

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053520.D
 Acq On : 03 Apr 2023 15:16
 Operator : JC/MD
 Sample : 02151-07ME
 Misc : 4.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C11B0ME

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: VU053520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	103	rVB	63562	96750	10.86%	1.380%
2	2.539	360	373	394	rVB	157854	257699	28.93%	3.675%
3	2.629	396	401	411	rBV7	2404	3666	0.41%	0.052%
4	2.867	470	475	481	rVB2	364	372	0.04%	0.005%
5	2.912	485	489	492	rVB2	452	350	0.04%	0.005%
6	3.031	515	526	546	rBV5	5796	14111	1.58%	0.201%
7	3.166	562	568	583	rBV4	1207	2866	0.32%	0.041%
8	3.440	651	653	659	rVB2	275	241	0.03%	0.003%
9	3.568	688	693	696	rBV2	384	353	0.04%	0.005%
10	3.674	719	726	730	rBV3	971	1184	0.13%	0.017%
11	3.781	755	759	762	rBV2	332	244	0.03%	0.003%
12	4.424	955	959	963	rVB2	278	233	0.03%	0.003%
13	4.533	987	993	997	rVB2	352	344	0.04%	0.005%
14	4.568	1001	1004	1009	rVB2	354	245	0.03%	0.003%
15	4.623	1009	1021	1046	rBV	55796	161742	18.16%	2.307%
16	5.054	1138	1155	1179	rBV	136602	321148	36.05%	4.580%
17	5.192	1195	1198	1200	rBV	337	209	0.02%	0.003%
18	5.260	1214	1219	1222	rVV	395	278	0.03%	0.004%
19	5.282	1222	1226	1231	rVV	361	330	0.04%	0.005%
20	5.440	1269	1275	1278	rVB2	611	433	0.05%	0.006%
21	5.578	1315	1318	1321	rBV	514	260	0.03%	0.004%
22	5.713	1340	1360	1387	rVV2	301285	788528	88.51%	11.246%
23	5.870	1407	1409	1413	rVB	460	219	0.02%	0.003%
24	5.903	1413	1419	1421	rBV	234	290	0.03%	0.004%
25	5.925	1423	1426	1430	rVV	405	314	0.04%	0.004%
26	5.970	1433	1440	1451	rVB5	1408	2868	0.32%	0.041%
27	6.112	1479	1484	1486	rBV3	470	444	0.05%	0.006%
28	6.240	1510	1524	1549	rBV	317471	623911	70.04%	8.899%
29	6.523	1603	1612	1623	rVB8	6901	13136	1.47%	0.187%
30	6.591	1627	1633	1635	rBV5	2209	2364	0.27%	0.034%
31	6.684	1648	1662	1680	rBV	179803	359381	40.34%	5.126%
32	6.790	1691	1695	1698	rBV2	448	407	0.05%	0.006%
33	6.806	1698	1700	1706	rVB2	580	480	0.05%	0.007%
34	7.179	1812	1816	1817	rBV3	871	584	0.07%	0.008%
35	7.562	1923	1935	1955	rVB2	99115	187165	21.01%	2.669%
36	7.732	1985	1988	1992	rBV	395	314	0.04%	0.004%

