

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039372.D
 Acq On : 19 Dec 2023 21:15
 Operator : JC/MD
 Sample : 05807-11ME
 Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ3

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: VX039372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.373	43	47	58	rBV	72719	112715	4.77%	1.295%
2	1.648	89	92	101	rVB	22317	30146	1.27%	0.346%
3	2.288	191	197	209	rBV	177793	284116	12.02%	3.263%
4	2.715	263	267	275	rBV	3528	8060	0.34%	0.093%
5	2.849	282	289	299	rVB	183413	370254	15.66%	4.252%
6	2.940	299	304	313	rVB2	5499	12842	0.54%	0.147%
7	3.068	321	325	327	rBV2	245	303	0.01%	0.003%
8	3.117	331	333	335	rBV2	380	370	0.02%	0.004%
9	3.135	335	336	340	rVB3	395	380	0.02%	0.004%
10	3.312	358	365	366	rBV4	735	1088	0.05%	0.012%
11	3.397	376	379	382	rBV2	335	354	0.01%	0.004%
12	3.477	390	392	395	rVB2	266	258	0.01%	0.003%
13	3.538	399	402	404	rBV2	191	209	0.01%	0.002%
14	3.769	435	440	443	rBV	325	501	0.02%	0.006%
15	4.019	477	481	482	rBV2	283	213	0.01%	0.002%
16	4.038	482	484	487	rVV	151	223	0.01%	0.003%
17	4.257	516	520	522	rBV	273	338	0.01%	0.004%
18	4.483	548	557	591	rBV	41865	204969	8.67%	2.354%
19	5.062	638	652	671	rBV2	98567	323832	13.69%	3.719%
20	5.220	676	678	682	rVV2	420	435	0.02%	0.005%
21	5.397	705	707	708	rBV	183	196	0.01%	0.002%
22	5.434	712	713	716	rBV2	292	294	0.01%	0.003%
