LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027068.D
Acq On : 29 Jul 2022 04:59
Operator : SY/MD
Sample : N3790-15ME
Misc : 5.21g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

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_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

Signal : TIC: VV027068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.208	48	52	58	rBV	10161	10073	0.43%	0.055%
2	1.301	74	81	113	rVB	219180	350219	15.09%	1.897%
3	1.558	155	161	170	rBV	97387	120750	5.20%	0.654%
4	2.079	313	323	340	rVB	587472	824986	35.55%	4.469%
5	2.433	424	433	444	rBV	26068	50625	2.18%	0.274%
6	2.610	477	488	505	rVB	13197	27405	1.18%	0.148%
7	2.806	547	549	554	rVB4	883	622	0.03%	0.003%
8	2.896	575	577	582	rVB2	607	405	0.02%	0.002%
9	2.928	584	587	590	rBV2	634	539	0.02%	0.003%
10	3.018	612	615	624	rVB5	675	755	0.03%	0.004%
11	3.146	646	655	656	rBV2	388	417	0.02%	0.002%
12	3.169	658	662	663	rBV3	628	501	0.02%	0.003%
13	3.256	683	689	691	rBV3	561	427	0.02%	0.002%
14	3.352	715	719	725	rBB3	328	352	0.02%	0.002%
15	3.407	729	736	740	rBV2	467	495	0.02%	0.003%
16	3.899	878	889	956	rBV2	115940	553535	23.86%	2.998%
17	4.339	1010	1026	1054	rBV	360094	910811	39.25%	4.934%
18	4.658	1123	1125	1130	rVB2	648	521	0.02%	0.003%
19	4.947	1211	1215	1220	rVB3	567	548	0.02%	0.003%
20	5.034	1225	1242	1271	rBV2	952007	2320322	100.00%	12.569%
21	5.294	1318	1323	1325	rBV3	517	404	0.02%	0.002%
22	5.336	1325	1336	1354	rBV4	11567	30372	1.31%	0.165%
23	5.423	1361	1363	1367	rVB4	1135	635	0.03%	0.003%
24	5.487	1380	1383	1391	rVB5	819	937	0.04%	0.005%
25	5.558	1398	1405	1407	rBV4	852	1003	0.04%	0.005%
26	5.609	1408	1421	1455	rBV	664747	1377218	59.35%	7.460%
27	5.899	1504	1511	1524	rVB5	16813	31970	1.38%	0.173%
28	6.063	1549	1562	1594	rVB	494924	1052468	45.36%	5.701%
29	6.638	1730	1741	1759	rBV9	4799	13434	0.58%	0.073%
30	6.748	1773	1775	1782	rVB5	1031	752	0.03%	0.004%
31	6.982	1837	1848	1876	rBV	216509	419496	18.08%	2.272%
32	7.310	1938	1950	1977	rBV	1014983	1797405	77.46%	9.736%
33	7.619	2035	2046	2079	rBV	149669	292144	12.59%	1.583%
34	7.886	2126	2129	2134	rVB5	630	555	0.02%	0.003%
35	7.973	2151	2156	2165	rVB8	2363	3408	0.15%	0.018%
36	8.037	2173	2176	2180	rBV3	560	399	0.02%	0.002%

LSC Area Percent Report

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Misc : 5.21g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

