

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
 Data File : VU053571.D
 Acq On : 04 Apr 2023 19:06
 Operator : JC/MD
 Sample : 02158-14DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-8S(20230330)DL

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\SFAMULM033123WMA.M

Title : VOC Analysis

Signal : TIC: VU053571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	95	rVB	101374	115567	14.27%	1.673%
2	1.909	170	177	194	rVB	81631	113361	14.00%	1.641%
3	2.565	369	381	401	rBV	146962	244655	30.21%	3.542%
4	2.945	497	499	504	rVV2	250	185	0.02%	0.003%
5	3.041	520	529	541	rVV2	4286	7543	0.93%	0.109%
6	3.347	615	624	642	rVB4	6897	13504	1.67%	0.195%
7	3.652	716	719	722	rBV	248	195	0.02%	0.003%
8	3.755	748	751	755	rVB	234	146	0.02%	0.002%
9	3.864	773	785	803	rVB2	11405	26954	3.33%	0.390%
10	3.974	814	819	820	rBV	448	366	0.05%	0.005%
11	4.096	854	857	861	rBV	177	146	0.02%	0.002%
12	4.173	877	881	887	rVB	296	301	0.04%	0.004%
13	4.253	904	906	912	rVV2	214	214	0.03%	0.003%
14	4.488	976	979	983	rBV	336	226	0.03%	0.003%
15	4.568	999	1004	1006	rBV	271	193	0.02%	0.003%
16	4.613	1006	1018	1024	rBV	73141	152076	18.78%	2.201%
17	4.858	1091	1094	1097	rBV2	211	204	0.03%	0.003%
18	4.957	1122	1125	1129	rBV2	257	225	0.03%	0.003%
19	4.980	1129	1132	1136	rVB2	335	265	0.03%	0.004%
20	5.057	1140	1156	1178	rBV	146292	323141	39.91%	4.678%