23	5.543	728	731	732	rBV2	251	274	0.01%	0.003%
24	5.647	745	748	750	rBV2	210	282	0.01%	0.003%
25	5.836	777	779	783	rVB2	195	200	0.01%	0.002%
26	5.964	789	800	830	rVV2	288819	907309	38.37%	10.420%
27	6.226	840	843	846	rVB3	267	399	0.02%	0.005%
28	6.763	921	931	946	rBV	190191	481977	20.38%	5.535%
29	6.891	951	952	953	rVB	524	196	0.01%	0.002%
30	6.988	965	968	969	rBV	251	289	0.01%	0.003%
31	7.104	983	987	994	rVB3	1504	3139	0.13%	0.036%
32	7.226	1004	1007	1009	rBV2	326	337	0.01%	0.004%
33	7.305	1011	1020	1036	rBV	163139	378416	16.00%	4.346%
34	7.458	1044	1045	1047	rBV2	241	214	0.01%	0.002%
35	7.488	1048	1050	1055	rVB2	611	953	0.04%	0.011%
36	7.647	1074	1076	1078	rBV	248	246	0.01%	0.003%

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 Title : VOC Analysis

37	7.689	1081	1083	1085	rVB2	262	216	0.01%	0.002%
38	7.714	1085	1087	1090	rBV	295	258	0.01%	0.003%
39	7.866	1111	1112	1115	rVB2	353	202	0.01%	0.002%
40	7.915	1115	1120	1123	rBV2	259	405	0.02%	0.005%
41	7.958	1126	1127	1129	rBV	332	236	0.01%	0.003%
42	8.165	1159	1161	1164	rVB2	270	278	0.01%	0.003%
43	8.262	1172	1177	1181	rBV2	3022	5369	0.23%	0.062%
44	8.323	1181	1187	1200	rVV	100992	179920	7.61%	2.066%
45	8.646	1234	1240	1250	rBV	400113	652819	27.61%	7.498%
46	8.951	1284	1290	1301	rBV	69136	116278	4.92%	1.335%
