

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
 Data File : VV031638.D
 Acq On : 03 Jul 2023 15:39
 Operator : SY/MD
 Sample : 03472-21ME
 Misc : 4.80g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46R2ME

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: VV031638.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	90	rVB	61599	88002	11.55%	1.250%
2	2.040	302	311	331	rVB	159369	235930	30.96%	3.352%
3	2.220	362	367	375	rBV5	852	1259	0.17%	0.018%
4	2.259	375	379	380	rBV2	937	597	0.08%	0.008%
5	2.346	403	406	407	rBV4	679	455	0.06%	0.006%
6	2.384	411	418	430	rVV2	8117	15802	2.07%	0.225%
7	2.558	459	472	484	rBV	13431	28390	3.73%	0.403%
8	2.883	567	573	577	rBV5	612	704	0.09%	0.010%
9	2.905	577	580	584	rVB3	512	458	0.06%	0.007%
10	2.979	601	603	610	rVB2	634	489	0.06%	0.007%
11	3.063	624	629	631	rBV3	501	381	0.05%	0.005%
12	3.092	636	638	644	rVV3	380	313	0.04%	0.004%
13	3.118	644	646	652	rVB3	520	372	0.05%	0.005%
14	3.163	656	660	666	rBV3	325	416	0.05%	0.006%
15	3.349	714	718	721	rBV2	384	336	0.04%	0.005%
16	3.433	740	744	751	rBV2	309	433	0.06%	0.006%
17	3.484	757	760	765	rVB2	564	443	0.06%	0.006%
18	3.661	812	815	819	rVV3	461	337	0.04%	0.005%
19	3.728	832	836	839	rBV2	443	355	0.05%	0.005%
20	3.802	848	859	900	rBV	55841	199770	26.22%	2.838%
