

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
 Data File : VX039423.D
 Acq On : 21 Dec 2023 12:47
 Operator : JC/MD
 Sample : 05808-10ME
 Misc : 4.90g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B04ME

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039423.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	67	rVB	60467	110628	11.62%	1.204%
2	1.648	89	92	99	rBV	20819	37199	3.91%	0.405%
3	2.288	190	197	211	rBV	158073	280416	29.46%	3.052%
4	2.575	242	244	245	rBV	294	232	0.02%	0.003%
5	2.684	260	262	263	rBV	364	219	0.02%	0.002%
6	2.843	281	288	299	rVB	148682	296727	31.17%	3.229%
7	2.947	299	305	311	rVB	5464	11661	1.23%	0.127%
8	3.093	327	329	331	rBV2	292	237	0.02%	0.003%
9	3.331	367	368	373	rVB	502	565	0.06%	0.006%
10	3.379	373	376	377	rBV2	320	393	0.04%	0.004%
11	3.428	381	384	385	rBV2	341	328	0.03%	0.004%
12	3.599	410	412	413	rBV	310	260	0.03%	0.003%
13	3.953	468	470	473	rBV	235	191	0.02%	0.002%
14	4.056	485	487	488	rBV2	255	209	0.02%	0.002%
15	4.483	547	557	586	rBV2	47419	241201	25.34%	2.625%
16	5.062	639	652	673	rBV	115224	376609	39.56%	4.099%
17	5.446	713	715	718	rVB	315	247	0.03%	0.003%
18	5.794	770	772	774	rBV2	285	231	0.02%	0.003%
19	5.964	786	800	820	rBV2	326230	951876	100.00%	10.360%
20	6.281	849	852	854	rVB2	269	306	0.03%	0.003%
21	6.550	894	896	897	rBV	283	194	0.02%	0.002%
22	6.678	916	917	921	rVB2	245	247	0.03%	0.003%
23	6.757	921	930	946	rBV	225703	559323	58.76%	6.087%
24	7.111	982	988	995	rVB5	1768	4174	0.44%	0.045%
25	7.306	1011	1020	1033	rBV	191405	434949	45.69%	4.734%
26	7.476	1046	1048	1053	rBV3	389	619	0.07%	0.007%
27	7.592	1064	1067	1070	rVB2	181	242	0.03%	0.003%
28	7.677	1079	1081	1087	rVB2	182	213	0.02%	0.002%
29	7.952	1124	1126	1128	rBV	235	223	0.02%	0.002%
30	8.263	1174	1177	1179	rBV	483	386	0.04%	0.004%
31	8.324	1181	1187	1201	rBV	119157	208457	21.90%	2.269%
32	8.525	1216	1220	1223	rVB2	399	562	0.06%	0.006%
33	8.647	1233	1240	1256	rBV	452332	726243	76.30%	7.904%
34	8.952	1285	1290	1305	rVB	84438	136732	14.36%	1.488%
35	9.122	1317	1318	1320	rBV	343	272	0.03%	0.003%
36	9.202	1329	1331	1335	rBV2	301	373	0.04%	0.004%

