

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102323\
 Data File : VU055849.D
 Acq On : 23 Oct 2023 12:38
 Operator : MD/SY
 Sample : VU1023MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK113

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: VU055849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	115	rBV	228227	260920	12.44%	1.656%
2	1.895	180	188	203	rVB	185241	257825	12.29%	1.637%
3	2.560	382	395	411	rBV	397201	650426	31.00%	4.129%
4	2.718	442	444	450	rVB5	1166	589	0.03%	0.004%
5	2.788	460	466	471	rBV4	1200	1457	0.07%	0.009%
6	2.949	509	516	519	rBV2	713	784	0.04%	0.005%
7	3.033	533	542	554	rBV3	5358	9483	0.45%	0.060%
8	3.177	574	587	610	rBV	18612	47522	2.26%	0.302%
9	3.258	610	612	616	rVB2	553	351	0.02%	0.002%
10	3.422	660	663	669	rVB2	427	430	0.02%	0.003%
11	3.570	704	709	712	rVV	418	459	0.02%	0.003%
12	3.644	725	732	735	rBV3	289	306	0.01%	0.002%
13	3.763	765	769	772	rBV	489	392	0.02%	0.002%
14	3.933	817	822	825	rVV	353	326	0.02%	0.002%
15	3.956	825	829	832	rVV	381	347	0.02%	0.002%
16	4.001	838	843	846	rVB2	407	320	0.02%	0.002%
17	4.303	936	937	947	rVB2	336	500	0.02%	0.003%
18	4.438	974	979	982	rVB2	562	386	0.02%	0.002%
19	4.509	996	1001	1004	rBV2	506	464	0.02%	0.003%
20	4.615	1021	1034	1074	rBV	160234	445110	21.21%	2.825%
21	5.055	1154	1171	1200	rBV	378910	854372	40.72%	5.423%
22	5.319	1249	1253	1254	rBV3	534	398	0.02%	0.003%
23	5.348	1260	1262	1267	rVB	382	332	0.02%	0.002%
24	5.608	1340	1343	1349	rVB2	340	313	0.01%	0.002%
25	5.718	1356	1377	1399	rBV2	762279	2098110	100.00%	13.318%
26	5.952	1448	1450	1453	rBV2	652	344	0.02%	0.002%
27	6.113	1496	1500	1507	rVB4	452	573	0.03%	0.004%
28	6.171	1515	1518	1523	rBV2	385	308	0.01%	0.002%
29	6.245	1527	1541	1566	rBV	576649	1113231	53.06%	7.066%
30	6.528	1618	1629	1642	rBV3	25899	50570	2.41%	0.321%
31	6.589	1645	1648	1651	rVB3	910	575	0.03%	0.004%
32	6.685	1662	1678	1706	rBV	481615	961477	45.83%	6.103%
33	6.904	1743	1746	1751	rBV3	420	344	0.02%	0.002%
34	6.968	1764	1766	1770	rVB2	473	295	0.01%	0.002%
35	7.094	1802	1805	1807	rBV2	501	341	0.02%	0.002%
36	7.190	1823	1835	1849	rBV3	7513	15527	0.74%	0.099%

