

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
 Data File : VU050619.D
 Acq On : 03 Sep 2022 17:57
 Operator : SY/MD
 Sample : N4345-19ME
 Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT7ME

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\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	39	44	49	rBV4	5132	5719	0.22%	0.035%
2	1.594	71	79	116	rBV	126157	266205	10.37%	1.644%
3	1.893	167	172	183	rBV	40485	58407	2.28%	0.361%
4	2.530	356	370	383	rBV	387279	635512	24.76%	3.925%
5	2.935	492	496	499	rBV3	667	579	0.02%	0.004%
6	3.031	515	526	538	rBV3	10031	20206	0.79%	0.125%
7	3.179	555	572	591	rBV	23886	66534	2.59%	0.411%
8	3.382	631	635	641	rVB4	821	818	0.03%	0.005%
9	3.665	719	723	724	rBV3	753	560	0.02%	0.003%
10	3.735	741	745	749	rBV2	314	304	0.01%	0.002%
11	3.806	761	767	768	rBV2	418	345	0.01%	0.002%
12	3.819	768	771	776	rVB3	421	304	0.01%	0.002%
13	4.128	864	867	872	rVB3	364	263	0.01%	0.002%
14	4.259	905	908	912	rBV3	309	325	0.01%	0.002%
15	4.423	952	959	960	rBV	336	265	0.01%	0.002%
16	4.485	973	978	984	rVB3	366	448	0.02%	0.003%
17	4.517	984	988	992	rBV2	330	242	0.01%	0.001%
18	4.649	1014	1029	1080	rBV	133024	544571	21.22%	3.363%
19	5.060	1137	1157	1183	rBV	304452	746304	29.08%	4.609%
20	5.285	1218	1227	1230	rBV5	1277	1715	0.07%	0.011%
21	5.372	1248	1254	1257	rBV	484	560	0.02%	0.003%
22	5.443	1274	1276	1282	rVB3	445	385	0.02%	0.002%
23	5.716	1339	1361	1396	rBV2	761402	1927139	75.09%	11.902%
24	5.983	1430	1444	1460	rBV4	14763	36163	1.41%	0.223%
