

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062424\
 Data File : VU059442.D
 Acq On : 24 Jun 2024 12:15
 Operator : MD/SY
 Sample : P2962-09ME
 Misc : 5.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COT81ME

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: VU059442.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	56	59	67	rVB4	1346	1396	0.21%	0.026%
2	1.592	87	94	119	rVB	29959	52382	7.78%	0.961%
3	1.872	136	181	187	rBV6	65186	342583	50.87%	6.287%
4	2.534	376	387	405	rVB	84803	138505	20.56%	2.542%
5	2.631	410	417	418	rBV3	1246	1231	0.18%	0.023%
6	2.702	437	439	443	rVB2	285	146	0.02%	0.003%
7	2.763	450	458	469	rVB3	1029	1832	0.27%	0.034%
8	2.805	469	471	474	rBV2	198	137	0.02%	0.003%
9	2.830	476	479	484	rVB3	337	256	0.04%	0.005%
10	2.875	487	493	496	rBV	328	323	0.05%	0.006%
11	2.949	513	516	518	rBV2	286	230	0.03%	0.004%
12	3.023	530	539	551	rBV3	5658	11925	1.77%	0.219%
13	3.178	572	587	600	rBV2	7485	18735	2.78%	0.344%
14	3.406	653	658	665	rBV2	342	438	0.07%	0.008%
15	3.718	752	755	758	rBV	158	131	0.02%	0.002%
16	4.100	869	874	876	rBV	192	192	0.03%	0.004%
17	4.329	942	945	950	rBV2	188	176	0.03%	0.003%
18	4.412	967	971	973	rBV	142	120	0.02%	0.002%
19	4.486	990	994	997	rBV	251	183	0.03%	0.003%
20	4.624	1023	1037	1066	rBV2	50984	156471	23.23%	2.871%
21	4.856	1106	1109	1114	rVB	263	203	0.03%	0.004%
22	4.904	1121	1124	1129	rVB3	194	139	0.02%	0.003%
23	4.975	1143	1146	1152	rBV3	302	350	0.05%	0.006%
24	5.052	1155	1170	1194	rVV	95860	216345	32.12%	3.970%
25	5.194	1212	1214	1221	rVB2	417	264	0.04%	0.005%
26	5.296	1243	1246	1249	rBV2	255	182	0.03%	0.003%
27	5.477	1299	1302	1305	rVB	253	139	0.02%	0.003%
28	5.544	1320	1323	1330	rVB2	242	260	0.04%	0.005%
29	5.579	1330	1334	1338	rBV2	152	135	0.02%	0.002%
30	5.711	1356	1375	1397	rBV3	193951	523746	77.76%	9.612%
31	5.981	1450	1459	1464	rBV5	1366	2518	0.37%	0.046%
32	6.113	1496	1500	1502	rBV	273	217	0.03%	0.004%
33	6.155	1506	1513	1517	rBV	328	340	0.05%	0.006%
34	6.239	1527	1539	1560	rBV	258485	509129	75.59%	9.343%
35	6.390	1584	1586	1588	rVB	314	124	0.02%	0.002%
36	6.457	1604	1607	1611	rBV2	230	179	0.03%	0.003%

