

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049752.D
 Acq On : 18 Jul 2022 11:12
 Operator : SY/MD
 Sample : VU0718MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK158

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.520	51	56	65	rBV3	2252	3402	0.43%	0.056%
2	1.597	72	80	95	rVB	76238	86898	11.07%	1.438%
3	1.777	133	136	138	rBV2	1415	1139	0.15%	0.019%
4	1.903	168	175	192	rVB	66671	88635	11.29%	1.467%
5	2.337	307	310	311	rBV	390	231	0.03%	0.004%
6	2.398	327	329	331	rBV2	499	223	0.03%	0.004%
7	2.562	369	380	397	rBV	126687	204588	26.06%	3.386%
8	2.632	397	402	411	rVB3	554	758	0.10%	0.013%
9	2.745	430	437	438	rBV	321	338	0.04%	0.006%
10	2.787	444	450	453	rBV3	713	699	0.09%	0.012%
11	2.841	462	467	469	rBV2	176	168	0.02%	0.003%
12	3.044	521	530	539	rBV2	3419	5506	0.70%	0.091%
13	3.173	566	570	574	rVB3	536	439	0.06%	0.007%
14	3.195	574	577	578	rBV2	281	163	0.02%	0.003%
15	3.401	637	641	644	rBV2	262	231	0.03%	0.004%
16	3.665	719	723	726	rBV2	210	158	0.02%	0.003%
17	3.832	772	775	779	rVB2	269	192	0.02%	0.003%
18	3.906	791	798	802	rVB2	213	262	0.03%	0.004%
19	4.157	867	876	882	rBV	212	249	0.03%	0.004%
20	4.285	911	916	920	rBV2	205	214	0.03%	0.004%
21	4.314	920	925	929	rVB2	239	260	0.03%	0.004%
22	4.349	929	936	938	rBV2	255	346	0.04%	0.006%
23	4.575	999	1006	1008	rBV2	239	285	0.04%	0.005%
