

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062218\
 Data File : VU024832.D
 Acq On : 22 Jun 2018 13:44
 Operator : MD/SY
 Sample : J3569-08ME
 Misc : 6.21g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 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	0.822	68	72	76	rBV	351	394	0.03%	0.004%
2	0.999	121	127	130	rBV2	332	382	0.03%	0.004%
3	1.082	137	153	178	rBV	1147043	1322768	100.00%	13.056%
4	1.397	243	251	266	rVB	78876	106091	8.02%	1.047%
5	1.545	289	297	298	rBV4	11338	10526	0.80%	0.104%
6	1.648	325	329	338	rVB	47364	58277	4.41%	0.575%
7	2.240	503	513	528	rVB	186893	291653	22.05%	2.879%
8	2.613	626	629	631	rBV3	973	770	0.06%	0.008%
9	2.834	686	698	710	rVB2	6160	13079	0.99%	0.129%
10	3.063	764	769	773	rBV4	441	475	0.04%	0.005%
11	3.098	778	780	785	rVB3	608	374	0.03%	0.004%
12	3.262	828	831	834	rBV	740	587	0.04%	0.006%
13	3.368	861	864	866	rBV3	680	470	0.04%	0.005%
14	3.513	903	909	911	rBV2	635	715	0.05%	0.007%
15	3.783	990	993	998	rVB2	717	666	0.05%	0.007%
16	3.812	998	1002	1005	rBV3	515	456	0.03%	0.005%
17	3.947	1039	1044	1049	rVB	571	542	0.04%	0.005%
18	3.998	1056	1060	1065	rBV4	567	495	0.04%	0.005%
19	4.034	1068	1071	1074	rBV2	743	554	0.04%	0.005%
20	4.056	1074	1078	1079	rBV2	741	568	0.04%	0.006%
21	4.127	1098	1100	1104	rBV2	534	443	0.03%	0.004%
22	4.195	1104	1121	1161	rVV	61532	235119	17.77%	2.321%
23	4.648	1244	1262	1289	rVB	151699	384861	29.10%	3.799%
24	4.982	1355	1366	1376	rVV8	2344	4951	0.37%	0.049%
25	5.050	1382	1387	1388	rBV2	569	436	0.03%	0.004%
26	5.194	1425	1432	1440	rBV4	885	1391	0.11%	0.014%
27	5.336	1451	1476	1498	rBV2	323707	954285	72.14%	9.419%
28	5.545	1536	1541	1543	rVV2	617	608	0.05%	0.006%
29	5.609	1551	1561	1565	rBV6	3534	5927	0.45%	0.059%
30	5.770	1607	1611	1614	rBV2	606	544	0.04%	0.005%
31	5.812	1622	1624	1630	rVB2	551	415	0.03%	0.004%
32	5.886	1631	1647	1670	rBV	389749	821268	62.09%	8.106%
33	6.085	1706	1709	1713	rVB3	631	442	0.03%	0.004%
34	6.114	1713	1718	1719	rBV2	612	474	0.04%	0.005%

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Instrument :
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 ClientSampleId :
 DAXQ9ME

