

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
 Data File : VV031639.D
 Acq On : 03 Jul 2023 16:02
 Operator : SY/MD
 Sample : 03472-22ME
 Misc : 4.03g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46R3ME

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: VV031639.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	92885	103680	12.31%	1.554%
2	1.532	147	153	170	rVB	94512	114320	13.57%	1.714%
3	2.063	308	318	332	rBV	174179	253256	30.06%	3.796%
4	2.336	401	403	405	rVB	500	205	0.02%	0.003%
5	2.452	430	439	450	rBV2	5201	8391	1.00%	0.126%
6	2.500	452	454	458	rVB4	470	249	0.03%	0.004%
7	2.606	484	487	490	rBV	393	239	0.03%	0.004%
8	2.629	490	494	495	rBV2	331	218	0.03%	0.003%
9	2.799	543	547	550	rBV	497	363	0.04%	0.005%
10	2.867	564	568	570	rBV2	302	228	0.03%	0.003%
11	2.931	586	588	591	rBV2	307	158	0.02%	0.002%
12	3.024	615	617	621	rBV2	218	176	0.02%	0.003%
13	3.060	624	628	631	rBV2	293	271	0.03%	0.004%
14	3.143	653	654	660	rVB	233	175	0.02%	0.003%
15	3.191	664	669	672	rBV2	379	326	0.04%	0.005%
16	3.343	713	716	720	rVB2	459	240	0.03%	0.004%
17	3.365	720	723	727	rBV2	240	165	0.02%	0.002%
18	3.445	746	748	751	rVV2	421	208	0.02%	0.003%
19	3.545	776	779	781	rVV	325	160	0.02%	0.002%
20	3.584	783	791	792	rBV2	328	301	0.04%	0.005%
21	3.661	812	815	818	rBV2	289	237	0.03%	0.004%
22	3.712	828	831	836	rVB	354	221	0.03%	0.003%
23	3.738	836	839	841	rBV	518	261	0.03%	0.004%
24	3.793	846	856	890	rBV	83952	227204	26.97%	3.406%
25	4.259	983	1001	1029	rBV2	143098	371577	44.11%	5.570%
26	4.552	1091	1092	1096	rVB	307	159	0.02%	0.002%
27	4.571	1096	1098	1100	rBV	370	195	0.02%	0.003%
28	4.600	1105	1107	1113	rVB3	621	502	0.06%	0.008%
29	4.642	1113	1120	1121	rBV	351	330	0.04%	0.005%
30	4.806	1169	1171	1174	rVB2	390	211	0.03%	0.003%
31	4.844	1180	1183	1186	rBV2	366	242	0.03%	0.004%
32	4.963	1202	1220	1249	rBV2	312543	842470	100.00%	12.629%
33	5.275	1312	1317	1320	rBV5	574	714	0.08%	0.011%
34	5.407	1353	1358	1363	rBV3	701	562	0.07%	0.008%
35	5.439	1365	1368	1371	rBV2	318	263	0.03%	0.004%
36	5.474	1376	1379	1380	rBV	383	165	0.02%	0.002%

