099	323	330	337	rVV5	2007	4605	0.00%	0.001%
13	3.343	369	370	374	rVB3	382	398	0.00%	0.000%
14	3.446	381	387	392	rVB5	1914	3525	0.00%	0.001%
15	3.891	457	460	463	rBV3	253	390	0.00%	0.000%
16	4.196	506	510	511	rBV3	317	402	0.00%	0.000%
17	4.306	517	528	544	rVB	43014	124336	0.08%	0.024%
18	4.464	544	554	563	rBV	107872	330670	0.21%	0.065%
19	4.568	564	571	595	rVB	79678	297042	0.19%	0.058%
20	4.861	617	619	620	rVB2	790	524	0.00%	0.000%
21	4.891	620	624	626	rBV3	469	762	0.00%	0.000%
22	5.074	638	654	677	rBV3	291656	1267979	0.81%	0.250%
23	5.300	688	691	692	rBV2	597	376	0.00%	0.000%
24	5.318	692	694	696	rVB3	491	412	0.00%	0.000%
25	5.379	702	704	706	rVV3	577	523	0.00%	0.000%
26	5.397	706	707	709	rVV2	712	575	0.00%	0.000%
27	5.470	709	719	730	rVV4	16751	54171	0.03%	0.011%
28	5.556	732	733	740	rVB3	1604	2554	0.00%	0.001%
29	5.678	740	753	767	rBV	109807	324146	0.21%	0.064%
30	5.818	773	776	777	rBV2	995	775	0.00%	0.000%
31	5.836	777	779	782	rVV3	956	1202	0.00%	0.000%
32	6.056	789	815	845	rBV	21550911	65387414	41.96%	12.874%
33	6.458	879	881	886	rVB5	1095	1581	0.00%	0.000%
34	6.598	902	904	905	rBV2	522	356	0.00%	0.000%
