

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059950.D
 Acq On : 15 Jul 2024 14:44
 Operator : MD/SY
 Sample : P3178-09ME
 Misc : 4.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4BT4ME

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: VU059950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	88	94	115	rVB	39140	65949	9.99%	1.227%
2	2.531	374	386	411	rBV	102438	178895	27.11%	3.327%
3	2.952	507	517	531	rBV2	6898	14014	2.12%	0.261%
4	3.174	574	586	587	rBV3	2882	4136	0.63%	0.077%
5	3.322	630	632	635	rBV2	161	124	0.02%	0.002%
6	3.428	662	665	667	rBV	202	132	0.02%	0.002%
7	3.444	667	670	674	rVV	286	233	0.04%	0.004%
8	3.509	686	690	692	rBV	176	131	0.02%	0.002%
9	3.605	715	720	723	rBV2	233	201	0.03%	0.004%
10	3.631	723	728	731	rBV	288	314	0.05%	0.006%
11	3.695	744	748	751	rBV2	385	257	0.04%	0.005%
12	3.724	751	757	760	rBV2	277	312	0.05%	0.006%
13	3.914	812	816	818	rBV2	209	164	0.02%	0.003%
14	4.116	876	879	885	rVB2	239	270	0.04%	0.005%
15	4.145	885	888	889	rBV	101	54	0.01%	0.001%
16	4.190	898	902	907	rBV	214	174	0.03%	0.003%
17	4.245	915	919	922	rBV	323	241	0.04%	0.004%
18	4.264	922	925	928	rVB	227	167	0.03%	0.003%
19	4.505	997	1000	1005	rVB2	268	197	0.03%	0.004%
20	4.537	1005	1010	1012	rBV	267	255	0.04%	0.005%
21	4.563	1015	1018	1023	rVB	255	181	0.03%	0.003%
22	4.627	1028	1038	1074	rBV	57904	168812	25.58%	3.140%
23	5.052	1154	1170	1197	rBV	110238	242730	36.78%	4.514%
24	5.197	1213	1215	1221	rVB3	518	346	0.05%	0.006%
25	5.242	1226	1229	1230	rBV	167	65	0.01%	0.001%
26	5.251	1230	1232	1234	rBV2	227	115	0.02%	0.002%
27	5.441	1289	1291	1293	rBV	135	90	0.01%	0.002%
28	5.476	1299	1302	1310	rVB2	257	316	0.05%	0.006%
29	5.512	1310	1313	1316	rBV2	254	223	0.03%	0.004%
30	5.627	1346	1349	1351	rBV2	204	144	0.02%	0.003%
31	5.714	1357	1376	1402	rBV3	226061	601333	91.12%	11.184%
32	5.891	1429	1431	1434	rBV	187	123	0.02%	0.002%
33	5.939	1444	1446	1447	rBV	221	55	0.01%	0.001%
34	6.116	1497	1501	1507	rVB2	298	304	0.05%	0.006%
35	6.161	1507	1515	1516	rBV	190	241	0.04%	0.004%
36	6.242	1527	1540	1563	rBV	261834	503387	76.28%	9.362%

