

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027814.D
 Acq On : 25 Oct 2018 21:35
 Operator : MD/SY
 Sample : J5635-23ME 20X
 Misc : 4.77g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40F9ME

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	1.398	64	70	79	rBV	42849	43436	1.61%	0.691%
2	1.678	149	157	171	rVB	31826	39892	1.47%	0.635%
3	2.273	331	342	356	rVV	65667	99674	3.69%	1.586%
4	2.476	403	405	410	rVB	264	140	0.01%	0.002%
5	2.623	446	451	455	rVB	279	302	0.01%	0.005%
6	3.315	664	666	672	rVV	163	177	0.01%	0.003%
7	3.344	672	675	678	rVB	168	132	0.00%	0.002%
8	3.366	679	682	685	rBB	168	137	0.01%	0.002%
9	3.810	817	820	829	rBV	167	310	0.01%	0.005%
10	4.180	922	935	961	rBV	30508	79140	2.93%	1.259%
11	4.369	989	994	997	rBV2	134	131	0.00%	0.002%
12	4.411	1003	1007	1014	rBV	183	134	0.00%	0.002%
13	4.479	1026	1028	1031	rBV	169	136	0.01%	0.002%
14	4.649	1066	1081	1102	rVV	54782	128141	4.74%	2.039%
15	4.746	1110	1111	1115	rVB	272	145	0.01%	0.002%
16	4.778	1118	1121	1123	rBV	171	141	0.01%	0.002%
17	4.820	1132	1134	1140	rVB	168	190	0.01%	0.003%
18	4.848	1140	1143	1146	rBV	153	149	0.01%	0.002%
19	4.916	1161	1164	1167	rBV	253	200	0.01%	0.003%
20	5.038	1200	1202	1208	rBB	133	163	0.01%	0.003%
21	5.106	1220	1223	1226	rBV	181	170	0.01%	0.003%
22	5.344	1274	1297	1320	rBV3	107770	324855	12.01%	5.168%
23	5.466	1333	1335	1339	rBB2	252	159	0.01%	0.003%
24	5.492	1340	1343	1348	rBV2	268	265	0.01%	0.004%
25	5.578	1367	1370	1376	rBV	143	220	0.01%	0.003%
26	5.643	1383	1390	1393	rBV	159	260	0.01%	0.004%
27	5.688	1401	1404	1407	rBV	153	149	0.01%	0.002%
28	5.826	1445	1447	1451	rBB	176	148	0.01%	0.002%
29	5.887	1452	1466	1486	rBV	130574	249042	9.21%	3.962%
30	5.993	1497	1499	1504	rVB2	355	318	0.01%	0.005%
31	6.022	1505	1508	1512	rBB	259	187	0.01%	0.003%
32	6.093	1523	1530	1531	rBV	174	225	0.01%	0.004%
33	6.128	1538	1541	1545	rBV	187	202	0.01%	0.003%
34	6.266	1580	1584	1587	rBB	158	151	0.01%	0.002%

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Integration Parameters: LSCINT.P