21	4.034	927	931	932	rBV2	624	489	0.06%	0.007%
22	4.253	981	999	1026	rBV	128077	334952	43.96%	4.759%
23	4.484	1069	1071	1074	rBV2	441	319	0.04%	0.005%
24	4.574	1092	1099	1106	rBV4	848	1525	0.20%	0.022%
25	4.635	1113	1118	1121	rBV2	360	363	0.05%	0.005%
26	4.825	1172	1177	1178	rBV	605	443	0.06%	0.006%
27	4.883	1188	1195	1197	rBV3	584	514	0.07%	0.007%
28	4.957	1201	1218	1244	rBV2	288793	755602	99.16%	10.735%
29	5.162	1278	1282	1283	rBV2	705	411	0.05%	0.006%
30	5.487	1377	1383	1386	rBV	398	420	0.06%	0.006%
31	5.539	1386	1399	1424	rBV	269111	571028	74.94%	8.113%
32	5.696	1445	1448	1451	rVB4	581	363	0.05%	0.005%
33	5.831	1481	1490	1503	rBV9	5025	10785	1.42%	0.153%
34	5.995	1526	1541	1572	rBV2	176189	377668	49.56%	5.366%
35	6.178	1593	1598	1604	rVB5	367	490	0.06%	0.007%
36	6.207	1604	1607	1612	rVB3	883	680	0.09%	0.010%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

37	6.230	1612	1614	1616	rBV	671	342	0.04%	0.005%
38	6.330	1641	1645	1647	rBV2	702	525	0.07%	0.007%
39	6.577	1718	1722	1724	rBV2	598	463	0.06%	0.007%
40	6.593	1726	1727	1733	rVB2	494	428	0.06%	0.006%
41	6.677	1749	1753	1758	rVB3	512	440	0.06%	0.006%
42	6.799	1787	1791	1792	rBV2	504	341	0.04%	0.005%
43	6.921	1817	1829	1858	rBV	84142	171349	22.49%	2.434%
