

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040919\
 Data File : VU030906.D
 Acq On : 08 Apr 2019 15:24
 Operator : JC/SP
 Sample : K2277-21ME
 Misc : 5.69g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BF2R5ME

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\SOMULM040519WMA.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	1.174	21	26	34	rVB2	21403	20215	0.46%	0.056%
2	1.389	86	93	109	rBV	513490	565286	12.87%	1.579%
3	1.637	164	170	194	rVB	607961	781946	17.80%	2.184%
4	2.167	330	335	341	rVB2	11744	14362	0.33%	0.040%
5	2.248	349	360	374	rVB	925561	1402663	31.93%	3.918%
6	2.553	449	455	458	rVB4	1172	941	0.02%	0.003%
7	2.579	461	463	468	rVB2	1335	914	0.02%	0.003%
8	2.605	468	471	474	rBV4	998	847	0.02%	0.002%
9	2.678	487	494	513	rBV7	4351	10105	0.23%	0.028%
10	2.746	513	515	520	rVB2	981	608	0.01%	0.002%
11	2.785	524	527	530	rBV2	675	616	0.01%	0.002%
12	2.823	534	539	542	rBV3	2012	2025	0.05%	0.006%
13	2.945	570	577	581	rBV7	1024	1292	0.03%	0.004%
14	2.968	581	584	588	rVV3	547	498	0.01%	0.001%
15	3.206	655	658	661	rVB3	960	680	0.02%	0.002%
16	3.235	661	667	670	rBV3	826	827	0.02%	0.002%
17	3.286	675	683	688	rBV6	1605	2074	0.05%	0.006%
18	3.415	721	723	727	rBV3	1055	759	0.02%	0.002%
19	3.431	727	728	732	rVV	843	481	0.01%	0.001%
20	3.531	754	759	760	rBV	955	710	0.02%	0.002%
21	3.559	766	768	774	rBV2	780	576	0.01%	0.002%
22	3.704	810	813	816	rBV	760	712	0.02%	0.002%
23	3.752	824	828	831	rBV2	669	602	0.01%	0.002%
24	3.804	838	844	849	rVB3	483	532	0.01%	0.001%
25	3.855	858	860	864	rVB3	854	602	0.01%	0.002%
26	3.900	867	874	877	rVB3	674	682	0.02%	0.002%
27	4.174	945	959	997	rBV	483659	1409501	32.09%	3.937%
28	4.505	1057	1062	1068	rVB6	954	1069	0.02%	0.003%
29	4.637	1085	1103	1128	rBV	687255	1710835	38.95%	4.779%
30	4.971	1204	1207	1209	rVV4	1098	604	0.01%	0.002%
31	5.090	1240	1244	1248	rBV5	813	564	0.01%	0.002%
32	5.199	1275	1278	1281	rVB2	788	544	0.01%	0.002%
33	5.328	1292	1318	1347	rBV2	1485741	4392632	100.00%	12.270%
34	5.775	1455	1457	1462	rVB5	676	512	0.01%	0.001%

