

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062923\
 Data File : VV031618.D
 Acq On : 29 Jun 2023 13:38
 Operator : SY/MD
 Sample : 03422-20ME
 Misc : 4.32g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46L7ME

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: VV031618.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	87849	118364	14.52%	1.707%
2	2.047	304	313	330	rVB	199232	286555	35.15%	4.133%
3	2.381	409	417	429	rBV	22583	41158	5.05%	0.594%
4	2.831	554	557	559	rBV2	278	197	0.02%	0.003%
5	2.850	559	563	565	rVV2	473	277	0.03%	0.004%
6	2.973	599	601	603	rVB	293	121	0.01%	0.002%
7	3.014	612	614	615	rBV	320	134	0.02%	0.002%
8	3.124	646	648	652	rBV3	246	131	0.02%	0.002%
9	3.223	677	679	680	rBV	210	89	0.01%	0.001%
10	3.249	685	687	688	rBV	231	84	0.01%	0.001%
11	3.294	699	701	706	rVB3	365	266	0.03%	0.004%
12	3.326	708	711	712	rBV3	377	178	0.02%	0.003%
13	3.359	720	721	722	rBV3	248	88	0.01%	0.001%
14	3.368	722	724	728	rVB3	502	266	0.03%	0.004%
15	3.400	729	734	737	rBV3	370	262	0.03%	0.004%
16	3.439	743	746	748	rBV2	510	333	0.04%	0.005%
17	3.481	754	759	762	rBV2	399	342	0.04%	0.005%
18	3.497	762	764	766	rVB2	367	151	0.02%	0.002%
19	3.513	766	769	773	rBV2	254	231	0.03%	0.003%
20	3.571	782	787	792	rBV	372	396	0.05%	0.006%
21	3.600	792	796	799	rBV3	472	344	0.04%	0.005%
22	3.651	810	812	815	rBV2	338	180	0.02%	0.003%
23	3.690	819	824	825	rBV2	448	345	0.04%	0.005%
24	3.744	839	841	843	rBV	371	163	0.02%	0.002%
25	3.760	843	846	847	rBV2	147	67	0.01%	0.001%
26	3.802	849	859	902	rBV2	50097	182138	22.34%	2.627%
27	4.252	983	999	1026	rBV	135421	355116	43.56%	5.122%
28	4.522	1080	1083	1086	rVB2	654	363	0.04%	0.005%
29	4.622	1111	1114	1117	rVB	522	349	0.04%	0.005%
30	4.645	1117	1121	1125	rBV2	449	492	0.06%	0.007%
31	4.680	1131	1132	1134	rVB	319	66	0.01%	0.001%
32	4.860	1184	1188	1190	rBV3	553	382	0.05%	0.006%
33	4.899	1199	1200	1202	rVB	281	104	0.01%	0.001%
34	4.960	1202	1219	1253	rBV2	310443	815210	100.00%	11.757%
35	5.227	1297	1302	1305	rBV3	410	423	0.05%	0.006%
36	5.284	1318	1320	1322	rBV3	326	177	0.02%	0.003%

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

37	5.310	1326	1328	1329	rBV	264	112	0.01%	0.002%
38	5.346	1337	1339	1341	rBV2	264	115	0.01%	0.002%
39	5.468	1373	1377	1378	rBV3	514	239	0.03%	0.003%
40	5.481	1378	1381	1386	rVB3	471	368	0.05%	0.005%
41	5.538	1386	1399	1422	rBV	291760	608859	74.69%	8.781%
42	5.915	1515	1516	1517	rBV	290	98	0.01%	0.001%
43	5.940	1522	1524	1527	rBV2	348	183	0.02%	0.003%
44	5.995	1528	1541	1570	rVV	187213	398865	48.93%	5.753%
45	6.204	1604	1606	1610	rVB4	581	386	0.05%	0.006%
46	6.243	1615	1618	1619	rBV2	475	286	0.04%	0.004%
47	6.268	1624	1626	1628	rVB2	433	198	0.02%	0.003%
48	6.291	1628	1633	1636	rBV3	674	675	0.08%	0.010%
49	6.323	1641	1643	1644	rBV3	286	97	0.01%	0.001%
50	6.378	1657	1660	1661	rBV2	359	181	0.02%	0.003%
51	6.439	1676	1679	1682	rBV2	373	262	0.03%	0.004%
52	6.455	1682	1684	1687	rVB3	328	200	0.02%	0.003%
53	6.493	1694	1696	1698	rBV	260	126	0.02%	0.002%
54	6.503	1698	1699	1703	rVV3	340	237	0.03%	0.003%
55	6.519	1703	1704	1707	rVV	326	148	0.02%	0.002%
56	6.558	1714	1716	1717	rBV	234	92	0.01%	0.001%
57	6.577	1717	1722	1726	rBV4	1008	1092	0.13%	0.016%
58	6.635	1737	1740	1743	rVB4	502	396	0.05%	0.006%
59	6.651	1743	1745	1746	rBV4	291	124	0.02%	0.002%
60	6.728	1766	1769	1772	rBV2	476	295	0.04%	0.004%
61	6.834	1793	1802	1805	rBV2	477	559	0.07%	0.008%
62	6.870	1811	1813	1817	rVB2	355	151	0.02%	0.002%
63	6.918	1817	1828	1848	rBV	88028	171964	21.09%	2.480%
64	7.085	1878	1880	1881	rBV2	428	206	0.03%	0.003%
65	7.249	1920	1931	1952	rBV	297664	518499	63.60%	7.478%
66	7.561	2018	2028	2058	rBV	63342	126768	15.55%	1.828%
67	7.725	2074	2079	2082	rBV4	669	599	0.07%	0.009%
68	7.796	2099	2101	2105	rVB2	425	262	0.03%	0.004%
69	7.815	2105	2107	2111	rVB2	530	425	0.05%	0.006%
70	7.837	2111	2114	2116	rBV2	414	234	0.03%	0.003%
71	7.969	2152	2155	2156	rBV	205	120	0.01%	0.002%
72	8.043	2166	2178	2209	rBV	178236	408519	50.11%	5.892%
73	8.493	2312	2318	2323	rBV4	783	834	0.10%	0.012%
74	8.638	2357	2363	2366	rBV2	657	770	0.09%	0.011%
75	8.731	2390	2392	2394	rBV2	532	280	0.03%	0.004%
76	8.792	2399	2411	2444	rVV	448165	761852	93.45%	10.988%

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 Title : VOC Analysis

77	9.226	2544	2546	2548	rBV2	400	184	0.02%	0.003%
78	9.310	2568	2572	2574	rBV	303	251	0.03%	0.004%
79	9.410	2600	2603	2605	rBV2	177	109	0.01%	0.002%
80	9.445	2612	2614	2618	rVB	493	226	0.03%	0.003%
81	9.484	2624	2626	2629	rBV2	676	362	0.04%	0.005%
82	9.542	2640	2644	2648	rBV4	525	501	0.06%	0.007%
83	9.590	2657	2659	2661	rBV2	433	167	0.02%	0.002%
84	9.696	2690	2692	2694	rBV	428	203	0.02%	0.003%
85	9.786	2717	2720	2721	rBV2	435	222	0.03%	0.003%
86	9.824	2728	2732	2736	rBV2	302	364	0.04%	0.005%
87	9.879	2745	2749	2752	rBV	627	593	0.07%	0.009%
88	9.911	2757	2759	2760	rBV	389	156	0.02%	0.002%
89	9.966	2775	2776	2778	rBV	257	128	0.02%	0.002%
90	10.066	2804	2807	2810	rBV2	379	211	0.03%	0.003%
91	10.162	2825	2837	2855	rBV	303997	490790	60.20%	7.078%
92	10.329	2883	2889	2892	rBV3	1376	1600	0.20%	0.023%
93	10.734	3012	3015	3017	rBV	431	306	0.04%	0.004%
94	10.908	3066	3069	3074	rBV4	731	645	0.08%	0.009%
95	11.075	3119	3121	3123	rBV2	514	289	0.04%	0.004%
96	11.120	3133	3135	3136	rBV	468	160	0.02%	0.002%
97	11.194	3146	3158	3181	rBV	499861	782333	95.97%	11.283%
98	11.567	3263	3274	3291	rBV	384459	605621	74.29%	8.735%
99	12.442	3542	3546	3550	rBV3	628	548	0.07%	0.008%
100	16.397	4767	4776	4792	rVB	156296	236425	29.00%	3.410%

