

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
 Data File : VV031640.D
 Acq On : 03 Jul 2023 16:28
 Operator : SY/MD
 Sample : 03472-13ME
 Misc : 4.68g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A46S5ME

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: VV031640.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	67	74	106	rVB2	74178	131755	11.21%	1.447%
2	2.037	300	310	327	rVB2	215720	344908	29.36%	3.788%
3	2.256	376	378	379	rBV	493	264	0.02%	0.003%
4	2.391	411	420	429	rBV2	8068	16986	1.45%	0.187%
5	2.439	430	435	449	rVB4	9469	16751	1.43%	0.184%
6	2.561	461	473	488	rBV2	9872	21143	1.80%	0.232%
7	2.690	503	513	525	rVB3	5886	11272	0.96%	0.124%
8	2.863	561	567	570	rBV5	353	382	0.03%	0.004%
9	2.934	584	589	590	rBV2	589	362	0.03%	0.004%
10	2.957	590	596	603	rVB6	1033	1617	0.14%	0.018%
11	3.108	630	643	654	rBV2	6992	15089	1.28%	0.166%
12	3.252	683	688	690	rBV2	626	499	0.04%	0.005%
13	3.326	709	711	716	rVV2	371	289	0.02%	0.003%
14	3.362	718	722	727	rVV	527	465	0.04%	0.005%
15	3.535	771	776	777	rBV2	354	241	0.02%	0.003%
16	3.667	813	817	822	rVB3	312	272	0.02%	0.003%
17	3.696	822	826	830	rBV3	315	308	0.03%	0.003%
18	3.812	845	862	898	rBV2	214139	601399	51.19%	6.606%
19	4.140	961	964	966	rBV3	507	262	0.02%	0.003%
20	4.252	982	999	1028	rBV	122459	327121	27.84%	3.593%
21	4.371	1033	1036	1037	rBV2	474	272	0.02%	0.003%
22	4.513	1060	1080	1099	rBV2	42054	110468	9.40%	1.213%
23	4.606	1107	1109	1113	rVB2	412	261	0.02%	0.003%
24	4.657	1120	1125	1128	rVB4	507	385	0.03%	0.004%
25	4.680	1128	1132	1136	rVB5	742	579	0.05%	0.006%
26	4.812	1167	1173	1175	rBV2	444	430	0.04%	0.005%
27	4.956	1200	1218	1244	rBV3	287955	743222	63.26%	8.163%
28	5.127	1267	1271	1272	rBV4	2752	1772	0.15%	0.019%
29	5.288	1319	1321	1324	rVB2	620	342	0.03%	0.004%
30	5.320	1329	1331	1337	rVB4	411	349	0.03%	0.004%
31	5.407	1350	1358	1367	rBV6	1162	1515	0.13%	0.017%
32	5.538	1384	1399	1425	rBV	281912	611488	52.05%	6.716%
33	5.754	1462	1466	1468	rBV2	358	331	0.03%	0.004%
34	5.837	1476	1492	1510	rBV6	37375	84857	7.22%	0.932%
35	5.940	1522	1524	1527	rBV2	519	373	0.03%	0.004%
36	5.995	1527	1541	1568	rVV	170461	372135	31.68%	4.087%

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Integrator: RTE

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

37	6.146	1585	1588	1592	rVB3	643	445	0.04%	0.005%
38	6.165	1592	1594	1596	rBV3	699	319	0.03%	0.004%
39	6.181	1596	1599	1602	rVB3	810	476	0.04%	0.005%
40	6.291	1631	1633	1636	rVB	571	279	0.02%	0.003%

41	6.381	1651	1661	1663	rBV4	1307	1538	0.13%	0.017%
42	6.461	1683	1686	1689	rBV	372	309	0.03%	0.003%
43	6.551	1709	1714	1715	rBV3	1082	893	0.08%	0.010%
44	6.583	1722	1724	1728	rVB3	586	376	0.03%	0.004%
45	6.638	1740	1741	1745	rBV2	364	268	0.02%	0.003%

