

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027811.D
 Acq On : 25 Oct 2018 19:39
 Operator : MD/SY
 Sample : J5635-26ME 10X
 Misc : 5.64g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G2ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	62	69	79	rBV	39162	42324	7.93%	1.185%
2	1.668	147	154	172	rVB	29851	40560	7.59%	1.136%
3	2.180	311	313	321	rVB5	915	1174	0.22%	0.033%
4	2.270	331	341	355	rBV	63908	97821	18.32%	2.740%
5	2.620	444	450	454	rVB2	236	254	0.05%	0.007%
6	2.765	488	495	498	rBV	219	354	0.07%	0.010%
7	2.836	511	517	524	rBV2	436	726	0.14%	0.020%
8	3.070	584	590	595	rBV	175	324	0.06%	0.009%
9	3.492	718	721	724	rBV	152	152	0.03%	0.004%
10	3.659	769	773	776	rBV	152	182	0.03%	0.005%
11	3.913	849	852	856	rBV	185	198	0.04%	0.006%
12	4.016	881	884	886	rBV	155	134	0.03%	0.004%
13	4.119	909	916	919	rBV	151	217	0.04%	0.006%
14	4.173	919	933	962	rVV	28790	76598	14.34%	2.145%
15	4.363	989	992	995	rBV	288	219	0.04%	0.006%
16	4.414	1005	1008	1016	rBB	159	227	0.04%	0.006%
17	4.514	1036	1039	1043	rBV	166	198	0.04%	0.006%
18	4.646	1064	1080	1104	rBV	54839	126962	23.77%	3.556%
19	4.836	1137	1139	1141	rBV	254	140	0.03%	0.004%
20	4.877	1149	1152	1157	rVB2	305	307	0.06%	0.009%
21	4.910	1159	1162	1165	rVB2	250	179	0.03%	0.005%
