

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042923\
 Data File : VU053976.D
 Acq On : 28 Apr 2023 17:57
 Operator : JC/MD
 Sample : 02526-09ME
 Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCF3ME

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: VU053976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.598	73	80	102	rVB	70800	104495	14.83%	1.822%
2	2.549	364	376	392	rBV	153940	244433	34.68%	4.263%
3	2.649	400	407	415	rVB2	3082	5787	0.82%	0.101%
4	2.765	439	443	446	rBV	355	284	0.04%	0.005%
5	2.887	477	481	485	rBV3	346	290	0.04%	0.005%
6	2.954	499	502	504	rBV	279	200	0.03%	0.003%
7	3.038	518	528	540	rBV4	4412	9844	1.40%	0.172%
8	3.575	690	695	697	rBV	180	222	0.03%	0.004%
9	3.588	697	699	702	rVB2	326	214	0.03%	0.004%
10	3.630	705	712	715	rBV	236	311	0.04%	0.005%
11	3.723	740	741	745	rVB	259	121	0.02%	0.002%
12	3.768	750	755	757	rBV	215	203	0.03%	0.004%
13	3.803	762	766	769	rVB2	166	154	0.02%	0.003%
14	3.851	778	781	786	rBV	211	134	0.02%	0.002%
15	3.877	786	789	791	rVV	193	124	0.02%	0.002%
16	4.003	825	828	830	rBV	225	183	0.03%	0.003%
17	4.067	844	848	852	rBV2	425	381	0.05%	0.007%
18	4.228	897	898	902	rVB	332	191	0.03%	0.003%
19	4.253	902	906	909	rBV	199	208	0.03%	0.004%
20	4.331	927	930	933	rBV2	267	207	0.03%	0.004%
21	4.366	939	941	945	rVB2	334	266	0.04%	0.005%
22	4.414	951	956	958	rBV	339	316	0.04%	0.006%
23	4.427	958	960	964	rVB	362	239	0.03%	0.004%
24	4.636	1014	1025	1049	rBV2	29329	95145	13.50%	1.659%
25	4.996	1134	1137	1139	rBB	263	165	0.02%	0.003%
26	5.057	1139	1156	1177	rBV	125576	291907	41.42%	5.091%
27	5.189	1193	1197	1199	rVB	566	470	0.07%	0.008%
28	5.208	1199	1203	1204	rBV	811	573	0.08%	0.010%
29	5.314	1233	1236	1237	rBV	309	171	0.02%	0.003%
30	5.337	1240	1243	1246	rVV3	372	270	0.04%	0.005%
31	5.421	1267	1269	1274	rVB	283	178	0.03%	0.003%
32	5.453	1275	1279	1282	rBV2	363	312	0.04%	0.005%
33	5.575	1314	1317	1321	rBB	204	190	0.03%	0.003%
34	5.597	1322	1324	1326	rBV	252	147	0.02%	0.003%
35	5.716	1341	1361	1385	rBV2	269585	704825	100.00%	12.292%
36	5.970	1435	1440	1441	rBV3	893	735	0.10%	0.013%

