

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU010719\
 Data File : VU029054.D
 Acq On : 07 Jan 2019 12:52
 Operator : MD/SY
 Sample : K1048-05
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0950

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	62	69	80	rBV	114792	113464	0.04%	0.012%
2	1.668	146	154	168	rVB	82019	103137	0.03%	0.011%
3	1.939	235	238	251	rVB6	2807	3485	0.00%	0.000%
4	1.990	252	254	257	rBV2	662	429	0.00%	0.000%
5	2.186	307	315	322	rBV4	1737	2838	0.00%	0.000%
6	2.266	329	340	351	rBV	167418	256908	0.08%	0.028%
7	2.321	351	357	373	rVB	21381	34754	0.01%	0.004%
8	2.447	385	396	418	rBV	27184	52530	0.02%	0.006%
9	2.623	448	451	457	rBV2	400	303	0.00%	0.000%
10	2.701	467	475	480	rBV5	3268	5351	0.00%	0.001%
11	2.787	494	502	510	rBV	14068	22879	0.01%	0.003%
12	2.993	555	566	579	rVV3	4492	8843	0.00%	0.001%
13	3.164	617	619	625	rVV2	227	250	0.00%	0.000%
14	3.302	651	662	675	rVB4	2946	5656	0.00%	0.001%
15	3.440	702	705	709	rVB2	267	179	0.00%	0.000%
16	3.540	732	736	742	rBV	138	173	0.00%	0.000%
17	3.971	864	870	872	rBV2	465	392	0.00%	0.000%
18	4.093	889	908	923	rBV2	73687	200147	0.06%	0.022%
19	4.176	923	934	965	rVB2	67647	192105	0.06%	0.021%
20	4.450	1013	1019	1025	rBV4	419	574	0.00%	0.000%
21	4.485	1028	1030	1032	rVB	393	163	0.00%	0.000%
22	4.501	1032	1035	1039	rBV2	213	189	0.00%	0.000%
23	4.668	1064	1087	1113	rBV2	392602	1090683	0.35%	0.119%
24	4.774	1119	1120	1125	rVB	404	254	0.00%	0.000%
25	4.877	1148	1152	1154	rBV3	255	213	0.00%	0.000%
26	4.993	1169	1188	1206	rVB3	30374	74236	0.02%	0.008%
27	5.135	1208	1232	1253	rBV	175446	402788	0.13%	0.044%
28	5.215	1254	1257	1258	rBV3	282	170	0.00%	0.000%
29	5.253	1264	1269	1272	rBV4	829	956	0.00%	0.000%
30	5.401	1273	1315	1350	rBV2	27535452	60553354	19.55%	6.632%
31	5.884	1452	1465	1490	rVB	222231	431539	0.14%	0.047%
32	6.064	1517	1521	1524	rVB2	293	207	0.00%	0.000%
33	6.083	1524	1527	1530	rBV	309	188	0.00%	0.000%
34	6.183	1546	1558	1559	rBV6	3560	3499	0.00%	0.000%

