

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040419\
 Data File : VU030637.D
 Acq On : 03 Apr 2019 19:05
 Operator : JC/SP
 Sample : K2101-16ME
 Misc : 4.47g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFOE7ME

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\SOMULM032319WMA.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	22	26	36	rVB3	14205	14020	0.75%	0.089%
2	1.392	87	94	106	rVB	216804	247403	13.26%	1.568%
3	1.637	166	170	181	rVB	159703	167248	8.97%	1.060%
4	2.238	347	357	372	rVB	402729	624118	33.46%	3.956%
5	2.595	464	468	471	rBV3	934	846	0.05%	0.005%
6	2.630	476	479	481	rBV4	949	738	0.04%	0.005%
7	2.662	485	489	490	rBV2	1574	1053	0.06%	0.007%
8	2.691	490	498	512	rVB7	4783	12123	0.65%	0.077%
9	2.775	521	524	527	rBV4	693	637	0.03%	0.004%
10	2.826	531	540	546	rBV6	3991	7168	0.38%	0.045%
11	2.965	580	583	594	rVB5	1657	2546	0.14%	0.016%
12	3.045	604	608	612	rVB5	659	541	0.03%	0.003%
13	3.138	632	637	639	rBV4	611	542	0.03%	0.003%
14	3.174	644	648	649	rBV	786	429	0.02%	0.003%
15	3.273	671	679	681	rBV4	2373	2755	0.15%	0.017%
16	3.408	716	721	724	rBV2	895	888	0.05%	0.006%
17	3.434	725	729	732	rVV3	791	696	0.04%	0.004%
18	3.456	732	736	739	rVV3	505	471	0.03%	0.003%
19	3.534	756	760	767	rVV6	916	979	0.05%	0.006%
20	3.598	775	780	783	rVB4	439	438	0.02%	0.003%
21	3.617	783	786	790	rBV2	645	493	0.03%	0.003%
22	3.794	837	841	844	rBV4	613	461	0.02%	0.003%
23	3.852	857	859	863	rVB	895	502	0.03%	0.003%
24	3.878	863	867	873	rBV3	371	455	0.02%	0.003%
25	3.942	883	887	890	rVB3	533	432	0.02%	0.003%
26	3.977	895	898	902	rBV2	801	662	0.04%	0.004%
27	4.132	944	946	950	rBV2	805	662	0.04%	0.004%
28	4.190	951	964	987	rBV	132537	432220	23.17%	2.740%
29	4.456	1045	1047	1051	rVB3	813	518	0.03%	0.003%
30	4.640	1084	1104	1136	rBV	256656	663118	35.55%	4.203%
31	4.794	1149	1152	1155	rBV5	821	518	0.03%	0.003%
32	4.874	1173	1177	1181	rBV3	861	1010	0.05%	0.006%
33	4.936	1193	1196	1198	rBV2	1082	714	0.04%	0.005%
34	5.051	1227	1232	1234	rBV3	882	716	0.04%	0.005%

