

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053501.D
 Acq On : 31 Mar 2023 18:58
 Operator : JC/MD
 Sample : 02121-07ME
 Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1180ME

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: VU053501.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	72	80	98	rBV	166746	238960	6.93%	1.720%
2	2.543	362	374	390	rVB	328454	529607	15.36%	3.812%
3	2.829	460	463	470	rBV2	547	552	0.02%	0.004%
4	2.941	491	498	512	rBV6	1647	3177	0.09%	0.023%
5	3.031	517	526	539	rBV4	4187	7996	0.23%	0.058%
6	3.115	550	552	555	rBV2	333	185	0.01%	0.001%
7	3.170	564	569	571	rBV2	641	622	0.02%	0.004%
8	3.266	595	599	602	rBV	275	234	0.01%	0.002%
9	3.285	602	605	606	rBV2	290	197	0.01%	0.001%
10	3.337	607	621	638	rVB2	32398	63839	1.85%	0.460%
11	3.568	691	693	695	rBV	293	185	0.01%	0.001%
12	3.678	717	727	732	rBV6	1248	2099	0.06%	0.015%
13	3.752	748	750	755	rVB	304	181	0.01%	0.001%
14	3.813	765	769	772	rBV2	280	228	0.01%	0.002%
15	3.922	799	803	806	rVB2	248	223	0.01%	0.002%
16	4.414	952	956	960	rBV2	244	243	0.01%	0.002%
17	4.456	966	969	974	rBV	198	196	0.01%	0.001%
18	4.652	1006	1030	1063	rBV2	1445310	3448099	100.00%	24.820%
19	4.925	1110	1115	1117	rBV	521	467	0.01%	0.003%
20	5.054	1138	1155	1179	rBV	258124	583738	16.93%	4.202%
21	5.327	1233	1240	1243	rBV2	478	733	0.02%	0.005%
22	5.382	1255	1257	1264	rVB	482	271	0.01%	0.002%
23	5.420	1264	1269	1273	rBV	329	299	0.01%	0.002%
24	5.575	1312	1317	1318	rBV2	599	483	0.01%	0.003%
25	5.713	1338	1360	1385	rBV2	537697	1411493	40.94%	10.160%
26	5.970	1433	1440	1447	rBV3	1175	1869	0.05%	0.013%
27	6.028	1454	1458	1463	rBV3	362	431	0.01%	0.003%
28	6.118	1476	1486	1489	rBV4	1221	1630	0.05%	0.012%
29	6.240	1511	1524	1550	rVV	274653	534652	15.51%	3.849%
30	6.523	1601	1612	1627	rBV9	8827	17860	0.52%	0.129%
31	6.597	1627	1635	1638	rBV4	1761	2596	0.08%	0.019%
32	6.684	1648	1662	1683	rBV	315241	623147	18.07%	4.486%
33	6.806	1697	1700	1710	rVB3	1354	1281	0.04%	0.009%
34	6.851	1712	1714	1719	rVB3	335	194	0.01%	0.001%
35	6.944	1739	1743	1749	rVB2	256	201	0.01%	0.001%
36	7.021	1764	1767	1771	rVB2	262	200	0.01%	0.001%