25	6.099	1474	1480	1483	rBV4	642	682	0.03%	0.004%
26	6.137	1491	1492	1500	rVB3	464	425	0.02%	0.003%
27	6.176	1500	1504	1507	rBV2	369	313	0.01%	0.002%
28	6.247	1511	1526	1556	rBV	520557	1073293	41.82%	6.628%
29	6.452	1588	1590	1594	rBV3	367	276	0.01%	0.002%
30	6.533	1604	1615	1628	rBV10	7607	17093	0.67%	0.106%
31	6.603	1628	1637	1649	rBV2	7418	14535	0.57%	0.090%
32	6.690	1650	1664	1687	rVB	417282	873345	34.03%	5.394%
33	6.848	1711	1713	1718	rVB4	560	314	0.01%	0.002%
34	6.925	1733	1737	1743	rBV4	521	454	0.02%	0.003%
35	6.954	1743	1746	1748	rBV2	494	306	0.01%	0.002%
36	6.976	1750	1753	1756	rVV2	666	482	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	7.070	1780	1782	1786	rVB2	456	262	0.01%	0.002%
38	7.108	1790	1794	1795	rBV	351	259	0.01%	0.002%
39	7.227	1809	1831	1835	rBV10	7254	15500	0.60%	0.096%
40	7.304	1852	1855	1859	rVB3	1078	854	0.03%	0.005%
41	7.343	1864	1867	1873	rVB5	789	608	0.02%	0.004%
42	7.430	1891	1894	1897	rBV2	392	243	0.01%	0.002%
43	7.468	1903	1906	1910	rVB	457	284	0.01%	0.002%
44	7.565	1923	1936	1963	rVV	167366	332830	12.97%	2.055%
45	7.796	2002	2008	2014	rBV4	819	1005	0.04%	0.006%
46	7.899	2025	2040	2061	rBV	771131	1410085	54.94%	8.708%
47	7.996	2062	2070	2083	rVB3	8284	18144	0.71%	0.112%
48	8.121	2107	2109	2112	rVB2	495	300	0.01%	0.002%
49	8.182	2116	2128	2150	rBV	105823	219861	8.57%	1.358%
50	8.346	2175	2179	2187	rBV5	1488	1881	0.07%	0.012%
51	8.478	2216	2220	2226	rVB3	502	428	0.02%	0.003%
52	8.552	2229	2243	2261	rBV	1497126	2566439	100.00%	15.850%
