

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
 Data File : VU054008.D
 Acq On : 29 Apr 2023 23:55
 Operator : JC/MD
 Sample : 02548-35ME
 Misc : 6.24g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCR5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

Signal : TIC: VU054008.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	101	rVB	87527	127872	13.84%	1.785%
2	1.906	170	176	190	rBV	48046	84944	9.20%	1.186%
3	2.549	364	376	395	rBV	196714	316853	34.30%	4.424%
4	2.954	496	502	503	rBV2	455	433	0.05%	0.006%
5	2.980	507	510	513	rBV3	498	373	0.04%	0.005%
6	3.038	519	528	536	rBV2	2421	4912	0.53%	0.069%
7	3.199	577	578	579	rBV2	143	37	0.00%	0.001%
8	3.607	702	705	708	rBV	271	177	0.02%	0.002%
9	3.806	765	767	768	rBV	211	85	0.01%	0.001%
10	3.948	807	811	815	rVB	189	137	0.01%	0.002%
11	3.977	815	820	824	rBV2	337	326	0.04%	0.005%
12	4.002	824	828	835	rVB2	279	369	0.04%	0.005%
13	4.192	885	887	890	rVB	206	99	0.01%	0.001%
14	4.244	900	903	904	rBV	206	141	0.02%	0.002%
15	4.398	948	951	955	rBV	231	211	0.02%	0.003%
16	4.427	955	960	964	rVV2	256	319	0.03%	0.004%
17	4.520	987	989	991	rBV	140	57	0.01%	0.001%
18	4.536	991	994	999	rBV2	242	221	0.02%	0.003%
19	4.633	1013	1024	1063	rBV2	42670	162301	17.57%	2.266%
20	5.054	1141	1155	1183	rVB	157079	358189	38.78%	5.001%
21	5.199	1198	1200	1201	rBV	645	287	0.03%	0.004%
22	5.266	1218	1221	1224	rBV2	269	229	0.02%	0.003%
23	5.350	1244	1247	1249	rVB	246	127	0.01%	0.002%
24	5.417	1266	1268	1271	rVB2	326	218	0.02%	0.003%
25	5.436	1271	1274	1278	rBV	399	406	0.04%	0.006%
26	5.584	1315	1320	1321	rBV	177	153	0.02%	0.002%
27	5.713	1340	1360	1382	rBV2	349121	923740	100.00%	12.898%
28	5.973	1432	1441	1449	rBV6	2189	4463	0.48%	0.062%
29	6.083	1473	1475	1477	rBV	189	83	0.01%	0.001%
30	6.240	1511	1524	1548	rBV	318808	624864	67.65%	8.725%
31	6.472	1594	1596	1600	rVB	393	191	0.02%	0.003%
32	6.488	1600	1601	1602	rBB	110	21	0.00%	0.000%
33	6.523	1603	1612	1623	rVV8	3436	6491	0.70%	0.091%
34	6.600	1627	1636	1648	rVV4	2297	5426	0.59%	0.076%
35	6.684	1649	1662	1690	rVB	207485	413461	44.76%	5.773%
36	6.951	1743	1745	1747	rBV	170	79	0.01%	0.001%

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 Title : VOC Analysis

37	6.983	1753	1755	1757	rVB	179	75	0.01%	0.001%
38	6.996	1757	1759	1761	rVB	132	69	0.01%	0.001%
39	7.018	1763	1766	1771	rVV2	200	224	0.02%	0.003%
40	7.073	1782	1783	1784	rBV2	104	24	0.00%	0.000%
41	7.195	1812	1821	1827	rBV4	1638	3040	0.33%	0.042%
42	7.340	1864	1866	1867	rBV	235	97	0.01%	0.001%
43	7.369	1873	1875	1877	rBV	203	109	0.01%	0.002%
44	7.440	1894	1897	1903	rVB2	196	233	0.03%	0.003%
45	7.472	1904	1907	1912	rVB2	285	262	0.03%	0.004%
46	7.497	1912	1915	1918	rBV2	312	235	0.03%	0.003%
47	7.562	1922	1935	1966	rVB	105669	204300	22.12%	2.853%
48	7.674	1967	1970	1972	rBV2	211	148	0.02%	0.002%
49	7.768	1995	1999	2003	rVB2	191	176	0.02%	0.002%
50	7.809	2009	2012	2013	rBV	204	134	0.01%	0.002%
51	7.893	2022	2038	2057	rBV	412112	749495	81.14%	10.465%
52	8.128	2109	2111	2112	rBV	145	56	0.01%	0.001%
53	8.176	2115	2126	2153	rVB	66519	140261	15.18%	1.958%
54	8.282	2156	2159	2164	rBV	240	193	0.02%	0.003%
55	8.369	2183	2186	2189	rBV2	378	225	0.02%	0.003%
56	8.391	2191	2193	2194	rBV	152	44	0.00%	0.001%
57	8.546	2233	2241	2251	rVB3	8128	13677	1.48%	0.191%
58	8.594	2252	2256	2259	rBV	229	166	0.02%	0.002%
59	8.655	2259	2275	2306	rBV	172271	370094	40.06%	5.167%
60	9.050	2394	2398	2399	rBV2	238	159	0.02%	0.002%
61	9.202	2442	2445	2450	rVB	242	167	0.02%	0.002%
62	9.295	2472	2474	2476	rBV	167	118	0.01%	0.002%
63	9.417	2498	2512	2534	rBV	396796	758090	82.07%	10.585%
64	9.758	2614	2618	2619	rBV	227	144	0.02%	0.002%
65	9.816	2633	2636	2639	rBV2	222	179	0.02%	0.002%
66	9.886	2655	2658	2661	rBV2	164	138	0.01%	0.002%
67	10.086	2718	2720	2722	rBV	379	199	0.02%	0.003%
68	10.179	2747	2749	2752	rBV	180	71	0.01%	0.001%
69	10.263	2772	2775	2779	rVB2	350	207	0.02%	0.003%
70	10.401	2815	2818	2824	rVB	257	165	0.02%	0.002%
71	10.452	2833	2834	2835	rBV	307	91	0.01%	0.001%
72	10.587	2872	2876	2881	rBV2	323	340	0.04%	0.005%
73	10.613	2881	2884	2885	rBV	233	119	0.01%	0.002%
74	10.758	2917	2929	2945	rBV	268387	436669	47.27%	6.097%
75	10.832	2950	2952	2954	rVB	425	161	0.02%	0.002%
76	10.925	2978	2981	2983	rBV2	297	229	0.02%	0.003%

