

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091818\
 Data File : VU026886.D
 Acq On : 19 Sep 2018 00:32
 Operator : MD/SY
 Sample : J4865-20ME
 Misc : 4.59g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB3P8ME

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\SOMULM091718WMA.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	62	68	86	rVB	62994	82489	1.80%	0.601%
2	2.234	320	330	344	rBV	133315	207985	4.55%	1.514%
3	2.344	355	364	389	rVB	38247	83733	1.83%	0.610%
4	2.620	439	450	489	rVB	287888	556550	12.18%	4.052%
5	3.019	572	574	578	rBV	169	70	0.00%	0.001%
6	3.064	584	588	592	rVB2	239	181	0.00%	0.001%
7	3.103	597	600	602	rBV	98	72	0.00%	0.001%
8	3.183	615	625	646	rVB5	2945	7224	0.16%	0.053%
9	3.279	651	655	657	rBV	282	191	0.00%	0.001%
10	3.501	721	724	729	rBV	141	142	0.00%	0.001%
11	3.742	791	799	801	rBV2	852	1006	0.02%	0.007%
12	3.980	870	873	877	rBV	103	77	0.00%	0.001%
13	4.103	906	911	914	rBV	151	121	0.00%	0.001%
14	4.125	914	918	920	rBV	78	64	0.00%	0.000%
15	4.144	920	924	926	rBV	135	107	0.00%	0.001%
16	4.196	926	940	960	rBV	48987	166976	3.65%	1.216%
17	4.475	1025	1027	1031	rVB2	243	164	0.00%	0.001%
18	4.492	1031	1032	1035	rBV2	240	115	0.00%	0.001%
19	4.530	1042	1044	1046	rBV	159	111	0.00%	0.001%
