

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062218\
 Data File : VU024836.D
 Acq On : 22 Jun 2018 15:26
 Operator : MD/SY
 Sample : J3569-08ME
 Misc : 6.21g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DAXQ9ME

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\SOMULM061518WMA.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	0.896	89	95	101	rVB2	463	593	0.04%	0.005%
2	1.082	135	153	171	rBV	1138536	1338879	100.00%	12.380%
3	1.397	243	251	267	rVB	81635	117399	8.77%	1.086%
4	1.651	326	330	344	rVB	50393	63735	4.76%	0.589%
5	2.243	504	514	529	rVB	202172	319631	23.87%	2.956%
6	2.831	685	697	710	rBV	6076	12284	0.92%	0.114%
7	2.969	732	740	751	rVB8	1257	2645	0.20%	0.024%
8	3.278	830	836	847	rVB4	2149	3990	0.30%	0.037%
9	3.535	913	916	920	rBV4	436	427	0.03%	0.004%
10	3.854	1010	1015	1017	rVV2	492	406	0.03%	0.004%
11	3.889	1021	1026	1031	rVB3	578	548	0.04%	0.005%
12	3.957	1041	1047	1051	rVB3	456	469	0.04%	0.004%
13	3.982	1051	1055	1057	rBV3	489	438	0.03%	0.004%
14	4.194	1103	1121	1168	rBV2	65888	258112	19.28%	2.387%
15	4.648	1244	1262	1287	rVV	165258	421169	31.46%	3.894%
16	4.780	1298	1303	1305	rBV	575	409	0.03%	0.004%
17	4.879	1328	1334	1336	rBV3	647	744	0.06%	0.007%
18	4.989	1350	1368	1379	rBV7	2965	7684	0.57%	0.071%
19	5.075	1392	1395	1403	rVB3	1255	1423	0.11%	0.013%
20	5.124	1408	1410	1414	rVB3	599	397	0.03%	0.004%
21	5.336	1450	1476	1505	rVV2	364608	1063650	79.44%	9.835%
22	5.574	1547	1550	1553	rBV2	590	573	0.04%	0.005%
23	5.619	1553	1564	1575	rVV7	3455	8259	0.62%	0.076%
24	5.770	1606	1611	1614	rBV4	728	820	0.06%	0.008%
25	5.886	1632	1647	1671	rBV	397989	827527	61.81%	7.652%
26	6.243	1752	1758	1759	rBV2	2375	1973	0.15%	0.018%
27	6.333	1771	1786	1803	rBV2	232141	487499	36.41%	4.508%
28	6.725	1901	1908	1913	rBV5	682	853	0.06%	0.008%
29	6.863	1944	1951	1952	rBV3	1308	1221	0.09%	0.011%
30	6.879	1952	1956	1957	rBV3	1244	779	0.06%	0.007%
31	7.165	2039	2045	2046	rBV3	726	506	0.04%	0.005%
32	7.230	2053	2065	2090	rVB	130504	263620	19.69%	2.438%
33	7.381	2103	2112	2114	rBV5	947	1302	0.10%	0.012%
34	7.477	2137	2142	2143	rBV2	619	514	0.04%	0.005%

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Integration Parameters: LSCINT.P

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

Filtering: 5
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061518WMA.M
 Title : VOC Analysis