21	5.256	1215	1218	1222	rBV	287	191	0.02%	0.003%
22	5.282	1223	1226	1229	rVB2	353	180	0.02%	0.003%
23	5.301	1229	1232	1234	rBV	245	178	0.02%	0.003%
24	5.372	1252	1254	1258	rVB2	199	171	0.02%	0.002%
25	5.482	1285	1288	1293	rVB2	223	155	0.02%	0.002%
26	5.507	1293	1296	1302	rVB	275	248	0.03%	0.004%
27	5.543	1302	1307	1310	rBV	283	254	0.03%	0.004%
28	5.613	1326	1329	1333	rVB	221	162	0.02%	0.002%
29	5.719	1342	1362	1394	rBV3	277921	787752	97.29%	11.404%
30	6.006	1447	1451	1452	rVB2	252	167	0.02%	0.002%
31	6.015	1452	1454	1458	rBV	403	296	0.04%	0.004%
32	6.047	1462	1464	1471	rVB2	206	209	0.03%	0.003%
33	6.244	1511	1525	1551	rBV	312074	592835	73.21%	8.582%
34	6.526	1604	1613	1626	rVB7	4357	8550	1.06%	0.124%
35	6.684	1647	1662	1684	rBV	181247	355324	43.88%	5.144%
36	6.948	1740	1744	1745	rBV2	237	156	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.012	1760	1764	1766	rBV	283	172	0.02%	0.002%
38	7.379	1874	1878	1884	rBV	158	151	0.02%	0.002%
39	7.562	1919	1935	1954	rBV	103617	179897	22.22%	2.604%
40	7.697	1972	1977	1981	rBV	685	732	0.09%	0.011%
41	7.748	1989	1993	1997	rVB2	221	216	0.03%	0.003%
42	7.780	1997	2003	2008	rBV2	368	374	0.05%	0.005%
43	7.822	2011	2016	2020	rBV2	308	317	0.04%	0.005%
44	7.893	2025	2038	2059	rBV	360781	626456	77.37%	9.069%
45	8.070	2089	2093	2098	rBV2	321	263	0.03%	0.004%
46	8.096	2098	2101	2104	rVB2	371	262	0.03%	0.004%
