

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
 Data File : VV031634.D
 Acq On : 03 Jul 2023 13:56
 Operator : SY/MD
 Sample : 03472-12ME
 Misc : 3.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46S4ME

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: VV031634.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	rVB2	74490	109078	8.72%	1.257%
2	2.043	302	312	328	rVB	193881	293856	23.50%	3.386%
3	2.224	365	368	369	rBV2	788	493	0.04%	0.006%
4	2.384	409	418	430	rBV	14264	27327	2.19%	0.315%
5	2.558	457	472	491	rBV2	9810	22912	1.83%	0.264%
6	2.693	507	514	521	rVB6	2346	4039	0.32%	0.047%
7	2.818	551	553	557	rVB2	585	340	0.03%	0.004%
8	2.834	557	558	564	rBV3	332	330	0.03%	0.004%
9	2.953	589	595	596	rBV2	732	666	0.05%	0.008%
10	3.053	622	626	628	rBV2	577	396	0.03%	0.005%
11	3.111	631	644	660	rBV2	10181	21103	1.69%	0.243%
12	3.397	727	733	739	rVB4	514	581	0.05%	0.007%
13	3.436	741	745	748	rBV3	357	330	0.03%	0.004%
14	3.812	849	862	897	rBV2	103309	331513	26.51%	3.819%
15	4.066	937	941	946	rBV5	729	723	0.06%	0.008%
16	4.252	982	999	1025	rBV	128925	334695	26.76%	3.856%
17	4.384	1036	1040	1043	rBV3	472	380	0.03%	0.004%
18	4.513	1063	1080	1098	rBV2	45814	119148	9.53%	1.373%
19	4.661	1122	1126	1130	rBV4	785	836	0.07%	0.010%
20	4.683	1130	1133	1138	rVV3	576	528	0.04%	0.006%
21	4.805	1166	1171	1172	rBV2	947	727	0.06%	0.008%
22	4.957	1200	1218	1247	rBV3	295061	766605	61.30%	8.832%
23	5.140	1270	1275	1289	rVB4	7080	15532	1.24%	0.179%
24	5.233	1300	1304	1307	rVB5	435	414	0.03%	0.005%
25	5.323	1328	1332	1337	rBV4	392	360	0.03%	0.004%
26	5.410	1351	1359	1360	rBV3	1433	1526	0.12%	0.018%
27	5.465	1370	1376	1377	rBV3	483	365	0.03%	0.004%
28	5.539	1386	1399	1428	rBV	282976	599410	47.93%	6.906%
29	5.725	1455	1457	1461	rVB3	949	636	0.05%	0.007%
30	5.789	1475	1477	1480	rVV2	773	451	0.04%	0.005%
31	5.838	1480	1492	1509	rVV6	28611	61809	4.94%	0.712%
32	5.995	1527	1541	1572	rVV	174937	381699	30.52%	4.398%
33	6.175	1593	1597	1598	rBV2	1230	843	0.07%	0.010%
34	6.346	1647	1650	1652	rBV2	552	332	0.03%	0.004%
35	6.365	1652	1656	1657	rBV2	1107	732	0.06%	0.008%
36	6.378	1657	1660	1661	rBV3	896	604	0.05%	0.007%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Max Peaks: 100