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 Title : VOC Analysis

37	7.283	1861	1864	1870	rVB4	488	399	0.02%	0.003%
38	7.328	1875	1878	1881	rVB2	495	332	0.02%	0.002%
39	7.348	1881	1884	1889	rBV2	365	331	0.02%	0.002%
40	7.418	1902	1906	1909	rBV2	441	361	0.02%	0.002%
41	7.447	1909	1915	1917	rBV2	361	312	0.01%	0.002%
42	7.563	1937	1951	1975	rBV	249485	461403	21.99%	2.929%
43	7.698	1985	1993	2011	rVB5	4287	8496	0.40%	0.054%
44	7.795	2020	2023	2024	rBV3	662	387	0.02%	0.002%
45	7.814	2027	2029	2034	rVB4	816	594	0.03%	0.004%
46	7.894	2038	2054	2081	rBV	935708	1638305	78.08%	10.399%
47	8.177	2130	2142	2163	rBV	175435	305708	14.57%	1.940%
48	8.344	2188	2194	2196	rBV3	354	342	0.02%	0.002%
49	8.515	2244	2247	2251	rBV3	527	426	0.02%	0.003%
50	8.550	2253	2258	2264	rVB3	1979	2342	0.11%	0.015%
51	8.634	2272	2284	2319	rBV3	363661	950904	45.32%	6.036%
52	8.904	2364	2368	2370	rVB3	636	394	0.02%	0.003%
53	8.920	2370	2373	2375	rBV	443	307	0.01%	0.002%
54	9.013	2398	2402	2405	rVB	607	411	0.02%	0.003%
55	9.081	2418	2423	2427	rBV4	455	535	0.03%	0.003%
56	9.132	2436	2439	2443	rVB3	429	296	0.01%	0.002%
57	9.155	2443	2446	2448	rBV2	500	295	0.01%	0.002%
58	9.216	2462	2465	2468	rBV	432	330	0.02%	0.002%
59	9.306	2490	2493	2496	rBV4	432	311	0.01%	0.002%
60	9.415	2509	2527	2558	rBV	824594	1415107	67.45%	8.982%
61	9.573	2573	2576	2580	rVB4	1544	1180	0.06%	0.007%
62	9.637	2592	2596	2598	rBV3	498	317	0.02%	0.002%
63	9.666	2602	2605	2607	rVB2	567	310	0.01%	0.002%
64	9.695	2607	2614	2617	rBV4	1018	1226	0.06%	0.008%
65	9.737	2624	2627	2632	rVB3	699	568	0.03%	0.004%
66	9.791	2640	2644	2649	rVV2	657	675	0.03%	0.004%
67	9.894	2673	2676	2680	rBV	514	393	0.02%	0.002%
68	10.110	2736	2743	2745	rBV2	1339	1491	0.07%	0.009%
69	10.229	2776	2780	2785	rBV	416	463	0.02%	0.003%
70	10.489	2852	2861	2868	rBV4	1173	1883	0.09%	0.012%
71	10.566	2882	2885	2892	rVB2	434	520	0.02%	0.003%
72	10.753	2930	2943	2963	rBV	720917	1185478	56.50%	7.525%
73	10.904	2988	2990	2998	rVB4	510	389	0.02%	0.002%
74	11.090	3045	3048	3051	rBV2	759	603	0.03%	0.004%
75	11.364	3128	3133	3136	rBV3	543	453	0.02%	0.003%
76	11.473	3160	3167	3168	rBV4	1572	1552	0.07%	0.010%

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77	11.711	3238	3241	3244	rBV2	605	422	0.02%	0.003%
78	11.749	3246	3253	3259	rBV4	2153	2887	0.14%	0.018%
79	11.811	3259	3272	3297	rBV	832120	1387011	66.11%	8.804%
80	12.113	3361	3366	3369	rBV4	469	416	0.02%	0.003%
81	12.190	3376	3390	3413	rBV	912535	1549884	73.87%	9.838%
82	12.550	3498	3502	3504	rBV3	765	578	0.03%	0.004%
83	12.624	3523	3525	3528	rVB2	677	353	0.02%	0.002%
84	12.692	3543	3546	3548	rBV2	496	343	0.02%	0.002%
85	12.701	3548	3549	3553	rVB2	753	392	0.02%	0.002%
86	12.814	3581	3584	3590	rBV4	469	600	0.03%	0.004%
87	13.042	3652	3655	3658	rBV2	559	404	0.02%	0.003%
88	13.228	3709	3713	3717	rBV5	1629	1709	0.08%	0.011%
89	13.325	3740	3743	3746	rBV2	469	361	0.02%	0.002%
90	13.515	3797	3802	3806	rBV4	669	761	0.04%	0.005%
91	13.595	3823	3827	3829	rBV2	932	779	0.04%	0.005%
92	13.640	3837	3841	3846	rBV3	821	737	0.04%	0.005%
93	13.708	3859	3862	3868	rBV3	673	655	0.03%	0.004%
94	13.855	3897	3908	3920	rBV8	6460	12071	0.58%	0.077%
95	14.100	3977	3984	3999	rBV6	7433	15876	0.76%	0.101%
96	14.338	4051	4058	4073	rVB5	6936	13458	0.64%	0.085%
97	14.495	4105	4107	4112	rVB4	742	516	0.02%	0.003%
98	15.032	4272	4274	4278	rBV3	1230	862	0.04%	0.005%
99	15.216	4328	4331	4334	rBV3	1168	1000	0.05%	0.006%
100	15.399	4386	4388	4392	rBV3	1012	745	0.04%	0.005%

