

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
 Data File : VU049677.D
 Acq On : 11 Jul 2022 15:44
 Operator : SY/MD
 Sample : N3598-01ME
 Misc : 5.37g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AG2ME

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: VU049677.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.514	51	54	58	rBV4	1427	1017	0.11%	0.013%
2	1.594	72	79	85	rBV	68530	86802	9.32%	1.149%
3	1.800	122	143	145	rBV3	14351	31043	3.33%	0.411%
4	1.871	161	165	174	rBV	34777	41318	4.44%	0.547%
5	2.527	356	369	385	rVB	178064	290186	31.16%	3.842%
6	2.745	432	437	449	rVB2	760	1178	0.13%	0.016%
7	2.919	487	491	492	rBV	258	187	0.02%	0.002%
8	3.028	516	525	536	rVB5	2902	5413	0.58%	0.072%
9	3.092	542	545	550	rBV3	246	197	0.02%	0.003%
10	3.176	559	571	584	rVB3	3048	6553	0.70%	0.087%
11	3.488	664	668	671	rVB2	236	189	0.02%	0.003%
12	3.510	671	675	679	rVB	303	223	0.02%	0.003%
13	4.022	831	834	842	rVB2	198	253	0.03%	0.003%
14	4.488	975	979	981	rBV	206	169	0.02%	0.002%
15	4.636	1011	1025	1067	rBV	80693	267993	28.78%	3.548%
16	5.060	1140	1157	1177	rBV	154478	358404	38.49%	4.745%
17	5.279	1221	1225	1226	rBV	307	219	0.02%	0.003%
18	5.369	1246	1253	1256	rBV2	621	715	0.08%	0.009%
19	5.533	1300	1304	1307	rBV	211	179	0.02%	0.002%
20	5.610	1326	1328	1333	rVB	285	178	0.02%	0.002%
21	5.716	1334	1361	1385	rBV2	362667	931216	100.00%	12.329%
22	5.800	1385	1387	1391	rVB3	303	178	0.02%	0.002%
23	5.977	1429	1442	1460	rBV3	9202	22188	2.38%	0.294%
24	6.157	1496	1498	1504	rVB2	328	255	0.03%	0.003%
25	6.186	1504	1507	1511	rVB2	249	180	0.02%	0.002%
26	6.243	1511	1525	1548	rBV	302795	605464	65.02%	8.016%
27	6.475	1594	1597	1601	rBV2	270	227	0.02%	0.003%
28	6.536	1601	1616	1626	rVV7	11300	23172	2.49%	0.307%
29	6.600	1628	1636	1649	rVV3	3915	8756	0.94%	0.116%
30	6.687	1649	1663	1686	rVB	210883	431906	46.38%	5.718%
31	6.784	1689	1693	1695	rBV3	379	286	0.03%	0.004%
32	7.115	1792	1796	1798	rBV	325	245	0.03%	0.003%
33	7.192	1809	1820	1821	rBV3	1857	2095	0.22%	0.028%
34	7.285	1846	1849	1854	rBV3	362	394	0.04%	0.005%
35	7.343	1864	1867	1871	rVB3	232	182	0.02%	0.002%
36	7.452	1898	1901	1905	rVV2	279	231	0.02%	0.003%

