

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059331.D
 Acq On : 18 Jun 2024 23:01
 Operator : MD/SY
 Sample : P2873-20ME
 Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SK9ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059331.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	65	rBV4	2201	2331	0.49%	0.056%
2	1.592	86	94	121	rVB	30593	58256	12.14%	1.401%
3	1.833	134	169	170	rBV4	43838	175594	36.58%	4.224%
4	2.534	375	387	404	rBV	86936	140534	29.28%	3.380%
5	2.795	465	468	471	rBV2	340	243	0.05%	0.006%
6	2.891	494	498	502	rVV3	443	450	0.09%	0.011%
7	3.026	529	540	559	rBV3	6705	14839	3.09%	0.357%
8	3.168	574	584	585	rBV2	1172	1414	0.29%	0.034%
9	3.255	606	611	614	rBV2	333	312	0.07%	0.008%
10	3.341	633	638	641	rBV2	333	286	0.06%	0.007%
11	3.965	825	832	834	rBV2	251	303	0.06%	0.007%
12	4.235	912	916	920	rVB2	280	275	0.06%	0.007%
13	4.271	924	927	930	rVV	328	285	0.06%	0.007%
14	4.290	930	933	936	rVV	337	292	0.06%	0.007%
15	4.335	940	947	951	rBV2	279	361	0.08%	0.009%
16	4.624	1027	1037	1077	rBV	40637	128466	26.76%	3.090%
17	4.898	1119	1122	1126	rBV2	283	217	0.05%	0.005%
18	4.917	1126	1128	1134	rVB2	285	208	0.04%	0.005%
19	4.978	1142	1147	1152	rBV3	403	505	0.11%	0.012%
20	5.052	1155	1170	1191	rBV	84092	189620	39.50%	4.561%
21	5.168	1202	1206	1210	rBV2	298	255	0.05%	0.006%
22	5.209	1217	1219	1226	rVB2	435	393	0.08%	0.009%
23	5.283	1240	1242	1248	rVB	331	254	0.05%	0.006%
24	5.502	1306	1310	1313	rBV2	288	271	0.06%	0.007%
25	5.608	1336	1343	1349	rVB2	260	346	0.07%	0.008%