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 Title : VOC Analysis

35	5.878	1473	1489	1518	rBV	1403245	2784867	63.40%	7.779%
36	6.177	1573	1582	1596	rVB10	17370	39846	0.91%	0.111%
37	6.325	1613	1628	1658	rBV	1000010	2032876	46.28%	5.678%
38	6.701	1743	1745	1750	rVB3	992	618	0.01%	0.002%
39	6.794	1771	1774	1779	rVB3	1053	814	0.02%	0.002%
40	6.820	1779	1782	1786	rBV	639	537	0.01%	0.001%
41	6.868	1791	1797	1799	rBV5	1059	1056	0.02%	0.003%
42	6.878	1799	1800	1803	rVV2	1064	816	0.02%	0.002%
43	6.907	1806	1809	1814	rBV4	1107	1146	0.03%	0.003%
44	7.022	1842	1845	1847	rVV2	855	542	0.01%	0.002%
45	7.045	1847	1852	1854	rVB4	722	519	0.01%	0.001%
46	7.100	1866	1869	1873	rBV2	577	503	0.01%	0.001%
47	7.148	1881	1884	1887	rBV3	711	487	0.01%	0.001%
48	7.222	1894	1907	1936	rBV	558834	1002820	22.83%	2.801%
49	7.559	1998	2012	2031	rBV	1936189	3355808	76.40%	9.374%
50	7.845	2086	2101	2120	rBV	407936	697771	15.89%	1.949%
51	8.019	2152	2155	2158	rBV4	1157	851	0.02%	0.002%
52	8.035	2158	2160	2163	rVB4	1373	758	0.02%	0.002%
53	8.167	2194	2201	2205	rBV6	1574	2140	0.05%	0.006%
54	8.225	2209	2219	2232	rVB2	39978	63528	1.45%	0.177%
55	8.308	2234	2245	2286	rBV	1763602	3080741	70.13%	8.605%
56	8.656	2351	2353	2357	rBV4	1309	786	0.02%	0.002%
57	8.707	2366	2369	2372	rVB3	942	541	0.01%	0.002%
58	8.794	2393	2396	2399	rBV3	1014	720	0.02%	0.002%
59	9.032	2466	2470	2474	rBV4	1083	955	0.02%	0.003%
60	9.087	2474	2487	2514	rBV	2109824	3495339	79.57%	9.763%
61	9.418	2588	2590	2592	rBV3	1064	549	0.01%	0.002%
62	9.447	2596	2599	2602	rVV3	1078	766	0.02%	0.002%
63	9.485	2609	2611	2617	rVB4	885	639	0.01%	0.002%
64	9.598	2643	2646	2650	rBV3	827	781	0.02%	0.002%
65	9.759	2692	2696	2702	rBV5	958	1148	0.03%	0.003%
66	9.974	2759	2763	2766	rVB4	721	539	0.01%	0.002%
67	10.080	2792	2796	2799	rBV3	675	508	0.01%	0.001%
68	10.122	2804	2809	2812	rBV3	736	789	0.02%	0.002%
69	10.186	2826	2829	2834	rBV4	770	761	0.02%	0.002%
70	10.267	2850	2854	2859	rBV3	578	687	0.02%	0.002%
71	10.337	2874	2876	2880	rVB3	735	487	0.01%	0.001%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

72	10.427	2891	2904	2928	rBV	1517084	2452223	55.83%	6.850%
73	10.601	2951	2958	2967	rBV7	4982	8046	0.18%	0.022%
74	10.704	2987	2990	2992	rBV2	891	570	0.01%	0.002%
75	10.797	3017	3019	3022	rVV3	997	707	0.02%	0.002%
76	10.813	3022	3024	3028	rVB3	959	611	0.01%	0.002%
77	10.951	3063	3067	3073	rVB4	1022	1293	0.03%	0.004%
78	10.980	3073	3076	3079	rBV3	871	692	0.02%	0.002%
79	11.086	3103	3109	3113	rBV6	1729	1626	0.04%	0.005%
80	11.334	3183	3186	3189	rBV2	714	505	0.01%	0.001%
81	11.363	3190	3195	3197	rBV3	1131	903	0.02%	0.003%
82	11.395	3201	3205	3206	rBV2	2139	1193	0.03%	0.003%
83	11.479	3219	3231	3256	rBV	2047999	3248566	73.95%	9.074%
84	11.855	3336	3348	3370	rBV	1910674	3133071	71.33%	8.751%
85	12.160	3440	3443	3447	rBV3	1670	1633	0.04%	0.005%
86	12.476	3533	3541	3555	rVB3	8716	16361	0.37%	0.046%
87	12.640	3589	3592	3598	rVB5	1643	1495	0.03%	0.004%
88	12.672	3599	3602	3605	rVB3	1362	794	0.02%	0.002%
89	12.691	3605	3608	3610	rBV3	1425	1122	0.03%	0.003%
90	12.861	3658	3661	3665	rBV3	1443	1173	0.03%	0.003%
91	12.884	3666	3668	3671	rVB3	1269	665	0.02%	0.002%
92	13.006	3704	3706	3714	rVB5	1287	1313	0.03%	0.004%
93	13.041	3714	3717	3720	rBV2	892	532	0.01%	0.001%
94	13.115	3738	3740	3744	rVB5	1409	653	0.01%	0.002%
95	13.312	3798	3801	3807	rBV6	1034	911	0.02%	0.003%
96	13.482	3849	3854	3858	rBV2	1351	1718	0.04%	0.005%
97	13.742	3933	3935	3939	rBV5	903	671	0.02%	0.002%
98	13.971	4003	4006	4009	rBV	1216	1041	0.02%	0.003%
99	14.273	4091	4100	4113	rBV2	9410	15924	0.36%	0.044%
100	14.681	4223	4227	4234	rBV6	1452	1714	0.04%	0.005%

