

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
 Data File : VV031635.D
 Acq On : 03 Jul 2023 14:17
 Operator : SY/MD
 Sample : 03452-21ME
 Misc : 4.59g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46Q0ME

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: VV031635.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	69	74	91	rVB	70159	98104	12.68%	1.504%
2	2.047	304	313	328	rVB	172031	248644	32.15%	3.813%
3	2.384	410	418	431	rBV2	20827	35651	4.61%	0.547%
4	2.796	543	546	548	rVB2	548	284	0.04%	0.004%
5	2.822	550	554	556	rBV	328	263	0.03%	0.004%
6	2.892	568	576	582	rBV5	1107	1827	0.24%	0.028%
7	3.040	619	622	626	rVB3	514	356	0.05%	0.005%
8	3.063	626	629	633	rVB2	404	293	0.04%	0.004%
9	3.134	648	651	653	rBV2	256	185	0.02%	0.003%
10	3.256	687	689	692	rVB2	361	144	0.02%	0.002%
11	3.275	692	695	698	rVB	289	225	0.03%	0.003%
12	3.294	698	701	704	rBV2	332	222	0.03%	0.003%
13	3.317	704	708	714	rVB2	351	288	0.04%	0.004%
14	3.371	721	725	729	rBV4	504	491	0.06%	0.008%
15	3.433	740	744	746	rBV2	295	248	0.03%	0.004%
16	3.558	778	783	789	rVB3	403	389	0.05%	0.006%
17	3.580	789	790	793	rBV2	405	174	0.02%	0.003%
18	3.635	804	807	811	rBV2	240	211	0.03%	0.003%
19	3.670	816	818	821	rVB	324	175	0.02%	0.003%
20	3.693	821	825	826	rBV	445	334	0.04%	0.005%
21	3.806	850	860	893	rBV2	54381	190325	24.61%	2.919%
22	4.166	970	972	973	rBV	373	158	0.02%	0.002%
23	4.252	985	999	1031	rVB2	124661	324828	42.00%	4.981%
24	4.490	1071	1073	1076	rBV2	519	273	0.04%	0.004%
25	4.574	1097	1099	1102	rBV2	374	273	0.04%	0.004%
26	4.641	1118	1120	1121	rBV2	325	142	0.02%	0.002%
27	4.815	1166	1174	1179	rBV4	421	562	0.07%	0.009%
28	4.960	1202	1219	1251	rBV2	287608	755057	97.62%	11.579%
29	5.204	1293	1295	1298	rBV2	289	222	0.03%	0.003%
30	5.288	1318	1321	1324	rBV3	361	221	0.03%	0.003%
31	5.323	1328	1332	1334	rBV2	433	240	0.03%	0.004%
32	5.336	1334	1336	1339	rVB2	357	178	0.02%	0.003%
33	5.371	1345	1347	1351	rVB2	287	209	0.03%	0.003%
34	5.391	1351	1353	1354	rBV	417	159	0.02%	0.002%
35	5.539	1386	1399	1427	rBV	273219	578413	74.78%	8.870%
36	5.834	1482	1491	1507	rVB4	5041	10641	1.38%	0.163%