37	8.098	2183	2195	2237	rBV	276871	964314	41.56%	5.224%
38	8.436	2294	2300	2310	rVB5	3375	5866	0.25%	0.032%
39	8.638	2360	2363	2365	rBV3	496	350	0.02%	0.002%
40	8.850	2412	2429	2459	rBV	989637	1710948	73.74%	9.268%
41	9.111	2507	2510	2511	rBV2	699	405	0.02%	0.002%
42	9.191	2532	2535	2538	rBV3	818	544	0.02%	0.003%
43	9.455	2612	2617	2624	rVB4	575	626	0.03%	0.003%
44	9.497	2624	2630	2633	rBV4	855	757	0.03%	0.004%
45	9.751	2701	2709	2722	rVB5	8130	14476	0.62%	0.078%
46	9.905	2743	2757	2770	rBV	503290	826093	35.60%	4.475%
47	10.085	2811	2813	2817	rVB3	838	453	0.02%	0.002%
48	10.111	2817	2821	2823	rBV4	906	657	0.03%	0.004%
49	10.140	2823	2830	2834	rBV7	3582	4393	0.19%	0.024%
50	10.217	2835	2854	2871	rVV	654977	1169241	50.39%	6.334%
51	10.420	2910	2917	2919	rBV4	587	591	0.03%	0.003%
52	10.538	2942	2954	2957	rVV2	9603	13592	0.59%	0.074%
53	10.577	2958	2966	2982	rVB	70929	116563	5.02%	0.631%
54	10.857	3049	3053	3054	rBV3	705	442	0.02%	0.002%
55	10.944	3068	3080	3095	rVB	67067	106630	4.60%	0.578%
56	11.059	3111	3116	3122	rVB8	845	1165	0.05%	0.006%
57	11.137	3135	3140	3143	rBV3	625	455	0.02%	0.002%
58	11.191	3143	3157	3164	rBV4	13754	21921	0.94%	0.119%
59	11.252	3164	3176	3198	rBV	1048081	1650417	71.13%	8.940%
60	11.538	3258	3265	3273	rVB9	2811	4200	0.18%	0.023%
61	11.625	3279	3292	3320	rBV	975256	1543332	66.51%	8.360%
62	11.799	3341	3346	3351	rVB4	814	1014	0.04%	0.005%
63	11.834	3351	3357	3358	rBV4	671	657	0.03%	0.004%
64	11.882	3366	3372	3373	rBV4	527	490	0.02%	0.003%
65	11.899	3373	3377	3379	rBV3	1126	828	0.04%	0.004%
66	12.095	3436	3438	3442	rVB2	600	407	0.02%	0.002%
67	12.120	3442	3446	3450	rBV3	572	617	0.03%	0.003%
68	12.355	3513	3519	3520	rVV4	1427	1264	0.05%	0.007%
69	12.381	3521	3527	3535	rVV6	3278	5526	0.24%	0.030%
70	12.651	3608	3611	3615	rVB4	522	460	0.02%	0.002%
71	12.741	3635	3639	3640	rBV2	515	367	0.02%	0.002%
72	12.815	3654	3662	3667	rVB7	1602	2304	0.10%	0.012%
73	12.882	3678	3683	3684	rBV3	627	423	0.02%	0.002%
74	13.011	3720	3723	3726	rVV4	492	364	0.02%	0.002%
75	13.069	3729	3741	3754	rVB3	16815	25284	1.09%	0.137%
76	13.124	3754	3758	3763	rVB3	543	410	0.02%	0.002%

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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

77	13.153	3763	3767	3769	rBV3	968	539	0.02%	0.003%
78	13.188	3772	3778	3779	rBV3	426	393	0.02%	0.002%
79	13.268	3797	3803	3811	rBV4	568	821	0.04%	0.004%
80	13.300	3811	3813	3816	rBV3	593	445	0.02%	0.002%
81	13.368	3832	3834	3840	rVB2	645	588	0.03%	0.003%
82	13.403	3840	3845	3849	rBV3	496	672	0.03%	0.004%
83	13.442	3849	3857	3862	rBV6	2349	3304	0.14%	0.018%
84	13.493	3871	3873	3875	rBV	671	378	0.02%	0.002%
85	13.516	3875	3880	3889	rVB5	1645	1962	0.08%	0.011%
86	13.606	3902	3908	3916	rVV4	1281	1983	0.09%	0.011%
87	13.699	3934	3937	3940	rVB3	640	507	0.02%	0.003%
88	13.902	3998	4000	4005	rVB4	969	767	0.03%	0.004%
89	14.329	4129	4133	4139	rBV5	976	1086	0.05%	0.006%
90	14.416	4150	4160	4172	rBV3	13402	19347	0.83%	0.105%
91	14.680	4239	4242	4245	rVB3	864	516	0.02%	0.003%
92	14.699	4245	4248	4251	rBV2	645	540	0.02%	0.003%
93	14.821	4280	4286	4290	rBV6	1034	1192	0.05%	0.006%
94	14.963	4328	4330	4334	rBV3	517	365	0.02%	0.002%
95	14.998	4338	4341	4342	rBV2	783	452	0.02%	0.002%
96	15.014	4342	4346	4350	rBV7	1803	1931	0.08%	0.010%
97	15.123	4378	4380	4383	rBV3	608	468	0.02%	0.003%
98	15.181	4390	4398	4410	rVB6	13428	20091	0.87%	0.109%
99	15.304	4434	4436	4439	rBV3	840	615	0.03%	0.003%
100	15.590	4520	4525	4534	rVB5	4332	5790	0.25%	0.031%