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

37	9.281	1339	1344	1348	rVB3	971	1457	0.15%	0.016%
38	9.397	1356	1363	1380	rBV	285818	552169	58.01%	6.010%
39	9.714	1411	1415	1419	rVB3	1011	1566	0.16%	0.017%
40	9.836	1433	1435	1438	rBV2	262	280	0.03%	0.003%
41	10.055	1465	1471	1486	rBV	459010	670568	70.45%	7.298%
42	10.250	1501	1503	1509	rBV3	419	554	0.06%	0.006%
43	10.305	1509	1512	1515	rBV3	609	779	0.08%	0.008%
44	10.592	1558	1559	1562	rBV2	238	282	0.03%	0.003%
45	10.646	1565	1568	1570	rBV2	662	771	0.08%	0.008%
46	10.903	1607	1610	1613	rBV2	190	228	0.02%	0.002%
47	10.945	1613	1617	1618	rVV2	503	469	0.05%	0.005%
48	10.970	1618	1621	1625	rVB2	704	890	0.09%	0.010%
49	11.098	1638	1642	1644	rBV2	322	405	0.04%	0.004%
50	11.195	1652	1658	1671	rVV	346754	455477	47.85%	4.957%
51	11.311	1673	1677	1681	rVB2	2723	3775	0.40%	0.041%
52	11.457	1697	1701	1702	rBV3	678	981	0.10%	0.011%
53	11.671	1734	1736	1738	rBV	222	213	0.02%	0.002%
54	11.762	1747	1751	1753	rBV2	693	851	0.09%	0.009%
55	11.866	1765	1768	1771	rBV3	208	258	0.03%	0.003%
56	11.969	1780	1785	1789	rBV	102112	128948	13.55%	1.403%
57	12.024	1789	1794	1806	rVB2	551697	810596	85.16%	8.822%
58	12.201	1820	1823	1826	rVB2	237	276	0.03%	0.003%
59	12.274	1832	1835	1837	rBV	223	297	0.03%	0.003%
60	12.323	1837	1843	1857	rBV2	585657	949492	99.75%	10.334%
61	12.640	1893	1895	1898	rBV2	333	449	0.05%	0.005%
62	12.762	1910	1915	1920	rVB2	6726	9098	0.96%	0.099%
63	12.805	1920	1922	1926	rBV2	149	243	0.03%	0.003%
64	12.866	1929	1932	1933	rBV	267	278	0.03%	0.003%
65	13.000	1952	1954	1956	rVB2	298	223	0.02%	0.002%
66	13.024	1956	1958	1959	rBV2	318	224	0.02%	0.002%
67	13.067	1959	1965	1970	rBV3	2207	3550	0.37%	0.039%
68	13.116	1970	1973	1978	rVV4	1323	1670	0.18%	0.018%
69	13.195	1984	1986	1991	rBV2	2054	2482	0.26%	0.027%
70	13.262	1995	1997	2001	rVB3	538	601	0.06%	0.007%
71	13.384	2013	2017	2019	rBV2	443	461	0.05%	0.005%
72	13.426	2023	2024	2027	rBV2	293	260	0.03%	0.003%
73	13.536	2040	2042	2045	rVB2	219	256	0.03%	0.003%
74	13.585	2045	2050	2065	rBV	553255	683737	71.83%	7.442%
75	13.701	2065	2069	2071	rVB2	278	355	0.04%	0.004%
76	13.780	2079	2082	2086	rVB2	684	821	0.09%	0.009%

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 Title : VOC Analysis

77	13.829	2088	2090	2091	rVB	277	185	0.02%	0.002%
78	13.957	2106	2111	2121	rBV	172770	224546	23.59%	2.444%
79	14.067	2127	2129	2132	rVB	383	361	0.04%	0.004%
80	14.128	2134	2139	2144	rBV	7296	9674	1.02%	0.105%
81	14.243	2155	2158	2159	rBV2	321	231	0.02%	0.003%
82	14.481	2195	2197	2199	rVB	372	263	0.03%	0.003%
83	14.536	2204	2206	2207	rBV2	311	202	0.02%	0.002%
84	14.621	2218	2220	2224	rBV3	418	658	0.07%	0.007%
85	14.688	2229	2231	2234	rVB3	243	258	0.03%	0.003%
86	14.719	2234	2236	2237	rBV	210	187	0.02%	0.002%
87	14.780	2239	2246	2253	rVB3	21556	38353	4.03%	0.417%
88	14.920	2267	2269	2272	rVB2	323	313	0.03%	0.003%
89	14.981	2278	2279	2282	rBV	367	306	0.03%	0.003%
90	15.018	2284	2285	2289	rVV2	307	316	0.03%	0.003%
91	15.243	2316	2322	2332	rBV	161755	228432	24.00%	2.486%
92	15.390	2342	2346	2352	rBV4	1667	2594	0.27%	0.028%
93	15.639	2385	2387	2389	rBV2	374	294	0.03%	0.003%
94	15.780	2409	2410	2413	rBV2	383	365	0.04%	0.004%
95	16.024	2448	2450	2452	rBV3	275	256	0.03%	0.003%
96	16.048	2452	2454	2457	rVV2	304	316	0.03%	0.003%
97	16.194	2475	2478	2480	rBV2	427	357	0.04%	0.004%
98	16.231	2482	2484	2488	rBV2	243	264	0.03%	0.003%
99	16.347	2501	2503	2505	rBV2	303	300	0.03%	0.003%
100	16.505	2524	2529	2537	rVB3	5789	9895	1.04%	0.108%