44	7.133	1891	1895	1898	rBV2	754	697	0.09%	0.010%
45	7.198	1906	1915	1920	rBV7	2734	4608	0.60%	0.065%
46	7.249	1920	1931	1954	rVV	268920	481000	63.12%	6.834%
47	7.561	2017	2028	2049	rBV	60446	121987	16.01%	1.733%
48	7.709	2071	2074	2077	rVB4	549	349	0.05%	0.005%
49	7.767	2089	2092	2095	rBV3	421	329	0.04%	0.005%
50	7.876	2119	2126	2128	rBV4	419	514	0.07%	0.007%
51	8.043	2167	2178	2203	rBV	188064	437375	57.40%	6.214%
52	8.336	2267	2269	2271	rBV3	660	395	0.05%	0.006%
53	8.413	2291	2293	2297	rVB2	711	392	0.05%	0.006%
54	8.436	2297	2300	2303	rBV3	423	330	0.04%	0.005%
55	8.493	2314	2318	2322	rBV3	521	509	0.07%	0.007%
56	8.555	2333	2337	2341	rBV5	747	558	0.07%	0.008%
57	8.728	2386	2391	2393	rBV2	616	522	0.07%	0.007%
58	8.793	2398	2411	2435	rBV	409767	712098	93.45%	10.117%
59	9.014	2475	2480	2485	rVB6	768	731	0.10%	0.010%
60	9.095	2500	2505	2508	rBV3	796	848	0.11%	0.012%
61	9.487	2624	2627	2630	rVV2	415	428	0.06%	0.006%
62	9.612	2664	2666	2670	rVB2	540	353	0.05%	0.005%
63	9.638	2670	2674	2676	rBV2	529	462	0.06%	0.007%
64	9.661	2676	2681	2686	rVB4	1428	1560	0.20%	0.022%
65	9.693	2689	2691	2695	rBV3	392	314	0.04%	0.004%
66	9.735	2699	2704	2706	rBV5	640	516	0.07%	0.007%
67	9.789	2718	2721	2723	rBV3	707	448	0.06%	0.006%