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

37	6.483	1611	1615	1618	rVV2	275	225	0.03%	0.004%
38	6.528	1619	1629	1639	rVB8	3967	7647	1.14%	0.140%
39	6.599	1639	1651	1663	rBV4	2343	5373	0.80%	0.099%
40	6.682	1664	1677	1699	rVV2	122859	244090	36.24%	4.479%
41	6.865	1730	1734	1738	rBV	250	211	0.03%	0.004%
42	6.927	1749	1753	1755	rBV2	246	184	0.03%	0.003%
43	6.988	1769	1772	1775	rBV2	172	141	0.02%	0.003%
44	7.193	1828	1836	1838	rBV2	1948	1970	0.29%	0.036%
45	7.335	1876	1880	1886	rBV2	290	258	0.04%	0.005%
46	7.486	1924	1927	1930	rVV2	283	201	0.03%	0.004%
47	7.521	1934	1938	1939	rBV2	163	116	0.02%	0.002%
48	7.560	1939	1950	1976	rVB	59411	108938	16.17%	1.999%
49	7.714	1989	1998	2003	rBV4	885	1607	0.24%	0.029%
50	7.788	2017	2021	2024	rBV	207	159	0.02%	0.003%
51	7.891	2041	2053	2071	rBV	210509	376367	55.88%	6.907%
52	8.036	2096	2098	2101	rVB	327	185	0.03%	0.003%
53	8.174	2131	2141	2171	rVB	40895	75398	11.19%	1.384%
54	8.364	2195	2200	2205	rBV2	530	693	0.10%	0.013%
55	8.467	2224	2232	2239	rVB3	485	811	0.12%	0.015%
56	8.547	2244	2257	2273	rBV2	77676	132368	19.65%	2.429%
57	8.640	2273	2286	2320	rBV2	141912	343898	51.06%	6.311%
58	8.878	2358	2360	2367	rBV3	164	183	0.03%	0.003%
59	9.152	2441	2445	2450	rBV2	227	214	0.03%	0.004%
60	9.412	2514	2526	2560	rVV	380637	673512	100.00%	12.360%
61	9.570	2566	2575	2587	rVB2	3965	6200	0.92%	0.114%
62	9.695	2602	2614	2625	rBV2	7391	12915	1.92%	0.237%
63	9.763	2632	2635	2639	rVB2	250	167	0.02%	0.003%
64	9.994	2703	2707	2714	rBV2	326	386	0.06%	0.007%
65	10.107	2734	2742	2748	rBV3	1974	2918	0.43%	0.054%
66	10.155	2755	2757	2762	rBV2	228	145	0.02%	0.003%
67	10.235	2780	2782	2785	rVB	312	169	0.03%	0.003%
68	10.258	2785	2789	2793	rBV2	194	201	0.03%	0.004%
69	10.312	2804	2806	2808	rBV2	285	183	0.03%	0.003%
70	10.496	2860	2863	2865	rVB2	266	170	0.03%	0.003%
71	10.512	2865	2868	2876	rVB	288	327	0.05%	0.006%
72	10.753	2930	2943	2961	rBV	224449	375640	55.77%	6.894%
73	10.881	2980	2983	2985	rBV2	408	335	0.05%	0.006%
74	10.917	2991	2994	2996	rBV2	307	204	0.03%	0.004%
75	11.042	3031	3033	3035	rVB	398	168	0.02%	0.003%
76	11.094	3042	3049	3057	rVB3	619	887	0.13%	0.016%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
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77	11.322	3118	3120	3122	rBV	223	125	0.02%	0.002%
78	11.367	3131	3134	3137	rBV	213	176	0.03%	0.003%
79	11.473	3160	3167	3176	rVB2	1935	2393	0.36%	0.044%
80	11.733	3245	3248	3249	rBV2	231	147	0.02%	0.003%
81	11.811	3260	3272	3292	rBV	387203	622146	92.37%	11.417%
82	11.987	3324	3327	3329	rBV2	242	159	0.02%	0.003%
83	12.029	3337	3340	3343	rBV3	335	186	0.03%	0.003%
84	12.097	3357	3361	3370	rVB4	587	589	0.09%	0.011%
85	12.190	3378	3390	3410	rBV	250373	407390	60.49%	7.476%
86	12.586	3509	3513	3518	rVB2	274	282	0.04%	0.005%
87	12.614	3518	3522	3529	rBV2	339	421	0.06%	0.008%
88	12.759	3564	3567	3569	rBV2	232	164	0.02%	0.003%
89	13.122	3677	3680	3688	rVB2	319	335	0.05%	0.006%
90	13.187	3698	3700	3704	rBV	230	156	0.02%	0.003%
91	13.229	3711	3713	3717	rBV	267	139	0.02%	0.003%
92	14.090	3970	3981	4002	rBV	27732	51754	7.68%	0.950%
93	14.216	4018	4020	4022	rBV	343	221	0.03%	0.004%
94	14.303	4044	4047	4048	rBV	251	166	0.02%	0.003%
95	14.364	4062	4066	4068	rBV2	415	362	0.05%	0.007%
96	14.460	4093	4096	4098	rBV2	321	221	0.03%	0.004%
97	14.518	4111	4114	4120	rBV3	281	316	0.05%	0.006%
98	15.241	4334	4339	4342	rBV5	1043	1194	0.18%	0.022%
99	15.418	4387	4394	4403	rBV4	1375	2383	0.35%	0.044%
100	16.193	4633	4635	4638	rVB2	589	281	0.04%	0.005%

