

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059954.D
 Acq On : 15 Jul 2024 16:18
 Operator : MD/SY
 Sample : P3230-10ME
 Misc : 5.26g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB49ME

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: VU059954.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	113	rBV	36293	60395	8.96%	1.124%
2	2.528	374	385	408	rBV	99347	170446	25.29%	3.171%
3	2.956	514	518	520	rBV2	393	345	0.05%	0.006%
4	3.075	552	555	557	rBV	225	125	0.02%	0.002%
5	3.316	627	630	631	rBV	128	75	0.01%	0.001%
6	3.936	820	823	829	rBV	280	238	0.04%	0.004%
7	3.991	837	840	843	rBV	184	128	0.02%	0.002%
8	4.026	847	851	854	rBV2	215	166	0.02%	0.003%
9	4.094	870	872	874	rBV2	121	74	0.01%	0.001%
10	4.222	909	912	914	rBV	164	79	0.01%	0.001%
11	4.238	914	917	923	rVB	234	214	0.03%	0.004%
12	4.271	924	927	930	rBV2	132	100	0.01%	0.002%
13	4.451	978	983	988	rBV2	191	269	0.04%	0.005%
14	4.518	999	1004	1007	rBV2	151	135	0.02%	0.003%
15	4.550	1012	1014	1016	rBV2	80	44	0.01%	0.001%
16	4.566	1016	1019	1021	rBV2	113	78	0.01%	0.001%
17	4.631	1029	1039	1078	rBV	61141	188633	27.98%	3.510%
18	4.988	1146	1150	1154	rBV2	292	305	0.05%	0.006%
19	5.052	1154	1170	1197	rVV	108847	242777	36.02%	4.517%
20	5.177	1207	1209	1212	rVB	265	134	0.02%	0.002%
21	5.193	1212	1214	1215	rBV	166	71	0.01%	0.001%
22	5.206	1215	1218	1219	rBV	184	109	0.02%	0.002%
23	5.383	1268	1273	1276	rBV2	227	262	0.04%	0.005%
24	5.460	1291	1297	1299	rBV	143	153	0.02%	0.003%
25	5.476	1299	1302	1304	rVV	114	60	0.01%	0.001%
26	5.489	1304	1306	1309	rVV2	199	118	0.02%	0.002%
27	5.566	1327	1330	1336	rBV2	258	232	0.03%	0.004%
28	5.644	1352	1354	1356	rBV	167	104	0.02%	0.002%
29	5.711	1357	1375	1397	rBV2	229314	599474	88.94%	11.153%
30	5.904	1432	1435	1436	rBV2	262	159	0.02%	0.003%
31	5.988	1456	1461	1465	rBV2	183	204	0.03%	0.004%
32	6.164	1514	1516	1518	rBV	84	48	0.01%	0.001%
33	6.242	1527	1540	1567	rBV	259092	512785	76.07%	9.540%
34	6.425	1595	1597	1600	rVB2	238	126	0.02%	0.002%
35	6.444	1600	1603	1604	rBV	180	84	0.01%	0.002%
36	6.476	1610	1613	1614	rBV	233	142	0.02%	0.003%

