

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
 Data File : VU057846.D
 Acq On : 07 Feb 2024 17:35
 Operator : MD/SY
 Sample : P1081-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0B38

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: VU057846.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	88	95	106	rBV	127543	149603	0.05%	0.019%
2	1.891	180	187	205	rVB	98524	139414	0.05%	0.017%
3	2.470	365	367	372	rVB3	510	437	0.00%	0.000%
4	2.493	372	374	378	rBV2	278	201	0.00%	0.000%
5	2.557	382	394	406	rBV	209068	342587	0.12%	0.043%
6	2.615	406	412	424	rVB	16413	27872	0.01%	0.003%
7	2.785	447	465	477	rBV2	7348	15451	0.01%	0.002%
8	2.895	496	499	504	rVB2	238	251	0.00%	0.000%
9	2.949	504	516	529	rBV3	1006	2063	0.00%	0.000%
10	3.036	529	543	555	rBV4	7804	16338	0.01%	0.002%
11	3.129	561	572	576	rBV2	24232	46138	0.02%	0.006%
12	3.174	577	586	623	rVB	109875	253126	0.09%	0.032%
13	3.351	631	641	653	rVB8	3871	8075	0.00%	0.001%
14	3.406	653	658	662	rVB2	243	253	0.00%	0.000%
15	3.679	737	743	744	rBV3	1039	780	0.00%	0.000%
16	3.859	797	799	804	rVV2	250	169	0.00%	0.000%
17	3.885	804	807	811	rVB2	199	147	0.00%	0.000%
18	4.033	848	853	857	rBV	126	130	0.00%	0.000%
19	4.087	867	870	874	rBV2	135	135	0.00%	0.000%
20	4.223	908	912	915	rBV	217	195	0.00%	0.000%
21	4.261	920	924	927	rVV2	195	196	0.00%	0.000%
22	4.309	935	939	945	rVV2	163	182	0.00%	0.000%
23	4.522	984	1005	1021	rBV3	99863	246241	0.08%	0.031%
24	4.621	1021	1036	1083	rVB4	70268	287574	0.10%	0.036%
25	5.055	1154	1171	1197	rVV3	189494	493810	0.17%	0.062%
26	5.187	1209	1212	1213	rBV2	259	155	0.00%	0.000%
27	5.267	1234	1237	1240	rVB3	314	181	0.00%	0.000%
28	5.300	1243	1247	1249	rBV2	418	392	0.00%	0.000%
29	5.325	1252	1255	1257	rVV2	363	294	0.00%	0.000%
30	5.380	1257	1272	1291	rVB2	48150	108469	0.04%	0.014%
31	5.480	1298	1303	1304	rBV	315	208	0.00%	0.000%
32	5.518	1304	1315	1324	rVV3	3610	7416	0.00%	0.001%
33	5.628	1339	1349	1357	rBV5	1133	2236	0.00%	0.000%
34	5.769	1357	1393	1425	rBV2	26611203	55750845	19.01%	6.987%
35	6.242	1528	1540	1563	rVB	321520	610555	0.21%	0.077%
36	6.383	1578	1584	1596	rVB4	1462	2588	0.00%	0.000%

