

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
 Data File : VU051488.D
 Acq On : 25 Oct 2022 16:02
 Operator : JC/MD
 Sample : N5258-02ME
 Misc : 6.41g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBLN3ME

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\SFAMULM102022WMA.M

Title : VOC Analysis

Signal : TIC: VU051488.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	129607	252814	10.47%	1.419%
2	1.768	119	133	134	rBV3	23101	38324	1.59%	0.215%
3	1.867	160	164	188	rVB	50007	93206	3.86%	0.523%
4	2.128	238	245	261	rVB2	40537	62025	2.57%	0.348%
5	2.526	356	369	388	rBV	349029	585266	24.24%	3.286%
6	2.745	433	437	440	rBV2	1014	886	0.04%	0.005%
7	2.874	472	477	479	rBV3	800	699	0.03%	0.004%
8	3.028	514	525	539	rBV6	5541	10686	0.44%	0.060%
9	3.118	548	553	555	rBV4	491	421	0.02%	0.002%
10	3.176	555	571	588	rBV	32678	78610	3.26%	0.441%
11	3.665	720	723	726	rBV2	524	404	0.02%	0.002%
12	3.684	726	729	731	rVV	612	449	0.02%	0.003%
13	3.752	745	750	755	rVB3	488	521	0.02%	0.003%
14	3.777	755	758	763	rVB	602	473	0.02%	0.003%
15	3.887	786	792	795	rBV2	399	416	0.02%	0.002%
16	3.999	823	827	835	rVB	538	569	0.02%	0.003%
17	4.150	871	874	878	rBV2	463	376	0.02%	0.002%
18	4.292	914	918	921	rBV	458	378	0.02%	0.002%
19	4.388	944	948	949	rBV	560	379	0.02%	0.002%
20	4.465	969	972	976	rVV3	561	438	0.02%	0.002%
21	4.520	985	989	994	rBV2	318	453	0.02%	0.003%
22	4.636	1004	1025	1064	rBV	144975	496699	20.57%	2.789%
23	5.057	1139	1156	1183	rBV	337554	775706	32.13%	4.355%
24	5.295	1219	1230	1234	rBV6	1983	2880	0.12%	0.016%
25	5.488	1287	1290	1296	rVB	475	499	0.02%	0.003%
26	5.636	1332	1336	1341	rBV3	470	510	0.02%	0.003%
27	5.716	1341	1361	1384	rBV2	770047	1953592	80.92%	10.969%
28	5.883	1411	1413	1419	rVB2	455	371	0.02%	0.002%
29	5.983	1437	1444	1454	rVV6	1520	2934	0.12%	0.016%
30	6.041	1460	1462	1467	rVB2	566	365	0.02%	0.002%
31	6.179	1499	1505	1508	rBV2	482	431	0.02%	0.002%
32	6.243	1508	1525	1550	rBV	633542	1273211	52.74%	7.149%
33	6.536	1603	1616	1628	rBV4	43608	86053	3.56%	0.483%
34	6.687	1649	1663	1688	rBV	448509	905239	37.49%	5.083%
35	6.800	1696	1698	1706	rVB4	1767	1676	0.07%	0.009%
36	6.870	1717	1720	1727	rVB2	504	488	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
 Title : VOC Analysis