20	4.646	1063	1080	1111	rBV	118518	299124	6.54%	2.178%
21	4.958	1174	1177	1179	rVB	148	83	0.00%	0.001%
22	4.971	1179	1181	1184	rVB	151	88	0.00%	0.001%
23	5.061	1204	1209	1212	rVB	98	87	0.00%	0.001%
24	5.109	1220	1224	1228	rBV	84	63	0.00%	0.000%
25	5.221	1256	1259	1262	rVB	110	72	0.00%	0.001%
26	5.334	1267	1294	1329	rVV2	249123	728595	15.94%	5.305%
27	5.488	1339	1342	1345	rBV2	192	112	0.00%	0.001%
28	5.559	1360	1364	1367	rBV	107	86	0.00%	0.001%
29	5.601	1367	1377	1386	rBV3	1078	2057	0.05%	0.015%
30	5.659	1392	1395	1397	rVB2	370	226	0.00%	0.002%
31	5.736	1417	1419	1422	rVB	164	66	0.00%	0.000%
32	5.774	1422	1431	1436	rBV4	939	1541	0.03%	0.011%
33	5.884	1450	1465	1495	rBV	257953	534210	11.69%	3.890%
34	6.045	1512	1515	1518	rBV3	220	147	0.00%	0.001%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
 Title : VOC Analysis

35	6.173	1549	1555	1562	rVV	701	961	0.02%	0.007%
36	6.331	1586	1604	1631	rBV	163664	347088	7.59%	2.527%
37	6.456	1635	1643	1645	rBV2	802	944	0.02%	0.007%
38	6.617	1690	1693	1697	rBV	91	68	0.00%	0.000%
39	6.649	1699	1703	1707	rBV	81	82	0.00%	0.001%
40	6.723	1720	1726	1728	rBV2	159	155	0.00%	0.001%
41	6.816	1751	1755	1757	rBV	507	406	0.01%	0.003%
42	6.868	1762	1771	1792	rVB7	4822	13277	0.29%	0.097%
