

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060619\
 Data File : VU032490.D
 Acq On : 06 Jun 2019 12:35
 Operator : JC/SP
 Sample : K3017-08ME
 Misc : 4.66g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A51E1ME

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\SOMULM060619WMA.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	1.392	87	94	111	rVB	51495	73244	10.91%	1.198%
2	2.228	345	354	370	rVB	143195	219475	32.69%	3.591%
3	2.617	467	475	491	rBV	15410	29367	4.37%	0.480%
4	2.823	528	539	555	rBV	15593	34794	5.18%	0.569%
5	3.093	620	623	627	rVB2	312	231	0.03%	0.004%
6	3.122	628	632	634	rVB	288	148	0.02%	0.002%
7	3.190	649	653	656	rBV2	206	195	0.03%	0.003%
8	3.241	667	669	672	rVB	257	158	0.02%	0.003%
9	3.321	692	694	697	rVB	220	112	0.02%	0.002%
10	3.347	697	702	703	rBV	246	149	0.02%	0.002%
11	3.428	720	727	732	rBV4	631	861	0.13%	0.014%
12	3.511	749	753	754	rBV	203	157	0.02%	0.003%
13	3.537	756	761	763	rBV	269	195	0.03%	0.003%
14	3.585	772	776	777	rBV	182	130	0.02%	0.002%
15	3.633	784	791	794	rBV3	629	908	0.14%	0.015%
16	3.691	806	809	812	rBV	303	204	0.03%	0.003%
17	3.791	835	840	842	rBV2	218	177	0.03%	0.003%
18	3.884	866	869	872	rBV	148	132	0.02%	0.002%
19	3.929	879	883	886	rBV	116	110	0.02%	0.002%
20	3.990	900	902	906	rVB	224	166	0.02%	0.003%
21	4.186	949	963	1023	rBV	44070	189905	28.29%	3.107%
22	4.559	1077	1079	1082	rBV2	329	184	0.03%	0.003%
23	4.637	1087	1103	1140	rVB	101922	257457	38.35%	4.212%
24	4.784	1142	1149	1152	rBV	404	534	0.08%	0.009%
25	4.884	1174	1180	1185	rBV4	550	692	0.10%	0.011%
26	5.000	1214	1216	1219	rVB2	232	123	0.02%	0.002%
27	5.196	1272	1277	1278	rBV	160	124	0.02%	0.002%
28	5.325	1296	1317	1348	rVV2	234338	671385	100.00%	10.984%
29	5.524	1376	1379	1383	rVB2	184	130	0.02%	0.002%
30	5.620	1402	1409	1410	rBV	561	421	0.06%	0.007%
31	5.730	1441	1443	1448	rVB	200	135	0.02%	0.002%
32	5.755	1448	1451	1454	rBV2	178	176	0.03%	0.003%
33	5.794	1460	1463	1467	rBV	332	368	0.05%	0.006%
34	5.874	1475	1488	1521	rBV	226676	477815	71.17%	7.817%

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Integration Parameters: LSCINT.P

Integrator: RTE
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 Title : VOC Analysis