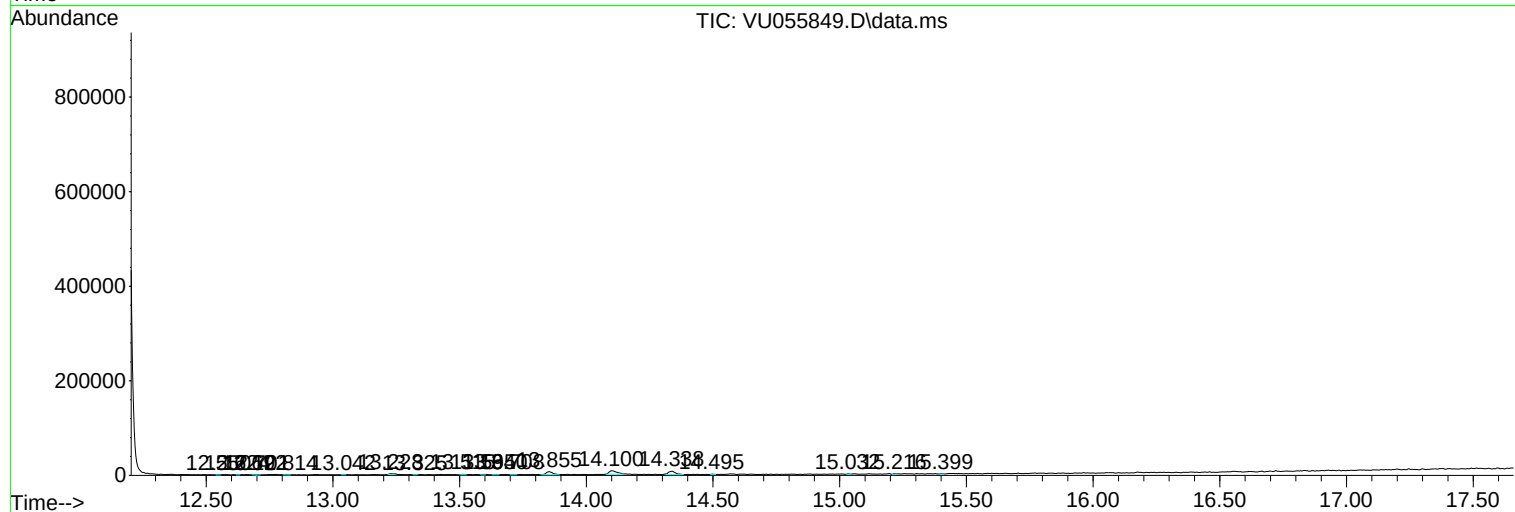
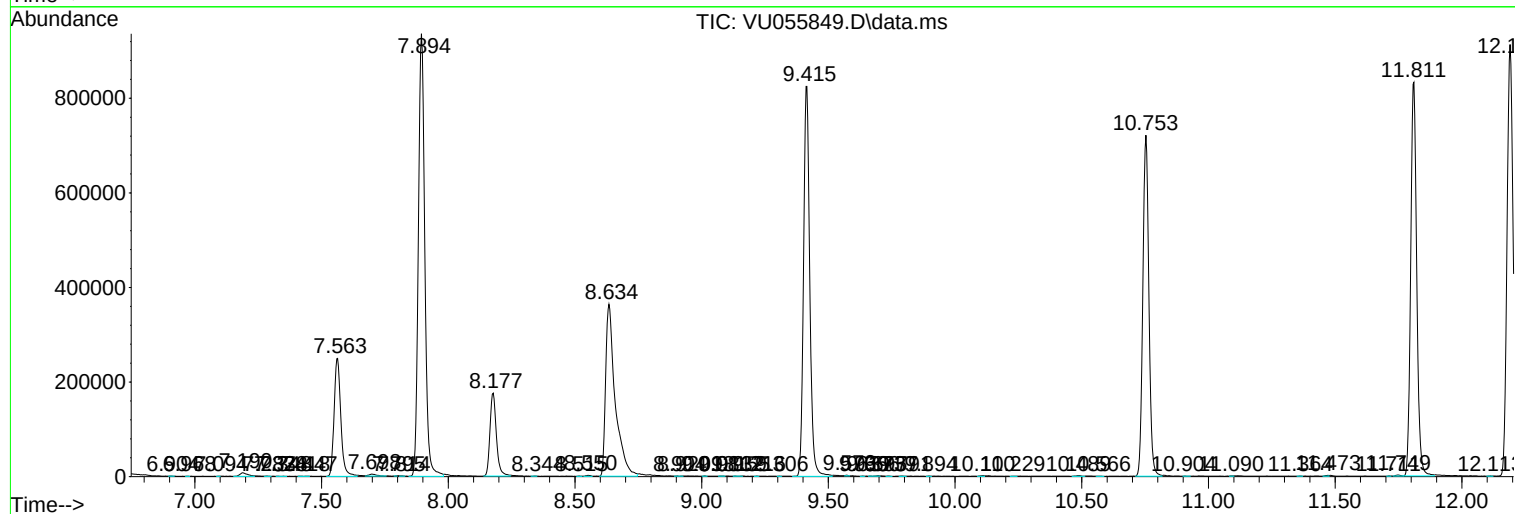
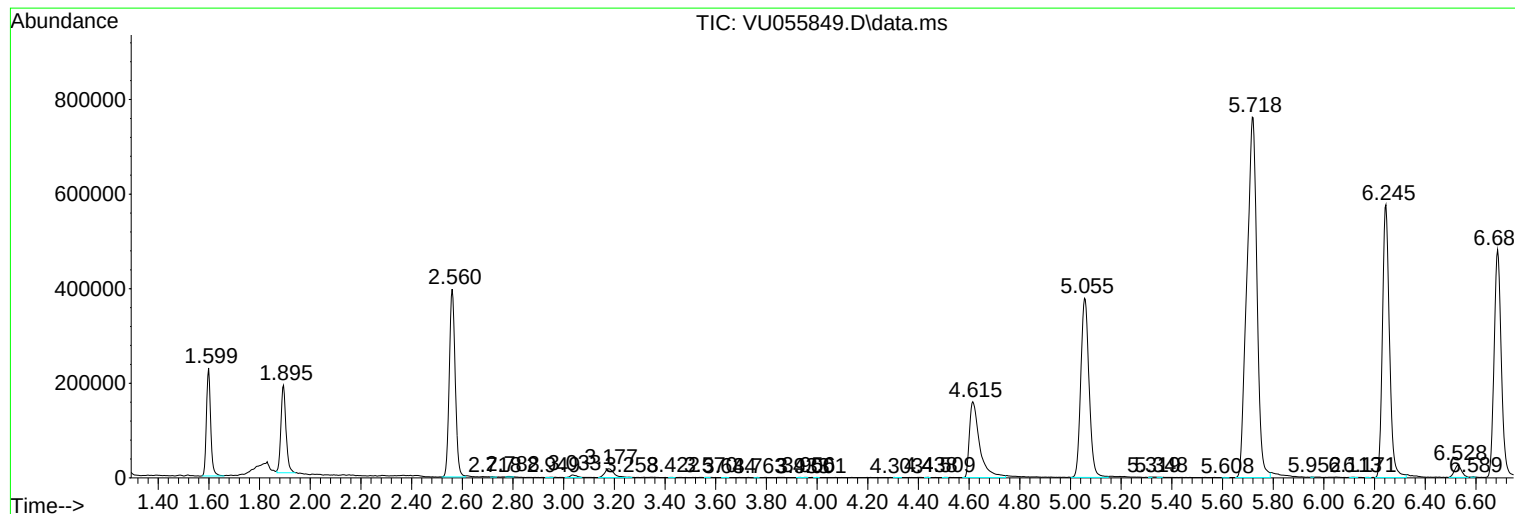
Sum of corrected areas: 15754456

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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
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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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