

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070623\
 Data File : VV031650.D
 Acq On : 06 Jul 2023 13:04
 Operator : SY/MD
 Sample : 03444-19ME
 Misc : 4.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46Y0ME

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\SFAMVLM061423WMA.M
 Title : VOC Analysis

Signal : TIC: VV031650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	91	rVB	46748	71476	8.75%	1.054%
2	1.484	134	138	140	rBV	21416	18572	2.27%	0.274%
3	2.040	301	311	326	rBV	123942	178407	21.84%	2.631%
4	2.124	330	337	348	rVB4	6159	10244	1.25%	0.151%
5	2.217	361	366	370	rBV4	891	881	0.11%	0.013%
6	2.269	376	382	389	rBV4	960	1457	0.18%	0.021%
7	2.381	408	417	428	rBV	13289	25700	3.15%	0.379%
8	2.500	452	454	458	rVB2	524	332	0.04%	0.005%
9	2.558	458	472	486	rBV2	10075	23643	2.89%	0.349%
10	2.895	567	577	581	rBV3	1264	1890	0.23%	0.028%
11	3.021	610	616	618	rBV2	617	446	0.05%	0.007%
12	3.037	618	621	624	rBV2	485	278	0.03%	0.004%
13	3.108	639	643	649	rVB2	531	394	0.05%	0.006%
14	3.220	674	678	682	rVV2	342	344	0.04%	0.005%
15	3.246	684	686	691	rVV3	291	254	0.03%	0.004%
16	3.548	773	780	784	rBV2	304	271	0.03%	0.004%
17	3.645	805	810	813	rBV2	252	248	0.03%	0.004%
18	3.805	850	860	898	rBV	47362	164925	20.19%	2.432%
19	4.252	982	999	1029	rBV2	105230	277867	34.02%	4.098%
20	4.465	1062	1065	1069	rBV2	504	446	0.05%	0.007%
21	4.587	1099	1103	1108	rVB4	774	611	0.07%	0.009%
22	4.956	1202	1218	1250	rBV2	230921	602490	73.77%	8.886%
23	5.143	1274	1276	1279	rVB3	488	279	0.03%	0.004%
24	5.268	1313	1315	1319	rBV3	426	331	0.04%	0.005%
25	5.387	1348	1352	1354	rBV3	394	283	0.03%	0.004%
26	5.439	1364	1368	1371	rBV	370	270	0.03%	0.004%
27	5.538	1386	1399	1431	rBV	257584	557998	68.32%	8.229%
28	5.831	1480	1490	1500	rBV9	6060	13229	1.62%	0.195%
29	5.921	1514	1518	1522	rBV2	296	341	0.04%	0.005%
30	5.995	1528	1541	1570	rBV	140142	308518	37.77%	4.550%
31	6.346	1648	1650	1655	rVB	403	267	0.03%	0.004%
32	6.464	1682	1687	1689	rBV2	337	267	0.03%	0.004%
33	6.580	1718	1723	1725	rBV2	621	511	0.06%	0.008%
34	6.632	1734	1739	1741	rBV2	591	532	0.07%	0.008%
35	6.702	1758	1761	1765	rVB2	556	288	0.04%	0.004%
36	6.850	1805	1807	1811	rVB2	506	346	0.04%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
 Title : VOC Analysis

