

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039391.D
 Acq On : 20 Dec 2023 10:54
 Operator : JC/MD
 Sample : 05807-12 5X
 Misc : 1.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ4

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	23	25	32	rBV3	2368	4483	0.69%	0.086%
2	1.368	43	46	55	rBV	52494	61762	9.50%	1.189%
3	1.648	89	92	104	rVB	43546	66141	10.17%	1.273%
4	2.300	193	199	209	rBV	96635	155764	23.95%	2.999%
5	2.562	240	242	245	rVB2	649	618	0.10%	0.012%
6	2.697	259	264	273	rVV4	1384	2988	0.46%	0.058%
7	2.788	275	279	284	rVV3	2370	4373	0.67%	0.084%
8	2.861	284	291	297	rVV	12217	22440	3.45%	0.432%
9	2.940	298	304	316	rVB	12559	30707	4.72%	0.591%
10	3.093	326	329	331	rBV2	268	300	0.05%	0.006%
11	3.562	404	406	408	rBV2	177	181	0.03%	0.003%
12	3.599	408	412	415	rVB2	211	240	0.04%	0.005%
13	3.715	430	431	435	rVB2	233	179	0.03%	0.003%
14	3.824	447	449	451	rVV	272	173	0.03%	0.003%
15	4.001	476	478	481	rBV2	188	211	0.03%	0.004%
16	4.087	488	492	493	rVB2	172	187	0.03%	0.004%
17	4.129	496	499	502	rVB2	196	233	0.04%	0.004%
18	4.452	543	552	568	rBV	62218	185195	28.47%	3.565%
19	4.958	632	635	636	rBV2	333	277	0.04%	0.005%
20	5.050	638	650	671	rBV2	81459	258229	39.70%	4.971%
21	5.318	692	694	699	rVB	191	238	0.04%	0.005%
