

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070623\
 Data File : VV031651.D
 Acq On : 06 Jul 2023 13:27
 Operator : SY/MD
 Sample : 03444-15ME
 Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46W0ME

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: VV031651.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	53469	77856	8.55%	1.009%
2	2.040	301	311	327	rBV	125317	189122	20.77%	2.452%
3	2.381	410	417	429	rBV2	15596	27072	2.97%	0.351%
4	2.555	460	471	485	rBV	11419	23805	2.61%	0.309%
5	2.889	568	575	578	rBV4	1112	1453	0.16%	0.019%
6	2.973	599	601	608	rVB3	238	168	0.02%	0.002%
7	3.005	608	611	613	rVB	405	233	0.03%	0.003%
8	3.021	613	616	619	rBV3	478	408	0.04%	0.005%
9	3.072	629	632	636	rBV	492	287	0.03%	0.004%
10	3.121	645	647	651	rVB	248	145	0.02%	0.002%
11	3.397	731	733	736	rVB2	325	160	0.02%	0.002%
12	3.568	781	786	791	rVB2	309	367	0.04%	0.005%
13	3.593	791	794	798	rBV2	261	182	0.02%	0.002%
14	3.619	798	802	804	rBV	223	160	0.02%	0.002%
15	3.693	822	825	828	rBV	216	156	0.02%	0.002%
16	3.712	829	831	835	rVB2	358	199	0.02%	0.003%
17	3.802	849	859	897	rBV	55445	187313	20.57%	2.428%
18	4.252	983	999	1026	rBV	115407	301258	33.08%	3.906%
19	4.468	1062	1066	1068	rBV	610	399	0.04%	0.005%
20	4.513	1076	1080	1083	rBV4	567	579	0.06%	0.008%
21	4.577	1098	1100	1103	rVB2	753	437	0.05%	0.006%
22	4.699	1136	1138	1142	rVV2	211	163	0.02%	0.002%
23	4.809	1169	1172	1178	rBV2	191	210	0.02%	0.003%
24	4.957	1202	1218	1247	rBV2	257645	664059	72.92%	8.609%
25	5.130	1270	1272	1276	rBV3	780	456	0.05%	0.006%
26	5.207	1293	1296	1297	rBV	314	145	0.02%	0.002%
27	5.265	1310	1314	1318	rVB3	391	332	0.04%	0.004%
28	5.294	1318	1323	1327	rVB2	295	259	0.03%	0.003%
29	5.313	1327	1329	1331	rBV2	239	140	0.02%	0.002%
30	5.384	1347	1351	1357	rVB2	294	161	0.02%	0.002%
31	5.413	1357	1360	1362	rBV	293	143	0.02%	0.002%
32	5.539	1386	1399	1435	rBV	266554	562748	61.79%	7.296%
33	5.838	1479	1492	1504	rBV	6524	16218	1.78%	0.210%
34	5.995	1527	1541	1570	rBV	155250	335744	36.87%	4.353%
35	6.182	1597	1599	1605	rBV2	478	468	0.05%	0.006%
36	6.259	1621	1623	1626	rBV2	348	174	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Max Peaks: 100

