

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027815.D
 Acq On : 25 Oct 2018 21:58
 Operator : MD/SY
 Sample : J5635-23MEDL 100X
 Misc : 4.77g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40F9MEDL

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	82	rBV	42433	43323	7.98%	1.214%
2	1.681	150	158	169	rVB	31003	38735	7.13%	1.086%
3	2.086	282	284	287	rBV	339	237	0.04%	0.007%
4	2.125	294	296	301	rBV3	408	299	0.06%	0.008%
5	2.183	311	314	315	rBV2	607	394	0.07%	0.011%
6	2.231	327	329	332	rBV	228	148	0.03%	0.004%
7	2.276	332	343	356	rVV	66670	100133	18.44%	2.807%
8	2.630	448	453	457	rBV2	217	212	0.04%	0.006%
9	2.964	554	557	562	rBV	102	112	0.02%	0.003%
10	3.302	659	662	664	rBV	197	168	0.03%	0.005%
11	3.356	676	679	682	rBV	217	188	0.03%	0.005%
12	3.514	725	728	733	rVB	189	192	0.04%	0.005%
13	3.556	733	741	744	rBV	166	285	0.05%	0.008%
14	3.672	774	777	780	rVB	174	141	0.03%	0.004%
15	3.704	783	787	791	rBB	179	191	0.04%	0.005%
16	3.836	825	828	830	rBV	170	140	0.03%	0.004%
17	3.906	845	850	853	rBV	157	168	0.03%	0.005%
18	4.080	898	904	910	rBB	197	306	0.06%	0.009%
19	4.109	910	913	916	rBB	161	127	0.02%	0.004%
20	4.176	922	934	959	rBV2	31740	83966	15.46%	2.354%
21	4.385	996	999	1002	rBV2	169	124	0.02%	0.003%
22	4.588	1060	1062	1066	rVB	141	117	0.02%	0.003%
23	4.652	1066	1082	1105	rBV	55322	129766	23.90%	3.638%
24	4.848	1137	1143	1148	rBB	310	426	0.08%	0.012%
25	4.884	1148	1154	1157	rBV2	275	296	0.05%	0.008%
26	5.022	1191	1197	1200	rBB	173	209	0.04%	0.006%
27	5.067	1208	1211	1214	rBV	144	146	0.03%	0.004%
28	5.221	1254	1259	1262	rBV	140	185	0.03%	0.005%
29	5.344	1273	1297	1319	rBV3	108462	326849	60.19%	9.162%
30	5.504	1341	1347	1351	rBV	203	291	0.05%	0.008%
31	5.572	1365	1368	1370	rBV	210	157	0.03%	0.004%
32	5.643	1383	1390	1391	rBV2	291	306	0.06%	0.009%
33	5.887	1453	1466	1492	rBV2	128575	251676	46.35%	7.055%
34	6.057	1515	1519	1521	rBB2	253	143	0.03%	0.004%