47	8.176	2113	2126	2145	rBV	71873	122401	15.12%	1.772%
48	8.465	2213	2216	2222	rBV2	213	212	0.03%	0.003%
49	8.494	2222	2225	2228	rBV	223	188	0.02%	0.003%
50	8.555	2238	2244	2248	rVB4	1171	1301	0.16%	0.019%
51	8.626	2255	2266	2299	rBV2	214402	394332	48.70%	5.708%
52	8.838	2328	2332	2334	rBV2	177	157	0.02%	0.002%
53	8.922	2356	2358	2361	rBV	253	152	0.02%	0.002%
54	8.980	2373	2376	2382	rBV	198	218	0.03%	0.003%
55	9.141	2420	2426	2429	rBV	197	182	0.02%	0.003%
56	9.157	2429	2431	2433	rVV	219	150	0.02%	0.002%
57	9.214	2444	2449	2453	rVB2	232	218	0.03%	0.003%
58	9.260	2460	2463	2466	rBV	174	145	0.02%	0.002%
59	9.298	2472	2475	2478	rBV	222	163	0.02%	0.002%
60	9.414	2497	2511	2539	rBV2	427843	809721	100.00%	11.722%
61	9.600	2566	2569	2572	rBV	219	160	0.02%	0.002%
62	9.694	2592	2598	2601	rBV4	758	846	0.10%	0.012%
63	9.745	2610	2614	2618	rBV2	214	194	0.02%	0.003%
64	9.858	2645	2649	2656	rVB	251	259	0.03%	0.004%
65	10.112	2725	2728	2732	rVV3	386	270	0.03%	0.004%
66	10.221	2757	2762	2765	rVB2	320	257	0.03%	0.004%
67	10.285	2779	2782	2786	rBV2	303	278	0.03%	0.004%
68	10.472	2836	2840	2845	rBV2	294	357	0.04%	0.005%
69	10.751	2914	2927	2946	rBV	275433	444131	54.85%	6.429%
70	10.896	2967	2972	2977	rBV2	265	298	0.04%	0.004%
71	10.948	2986	2988	2992	rVB2	294	183	0.02%	0.003%
72	11.041	3012	3017	3022	rBV2	281	301	0.04%	0.004%
73	11.099	3030	3035	3037	rBV2	287	217	0.03%	0.003%