35	6.763	921	931	949	rBV	457519	1089560	0.70%	0.215%
36	6.964	962	964	967	rBV3	513	483	0.00%	0.000%

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 Title : VOC Analysis

37	7.129	983	991	998	rVB9	3905	10200	0.01%	0.002%
38	7.305	1010	1020	1030	rBV	332415	744435	0.48%	0.147%
39	7.476	1045	1048	1057	rBV8	875	1891	0.00%	0.000%
40	7.659	1073	1078	1084	rVB6	2122	3930	0.00%	0.001%
41	7.744	1091	1092	1095	rBV2	516	367	0.00%	0.000%
42	7.830	1100	1106	1111	rBV4	2203	4444	0.00%	0.001%
43	7.903	1115	1118	1121	rBV3	371	490	0.00%	0.000%
44	7.946	1121	1125	1130	rBV4	1611	3363	0.00%	0.001%
45	8.116	1148	1153	1157	rVB4	1635	2923	0.00%	0.001%
46	8.324	1180	1187	1199	rBV	208762	339007	0.22%	0.067%
47	8.494	1212	1215	1224	rVB6	1072	2830	0.00%	0.001%
48	8.580	1225	1229	1233	rVB4	523	957	0.00%	0.000%
49	8.647	1234	1240	1248	rBV	805926	1312677	0.84%	0.258%
50	8.720	1248	1252	1259	rVB	15163	26819	0.02%	0.005%
51	8.872	1274	1277	1280	rBV2	275	435	0.00%	0.000%
52	8.951	1284	1290	1302	rBV	145477	220070	0.14%	0.043%
53	9.275	1337	1343	1351	rVB2	14442	23045	0.01%	0.005%
54	9.348	1351	1355	1356	rBV3	482	503	0.00%	0.000%
55	9.390	1356	1362	1376	rBV	483260	735480	0.47%	0.145%