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 Title : VOC Analysis

37	6.447	1602	1604	1611	rVB2	618	514	0.08%	0.010%
38	6.476	1611	1613	1615	rBV	89	56	0.01%	0.001%
39	6.521	1621	1627	1628	rBV2	1906	1401	0.21%	0.026%
40	6.598	1640	1651	1661	rBV6	1729	3558	0.54%	0.066%
41	6.682	1665	1677	1699	rVB	136959	273365	41.42%	5.084%
42	6.791	1710	1711	1712	rVB	294	57	0.01%	0.001%
43	6.811	1712	1717	1719	rBV2	279	193	0.03%	0.004%
44	6.827	1721	1722	1726	rBV	198	114	0.02%	0.002%
45	6.891	1736	1742	1746	rBV2	235	289	0.04%	0.005%
46	6.910	1746	1748	1753	rVV2	180	142	0.02%	0.003%
47	6.965	1762	1765	1767	rBV2	133	83	0.01%	0.002%
48	6.991	1771	1773	1777	rVB2	171	109	0.02%	0.002%
49	7.097	1797	1806	1808	rBV2	262	346	0.05%	0.006%
50	7.222	1834	1845	1848	rBV5	1092	1726	0.26%	0.032%
51	7.274	1858	1861	1862	rBV	275	176	0.03%	0.003%
52	7.309	1869	1872	1873	rBV	153	85	0.01%	0.002%
53	7.354	1882	1886	1888	rBV	258	197	0.03%	0.004%
54	7.402	1898	1901	1903	rBV	168	115	0.02%	0.002%
55	7.563	1940	1951	1971	rBV	71511	127181	19.27%	2.365%
56	7.676	1983	1986	1992	rBV2	296	322	0.05%	0.006%
57	7.704	1992	1995	1996	rBV2	243	116	0.02%	0.002%
58	7.798	2018	2024	2028	rBV3	393	468	0.07%	0.009%
59	7.891	2041	2053	2072	rBV	259005	452034	68.50%	8.407%
60	8.177	2132	2142	2158	rBV	48923	86132	13.05%	1.602%
61	8.290	2174	2177	2179	rBV	164	89	0.01%	0.002%
62	8.409	2210	2214	2217	rBV2	199	183	0.03%	0.003%
63	8.470	2225	2233	2234	rBV	407	607	0.09%	0.011%
64	8.550	2249	2258	2271	rBV	12521	20966	3.18%	0.390%
65	8.637	2274	2285	2316	rBV	185723	379471	57.50%	7.057%
66	8.875	2356	2359	2361	rVB2	309	189	0.03%	0.004%
67	8.888	2361	2363	2366	rVB2	299	170	0.03%	0.003%
68	8.930	2366	2376	2381	rBV2	726	937	0.14%	0.017%
69	8.968	2386	2388	2389	rBV	298	100	0.02%	0.002%
70	8.978	2389	2391	2398	rBV	226	196	0.03%	0.004%
71	9.058	2410	2416	2419	rBV2	312	368	0.06%	0.007%
72	9.077	2419	2422	2426	rVV2	387	275	0.04%	0.005%
73	9.177	2450	2453	2456	rBV2	247	151	0.02%	0.003%
74	9.270	2477	2482	2487	rVB2	207	231	0.04%	0.004%
75	9.299	2487	2491	2499	rVB2	258	278	0.04%	0.005%
76	9.338	2499	2503	2504	rBV2	141	94	0.01%	0.002%

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77	9.348	2504	2506	2512	rVB	271	211	0.03%	0.004%
78	9.415	2512	2527	2545	rBV	386026	659929	100.00%	12.273%
79	9.569	2571	2575	2582	rBV4	779	1096	0.17%	0.020%
80	9.630	2593	2594	2599	rBV2	163	114	0.02%	0.002%
81	9.701	2608	2616	2627	rVB4	1420	2376	0.36%	0.044%
82	9.875	2667	2670	2672	rBV	135	99	0.02%	0.002%
83	9.891	2672	2675	2677	rVV	173	101	0.02%	0.002%
84	9.936	2687	2689	2695	rVB2	266	154	0.02%	0.003%
85	9.984	2700	2704	2706	rBV2	374	298	0.05%	0.006%
86	10.100	2730	2740	2741	rBV2	457	570	0.09%	0.011%
87	10.148	2754	2755	2756	rBV2	156	53	0.01%	0.001%
88	10.405	2832	2835	2838	rBV	196	137	0.02%	0.003%
89	10.756	2932	2944	2969	rVB	260028	422211	63.98%	7.852%
90	10.891	2979	2986	2995	rBV4	2278	3397	0.51%	0.063%
91	11.064	3037	3040	3042	rVB2	161	80	0.01%	0.001%
92	11.084	3042	3046	3049	rBV	362	305	0.05%	0.006%
93	11.126	3056	3059	3062	rBV2	255	189	0.03%	0.004%
94	11.460	3160	3163	3165	rBV2	335	225	0.03%	0.004%
95	11.592	3201	3204	3210	rBV2	212	209	0.03%	0.004%
96	11.810	3260	3272	3300	rBV	407324	658669	99.81%	12.250%
97	12.061	3348	3350	3354	rVB2	264	154	0.02%	0.003%
98	12.193	3378	3391	3411	rBV	297091	486096	73.66%	9.040%
99	12.646	3528	3532	3536	rBV2	360	293	0.04%	0.005%
100	13.627	3828	3837	3845	rVB5	1167	2141	0.32%	0.040%