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

37	7.047	1771	1775	1778	rBV	298	251	0.01%	0.002%
38	7.275	1843	1846	1848	rBV	268	194	0.01%	0.001%
39	7.292	1849	1851	1860	rVB2	468	511	0.01%	0.004%
40	7.372	1869	1876	1879	rBV2	454	480	0.01%	0.003%
41	7.404	1884	1886	1889	rBV	310	245	0.01%	0.002%
42	7.491	1909	1913	1917	rVB	777	588	0.02%	0.004%
43	7.562	1922	1935	1956	rVV	181640	339617	9.85%	2.445%
44	7.645	1957	1961	1970	rVB6	1235	1726	0.05%	0.012%
45	7.838	2018	2021	2024	rBV2	322	262	0.01%	0.002%
46	7.893	2024	2038	2054	rBV	710156	1245335	36.12%	8.964%
47	8.124	2103	2110	2115	rBV3	2059	2700	0.08%	0.019%
48	8.176	2115	2126	2151	rVB	126982	236346	6.85%	1.701%
49	8.320	2166	2171	2174	rBV2	182	176	0.01%	0.001%
50	8.353	2179	2181	2182	rBV	375	175	0.01%	0.001%
51	8.449	2204	2211	2212	rBV	373	317	0.01%	0.002%
52	8.549	2239	2242	2248	rVB3	1198	1215	0.04%	0.009%
53	8.578	2248	2251	2253	rBV	268	201	0.01%	0.001%
54	8.642	2258	2271	2298	rVV	356311	676233	19.61%	4.868%
55	9.163	2428	2433	2441	rVV5	1557	2232	0.06%	0.016%
56	9.208	2441	2447	2458	rVB8	2534	4396	0.13%	0.032%
57	9.330	2477	2485	2495	rBV5	2808	3983	0.12%	0.029%
58	9.414	2495	2511	2533	rBV	384705	687160	19.93%	4.946%
59	9.517	2541	2543	2546	rBV2	475	274	0.01%	0.002%
60	9.568	2552	2559	2570	rVB2	3118	5039	0.15%	0.036%
61	9.693	2587	2598	2607	rBV	15664	28953	0.84%	0.208%
62	9.812	2630	2635	2638	rVB2	439	306	0.01%	0.002%
63	9.835	2639	2642	2647	rVB2	334	245	0.01%	0.002%
64	9.861	2647	2650	2654	rBV	364	220	0.01%	0.002%
65	9.954	2676	2679	2682	rVB3	347	211	0.01%	0.002%
66	10.012	2693	2697	2699	rBV2	803	536	0.02%	0.004%
67	10.102	2715	2725	2738	rVB2	15429	27428	0.80%	0.197%
68	10.250	2763	2771	2776	rBV5	1243	1837	0.05%	0.013%
69	10.320	2788	2793	2794	rBV	321	216	0.01%	0.002%
70	10.330	2794	2796	2798	rBV2	799	423	0.01%	0.003%
71	10.446	2829	2832	2833	rBV2	331	183	0.01%	0.001%
72	10.455	2833	2835	2837	rBV	575	297	0.01%	0.002%
73	10.552	2856	2865	2866	rBV5	2125	2441	0.07%	0.018%
74	10.687	2904	2907	2910	rVB2	329	192	0.01%	0.001%
75	10.754	2914	2928	2943	rBV	536341	847917	24.59%	6.104%
76	10.864	2959	2962	2964	rBV2	404	236	0.01%	0.002%

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Integrator: RTE

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Peak Location: TOP

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

77	11.008	2998	3007	3009	rBV2	643	848	0.02%	0.006%
78	11.044	3015	3018	3020	rBV2	591	356	0.01%	0.003%
79	11.060	3021	3023	3028	rVB3	599	380	0.01%	0.003%
80	11.195	3062	3065	3068	rBV3	441	406	0.01%	0.003%
81	11.291	3092	3095	3096	rBV3	690	446	0.01%	0.003%
82	11.311	3097	3101	3106	rVV7	2539	2926	0.08%	0.021%
83	11.369	3110	3119	3127	rBV7	1486	2814	0.08%	0.020%
84	11.465	3146	3149	3156	rVB4	2018	2225	0.06%	0.016%
85	11.555	3175	3177	3178	rBV	370	202	0.01%	0.001%
86	11.565	3178	3180	3186	rVB4	696	554	0.02%	0.004%
87	11.635	3199	3202	3206	rBV2	1166	864	0.03%	0.006%
88	11.655	3206	3208	3213	rVB4	802	484	0.01%	0.003%
89	11.745	3228	3236	3242	rBV6	2636	3565	0.10%	0.026%
90	11.809	3244	3256	3275	rVV	514300	813490	23.59%	5.856%
91	11.999	3308	3315	3322	rVB7	1993	2777	0.08%	0.020%
92	12.192	3360	3375	3402	rBV	842493	1393676	40.42%	10.032%
93	12.324	3411	3416	3428	rVB7	5351	7885	0.23%	0.057%
94	12.777	3555	3557	3558	rBV	510	257	0.01%	0.002%
95	12.896	3588	3594	3597	rBV5	1435	1735	0.05%	0.012%
96	13.127	3661	3666	3673	rVB7	1527	1986	0.06%	0.014%
97	13.368	3738	3741	3745	rBV5	817	626	0.02%	0.005%
98	13.423	3749	3758	3768	rBV7	6494	10954	0.32%	0.079%
99	14.089	3958	3965	3978	rVB	14297	23443	0.68%	0.169%
100	15.227	4306	4319	4332	rBV3	9369	19607	0.57%	0.141%

