

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030622.D
 Acq On : 15 Aug 2022 12:51
 Operator : JC/MD
 Sample : N4168-14
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9C1

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030622.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	13	rVB	6059	5942	0.49%	0.068%
2	1.368	42	46	56	rVB	99389	152120	12.47%	1.734%
3	1.612	83	86	87	rBV2	2741	3080	0.25%	0.035%
4	1.672	91	96	105	rVV	57348	111325	9.13%	1.269%
5	2.270	188	194	211	rVB	243547	404576	33.16%	4.613%
6	2.666	257	259	261	rVB2	688	595	0.05%	0.007%
7	2.703	263	265	268	rBV	562	866	0.07%	0.010%
8	2.837	281	287	297	rVB	19137	39361	3.23%	0.449%
9	2.947	297	305	318	rBV2	9881	28148	2.31%	0.321%
10	3.197	344	346	348	rBV2	587	526	0.04%	0.006%
11	3.355	370	372	374	rBV	819	649	0.05%	0.007%
12	3.410	378	381	382	rBV3	831	1033	0.08%	0.012%
13	3.727	431	433	438	rVB2	394	554	0.05%	0.006%
14	3.788	442	443	448	rBV3	650	924	0.08%	0.011%
15	3.831	448	450	453	rBV2	420	486	0.04%	0.006%
16	3.989	474	476	482	rBV2	510	787	0.06%	0.009%
17	4.288	523	525	527	rVB2	525	453	0.04%	0.005%
18	4.519	551	563	590	rBV2	42562	229650	18.82%	2.618%
19	4.922	628	629	631	rVB2	787	464	0.04%	0.005%
20	4.940	631	632	634	rBV	562	564	0.05%	0.006%
21	5.056	640	651	668	rVB	156766	486249	39.86%	5.544%
22	5.550	725	732	742	rVV3	1688	4118	0.34%	0.047%
23	5.964	787	800	817	rBV2	438369	1219951	100.00%	13.909%
24	6.355	862	864	865	rBV	765	516	0.04%	0.006%
25	6.379	865	868	869	rBV2	925	1052	0.09%	0.012%
26	6.763	921	931	948	rBV	294894	716528	58.73%	8.170%
27	7.111	979	988	998	rBV5	7971	19878	1.63%	0.227%
28	7.226	998	1007	1012	rBV2	3026	7489	0.61%	0.085%
29	7.312	1012	1021	1034	rVB	248524	547067	44.84%	6.237%
30	7.470	1045	1047	1048	rBV	1008	619	0.05%	0.007%
31	7.488	1048	1050	1054	rVV2	694	983	0.08%	0.011%
32	7.702	1082	1085	1089	rVB3	486	698	0.06%	0.008%
33	7.751	1089	1093	1096	rBV3	489	645	0.05%	0.007%
34	7.964	1121	1128	1138	rVB7	2373	6445	0.53%	0.073%
35	8.031	1138	1139	1141	rBV	589	520	0.04%	0.006%
36	8.055	1141	1143	1145	rVB2	653	657	0.05%	0.007%

