

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
 Data File : VV024379.D
 Acq On : 17 Jan 2022 16:44
 Operator : SY/MD
 Sample : N1115-11ME
 Misc : 7.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLS1ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	48	54	60	rBV2	24693	22365	1.11%	0.137%
2	1.307	73	83	98	rBV	218234	254136	12.66%	1.560%
3	1.384	103	107	111	rVB2	1589	1699	0.08%	0.010%
4	1.532	149	153	155	rBV4	1879	1571	0.08%	0.010%
5	1.568	156	164	178	rBV	162450	226788	11.30%	1.392%
6	2.031	305	308	309	rBV2	573	342	0.02%	0.002%
7	2.095	316	328	352	rBV	446781	667371	33.25%	4.097%
8	2.320	391	398	401	rBB	365	345	0.02%	0.002%
9	2.400	415	423	425	rBV2	280	366	0.02%	0.002%
10	2.429	430	432	434	rVV2	518	310	0.02%	0.002%
11	2.445	434	437	442	rVV3	899	900	0.04%	0.006%
12	2.506	446	456	463	rBV5	1748	2799	0.14%	0.017%
13	2.616	477	490	499	rVV2	3398	7507	0.37%	0.046%
14	2.744	527	530	532	rBV2	433	317	0.02%	0.002%
15	2.757	532	534	538	rVB3	441	262	0.01%	0.002%
16	2.844	559	561	568	rBV2	326	314	0.02%	0.002%
17	2.886	571	574	583	rVB3	568	706	0.04%	0.004%
18	2.944	583	592	603	rBV9	5650	11014	0.55%	0.068%
19	3.182	659	666	667	rBV2	1392	1198	0.06%	0.007%
20	3.281	693	697	700	rBV	276	287	0.01%	0.002%
21	3.452	745	750	754	rBV2	212	263	0.01%	0.002%
22	3.529	772	774	780	rVB	297	262	0.01%	0.002%
23	3.719	830	833	837	rVV3	341	359	0.02%	0.002%
24	3.735	837	838	842	rVV	369	266	0.01%	0.002%
25	3.886	874	885	922	rBV2	94777	349003	17.39%	2.143%
26	4.339	1010	1026	1059	rVB	332188	819121	40.82%	5.029%
27	4.493	1072	1074	1078	rVB4	678	317	0.02%	0.002%
28	4.535	1083	1087	1091	rBV4	395	337	0.02%	0.002%
29	4.603	1097	1108	1123	rVB6	4188	9614	0.48%	0.059%
30	4.699	1134	1138	1144	rVB4	551	500	0.02%	0.003%
31	4.899	1196	1200	1205	rVB3	368	416	0.02%	0.003%
32	4.969	1217	1222	1224	rBV2	331	279	0.01%	0.002%
33	5.037	1225	1243	1270	rBV2	794442	2006871	100.00%	12.320%
34	5.239	1304	1306	1312	rBV2	331	280	0.01%	0.002%
35	5.339	1320	1337	1346	rBV7	3804	10971	0.55%	0.067%
36	5.403	1354	1357	1365	rVB6	720	731	0.04%	0.004%

