

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081222\
 Data File : VX030600.D
 Acq On : 12 Aug 2022 17:31
 Operator : JC/MD
 Sample : N4131-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5E41

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	52	rVB	111572	115072	10.39%	1.248%
2	1.666	91	95	105	rVB	90929	118304	10.68%	1.283%
3	2.306	194	200	210	rVB	213216	326443	29.46%	3.540%
4	2.398	212	215	222	rVB2	2359	4792	0.43%	0.052%
5	2.648	254	256	258	rBV3	692	418	0.04%	0.005%
6	2.788	274	279	286	rBV	7250	12603	1.14%	0.137%
7	2.934	300	303	305	rBV2	497	594	0.05%	0.006%
8	3.075	324	326	327	rBV2	556	434	0.04%	0.005%
9	3.099	327	330	336	rVB5	968	1396	0.13%	0.015%
10	3.233	348	352	354	rBV	584	880	0.08%	0.010%
11	3.398	376	379	380	rBV	535	432	0.04%	0.005%
12	3.538	400	402	403	rBV	773	506	0.05%	0.005%
13	3.593	408	411	413	rVV	402	416	0.04%	0.005%
14	3.855	453	454	458	rBV2	311	498	0.04%	0.005%
15	3.904	460	462	465	rBV	461	442	0.04%	0.005%
16	4.044	482	485	486	rBV	571	509	0.05%	0.006%
17	4.129	496	499	503	rVV2	331	624	0.06%	0.007%
18	4.208	509	512	515	rVV2	255	408	0.04%	0.004%
19	4.477	547	556	572	rBV	109636	333961	30.14%	3.622%
20	4.733	589	598	601	rBV5	2808	6030	0.54%	0.065%
21	5.068	639	653	671	rBV	151998	463402	41.82%	5.026%
22	5.214	675	677	679	rBV	745	480	0.04%	0.005%
23	5.391	702	706	710	rBV4	513	1028	0.09%	0.011%
24	5.495	720	723	724	rBV2	445	413	0.04%	0.004%
25	5.544	728	731	732	rBV2	404	512	0.05%	0.006%
26	5.556	732	733	738	rVV3	933	1461	0.13%	0.016%
27	5.598	738	740	742	rVB	671	550	0.05%	0.006%
28	5.781	768	770	773	rVB2	409	483	0.04%	0.005%
29	5.976	790	802	816	rBV3	379212	1108038	100.00%	12.017%
30	6.336	857	861	863	rBV2	583	806	0.07%	0.009%
31	6.556	893	897	900	rVB3	569	785	0.07%	0.009%
32	6.769	922	932	945	rBV	269609	643069	58.04%	6.974%
33	6.995	967	969	971	rBV	519	431	0.04%	0.005%
34	7.037	974	976	980	rVV	624	584	0.05%	0.006%
35	7.117	980	989	1000	rVB4	14539	35959	3.25%	0.390%
36	7.202	1000	1003	1006	rBV3	985	949	0.09%	0.010%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
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37	7.318	1012	1022	1040	rVB	243474	531264	47.95%	5.762%
38	7.446	1040	1043	1044	rBV	573	480	0.04%	0.005%
39	7.488	1047	1050	1054	rVV3	1103	1486	0.13%	0.016%
40	7.549	1058	1060	1062	rVB2	617	501	0.05%	0.005%

41	7.671	1076	1080	1081	rBV	432	438	0.04%	0.005%
42	7.818	1100	1104	1108	rBV5	1231	2282	0.21%	0.025%
43	7.940	1118	1124	1131	rBV4	1623	3392	0.31%	0.037%
44	8.061	1141	1144	1147	rVB2	453	478	0.04%	0.005%
45	8.135	1152	1156	1157	rBV	584	433	0.04%	0.005%

46	8.330	1182	1188	1201	rVV	152407	252458	22.78%	2.738%
47	8.482	1211	1213	1220	rVB4	1639	2605	0.24%	0.028%
48	8.586	1224	1230	1233	rBV2	3303	5335	0.48%	0.058%
49	8.653	1234	1241	1251	rBV	545880	821458	74.14%	8.909%
50	8.952	1285	1290	1308	rBV	112035	174340	15.73%	1.891%

