

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060619\
 Data File : VU032466.D
 Acq On : 05 Jun 2019 17:25
 Operator : JC/SP
 Sample : K3017-08ME
 Misc : 4.66g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 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	1.389	87	93	108	rVB	69319	88864	13.29%	1.472%
2	2.228	345	354	369	rVB	163974	248344	37.15%	4.115%
3	2.479	429	432	434	rBV	438	283	0.04%	0.005%
4	2.620	468	476	490	rBV	14765	26960	4.03%	0.447%
5	2.823	528	539	557	rBV	15360	34554	5.17%	0.573%
6	3.064	610	614	616	rBV2	248	168	0.03%	0.003%
7	3.167	643	646	648	rBV2	320	187	0.03%	0.003%
8	3.344	698	701	706	rBV	390	298	0.04%	0.005%
9	3.386	712	714	717	rVB	285	145	0.02%	0.002%
10	3.421	717	725	727	rBV	503	628	0.09%	0.010%
11	3.505	749	751	754	rBV	166	108	0.02%	0.002%
12	3.630	782	790	795	rBV3	657	1063	0.16%	0.018%
13	3.784	836	838	842	rVV	214	114	0.02%	0.002%
14	3.929	879	883	885	rVV2	233	153	0.02%	0.003%
15	3.997	899	904	908	rBV2	236	296	0.04%	0.005%
16	4.103	934	937	941	rBV	178	158	0.02%	0.003%
17	4.189	952	964	1019	rVV2	42011	189699	28.38%	3.143%
18	4.524	1066	1068	1074	rVB3	382	229	0.03%	0.004%
19	4.553	1074	1077	1079	rBV	325	222	0.03%	0.004%
20	4.636	1086	1103	1131	rBV	102769	257321	38.49%	4.264%
21	4.881	1176	1179	1184	rBV2	548	497	0.07%	0.008%
22	4.984	1207	1211	1212	rVB2	434	263	0.04%	0.004%
23	4.997	1212	1215	1219	rVB2	283	245	0.04%	0.004%
24	5.038	1223	1228	1232	rBV2	346	396	0.06%	0.007%
25	5.244	1290	1292	1296	rBV2	151	122	0.02%	0.002%
26	5.324	1296	1317	1347	rVV2	233469	668472	100.00%	11.076%
27	5.575	1392	1395	1400	rBV2	193	172	0.03%	0.003%
28	5.624	1407	1410	1414	rVB2	360	285	0.04%	0.005%
29	5.656	1417	1420	1422	rVV2	187	136	0.02%	0.002%
30	5.804	1463	1466	1468	rBV2	411	272	0.04%	0.005%
31	5.874	1475	1488	1520	rBV	221038	462081	69.12%	7.656%
32	6.109	1559	1561	1564	rBV2	282	153	0.02%	0.003%
33	6.167	1573	1579	1597	rVB6	2795	6122	0.92%	0.101%
34	6.321	1614	1627	1659	rVB2	140225	299124	44.75%	4.956%

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Integration Parameters: LSCINT.P

Integrator: RTE
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 Title : VOC Analysis