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

37	6.115	1481	1485	1489	rBV2	328	291	0.04%	0.005%
38	6.134	1489	1491	1494	rVB	226	136	0.02%	0.002%
39	6.240	1509	1524	1555	rBV	276057	543848	77.16%	9.485%
40	6.404	1572	1575	1576	rBV2	389	264	0.04%	0.005%
41	6.488	1598	1601	1604	rVB2	311	268	0.04%	0.005%
42	6.523	1604	1612	1623	rBV10	2804	5397	0.77%	0.094%
43	6.594	1627	1634	1635	rBV3	1291	1182	0.17%	0.021%
44	6.684	1648	1662	1683	rBV	158871	311572	44.21%	5.434%
45	6.900	1724	1729	1732	rBB	174	179	0.03%	0.003%
46	6.932	1733	1739	1743	rBV2	270	344	0.05%	0.006%
47	7.022	1764	1767	1770	rBV	247	220	0.03%	0.004%
48	7.092	1784	1789	1792	rBV	169	188	0.03%	0.003%
49	7.160	1808	1810	1814	rBV	199	196	0.03%	0.003%
50	7.186	1814	1818	1823	rBV6	671	886	0.13%	0.015%
51	7.311	1854	1857	1859	rBV	148	132	0.02%	0.002%
52	7.343	1863	1867	1868	rBV	225	122	0.02%	0.002%
53	7.408	1884	1887	1891	rBV	261	266	0.04%	0.005%
54	7.562	1923	1935	1961	rVB	84905	161298	22.88%	2.813%
55	7.893	2023	2038	2058	rBV	329629	591405	83.91%	10.314%
56	8.179	2115	2127	2148	rBV	49106	108287	15.36%	1.889%
57	8.269	2152	2155	2159	rVB	432	332	0.05%	0.006%
58	8.298	2159	2164	2168	rBV	232	340	0.05%	0.006%
59	8.465	2211	2216	2222	rBB2	452	559	0.08%	0.010%
60	8.549	2233	2242	2252	rVB4	11866	19943	2.83%	0.348%
61	8.658	2261	2276	2306	rBV2	123909	256414	36.38%	4.472%
62	8.803	2318	2321	2322	rBV2	412	205	0.03%	0.004%
63	8.858	2333	2338	2340	rBV	209	221	0.03%	0.004%
64	9.211	2443	2448	2451	rBV	380	368	0.05%	0.006%
65	9.253	2455	2461	2462	rBV	279	242	0.03%	0.004%
66	9.417	2498	2512	2533	rBV	346267	664330	94.25%	11.586%
67	9.658	2584	2587	2590	rVV	273	200	0.03%	0.003%
68	9.761	2616	2619	2621	rBV	264	156	0.02%	0.003%
69	9.880	2650	2656	2663	rBV2	327	500	0.07%	0.009%
70	9.967	2680	2683	2689	rBV2	387	376	0.05%	0.007%
71	10.179	2747	2749	2750	rBV	361	121	0.02%	0.002%
72	10.253	2768	2772	2776	rBV	150	131	0.02%	0.002%
73	10.276	2776	2779	2782	rBV	260	225	0.03%	0.004%
74	10.337	2793	2798	2801	rBV	306	344	0.05%	0.006%
75	10.591	2875	2877	2881	rBV	299	175	0.02%	0.003%
76	10.616	2882	2885	2888	rVV2	410	243	0.03%	0.004%

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77	10.652	2893	2896	2898	rVB2	345	178	0.03%	0.003%
78	10.761	2916	2930	2945	rBV	229751	371927	52.77%	6.487%
79	10.960	2989	2992	2998	rVB	268	268	0.04%	0.005%
80	10.996	2998	3003	3007	rBV2	302	263	0.04%	0.005%
81	11.054	3017	3021	3025	rBV2	259	188	0.03%	0.003%
82	11.115	3033	3040	3045	rBV4	745	893	0.13%	0.016%
83	11.369	3117	3119	3124	rVB2	459	328	0.05%	0.006%
84	11.494	3154	3158	3160	rBV	222	220	0.03%	0.004%
85	11.575	3181	3183	3185	rBV	233	128	0.02%	0.002%
86	11.809	3244	3256	3275	rBV	415072	655441	92.99%	11.431%
87	12.192	3362	3375	3390	rBV	355225	565023	80.17%	9.854%
88	12.359	3424	3427	3430	rBV2	255	185	0.03%	0.003%
89	12.858	3579	3582	3584	rBV	217	155	0.02%	0.003%
90	12.909	3596	3598	3600	rBV2	208	126	0.02%	0.002%
91	13.124	3661	3665	3666	rBV2	180	127	0.02%	0.002%
92	13.356	3734	3737	3739	rBV2	249	158	0.02%	0.003%
93	13.629	3820	3822	3825	rBV	300	147	0.02%	0.003%
94	13.742	3852	3857	3860	rBV	325	337	0.05%	0.006%
95	13.931	3913	3916	3919	rBV	222	133	0.02%	0.002%
96	14.163	3984	3988	3991	rBV2	312	249	0.04%	0.004%
97	14.192	3994	3997	4000	rBV	476	268	0.04%	0.005%
98	14.407	4061	4064	4070	rBV3	441	446	0.06%	0.008%
99	14.603	4121	4125	4127	rBV	380	249	0.04%	0.004%
100	15.259	4325	4329	4334	rBV2	519	566	0.08%	0.010%