Integration Parameters: LSCINT.P

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

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

35	6.169	1726	1735	1745	rBV8	3027	5583	0.42%	0.055%
36	6.256	1751	1762	1771	rVB4	2562	5317	0.40%	0.052%
37	6.333	1771	1786	1803	rBV	207975	442457	33.45%	4.367%
38	6.738	1906	1912	1916	rBV3	583	769	0.06%	0.008%
39	6.876	1944	1955	1956	rBV4	2419	3746	0.28%	0.037%
40	7.014	1994	1998	2002	rVB5	451	398	0.03%	0.004%
41	7.050	2003	2009	2015	rVB4	1168	1480	0.11%	0.015%
42	7.156	2039	2042	2044	rBV2	620	410	0.03%	0.004%
43	7.230	2053	2065	2087	rVB2	119068	234835	17.75%	2.318%
44	7.378	2108	2111	2117	rBV5	777	711	0.05%	0.007%
45	7.448	2130	2133	2135	rBV	439	353	0.03%	0.003%
46	7.516	2152	2154	2156	rBV3	649	353	0.03%	0.003%
47	7.567	2156	2170	2186	rBV	445093	804511	60.82%	7.941%
48	7.854	2244	2259	2289	rVB2	81385	165803	12.53%	1.637%
49	7.979	2294	2298	2305	rBV4	592	617	0.05%	0.006%
50	8.329	2389	2407	2431	rBV	288721	598539	45.25%	5.908%
51	8.535	2467	2471	2473	rBV3	655	601	0.05%	0.006%
52	8.606	2482	2493	2496	rBV5	1198	1749	0.13%	0.017%
53	8.818	2553	2559	2566	rVV4	1036	1269	0.10%	0.013%
54	8.892	2578	2582	2586	rBV2	432	390	0.03%	0.004%
55	9.095	2632	2645	2673	rBV	552110	1008653	76.25%	9.956%
56	9.259	2690	2696	2704	rBV3	968	1474	0.11%	0.015%
57	9.384	2726	2735	2743	rBV3	5056	8330	0.63%	0.082%
58	9.442	2750	2753	2761	rVB5	1097	1346	0.10%	0.013%
59	9.664	2814	2822	2828	rBV4	573	880	0.07%	0.009%
60	9.789	2854	2861	2873	rVV5	4374	8012	0.61%	0.079%
61	9.966	2913	2916	2920	rVB2	533	398	0.03%	0.004%
62	10.156	2964	2975	2990	rVB2	36134	60120	4.55%	0.593%
63	10.262	3002	3008	3012	rBV4	880	922	0.07%	0.009%
64	10.326	3021	3028	3032	rVV4	902	1037	0.08%	0.010%
65	10.371	3040	3042	3046	rVV	470	396	0.03%	0.004%
66	10.394	3046	3049	3051	rVV2	612	429	0.03%	0.004%
67	10.442	3051	3064	3082	rVB	349761	566667	42.84%	5.593%
68	10.609	3109	3116	3125	rVB5	1399	2518	0.19%	0.025%
69	10.689	3135	3141	3146	rBV3	930	1028	0.08%	0.010%
70	10.722	3146	3151	3156	rVB5	764	741	0.06%	0.007%
71	10.779	3163	3169	3174	rBV4	1014	1407	0.11%	0.014%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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 Title : VOC Analysis

72	10.821	3176	3182	3190	rVB4	2478	3315	0.25%	0.033%
73	10.963	3221	3226	3227	rBV	695	391	0.03%	0.004%
74	11.156	3279	3286	3298	rVB6	3066	5272	0.40%	0.052%
75	11.410	3362	3365	3367	rBV	669	524	0.04%	0.005%
76	11.435	3367	3373	3378	rVB6	3195	3855	0.29%	0.038%
77	11.490	3378	3390	3408	rBV	644984	1015967	76.81%	10.028%
78	11.786	3480	3482	3485	rBV	612	386	0.03%	0.004%
79	11.866	3492	3507	3529	rBV	501688	815360	61.64%	8.048%
80	11.982	3540	3543	3545	rBV3	630	434	0.03%	0.004%
81	12.030	3549	3558	3567	rBV6	2005	3227	0.24%	0.032%
82	12.339	3651	3654	3656	rBV2	480	355	0.03%	0.004%
83	12.484	3691	3699	3713	rVB2	2717	5098	0.39%	0.050%
84	12.567	3719	3725	3726	rBV4	587	563	0.04%	0.006%
85	13.127	3891	3899	3908	rVB7	2033	3272	0.25%	0.032%
86	13.197	3918	3921	3924	rBV2	763	461	0.03%	0.005%
87	13.275	3940	3945	3952	rBV5	1234	1764	0.13%	0.017%
88	13.757	4088	4095	4103	rVB3	2891	4432	0.34%	0.044%
89	13.992	4166	4168	4174	rBV3	678	513	0.04%	0.005%
90	14.146	4208	4216	4224	rBV5	1653	2248	0.17%	0.022%
91	14.281	4248	4258	4266	rBV	5703	10462	0.79%	0.103%
92	14.654	4367	4374	4378	rBV5	988	1337	0.10%	0.013%
93	14.882	4441	4445	4446	rBV2	1096	780	0.06%	0.008%
94	15.040	4492	4494	4497	rBV	581	397	0.03%	0.004%
95	15.069	4500	4503	4504	rBV3	1024	589	0.04%	0.006%
96	15.287	4566	4571	4583	rVB7	4186	6063	0.46%	0.060%
97	15.657	4683	4686	4688	rBV4	1169	860	0.07%	0.008%
98	15.853	4737	4747	4769	rBV8	29556	55646	4.21%	0.549%
99	16.175	4839	4847	4854	rBV7	5923	11057	0.84%	0.109%
100	16.557	4958	4966	4974	rVB5	14380	21599	1.63%	0.213%