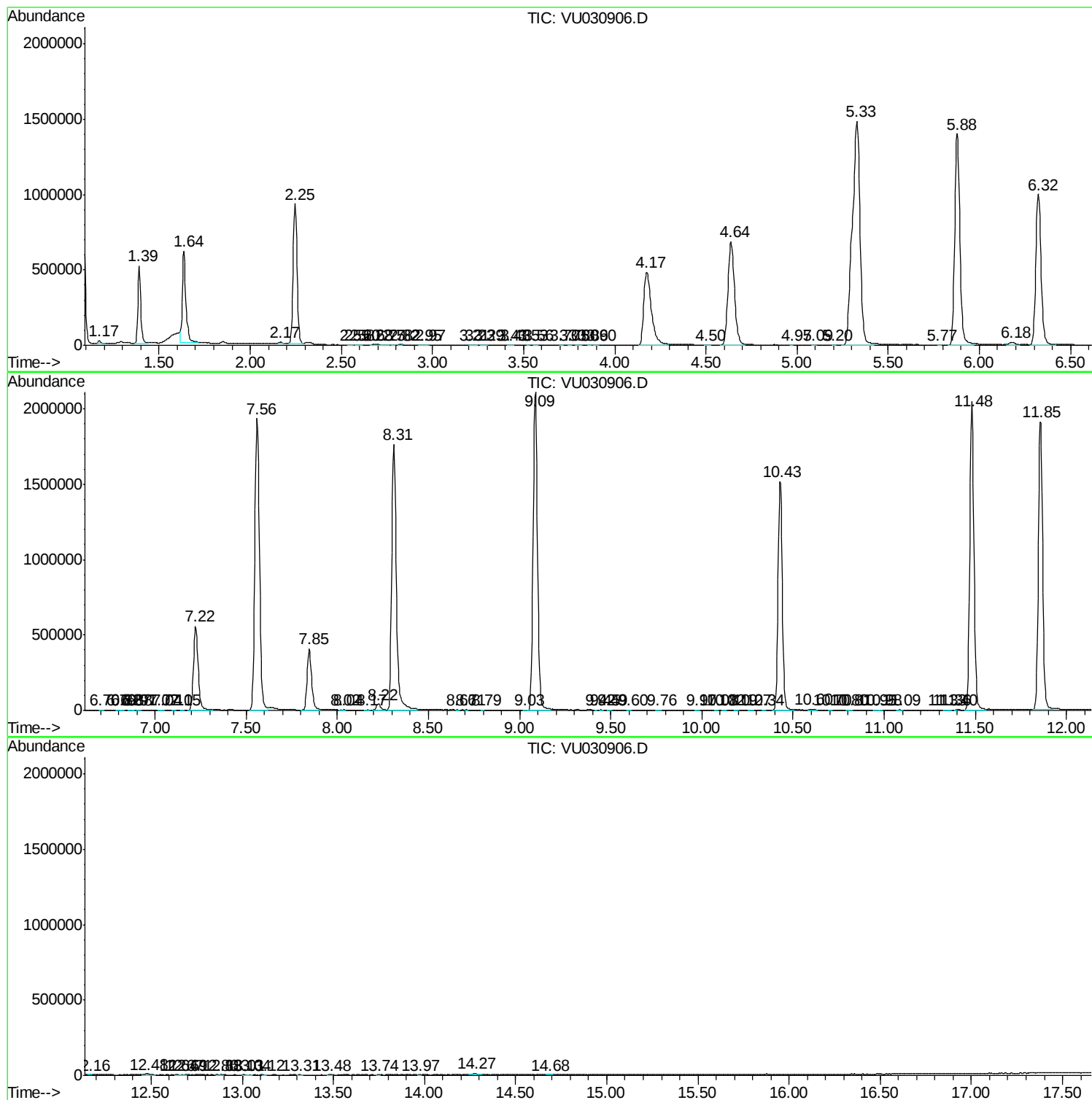
Sum of corrected areas: 35800581

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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