22	5.464	714	718	720	rBV	245	288	0.04%	0.006%
23	5.550	727	732	733	rBV3	413	587	0.09%	0.011%
24	5.586	736	738	741	rVB	303	300	0.05%	0.006%
25	5.623	743	744	746	rBV	277	194	0.03%	0.004%
26	5.964	789	800	809	rBV2	212765	650395	100.00%	12.521%
27	6.287	851	853	854	rVV2	264	197	0.03%	0.004%
28	6.306	854	856	859	rVB	263	205	0.03%	0.004%
29	6.361	861	865	869	rBV2	279	537	0.08%	0.010%
30	6.489	884	886	889	rVB2	257	209	0.03%	0.004%
31	6.665	912	915	919	rVB2	188	269	0.04%	0.005%
32	6.757	922	930	953	rVB	173210	423423	65.10%	8.151%
33	6.915	953	956	959	rVB2	417	448	0.07%	0.009%
34	7.025	972	974	977	rVB2	236	217	0.03%	0.004%
35	7.116	982	989	994	rVB4	1308	2509	0.39%	0.048%
36	7.305	1011	1020	1039	rBV2	136781	302627	46.53%	5.826%

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 Title : VOC Analysis

37	7.433	1039	1041	1044	rVB4	297	363	0.06%	0.007%
38	7.482	1047	1049	1050	rBV	442	231	0.04%	0.004%
39	7.665	1078	1079	1083	rVB2	241	268	0.04%	0.005%
40	7.903	1117	1118	1121	rBV2	262	301	0.05%	0.006%
41	7.970	1127	1129	1133	rBV	256	241	0.04%	0.005%
42	8.025	1136	1138	1140	rVB	240	206	0.03%	0.004%
43	8.196	1164	1166	1169	rVB2	155	177	0.03%	0.003%
44	8.263	1174	1177	1181	rVB2	218	295	0.05%	0.006%
45	8.324	1181	1187	1202	rBV	83702	142873	21.97%	2.750%
46	8.543	1220	1223	1224	rBV2	185	198	0.03%	0.004%
