

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
 Data File : VU055728.D
 Acq On : 10 Oct 2023 18:01
 Operator : MD/SY
 Sample : 04747-06ME
 Misc : 4.40g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX841ME

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	54	59	66	rBV3	4781	5272	0.23%	0.031%
2	1.596	87	95	126	rVB	162865	322845	14.24%	1.889%
3	2.531	374	386	403	rBV	445797	742028	32.74%	4.341%
4	2.856	483	487	488	rBV3	734	565	0.02%	0.003%
5	2.878	492	494	499	rVB4	791	597	0.03%	0.003%
6	3.026	529	540	558	rBV5	8797	20867	0.92%	0.122%
7	3.174	571	586	598	rBV2	23534	56212	2.48%	0.329%
8	3.280	617	619	623	rVB2	845	404	0.02%	0.002%
9	3.380	645	650	652	rBV3	496	451	0.02%	0.003%
10	3.409	655	659	660	rBV	865	577	0.03%	0.003%
11	3.435	662	667	669	rBV2	3002	2857	0.13%	0.017%
12	3.518	690	693	696	rBV2	586	398	0.02%	0.002%
13	3.583	709	713	719	rVB3	677	701	0.03%	0.004%
14	3.666	730	739	741	rBV6	1053	1407	0.06%	0.008%
15	3.679	741	743	747	rVV4	1214	908	0.04%	0.005%
16	3.779	770	774	776	rBV2	607	368	0.02%	0.002%
17	3.878	802	805	811	rVV2	508	458	0.02%	0.003%
18	3.907	811	814	820	rVB2	443	464	0.02%	0.003%
19	4.055	856	860	862	rBV	510	439	0.02%	0.003%
20	4.631	1025	1039	1095	rBV	146519	575145	25.37%	3.365%
21	5.055	1153	1171	1198	rBV	374004	905996	39.97%	5.301%
22	5.193	1212	1214	1216	rBV3	743	409	0.02%	0.002%
23	5.248	1227	1231	1233	rBV3	509	409	0.02%	0.002%
24	5.293	1239	1245	1249	rBV5	854	959	0.04%	0.006%
25	5.338	1249	1259	1271	rVB6	3260	6946	0.31%	0.041%
