

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121818\
 Data File : VU028769.D
 Acq On : 18 Dec 2018 14:52
 Operator : MD/SY
 Sample : J6441-03
 Misc : 5.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE814

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.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	1.395	62	69	84	rVB	89214	98704	15.56%	1.887%
2	1.640	141	145	154	rVB	60436	59356	9.36%	1.135%
3	2.238	321	331	346	rBV	141874	209907	33.08%	4.014%
4	2.829	508	515	525	rVB3	2233	4385	0.69%	0.084%
5	2.926	542	545	549	rBV	192	104	0.02%	0.002%
6	3.006	567	570	575	rBV	225	233	0.04%	0.004%
7	3.167	615	620	623	rBV2	181	205	0.03%	0.004%
8	3.199	628	630	634	rVB	161	133	0.02%	0.003%
9	3.276	646	654	664	rVB5	934	1665	0.26%	0.032%
10	3.318	664	667	669	rBV	215	116	0.02%	0.002%
11	3.341	669	674	676	rBV	122	94	0.01%	0.002%
12	3.370	681	683	686	rVV	211	99	0.02%	0.002%
13	3.386	686	688	692	rVB	155	97	0.02%	0.002%
14	3.453	704	709	713	rBV2	227	175	0.03%	0.003%
15	3.550	736	739	743	rVB2	172	157	0.02%	0.003%
16	3.572	743	746	749	rBV	174	97	0.02%	0.002%
17	3.707	786	788	792	rVV	179	88	0.01%	0.002%
18	3.730	792	795	799	rVB	219	180	0.03%	0.003%
19	3.759	799	804	808	rVB	167	162	0.03%	0.003%
20	3.855	830	834	839	rBV	138	150	0.02%	0.003%
21	3.971	866	870	872	rBV2	513	349	0.06%	0.007%
22	4.099	907	910	914	rVB2	185	136	0.02%	0.003%
23	4.189	922	938	981	rBV	44766	152014	23.96%	2.907%
24	4.505	1030	1036	1038	rBV	115	129	0.02%	0.002%
25	4.550	1048	1050	1056	rVB	200	115	0.02%	0.002%
26	4.640	1060	1078	1104	rVV	94973	230701	36.36%	4.411%
27	4.755	1110	1114	1117	rBV2	258	154	0.02%	0.003%
28	4.771	1117	1119	1125	rVB	239	172	0.03%	0.003%
29	4.858	1144	1146	1148	rBV	166	94	0.01%	0.002%
30	4.881	1148	1153	1161	rVB2	426	540	0.09%	0.010%
31	4.919	1161	1165	1167	rBV	136	101	0.02%	0.002%
32	4.948	1170	1174	1179	rVB	144	155	0.02%	0.003%
33	5.119	1223	1227	1229	rBV2	175	114	0.02%	0.002%
34	5.189	1245	1249	1252	rBV	137	122	0.02%	0.002%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.M
 Title : VOC Analysis