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 Title : VOC Analysis

37	7.475	1905	1908	1911	rVV	249	174	0.02%	0.002%
38	7.565	1916	1936	1959	rBV2	105679	201693	21.66%	2.670%
39	7.793	1999	2007	2008	rBV2	372	349	0.04%	0.005%
40	7.896	2025	2039	2058	rBV	390468	701433	75.32%	9.287%
41	7.989	2058	2068	2084	rVB4	5209	12600	1.35%	0.167%
42	8.073	2092	2094	2100	rVB3	512	375	0.04%	0.005%
43	8.128	2110	2111	2116	rVB	246	170	0.02%	0.002%
44	8.182	2116	2128	2154	rBV2	65178	130948	14.06%	1.734%
45	8.321	2167	2171	2174	rVB3	301	234	0.03%	0.003%
46	8.349	2174	2180	2184	rBV3	865	980	0.11%	0.013%
47	8.420	2198	2202	2211	rVB2	389	544	0.06%	0.007%
48	8.465	2211	2216	2219	rBV3	421	394	0.04%	0.005%
49	8.552	2230	2243	2257	rBV2	127440	217477	23.35%	2.879%
50	8.652	2257	2274	2306	rBV2	229774	570156	61.23%	7.549%
51	8.796	2315	2319	2330	rVB6	3585	5584	0.60%	0.074%
52	8.841	2330	2333	2336	rBV3	286	240	0.03%	0.003%
53	8.919	2354	2357	2361	rBV	238	214	0.02%	0.003%
54	9.050	2392	2398	2402	rBV2	214	248	0.03%	0.003%
55	9.218	2446	2450	2453	rVB	273	208	0.02%	0.003%
56	9.263	2461	2464	2469	rBV	347	296	0.03%	0.004%
57	9.420	2499	2513	2539	rBV	404490	744513	79.95%	9.857%
58	9.755	2614	2617	2624	rBV	264	313	0.03%	0.004%
59	9.893	2656	2660	2666	rBV	301	286	0.03%	0.004%
60	10.128	2729	2733	2736	rVV2	296	203	0.02%	0.003%
61	10.388	2811	2814	2817	rBV	255	237	0.03%	0.003%
62	10.423	2822	2825	2832	rVB	193	195	0.02%	0.003%
63	10.491	2840	2846	2850	rBV2	447	446	0.05%	0.006%
64	10.555	2863	2866	2872	rVB2	375	331	0.04%	0.004%
65	10.619	2883	2886	2889	rVV2	613	552	0.06%	0.007%
66	10.648	2892	2895	2901	rVB4	811	773	0.08%	0.010%
67	10.761	2917	2930	2950	rBV	308323	505293	54.26%	6.690%
68	10.976	2995	2997	3004	rVB	249	219	0.02%	0.003%
69	11.009	3004	3007	3009	rBV	264	181	0.02%	0.002%
70	11.066	3018	3025	3027	rBV2	274	344	0.04%	0.005%
71	11.111	3035	3039	3046	rBV3	1438	1774	0.19%	0.023%
72	11.311	3099	3101	3106	rVB2	328	210	0.02%	0.003%
73	11.472	3147	3151	3152	rBV2	440	328	0.04%	0.004%
74	11.545	3170	3174	3176	rBV	276	216	0.02%	0.003%
75	11.642	3200	3204	3207	rBV	242	193	0.02%	0.003%
76	11.751	3232	3238	3240	rBV3	334	342	0.04%	0.005%

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 Title : VOC Analysis

77	11.816	3245	3258	3276	rBV	441074	703322	75.53%	9.312%
78	11.957	3300	3302	3308	rVB2	402	269	0.03%	0.004%
79	11.989	3308	3312	3315	rBV	247	234	0.03%	0.003%
80	12.195	3363	3376	3392	rBV	378547	620860	66.67%	8.220%
81	12.324	3410	3416	3418	rBV	341	340	0.04%	0.005%
82	12.507	3470	3473	3475	rBV	201	168	0.02%	0.002%
83	12.896	3591	3594	3599	rBV2	341	293	0.03%	0.004%
84	12.938	3604	3607	3612	rVV2	296	236	0.03%	0.003%
85	13.108	3656	3660	3663	rBV2	299	257	0.03%	0.003%
86	13.314	3720	3724	3726	rBV2	295	220	0.02%	0.003%
87	13.330	3726	3729	3733	rVV2	331	289	0.03%	0.004%
88	13.362	3737	3739	3742	rVB2	374	181	0.02%	0.002%
89	13.491	3774	3779	3782	rBV2	272	264	0.03%	0.003%
90	13.677	3833	3837	3840	rBV2	379	304	0.03%	0.004%
91	14.095	3958	3967	3972	rBV4	1845	2544	0.27%	0.034%
92	14.150	3981	3984	3987	rBV3	385	263	0.03%	0.003%
93	14.230	4006	4009	4011	rBV2	383	262	0.03%	0.003%
94	14.295	4026	4029	4033	rBV	459	411	0.04%	0.005%
95	14.410	4062	4065	4066	rBV	292	173	0.02%	0.002%
96	14.568	4112	4114	4117	rBV2	459	300	0.03%	0.004%
97	14.616	4127	4129	4132	rBV2	276	217	0.02%	0.003%
98	15.661	4452	4454	4457	rBV	403	193	0.02%	0.003%
99	15.677	4457	4459	4463	rBV3	426	357	0.04%	0.005%
100	16.211	4623	4625	4628	rBV2	638	375	0.04%	0.005%

