

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027812.D
 Acq On : 25 Oct 2018 20:26
 Operator : MD/SY
 Sample : J5657-01ME 20X
 Misc : 4.65µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G4ME

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	63	70	83	rBV	43065	43426	7.80%	1.215%
2	1.675	148	156	170	rVB	29547	37515	6.74%	1.050%
3	1.881	217	220	227	rBV3	1063	1130	0.20%	0.032%
4	2.183	311	314	315	rBV2	433	263	0.05%	0.007%
5	2.273	332	342	357	rBV	63507	95936	17.24%	2.684%
6	2.395	377	380	385	rBV	170	162	0.03%	0.005%
7	2.620	446	450	452	rBV2	217	169	0.03%	0.005%
8	2.701	469	475	483	rBV3	1284	1732	0.31%	0.048%
9	2.839	514	518	523	rBV2	316	322	0.06%	0.009%
10	3.099	597	599	602	rBV	160	133	0.02%	0.004%
11	3.199	628	630	634	rBV	135	143	0.03%	0.004%
12	3.768	804	807	810	rVB	250	204	0.04%	0.006%
13	4.038	888	891	894	rBV	133	137	0.02%	0.004%
14	4.115	912	915	917	rBV	151	129	0.02%	0.004%
15	4.180	921	935	963	rVV	31435	81206	14.59%	2.272%
16	4.379	994	997	999	rVB	242	138	0.02%	0.004%
17	4.395	999	1002	1005	rBV	177	178	0.03%	0.005%
18	4.453	1018	1020	1025	rBB	162	161	0.03%	0.005%
19	4.649	1066	1081	1107	rBV	53162	125062	22.47%	3.499%
20	4.897	1156	1158	1161	rBV	237	152	0.03%	0.004%
21	4.987	1183	1186	1189	rBB	157	128	0.02%	0.004%
22	5.009	1189	1193	1195	rBV	122	135	0.02%	0.004%
23	5.151	1233	1237	1240	rBV	150	179	0.03%	0.005%
24	5.340	1273	1296	1324	rBV2	106098	316837	56.94%	8.865%
25	5.652	1390	1393	1396	rBV	144	145	0.03%	0.004%
26	5.887	1452	1466	1484	rBV	127499	246686	44.33%	6.902%
27	6.006	1500	1503	1508	rVV2	174	194	0.03%	0.005%
28	6.176	1552	1556	1561	rBB	263	196	0.04%	0.005%
29	6.244	1571	1577	1582	rBB	155	244	0.04%	0.007%
30	6.334	1592	1605	1623	rVB	73609	147479	26.50%	4.126%
31	6.401	1623	1626	1628	rBV	279	193	0.03%	0.005%
32	6.453	1636	1642	1644	rBV	163	218	0.04%	0.006%
33	6.514	1658	1661	1666	rBV	156	197	0.04%	0.006%
34	6.562	1671	1676	1681	rBV	140	218	0.04%	0.006%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027812.D
 Acq On : 25 Oct 2018 20:26
 Operator : MD/SY
 Sample : J5657-01ME 20X
 Misc : 4.65µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G4ME

