

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
 Data File : VU027834.D
 Acq On : 26 Oct 2018 15:28
 Operator : MD/SY
 Sample : J5668-08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETBR3

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	1.402	64	71	86	rBV2	82839	92391	21.45%	2.209%
2	1.681	151	158	173	rVB	40461	53103	12.33%	1.269%
3	2.276	332	343	354	rBV	83466	127203	29.53%	3.041%
4	2.447	386	396	413	rVB2	5927	10699	2.48%	0.256%
5	2.620	447	450	453	rVB2	244	173	0.04%	0.004%
6	2.845	510	520	526	rVB2	502	913	0.21%	0.022%
7	2.987	557	564	579	rVB3	1419	2370	0.55%	0.057%
8	3.453	699	709	717	rVB2	833	1592	0.37%	0.038%
9	3.813	819	821	824	rBB	135	94	0.02%	0.002%
10	3.836	825	828	831	rBV	179	182	0.04%	0.004%
11	4.183	922	936	938	rBV	51668	84974	19.72%	2.031%
12	4.446	1014	1018	1019	rBV	170	143	0.03%	0.003%
13	4.591	1060	1063	1065	rBV	394	320	0.07%	0.008%
14	4.652	1065	1082	1113	rVB	72394	170783	39.64%	4.083%
15	4.762	1113	1116	1118	rBV2	195	150	0.03%	0.004%
16	4.803	1124	1129	1132	rBV2	182	203	0.05%	0.005%
17	4.916	1160	1164	1174	rVB3	675	954	0.22%	0.023%
18	5.054	1204	1207	1210	rVB2	172	148	0.03%	0.004%
19	5.109	1220	1224	1231	rVB	247	167	0.04%	0.004%
20	5.344	1273	1297	1323	rBV3	143262	430814	100.00%	10.299%
21	5.691	1401	1405	1408	rBV	164	176	0.04%	0.004%
22	5.720	1411	1414	1417	rVV	217	197	0.05%	0.005%