35	5.328	1269	1292	1324	rBV2	225380	634452	100.00%	12.132%
36	5.614	1375	1381	1390	rVB4	1144	1884	0.30%	0.036%
37	5.784	1431	1434	1437	rVB	257	150	0.02%	0.003%
38	5.826	1443	1447	1448	rBV	200	123	0.02%	0.002%
39	5.881	1450	1464	1484	rBV	221632	444389	70.04%	8.497%
40	6.090	1527	1529	1535	rBV3	229	234	0.04%	0.004%
41	6.141	1541	1545	1547	rBV2	175	147	0.02%	0.003%
42	6.167	1551	1553	1555	rBV2	366	198	0.03%	0.004%
43	6.241	1569	1576	1588	rBV5	1595	3189	0.50%	0.061%
44	6.324	1588	1602	1627	rVB	138288	288495	45.47%	5.516%
45	6.440	1634	1638	1639	rVB2	241	127	0.02%	0.002%
46	6.456	1640	1643	1644	rBV2	232	112	0.02%	0.002%
47	6.485	1650	1652	1656	rVB	227	124	0.02%	0.002%
48	6.585	1680	1683	1685	rBV	229	108	0.02%	0.002%
49	6.623	1693	1695	1699	rVB	257	134	0.02%	0.003%
50	6.762	1732	1738	1742	rBV	227	178	0.03%	0.003%
51	6.849	1762	1765	1767	rBV2	140	89	0.01%	0.002%
52	6.890	1768	1778	1784	rVB4	757	1183	0.19%	0.023%
53	6.942	1790	1794	1797	rBV	123	95	0.01%	0.002%
54	7.038	1820	1824	1825	rBV	153	91	0.01%	0.002%
55	7.154	1857	1860	1869	rVB	172	137	0.02%	0.003%
56	7.225	1869	1882	1906	rBV	78648	149844	23.62%	2.865%
57	7.357	1921	1923	1926	rBV2	215	139	0.02%	0.003%
58	7.562	1972	1987	2004	rBV	284985	509689	80.34%	9.746%
59	7.771	2050	2052	2055	rVB2	174	110	0.02%	0.002%
60	7.848	2065	2076	2099	rBV	52211	100319	15.81%	1.918%
61	7.942	2103	2105	2109	rVB	367	199	0.03%	0.004%
62	8.000	2121	2123	2125	rBV2	261	127	0.02%	0.002%
63	8.025	2128	2131	2133	rVV3	271	132	0.02%	0.003%
64	8.038	2133	2135	2139	rVB	286	176	0.03%	0.003%
65	8.064	2139	2143	2145	rBV	108	94	0.01%	0.002%
66	8.228	2191	2194	2197	rBV	168	128	0.02%	0.002%
67	8.321	2210	2223	2252	rVV	201703	383851	60.50%	7.340%
68	8.524	2283	2286	2288	rBV	288	118	0.02%	0.002%
69	8.569	2297	2300	2304	rVB	221	137	0.02%	0.003%
70	8.598	2306	2309	2312	rVV2	268	146	0.02%	0.003%
71	8.630	2314	2319	2325	rBV2	995	1020	0.16%	0.020%

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 Title : VOC Analysis

72	8.675	2330	2333	2338	rVB3	264	215	0.03%	0.004%
73	8.749	2354	2356	2362	rVB	220	113	0.02%	0.002%
74	8.893	2398	2401	2406	rVB2	284	240	0.04%	0.005%
75	9.090	2448	2462	2491	rBV	321110	561766	88.54%	10.742%
76	9.250	2509	2512	2517	rBV2	244	281	0.04%	0.005%
77	9.299	2524	2527	2531	rVB	235	160	0.03%	0.003%
78	9.331	2531	2537	2540	rBV2	230	198	0.03%	0.004%
79	9.373	2547	2550	2551	rBV	327	207	0.03%	0.004%
80	9.453	2571	2575	2580	rBV2	232	237	0.04%	0.005%
81	9.617	2620	2626	2629	rBV	114	145	0.02%	0.003%
82	9.704	2651	2653	2657	rVV	161	94	0.01%	0.002%
83	9.787	2671	2679	2688	rVB2	475	686	0.11%	0.013%
84	9.832	2688	2693	2699	rVB	275	247	0.04%	0.005%
85	10.102	2773	2777	2780	rBV	256	164	0.03%	0.003%
86	10.147	2787	2791	2792	rBV	158	106	0.02%	0.002%
87	10.366	2857	2859	2862	rVV2	179	105	0.02%	0.002%
88	10.434	2868	2880	2895	rBV	220051	350535	55.25%	6.703%
89	10.771	2982	2985	2989	rBV2	294	233	0.04%	0.004%
90	10.810	2995	2997	3000	rVB	420	218	0.03%	0.004%
91	10.980	3043	3050	3053	rBV2	252	266	0.04%	0.005%
92	11.128	3092	3096	3097	rBV2	199	135	0.02%	0.003%
93	11.440	3190	3193	3195	rBV2	198	146	0.02%	0.003%
94	11.485	3195	3207	3228	rVV	351492	547489	86.29%	10.469%
95	11.643	3252	3256	3261	rBV	248	333	0.05%	0.006%
96	11.694	3269	3272	3275	rBV	210	122	0.02%	0.002%
97	11.861	3308	3324	3349	rBV	300070	481675	75.92%	9.210%
98	12.215	3431	3434	3438	rBV2	326	270	0.04%	0.005%
99	12.234	3438	3440	3444	rVB	265	137	0.02%	0.003%
100	12.688	3576	3581	3584	rBV	303	357	0.06%	0.007%