53	8.668	2261	2279	2312	rVB5	318501	1050602	40.94%	6.488%
54	8.986	2372	2378	2381	rBV4	484	442	0.02%	0.003%
55	9.031	2390	2392	2395	rVV2	451	274	0.01%	0.002%
56	9.102	2410	2414	2423	rVB4	675	962	0.04%	0.006%
57	9.156	2426	2431	2433	rBV3	322	256	0.01%	0.002%
58	9.208	2441	2447	2449	rBV3	311	278	0.01%	0.002%
59	9.353	2488	2492	2498	rBV3	782	811	0.03%	0.005%
60	9.420	2499	2513	2537	rBV	653387	1264518	49.27%	7.809%
61	9.664	2583	2589	2591	rBV3	363	296	0.01%	0.002%
62	9.787	2623	2627	2633	rBV3	453	530	0.02%	0.003%
63	9.832	2636	2641	2643	rBV2	322	257	0.01%	0.002%
64	9.902	2661	2663	2667	rVB	428	271	0.01%	0.002%
65	9.938	2670	2674	2679	rVB2	372	333	0.01%	0.002%
66	9.967	2679	2683	2686	rBV2	602	476	0.02%	0.003%
67	10.034	2700	2704	2711	rBV2	406	520	0.02%	0.003%
68	10.115	2727	2729	2735	rVB2	914	814	0.03%	0.005%
69	10.211	2753	2759	2762	rBV3	217	256	0.01%	0.002%
70	10.391	2811	2815	2817	rBV2	343	260	0.01%	0.002%
71	10.623	2882	2887	2891	rBV2	665	802	0.03%	0.005%
72	10.767	2916	2932	2948	rBV	548060	947545	36.92%	5.852%
73	10.880	2965	2967	2974	rVB3	350	309	0.01%	0.002%
74	10.967	2987	2994	2996	rBV2	374	460	0.02%	0.003%
75	11.118	3034	3041	3048	rVV5	3057	3874	0.15%	0.024%
76	11.160	3051	3054	3057	rBV2	329	238	0.01%	0.001%

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 Title : VOC Analysis

77	11.314	3098	3102	3106	rBV3	737	674	0.03%	0.004%
78	11.375	3117	3121	3123	rBV3	647	476	0.02%	0.003%
79	11.417	3131	3134	3137	rBV2	546	335	0.01%	0.002%
80	11.475	3147	3152	3158	rVB4	908	1063	0.04%	0.007%