46	6.763	1773	1780	1783	rBV6	826	916	0.08%	0.010%
47	6.780	1783	1785	1789	rBV2	455	361	0.03%	0.004%
48	6.808	1789	1794	1796	rBV4	860	753	0.06%	0.008%
49	6.921	1813	1829	1858	rBV2	82369	174694	14.87%	1.919%
50	7.088	1877	1881	1883	rBV3	1054	711	0.06%	0.008%

51	7.194	1905	1914	1919	rBV6	2199	3331	0.28%	0.037%
52	7.249	1919	1931	1950	rBV	280464	507413	43.19%	5.573%
53	7.400	1977	1978	1982	rVB3	771	387	0.03%	0.004%
54	7.484	2000	2004	2006	rBV4	615	432	0.04%	0.005%
55	7.500	2006	2009	2010	rBV3	951	561	0.05%	0.006%

56	7.561	2019	2028	2053	rBV3	58842	125802	10.71%	1.382%
57	7.722	2073	2078	2088	rVB6	2997	4169	0.35%	0.046%
58	7.776	2089	2095	2097	rBV4	1172	1061	0.09%	0.012%
59	7.911	2124	2137	2154	rBV	196613	337796	28.75%	3.710%
60	8.046	2166	2179	2204	rBV	154253	404858	34.46%	4.447%

61	8.159	2207	2214	2223	rVB2	14124	23617	2.01%	0.259%
62	8.287	2245	2254	2263	rBV4	16816	33420	2.84%	0.367%
63	8.445	2296	2303	2314	rVB9	5789	10140	0.86%	0.111%
64	8.532	2319	2330	2339	rBV3	20042	36679	3.12%	0.403%
65	8.686	2376	2378	2383	rBV2	412	253	0.02%	0.003%

66	8.722	2386	2389	2392	rBV2	518	422	0.04%	0.005%
67	8.792	2399	2411	2438	rBV	438080	788885	67.15%	8.665%
68	8.931	2447	2454	2468	rVB9	9251	18959	1.61%	0.208%
69	9.001	2470	2476	2482	rBV9	3559	4689	0.40%	0.052%
70	9.046	2485	2490	2497	rBV7	6221	9124	0.78%	0.100%

71	9.143	2514	2520	2533	rVB7	4756	9932	0.85%	0.109%
72	9.255	2547	2555	2564	rBV8	4492	7461	0.64%	0.082%
73	9.323	2573	2576	2578	rBV3	417	260	0.02%	0.003%
74	9.355	2584	2586	2587	rBV3	712	307	0.03%	0.003%
75	9.413	2587	2604	2623	rVV9	22422	62948	5.36%	0.691%

76	9.493	2623	2629	2636	rBV6	2866	4866	0.41%	0.053%
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Integrator: RTE

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 Title : VOC Analysis

77	9.619	2659	2668	2673	rBV9	4923	8790	0.75%	0.097%
78	9.686	2686	2689	2692	rBV5	1767	1671	0.14%	0.018%
79	9.921	2752	2762	2770	rBV7	13854	25687	2.19%	0.282%
80	10.072	2799	2809	2815	rBV7	8056	12652	1.08%	0.139%
81	10.165	2826	2838	2855	rBV	285103	529027	45.03%	5.811%
82	10.284	2870	2875	2879	rBV7	2696	2826	0.24%	0.031%
83	10.329	2881	2889	2891	rBV2	8805	12191	1.04%	0.134%
84	10.558	2952	2960	2972	rVB9	14998	28378	2.42%	0.312%
85	10.670	2984	2995	3002	rBV7	9408	21404	1.82%	0.235%
86	10.840	3038	3048	3055	rBV7	9940	22180	1.89%	0.244%
87	10.975	3076	3090	3094	rBV7	5956	13117	1.12%	0.144%
88	11.194	3147	3158	3179	rBV	567044	905993	77.12%	9.951%
89	11.496	3238	3252	3259	rBV10	6369	14605	1.24%	0.160%
90	11.574	3261	3276	3295	rVV2	508472	1174841	100.00%	12.904%
91	11.934	3381	3388	3390	rBV6	3410	4045	0.34%	0.044%
92	12.184	3460	3466	3480	rVB7	8658	19750	1.68%	0.217%
93	12.310	3498	3505	3506	rBV6	3953	4084	0.35%	0.045%
94	12.419	3531	3539	3548	rBV6	5138	8312	0.71%	0.091%
95	12.705	3625	3628	3633	rBV5	1100	1034	0.09%	0.011%
96	12.728	3633	3635	3636	rBV2	1257	577	0.05%	0.006%
97	12.802	3656	3658	3660	rBV2	914	556	0.05%	0.006%
98	13.210	3776	3785	3791	rBV4	16338	24762	2.11%	0.272%
99	16.397	4767	4776	4787	rBV	45795	69543	5.92%	0.764%
100	17.480	5103	5113	5128	rVB3	113559	198035	16.86%	2.175%

