LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062923\
Data File : VV031626.D
Acq On : 29 Jun 2023 17:20
Operator : SY/MD
Sample : 03458-13ME
Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46M6ME

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: VV031626.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	93	rVB	67784	97918	12.50%	1.286%
2	1.497	137	142	144	rBV	15298	14402	1.84%	0.189%
3	1.519	145	149	157	rVV	32247	39719	5.07%	0.522%
4	2.047	302	313	331	rBV	170683	253040	32.31%	3.324%
5	2.227	361	369	378	rBV3	2012	2852	0.36%	0.037%
6	2.336	399	403	405	rBV3	688	556	0.07%	0.007%
7	2.384	409	418	428	rBV	20807	39480	5.04%	0.519%
8	2.564	462	474	486	rBV4	4342	9283	1.19%	0.122%
9	2.699	508	516	519	rBV6	2481	3729	0.48%	0.049%
10	2.889	566	575	576	rBV6	878	1133	0.14%	0.015%
11	2.976	599	602	605	rBV3	520	406	0.05%	0.005%
12	3.060	624	628	630	rBV2	502	448	0.06%	0.006%
13	3.146	652	655	661	rBV3	323	344	0.04%	0.005%
14	3.304	701	704	709	rVB	358	316	0.04%	0.004%
15	3.336	713	714	719	rVV2	385	310	0.04%	0.004%
16	3.371	721	725	731	rVB3	503	417	0.05%	0.005%
17	3.397	731	733	738	rBV3	496	337	0.04%	0.004%
18	3.516	767	770	776	rBV3	379	352	0.04%	0.005%
19	3.674	815	819	821	rBV	360	313	0.04%	0.004%
20	3.809	851	861	888	rBV2	51028	180712	23.08%	2.374%
21	4.256	983	1000	1022	rBV	128524	339475	43.35%	4.459%
22	4.584	1100	1102	1107	rVB	800	586	0.07%	0.008%
23	4.696	1133	1137	1141	rVB4	578	393	0.05%	0.005%
24	4.738	1144	1150	1153	rBV4	822	655	0.08%	0.009%
25	4.818	1172	1175	1177	rBV2	520	335	0.04%	0.004%
26	4.960	1203	1219	1252	rBV2	302467	783078	100.00%	10.286%
27	5.175	1282	1286	1296	rVB5	761	835	0.11%	0.011%
28	5.220	1296	1300	1304	rVB3	564	332	0.04%	0.004%
29	5.333	1333	1335	1337	rBV	489	297	0.04%	0.004%
30	5.539	1387	1399	1433	rBV	276564	595454	76.04%	7.822%
31	5.834	1481	1491	1504	rVB10	3772	7944	1.01%	0.104%
32	5.995	1528	1541	1570	rBV	180111	389848	49.78%	5.121%
33	6.095	1570	1572	1576	rVV2	485	372	0.05%	0.005%
34	6.114	1576	1578	1584	rVV3	489	347	0.04%	0.005%
35	6.178	1595	1598	1600	rBV3	525	319	0.04%	0.004%
36	6.214	1605	1609	1613	rVB3	648	527	0.07%	0.007%

LSC Area Percent Report

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Sample : 03458-13ME
Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46M6ME