68	9.879	2745	2749	2753	rVB2	642	681	0.09%	0.010%
69	9.908	2753	2758	2763	rBV4	617	696	0.09%	0.010%
70	10.162	2824	2837	2857	rBV	298480	485176	63.67%	6.893%
71	10.284	2873	2875	2878	rBV	583	321	0.04%	0.005%
72	10.317	2878	2885	2887	rBV5	709	726	0.10%	0.010%
73	10.339	2889	2892	2894	rVV2	727	444	0.06%	0.006%
74	10.442	2921	2924	2926	rBV2	818	526	0.07%	0.007%
75	10.487	2934	2938	2940	rBV4	687	568	0.07%	0.008%
76	10.545	2952	2956	2957	rBV2	611	425	0.06%	0.006%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMVLM061423WMA.M
 Title : VOC Analysis

77	10.625	2977	2981	2984	rBV6	577	538	0.07%	0.008%
78	10.667	2988	2994	2996	rBV5	640	557	0.07%	0.008%
79	10.699	3001	3004	3006	rBV4	610	419	0.05%	0.006%
80	10.773	3023	3027	3032	rVB5	1191	1142	0.15%	0.016%
81	10.818	3037	3041	3042	rBV5	554	337	0.04%	0.005%
82	10.831	3043	3045	3047	rBV3	600	321	0.04%	0.005%
83	10.982	3084	3092	3095	rBV5	1346	1737	0.23%	0.025%
84	11.133	3137	3139	3141	rBV3	1068	637	0.08%	0.009%
85	11.194	3147	3158	3177	rBV	491571	761991	100.00%	10.826%
86	11.323	3196	3198	3200	rBV3	1272	693	0.09%	0.010%
87	11.416	3224	3227	3230	rBV4	679	510	0.07%	0.007%
88	11.435	3230	3233	3234	rBV2	825	449	0.06%	0.006%
89	11.477	3240	3246	3247	rBV4	1365	1328	0.17%	0.019%
90	11.567	3261	3274	3293	rBV	376514	602306	79.04%	8.557%