Sum of corrected areas: 9104334

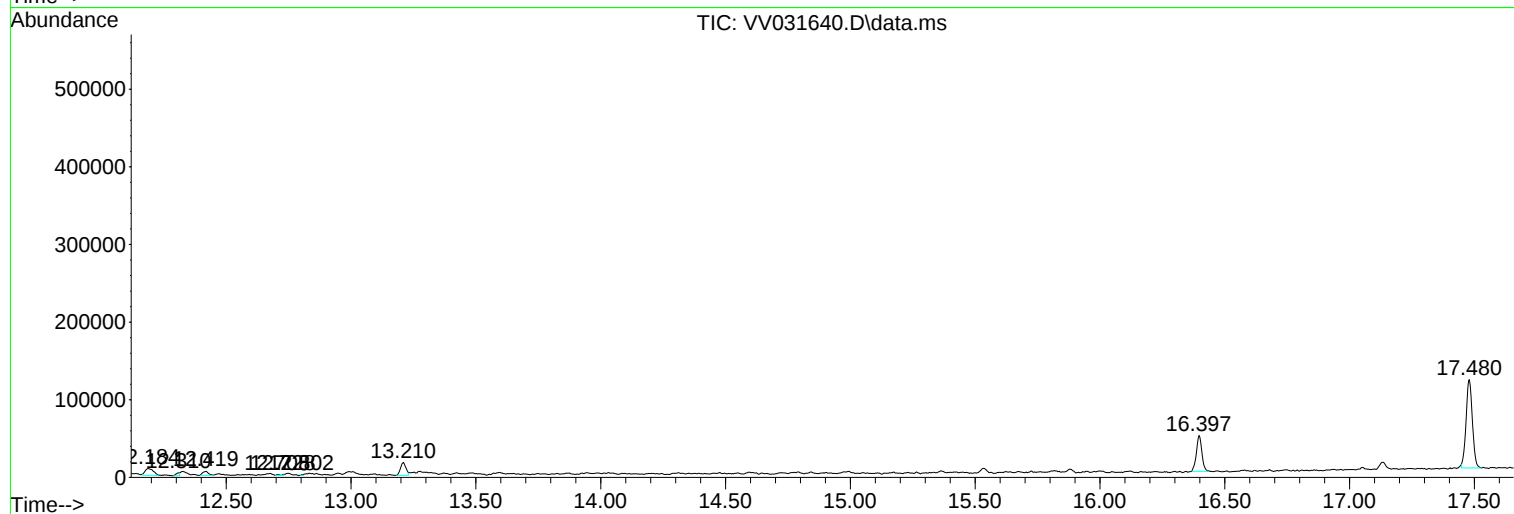
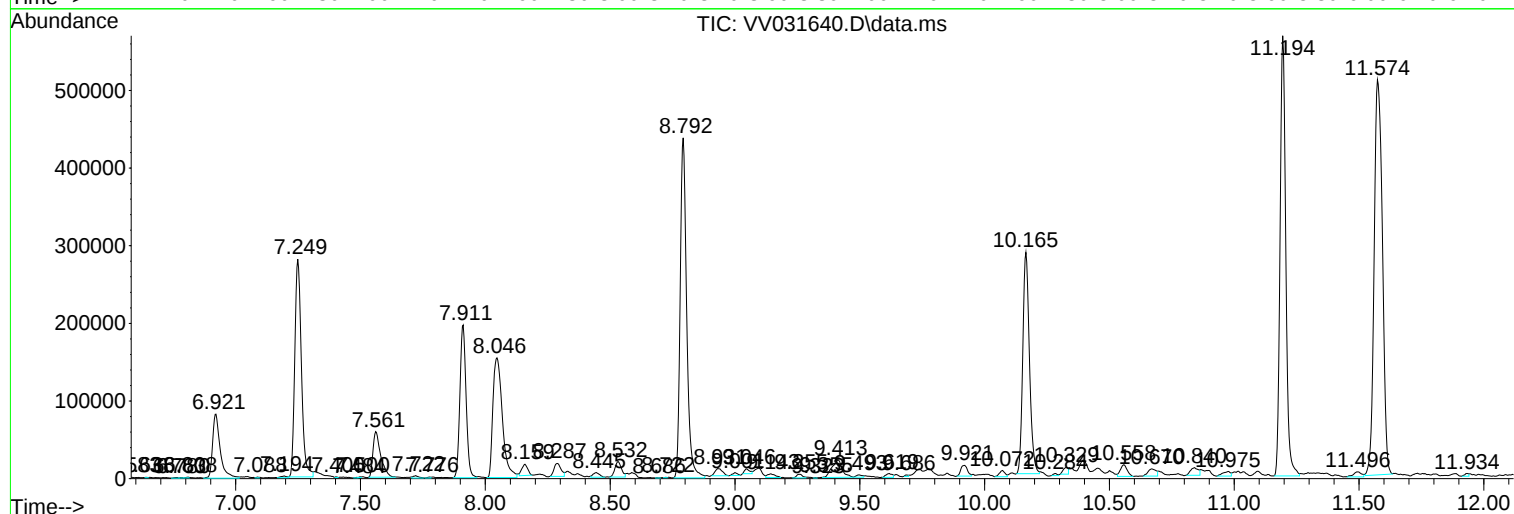