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37	5.455	1371	1373	1376	rVB3	533	352	0.02%	0.002%
38	5.484	1379	1382	1385	rVB2	456	332	0.02%	0.002%
39	5.503	1385	1388	1391	rBV2	611	288	0.01%	0.002%
40	5.532	1394	1397	1402	rBV4	358	344	0.02%	0.002%
41	5.609	1408	1421	1451	rBV	449372	907228	45.21%	5.570%
42	5.905	1500	1513	1532	rVV5	33464	78479	3.91%	0.482%
43	6.063	1548	1562	1589	rBV	436948	890602	44.38%	5.467%
44	6.297	1631	1635	1636	rBV	647	399	0.02%	0.002%
45	6.310	1636	1639	1640	rBV	758	435	0.02%	0.003%
46	6.519	1702	1704	1707	rVB3	485	266	0.01%	0.002%
47	6.632	1731	1739	1745	rBV6	2513	4413	0.22%	0.027%
48	6.760	1776	1779	1781	rBV3	542	454	0.02%	0.003%
49	6.789	1785	1788	1790	rVV3	673	472	0.02%	0.003%
50	6.886	1814	1818	1820	rBV	275	256	0.01%	0.002%
51	6.915	1824	1827	1835	rVB2	847	743	0.04%	0.005%
52	6.982	1835	1848	1877	rBV	271029	503925	25.11%	3.094%
53	7.310	1938	1950	1968	rBV	1016562	1750095	87.21%	10.744%
54	7.619	2035	2046	2076	rBV	179671	343372	17.11%	2.108%
55	7.792	2096	2100	2108	rVB4	887	894	0.04%	0.005%
56	7.892	2129	2131	2133	rBV2	443	268	0.01%	0.002%
57	7.924	2136	2141	2144	rVB2	339	278	0.01%	0.002%
58	7.972	2144	2156	2177	rVB	87917	152371	7.59%	0.935%
59	8.117	2182	2201	2237	rBV2	261145	894609	44.58%	5.492%
60	8.265	2245	2247	2255	rVB7	1222	1204	0.06%	0.007%
61	8.390	2282	2286	2292	rBV6	708	716	0.04%	0.004%
62	8.439	2299	2301	2304	rBV2	458	309	0.02%	0.002%
63	8.500	2318	2320	2325	rVB2	466	323	0.02%	0.002%
64	8.567	2334	2341	2343	rBV4	835	835	0.04%	0.005%
65	8.612	2353	2355	2359	rBV3	495	424	0.02%	0.003%
66	8.664	2362	2371	2384	rVB4	4559	8302	0.41%	0.051%
67	8.786	2395	2409	2418	rBV3	4189	7192	0.36%	0.044%
68	8.850	2418	2429	2452	rBV	633741	1109387	55.28%	6.811%
69	9.014	2474	2480	2484	rBV5	966	1221	0.06%	0.007%
70	9.098	2502	2506	2508	rBV3	1103	962	0.05%	0.006%
71	9.149	2516	2522	2531	rVB6	3008	4253	0.21%	0.026%
72	9.410	2593	2603	2605	rBV4	1489	2063	0.10%	0.013%
73	9.477	2616	2624	2633	rVB4	6544	9665	0.48%	0.059%
74	9.548	2640	2646	2648	rBV5	1950	2079	0.10%	0.013%
75	9.574	2648	2654	2666	rVB6	5559	10110	0.50%	0.062%
76	9.670	2680	2684	2686	rBV3	1926	1683	0.08%	0.010%

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 Title : VOC Analysis

77	9.709	2688	2696	2707	rVB3	16304	26882	1.34%	0.165%
78	9.767	2709	2714	2715	rBV3	2735	2299	0.11%	0.014%
79	9.799	2719	2724	2732	rVV8	5749	8533	0.43%	0.052%
80	9.908	2754	2758	2762	rBV5	1898	2127	0.11%	0.013%
81	10.017	2784	2792	2800	rBV6	11938	19952	0.99%	0.122%
82	10.220	2836	2855	2873	rBV	563262	995104	49.58%	6.109%
83	10.509	2936	2945	2953	rBV4	18102	30320	1.51%	0.186%
84	10.879	3052	3060	3066	rBV2	35918	52579	2.62%	0.323%
85	11.030	3100	3107	3115	rBV3	15560	25847	1.29%	0.159%
86	11.149	3137	3144	3154	rVB6	33355	50485	2.52%	0.310%
87	11.252	3165	3176	3195	rBV	770258	1228071	61.19%	7.539%
88	11.625	3281	3292	3311	rVB	1107939	1744257	86.91%	10.708%
89	12.368	3514	3523	3531	rBV6	20220	39261	1.96%	0.241%
90	12.467	3547	3554	3562	rBV5	18859	30249	1.51%	0.186%
91	12.728	3630	3635	3646	rVB4	9897	14068	0.70%	0.086%
92	12.795	3650	3656	3657	rBV4	6741	5900	0.29%	0.036%
93	13.001	3716	3720	3725	rBV	5587	5582	0.28%	0.034%
94	13.217	3781	3787	3795	rVB5	5339	7966	0.40%	0.049%
95	13.271	3796	3804	3810	rBV4	14280	22129	1.10%	0.136%
96	14.361	4134	4143	4154	rBV4	7985	14996	0.75%	0.092%
97	14.818	4278	4285	4295	rVB2	31543	47410	2.36%	0.291%
98	15.667	4538	4549	4569	rBV	237660	416557	20.76%	2.557%
99	15.811	4585	4594	4601	rBV	212666	328593	16.37%	2.017%
100	16.290	4736	4743	4755	rVB2	45557	78160	3.89%	0.480%

