

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035196.D
 Acq On : 20 Apr 2023 01:53
 Operator : JC/MD
 Sample : 02378-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMK7

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	30	rBV2	2732	2531	0.00%	0.000%
2	1.319	32	38	42	rVV	8924	21628	0.01%	0.003%
3	1.368	42	46	57	rVB	178289	201630	0.09%	0.024%
4	1.496	64	67	73	rVB4	1498	2400	0.00%	0.000%
5	1.624	84	88	89	rBV4	1556	2261	0.00%	0.000%
6	1.673	91	96	106	rVV	134519	189094	0.08%	0.022%
7	1.752	106	109	114	rVB3	6113	8838	0.00%	0.001%
8	1.959	138	143	147	rVB2	3214	5134	0.00%	0.001%
9	2.307	193	200	208	rVV	353489	556124	0.24%	0.065%
10	2.392	208	214	224	rVB	29235	62055	0.03%	0.007%
11	2.514	229	234	239	rVB4	1060	2272	0.00%	0.000%
12	2.788	268	279	282	rBV5	7800	15719	0.01%	0.002%
13	2.867	286	292	298	rVV	49343	100357	0.04%	0.012%
14	2.941	298	304	318	rVB	41329	95417	0.04%	0.011%
15	3.099	324	330	338	rVB2	5513	11930	0.01%	0.001%
16	3.447	380	387	394	rBV4	3255	7619	0.00%	0.001%
17	4.306	514	528	542	rBV	137230	400504	0.17%	0.047%
18	4.459	544	553	565	rBV	112875	347539	0.15%	0.041%
19	4.568	565	571	585	rVV2	20235	76790	0.03%	0.009%
20	4.684	588	590	594	rVV4	1217	1851	0.00%	0.000%
21	5.087	639	656	673	rBV2	568444	2252115	0.97%	0.264%