47	9.189	1327	1329	1331	rBV	215	222	0.01%	0.003%
48	9.268	1340	1342	1347	rVB3	1038	1097	0.05%	0.013%
49	9.396	1357	1363	1383	rBV	253417	464348	19.64%	5.333%
50	9.616	1395	1399	1401	rBV2	404	574	0.02%	0.007%
51	9.707	1411	1414	1415	rBV3	547	565	0.02%	0.006%
52	9.841	1434	1436	1440	rBV2	297	250	0.01%	0.003%
53	10.079	1465	1475	1493	rBV2	1255494	2364656	100.00%	27.158%
54	10.274	1504	1507	1509	rBV2	279	288	0.01%	0.003%
55	10.305	1510	1512	1514	rVV3	562	422	0.02%	0.005%
56	10.378	1522	1524	1527	rVB2	195	246	0.01%	0.003%
57	10.414	1527	1530	1533	rBV2	267	380	0.02%	0.004%
58	10.652	1565	1569	1571	rBV2	473	629	0.03%	0.007%
59	10.683	1571	1574	1575	rVV2	267	294	0.01%	0.003%
60	10.945	1614	1617	1619	rBV3	503	665	0.03%	0.008%
61	10.969	1619	1621	1626	rVB2	764	826	0.03%	0.009%
62	11.195	1652	1658	1670	rBV	289446	378008	15.99%	4.341%
63	11.311	1674	1677	1682	rVB3	2202	3028	0.13%	0.035%
64	11.481	1696	1705	1709	rVV4	2281	3880	0.16%	0.045%
65	11.756	1747	1750	1755	rVB3	477	928	0.04%	0.011%
66	11.804	1755	1758	1760	rBV3	180	263	0.01%	0.003%
67	11.896	1771	1773	1775	rBV	221	206	0.01%	0.002%
68	11.969	1780	1785	1789	rBV	42141	55255	2.34%	0.635%
69	12.024	1789	1794	1796	rBV	498130	760968	32.18%	8.740%
70	12.323	1837	1843	1854	rVV	435147	564417	23.87%	6.482%
71	12.762	1910	1915	1919	rVB2	4324	5634	0.24%	0.065%
72	12.963	1944	1948	1949	rBV	234	211	0.01%	0.002%