22	5.337	1272	1295	1320	rBV2	106062	319753	59.87%	8.956%
23	5.517	1349	1351	1357	rBB	175	206	0.04%	0.006%
24	5.884	1452	1465	1486	rBV	123276	246905	46.23%	6.916%
25	6.106	1527	1534	1537	rBB	168	224	0.04%	0.006%
26	6.122	1537	1539	1541	rBV	316	188	0.04%	0.005%
27	6.247	1572	1578	1580	rBV	144	191	0.04%	0.005%
28	6.331	1590	1604	1625	rBV	73588	150533	28.19%	4.216%
29	6.517	1658	1662	1664	rBB	158	129	0.02%	0.004%
30	6.601	1684	1688	1689	rBV	152	127	0.02%	0.004%
31	6.665	1704	1708	1711	rBB	151	149	0.03%	0.004%
32	6.684	1711	1714	1716	rBV	146	131	0.02%	0.004%
33	6.717	1719	1724	1728	rBB	142	165	0.03%	0.005%
34	6.778	1740	1743	1746	rBV	164	157	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
 Title : VOC Analysis

35	6.855	1760	1767	1780	rBV3	3023	5166	0.97%	0.145%
36	6.900	1780	1781	1786	rVB	397	228	0.04%	0.006%
37	7.019	1815	1818	1823	rBV	147	199	0.04%	0.006%
38	7.112	1842	1847	1851	rBV	140	187	0.04%	0.005%
39	7.228	1872	1883	1903	rBV	42884	76153	14.26%	2.133%
40	7.389	1930	1933	1939	rBV2	243	266	0.05%	0.007%
41	7.466	1953	1957	1958	rBV	168	136	0.03%	0.004%
42	7.565	1975	1988	2017	rBV	142077	250779	46.96%	7.024%
43	7.848	2067	2076	2097	rBV	29439	50946	9.54%	1.427%
44	7.922	2097	2099	2103	rVB	440	200	0.04%	0.006%