22	5.385	699	705	707	rBV4	1238	2068	0.00%	0.000%
23	5.471	707	719	731	rVV	54617	170941	0.07%	0.020%
24	5.678	740	753	773	rBV	433701	1308069	0.56%	0.153%
25	5.830	773	778	779	rBV3	2476	3365	0.00%	0.000%
26	6.074	788	818	843	rBV2	35581929	129593925	55.62%	15.183%
27	6.361	860	865	872	rVB7	6940	16942	0.01%	0.002%
28	6.763	921	931	948	rBV	421727	996828	0.43%	0.117%
29	7.129	982	991	1002	rVB4	10676	25817	0.01%	0.003%
30	7.312	1011	1021	1028	rBV	345140	777394	0.33%	0.091%
31	7.489	1048	1050	1054	rVB3	1203	1389	0.00%	0.000%
32	7.653	1069	1077	1083	rBV5	4595	9518	0.00%	0.001%
33	7.824	1098	1105	1114	rBV2	9467	19415	0.01%	0.002%
34	7.934	1119	1123	1125	rBV5	1763	2503	0.00%	0.000%
35	8.110	1148	1152	1159	rVB5	2906	4875	0.00%	0.001%
36	8.324	1181	1187	1206	rBV	214162	360017	0.15%	0.042%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

37	8.470	1206	1211	1212	rBV4	528	897	0.00%	0.000%
38	8.488	1212	1214	1220	rVV5	1125	2005	0.00%	0.000%
39	8.586	1225	1230	1234	rVV3	2039	3516	0.00%	0.000%
40	8.653	1234	1241	1248	rVV	835645	1370054	0.59%	0.161%
41	8.720	1248	1252	1264	rVB	36653	62887	0.03%	0.007%
42	8.952	1283	1290	1300	rBV	151842	231047	0.10%	0.027%
43	9.025	1301	1302	1305	rVV2	1110	805	0.00%	0.000%