56	9.628	1400	1401	1405	rVB3	553	416	0.00%	0.000%
57	9.701	1411	1413	1415	rVB3	544	428	0.00%	0.000%
58	9.951	1452	1454	1457	rVB3	283	349	0.00%	0.000%
59	10.110	1466	1480	1486	rBV2	55631846	155815733	100.00%	30.677%
60	10.762	1585	1587	1590	rBV3	680	643	0.00%	0.000%
61	11.195	1652	1658	1670	rVB	622216	822538	0.53%	0.162%
62	11.317	1675	1678	1682	rVB4	1423	1666	0.00%	0.000%
63	11.366	1682	1686	1691	rVB	23949	31373	0.02%	0.006%
64	11.421	1693	1695	1697	rVV3	1059	724	0.00%	0.000%
65	11.457	1697	1701	1709	rVB	11596	15363	0.01%	0.003%
66	11.670	1734	1736	1737	rBV2	446	395	0.00%	0.000%
67	11.719	1740	1744	1748	rVV5	1572	2276	0.00%	0.000%
68	11.762	1748	1751	1756	rVB6	808	1308	0.00%	0.000%
69	11.823	1758	1761	1764	rBV4	610	838	0.00%	0.000%
70	11.878	1769	1770	1773	rVB2	404	350	0.00%	0.000%
71	11.969	1780	1785	1791	rBV	11234262	15241375	9.78%	3.001%
72	12.061	1791	1800	1804	rVV	51986955	93345799	59.91%	18.378%
73	12.353	1838	1848	1853	rBV	50594130	89650895	57.54%	17.651%
74	12.707	1902	1906	1911	rVB2	11110	15419	0.01%	0.003%
75	12.878	1929	1934	1936	rBV3	15523	20864	0.01%	0.004%
76	12.920	1936	1941	1953	rVB	652793	790016	0.51%	0.156%