26	5.711	1357	1375	1394	rBV2	182233	479991	100.00%	11.546%
27	5.898	1429	1433	1437	rVB2	415	397	0.08%	0.010%
28	5.978	1449	1458	1465	rBV6	1481	2804	0.58%	0.067%
29	6.242	1526	1540	1574	rBV	185773	367103	76.48%	8.830%
30	6.479	1610	1614	1620	rVV2	277	344	0.07%	0.008%
31	6.525	1620	1628	1641	rVB7	4225	7779	1.62%	0.187%
32	6.598	1641	1651	1663	rBV5	1969	4403	0.92%	0.106%
33	6.682	1664	1677	1696	rVV	108629	217294	45.27%	5.227%
34	7.007	1774	1778	1782	rBV	284	274	0.06%	0.007%
35	7.190	1830	1835	1838	rBV2	1227	1450	0.30%	0.035%
36	7.380	1890	1894	1897	rBV2	265	237	0.05%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.505	1930	1933	1939	rBV2	239	218	0.05%	0.005%
38	7.560	1939	1950	1968	rBV	49890	91940	19.15%	2.212%
39	7.714	1991	1998	2004	rVB4	626	1030	0.21%	0.025%
40	7.891	2041	2053	2073	rBV	189280	342410	71.34%	8.236%
41	7.984	2079	2082	2095	rVB6	1901	3242	0.68%	0.078%
42	8.177	2132	2142	2161	rVV	32719	62151	12.95%	1.495%
43	8.367	2199	2201	2207	rVB2	229	234	0.05%	0.006%
44	8.467	2223	2232	2238	rBV3	465	763	0.16%	0.018%
45	8.547	2248	2257	2273	rBV3	13243	22197	4.62%	0.534%
46	8.640	2274	2286	2321	rBV	112498	271793	56.62%	6.538%
47	8.913	2368	2371	2377	rVB2	406	359	0.07%	0.009%
48	8.946	2377	2381	2388	rBV2	391	468	0.10%	0.011%
49	9.029	2401	2407	2410	rBV	343	375	0.08%	0.009%
50	9.299	2487	2491	2495	rBV2	283	322	0.07%	0.008%
51	9.415	2514	2527	2551	rBV	257568	462696	96.40%	11.130%
52	9.569	2571	2575	2576	rBV	570	360	0.08%	0.009%
