

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
 Data File : VU057847.D
 Acq On : 07 Feb 2024 18:00
 Operator : MD/SY
 Sample : P1081-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0B39

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_U\Method\SFAMULM020724WMA.M

Title : VOC Analysis

Signal : TIC: VU057847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	111	rVB	131330	165087	0.05%	0.017%
2	1.879	176	183	200	rVB	98132	144641	0.05%	0.015%
3	2.554	381	393	406	rBV	214432	352322	0.11%	0.037%
4	2.618	408	413	423	rVB	8266	13614	0.00%	0.001%
5	2.779	456	463	476	rVB2	4305	7086	0.00%	0.001%
6	2.904	498	502	508	rVB4	250	238	0.00%	0.000%
7	2.959	516	519	521	rVB2	410	213	0.00%	0.000%
8	3.033	532	542	558	rBV3	7952	17501	0.01%	0.002%
9	3.123	558	570	578	rBV2	21906	42690	0.01%	0.004%
10	3.348	630	640	651	rVB8	2735	5543	0.00%	0.001%
11	3.419	659	662	669	rVB3	339	367	0.00%	0.000%
12	3.538	694	699	703	rBV2	291	264	0.00%	0.000%
13	3.689	739	746	758	rVB7	1607	2996	0.00%	0.000%
14	3.779	770	774	780	rBV3	341	341	0.00%	0.000%
15	3.833	785	791	795	rVB3	215	242	0.00%	0.000%
16	3.869	795	802	805	rBV3	312	320	0.00%	0.000%
17	3.965	827	832	834	rBV3	226	152	0.00%	0.000%
18	4.014	843	847	851	rVB2	278	226	0.00%	0.000%
19	4.046	851	857	861	rBV3	330	456	0.00%	0.000%
20	4.165	892	894	898	rBV2	244	164	0.00%	0.000%
21	4.213	907	909	914	rBV3	197	169	0.00%	0.000%
22	4.409	965	970	974	rBV2	393	271	0.00%	0.000%
23	4.518	983	1004	1021	rBV2	70544	172137	0.05%	0.018%
24	4.624	1025	1037	1079	rBV4	58109	221011	0.07%	0.023%
25	4.827	1098	1100	1105	rVB3	551	371	0.00%	0.000%
26	4.988	1147	1150	1154	rBV2	238	210	0.00%	0.000%
27	5.065	1154	1174	1198	rBV5	244909	776088	0.24%	0.081%
28	5.190	1209	1213	1217	rBV5	599	619	0.00%	0.000%
29	5.251	1226	1232	1234	rBV3	459	440	0.00%	0.000%
30	5.264	1234	1236	1240	rVB2	296	181	0.00%	0.000%
31	5.313	1248	1251	1252	rBV	513	220	0.00%	0.000%
32	5.325	1252	1255	1256	rVV2	471	291	0.00%	0.000%
33	5.380	1257	1272	1287	rVB3	37201	84398	0.03%	0.009%
34	5.515	1300	1314	1330	rBV2	30018	66635	0.02%	0.007%
35	5.634	1339	1351	1352	rBV5	1054	1679	0.00%	0.000%
36	5.776	1357	1395	1430	rBV2	44962571	104210896	32.60%	10.934%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
 Title : VOC Analysis

