

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011822\
 Data File : VV024395.D
 Acq On : 18 Jan 2022 15:44
 Operator : SY/MD
 Sample : N1129-08ME
 Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBM01ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024395.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	50	54	59	rBV2	11443	9366	0.71%	0.100%
2	1.307	76	83	102	rVB	132544	158723	12.08%	1.702%
3	1.568	157	164	179	rBV	93505	134477	10.23%	1.442%
4	2.092	318	327	338	rBV	288110	403759	30.72%	4.330%
5	2.359	408	410	414	rBV3	358	272	0.02%	0.003%
6	2.394	419	421	424	rVB2	538	213	0.02%	0.002%
7	2.445	428	437	442	rBV4	1244	2115	0.16%	0.023%
8	2.581	477	479	481	rBV	419	257	0.02%	0.003%
9	2.619	481	491	499	rVV7	2386	4702	0.36%	0.050%
10	2.677	507	509	511	rBV	344	152	0.01%	0.002%
11	2.799	545	547	551	rVB	299	167	0.01%	0.002%
12	2.947	585	593	601	rBV4	2171	3814	0.29%	0.041%
13	3.134	648	651	654	rVB2	380	258	0.02%	0.003%
14	3.153	654	657	660	rBV	380	193	0.01%	0.002%
15	3.175	660	664	665	rVV	277	142	0.01%	0.002%
16	3.185	665	667	672	rVB2	216	141	0.01%	0.002%
17	3.249	684	687	690	rBV2	241	137	0.01%	0.001%
18	3.298	699	702	704	rBV2	202	168	0.01%	0.002%
19	3.362	720	722	726	rVB2	205	142	0.01%	0.002%
20	3.417	734	739	740	rBV2	179	157	0.01%	0.002%
21	3.529	770	774	776	rVB	169	134	0.01%	0.001%
22	3.584	785	791	793	rBV3	407	379	0.03%	0.004%
23	3.616	798	801	806	rVB2	362	271	0.02%	0.003%
24	3.738	834	839	841	rBV2	181	153	0.01%	0.002%
25	3.757	841	845	847	rVB2	271	149	0.01%	0.002%
26	3.773	847	850	852	rBV	352	170	0.01%	0.002%
27	3.902	879	890	910	rBV	57704	195415	14.87%	2.096%
28	4.346	1014	1028	1057	rVB2	214090	534502	40.67%	5.732%
29	4.587	1100	1103	1107	rBV4	473	405	0.03%	0.004%
30	4.696	1134	1137	1141	rVV2	406	358	0.03%	0.004%
31	4.725	1144	1146	1148	rVV	381	216	0.02%	0.002%
32	4.767	1155	1159	1162	rVB3	360	258	0.02%	0.003%
33	4.786	1162	1165	1166	rBV	380	144	0.01%	0.002%
34	4.838	1177	1181	1182	rVV3	319	225	0.02%	0.002%
35	5.040	1227	1244	1274	rBV2	525548	1314365	100.00%	14.096%
36	5.330	1326	1334	1336	rBV2	4949	5729	0.44%	0.061%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