24	4.623	1008	1021	1049	rBV	108975	269148	34.28%	4.454%
25	4.819	1079	1082	1093	rBV2	415	647	0.08%	0.011%
26	5.063	1142	1158	1183	rBV2	149443	328739	41.87%	5.441%
27	5.156	1183	1187	1191	rBV3	377	293	0.04%	0.005%
28	5.285	1222	1227	1230	rBV2	589	670	0.09%	0.011%
29	5.362	1248	1251	1253	rVV2	253	175	0.02%	0.003%
30	5.372	1253	1254	1260	rVV3	342	286	0.04%	0.005%
31	5.722	1341	1363	1395	rBV2	285771	785192	100.00%	12.995%
32	5.835	1395	1398	1401	rVB2	290	179	0.02%	0.003%
33	5.873	1407	1410	1412	rVB2	379	223	0.03%	0.004%
34	5.886	1412	1414	1421	rBV3	193	244	0.03%	0.004%
35	6.079	1470	1474	1478	rBV2	307	317	0.04%	0.005%
36	6.124	1486	1488	1492	rBV2	259	238	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.173	1500	1503	1505	rVB2	270	162	0.02%	0.003%
38	6.246	1513	1526	1542	rBV	249468	468176	59.63%	7.748%
39	6.420	1576	1580	1586	rVB2	343	308	0.04%	0.005%
40	6.446	1586	1588	1591	rVB2	310	179	0.02%	0.003%
41	6.465	1591	1594	1596	rBV	287	212	0.03%	0.004%
42	6.529	1606	1614	1626	rVB4	2253	4237	0.54%	0.070%
43	6.594	1631	1634	1639	rBV2	260	242	0.03%	0.004%
44	6.690	1650	1664	1684	rBV2	199650	383559	48.85%	6.348%
45	6.809	1697	1701	1707	rVB3	439	505	0.06%	0.008%
46	7.150	1803	1807	1811	rBV2	193	164	0.02%	0.003%
47	7.179	1811	1816	1817	rBV	1300	995	0.13%	0.016%
48	7.291	1844	1851	1854	rVB	214	198	0.03%	0.003%
