

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051975.D
 Acq On : 20 Nov 2022 15:38
 Operator : JC/MD
 Sample : N5683-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ESQT1

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\SFAMULM111522WMA.M

Title : VOC Analysis

Signal : TIC: VU051975.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	91	rBV	102499	118141	9.91%	1.204%
2	1.906	168	176	202	rVB	103767	158253	13.27%	1.613%
3	2.565	369	381	393	rBV	155420	252837	21.21%	2.577%
4	3.051	524	532	541	rVB6	1692	3267	0.27%	0.033%
5	3.109	548	550	553	rBV2	317	137	0.01%	0.001%
6	3.295	605	608	612	rBV2	354	268	0.02%	0.003%
7	3.353	623	626	629	rBV2	135	121	0.01%	0.001%
8	3.549	683	687	690	rBV2	242	221	0.02%	0.002%
9	3.604	698	704	705	rBV2	194	190	0.02%	0.002%
10	3.790	760	762	770	rBV	277	242	0.02%	0.002%
11	3.835	773	776	780	rBV	197	154	0.01%	0.002%
12	3.909	797	799	802	rBV	114	82	0.01%	0.001%
13	4.092	853	856	860	rVB2	195	149	0.01%	0.002%
14	4.118	860	864	866	rBV2	359	241	0.02%	0.002%
15	4.202	883	890	897	rBV2	195	272	0.02%	0.003%
16	4.282	912	915	917	rBV	110	59	0.00%	0.001%
17	4.298	917	920	923	rVV	321	187	0.02%	0.002%
18	4.346	932	935	938	rBV2	147	101	0.01%	0.001%
19	4.362	938	940	943	rVB	124	62	0.01%	0.001%
20	4.379	943	945	947	rBV	139	62	0.01%	0.001%
21	4.453	964	968	971	rBV	224	247	0.02%	0.003%
22	4.491	977	980	984	rBV2	169	149	0.01%	0.002%
23	4.543	994	996	998	rBV	92	50	0.00%	0.001%
24	4.575	1004	1006	1007	rBV	148	70	0.01%	0.001%
25	4.617	1007	1019	1045	rBV	174984	426784	35.80%	4.350%
26	5.060	1141	1157	1179	rBV	241433	534617	44.84%	5.449%
27	5.237	1209	1212	1214	rVB2	442	229	0.02%	0.002%
28	5.269	1219	1222	1224	rBV2	486	300	0.03%	0.003%
29	5.333	1240	1242	1244	rBV2	227	108	0.01%	0.001%
30	5.356	1247	1249	1251	rBV	90	48	0.00%	0.000%
31	5.375	1251	1255	1260	rBV3	570	681	0.06%	0.007%
32	5.443	1275	1276	1279	rBV2	159	88	0.01%	0.001%
33	5.459	1279	1281	1288	rVB2	275	204	0.02%	0.002%
34	5.501	1288	1294	1298	rBV2	337	419	0.04%	0.004%
35	5.571	1311	1316	1319	rBV2	258	258	0.02%	0.003%
36	5.604	1325	1326	1329	rBV	161	77	0.01%	0.001%