37	6.921	1818	1829	1862	rBV	68949	139021	17.02%	2.050%
38	7.069	1871	1875	1879	rVB2	488	444	0.05%	0.007%
39	7.181	1907	1910	1912	rBV3	377	258	0.03%	0.004%
40	7.204	1914	1917	1919	rBV3	498	316	0.04%	0.005%
41	7.249	1919	1931	1949	rBV	214589	385141	47.16%	5.680%
42	7.513	2010	2013	2017	rVB3	474	342	0.04%	0.005%
43	7.561	2017	2028	2049	rBV2	48340	99391	12.17%	1.466%
44	7.673	2061	2063	2069	rVB2	495	383	0.05%	0.006%
45	7.706	2069	2073	2077	rVB2	388	408	0.05%	0.006%
46	7.789	2095	2099	2104	rBV3	297	306	0.04%	0.005%
47	7.873	2120	2125	2127	rVV	430	343	0.04%	0.005%
48	7.895	2127	2132	2134	rVV2	616	574	0.07%	0.008%
49	7.915	2135	2138	2144	rVB5	820	581	0.07%	0.009%
50	8.046	2167	2179	2214	rBV2	144782	365392	44.74%	5.389%
51	8.281	2249	2252	2253	rBV2	898	405	0.05%	0.006%
52	8.384	2274	2284	2289	rBV5	2746	4203	0.51%	0.062%
53	8.471	2304	2311	2315	rBV3	553	663	0.08%	0.010%
54	8.503	2318	2321	2324	rBV3	565	368	0.05%	0.005%
55	8.548	2333	2335	2339	rBV2	483	271	0.03%	0.004%
56	8.570	2339	2342	2346	rBV3	553	499	0.06%	0.007%
57	8.722	2385	2389	2393	rBV3	579	670	0.08%	0.010%
58	8.792	2398	2411	2433	rBV	407269	698337	85.50%	10.299%
59	8.927	2451	2453	2455	rBV2	600	281	0.03%	0.004%
60	8.963	2461	2464	2465	rBV2	723	401	0.05%	0.006%
61	9.001	2473	2476	2479	rVB2	360	249	0.03%	0.004%
62	9.046	2486	2490	2494	rVB5	504	391	0.05%	0.006%
63	9.091	2495	2504	2505	rBV6	1855	2345	0.29%	0.035%
64	9.130	2513	2516	2518	rBV4	507	292	0.04%	0.004%
65	9.146	2518	2521	2527	rVB4	490	420	0.05%	0.006%
66	9.185	2529	2533	2536	rVB	378	316	0.04%	0.005%
67	9.339	2576	2581	2587	rBV3	510	703	0.09%	0.010%
68	9.416	2596	2605	2610	rVV6	1558	2327	0.28%	0.034%
69	9.490	2624	2628	2630	rBV2	1000	894	0.11%	0.013%
70	9.516	2634	2636	2641	rVV4	1488	1248	0.15%	0.018%
71	9.577	2650	2655	2657	rVV3	591	510	0.06%	0.008%
72	9.615	2663	2667	2669	rBV3	477	302	0.04%	0.004%
73	9.648	2669	2677	2687	rVV9	2444	4219	0.52%	0.062%
74	9.718	2693	2699	2702	rBV5	1546	1912	0.23%	0.028%
75	9.744	2703	2707	2714	rVV8	2699	3701	0.45%	0.055%
76	9.792	2715	2722	2734	rVB6	2614	4577	0.56%	0.068%

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Integrator: RTE

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 Title : VOC Analysis

77	9.850	2736	2740	2746	rBV5	631	719	0.09%	0.011%
78	9.876	2746	2748	2753	rVB3	938	540	0.07%	0.008%
79	9.918	2759	2761	2765	rVB4	925	512	0.06%	0.008%
80	9.963	2765	2775	2781	rBV8	2141	3974	0.49%	0.059%
81	10.066	2805	2807	2814	rVB4	1817	1843	0.23%	0.027%
82	10.162	2819	2837	2857	rBV	247543	413140	50.58%	6.093%
83	10.294	2876	2878	2880	rBV3	616	321	0.04%	0.005%
84	10.332	2885	2890	2893	rBV5	1398	1480	0.18%	0.022%
85	10.397	2904	2910	2913	rBV7	1683	1787	0.22%	0.026%
86	10.448	2920	2926	2935	rBV9	3364	5237	0.64%	0.077%
87	10.619	2974	2979	2983	rBV5	972	1001	0.12%	0.015%
88	10.667	2992	2994	2996	rBV3	751	387	0.05%	0.006%
89	10.824	3036	3043	3050	rBV7	5347	8603	1.05%	0.127%
90	10.982	3084	3092	3094	rBV5	3208	3831	0.47%	0.057%
91	11.098	3119	3128	3135	rBV7	7103	12293	1.51%	0.181%
92	11.194	3147	3158	3177	rBV	522298	816732	100.00%	12.045%
93	11.471	3241	3244	3246	rBV4	1158	903	0.11%	0.013%
94	11.570	3263	3275	3291	rBV	344502	551755	67.56%	8.137%
95	11.882	3362	3372	3380	rBV10	7556	14836	1.82%	0.219%
96	12.316	3497	3507	3517	rBV10	12353	28026	3.43%	0.413%
97	12.416	3530	3538	3547	rVB10	12435	18070	2.21%	0.267%
98	12.744	3631	3640	3648	rBV9	5841	11358	1.39%	0.168%
99	16.397	4766	4776	4792	rBV	432484	651524	79.77%	9.609%
100	17.477	5102	5112	5127	rVB	142787	243568	29.82%	3.592%

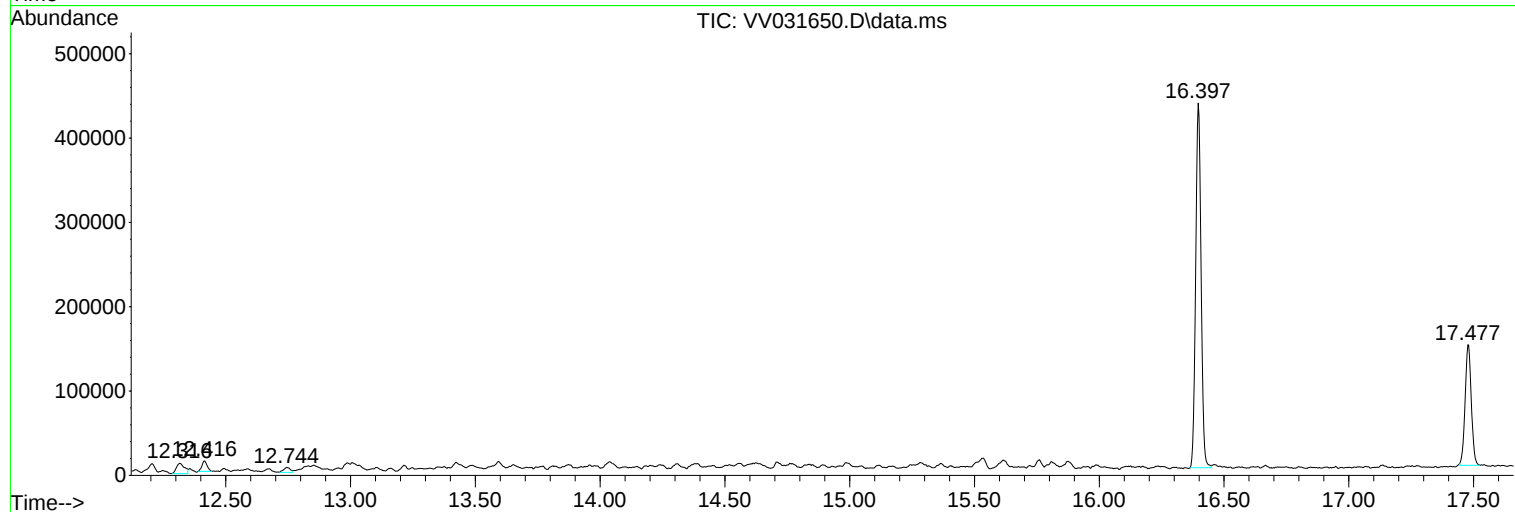
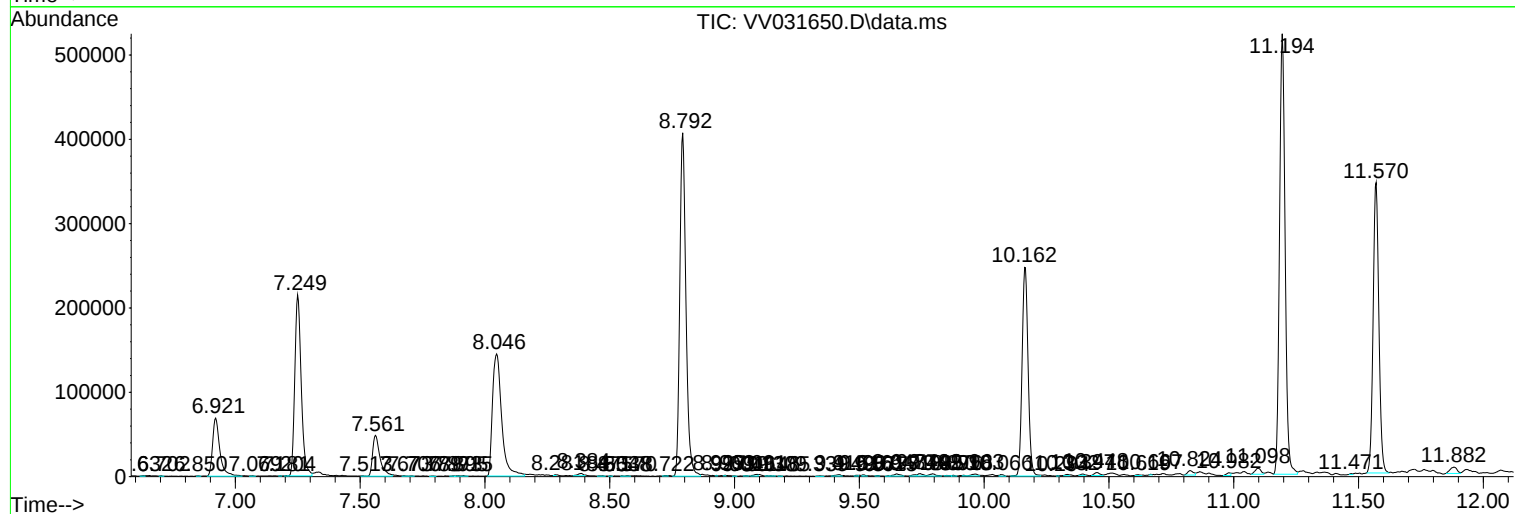