43	6.977	1803	1805	1810	rVB	177	83	0.00%	0.001%
44	7.003	1810	1813	1815	rBV	226	143	0.00%	0.001%
45	7.038	1821	1824	1827	rBV	195	137	0.00%	0.001%
46	7.067	1831	1833	1836	rVB2	142	78	0.00%	0.001%
47	7.115	1844	1848	1849	rBV	179	127	0.00%	0.001%
48	7.228	1871	1883	1907	rBV2	75296	147193	3.22%	1.072%
49	7.324	1911	1913	1915	rBV2	143	78	0.00%	0.001%
50	7.350	1919	1921	1927	rBV2	253	172	0.00%	0.001%
51	7.376	1927	1929	1930	rBV2	233	101	0.00%	0.001%
52	7.456	1953	1954	1956	rBV	112	63	0.00%	0.000%
53	7.472	1956	1959	1962	rBV	669	620	0.01%	0.005%
54	7.565	1974	1988	2008	rBV	287786	521336	11.41%	3.796%
55	7.784	2051	2056	2058	rBV2	213	177	0.00%	0.001%
56	7.797	2058	2060	2062	rBV	233	158	0.00%	0.001%
57	7.855	2067	2078	2100	rVB	53081	106553	2.33%	0.776%
58	7.961	2107	2111	2116	rVB4	325	333	0.01%	0.002%
59	8.003	2122	2124	2127	rBV2	126	94	0.00%	0.001%
60	8.061	2139	2142	2146	rBV	207	181	0.00%	0.001%
61	8.083	2146	2149	2151	rVB	213	97	0.00%	0.001%
62	8.327	2213	2225	2256	rBV	236109	431677	9.44%	3.143%
63	8.630	2311	2319	2332	rVB2	3169	5465	0.12%	0.040%
64	8.691	2332	2338	2339	rBV2	932	671	0.01%	0.005%
65	8.771	2359	2363	2368	rVB2	243	240	0.01%	0.002%
66	8.797	2368	2371	2374	rBV2	191	132	0.00%	0.001%