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

35	6.675	1709	1711	1714	rBV	164	136	0.02%	0.004%
36	6.803	1748	1751	1754	rBV	164	151	0.03%	0.004%
37	6.855	1762	1767	1768	rBV2	1182	860	0.15%	0.024%
38	7.054	1824	1829	1831	rBV	149	177	0.03%	0.005%
39	7.170	1861	1865	1871	rBV	182	293	0.05%	0.008%
40	7.228	1871	1883	1902	rVB	42963	75426	13.55%	2.110%
41	7.376	1926	1929	1930	rBV	279	172	0.03%	0.005%
42	7.433	1945	1947	1953	rVB	187	198	0.04%	0.006%
43	7.565	1975	1988	2005	rBV	141840	244581	43.95%	6.843%
44	7.671	2016	2021	2025	rVB	311	236	0.04%	0.007%
45	7.752	2043	2046	2048	rBV	156	126	0.02%	0.004%
46	7.851	2067	2077	2094	rBV2	30873	49885	8.96%	1.396%
47	7.935	2099	2103	2104	rBV	193	159	0.03%	0.004%
48	8.183	2164	2180	2191	rBV	21625	49410	8.88%	1.382%
49	8.311	2211	2220	2245	rVB	116351	196318	35.28%	5.493%
50	8.585	2302	2305	2308	rVB	285	180	0.03%	0.005%
51	8.617	2309	2315	2316	rBV	933	889	0.16%	0.025%
52	8.659	2323	2328	2330	rBV	267	231	0.04%	0.006%
53	8.755	2355	2358	2361	rBV	235	168	0.03%	0.005%
54	8.777	2361	2365	2368	rBV2	302	281	0.05%	0.008%
55	8.797	2368	2371	2374	rVB2	318	211	0.04%	0.006%
56	8.980	2426	2428	2430	rBV2	384	232	0.04%	0.006%
57	9.089	2450	2462	2480	rBV	191963	311473	55.97%	8.715%
58	10.006	2744	2747	2750	rVB2	237	147	0.03%	0.004%
59	10.163	2793	2796	2801	rVB2	166	145	0.03%	0.004%
60	10.433	2867	2880	2897	rVV	96509	152260	27.36%	4.260%
61	10.613	2925	2936	2952	rBV3	7763	15145	2.72%	0.424%
62	10.777	2982	2987	2992	rBV3	423	427	0.08%	0.012%
63	10.874	3011	3017	3027	rVB2	535	889	0.16%	0.025%
64	10.925	3027	3033	3039	rBV	140	219	0.04%	0.006%
65	11.150	3100	3103	3105	rBV2	225	166	0.03%	0.005%
66	11.420	3180	3187	3194	rVB	1976	2616	0.47%	0.073%
67	11.485	3194	3207	3225	rBV	197815	333303	59.90%	9.326%
68	11.562	3228	3231	3232	rVV	356	167	0.03%	0.005%
69	11.568	3232	3233	3237	rVB2	340	192	0.03%	0.005%