23	5.771	1428	1430	1433	rBV	226	183	0.04%	0.004%
24	5.797	1435	1438	1442	rBV2	174	158	0.04%	0.004%
25	5.890	1450	1467	1491	rBV	149306	296050	68.72%	7.077%
26	6.154	1546	1549	1550	rBV	159	110	0.03%	0.003%
27	6.189	1550	1560	1575	rVV2	15554	28824	6.69%	0.689%
28	6.247	1575	1578	1583	rVV	135	140	0.03%	0.003%
29	6.276	1584	1587	1591	rVV	113	105	0.02%	0.003%
30	6.334	1591	1605	1628	rVV	102770	204148	47.39%	4.880%
31	6.675	1703	1711	1713	rBV	193	307	0.07%	0.007%
32	6.864	1763	1770	1778	rVB4	1163	1857	0.43%	0.044%
33	7.122	1847	1850	1852	rVB	189	128	0.03%	0.003%
34	7.138	1852	1855	1857	rBV	144	123	0.03%	0.003%

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 Title : VOC Analysis

35	7.228	1872	1883	1903	rBV2	58045	103289	23.98%	2.469%
36	7.376	1926	1929	1930	rBV2	250	157	0.04%	0.004%
37	7.398	1933	1936	1939	rVB2	321	223	0.05%	0.005%
38	7.517	1969	1973	1976	rBV	113	96	0.02%	0.002%
39	7.565	1976	1988	2008	rBV	186989	325209	75.49%	7.774%
40	7.765	2046	2050	2053	rBV	89	92	0.02%	0.002%
41	7.851	2066	2077	2098	rVB	40508	68261	15.84%	1.632%
42	7.929	2098	2101	2104	rBV2	307	183	0.04%	0.004%
43	7.958	2108	2110	2112	rBV	182	125	0.03%	0.003%
44	8.183	2165	2180	2186	rBV2	35519	70239	16.30%	1.679%
45	8.228	2186	2194	2209	rVV	112440	246451	57.21%	5.892%
46	8.311	2212	2220	2247	rVB	178247	310557	72.09%	7.424%
47	8.523	2283	2286	2293	rBV	105	115	0.03%	0.003%