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

35	6.331	1590	1604	1624	rVV	76230	151756	5.61%	2.414%
36	6.424	1630	1633	1637	rBB	153	161	0.01%	0.003%
37	6.456	1640	1643	1646	rBV	162	162	0.01%	0.003%
38	6.575	1676	1680	1683	rBV	166	189	0.01%	0.003%
39	6.700	1713	1719	1725	rBV	177	345	0.01%	0.005%
40	6.778	1739	1743	1745	rBV	165	161	0.01%	0.003%
41	6.858	1762	1768	1778	rBV3	1207	2037	0.08%	0.032%
42	6.900	1778	1781	1784	rVB	163	137	0.01%	0.002%
43	7.138	1852	1855	1859	rVB	168	164	0.01%	0.003%
44	7.163	1859	1863	1868	rBV	192	252	0.01%	0.004%
45	7.228	1871	1883	1900	rBV	45384	77690	2.87%	1.236%
46	7.565	1975	1988	2012	rBV	148480	254987	9.43%	4.057%
47	7.784	2053	2056	2060	rVB	176	172	0.01%	0.003%
48	7.813	2061	2065	2067	rBV	196	188	0.01%	0.003%
49	7.852	2067	2077	2101	rVB	31182	52151	1.93%	0.830%
50	7.938	2101	2104	2106	rBV	273	164	0.01%	0.003%
51	7.993	2118	2121	2128	rVB2	331	461	0.02%	0.007%
52	8.183	2167	2180	2191	rBV2	21100	50258	1.86%	0.800%
53	8.311	2211	2220	2248	rVB	113555	193959	7.17%	3.086%
54	8.450	2260	2263	2266	rBV2	202	150	0.01%	0.002%
55	8.466	2266	2268	2275	rVB	192	145	0.01%	0.002%
56	8.591	2302	2307	2310	rBV	162	216	0.01%	0.003%
57	8.623	2310	2317	2321	rVV	466	648	0.02%	0.010%
58	8.871	2391	2394	2398	rVB2	232	167	0.01%	0.003%
59	8.903	2398	2404	2407	rBV2	204	286	0.01%	0.005%
60	9.019	2437	2440	2443	rVB2	277	213	0.01%	0.003%
61	9.089	2450	2462	2483	rBV	192461	314320	11.62%	5.001%
62	9.208	2497	2499	2502	rBV2	480	317	0.01%	0.005%
63	9.694	2647	2650	2653	rVB2	384	229	0.01%	0.004%
64	9.733	2659	2662	2665	rVB3	463	351	0.01%	0.006%
65	9.752	2665	2668	2671	rBV3	252	190	0.01%	0.003%
66	9.948	2725	2729	2734	rVB2	500	553	0.02%	0.009%
67	10.433	2868	2880	2895	rBV	97713	154566	5.71%	2.459%
68	10.617	2926	2937	2949	rVV3	8051	15700	0.58%	0.250%