70	11.858	3311	3323	3337	rBV	144914	231459	41.60%	6.476%
71	12.289	3406	3457	3458	rBV5	22977	91574	16.46%	2.562%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027812.D
 Acq On : 25 Oct 2018 20:26
 Operator : MD/SY
 Sample : J5657-01ME 20X
 Misc : 4.65µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G4ME

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

72	12.626	3559	3562	3565	rBV2	236	217	0.04%	0.006%
73	12.713	3587	3589	3591	rVV	400	194	0.03%	0.005%
74	12.726	3591	3593	3599	rVB2	331	246	0.04%	0.007%
75	12.758	3599	3603	3606	rVB2	303	215	0.04%	0.006%
76	12.777	3606	3609	3614	rBV2	210	169	0.03%	0.005%
77	13.707	3895	3898	3903	rBV	147	129	0.02%	0.004%
78	13.957	3974	3976	3979	rBV	189	159	0.03%	0.004%
79	14.215	4042	4056	4057	rBV2	1260	2061	0.37%	0.058%
80	14.276	4066	4075	4087	rVB2	5715	11477	2.06%	0.321%
81	14.346	4093	4097	4101	rBV2	283	284	0.05%	0.008%
82	14.407	4114	4116	4121	rVB	277	172	0.03%	0.005%
83	14.584	4149	4171	4173	rBV4	10383	20749	3.73%	0.581%
84	14.784	4227	4233	4240	rBV4	3649	4430	0.80%	0.124%
85	14.832	4240	4248	4259	rVB3	5377	8005	1.44%	0.224%
86	14.887	4259	4265	4275	rVB4	512	857	0.15%	0.024%
87	14.928	4275	4278	4281	rBV	250	193	0.03%	0.005%
88	15.009	4296	4303	4311	rBV4	6146	9744	1.75%	0.273%
89	15.060	4312	4319	4324	rBV3	9004	12019	2.16%	0.336%
90	15.179	4351	4356	4367	rVB4	1599	2054	0.37%	0.057%
91	15.616	4484	4492	4499	rBV3	2827	4566	0.82%	0.128%
92	15.665	4502	4507	4508	rBV2	1054	769	0.14%	0.022%
93	15.880	4565	4574	4584	rBV2	3255	5418	0.97%	0.152%
94	16.459	4742	4754	4765	rBV10	3097	9040	1.62%	0.253%
95	16.552	4772	4783	4800	rVB	371085	556453	100.00%	15.570%
96	16.632	4804	4808	4809	rBV2	736	473	0.09%	0.013%
97	16.703	4820	4830	4841	rVB	28351	42572	7.65%	1.191%
98	16.899	4889	4891	4899	rBV4	445	361	0.06%	0.010%
99	17.276	5004	5008	5021	rVB6	3683	5235	0.94%	0.146%
100	17.485	5066	5073	5085	rVB4	8667	13875	2.49%	0.388%