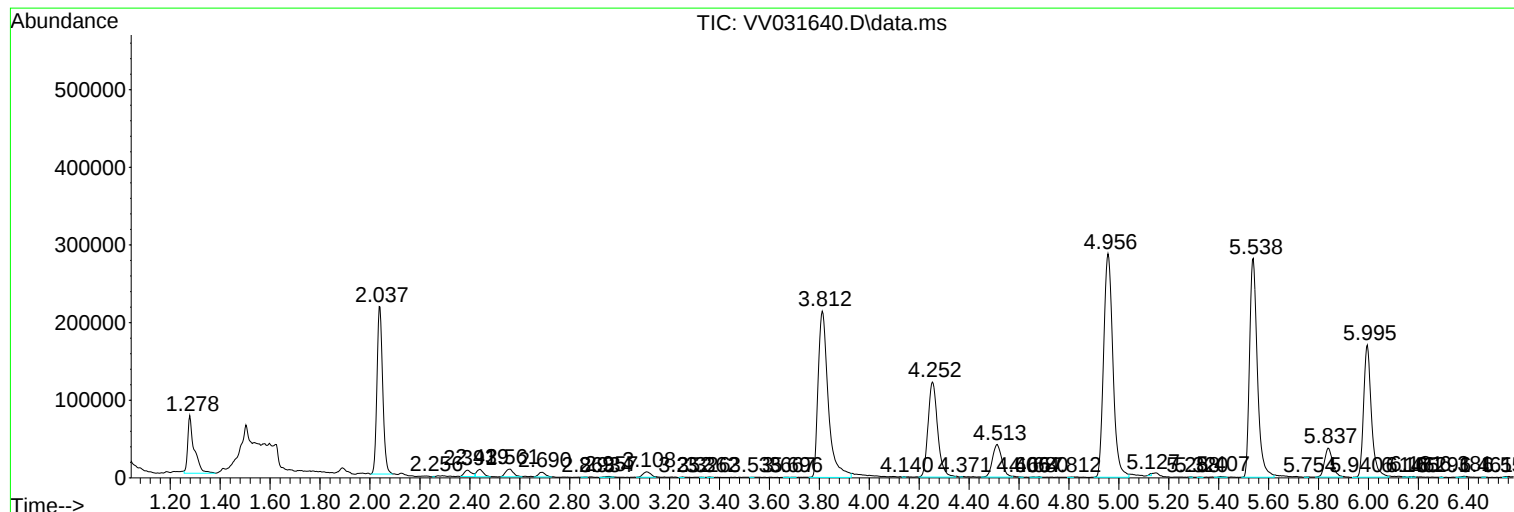
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46S5ME