73	13.103	1967	1971	1972	rVV	197	271	0.01%	0.003%
74	13.115	1972	1973	1978	rVB	423	360	0.02%	0.004%
75	13.268	1994	1998	2003	rVB3	432	630	0.03%	0.007%
76	13.438	2024	2026	2029	rBV	152	195	0.01%	0.002%

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 Title : VOC Analysis

77	13.463	2029	2030	2034	rVV	316	263	0.01%	0.003%
78	13.591	2048	2051	2055	rVB2	1416	1884	0.08%	0.022%
79	13.725	2072	2073	2077	rBV2	299	358	0.02%	0.004%
80	13.786	2079	2083	2092	rVV3	548	1287	0.05%	0.015%
81	13.963	2109	2112	2115	rVB2	745	886	0.04%	0.010%
82	14.048	2121	2126	2128	rVB2	273	337	0.01%	0.004%
83	14.127	2135	2139	2144	rVV	3050	4025	0.17%	0.046%
84	14.182	2146	2148	2152	rVB2	194	200	0.01%	0.002%
85	14.225	2154	2155	2157	rBV2	244	191	0.01%	0.002%
86	14.639	2222	2223	2226	rBV2	261	261	0.01%	0.003%
87	14.975	2276	2278	2279	rVB2	321	208	0.01%	0.002%
88	14.993	2279	2281	2284	rBV3	346	291	0.01%	0.003%
89	15.285	2327	2329	2331	rBV	217	211	0.01%	0.002%
90	15.383	2343	2345	2352	rVB6	950	1560	0.07%	0.018%
91	15.450	2352	2356	2359	rBV3	290	359	0.02%	0.004%
92	15.816	2414	2416	2417	rBV	304	197	0.01%	0.002%
93	15.883	2426	2427	2429	rVB	471	195	0.01%	0.002%
94	15.913	2429	2432	2434	rBV2	440	380	0.02%	0.004%
95	16.151	2469	2471	2475	rVB2	398	384	0.02%	0.004%
96	16.182	2475	2476	2478	rBV2	255	258	0.01%	0.003%