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

37	6.693	1752	1758	1762	rBV5	805	768	0.06%	0.009%
38	6.709	1762	1763	1768	rVB4	514	376	0.03%	0.004%
39	6.760	1768	1779	1780	rBV4	1586	1512	0.12%	0.017%
40	6.854	1801	1808	1813	rVB6	1112	1382	0.11%	0.016%
41	6.918	1816	1828	1851	rBV2	85677	170088	13.60%	1.960%
42	7.130	1891	1894	1895	rBV2	566	355	0.03%	0.004%
43	7.194	1903	1914	1919	rBV5	9714	17017	1.36%	0.196%
44	7.249	1920	1931	1954	rVB	285056	514845	41.17%	5.932%
45	7.503	2004	2010	2011	rBV2	1467	1180	0.09%	0.014%
46	7.561	2017	2028	2053	rBV2	60867	135859	10.86%	1.565%
47	7.722	2066	2078	2092	rVB9	8272	16060	1.28%	0.185%
48	7.783	2092	2097	2102	rVB6	1085	1226	0.10%	0.014%
49	7.911	2126	2137	2155	rVB2	56226	98928	7.91%	1.140%
50	8.043	2164	2178	2207	rBV	177669	421569	33.71%	4.857%
51	8.223	2227	2234	2244	rVB4	9902	15672	1.25%	0.181%
52	8.288	2245	2254	2262	rBV8	10234	16820	1.34%	0.194%
53	8.532	2320	2330	2338	rVV9	4611	8598	0.69%	0.099%
54	8.587	2341	2347	2355	rVB7	1523	2241	0.18%	0.026%
55	8.670	2369	2373	2377	rVB3	739	543	0.04%	0.006%
56	8.728	2385	2391	2392	rBV3	533	413	0.03%	0.005%
57	8.738	2392	2394	2398	rVB3	615	358	0.03%	0.004%
58	8.792	2398	2411	2432	rBV	438050	754452	60.33%	8.692%
59	8.937	2447	2456	2468	rBV	4248	9877	0.79%	0.114%
60	8.995	2471	2474	2479	rBV6	1602	1394	0.11%	0.016%
61	9.056	2484	2493	2494	rBV7	3779	4897	0.39%	0.056%
62	9.178	2529	2531	2534	rVB3	1041	602	0.05%	0.007%
63	9.255	2544	2555	2563	rVB6	3779	6120	0.49%	0.071%
64	9.419	2590	2606	2622	rBV8	11379	29759	2.38%	0.343%
65	9.493	2623	2629	2630	rBV3	2496	2204	0.18%	0.025%
66	9.571	2649	2653	2654	rVV3	553	431	0.03%	0.005%
67	9.583	2655	2657	2658	rVV2	1073	505	0.04%	0.006%
68	9.644	2659	2676	2687	rVB6	12171	26477	2.12%	0.305%
69	9.741	2692	2706	2718	rBV6	8439	19321	1.54%	0.223%
70	9.876	2745	2748	2750	rBV4	596	405	0.03%	0.005%
71	9.902	2752	2756	2757	rBV3	998	737	0.06%	0.008%
72	9.956	2771	2773	2778	rVB5	1412	880	0.07%	0.010%
73	9.982	2778	2781	2787	rVB4	410	428	0.03%	0.005%
74	10.066	2799	2807	2817	rVB6	6826	10622	0.85%	0.122%
75	10.104	2817	2819	2822	rBV4	538	316	0.03%	0.004%
76	10.162	2822	2837	2857	rBV	292148	488195	39.04%	5.625%

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 Title : VOC Analysis

77	10.323	2885	2887	2890	rBV2	735	514	0.04%	0.006%
78	10.390	2903	2908	2909	rBV3	2499	1952	0.16%	0.022%
79	10.455	2919	2928	2931	rBV8	2879	3743	0.30%	0.043%
80	10.641	2984	2986	2989	rBV4	580	355	0.03%	0.004%
81	10.677	2989	2997	3007	rVV8	3499	6731	0.54%	0.078%
82	10.828	3036	3044	3052	rBV8	3098	6145	0.49%	0.071%
83	10.963	3079	3086	3088	rBV3	1907	2117	0.17%	0.024%
84	11.011	3094	3101	3102	rBV5	1891	2008	0.16%	0.023%
85	11.033	3102	3108	3118	rVB2	8614	13794	1.10%	0.159%
86	11.075	3118	3121	3122	rBV2	766	491	0.04%	0.006%
87	11.194	3146	3158	3179	rBV	528730	839519	67.13%	9.672%
88	11.490	3241	3250	3259	rBV8	6661	11800	0.94%	0.136%
89	11.577	3262	3277	3296	rVV3	534433	1250624	100.00%	14.409%
90	11.879	3366	3371	3380	rVB9	3645	5143	0.41%	0.059%
91	11.934	3381	3388	3397	rVV10	4824	7379	0.59%	0.085%
92	12.066	3424	3429	3433	rBV6	2582	3171	0.25%	0.037%
93	12.204	3461	3472	3480	rVB6	5390	11593	0.93%	0.134%
94	12.316	3496	3507	3508	rBV5	6267	7700	0.62%	0.089%
95	12.744	3634	3640	3648	rBV8	3219	4404	0.35%	0.051%
96	13.136	3759	3762	3763	rBV3	1028	567	0.05%	0.007%
97	13.207	3777	3784	3794	rBV5	15906	24964	2.00%	0.288%
98	15.422	4461	4473	4494	rVB5	86754	229222	18.33%	2.641%
99	16.397	4767	4776	4789	rBV	85539	133221	10.65%	1.535%
100	17.480	5104	5113	5125	rVB	136866	227650	18.20%	2.623%