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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ALS Vial : 12 Sample Multiplier: 1

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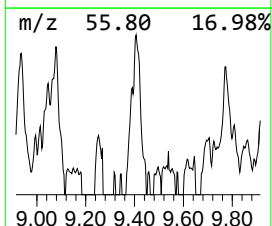
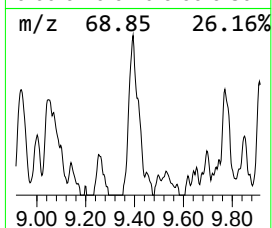
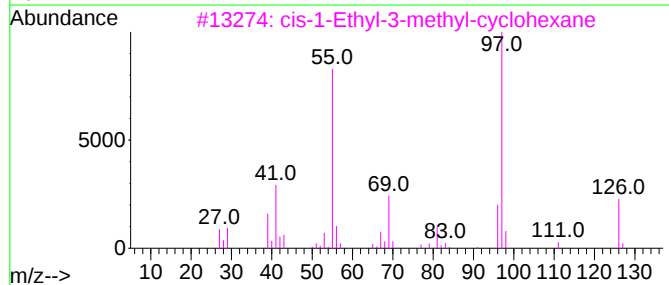
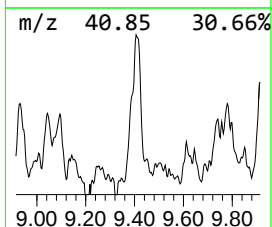
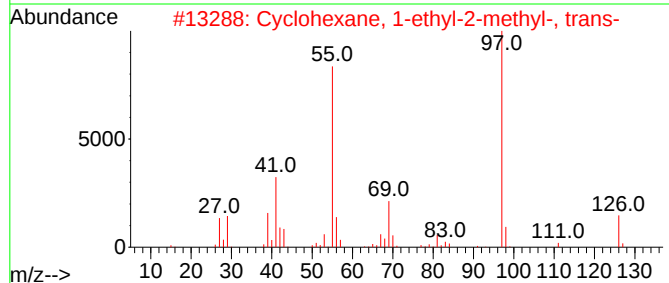
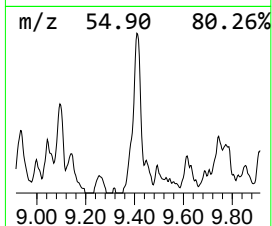
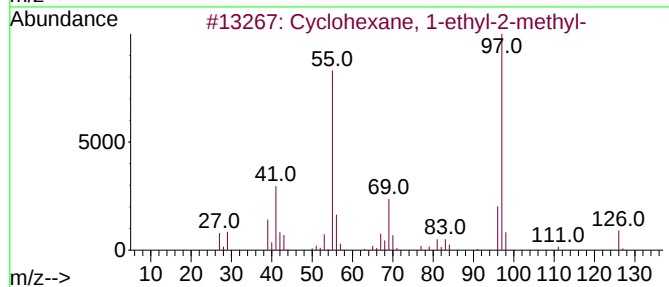
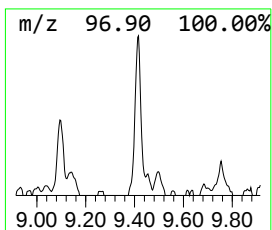
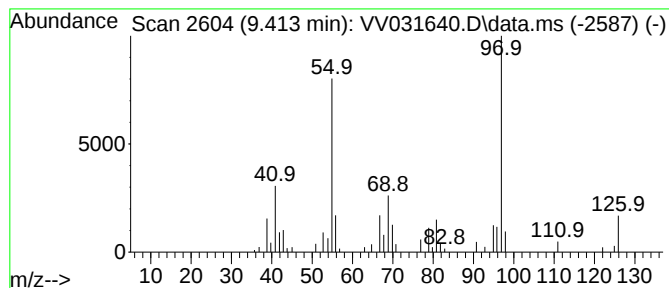
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic9.413 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.413	3.99 ug/L	62948	Chlorobenzene-d5	8.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	64
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
3			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	64
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	64
5			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	64