35	6.087	1551	1554	1558	rBV2	266	210	0.03%	0.003%
36	6.173	1568	1581	1592	rVB5	3766	7682	1.14%	0.126%
37	6.241	1601	1602	1605	rBV	235	159	0.02%	0.003%
38	6.260	1605	1608	1610	rVV	449	391	0.06%	0.006%
39	6.321	1614	1627	1656	rVB	140861	303276	45.17%	4.962%
40	6.473	1671	1674	1676	rVB	308	209	0.03%	0.003%
41	6.559	1695	1701	1704	rBV	169	154	0.02%	0.003%
42	6.672	1732	1736	1741	rBV2	202	229	0.03%	0.004%
43	6.743	1755	1758	1761	rBV2	206	138	0.02%	0.002%
44	6.874	1796	1799	1800	rBV	412	205	0.03%	0.003%
45	6.890	1800	1804	1808	rVV5	807	863	0.13%	0.014%
46	6.968	1825	1828	1833	rVB2	278	255	0.04%	0.004%
47	7.026	1842	1846	1848	rBV2	176	131	0.02%	0.002%
48	7.042	1848	1851	1858	rVB	203	184	0.03%	0.003%
49	7.090	1863	1866	1869	rBV	239	148	0.02%	0.002%
50	7.106	1869	1871	1874	rVV2	223	115	0.02%	0.002%
51	7.222	1895	1907	1938	rBV2	81984	164052	24.43%	2.684%
52	7.424	1964	1970	1974	rBV4	354	452	0.07%	0.007%
53	7.556	1998	2011	2033	rBV	310904	569728	84.86%	9.321%
54	7.749	2069	2071	2073	rBV2	278	146	0.02%	0.002%
55	7.762	2073	2075	2079	rVV4	423	289	0.04%	0.005%
56	7.794	2081	2085	2086	rBV2	331	191	0.03%	0.003%
57	7.849	2091	2102	2126	rBV	54068	110482	16.46%	1.808%
58	8.035	2157	2160	2162	rBV	184	117	0.02%	0.002%
59	8.106	2179	2182	2185	rBV	169	118	0.02%	0.002%
60	8.318	2237	2248	2292	rBV	200341	425074	63.31%	6.954%
61	8.614	2337	2340	2341	rBV	575	321	0.05%	0.005%
62	8.685	2359	2362	2364	rBV	197	143	0.02%	0.002%
63	8.717	2367	2372	2376	rBV	398	327	0.05%	0.005%
64	8.784	2392	2393	2398	rBV	130	113	0.02%	0.002%
65	8.820	2400	2404	2410	rBV	192	134	0.02%	0.002%
66	8.849	2410	2413	2416	rVB2	162	119	0.02%	0.002%
67	8.906	2428	2431	2436	rVV	264	180	0.03%	0.003%
68	9.032	2467	2470	2473	rBV2	171	140	0.02%	0.002%
69	9.087	2474	2487	2522	rBV	344463	611477	91.08%	10.004%
70	9.366	2572	2574	2580	rVB2	259	112	0.02%	0.002%
71	9.395	2580	2583	2588	rBV2	180	194	0.03%	0.003%

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72	9.578	2638	2640	2644	rVB	224	113	0.02%	0.002%
73	9.611	2644	2650	2655	rBV	153	188	0.03%	0.003%
74	9.701	2675	2678	2681	rVB	210	155	0.02%	0.003%
75	9.720	2681	2684	2687	rBV	207	175	0.03%	0.003%
76	9.771	2697	2700	2701	rBV	219	125	0.02%	0.002%
77	9.823	2711	2716	2719	rVB2	201	206	0.03%	0.003%
78	9.849	2720	2724	2726	rBV2	222	163	0.02%	0.003%
79	9.990	2763	2768	2770	rBV2	560	491	0.07%	0.008%
80	10.045	2779	2785	2788	rBV2	269	276	0.04%	0.005%
81	10.144	2802	2816	2838	rBV	60165	107062	15.95%	1.752%
82	10.321	2867	2871	2876	rBV2	187	222	0.03%	0.004%
83	10.431	2891	2905	2926	rBV	252416	413816	61.64%	6.770%
84	10.601	2954	2958	2971	rVB4	1059	1641	0.24%	0.027%
85	10.746	2998	3003	3006	rBV2	246	199	0.03%	0.003%
86	10.816	3014	3025	3044	rVV	67060	112966	16.83%	1.848%
87	10.993	3076	3080	3084	rBV2	269	269	0.04%	0.004%
88	11.038	3092	3094	3097	rVB	174	116	0.02%	0.002%
89	11.061	3098	3101	3103	rVB2	220	129	0.02%	0.002%
90	11.093	3103	3111	3116	rBV2	1389	2280	0.34%	0.037%
91	11.160	3124	3132	3144	rBV3	9605	16776	2.50%	0.274%
92	11.424	3207	3214	3220	rBV4	5740	7431	1.11%	0.122%
93	11.482	3220	3232	3252	rVV	419756	668208	99.53%	10.932%
94	11.736	3310	3311	3314	rBV	417	161	0.02%	0.003%
95	11.858	3330	3349	3372	rBV	372205	618707	92.15%	10.122%
96	12.135	3433	3435	3442	rVB4	687	586	0.09%	0.010%
97	12.636	3587	3591	3595	rBV2	254	264	0.04%	0.004%
98	12.768	3630	3632	3634	rVB	338	136	0.02%	0.002%
99	13.138	3742	3747	3749	rBV2	392	309	0.05%	0.005%
100	13.533	3867	3870	3871	rBV2	730	433	0.06%	0.007%