37	6.242	1528	1540	1563	rVB	336420	645980	0.20%	0.068%
38	6.541	1622	1633	1644	rBV5	7156	13415	0.00%	0.001%
39	6.592	1647	1649	1654	rBV3	422	293	0.00%	0.000%
40	6.682	1664	1677	1693	rBV	226686	458631	0.14%	0.048%
41	6.923	1749	1752	1756	rBV3	305	245	0.00%	0.000%
42	6.972	1759	1767	1779	rVB7	1655	2787	0.00%	0.000%
43	7.062	1791	1795	1798	rVB	279	193	0.00%	0.000%
44	7.100	1798	1807	1813	rBV3	767	1397	0.00%	0.000%
45	7.145	1817	1821	1825	rVB3	274	294	0.00%	0.000%
46	7.174	1825	1830	1831	rBV2	593	465	0.00%	0.000%
47	7.303	1867	1870	1874	rBV2	361	290	0.00%	0.000%
48	7.357	1883	1887	1890	rBV2	256	224	0.00%	0.000%
49	7.438	1909	1912	1916	rVB2	270	186	0.00%	0.000%
50	7.496	1926	1930	1936	rVB4	460	302	0.00%	0.000%
51	7.560	1936	1950	1968	rBV	136418	247283	0.08%	0.026%
52	7.624	1968	1970	1973	rBV2	415	268	0.00%	0.000%
53	7.740	2003	2006	2012	rVB2	544	468	0.00%	0.000%
54	7.811	2019	2028	2034	rBV4	1172	1724	0.00%	0.000%
55	7.840	2034	2037	2041	rBV2	243	185	0.00%	0.000%
56	7.891	2041	2053	2068	rBV	468683	825610	0.26%	0.087%
57	7.968	2069	2077	2094	rVB2	25139	48523	0.02%	0.005%
58	8.177	2130	2142	2163	rBV	94090	169701	0.05%	0.018%
59	8.415	2213	2216	2218	rBV3	345	207	0.00%	0.000%
60	8.470	2224	2233	2243	rVB3	1996	3460	0.00%	0.000%
61	8.550	2248	2258	2273	rBV4	13508	24058	0.01%	0.003%
62	8.637	2273	2285	2315	rBV	286571	568838	0.18%	0.060%
63	8.862	2351	2355	2358	rVB3	415	286	0.00%	0.000%
64	8.910	2365	2370	2372	rBV2	203	147	0.00%	0.000%
65	8.978	2387	2391	2396	rBV3	275	245	0.00%	0.000%
66	9.087	2423	2425	2430	rVB3	316	213	0.00%	0.000%
67	9.119	2431	2435	2439	rVB3	250	203	0.00%	0.000%
68	9.155	2444	2446	2451	rVB2	311	186	0.00%	0.000%
69	9.216	2461	2465	2469	rVB4	364	335	0.00%	0.000%
70	9.290	2485	2488	2493	rVB	270	187	0.00%	0.000%
71	9.338	2499	2503	2505	rBV	357	245	0.00%	0.000%
72	9.370	2509	2513	2515	rBV	382	284	0.00%	0.000%
73	9.489	2515	2550	2606	rBV6	83837896	319637283	100.00%	33.535%
74	10.753	2931	2943	2971	rBV2	352010	829289	0.26%	0.087%
75	10.894	2980	2987	2995	rVB5	2844	3797	0.00%	0.000%
76	10.988	3005	3016	3030	rBV2	43181	74267	0.02%	0.008%

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 Title : VOC Analysis

77	11.052	3031	3036	3040	rVV5	1475	1742	0.00%	0.000%
78	11.100	3043	3051	3071	rVB2	22294	39801	0.01%	0.004%
79	11.354	3127	3130	3131	rBV	471	222	0.00%	0.000%
80	11.367	3132	3134	3138	rVB2	714	448	0.00%	0.000%
81	11.418	3145	3150	3151	rBV2	635	468	0.00%	0.000%
82	11.476	3160	3168	3172	rBV4	1363	2161	0.00%	0.000%
83	11.589	3199	3203	3207	rVB3	377	319	0.00%	0.000%
84	11.611	3207	3210	3214	rVB4	512	352	0.00%	0.000%
85	11.637	3215	3218	3220	rBV	546	328	0.00%	0.000%
86	11.750	3236	3253	3267	rBV	25396408	44030527	13.78%	4.620%
87	11.865	3267	3289	3333	rVB4	84724864	221682124	69.35%	23.258%
88	12.245	3380	3407	3443	rBV4	83802409	219564365	68.69%	23.036%
89	12.685	3539	3544	3553	rVB3	9378	13416	0.00%	0.001%
90	12.965	3621	3631	3648	rVB	200770	319738	0.10%	0.034%
91	13.148	3677	3688	3699	rBV3	26033	57950	0.02%	0.006%
92	13.209	3700	3707	3725	rVB4	23300	45359	0.01%	0.005%
93	13.325	3732	3743	3759	rVB	115233	185954	0.06%	0.020%
94	13.573	3812	3820	3832	rVB3	4870	8069	0.00%	0.001%
95	13.840	3887	3903	3927	rBV	18029092	28527140	8.92%	2.993%
96	14.087	3971	3980	3990	rVB	10710	17868	0.01%	0.002%
97	14.325	4039	4054	4077	rBV	5467958	8685172	2.72%	0.911%
98	14.733	4176	4181	4188	rBV5	2729	3809	0.00%	0.000%
99	15.415	4383	4393	4402	rVB3	22726	36354	0.01%	0.004%
100	15.997	4564	4574	4594	rVB2	35443	57864	0.02%	0.006%