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 Title : VOC Analysis

35	6.253	1577	1580	1586	rVB2	263	195	0.00%	0.000%
36	6.327	1588	1603	1617	rBV	163452	324724	0.10%	0.036%
37	6.472	1645	1648	1656	rVB2	370	232	0.00%	0.000%
38	6.639	1692	1700	1709	rVB4	2288	3958	0.00%	0.000%
39	6.755	1720	1736	1748	rBV4	4902	8979	0.00%	0.001%
40	6.829	1756	1759	1765	rBV2	209	201	0.00%	0.000%
41	7.067	1828	1833	1837	rBV4	702	677	0.00%	0.000%
42	7.224	1870	1882	1901	rBV	97408	169879	0.05%	0.019%
43	7.392	1924	1934	1941	rBV4	1980	2773	0.00%	0.000%
44	7.469	1952	1958	1965	rBV2	487	857	0.00%	0.000%
45	7.565	1972	1988	2003	rBV	351348	606508	0.20%	0.066%
46	7.639	2004	2011	2032	rVB	11722	21815	0.01%	0.002%
47	7.848	2065	2076	2093	rBV	66934	113909	0.04%	0.012%
48	7.935	2099	2103	2108	rVB3	228	203	0.00%	0.000%
49	8.179	2169	2179	2185	rBV2	631	1041	0.00%	0.000%
50	8.228	2185	2194	2206	rVB3	10523	16473	0.01%	0.002%
51	8.314	2209	2221	2248	rBV	197779	359027	0.12%	0.039%
52	8.459	2263	2266	2267	rBV2	564	312	0.00%	0.000%
53	8.478	2267	2272	2279	rVB3	1368	1782	0.00%	0.000%
54	8.530	2285	2288	2292	rVB3	280	222	0.00%	0.000%
55	8.855	2385	2389	2397	rBV	108	174	0.00%	0.000%
56	9.183	2452	2491	2514	rBV4	80221342	309708108	100.00%	33.918%
57	9.787	2671	2679	2689	rBV8	2422	3748	0.00%	0.000%
58	9.964	2729	2734	2738	rVB4	764	787	0.00%	0.000%
59	9.983	2738	2740	2745	rVV3	199	171	0.00%	0.000%
60	10.048	2758	2760	2764	rVB2	312	190	0.00%	0.000%
61	10.076	2764	2769	2772	rBV3	316	330	0.00%	0.000%
62	10.118	2778	2782	2784	rBV	271	261	0.00%	0.000%
63	10.170	2794	2798	2799	rBV2	271	169	0.00%	0.000%
64	10.205	2806	2809	2811	rBV2	290	176	0.00%	0.000%
65	10.234	2815	2818	2823	rBV2	351	337	0.00%	0.000%
66	10.260	2823	2826	2827	rBV2	536	274	0.00%	0.000%
67	10.321	2837	2845	2848	rBV3	766	777	0.00%	0.000%
68	10.433	2867	2880	2905	rVV2	253463	523042	0.17%	0.057%
69	10.575	2920	2924	2925	rBV	370	213	0.00%	0.000%
70	10.662	2940	2951	2964	rVB	19895	32004	0.01%	0.004%
71	10.710	2964	2966	2968	rBV2	348	188	0.00%	0.000%

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 Title : VOC Analysis

72	10.774	2977	2986	2999	rBV2	9602	14704	0.00%	0.002%
73	11.025	3061	3064	3068	rVV	431	340	0.00%	0.000%
74	11.064	3073	3076	3079	rVV2	353	229	0.00%	0.000%
75	11.105	3082	3089	3094	rVV2	1566	1879	0.00%	0.000%
76	11.160	3100	3106	3114	rBV3	454	579	0.00%	0.000%
77	11.366	3166	3170	3172	rBV	287	189	0.00%	0.000%
78	11.427	3172	3189	3202	rBV	13588569	23832013	7.69%	2.610%
79	11.549	3202	3227	3244	rVB4	81306138	203205411	65.61%	22.254%
80	11.932	3313	3346	3371	rBV4	86305388	248648343	80.28%	27.231%
81	12.353	3470	3477	3485	rVB4	5004	7872	0.00%	0.001%
82	12.436	3500	3503	3510	rBV5	607	704	0.00%	0.000%
83	12.575	3540	3546	3554	rBV7	2112	3169	0.00%	0.000%
84	12.633	3554	3564	3579	rVB	159416	243693	0.08%	0.027%
85	12.816	3609	3621	3628	rVV3	38961	85334	0.03%	0.009%
86	12.861	3629	3635	3656	rVB2	79201	151911	0.05%	0.017%
87	12.986	3663	3674	3696	rVB	82804	134621	0.04%	0.015%
88	13.237	3739	3752	3766	rBV3	7344	12405	0.00%	0.001%
89	13.314	3774	3776	3785	rVB5	1586	1843	0.00%	0.000%
90	13.517	3820	3839	3873	rBV	31208721	48897489	15.79%	5.355%
91	13.745	3904	3910	3921	rVB	5961	8850	0.00%	0.001%
92	13.989	3970	3986	4019	rBV	7094212	10819946	3.49%	1.185%
93	14.382	4099	4108	4128	rBV4	16669	31041	0.01%	0.003%
94	14.539	4141	4157	4168	rVB7	5096	11905	0.00%	0.001%
95	14.700	4199	4207	4214	rBV8	1058	1979	0.00%	0.000%
96	14.755	4218	4224	4231	rVB3	1235	1605	0.00%	0.000%
97	14.858	4252	4256	4266	rBV8	1495	2180	0.00%	0.000%
98	15.070	4305	4322	4340	rBV	262374	454339	0.15%	0.050%
99	15.452	4439	4441	4445	rBV3	474	354	0.00%	0.000%
100	15.645	4489	4501	4526	rBV	655322	1066709	0.34%	0.117%