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 Title : VOC Analysis

37	5.892	1507	1509	1513	rVB2	602	362	0.05%	0.006%
38	5.931	1518	1521	1523	rBV2	363	237	0.03%	0.004%
39	5.995	1527	1541	1562	rBV	174557	371452	48.02%	5.696%
40	6.211	1605	1608	1613	rVB2	383	280	0.04%	0.004%
41	6.239	1613	1617	1618	rBV	280	161	0.02%	0.002%
42	6.313	1637	1640	1641	rBV	248	153	0.02%	0.002%
43	6.323	1641	1643	1647	rVB3	449	182	0.02%	0.003%
44	6.346	1647	1650	1653	rBV2	317	197	0.03%	0.003%
45	6.387	1660	1663	1666	rVB	308	184	0.02%	0.003%
46	6.407	1666	1669	1670	rBV	284	184	0.02%	0.003%
47	6.429	1674	1676	1678	rBV2	332	191	0.02%	0.003%
48	6.445	1678	1681	1691	rVV5	338	524	0.07%	0.008%
49	6.577	1716	1722	1724	rBV3	751	600	0.08%	0.009%
50	6.683	1752	1755	1760	rVB3	440	303	0.04%	0.005%
51	6.719	1760	1766	1768	rBV2	661	666	0.09%	0.010%
52	6.744	1772	1774	1778	rBV	328	210	0.03%	0.003%
53	6.844	1803	1805	1810	rBV3	430	414	0.05%	0.006%
54	6.921	1813	1829	1855	rBV	85848	167912	21.71%	2.575%
55	7.079	1875	1878	1882	rBV3	627	389	0.05%	0.006%
56	7.127	1891	1893	1897	rBV2	477	299	0.04%	0.005%
57	7.182	1905	1910	1911	rBV3	681	489	0.06%	0.007%
58	7.249	1920	1931	1953	rBV	278054	490908	63.47%	7.528%
59	7.561	2018	2028	2058	rBV	59867	122280	15.81%	1.875%
60	7.690	2065	2068	2070	rBV2	686	408	0.05%	0.006%
61	7.792	2098	2100	2103	rBV	419	152	0.02%	0.002%
62	7.998	2162	2164	2166	rBV2	373	205	0.03%	0.003%
63	8.043	2167	2178	2206	rBV	192568	432973	55.98%	6.640%
64	8.571	2340	2342	2343	rBV	411	154	0.02%	0.002%
65	8.600	2348	2351	2354	rBV2	614	303	0.04%	0.005%
66	8.792	2399	2411	2439	rBV	422427	712750	92.15%	10.930%
67	8.995	2472	2474	2478	rVB3	648	332	0.04%	0.005%
68	9.014	2478	2480	2483	rBV3	392	224	0.03%	0.003%
69	9.030	2483	2485	2489	rVV4	345	238	0.03%	0.004%
70	9.066	2494	2496	2499	rBV2	328	182	0.02%	0.003%
71	9.082	2499	2501	2503	rBV	509	315	0.04%	0.005%
72	9.181	2531	2532	2534	rBV	330	148	0.02%	0.002%
73	9.516	2634	2636	2639	rBV2	382	197	0.03%	0.003%
74	9.850	2737	2740	2744	rBV3	739	601	0.08%	0.009%
75	9.870	2744	2746	2749	rBV3	472	321	0.04%	0.005%
76	9.902	2754	2756	2760	rBV3	535	324	0.04%	0.005%

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 Title : VOC Analysis

77	9.963	2772	2775	2779	rBV3	259	242	0.03%	0.004%
78	10.162	2824	2837	2859	rBV	298985	479140	61.95%	7.348%
79	10.288	2873	2876	2880	rBV4	694	439	0.06%	0.007%
80	10.323	2884	2887	2888	rBV	739	390	0.05%	0.006%
81	10.419	2915	2917	2920	rVB	415	140	0.02%	0.002%
82	10.542	2952	2955	2956	rBV	408	177	0.02%	0.003%
83	10.603	2970	2974	2976	rBV2	353	323	0.04%	0.005%
84	10.644	2985	2987	2991	rBV3	468	274	0.04%	0.004%
85	10.747	3016	3019	3021	rBV2	316	225	0.03%	0.003%
86	10.789	3030	3032	3036	rVV2	318	260	0.03%	0.004%
87	10.812	3036	3039	3041	rVB3	303	193	0.02%	0.003%
88	10.972	3087	3089	3090	rBV	363	142	0.02%	0.002%
89	11.194	3145	3158	3184	rBV	499277	773478	100.00%	11.862%
90	11.419	3227	3228	3230	rBV2	325	139	0.02%	0.002%
91	11.484	3245	3248	3250	rBV	554	307	0.04%	0.005%
92	11.570	3263	3275	3289	rBV	382974	598579	77.39%	9.179%
93	12.014	3409	3413	3414	rBV2	461	361	0.05%	0.006%
94	12.519	3568	3570	3575	rVB3	606	381	0.05%	0.006%
95	12.734	3635	3637	3640	rBV2	713	458	0.06%	0.007%
96	12.754	3640	3643	3646	rBV4	718	525	0.07%	0.008%
97	12.841	3663	3670	3675	rBV5	995	1356	0.18%	0.021%
98	13.249	3795	3797	3799	rBV2	441	217	0.03%	0.003%
99	13.998	4018	4030	4034	rBV5	2194	4029	0.52%	0.062%
100	16.397	4768	4776	4789	rBV2	66473	100310	12.97%	1.538%

