

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050523\
 Data File : VU054071.D
 Acq On : 05 May 2023 16:02
 Operator : JC/MD
 Sample : 02589-18ME
 Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JRED6ME

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: VU054071.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	100	rBV	80036	96816	11.52%	1.498%
2	1.909	169	177	195	rVB	70199	96863	11.52%	1.498%
3	2.086	230	232	235	rBV	542	286	0.03%	0.004%
4	2.298	295	298	303	rBV2	422	398	0.05%	0.006%
5	2.565	369	381	396	rBV	150234	247111	29.39%	3.823%
6	2.787	444	450	451	rBV	559	443	0.05%	0.007%
7	2.928	492	494	505	rVB2	250	282	0.03%	0.004%
8	3.041	520	529	541	rVB3	4161	7592	0.90%	0.117%
9	3.099	543	547	551	rBV2	302	294	0.03%	0.005%
10	3.125	551	555	557	rBV	246	214	0.03%	0.003%
11	3.182	561	573	587	rVB2	3962	8464	1.01%	0.131%
12	3.295	602	608	610	rBV2	205	215	0.03%	0.003%
13	3.363	624	629	630	rBV	348	259	0.03%	0.004%
14	3.504	669	673	676	rVB2	372	258	0.03%	0.004%
15	3.694	729	732	737	rVV2	203	229	0.03%	0.004%
16	3.835	773	776	780	rVB	275	183	0.02%	0.003%
17	3.993	816	825	828	rBV2	361	383	0.05%	0.006%
18	4.227	894	898	900	rBV	250	199	0.02%	0.003%
19	4.462	966	971	973	rBV2	147	174	0.02%	0.003%
20	4.514	985	987	991	rVB2	278	224	0.03%	0.003%
21	4.546	992	997	998	rBV2	365	334	0.04%	0.005%
22	4.620	1008	1020	1050	rBV	68744	175901	20.92%	2.721%
23	4.928	1113	1116	1118	rBV2	276	214	0.03%	0.003%
24	4.967	1125	1128	1130	rBV	280	212	0.03%	0.003%
25	5.057	1140	1156	1181	rBV	153070	339541	40.39%	5.253%
26	5.276	1218	1224	1226	rBV2	341	264	0.03%	0.004%
27	5.308	1230	1234	1238	rVB	233	241	0.03%	0.004%
28	5.334	1238	1242	1243	rBV2	294	186	0.02%	0.003%
29	5.359	1247	1250	1252	rBV	262	207	0.02%	0.003%
30	5.478	1285	1287	1290	rVV	311	196	0.02%	0.003%
31	5.639	1333	1337	1340	rBV2	176	165	0.02%	0.003%
32	5.719	1340	1362	1383	rBV2	302586	840681	100.00%	13.005%
33	5.977	1438	1442	1445	rBV	160	171	0.02%	0.003%
34	6.025	1453	1457	1459	rBV	389	353	0.04%	0.005%
35	6.115	1480	1485	1486	rBV2	252	222	0.03%	0.003%
36	6.243	1512	1525	1554	rBV	263127	506257	60.22%	7.832%

