

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083122\
 Data File : VU050571.D
 Acq On : 01 Sep 2022 00:02
 Operator : SY/MD
 Sample : N4345-08ME
 Misc : 5.45g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVS8ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	39	43	47	rBV2	3121	3212	0.21%	0.030%
2	1.594	71	79	89	rBV	92231	134081	8.57%	1.257%
3	1.890	166	171	179	rBV	35174	46546	2.97%	0.437%
4	2.533	359	371	391	rVB	290613	470358	30.06%	4.411%
5	2.649	400	407	419	rBV6	1591	3387	0.22%	0.032%
6	2.745	435	437	439	rBV2	305	177	0.01%	0.002%
7	2.768	442	444	452	rVB4	841	627	0.04%	0.006%
8	2.929	489	494	498	rBV4	516	589	0.04%	0.006%
9	2.954	499	502	506	rBV2	378	310	0.02%	0.003%
10	3.028	516	525	541	rBV3	9412	17901	1.14%	0.168%
11	3.179	557	572	597	rBV2	18090	51361	3.28%	0.482%
12	3.392	636	638	642	rVB2	555	344	0.02%	0.003%
13	3.417	642	646	651	rBV	259	250	0.02%	0.002%
14	3.556	683	689	692	rBV3	269	293	0.02%	0.003%
15	3.678	720	727	732	rVB4	899	1134	0.07%	0.011%
16	3.810	765	768	770	rBV	210	163	0.01%	0.002%
17	4.057	841	845	848	rVB	354	249	0.02%	0.002%
18	4.211	890	893	898	rVV2	353	326	0.02%	0.003%
19	4.237	899	901	907	rVB	362	327	0.02%	0.003%
20	4.269	907	911	913	rBV	336	239	0.02%	0.002%
21	4.375	942	944	949	rBV	225	191	0.01%	0.002%
22	4.411	949	955	956	rBV2	224	210	0.01%	0.002%
23	4.504	980	984	987	rBV2	267	207	0.01%	0.002%
24	4.565	997	1003	1007	rBV	234	249	0.02%	0.002%
25	4.645	1014	1028	1076	rBV	110606	412819	26.38%	3.871%