48	8.774	2360	2364	2369	rBV	148	134	0.03%	0.003%
49	8.958	2419	2421	2424	rBV	177	97	0.02%	0.002%
50	8.986	2428	2430	2433	rVB2	203	123	0.03%	0.003%
51	9.003	2433	2435	2440	rBV	167	124	0.03%	0.003%
52	9.038	2444	2446	2450	rBV2	192	117	0.03%	0.003%
53	9.089	2450	2462	2480	rBV	218654	353240	81.99%	8.444%
54	9.192	2492	2494	2496	rBV	208	107	0.02%	0.003%
55	9.305	2527	2529	2532	rBV4	392	300	0.07%	0.007%
56	9.787	2676	2679	2681	rBV2	268	195	0.05%	0.005%
57	9.957	2729	2732	2737	rVB2	386	256	0.06%	0.006%
58	9.986	2737	2741	2744	rBV	289	145	0.03%	0.003%
59	10.019	2749	2751	2756	rVB	189	108	0.03%	0.003%
60	10.430	2868	2879	2898	rBV	138164	218781	50.78%	5.230%
61	10.617	2925	2937	2952	rVB2	20316	42030	9.76%	1.005%
62	10.739	2972	2975	2978	rVB	175	105	0.02%	0.003%
63	10.871	3010	3016	3025	rVB2	1255	1682	0.39%	0.040%
64	11.485	3195	3207	3226	rBV	207423	323183	75.02%	7.726%
65	11.752	3285	3290	3299	rVB3	702	1050	0.24%	0.025%
66	11.861	3311	3324	3341	rBV	187629	296102	68.73%	7.079%
67	11.954	3349	3353	3356	rBV2	236	194	0.05%	0.005%
68	12.102	3395	3399	3402	rBV	234	205	0.05%	0.005%
69	12.285	3406	3456	3458	rBV7	29339	118104	27.41%	2.823%
70	12.613	3554	3558	3560	rBV2	363	254	0.06%	0.006%
71	12.629	3560	3563	3565	rVV3	194	153	0.04%	0.004%

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72	12.697	3581	3584	3587	rBB2	197	116	0.03%	0.003%