35	6.443	1663	1665	1667	rBV2	287	136	0.02%	0.002%
36	6.646	1721	1728	1733	rVB2	340	365	0.05%	0.006%
37	6.675	1733	1737	1742	rBV	185	232	0.03%	0.004%
38	6.730	1751	1754	1756	rBV	211	130	0.02%	0.002%
39	6.832	1784	1786	1789	rBV	272	128	0.02%	0.002%
40	6.894	1799	1805	1811	rBV3	518	809	0.12%	0.013%
41	6.990	1833	1835	1836	rVV3	336	111	0.02%	0.002%
42	7.029	1843	1847	1849	rBV2	179	114	0.02%	0.002%
43	7.067	1857	1859	1862	rBV2	197	109	0.02%	0.002%
44	7.222	1895	1907	1934	rBV	81782	161524	24.16%	2.676%
45	7.411	1963	1966	1968	rBV	170	131	0.02%	0.002%
46	7.482	1979	1988	1994	rBV4	1142	2164	0.32%	0.036%
47	7.559	1999	2012	2035	rBV	308252	560601	83.86%	9.289%
48	7.746	2068	2070	2076	rVB3	321	247	0.04%	0.004%
49	7.771	2076	2078	2080	rBV	346	153	0.02%	0.003%
50	7.810	2086	2090	2091	rBV2	226	137	0.02%	0.002%
51	7.849	2091	2102	2124	rVV	54961	108221	16.19%	1.793%
52	8.025	2154	2157	2158	rBV	296	119	0.02%	0.002%
53	8.093	2175	2178	2181	rVB2	287	155	0.02%	0.003%
54	8.164	2196	2200	2201	rBV2	361	241	0.04%	0.004%
55	8.279	2232	2236	2237	rBV	153	117	0.02%	0.002%
56	8.318	2237	2248	2284	rVV	198451	416103	62.25%	6.895%
57	8.585	2329	2331	2336	rVB3	309	139	0.02%	0.002%
58	8.630	2337	2345	2354	rBV4	1405	2737	0.41%	0.045%
59	8.742	2378	2380	2384	rBV	160	112	0.02%	0.002%
60	8.768	2384	2388	2392	rVB2	326	236	0.04%	0.004%
61	8.887	2422	2425	2427	rBV	229	190	0.03%	0.003%
62	8.967	2446	2450	2453	rVB2	173	135	0.02%	0.002%
63	9.045	2470	2474	2475	rBV2	179	121	0.02%	0.002%
64	9.086	2475	2487	2515	rBV	338625	589433	88.18%	9.766%
65	9.302	2552	2554	2558	rBV2	169	138	0.02%	0.002%
66	9.453	2599	2601	2606	rVB2	199	143	0.02%	0.002%
67	9.604	2645	2648	2650	rVB	202	114	0.02%	0.002%
68	9.620	2650	2653	2655	rBV	175	113	0.02%	0.002%
69	9.652	2660	2663	2665	rBV2	229	157	0.02%	0.003%
70	9.704	2676	2679	2683	rVB2	336	180	0.03%	0.003%
71	9.729	2683	2687	2689	rBV2	177	152	0.02%	0.003%

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Integration Parameters: LSCINT.P

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72	9.958	2756	2758	2763	rBV2	172	181	0.03%	0.003%
73	9.993	2765	2769	2777	rVV3	949	1237	0.19%	0.020%
74	10.028	2777	2780	2783	rVB3	303	193	0.03%	0.003%
75	10.144	2805	2816	2835	rBV	63411	107802	16.13%	1.786%
76	10.279	2856	2858	2860	rBV	192	121	0.02%	0.002%
77	10.311	2864	2868	2873	rBV2	255	250	0.04%	0.004%
78	10.373	2885	2887	2890	rVB	256	109	0.02%	0.002%
79	10.430	2892	2905	2928	rVV	243869	397589	59.48%	6.588%
80	10.610	2953	2961	2964	rBV2	461	720	0.11%	0.012%
81	10.684	2981	2984	2986	rVB2	228	129	0.02%	0.002%
82	10.768	3008	3010	3013	rBV2	174	114	0.02%	0.002%
83	10.819	3014	3026	3043	rVB2	69992	115385	17.26%	1.912%
84	11.096	3100	3112	3121	rBV3	1474	3175	0.47%	0.053%
85	11.160	3123	3132	3151	rVV	10041	19221	2.88%	0.318%
86	11.372	3195	3198	3202	rBV2	647	512	0.08%	0.008%
87	11.427	3207	3215	3220	rVV5	6418	8647	1.29%	0.143%
88	11.479	3221	3231	3254	rVV	407432	653060	97.69%	10.821%
89	11.768	3315	3321	3324	rBV3	510	545	0.08%	0.009%
90	11.858	3336	3349	3378	rBV	348776	587589	87.90%	9.736%
91	12.122	3428	3431	3433	rBV2	350	253	0.04%	0.004%
92	12.138	3433	3436	3442	rVB4	922	802	0.12%	0.013%
93	12.163	3442	3444	3447	rBV2	359	166	0.02%	0.003%
94	12.186	3447	3451	3454	rBV2	251	186	0.03%	0.003%
95	12.237	3464	3467	3469	rBV2	283	166	0.02%	0.003%
96	12.475	3535	3541	3547	rBV4	657	887	0.13%	0.015%
97	12.816	3645	3647	3651	rBV	284	165	0.02%	0.003%
98	12.897	3666	3672	3676	rBV6	1112	1402	0.21%	0.023%
99	13.025	3710	3712	3714	rBV	337	138	0.02%	0.002%
100	13.109	3735	3738	3740	rBV	339	243	0.04%	0.004%