51	9.153	1321	1323	1327	rVB3	480	492	0.04%	0.005%
52	9.220	1332	1334	1339	rVB	715	899	0.08%	0.010%
53	9.281	1342	1344	1345	rBV2	490	515	0.05%	0.006%
54	9.390	1356	1362	1375	rBV	501194	711343	64.20%	7.715%
55	9.586	1392	1394	1400	rVB5	2302	3529	0.32%	0.038%

56	10.055	1465	1471	1482	rBV	544996	753983	68.05%	8.177%
57	10.262	1504	1505	1509	rVB2	1032	756	0.07%	0.008%
58	10.299	1509	1511	1512	rBV2	720	460	0.04%	0.005%
59	10.683	1568	1574	1580	rVB3	651	1660	0.15%	0.018%
60	10.774	1585	1589	1594	rBV5	1178	2123	0.19%	0.023%

61	10.890	1607	1608	1613	rVB3	479	458	0.04%	0.005%
62	11.073	1633	1638	1639	rBV	466	800	0.07%	0.009%
63	11.195	1651	1658	1668	rBV	427498	548039	49.46%	5.944%
64	11.421	1693	1695	1700	rBV3	552	925	0.08%	0.010%
65	11.518	1707	1711	1716	rVB3	11874	15078	1.36%	0.164%

66	11.756	1743	1750	1751	rBV4	1553	3243	0.29%	0.035%
67	11.817	1757	1760	1761	rBV2	562	665	0.06%	0.007%
68	11.975	1777	1786	1789	rBV6	6621	13153	1.19%	0.143%
69	12.024	1789	1794	1802	rVV	565497	695417	62.76%	7.542%
70	12.103	1802	1807	1812	rVB3	35773	51932	4.69%	0.563%

71	12.225	1822	1827	1837	rBV3	13040	25223	2.28%	0.274%
72	12.323	1838	1843	1850	rVB	600673	757710	68.38%	8.218%
73	12.463	1861	1866	1867	rBV4	675	921	0.08%	0.010%
74	12.524	1874	1876	1881	rVB5	2427	3122	0.28%	0.034%
75	12.701	1903	1905	1908	rVB3	642	470	0.04%	0.005%

76	12.731	1908	1910	1912	rBV2	473	450	0.04%	0.005%
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77	12.774	1914	1917	1918	rBV2	1355	1338	0.12%	0.015%
78	12.823	1920	1925	1936	rBV	437980	535213	48.30%	5.805%
79	13.311	2001	2005	2009	rBV4	720	1322	0.12%	0.014%
80	13.384	2015	2017	2019	rBV	1013	684	0.06%	0.007%
81	13.426	2022	2024	2025	rVV2	752	549	0.05%	0.006%
82	13.451	2025	2028	2033	rVV6	1851	3948	0.36%	0.043%
83	13.512	2033	2038	2045	rVV2	17213	25420	2.29%	0.276%
84	13.585	2045	2050	2055	rVV	24048	32937	2.97%	0.357%
85	13.658	2059	2062	2067	rVV4	2591	4300	0.39%	0.047%
86	13.731	2070	2074	2085	rVB5	18528	26146	2.36%	0.284%
87	13.963	2108	2112	2113	rBV3	1203	1503	0.14%	0.016%
88	14.079	2129	2131	2134	rBV3	627	649	0.06%	0.007%
89	14.134	2136	2140	2144	rBV2	2615	3488	0.31%	0.038%
90	14.274	2161	2163	2169	rVB4	997	903	0.08%	0.010%
91	14.390	2179	2182	2185	rBV3	587	757	0.07%	0.008%
92	14.444	2189	2191	2192	rBV	770	609	0.05%	0.007%
93	14.627	2219	2221	2222	rBV	773	417	0.04%	0.005%
94	14.707	2233	2234	2237	rBV3	853	660	0.06%	0.007%
95	14.993	2278	2281	2283	rBV4	1016	1361	0.12%	0.015%
96	15.231	2318	2320	2323	rBV3	902	750	0.07%	0.008%
97	15.359	2340	2341	2344	rBV4	719	832	0.08%	0.009%
98	15.694	2395	2396	2398	rBV2	774	646	0.06%	0.007%
99	16.145	2468	2470	2472	rBV2	776	965	0.09%	0.010%
100	16.225	2480	2483	2485	rBV3	827	1147	0.10%	0.012%

