LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062923\
Data File : VV031621.D
Acq On : 29 Jun 2023 15:15
Operator : SY/MD
Sample : 03422-22ME
Misc : 4.48/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46G1ME

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: VV031621.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	78712	112643	13.90%	1.457%
2	2.043	303	312	330	rVB	195253	282973	34.91%	3.660%
3	2.211	362	364	365	rBV2	748	274	0.03%	0.004%
4	2.249	374	376	379	rVB2	562	292	0.04%	0.004%
5	2.384	409	418	429	rBV	21813	42438	5.24%	0.549%
6	2.513	455	458	460	rBV3	605	341	0.04%	0.004%
7	2.558	462	472	480	rBV4	3662	6997	0.86%	0.091%
8	2.764	534	536	540	rVB2	725	377	0.05%	0.005%
9	2.969	597	600	603	rBV3	393	264	0.03%	0.003%
10	2.989	603	606	615	rVB3	658	632	0.08%	0.008%
11	3.117	640	646	650	rBV3	667	778	0.10%	0.010%
12	3.156	654	658	661	rVB	352	262	0.03%	0.003%
13	3.217	671	677	681	rBV4	563	447	0.06%	0.006%
14	3.654	809	813	817	rVB2	473	328	0.04%	0.004%
15	3.677	817	820	823	rBV2	489	434	0.05%	0.006%
16	3.805	850	860	891	rBV2	48689	174498	21.53%	2.257%
17	4.137	957	963	965	rBV2	397	446	0.06%	0.006%
18	4.185	976	978	982	rBV3	361	285	0.04%	0.004%
19	4.252	983	999	1024	rBV	132889	350857	43.29%	4.538%
20	4.513	1078	1080	1085	rVB4	701	476	0.06%	0.006%
21	4.574	1093	1099	1102	rBV5	939	795	0.10%	0.010%
22	4.744	1150	1152	1157	rBV2	600	462	0.06%	0.006%
23	4.818	1172	1175	1177	rBV2	559	332	0.04%	0.004%
24	4.850	1180	1185	1188	rBV3	394	294	0.04%	0.004%
25	4.960	1202	1219	1248	rBV2	306228	806258	99.47%	10.429%
26	5.278	1316	1318	1324	rVB3	482	409	0.05%	0.005%
27	5.307	1324	1327	1329	rBV	552	377	0.05%	0.005%
28	5.320	1329	1331	1332	rVV3	645	306	0.04%	0.004%
29	5.538	1386	1399	1436	rBV	287617	618895	76.35%	8.006%
30	5.741	1458	1462	1465	rVB3	480	292	0.04%	0.004%
31	5.770	1468	1471	1472	rBV2	558	340	0.04%	0.004%
32	5.828	1481	1489	1496	rBV8	2519	4366	0.54%	0.056%
33	5.931	1517	1521	1526	rBV6	582	687	0.08%	0.009%
34	5.995	1526	1541	1562	rBV2	183035	395045	48.74%	5.110%
35	6.153	1586	1590	1596	rVB6	995	1123	0.14%	0.015%
36	6.191	1600	1602	1607	rVB4	655	427	0.05%	0.006%

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Misc : 4.48/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46G1ME