45	7.942	2103	2105	2109	rBV	244	183	0.03%	0.005%
46	8.077	2144	2147	2148	rBV	244	146	0.03%	0.004%
47	8.183	2164	2180	2192	rBV2	28321	70042	13.12%	1.962%
48	8.311	2211	2220	2245	rVB	111375	194329	36.39%	5.443%
49	8.540	2289	2291	2293	rBV	311	129	0.02%	0.004%
50	8.552	2293	2295	2299	rVB	245	147	0.03%	0.004%
51	8.578	2299	2303	2307	rVB2	230	214	0.04%	0.006%
52	8.620	2307	2316	2321	rBV2	1119	1745	0.33%	0.049%
53	8.736	2350	2352	2356	rVB2	298	196	0.04%	0.005%
54	8.761	2356	2360	2361	rBV2	341	259	0.05%	0.007%
55	8.816	2375	2377	2380	rVB3	323	200	0.04%	0.006%
56	8.880	2393	2397	2399	rBV2	449	340	0.06%	0.010%
57	8.919	2406	2409	2413	rBV	335	344	0.06%	0.010%
58	8.948	2415	2418	2420	rVV2	301	222	0.04%	0.006%
59	8.977	2424	2427	2433	rBV3	284	287	0.05%	0.008%
60	9.025	2439	2442	2446	rBV3	240	220	0.04%	0.006%
61	9.089	2450	2462	2488	rBV	195159	321687	60.24%	9.010%
62	9.585	2611	2616	2618	rBV	162	183	0.03%	0.005%
63	9.687	2646	2648	2651	rBV	179	153	0.03%	0.004%
64	9.954	2725	2731	2737	rBV3	420	580	0.11%	0.016%
65	10.170	2792	2798	2803	rBV	375	524	0.10%	0.015%
66	10.347	2851	2853	2857	rVV	160	143	0.03%	0.004%
67	10.379	2860	2863	2868	rVV	168	224	0.04%	0.006%
68	10.433	2868	2880	2897	rVB	96289	152649	28.58%	4.276%
69	10.517	2902	2906	2911	rBV	177	258	0.05%	0.007%