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 Title : VOC Analysis

37	5.542	1387	1400	1430	rBV	246002	512977	60.89%	7.690%
38	5.773	1470	1472	1473	rBV	415	193	0.02%	0.003%
39	5.908	1507	1514	1515	rBV3	714	641	0.08%	0.010%
40	5.995	1525	1541	1565	rBV	203346	424447	50.38%	6.363%
41	6.175	1594	1597	1601	rVB2	524	318	0.04%	0.005%
42	6.259	1619	1623	1624	rBV	305	190	0.02%	0.003%
43	6.381	1658	1661	1667	rBV3	474	347	0.04%	0.005%
44	6.416	1667	1672	1674	rVB2	330	271	0.03%	0.004%
45	6.503	1697	1699	1701	rBV2	257	164	0.02%	0.002%
46	6.539	1707	1710	1713	rBV3	298	236	0.03%	0.004%
47	6.706	1758	1762	1765	rBV3	413	359	0.04%	0.005%
48	6.744	1770	1774	1776	rVV3	310	203	0.02%	0.003%
49	6.777	1782	1784	1788	rBV2	314	244	0.03%	0.004%
50	6.809	1792	1794	1796	rVB	339	160	0.02%	0.002%
51	6.918	1817	1828	1849	rBV	93925	178979	21.24%	2.683%
52	7.195	1912	1914	1916	rVB	370	185	0.02%	0.003%
53	7.249	1920	1931	1967	rBV	298185	536651	63.70%	8.045%
54	7.558	2018	2027	2043	rBV	69972	125318	14.88%	1.879%
55	7.731	2079	2081	2084	rBV2	572	307	0.04%	0.005%
56	7.770	2091	2093	2095	rBV	449	264	0.03%	0.004%
57	7.918	2135	2139	2143	rBV3	804	680	0.08%	0.010%
58	7.985	2158	2160	2164	rBV2	271	186	0.02%	0.003%
59	8.031	2164	2174	2205	rBV	262398	479294	56.89%	7.185%
60	8.542	2331	2333	2339	rVB2	442	421	0.05%	0.006%
61	8.574	2339	2343	2349	rBV3	620	650	0.08%	0.010%
62	8.600	2349	2351	2358	rVB3	437	353	0.04%	0.005%
63	8.629	2358	2360	2362	rBV	344	162	0.02%	0.002%
64	8.680	2373	2376	2379	rBV3	402	296	0.04%	0.004%
65	8.793	2398	2411	2445	rVV	374749	635752	75.46%	9.530%
66	9.043	2487	2489	2492	rBV2	374	181	0.02%	0.003%
67	9.204	2535	2539	2546	rVB4	590	675	0.08%	0.010%
68	9.243	2546	2551	2554	rBV3	456	392	0.05%	0.006%
69	9.355	2583	2586	2590	rVB3	466	269	0.03%	0.004%
70	9.564	2646	2651	2652	rBV	372	286	0.03%	0.004%
71	9.596	2658	2661	2665	rBV2	206	175	0.02%	0.003%
72	9.616	2665	2667	2669	rBV	287	158	0.02%	0.002%
73	9.677	2684	2686	2692	rVB3	371	254	0.03%	0.004%
74	9.722	2698	2700	2702	rVB2	405	160	0.02%	0.002%
75	9.738	2702	2705	2707	rVB	365	213	0.03%	0.003%
76	9.809	2723	2727	2729	rBV	286	288	0.03%	0.004%

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 Title : VOC Analysis

77	9.873	2743	2747	2749	rBV	397	309	0.04%	0.005%
78	10.018	2789	2792	2794	rBV2	416	215	0.03%	0.003%
79	10.059	2802	2805	2810	rBV2	518	397	0.05%	0.006%
80	10.159	2824	2836	2854	rBV	321613	505932	60.05%	7.584%
81	10.304	2879	2881	2885	rBV3	339	259	0.03%	0.004%
82	10.365	2896	2900	2902	rBV3	350	272	0.03%	0.004%
83	10.481	2932	2936	2941	rBV3	463	517	0.06%	0.008%
84	10.529	2949	2951	2954	rBV2	330	203	0.02%	0.003%
85	10.596	2970	2972	2973	rBV	363	176	0.02%	0.003%
86	10.632	2980	2983	2985	rVB2	518	273	0.03%	0.004%
87	10.648	2985	2988	2992	rVB2	256	183	0.02%	0.003%
88	10.686	2997	3000	3003	rVV2	492	289	0.03%	0.004%
89	10.818	3038	3041	3046	rBV2	470	417	0.05%	0.006%
90	11.037	3105	3109	3110	rBV	437	295	0.04%	0.004%
91	11.191	3146	3157	3181	rBV	392306	607761	72.14%	9.111%
92	11.345	3203	3205	3212	rVB3	608	417	0.05%	0.006%
93	11.567	3263	3274	3300	rBV	370735	586739	69.65%	8.796%
94	11.709	3316	3318	3320	rBV2	491	241	0.03%	0.004%
95	12.014	3411	3413	3418	rBV2	453	256	0.03%	0.004%
96	12.477	3554	3557	3560	rBV2	554	445	0.05%	0.007%
97	12.763	3644	3646	3650	rBV2	649	425	0.05%	0.006%
98	12.857	3671	3675	3678	rBV2	424	389	0.05%	0.006%
99	13.156	3764	3768	3774	rBV2	633	782	0.09%	0.012%
100	16.397	4768	4776	4791	rVB	85285	131657	15.63%	1.974%