67	8.845	2384	2386	2390	rVB	235	119	0.00%	0.001%
68	8.897	2400	2402	2407	rBB	165	71	0.00%	0.001%
69	8.983	2426	2429	2432	rVB	199	160	0.00%	0.001%
70	9.044	2446	2448	2450	rBV2	132	67	0.00%	0.000%
71	9.093	2450	2463	2493	rVV	384518	677027	14.81%	4.929%

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72	9.224	2498	2504	2506	rBV2	379	354	0.01%	0.003%
73	9.315	2528	2532	2534	rBV	230	153	0.00%	0.001%
74	9.382	2545	2553	2563	rVB5	3534	5709	0.12%	0.042%
75	9.498	2587	2589	2593	rVB	174	93	0.00%	0.001%
76	9.552	2604	2606	2610	rBV	145	73	0.00%	0.001%
77	9.601	2619	2621	2625	rBV	159	77	0.00%	0.001%
78	9.884	2707	2709	2712	rVV	179	122	0.00%	0.001%
79	10.003	2739	2746	2758	rVB4	2904	4921	0.11%	0.036%
80	10.154	2778	2793	2814	rBV	2863607	4570501	100.00%	33.278%
81	10.437	2870	2881	2901	rVB	344379	559982	12.25%	4.077%
82	10.607	2929	2934	2946	rVB4	1506	2463	0.05%	0.018%
83	10.732	2971	2973	2975	rVB	185	74	0.00%	0.001%
84	10.755	2975	2980	2983	rBV	421	356	0.01%	0.003%
85	10.826	2988	3002	3032	rBV	915312	1503413	32.89%	10.946%
86	10.983	3048	3051	3052	rBV	275	182	0.00%	0.001%
87	11.138	3089	3099	3104	rBV3	7704	13689	0.30%	0.100%
88	11.298	3140	3149	3160	rVB6	10499	15787	0.35%	0.115%
89	11.433	3177	3191	3198	rBV	57433	91469	2.00%	0.666%