26	5.460	1294	1297	1301	rBV3	452	390	0.02%	0.002%
27	5.509	1310	1312	1316	rVB2	644	406	0.02%	0.002%
28	5.714	1352	1376	1407	rBV2	864834	2266766	100.00%	13.262%
29	5.975	1449	1457	1466	rBV9	2767	5891	0.26%	0.034%
30	6.242	1525	1540	1566	rBV	578766	1213964	53.55%	7.102%
31	6.525	1617	1628	1642	rVV7	13869	29143	1.29%	0.171%
32	6.599	1642	1651	1664	rVV7	5150	11916	0.53%	0.070%
33	6.685	1664	1678	1704	rVV	481713	1016390	44.84%	5.946%
34	6.846	1725	1728	1732	rVB2	1385	1013	0.04%	0.006%
35	6.972	1762	1767	1769	rBV	449	428	0.02%	0.003%
36	7.193	1825	1836	1841	rBV5	3121	5147	0.23%	0.030%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	7.486	1923	1927	1930	rBV3	714	602	0.03%	0.004%
38	7.563	1936	1951	1981	rBV	250104	517914	22.85%	3.030%
39	7.682	1984	1988	1989	rBV3	584	441	0.02%	0.003%
40	7.782	2015	2019	2020	rBV2	674	440	0.02%	0.003%
41	7.827	2030	2033	2038	rVB5	757	718	0.03%	0.004%
42	7.894	2040	2054	2075	rBV	957443	1818812	80.24%	10.641%
43	8.087	2112	2114	2118	rVB3	609	368	0.02%	0.002%
44	8.181	2130	2143	2168	rBV2	156018	354205	15.63%	2.072%
45	8.341	2187	2193	2198	rBV6	1191	1607	0.07%	0.009%
46	8.454	2224	2228	2231	rVB3	506	444	0.02%	0.003%
47	8.547	2254	2257	2261	rBV5	1954	1594	0.07%	0.009%
48	8.660	2273	2292	2325	rBV2	530344	1377589	60.77%	8.060%
49	8.856	2349	2353	2356	rBV6	693	635	0.03%	0.004%
50	8.920	2371	2373	2376	rVB3	854	511	0.02%	0.003%
51	8.943	2376	2380	2383	rVB2	1004	650	0.03%	0.004%
52	8.968	2385	2388	2392	rVB3	655	405	0.02%	0.002%