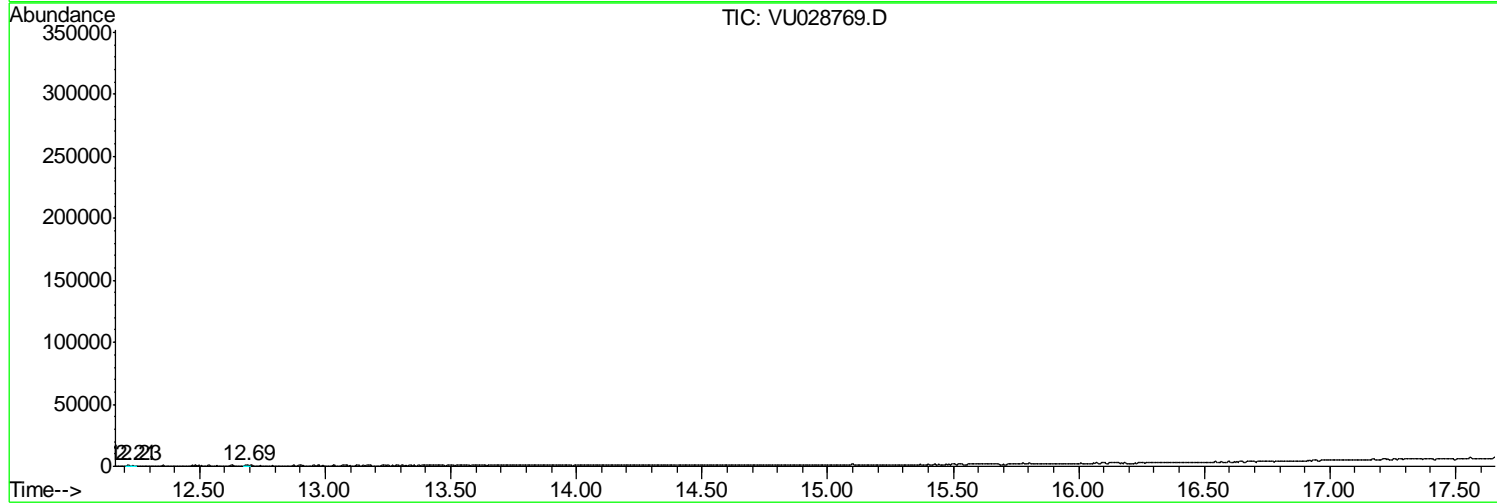
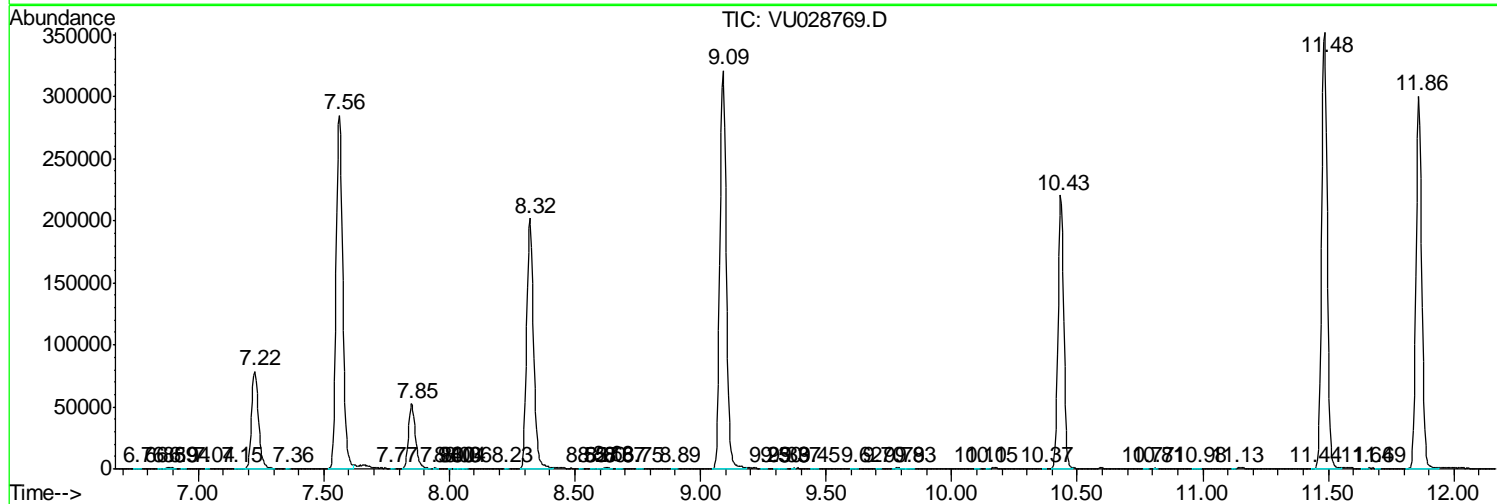