35	7.490	2143	2146	2152	rVB3	539	510	0.04%	0.005%
36	7.567	2152	2170	2186	rBV	491648	896944	66.99%	8.294%
37	7.641	2188	2193	2206	rVB2	8592	15079	1.13%	0.139%
38	7.776	2230	2235	2239	rBV3	561	592	0.04%	0.005%
39	7.853	2243	2259	2277	rBV	89790	182995	13.67%	1.692%
40	7.944	2286	2287	2294	rVB3	610	428	0.03%	0.004%
41	8.046	2310	2319	2326	rBV5	982	1914	0.14%	0.018%
42	8.333	2392	2408	2427	rBV	311901	629562	47.02%	5.821%
43	8.551	2467	2476	2486	rBV7	1094	2002	0.15%	0.019%
44	8.606	2486	2493	2498	rBV6	1554	2067	0.15%	0.019%
45	8.683	2515	2517	2523	rVB2	581	477	0.04%	0.004%
46	8.725	2523	2530	2534	rBV2	518	625	0.05%	0.006%
47	8.773	2541	2545	2551	rVB3	543	611	0.05%	0.006%
48	8.808	2551	2556	2558	rBV3	1270	1022	0.08%	0.009%
49	9.095	2631	2645	2667	rBV	549756	1008822	75.35%	9.328%
50	9.259	2688	2696	2703	rBV3	1134	1764	0.13%	0.016%
51	9.384	2721	2735	2749	rBV4	6137	11707	0.87%	0.108%
52	9.445	2749	2754	2762	rVB5	1765	2279	0.17%	0.021%
53	9.548	2782	2786	2792	rVB2	497	530	0.04%	0.005%
54	9.792	2849	2862	2877	rVV5	5348	10666	0.80%	0.099%
55	9.953	2906	2912	2918	rVB5	1381	1896	0.14%	0.018%
56	9.988	2918	2923	2928	rBV3	346	422	0.03%	0.004%
57	10.040	2934	2939	2943	rBV4	904	838	0.06%	0.008%
58	10.095	2953	2956	2964	rVB2	626	641	0.05%	0.006%
59	10.156	2964	2975	2987	rVB	39271	65104	4.86%	0.602%
60	10.300	3015	3020	3023	rBV2	367	438	0.03%	0.004%
61	10.323	3023	3027	3031	rBV3	1060	1012	0.08%	0.009%
62	10.361	3037	3039	3043	rVB3	819	524	0.04%	0.005%
63	10.390	3044	3048	3050	rBV2	698	575	0.04%	0.005%
64	10.442	3052	3064	3080	rVB	380651	620950	46.38%	5.742%
65	10.609	3113	3116	3122	rVB3	953	1087	0.08%	0.010%
66	10.686	3133	3140	3143	rBV3	738	907	0.07%	0.008%
67	10.760	3158	3163	3165	rBV	1223	1000	0.07%	0.009%
68	10.815	3176	3180	3192	rVB6	2482	3922	0.29%	0.036%
69	11.111	3268	3272	3273	rBV2	1160	715	0.05%	0.007%
70	11.156	3280	3286	3295	rVB6	3736	5102	0.38%	0.047%
71	11.287	3322	3327	3329	rBV2	483	468	0.03%	0.004%

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Instrument :
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 ClientSampleId :
 DAXQ9ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
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 Title : VOC Analysis

72	11.435	3361	3373	3378	rBV8	4324	6433	0.48%	0.059%
73	11.490	3378	3390	3408	rVB	678096	1057494	78.98%	9.779%
74	11.577	3414	3417	3426	rVB5	2086	2003	0.15%	0.019%
75	11.670	3443	3446	3449	rVB2	709	448	0.03%	0.004%
76	11.866	3495	3507	3526	rBV	583523	926133	69.17%	8.564%
77	11.959	3532	3536	3539	rBV3	743	602	0.04%	0.006%
78	12.030	3551	3558	3564	rVB6	2162	3094	0.23%	0.029%
79	12.188	3605	3607	3615	rVB4	637	723	0.05%	0.007%
80	12.477	3693	3697	3698	rBV2	1688	1184	0.09%	0.011%
81	12.580	3724	3729	3732	rBV4	1010	1056	0.08%	0.010%
82	12.680	3756	3760	3765	rBV3	537	482	0.04%	0.004%
83	12.937	3835	3840	3847	rBV4	646	831	0.06%	0.008%
84	13.133	3897	3901	3904	rBV4	1002	889	0.07%	0.008%
85	13.278	3939	3946	3947	rBV2	998	927	0.07%	0.009%
86	13.615	4049	4051	4056	rBV2	607	558	0.04%	0.005%
87	13.754	4089	4094	4103	rBV2	3876	4533	0.34%	0.042%
88	13.840	4117	4121	4125	rBV4	1002	763	0.06%	0.007%
89	13.879	4130	4133	4134	rBV2	800	438	0.03%	0.004%
90	13.985	4163	4166	4171	rVB3	599	494	0.04%	0.005%
91	14.091	4196	4199	4202	rBV2	549	431	0.03%	0.004%
92	14.143	4211	4215	4222	rVB6	1171	1766	0.13%	0.016%
93	14.281	4250	4258	4269	rVB2	6251	9975	0.75%	0.092%
94	14.898	4442	4450	4461	rVB9	2595	5341	0.40%	0.049%
95	15.284	4566	4570	4579	rVB6	3873	4870	0.36%	0.045%
96	15.512	4637	4641	4645	rBV3	763	894	0.07%	0.008%
97	15.856	4738	4748	4766	rVB7	35156	62074	4.64%	0.574%
98	15.985	4784	4788	4797	rVB5	1511	1722	0.13%	0.016%
99	16.171	4840	4846	4853	rBV7	7160	10925	0.82%	0.101%
100	16.557	4959	4966	4974	rVB6	13546	20714	1.55%	0.192%