49	7.324	1854	1861	1864	rBV2	251	267	0.03%	0.004%
50	7.375	1873	1877	1885	rBV2	204	298	0.04%	0.005%
51	7.443	1894	1898	1901	rBV	199	204	0.03%	0.003%
52	7.484	1909	1911	1915	rVB	336	261	0.03%	0.004%
53	7.565	1919	1936	1951	rBV	100204	175897	22.40%	2.911%
54	7.687	1968	1974	1981	rBV3	837	1290	0.16%	0.021%
55	7.793	2001	2007	2011	rBV3	586	625	0.08%	0.010%
56	7.896	2021	2039	2056	rBV	314416	542392	69.08%	8.977%
57	8.179	2115	2127	2148	rBV	68328	115556	14.72%	1.912%
58	8.452	2207	2212	2215	rBV	273	187	0.02%	0.003%
59	8.632	2253	2268	2299	rBV2	282746	556091	70.82%	9.203%
60	8.828	2326	2329	2332	rBV2	197	152	0.02%	0.003%
61	9.208	2444	2447	2451	rVB	244	181	0.02%	0.003%
62	9.317	2478	2481	2485	rVB2	326	312	0.04%	0.005%
63	9.349	2485	2491	2498	rBV2	467	844	0.11%	0.014%
64	9.417	2498	2512	2533	rBV	339791	564742	71.92%	9.346%
65	9.770	2617	2622	2623	rBV	308	274	0.03%	0.005%
66	9.922	2667	2669	2672	rVB	280	163	0.02%	0.003%
67	10.102	2720	2725	2726	rBV	544	324	0.04%	0.005%
68	10.256	2764	2773	2778	rBV2	199	317	0.04%	0.005%
69	10.323	2788	2794	2797	rBV2	198	194	0.02%	0.003%
70	10.430	2824	2827	2832	rBV2	201	186	0.02%	0.003%
71	10.487	2840	2845	2849	rBV	412	464	0.06%	0.008%
72	10.603	2872	2881	2884	rBV2	253	399	0.05%	0.007%
73	10.626	2884	2888	2889	rBV3	844	544	0.07%	0.009%
74	10.754	2915	2928	2947	rVV	285772	456189	58.10%	7.550%