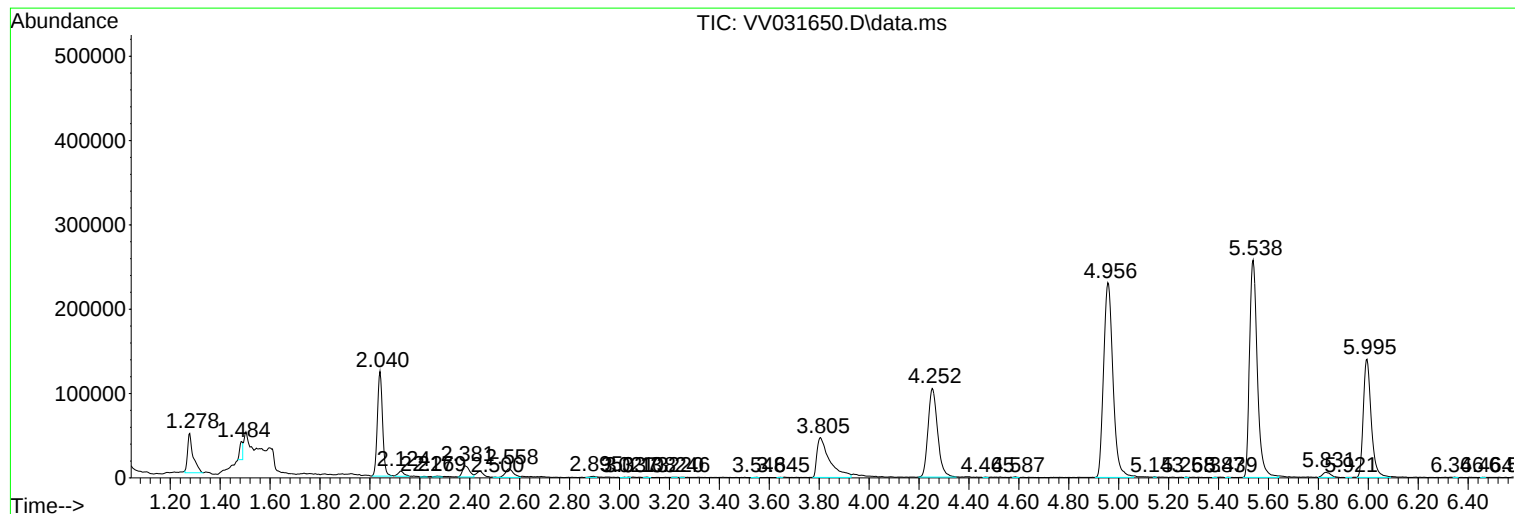
Sum of corrected areas: 6780480