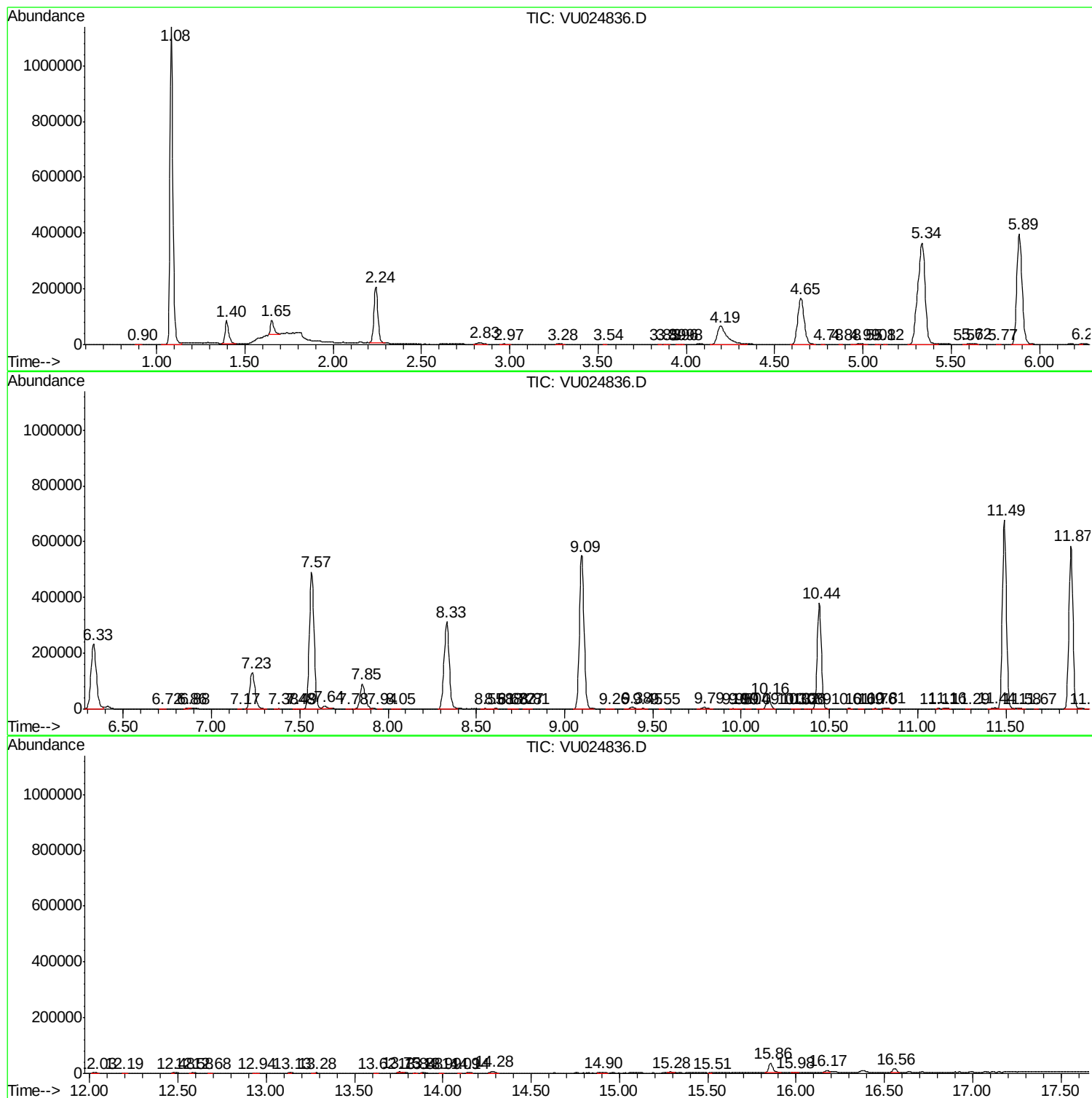
Sum of corrected areas: 10814472

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DAXQ9ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061518WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
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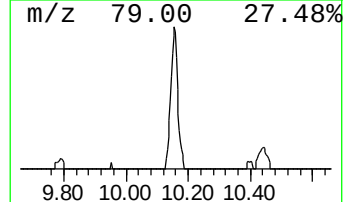
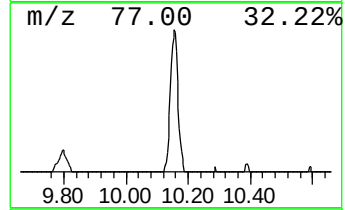
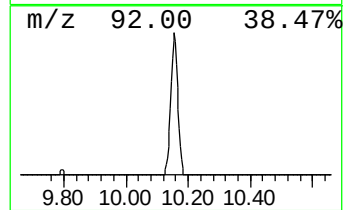
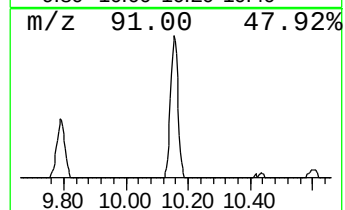
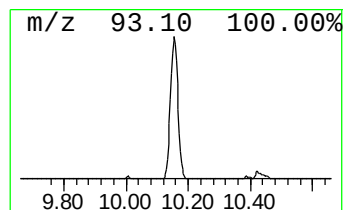