90	11.488	3198	3208	3232	rVV2	491589	882634	19.31%	6.426%
91	11.594	3234	3241	3262	rVB3	16688	26939	0.59%	0.196%
92	11.777	3291	3298	3307	rVB5	4225	5489	0.12%	0.040%
93	11.864	3312	3325	3345	rBV	394978	626826	13.71%	4.564%
94	12.028	3367	3376	3385	rVB3	12045	17444	0.38%	0.127%
95	12.115	3400	3403	3404	rBV	231	121	0.00%	0.001%
96	12.141	3404	3411	3420	rVV4	7925	11046	0.24%	0.080%
97	12.601	3546	3554	3570	rBV	6514	12032	0.26%	0.088%
98	12.781	3608	3610	3612	rBV	259	142	0.00%	0.001%
99	13.395	3796	3801	3811	rVB4	1131	1667	0.04%	0.012%
100	14.649	4173	4191	4213	rBV	260990	450355	9.85%	3.279%

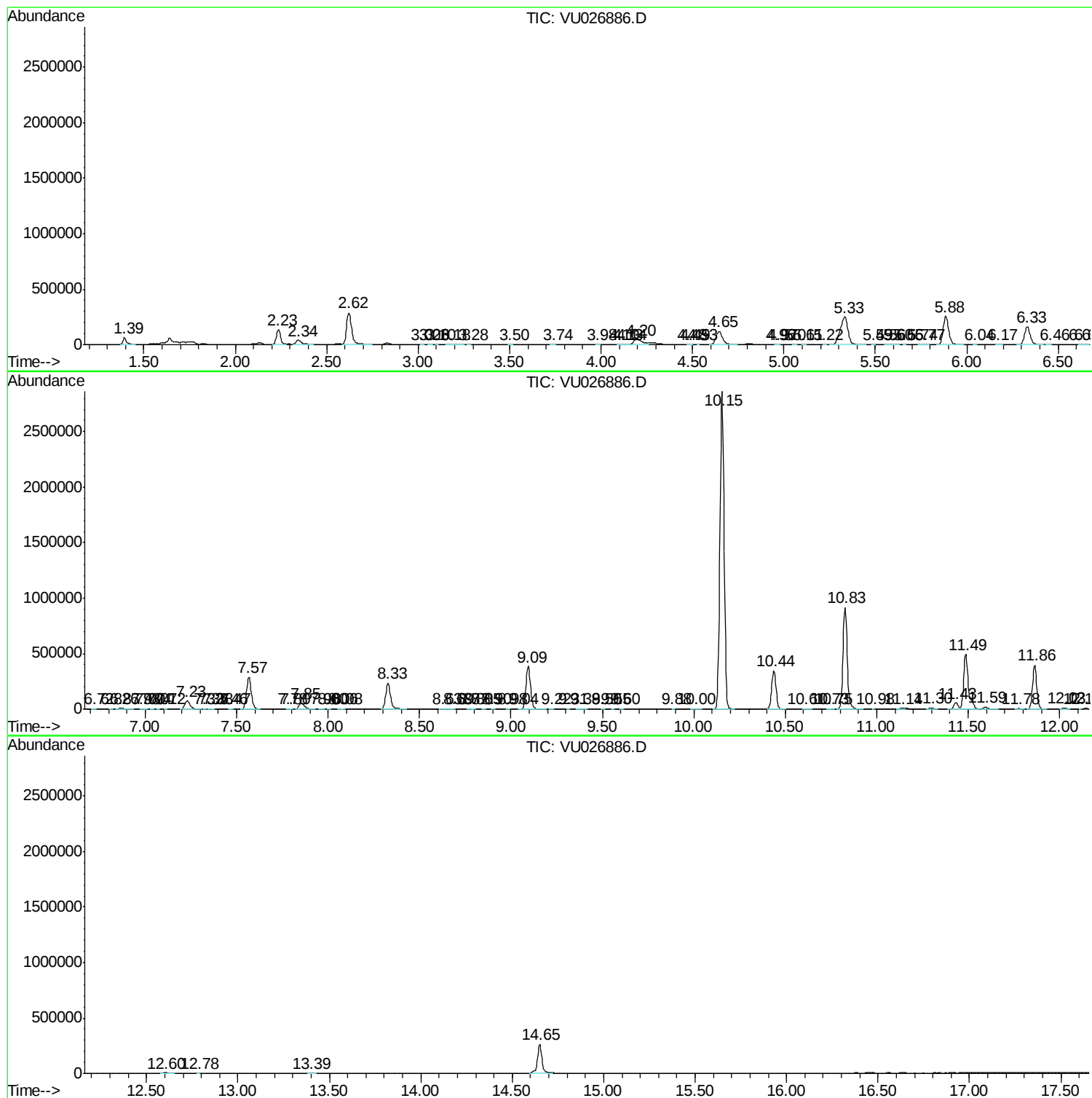
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 44 Sample Multiplier: 1

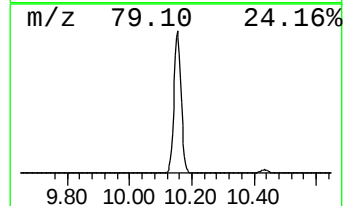
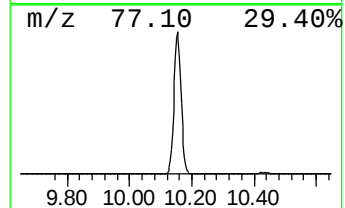
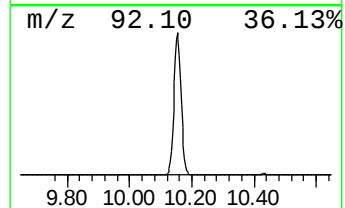
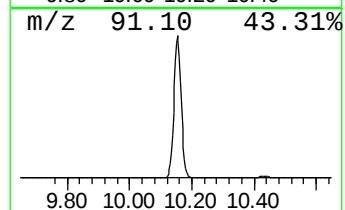
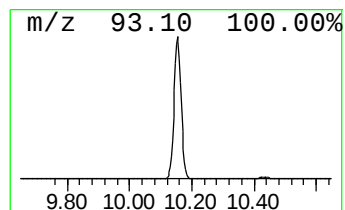
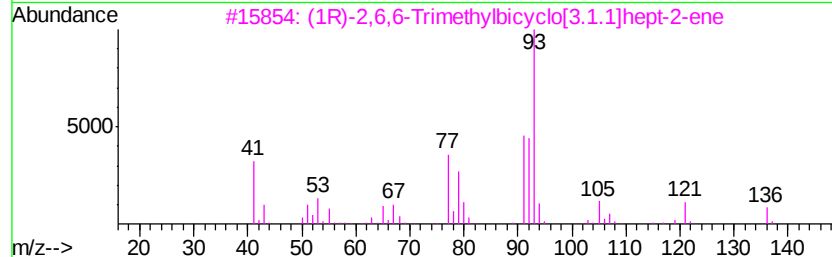
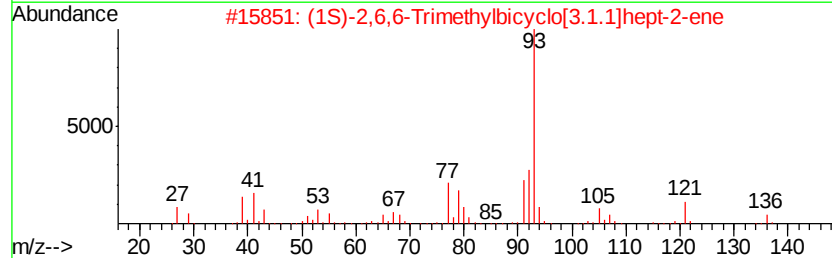
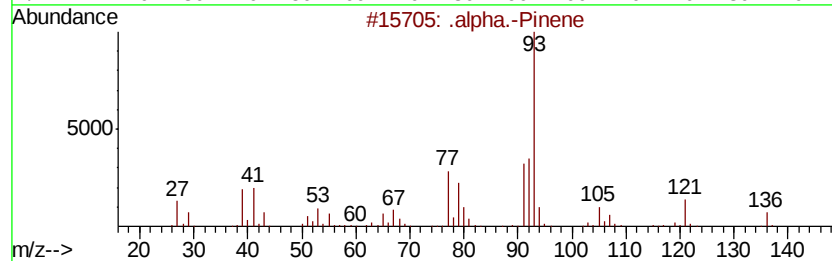
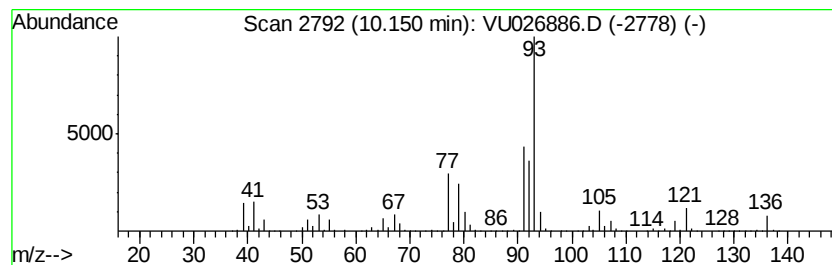
Instrument :
MSVOA_U
ClientSampleId :
DB3P8ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.15	337.54 ug/L	4570500	Chlorobenzene-d5	9.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	97