Sum of corrected areas: 18460506

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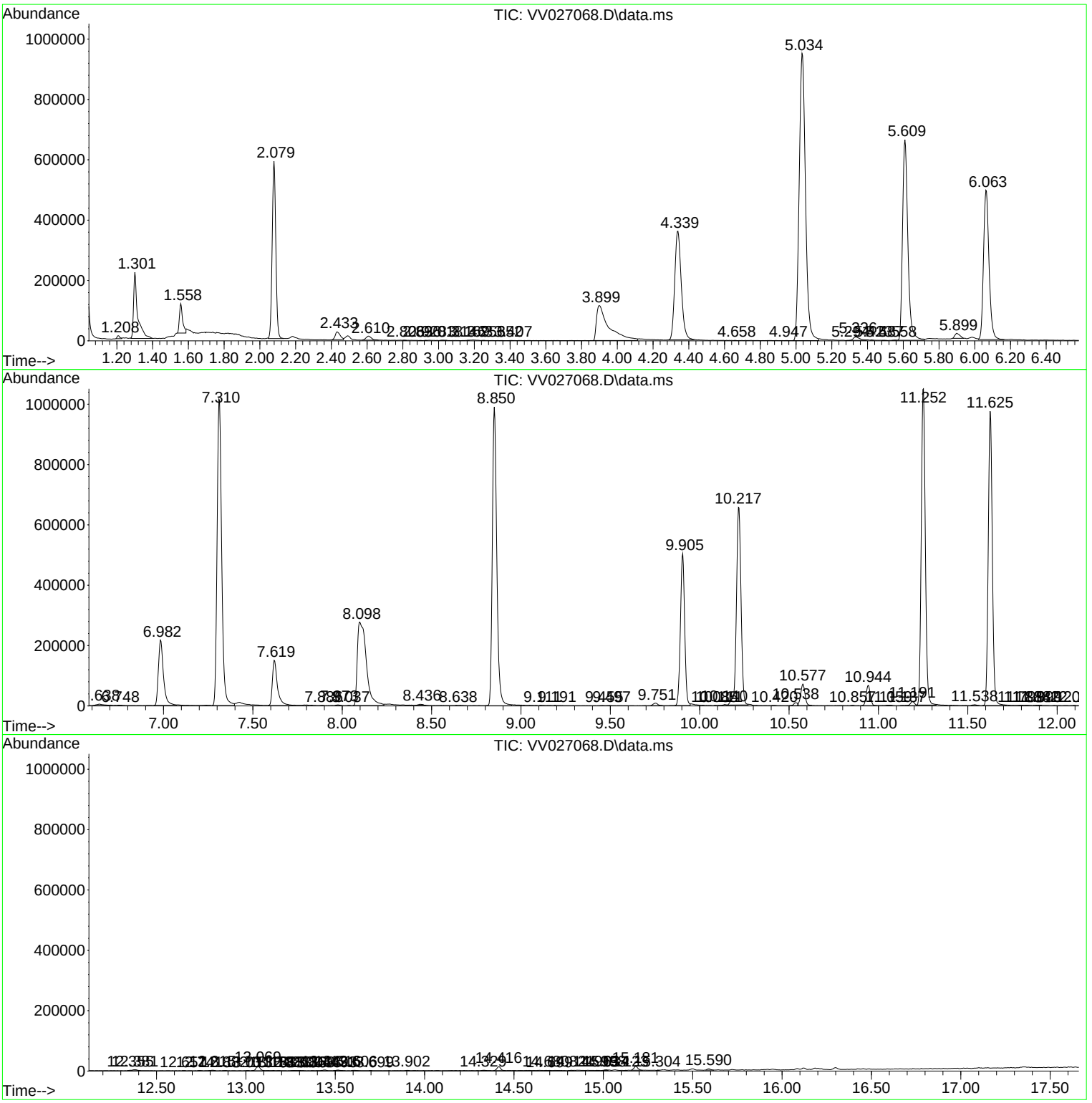
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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