Sum of corrected areas: 16289117

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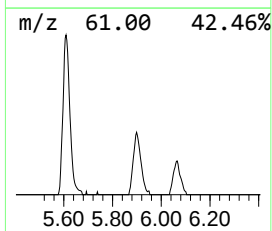
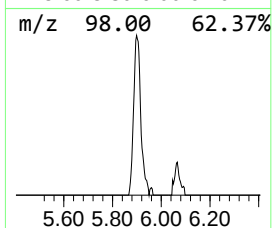
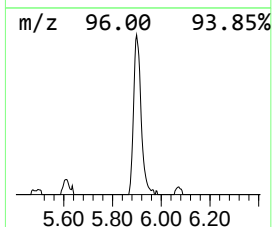
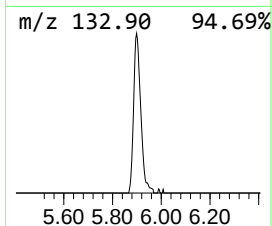
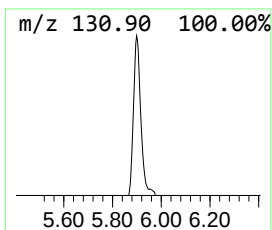
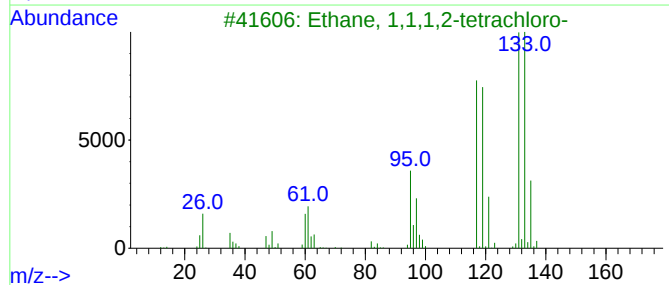
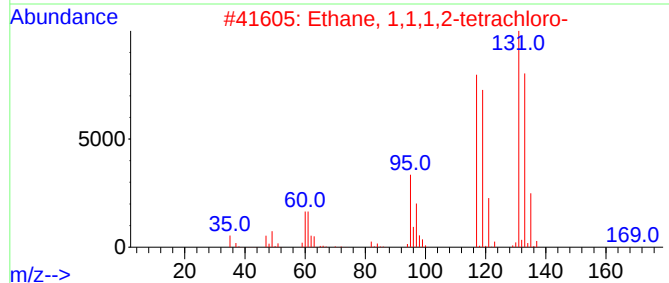
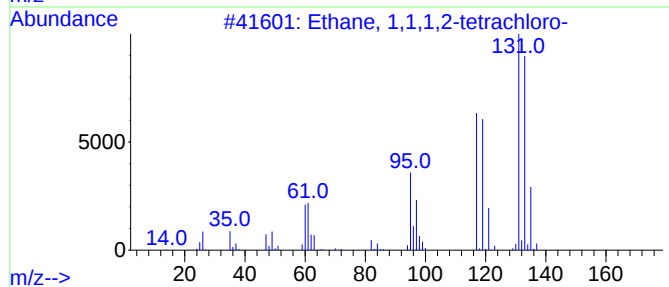
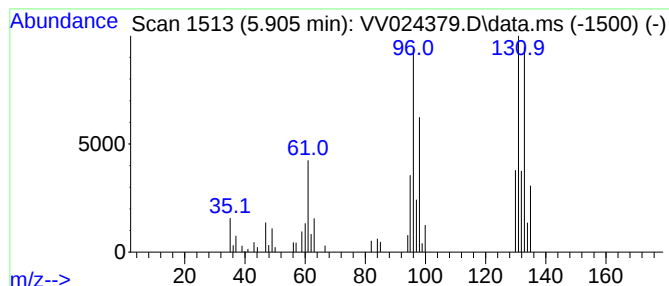
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	4.33 ug/L	78479	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	47
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
4			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	25