73	12.748	3597	3600	3604	rVB	215	136	0.03%	0.003%
74	12.771	3604	3607	3611	rBV	198	142	0.03%	0.003%
75	13.154	3722	3726	3727	rBV	266	196	0.05%	0.005%
76	13.186	3731	3736	3738	rBV2	447	451	0.10%	0.011%
77	13.398	3798	3802	3808	rBV2	241	227	0.05%	0.005%
78	13.436	3811	3814	3819	rBV	227	135	0.03%	0.003%
79	13.494	3829	3832	3835	rBV	178	150	0.03%	0.004%
80	13.620	3868	3871	3873	rBV	167	99	0.02%	0.002%
81	13.636	3873	3876	3886	rVB	368	292	0.07%	0.007%
82	13.768	3913	3917	3918	rBV	164	103	0.02%	0.002%
83	13.919	3962	3964	3967	rVB2	195	112	0.03%	0.003%
84	14.102	4018	4021	4025	rVB2	172	140	0.03%	0.003%
85	14.157	4035	4038	4042	rVB2	269	234	0.05%	0.006%
86	14.215	4042	4056	4057	rBV3	2294	3399	0.79%	0.081%
87	14.279	4069	4076	4090	rVB	20693	32975	7.65%	0.788%
88	14.356	4098	4100	4102	rBV	332	135	0.03%	0.003%
89	14.417	4115	4119	4121	rBV2	295	256	0.06%	0.006%
90	14.478	4136	4138	4142	rVB2	146	114	0.03%	0.003%
91	14.507	4145	4147	4149	rBV	204	102	0.02%	0.002%
92	14.597	4149	4175	4201	rBV5	19291	86273	20.03%	2.062%
93	14.825	4243	4246	4247	rBV2	234	148	0.03%	0.004%
94	14.896	4266	4268	4269	rBV2	270	120	0.03%	0.003%
95	15.350	4408	4409	4412	rBV	212	127	0.03%	0.003%
96	15.681	4498	4512	4529	rVB6	3730	10896	2.53%	0.260%
97	15.880	4564	4574	4585	rVB2	13526	21786	5.06%	0.521%
98	16.166	4661	4663	4667	rBV2	244	176	0.04%	0.004%
99	16.452	4739	4752	4765	rBV8	9851	32145	7.46%	0.768%