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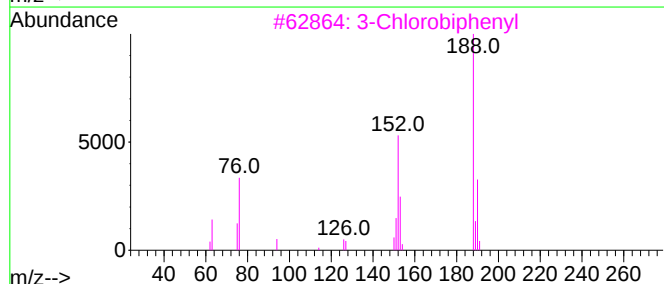
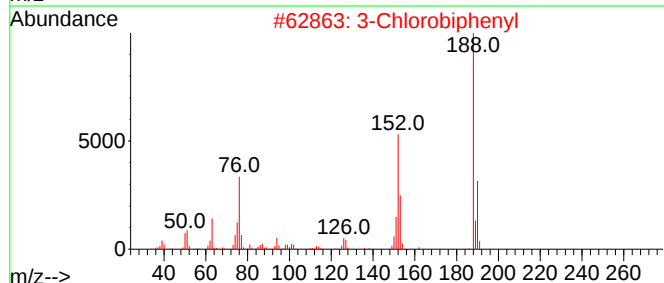
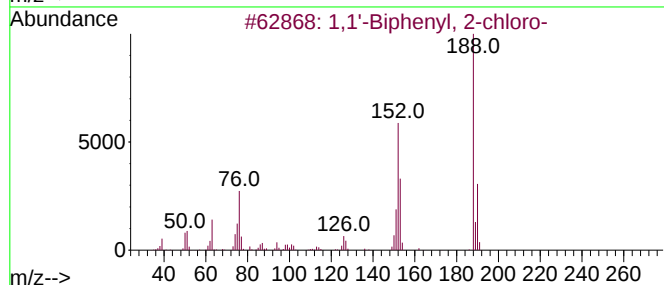
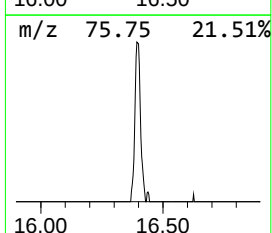
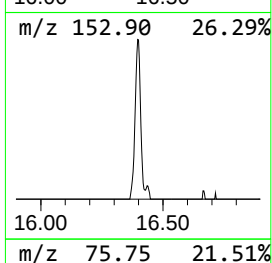
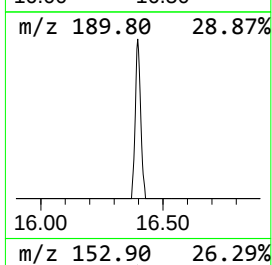
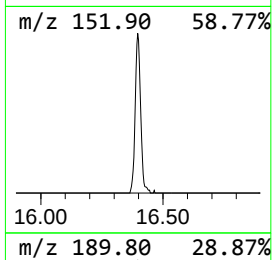
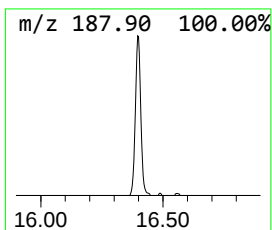
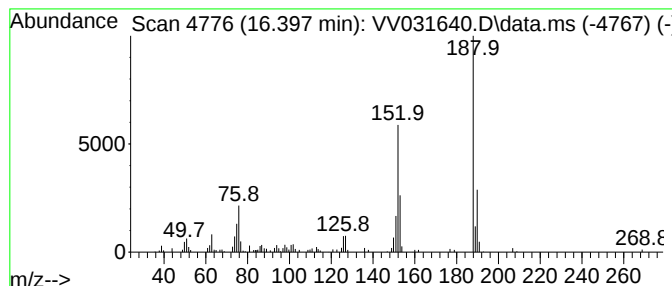
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Quant Title : VOC Analysis

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

Peak Number 3 1,1'-Biphenyl, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	3.84 ug/L	69543	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	96
2			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
3			3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
4			1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96
5			1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	94