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

37	7.800	2006	2009	2013	rVB	287	233	0.03%	0.003%
38	7.822	2013	2016	2022	rBV2	243	268	0.03%	0.004%
39	7.893	2024	2038	2055	rBV	370841	661094	74.21%	9.429%
40	8.089	2095	2099	2102	rBV2	356	230	0.03%	0.003%
41	8.124	2105	2110	2114	rVV3	414	464	0.05%	0.007%
42	8.176	2114	2126	2145	rVV	67724	130149	14.61%	1.856%
43	8.259	2149	2152	2156	rVB3	631	424	0.05%	0.006%
44	8.282	2156	2159	2162	rBV	408	239	0.03%	0.003%
45	8.462	2211	2215	2217	rBV3	614	521	0.06%	0.007%
46	8.549	2236	2242	2249	rVB6	2139	2923	0.33%	0.042%
47	8.642	2258	2271	2302	rBV2	206073	404715	45.43%	5.772%
48	8.806	2313	2322	2329	rBV7	1496	2461	0.28%	0.035%
49	8.922	2355	2358	2360	rVV2	376	263	0.03%	0.004%
50	8.941	2360	2364	2366	rVB2	298	219	0.02%	0.003%
51	9.015	2383	2387	2390	rBV	284	248	0.03%	0.004%
52	9.034	2390	2393	2397	rBV2	280	243	0.03%	0.003%
53	9.118	2417	2419	2425	rVB2	271	224	0.03%	0.003%
54	9.198	2438	2444	2447	rBV3	306	267	0.03%	0.004%
55	9.224	2450	2452	2457	rVB	393	221	0.02%	0.003%
56	9.417	2498	2512	2537	rBV	434417	774402	86.93%	11.045%
57	9.687	2589	2596	2597	rBV	1785	1320	0.15%	0.019%
58	9.745	2609	2614	2620	rBV4	553	647	0.07%	0.009%
59	9.793	2626	2629	2633	rBV2	313	235	0.03%	0.003%
60	10.015	2695	2698	2704	rVB2	254	261	0.03%	0.004%
61	10.099	2718	2724	2725	rBV2	775	596	0.07%	0.009%
62	10.247	2768	2770	2774	rVB2	455	255	0.03%	0.004%
63	10.481	2839	2843	2844	rBV	328	231	0.03%	0.003%
64	10.562	2863	2868	2870	rBV2	284	226	0.03%	0.003%
65	10.645	2892	2894	2896	rBV2	412	233	0.03%	0.003%
66	10.758	2916	2929	2946	rBV	318643	508905	57.13%	7.258%
67	10.883	2962	2968	2970	rBV3	495	470	0.05%	0.007%
68	10.896	2970	2972	2975	rBV2	437	277	0.03%	0.004%
69	10.954	2987	2990	2994	rBV	336	247	0.03%	0.004%
70	11.009	3004	3007	3009	rBV3	313	228	0.03%	0.003%
71	11.054	3018	3021	3023	rBV3	472	286	0.03%	0.004%
72	11.163	3052	3055	3059	rBV3	454	363	0.04%	0.005%
73	11.214	3068	3071	3078	rVB2	366	387	0.04%	0.006%
74	11.320	3097	3104	3111	rVB6	2333	3452	0.39%	0.049%
75	11.365	3111	3118	3119	rBV2	463	563	0.06%	0.008%
76	11.417	3126	3134	3139	rBV3	905	1159	0.13%	0.017%

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

77	11.607	3187	3193	3198	rVB3	1625	1772	0.20%	0.025%
78	11.645	3202	3205	3210	rVB2	316	289	0.03%	0.004%
79	11.745	3231	3236	3241	rBV4	879	1029	0.12%	0.015%
80	11.809	3244	3256	3277	rBV	565102	890849	100.00%	12.706%
81	11.938	3295	3296	3302	rBV	457	277	0.03%	0.004%
82	12.041	3324	3328	3334	rVB2	308	265	0.03%	0.004%
83	12.079	3334	3340	3341	rBV2	1974	1403	0.16%	0.020%
84	12.192	3361	3375	3396	rBV	465517	749479	84.13%	10.689%
85	12.320	3411	3415	3417	rBV4	1370	1219	0.14%	0.017%
86	12.455	3455	3457	3460	rBV	412	233	0.03%	0.003%
87	12.504	3467	3472	3474	rBV	336	312	0.04%	0.004%
88	12.828	3568	3573	3579	rBV3	519	563	0.06%	0.008%
89	12.899	3589	3595	3599	rBV4	1079	1226	0.14%	0.017%
90	12.999	3624	3626	3630	rVB2	451	291	0.03%	0.004%
91	13.166	3675	3678	3683	rBV2	305	274	0.03%	0.004%
92	13.230	3694	3698	3700	rBV2	358	270	0.03%	0.004%
93	13.426	3750	3759	3766	rBV4	2733	4042	0.45%	0.058%
94	13.533	3788	3792	3796	rBV2	373	296	0.03%	0.004%
95	13.703	3842	3845	3848	rBV	476	350	0.04%	0.005%
96	13.841	3884	3888	3889	rBV2	1050	607	0.07%	0.009%
97	14.089	3959	3965	3975	rBV4	4313	7155	0.80%	0.102%
98	14.295	4027	4029	4033	rBV2	362	240	0.03%	0.003%
99	14.446	4070	4076	4084	rVB5	3582	4605	0.52%	0.066%
100	15.860	4512	4516	4517	rBV2	1041	718	0.08%	0.010%