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 Title : VOC Analysis

35	6.083	1521	1527	1529	rBV	148	207	0.04%	0.006%
36	6.115	1534	1537	1538	rBV	167	117	0.02%	0.003%
37	6.186	1556	1559	1564	rBB	168	162	0.03%	0.005%
38	6.215	1565	1568	1572	rBB	185	171	0.03%	0.005%
39	6.241	1573	1576	1578	rBV	141	119	0.02%	0.003%
40	6.334	1591	1605	1626	rVV2	78530	155355	28.61%	4.355%
41	6.520	1657	1663	1667	rBV	154	230	0.04%	0.006%
42	6.720	1723	1725	1730	rBV	133	162	0.03%	0.005%
43	6.855	1761	1767	1775	rBV3	908	1552	0.29%	0.044%
44	7.067	1830	1833	1837	rBB	197	185	0.03%	0.005%
45	7.228	1871	1883	1910	rVB	44114	77933	14.35%	2.185%
46	7.398	1932	1936	1941	rBB	150	149	0.03%	0.004%
47	7.427	1942	1945	1947	rBV	148	131	0.02%	0.004%
48	7.501	1965	1968	1973	rBB	171	185	0.03%	0.005%
49	7.565	1975	1988	2016	rVV	146968	256885	47.31%	7.201%
50	7.688	2023	2026	2029	rVB	263	176	0.03%	0.005%
51	7.774	2051	2053	2056	rBV	142	119	0.02%	0.003%
52	7.797	2056	2060	2063	rVV	143	119	0.02%	0.003%
53	7.851	2067	2077	2092	rVV2	31603	51701	9.52%	1.449%
54	8.183	2165	2180	2193	rBV	23044	58652	10.80%	1.644%
55	8.311	2211	2220	2242	rVB	115131	198220	36.50%	5.557%
56	8.482	2268	2273	2278	rBV	216	314	0.06%	0.009%
57	8.562	2292	2298	2301	rBV	180	226	0.04%	0.006%
58	8.614	2310	2314	2315	rBV	589	369	0.07%	0.010%
59	8.671	2329	2332	2333	rBV	157	109	0.02%	0.003%
60	8.729	2347	2350	2356	rBV	171	245	0.05%	0.007%
61	8.777	2361	2365	2369	rBV2	280	316	0.06%	0.009%
62	8.913	2404	2407	2410	rBV	152	117	0.02%	0.003%
63	8.983	2426	2429	2433	rBV2	228	201	0.04%	0.006%
64	9.012	2436	2438	2441	rVV2	274	150	0.03%	0.004%
65	9.089	2450	2462	2482	rBV	194166	316198	58.23%	8.864%
66	9.977	2735	2738	2740	rVB	174	118	0.02%	0.003%
67	10.430	2868	2879	2896	rBV	99429	156346	28.79%	4.383%
68	10.617	2924	2937	2949	rBV3	8423	17373	3.20%	0.487%
69	10.874	3010	3017	3025	rBV2	530	807	0.15%	0.023%
70	11.302	3148	3150	3158	rVB	142	158	0.03%	0.004%
71	11.485	3195	3207	3226	rVB	197431	315981	58.19%	8.858%

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 Title : VOC Analysis

72	11.568	3230	3233	3235	rVB2	186	109	0.02%	0.003%
73	11.861	3312	3324	3345	rVB	151435	240520	44.29%	6.742%
74	11.941	3345	3349	3352	rBV	247	154	0.03%	0.004%
75	12.019	3369	3373	3377	rBV	143	147	0.03%	0.004%
76	12.150	3409	3414	3416	rBV	238	239	0.04%	0.007%
77	12.182	3416	3424	3426	rBV2	917	1056	0.19%	0.030%
78	12.211	3427	3433	3435	rBV3	1368	1435	0.26%	0.040%
79	12.539	3533	3535	3538	rBV	129	115	0.02%	0.003%
80	12.842	3626	3629	3634	rVB	210	183	0.03%	0.005%
81	13.060	3694	3697	3702	rVB	149	133	0.02%	0.004%
82	13.160	3724	3728	3729	rBV	247	188	0.03%	0.005%
83	13.501	3822	3834	3855	rBV	345000	543000	100.00%	15.221%
84	13.642	3874	3878	3881	rBV3	236	228	0.04%	0.006%
85	13.716	3899	3901	3906	rVB	211	139	0.03%	0.004%
86	13.986	3974	3985	4000	rBV2	71761	113968	20.99%	3.195%
87	14.211	4045	4055	4058	rBV2	1060	1817	0.33%	0.051%
88	14.279	4069	4076	4085	rVB2	6270	9802	1.81%	0.275%
89	14.314	4085	4087	4090	rVB	407	181	0.03%	0.005%
90	14.465	4130	4134	4139	rVB	211	206	0.04%	0.006%
91	14.597	4149	4175	4190	rBV7	9477	35944	6.62%	1.008%
92	14.838	4247	4250	4254	rBV2	352	278	0.05%	0.008%
93	14.874	4259	4261	4264	rBV	223	165	0.03%	0.005%
94	15.102	4327	4332	4339	rBV2	299	513	0.09%	0.014%
95	15.137	4339	4343	4348	rBV	240	291	0.05%	0.008%
96	15.674	4504	4510	4512	rBV4	895	939	0.17%	0.026%
97	15.877	4569	4573	4584	rVB3	2060	3113	0.57%	0.087%
98	16.420	4740	4742	4743	rBV2	510	277	0.05%	0.008%
99	16.462	4743	4755	4766	rVV2	3971	10862	2.00%	0.304%
100	16.706	4823	4831	4843	rVB2	5950	9608	1.77%	0.269%