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 Title : VOC Analysis

37	6.537	1622	1632	1644	rVB8	3261	7125	1.06%	0.133%
38	6.582	1644	1646	1648	rVB	77	32	0.00%	0.001%
39	6.602	1648	1652	1656	rBV2	496	476	0.07%	0.009%
40	6.682	1664	1677	1703	rBV	140313	276222	40.98%	5.139%
41	6.798	1710	1713	1714	rBV2	297	171	0.03%	0.003%
42	6.965	1762	1765	1767	rBV	202	152	0.02%	0.003%
43	6.991	1771	1773	1775	rBV2	134	66	0.01%	0.001%
44	7.004	1775	1777	1780	rBV	290	157	0.02%	0.003%
45	7.023	1780	1783	1786	rBV	235	126	0.02%	0.002%
46	7.045	1786	1790	1794	rVB	178	132	0.02%	0.002%
47	7.094	1802	1805	1806	rBV	52	25	0.00%	0.000%
48	7.107	1806	1809	1810	rBV	75	31	0.00%	0.001%
49	7.203	1831	1839	1840	rBV2	859	872	0.13%	0.016%
50	7.361	1883	1888	1893	rBV2	263	260	0.04%	0.005%
51	7.393	1895	1898	1903	rBV2	159	141	0.02%	0.003%
52	7.476	1922	1924	1927	rVB	257	147	0.02%	0.003%
53	7.563	1940	1951	1973	rBV	69710	127073	18.85%	2.364%
54	7.669	1982	1984	1986	rBV2	211	77	0.01%	0.001%
55	7.717	1996	1999	2006	rBV2	338	369	0.05%	0.007%
56	7.785	2013	2020	2024	rBV3	435	551	0.08%	0.010%
57	7.833	2032	2035	2037	rBV2	119	70	0.01%	0.001%
58	7.891	2041	2053	2074	rBV	252933	445832	66.14%	8.295%
59	8.177	2132	2142	2162	rBV	48312	86182	12.79%	1.603%
60	8.293	2176	2178	2180	rBV	146	63	0.01%	0.001%
61	8.325	2184	2188	2190	rBV	193	142	0.02%	0.003%
62	8.460	2225	2230	2232	rBV	515	484	0.07%	0.009%
63	8.550	2247	2258	2270	rVB	35066	58416	8.67%	1.087%
64	8.640	2274	2286	2314	rBV	179448	377574	56.02%	7.025%
65	8.885	2360	2362	2364	rVB2	242	99	0.01%	0.002%
66	8.901	2364	2367	2368	rBV2	350	217	0.03%	0.004%
67	9.058	2413	2416	2419	rBV2	159	108	0.02%	0.002%
68	9.097	2424	2428	2431	rVB2	398	276	0.04%	0.005%
69	9.135	2437	2440	2442	rBV	159	100	0.01%	0.002%
70	9.245	2467	2474	2475	rBV2	176	216	0.03%	0.004%
71	9.274	2480	2483	2485	rBV	241	159	0.02%	0.003%
72	9.341	2502	2504	2506	rBV	133	77	0.01%	0.001%
73	9.415	2512	2527	2552	rBV	387087	674054	100.00%	12.541%
74	9.566	2572	2574	2577	rBV	299	168	0.02%	0.003%
75	9.627	2591	2593	2596	rBV2	275	156	0.02%	0.003%
76	9.650	2597	2600	2602	rBV2	167	100	0.01%	0.002%

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77	9.695	2609	2614	2616	rBV2	654	555	0.08%	0.010%
78	9.868	2664	2668	2670	rBV2	222	184	0.03%	0.003%
79	9.971	2697	2700	2702	rBV2	153	80	0.01%	0.001%
80	10.132	2746	2750	2755	rBV	275	255	0.04%	0.005%
81	10.438	2842	2845	2847	rBV2	135	80	0.01%	0.001%
82	10.685	2918	2922	2924	rBV	290	237	0.04%	0.004%
83	10.756	2931	2944	2961	rBV	253987	419505	62.24%	7.805%
84	10.971	3007	3011	3013	rBV	293	174	0.03%	0.003%
85	11.190	3076	3079	3080	rBV	217	129	0.02%	0.002%
86	11.232	3089	3092	3094	rBV2	211	147	0.02%	0.003%
87	11.811	3260	3272	3294	rBV	401308	643833	95.52%	11.979%
88	12.045	3341	3345	3350	rBV2	389	382	0.06%	0.007%
89	12.193	3378	3391	3412	rBV	284977	471185	69.90%	8.767%
90	12.373	3445	3447	3448	rBV	278	132	0.02%	0.002%
91	12.704	3547	3550	3552	rBV	259	163	0.02%	0.003%
92	12.743	3559	3562	3564	rBV	265	196	0.03%	0.004%