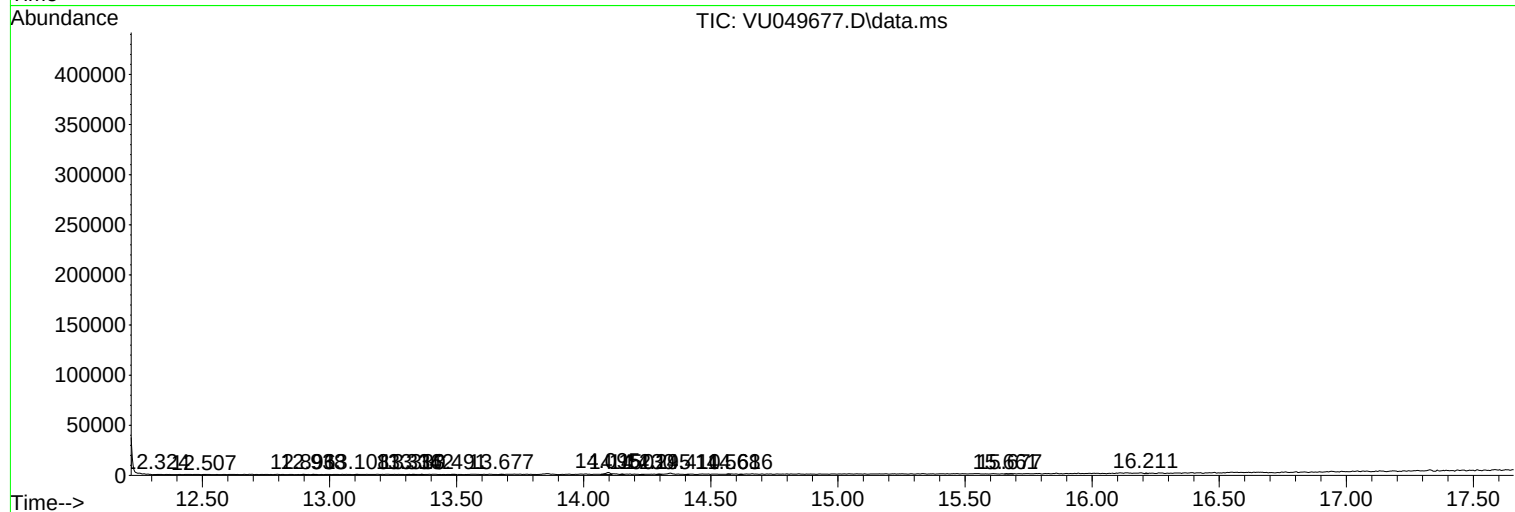
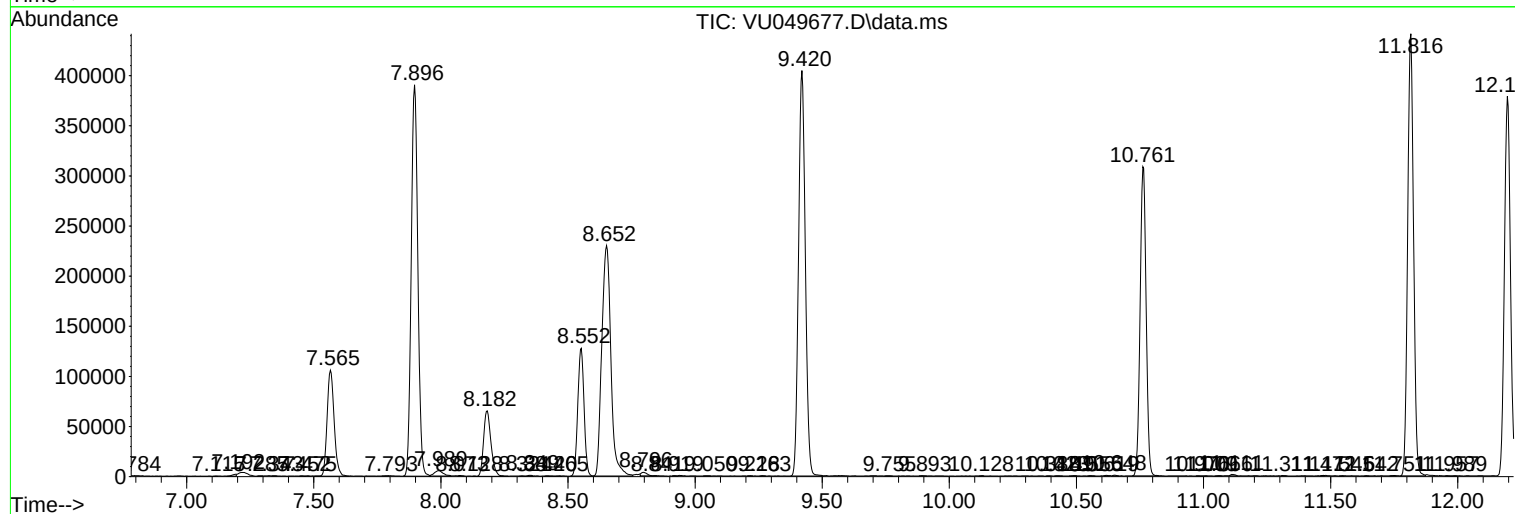