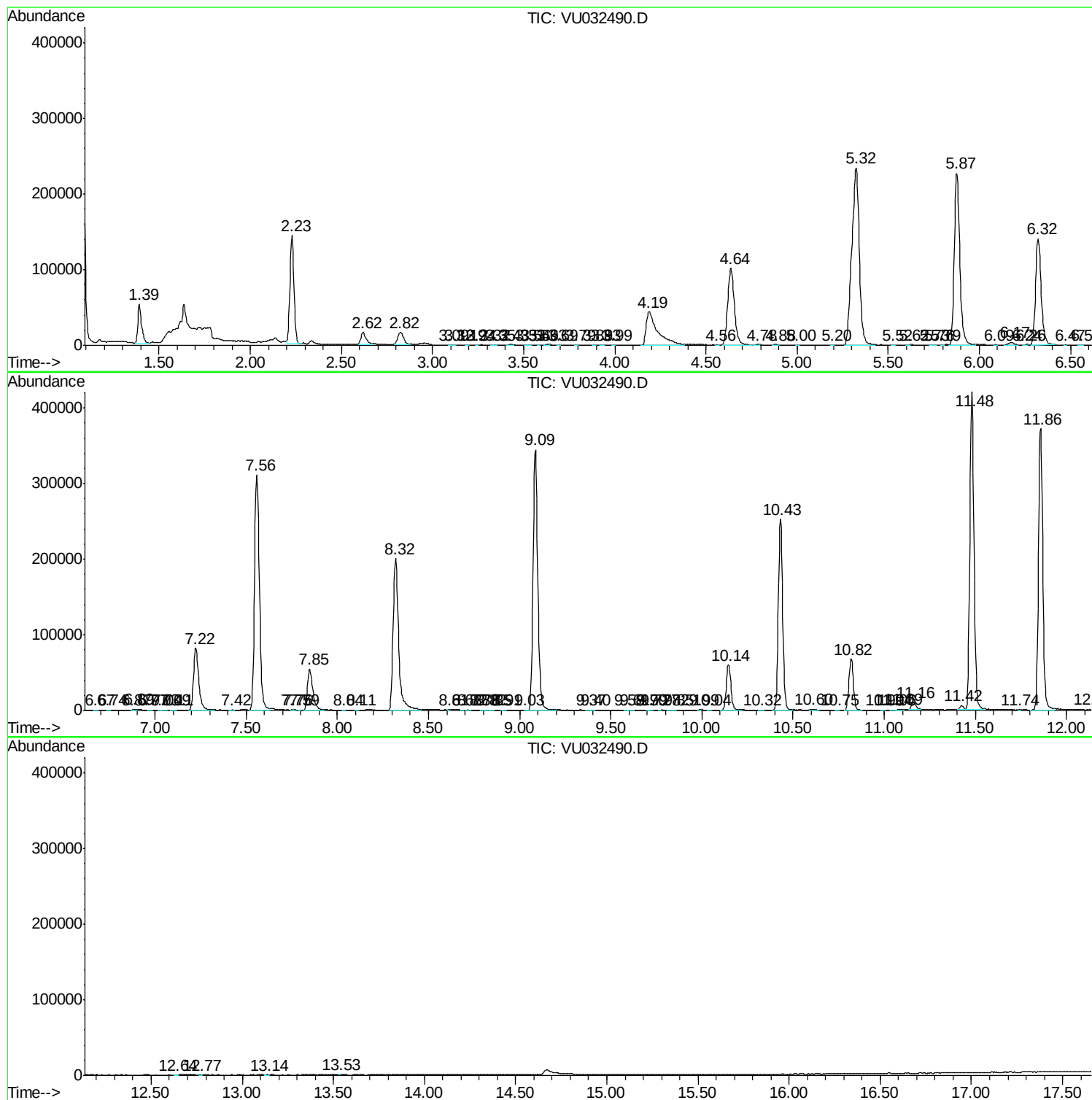
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 9 Sample Multiplier: 1