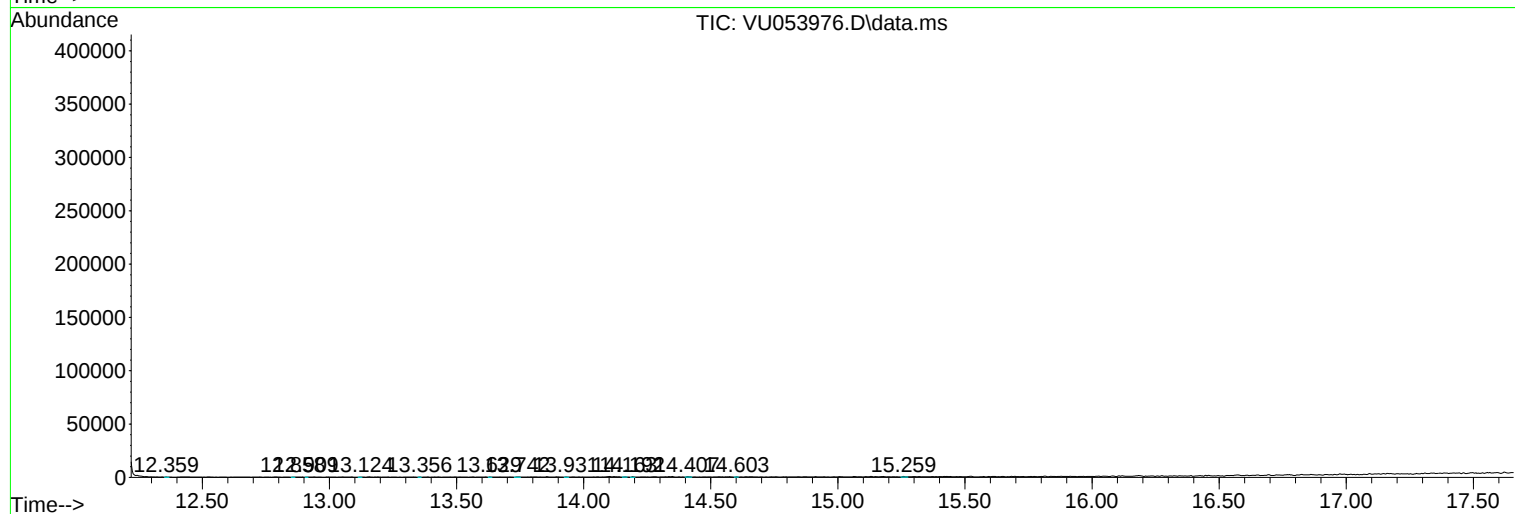
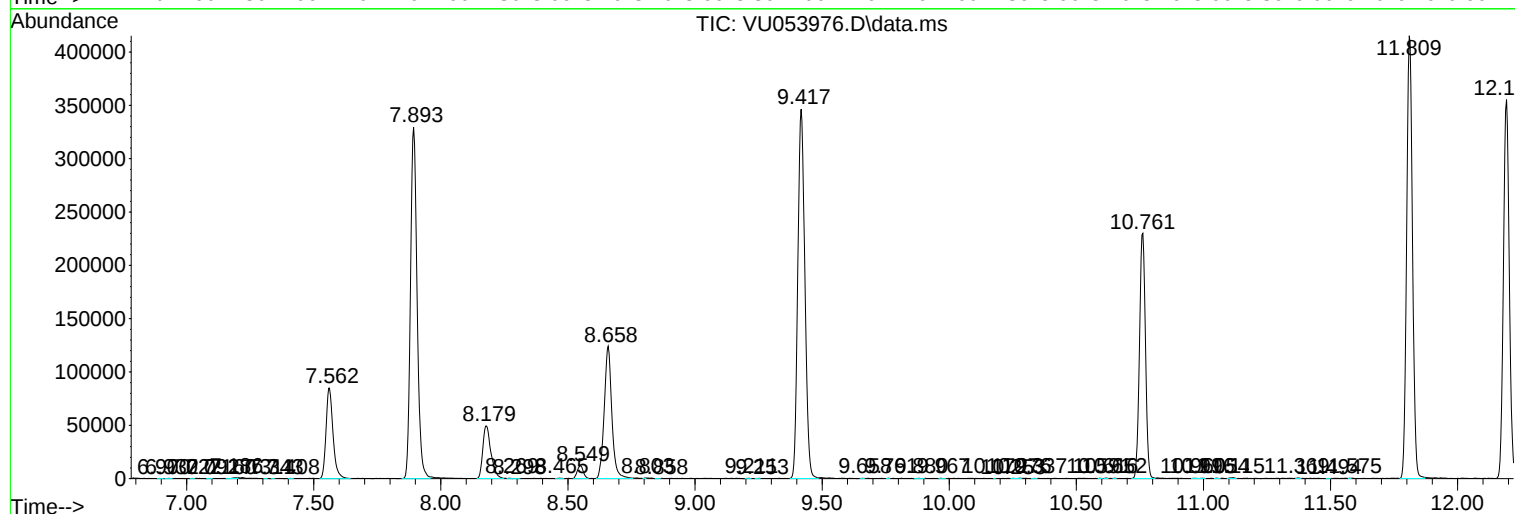
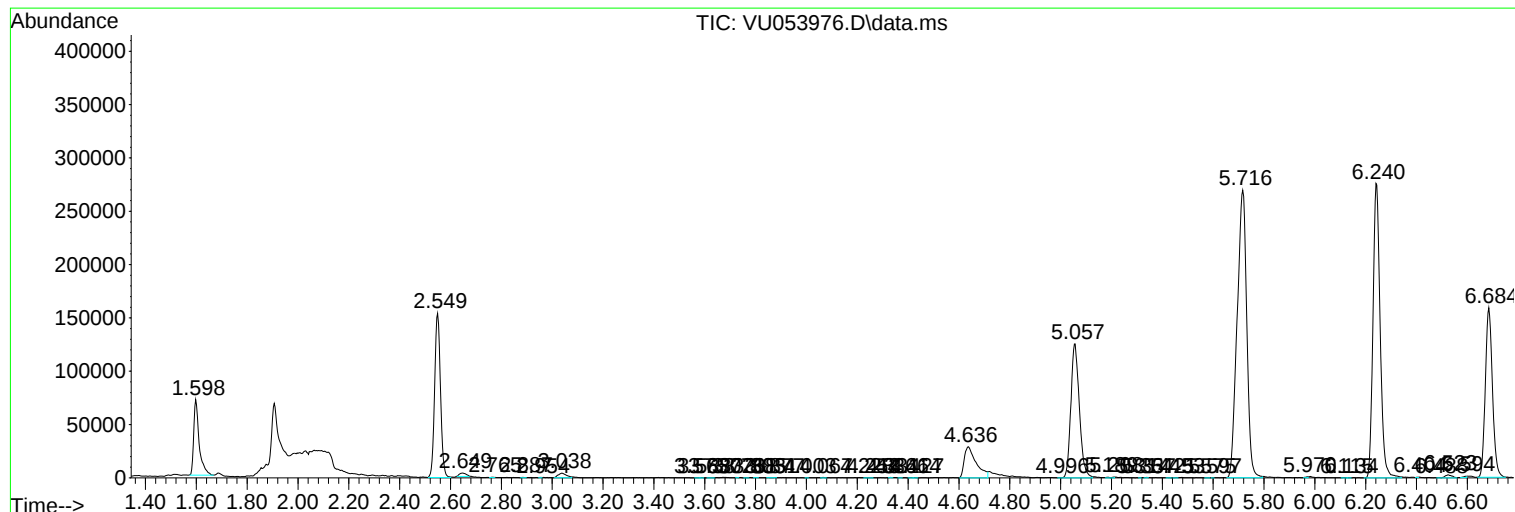
Sum of corrected areas: 5733804

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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



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

TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc