

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
 Data File : VX039420.D
 Acq On : 21 Dec 2023 11:39
 Operator : JC/MD
 Sample : 05807-16
 Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B01

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: VX039420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	64	rVB	54861	94226	10.74%	1.171%
2	1.575	72	80	81	rBV4	5945	13554	1.54%	0.168%
3	1.648	89	92	99	rBV	21621	36903	4.20%	0.459%
4	2.288	191	197	212	rBV	142927	238116	27.13%	2.959%
5	2.629	251	253	254	rBV2	380	210	0.02%	0.003%
6	2.727	263	269	270	rBV4	1393	1857	0.21%	0.023%
7	2.843	281	288	300	rVB	406547	824304	93.92%	10.243%
8	3.075	323	326	328	rBV3	455	575	0.07%	0.007%
9	3.123	332	334	337	rVV2	559	648	0.07%	0.008%
10	3.300	359	363	369	rBV4	950	2049	0.23%	0.025%
11	3.398	378	379	381	rBV	244	219	0.02%	0.003%
12	3.428	381	384	388	rVV3	1115	1677	0.19%	0.021%
13	3.574	405	408	409	rBV2	315	281	0.03%	0.003%
14	3.678	421	425	427	rVB2	382	407	0.05%	0.005%
15	4.068	487	489	492	rVB	334	299	0.03%	0.004%
16	4.099	492	494	498	rVV	155	222	0.03%	0.003%
17	4.257	518	520	522	rVB2	252	234	0.03%	0.003%
18	4.337	532	533	536	rVB2	518	283	0.03%	0.004%
19	4.477	546	556	583	rBV	42133	198158	22.58%	2.462%
20	5.056	637	651	671	rBV	90541	304614	34.71%	3.785%
21	5.373	699	703	704	rBV2	231	273	0.03%	0.003%