44	9.159	1319	1324	1326	rBV3	655	984	0.00%	0.000%
45	9.190	1326	1329	1335	rVB3	697	1488	0.00%	0.000%
46	9.275	1335	1343	1349	rBV2	22107	35927	0.02%	0.004%
47	9.391	1356	1362	1379	rBV	450732	763427	0.33%	0.089%
48	9.525	1379	1384	1392	rVB2	7401	12721	0.01%	0.001%
49	10.116	1466	1481	1486	rBV5	57119963	233010354	100.00%	27.299%
50	10.647	1565	1568	1574	rVB4	5504	8795	0.00%	0.001%
51	10.805	1590	1594	1603	rVB8	3638	7043	0.00%	0.001%
52	10.866	1603	1604	1610	rVB5	804	1260	0.00%	0.000%
53	11.049	1632	1634	1636	rVV3	1387	1204	0.00%	0.000%
54	11.195	1651	1658	1673	rVV2	824135	1126312	0.48%	0.132%
55	11.311	1673	1677	1681	rVV6	1896	3549	0.00%	0.000%
56	11.366	1681	1686	1692	rVV	59012	82597	0.04%	0.010%
57	11.427	1692	1696	1697	rVV4	2939	3893	0.00%	0.000%
58	11.457	1697	1701	1709	rVV	25953	40055	0.02%	0.005%
59	11.579	1717	1721	1722	rBV3	780	921	0.00%	0.000%
60	11.683	1736	1738	1741	rBV3	821	999	0.00%	0.000%
61	11.726	1741	1745	1749	rVV4	6788	9149	0.00%	0.001%
62	11.982	1780	1787	1793	rBV	25955393	42825195	18.38%	5.017%
63	12.073	1793	1802	1803	rBV2	61538579	141467986	60.71%	16.574%
64	12.378	1839	1852	1856	rBV2	62391616	178683905	76.68%	20.934%
65	12.549	1876	1880	1890	rVB9	10785	22907	0.01%	0.003%
66	12.707	1903	1906	1911	rVB2	15099	20182	0.01%	0.002%