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Instrument :
MSVOA_V
ClientSampleId :
A46Y0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y0ME

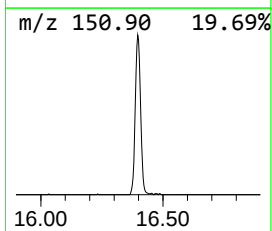
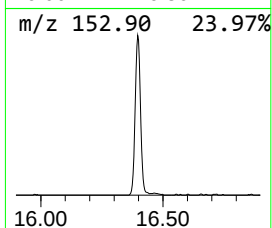
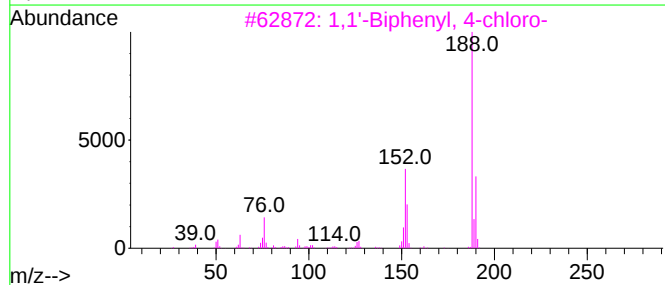
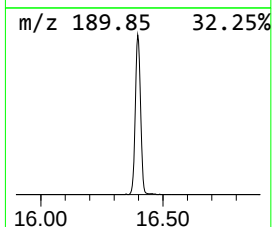
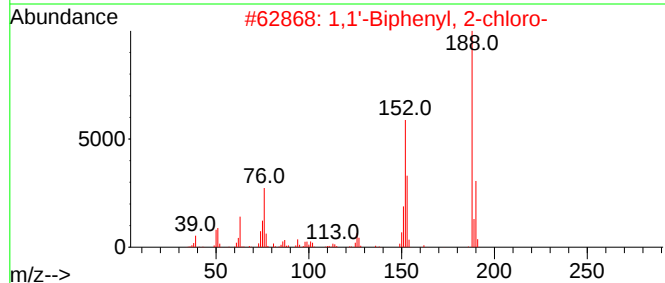
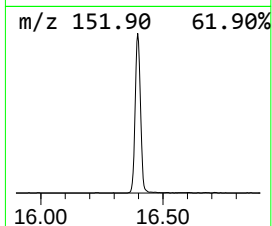
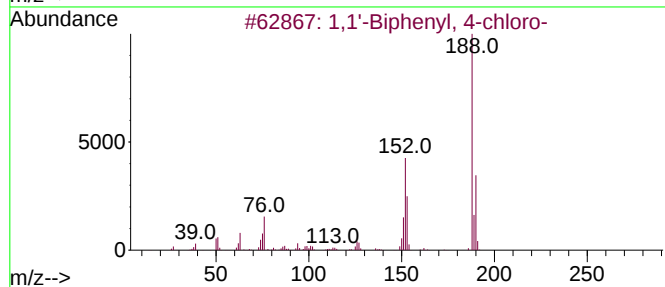
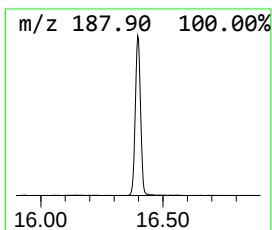
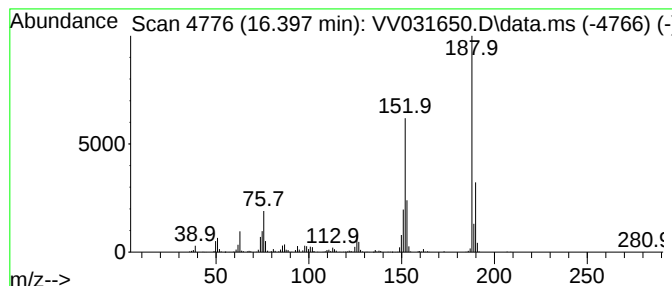
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1,1'-Biphenyl, 4-chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	39.89 ug/L	651524	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	97
2	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	97
3	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	94
4	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	94
5	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	93