Stop Thrs : 0

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

37	6.333	1642	1646	1648	rBV2	365	221	0.02%	0.003%
38	6.346	1648	1650	1657	rVB3	274	198	0.02%	0.003%
39	6.384	1659	1662	1667	rVB2	293	257	0.03%	0.003%
40	6.452	1680	1683	1685	rBV2	210	150	0.02%	0.002%
41	6.506	1698	1700	1705	rVB	274	178	0.02%	0.002%
42	6.532	1705	1708	1711	rBV2	300	248	0.03%	0.003%
43	6.731	1766	1770	1772	rBV3	295	206	0.02%	0.003%
44	6.796	1787	1790	1793	rVB2	270	165	0.02%	0.002%
45	6.825	1794	1799	1800	rBV	202	156	0.02%	0.002%
46	6.921	1818	1829	1855	rBV	74828	149850	16.45%	1.943%
47	7.050	1867	1869	1873	rVB2	480	214	0.02%	0.003%
48	7.249	1919	1931	1949	rBV	238504	426844	46.87%	5.534%
49	7.506	2008	2011	2017	rBV3	425	346	0.04%	0.004%
50	7.561	2017	2028	2048	rBV2	55301	108658	11.93%	1.409%
51	7.757	2086	2089	2092	rBV	254	209	0.02%	0.003%
52	7.825	2108	2110	2113	rBV2	293	154	0.02%	0.002%
53	7.918	2137	2139	2145	rVB4	779	545	0.06%	0.007%
54	7.960	2149	2152	2158	rVB3	385	254	0.03%	0.003%
55	7.998	2160	2164	2166	rBV2	207	148	0.02%	0.002%
56	8.043	2166	2178	2218	rBV	180849	415356	45.61%	5.385%
57	8.313	2260	2262	2264	rBV2	717	363	0.04%	0.005%
58	8.384	2274	2284	2296	rVB5	3246	6236	0.68%	0.081%
59	8.606	2349	2353	2358	rVB3	407	401	0.04%	0.005%
60	8.696	2378	2381	2384	rBV	285	179	0.02%	0.002%
61	8.792	2399	2411	2439	rBV	410489	693916	76.20%	8.996%
62	9.014	2478	2480	2485	rVB5	604	416	0.05%	0.005%
63	9.127	2513	2515	2517	rBV2	338	168	0.02%	0.002%
64	9.165	2524	2527	2529	rBV2	331	218	0.02%	0.003%
65	9.259	2551	2556	2559	rBV3	423	377	0.04%	0.005%
66	9.317	2566	2574	2578	rBV2	188	298	0.03%	0.004%
67	9.339	2578	2581	2583	rBV	261	143	0.02%	0.002%
68	9.413	2599	2604	2612	rVB4	747	1047	0.11%	0.014%
69	9.452	2614	2616	2618	rVV2	322	146	0.02%	0.002%
70	9.493	2620	2629	2638	rVV3	2362	3537	0.39%	0.046%
71	9.529	2638	2640	2642	rVB2	403	184	0.02%	0.002%
72	9.683	2685	2688	2691	rBV2	341	267	0.03%	0.003%
73	9.828	2731	2733	2735	rBV2	262	145	0.02%	0.002%
74	9.956	2769	2773	2774	rBV3	546	325	0.04%	0.004%
75	10.005	2786	2788	2791	rBV2	325	178	0.02%	0.002%
76	10.162	2826	2837	2857	rBV	278270	441316	48.46%	5.721%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

77	10.448	2920	2926	2934	rBV6	1337	1766	0.19%	0.023%
78	10.484	2934	2937	2939	rBV3	602	471	0.05%	0.006%
79	10.609	2973	2976	2978	rBV2	375	303	0.03%	0.004%
80	10.648	2985	2988	2990	rBV	267	154	0.02%	0.002%
81	10.664	2990	2993	2999	rVV2	654	808	0.09%	0.010%
82	10.689	2999	3001	3004	rVB	669	237	0.03%	0.003%
83	10.744	3016	3018	3022	rBV2	491	353	0.04%	0.005%
84	10.783	3028	3030	3034	rVB3	799	456	0.05%	0.006%
85	10.825	3036	3043	3051	rBV6	1690	2938	0.32%	0.038%
86	10.866	3051	3056	3065	rVB7	2486	2790	0.31%	0.036%
87	10.972	3086	3089	3091	rBV2	478	345	0.04%	0.004%
88	11.008	3098	3100	3101	rBV2	469	260	0.03%	0.003%
89	11.095	3122	3127	3128	rBV4	1590	1181	0.13%	0.015%
90	11.194	3147	3158	3181	rBV	510159	789856	86.73%	10.240%
91	11.413	3224	3226	3229	rVB2	974	374	0.04%	0.005%
92	11.570	3263	3275	3289	rBV	370697	585320	64.27%	7.588%
93	11.831	3354	3356	3359	rVB	555	256	0.03%	0.003%
94	12.313	3498	3506	3507	rBV4	2956	3176	0.35%	0.041%
95	12.413	3530	3537	3546	rBV6	5112	7588	0.83%	0.098%
96	12.468	3552	3554	3559	rBV5	943	666	0.07%	0.009%
97	12.943	3699	3702	3706	rBV4	1780	1430	0.16%	0.019%
98	13.545	3887	3889	3891	rBV2	1218	797	0.09%	0.010%
99	16.400	4766	4777	4791	rBV	618127	910679	100.00%	11.807%
100	17.480	5104	5113	5129	rVB	450414	753700	82.76%	9.771%