70	10.613	2924	2936	2952	rVB2	12704	24929	4.67%	0.698%
71	10.874	3011	3017	3024	rVB2	736	1022	0.19%	0.029%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

72	11.421	3181	3187	3195	rBV2	2434	3363	0.63%	0.094%
73	11.485	3195	3207	3225	rVV	202078	342076	64.05%	9.581%
74	11.671	3261	3265	3269	rBV2	167	144	0.03%	0.004%
75	11.861	3312	3324	3343	rVV	149212	235261	44.05%	6.590%
76	12.019	3362	3373	3376	rBV	982	1432	0.27%	0.040%
77	12.482	3506	3517	3528	rVB2	6650	11680	2.19%	0.327%
78	12.575	3542	3546	3549	rVV2	183	133	0.02%	0.004%
79	12.597	3549	3553	3558	rVV2	186	188	0.04%	0.005%
80	12.620	3558	3560	3566	rVB	247	158	0.03%	0.004%
81	14.154	4029	4037	4038	rBV2	757	953	0.18%	0.027%
82	14.179	4043	4045	4047	rBV2	537	288	0.05%	0.008%
83	14.279	4068	4076	4087	rVB	5573	8655	1.62%	0.242%
84	14.372	4100	4105	4114	rVB2	396	440	0.08%	0.012%
85	14.488	4139	4141	4142	rBV	335	130	0.02%	0.004%
86	14.555	4144	4162	4169	rBV8	6426	19494	3.65%	0.546%
87	14.787	4228	4234	4241	rBV4	2311	2923	0.55%	0.082%
88	14.832	4241	4248	4255	rBV4	3345	4795	0.90%	0.134%
89	14.887	4262	4265	4270	rBV3	786	735	0.14%	0.021%
90	15.015	4297	4305	4315	rVB5	2948	5011	0.94%	0.140%
91	15.089	4321	4328	4336	rVB3	4038	5251	0.98%	0.147%
92	15.179	4351	4356	4364	rBV2	1767	2353	0.44%	0.066%