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

37	6.323	1640	1643	1648	rBV2	356	343	0.04%	0.005%
38	6.458	1682	1685	1687	rVB2	457	318	0.04%	0.004%
39	6.522	1697	1705	1706	rBV2	683	613	0.08%	0.008%
40	6.587	1721	1725	1730	rVV3	582	702	0.09%	0.009%
41	6.638	1737	1741	1744	rVB4	554	413	0.05%	0.005%
42	6.664	1746	1749	1755	rBV3	515	468	0.06%	0.006%
43	6.783	1784	1786	1790	rVB4	609	309	0.04%	0.004%
44	6.921	1818	1829	1848	rBV	85710	172477	22.03%	2.266%
45	7.188	1907	1912	1915	rBV3	1076	1318	0.17%	0.017%
46	7.249	1919	1931	1949	rBV	280081	499609	63.80%	6.563%
47	7.400	1975	1978	1983	rVB4	1140	841	0.11%	0.011%
48	7.561	2018	2028	2056	rBV	62385	126961	16.21%	1.668%
49	7.780	2092	2096	2100	rBV4	738	662	0.08%	0.009%
50	7.876	2122	2126	2128	rBV2	1056	832	0.11%	0.011%
51	7.915	2134	2138	2145	rVB5	779	1055	0.13%	0.014%
52	8.053	2167	2181	2215	rBV	147211	426501	54.46%	5.602%
53	8.272	2247	2249	2252	rBV4	587	483	0.06%	0.006%
54	8.358	2273	2276	2277	rBV3	1095	553	0.07%	0.007%
55	8.503	2316	2321	2325	rVB5	628	664	0.08%	0.009%
56	8.529	2326	2329	2337	rVB5	792	984	0.13%	0.013%
57	8.583	2342	2346	2351	rBV2	595	582	0.07%	0.008%
58	8.619	2355	2357	2363	rVB3	546	346	0.04%	0.005%
59	8.674	2371	2374	2377	rVB2	613	442	0.06%	0.006%
60	8.699	2377	2382	2383	rBV2	456	314	0.04%	0.004%
61	8.738	2390	2394	2396	rBV4	517	295	0.04%	0.004%
62	8.792	2399	2411	2433	rBV	419858	728349	93.01%	9.568%
63	8.944	2455	2458	2460	rBV2	642	469	0.06%	0.006%
64	8.963	2461	2464	2472	rVB5	1358	1483	0.19%	0.019%
65	9.088	2498	2503	2504	rBV3	1428	1160	0.15%	0.015%
66	9.156	2521	2524	2530	rVB5	702	571	0.07%	0.008%
67	9.381	2592	2594	2597	rVB3	558	293	0.04%	0.004%
68	9.410	2599	2603	2604	rBV	814	572	0.07%	0.008%
69	9.490	2623	2628	2629	rBV	1223	814	0.10%	0.011%
70	9.596	2659	2661	2664	rBV	462	369	0.05%	0.005%
71	9.651	2674	2678	2694	rVB6	1744	2976	0.38%	0.039%
72	9.731	2698	2703	2704	rBV4	1484	1222	0.16%	0.016%
73	9.879	2745	2749	2752	rBV3	807	801	0.10%	0.011%
74	9.960	2766	2774	2777	rBV5	1852	2048	0.26%	0.027%
75	10.069	2804	2808	2810	rBV3	1030	694	0.09%	0.009%
76	10.120	2820	2824	2825	rBV2	740	508	0.06%	0.007%

LSC Area Percent Report

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Sample : 03458-13ME
Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46M6ME

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

77	10.165	2826	2838	2853	rVV	279575	470886	60.13%	6.186%
78	10.333	2882	2890	2899	rVB5	3794	6318	0.81%	0.083%
79	10.378	2899	2904	2905	rBV3	803	640	0.08%	0.008%
80	10.397	2905	2910	2916	rVB7	1852	2215	0.28%	0.029%
81	10.452	2920	2927	2928	rBV3	1779	1761	0.22%	0.023%
82	10.516	2943	2947	2953	rVB6	1667	1913	0.24%	0.025%
83	10.561	2959	2961	2964	rVB3	1242	610	0.08%	0.008%
84	10.667	2992	2994	2998	rVB4	634	341	0.04%	0.004%
85	10.706	3003	3006	3008	rBV3	888	719	0.09%	0.009%
86	10.825	3038	3043	3047	rBV6	1331	1610	0.21%	0.021%
87	10.863	3052	3055	3060	rVV6	1345	1258	0.16%	0.017%
88	10.982	3082	3092	3097	rBV7	1981	3297	0.42%	0.043%
89	11.008	3097	3100	3104	rBV5	1488	1251	0.16%	0.016%
90	11.091	3121	3126	3135	rBV8	3812	6110	0.78%	0.080%
91	11.194	3147	3158	3181	rBV	476275	748627	95.60%	9.834%
92	11.474	3242	3245	3246	rBV2	1459	813	0.10%	0.011%
93	11.570	3263	3275	3294	rVB	364030	581234	74.22%	7.635%
94	12.201	3460	3471	3480	rBV	8166	15447	1.97%	0.203%
95	12.316	3498	3507	3517	rBV	10174	22238	2.84%	0.292%
96	12.413	3532	3537	3547	rVB7	6088	8835	1.13%	0.116%
97	13.214	3779	3786	3793	rBV9	8024	11363	1.45%	0.149%
98	13.426	3847	3852	3854	rBV5	5372	5805	0.74%	0.076%
99	16.397	4765	4776	4793	rBV	488402	748694	95.61%	9.835%
100	17.480	5104	5113	5127	rVB2	130638	223437	28.53%	2.935%