75	10.889	2967	2970	2975	rVB2	321	300	0.04%	0.005%
76	10.967	2991	2994	2998	rVB2	345	283	0.04%	0.005%

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 Title : VOC Analysis

77	10.992	2998	3002	3003	rBV	236	196	0.02%	0.003%
78	11.153	3048	3052	3054	rBV	257	249	0.03%	0.004%
79	11.311	3094	3101	3104	rBV2	217	317	0.04%	0.005%
80	11.365	3114	3118	3123	rBV2	395	502	0.06%	0.008%
81	11.433	3135	3139	3141	rBV2	184	182	0.02%	0.003%
82	11.465	3146	3149	3150	rBV2	454	284	0.04%	0.005%
83	11.536	3168	3171	3174	rBV2	231	176	0.02%	0.003%
84	11.741	3232	3235	3245	rVB3	636	883	0.11%	0.015%
85	11.812	3245	3257	3279	rBV	294384	470960	59.98%	7.794%
86	12.192	3362	3375	3393	rBV	297033	483661	61.60%	8.005%
87	12.867	3579	3585	3586	rBV	257	265	0.03%	0.004%
88	13.050	3639	3642	3645	rBV	264	210	0.03%	0.003%
89	13.224	3690	3696	3704	rBV4	1204	1541	0.20%	0.026%
90	13.285	3713	3715	3719	rVB2	296	178	0.02%	0.003%
91	13.468	3769	3772	3775	rBV	216	180	0.02%	0.003%
92	13.822	3878	3882	3883	rBV3	347	234	0.03%	0.004%
93	13.844	3883	3889	3900	rVB4	2759	4016	0.51%	0.066%
94	13.941	3916	3919	3922	rVV	368	238	0.03%	0.004%
95	13.973	3926	3929	3932	rBV	343	197	0.03%	0.003%
96	14.040	3947	3950	3953	rBV2	286	257	0.03%	0.004%
97	14.089	3955	3965	3979	rVV	6791	11426	1.46%	0.189%
98	14.333	4032	4041	4052	rBV4	3642	5738	0.73%	0.095%