69	10.874	3010	3017	3025	rVB2	824	1021	0.04%	0.016%
70	11.208	3113	3121	3128	rBV	112	230	0.01%	0.004%
71	11.388	3170	3177	3180	rBV4	398	429	0.02%	0.007%

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 Title : VOC Analysis

72	11.417	3182	3186	3195	rVB4	1256	1545	0.06%	0.025%
73	11.482	3195	3206	3226	rBV2	202582	355431	13.14%	5.655%
74	11.633	3250	3253	3255	rVV	264	180	0.01%	0.003%
75	11.671	3260	3265	3277	rVB3	643	704	0.03%	0.011%
76	11.858	3312	3323	3339	rBV	154713	247258	9.14%	3.934%
77	12.260	3403	3448	3451	rBV2	18217	61426	2.27%	0.977%
78	12.520	3527	3529	3533	rVB2	244	137	0.01%	0.002%
79	12.543	3533	3536	3540	rVB	258	193	0.01%	0.003%
80	12.732	3591	3595	3599	rBV	141	160	0.01%	0.003%
81	12.810	3614	3619	3621	rVV	505	393	0.01%	0.006%
82	12.839	3621	3628	3638	rVB4	1715	2830	0.10%	0.045%
83	13.125	3714	3717	3721	rBV	146	131	0.00%	0.002%
84	13.147	3721	3724	3726	rVB2	298	156	0.01%	0.002%
85	13.228	3745	3749	3750	rBV2	438	309	0.01%	0.005%
86	13.504	3821	3835	3867	rVV	1768269	2704724	100.00%	43.029%
87	13.845	3934	3941	3946	rBV	187	260	0.01%	0.004%
88	13.986	3973	3985	4001	rBV	360334	564058	20.85%	8.974%
89	14.115	4023	4025	4028	rVB	264	131	0.00%	0.002%
90	14.218	4038	4057	4059	rBV4	1656	3528	0.13%	0.056%
91	14.334	4090	4093	4096	rBV2	216	147	0.01%	0.002%
92	14.356	4096	4100	4103	rBV2	266	179	0.01%	0.003%
93	14.597	4147	4175	4203	rBV5	11264	50940	1.88%	0.810%
94	14.781	4229	4232	4233	rBV	230	154	0.01%	0.002%
95	14.854	4250	4255	4257	rBV2	244	290	0.01%	0.005%
96	15.063	4317	4320	4321	rBV2	757	374	0.01%	0.006%
97	15.662	4503	4506	4510	rBV2	1023	1104	0.04%	0.018%
98	15.883	4567	4575	4587	rVB2	2058	3657	0.14%	0.058%
99	16.456	4737	4753	4763	rBV2	4677	14819	0.55%	0.236%
100	16.706	4821	4831	4840	rBV2	16738	26205	0.97%	0.417%