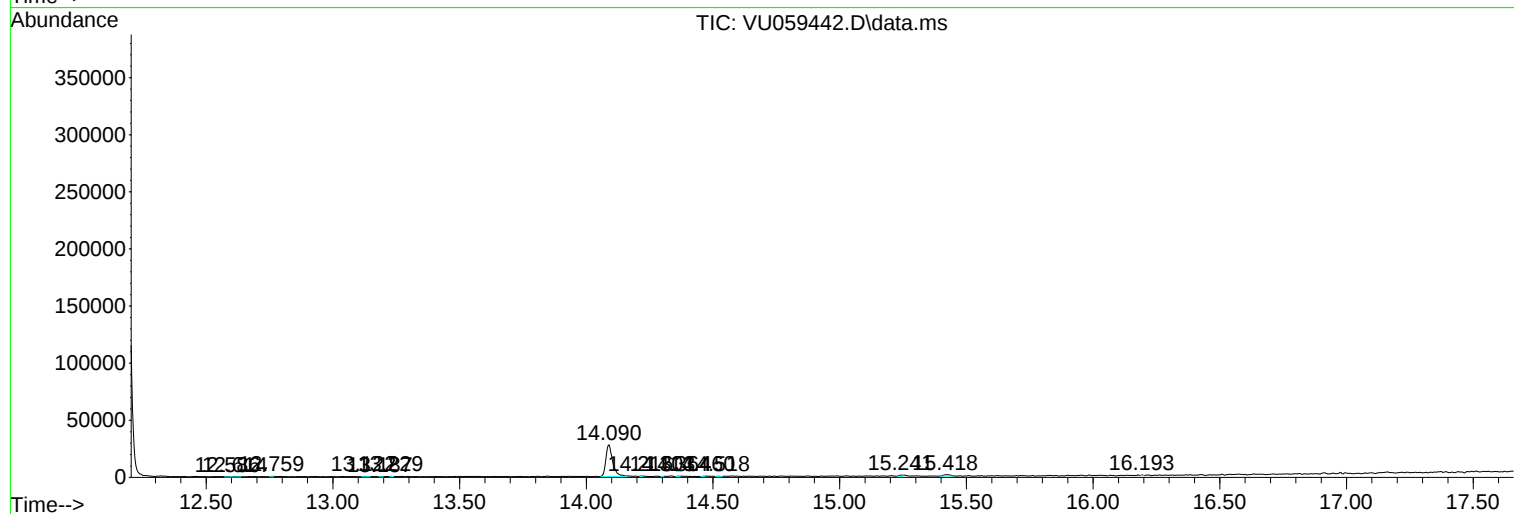
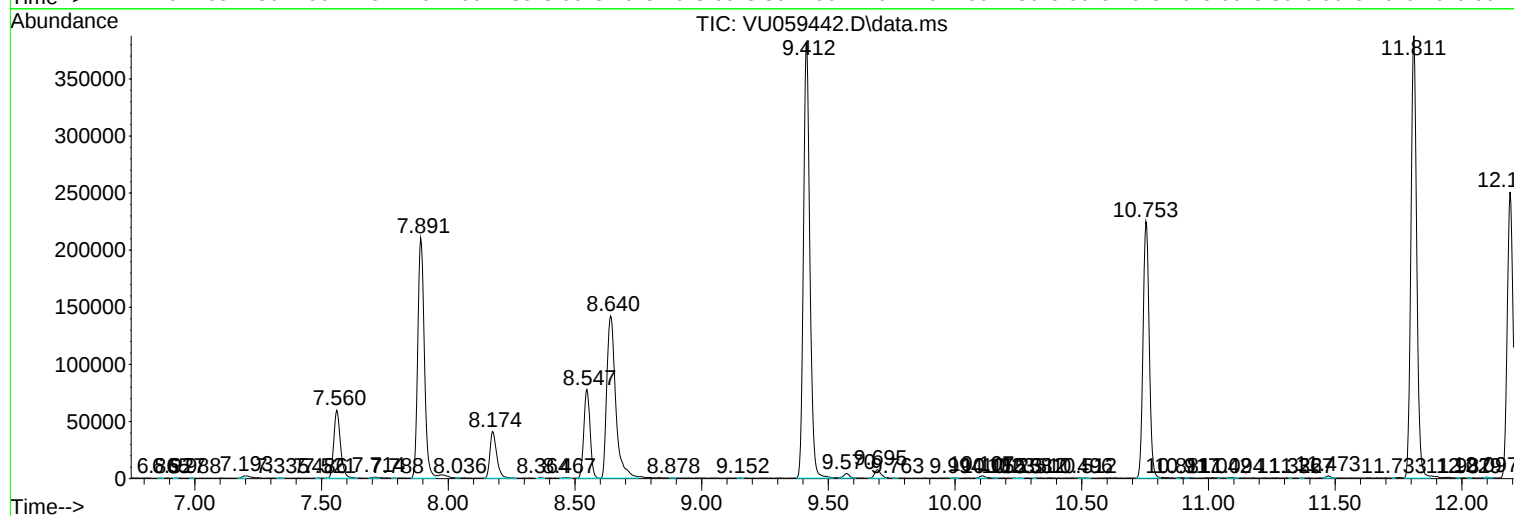
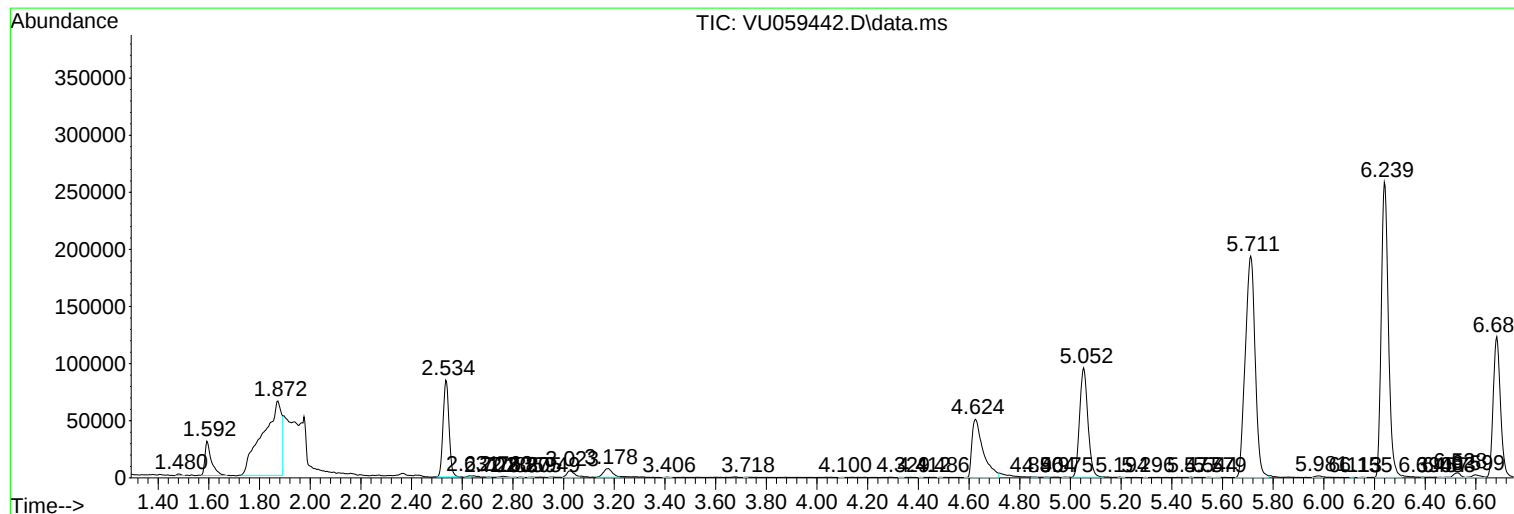
Sum of corrected areas: 5449132

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COT81ME

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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Instrument :
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C0T81ME

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 Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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