74	11.179	3057	3060	3068	rVB	182	179	0.02%	0.003%
75	11.417	3127	3134	3144	rVB3	2631	3642	0.45%	0.053%
76	11.468	3144	3150	3154	rBV	516	613	0.08%	0.009%

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 Title : VOC Analysis

77	11.491	3154	3157	3160	rVB	308	166	0.02%	0.002%
78	11.697	3218	3221	3224	rBV2	308	194	0.02%	0.003%
79	11.742	3224	3235	3244	rBV	90236	145801	18.01%	2.111%
80	11.809	3245	3256	3258	rBV	528680	696624	86.03%	10.084%
81	12.189	3361	3374	3396	rVV	405953	665303	82.16%	9.631%
82	12.346	3418	3423	3427	rVB2	393	353	0.04%	0.005%
83	12.382	3431	3434	3437	rVV	229	143	0.02%	0.002%
84	12.401	3437	3440	3445	rVB3	363	328	0.04%	0.005%
85	12.436	3448	3451	3456	rVB	267	182	0.02%	0.003%
86	12.513	3472	3475	3479	rBV	275	218	0.03%	0.003%
87	12.591	3496	3499	3501	rBV	269	151	0.02%	0.002%
88	12.677	3523	3526	3527	rBV	251	150	0.02%	0.002%
89	12.764	3549	3553	3554	rBV	233	167	0.02%	0.002%
90	12.812	3564	3568	3572	rBV	273	246	0.03%	0.004%
91	12.973	3615	3618	3619	rBV	239	154	0.02%	0.002%
92	13.272	3707	3711	3714	rBV	355	306	0.04%	0.004%
93	13.291	3714	3717	3721	rVV2	340	279	0.03%	0.004%
94	13.481	3773	3776	3782	rBV3	407	406	0.05%	0.006%
95	13.713	3845	3848	3860	rVB3	501	889	0.11%	0.013%
96	13.774	3864	3867	3868	rBV	411	219	0.03%	0.003%
97	13.838	3878	3887	3901	rBV2	33368	54512	6.73%	0.789%