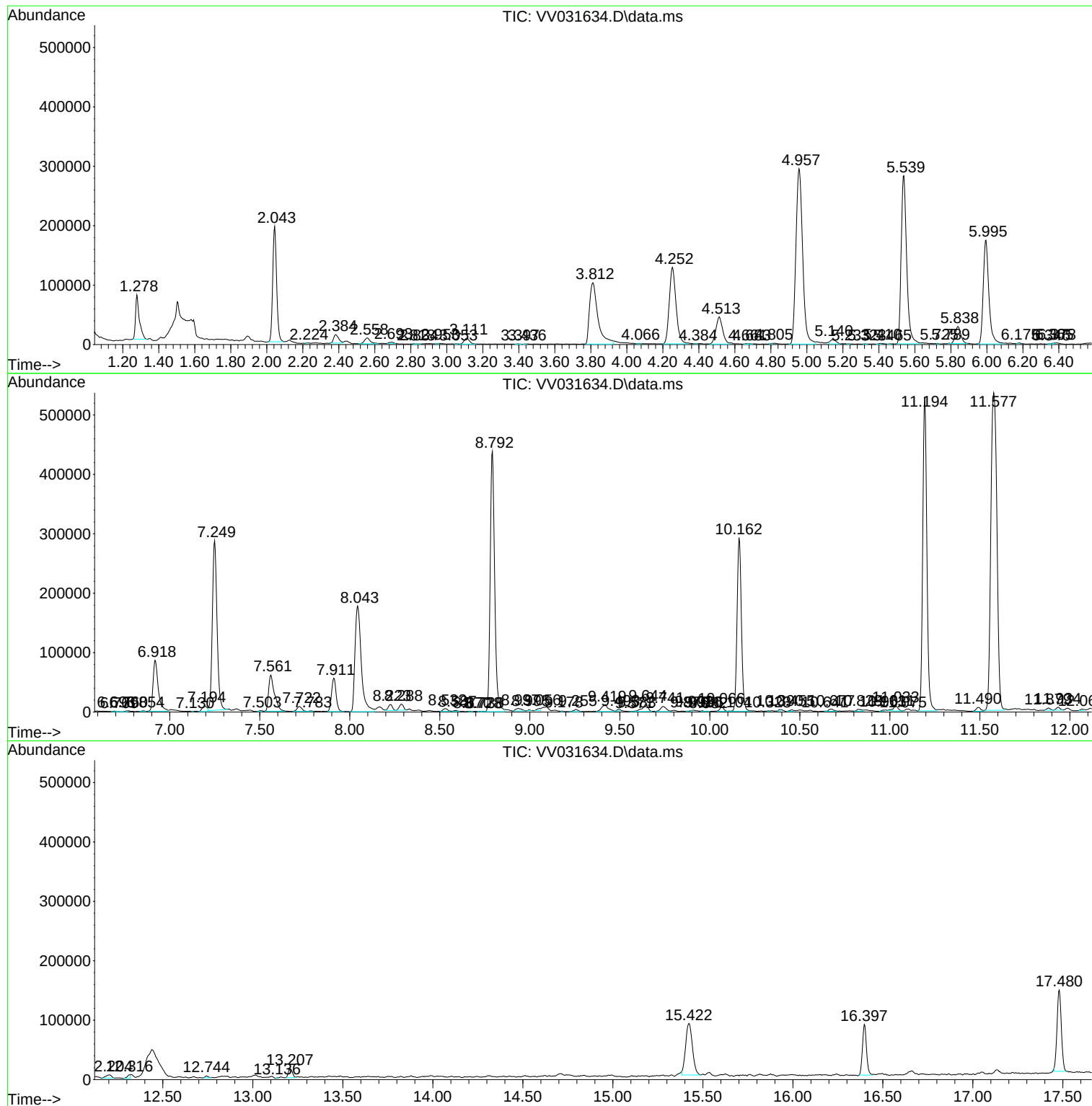
Sum of corrected areas: 8679558

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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