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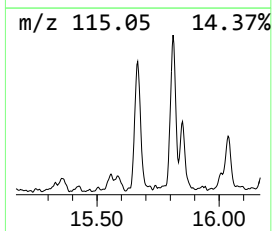
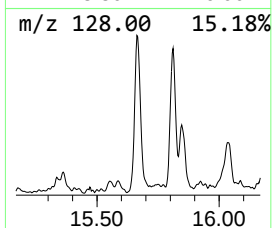
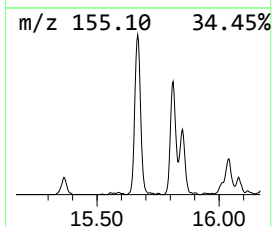
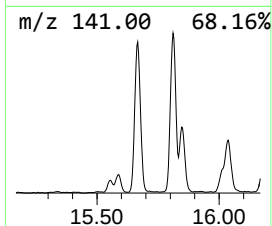
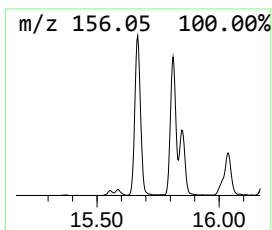
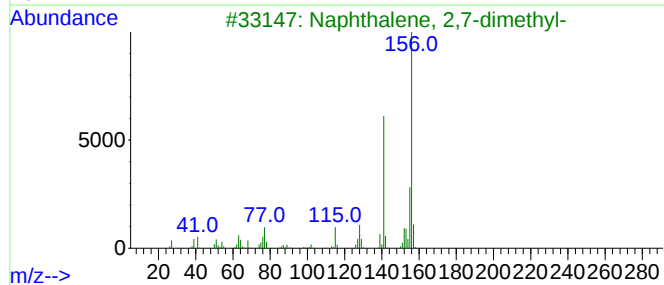
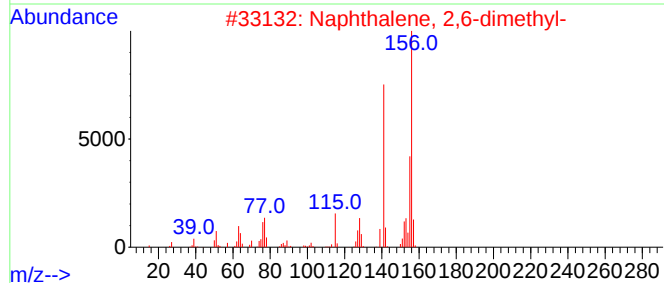
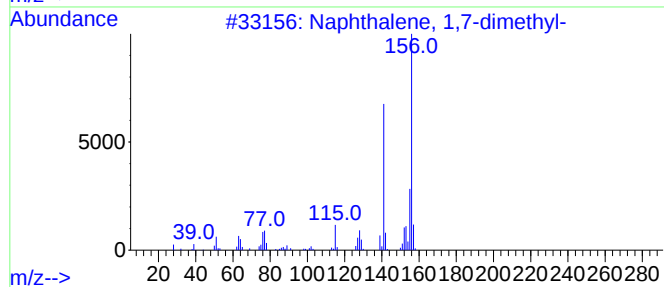
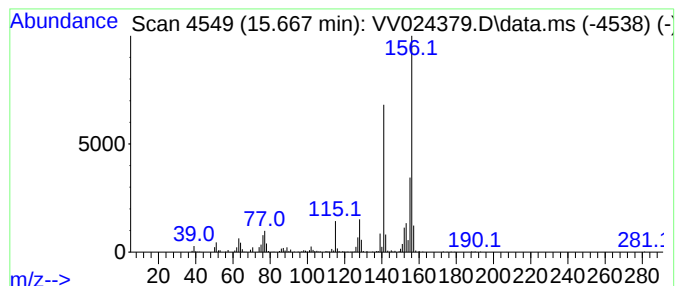
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 1,7-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.667	16.96 ug/L	416557	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