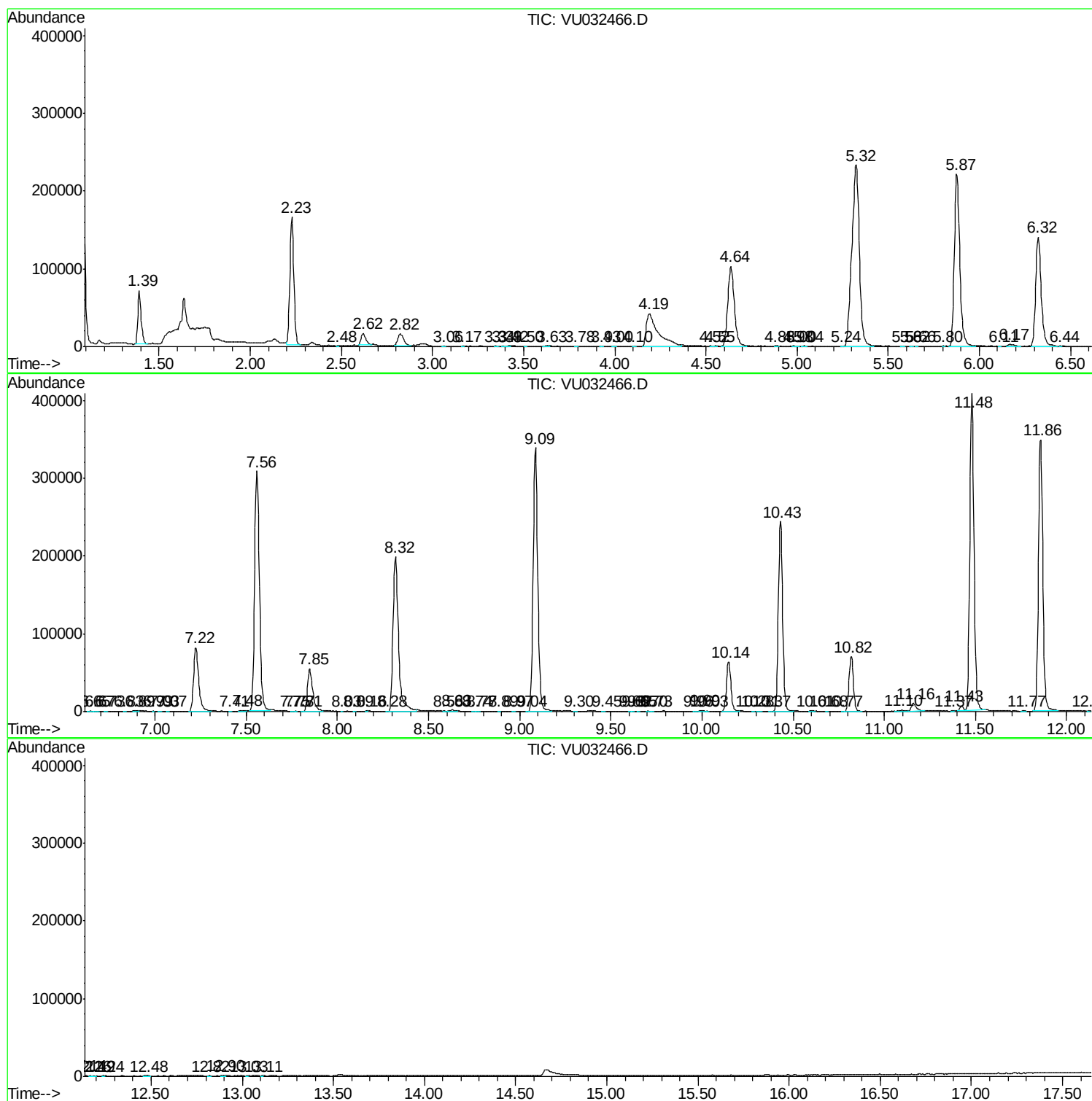
Sum of corrected areas: 6035268

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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 : 12 Sample Multiplier: 1