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MSVOA_V
ClientSampleId :
DBUK9ME

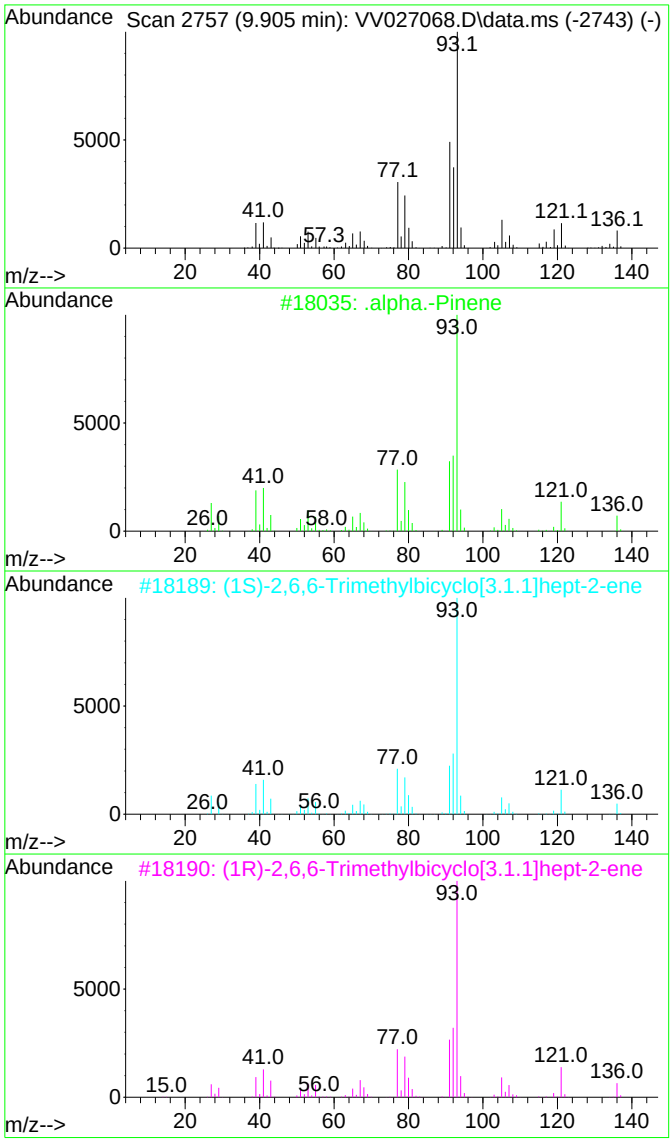
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

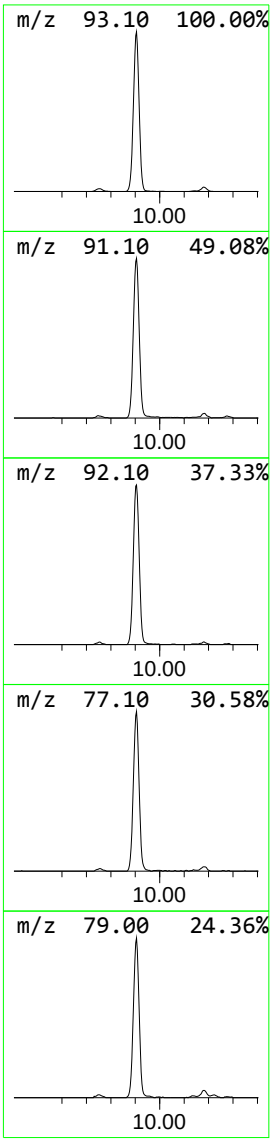
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.905	24.14 ug/L	826093	Chlorobenzene-d5	8.850