99	14.420	4064	4068	4074	rBV2	345	350	0.04%	0.006%
100	15.645	4445	4449	4453	rBV	459	444	0.06%	0.007%

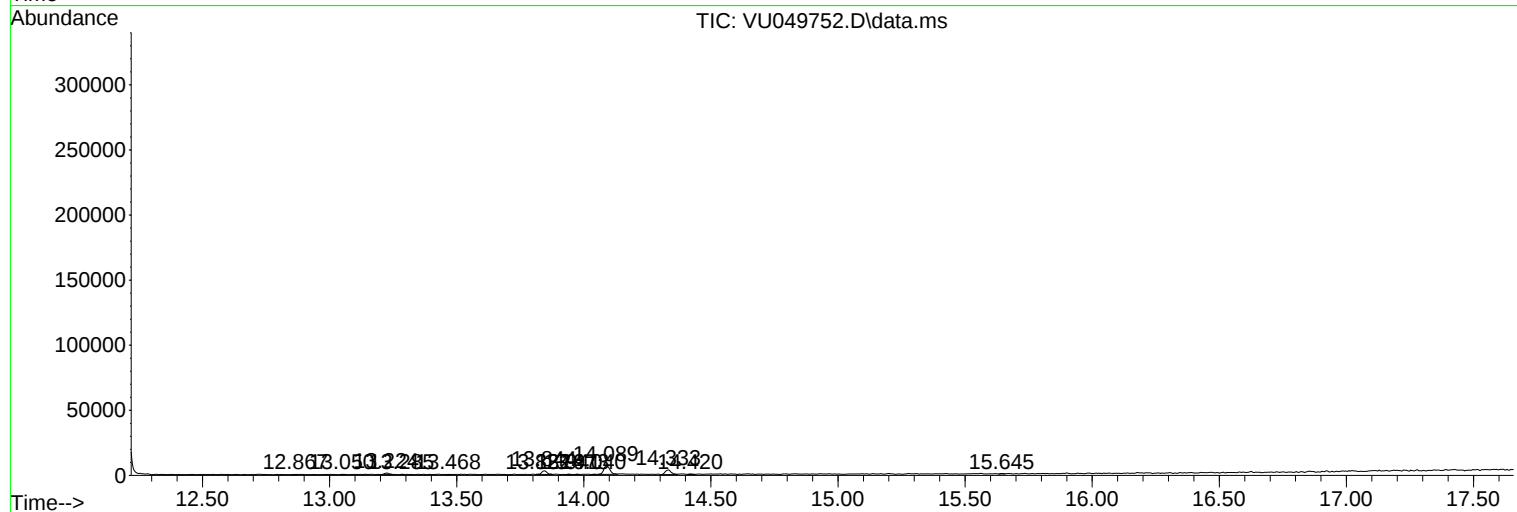
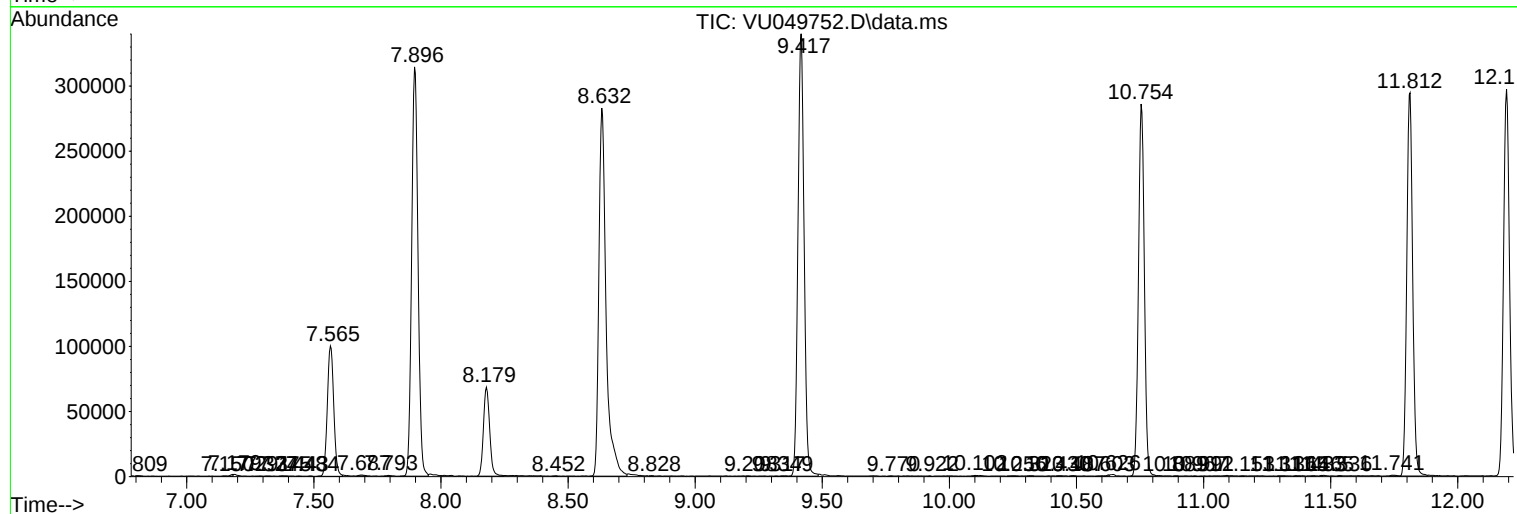
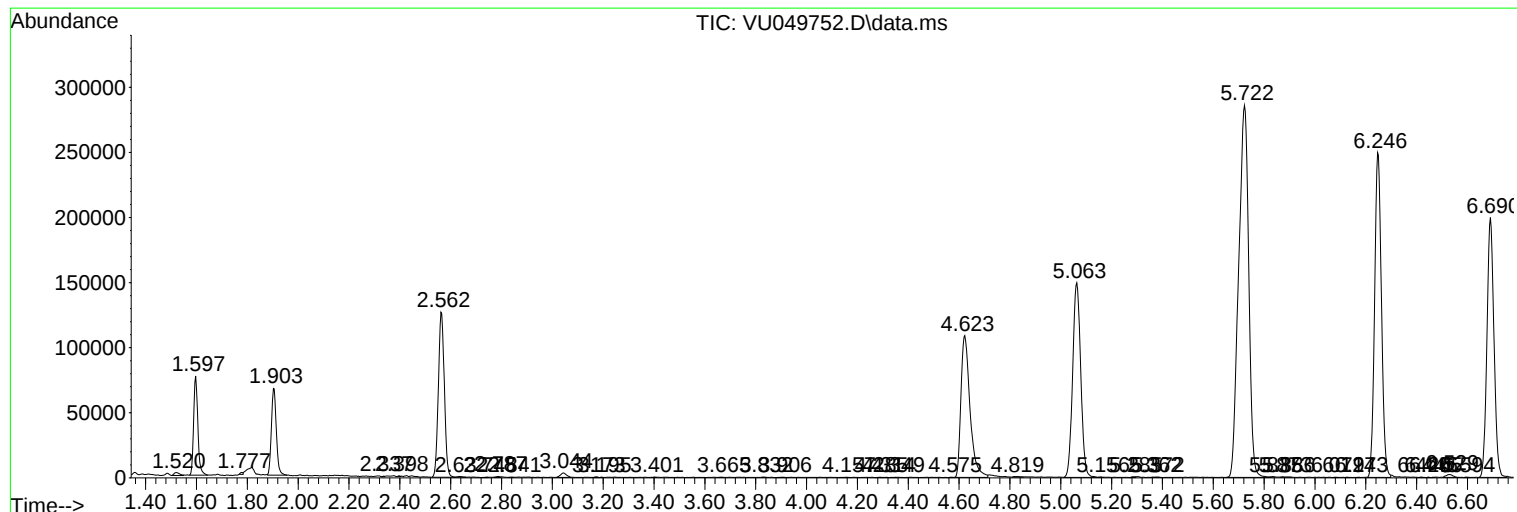
Sum of corrected areas: 6042292

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ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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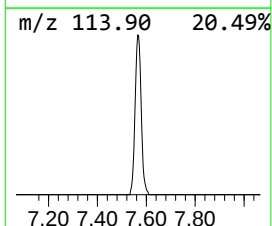
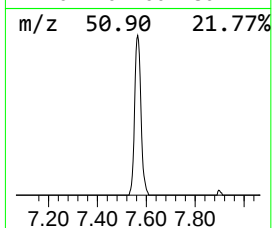
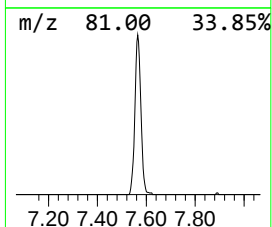
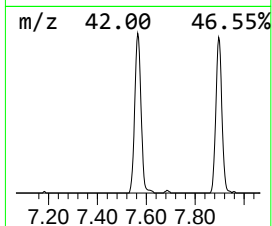
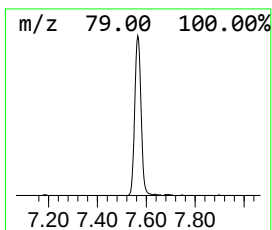
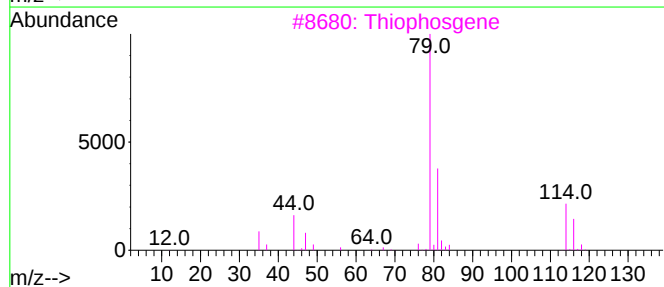
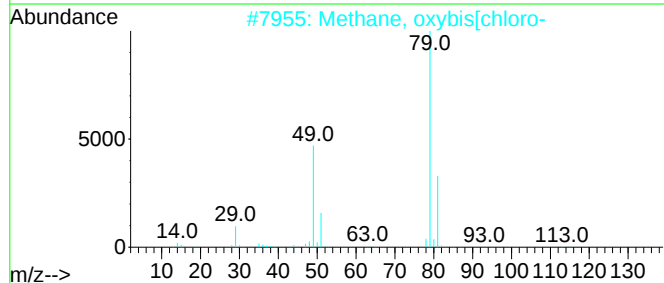
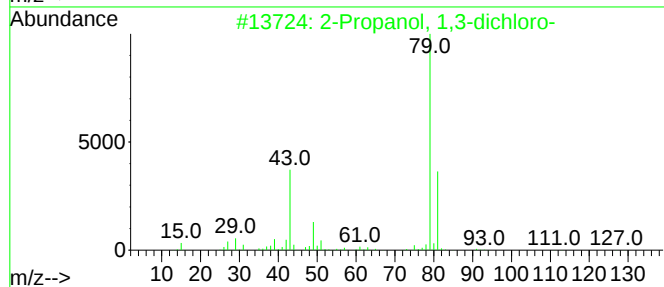
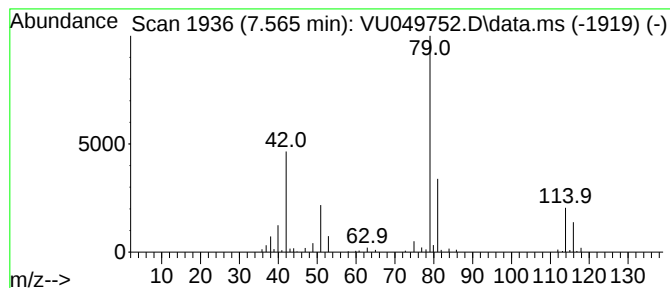
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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.
7.565	18.79 ug/L	175897	1,4-Difluorobenzene	6.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,3-dichloro-			128	C3H6Cl2O	000096-23-1	23
2	Methane, oxybis[chloro-			114	C2H4Cl2O	000542-88-1	23
3	Thiophosgene			114	CCl2S	000463-71-8	16
4	3-Thiatricyclo[3.1.1.0(2,4)]heptane			112	C6H8S	1000221-37-0	9
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	7.565	18.8	ug/L	175897	1	6.246	468176	50.0