2	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	95
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
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	91



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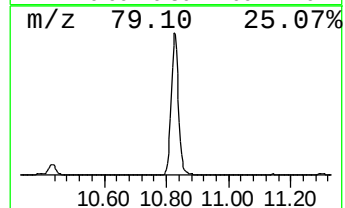
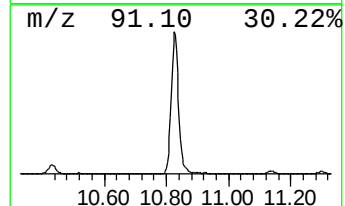
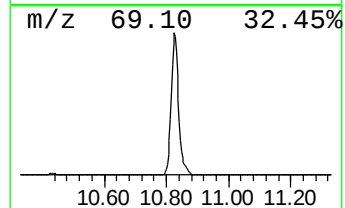
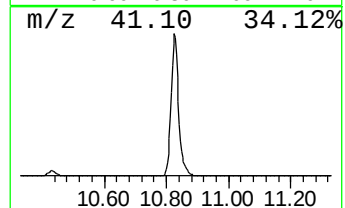
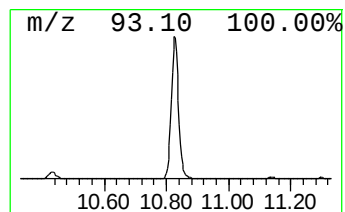
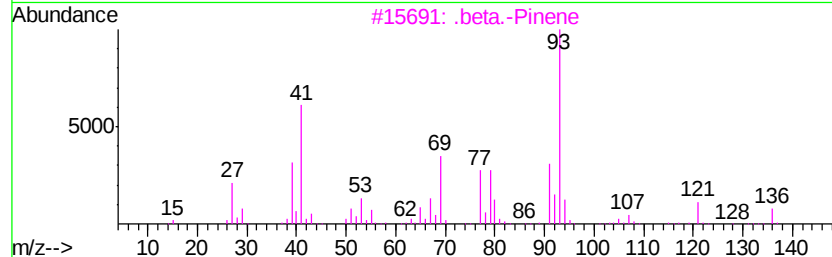
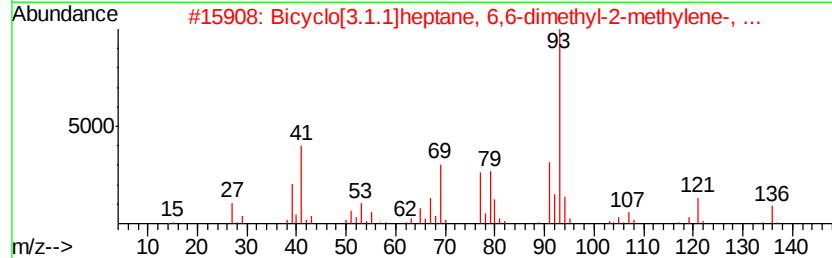
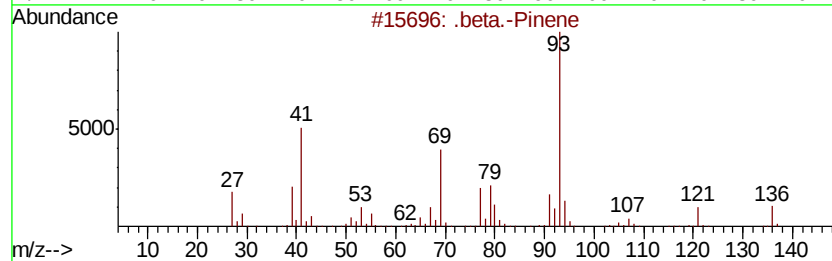
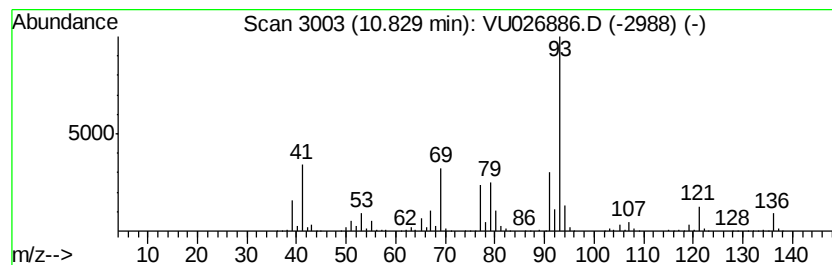
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Quant Title : VOC Analysis

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

Peak Number 3 .beta.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	85.17 ug/L	1503410	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Pinene	136 C10H16	000127-91-3 97
2		Bicyclo[3.1.1]heptane, 6,6-dimet...	136 C10H16	018172-67-3 96
3		.beta.-Pinene	136 C10H16	000127-91-3 96
4		.beta.-Pinene	136 C10H16	000127-91-3 94
5		.alpha.-Pinene	136 C10H16	000080-56-8 93



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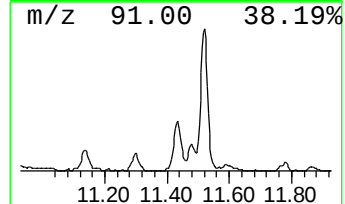