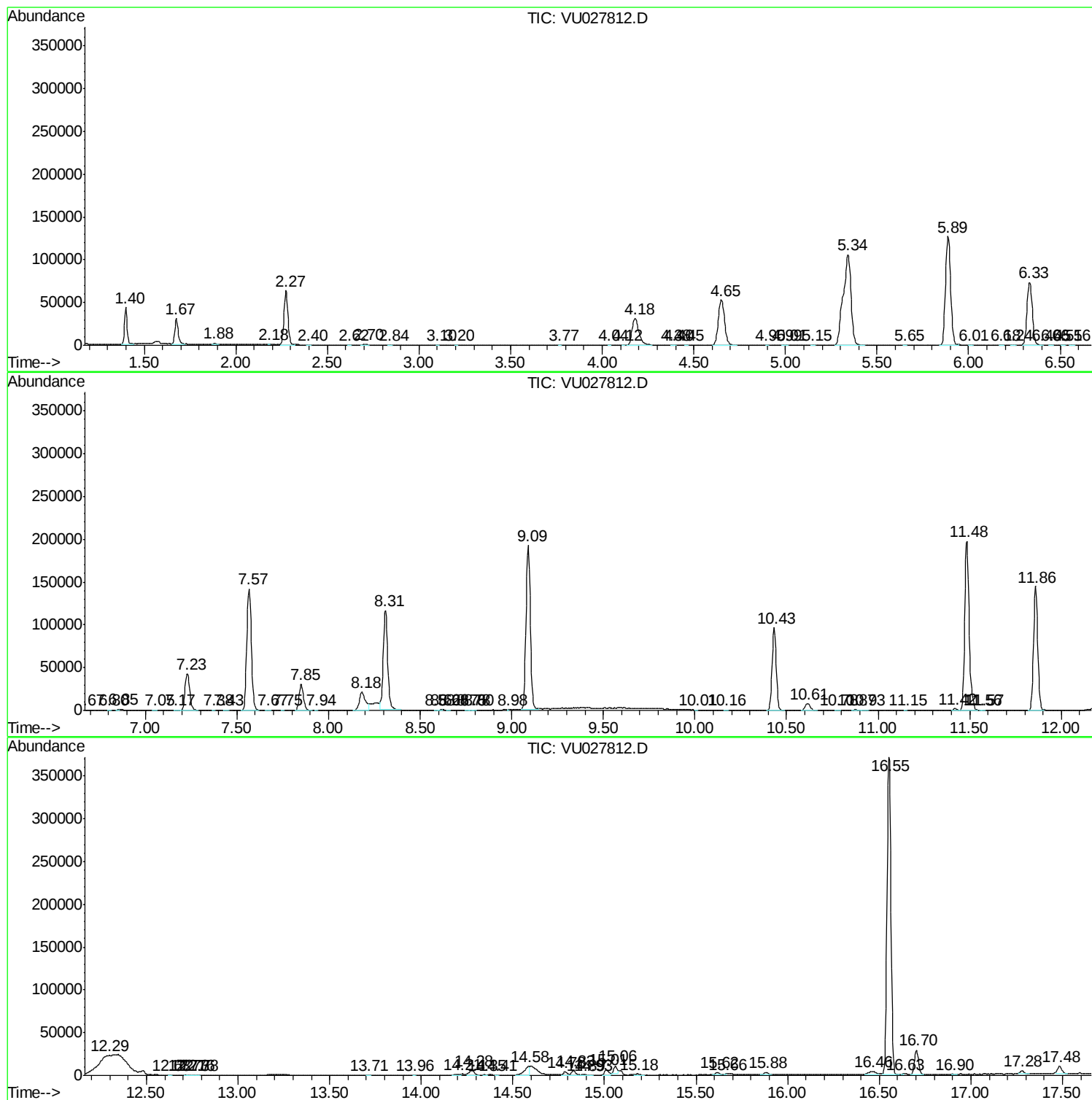
Sum of corrected areas: 3573985

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65u/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G4ME

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65u/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

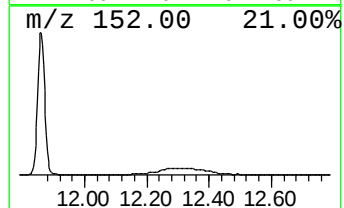