53	9.078	2418	2422	2425	rBV2	408	372	0.02%	0.002%
54	9.119	2432	2435	2439	rVB3	572	443	0.02%	0.003%
55	9.200	2456	2460	2461	rBV	632	387	0.02%	0.002%
56	9.225	2467	2468	2472	rVB2	1062	482	0.02%	0.003%
57	9.418	2514	2528	2561	rBV	729445	1581627	69.77%	9.253%
58	9.705	2611	2617	2619	rBV4	871	880	0.04%	0.005%
59	9.779	2637	2640	2643	rVV	681	387	0.02%	0.002%
60	9.852	2658	2663	2666	rVV2	652	512	0.02%	0.003%
61	9.991	2702	2706	2707	rBV	765	510	0.02%	0.003%
62	10.113	2736	2744	2745	rBV	644	612	0.03%	0.004%
63	10.203	2767	2772	2779	rVB3	568	853	0.04%	0.005%
64	10.370	2820	2824	2828	rBV3	634	626	0.03%	0.004%
65	10.441	2841	2846	2852	rBV2	385	430	0.02%	0.003%
66	10.492	2860	2862	2867	rVB2	813	571	0.03%	0.003%
67	10.762	2931	2946	2973	rBV	776016	1289015	56.87%	7.541%
68	11.158	3067	3069	3075	rVB2	494	390	0.02%	0.002%
69	11.254	3095	3099	3103	rBV3	401	389	0.02%	0.002%
70	11.315	3116	3118	3126	rVB3	921	785	0.03%	0.005%
71	11.377	3134	3137	3140	rVB2	764	504	0.02%	0.003%
72	11.415	3140	3149	3153	rBV6	1080	1731	0.08%	0.010%
73	11.473	3162	3167	3171	rBV2	941	901	0.04%	0.005%
74	11.682	3228	3232	3233	rBV	545	368	0.02%	0.002%
75	11.737	3241	3249	3253	rBV2	613	966	0.04%	0.006%
76	11.756	3253	3255	3259	rVB2	1320	806	0.04%	0.005%

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77	11.814	3260	3273	3294	rBV	875581	1402222	61.86%	8.204%
78	12.061	3347	3350	3356	rVB4	624	543	0.02%	0.003%
79	12.193	3378	3391	3411	rBV	929585	1518034	66.97%	8.881%