91	11.927	3383	3386	3387	rBV2	1466	977	0.13%	0.014%
92	12.201	3461	3471	3479	rBV2	5029	9898	1.30%	0.141%
93	12.310	3500	3505	3518	rBV2	3842	8216	1.08%	0.117%
94	12.416	3531	3538	3549	rVB2	4681	7427	0.97%	0.106%
95	13.149	3762	3766	3768	rBV5	1463	1250	0.16%	0.018%
96	13.426	3846	3852	3857	rBV9	4047	6298	0.83%	0.089%
97	14.037	4034	4042	4045	rBV9	3996	5916	0.78%	0.084%
98	14.310	4122	4127	4135	rVB9	4299	5286	0.69%	0.075%
99	16.397	4766	4776	4791	rBV	226062	343571	45.09%	4.881%
100	17.480	5103	5113	5128	rVB	127113	214520	28.15%	3.048%

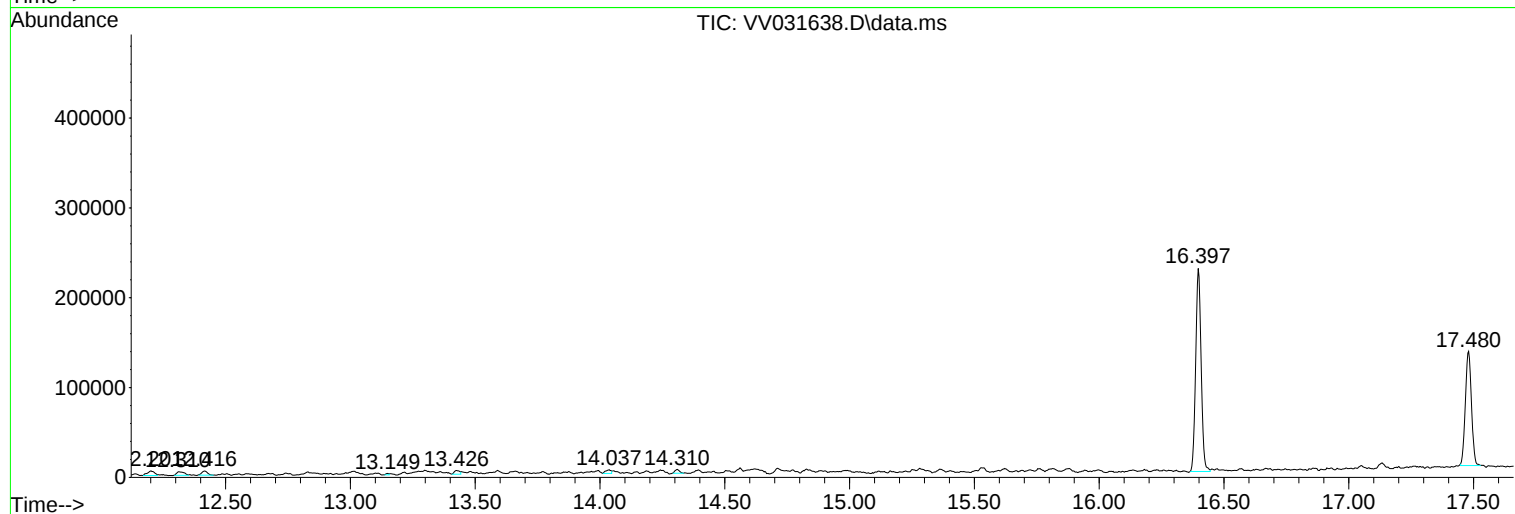
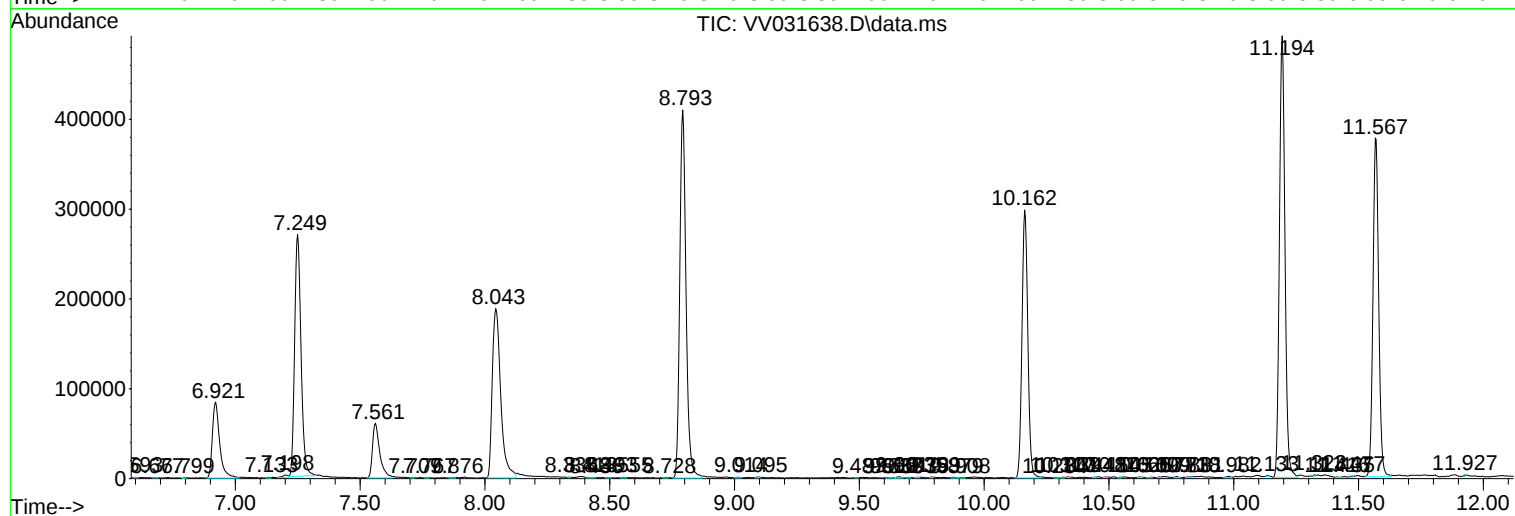
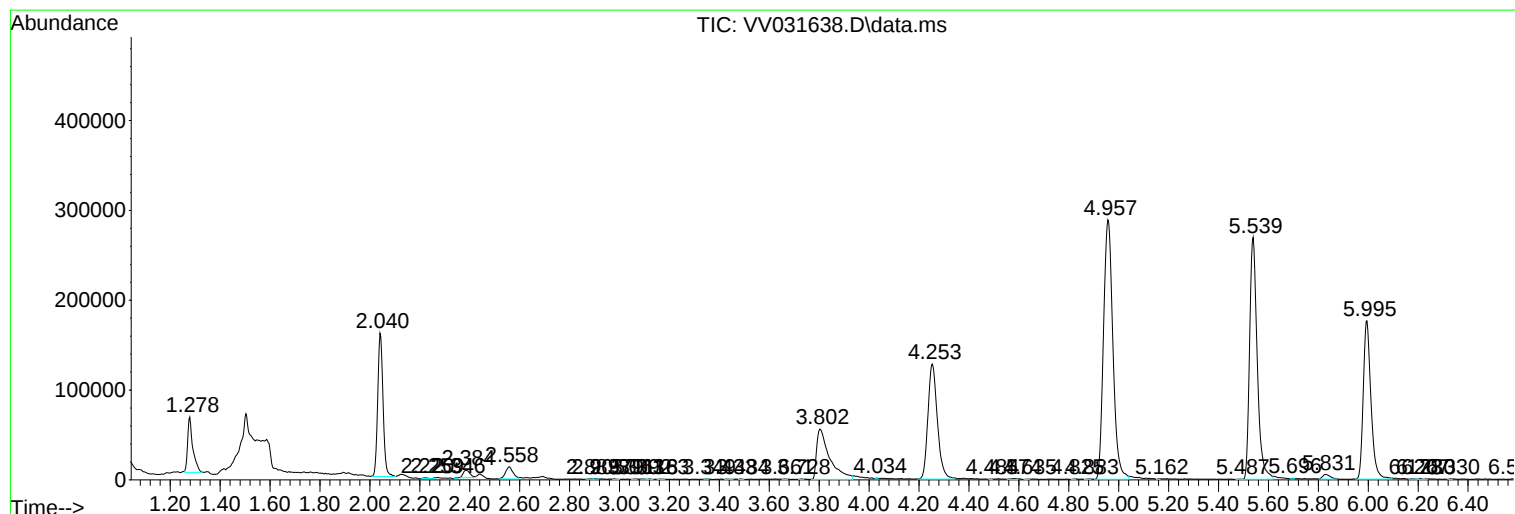
Sum of corrected areas: 7038392

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Instrument :
MSVOA_V
ClientSampleId :
A46R2ME

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 :
A46R2ME

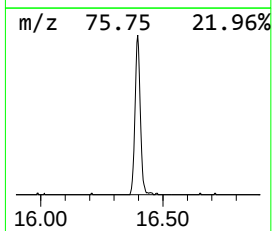
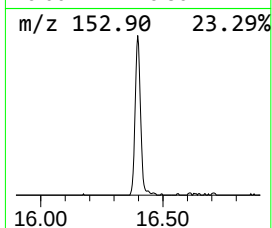
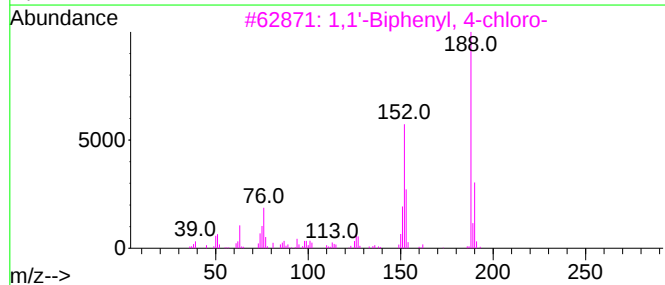
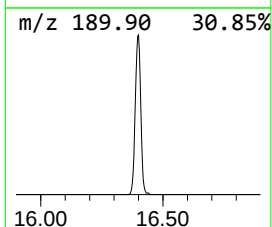
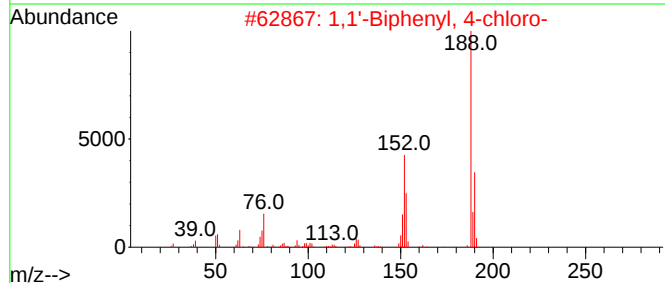
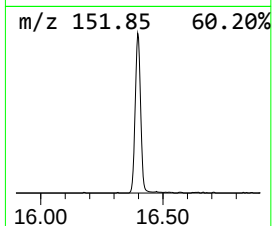
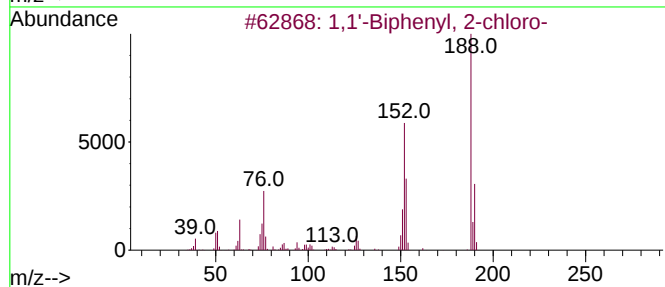
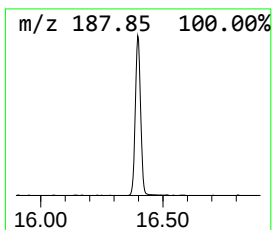
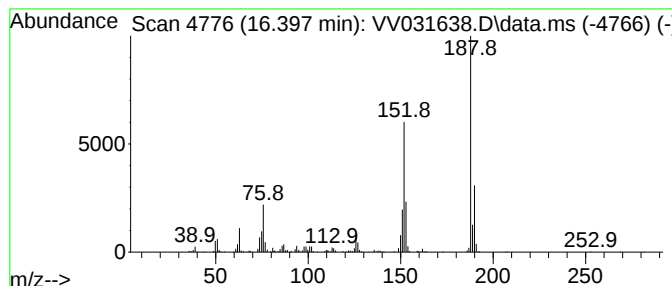