Sum of corrected areas: 7612700

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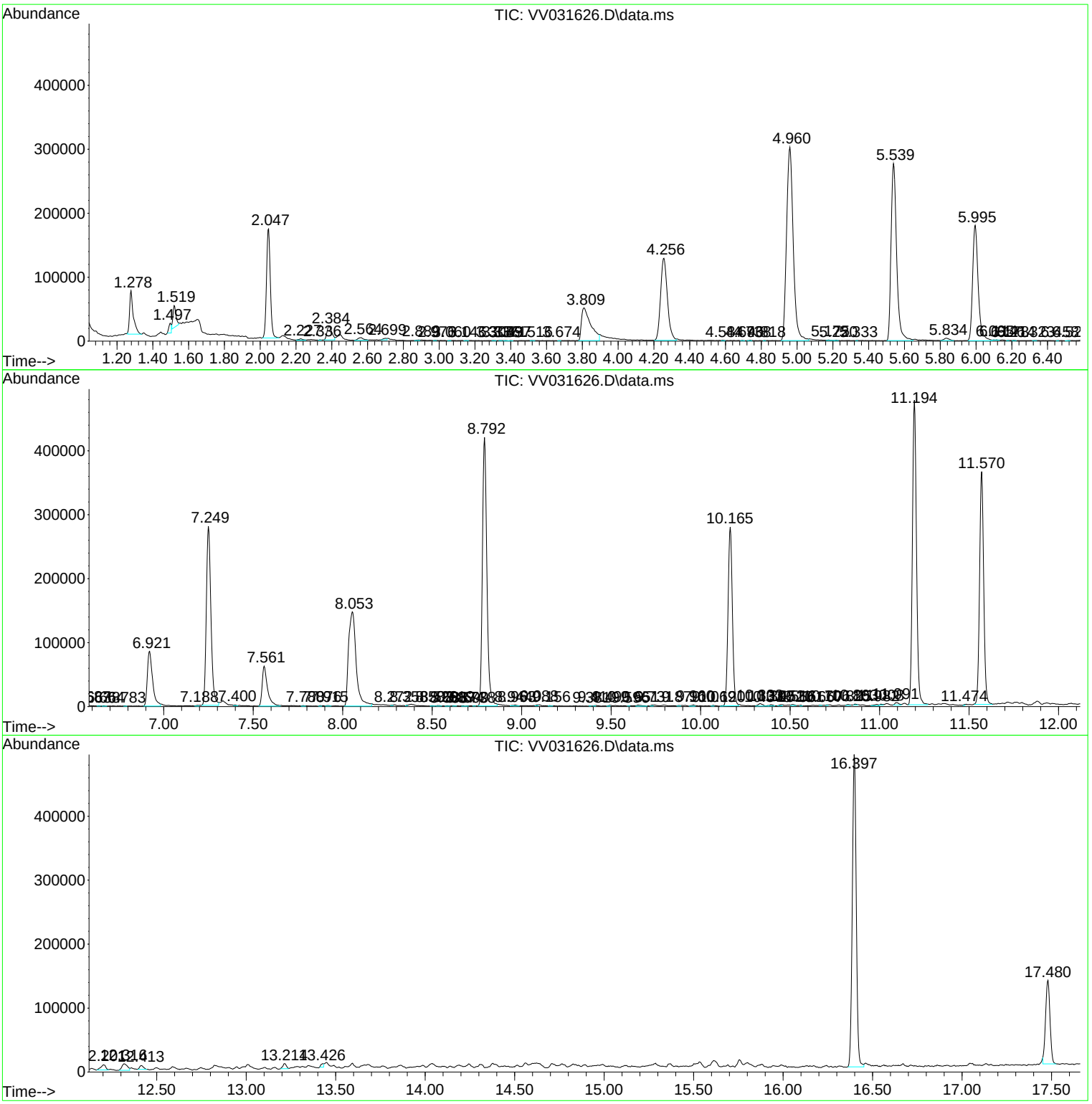
Instrument :
MSVOA_V
ClientSampleId :
A46M6ME