93	15.613	4483	4491	4497	rBV5	4293	6656	1.25%	0.186%
94	15.880	4567	4574	4584	rVB3	2853	4355	0.82%	0.122%
95	16.375	4725	4728	4730	rBV2	441	237	0.04%	0.007%
96	16.436	4738	4747	4749	rBV5	2254	3106	0.58%	0.087%
97	16.555	4773	4784	4804	rVB	362603	534046	100.00%	14.958%
98	16.703	4820	4830	4842	rBV	61116	92419	17.31%	2.589%
99	17.279	5002	5009	5017	rBV5	3397	4607	0.86%	0.129%
100	17.485	5066	5073	5085	rVB4	9225	15626	2.93%	0.438%

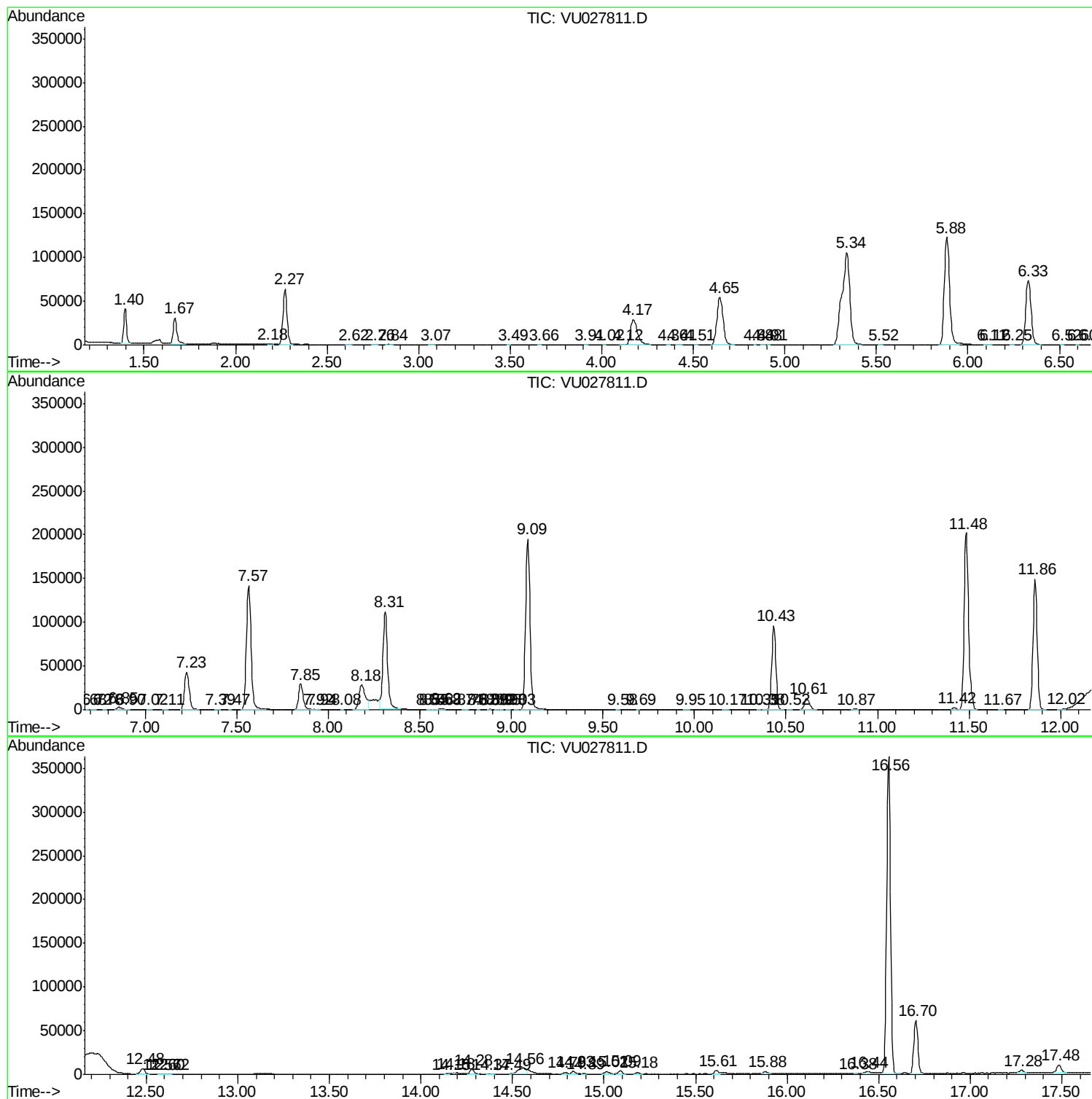
Sum of corrected areas: 3570238

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Instrument :
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ClientSampleId :
A40G2ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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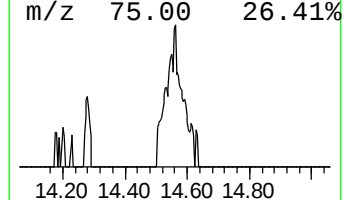
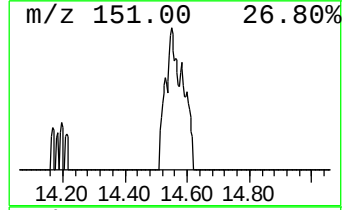
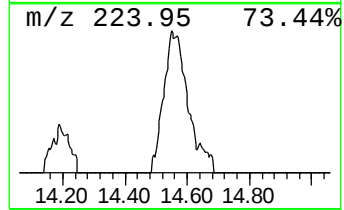
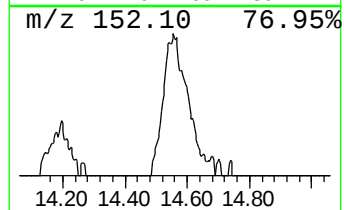
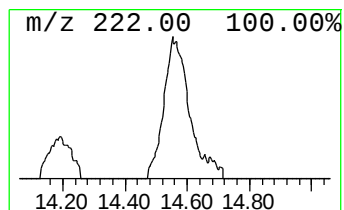
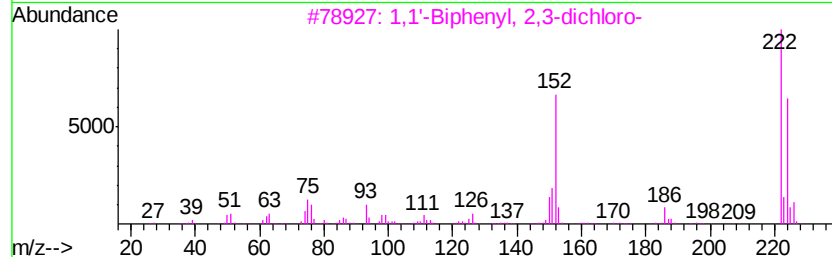
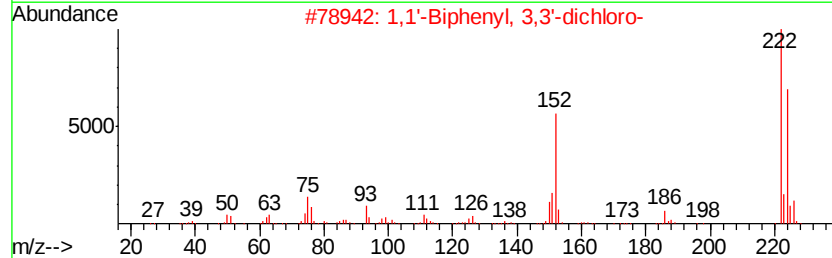
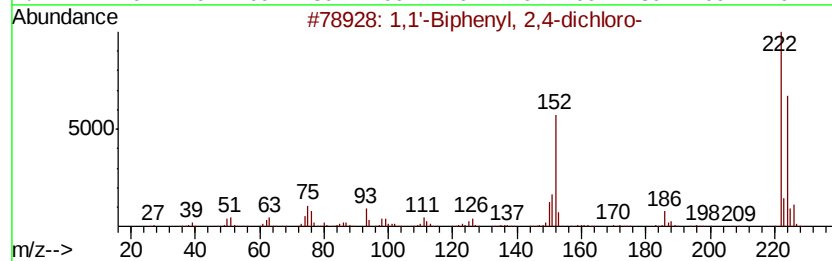
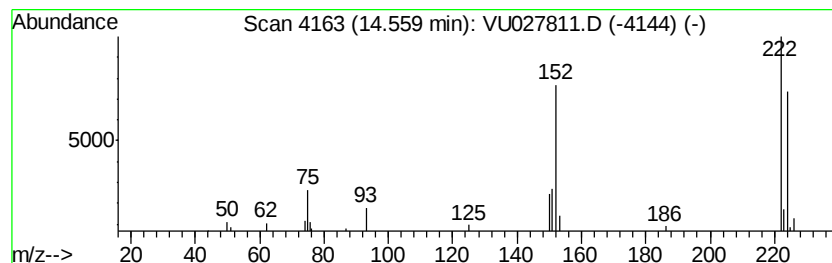