53	9.621	2585	2591	2593	rBV2	281	252	0.05%	0.006%
54	9.698	2605	2615	2629	rBV4	1811	3445	0.72%	0.083%
55	9.859	2659	2665	2669	rBV2	286	386	0.08%	0.009%
56	9.884	2669	2673	2677	rBV	250	269	0.06%	0.006%
57	9.975	2697	2701	2706	rVV2	234	261	0.05%	0.006%
58	10.023	2713	2716	2722	rVB2	302	321	0.07%	0.008%
59	10.187	2764	2767	2777	rBV2	267	360	0.08%	0.009%
60	10.647	2907	2910	2913	rVB	314	211	0.04%	0.005%
61	10.666	2913	2916	2918	rBV	383	297	0.06%	0.007%
62	10.756	2931	2944	2963	rBV	179863	297890	62.06%	7.165%
63	10.888	2976	2985	2994	rBV4	1298	2157	0.45%	0.052%
64	11.158	3066	3069	3074	rVB2	409	372	0.08%	0.009%
65	11.264	3099	3102	3107	rBV2	224	227	0.05%	0.005%
66	11.328	3113	3122	3128	rBV5	938	1488	0.31%	0.036%
67	11.447	3154	3159	3163	rBV2	219	253	0.05%	0.006%
68	11.479	3163	3169	3174	rVV4	403	500	0.10%	0.012%
69	11.672	3225	3229	3234	rBV2	271	298	0.06%	0.007%
70	11.753	3251	3254	3257	rVB3	340	225	0.05%	0.005%
71	11.810	3260	3272	3290	rBV	261732	431781	89.96%	10.386%
72	12.081	3351	3356	3358	rBV2	274	323	0.07%	0.008%
73	12.193	3379	3391	3411	rBV	194058	325093	67.73%	7.820%
74	12.331	3432	3434	3439	rVB2	369	269	0.06%	0.006%
75	12.499	3483	3486	3490	rBV2	277	254	0.05%	0.006%
76	12.765	3565	3569	3576	rVV2	804	996	0.21%	0.024%

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 Title : VOC Analysis

77	12.794	3576	3578	3582	rVB2	304	212	0.04%	0.005%
78	12.888	3601	3607	3612	rBV2	319	451	0.09%	0.011%
79	13.061	3656	3661	3665	rBV2	288	328	0.07%	0.008%
80	13.193	3699	3702	3710	rBV	320	400	0.08%	0.010%