37	5.613	1411	1422	1453	rBV	344537	700144	53.27%	7.509%
38	5.905	1502	1513	1530	rBV2	19941	44845	3.41%	0.481%
39	6.066	1551	1563	1600	rVB	282917	588771	44.80%	6.314%
40	6.317	1637	1641	1643	rBV3	1184	1116	0.08%	0.012%
41	6.715	1763	1765	1767	rBV2	545	361	0.03%	0.004%
42	6.873	1811	1814	1817	rVB	440	206	0.02%	0.002%
43	6.892	1817	1820	1822	rBV	290	225	0.02%	0.002%
44	6.986	1838	1849	1878	rBV	160183	316786	24.10%	3.397%
45	7.182	1908	1910	1911	rBV	511	203	0.02%	0.002%
46	7.313	1939	1951	1971	rBV	621244	1103327	83.94%	11.833%
47	7.622	2036	2047	2073	rBV2	99659	211842	16.12%	2.272%
48	7.957	2148	2151	2153	rBV	286	178	0.01%	0.002%
49	7.985	2153	2160	2170	rVB7	1158	1670	0.13%	0.018%
50	8.098	2185	2195	2196	rBV2	84273	101772	7.74%	1.091%
51	8.365	2276	2278	2281	rVB2	382	227	0.02%	0.002%
52	8.555	2334	2337	2341	rBV2	259	226	0.02%	0.002%
53	8.574	2341	2343	2345	rBV	300	147	0.01%	0.002%
54	8.854	2418	2430	2466	rBV	428033	847332	64.47%	9.088%
55	9.082	2499	2501	2505	rBV2	298	168	0.01%	0.002%
56	9.104	2505	2508	2511	rVB2	236	163	0.01%	0.002%
57	9.339	2578	2581	2584	rBV2	264	202	0.02%	0.002%
58	9.416	2601	2605	2607	rBV	337	229	0.02%	0.002%
59	9.616	2665	2667	2668	rBV	353	164	0.01%	0.002%
60	9.712	2694	2697	2701	rBV2	254	180	0.01%	0.002%
61	9.744	2704	2707	2709	rBV3	399	209	0.02%	0.002%
62	9.796	2721	2723	2728	rVB3	395	270	0.02%	0.003%
63	9.905	2745	2757	2774	rVB	63413	103447	7.87%	1.109%
64	10.018	2784	2792	2794	rBV2	386	421	0.03%	0.005%
65	10.127	2819	2826	2836	rVB4	3698	6577	0.50%	0.071%
66	10.227	2836	2857	2875	rBV	322568	597641	45.47%	6.410%
67	10.577	2960	2966	2981	rVB5	5637	9200	0.70%	0.099%
68	10.661	2987	2992	2997	rBV2	879	881	0.07%	0.009%
69	10.828	3042	3044	3046	rBV	604	377	0.03%	0.004%
70	10.870	3053	3057	3059	rBV2	798	526	0.04%	0.006%
71	10.918	3066	3072	3084	rVB7	4093	6467	0.49%	0.069%
72	10.966	3084	3087	3089	rBV	445	275	0.02%	0.003%
73	11.082	3119	3123	3125	rBV	346	291	0.02%	0.003%
74	11.252	3164	3176	3193	rBV	531128	834945	63.52%	8.955%
75	11.464	3239	3242	3246	rBV2	483	453	0.03%	0.005%
76	11.538	3259	3265	3267	rBV4	1281	1230	0.09%	0.013%

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Integration Parameters: LSCINT.P

Integrator: RTE

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77	11.628	3280	3293	3314	rBV	642966	1032616	78.56%	11.075%
78	11.789	3337	3343	3351	rVB6	5732	8485	0.65%	0.091%
79	11.850	3356	3362	3369	rVB4	1234	1828	0.14%	0.020%
80	11.905	3375	3379	3382	rBV2	520	359	0.03%	0.004%
81	11.953	3389	3394	3397	rBV2	560	591	0.04%	0.006%
82	11.989	3402	3405	3409	rBV3	347	219	0.02%	0.002%
83	12.040	3419	3421	3424	rBV	259	171	0.01%	0.002%
84	12.159	3454	3458	3460	rBV2	387	295	0.02%	0.003%
85	12.313	3504	3506	3509	rBV	359	225	0.02%	0.002%
86	12.355	3513	3519	3525	rVB5	2080	3035	0.23%	0.033%
87	12.426	3538	3541	3543	rBV2	424	222	0.02%	0.002%
88	12.439	3543	3545	3548	rVB2	622	277	0.02%	0.003%
89	12.532	3572	3574	3577	rBV2	315	160	0.01%	0.002%
90	12.625	3601	3603	3609	rVB	292	131	0.01%	0.001%
91	12.911	3690	3692	3696	rBV	386	196	0.01%	0.002%
92	13.075	3741	3743	3748	rVB3	845	613	0.05%	0.007%
93	13.201	3781	3782	3785	rVB	555	179	0.01%	0.002%
94	13.281	3803	3807	3810	rBV	419	368	0.03%	0.004%
95	13.333	3821	3823	3826	rBV3	381	254	0.02%	0.003%
96	13.503	3873	3876	3877	rBV	292	158	0.01%	0.002%
97	13.677	3927	3930	3934	rBV2	363	351	0.03%	0.004%
98	13.824	3972	3976	3977	rBV	361	243	0.02%	0.003%
99	13.931	4006	4009	4012	rBV4	420	375	0.03%	0.004%
100	15.590	4520	4525	4535	rVB5	12381	16868	1.28%	0.181%