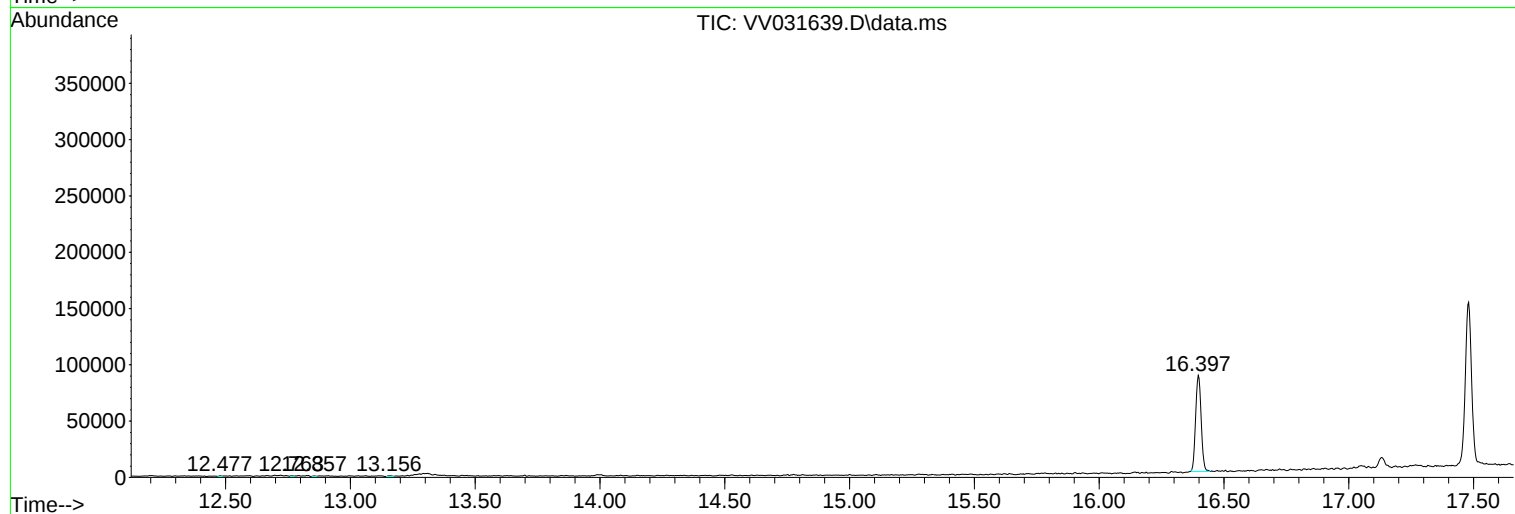
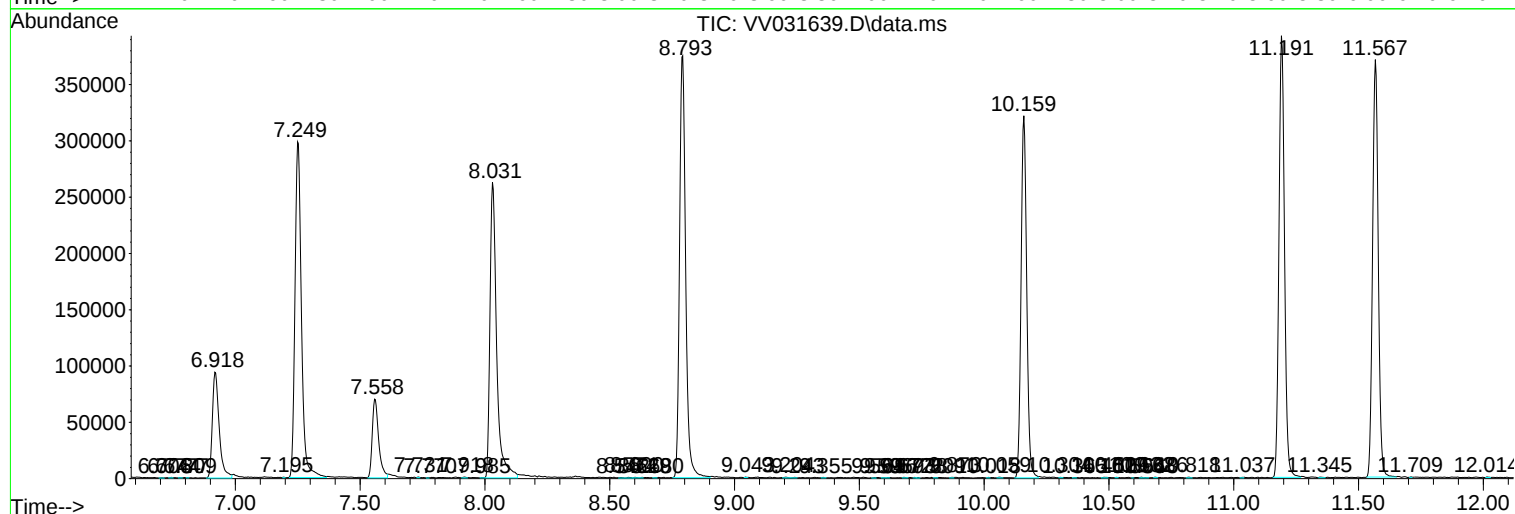