80	12.515	3487	3491	3493	rVB4	718	492	0.02%	0.003%
81	12.534	3493	3497	3500	rBV3	512	374	0.02%	0.002%
82	12.695	3544	3547	3550	rBV2	650	520	0.02%	0.003%
83	12.746	3560	3563	3567	rVB3	555	423	0.02%	0.002%
84	12.766	3567	3569	3572	rBV2	578	422	0.02%	0.002%
85	12.862	3595	3599	3601	rBV	865	672	0.03%	0.004%
86	12.926	3615	3619	3621	rBV	586	401	0.02%	0.002%
87	12.975	3632	3634	3638	rVB2	650	404	0.02%	0.002%
88	13.036	3649	3653	3656	rBV4	522	435	0.02%	0.003%
89	13.174	3693	3696	3699	rBV3	442	380	0.02%	0.002%
90	13.454	3779	3783	3786	rBV2	656	595	0.03%	0.003%
91	13.862	3904	3910	3912	rBV3	1399	1227	0.05%	0.007%
92	14.267	4034	4036	4039	rBV2	728	432	0.02%	0.003%
93	14.421	4081	4084	4086	rBV2	698	523	0.02%	0.003%
94	14.505	4107	4110	4112	rBV2	484	375	0.02%	0.002%
95	14.560	4124	4127	4129	rBV	797	501	0.02%	0.003%
96	14.939	4243	4245	4250	rBV2	865	569	0.03%	0.003%
97	15.016	4266	4269	4273	rBV4	705	468	0.02%	0.003%
98	15.106	4295	4297	4301	rBV2	1028	620	0.03%	0.004%
99	15.325	4363	4365	4366	rBV2	812	368	0.02%	0.002%
100	15.492	4414	4417	4418	rBV2	1291	677	0.03%	0.004%

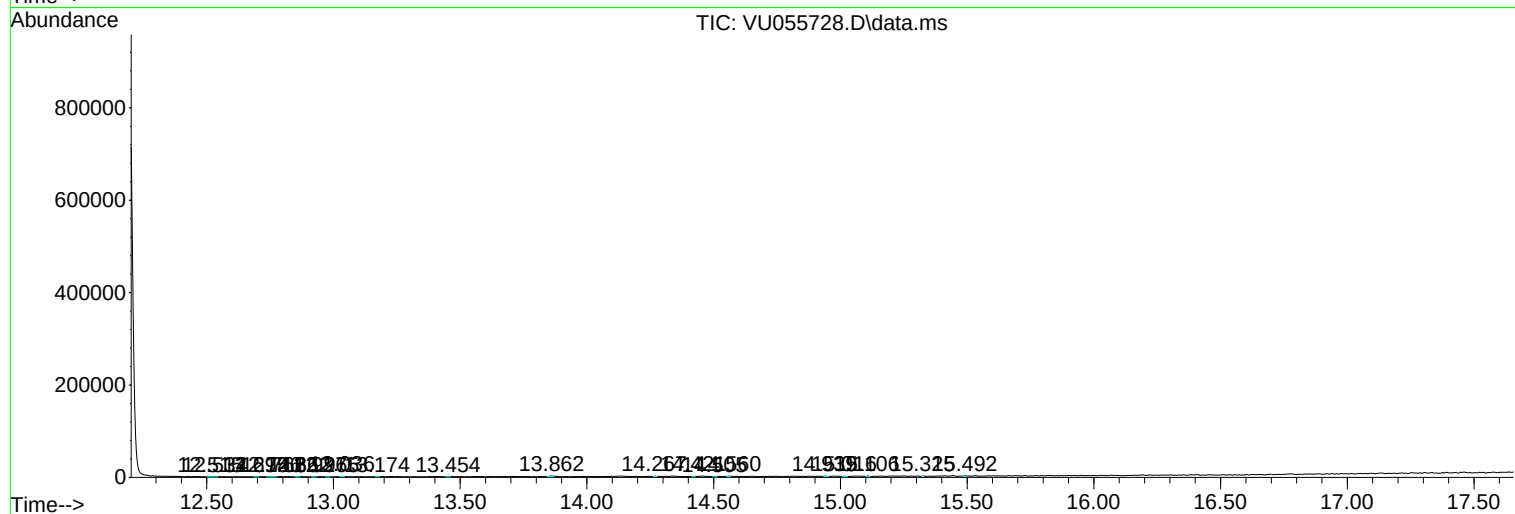
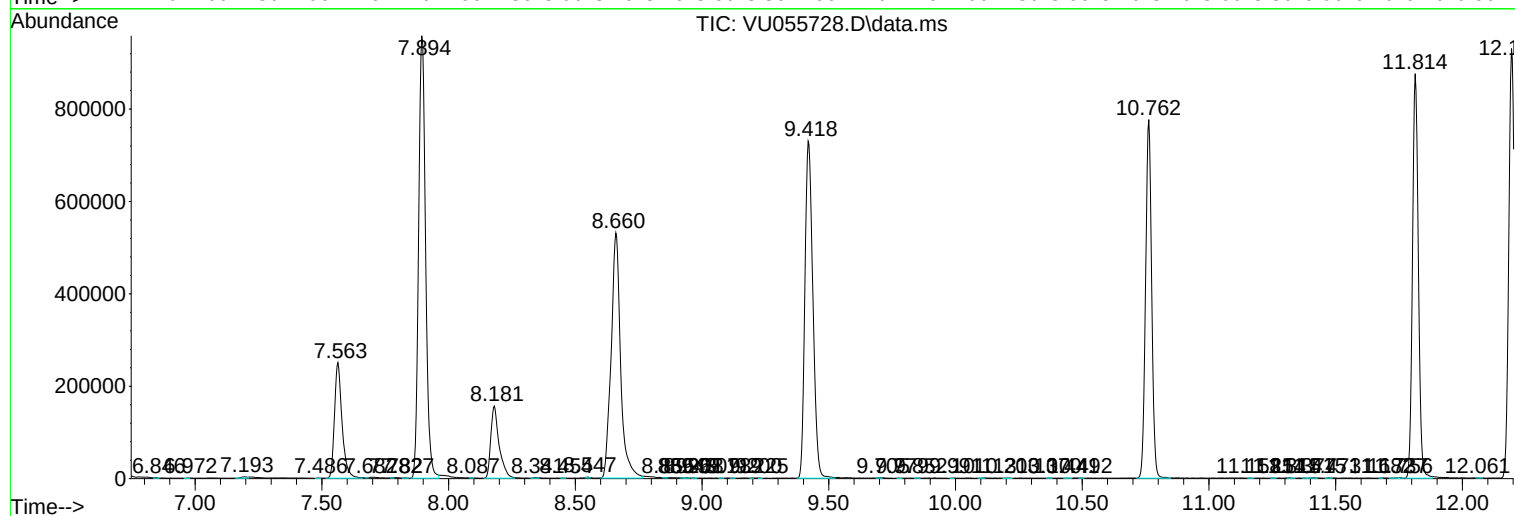
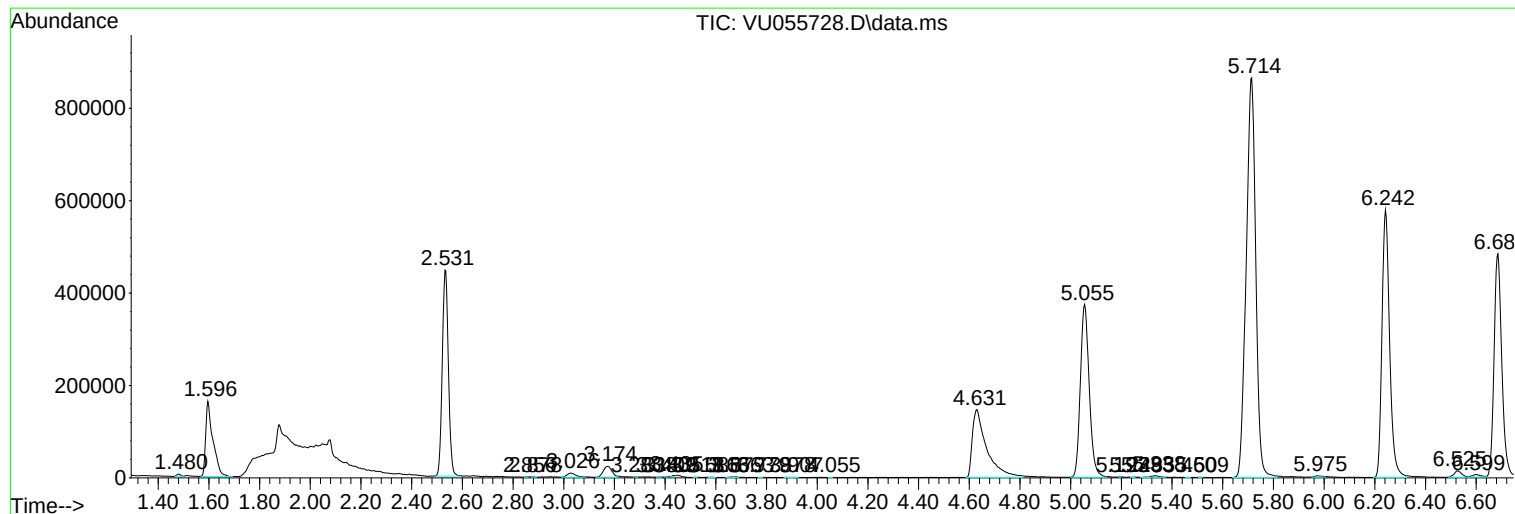
Sum of corrected areas: 17092295

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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\SFAMULM101023WMA.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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