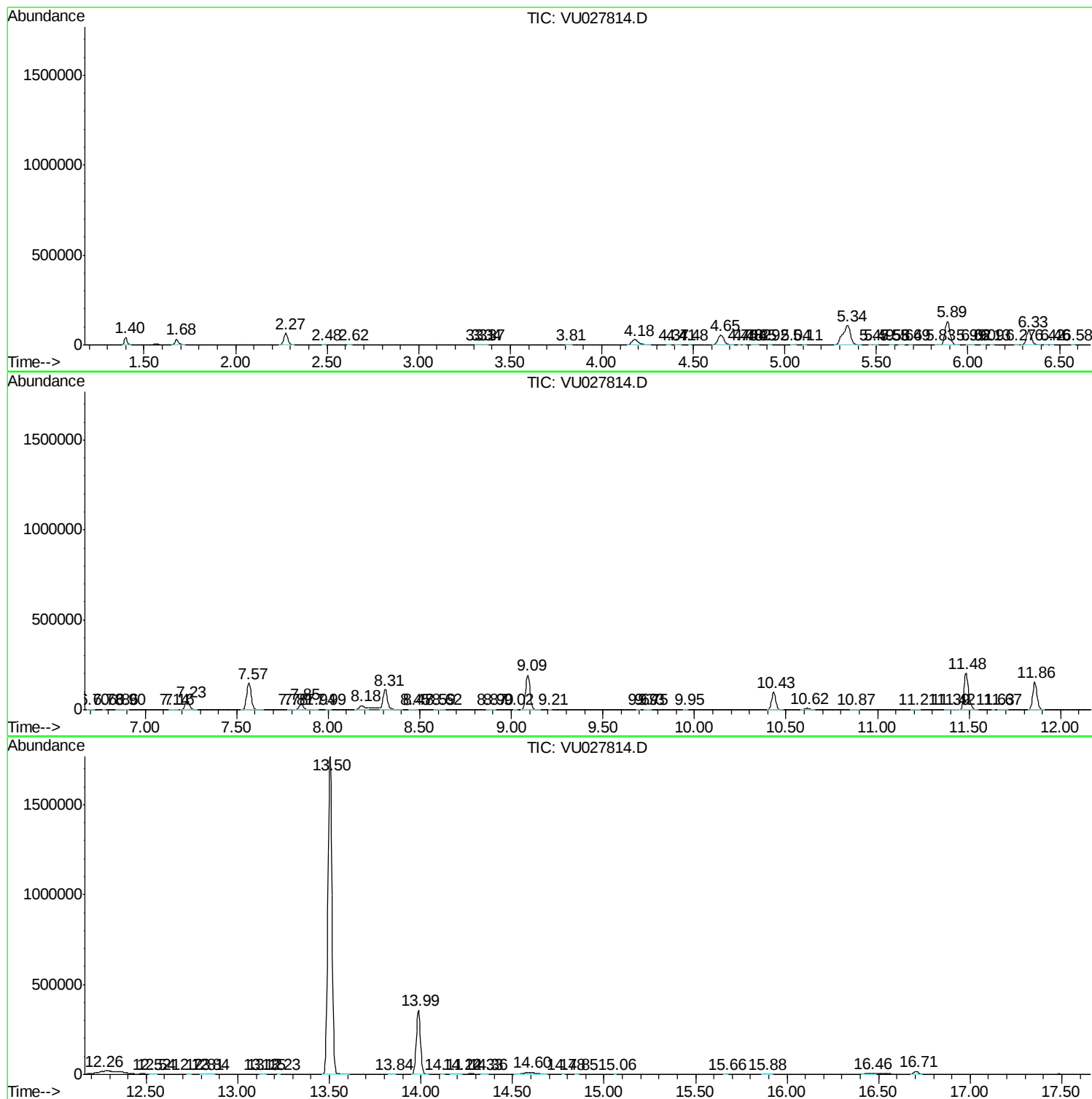
Sum of corrected areas: 6285769

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Instrument :
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ClientSampleId :
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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



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Sample : J5635-23ME 20X
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ALS Vial : 13 Sample Multiplier: 1

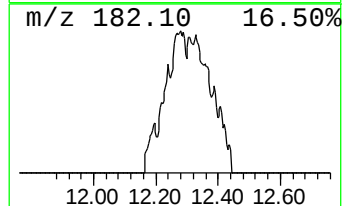
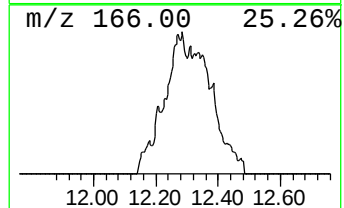
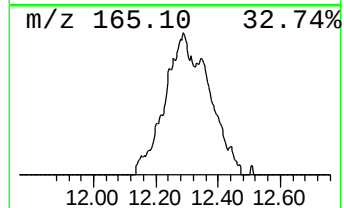
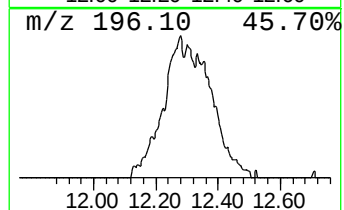
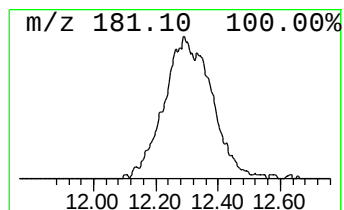