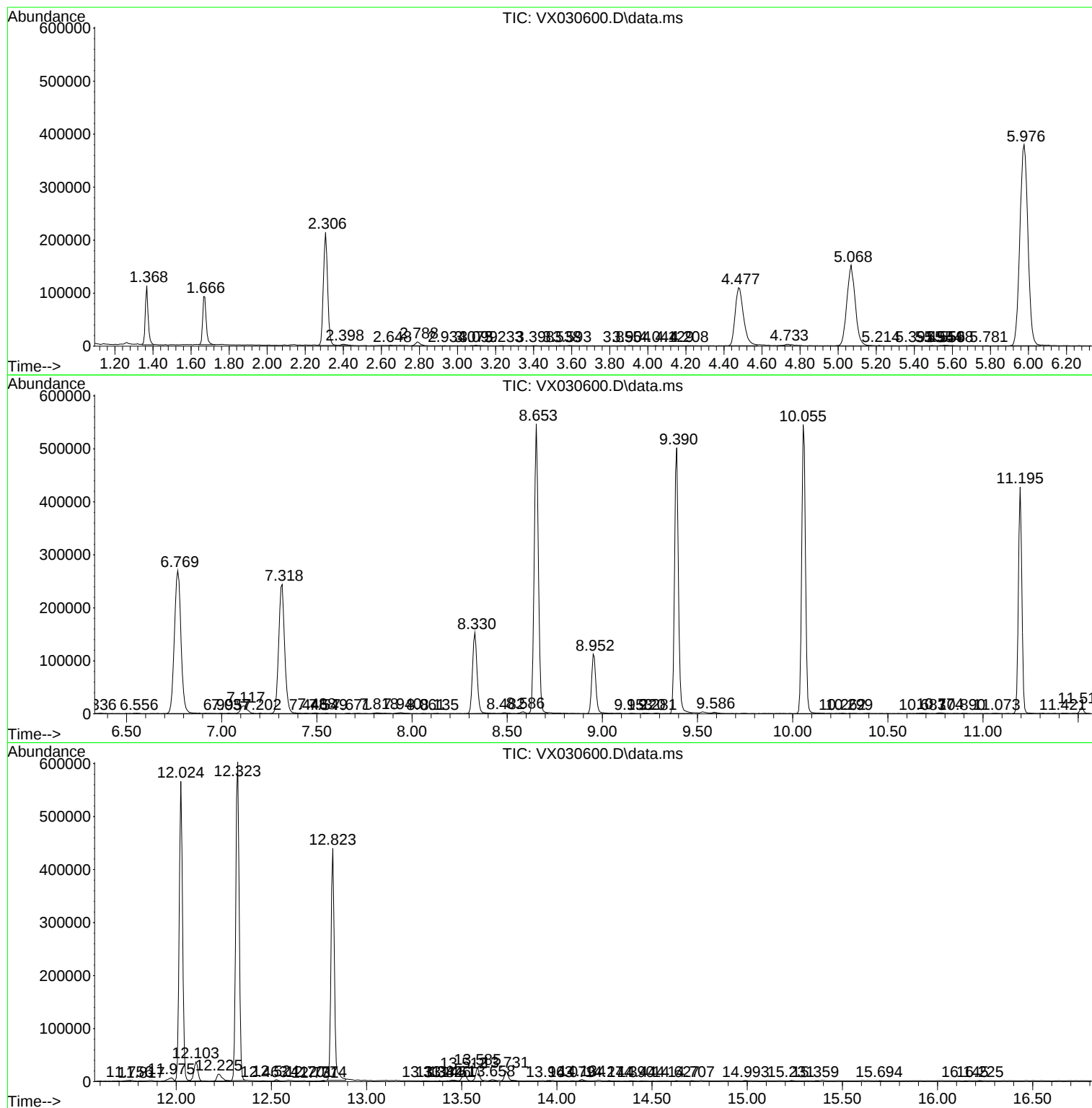
Sum of corrected areas: 9220572

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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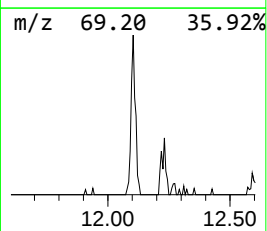
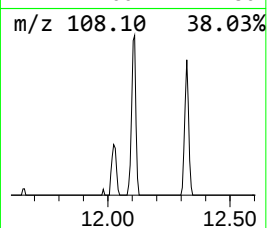
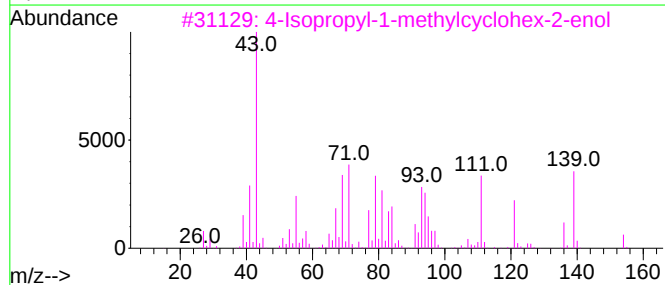
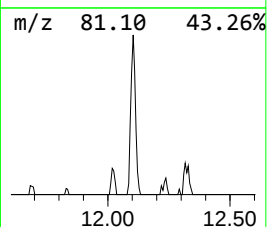
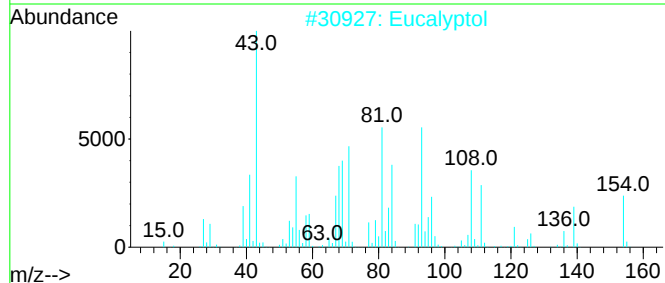
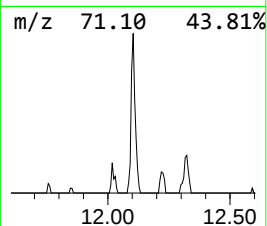
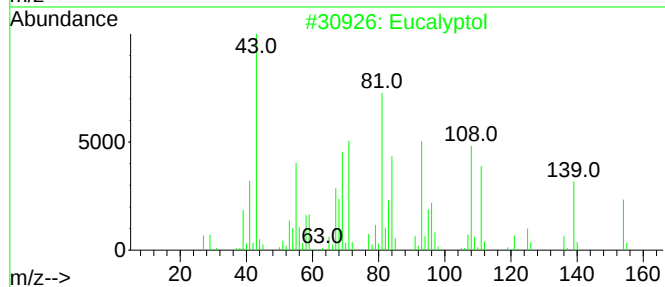
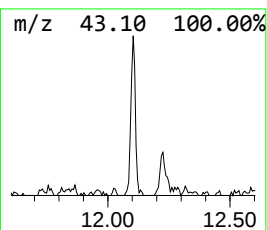
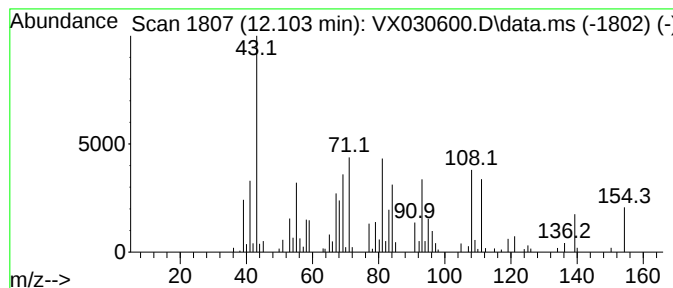
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	3.73 ug/L	51932	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	52
2			Eucalyptol	154	C10H18O	000470-82-6	40
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32
4			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	27
5			2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	16