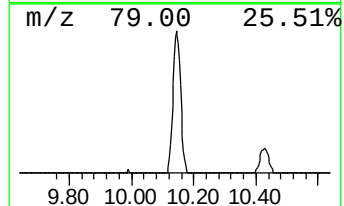
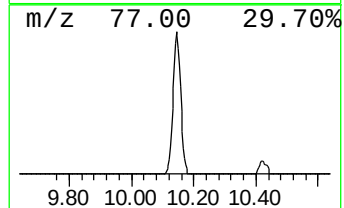
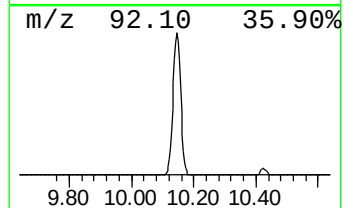
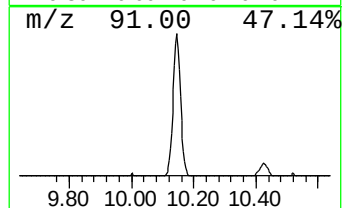
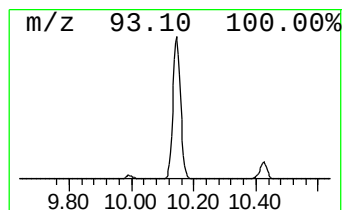
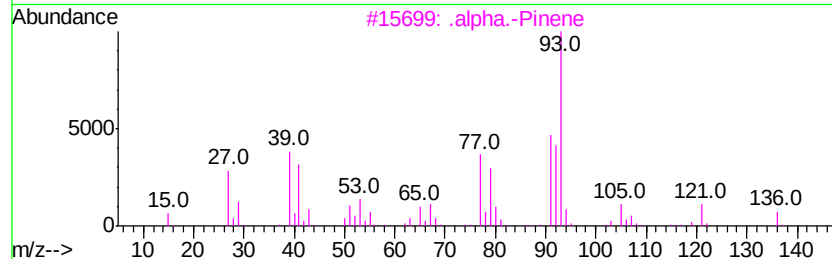
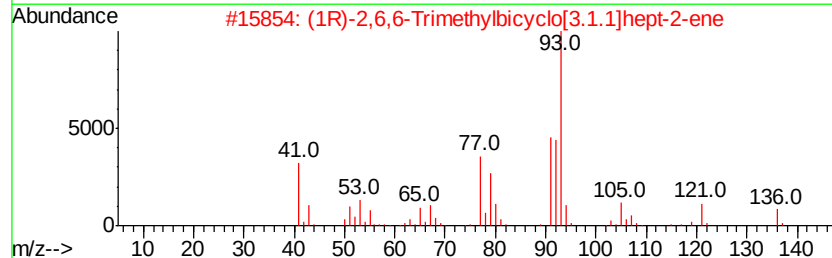
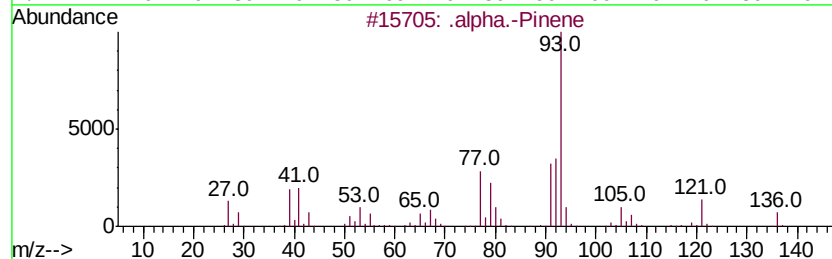
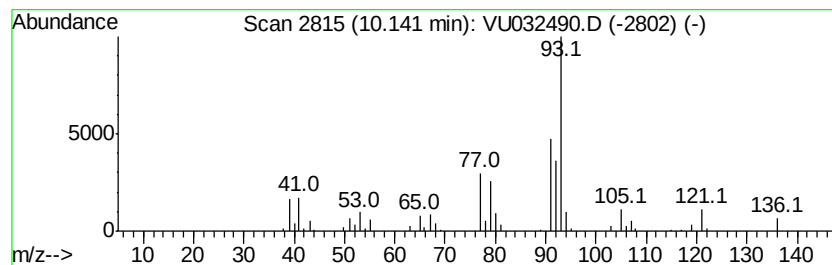
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.14	8.75 ug/L	107062	Chlorobenzene-d5	9.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	96
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
3	.alpha.-Pinene	136	C10H16	000080-56-8	95
4	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
5	.alpha.-Pinene	136	C10H16	000080-56-8	93