26	5.060	1139	1157	1181	rBV	256154	603502	38.57%	5.660%
27	5.227	1206	1209	1213	rVB3	437	312	0.02%	0.003%
28	5.292	1221	1229	1238	rVB3	1147	2228	0.14%	0.021%
29	5.369	1247	1253	1260	rVB2	550	698	0.04%	0.007%
30	5.501	1291	1294	1298	rVB2	268	203	0.01%	0.002%
31	5.607	1324	1327	1331	rBV2	228	163	0.01%	0.002%
32	5.633	1331	1335	1337	rBV	230	172	0.01%	0.002%
33	5.716	1341	1361	1385	rBV2	610773	1564668	100.00%	14.673%
34	5.980	1431	1443	1460	rBV3	10643	25831	1.65%	0.242%
35	6.070	1469	1471	1476	rVB	672	404	0.03%	0.004%
36	6.247	1511	1526	1553	rBV	459453	931459	59.53%	8.735%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
 Title : VOC Analysis

37	6.436	1582	1585	1591	rVB2	413	340	0.02%	0.003%
38	6.481	1595	1599	1604	rVV3	617	811	0.05%	0.008%
39	6.530	1605	1614	1627	rVV6	5076	9975	0.64%	0.094%
40	6.604	1627	1637	1649	rVV3	5167	10262	0.66%	0.096%
41	6.690	1649	1664	1689	rVB	348429	719402	45.98%	6.746%
42	7.160	1806	1810	1814	rBV2	434	321	0.02%	0.003%
43	7.227	1814	1831	1847	rBV10	4354	11644	0.74%	0.109%
44	7.308	1852	1856	1858	rVB	546	370	0.02%	0.003%
45	7.324	1858	1861	1865	rBV2	177	175	0.01%	0.002%
46	7.501	1911	1916	1923	rBV4	368	370	0.02%	0.003%
47	7.565	1923	1936	1963	rBV	129890	247859	15.84%	2.324%
48	7.697	1972	1977	1982	rBV3	553	675	0.04%	0.006%
49	7.745	1989	1992	1997	rBV	192	203	0.01%	0.002%
50	7.896	2025	2039	2061	rBV	541628	973912	62.24%	9.133%
51	8.060	2088	2090	2092	rBV2	467	280	0.02%	0.003%
52	8.182	2116	2128	2150	rBV	79537	162311	10.37%	1.522%