47	8.580	1226	1229	1232	rBV2	426	533	0.08%	0.010%
48	8.647	1234	1240	1251	rBV	273532	432588	66.51%	8.328%
49	8.817	1266	1268	1273	rVB3	315	355	0.05%	0.007%
50	8.952	1284	1290	1299	rBV	59935	93565	14.39%	1.801%
51	9.104	1312	1315	1320	rVB2	265	387	0.06%	0.007%
52	9.269	1339	1342	1347	rBV3	799	1343	0.21%	0.026%
53	9.384	1356	1361	1378	rBV	311311	450095	69.20%	8.665%
54	9.640	1398	1403	1405	rBV3	334	470	0.07%	0.009%
55	9.701	1411	1413	1418	rBV4	988	1509	0.23%	0.029%
56	9.823	1431	1433	1436	rVV2	251	178	0.03%	0.003%
57	9.915	1445	1448	1450	rBV	214	235	0.04%	0.005%
58	10.055	1465	1471	1472	rBV	393719	510330	78.46%	9.824%
59	10.232	1499	1500	1501	rBV	338	189	0.03%	0.004%
60	10.311	1510	1513	1518	rVB4	401	507	0.08%	0.010%
61	10.646	1566	1568	1571	rBV3	247	369	0.06%	0.007%
62	10.829	1597	1598	1602	rBV	247	244	0.04%	0.005%
63	10.921	1610	1613	1615	rVV	167	173	0.03%	0.003%
64	10.963	1618	1620	1624	rBV3	374	518	0.08%	0.010%
65	11.037	1630	1632	1635	rBV2	172	253	0.04%	0.005%
66	11.091	1639	1641	1643	rBV	285	333	0.05%	0.006%
67	11.189	1651	1657	1668	rBV	270529	359152	55.22%	6.914%
68	11.311	1675	1677	1680	rVB	402	384	0.06%	0.007%
69	11.451	1696	1700	1701	rBV2	317	264	0.04%	0.005%
70	11.603	1722	1725	1728	rVB2	180	234	0.04%	0.005%