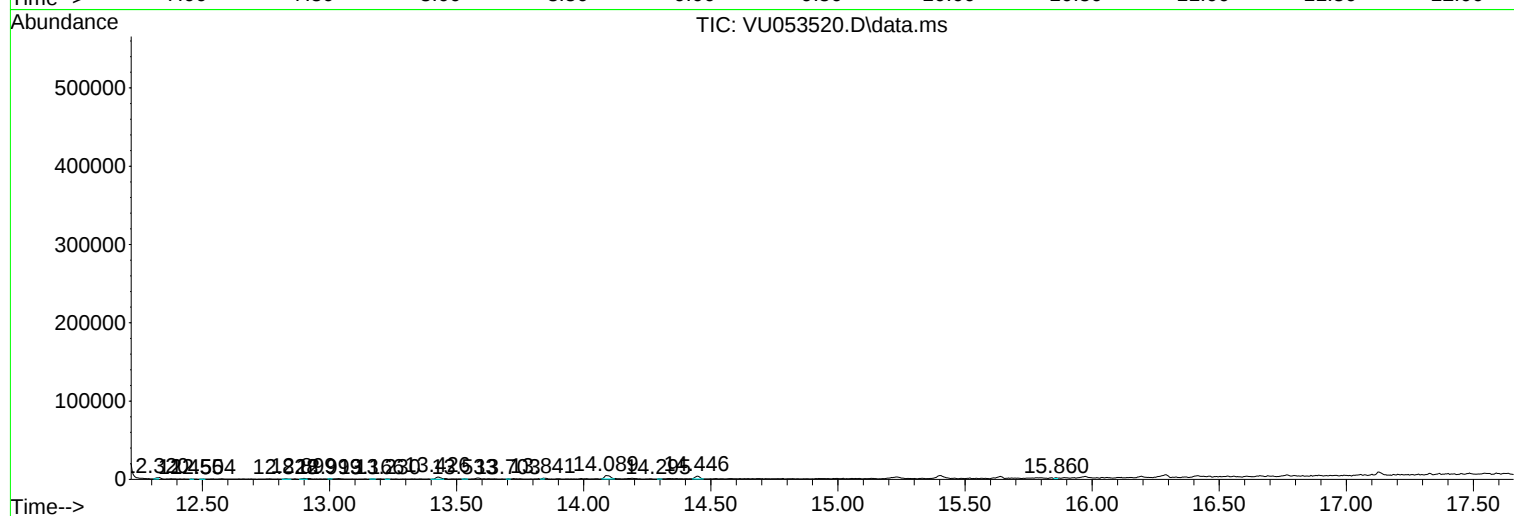
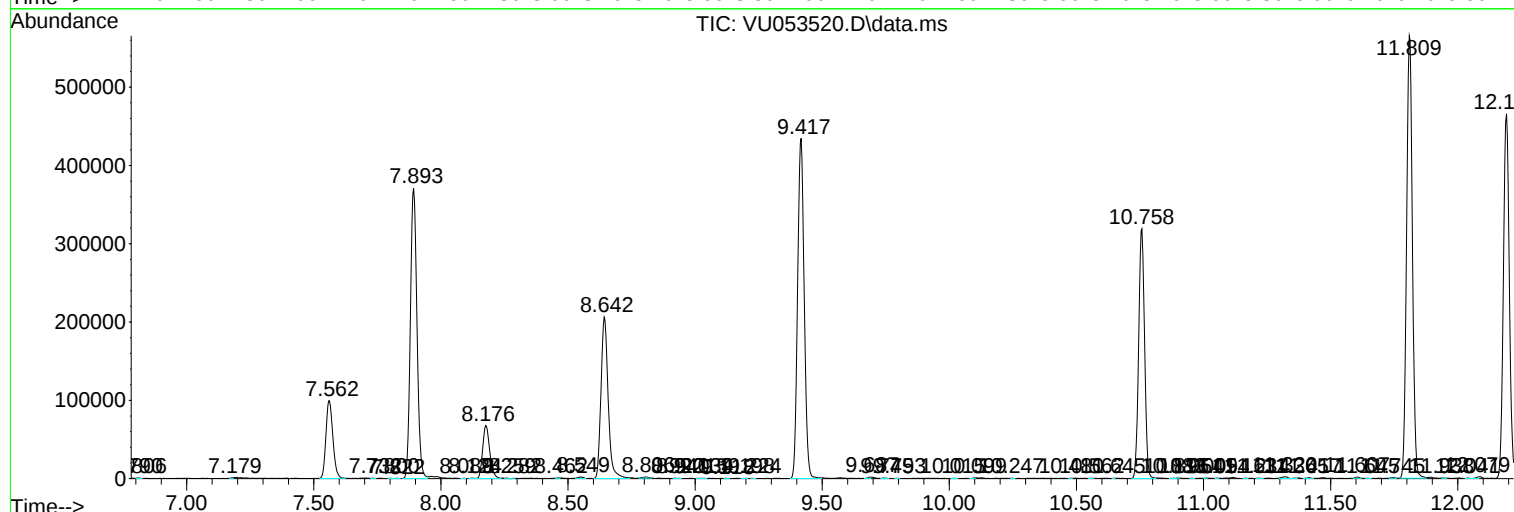
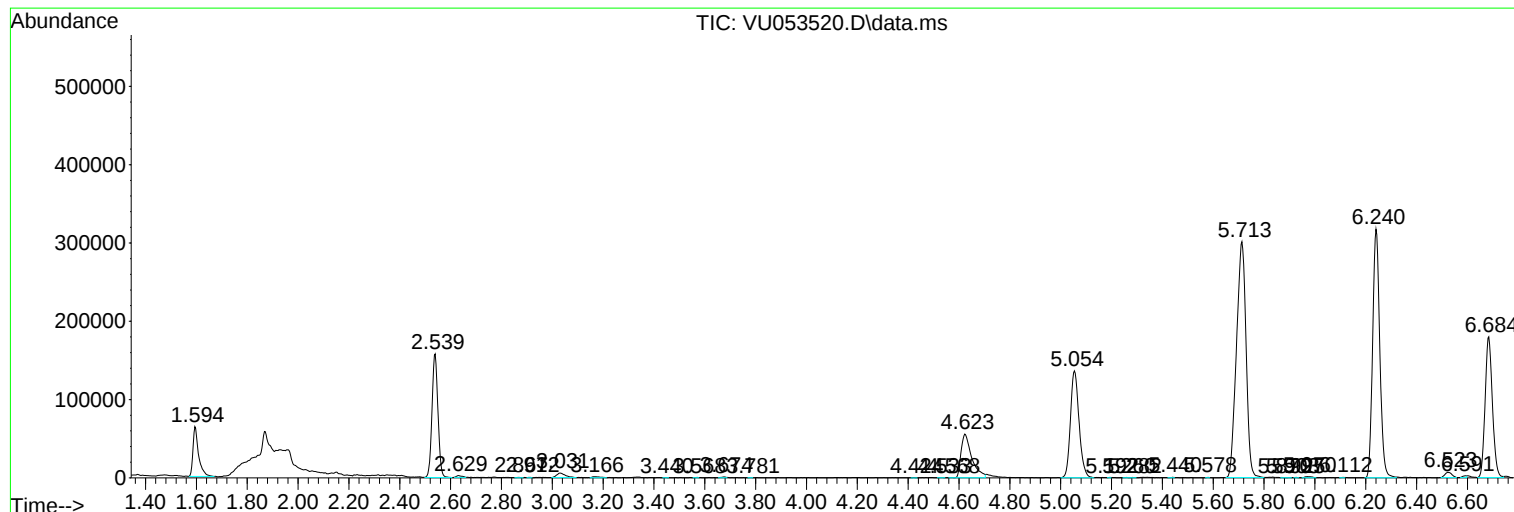
Sum of corrected areas: 7011376

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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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Instrument :
MSVOA_U
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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