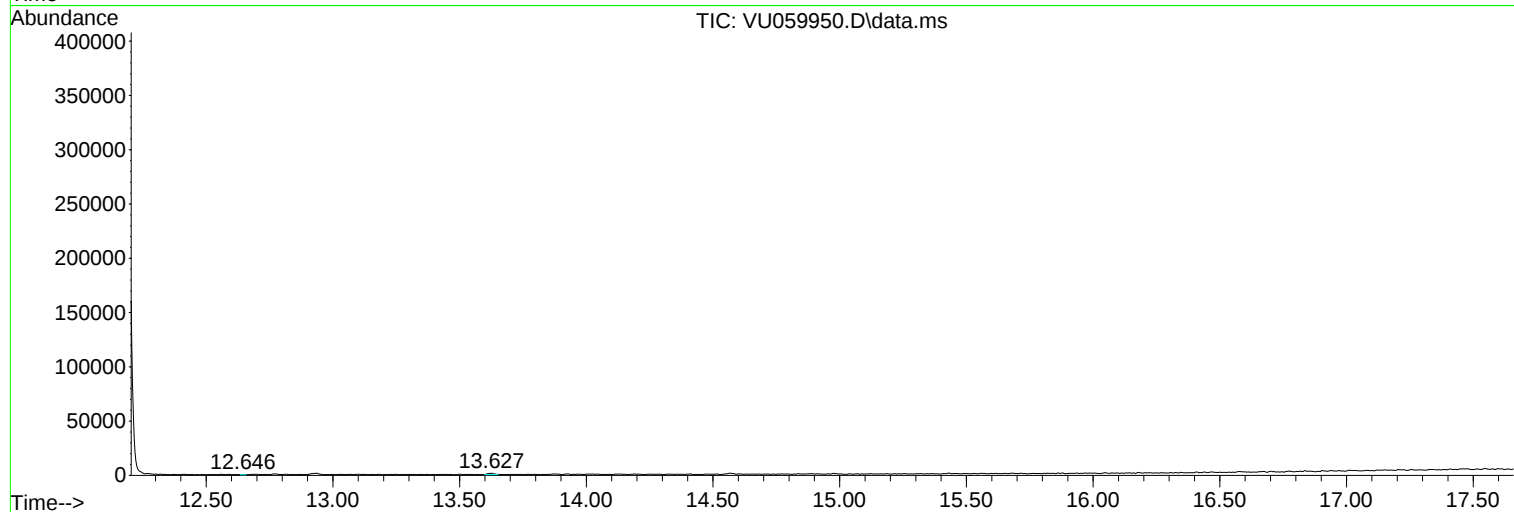
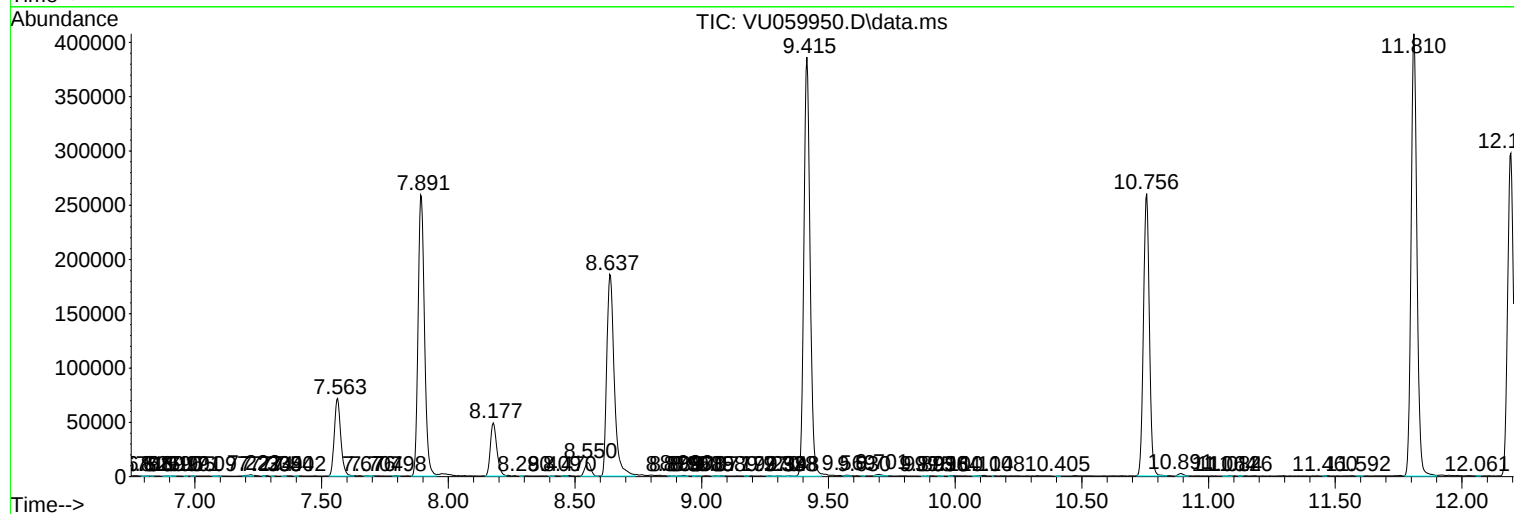
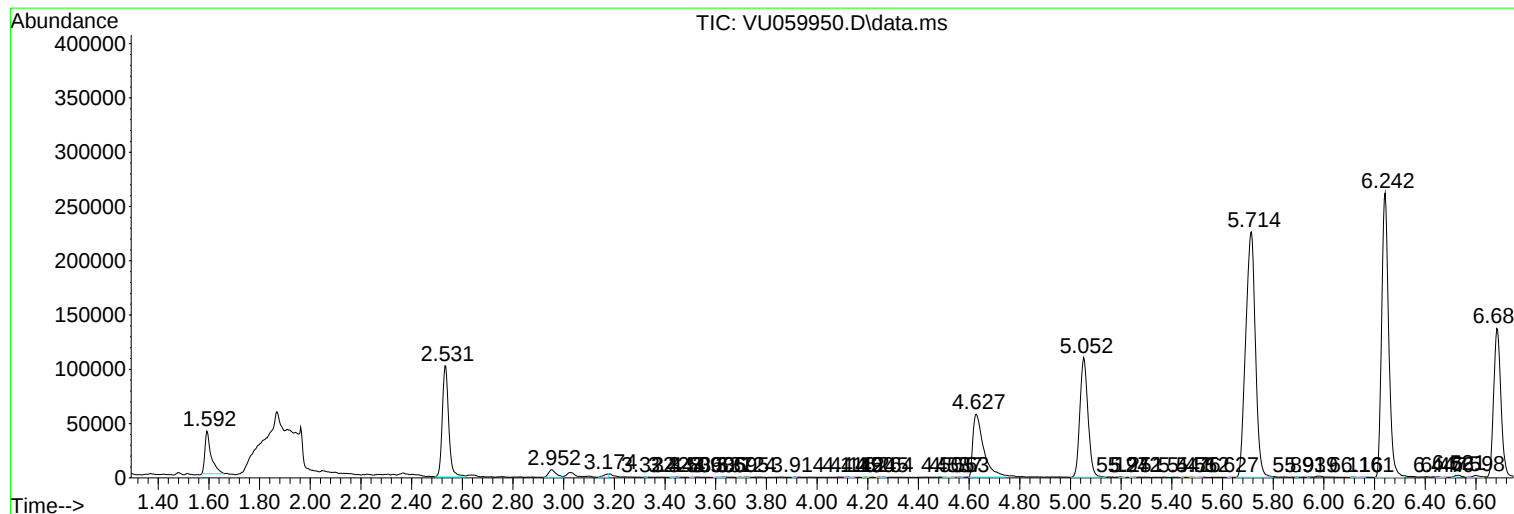
Sum of corrected areas: 5376876

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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



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