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

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Peak separation: 5

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

37	6.220	1607	1611	1613	rBV2	636	370	0.05%	0.005%
38	6.307	1634	1638	1642	rVB	465	378	0.05%	0.005%
39	6.490	1691	1695	1701	rBV3	337	372	0.05%	0.005%
40	6.593	1723	1727	1732	rBV4	663	726	0.09%	0.009%
41	6.654	1743	1746	1747	rBV2	486	282	0.03%	0.004%
42	6.673	1750	1752	1754	rVV2	578	324	0.04%	0.004%
43	6.690	1754	1757	1759	rVB2	629	340	0.04%	0.004%
44	6.735	1767	1771	1773	rBV3	489	387	0.05%	0.005%
45	6.866	1809	1812	1815	rBV	520	338	0.04%	0.004%
46	6.921	1815	1829	1855	rBV2	84105	174383	21.51%	2.256%
47	7.140	1894	1897	1899	rBV3	600	401	0.05%	0.005%
48	7.249	1919	1931	1951	rBV	292980	522971	64.52%	6.765%
49	7.493	2002	2007	2011	rVB5	589	624	0.08%	0.008%
50	7.561	2019	2028	2050	rBV	62263	126186	15.57%	1.632%
51	7.760	2085	2090	2091	rBV3	401	288	0.04%	0.004%
52	7.776	2093	2095	2098	rVB4	717	377	0.05%	0.005%
53	7.799	2098	2102	2104	rBV2	463	422	0.05%	0.005%
54	7.834	2108	2113	2115	rBV3	676	596	0.07%	0.008%
55	7.889	2125	2130	2131	rBV2	593	500	0.06%	0.006%
56	8.050	2167	2180	2204	rBV2	160023	403413	49.77%	5.218%
57	8.378	2280	2282	2283	rBV2	768	342	0.04%	0.004%
58	8.513	2321	2324	2329	rVB4	782	631	0.08%	0.008%
59	8.590	2346	2348	2350	rBV2	633	351	0.04%	0.005%
60	8.628	2358	2360	2366	rVB4	520	339	0.04%	0.004%
61	8.725	2388	2390	2397	rBV5	629	614	0.08%	0.008%
62	8.792	2399	2411	2434	rBV	443663	770230	95.02%	9.963%
63	9.037	2485	2487	2493	rVB3	600	444	0.05%	0.006%
64	9.091	2500	2504	2511	rVB4	1396	1445	0.18%	0.019%
65	9.223	2540	2545	2547	rBV3	579	519	0.06%	0.007%
66	9.310	2566	2572	2573	rBV2	559	385	0.05%	0.005%
67	9.378	2589	2593	2594	rBV2	356	302	0.04%	0.004%
68	9.397	2594	2599	2600	rBV3	412	366	0.05%	0.005%
69	9.461	2617	2619	2623	rVB2	468	313	0.04%	0.004%
70	9.487	2623	2627	2628	rBV3	919	650	0.08%	0.008%
71	9.622	2663	2669	2673	rBV2	1180	1511	0.19%	0.020%
72	9.654	2673	2679	2687	rVB8	2062	3017	0.37%	0.039%
73	9.738	2700	2705	2712	rVV5	2002	2821	0.35%	0.036%
74	9.796	2716	2723	2730	rVB5	1361	1943	0.24%	0.025%
75	9.956	2768	2773	2778	rBV4	975	1291	0.16%	0.017%
76	10.165	2816	2838	2854	rBV	298360	499227	61.59%	6.458%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
A46G1ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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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	10.259	2865	2867	2870	rBV2	430	355	0.04%	0.005%
78	10.332	2883	2890	2897	rVV3	4235	5625	0.69%	0.073%
79	10.361	2897	2899	2902	rVB3	548	275	0.03%	0.004%
80	10.394	2902	2909	2916	rVB8	1698	2377	0.29%	0.031%
81	10.455	2916	2928	2933	rBV6	3085	4356	0.54%	0.056%
82	10.615	2976	2978	2981	rBV3	710	518	0.06%	0.007%
83	10.660	2987	2992	2995	rBV5	1191	1057	0.13%	0.014%
84	10.680	2996	2998	3002	rVV4	618	518	0.06%	0.007%
85	10.750	3017	3020	3023	rBV3	687	469	0.06%	0.006%
86	10.773	3023	3027	3030	rVB4	1109	935	0.12%	0.012%
87	10.824	3035	3043	3044	rBV3	1861	1689	0.21%	0.022%
88	10.943	3078	3080	3083	rBV3	476	362	0.04%	0.005%
89	10.972	3083	3089	3091	rBV4	2166	2070	0.26%	0.027%
90	11.098	3121	3128	3134	rVB8	4263	5975	0.74%	0.077%
91	11.136	3135	3140	3146	rVB8	1967	2493	0.31%	0.032%
92	11.194	3147	3158	3177	rBV	521462	810557	100.00%	10.485%
93	11.400	3220	3222	3223	rBV2	796	262	0.03%	0.003%
94	11.480	3243	3247	3249	rBV4	1641	1312	0.16%	0.017%
95	11.570	3261	3275	3293	rBV	398329	632976	78.09%	8.188%
96	12.316	3498	3507	3520	rBV	10808	26415	3.26%	0.342%
97	12.413	3531	3537	3545	rBV9	7233	10809	1.33%	0.140%
98	13.217	3779	3787	3793	rBV9	6834	11471	1.42%	0.148%
99	16.397	4765	4776	4791	rBV	456901	701920	86.60%	9.079%
100	17.480	5104	5113	5126	rVB2	102572	179184	22.11%	2.318%