71	11.975	1781	1786	1788	rBV2	2953	3773	0.58%	0.073%
72	12.024	1788	1794	1803	rVV	407825	579344	89.08%	11.153%
73	12.219	1823	1826	1829	rVB2	272	321	0.05%	0.006%
74	12.250	1829	1831	1832	rBV	214	193	0.03%	0.004%
75	12.317	1837	1842	1851	rBV	324177	420392	64.64%	8.093%
76	12.506	1872	1873	1877	rVB2	183	174	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	12.561	1880	1882	1887	rBV2	206	298	0.05%	0.006%
78	12.652	1894	1897	1899	rBV2	166	177	0.03%	0.003%
79	12.762	1912	1915	1919	rVB2	2493	3120	0.48%	0.060%
80	12.920	1939	1941	1943	rBV2	187	234	0.04%	0.005%
81	13.115	1971	1973	1975	rVB	255	238	0.04%	0.005%
82	13.140	1975	1977	1978	rBV	186	180	0.03%	0.003%
83	13.518	2035	2039	2040	rBV2	217	304	0.05%	0.006%
84	13.597	2048	2052	2056	rVV2	735	814	0.13%	0.016%
85	13.664	2061	2063	2065	rBV	490	282	0.04%	0.005%
86	13.786	2081	2083	2085	rBV	327	329	0.05%	0.006%
87	14.030	2121	2123	2125	rVV2	322	257	0.04%	0.005%
88	14.134	2134	2140	2147	rVB2	3175	4778	0.73%	0.092%
89	14.444	2189	2191	2193	rVB	310	191	0.03%	0.004%
90	14.505	2198	2201	2202	rBV2	218	254	0.04%	0.005%
91	14.524	2202	2204	2208	rVB2	246	275	0.04%	0.005%
92	14.597	2212	2216	2217	rBV2	161	179	0.03%	0.003%
93	14.664	2225	2227	2228	rVB2	291	210	0.03%	0.004%
94	14.694	2228	2232	2234	rBV2	160	281	0.04%	0.005%