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 Title : VOC Analysis

37	6.538	1622	1632	1645	rVB3	8492	16425	0.01%	0.002%
38	6.631	1657	1661	1662	rBV	305	190	0.00%	0.000%
39	6.682	1663	1677	1694	rBV	221509	447875	0.15%	0.056%
40	6.952	1757	1761	1763	rBV2	353	205	0.00%	0.000%
41	6.972	1763	1767	1772	rBV4	561	451	0.00%	0.000%
42	7.097	1803	1806	1807	rBV	207	133	0.00%	0.000%
43	7.171	1826	1829	1832	rBV2	263	246	0.00%	0.000%
44	7.193	1832	1836	1839	rVB3	349	272	0.00%	0.000%
45	7.406	1893	1902	1908	rBV4	1636	2327	0.00%	0.000%
46	7.464	1916	1920	1925	rVB2	306	285	0.00%	0.000%
47	7.505	1925	1933	1936	rBV2	248	325	0.00%	0.000%
48	7.560	1936	1950	1968	rBV	130553	235586	0.08%	0.030%
49	7.727	2000	2002	2007	rVB2	321	157	0.00%	0.000%
50	7.798	2019	2024	2025	rBV	200	168	0.00%	0.000%
51	7.894	2041	2054	2067	rBV	473590	824125	0.28%	0.103%
52	7.965	2068	2076	2092	rVB	79205	142565	0.05%	0.018%
53	8.177	2128	2142	2160	rBV	90523	160316	0.05%	0.020%
54	8.338	2188	2192	2196	rBV2	137	127	0.00%	0.000%
55	8.373	2196	2203	2206	rBV	210	318	0.00%	0.000%
56	8.454	2224	2228	2229	rBV2	262	157	0.00%	0.000%
57	8.473	2231	2234	2242	rVB3	711	740	0.00%	0.000%
58	8.550	2248	2258	2270	rVB4	16728	28650	0.01%	0.004%
59	8.637	2273	2285	2319	rBV	268850	539931	0.18%	0.068%
60	8.798	2333	2335	2337	rVB	338	139	0.00%	0.000%
61	8.869	2354	2357	2360	rBV2	222	146	0.00%	0.000%
62	8.955	2381	2384	2390	rBV2	328	284	0.00%	0.000%
63	9.042	2406	2411	2413	rBV	164	156	0.00%	0.000%
64	9.081	2420	2423	2424	rBV2	318	181	0.00%	0.000%
65	9.187	2453	2456	2459	rVB2	268	172	0.00%	0.000%
66	9.274	2480	2483	2486	rVB	185	126	0.00%	0.000%
67	9.296	2486	2490	2495	rBV2	307	317	0.00%	0.000%
68	9.322	2495	2498	2501	rBV2	205	151	0.00%	0.000%
69	9.341	2501	2504	2508	rVB	194	128	0.00%	0.000%
70	9.489	2513	2550	2554	rBV6	82815329	293291082	100.00%	36.757%
71	10.753	2931	2943	2970	rBV2	338529	772571	0.26%	0.097%
72	10.984	3006	3015	3028	rVB	29142	47857	0.02%	0.006%
73	11.100	3043	3051	3063	rVB2	14407	24982	0.01%	0.003%
74	11.164	3068	3071	3073	rBV3	231	150	0.00%	0.000%
75	11.203	3079	3083	3086	rBV4	652	569	0.00%	0.000%
76	11.280	3103	3107	3108	rBV2	425	344	0.00%	0.000%

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77	11.312	3114	3117	3122	rBV3	408	399	0.00%	0.000%
78	11.399	3142	3144	3146	rVB2	301	136	0.00%	0.000%
79	11.418	3146	3150	3152	rBV3	748	554	0.00%	0.000%
80	11.473	3159	3167	3173	rBV5	1552	2552	0.00%	0.000%
81	11.553	3189	3192	3196	rBV	381	269	0.00%	0.000%
82	11.750	3237	3253	3266	rBV	13055822	22472209	7.66%	2.816%
83	11.862	3266	3288	3322	rVB4	81478769	206641099	70.46%	25.897%
84	12.241	3380	3406	3448	rBV4	81027380	203627878	69.43%	25.520%
85	12.682	3538	3543	3553	rVB3	8063	11649	0.00%	0.001%
86	12.901	3608	3611	3618	rVV6	1698	2218	0.00%	0.000%
87	12.965	3621	3631	3648	rVB2	104755	171926	0.06%	0.022%
88	13.090	3666	3670	3677	rVB6	1264	1625	0.00%	0.000%
89	13.148	3680	3688	3689	rBV4	5265	5825	0.00%	0.001%
90	13.219	3705	3710	3719	rVB6	4343	6115	0.00%	0.001%
91	13.325	3733	3743	3758	rVB2	52548	83703	0.03%	0.010%
92	13.495	3790	3796	3801	rBV6	779	1125	0.00%	0.000%
93	13.569	3814	3819	3822	rBV3	1344	1587	0.00%	0.000%
94	13.672	3849	3851	3854	rBV2	426	291	0.00%	0.000%
95	13.836	3887	3902	3927	rBV	5022153	7927154	2.70%	0.993%
96	14.087	3972	3980	3991	rVB	11754	19681	0.01%	0.002%
97	14.325	4041	4054	4083	rVB	1173173	1883097	0.64%	0.236%
98	14.489	4102	4105	4109	rBV3	463	469	0.00%	0.000%
99	15.415	4389	4393	4402	rVB5	1495	1449	0.00%	0.000%
100	15.675	4470	4474	4477	rBV4	704	740	0.00%	0.000%