53	8.330	2171	2174	2175	rBV	352	191	0.01%	0.002%
54	8.346	2175	2179	2180	rBV4	687	403	0.03%	0.004%
55	8.411	2197	2199	2203	rVB2	246	152	0.01%	0.001%
56	8.449	2203	2211	2215	rBV3	471	676	0.04%	0.006%
57	8.472	2215	2218	2222	rBV4	394	271	0.02%	0.003%
58	8.552	2232	2243	2259	rVB2	62156	103598	6.62%	0.972%
59	8.661	2259	2277	2308	rBV2	279108	765840	48.95%	7.182%
60	8.944	2363	2365	2369	rVB3	551	369	0.02%	0.003%
61	8.970	2369	2373	2386	rVB2	302	604	0.04%	0.006%
62	9.195	2436	2443	2448	rBV2	272	343	0.02%	0.003%
63	9.224	2448	2452	2458	rBV	196	243	0.02%	0.002%
64	9.279	2464	2469	2473	rVB2	289	208	0.01%	0.002%
65	9.420	2499	2513	2538	rBV	437053	832694	53.22%	7.809%
66	9.616	2570	2574	2577	rBV	231	195	0.01%	0.002%
67	9.645	2581	2583	2586	rVB	332	172	0.01%	0.002%
68	9.694	2595	2598	2601	rBV2	306	179	0.01%	0.002%
69	9.745	2611	2614	2620	rVB2	312	288	0.02%	0.003%
70	9.880	2652	2656	2659	rBV2	318	286	0.02%	0.003%
71	9.944	2673	2676	2681	rVB2	244	210	0.01%	0.002%
72	10.317	2789	2792	2795	rBV	306	199	0.01%	0.002%
73	10.620	2883	2886	2888	rBV2	318	188	0.01%	0.002%
74	10.652	2894	2896	2899	rVB2	302	158	0.01%	0.001%
75	10.764	2917	2931	2946	rBV	491685	832355	53.20%	7.806%
76	10.890	2967	2970	2972	rBV3	257	169	0.01%	0.002%

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 Title : VOC Analysis

77	10.973	2991	2996	3000	rBV2	280	338	0.02%	0.003%
78	11.044	3015	3018	3024	rVB	309	315	0.02%	0.003%
79	11.115	3034	3040	3043	rBV2	1209	1187	0.08%	0.011%
80	11.365	3115	3118	3121	rBV3	232	160	0.01%	0.002%