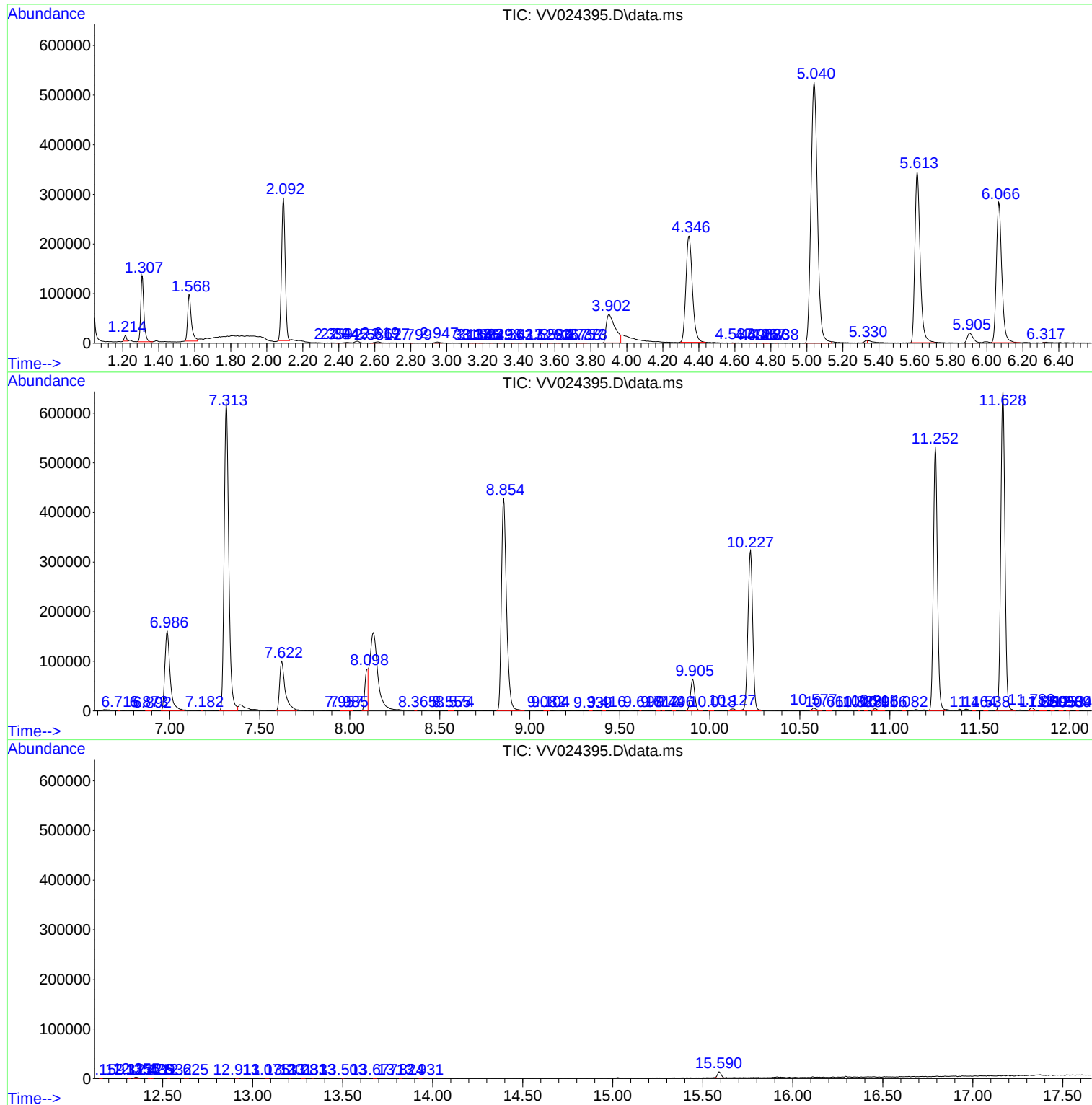
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBM01ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
ClientSampleId :
DBM01ME