22	5.409	707	709	711	rVB	343	250	0.03%	0.003%
23	5.458	711	717	719	rBV3	482	864	0.10%	0.011%
24	5.964	788	800	817	rVV2	265745	779322	88.80%	9.684%
25	6.165	831	833	835	rBV	272	248	0.03%	0.003%
26	6.293	851	854	856	rBV	250	427	0.05%	0.005%
27	6.440	874	878	881	rBV2	254	337	0.04%	0.004%
28	6.610	903	906	909	rVB2	212	258	0.03%	0.003%
29	6.757	921	930	947	rBV	188360	467462	53.26%	5.809%
30	7.110	982	988	995	rVB6	1244	3001	0.34%	0.037%
31	7.165	995	997	999	rVB	303	217	0.02%	0.003%
32	7.305	1012	1020	1038	rVV	158361	355376	40.49%	4.416%
33	7.872	1108	1113	1115	rBV2	140	253	0.03%	0.003%
34	7.952	1124	1126	1128	rBV	269	287	0.03%	0.004%
35	8.031	1136	1139	1142	rVB2	211	267	0.03%	0.003%
36	8.263	1175	1177	1180	rVB2	361	321	0.04%	0.004%

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 Title : VOC Analysis

37	8.324	1180	1187	1201	rBV	95685	172364	19.64%	2.142%
38	8.513	1215	1218	1220	rBV2	288	353	0.04%	0.004%
39	8.647	1233	1240	1249	rBV	370616	603540	68.77%	7.500%
40	8.952	1285	1290	1301	rBV	68511	110579	12.60%	1.374%
41	9.128	1317	1319	1322	rVB2	290	293	0.03%	0.004%
42	9.220	1330	1334	1337	rVB	171	214	0.02%	0.003%
43	9.275	1337	1343	1350	rBV	1553	2268	0.26%	0.028%
44	9.397	1357	1363	1380	rBV	246990	452803	51.59%	5.627%
45	9.647	1401	1404	1411	rVB4	1973	2979	0.34%	0.037%