97	16.291	2492	2494	2495	rBV	378	223	0.01%	0.003%
98	16.316	2496	2498	2501	rBV3	234	288	0.01%	0.003%
99	16.651	2549	2553	2556	rBV2	410	467	0.02%	0.005%
100	16.682	2556	2558	2562	rVV3	309	316	0.01%	0.004%

Sum of corrected areas: 8707053

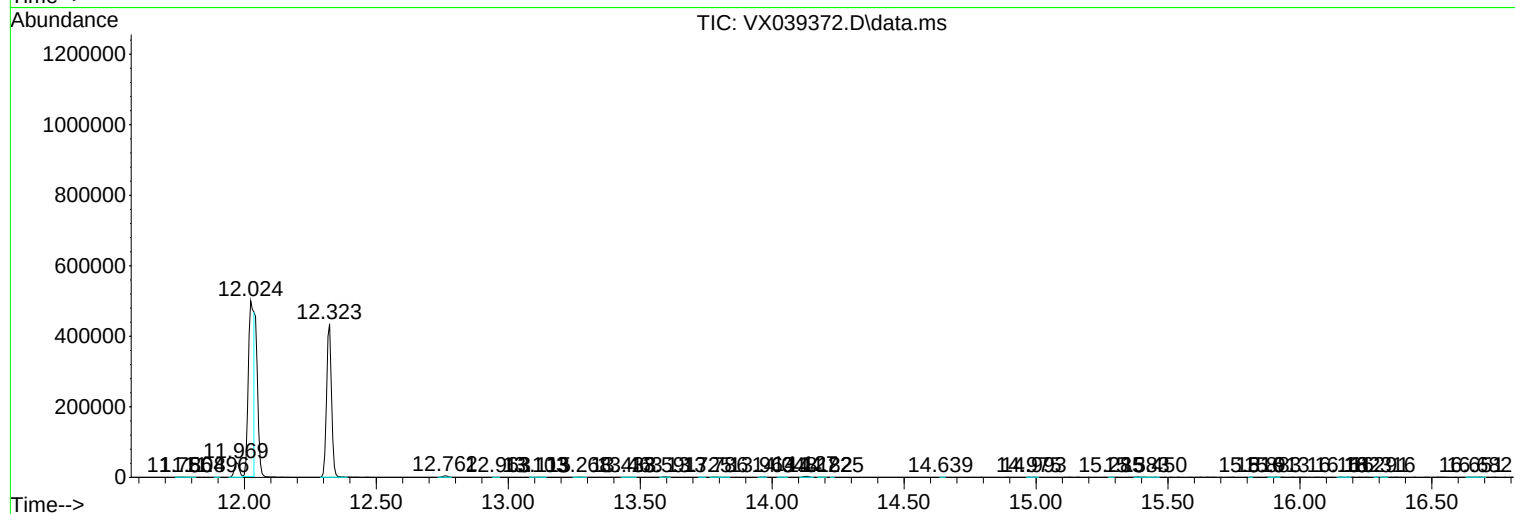
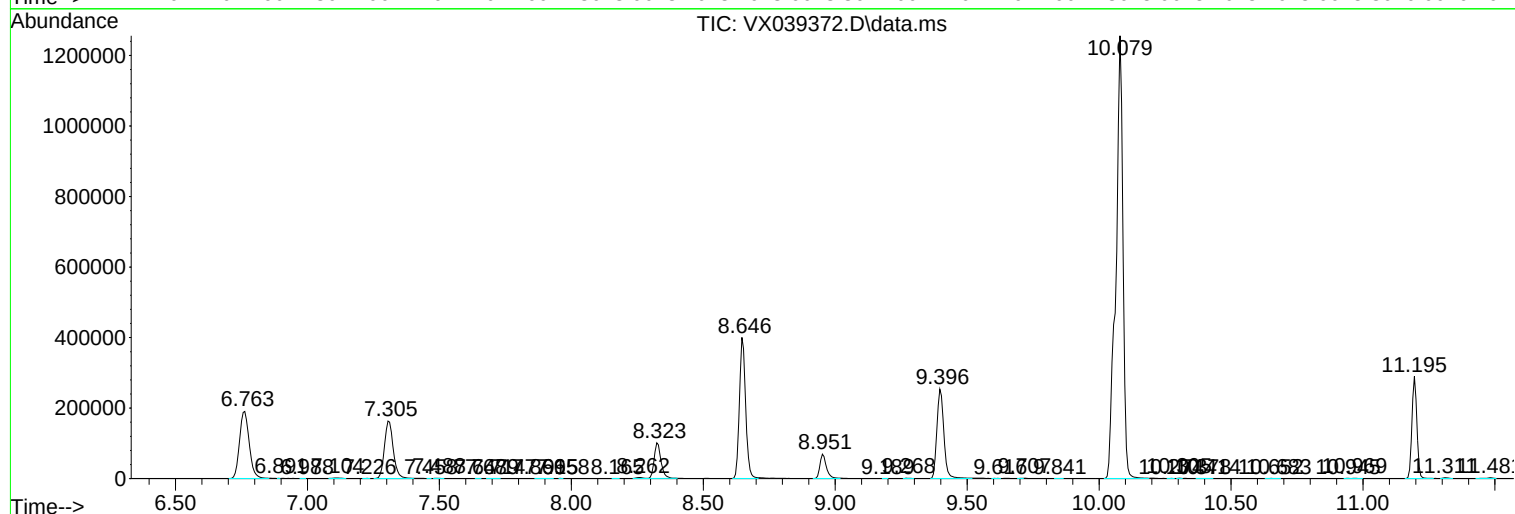
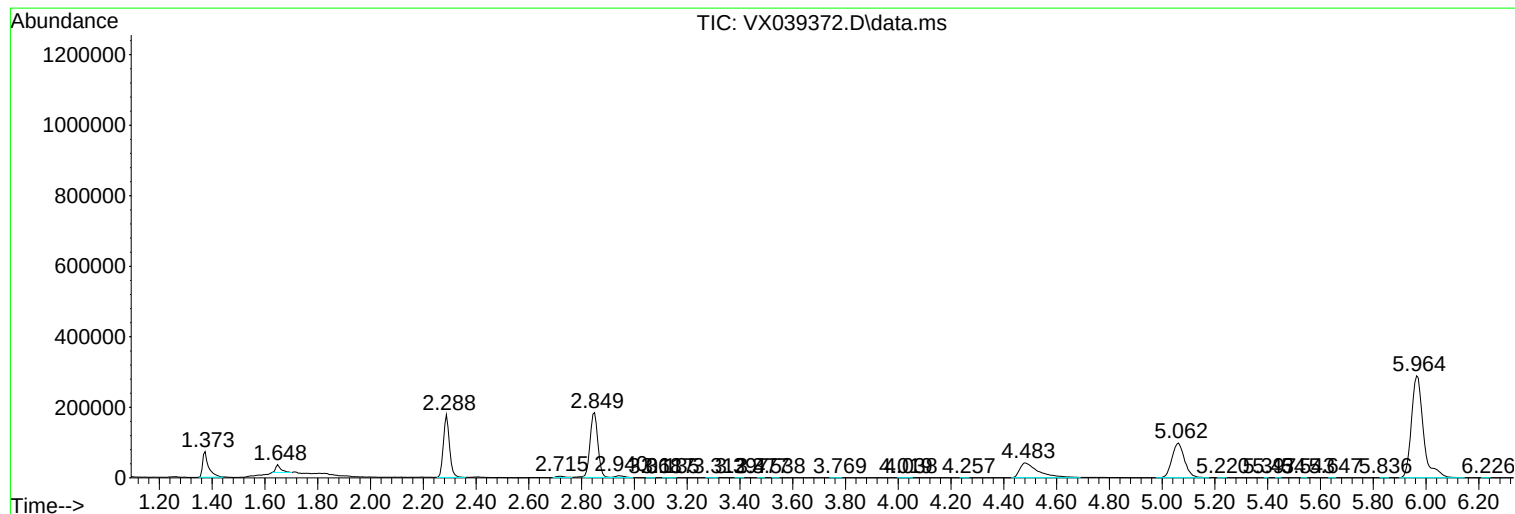
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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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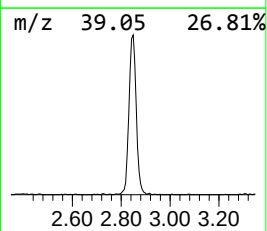
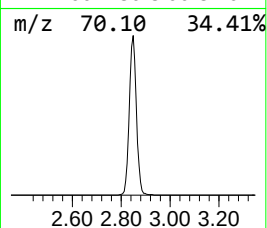
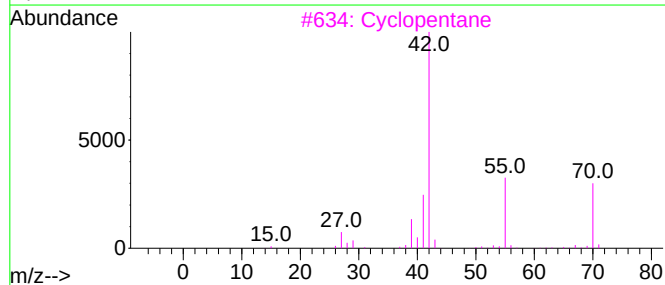
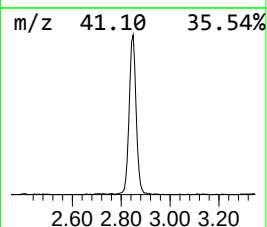
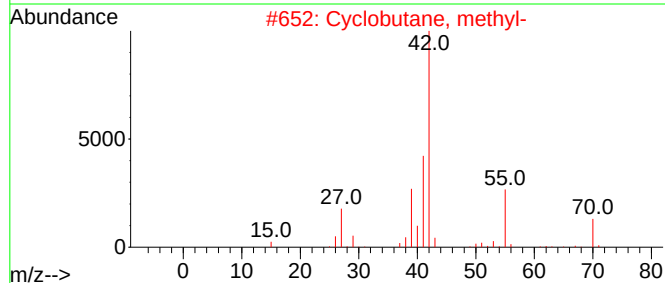
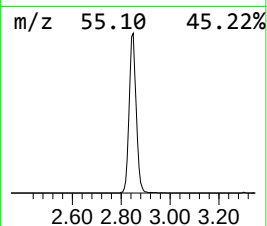
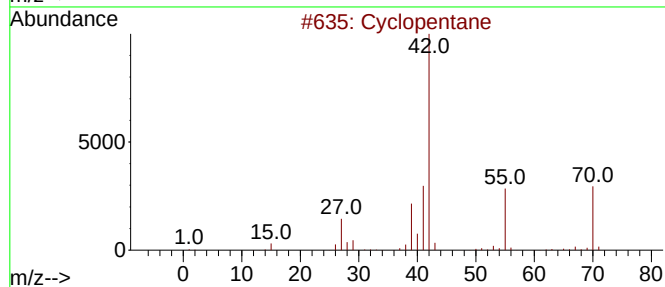
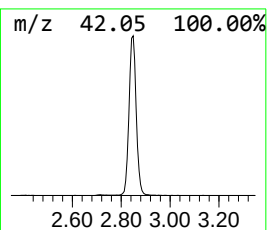
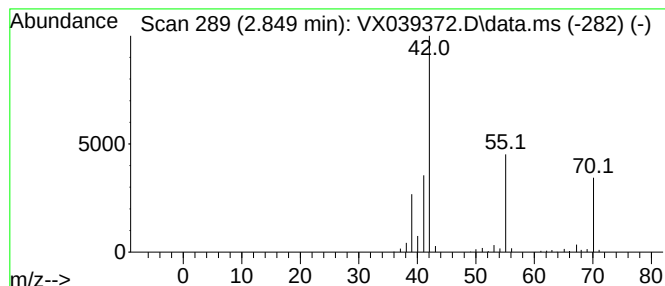
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic2.849 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.849	38.41 ug/L	370254	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	78
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3			Cyclopentane	70	C5H10	000287-92-3	72
4			Cyclopentane	70	C5H10	000287-92-3	72
5			1-Pentene	70	C5H10	000109-67-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.849	38.4	ug/L	370254	1	6.763	481977	50.0