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	22.54 ug/L	343571	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	99
2	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	96
3	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	95
4	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	94
5	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	94



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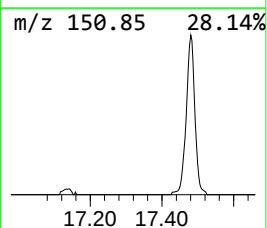
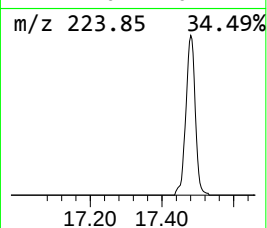
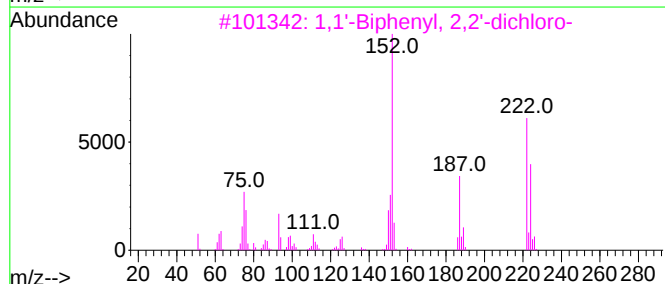
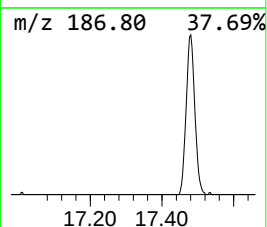
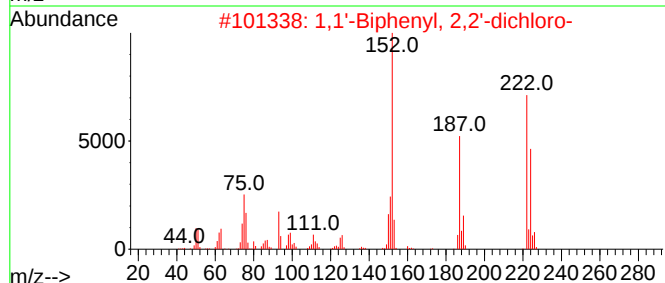
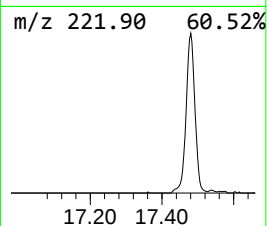
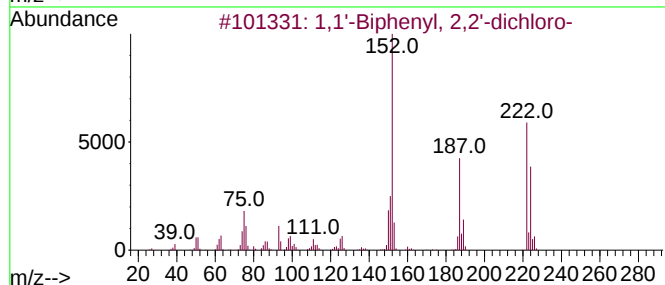
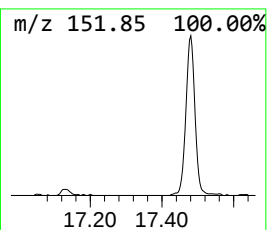
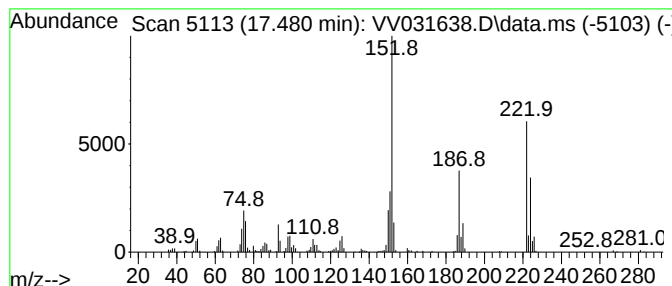
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	14.08 ug/L	214520	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	98		
4	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	98		
5	1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-90-5	98		



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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	22.5	ug/L	343571	3	11.194	761991	50.0
1,1'-Biphenyl, ...	17.480	14.1	ug/L	214520	3	11.194	761991	50.0