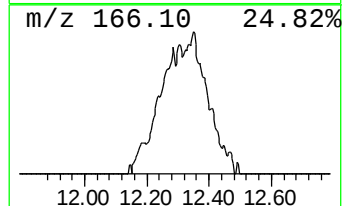
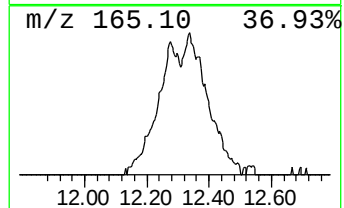
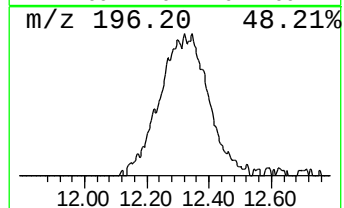
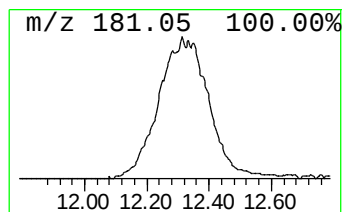
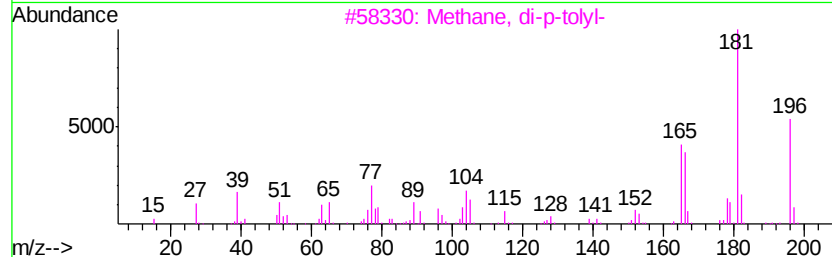
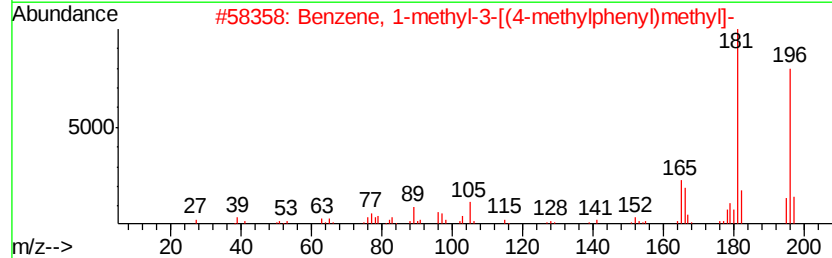
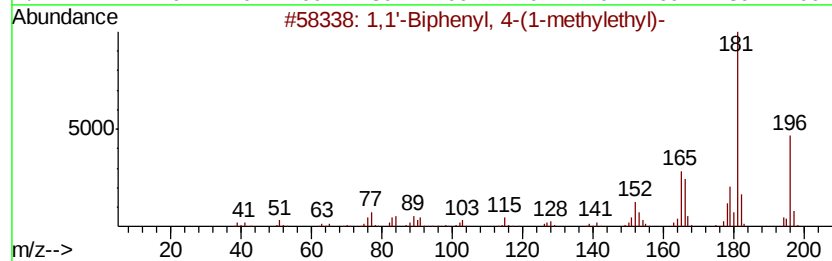
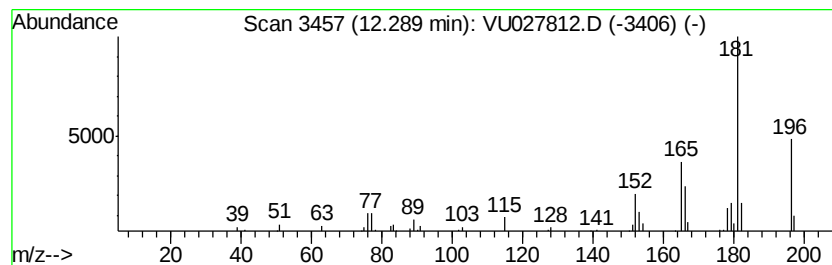
Instrument :
MSVOA_U
ClientSampleId :
A40G4ME