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77	11.201	3062	3067	3072	rBV2	272	364	0.04%	0.005%
78	11.436	3137	3140	3144	rBV2	317	333	0.04%	0.005%
79	11.742	3233	3235	3237	rBV	395	237	0.03%	0.003%
80	11.809	3244	3256	3275	rBV	472952	748381	81.02%	10.449%
81	12.076	3335	3339	3341	rBV	354	272	0.03%	0.004%
82	12.192	3362	3375	3394	rBV	436992	692570	74.97%	9.670%
83	12.452	3452	3456	3460	rBV2	349	253	0.03%	0.004%
84	12.642	3513	3515	3516	rBV	264	89	0.01%	0.001%
85	13.115	3659	3662	3664	rBV	261	170	0.02%	0.002%
86	13.661	3830	3832	3837	rBV2	531	431	0.05%	0.006%

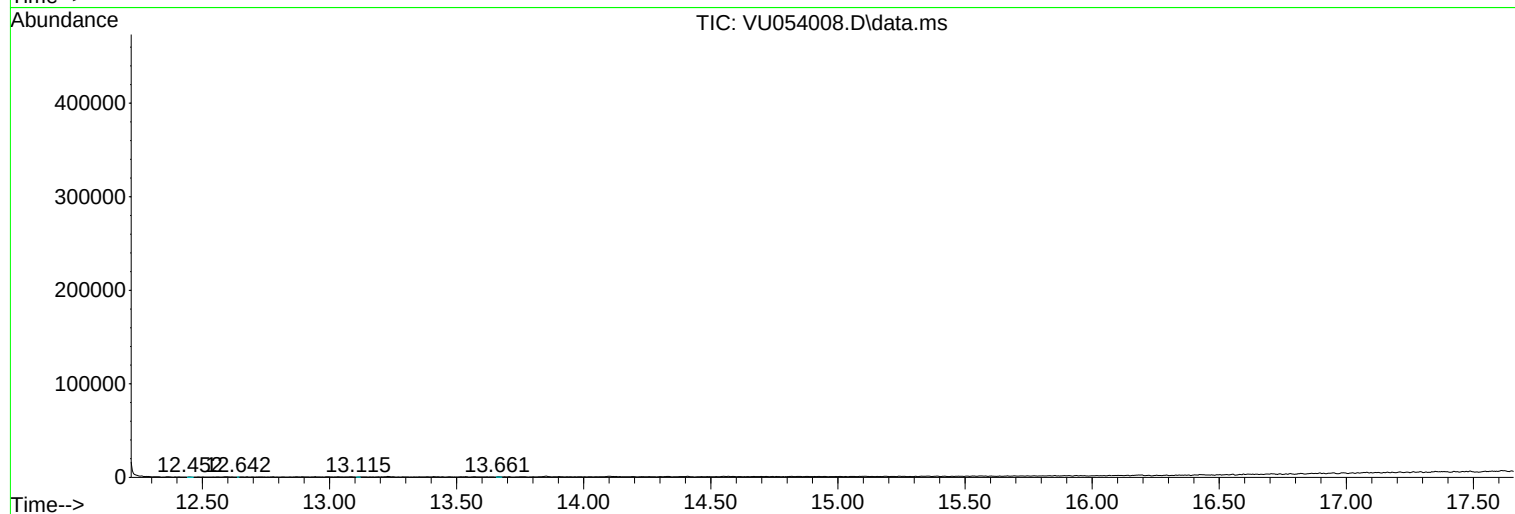
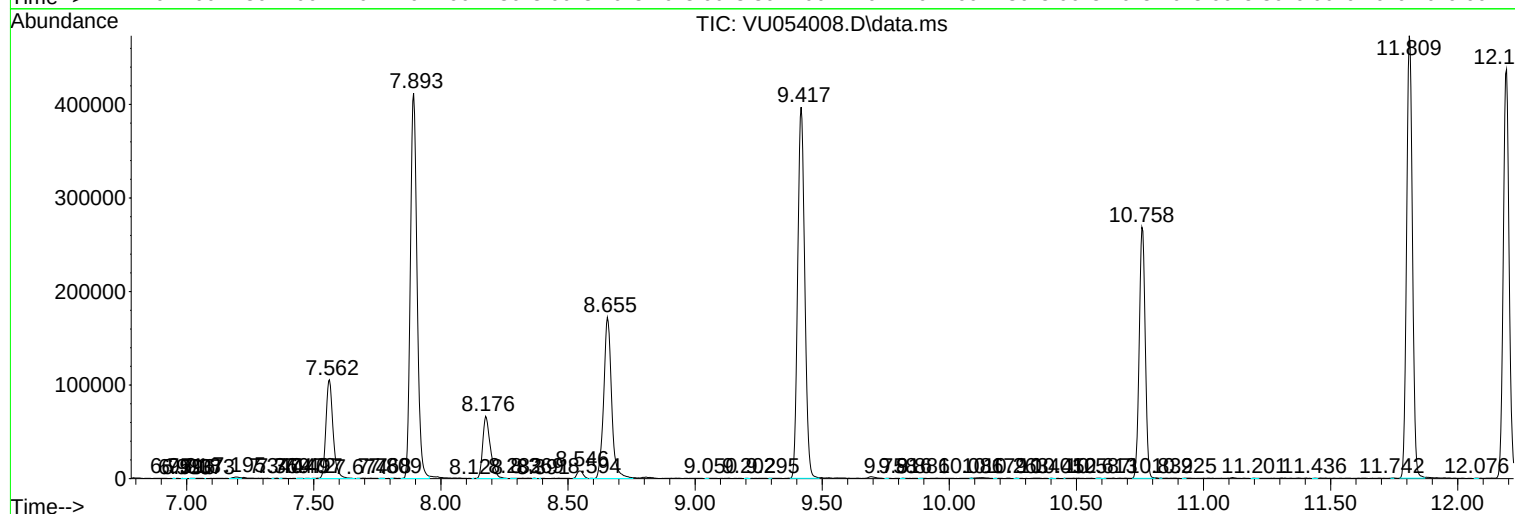
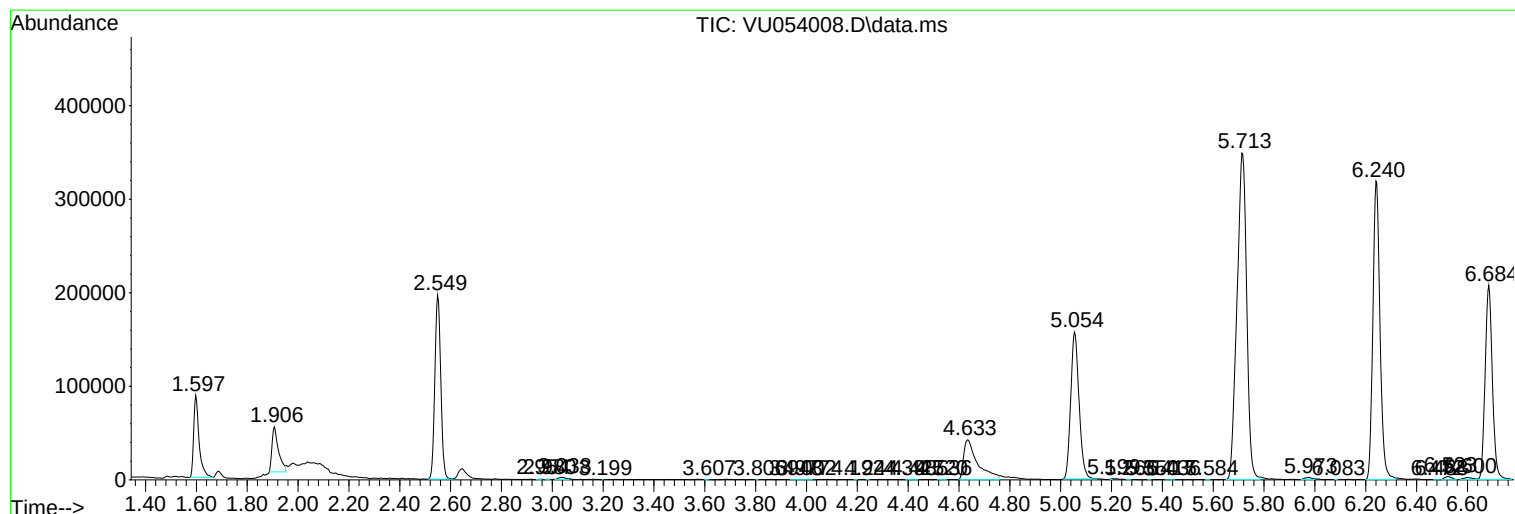
Sum of corrected areas: 7161978

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



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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	#	RT	Resp	Conc
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