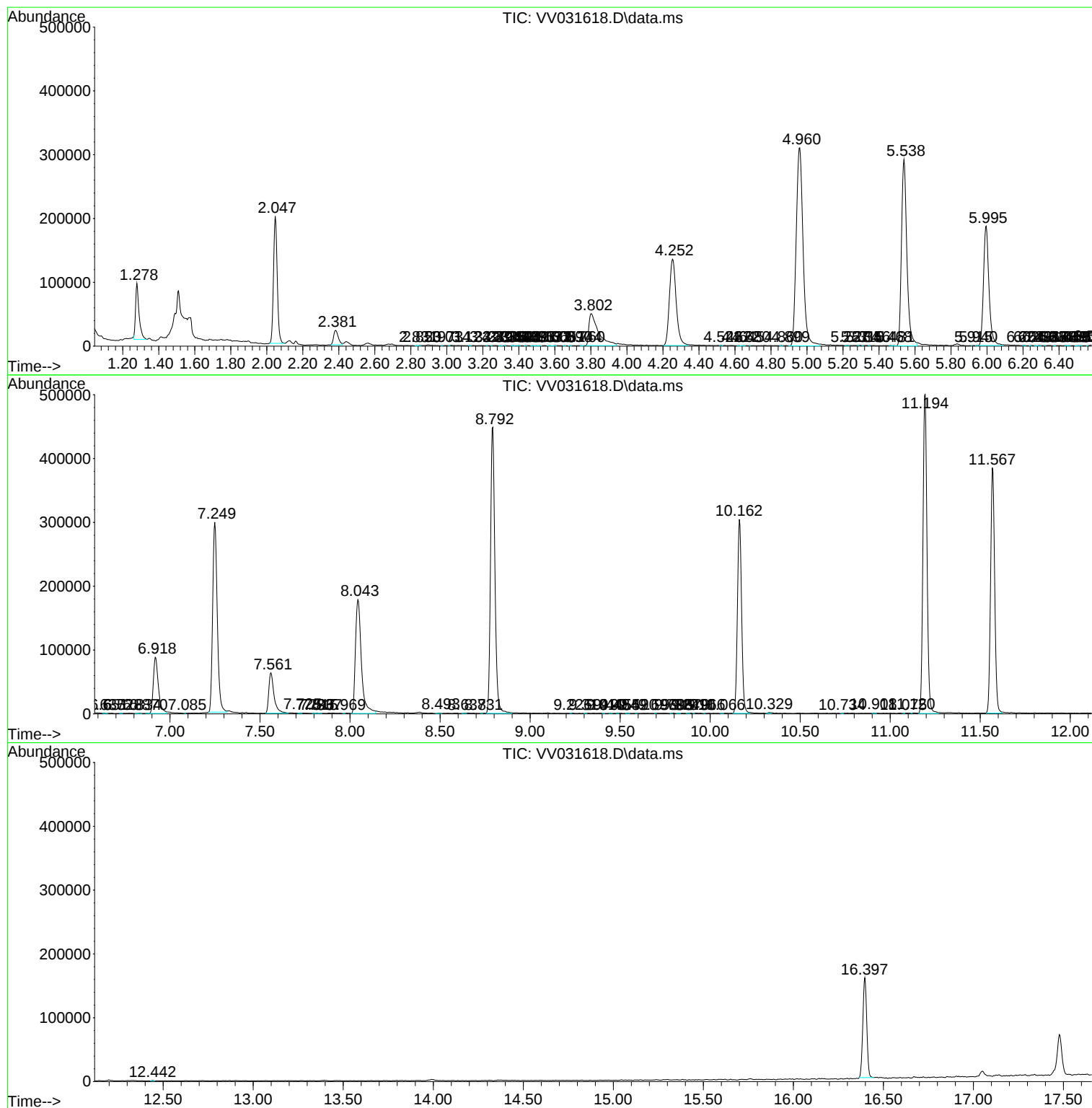
Sum of corrected areas: 6933612

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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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MSVOA_V
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A46L7ME