100	16.703	4828	4830	4832	rBV	439	245	0.06%	0.006%

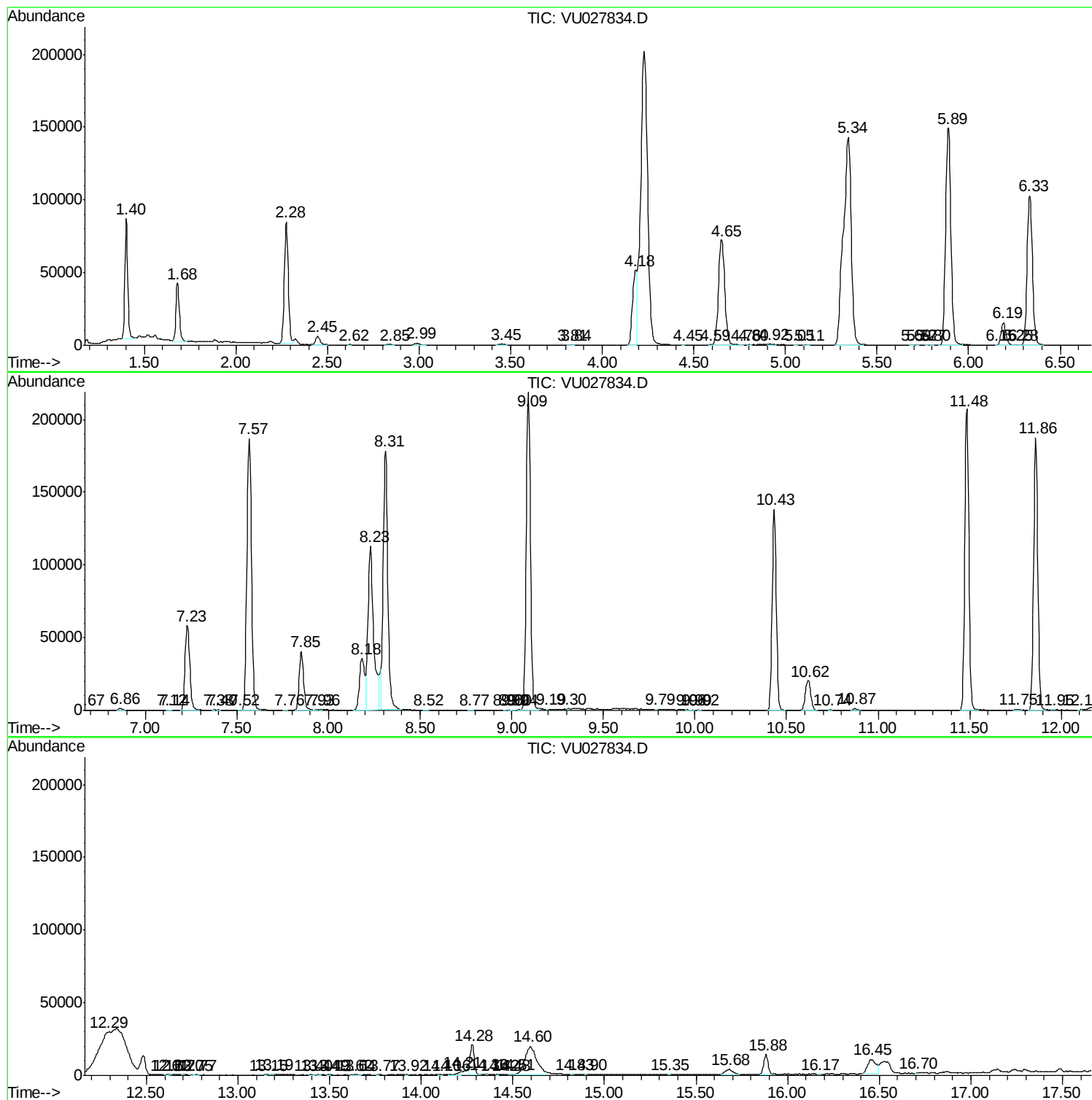
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
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ALS Vial : 18 Sample Multiplier: 1

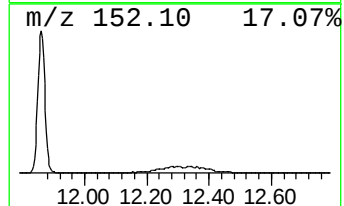
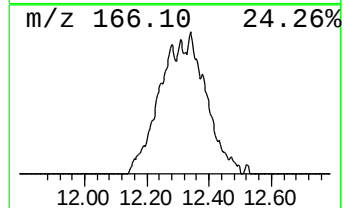
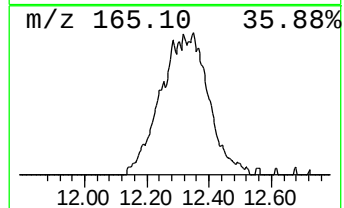
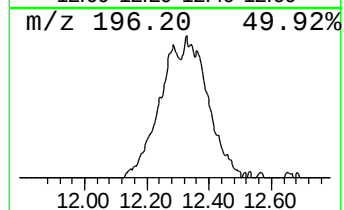
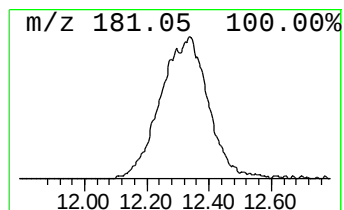
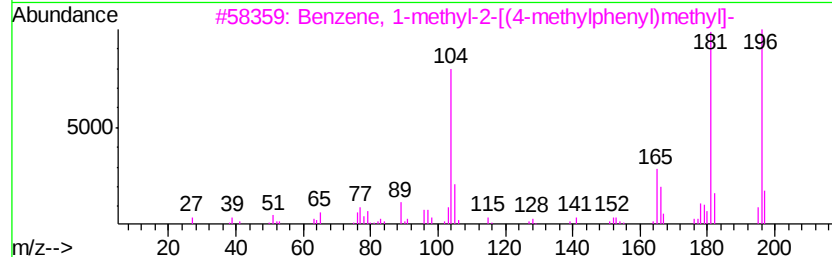
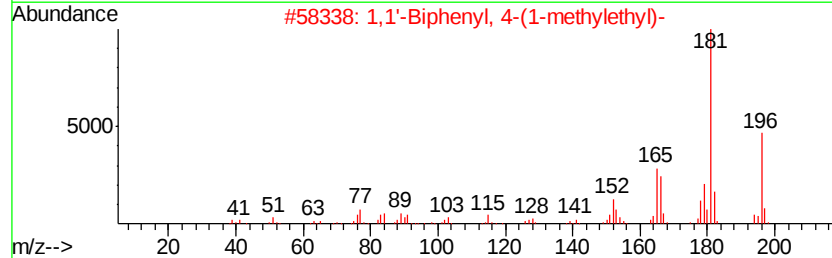
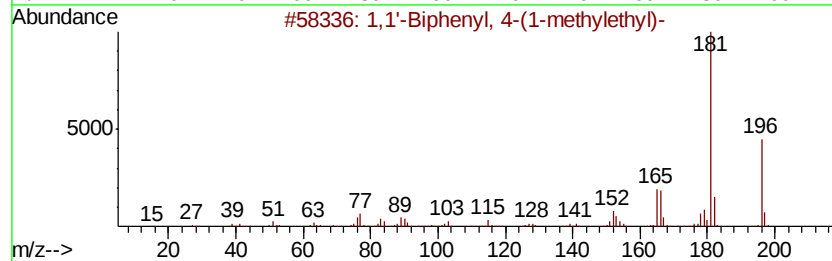
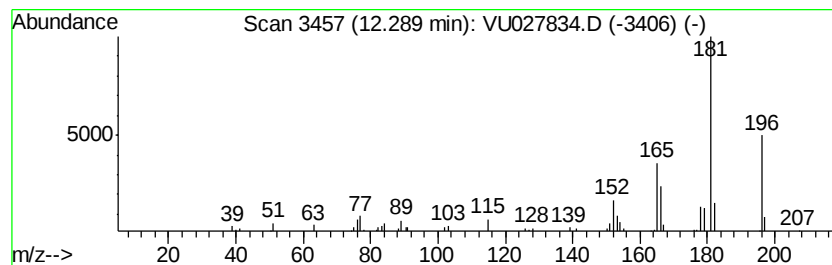
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.29	18.27 ug/L	118104	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	94
2	1,1'-Biphenyl, 4-(1-methylethyl)-	196	C15H16	007116-95-2	94
3	Benzene, 1-methyl-2-[(4-methylph...	196	C15H16	021895-17-0	91
4	Methane, di-p-tolyl-	196	C15H16	004957-14-6	91
5	Methane, di-p-tolyl-	196	C15H16	004957-14-6	87



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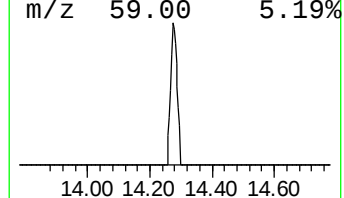
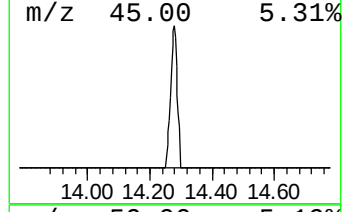
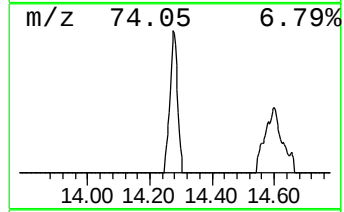
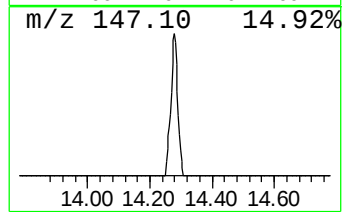
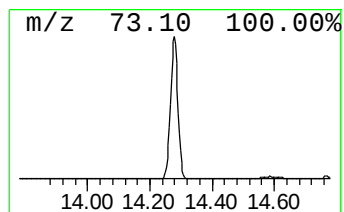
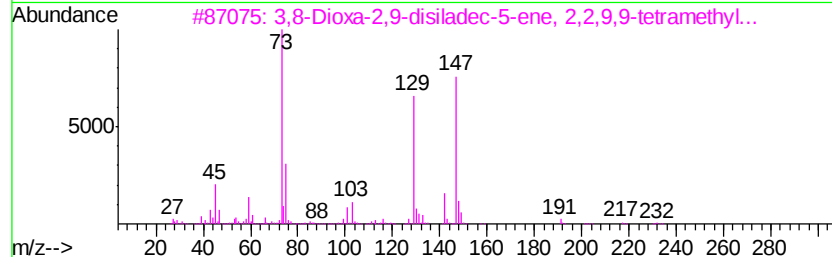
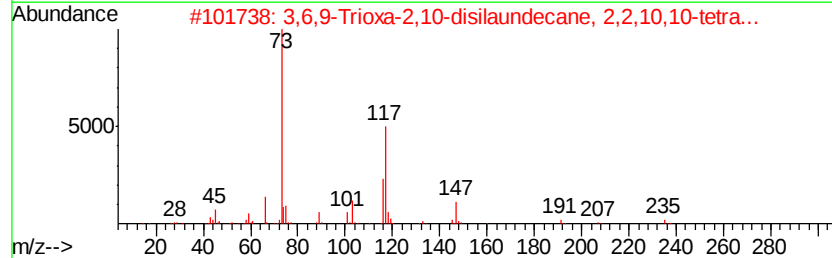
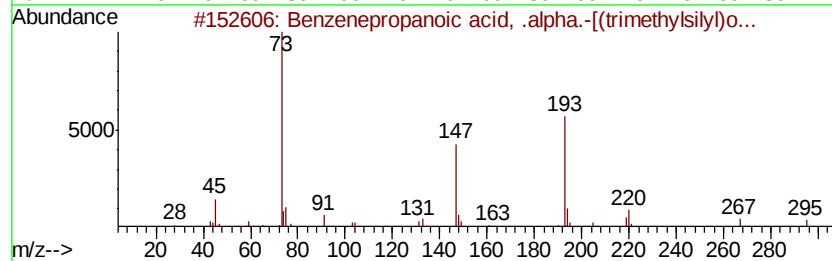