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 Title : VOC Analysis

35	5.087	1241	1243	1250	rVB4	526	589	0.03%	0.004%
36	5.196	1274	1277	1280	rBV3	1514	1402	0.08%	0.009%
37	5.328	1294	1318	1354	rBV2	616353	1768168	94.80%	11.207%
38	5.579	1392	1396	1398	rBV4	1182	1006	0.05%	0.006%
39	5.614	1398	1407	1421	rVV10	4635	11561	0.62%	0.073%
40	5.669	1422	1424	1431	rVB6	1898	1543	0.08%	0.010%
41	5.723	1437	1441	1442	rBV2	1114	787	0.04%	0.005%
42	5.759	1446	1452	1456	rBV4	744	841	0.05%	0.005%
43	5.788	1459	1461	1465	rVB4	1812	1162	0.06%	0.007%
44	5.810	1465	1468	1472	rVB4	971	569	0.03%	0.004%
45	5.878	1474	1489	1516	rBV	703860	1475611	79.12%	9.353%
46	6.083	1549	1553	1555	rBV3	853	518	0.03%	0.003%
47	6.112	1558	1562	1565	rBV4	924	958	0.05%	0.006%
48	6.170	1573	1580	1581	rBV4	3077	2615	0.14%	0.017%
49	6.247	1597	1604	1614	rBV5	4387	8299	0.44%	0.053%
50	6.325	1614	1628	1650	rBV	372419	779366	41.79%	4.940%
51	6.524	1685	1690	1694	rBV5	1647	1744	0.09%	0.011%
52	6.624	1717	1721	1723	rBV2	681	561	0.03%	0.004%
53	6.678	1734	1738	1744	rBV2	1227	981	0.05%	0.006%
54	6.717	1745	1750	1754	rVV4	688	782	0.04%	0.005%
55	6.865	1792	1796	1797	rBV3	735	603	0.03%	0.004%
56	6.897	1797	1806	1807	rBV5	2988	3587	0.19%	0.023%
57	6.984	1830	1833	1835	rBV	704	495	0.03%	0.003%
58	7.032	1845	1848	1854	rVV4	1338	1441	0.08%	0.009%
59	7.080	1859	1863	1866	rBV5	918	736	0.04%	0.005%
60	7.099	1866	1869	1873	rVB4	1402	1171	0.06%	0.007%
61	7.141	1879	1882	1883	rBV2	905	480	0.03%	0.003%
62	7.177	1885	1893	1897	rVV5	7418	10523	0.56%	0.067%
63	7.225	1897	1908	1935	rVB	203969	397663	21.32%	2.521%
64	7.421	1966	1969	1972	rBV2	822	642	0.03%	0.004%
65	7.437	1972	1974	1978	rVB3	773	480	0.03%	0.003%
66	7.463	1978	1982	1986	rBV5	864	758	0.04%	0.005%
67	7.562	1991	2013	2038	rBV	763437	1407125	75.44%	8.919%
68	7.849	2092	2102	2132	rBV2	131429	258869	13.88%	1.641%
69	8.032	2153	2159	2163	rBV5	2156	3125	0.17%	0.020%
70	8.115	2181	2185	2186	rBV4	723	565	0.03%	0.004%
71	8.164	2198	2200	2203	rBV3	1078	620	0.03%	0.004%

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 ClientSampleId :
 BFOE7ME

Integration Parameters: LSCINT.P

Integrator: RTE
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72	8.225	2208	2219	2231	rBV	107634	185176	9.93%	1.174%
73	8.318	2237	2248	2276	rBV	571731	1075557	57.67%	6.817%
74	8.588	2329	2332	2333	rBV4	1602	980	0.05%	0.006%
75	8.810	2391	2401	2409	rBV9	4760	10228	0.55%	0.065%
76	8.903	2424	2430	2443	rVB3	14087	23327	1.25%	0.148%
77	9.029	2459	2469	2476	rBV4	12630	22513	1.21%	0.143%
78	9.090	2476	2488	2513	rVV	1044681	1822106	97.69%	11.549%
79	9.328	2558	2562	2564	rBV5	1864	1465	0.08%	0.009%
80	9.340	2564	2566	2568	rVV2	1336	767	0.04%	0.005%
81	9.443	2592	2598	2608	rBV10	4774	8073	0.43%	0.051%
82	9.604	2643	2648	2651	rBV5	857	679	0.04%	0.004%
83	9.646	2659	2661	2665	rVB3	935	567	0.03%	0.004%
84	9.675	2669	2670	2672	rBV2	807	427	0.02%	0.003%
85	9.784	2702	2704	2706	rBV3	902	470	0.03%	0.003%
86	9.807	2708	2711	2712	rBV2	2230	1231	0.07%	0.008%
87	9.906	2738	2742	2744	rBV4	1354	1057	0.06%	0.007%
88	9.951	2749	2756	2764	rVB4	11032	16420	0.88%	0.104%
89	10.003	2767	2772	2776	rBV7	1837	2380	0.13%	0.015%
90	10.045	2779	2785	2792	rVB9	4969	7254	0.39%	0.046%
91	10.430	2894	2905	2931	rBV	567471	925425	49.62%	5.866%
92	10.591	2950	2955	2958	rBV6	2781	3101	0.17%	0.020%
93	10.752	2998	3005	3011	rBV9	5804	9116	0.49%	0.058%
94	10.813	3017	3024	3035	rVB9	7582	14064	0.75%	0.089%
95	10.858	3035	3038	3046	rVB9	1819	1820	0.10%	0.012%
96	11.112	3111	3117	3125	rBV7	8826	12406	0.67%	0.079%
97	11.482	3221	3232	3253	rBV	1179105	1865134	100.00%	11.822%
98	11.858	3337	3349	3370	rBV	786566	1314742	70.49%	8.333%
99	13.880	3972	3978	3990	rVB4	34636	53813	2.89%	0.341%
100	14.893	4287	4293	4308	rVB4	35925	60726	3.26%	0.385%

