

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071124\
 Data File : VU059906.D
 Acq On : 11 Jul 2024 13:42
 Operator : MD/SY
 Sample : P3177-09ME
 Misc : 4.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4BS7ME

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\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU059906.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	86	95	117	rBV	56961	91510	12.64%	1.555%
2	1.865	145	179	182	rBV2	38016	111633	15.42%	1.897%
3	1.894	183	188	204	rVB	45724	83478	11.53%	1.418%
4	2.547	379	391	407	rBV	133021	215721	29.79%	3.666%
5	2.634	411	418	420	rBV2	970	1234	0.17%	0.021%
6	2.766	454	459	462	rVV3	473	563	0.08%	0.010%
7	2.798	466	469	475	rVB3	464	355	0.05%	0.006%
8	2.865	485	490	491	rBV	263	233	0.03%	0.004%
9	2.949	504	516	534	rBV2	11409	26198	3.62%	0.445%
10	3.033	536	542	544	rBV3	1627	1923	0.27%	0.033%
11	3.116	558	568	576	rBV3	4899	9245	1.28%	0.157%
12	3.174	578	586	601	rVB3	5661	12712	1.76%	0.216%
13	3.399	651	656	660	rVV3	417	384	0.05%	0.007%
14	3.576	707	711	715	rBV2	564	594	0.08%	0.010%
15	4.209	903	908	913	rBV2	252	210	0.03%	0.004%
16	4.492	991	996	1001	rVB2	304	263	0.04%	0.004%
17	4.563	1015	1018	1027	rVB2	241	271	0.04%	0.005%
18	4.627	1027	1038	1070	rBV2	48135	149538	20.65%	2.541%
19	4.894	1118	1121	1128	rVB3	300	344	0.05%	0.006%
20	5.052	1155	1170	1194	rBV2	121047	272008	37.57%	4.622%
21	5.155	1200	1202	1206	rVB	348	210	0.03%	0.004%
22	5.505	1306	1311	1313	rBV	219	195	0.03%	0.003%
23	5.573	1326	1332	1334	rBV2	218	210	0.03%	0.004%
24	5.608	1340	1343	1348	rVB2	214	186	0.03%	0.003%
25	5.714	1357	1376	1407	rBV2	258209	684790	94.58%	11.636%
26	6.241	1527	1540	1566	rBV	286572	559154	77.22%	9.501%
27	6.409	1589	1592	1594	rBV2	280	184	0.03%	0.003%
28	6.473	1608	1612	1614	rBV2	295	226	0.03%	0.004%
29	6.531	1621	1630	1636	rBV5	1325	2284	0.32%	0.039%
30	6.682	1664	1677	1703	rBV	155586	307373	42.45%	5.223%
31	6.801	1711	1714	1715	rBV2	343	189	0.03%	0.003%
32	6.891	1738	1742	1747	rBV2	236	274	0.04%	0.005%
33	7.013	1771	1780	1783	rBV2	227	290	0.04%	0.005%
34	7.212	1833	1842	1844	rVV7	1081	1482	0.20%	0.025%
35	7.235	1847	1849	1857	rVB2	744	537	0.07%	0.009%
36	7.508	1927	1934	1937	rBV2	161	231	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

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Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