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 Title : VOC Analysis

77	13.060	1957	1964	1969	rBV	247626	479690	0.31%	0.094%
78	13.109	1969	1972	1979	rVV2	117060	167843	0.11%	0.033%
79	13.195	1981	1986	1995	rVB	318098	403939	0.26%	0.080%
80	13.384	2012	2017	2025	rVB	54616	73309	0.05%	0.014%
81	13.597	2045	2052	2057	rBV	40030679	56861811	36.49%	11.195%
82	13.780	2078	2082	2086	rVB	13894	16960	0.01%	0.003%
83	13.963	2106	2112	2129	rBV	13639173	17289414	11.10%	3.404%
84	14.207	2150	2152	2155	rVB4	2499	2594	0.00%	0.001%
85	14.261	2157	2161	2166	rVB2	13256	16101	0.01%	0.003%
86	14.377	2175	2180	2188	rVB3	15168	30320	0.02%	0.006%
87	14.475	2193	2196	2197	rBV3	1097	924	0.00%	0.000%
88	14.505	2199	2201	2203	rVV3	2247	2150	0.00%	0.000%
89	14.542	2203	2207	2211	rVV4	10913	14814	0.01%	0.003%
90	14.585	2211	2214	2217	rVV5	4346	5799	0.00%	0.001%
91	14.621	2217	2220	2227	rVB3	15866	22161	0.01%	0.004%
92	14.780	2235	2246	2253	rBV	569424	828813	0.53%	0.163%
93	14.920	2266	2269	2275	rVB5	6169	8057	0.01%	0.002%
94	15.145	2304	2306	2309	rBV4	607	598	0.00%	0.000%
95	15.249	2317	2323	2334	rBV	1680580	2293736	1.47%	0.452%
96	15.469	2357	2359	2363	rVB5	774	939	0.00%	0.000%