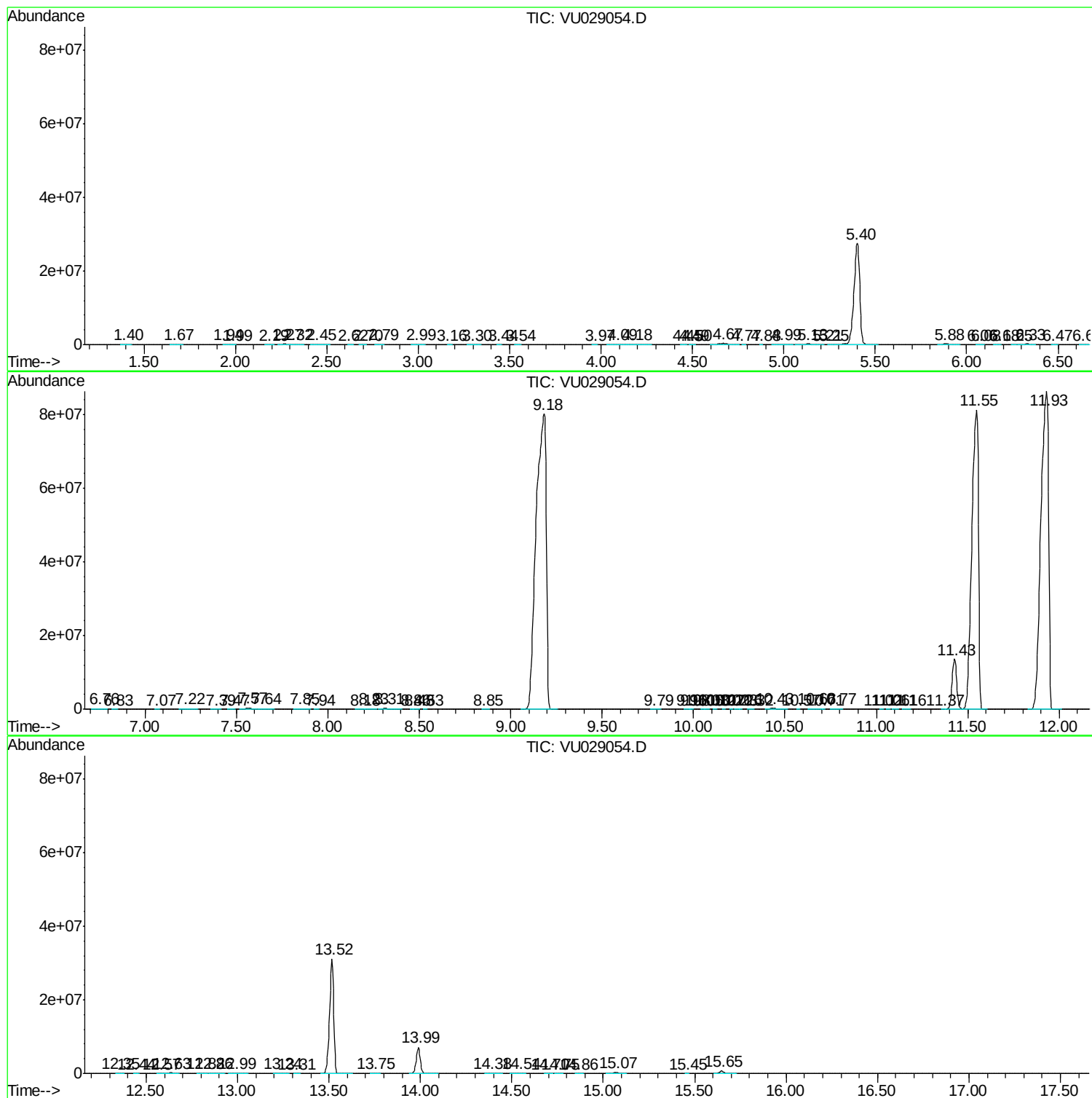
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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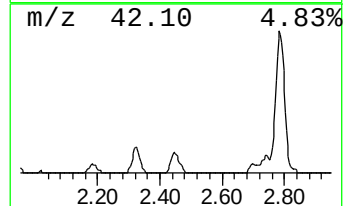
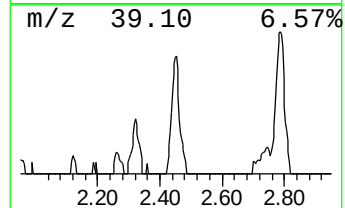
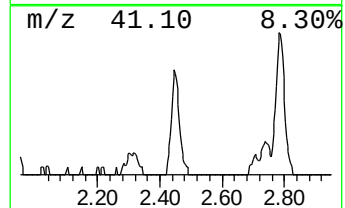
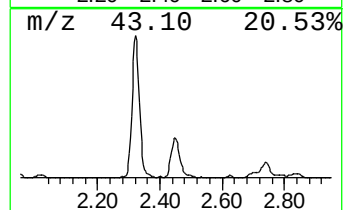
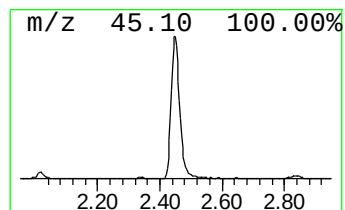