Sum of corrected areas: 7730849

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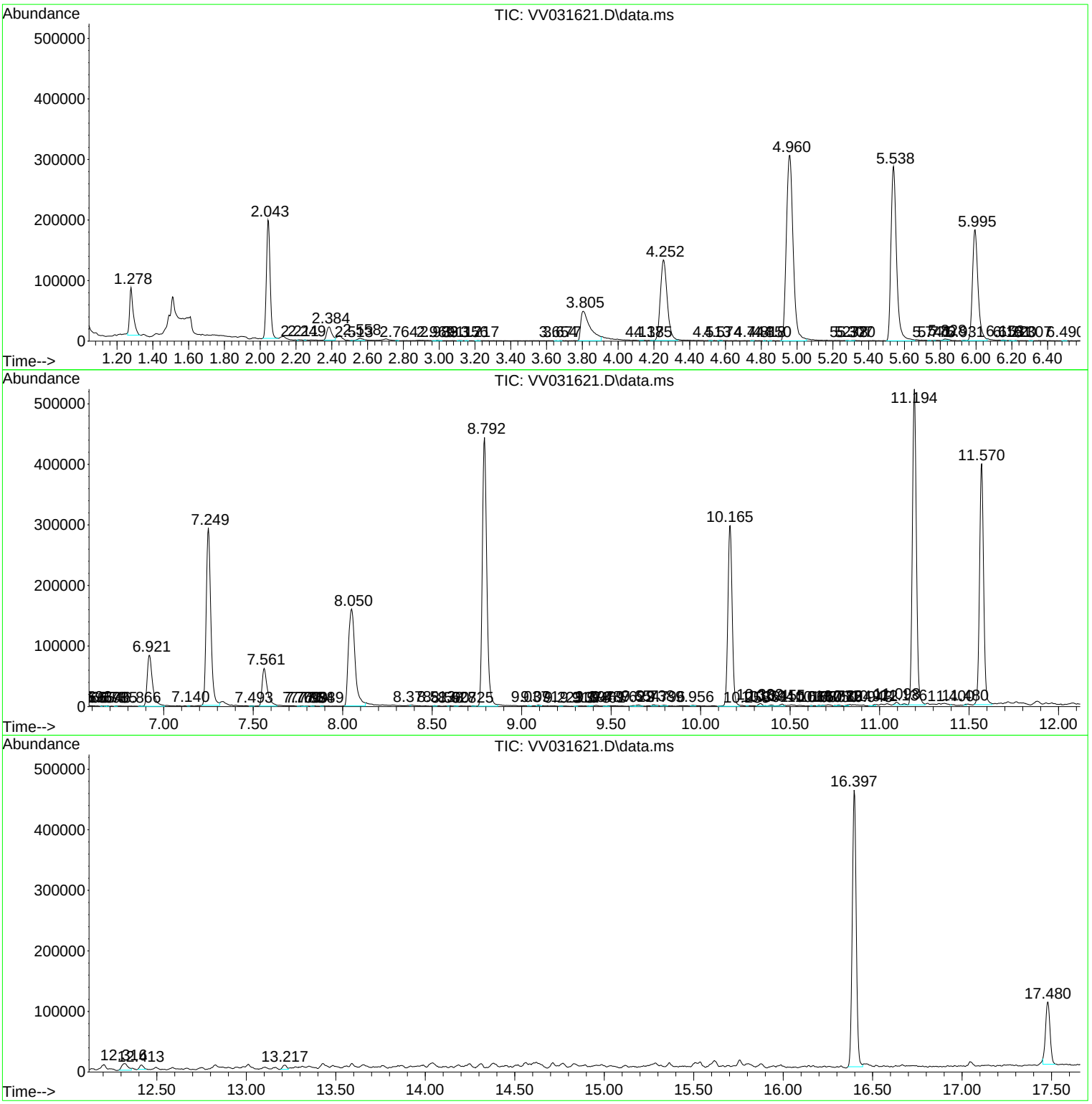
ClientSampleId :
A46G1ME