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 Title : VOC Analysis

37	5.723	1339	1363	1396	rBV2	412740	1192257	100.00%	12.152%
38	5.960	1434	1437	1439	rBV2	317	186	0.02%	0.002%
39	6.009	1450	1452	1456	rVB	238	100	0.01%	0.001%
40	6.044	1457	1463	1464	rBV2	521	412	0.03%	0.004%
41	6.247	1512	1526	1554	rBV	457054	886229	74.33%	9.033%
42	6.539	1605	1617	1627	rVB10	2307	4822	0.40%	0.049%
43	6.575	1627	1628	1632	rVB2	226	113	0.01%	0.001%
44	6.604	1632	1637	1638	rBV	362	316	0.03%	0.003%
45	6.687	1649	1663	1689	rBV	311395	609448	51.12%	6.212%
46	6.858	1713	1716	1721	rVB2	450	402	0.03%	0.004%
47	6.883	1721	1724	1727	rBV2	394	294	0.02%	0.003%
48	6.899	1727	1729	1732	rVV	205	104	0.01%	0.001%
49	6.938	1738	1741	1743	rBV	218	148	0.01%	0.002%
50	7.002	1758	1761	1763	rBV	243	168	0.01%	0.002%
51	7.047	1770	1775	1783	rBV2	389	441	0.04%	0.004%
52	7.086	1784	1787	1788	rBV	185	106	0.01%	0.001%
53	7.189	1810	1819	1831	rBV3	5457	10379	0.87%	0.106%
54	7.311	1852	1857	1859	rBV2	220	176	0.01%	0.002%
55	7.391	1879	1882	1886	rBV2	230	180	0.02%	0.002%
56	7.478	1906	1909	1913	rBV2	279	239	0.02%	0.002%
57	7.562	1924	1935	1955	rBV	125105	223295	18.73%	2.276%
58	7.694	1968	1976	1985	rBV5	3504	6412	0.54%	0.065%
59	7.835	2017	2020	2022	rBV	153	109	0.01%	0.001%
60	7.848	2022	2024	2026	rBV	279	164	0.01%	0.002%
61	7.896	2026	2039	2057	rBV	392549	680712	57.09%	6.938%
62	8.176	2115	2126	2144	rBV	88915	154349	12.95%	1.573%
63	8.420	2199	2202	2207	rVB2	405	303	0.03%	0.003%
64	8.462	2211	2215	2216	rBV	672	379	0.03%	0.004%
65	8.501	2225	2227	2230	rVB	373	139	0.01%	0.001%
66	8.520	2231	2233	2235	rVB	206	92	0.01%	0.001%
67	8.536	2235	2238	2240	rBV2	287	190	0.02%	0.002%
68	8.629	2256	2267	2293	rBV2	480478	920126	77.18%	9.378%
69	9.025	2388	2390	2392	rBV	236	126	0.01%	0.001%
70	9.038	2392	2394	2396	rVV2	335	170	0.01%	0.002%
71	9.095	2408	2412	2415	rBV	346	300	0.03%	0.003%
72	9.144	2425	2427	2429	rBV	169	57	0.00%	0.001%
73	9.288	2467	2472	2474	rBV2	111	103	0.01%	0.001%
74	9.304	2474	2477	2481	rBV	240	227	0.02%	0.002%
75	9.414	2498	2511	2539	rBV	673856	1107028	92.85%	11.283%
76	9.735	2607	2611	2613	rBV	216	169	0.01%	0.002%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

77	9.767	2617	2621	2623	rBV	281	171	0.01%	0.002%
78	9.780	2623	2625	2628	rVB	303	118	0.01%	0.001%
79	9.835	2638	2642	2646	rBV2	426	394	0.03%	0.004%
80	9.867	2650	2652	2659	rVB2	378	301	0.03%	0.003%
81	10.089	2718	2721	2725	rVB2	316	257	0.02%	0.003%
82	10.108	2725	2727	2729	rBV	178	72	0.01%	0.001%
83	10.320	2790	2793	2799	rBV	306	371	0.03%	0.004%
84	10.594	2875	2878	2880	rBV	260	190	0.02%	0.002%
85	10.755	2915	2928	2950	rBV	587496	953663	79.99%	9.720%
86	10.999	3002	3004	3007	rBV	263	153	0.01%	0.002%
87	11.745	3234	3236	3238	rBV	321	141	0.01%	0.001%
88	11.809	3244	3256	3283	rBV	479904	777327	65.20%	7.923%
89	12.070	3332	3337	3338	rBV4	1145	871	0.07%	0.009%
90	12.189	3361	3374	3401	rBV	465770	776503	65.13%	7.915%
91	12.558	3486	3489	3490	rBV	394	231	0.02%	0.002%