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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.29	13.74 ug/L	91574	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	Benzene, 1-methyl-3-[(4-methylph...	196	C15H16	021895-16-9	90
3	Methane, di-p-tolyl-	196	C15H16	004957-14-6	90
4	1,1'-Biphenyl, 4-(1-methylethyl)-	196	C15H16	007116-95-2	90
5	Benzene, 1,2-dimethyl-4-(phenylm...	196	C15H16	013540-56-2	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65u/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
A40G4ME

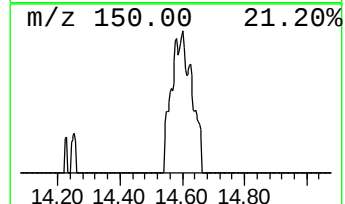
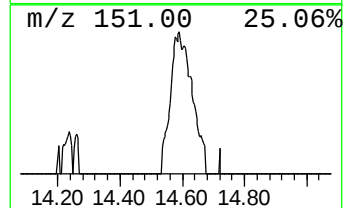
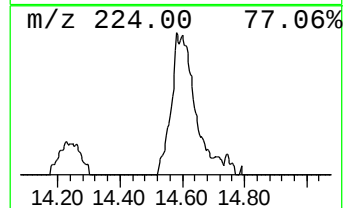
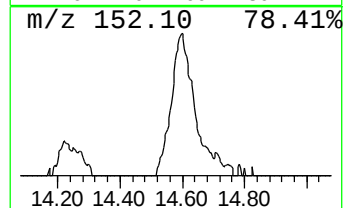
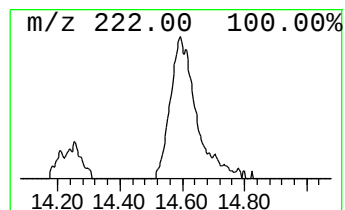
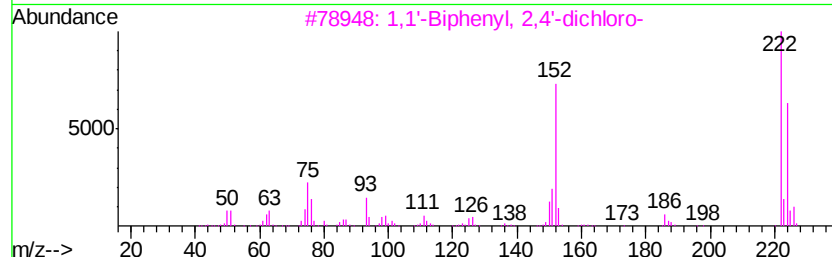
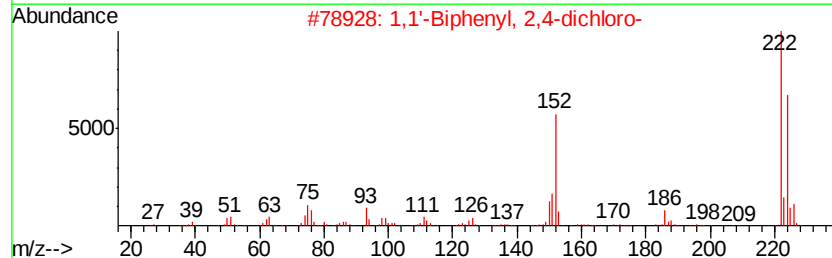
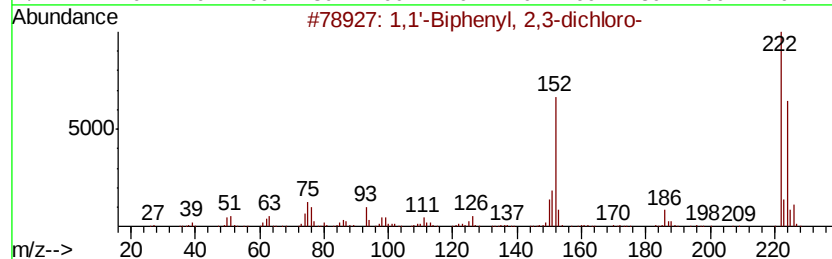
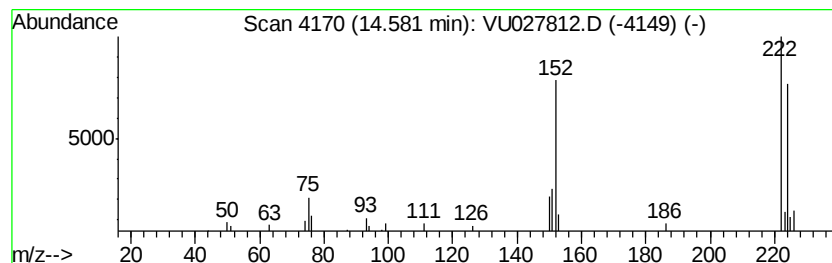
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,1'-Biphenyl, 2,3-dichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	3.11 ug/L	20749	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	98
2		1,1'-Biphenyl, 2,4-dichloro-	222	C12H8Cl2	033284-50-3	98
3		1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98
4		1,1'-Biphenyl 2,3'-dichloro-	222	C12H8Cl2	025569-80-6	98
5		1,1'-Biphenyl, 4,4'-dichloro-	222	C12H8Cl2	002050-68-2	98