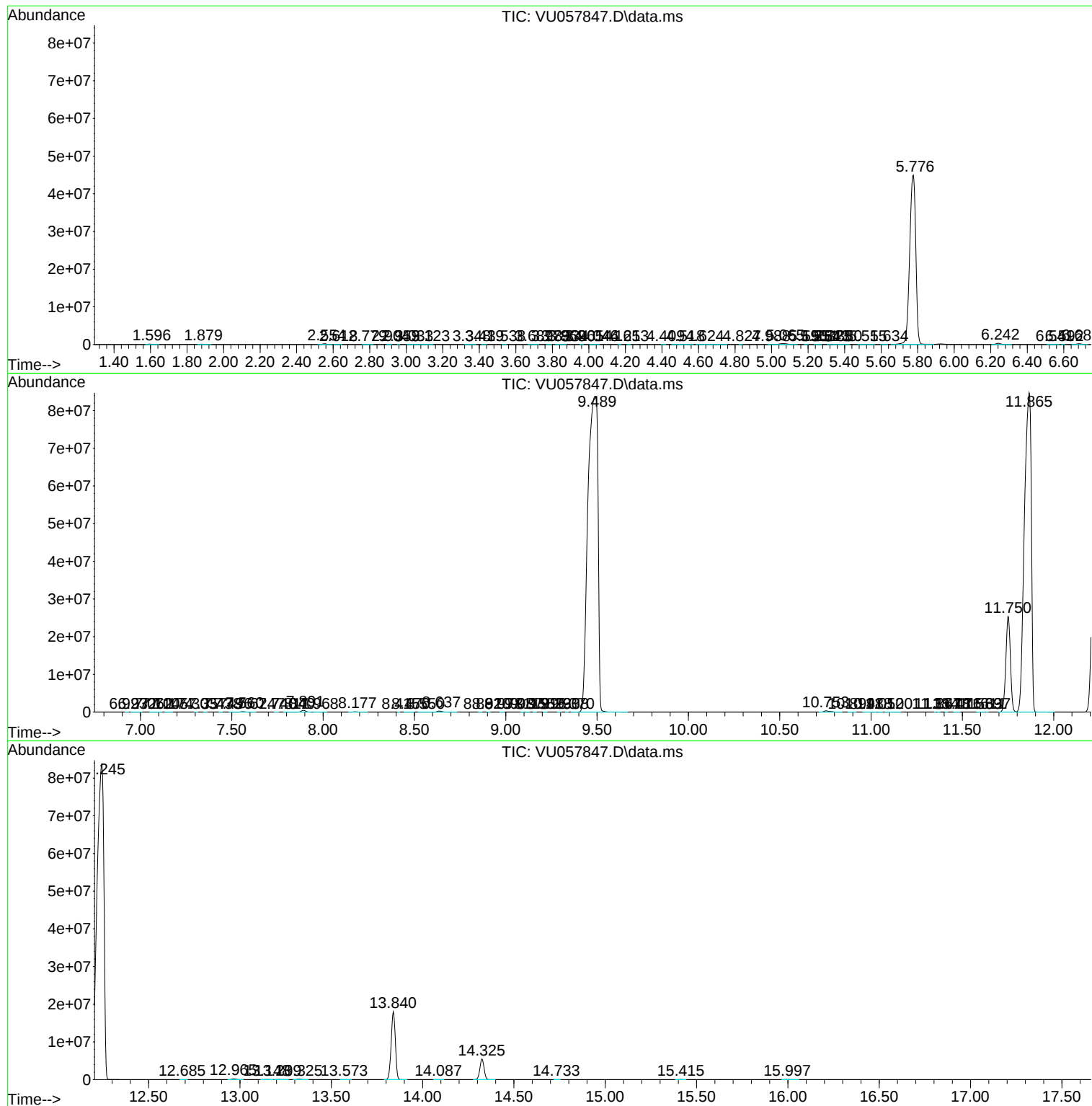
Sum of corrected areas: 953133623

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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