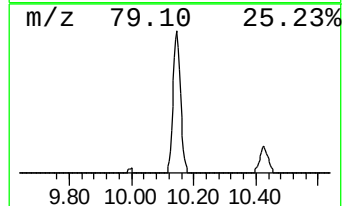
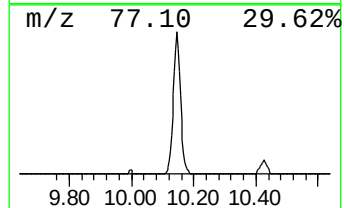
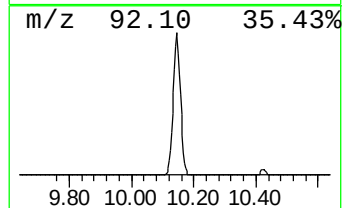
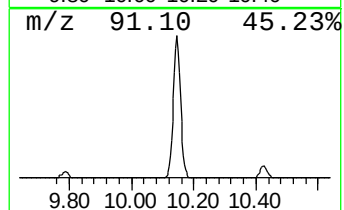
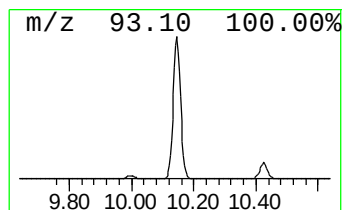
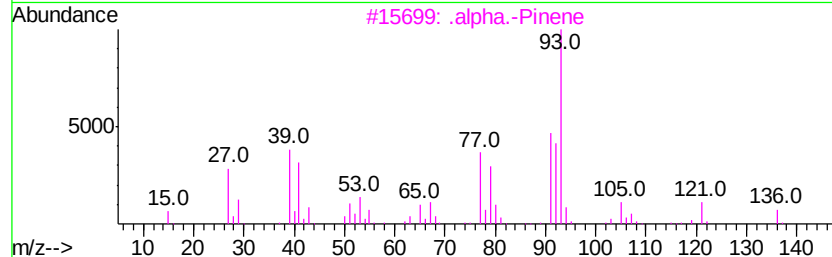
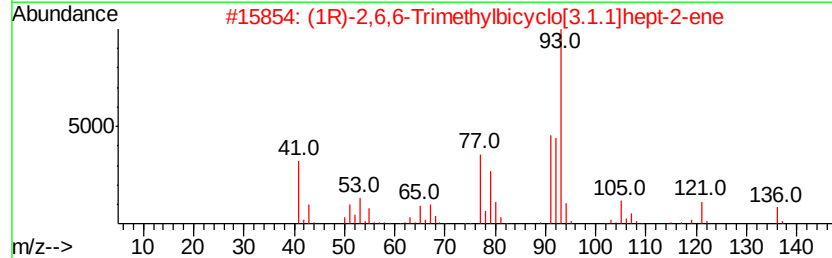
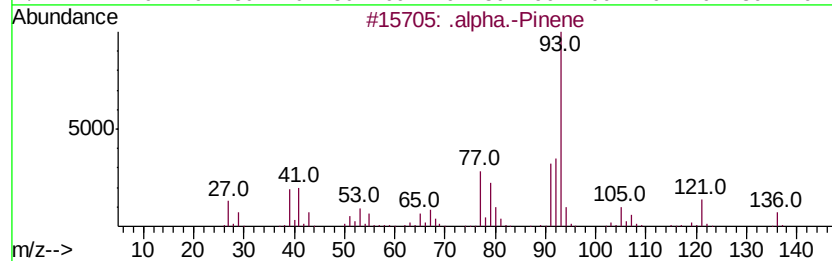
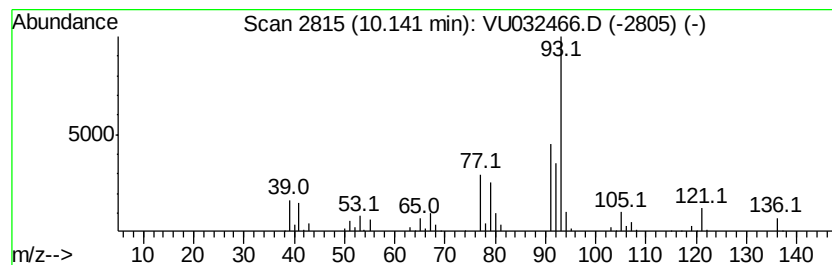
Instrument :
MSVOA_U
ClientSampleId :
A51E1ME

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	9.14 ug/L	107802	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	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94