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G4ME

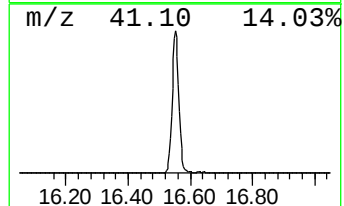
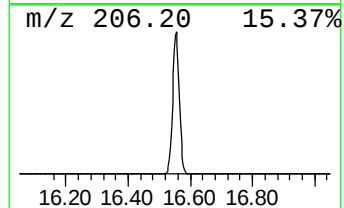
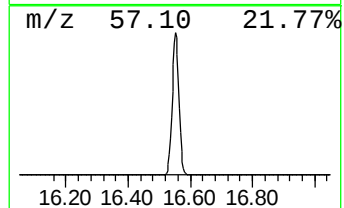
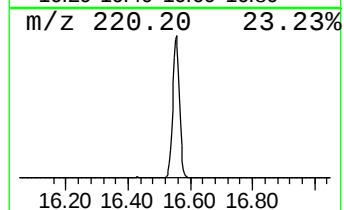
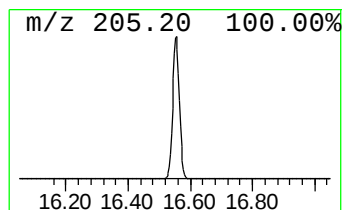
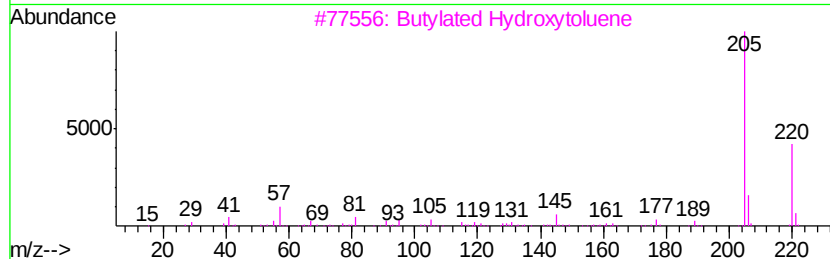
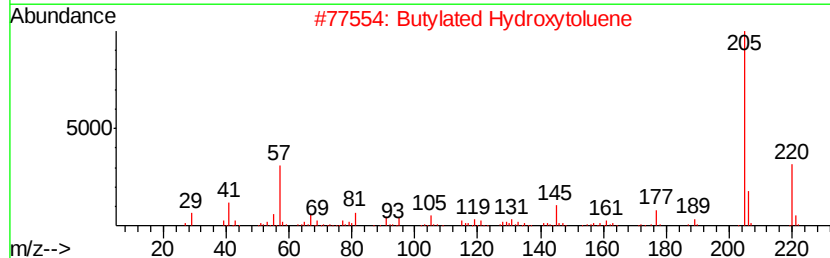
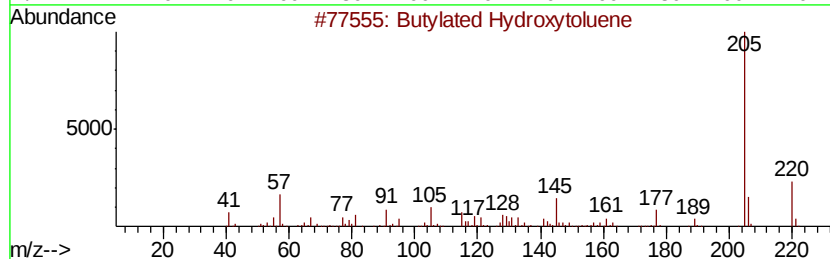
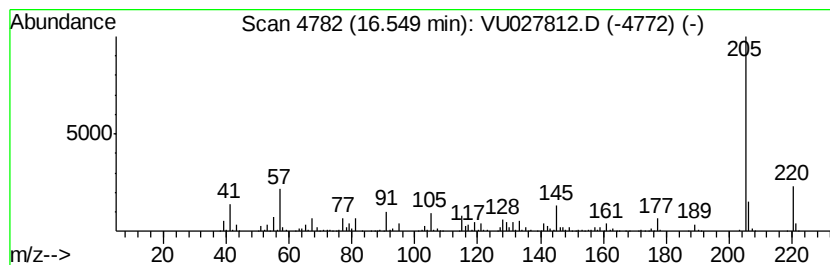
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	83.48 ug/L	556453	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
3		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
5		Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65u/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G4ME