46	9.707	1411	1414	1419	rBV4	998	1616	0.18%	0.020%
47	10.055	1465	1471	1481	rBV	393951	579886	66.07%	7.206%
48	10.201	1490	1495	1501	rVB6	757	1563	0.18%	0.019%
49	10.262	1503	1505	1507	rBV	280	272	0.03%	0.003%
50	10.287	1507	1509	1510	rBV2	299	227	0.03%	0.003%
51	10.311	1510	1513	1518	rVB2	743	1025	0.12%	0.013%
52	10.646	1564	1568	1570	rBV4	444	589	0.07%	0.007%
53	10.939	1614	1616	1617	rBV	327	262	0.03%	0.003%
54	11.097	1640	1642	1646	rVB2	332	387	0.04%	0.005%
55	11.195	1653	1658	1669	rVV	286553	376976	42.95%	4.685%
56	11.317	1673	1678	1683	rVB2	2923	4170	0.48%	0.052%
57	11.414	1692	1694	1697	rBV2	243	352	0.04%	0.004%
58	11.482	1698	1705	1710	rVB3	5051	8046	0.92%	0.100%
59	11.610	1723	1726	1729	rBV2	185	265	0.03%	0.003%
60	11.707	1740	1742	1744	rBV2	305	333	0.04%	0.004%
61	11.756	1747	1750	1754	rVV2	782	982	0.11%	0.012%
62	11.805	1756	1758	1761	rBV2	234	215	0.02%	0.003%
63	11.884	1768	1771	1772	rBV3	390	344	0.04%	0.004%
64	11.969	1780	1785	1789	rBV	17117	21621	2.46%	0.269%
65	12.024	1789	1794	1808	rVB2	495567	877628	100.00%	10.906%
66	12.323	1837	1843	1851	rBV2	438023	643321	73.30%	7.994%
67	12.420	1857	1859	1863	rVB4	1575	2120	0.24%	0.026%
68	12.457	1863	1865	1870	rVB2	641	721	0.08%	0.009%
69	12.500	1870	1872	1874	rBV2	278	294	0.03%	0.004%
70	12.628	1891	1893	1896	rVB2	281	261	0.03%	0.003%