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 2,4-dichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.85 ug/L	19494	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,4-dichloro-	222	C12H8Cl2	033284-50-3	97
2		1,1'-Biphenyl, 3,3'-dichloro-	222	C12H8Cl2	002050-67-1	97
3		1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	96
4		1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	95
5		1,1'-Biphenyl 2,3'-dichloro-	222	C12H8Cl2	025569-80-6	95



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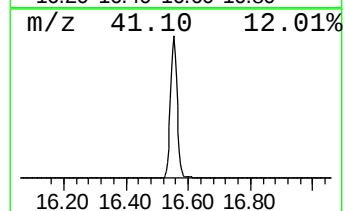
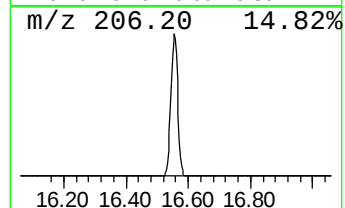
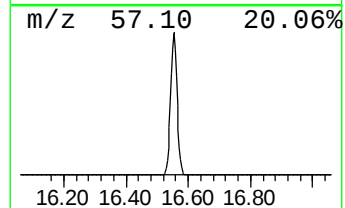
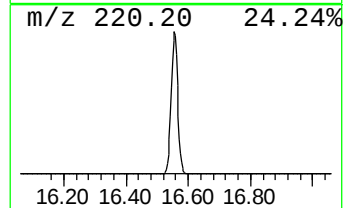
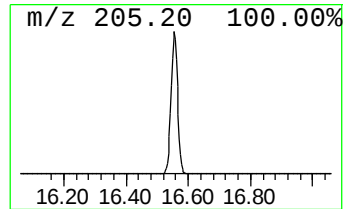
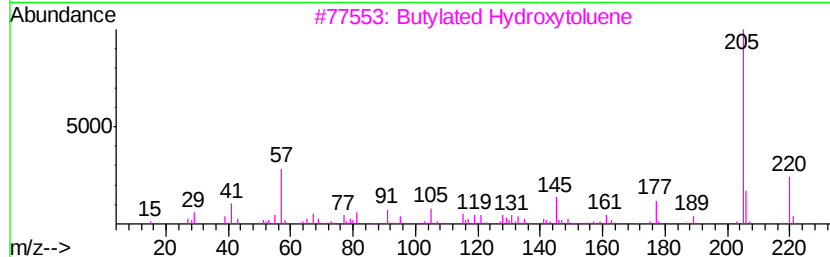
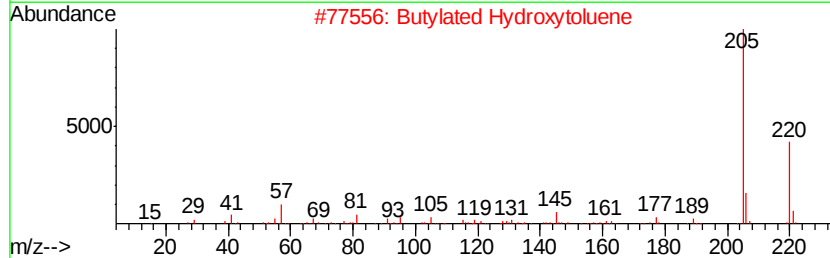
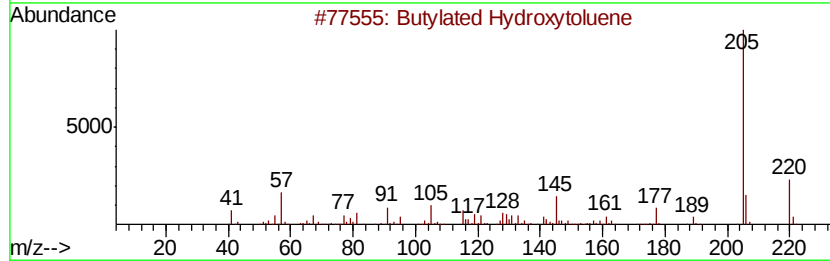
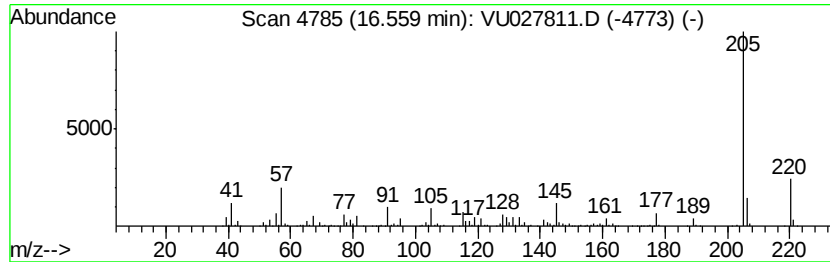
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.56	78.06 ug/L	534046	1,4-Dichlorobenzene-d4	11.48		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated	Hvdroxytoluene	220	C15H24O	000128-37-0	98
2	Butylated	Hvdroxytoluene	220	C15H24O	000128-37-0	94
3	Butylated	Hvdroxytoluene	220	C15H24O	000128-37-0	93
4	Phenol, 2,4,6-tris(1-methylethyl)-		220	C15H24O	002934-07-8	87
5	Phenol, 4,6-di(1,1-dimethylethyl)-		220	C15H24O	000616-55-7	81