81	11.558	3176	3178	3180	rBV2	265	164	0.01%	0.002%
82	11.816	3245	3258	3280	rBV	510194	810120	51.78%	7.597%
83	12.195	3363	3376	3394	rBV	545078	891725	56.99%	8.362%
84	12.436	3448	3451	3453	rBV2	309	230	0.01%	0.002%
85	12.597	3498	3501	3505	rBV2	338	224	0.01%	0.002%
86	12.645	3513	3516	3517	rBV	365	201	0.01%	0.002%
87	12.729	3540	3542	3547	rVB3	410	321	0.02%	0.003%
88	12.777	3553	3557	3560	rBV3	318	253	0.02%	0.002%
89	12.796	3560	3563	3567	rBV2	535	486	0.03%	0.005%
90	12.902	3590	3596	3597	rBV3	309	277	0.02%	0.003%
91	12.935	3603	3606	3609	rBV2	450	321	0.02%	0.003%
92	12.989	3618	3623	3629	rBV3	488	643	0.04%	0.006%
93	13.066	3645	3647	3650	rVB	368	220	0.01%	0.002%
94	13.089	3650	3654	3657	rVB2	385	301	0.02%	0.003%
95	13.115	3659	3662	3666	rBV2	400	391	0.02%	0.004%
96	13.214	3691	3693	3695	rBV	335	182	0.01%	0.002%
97	13.230	3695	3698	3702	rVV2	393	315	0.02%	0.003%
98	13.597	3808	3812	3814	rBV2	323	246	0.02%	0.002%
99	13.844	3886	3889	3894	rBV2	494	406	0.03%	0.004%
100	15.041	4258	4261	4263	rBV3	537	316	0.02%	0.003%

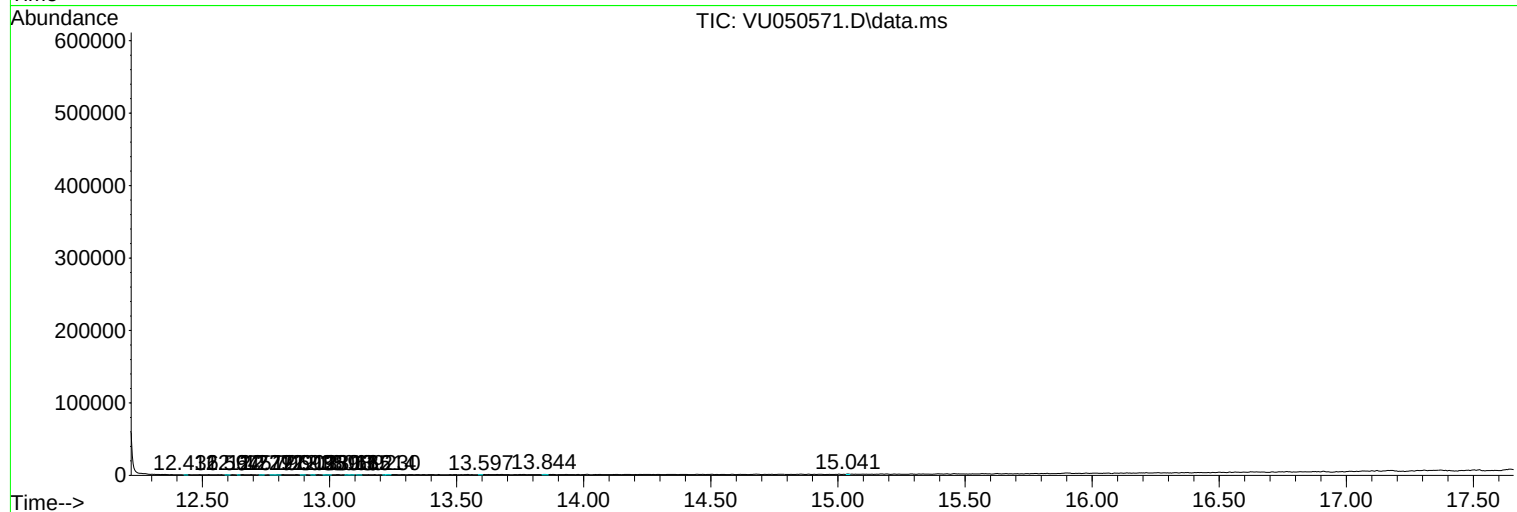
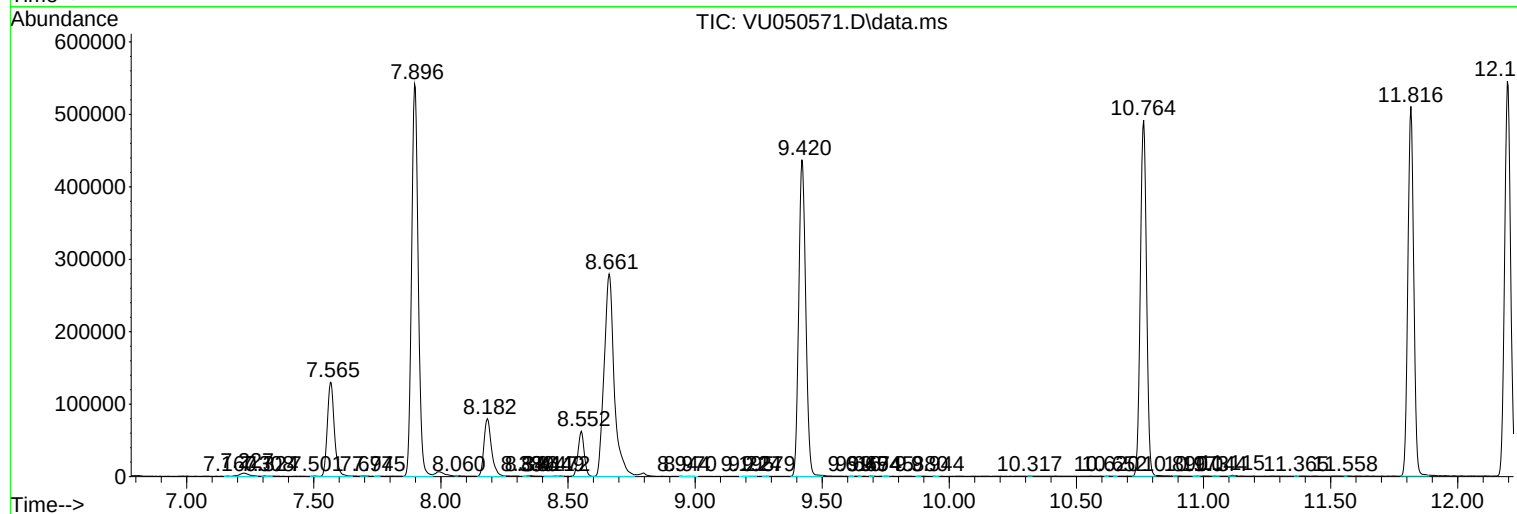
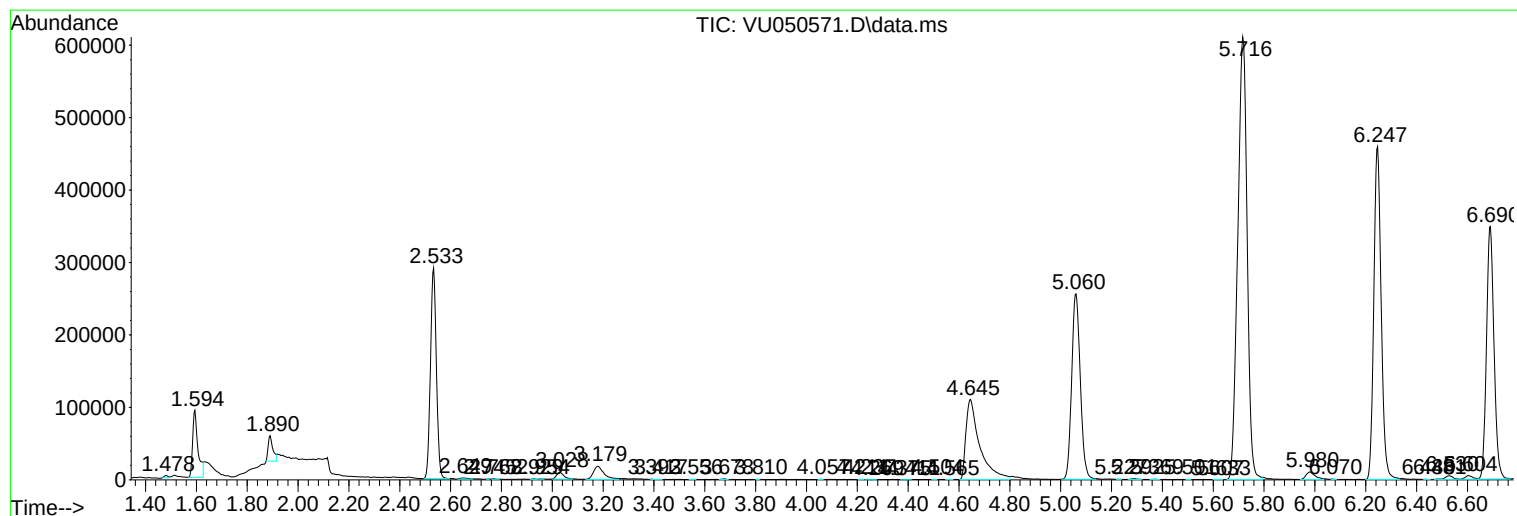
Sum of corrected areas: 10663433

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DBVS8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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\SFAMULM083022WMA.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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