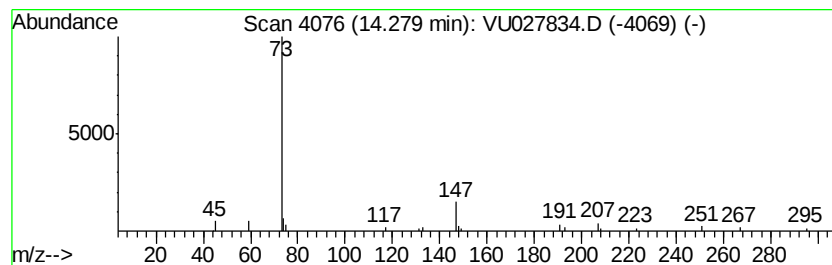
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzenepropanoic acid, .alp... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	5.10 ug/L	32975	1,4-Dichlorobenzene-d4	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenepropanoic acid, .alpha.-[...]	310	C15H26O3Si2	027750-45-4	50
2		3,6,9-Trioxa-2,10-disilaundecane...	250	C10H26O3Si2	016654-74-3	36
3		3,8-Dioxa-2,9-disiladec-5-ene, 2...	232	C10H24O2Si2	053326-59-3	28
4		Inosose, 2-desoxy-, 0-methvloxim...	479	C19H45N05Si4	1000149-50-8	28
5		3-Oxa-6-thia-2,7-disilaooctane, 2...	222	C8H22O5Si2	078921-31-0	23



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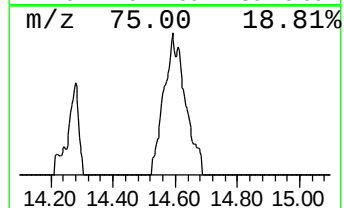
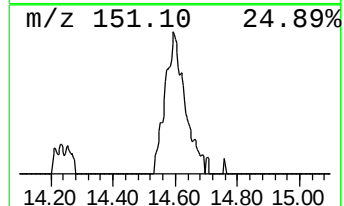
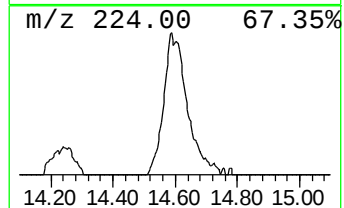
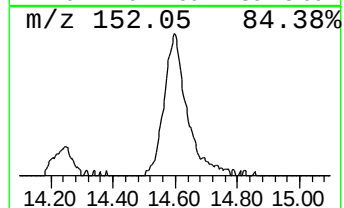
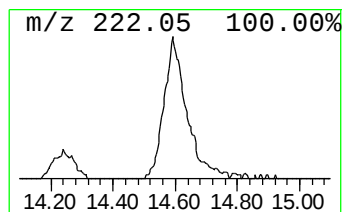
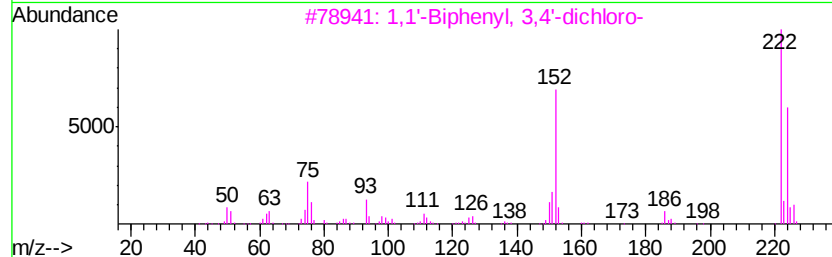
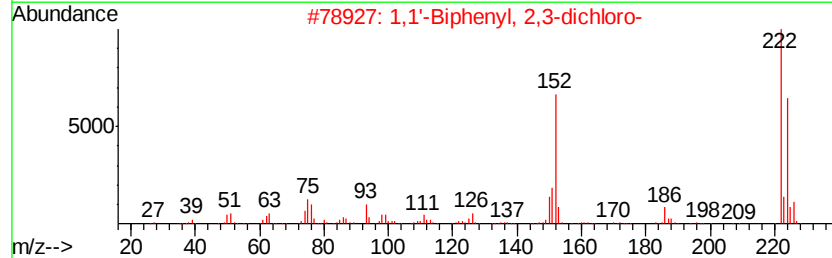
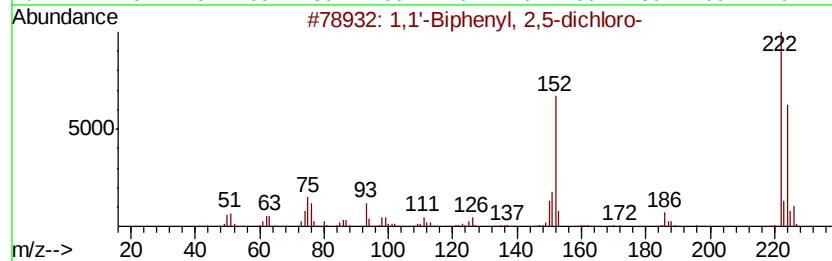
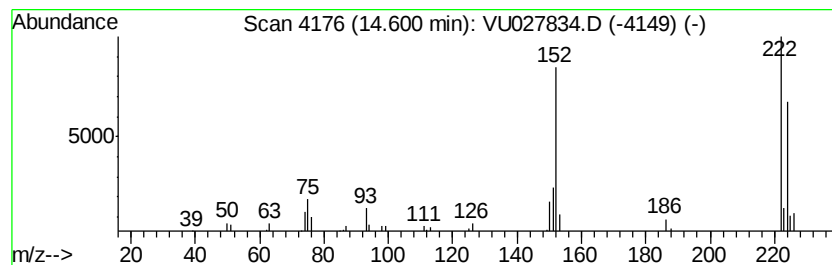
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 1,1'-Biphenyl, 2,5-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	13.35 ug/L	86273	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	99
2		1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	99
3		1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-90-5	99
