

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052218\
 Data File : VU024007.D
 Acq On : 22 May 2018 11:16
 Operator : MD/SY
 Sample : J2959-03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM051218WMA.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	0.658	15	21	25	rBV	114	141	0.01%	0.001%
2	0.741	43	47	49	rBV2	168	126	0.01%	0.001%
3	0.793	56	63	64	rBV2	164	144	0.01%	0.002%
4	0.850	77	81	85	rVB2	150	148	0.01%	0.002%
5	0.905	94	98	101	rBV2	278	223	0.02%	0.002%
6	0.985	120	123	125	rBV	193	163	0.01%	0.002%
7	1.088	137	155	175	rBV	269047	313671	25.74%	3.295%
8	1.182	180	184	191	rVB	5716	5844	0.48%	0.061%
9	1.397	245	251	268	rBV	158695	164609	13.51%	1.729%
10	1.680	331	339	352	rBV	126082	156769	12.87%	1.647%
11	2.272	512	523	535	rBV	266943	403429	33.11%	4.238%
12	2.477	585	587	594	rVB2	962	855	0.07%	0.009%
13	2.699	645	656	670	rVB3	8168	14573	1.20%	0.153%
14	2.834	690	698	700	rBV2	780	1039	0.09%	0.011%
15	2.960	733	737	740	rBV	221	229	0.02%	0.002%
16	2.982	740	744	745	rBV2	350	211	0.02%	0.002%
17	3.506	902	907	910	rBV	272	293	0.02%	0.003%
18	3.699	961	967	973	rBV2	280	467	0.04%	0.005%
19	3.812	999	1002	1004	rBV2	165	108	0.01%	0.001%
20	3.892	1025	1027	1030	rVV	230	156	0.01%	0.002%
21	3.921	1033	1036	1038	rVB2	203	126	0.01%	0.001%
22	3.940	1038	1042	1045	rBV2	204	154	0.01%	0.002%
23	3.976	1051	1053	1056	rBV	164	116	0.01%	0.001%
24	4.030	1064	1070	1073	rBV	193	203	0.02%	0.002%
25	4.178	1101	1116	1162	rBV	112522	303501	24.91%	3.189%
26	4.551	1228	1232	1235	rBV2	196	201	0.02%	0.002%
27	4.651	1246	1263	1287	rBV	205659	487730	40.03%	5.124%
28	4.815	1312	1314	1318	rVB2	366	246	0.02%	0.003%
29	4.879	1330	1334	1337	rBV3	489	461	0.04%	0.005%
30	4.937	1348	1352	1355	rVV	176	164	0.01%	0.002%
31	4.972	1361	1363	1367	rVV2	211	168	0.01%	0.002%
32	4.998	1367	1371	1375	rVB2	337	354	0.03%	0.004%
33	5.024	1375	1379	1382	rBV2	151	137	0.01%	0.001%
34	5.046	1382	1386	1391	rVB2	211	218	0.02%	0.002%