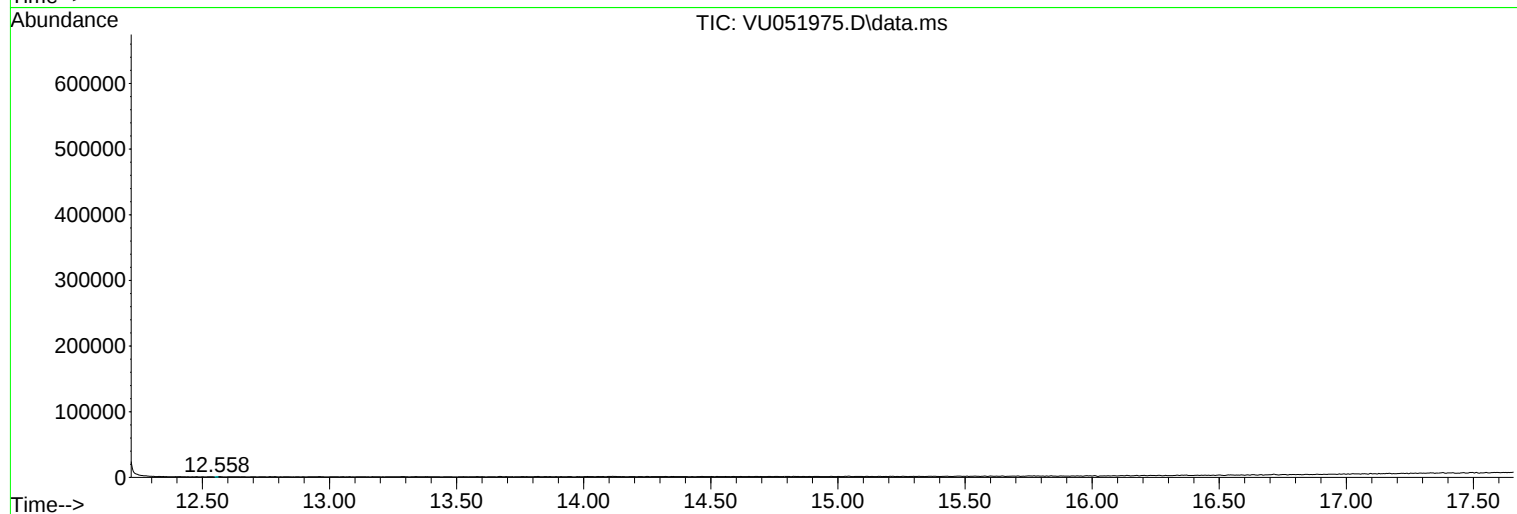
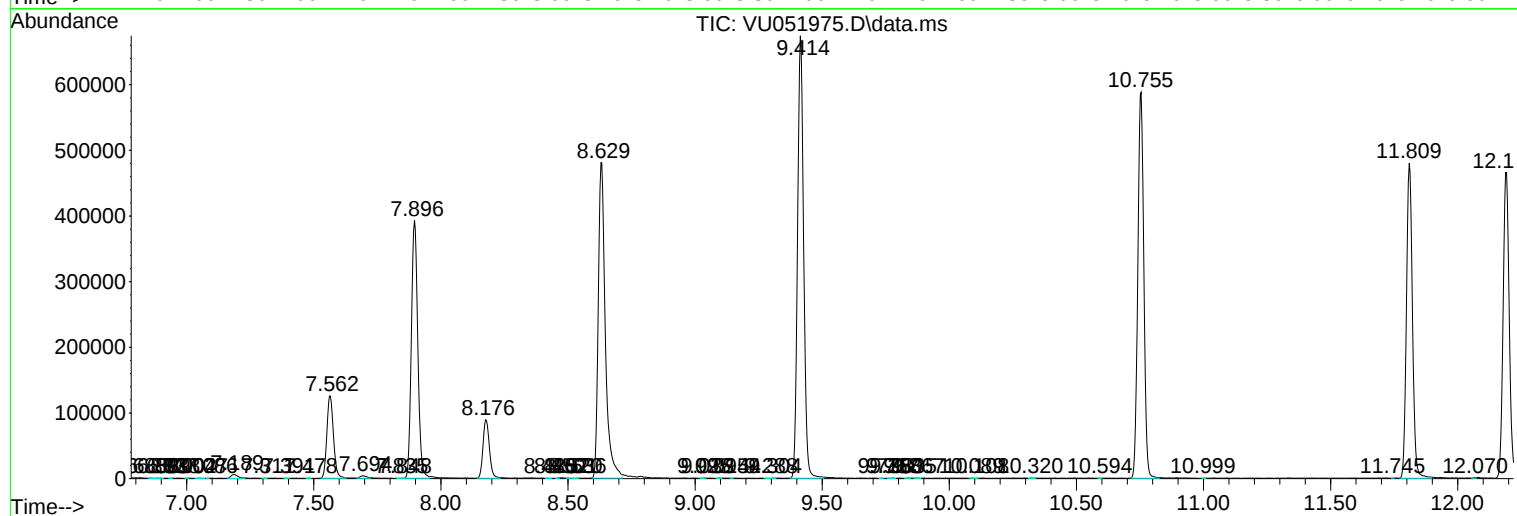