97	15.505	2363	2365	2367	rBV2	645	787	0.00%	0.000%
98	15.706	2396	2398	2400	rBV3	678	568	0.00%	0.000%
99	15.834	2417	2419	2421	rBV2	595	607	0.00%	0.000%
100	16.511	2524	2530	2537	rBV3	23196	42184	0.03%	0.008%

Sum of corrected areas: 507917627

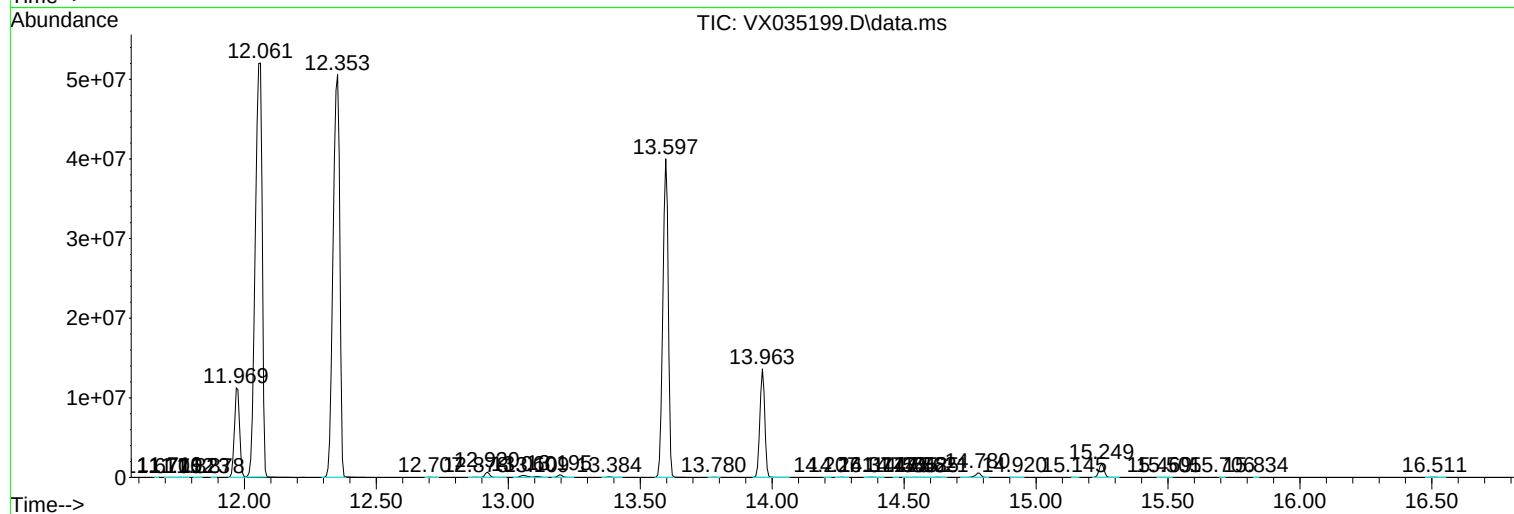
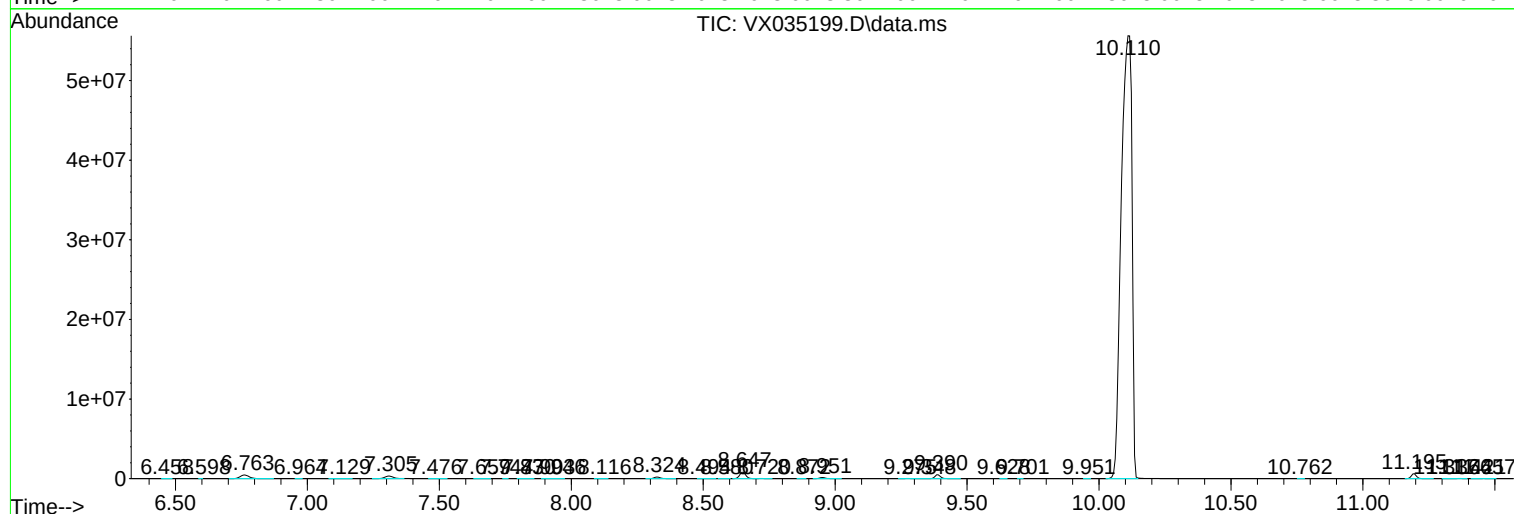
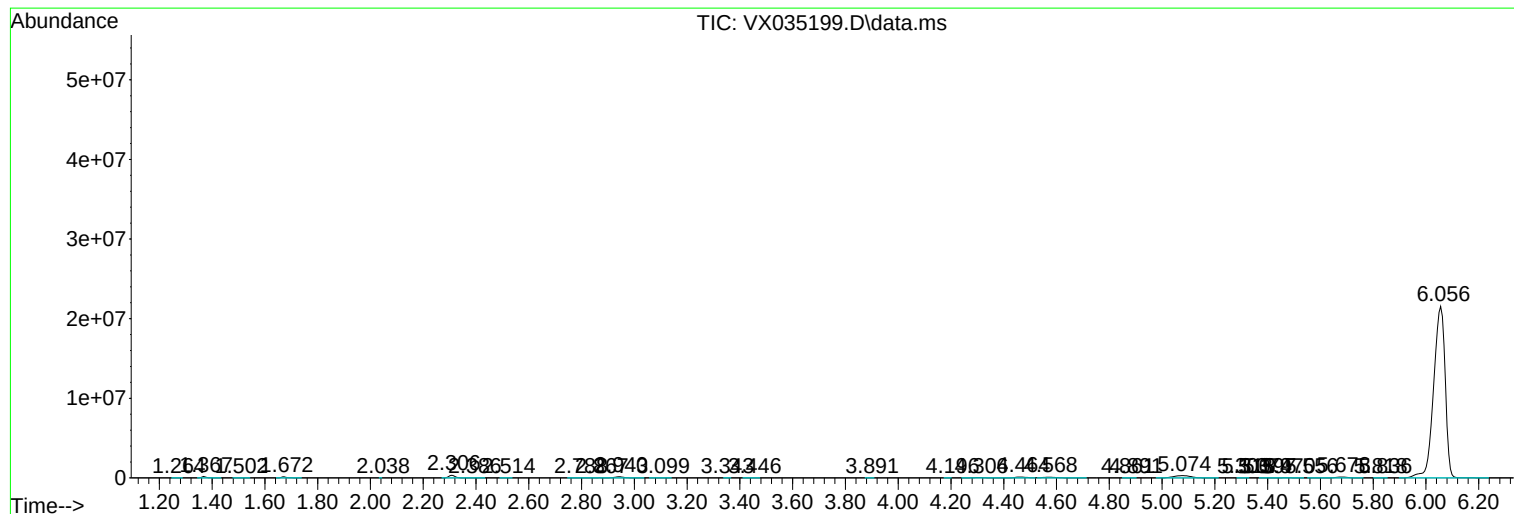
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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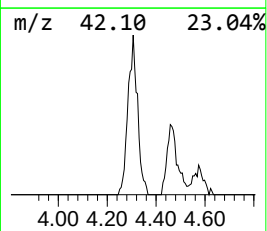
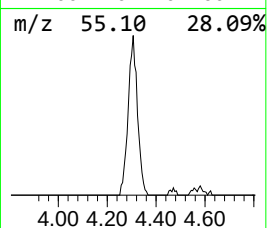
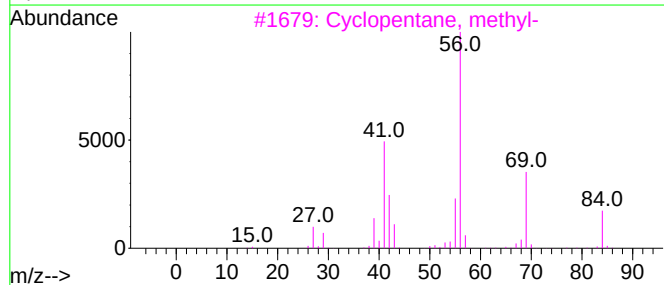
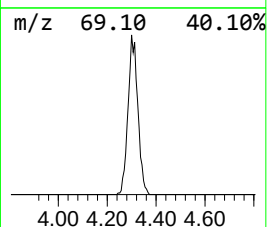
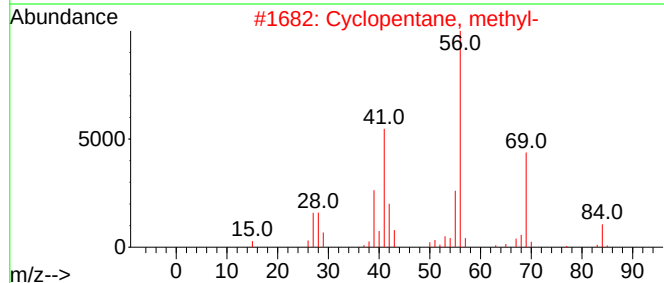
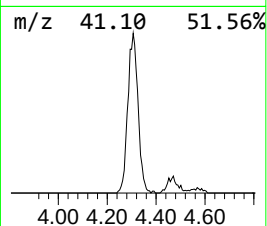
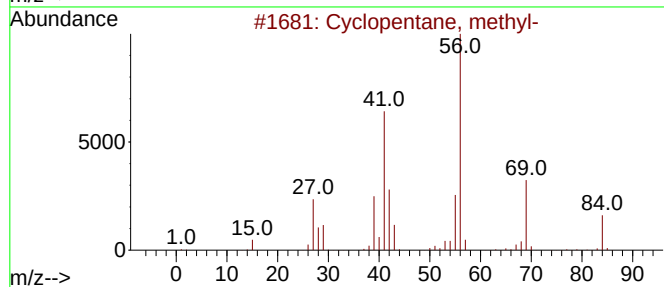
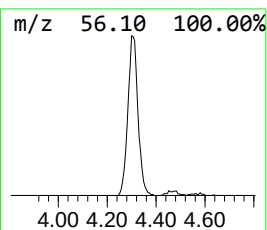
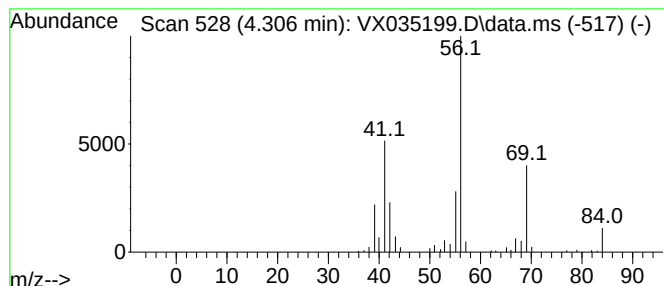
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.306 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.71 ug/L	124336	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	83
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	4.306	5.7	ug/L	124336	1	6.763	1089560	50.0