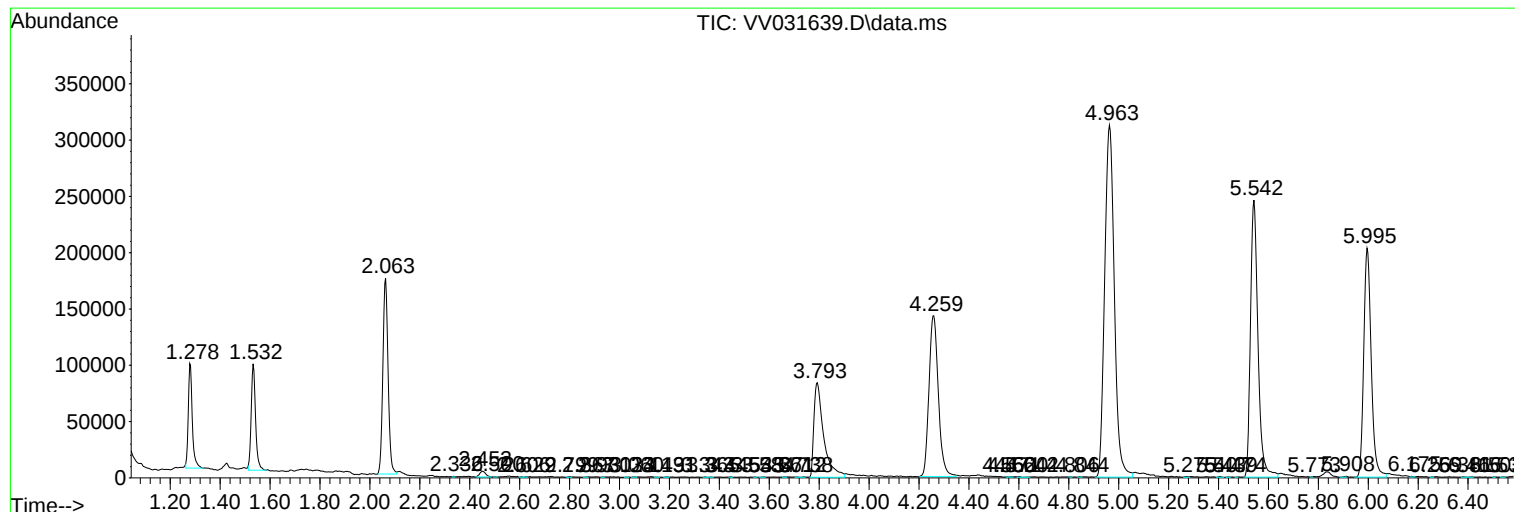
Sum of corrected areas: 6670790