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 Title : VOC Analysis

37	8.129	1153	1155	1157	rBV2	874	918	0.08%	0.010%
38	8.147	1157	1158	1167	rVB3	1614	3029	0.25%	0.035%
39	8.324	1181	1187	1197	rBV	158721	270919	22.21%	3.089%
40	8.647	1233	1240	1250	rBV	599494	967345	79.29%	11.029%
41	8.866	1273	1276	1279	rBV2	1070	1684	0.14%	0.019%
42	8.915	1279	1284	1285	rVV4	3055	4856	0.40%	0.055%
43	8.952	1285	1290	1301	rVB	116400	176747	14.49%	2.015%
44	9.116	1315	1317	1322	rBV4	651	1004	0.08%	0.011%
45	9.232	1334	1336	1341	rBV3	399	596	0.05%	0.007%
46	9.281	1341	1344	1345	rBV2	735	599	0.05%	0.007%
47	9.403	1357	1364	1380	rBV	171363	498485	40.86%	5.683%
48	9.732	1416	1418	1423	rVB2	1672	1679	0.14%	0.019%
49	9.860	1435	1439	1442	rBV5	1679	2206	0.18%	0.025%
50	10.055	1465	1471	1483	rBV	577830	808224	66.25%	9.215%
51	10.195	1491	1494	1498	rBV4	746	1023	0.08%	0.012%
52	10.305	1507	1512	1515	rBV5	1232	2181	0.18%	0.025%
53	10.640	1566	1567	1572	rVV3	757	1134	0.09%	0.013%
54	10.835	1598	1599	1604	rVB2	568	582	0.05%	0.007%
55	10.951	1612	1618	1623	rVB5	2255	3473	0.28%	0.040%
56	11.201	1653	1659	1666	rBV	329450	469128	38.45%	5.349%
57	11.317	1674	1678	1683	rVB5	2751	3866	0.32%	0.044%
58	11.360	1683	1685	1687	rVB2	573	422	0.03%	0.005%
59	11.396	1687	1691	1693	rBV2	586	942	0.08%	0.011%
60	11.415	1693	1694	1697	rBV	473	441	0.04%	0.005%
61	11.482	1701	1705	1710	rBV2	4676	7203	0.59%	0.082%
62	11.756	1748	1750	1757	rVB4	839	1286	0.11%	0.015%
63	11.884	1764	1771	1773	rBV3	1051	1631	0.13%	0.019%
64	11.933	1775	1779	1780	rBV2	553	598	0.05%	0.007%
65	12.024	1789	1794	1806	rBV	552224	734096	60.17%	8.370%
66	12.232	1824	1828	1831	rBV3	2147	3402	0.28%	0.039%
67	12.323	1838	1843	1853	rBV	597576	729011	59.76%	8.312%
68	12.512	1872	1874	1877	rBV4	853	691	0.06%	0.008%
69	12.585	1882	1886	1888	rBV5	1103	1736	0.14%	0.020%
70	12.762	1907	1915	1920	rVV	6228	10662	0.87%	0.122%
71	12.859	1929	1931	1935	rVB2	1155	1250	0.10%	0.014%
72	12.939	1943	1944	1948	rVB3	592	482	0.04%	0.005%
73	13.103	1966	1971	1976	rBV	9754	13191	1.08%	0.150%
74	13.164	1979	1981	1983	rBV2	419	443	0.04%	0.005%
75	13.244	1991	1994	1995	rBV3	845	749	0.06%	0.009%
76	13.268	1995	1998	2004	rVV3	2172	3094	0.25%	0.035%

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 Title : VOC Analysis

77	13.323	2004	2007	2008	rVB2	691	601	0.05%	0.007%
78	13.451	2026	2028	2031	rVB3	527	588	0.05%	0.007%
79	13.487	2031	2034	2036	rBV2	843	1011	0.08%	0.012%
80	13.719	2070	2072	2075	rBV2	772	703	0.06%	0.008%
81	13.762	2075	2079	2080	rBV3	818	1061	0.09%	0.012%
82	13.798	2081	2085	2089	rVV4	3907	5338	0.44%	0.061%
83	13.890	2097	2100	2103	rBV2	454	645	0.05%	0.007%
84	13.926	2103	2106	2109	rBV3	1991	2606	0.21%	0.030%
85	13.987	2114	2116	2120	rBV2	644	1222	0.10%	0.014%
86	14.073	2127	2130	2131	rBV2	419	455	0.04%	0.005%
87	14.134	2136	2140	2147	rVB	6330	8959	0.73%	0.102%
88	14.262	2156	2161	2164	rBV3	2420	3456	0.28%	0.039%
89	14.323	2170	2171	2177	rBV5	1300	1872	0.15%	0.021%
90	14.378	2177	2180	2183	rBV4	1280	1509	0.12%	0.017%
91	14.627	2219	2221	2223	rVB3	579	488	0.04%	0.006%
92	14.755	2240	2242	2246	rBV3	1515	1527	0.13%	0.017%
93	14.920	2268	2269	2271	rBV	745	738	0.06%	0.008%
94	15.524	2365	2368	2372	rVB4	2184	2977	0.24%	0.034%
95	15.810	2413	2415	2417	rBV3	1121	1175	0.10%	0.013%
96	15.896	2425	2429	2433	rVB5	3352	4708	0.39%	0.054%
97	16.200	2478	2479	2482	rVB2	935	501	0.04%	0.006%
98	16.328	2499	2500	2504	rBV3	949	848	0.07%	0.010%
99	16.469	2521	2523	2524	rBV2	756	673	0.06%	0.008%
100	16.633	2549	2550	2552	rBV2	627	565	0.05%	0.006%