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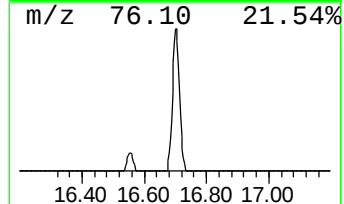
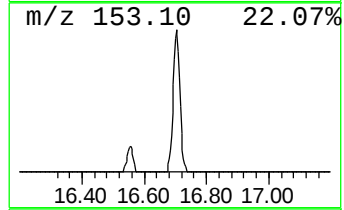
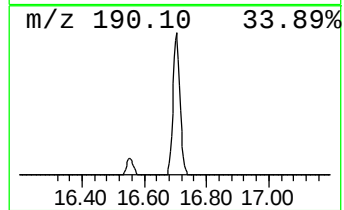
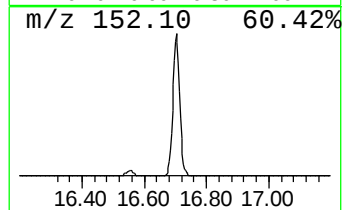
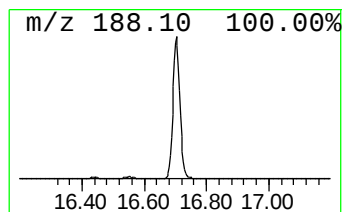
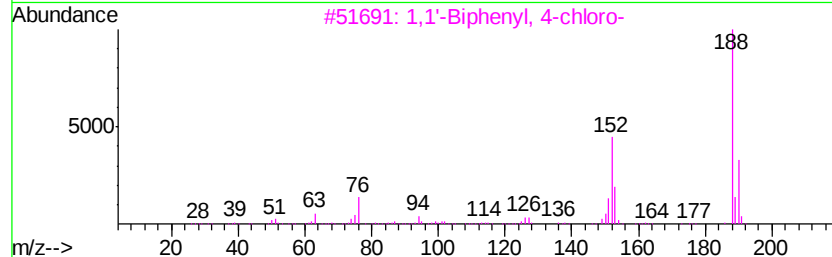
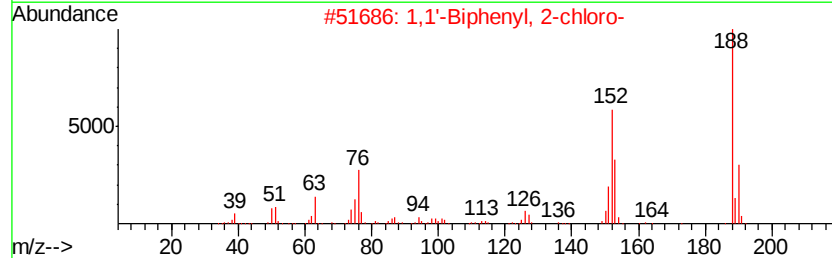
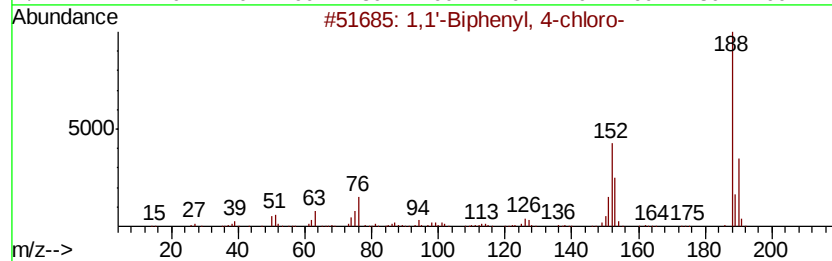
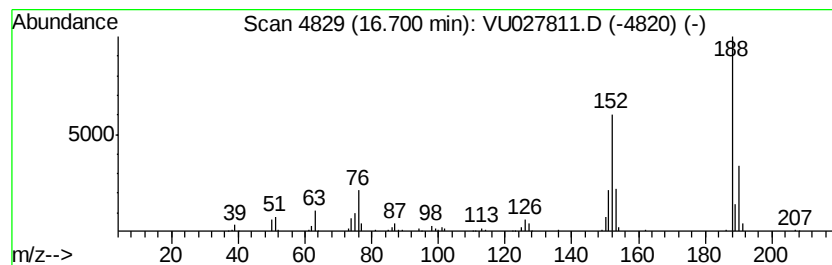
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,1'-Biphenyl, 4-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	13.51 ug/L	92419	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96
2		1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	94
3		1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	94
4		1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	94
5		3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU102518\
Data File : VU027811.D
Acq On : 25 Oct 2018 19:39
Operator : MD/SY
Sample : J5635-26ME 10X
Misc : 5.64g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G2ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, 2,...	14.56	2.9	ug/L	19494	3	11.48	342076	50.0
Butylated Hydroxy...	16.56	78.1	ug/L	534046	3	11.48	342076	50.0
1,1'-Biphenyl, 4-...	16.70	13.5	ug/L	92419	3	11.48	342076	50.0