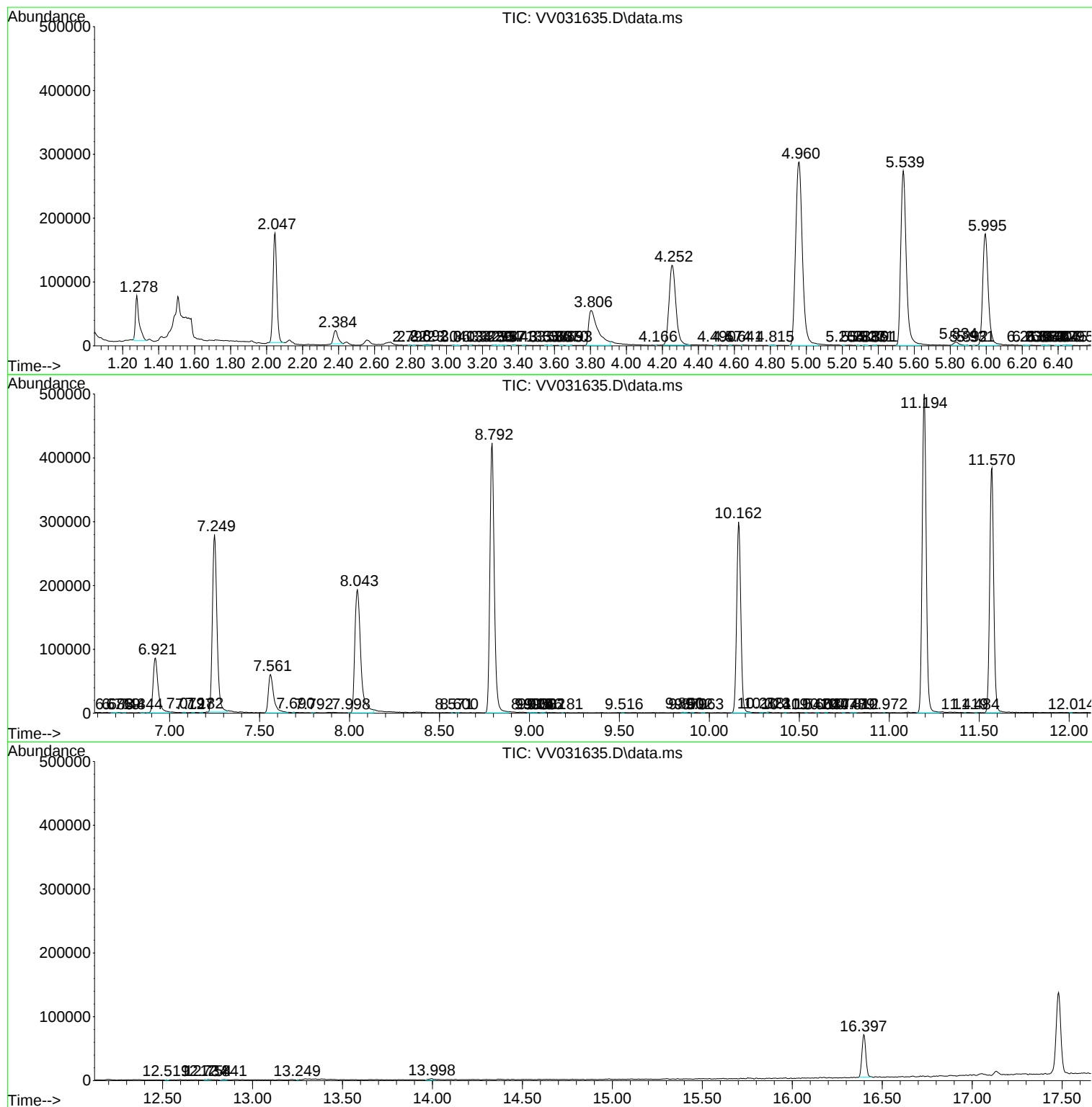
Sum of corrected areas: 6520898

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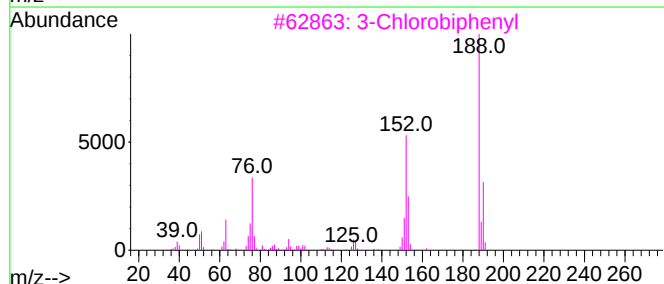
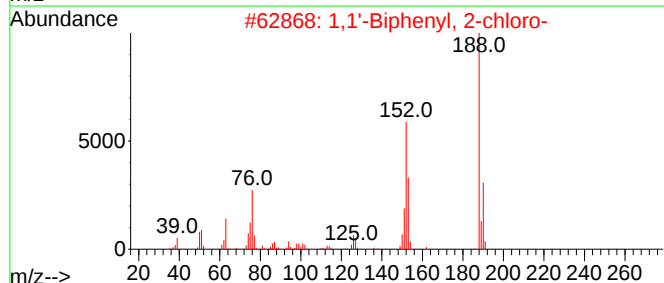
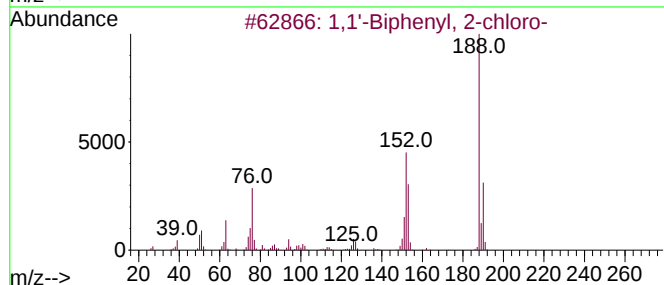
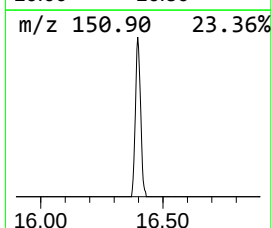
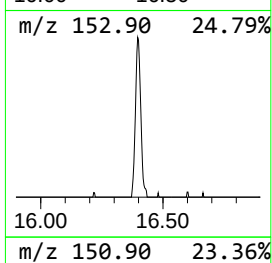
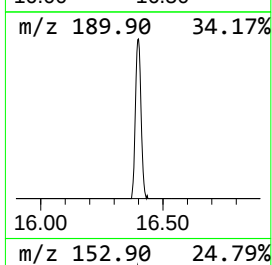
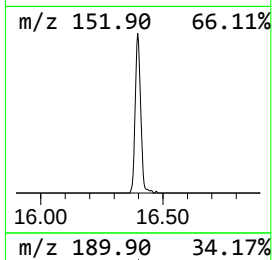
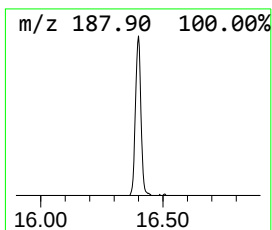
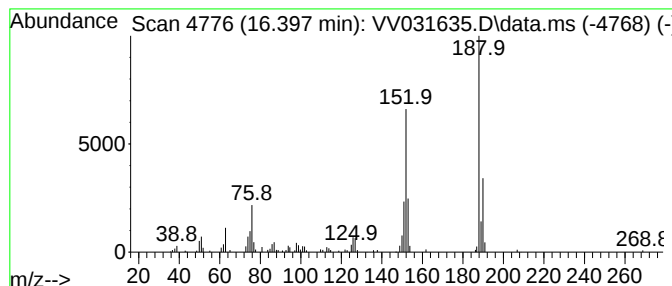
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	6.48 ug/L	100310	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, 2-chloro-	188	C12H9Cl	002051-60-7	97
3			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
4			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
5			1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	6.5	ug/L	100310	3	11.194	773478	50.0