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 Title : VOC Analysis

35	5.075	1391	1395	1398	rBV2	285	306	0.03%	0.003%
36	5.127	1408	1411	1416	rVB2	174	135	0.01%	0.001%
37	5.204	1432	1435	1440	rBV2	231	270	0.02%	0.003%
38	5.233	1440	1444	1445	rBV2	202	143	0.01%	0.002%
39	5.345	1451	1479	1521	rBV2	394523	1218406	100.00%	12.800%
40	5.673	1576	1581	1589	rVB4	516	745	0.06%	0.008%
41	5.709	1589	1592	1594	rBV2	289	193	0.02%	0.002%
42	5.760	1606	1608	1611	rVB2	260	149	0.01%	0.002%
43	5.779	1611	1614	1617	rBV2	295	233	0.02%	0.002%
44	5.808	1622	1623	1628	rVB2	220	136	0.01%	0.001%
45	5.841	1628	1633	1634	rBV2	263	192	0.02%	0.002%
46	5.889	1634	1648	1688	rBV	312040	641930	52.69%	6.744%
47	6.085	1707	1709	1712	rVB2	415	205	0.02%	0.002%
48	6.175	1732	1737	1749	rVB5	1204	2295	0.19%	0.024%
49	6.275	1766	1768	1771	rVB	239	117	0.01%	0.001%
50	6.336	1771	1787	1819	rBV	281544	576880	47.35%	6.061%
51	6.683	1891	1895	1898	rVB	232	189	0.02%	0.002%
52	6.702	1898	1901	1904	rBV	215	224	0.02%	0.002%
53	6.808	1930	1934	1937	rBV	216	245	0.02%	0.003%
54	6.876	1952	1955	1958	rBV	231	176	0.01%	0.002%
55	6.931	1969	1972	1974	rVB2	189	104	0.01%	0.001%
56	6.950	1974	1978	1980	rBV2	202	180	0.01%	0.002%
57	6.979	1984	1987	1993	rVV2	163	206	0.02%	0.002%
58	7.050	2006	2009	2018	rVB	206	286	0.02%	0.003%
59	7.091	2018	2022	2025	rBV2	150	158	0.01%	0.002%
60	7.136	2032	2036	2038	rBV2	211	184	0.02%	0.002%
61	7.233	2051	2066	2089	rBV	142930	261547	21.47%	2.748%
62	7.390	2111	2115	2117	rBV2	202	144	0.01%	0.002%
63	7.403	2117	2119	2122	rBV2	256	172	0.01%	0.002%
64	7.471	2135	2140	2148	rVB3	644	987	0.08%	0.010%
65	7.506	2148	2151	2154	rBV	235	184	0.02%	0.002%
66	7.570	2154	2171	2187	rBV	528802	936173	76.84%	9.835%
67	7.853	2245	2259	2283	rBV	102912	177488	14.57%	1.865%
68	8.062	2320	2324	2329	rBV2	285	280	0.02%	0.003%
69	8.104	2334	2337	2342	rVB2	278	253	0.02%	0.003%
70	8.181	2351	2361	2373	rBV3	4501	7985	0.66%	0.084%
71	8.313	2387	2402	2446	rBV	379706	677663	55.62%	7.119%