98	13.928	3912	3915	3918	rBV	289	219	0.03%	0.003%
99	14.156	3983	3986	3989	rBV2	315	210	0.03%	0.003%
100	14.330	4036	4040	4051	rVB5	2711	3840	0.47%	0.056%

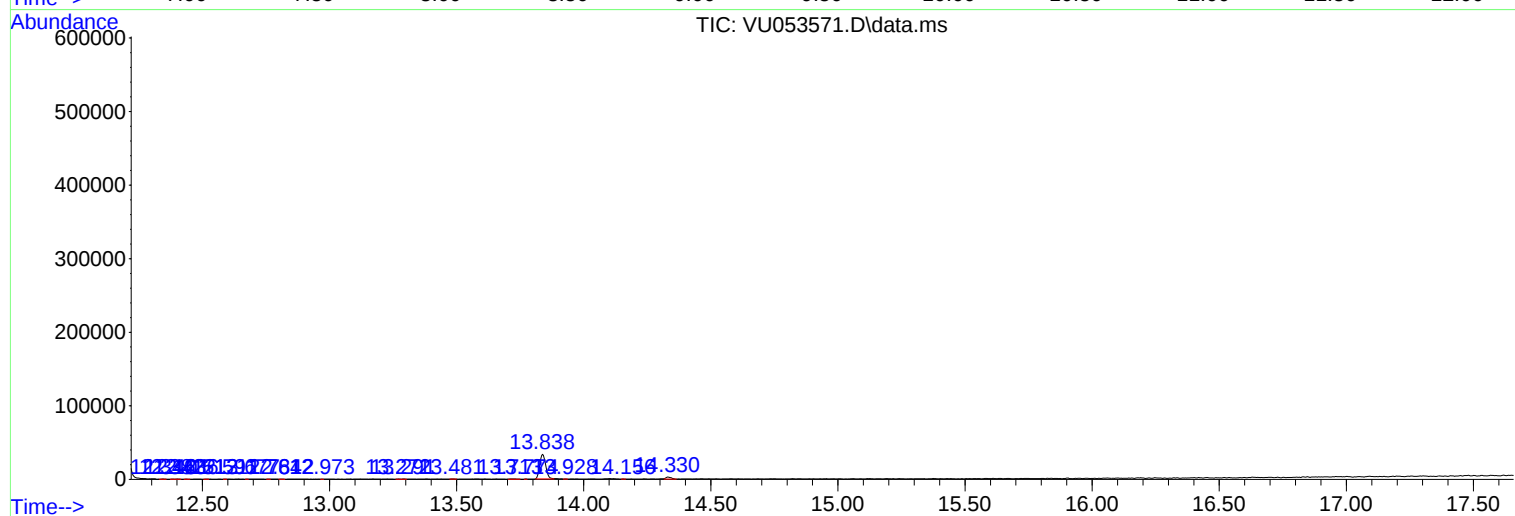
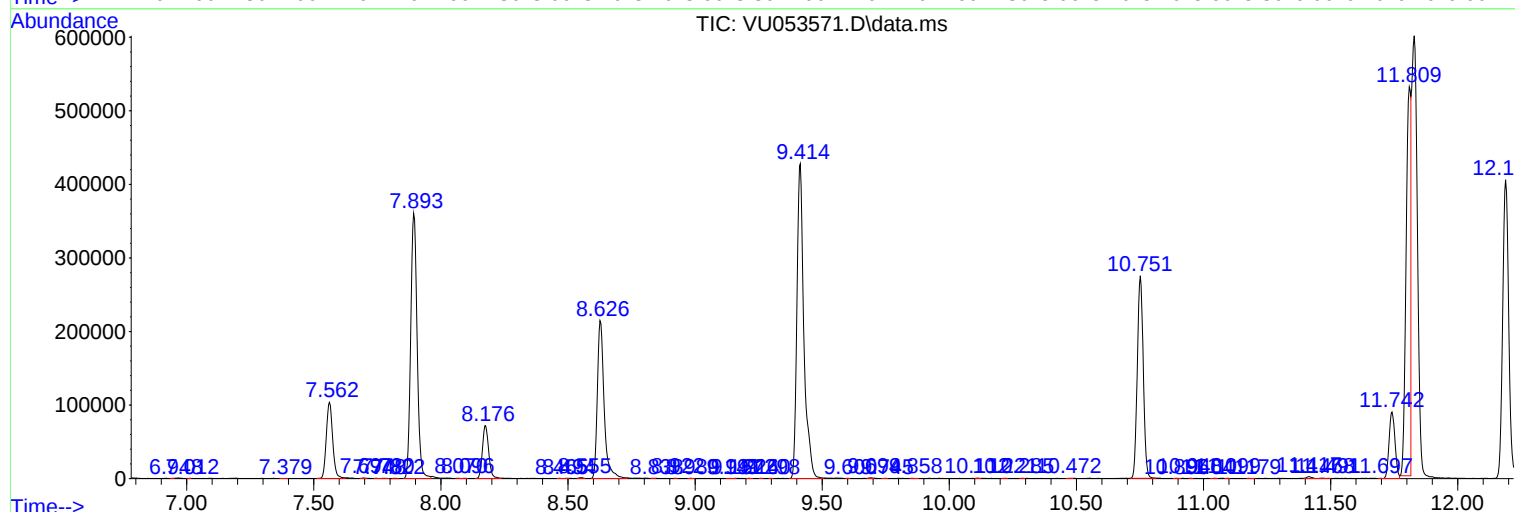
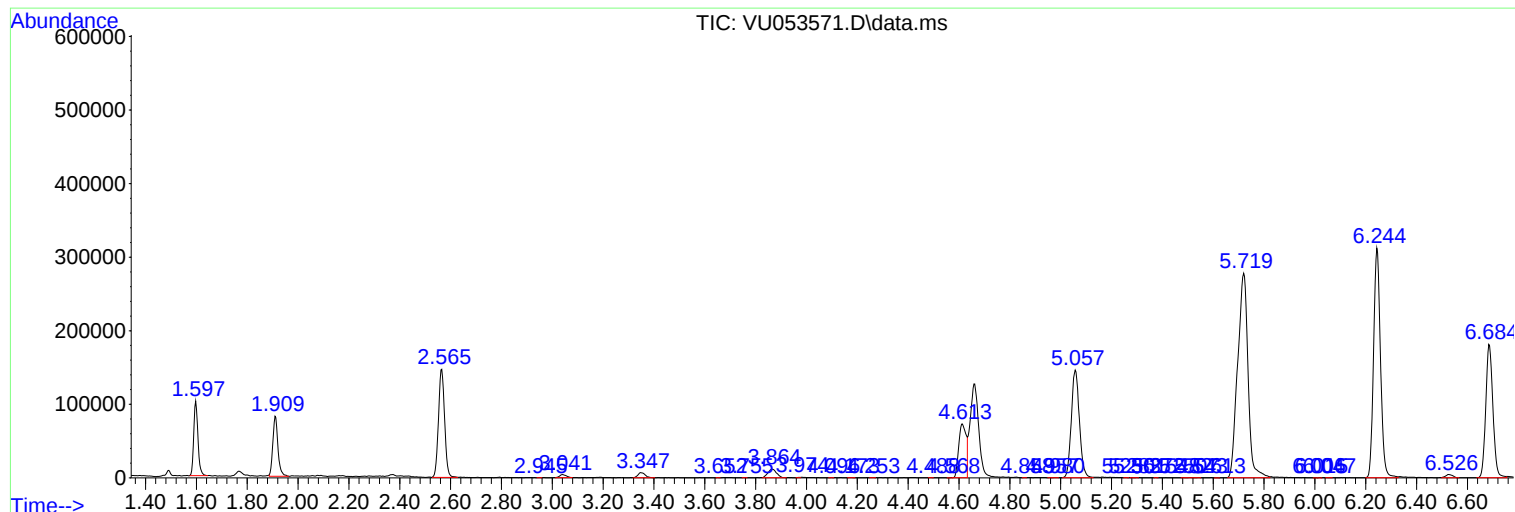
Sum of corrected areas: 6907920

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PMW-8S(20230330)DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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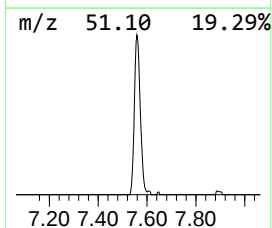
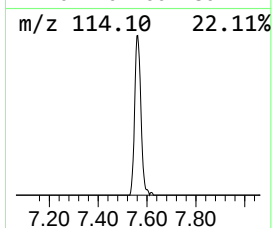
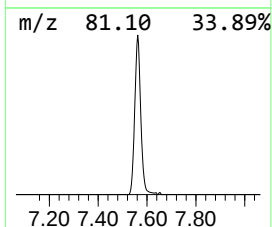
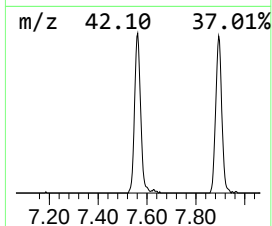
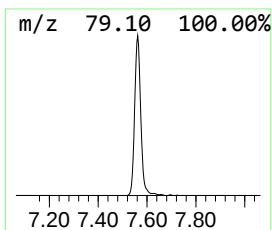
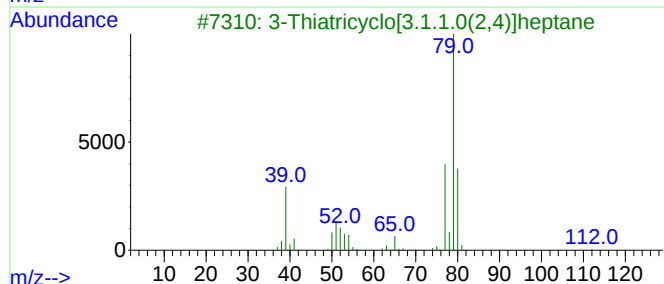
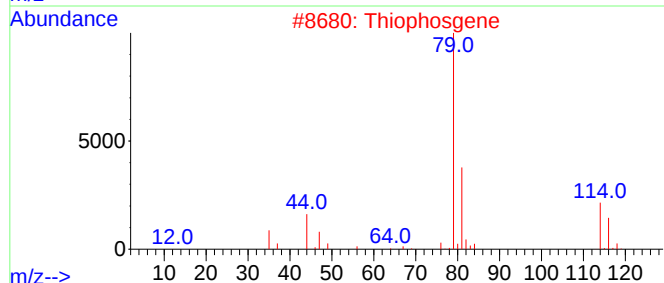
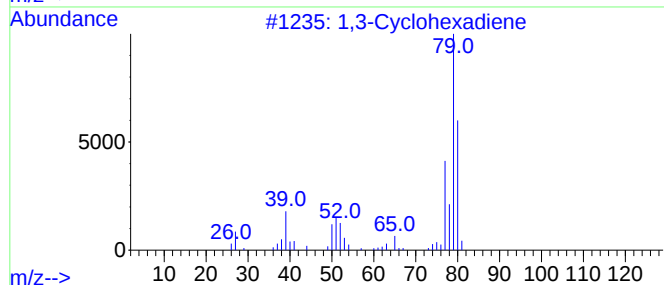
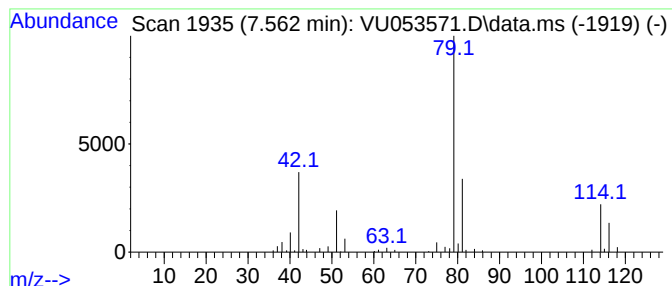
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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	15.17 ug/L	179897	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclohexadiene	80	C6H8	000592-57-4	47
2			Thiophosgene	114	CCl2S	000463-71-8	42
3			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	38
4			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
5			3-Methylenecyclopentene	80	C6H8	000930-26-7	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.562	15.2	ug/L	179897	1	6.244	592835	50.0