37	6.922	1733	1736	1741	rBV2	511	427	0.02%	0.002%
38	6.951	1741	1745	1749	rVB4	410	374	0.02%	0.002%
39	6.999	1756	1760	1765	rBV3	307	404	0.02%	0.002%
40	7.083	1784	1786	1791	rVB2	419	382	0.02%	0.002%
41	7.192	1810	1820	1838	rBV3	5513	13779	0.57%	0.077%
42	7.378	1871	1878	1884	rBV4	857	1442	0.06%	0.008%
43	7.484	1909	1911	1917	rVB2	695	500	0.02%	0.003%
44	7.565	1921	1936	1967	rBV	213015	402013	16.65%	2.257%
45	7.687	1970	1974	1975	rBV4	563	399	0.02%	0.002%
46	7.703	1975	1979	1983	rVB3	930	813	0.03%	0.005%
47	7.790	1999	2006	2007	rBV3	1141	1216	0.05%	0.007%
48	7.896	2025	2039	2065	rBV	813003	1458556	60.41%	8.189%
49	8.073	2091	2094	2095	rBV2	780	391	0.02%	0.002%
50	8.179	2114	2127	2150	rBV	138989	272916	11.30%	1.532%
51	8.349	2174	2180	2183	rBV4	728	579	0.02%	0.003%
52	8.388	2188	2192	2198	rBV3	615	796	0.03%	0.004%
53	8.459	2211	2214	2216	rBV2	604	388	0.02%	0.002%
54	8.504	2224	2228	2229	rBV2	746	537	0.02%	0.003%
55	8.549	2229	2242	2260	rVV	1412419	2414340	100.00%	13.556%
56	8.648	2260	2273	2311	rVB	535966	1102860	45.68%	6.192%
57	8.854	2335	2337	2341	rVB5	1062	665	0.03%	0.004%
58	8.918	2353	2357	2369	rVB6	1553	2597	0.11%	0.015%
59	9.009	2383	2385	2389	rVB2	556	385	0.02%	0.002%
60	9.034	2389	2393	2395	rBV3	720	588	0.02%	0.003%
61	9.301	2472	2476	2481	rVB3	424	402	0.02%	0.002%
62	9.340	2481	2488	2491	rBV3	608	696	0.03%	0.004%
63	9.420	2499	2513	2536	rBV	897674	1609608	66.67%	9.037%
64	9.549	2551	2553	2555	rBV2	660	363	0.02%	0.002%
65	9.568	2555	2559	2567	rVB6	1193	1701	0.07%	0.010%
66	9.632	2575	2579	2581	rBV2	770	562	0.02%	0.003%
67	9.706	2597	2602	2610	rVB3	1088	1481	0.06%	0.008%
68	9.758	2614	2618	2621	rBV2	364	373	0.02%	0.002%
69	9.816	2633	2636	2642	rVB	494	487	0.02%	0.003%
70	10.021	2696	2700	2705	rVV2	424	504	0.02%	0.003%
71	10.095	2720	2723	2731	rBV2	625	551	0.02%	0.003%
72	10.198	2751	2755	2758	rBV2	538	446	0.02%	0.003%
73	10.221	2758	2762	2771	rBV3	390	605	0.03%	0.003%
74	10.291	2781	2784	2790	rVB2	445	375	0.02%	0.002%
75	10.324	2790	2794	2797	rVB3	577	475	0.02%	0.003%
76	10.356	2797	2804	2807	rBV2	503	593	0.02%	0.003%

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 Title : VOC Analysis

77	10.420	2819	2824	2826	rBV2	384	361	0.01%	0.002%
78	10.497	2844	2848	2853	rBV2	588	586	0.02%	0.003%
79	10.523	2853	2856	2861	rVB3	453	478	0.02%	0.003%
80	10.574	2866	2872	2875	rBV2	545	548	0.02%	0.003%
81	10.761	2914	2930	2948	rBV	755785	1208103	50.04%	6.783%
82	11.356	3111	3115	3119	rBV2	805	845	0.03%	0.005%
83	11.516	3162	3165	3168	rBV2	438	391	0.02%	0.002%
84	11.574	3179	3183	3187	rBV2	396	391	0.02%	0.002%
85	11.748	3230	3237	3241	rBV4	810	1045	0.04%	0.006%
86	11.812	3245	3257	3281	rBV	819523	1332886	55.21%	7.484%
87	12.073	3330	3338	3345	rBV8	2992	5642	0.23%	0.032%
88	12.195	3362	3376	3397	rBV	821511	1325029	54.88%	7.440%
89	12.642	3511	3515	3520	rBV2	700	704	0.03%	0.004%
90	12.909	3594	3598	3602	rVV2	618	494	0.02%	0.003%
91	12.931	3602	3605	3609	rVB2	667	545	0.02%	0.003%
92	12.967	3613	3616	3618	rBV2	737	510	0.02%	0.003%
93	13.008	3626	3629	3631	rBV	567	371	0.02%	0.002%
94	13.153	3670	3674	3678	rBV	1066	849	0.04%	0.005%
95	14.089	3962	3965	3966	rBV2	1074	596	0.02%	0.003%
96	14.259	4016	4018	4024	rBV3	524	389	0.02%	0.002%
97	14.291	4024	4028	4029	rBV3	859	566	0.02%	0.003%
98	14.340	4037	4043	4053	rVB5	1372	2124	0.09%	0.012%
99	14.455	4074	4079	4084	rBV4	1102	1180	0.05%	0.007%
100	15.028	4253	4257	4260	rBV4	977	907	0.04%	0.005%