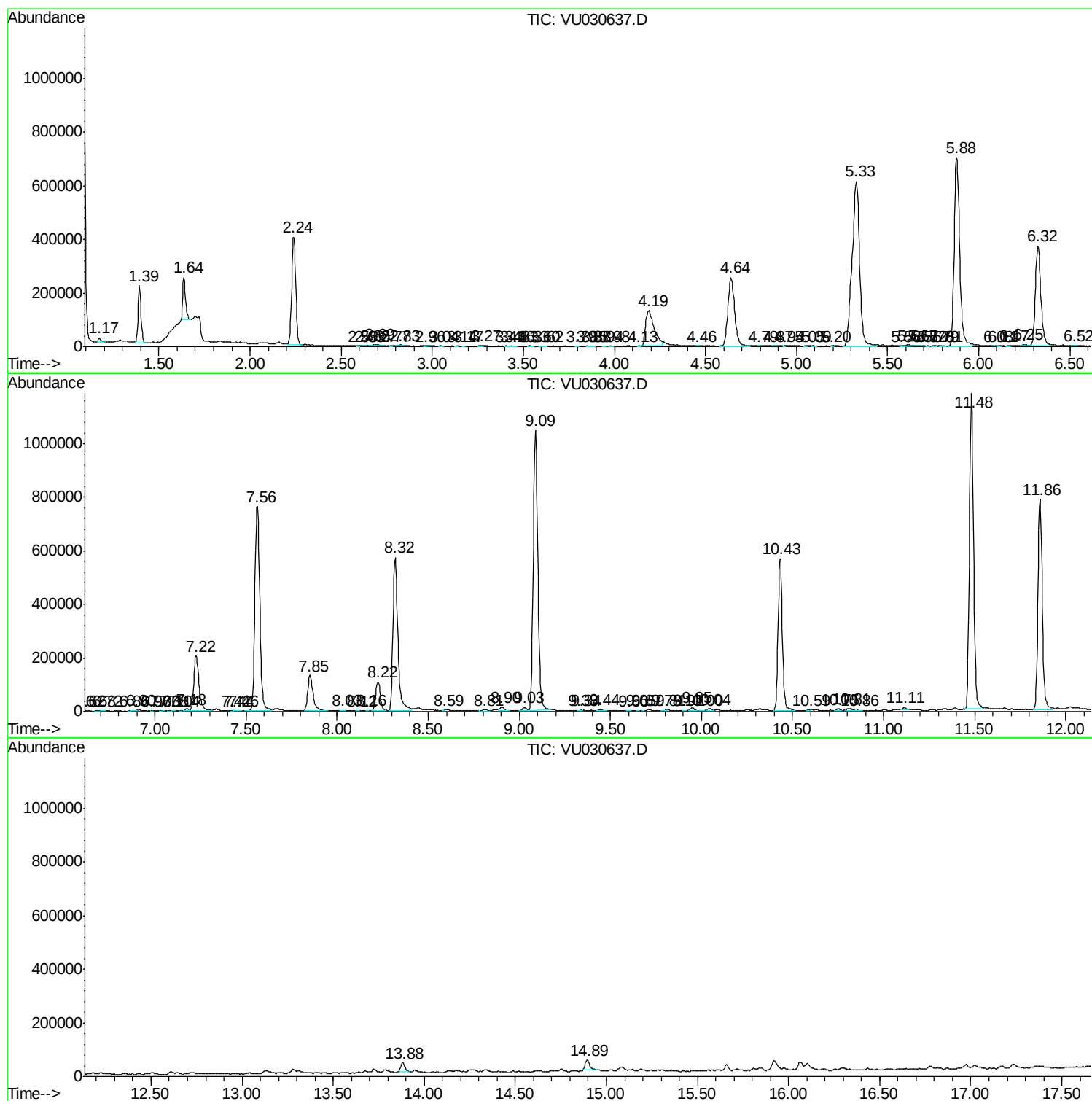
Sum of corrected areas: 15777090

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Misc : 4.47a/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
BF0E7ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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