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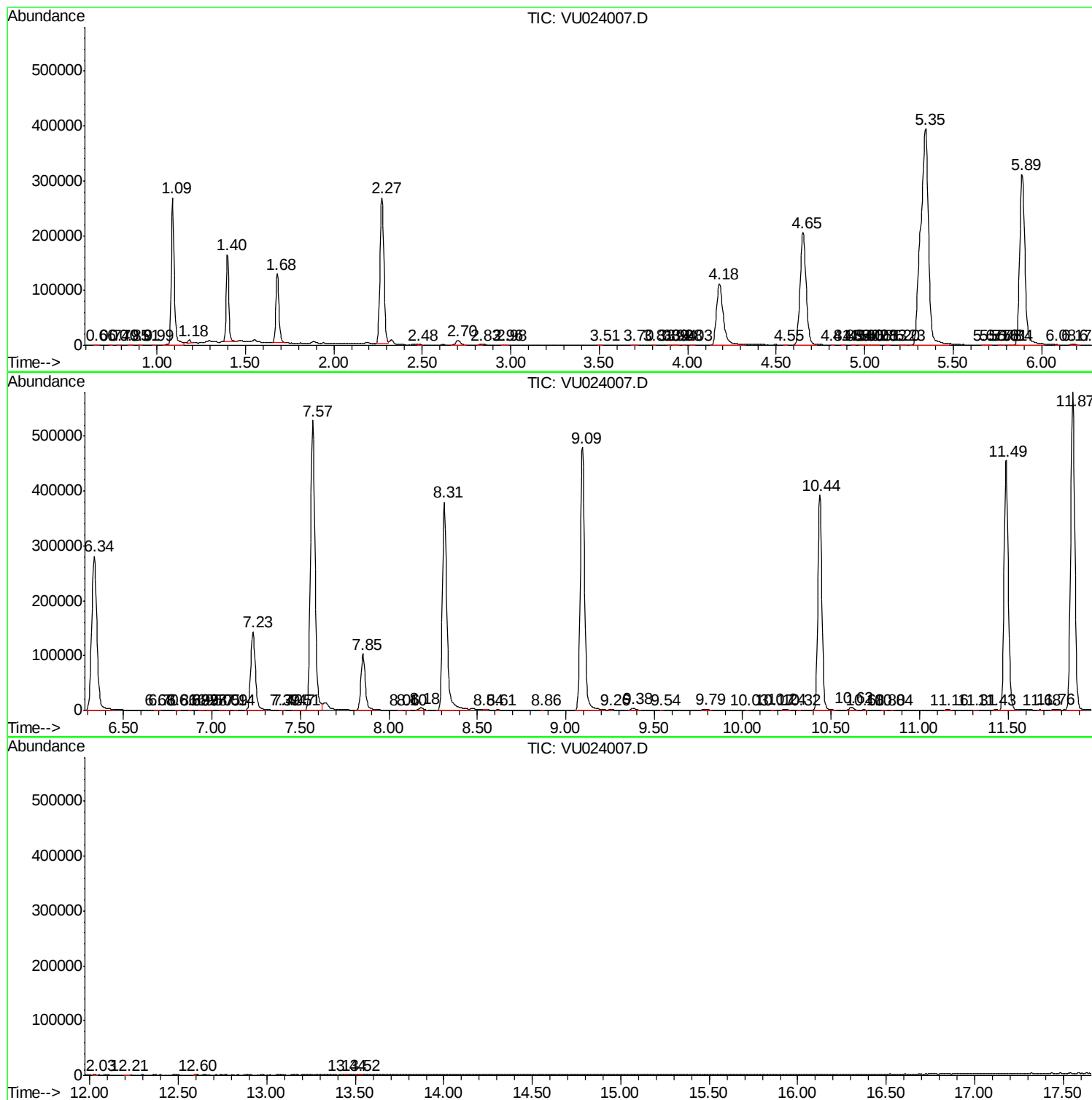
72	8.538	2470	2472	2477	rVB3	498	306	0.03%	0.003%
73	8.612	2492	2495	2499	rBV2	492	420	0.03%	0.004%
74	8.863	2571	2573	2578	rBV2	145	151	0.01%	0.002%
75	9.094	2632	2645	2683	rBV	479168	813875	66.80%	8.550%
76	9.255	2689	2695	2696	rBV	1006	900	0.07%	0.009%
77	9.384	2725	2735	2747	rVB4	3493	6108	0.50%	0.064%
78	9.541	2782	2784	2787	rBV	171	128	0.01%	0.001%
79	9.792	2853	2862	2872	rVB6	2008	3569	0.29%	0.037%
80	10.027	2932	2935	2938	rBV2	192	152	0.01%	0.002%
81	10.168	2976	2979	2984	rBV2	280	227	0.02%	0.002%
82	10.239	2995	3001	3010	rVB4	1735	2452	0.20%	0.026%
83	10.320	3023	3026	3028	rBV	206	122	0.01%	0.001%
84	10.435	3049	3062	3090	rBV	392355	631854	51.86%	6.638%
85	10.615	3109	3118	3127	rBV4	4539	7668	0.63%	0.081%
86	10.683	3137	3139	3146	rVB3	411	413	0.03%	0.004%
87	10.795	3171	3174	3179	rBV2	165	198	0.02%	0.002%
88	10.844	3186	3189	3192	rBV	285	234	0.02%	0.002%
89	11.156	3281	3286	3294	rVB	946	1138	0.09%	0.012%
90	11.313	3331	3335	3341	rBV2	236	285	0.02%	0.003%
91	11.426	3368	3370	3377	rVB4	503	537	0.04%	0.006%
92	11.490	3377	3390	3410	rBV	455508	747463	61.35%	7.853%
93	11.680	3444	3449	3452	rBV2	399	309	0.03%	0.003%
94	11.760	3468	3474	3484	rBV5	1726	2674	0.22%	0.028%
95	11.866	3494	3507	3524	rBV	580002	930792	76.39%	9.779%
96	12.027	3552	3557	3561	rBV2	525	617	0.05%	0.006%
97	12.210	3609	3614	3618	rBV2	269	321	0.03%	0.003%
98	12.596	3730	3734	3735	rBV	299	216	0.02%	0.002%
99	13.442	3994	3997	4003	rBV	593	594	0.05%	0.006%
100	13.519	4016	4021	4027	rBV3	551	737	0.06%	0.008%

Sum of corrected areas: 9518600

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Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM051218WMA.M
Quant Title : VOC Analysis