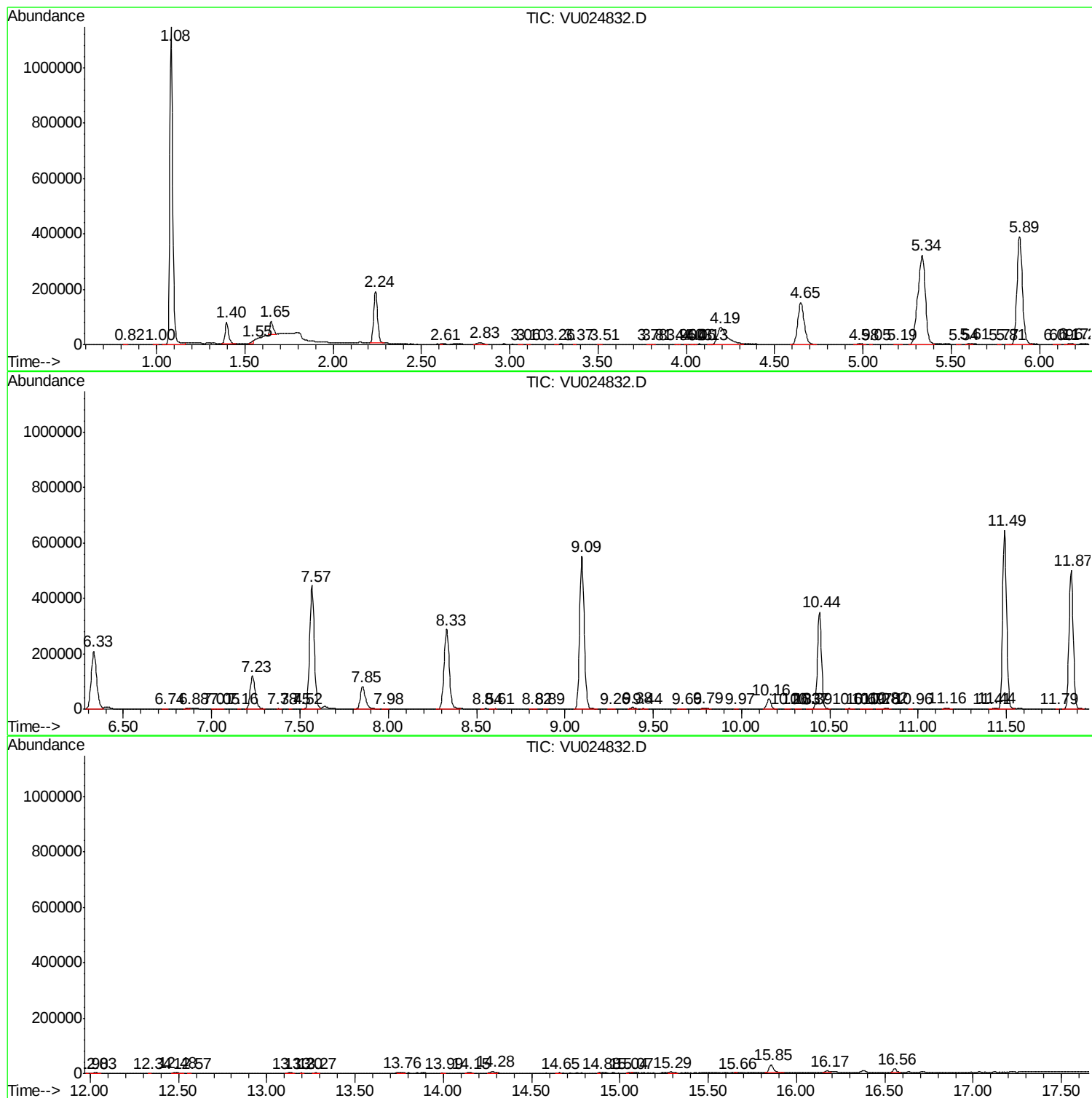
Sum of corrected areas: 10131482

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062218\
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ALS Vial : 6 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 :
DAXQ9ME