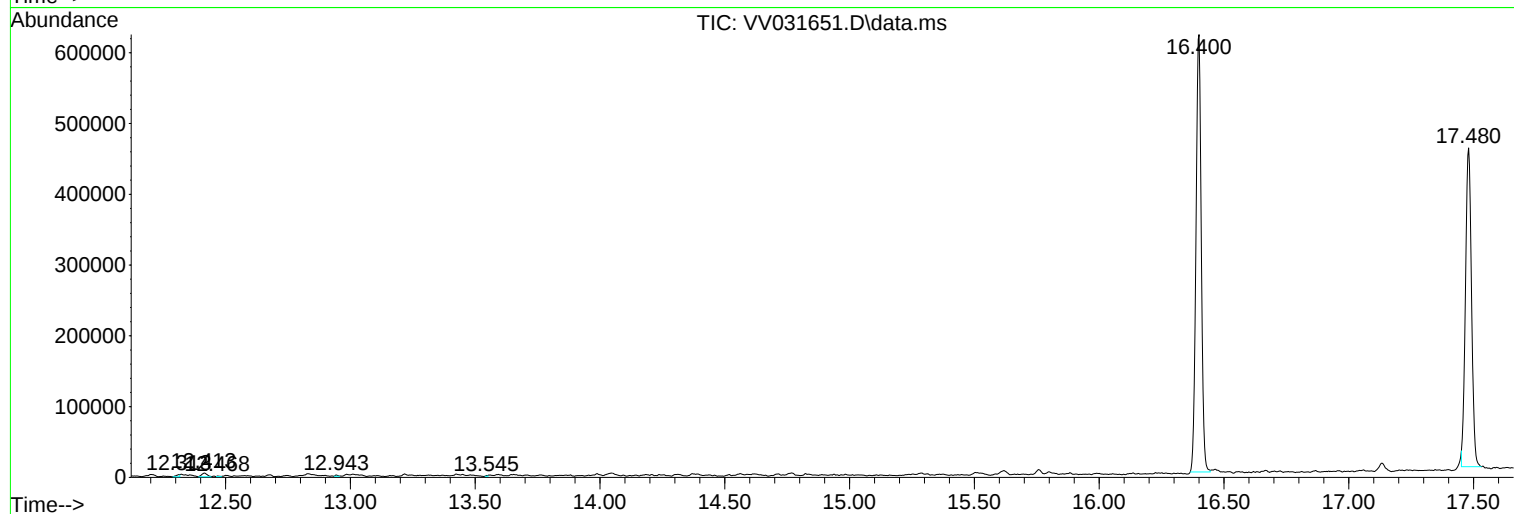
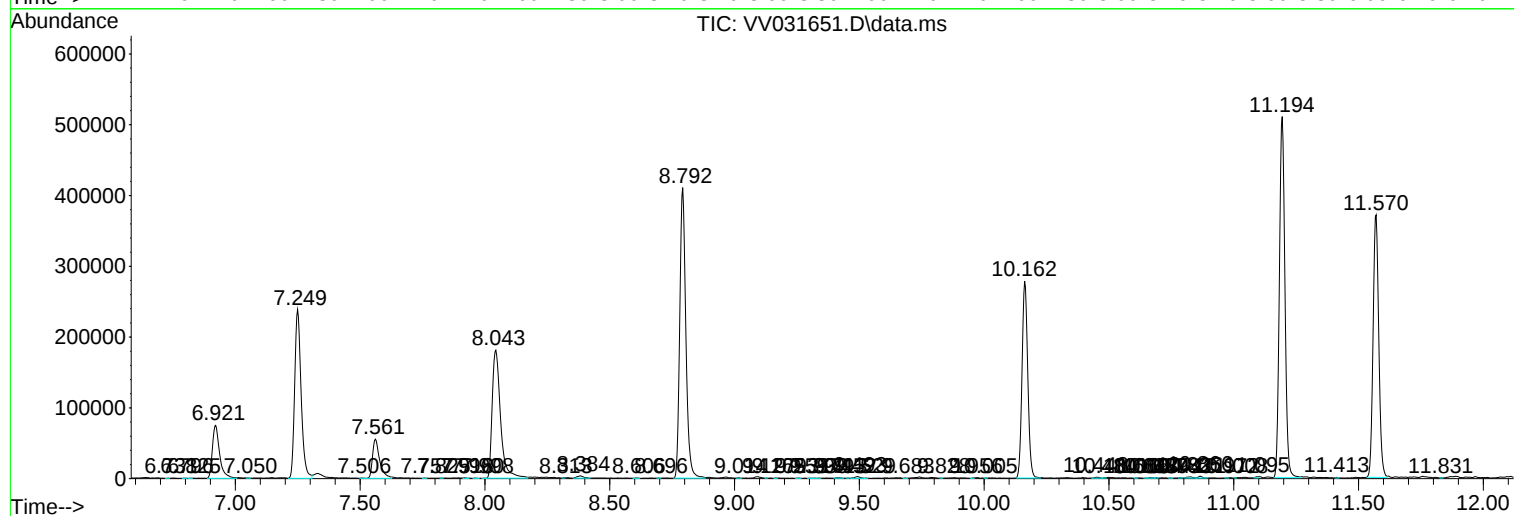