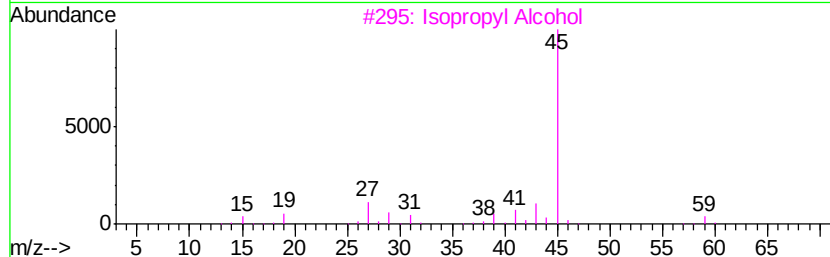
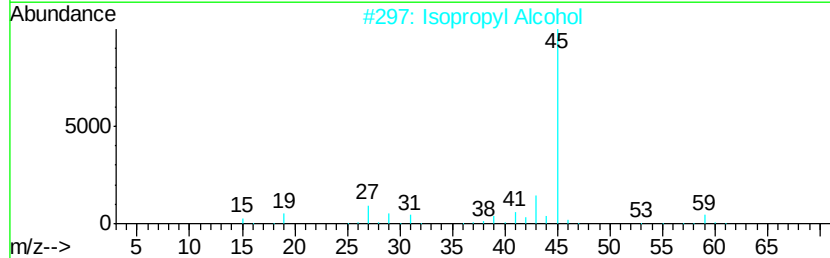
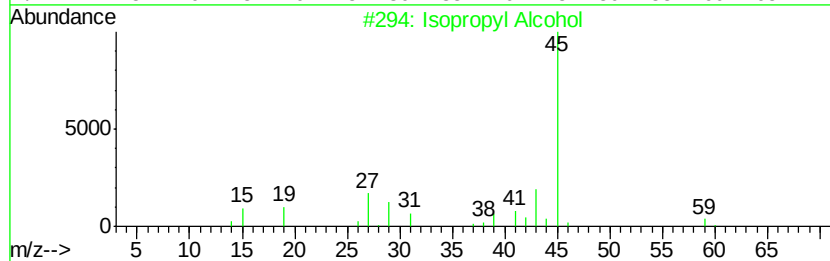
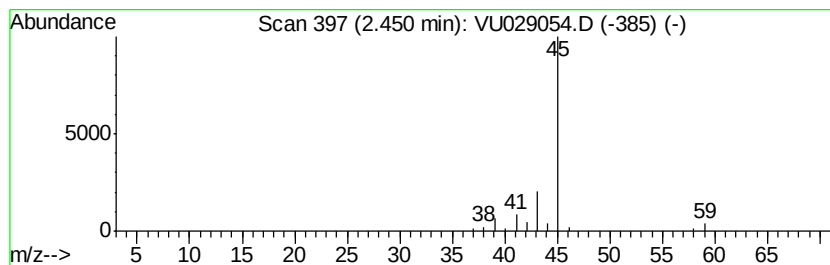
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	6.09 ug/L	52530	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Ethylamine	45	C2H7N	000075-04-7	5