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 :
A46M6ME

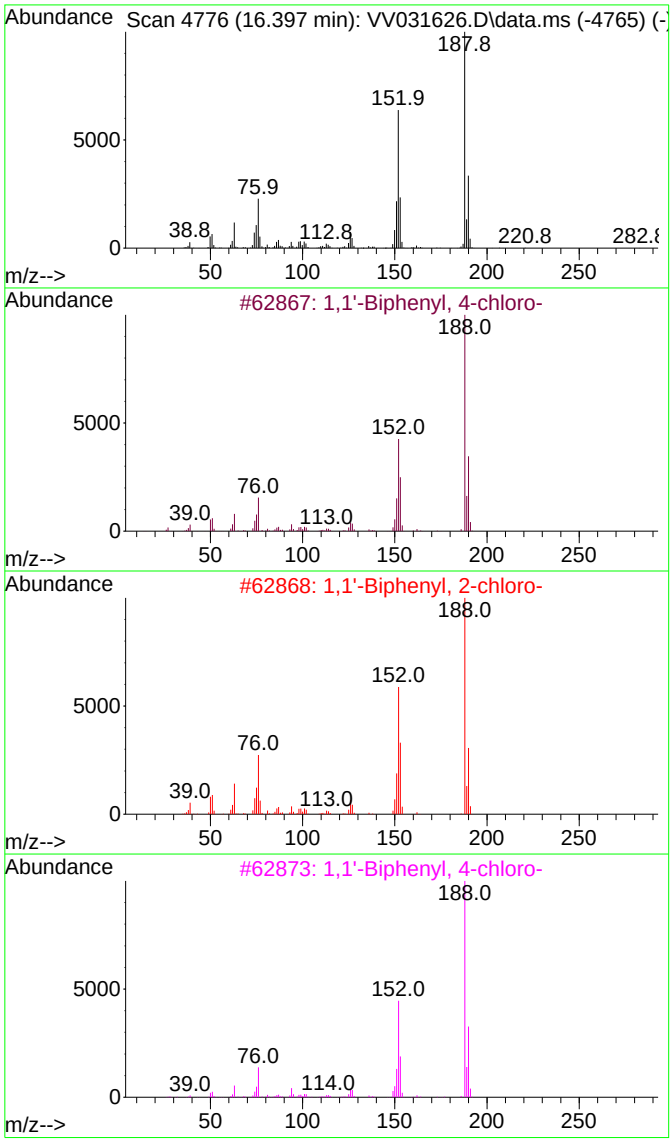
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

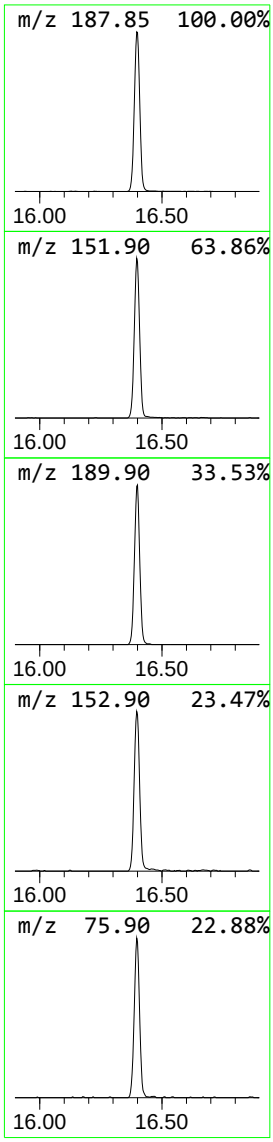
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	50.00 ug/L	748694	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	96
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	3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062923\
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Acq On : 29 Jun 2023 17:20
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46M6ME