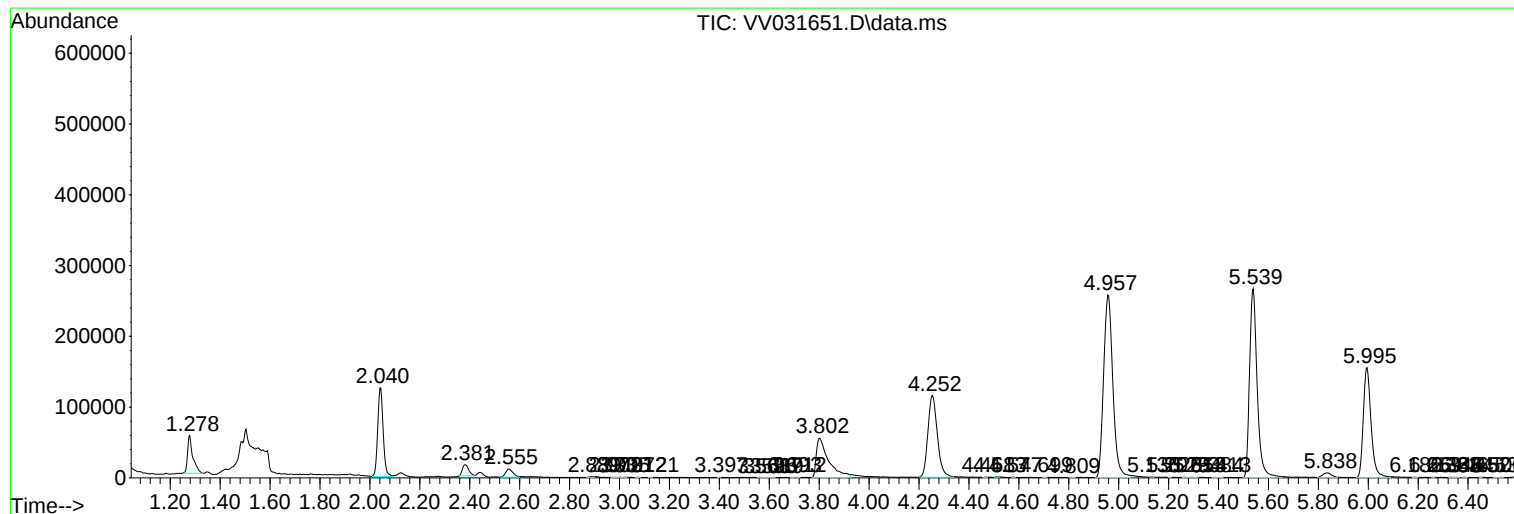
Sum of corrected areas: 7713300