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Instrument :
MSVOA_V
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A46R3ME

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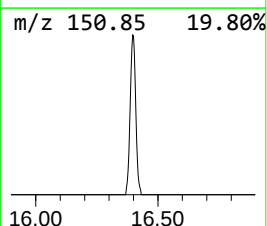
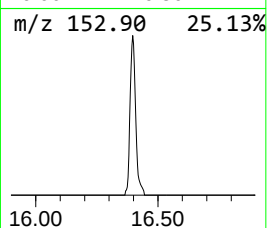
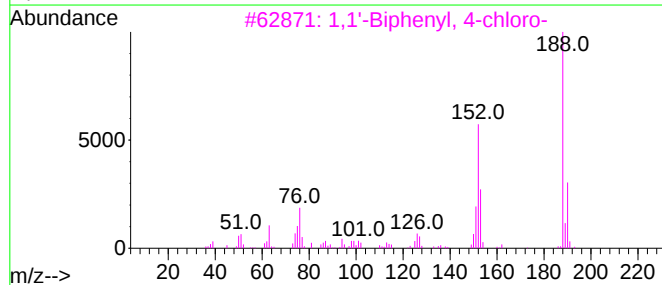
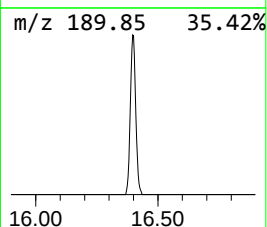
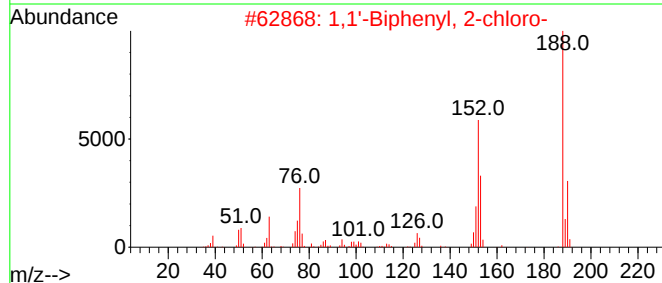
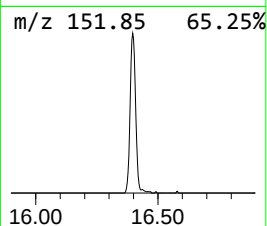
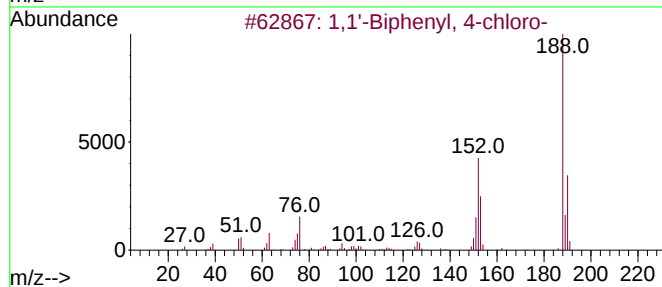
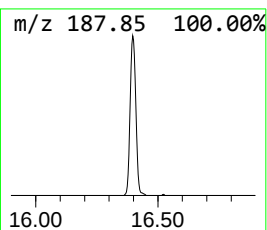
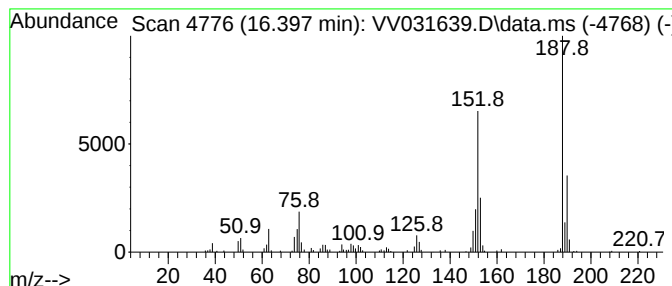
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	10.83 ug/L	131657	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	97
2	1,1'-Biphenyl, 2-chloro-			188	C12H9Cl	002051-60-7	97
3	1,1'-Biphenyl, 4-chloro-			188	C12H9Cl	002051-62-9	97
4	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	97
5	3-Chlorobiphenyl			188	C12H9Cl	002051-61-8	97



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, ...	16.397	10.8	ug/L	131657	3	11.191	607761	50.0