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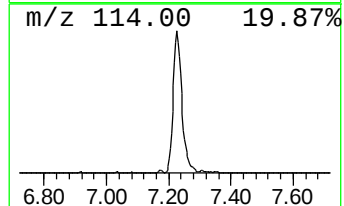
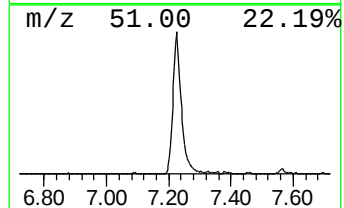
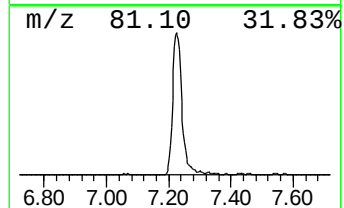
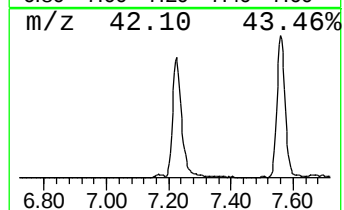
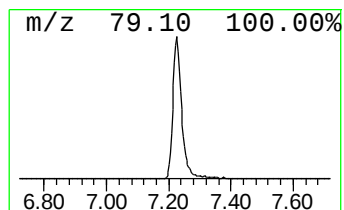
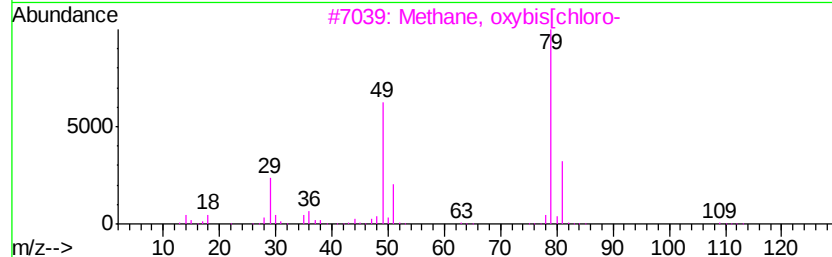
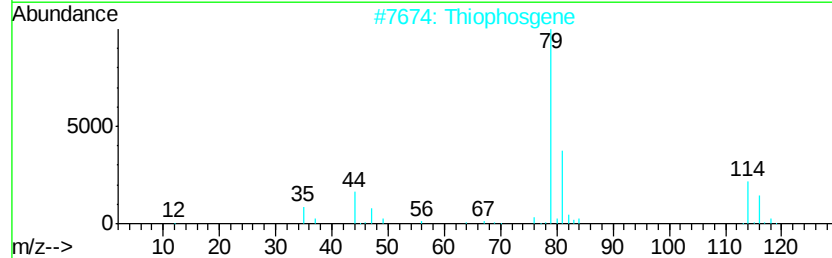
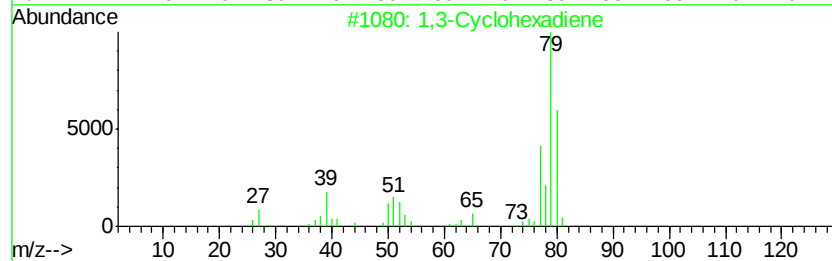
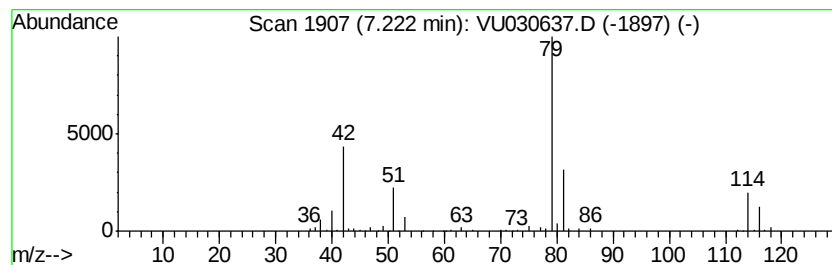
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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	13.47 ug/L	397663	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclohexadiene	80	C6H8	000592-57-4	32
2		Thiophosgene	114	CCl2S	000463-71-8	27
3		Methane, oxvbis[chloro-	114	C2H4Cl2O	000542-88-1	25
4		3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	25
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	13.5	ug/L	397663	1	5.88	1475610	50.0