81	11.561	3175	3179	3183	rBV2	399	302	0.01%	0.002%
82	11.590	3183	3188	3189	rBV2	339	327	0.01%	0.002%
83	11.651	3203	3207	3213	rBV3	493	606	0.02%	0.004%
84	11.758	3235	3240	3245	rVB4	917	963	0.04%	0.006%
85	11.815	3245	3258	3279	rBV	612742	983603	38.33%	6.075%
86	12.034	3323	3326	3331	rVB2	636	488	0.02%	0.003%
87	12.086	3339	3342	3345	rBV2	477	296	0.01%	0.002%
88	12.195	3363	3376	3397	rBV	657845	1059236	41.27%	6.542%
89	12.397	3433	3439	3442	rBV3	538	603	0.02%	0.004%
90	12.455	3454	3457	3461	rBV3	283	262	0.01%	0.002%
91	12.513	3472	3475	3477	rBV2	443	312	0.01%	0.002%
92	12.706	3532	3535	3538	rBV	331	284	0.01%	0.002%
93	12.767	3552	3554	3559	rVB2	436	313	0.01%	0.002%
94	12.983	3619	3621	3623	rBV2	398	244	0.01%	0.002%
95	12.999	3623	3626	3630	rVB3	607	462	0.02%	0.003%
96	13.282	3711	3714	3716	rVB2	404	239	0.01%	0.001%
97	13.610	3813	3816	3820	rBV2	484	327	0.01%	0.002%
98	13.957	3921	3924	3926	rBV2	439	276	0.01%	0.002%
99	14.050	3951	3953	3957	rBV2	403	301	0.01%	0.002%
100	15.883	4521	4523	4525	rBV3	1027	483	0.02%	0.003%

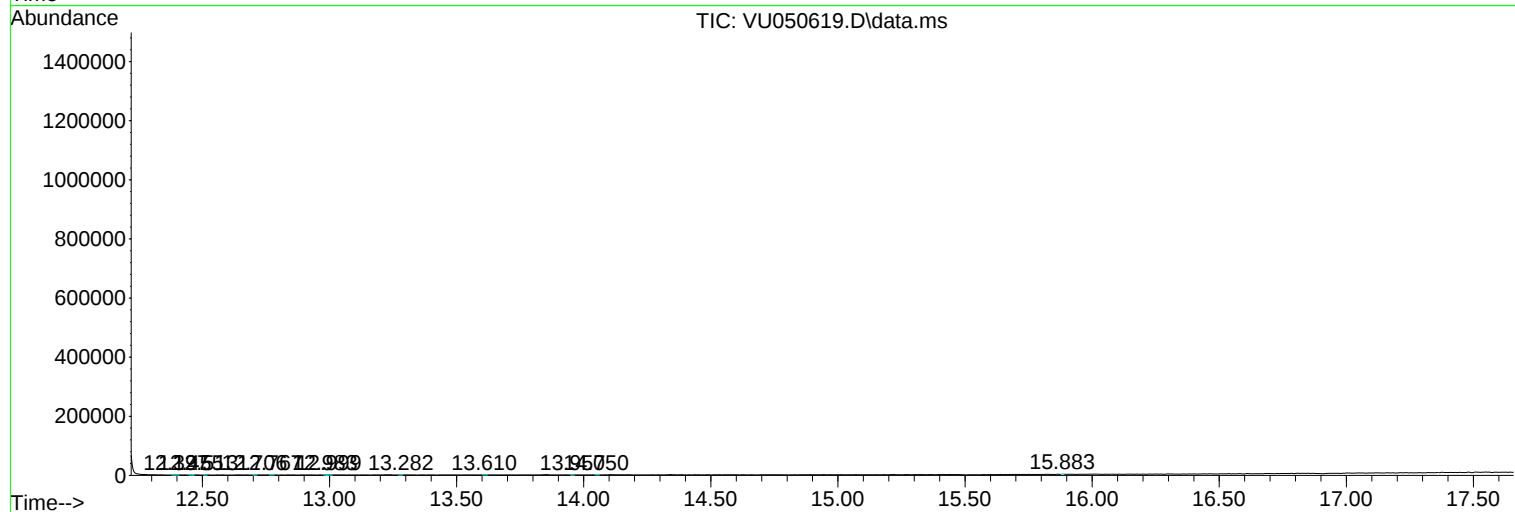
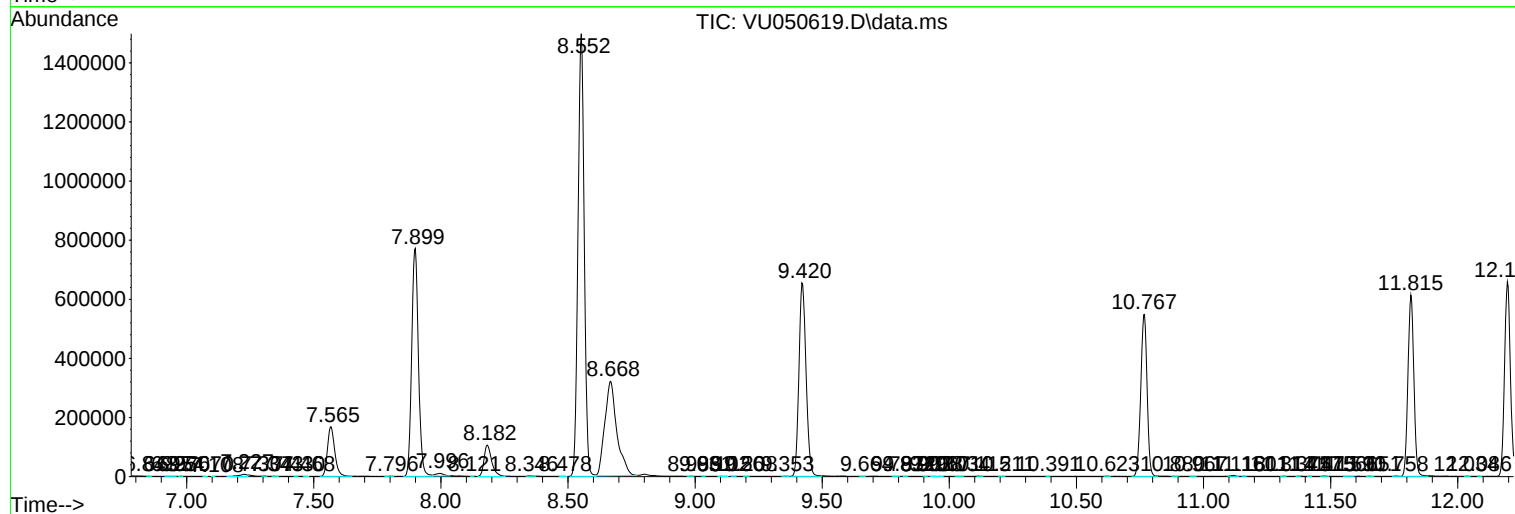
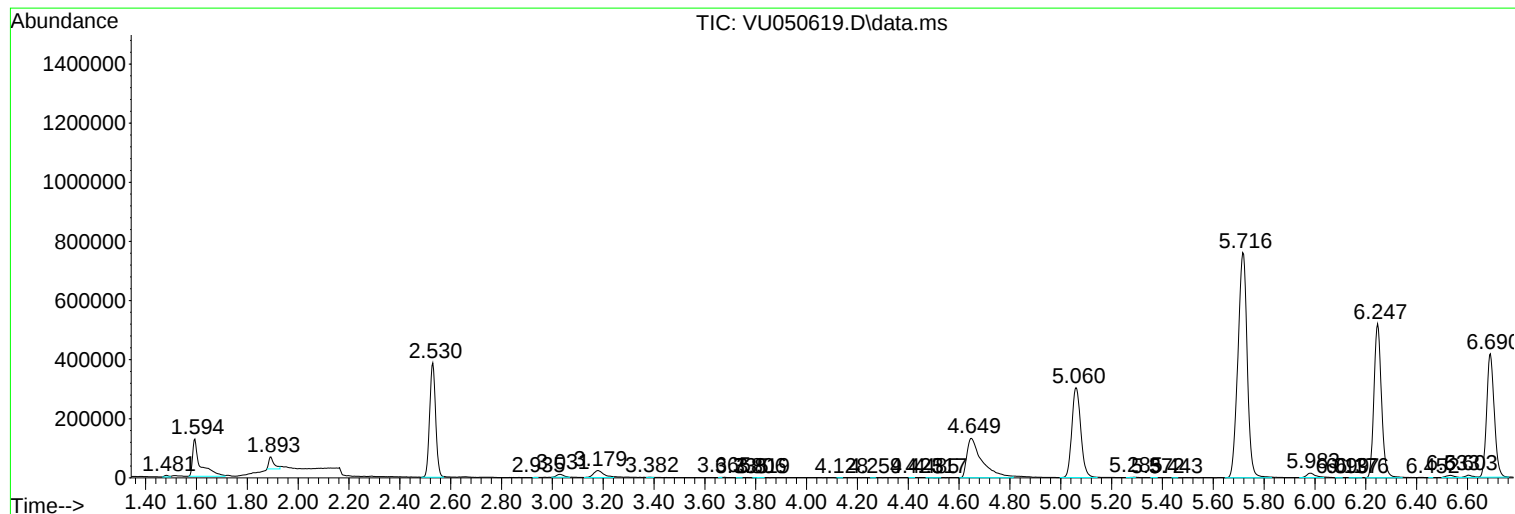
Sum of corrected areas: 16192233

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ClientSampleId :
DBVT7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
DBVT7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.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	#	RT	Resp	Conc
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