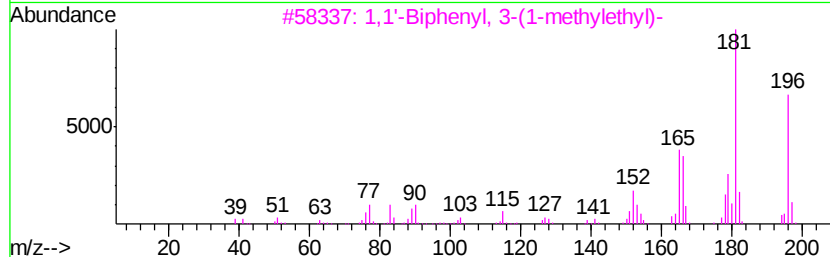
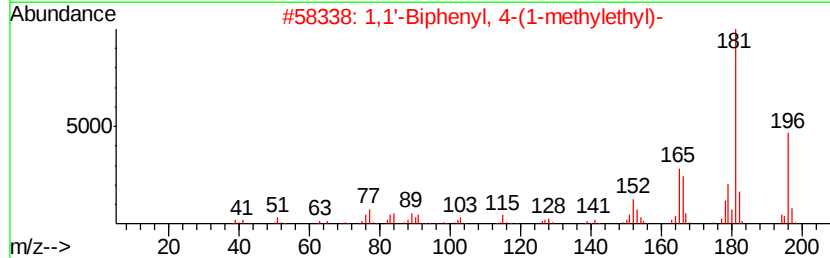
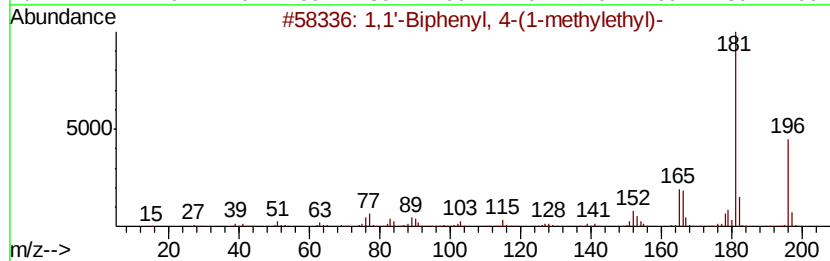
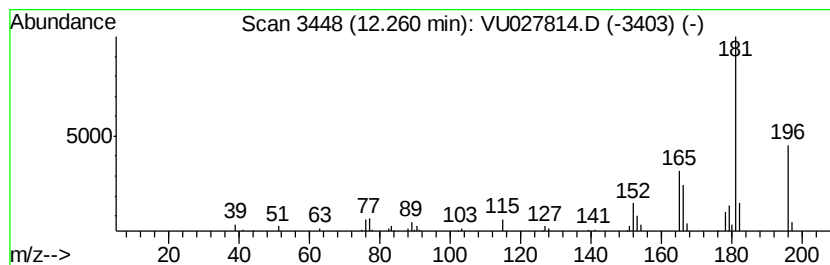
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,1'-Biphenyl, 4-(1-methyle... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.26	8.64 ug/L	61426	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-(1-methylethyl)-	196	C15H16	007116-95-2	96
2	1,1'-Biphenyl, 4-(1-methylethyl)-	196	C15H16	007116-95-2	96
3	1,1'-Biphenyl, 3-(1-methylethyl)-	196	C15H16	020282-30-8	93
4	Methane, di-p-tolyl-	196	C15H16	004957-14-6	91
5	Benzene, 2,4-dimethyl-1-(phenylm...	196	C15H16	028122-28-3	91