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	.alpha.-Pinene	136	C10H16	000080-56-8	94
5	.alpha.-Pinene	136	C10H16	000080-56-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027068.D
Acq On : 29 Jul 2022 04:59
Operator : SY/MD
Sample : N3790-15ME
Misc : 5.21g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

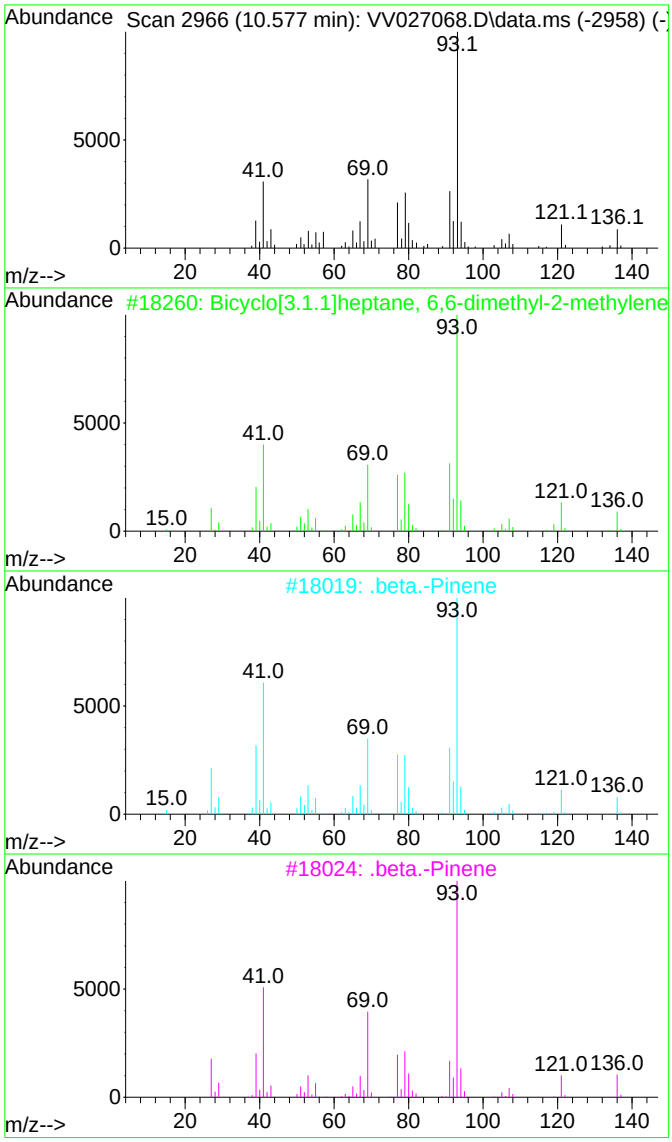
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

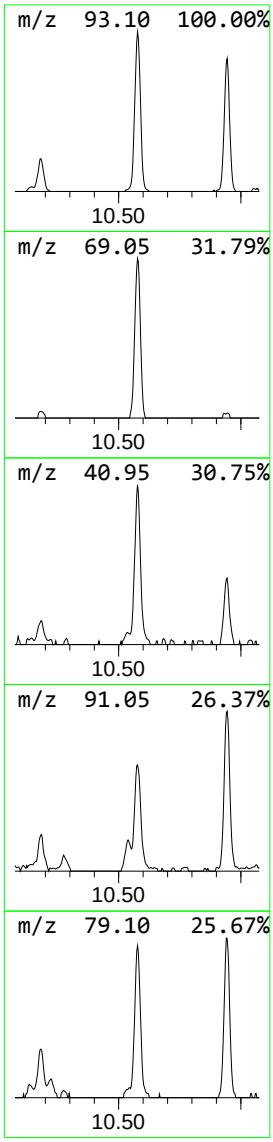
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.577	3.53 ug/L	116563	1,4-Dichlorobenzene-d4	11.252

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	95
3	.beta.-Pinene	136	C10H16	000127-91-3	94
4	.beta.-Pinene	136	C10H16	000127-91-3	94
5	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	94





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Instrument :
MSVOA_V
ClientSampleId :
DBUK9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