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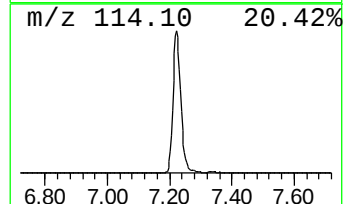
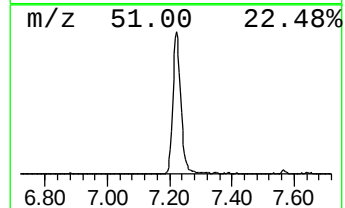
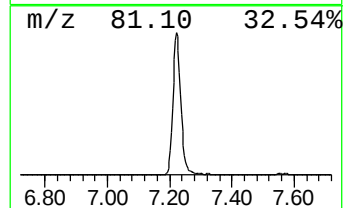
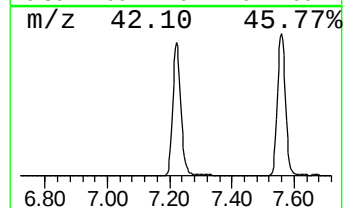
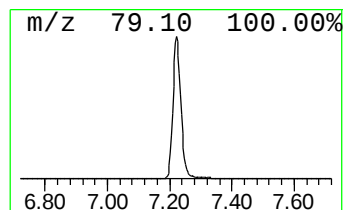
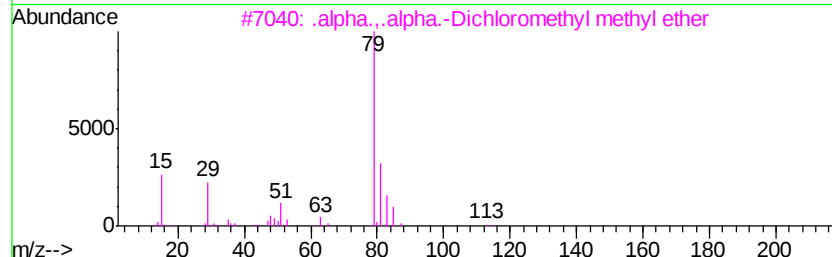
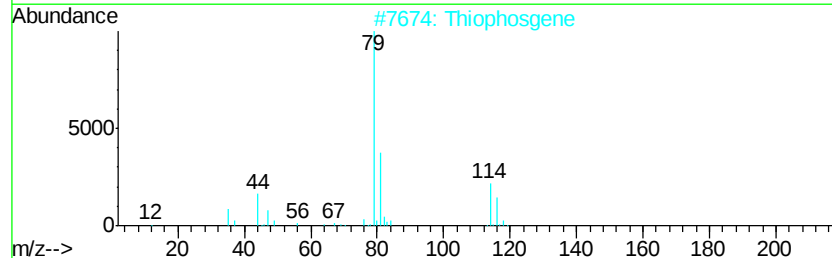
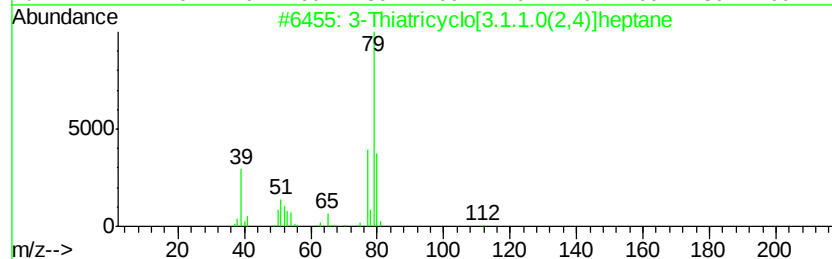
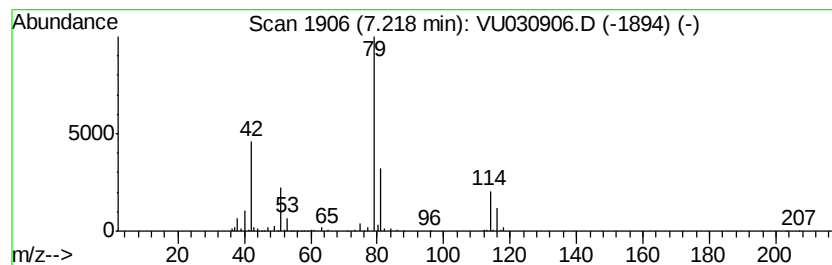
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	18.00 ug/L	1002820	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	32
2		Thiophosgene	114	CCl2S	000463-71-8	28
3		.alpha.,.alpha.-Dichloromethyl m...	114	C2H4Cl2O	004885-02-3	25
4		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
5		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.22	18.0	ug/L	1002820	1	5.88	2784870	50.0