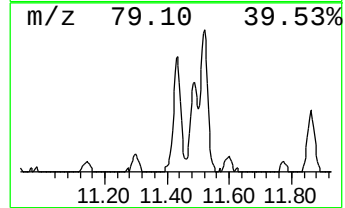
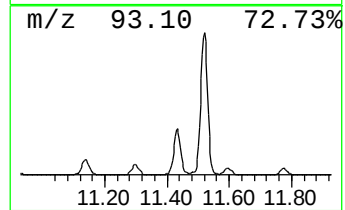
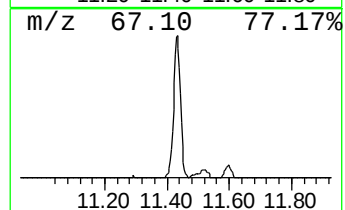
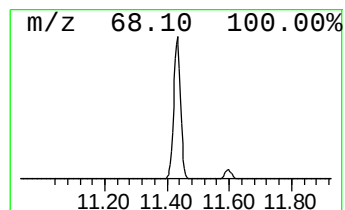
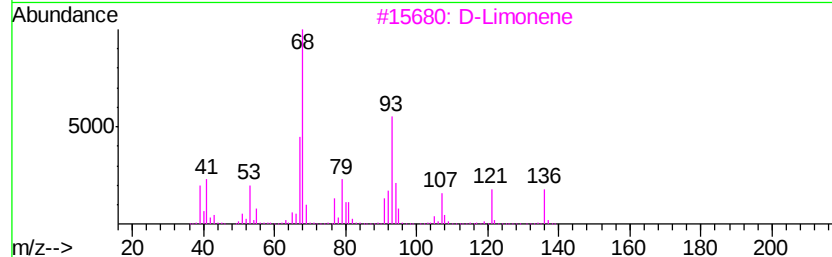
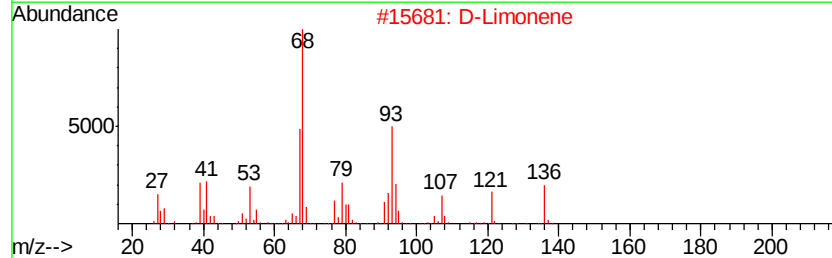
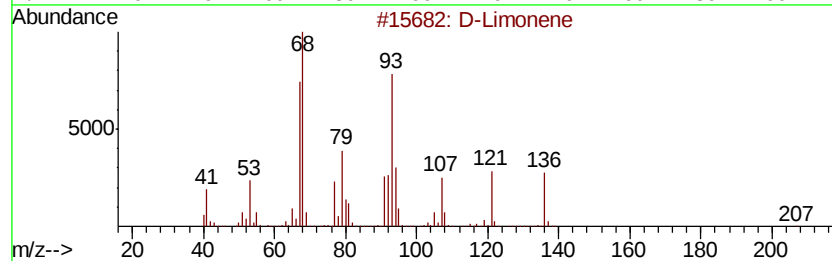
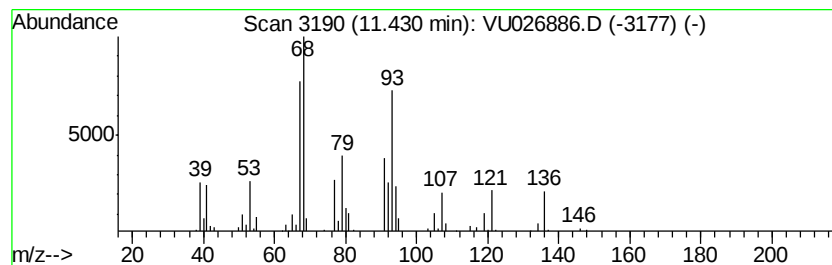
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Quant Title : VOC Analysis

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

Peak Number 4 D-Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.43	5.18 ug/L	91469	1,4-Dichlorobenzene-d4	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	D-Limonene	136	C10H16	005989-27-5	94
3	D-Limonene	136	C10H16	005989-27-5	94
4	Limonene	136	C10H16	000138-86-3	94
5	D-Limonene	136	C10H16	005989-27-5	76



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091818\
Data File : VU026886.D
Acq On : 19 Sep 2018 00:32
Operator : MD/SY
Sample : J4865-20ME
Misc : 4.59µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

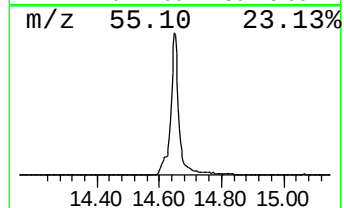
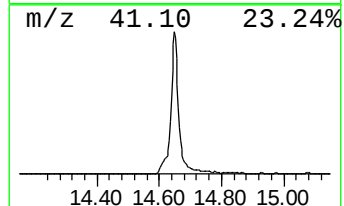
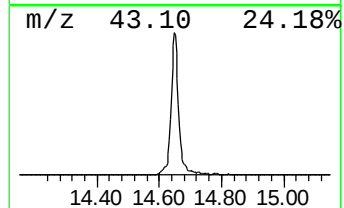
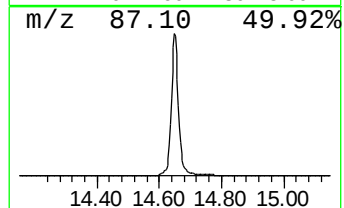
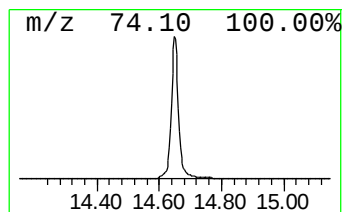