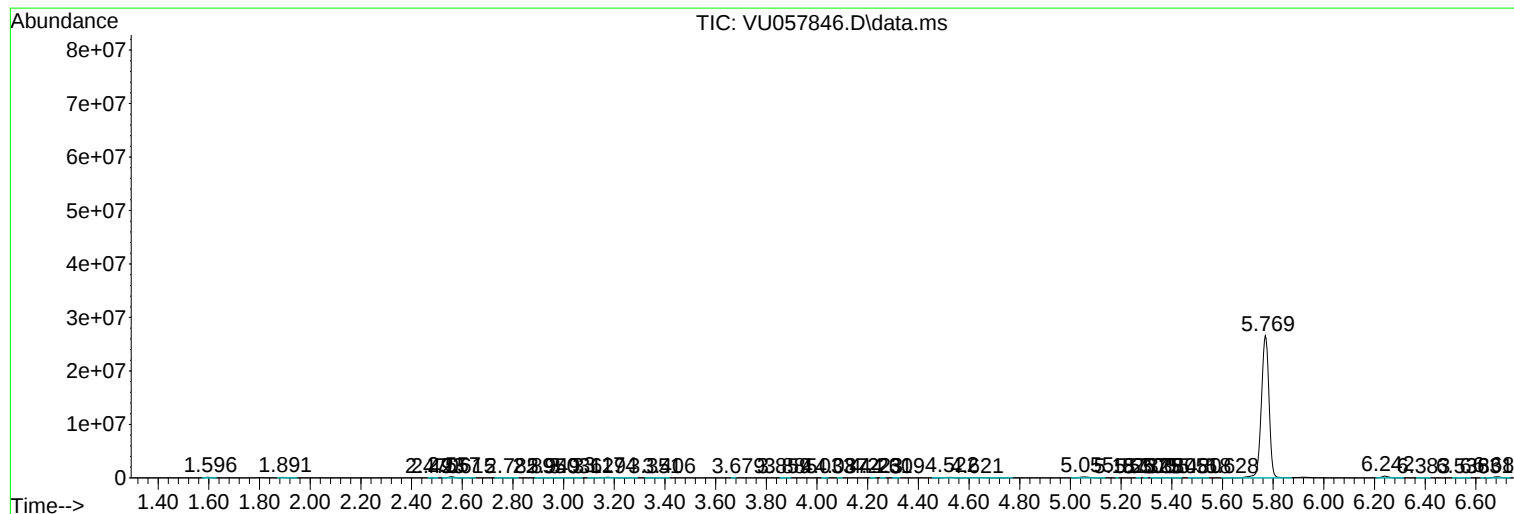
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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