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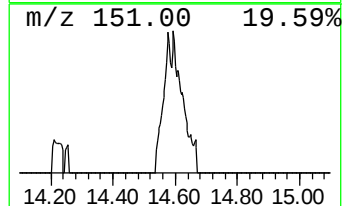
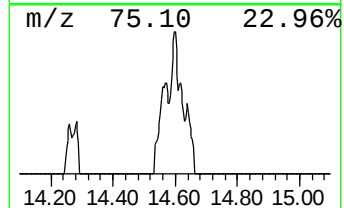
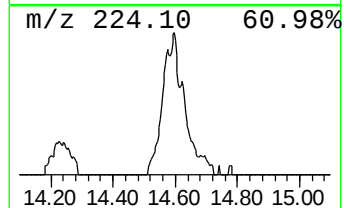
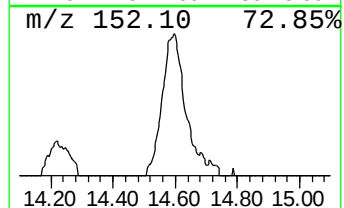
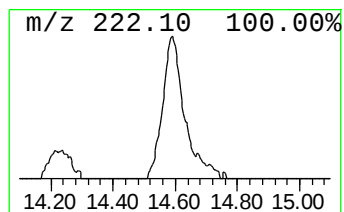
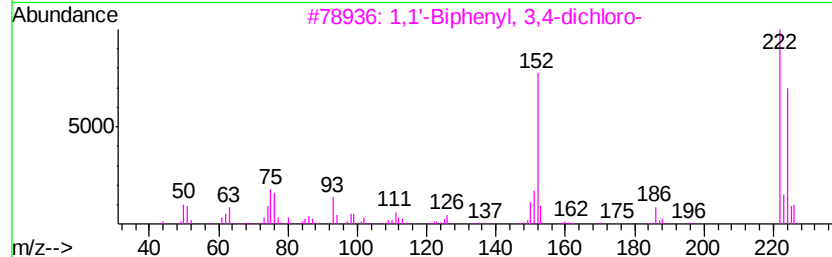
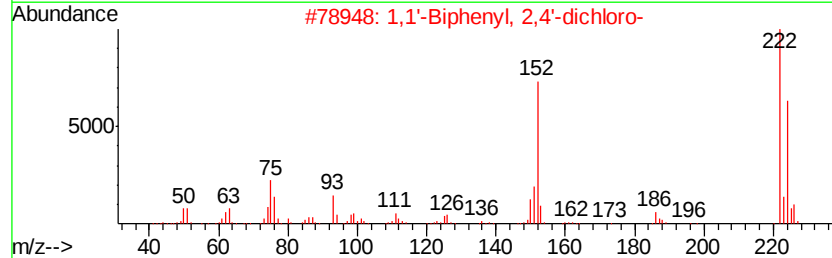
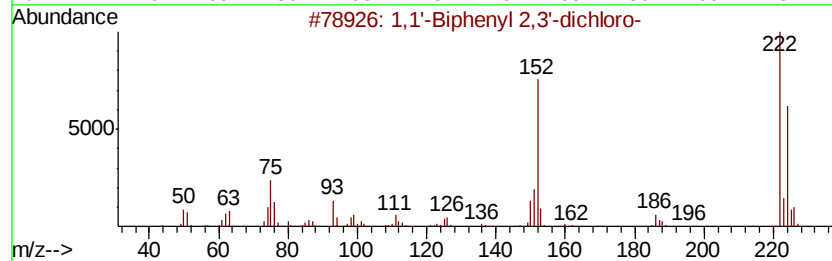
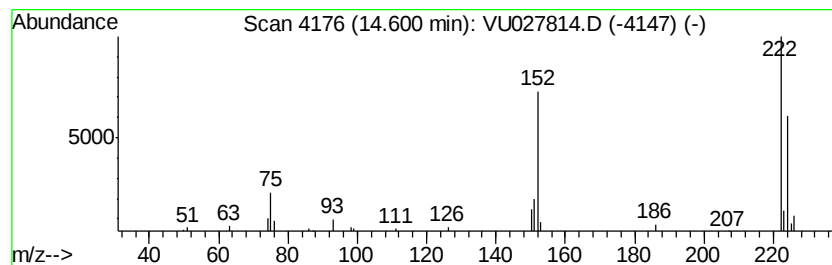
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	7.17 ug/L	50940	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl 2,3'-dichloro-	222	C12H8Cl2	025569-80-6	98
2		1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98
3		1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-92-7	98
4		1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-90-5	98
5		1,1'-Biphenyl, 2,6'-dichloro-	222	C12H8Cl2	033146-45-1	98