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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MSVOA_V
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A46G1ME

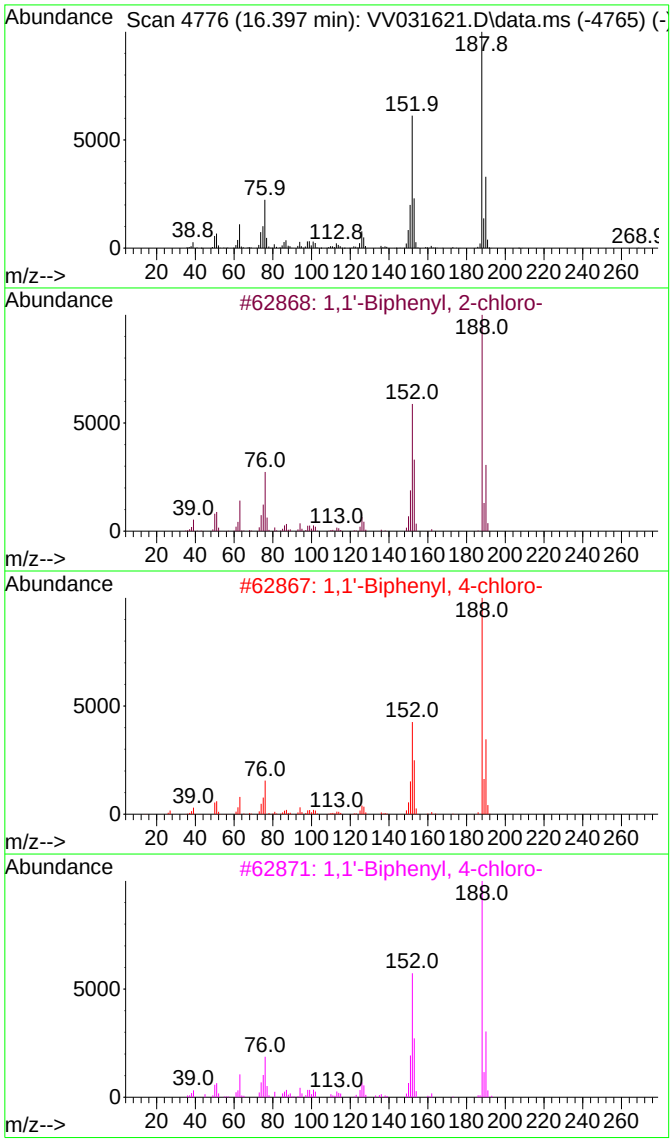
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

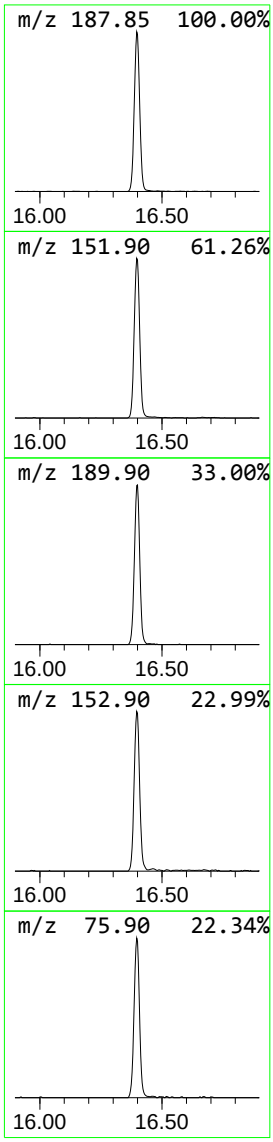
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	43.30 ug/L	701920	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	97
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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A46G1ME