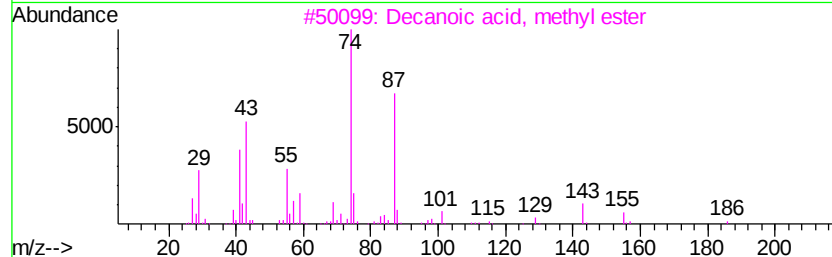
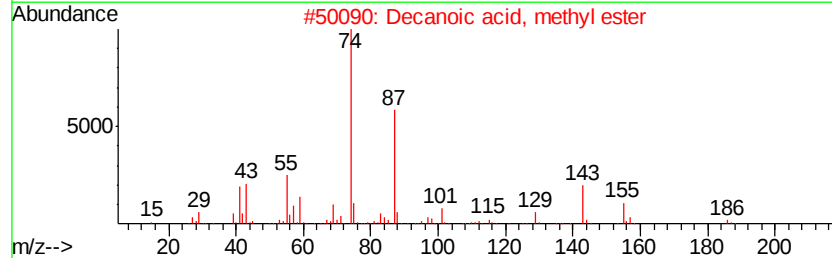
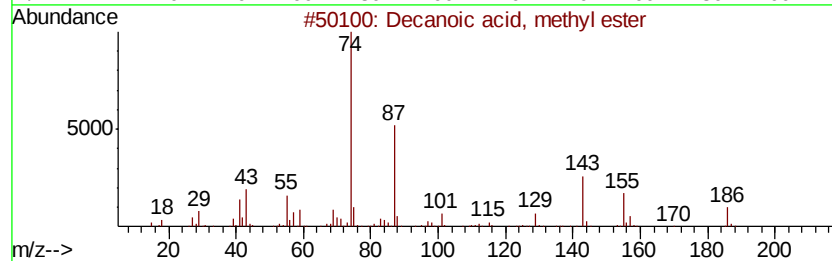
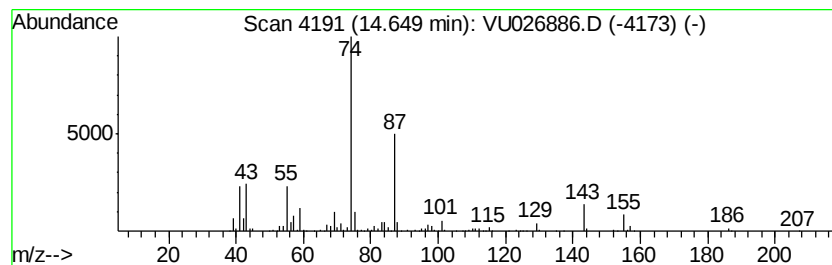
Instrument :
MSVOA_U
ClientSampleId :
DB3P8ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Decanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	25.51 ug/L	450355	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decanoic acid, methyl ester	186 C11H22O2	000110-42-9 97
2		Decanoic acid, methyl ester	186 C11H22O2	000110-42-9 96
3		Decanoic acid, methyl ester	186 C11H22O2	000110-42-9 94
4		Undecanoic acid, methyl ester	200 C12H24O2	001731-86-8 78
5		Nonanoic acid, methyl ester	172 C10H20O2	001731-84-6 78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU091818\
Data File : VU026886.D
Acq On : 19 Sep 2018 00:32
Operator : MD/SY
Sample : J4865-20ME
Misc : 4.59g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB3P8ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.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
.alpha.-Pinene	10.15	337.5	ug/L	4570500	2	9.10	677027	50.0
.beta.-Pinene	10.83	85.2	ug/L	1503410	3	11.49	882634	50.0
D-Limonene	11.43	5.2	ug/L	91469	3	11.49	882634	50.0
Decanoic acid, me...	14.65	25.5	ug/L	450355	3	11.49	882634	50.0