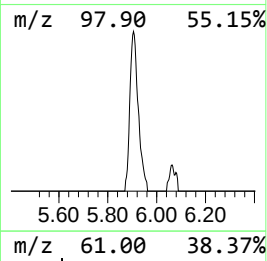
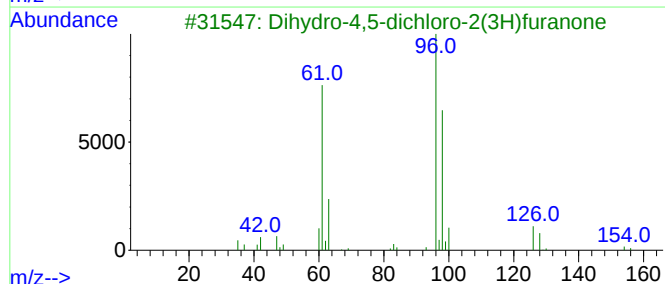
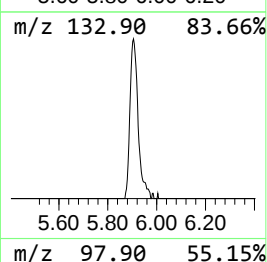
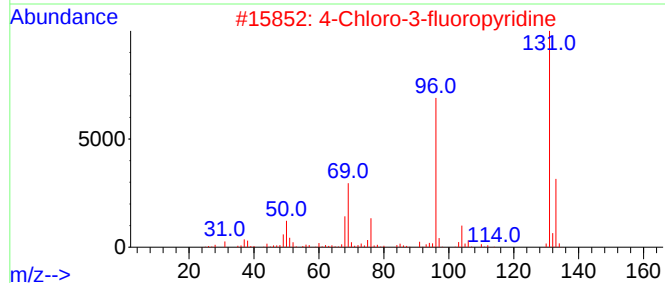
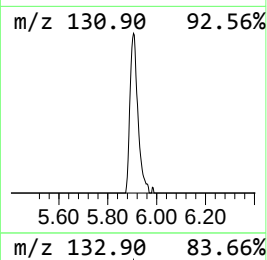
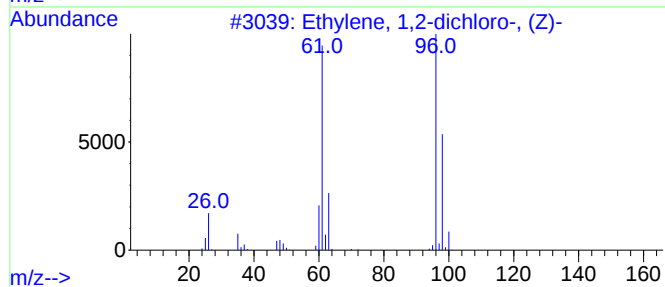
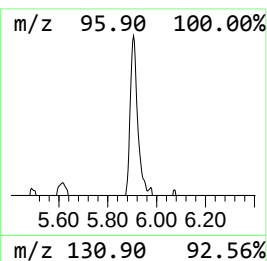
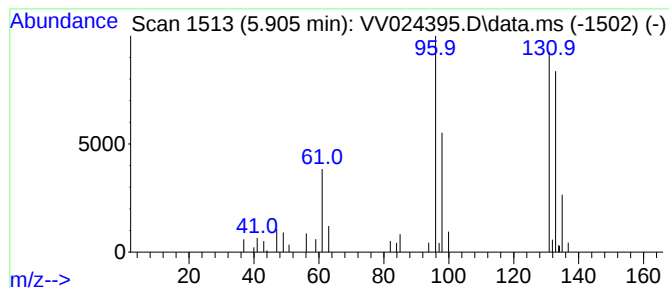
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	3.20 ug/L	44845	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	25
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	25