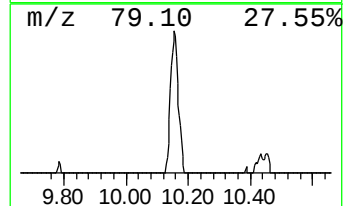
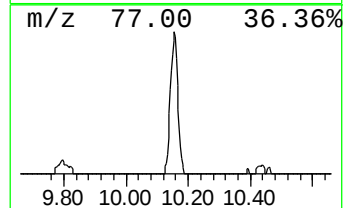
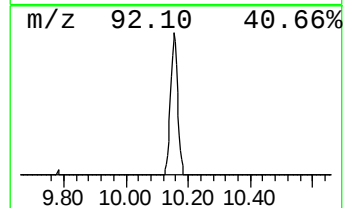
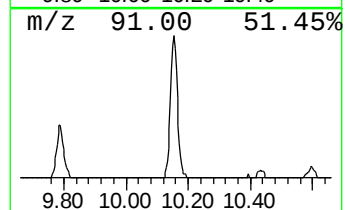
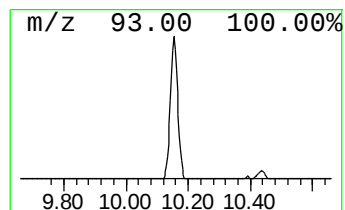
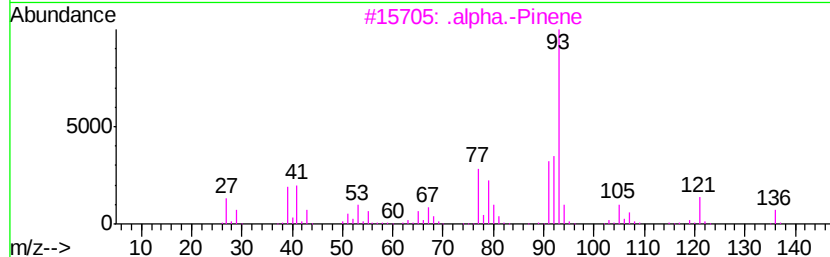
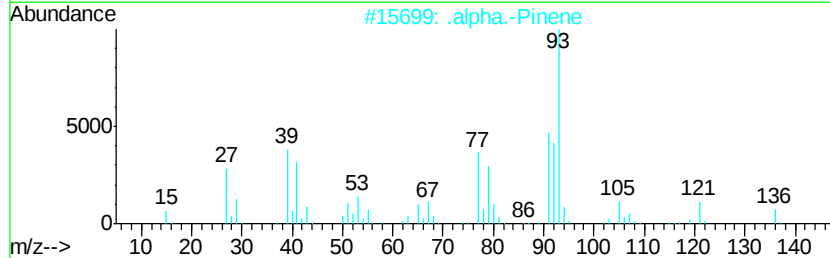
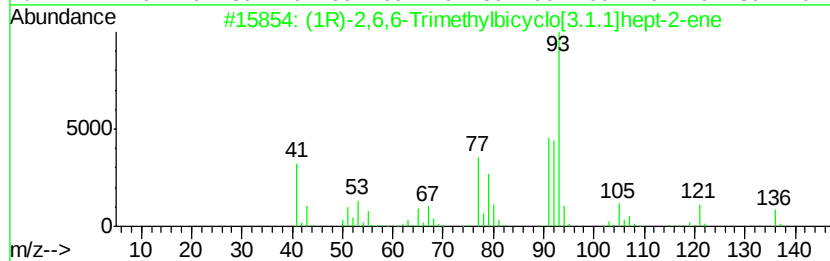
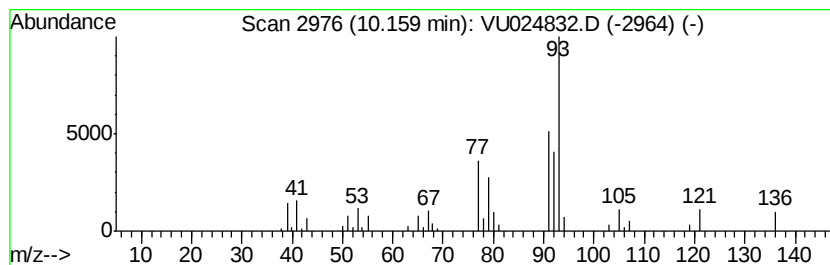
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061518WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.98 ug/L	60120	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	97
2		.alpha.-Pinene	136	C10H16	000080-56-8	95
3		.alpha.-Pinene	136	C10H16	000080-56-8	94
4		(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	91
5		.alpha.-Pinene	136	C10H16	000080-56-8	91