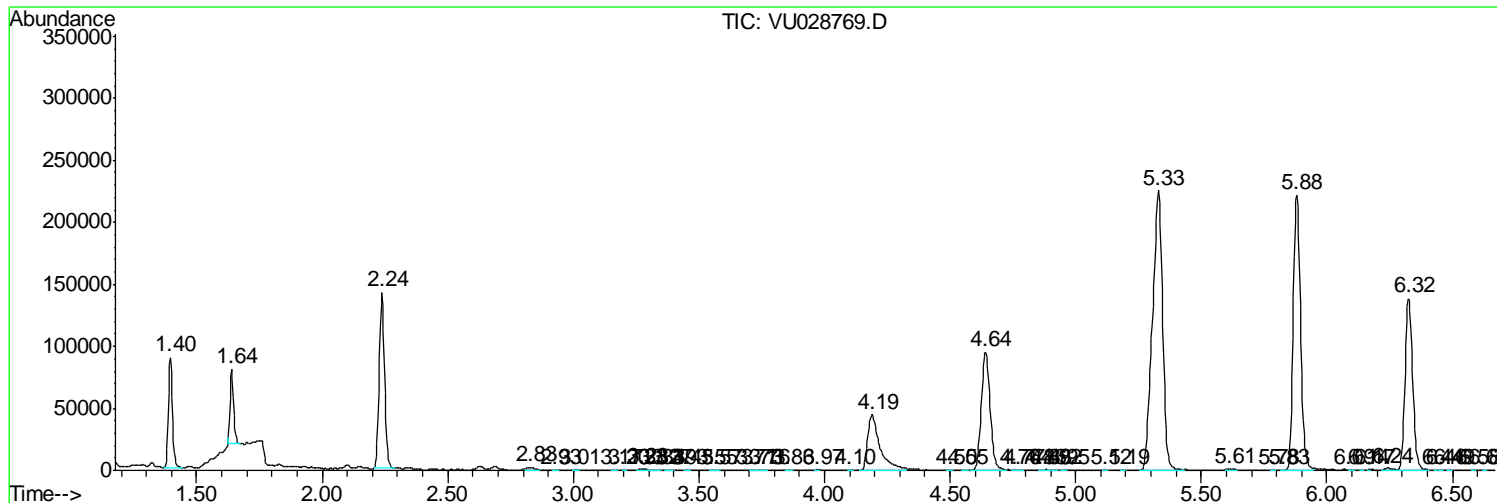
Sum of corrected areas: 5229751