95	14.761	2240	2243	2244	rBV	180	175	0.03%	0.003%
96	15.011	2281	2284	2285	rBV2	218	204	0.03%	0.004%
97	15.664	2390	2391	2395	rBV3	265	284	0.04%	0.005%
98	16.133	2467	2468	2470	rBV2	230	203	0.03%	0.004%
99	16.261	2488	2489	2491	rBV	210	189	0.03%	0.004%
100	16.462	2520	2522	2525	rBV3	293	267	0.04%	0.005%

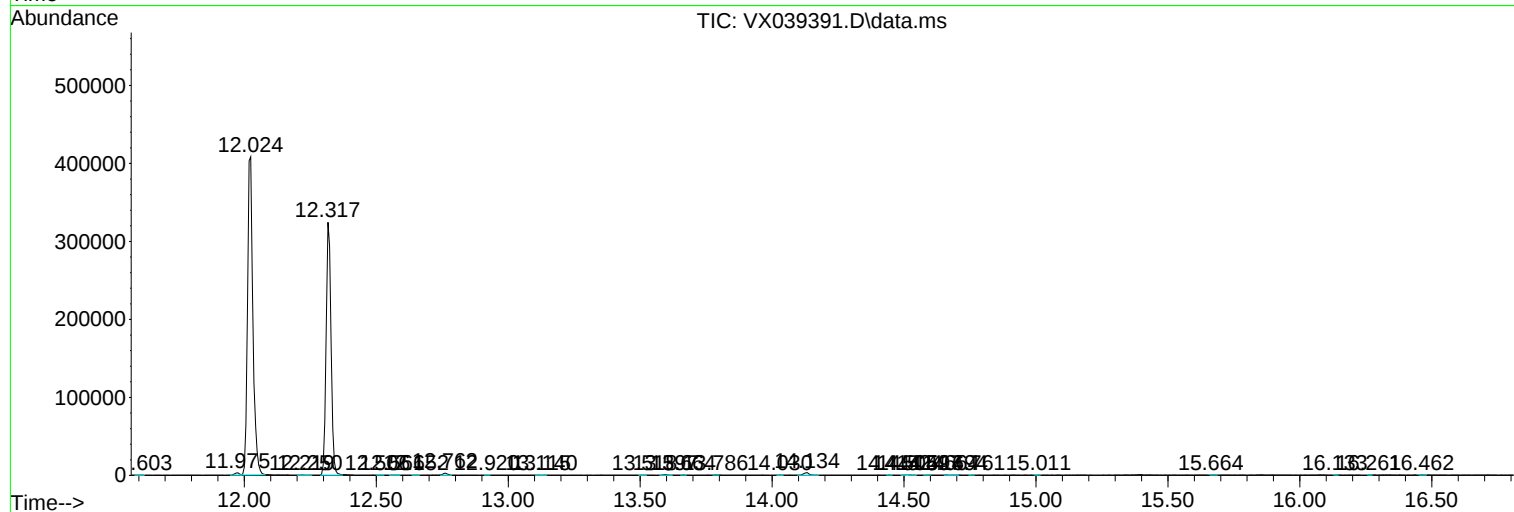
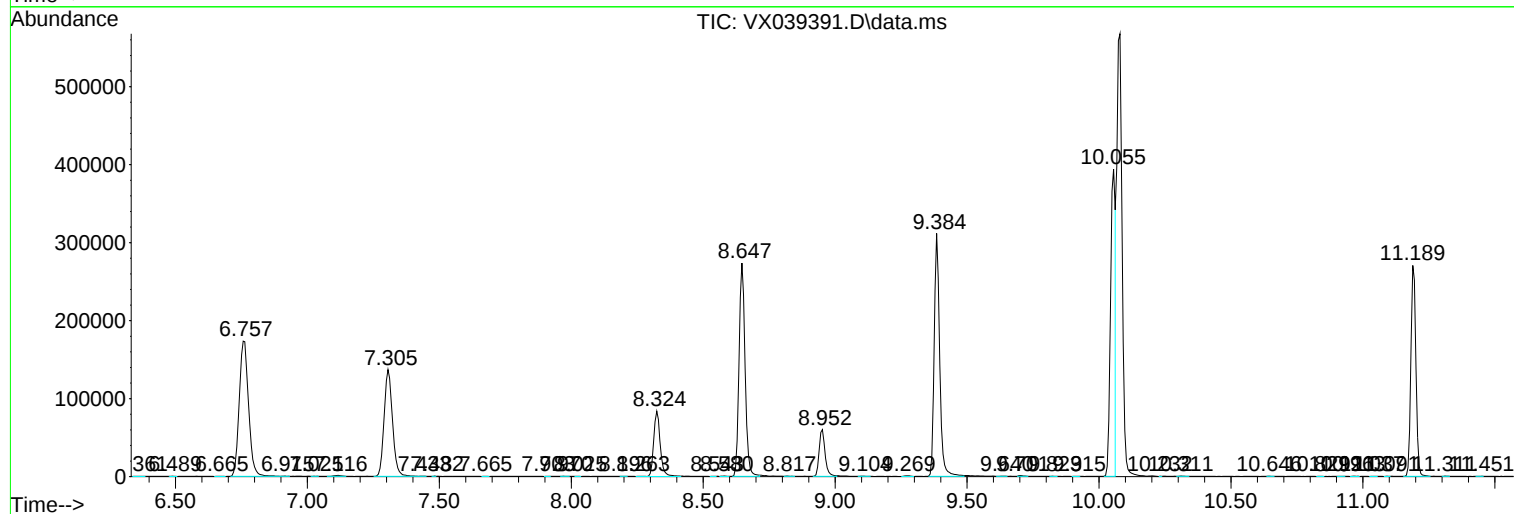
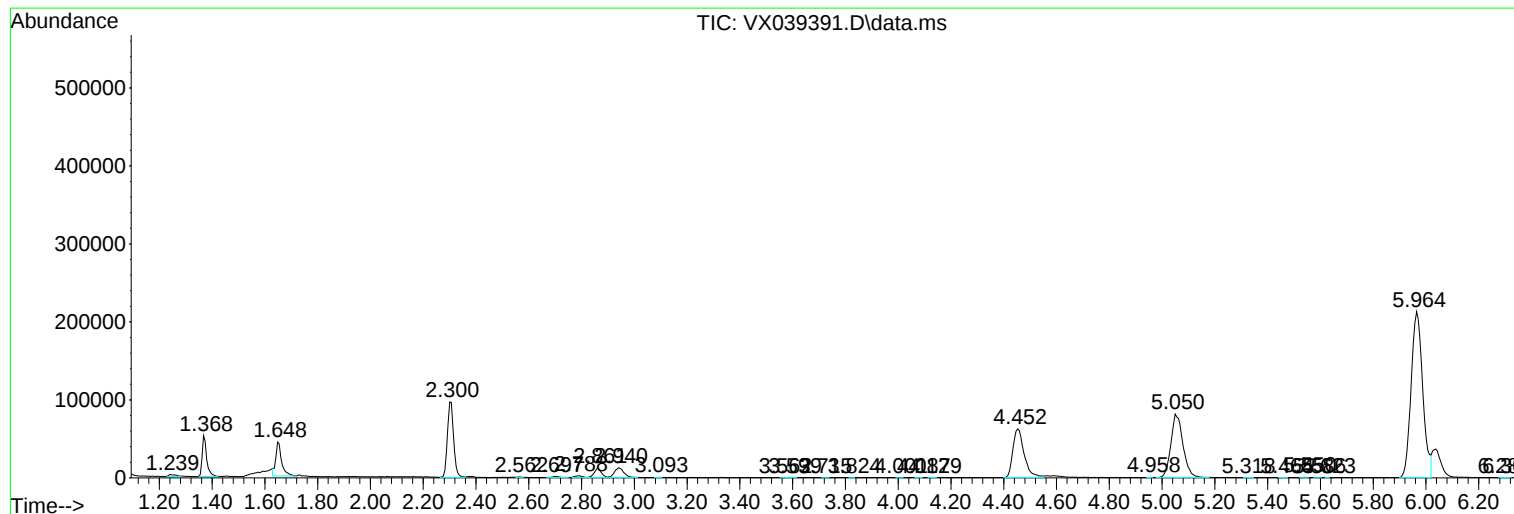
Sum of corrected areas: 5194605

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



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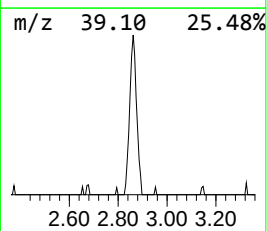
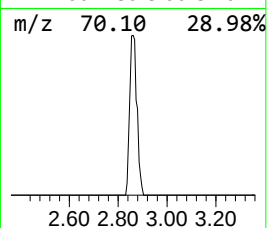
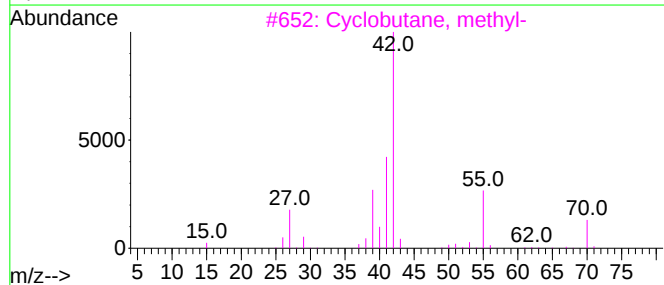
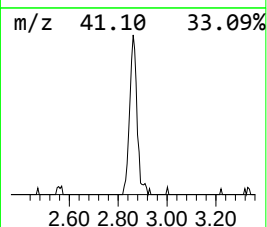
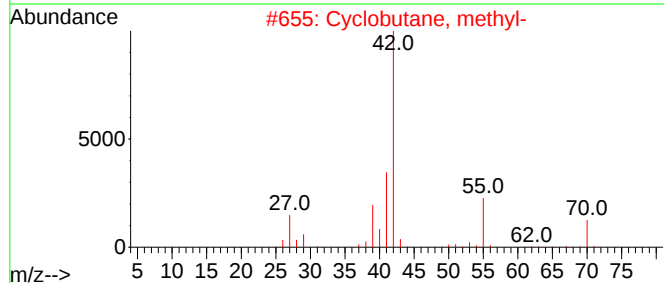
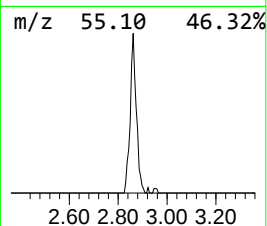
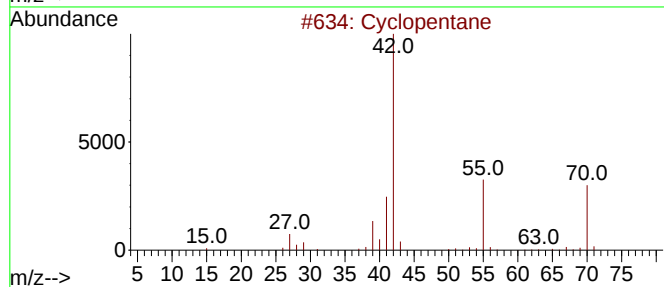
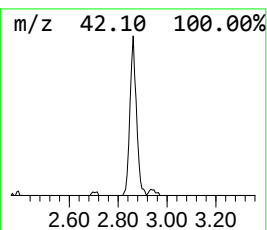
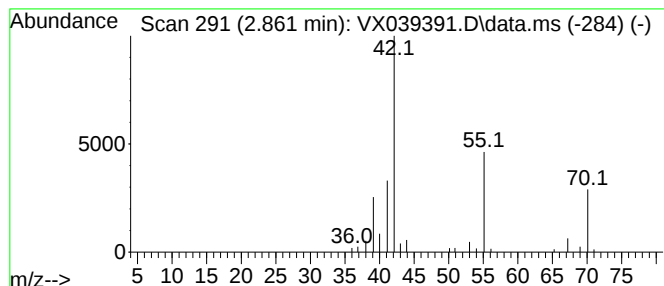
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic2.861 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.861	2.65 ug/L	22440	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	78
4			Cyclopentane	70	C5H10	000287-92-3	64
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.861	2.6	ug/L	22440	1	6.763	423423	50.0