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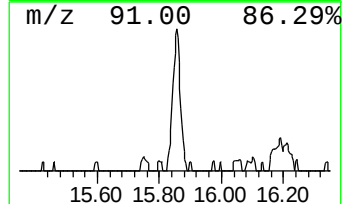
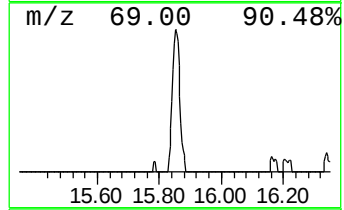
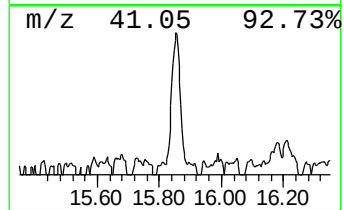
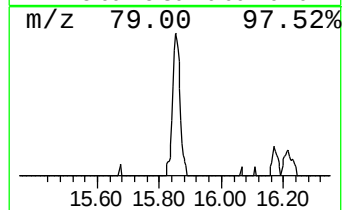
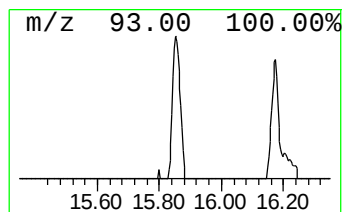
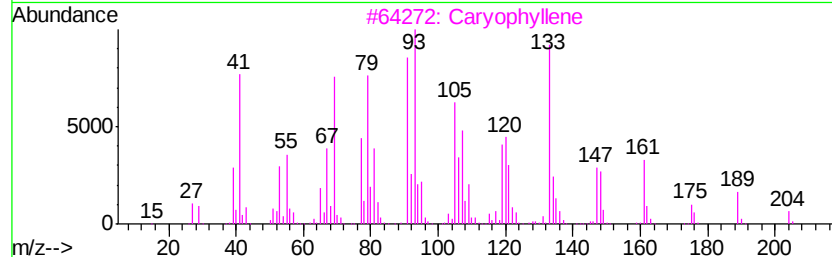
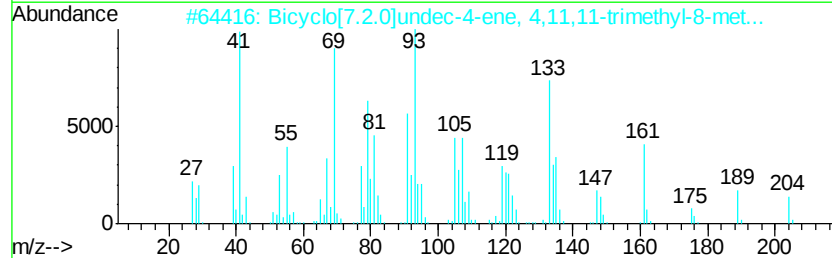
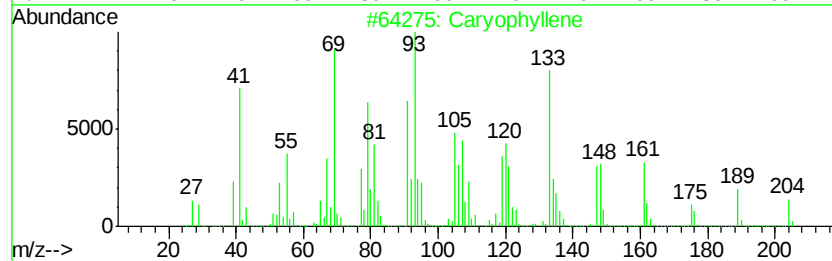
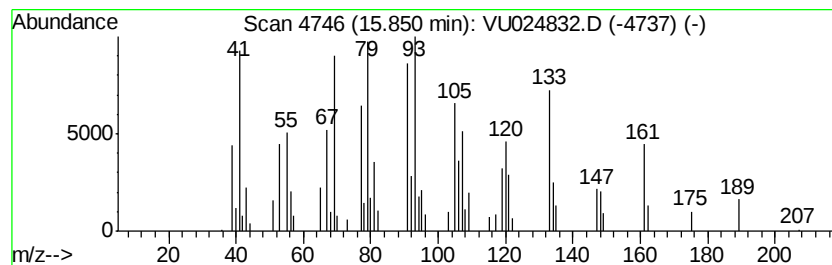
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Quant Title : VOC Analysis

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.
15.85	2.74 ug/L	55646	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Caryophyllene	204 C15H24	000087-44-5 64
2		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	013877-93-5 60
3		Caryophyllene	204 C15H24	000087-44-5 60
4		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	013877-93-5 53
5		Caryophyllene	204 C15H24	000087-44-5 53



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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	3.0	ug/L	60120	2	9.09	1008650	50.0
Caryophyllene	15.85	2.7	ug/L	55646	3	11.49	1015970	50.0