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

37	6.427	1579	1582	1586	rVB	318	313	0.04%	0.005%
38	6.452	1586	1590	1594	rBV2	306	400	0.05%	0.006%
39	6.526	1605	1613	1614	rBV3	2084	2209	0.26%	0.034%
40	6.629	1641	1645	1647	rBV	193	194	0.02%	0.003%
41	6.687	1650	1663	1686	rBV	198404	392970	46.74%	6.079%
42	7.054	1771	1777	1783	rBV2	319	384	0.05%	0.006%
43	7.115	1790	1796	1798	rBV	137	173	0.02%	0.003%
44	7.189	1812	1819	1829	rVB3	842	1076	0.13%	0.017%
45	7.337	1857	1865	1871	rVB2	306	466	0.06%	0.007%
46	7.369	1871	1875	1878	rBV2	228	201	0.02%	0.003%
47	7.501	1913	1916	1919	rBV	202	182	0.02%	0.003%
48	7.562	1919	1935	1958	rBV	108515	194423	23.13%	3.008%
49	7.694	1972	1976	1981	rVB3	580	543	0.06%	0.008%
50	7.796	1998	2008	2020	rBV5	2922	5376	0.64%	0.083%
51	7.893	2024	2038	2057	rBV	368100	643616	76.56%	9.957%
52	8.015	2074	2076	2079	rBV2	321	233	0.03%	0.004%
53	8.176	2114	2126	2152	rVV	77363	134072	15.95%	2.074%
54	8.333	2172	2175	2177	rBV	209	164	0.02%	0.003%
55	8.366	2182	2185	2188	rBV	239	187	0.02%	0.003%
56	8.436	2205	2207	2213	rVV2	327	338	0.04%	0.005%
57	8.465	2213	2216	2220	rVV	393	291	0.03%	0.005%
58	8.552	2238	2243	2249	rVB4	775	840	0.10%	0.013%
59	8.629	2256	2267	2298	rBV2	199380	388125	46.17%	6.004%
60	8.787	2314	2316	2322	rVB	287	255	0.03%	0.004%
61	8.812	2322	2324	2328	rBV2	368	254	0.03%	0.004%
62	8.954	2364	2368	2371	rBV2	235	249	0.03%	0.004%
63	9.083	2406	2408	2412	rVB	252	172	0.02%	0.003%
64	9.414	2496	2511	2534	rBV	360769	608260	72.35%	9.410%
65	9.568	2554	2559	2572	rVB3	1616	2320	0.28%	0.036%
66	9.648	2582	2584	2589	rVB2	311	206	0.02%	0.003%
67	9.697	2589	2599	2606	rBV4	1706	2706	0.32%	0.042%
68	9.767	2615	2621	2624	rBV	275	312	0.04%	0.005%
69	9.954	2674	2679	2682	rBV	234	241	0.03%	0.004%
70	10.108	2717	2727	2729	rBV4	2487	3136	0.37%	0.049%
71	10.201	2753	2756	2759	rVB2	257	198	0.02%	0.003%
72	10.221	2759	2762	2766	rBV	170	164	0.02%	0.003%
73	10.311	2786	2790	2793	rBV2	196	177	0.02%	0.003%
74	10.378	2808	2811	2816	rVB2	284	289	0.03%	0.004%
75	10.417	2816	2823	2825	rBV2	220	249	0.03%	0.004%
76	10.484	2830	2844	2851	rBV4	2366	3965	0.47%	0.061%

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 Title : VOC Analysis

77	10.751	2914	2927	2945	rBV	273793	440931	52.45%	6.821%
78	10.944	2983	2987	2990	rBV	209	214	0.03%	0.003%
79	10.996	3000	3003	3007	rBV2	211	221	0.03%	0.003%
80	11.086	3024	3031	3040	rVB4	1743	2698	0.32%	0.042%
81	11.465	3142	3149	3159	rVB2	2131	3349	0.40%	0.052%
82	11.742	3228	3235	3244	rBV6	4100	6179	0.73%	0.096%
83	11.806	3244	3255	3277	rVV	373144	605055	71.97%	9.360%
84	11.941	3294	3297	3299	rBV	262	179	0.02%	0.003%
85	12.189	3360	3374	3394	rBV	388363	630538	75.00%	9.754%
86	12.433	3442	3450	3453	rBV2	291	413	0.05%	0.006%
87	12.835	3571	3575	3577	rBV2	231	176	0.02%	0.003%
88	13.025	3629	3634	3636	rBV2	254	265	0.03%	0.004%
89	13.221	3687	3695	3706	rVB3	5166	7683	0.91%	0.119%
90	13.307	3717	3722	3723	rBV3	359	261	0.03%	0.004%
91	13.581	3803	3807	3811	rBV2	450	518	0.06%	0.008%
92	13.754	3855	3861	3870	rBV2	558	1020	0.12%	0.016%
93	13.838	3879	3887	3898	rBV4	9429	15218	1.81%	0.235%
94	13.883	3898	3901	3904	rBV2	261	168	0.02%	0.003%
95	13.934	3915	3917	3920	rBV2	294	211	0.03%	0.003%
96	14.089	3954	3965	3982	rBV2	8428	15574	1.85%	0.241%
97	14.327	4031	4039	4052	rBV2	9825	16227	1.93%	0.251%
98	14.417	4064	4067	4069	rBV2	360	235	0.03%	0.004%
99	14.558	4107	4111	4112	rBV2	350	238	0.03%	0.004%
100	15.896	4522	4527	4528	rBV2	733	635	0.08%	0.010%