67	12.811	1921	1923	1926	rVB4	2254	2427	0.00%	0.000%
68	12.878	1929	1934	1937	rVV2	20054	27601	0.01%	0.003%
69	12.921	1937	1941	1952	rVB	813388	1030895	0.44%	0.121%
70	13.061	1958	1964	1969	rBV2	317459	612424	0.26%	0.072%
71	13.110	1969	1972	1981	rVV3	226210	331344	0.14%	0.039%
72	13.195	1981	1986	1997	rVB	419528	556356	0.24%	0.065%
73	13.335	2006	2009	2012	rVV5	1369	1902	0.00%	0.000%
74	13.384	2012	2017	2025	rVB	71045	97295	0.04%	0.011%
75	13.603	2045	2053	2058	rBV	50578813	81574032	35.01%	9.557%
76	13.780	2078	2082	2088	rVB2	13489	19062	0.01%	0.002%

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 Title : VOC Analysis

77	13.969	2106	2113	2118	rBV	20513362	27715442	11.89%	3.247%
78	14.170	2142	2146	2151	rBV7	5428	11534	0.00%	0.001%
79	14.213	2151	2153	2156	rVB3	4566	3672	0.00%	0.000%
80	14.262	2156	2161	2170	rBV2	88554	122540	0.05%	0.014%
81	14.384	2171	2181	2185	rVB5	23434	54525	0.02%	0.006%
82	14.469	2192	2195	2197	rBV4	1127	1602	0.00%	0.000%
83	14.506	2197	2201	2204	rVV4	9727	15657	0.01%	0.002%
84	14.542	2204	2207	2211	rVV2	18038	22587	0.01%	0.003%
85	14.585	2211	2214	2217	rVV4	6042	8204	0.00%	0.001%
86	14.628	2217	2221	2226	rVB2	23906	33134	0.01%	0.004%
87	14.780	2236	2246	2255	rBV	667776	999131	0.43%	0.117%