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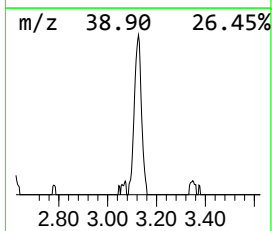
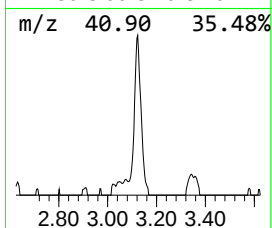
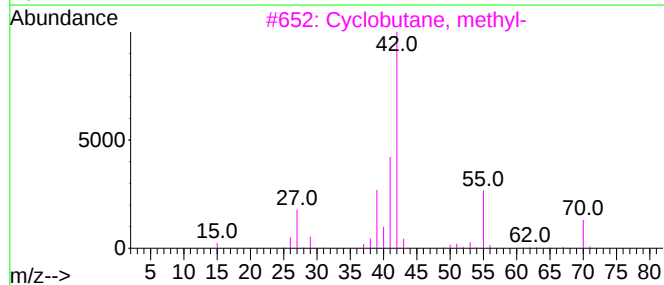
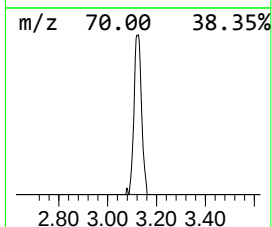
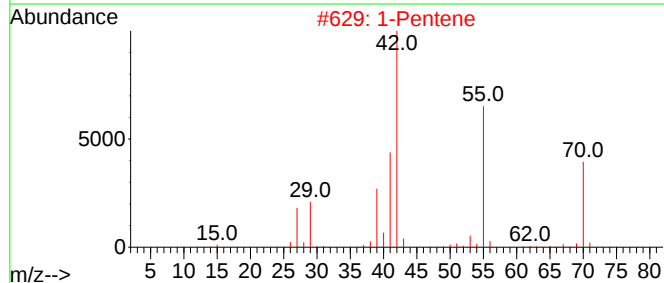
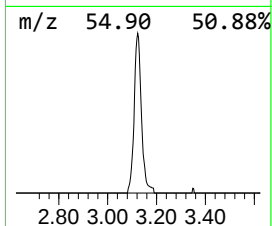
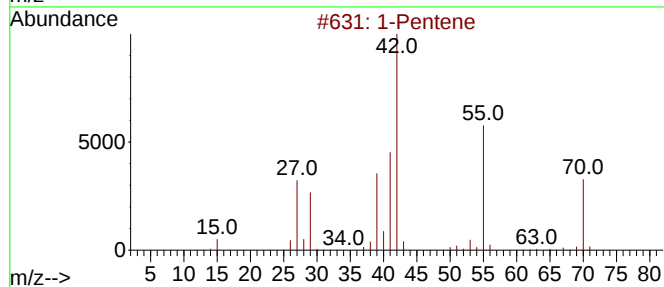
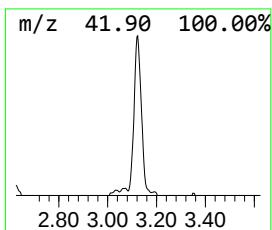
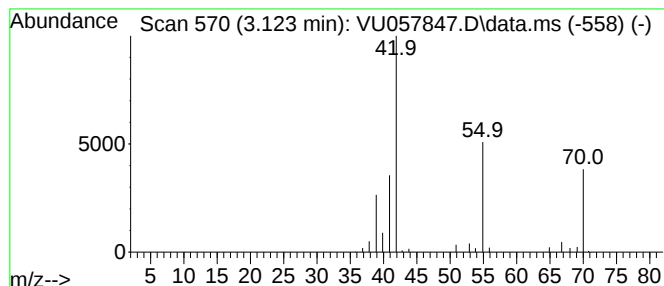
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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.
3.123	3.30 ug/L	42690	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	86
2		1-Pentene	70	C5H10	000109-67-1	86
3		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
4		Cyclopentane	70	C5H10	000287-92-3	78
5		Cyclopentane	70	C5H10	000287-92-3	56