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070623\
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46W0ME

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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Instrument :
MSVOA_V
ClientSampleId :
A46W0ME

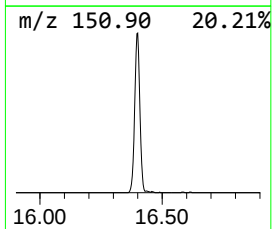
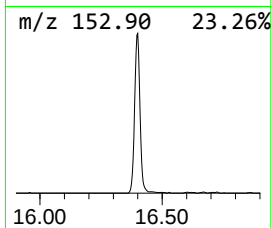
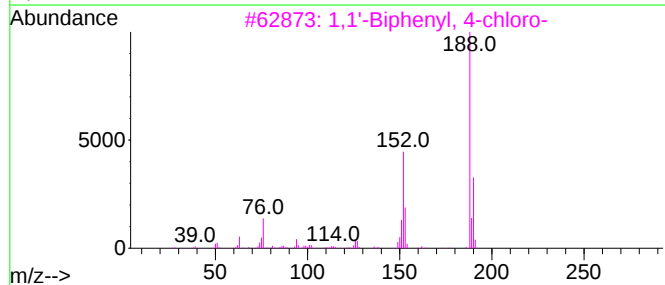
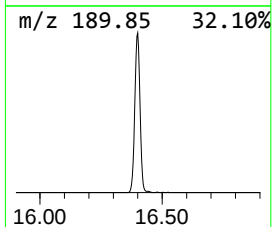
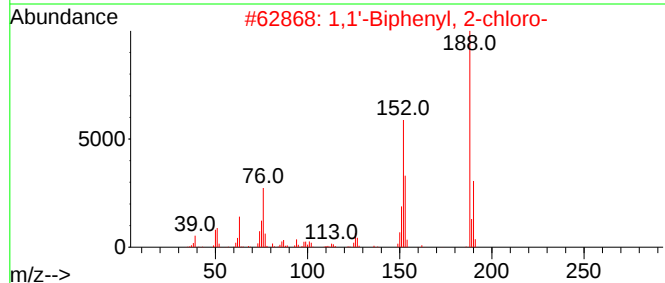
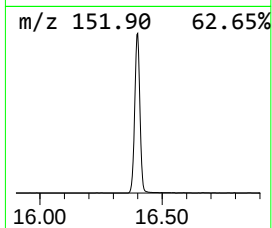
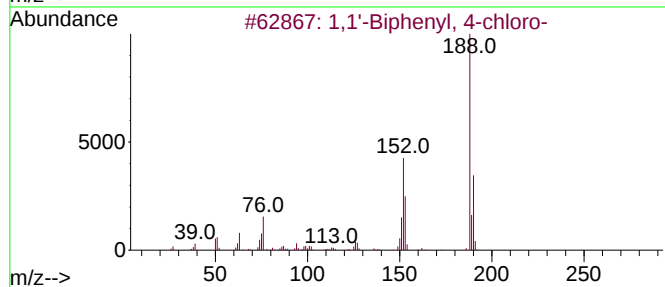
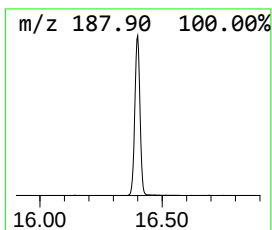
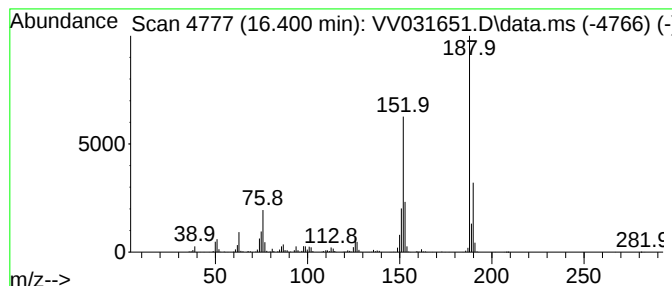
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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.
16.400	57.65 ug/L	910679	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	96
2	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	95
3	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	94
4	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	93
5	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	93