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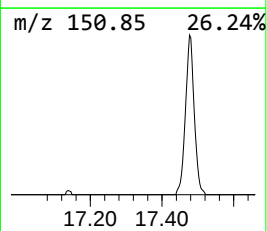
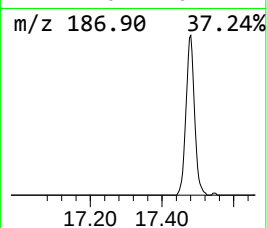
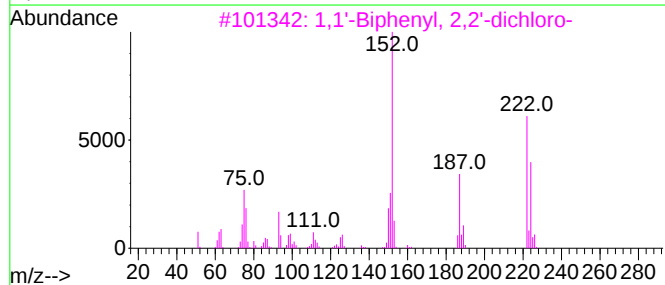
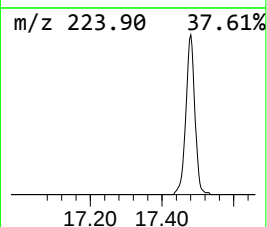
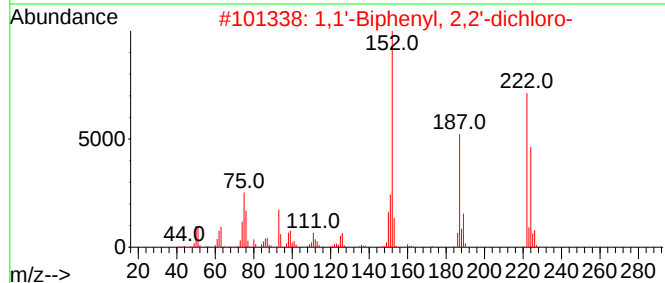
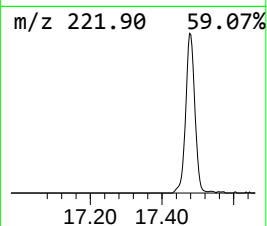
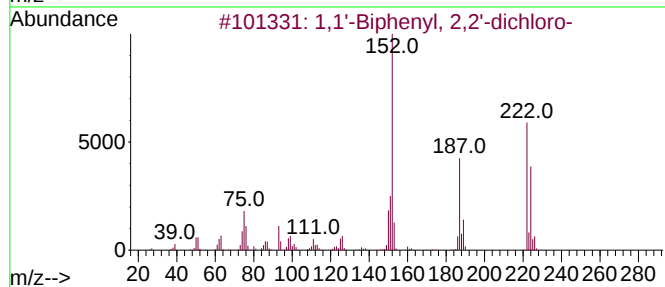
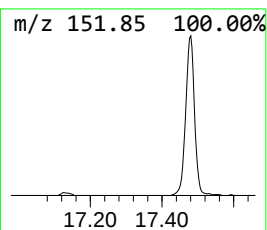
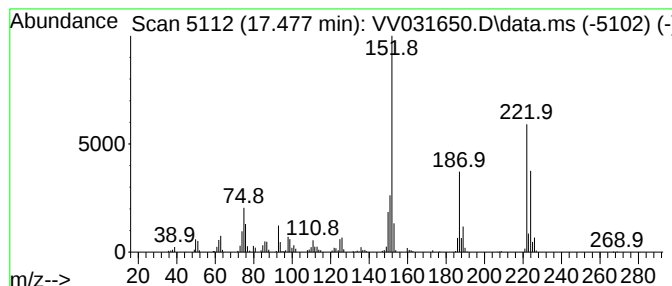
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,1'-Biphenyl, 2,2'-dichloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.477	14.91 ug/L	243568	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	99		
2	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	99		
3	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	99		
4	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	98		
5	1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98		



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Quant Title : VOC Analysis

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	39.9	ug/L	651524	3	11.194	816732	50.0
1,1'-Biphenyl, ...	17.477	14.9	ug/L	243568	3	11.194	816732	50.0