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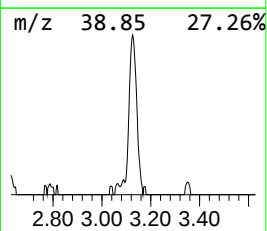
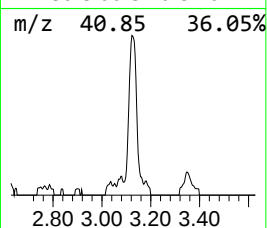
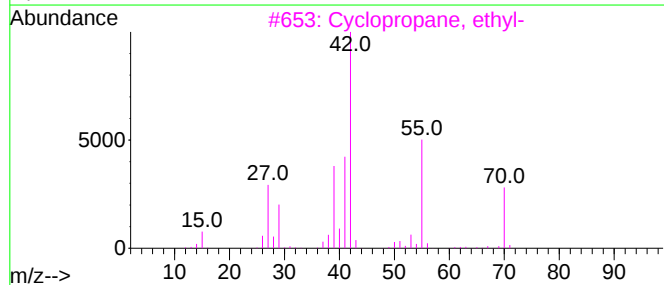
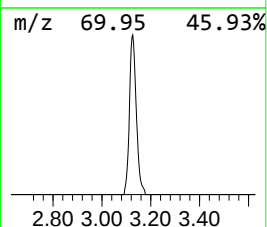
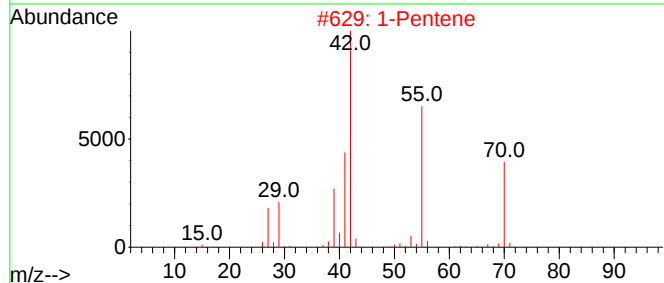
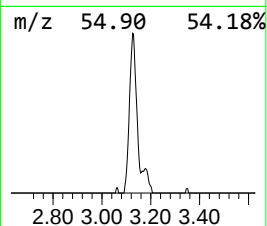
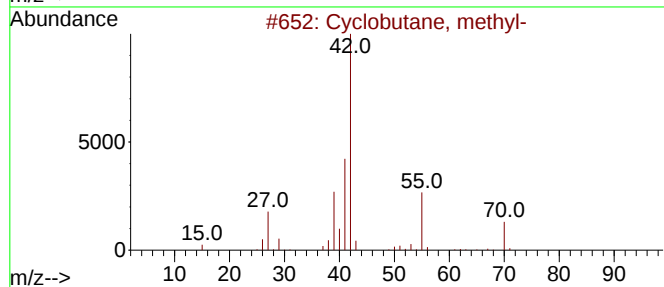
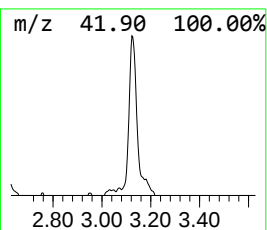
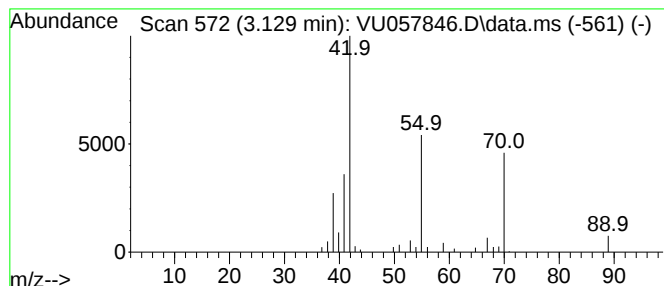
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic3.129 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.129	3.78 ug/L	46138	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2		1-Pentene	70	C5H10	000109-67-1	72
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	53
4		1-Pentene	70	C5H10	000109-67-1	53
5		1-Pentene	70	C5H10	000109-67-1	45