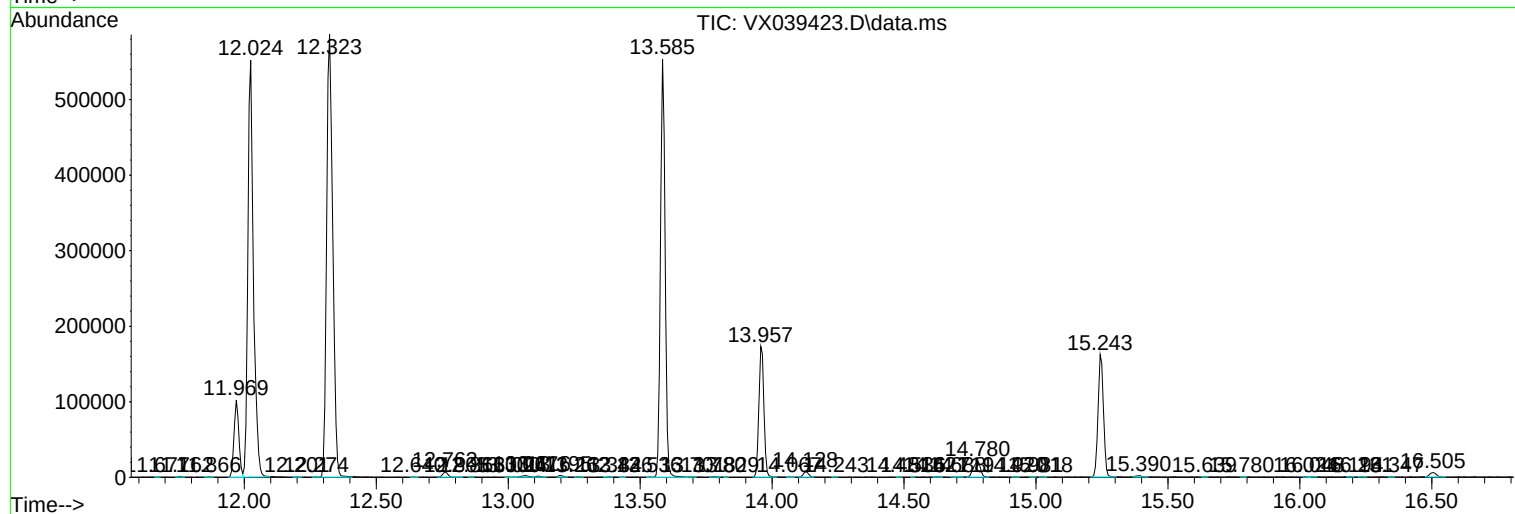
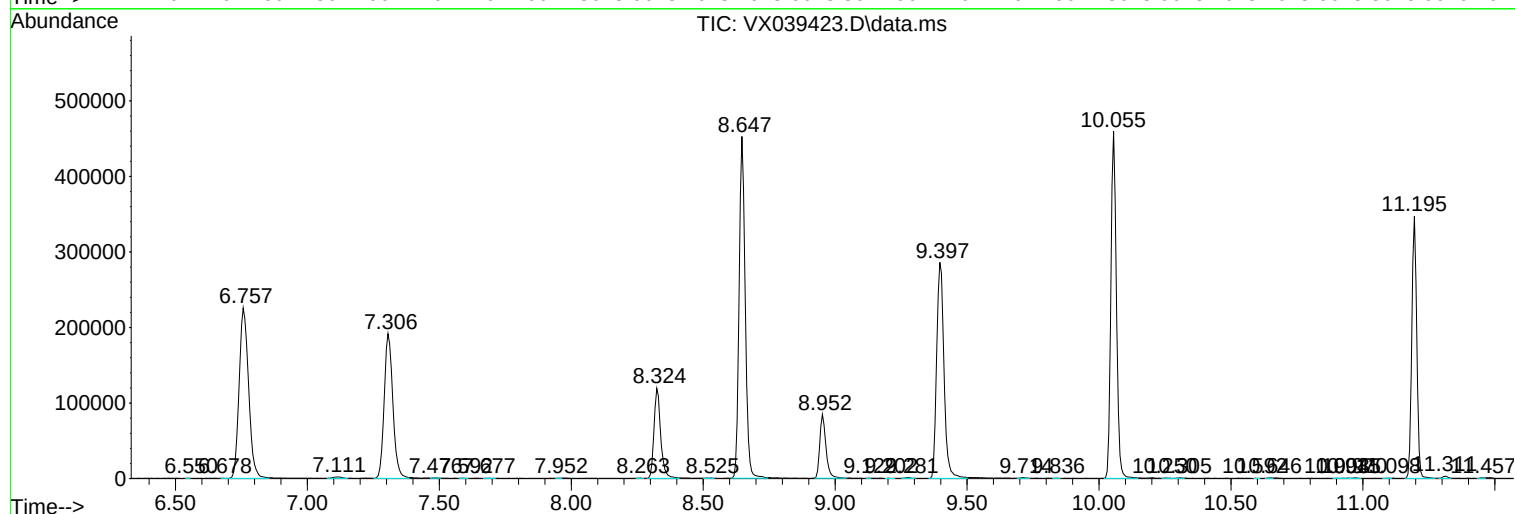