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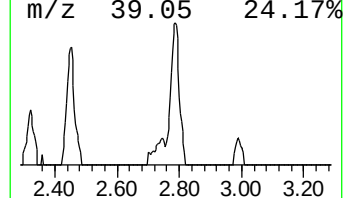
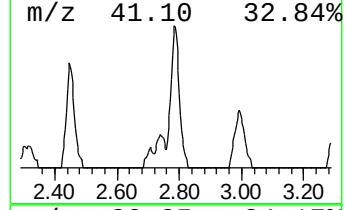
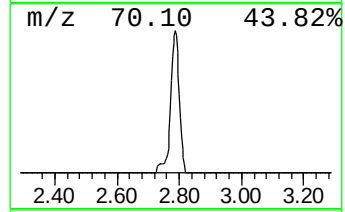
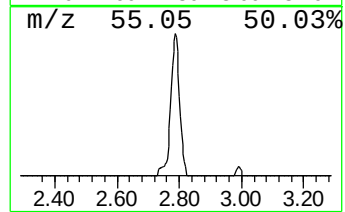
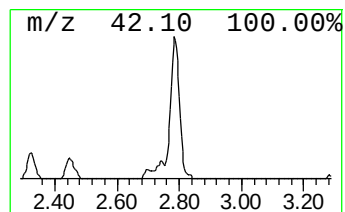
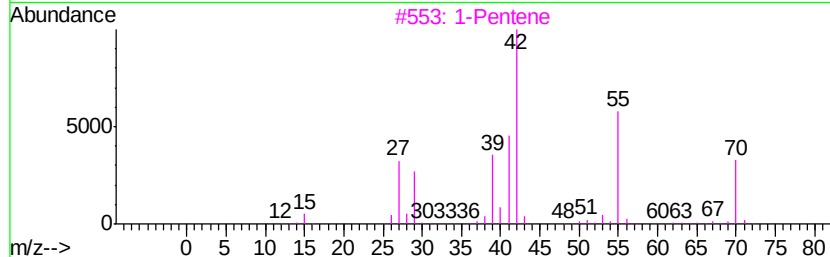
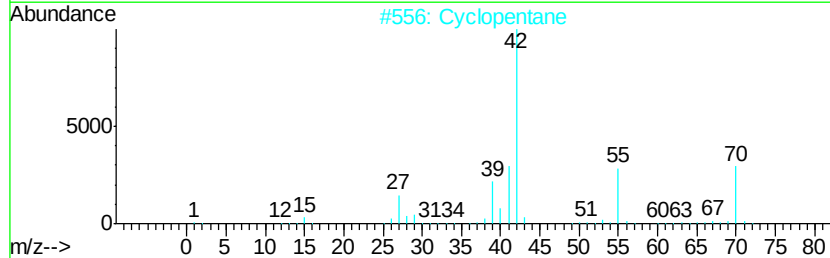
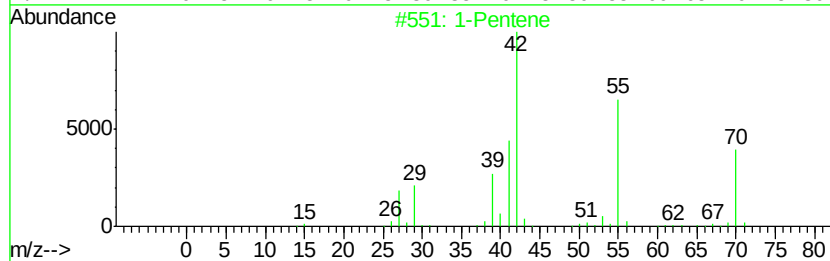
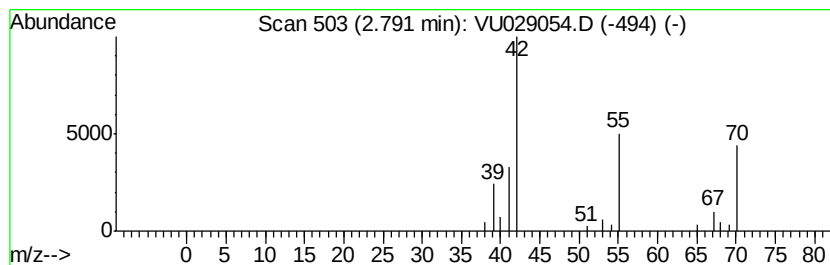
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic2.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	2.65 ug/L	22879	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	86
2			Cyclopentane	70	C5H10	000287-92-3	78
3			1-Pentene	70	C5H10	000109-67-1	56
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	23
5			Cyclopentane	70	C5H10	000287-92-3	9