88	14.920	2265	2269	2274	rVB3	8753	11353	0.00%	0.001%
89	15.182	2309	2312	2313	rBV3	951	889	0.00%	0.000%
90	15.249	2316	2323	2333	rBV	1965132	2769149	1.19%	0.324%
91	15.353	2337	2340	2343	rBV4	1446	1241	0.00%	0.000%
92	15.536	2366	2370	2373	rBV5	1000	1483	0.00%	0.000%
93	15.865	2421	2424	2425	rBV2	994	1084	0.00%	0.000%
94	15.969	2439	2441	2445	rVV5	895	871	0.00%	0.000%
95	16.261	2487	2489	2494	rVB4	956	1335	0.00%	0.000%
96	16.304	2494	2496	2498	rBV3	945	1182	0.00%	0.000%
97	16.383	2506	2509	2511	rVV3	754	982	0.00%	0.000%
98	16.505	2523	2529	2537	rVV3	31279	60517	0.03%	0.007%
99	16.658	2551	2554	2556	rVB3	743	813	0.00%	0.000%
100	16.743	2566	2568	2570	rBV3	852	793	0.00%	0.000%

Sum of corrected areas: 853551996

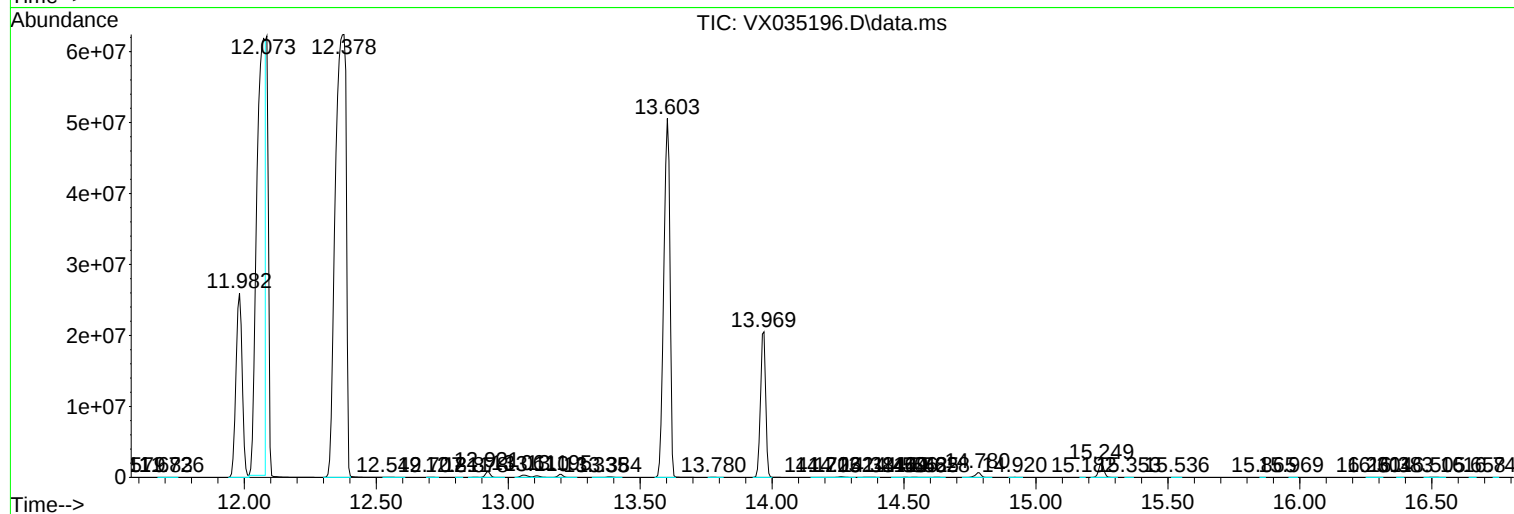
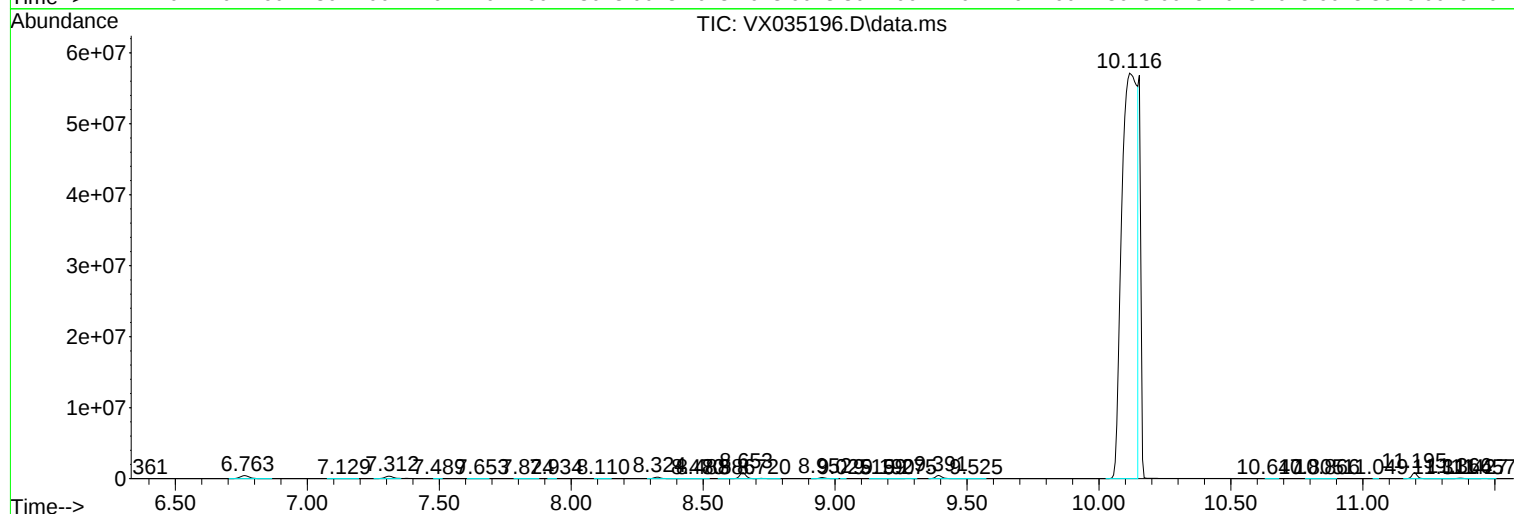
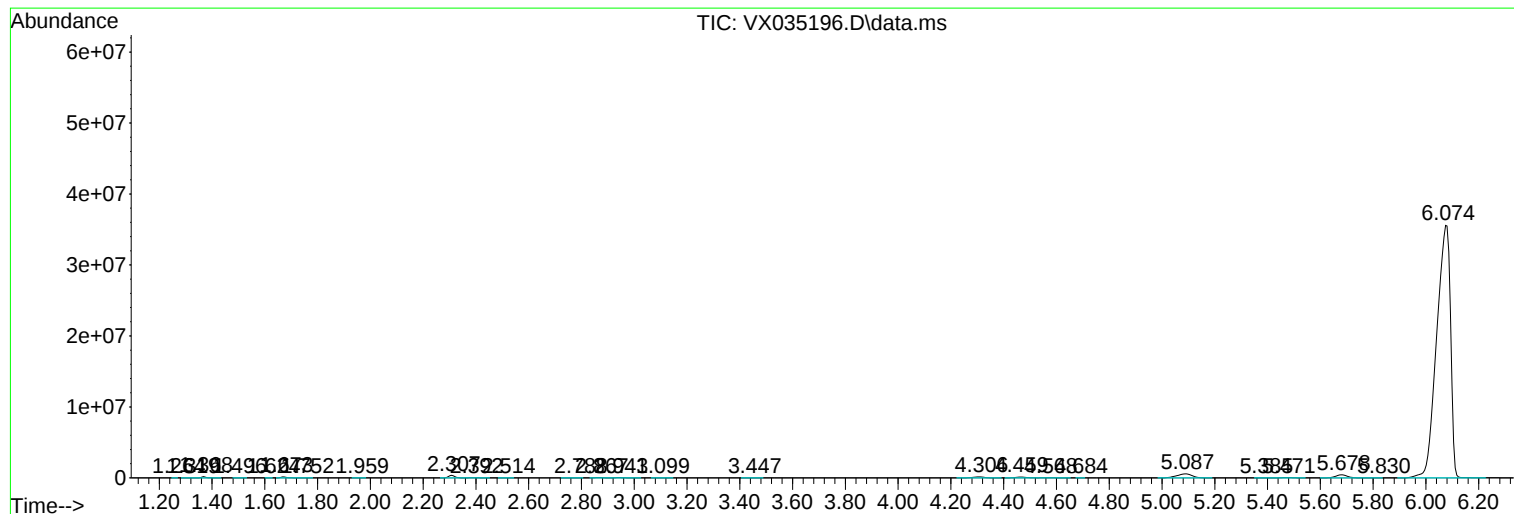
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
COMK7

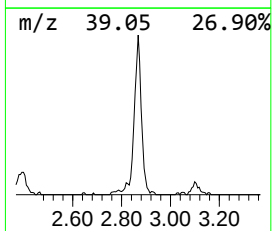
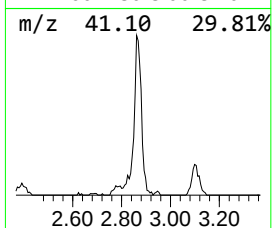
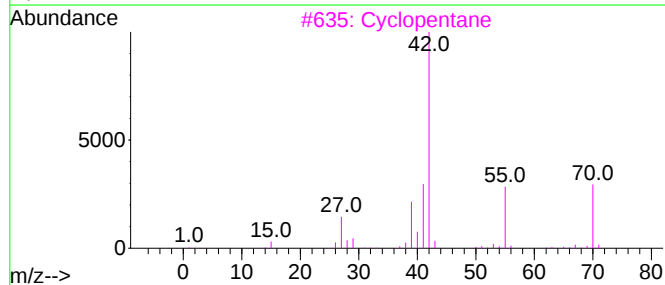
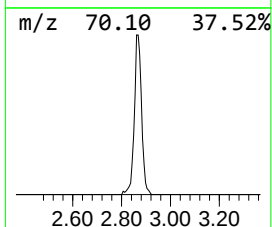
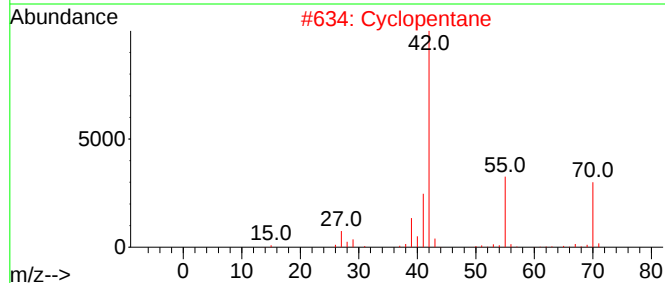
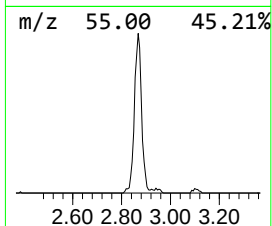
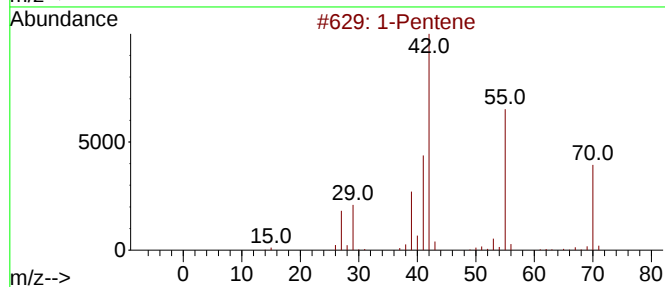
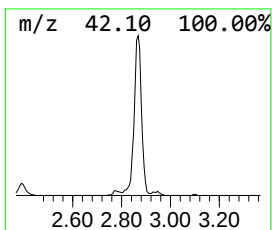