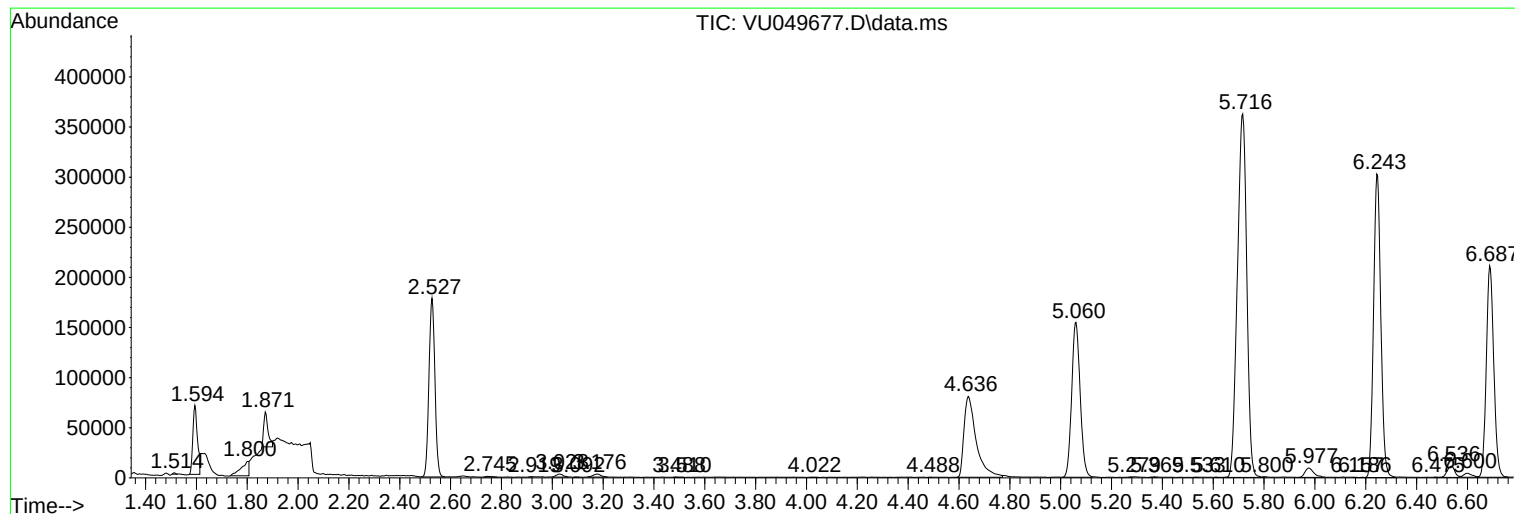
Sum of corrected areas: 7552989