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Instrument :
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ClientSampleId :
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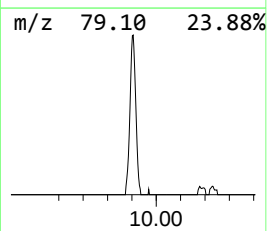
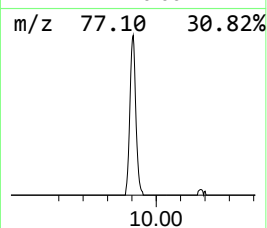
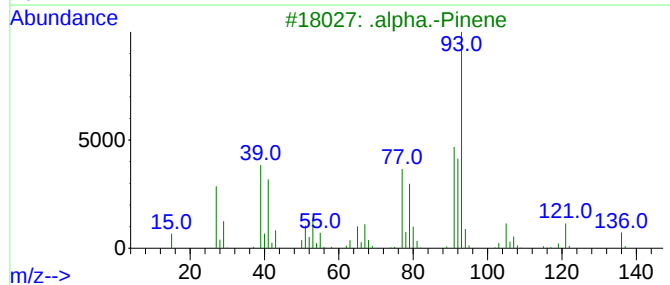
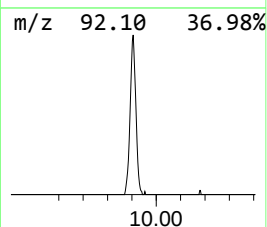
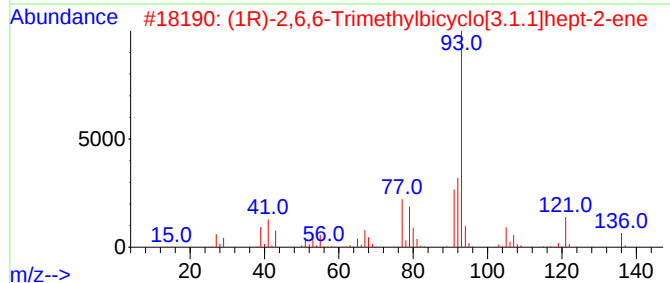
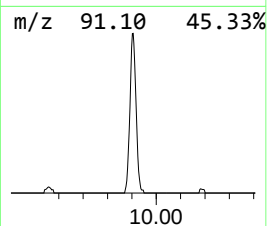
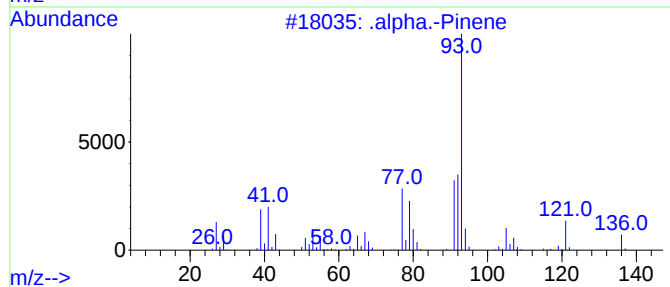
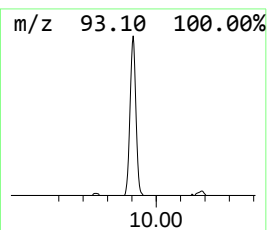
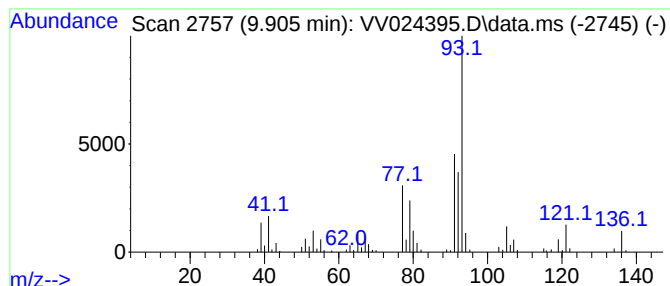
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.905	6.10 ug/L	103447	Chlorobenzene-d5	8.854

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	95
2	(1R)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-70-8	94
3	.		.alpha.-Pinene	136	C10H16	000080-56-8	94
4	.		.alpha.-Pinene	136	C10H16	000080-56-8	93
5	(1S)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-26-4	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	3.2	ug/L	44845	1	5.613	700144	50.0
.alpha.-Pinene	9.905	6.1	ug/L	103447	2	8.854	847332	50.0