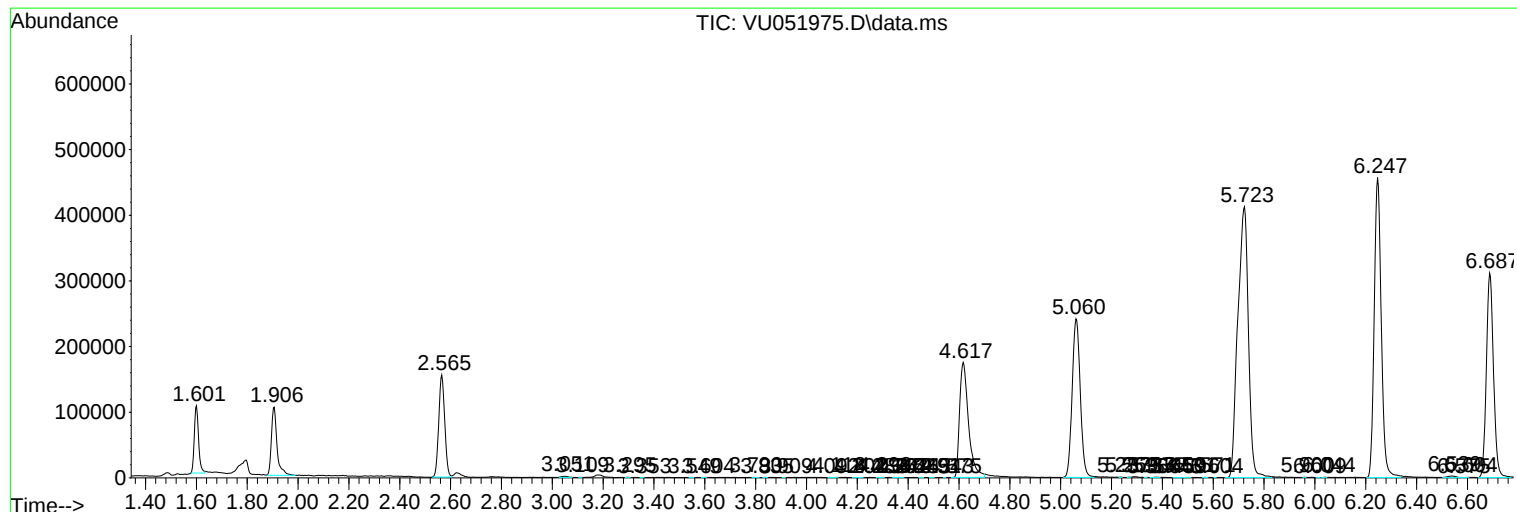
Sum of corrected areas: 9811108