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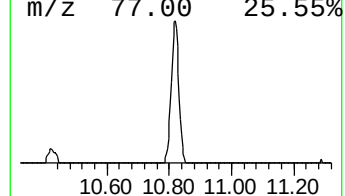
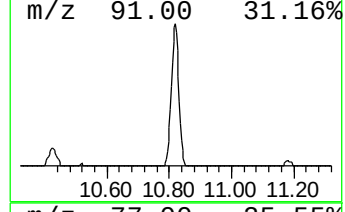
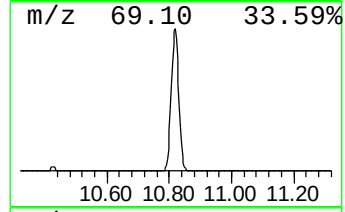
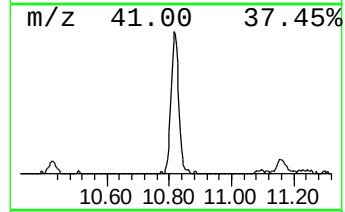
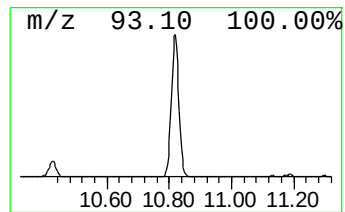
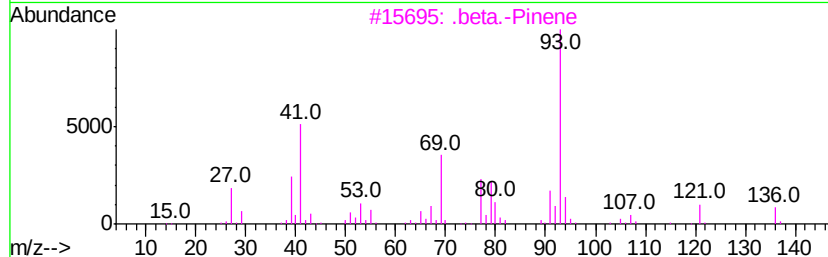
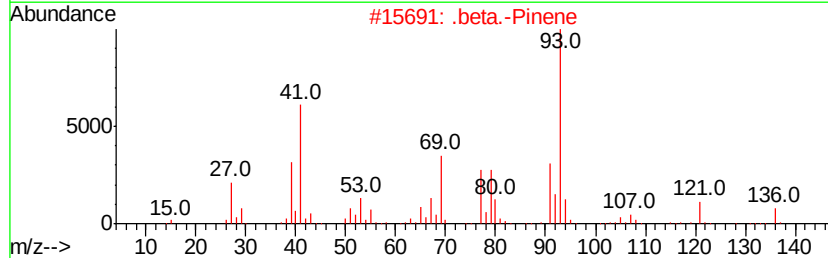
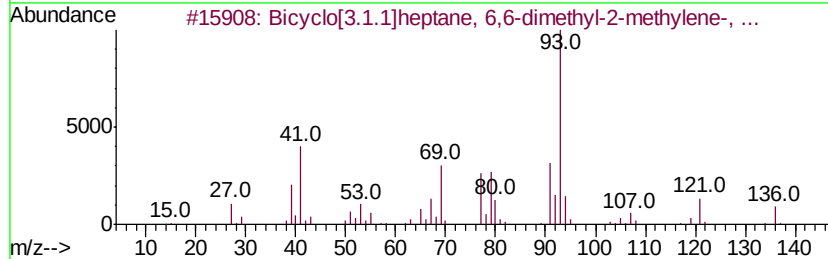
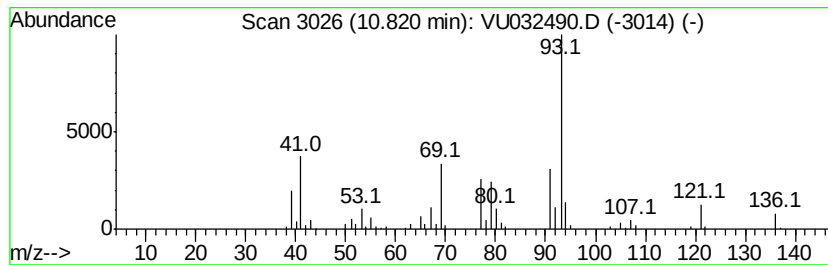
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Quant Title : VOC Analysis

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

Peak Number 4 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	8.45 ug/L	112966	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bicyclo[3.1.1]heptane, 6,6-dimet...	136 C10H16	018172-67-3 97
2		.beta.-Pinene	136 C10H16	000127-91-3 96
3		.beta.-Pinene	136 C10H16	000127-91-3 95
4		.beta.-Pinene	136 C10H16	000127-91-3 91
5		(1R)-2,6,6-Trimethylbicyclo[3.1....	136 C10H16	007785-70-8 91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
.alpha.-Pinene	10.14	8.8	ug/L	107062	2	9.09	611477	50.0
Bicyclo[3.1.1]hep...	10.82	8.4	ug/L	112966	3	11.48	668208	50.0