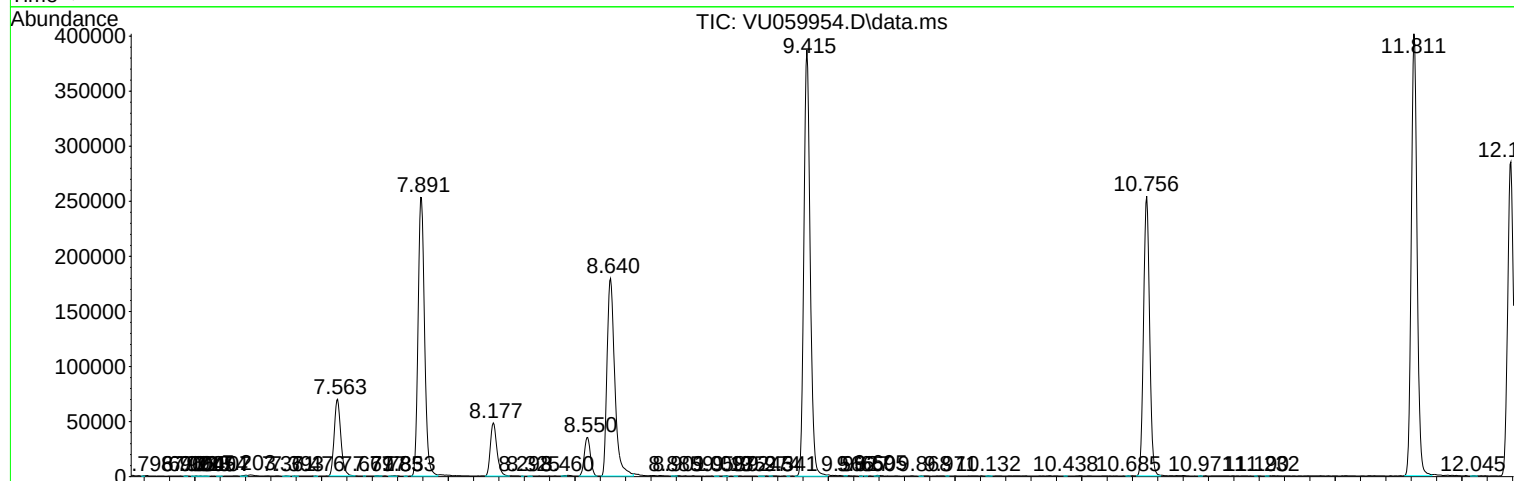
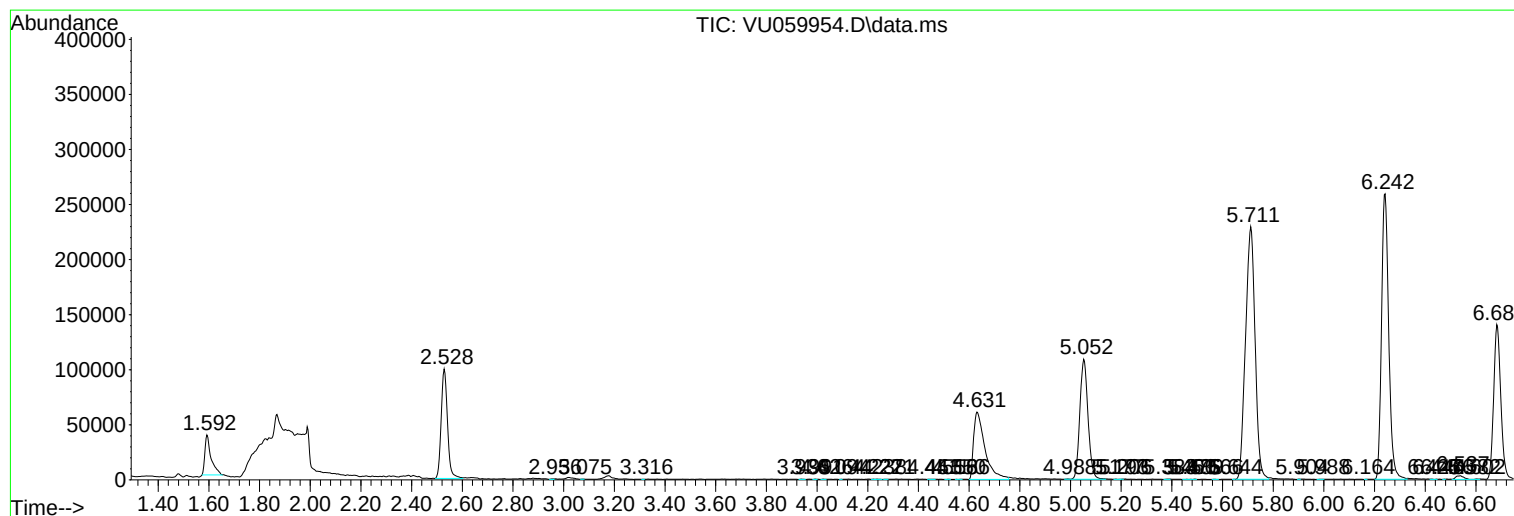
Sum of corrected areas: 5374826

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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	--Internal Standard--			
					#	RT	Resp	Conc