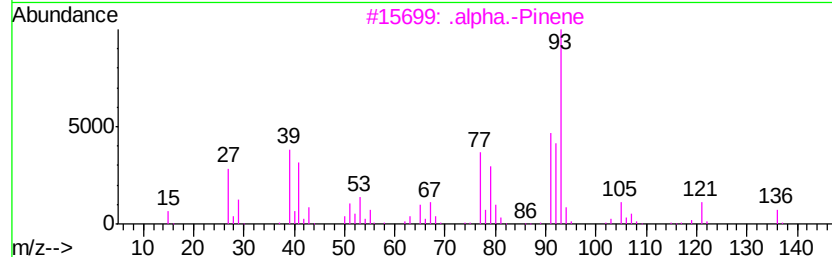
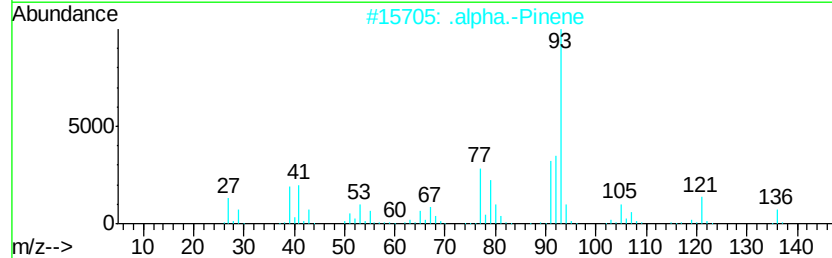
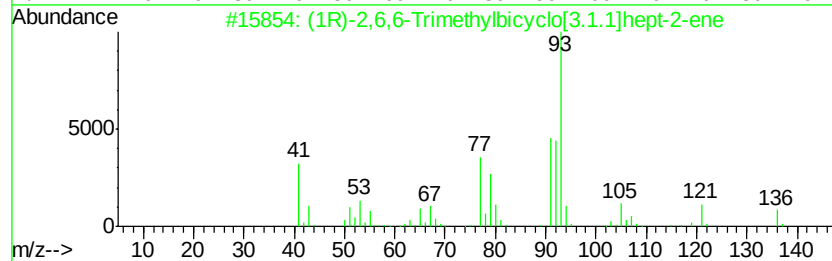
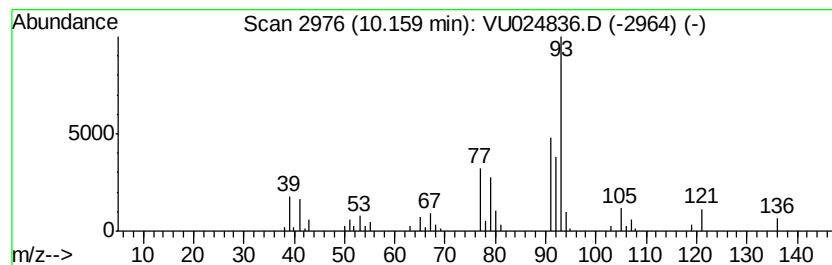
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061518WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	3.23 ug/L	65104	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	96
2		.alpha.-Pinene	136	C10H16	000080-56-8	95
3		.alpha.-Pinene	136	C10H16	000080-56-8	95
4		(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91