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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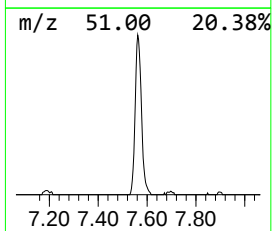
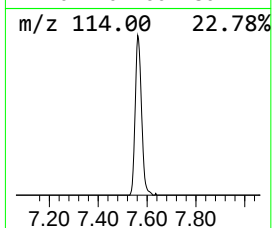
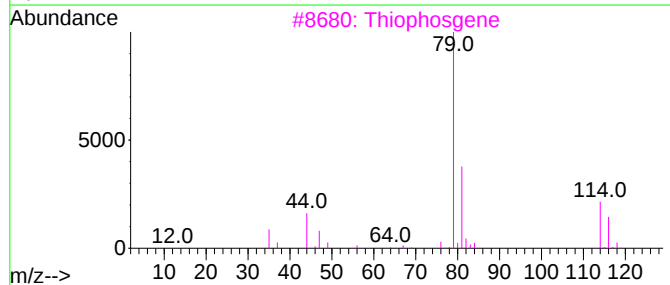
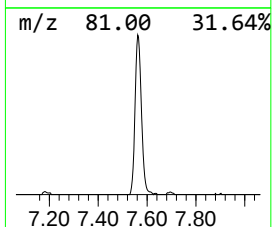
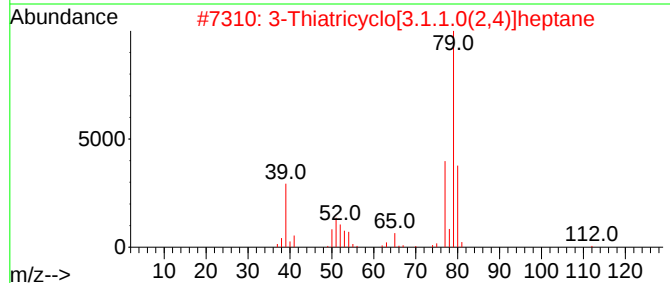
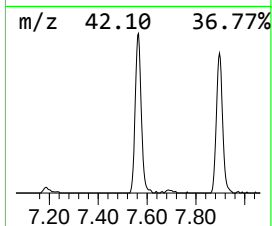
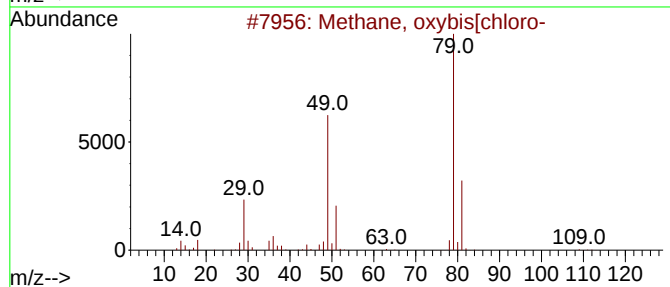
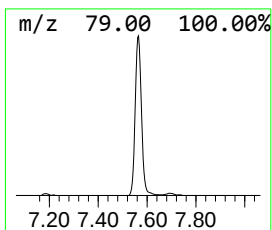
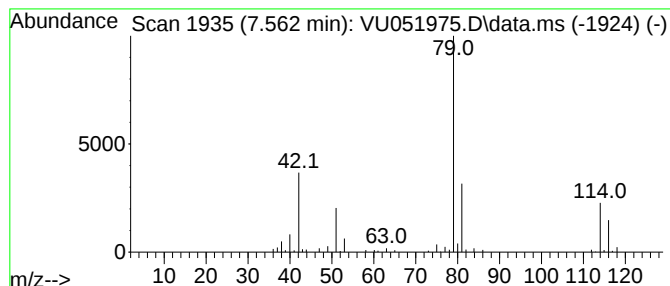
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.562	12.60 ug/L	223295	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	40
2			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	38
3			Thiophosgene	114	CCl2S	000463-71-8	35
4			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
5			1,3-Cyclohexadiene	80	C6H8	000592-57-4	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.562	12.6	ug/L	223295	1	6.247	886229	50.0