4		1,1'-Biphenyl, 3,4-dichloro-	222	C12H8Cl2	002974-92-7	99
5		1,1'-Biphenyl, 2,6-dichloro-	222	C12H8Cl2	033146-45-1	99



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027834.D
Acq On : 26 Oct 2018 15:28
Operator : MD/SY
Sample : J5668-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBR3

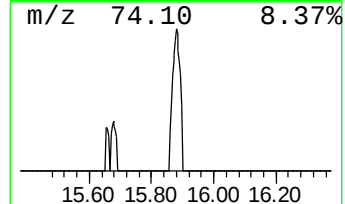
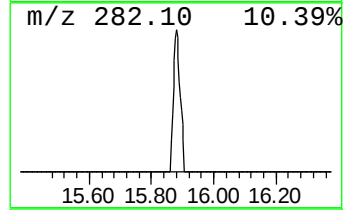
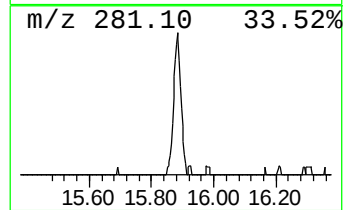
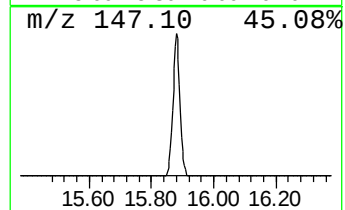
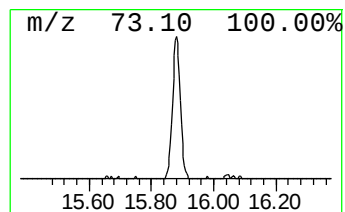
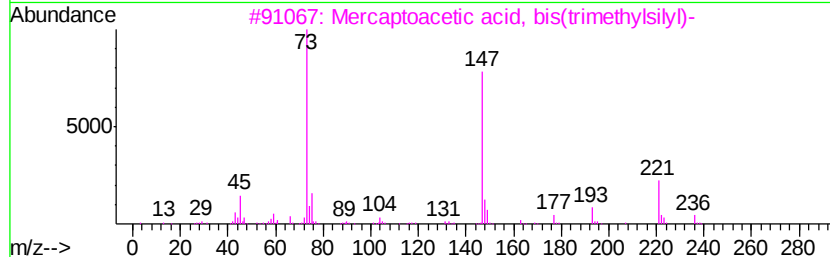
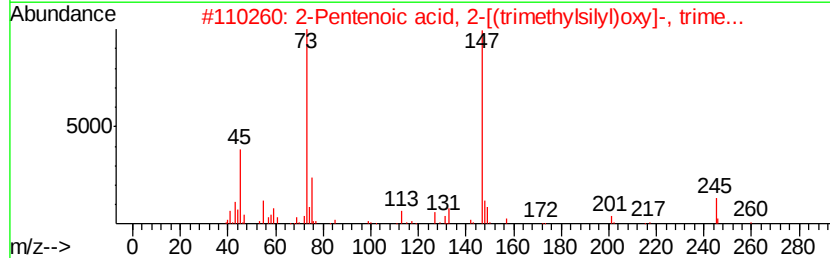
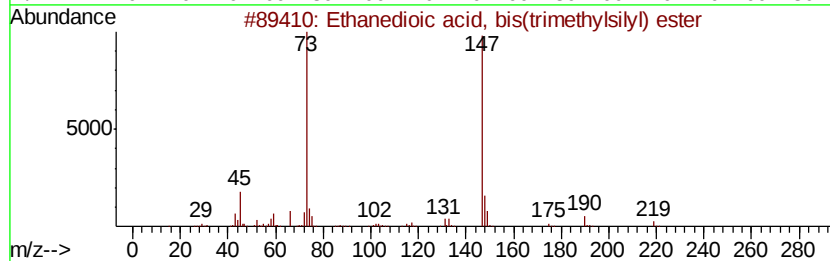
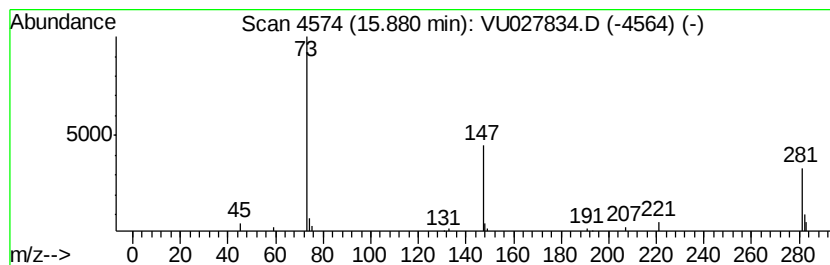
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.37 ug/L	21786	1,4-Dichlorobenzene-d4	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanedioic acid, bis(trimethyls...	234	C8H1804Si2	018294-04-7	28
2		2-Pentenoic acid, 2-[(trimethyls...	260	C11H2403Si2	055045-17-5	28
3		Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	23
4		Ethanedioic acid, bis(trimethyls...	234	C8H1804Si2	018294-04-7	23
5		2-Phenyl-1,2-bis(trimethylsilylo...	296	C15H2802Si2	294847-15-7	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027834.D
Acq On : 26 Oct 2018 15:28
Operator : MD/SY
Sample : J5668-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBR3