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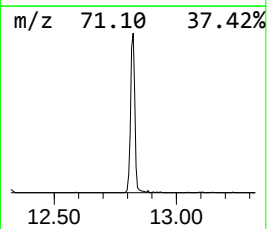
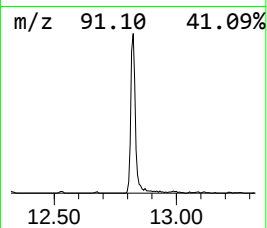
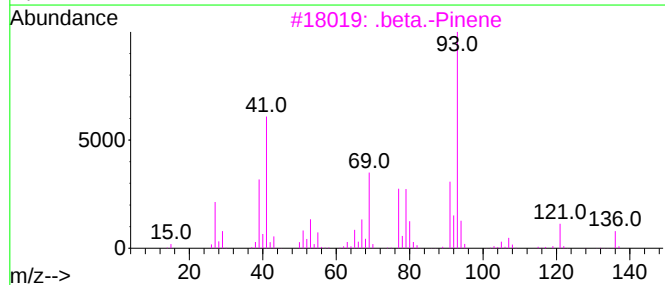
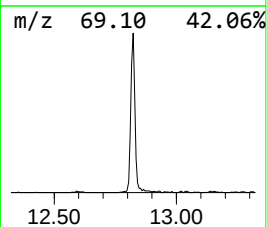
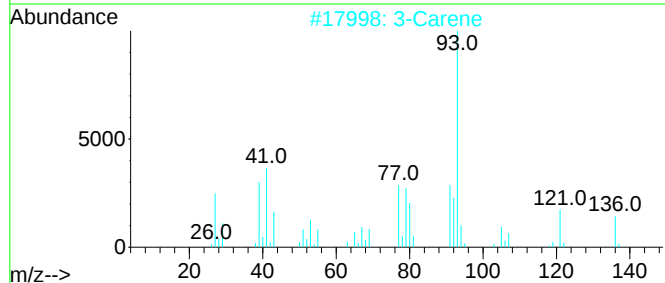
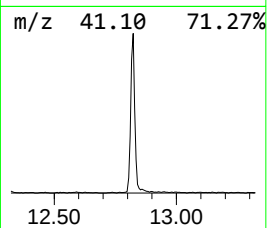
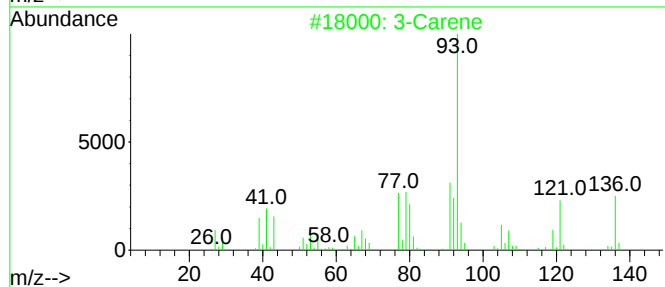
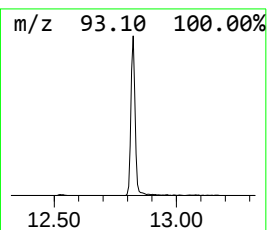
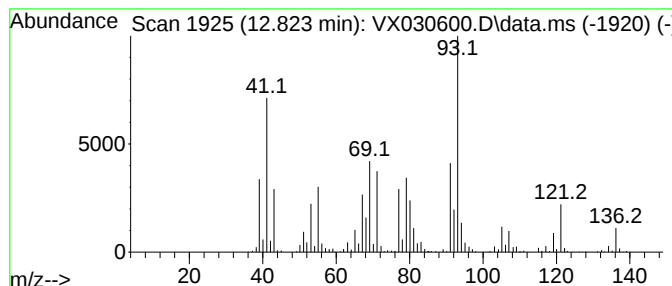
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Carene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.823	38.48 ug/L	535213	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	87
2			3-Carene	136	C10H16	013466-78-9	87
3			.beta.-Pinene	136	C10H16	000127-91-3	81
4			Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	76
5			Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	76



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	12.103	3.7	ug/L	51932	3	12.024	695417	50.0
3-Carene	12.823	38.5	ug/L	535213	3	12.024	695417	50.0