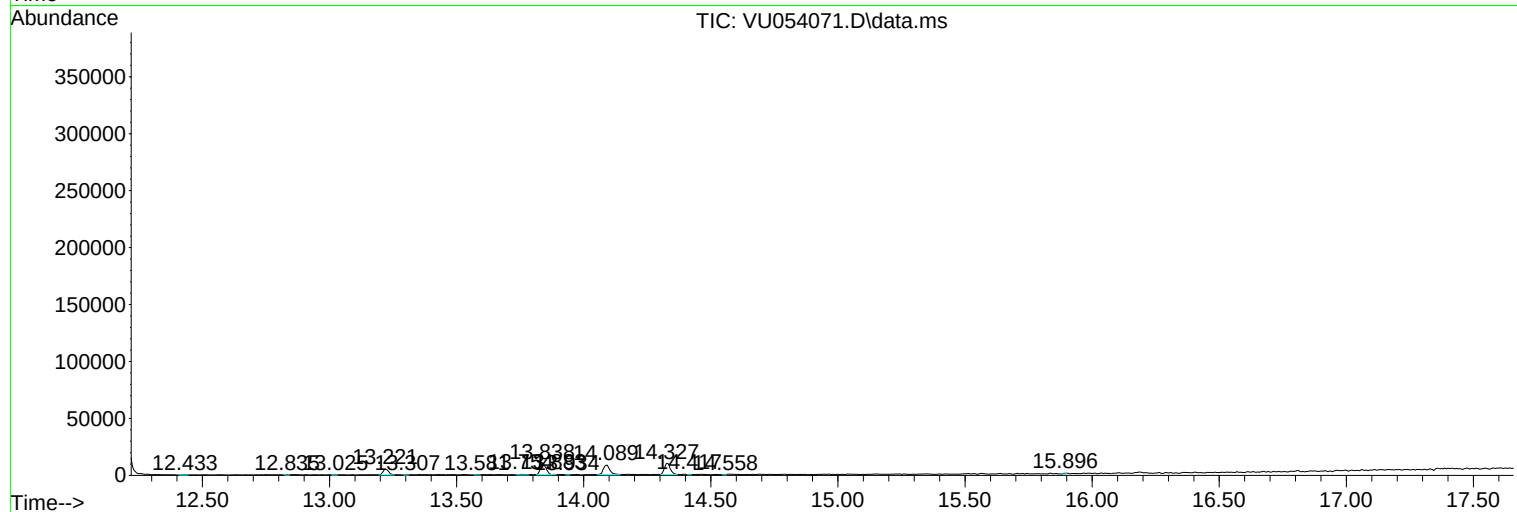
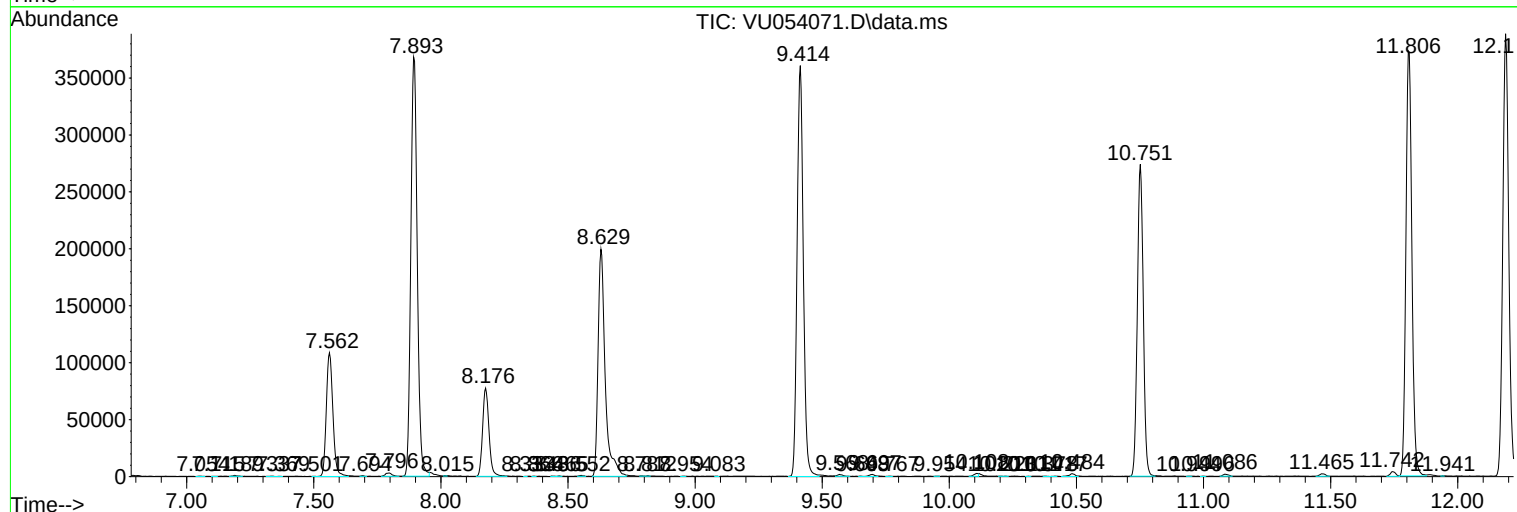
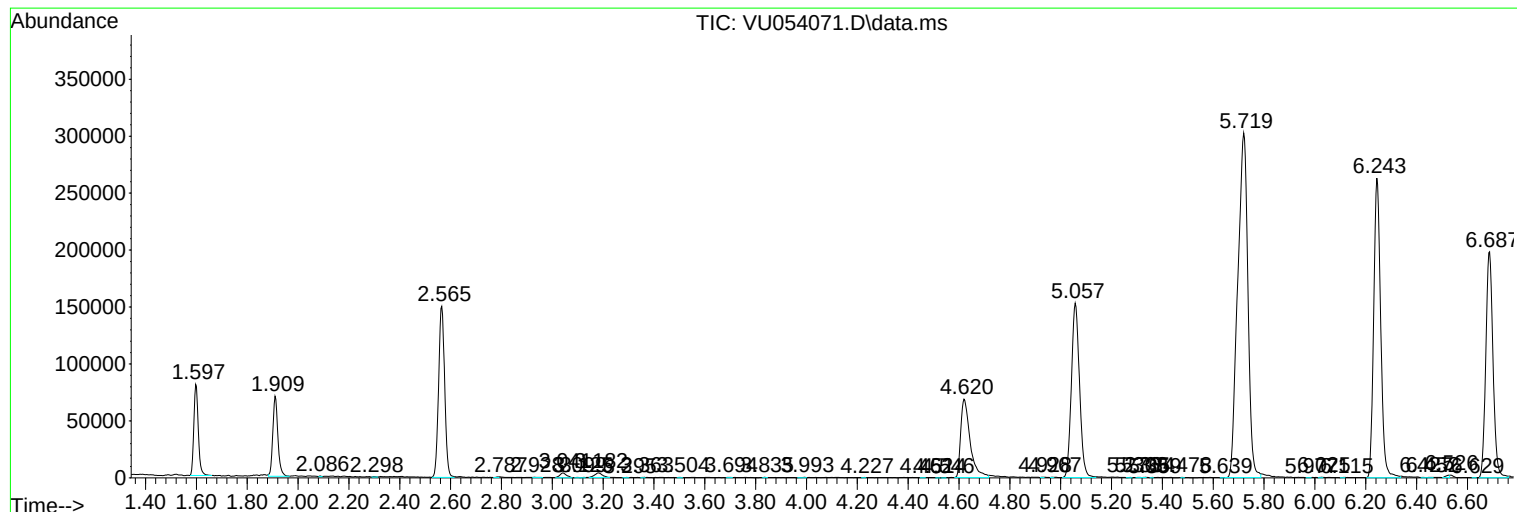
Sum of corrected areas: 6464167

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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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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.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	#	RT	Resp	Conc
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