71	12.762	1910	1915	1923	rVB2	6361	9019	1.03%	0.112%
72	12.817	1923	1924	1927	rBV	291	325	0.04%	0.004%
73	12.872	1930	1933	1934	rVV2	334	305	0.03%	0.004%
74	12.902	1936	1938	1939	rVV	268	225	0.03%	0.003%
75	12.926	1939	1942	1949	rVV3	2619	3926	0.45%	0.049%
76	13.061	1957	1964	1971	rBV2	2698	5270	0.60%	0.065%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	13.115	1971	1973	1978	rVV4	1182	1380	0.16%	0.017%
78	13.201	1981	1987	1990	rVV3	1811	2590	0.30%	0.032%
79	13.268	1994	1998	2003	rBV2	1477	1889	0.22%	0.023%
80	13.384	2016	2017	2019	rVB	380	243	0.03%	0.003%
81	13.420	2019	2023	2026	rBV2	180	312	0.04%	0.004%
82	13.585	2045	2050	2061	rBV	483652	608331	69.32%	7.560%
83	13.774	2079	2081	2088	rVB2	724	1101	0.13%	0.014%
84	13.823	2088	2089	2092	rBV2	234	209	0.02%	0.003%
85	13.957	2105	2111	2119	rBV	101742	133893	15.26%	1.664%
86	14.036	2122	2124	2127	rVB2	332	247	0.03%	0.003%
87	14.127	2134	2139	2144	rVB	9123	12435	1.42%	0.155%
88	14.262	2158	2161	2164	rBV	193	260	0.03%	0.003%
89	14.304	2167	2168	2173	rBV2	227	262	0.03%	0.003%
90	14.554	2207	2209	2213	rVB	284	241	0.03%	0.003%
91	14.597	2213	2216	2218	rBV3	179	283	0.03%	0.004%
92	14.780	2240	2246	2253	rVB2	8168	12401	1.41%	0.154%
93	15.243	2317	2322	2332	rBV	31237	46888	5.34%	0.583%
94	15.389	2340	2346	2351	rBV	2465	3845	0.44%	0.048%
95	15.584	2377	2378	2380	rBV2	306	210	0.02%	0.003%