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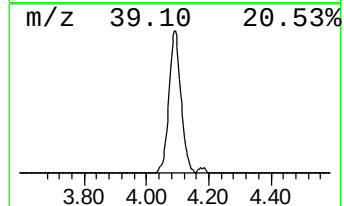
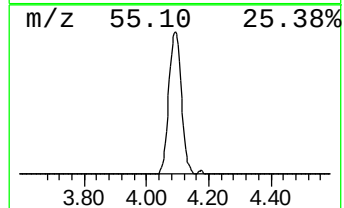
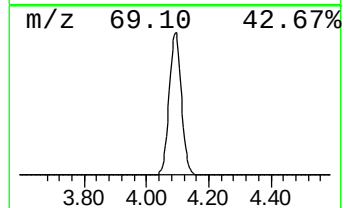
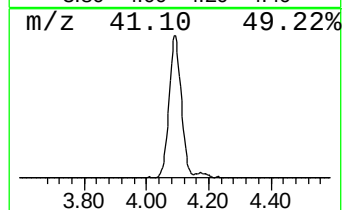
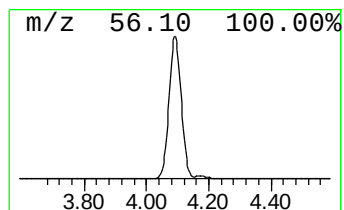
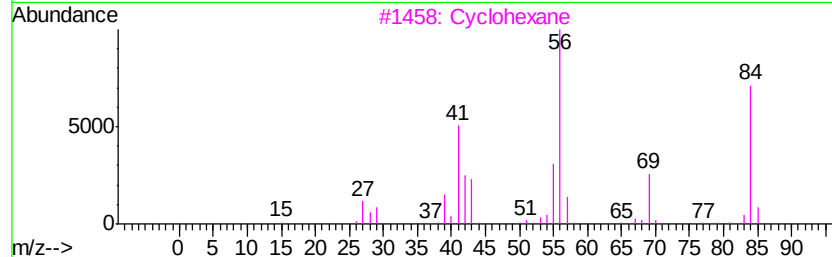
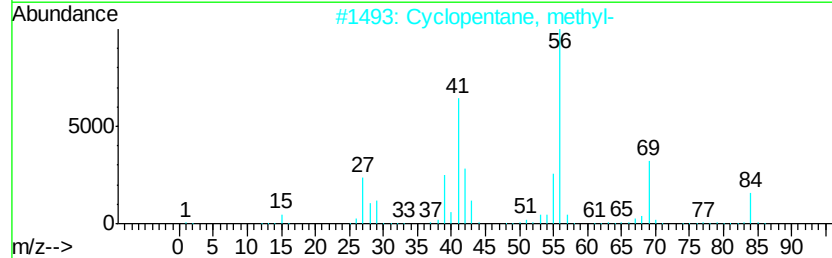
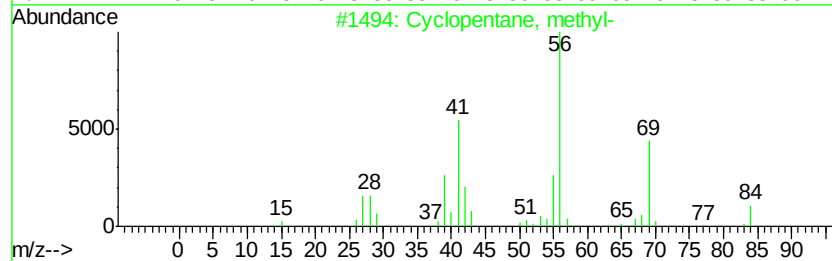
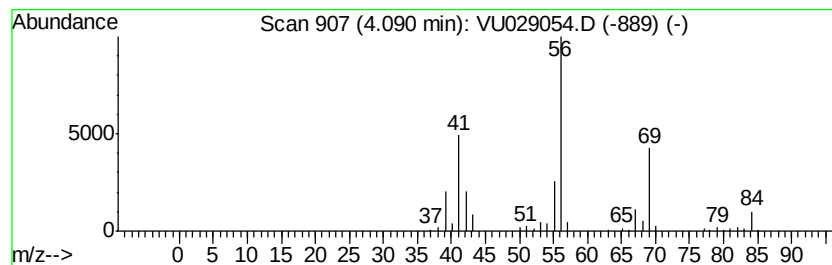
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic4.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	23.19 ug/L	200147	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3		Cyclohexane	84	C6H12	000110-82-7	78
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	72



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Operator : MD/SY
Sample : K1048-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0950

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.45	6.1	ug/L	52530	1	5.88	431539	50.0
(DEL) Alkane: Cyc...	2.79	2.6	ug/L	22879	1	5.88	431539	50.0
(DEL) Alkane: Cyc...	4.09	23.2	ug/L	200147	1	5.88	431539	50.0