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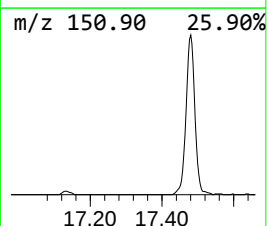
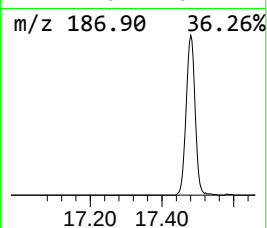
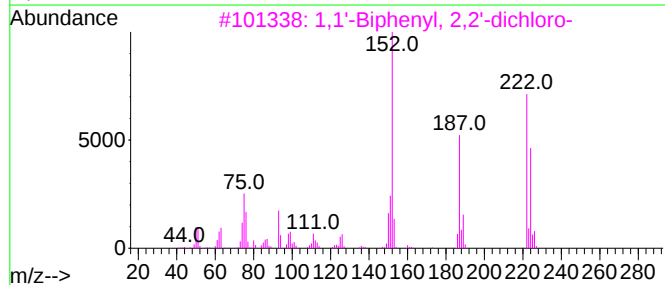
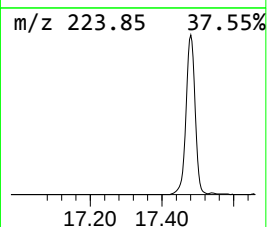
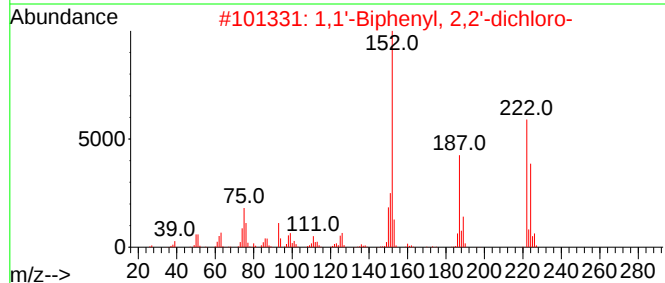
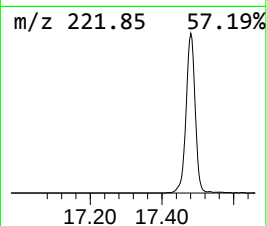
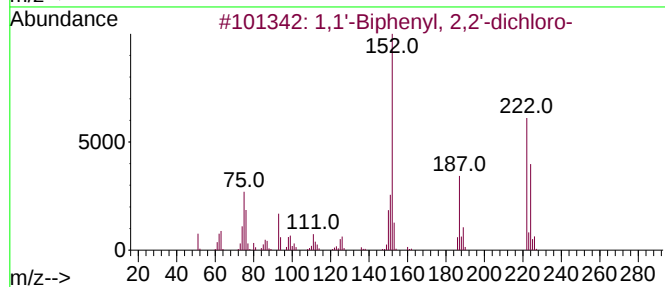
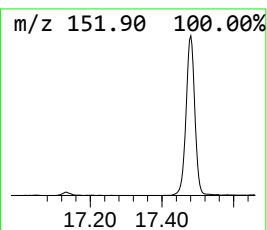
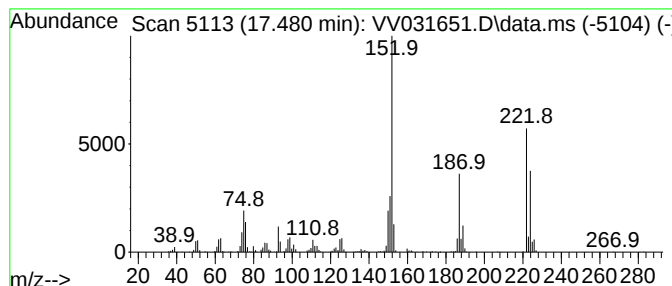
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Quant Title : VOC Analysis

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.
17.480	47.71 ug/L	753700	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	99		
5	1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	98		



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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, ...	16.400	57.6	ug/L	910679	3	11.194	789856	50.0
1,1'-Biphenyl, ...	17.480	47.7	ug/L	753700	3	11.194	789856	50.0