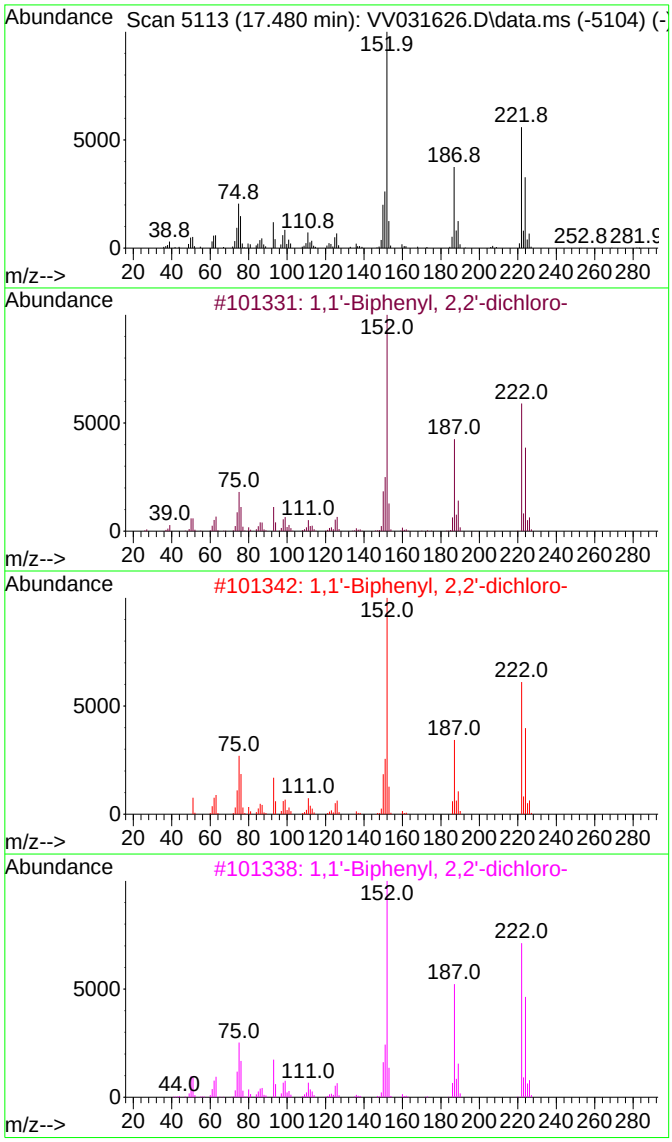
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

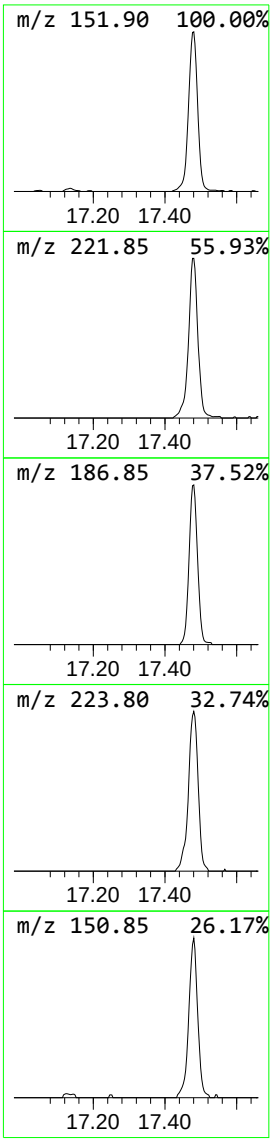
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	14.92 ug/L	223437	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, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	97
5	1,1'-Biphenyl 2,3'-dichloro-	222	C12H8Cl2	025569-80-6	97





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	50.0	ug/L	748694	3	11.194	748627	50.0
1,1'-Biphenyl, ...	17.480	14.9	ug/L	223437	3	11.194	748627	50.0