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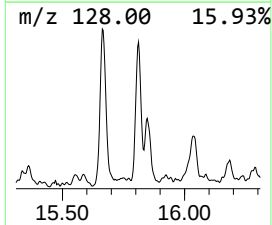
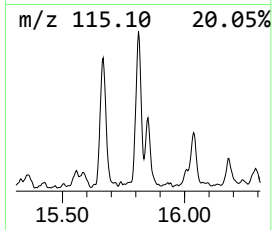
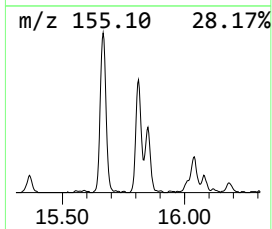
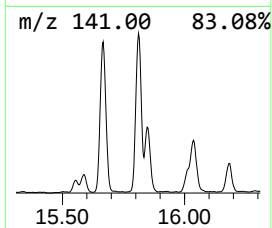
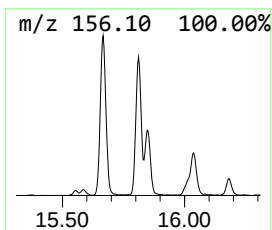
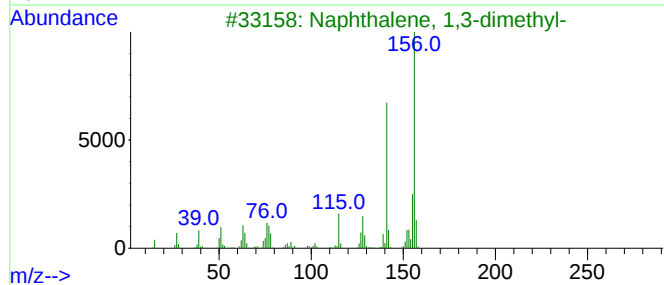
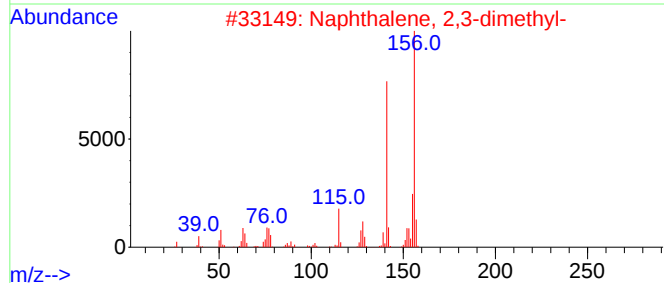
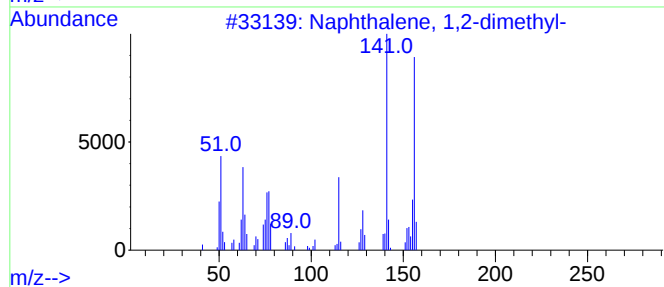
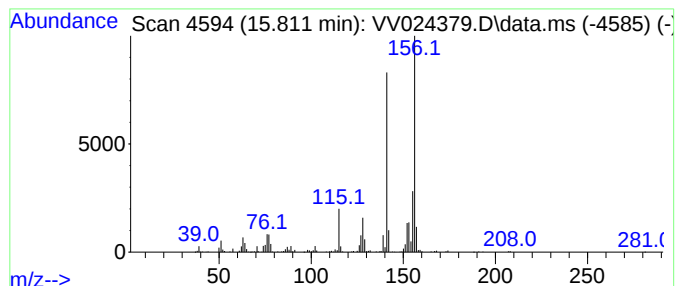
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Naphthalene, 1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.811	13.38 ug/L	328593	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



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Operator : SY/MD
Sample : N1115-11ME
Misc : 7.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLS1ME