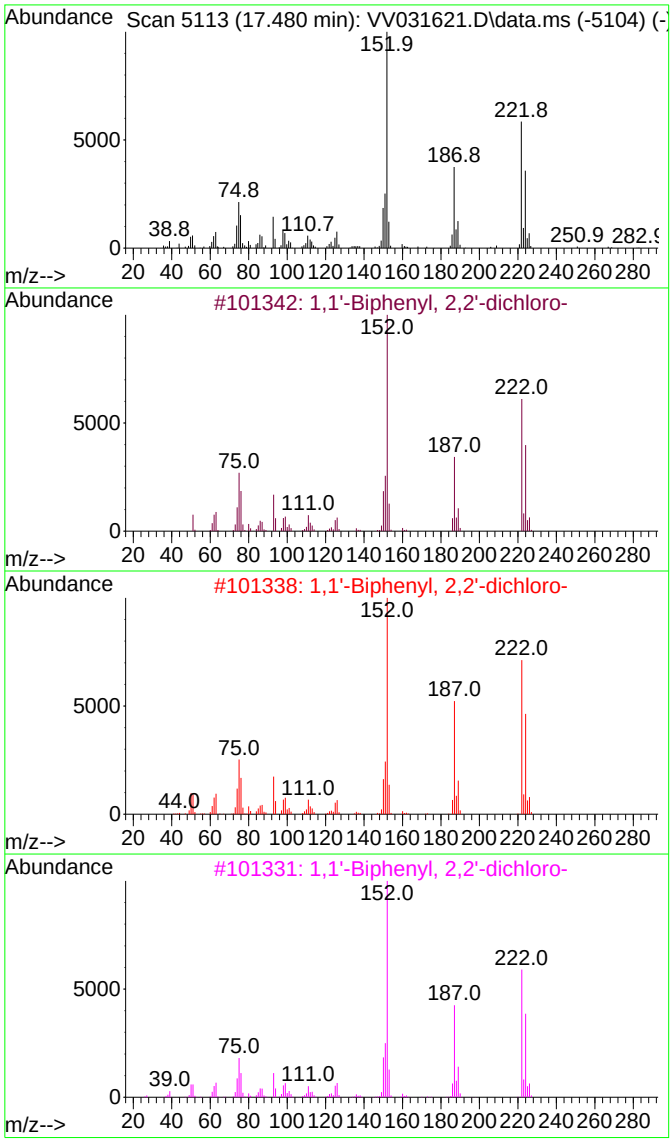
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

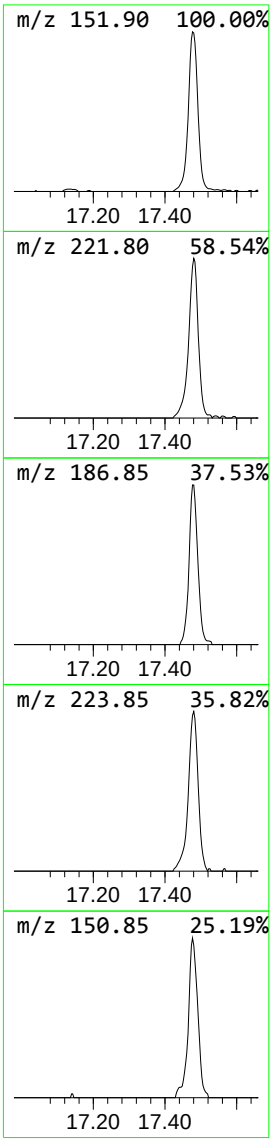
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	11.05 ug/L	179184	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, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98





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	43.3	ug/L	701920	3	11.194	810557	50.0
1,1'-Biphenyl, ...	17.480	11.1	ug/L	179184	3	11.194	810557	50.0