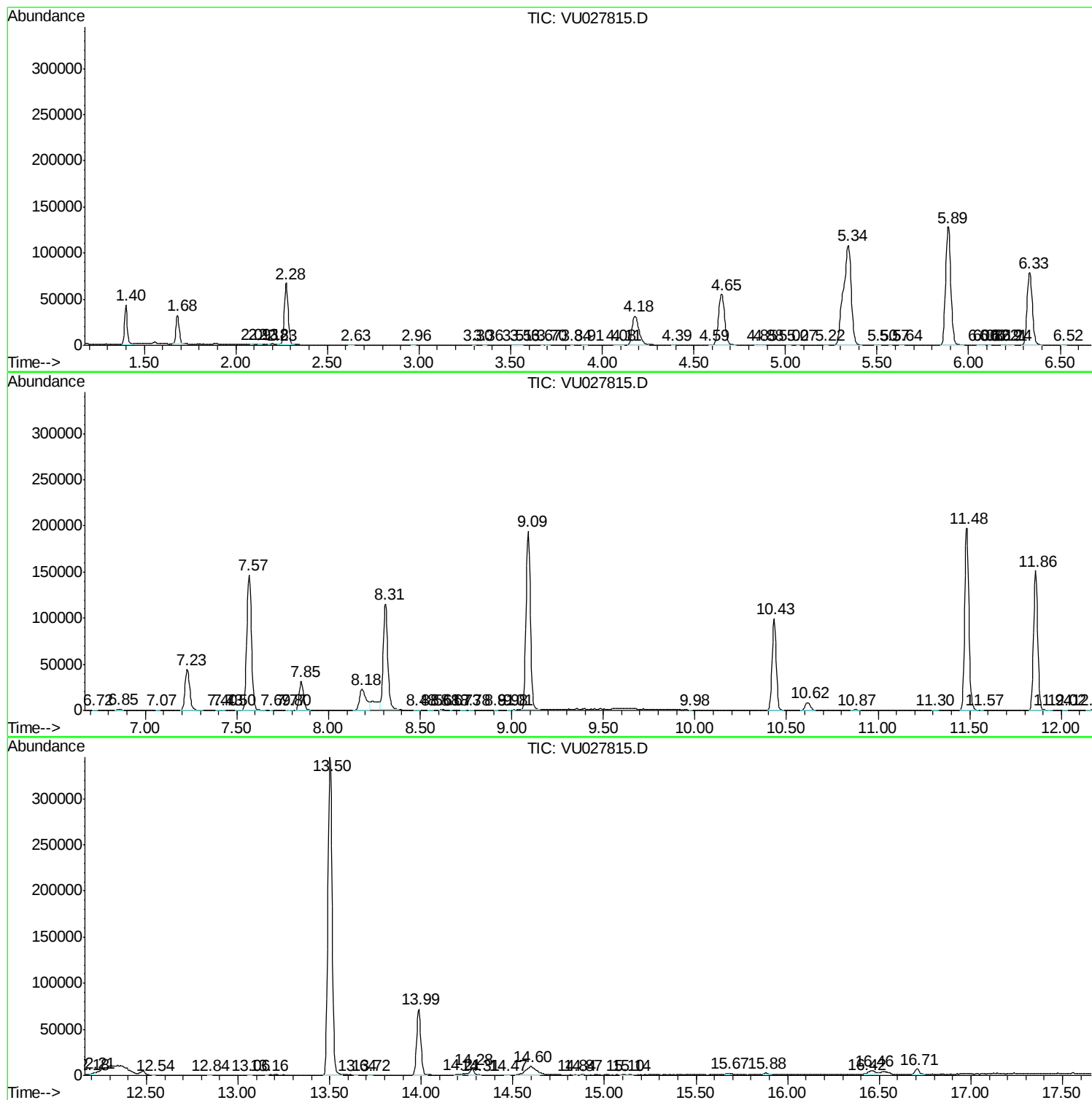
Sum of corrected areas: 3567324

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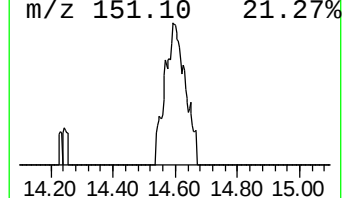
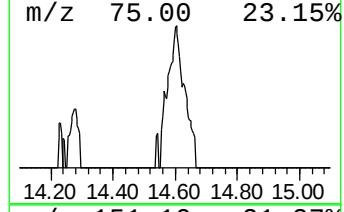
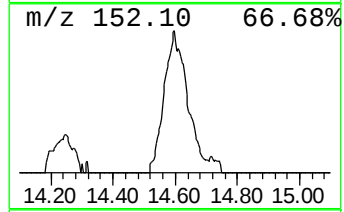
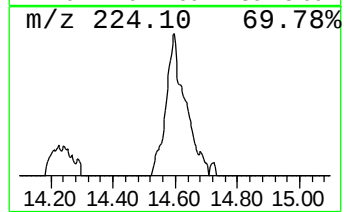
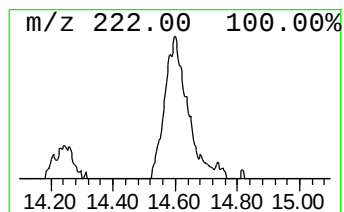
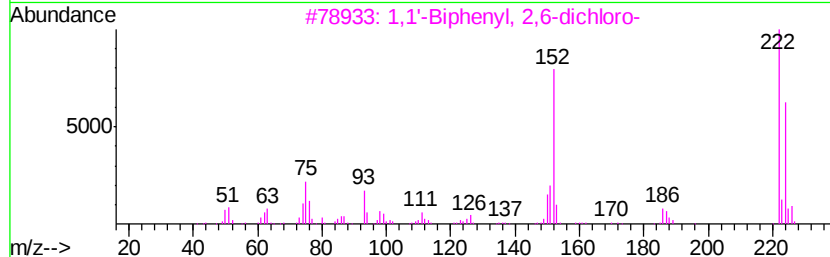
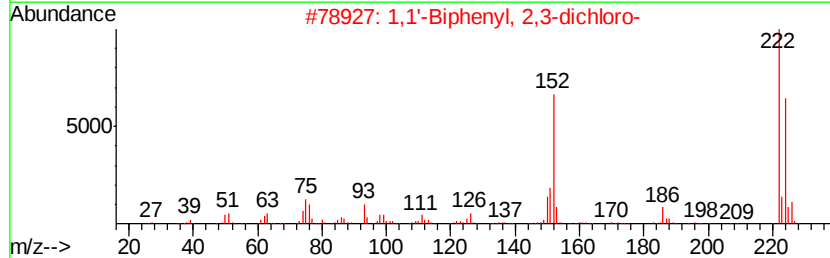
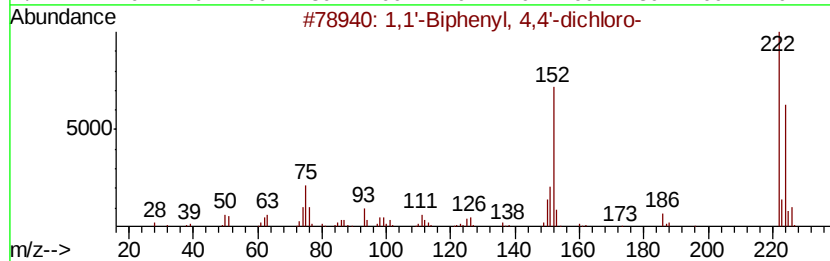
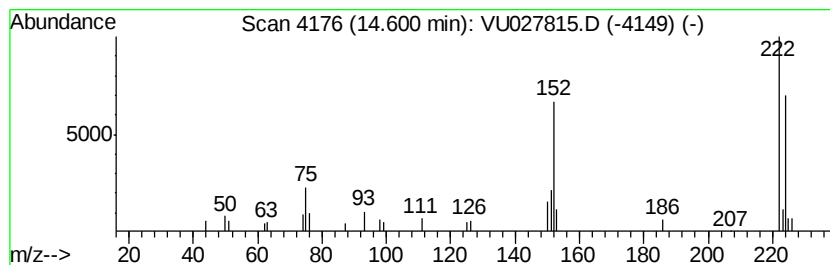
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	5.69 ug/L	35944	1,4-Dichlorobenzene-d4	11.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Biphenyl, 4,4'-dichloro-	222	C12H8Cl2	002050-68-2	97
2			1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	96
3			1,1'-Biphenyl, 2,6-dichloro-	222	C12H8Cl2	033146-45-1	95
4			1,1'-Biphenyl, 3,4-dichloro-	222	C12H8Cl2	002974-92-7	95
5			1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, 4,...	14.60	5.7	ug/L	35944	3	11.48	315981	50.0