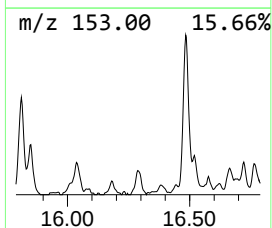
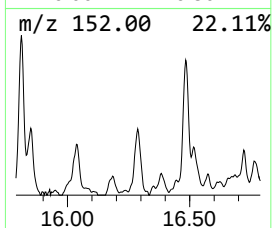
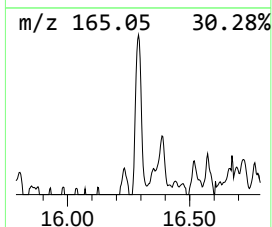
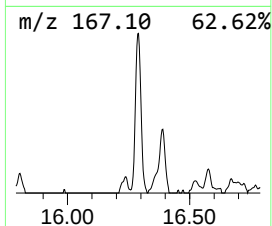
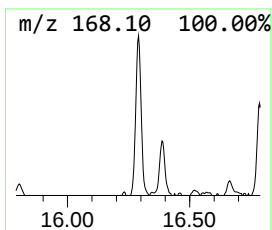
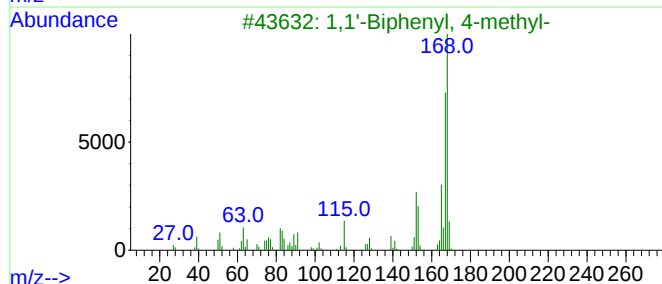
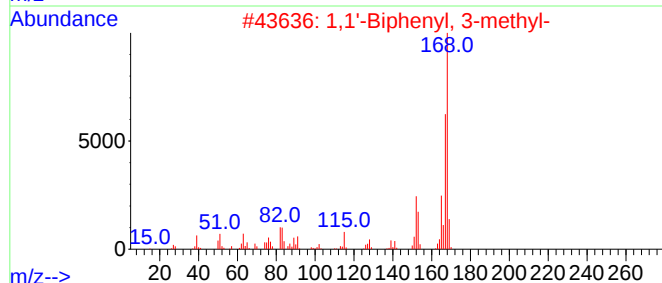
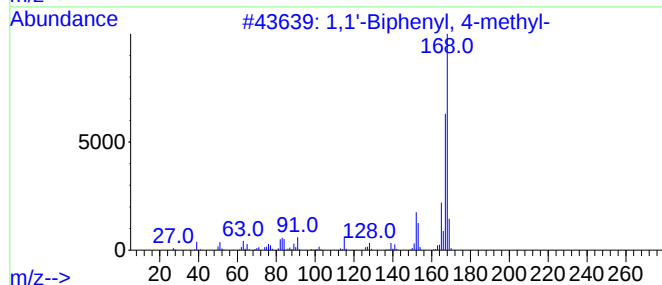
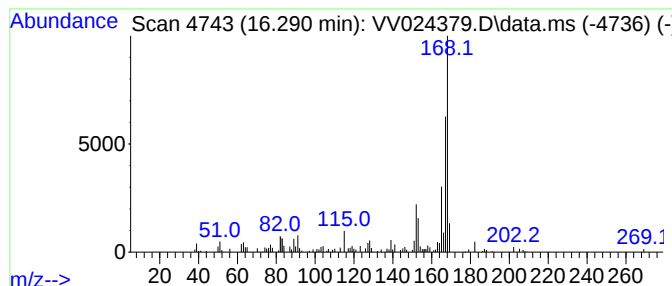
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Quant Title : VOC Analysis

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

Peak Number 5 1,1'-Biphenyl, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.290	3.18 ug/L	78160	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	95		
2	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	95		
3	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	93		
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	93		
5	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	91		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
Data File : VV024379.D
Acq On : 17 Jan 2022 16:44
Operator : SY/MD
Sample : N1115-11ME
Misc : 7.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLS1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.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
unknown-01	5.905	4.3	ug/L	78479	1	5.609	907228	50.0
Naphthalene, 1,...	15.667	17.0	ug/L	416557	3	11.252	1228070	50.0
Naphthalene, 1,...	15.811	13.4	ug/L	328593	3	11.252	1228070	50.0
1,1'-Biphenyl, ...	16.290	3.2	ug/L	78160	3	11.252	1228070	50.0