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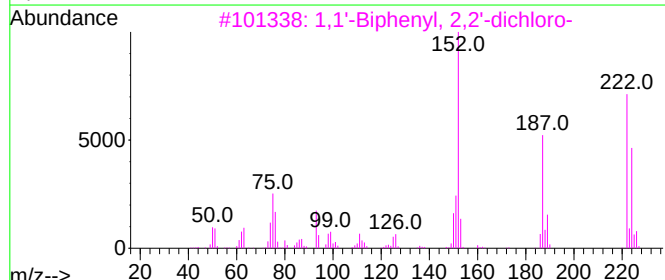
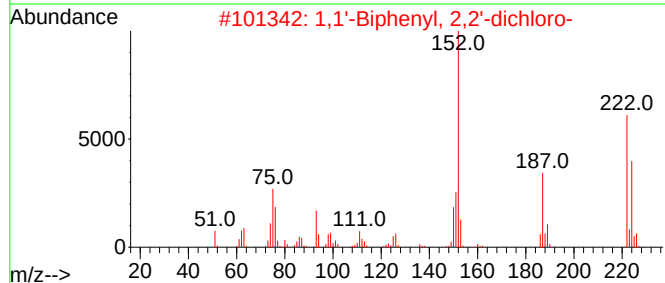
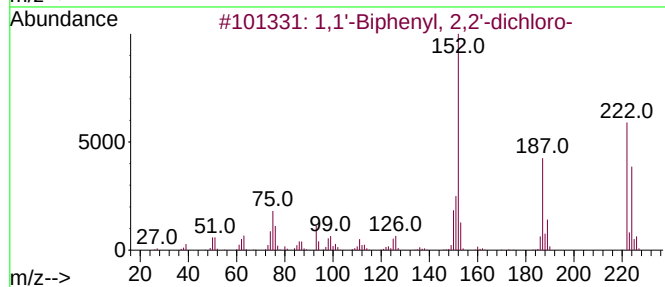
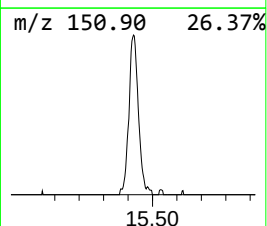
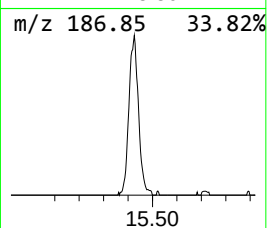
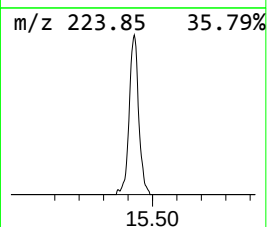
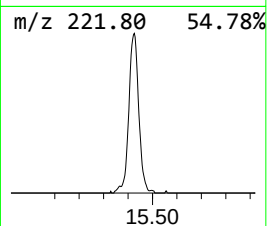
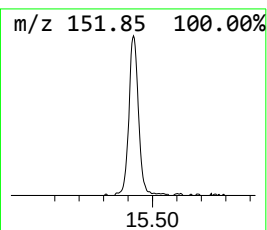
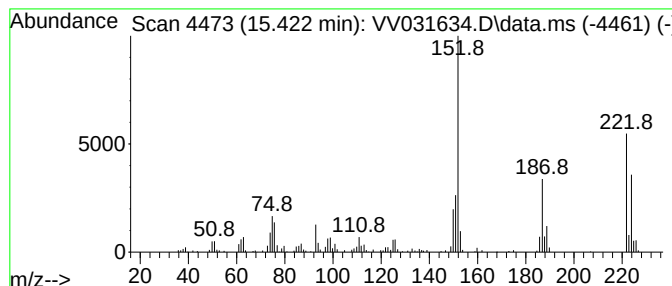
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.422	13.65 ug/L	229222	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	98		
3	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	98		
4	1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98		
5	1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	98		