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Instrument :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.M
 Quant Title : VOC Analysis

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



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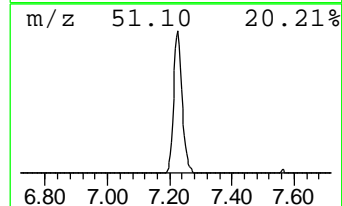
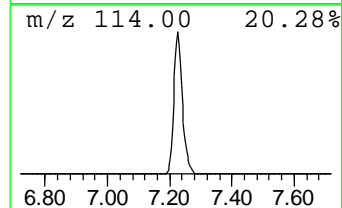
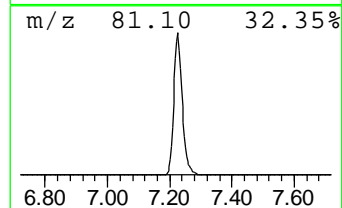
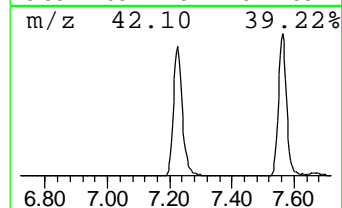
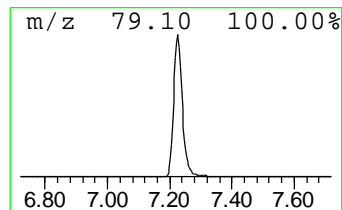
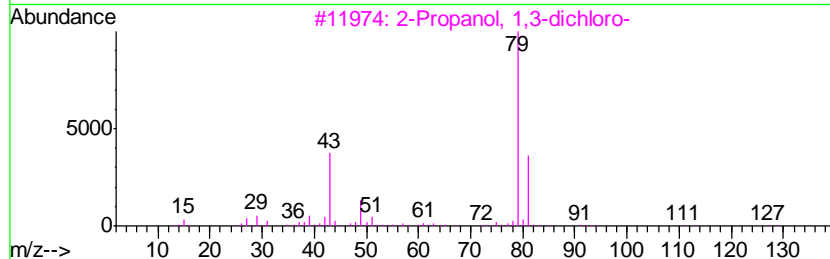
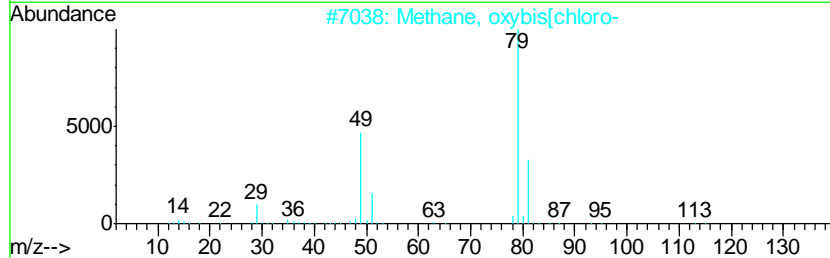
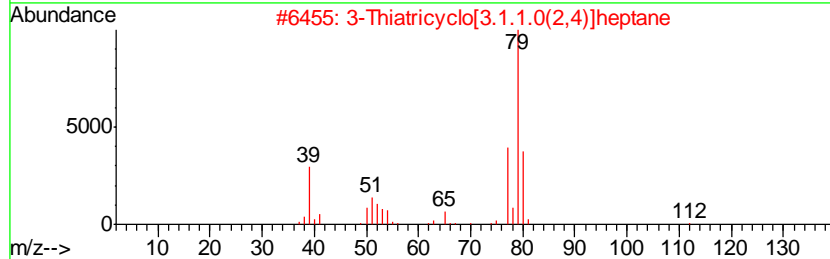
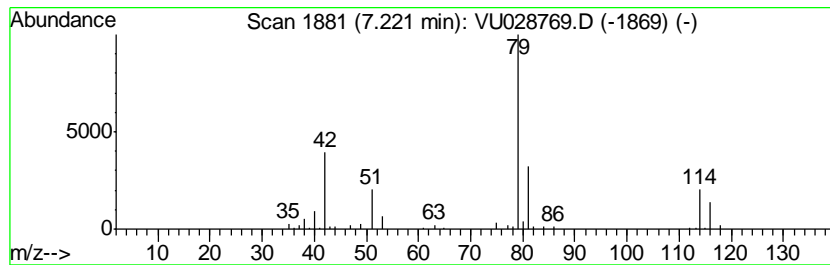
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.M
 Quant Title : VOC Analysis

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	16.86 ug/L	149844	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	25
2		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
3		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
4		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9
5		1,3-Cyclohexadiene	80	C6H8	000592-57-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.22	16.9	ug/L	149844	1	5.88	444389	50.0