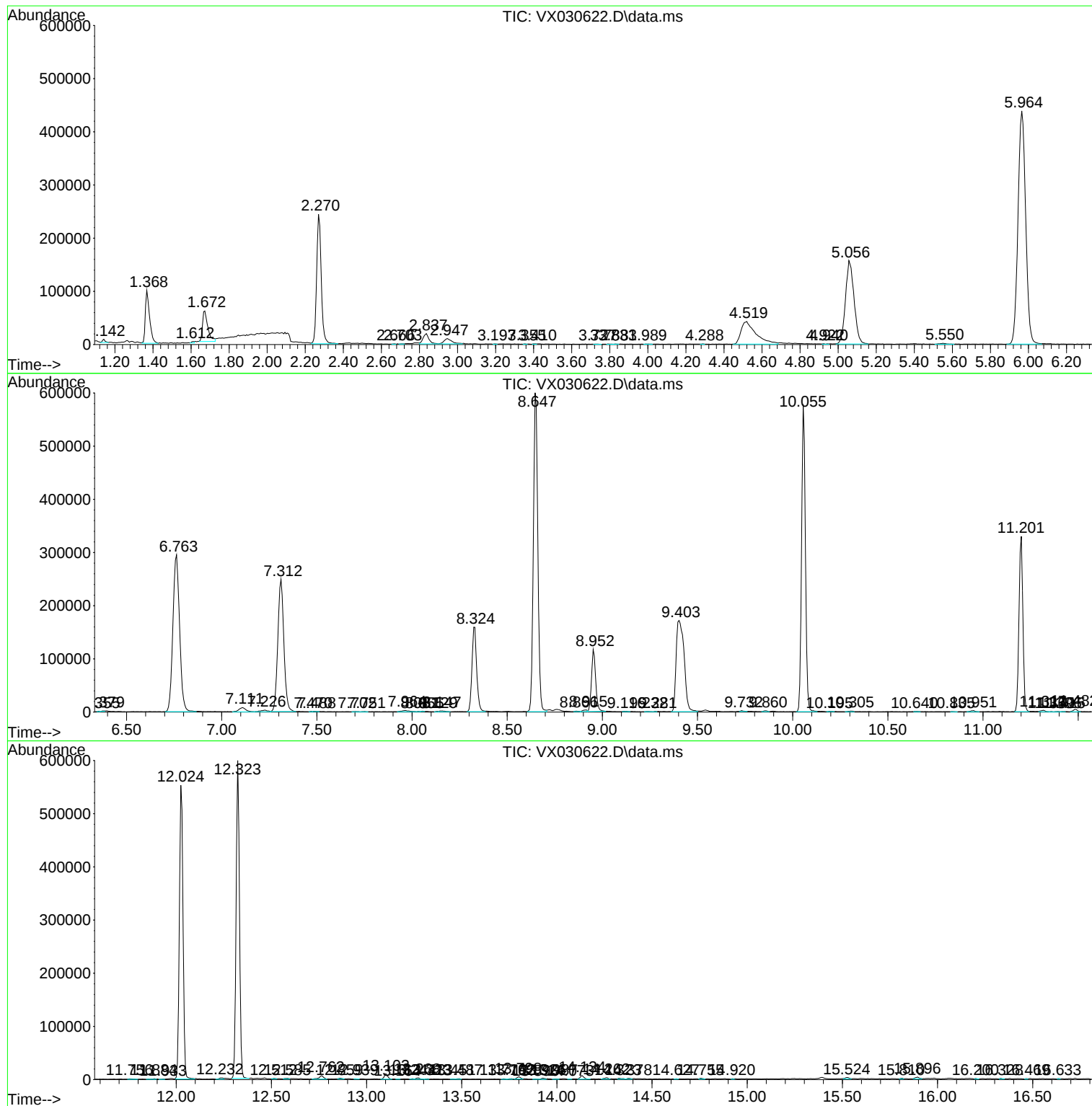
Sum of corrected areas: 8770752

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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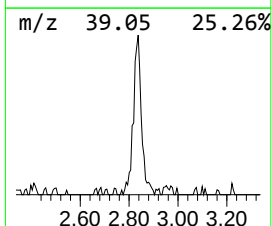
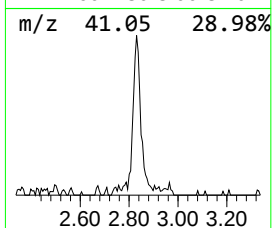
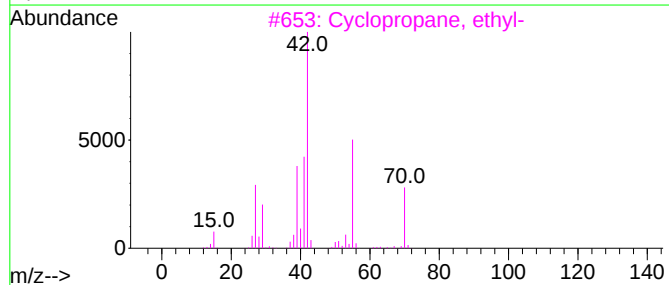
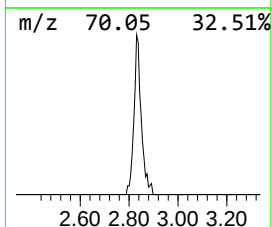
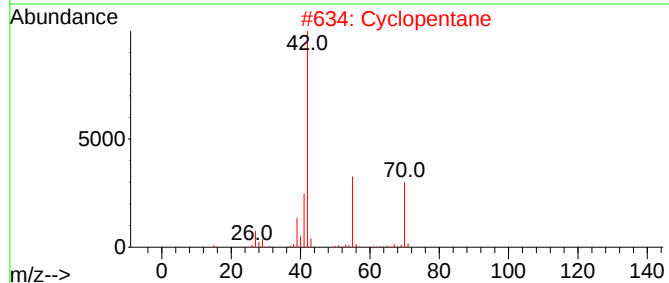
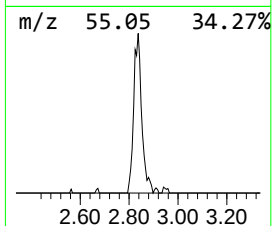
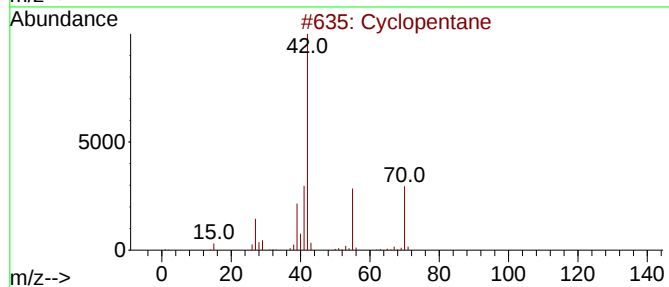
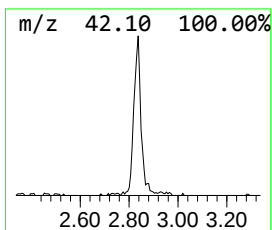
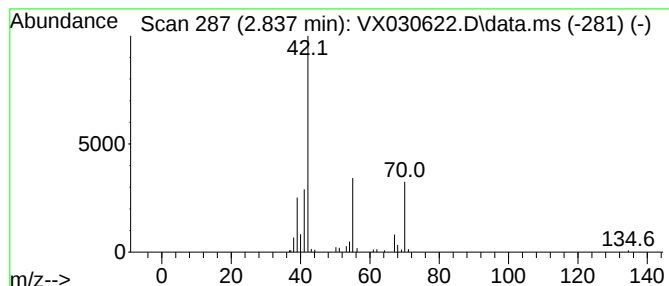
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic2.837 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.837	2.75 ug/L	39361	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			Cyclopentane	70	C5H10	000287-92-3	72
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
4			Cyclopentane	70	C5H10	000287-92-3	64
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.837	2.8	ug/L	39361	1	6.763	716528	50.0