96	15.853	2420	2422	2424	rVB2	405	224	0.03%	0.003%
97	16.127	2465	2467	2470	rBV3	244	324	0.04%	0.004%
98	16.353	2503	2504	2508	rBV2	318	397	0.05%	0.005%
99	16.456	2518	2521	2522	rBV	296	264	0.03%	0.003%
100	16.505	2526	2529	2536	rVB4	1667	3019	0.34%	0.038%

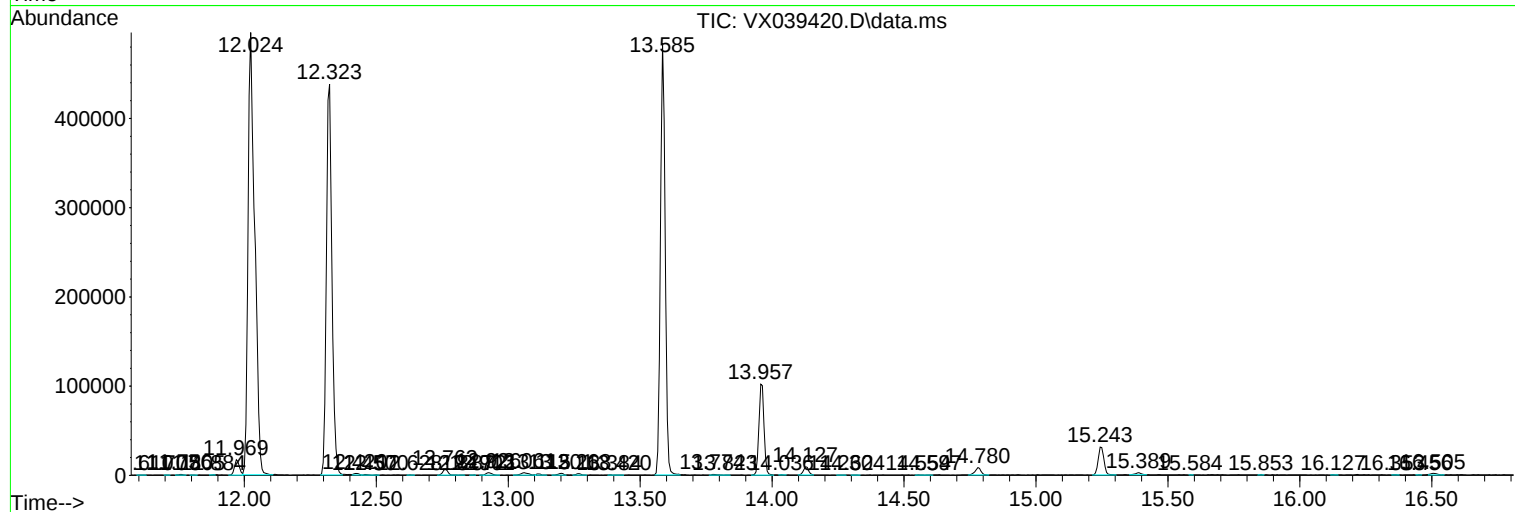
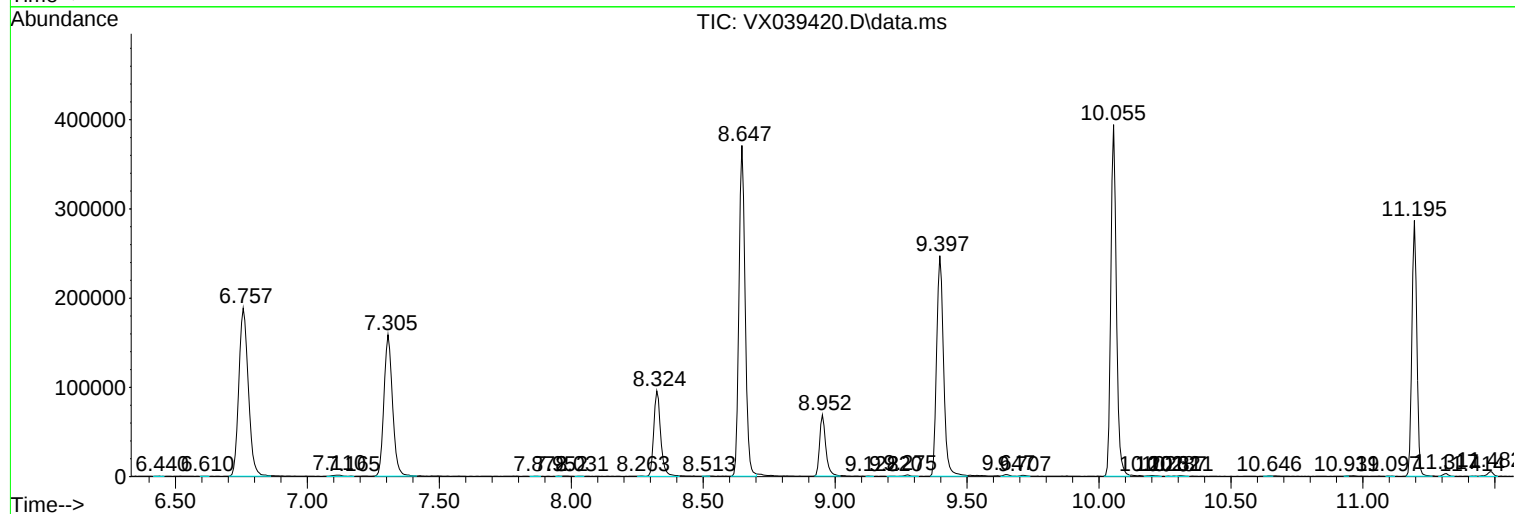
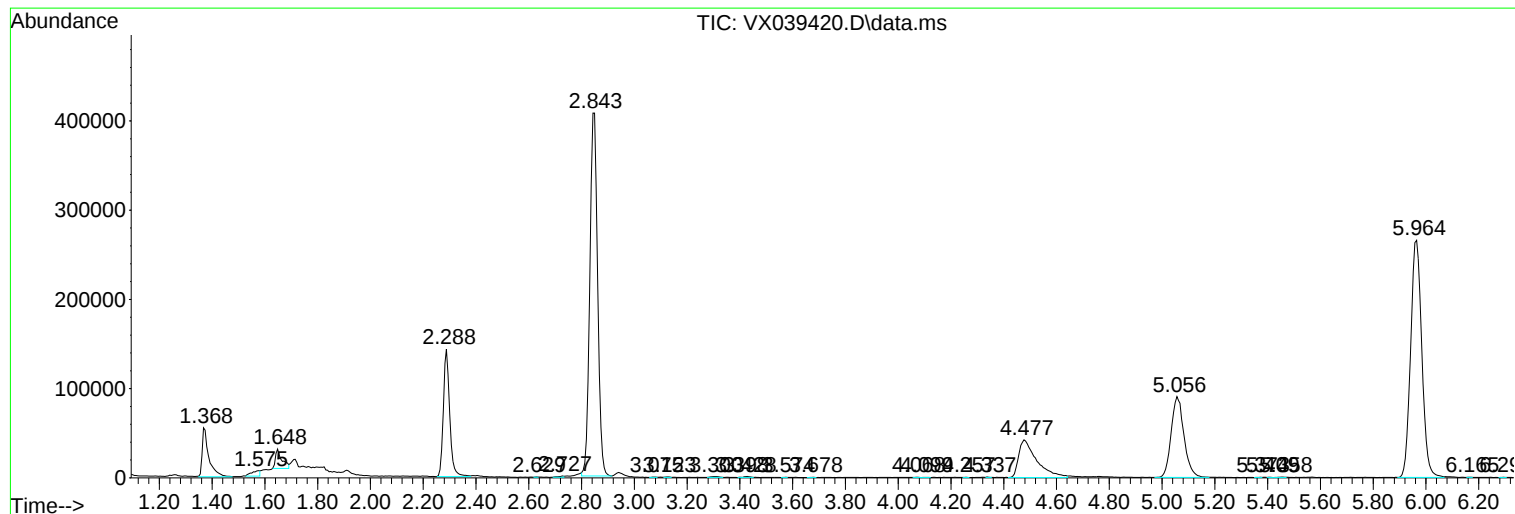
Sum of corrected areas: 8047186

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ALS Vial : 7 Sample Multiplier: 1

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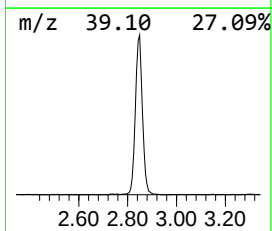
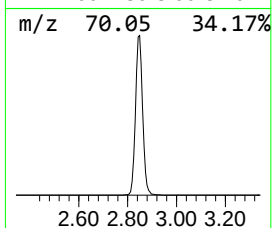
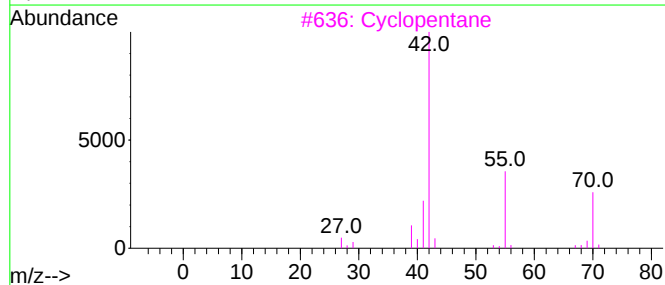
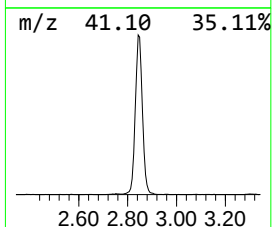
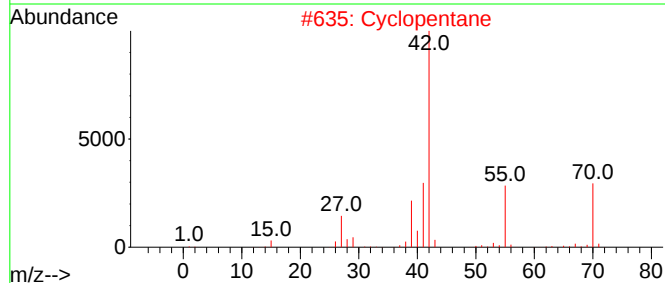
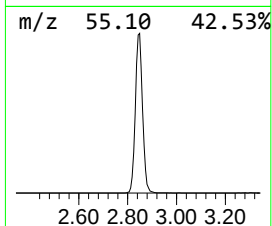
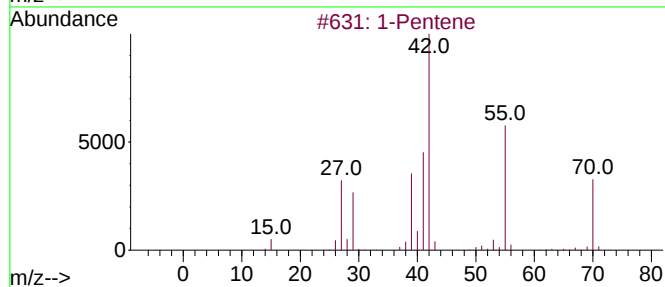
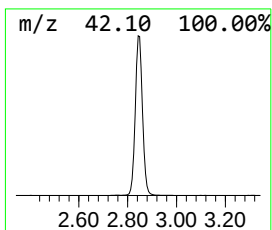
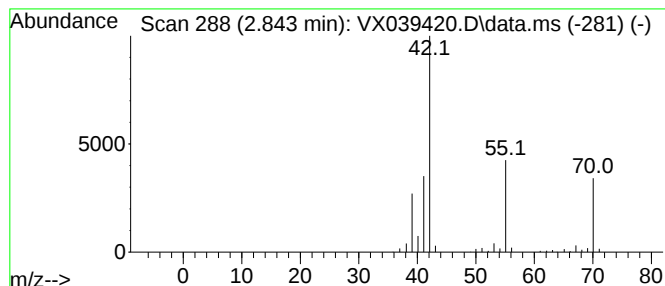
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.843	88.17 ug/L	824304	1,4-Difluorobenzene	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	91
2		Cyclopentane	70	C5H10	000287-92-3	90
3		Cyclopentane	70	C5H10	000287-92-3	80
4		Cyclopentane	70	C5H10	000287-92-3	78
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.843	88.2	ug/L	824304	1	6.757	467462	50.0