37	7.560	1937	1950	1969	rBV	74844	142396	19.67%	2.420%
38	7.704	1990	1995	2001	rVB2	415	447	0.06%	0.008%
39	7.733	2001	2004	2010	rBV2	204	225	0.03%	0.004%
40	7.804	2022	2026	2030	rVB3	236	248	0.03%	0.004%
41	7.827	2030	2033	2040	rVB3	202	202	0.03%	0.003%
42	7.891	2040	2053	2074	rBV	295897	528652	73.01%	8.983%
43	8.065	2103	2107	2111	rBV2	220	237	0.03%	0.004%
44	8.177	2130	2142	2167	rBV2	52430	97746	13.50%	1.661%
45	8.261	2167	2168	2175	rVB2	322	276	0.04%	0.005%
46	8.466	2222	2232	2241	rVB	1224	1723	0.24%	0.029%
47	8.537	2250	2254	2256	rVV2	563	373	0.05%	0.006%
48	8.547	2256	2257	2263	rVB3	711	518	0.07%	0.009%
49	8.646	2274	2288	2322	rBV	121140	322608	44.56%	5.482%
50	8.839	2345	2348	2352	rVB2	266	226	0.03%	0.004%
51	8.872	2353	2358	2361	rBV3	347	301	0.04%	0.005%
52	8.913	2369	2371	2373	rBV2	328	185	0.03%	0.003%
53	9.013	2399	2402	2407	rVV3	254	256	0.04%	0.004%
54	9.084	2420	2424	2428	rVB	227	176	0.02%	0.003%
55	9.126	2428	2437	2442	rBV2	234	368	0.05%	0.006%
56	9.351	2501	2507	2511	rBV2	257	282	0.04%	0.005%
57	9.412	2513	2526	2551	rBV	411697	724059	100.00%	12.303%
58	9.544	2565	2567	2570	rVB3	378	166	0.02%	0.003%
59	9.704	2605	2617	2624	rBV5	841	1742	0.24%	0.030%
60	9.762	2631	2635	2639	rBV2	226	192	0.03%	0.003%
61	10.055	2723	2726	2732	rVB2	273	280	0.04%	0.005%
62	10.254	2786	2788	2794	rVB	209	195	0.03%	0.003%
63	10.338	2811	2814	2817	rBV	266	181	0.02%	0.003%
64	10.437	2839	2845	2849	rBV2	306	317	0.04%	0.005%
65	10.463	2850	2853	2854	rVV2	299	181	0.02%	0.003%
66	10.476	2854	2857	2863	rVB3	892	843	0.12%	0.014%
67	10.572	2883	2887	2891	rBV2	201	223	0.03%	0.004%
68	10.621	2899	2902	2905	rVB2	269	179	0.02%	0.003%
69	10.701	2924	2927	2930	rBV2	197	181	0.02%	0.003%
70	10.756	2930	2944	2961	rVV	231743	393517	54.35%	6.687%
71	10.830	2965	2967	2973	rVB2	353	300	0.04%	0.005%
72	10.884	2978	2984	2993	rBV3	1133	1959	0.27%	0.033%
73	10.968	3007	3010	3014	rVV2	236	207	0.03%	0.004%
74	10.990	3014	3017	3022	rVB2	334	239	0.03%	0.004%
75	11.087	3043	3047	3050	rBV2	265	283	0.04%	0.005%
76	11.251	3094	3098	3102	rBV2	261	255	0.04%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

77	11.386	3134	3140	3146	rBV2	349	386	0.05%	0.007%
78	11.714	3237	3242	3245	rBV2	226	210	0.03%	0.004%
79	11.762	3254	3257	3259	rBV2	325	232	0.03%	0.004%
80	11.807	3260	3271	3291	rBV	393285	637632	88.06%	10.835%
81	12.061	3348	3350	3356	rVB	393	243	0.03%	0.004%
82	12.190	3378	3390	3411	rVV	289645	478166	66.04%	8.125%
83	12.370	3443	3446	3449	rVV2	275	199	0.03%	0.003%
84	12.769	3562	3570	3579	rVB2	919	1398	0.19%	0.024%
85	12.923	3613	3618	3629	rBV2	1400	1617	0.22%	0.027%
86	13.042	3653	3655	3660	rVB	322	257	0.04%	0.004%
87	13.170	3691	3695	3701	rBV2	248	278	0.04%	0.005%
88	13.556	3812	3815	3820	rVB2	300	188	0.03%	0.003%
89	13.617	3828	3834	3840	rBV4	1054	1302	0.18%	0.022%
90	13.855	3904	3908	3917	rBV	322	561	0.08%	0.010%
91	14.203	4012	4016	4018	rBV2	351	305	0.04%	0.005%
92	14.367	4064	4067	4070	rBV	290	165	0.02%	0.003%
93	14.559	4123	4127	4128	rBV2	499	340	0.05%	0.006%
94	14.630	4146	4149	4152	rBV2	340	330	0.05%	0.006%
95	15.186	4319	4322	4325	rBV2	481	337	0.05%	0.006%
96	15.212	4328	4330	4333	rBV2	343	183	0.03%	0.003%
97	15.524	4424	4427	4429	rBV2	429	302	0.04%	0.005%
98	15.611	4450	4454	4459	rBV3	515	444	0.06%	0.008%
99	15.707	4481	4484	4489	rBV3	584	475	0.07%	0.008%
100	15.858	4529	4531	4534	rBV3	435	283	0.04%	0.005%