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AG2ME

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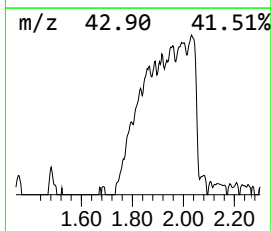
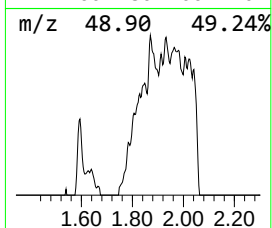
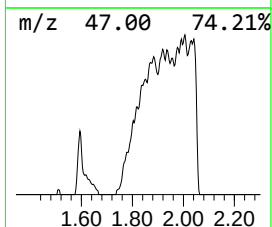
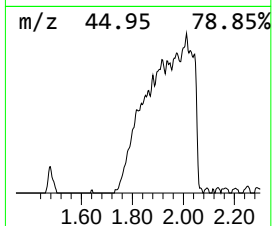
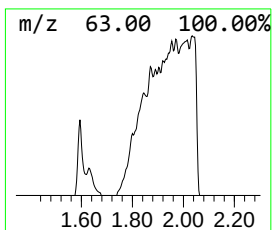
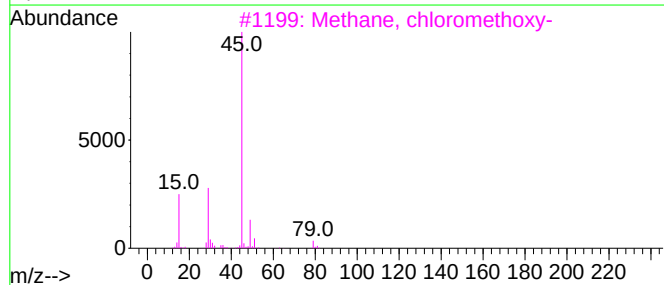
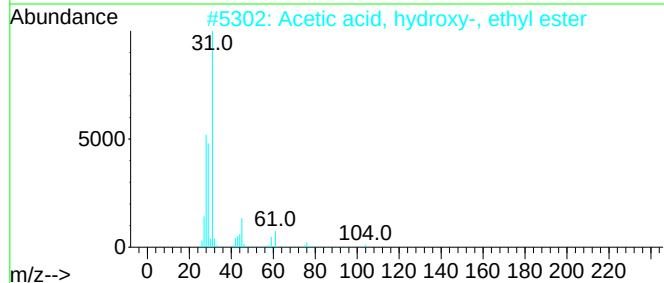
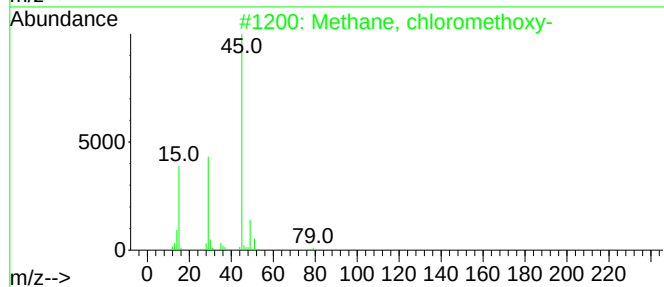
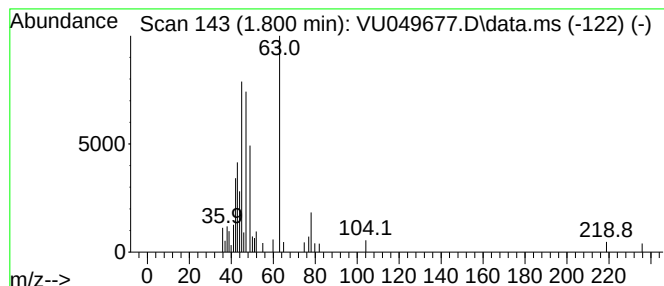
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.800	2.56 ug/L	31043	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
2			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	7
3			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	7
4			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	7
5			2-Chloroethyl methyl sulfone	142	C3H7ClO2S	050890-51-2	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.800	2.6	ug/L	31043	1	6.247	605464	50.0