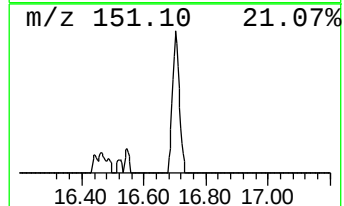
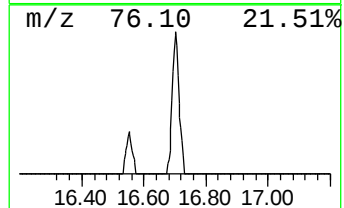
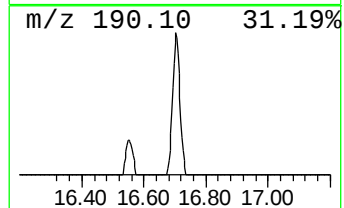
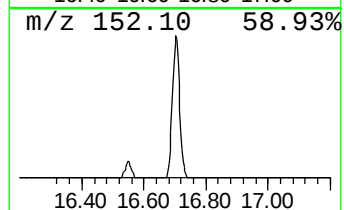
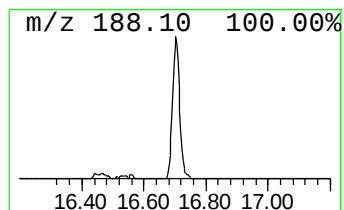
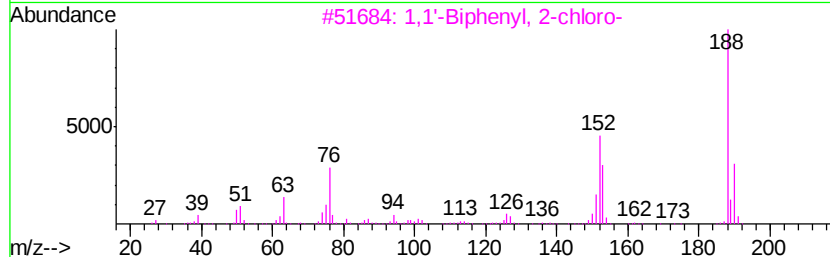
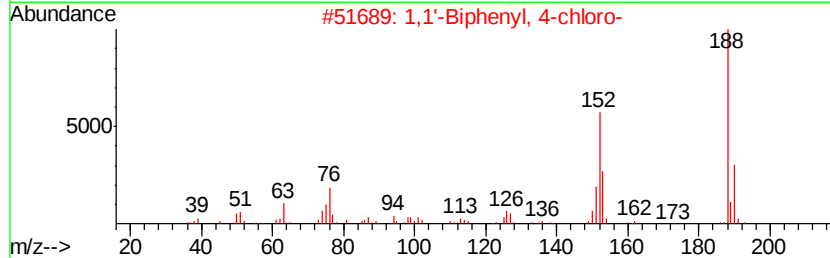
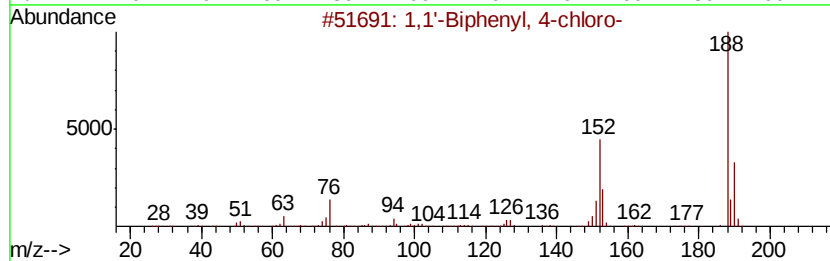
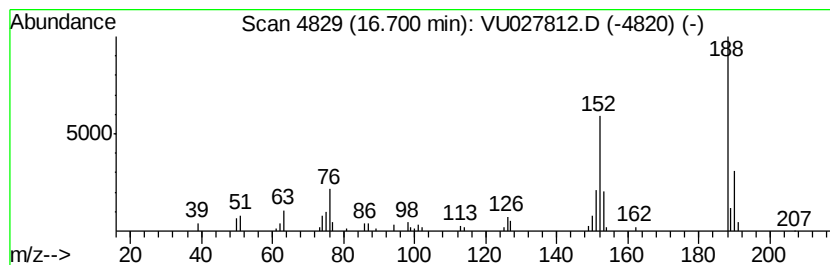
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 1,1'-Biphenyl, 4-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	6.39 ug/L	42572	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	94
2		1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	93
3		1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	93
4		3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	87
5		1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU102518\
Data File : VU027812.D
Acq On : 25 Oct 2018 20:26
Operator : MD/SY
Sample : J5657-01ME 20X
Misc : 4.65g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G4ME

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-...	12.29	13.7	ug/L	91574	3	11.48	333303	50.0
1,1'-Biphenyl, 2,...	14.58	3.1	ug/L	20749	3	11.48	333303	50.0
Butylated Hydroxy...	16.55	83.5	ug/L	556453	3	11.48	333303	50.0
1,1'-Biphenyl, 4-...	16.70	6.4	ug/L	42572	3	11.48	333303	50.0