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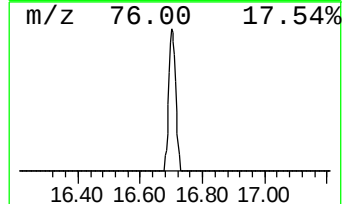
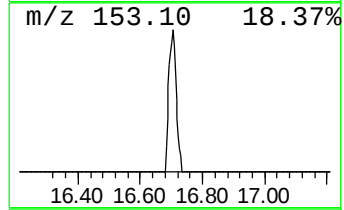
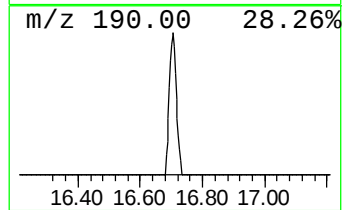
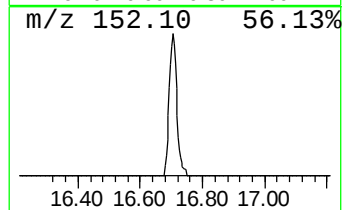
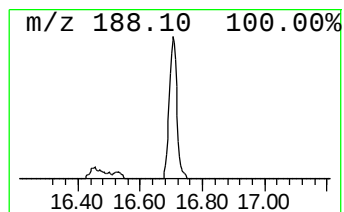
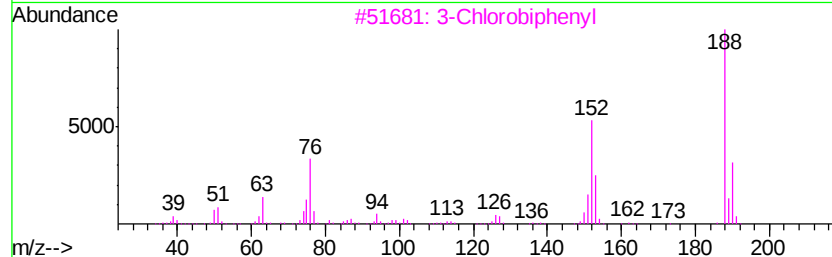
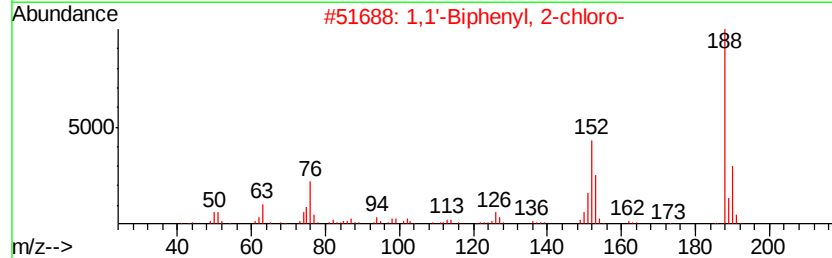
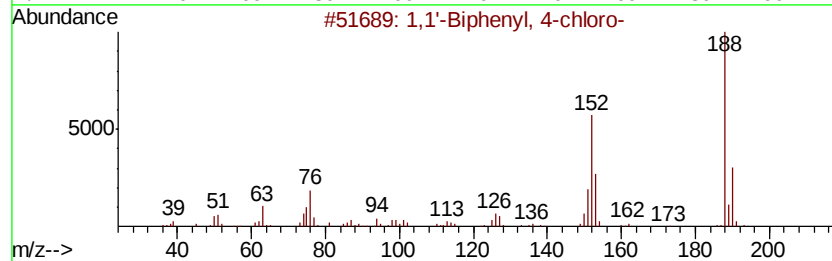
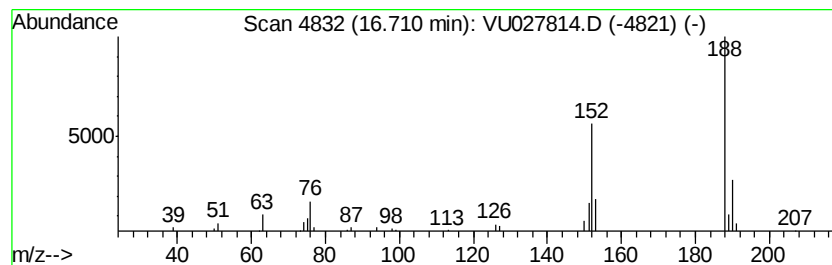
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	3.69 ug/L	26205	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	97
2		1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	96
3		3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	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 : VU027814.D
Acq On : 25 Oct 2018 21:35
Operator : MD/SY
Sample : J5635-23ME 20X
Misc : 4.77g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40F9ME

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, 4-...	12.26	8.6	ug/L	61426	3	11.48	355431	50.0	
1,1'-Biphenyl 2,3...	14.60	7.2	ug/L	50940	3	11.48	355431	50.0	
1,1'-Biphenyl, 4-...	16.71	3.7	ug/L	26205	3	11.48	355431	50.0	