Sum of corrected areas: 5885009

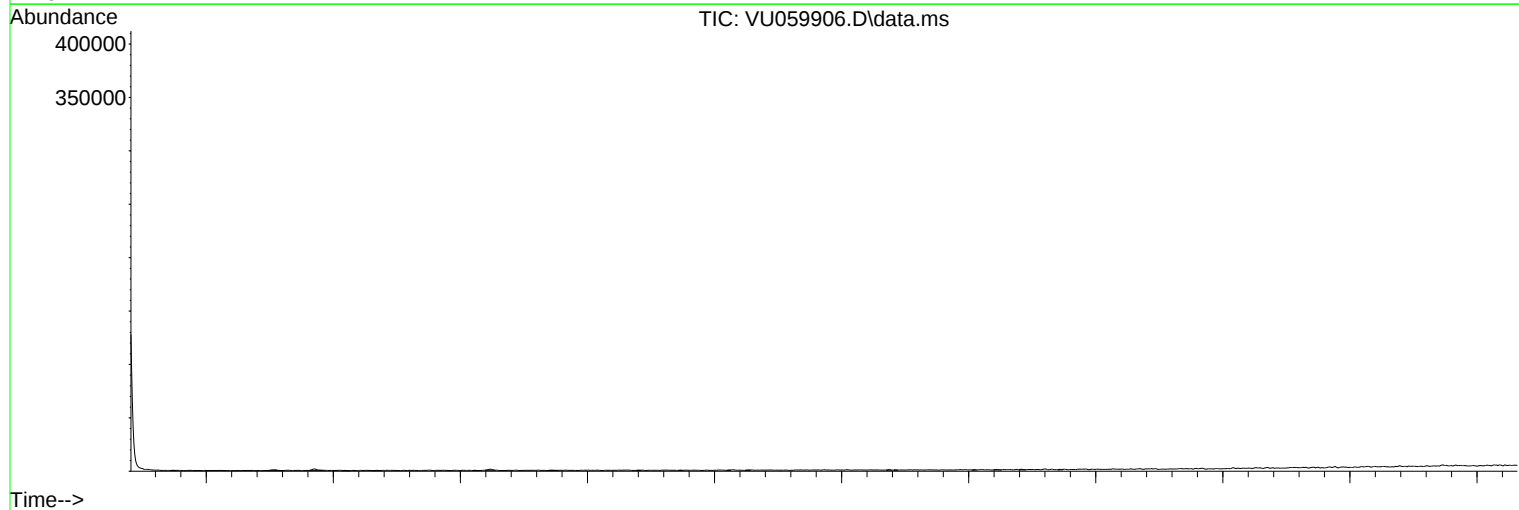
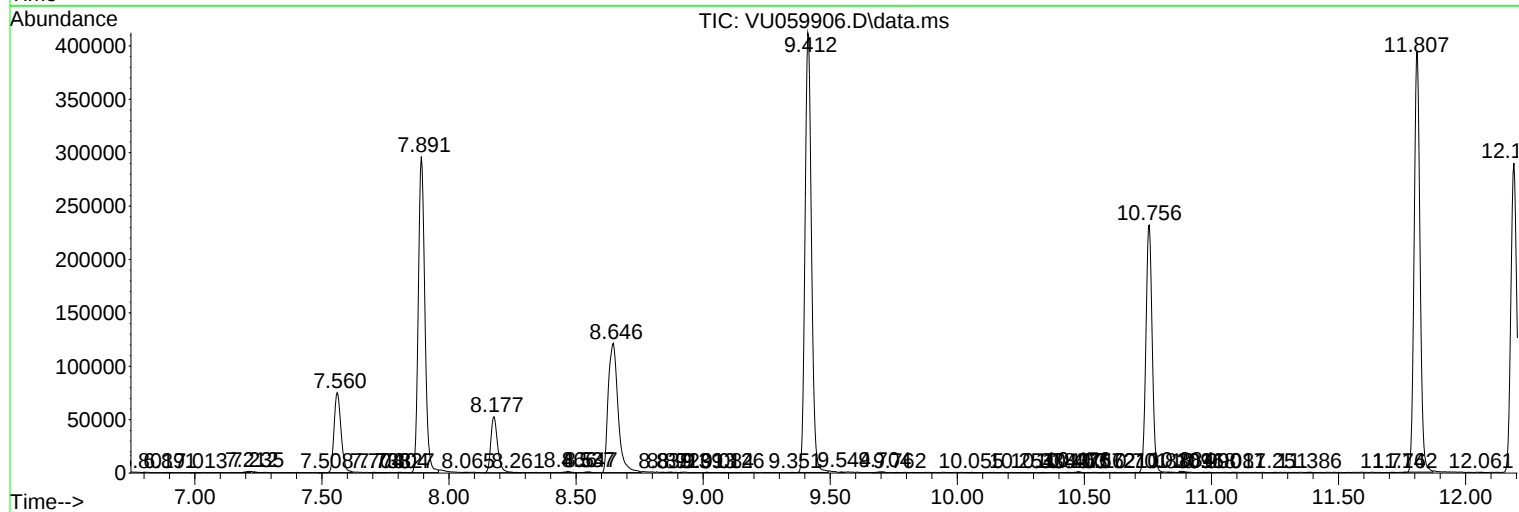
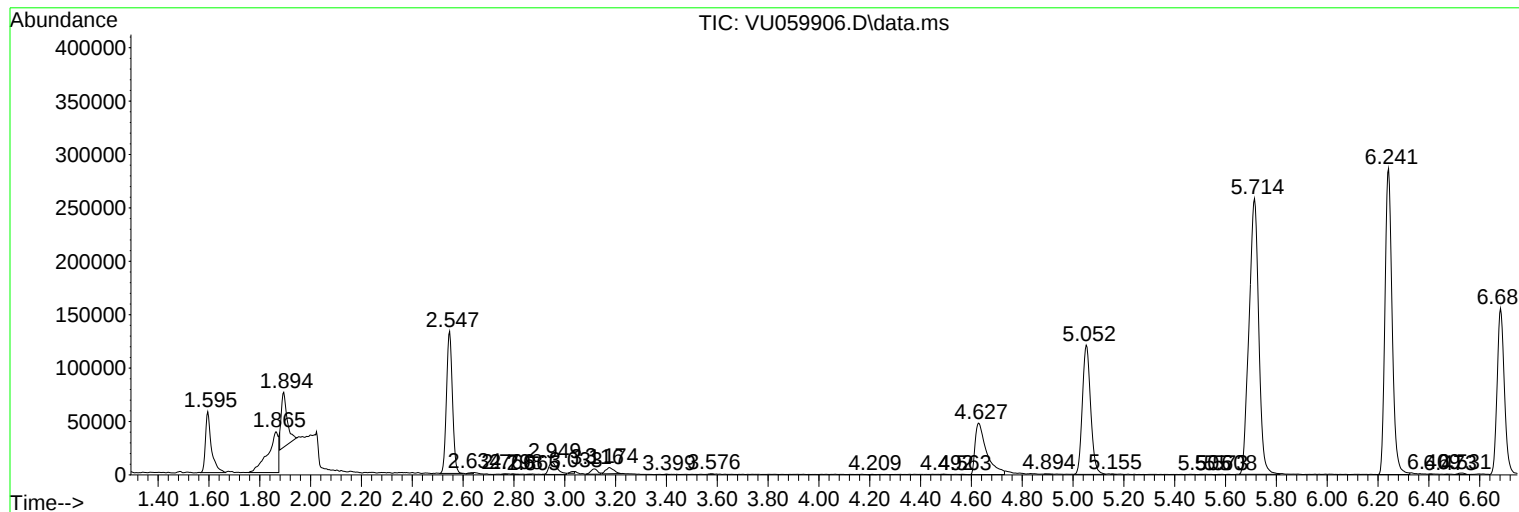
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Instrument :
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ClientSampleId :
A4BS7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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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