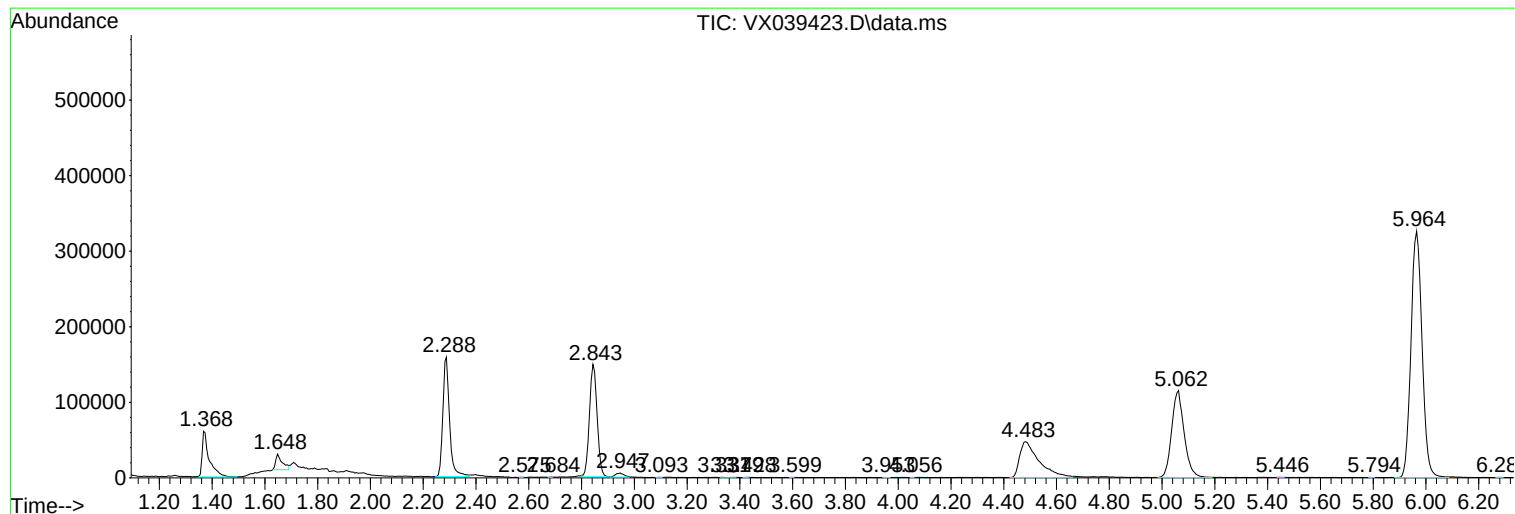
Sum of corrected areas: 9188160