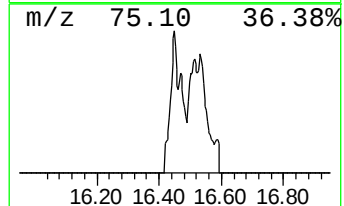
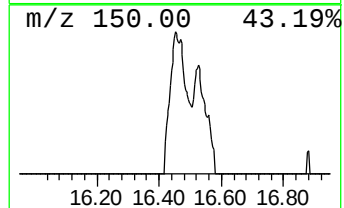
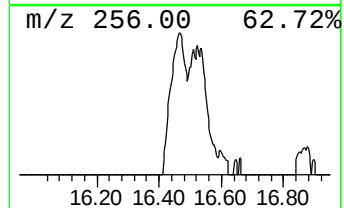
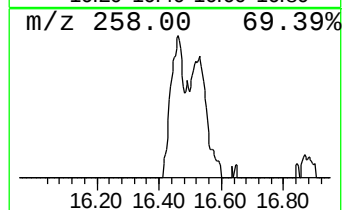
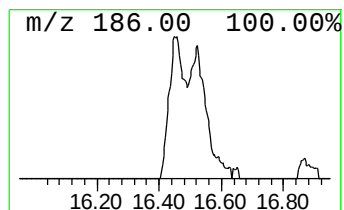
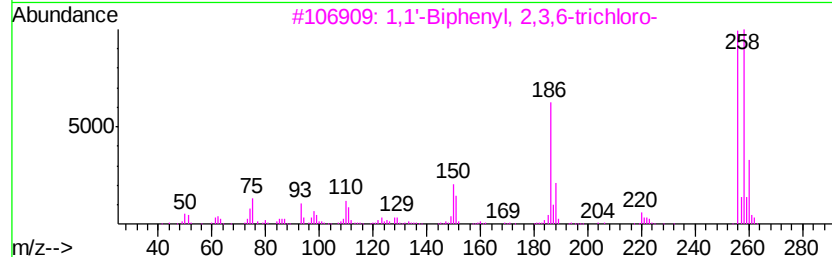
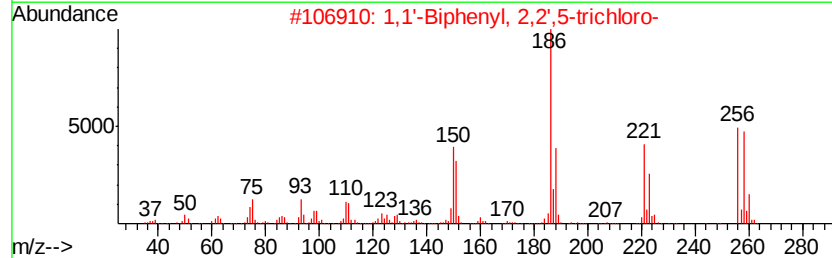
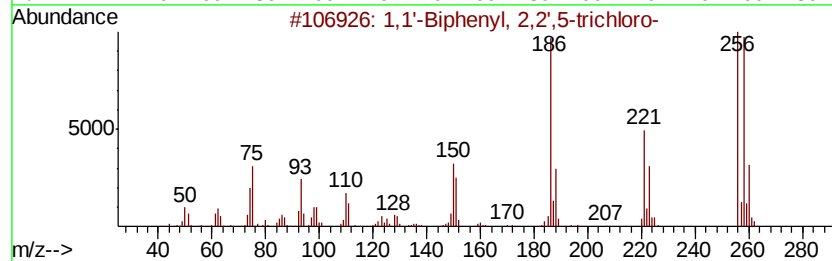
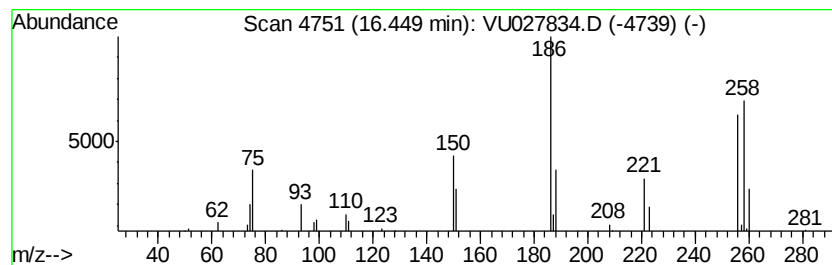
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 1,1'-Biphenyl, 2,2',5-trich... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	4.97 ug/L	32145	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	97
2		1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	96
3		1,1'-Biphenyl, 2,3,6-trichloro-	256	C12H7Cl3	055702-45-9	95
4		1,1'-Biphenyl, 2,3,3'-trichloro-	256	C12H7Cl3	038444-84-7	95
5		1,1'-Biphenyl, 3,4',5-trichloro-	256	C12H7Cl3	038444-88-1	95



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027834.D
Acq On : 26 Oct 2018 15:28
Operator : MD/SY
Sample : J5668-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBR3

Quant Method : Z:\VOASRV\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	18.3	ug/L	118104	3	11.48	323183	50.0
Benzenepropanoic ...	14.28	5.1	ug/L	32975	3	11.48	323183	50.0
1,1'-Biphenyl, 2,...	14.60	13.4	ug/L	86273	3	11.48	323183	50.0
unknown-01	15.88	3.4	ug/L	21786	3	11.48	323183	50.0
1,1'-Biphenyl, 2,...	16.45	5.0	ug/L	32145	3	11.48	323183	50.0