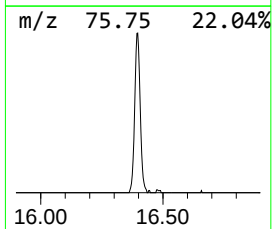
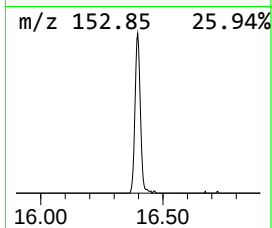
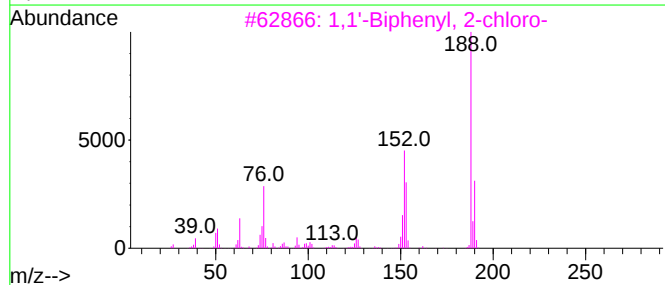
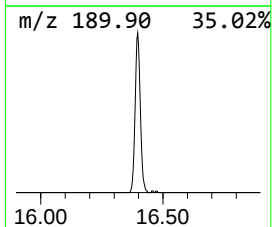
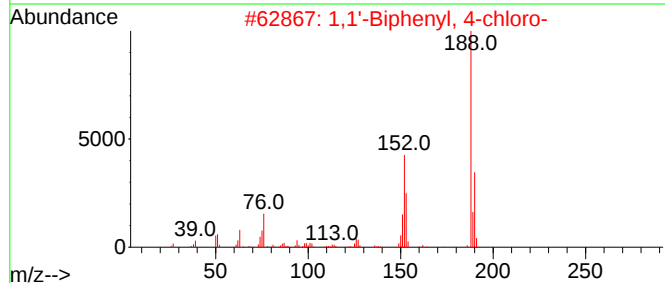
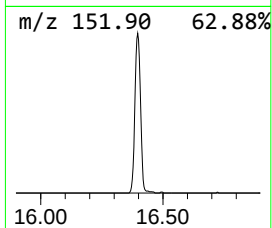
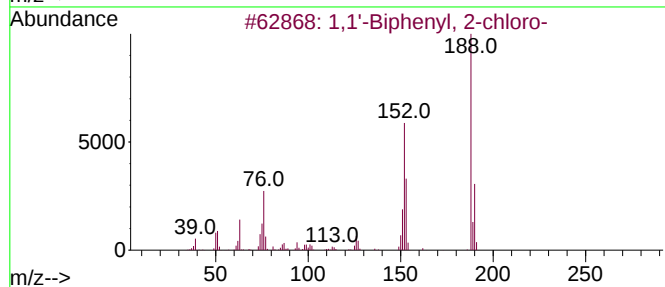
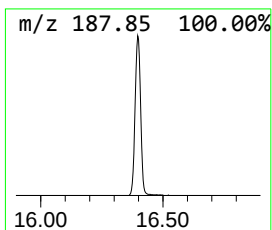
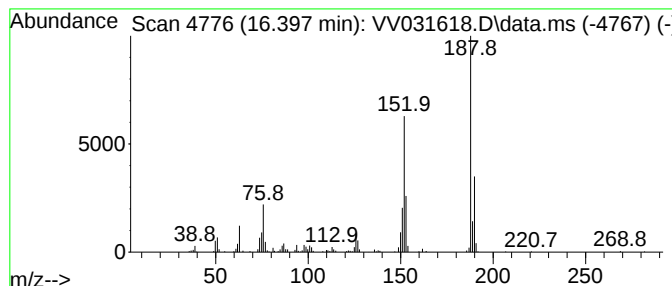
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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	15.11 ug/L	236425	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	98
2	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	96
3	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	94
4	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	94
5	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	15.1	ug/L	236425	3	11.194	782333	50.0