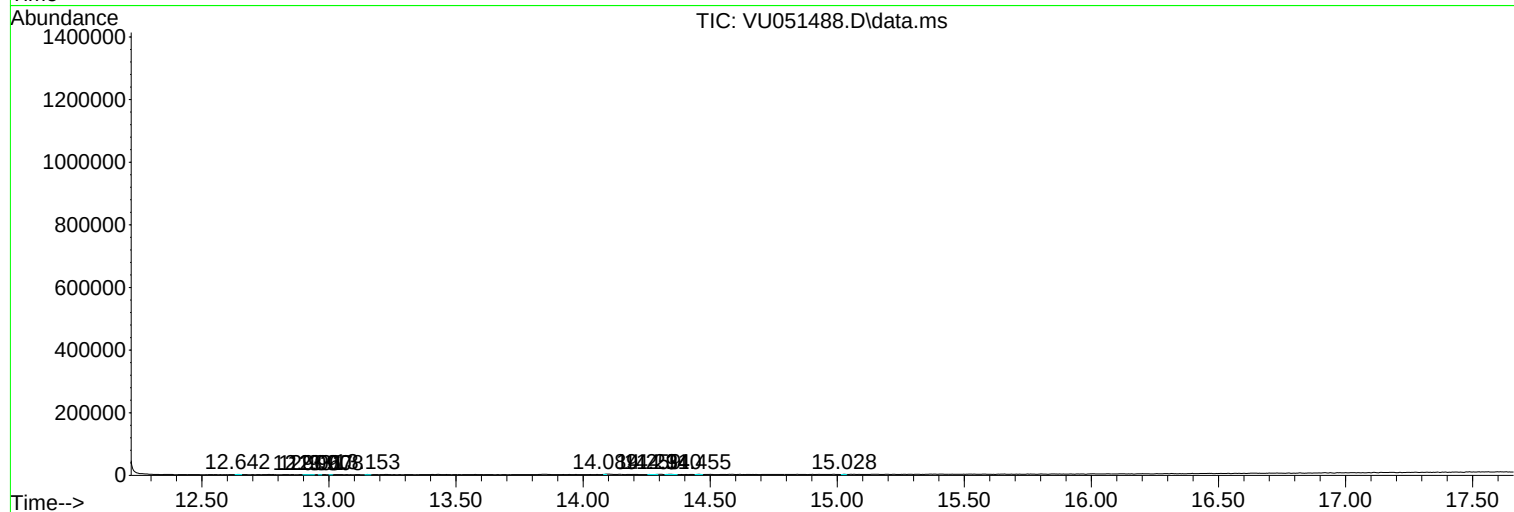
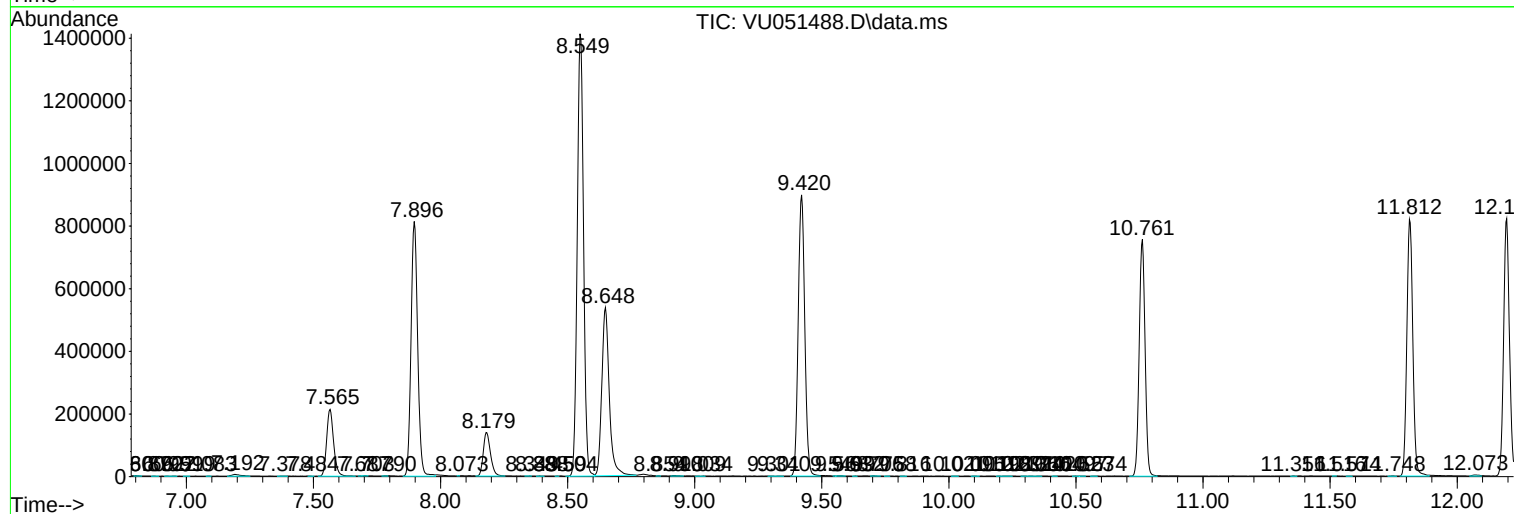
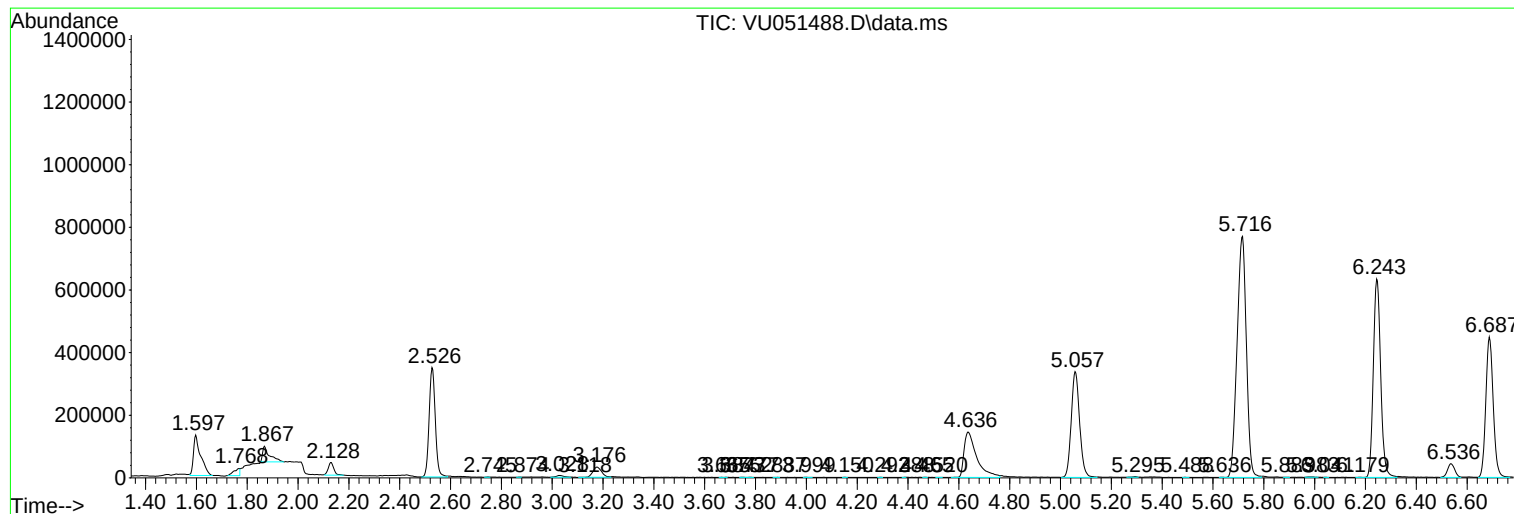
Sum of corrected areas: 17810556

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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