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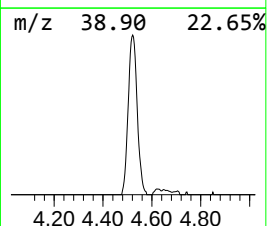
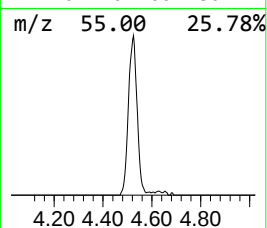
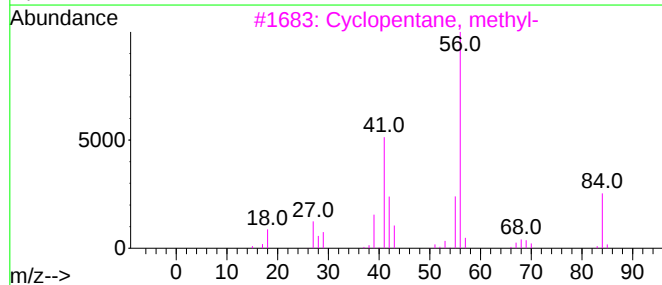
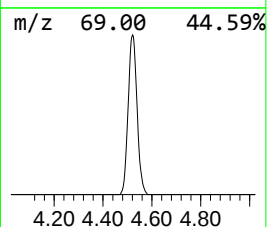
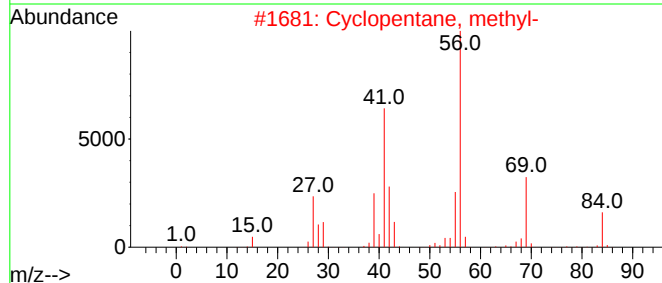
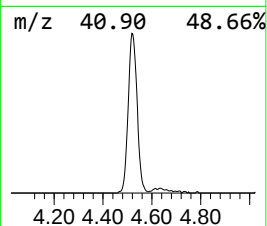
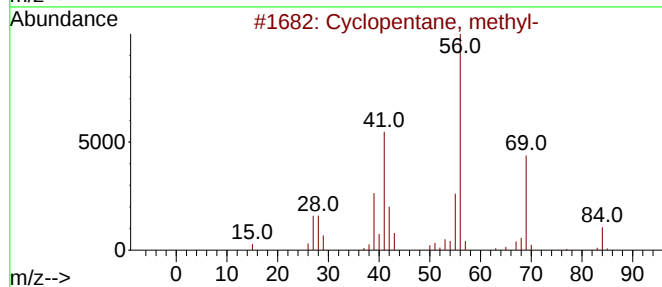
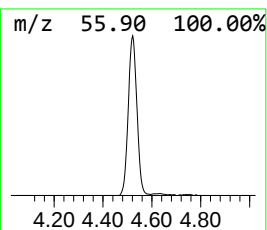
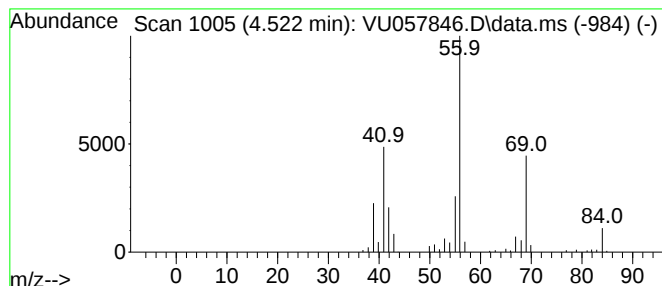
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic4.522 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.522	20.17 ug/L	246241	1,4-Difluorobenzene	6.242

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	90
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
4			Cyclohexane	84	C6H12	000110-82-7	78
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72



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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: C...	3.129	3.8	ug/L	46138	1	6.242	610555	50.0
(DEL) Alkane: C...	4.522	20.2	ug/L	246241	1	6.242	610555	50.0