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B04ME

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

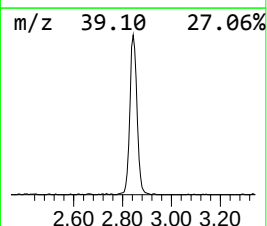
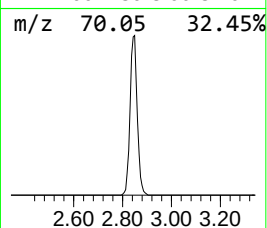
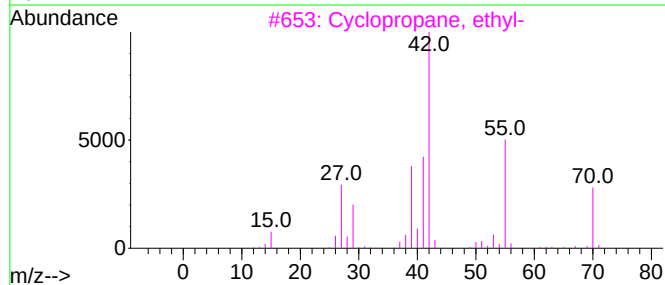
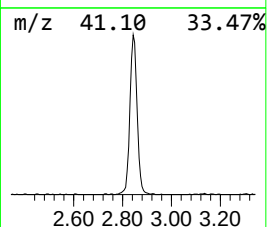
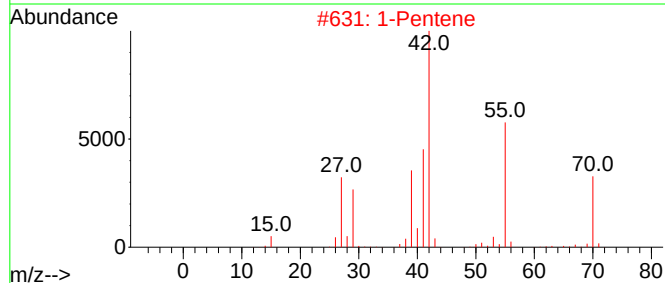
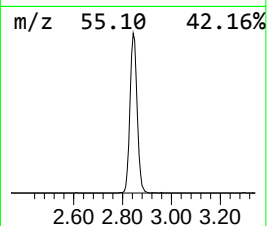
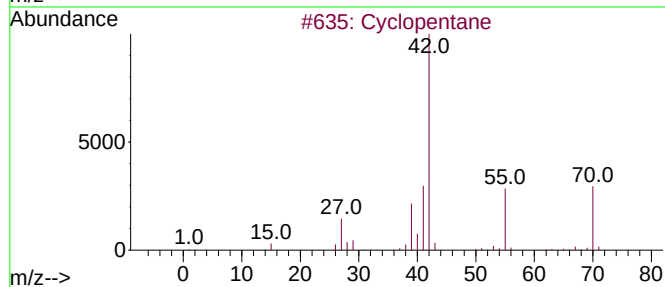
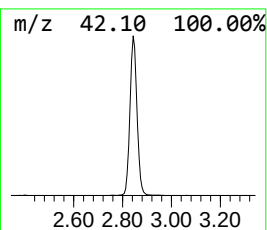
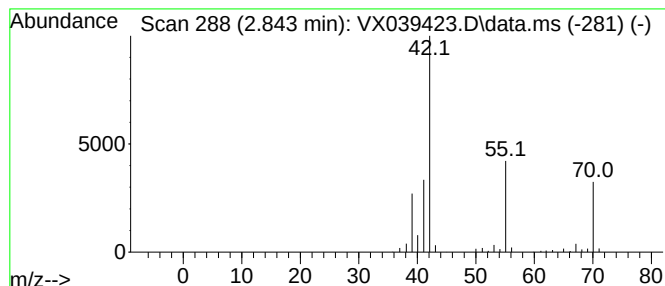
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Cyclic2.843 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.843	26.53 ug/L	296727	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	90
2			1-Pentene	70	C5H10	000109-67-1	87
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
5			Cyclopentane	70	C5H10	000287-92-3	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.843	26.5	ug/L	296727	1	6.757	559323	50.0