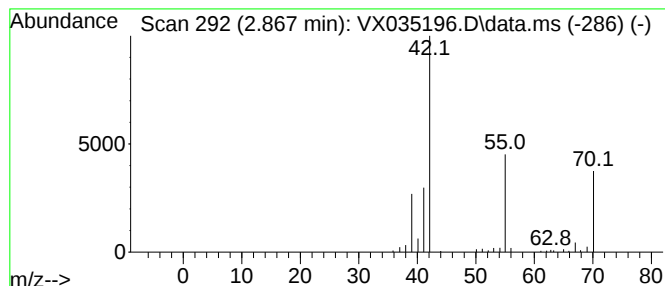
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.03 ug/L	100357	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	80
2		Cyclopentane	70	C5H10	000287-92-3	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO41923\
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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
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ClientSampleId :
COMK7

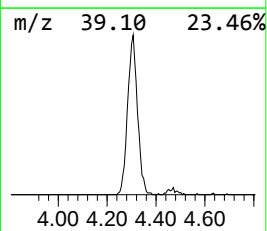
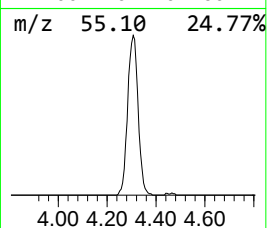
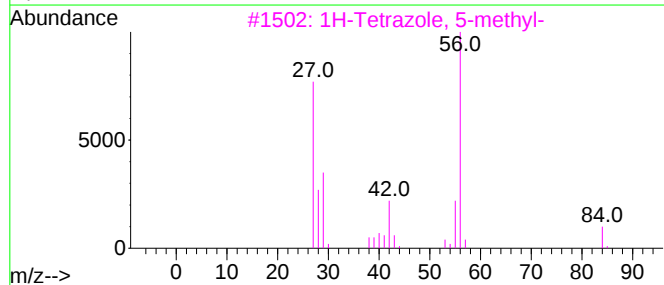
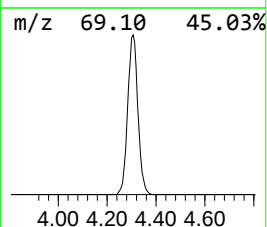
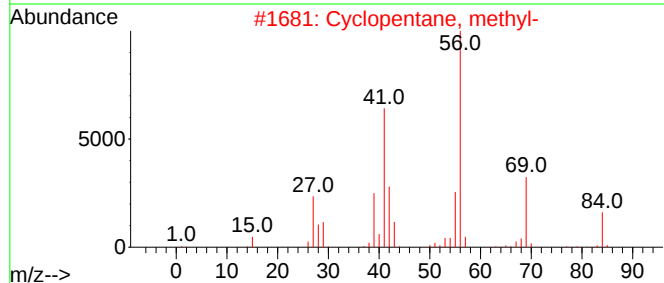
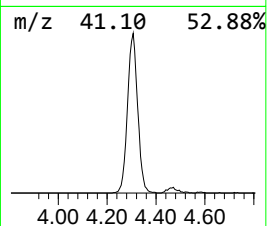
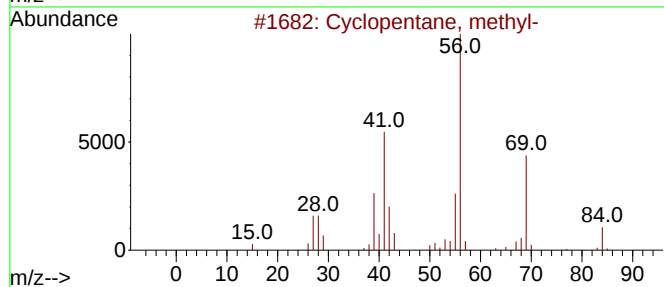
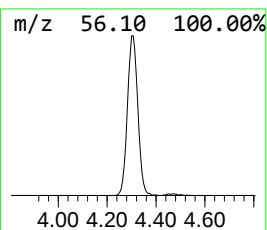
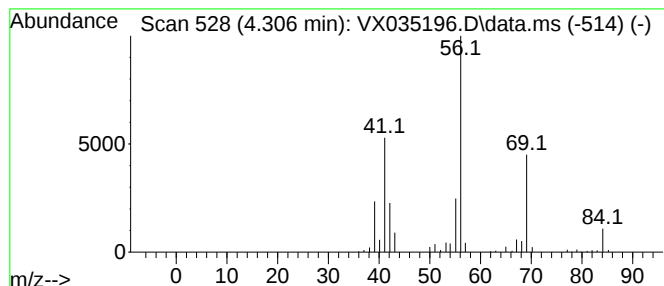
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic4.306 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	20.09 ug/L	400504	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5		Cyclohexane	84	C6H12	000110-82-7	78



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C0MK7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.867	5.0	ug/L	100357	1	6.763	996828	50.0
(DEL) Alkane: C...	4.306	20.1	ug/L	400504	1	6.763	996828	50.0