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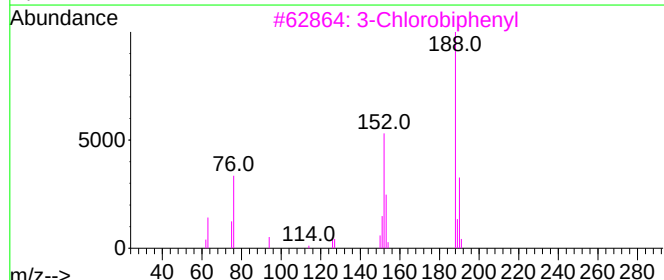
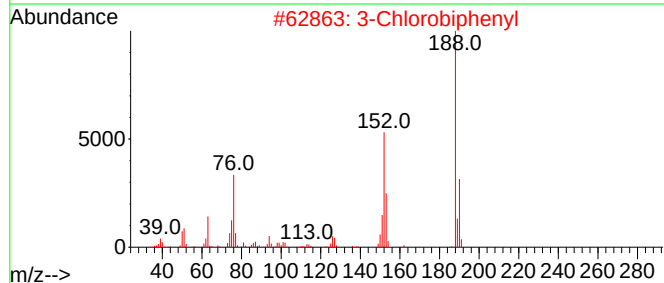
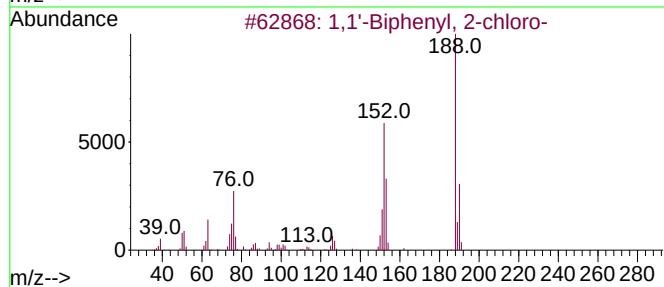
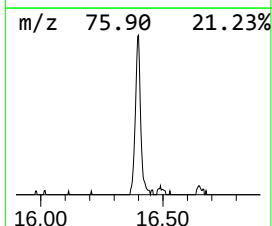
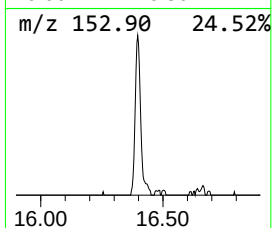
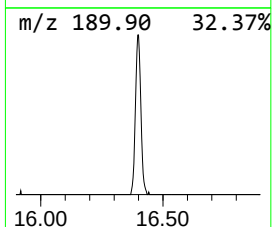
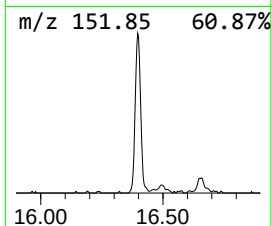
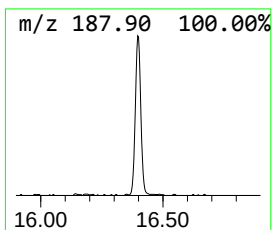
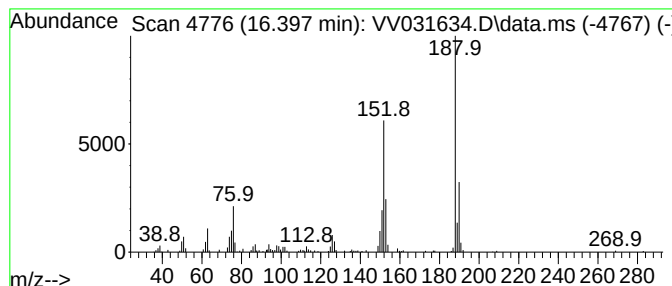
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Quant Title : VOC Analysis

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

Peak Number 3 1,1'-Biphenyl, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	7.93 ug/L	133221	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			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	97
3			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	97
4			1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96
5			1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	95



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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, ...	15.422	13.7	ug/L	229222	3	11.194	839519	50.0
1,1'-Biphenyl, ...	16.397	7.9	ug/L	133221	3	11.194	839519	50.0