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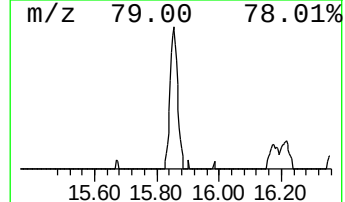
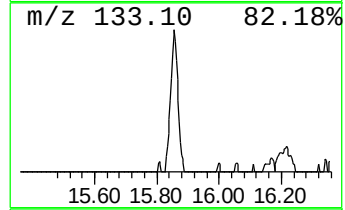
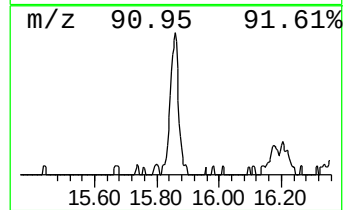
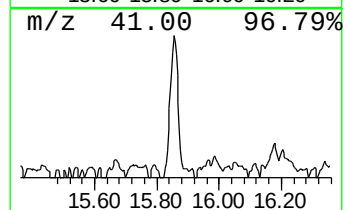
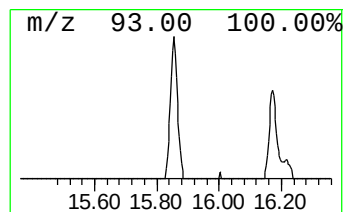
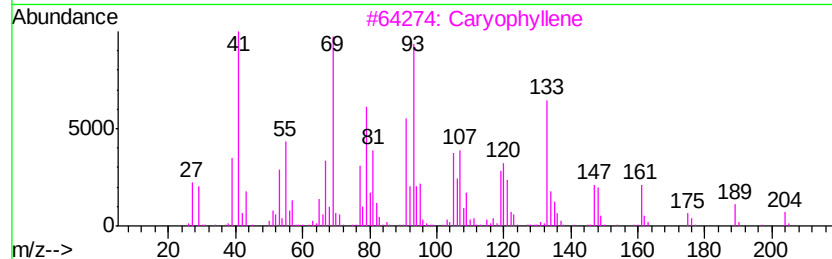
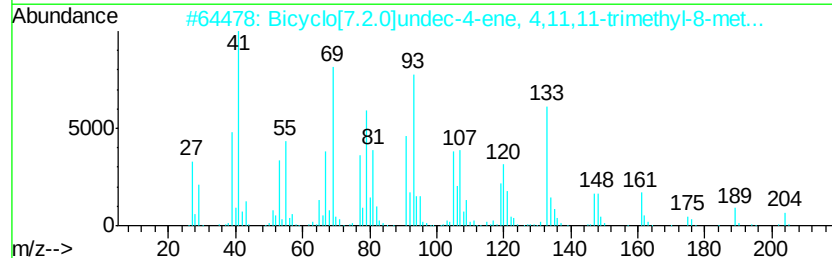
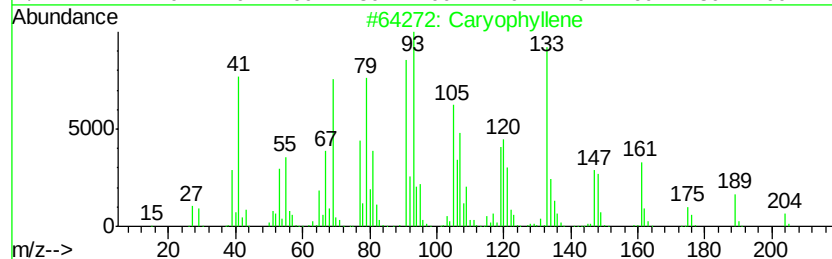
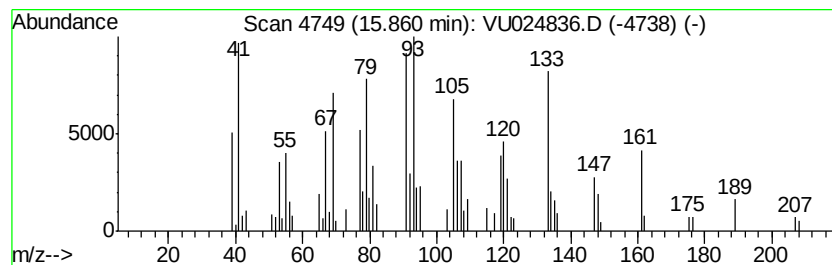
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Quant Title : VOC Analysis

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

Peak Number 4 Caryophyllene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.93 ug/L	62074	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Caryophyllene	204 C15H24	000087-44-5 91
2		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	000118-65-0 74
3		Caryophyllene	204 C15H24	000087-44-5 64
4		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	013877-93-5 58
5		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	000118-65-0 52



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(1R)-2,6,6-Trimet...	10.16	3.2	ug/L	65104	2	9.09	1008820	50.0
Caryophyllene	15.86	2.9	ug/L	62074	3	11.49	1057490	50.0