81	13.267	3722	3725	3729	rBV	281	249	0.05%	0.006%
82	13.508	3795	3800	3802	rBV	210	253	0.05%	0.006%
83	13.640	3836	3841	3847	rBV2	530	721	0.15%	0.017%
84	13.669	3847	3850	3853	rVB	316	220	0.05%	0.005%
85	13.801	3885	3891	3893	rBV2	245	256	0.05%	0.006%
86	13.852	3905	3907	3911	rVB2	393	253	0.05%	0.006%
87	13.929	3927	3931	3932	rBV	325	236	0.05%	0.006%
88	14.097	3972	3983	3998	rBV2	9848	18498	3.85%	0.445%
89	14.399	4072	4077	4079	rBV2	427	368	0.08%	0.009%
90	14.479	4098	4102	4104	rBV	326	255	0.05%	0.006%
91	14.515	4110	4113	4116	rVB2	371	272	0.06%	0.007%
92	14.569	4124	4130	4138	rVB3	1302	1814	0.38%	0.044%
93	14.643	4150	4153	4159	rVB2	393	328	0.07%	0.008%
94	14.717	4170	4176	4178	rBV2	480	484	0.10%	0.012%
95	14.772	4185	4193	4195	rBV3	345	509	0.11%	0.012%
96	14.859	4217	4220	4225	rBV2	520	607	0.13%	0.015%
97	15.248	4336	4341	4347	rBV4	849	1183	0.25%	0.028%
98	15.421	4389	4395	4403	rBV4	875	1591	0.33%	0.038%
99	15.852	4526	4529	4534	rBV3	605	480	0.10%	0.012%
100	16.260	4654	4656	4661	rBV3	501	504	0.11%	0.012%

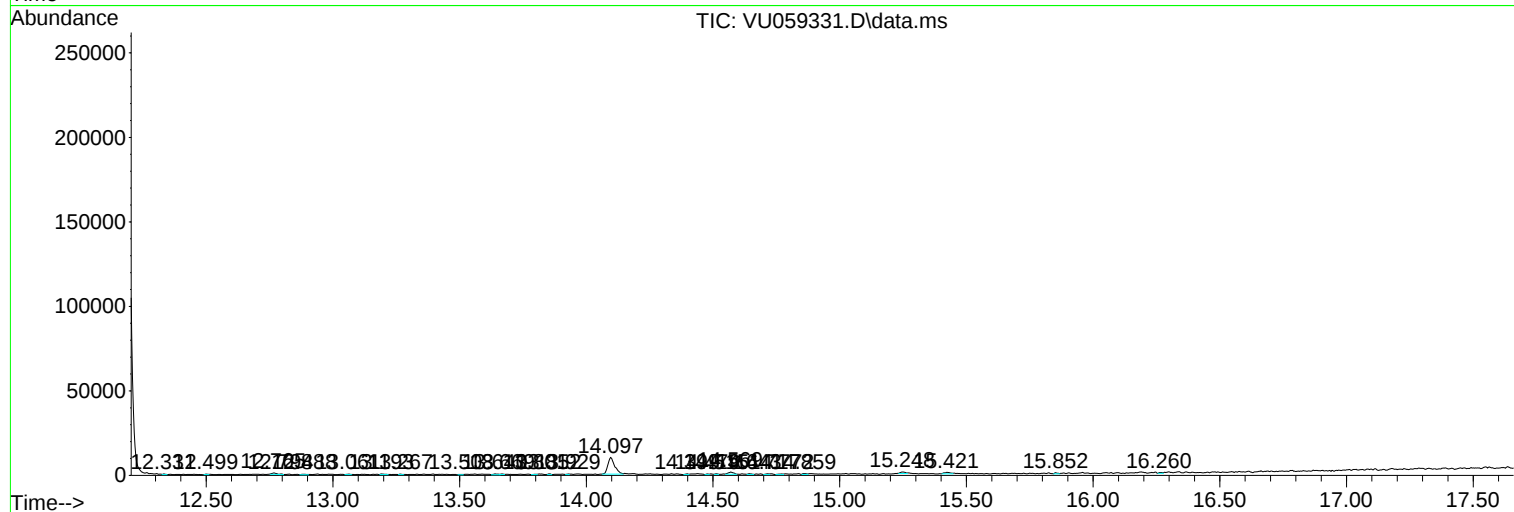
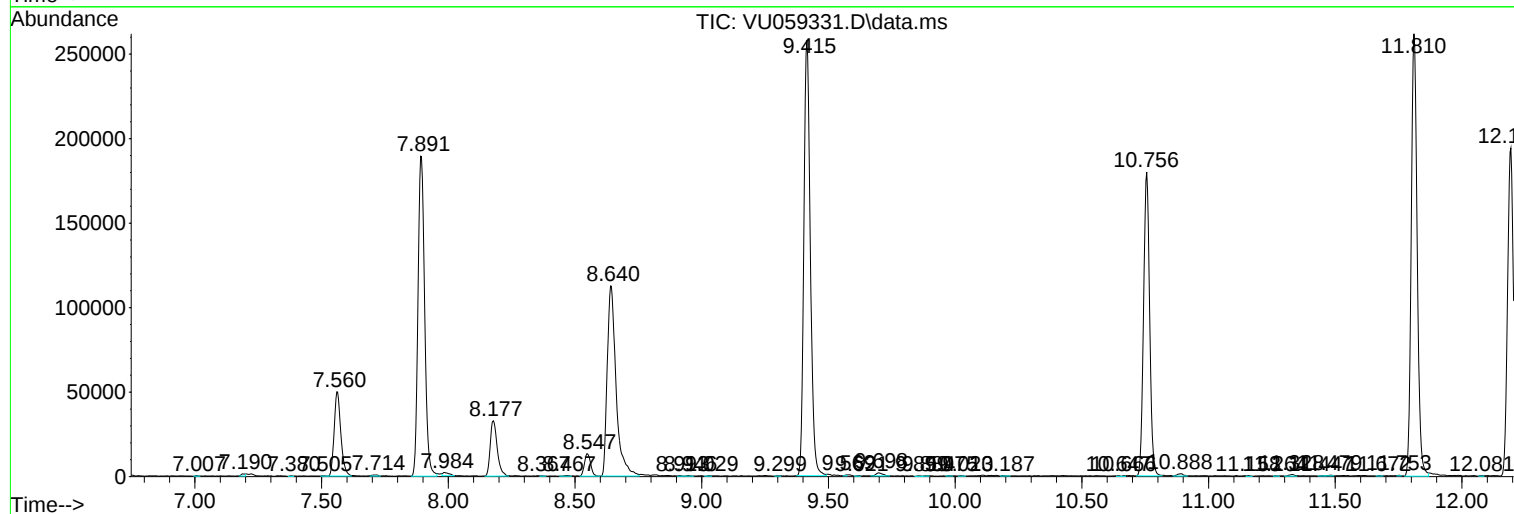
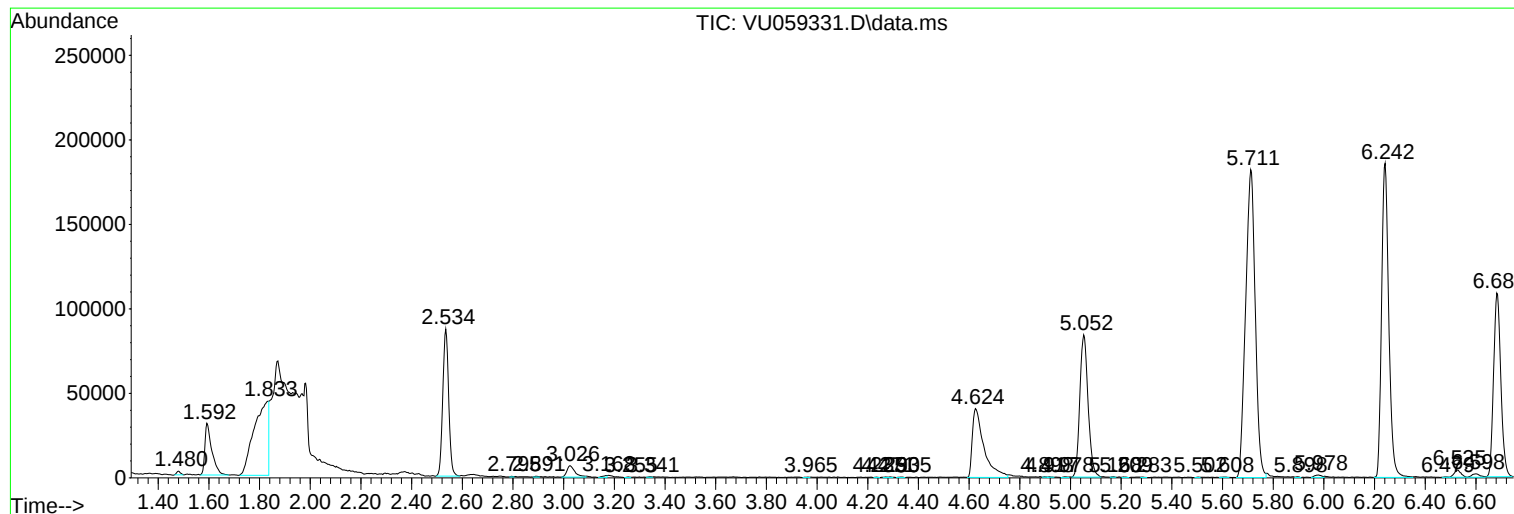
Sum of corrected areas: 4157344

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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\SFAMULM052924WMA.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 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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