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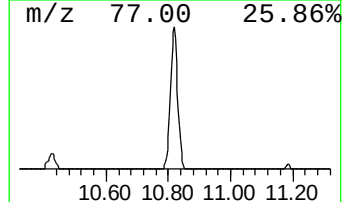
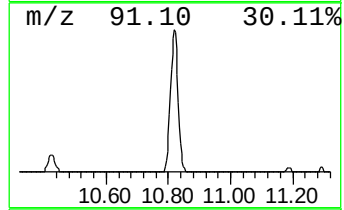
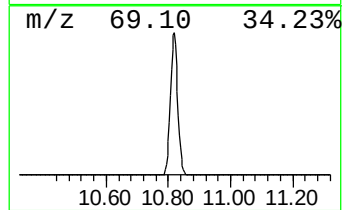
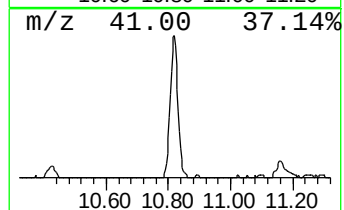
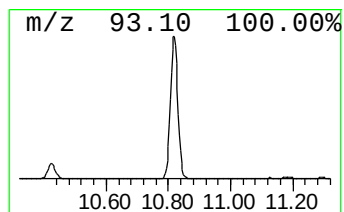
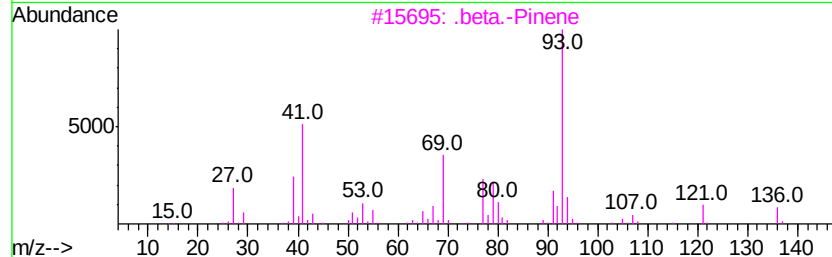
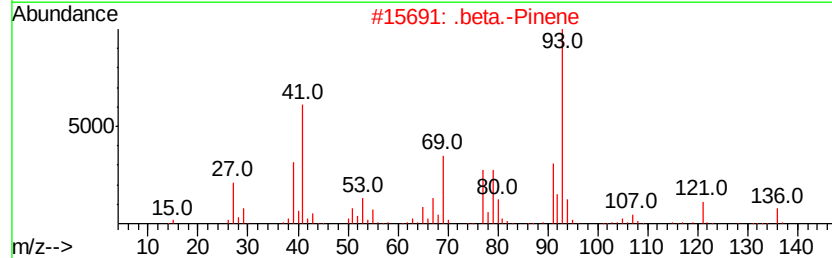
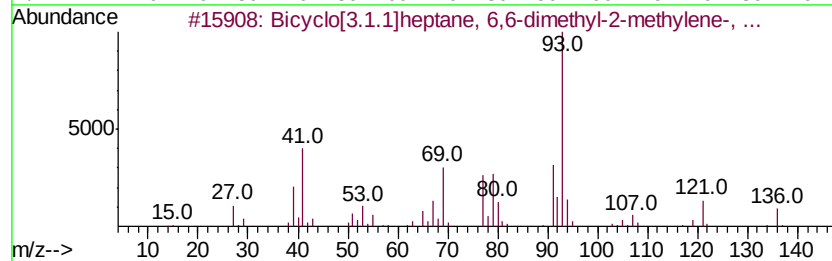
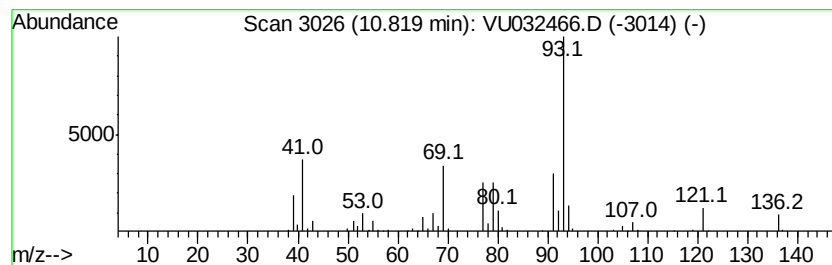
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Quant Title : VOC Analysis

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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	8.83 ug/L	115385	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 94
5		Bicyclo[3.1.0]hexane, 4-methylen...	136 C10H16	003387-41-5 87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
.alpha.-Pinene	10.14	9.1	ug/L	107802	2	9.09	589433	50.0
Bicyclo[3.1.1]hep...	10.82	8.8	ug/L	115385	3	11.48	653060	50.0