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



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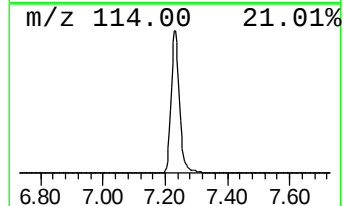
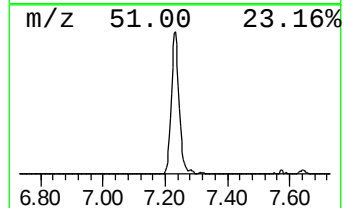
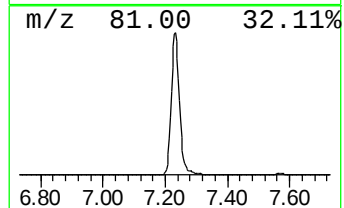
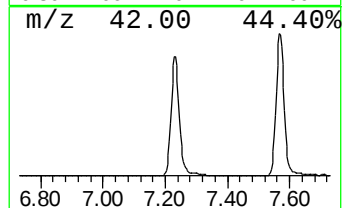
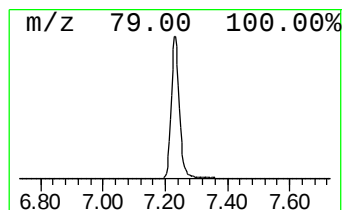
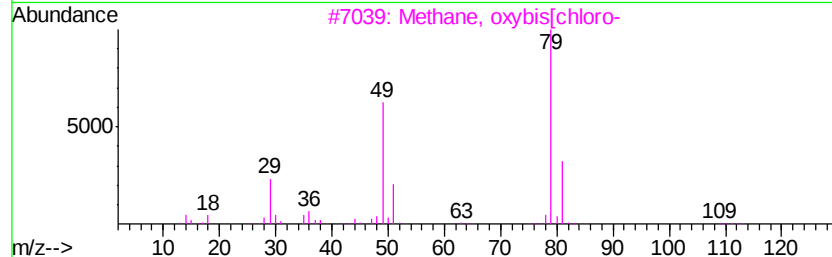
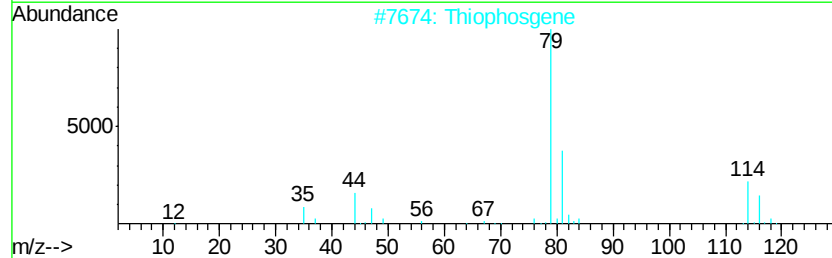
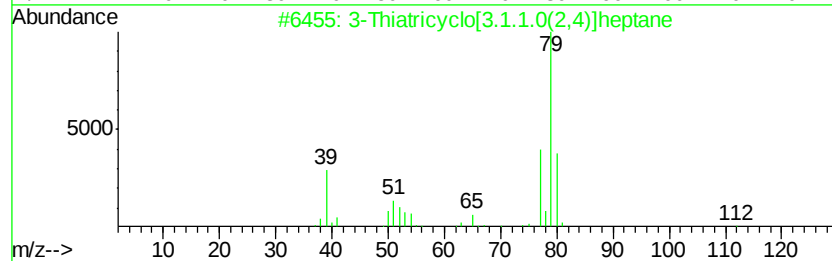
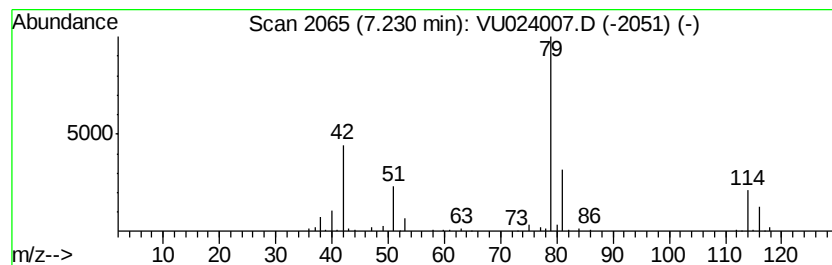
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM051218WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	20.37 ug/L	261547	1,4-Difluorobenzene	5.89

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		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
4		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23
5		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.23	20.4	ug/L	261547	1	5.89	641930	50.0