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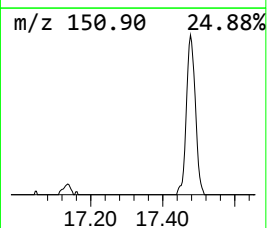
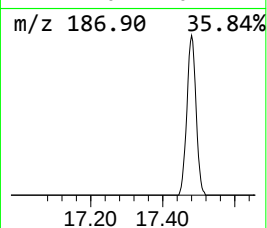
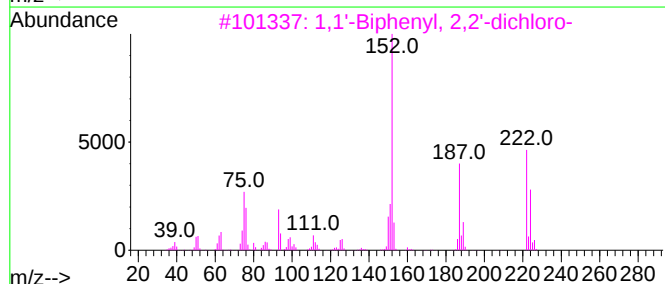
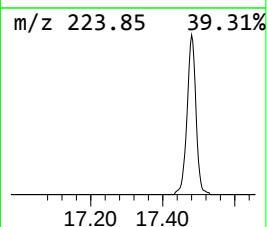
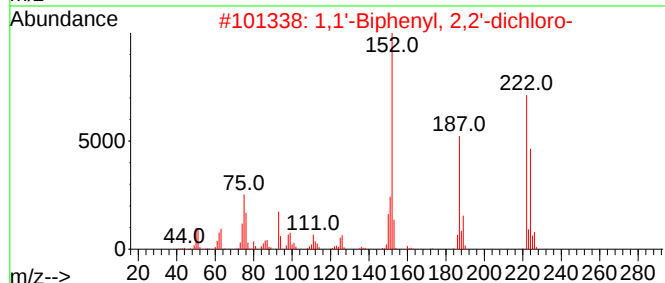
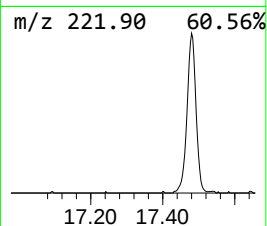
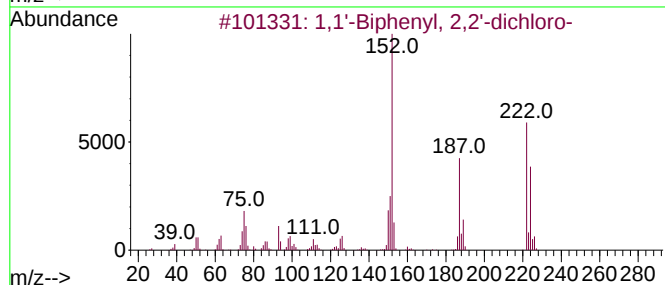
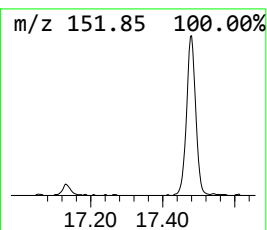
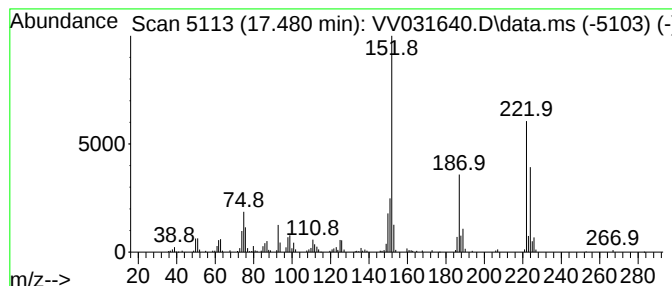
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	10.93 ug/L	198035	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, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	98		
5	1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	98		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031640.D
Acq On : 03 Jul 2023 16:28
Operator : SY/MD
Sample : 03472-13ME
Misc : 4.68g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46S5ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	9.413	4.0	ug/L	62948	2	8.792	788885	50.0
1,1'-Biphenyl, ...	16.397	3.8	ug/L	69543	3	11.194	905993	50.0
1,1'-Biphenyl, ...	17.480	10.9	ug/L	198035	3	11.194	905993	50.0