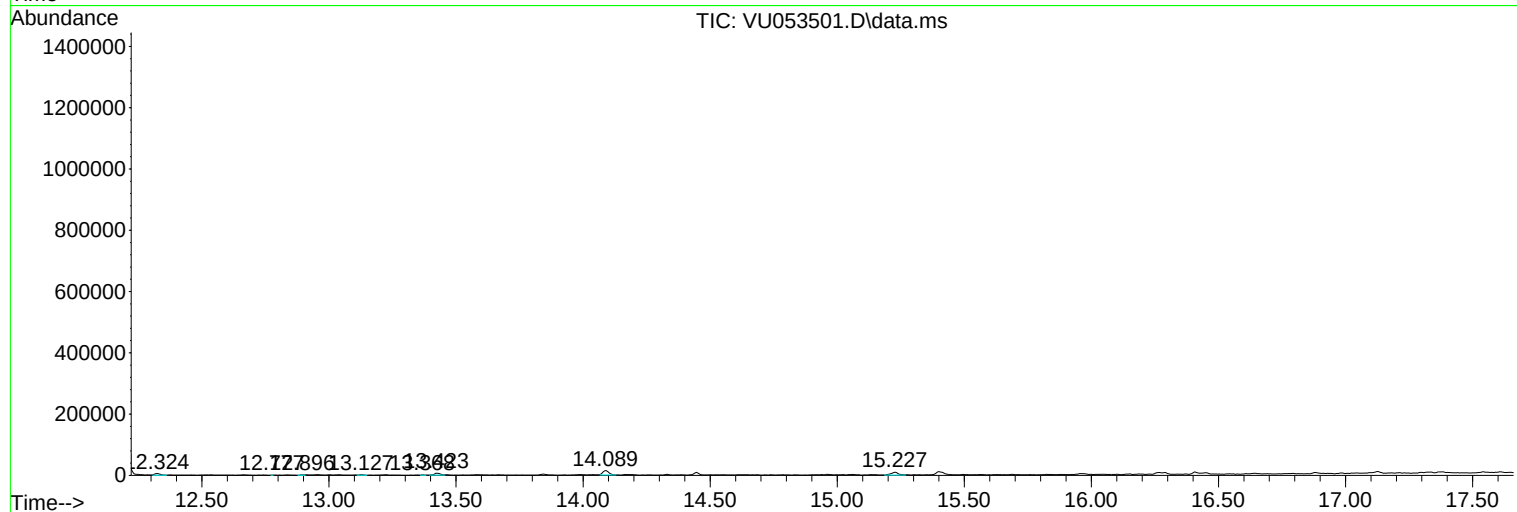
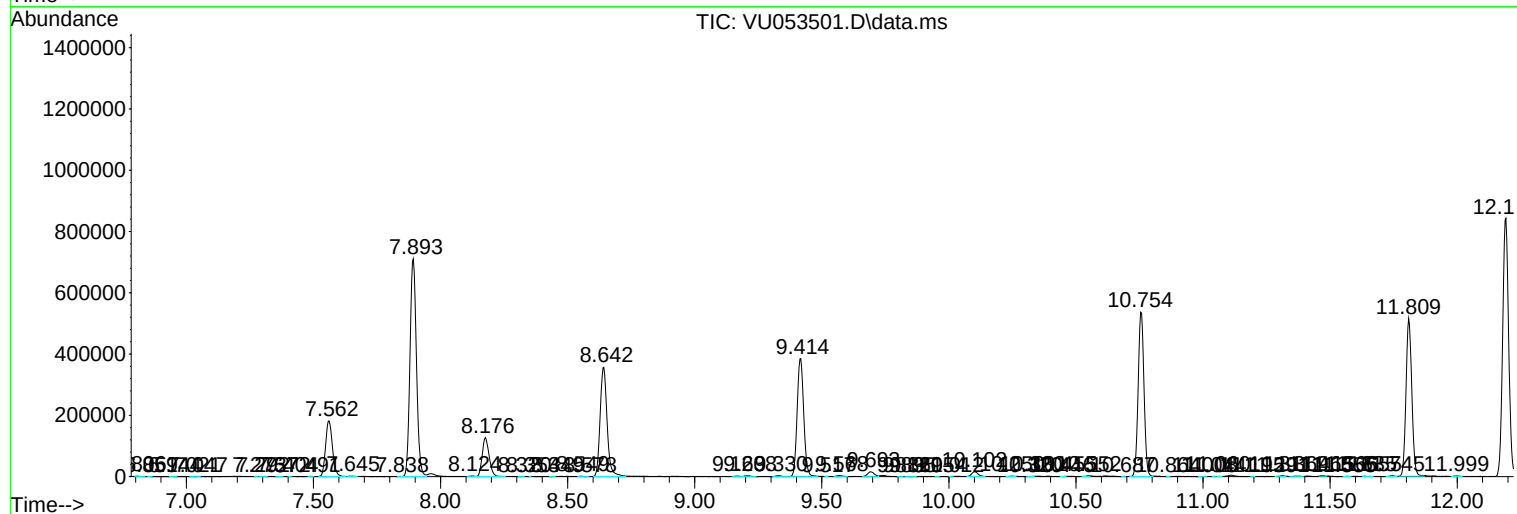
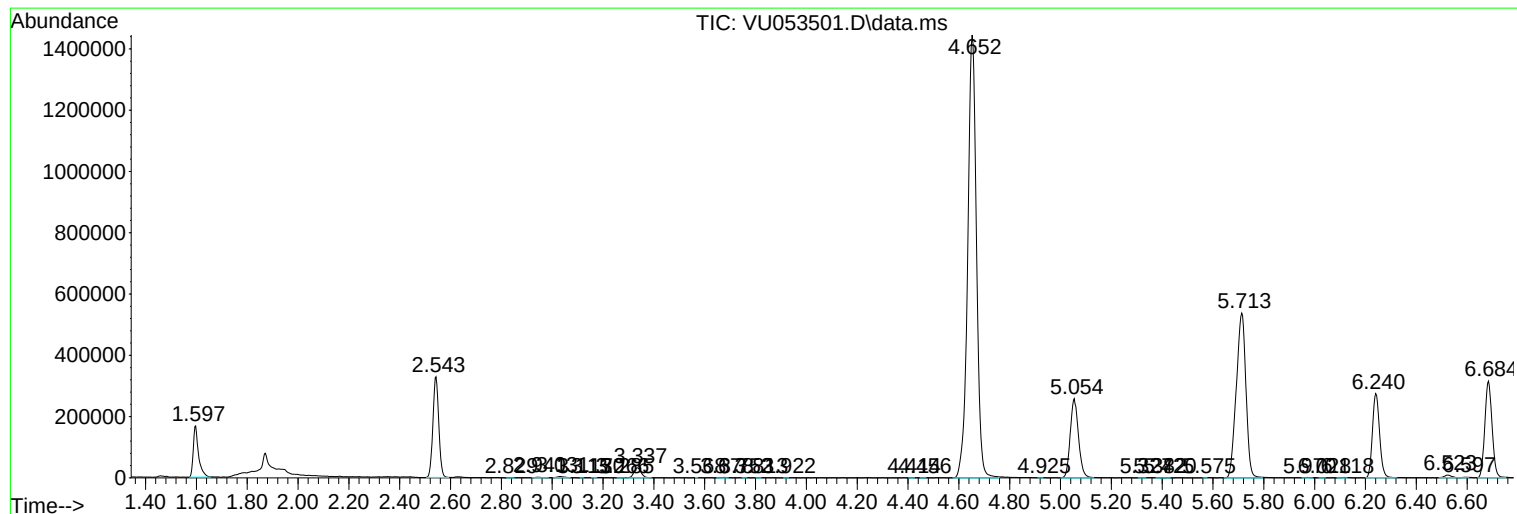
Sum of corrected areas: 13892171

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Instrument :
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ClientSampleId :
C1180ME

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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C1180ME

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

No Library Search Compounds Detected

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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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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