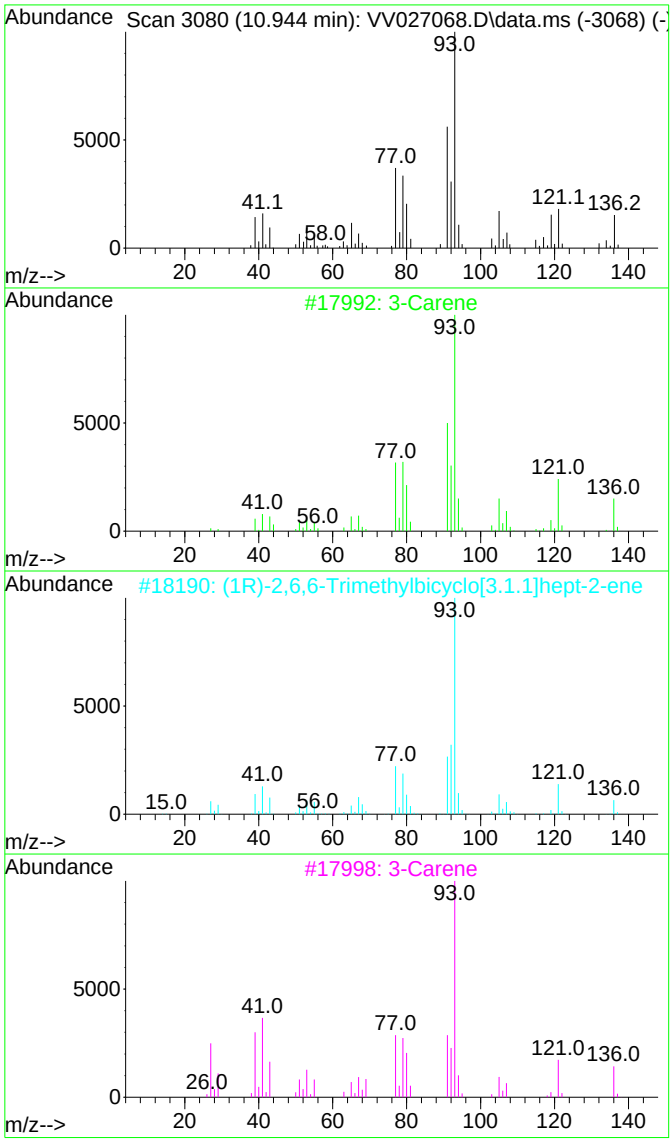
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

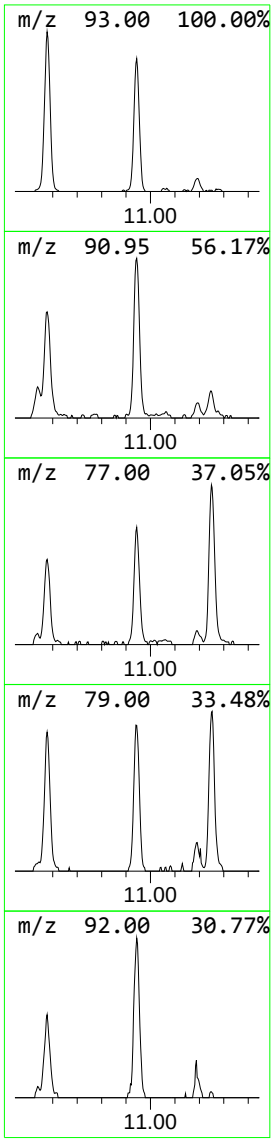
****

Peak Number 4 3-Carene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.944	3.23 ug/L	106630	1,4-Dichlorobenzene-d4	11.252

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Carene	136	C10H16	013466-78-9	94
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	93
3	3-Carene	136	C10H16	013466-78-9	93
4	4-Carene, (1S,3R,6R)-(-)-	136	C10H16	005208-49-1	90
5	Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	90





Tentatively Identified Compound (LSC) summary

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MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
.alpha.-Pinene	9.905	24.1	ug/L	826093	2	8.850	1710950	50.0
Bicyclo[3.1.1]h...	10.577	3.5	ug/L	116563	3	11.252	1650420	50.0
3-Carene	10.944	3.2	ug/L	106630	3	11.252	1650420	50.0