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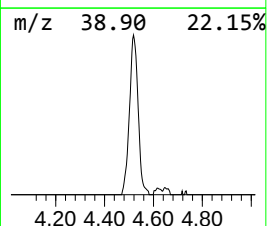
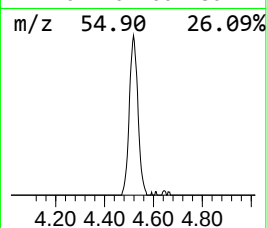
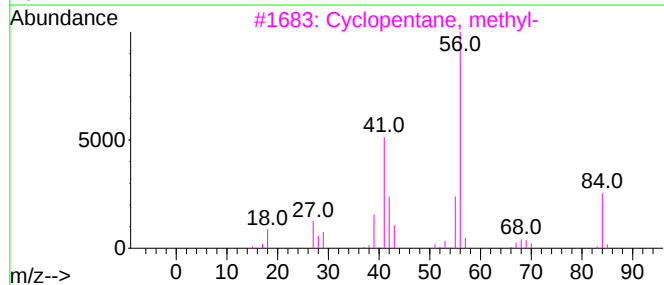
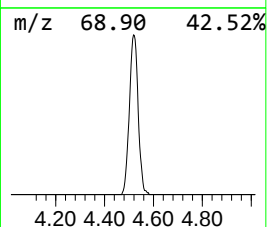
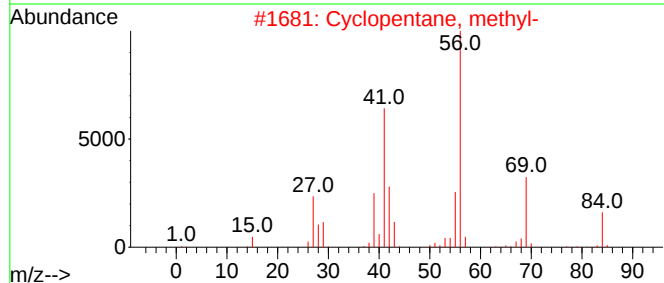
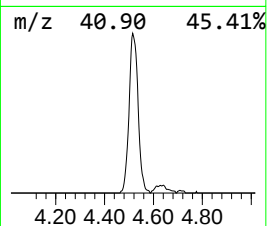
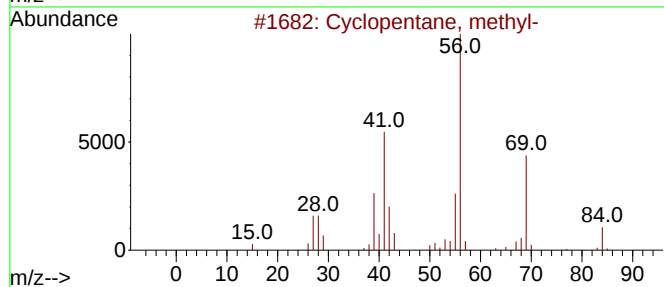
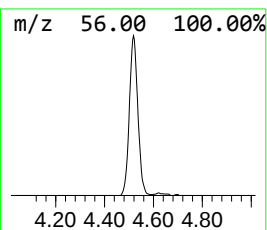
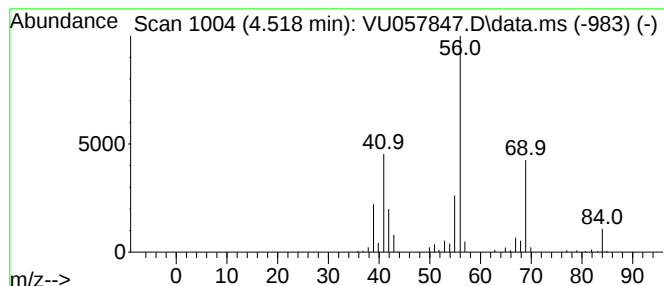
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Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.518 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.518	13.32 ug/L	172137	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
4			Cyclohexane	84	C6H12	000110-82-7	78
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	78



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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...	3.123	3.3	ug/L	42690	1	6.242	645980	50.0
(DEL) Alkane: C...	4.518	13.3	ug/L	172137	1	6.242	645980	50.0