

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058976.D
 Acq On : 24 May 2024 17:20
 Operator : MD/SY
 Sample : P2547-16ME
 Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5X3ME

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\SFAMULM052324WMA.M
 Title : VOC Analysis

Signal : TIC: VU058976.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	87	94	120	rVB	68828	120157	13.95%	1.942%
2	2.531	375	386	398	rBV	163110	263834	30.63%	4.265%
3	3.023	532	539	555	rVB3	7370	13915	1.62%	0.225%
4	3.419	660	662	664	rBV2	161	49	0.01%	0.001%
5	3.448	668	671	674	rVB	309	174	0.02%	0.003%
6	3.473	674	679	684	rVB2	386	361	0.04%	0.006%
7	3.499	684	687	688	rBV2	152	97	0.01%	0.002%
8	3.624	723	726	728	rBV2	151	76	0.01%	0.001%
9	3.676	737	742	748	rBV3	449	528	0.06%	0.009%
10	3.721	753	756	758	rBV	216	161	0.02%	0.003%
11	3.795	773	779	781	rBV2	230	219	0.03%	0.004%
12	3.817	784	786	789	rVV2	134	76	0.01%	0.001%
13	3.859	796	799	801	rBV	133	76	0.01%	0.001%
14	3.914	813	816	823	rBV2	258	238	0.03%	0.004%
15	3.962	827	831	832	rBV2	288	154	0.02%	0.002%
16	4.103	871	875	878	rBV2	282	217	0.03%	0.004%
17	4.158	890	892	894	rBV	103	49	0.01%	0.001%
18	4.177	894	898	900	rBV2	211	168	0.02%	0.003%
19	4.280	927	930	934	rVB2	206	162	0.02%	0.003%
20	4.306	934	938	940	rBV	259	156	0.02%	0.003%
21	4.492	994	996	998	rBV	102	49	0.01%	0.001%
22	4.512	998	1002	1003	rBV2	196	131	0.02%	0.002%
23	4.624	1026	1037	1075	rBV2	70125	228068	26.48%	3.687%
24	5.052	1148	1170	1191	rBV	145148	332461	38.60%	5.374%
25	5.171	1206	1207	1209	rVB	137	28	0.00%	0.000%
26	5.190	1209	1213	1215	rBV	314	218	0.03%	0.004%
27	5.203	1215	1217	1218	rVV	146	39	0.00%	0.001%
28	5.303	1242	1248	1252	rBV2	232	287	0.03%	0.005%
29	5.348	1259	1262	1264	rBV	191	138	0.02%	0.002%
30	5.467	1297	1299	1301	rVB2	82	33	0.00%	0.001%
31	5.489	1301	1306	1310	rBV2	379	404	0.05%	0.007%
32	5.563	1324	1329	1331	rBV	255	224	0.03%	0.004%
33	5.605	1339	1342	1344	rBV	139	82	0.01%	0.001%
34	5.711	1355	1375	1404	rBV2	327805	861326	100.00%	13.924%
35	5.978	1448	1458	1473	rBV5	2813	6801	0.79%	0.110%
36	6.033	1473	1475	1478	rVB	643	353	0.04%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

37	6.049	1478	1480	1482	rBV2	143	78	0.01%	0.001%
38	6.065	1483	1485	1486	rBV	259	97	0.01%	0.002%
39	6.123	1496	1503	1505	rBV2	284	299	0.03%	0.005%
40	6.238	1526	1539	1558	rBV	235959	463963	53.87%	7.500%
41	6.476	1611	1613	1618	rBV2	195	114	0.01%	0.002%
42	6.531	1618	1630	1642	rBV8	7956	17956	2.08%	0.290%
43	6.595	1643	1650	1662	rVV3	3827	7365	0.86%	0.119%
44	6.682	1664	1677	1702	rVB	194224	394272	45.78%	6.374%
45	6.811	1714	1717	1719	rVB	297	158	0.02%	0.003%
46	6.824	1719	1721	1722	rBV	228	82	0.01%	0.001%
47	6.869	1730	1735	1737	rBV2	244	220	0.03%	0.004%
48	6.888	1737	1741	1744	rBV2	223	230	0.03%	0.004%
49	7.033	1783	1786	1789	rBV2	150	106	0.01%	0.002%
50	7.081	1798	1801	1805	rVB2	199	142	0.02%	0.002%
51	7.107	1805	1809	1812	rBV2	249	171	0.02%	0.003%
52	7.145	1817	1821	1824	rBV	150	108	0.01%	0.002%
53	7.213	1831	1842	1843	rBV4	910	1182	0.14%	0.019%
54	7.290	1864	1866	1868	rBV2	190	70	0.01%	0.001%
55	7.364	1887	1889	1894	rVB2	166	103	0.01%	0.002%
56	7.399	1897	1900	1903	rVB	220	125	0.01%	0.002%
57	7.434	1906	1911	1913	rVB3	228	193	0.02%	0.003%
58	7.479	1920	1925	1926	rBV	417	243	0.03%	0.004%
59	7.560	1938	1950	1972	rBV	96170	176159	20.45%	2.848%
60	7.750	2007	2009	2011	rBV	149	66	0.01%	0.001%
61	7.782	2015	2019	2021	rBV3	478	385	0.04%	0.006%
62	7.891	2040	2053	2074	rBV	356788	629976	73.14%	10.184%
63	8.061	2104	2106	2108	rVB2	351	139	0.02%	0.002%
64	8.087	2112	2114	2117	rVB	305	166	0.02%	0.003%
65	8.113	2119	2122	2123	rBV2	236	119	0.01%	0.002%
66	8.174	2131	2141	2160	rBV	63304	120467	13.99%	1.947%
67	8.319	2184	2186	2189	rBV	153	69	0.01%	0.001%
68	8.348	2193	2195	2201	rVB2	528	465	0.05%	0.008%
69	8.377	2201	2204	2205	rBV	188	100	0.01%	0.002%
70	8.467	2225	2232	2235	rBV2	765	936	0.11%	0.015%
71	8.566	2261	2263	2265	rBV2	111	64	0.01%	0.001%
72	8.640	2273	2286	2319	rBV	187660	472122	54.81%	7.632%
73	9.071	2417	2420	2421	rBV	162	103	0.01%	0.002%
74	9.084	2422	2424	2425	rBV	228	85	0.01%	0.001%
75	9.248	2472	2475	2477	rBV	209	167	0.02%	0.003%
76	9.328	2497	2500	2502	rBV2	272	158	0.02%	0.003%

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77	9.415	2513	2527	2560	rBV	332370	583474	67.74%	9.432%
78	9.698	2603	2615	2624	rBV6	2005	3996	0.46%	0.065%
79	9.753	2631	2632	2633	rBV6	145	44	0.01%	0.001%
80	9.955	2691	2695	2696	rBV	210	147	0.02%	0.002%
81	9.997	2703	2708	2710	rBV2	178	193	0.02%	0.003%
82	10.132	2748	2750	2755	rVB2	306	242	0.03%	0.004%
83	10.167	2759	2761	2766	rVB3	226	116	0.01%	0.002%
84	10.261	2787	2790	2791	rBV	240	154	0.02%	0.002%
85	10.669	2916	2917	2919	rBV	154	60	0.01%	0.001%
86	10.756	2931	2944	2963	rBV	273996	466575	54.17%	7.543%
87	11.460	3160	3163	3165	rBV2	226	156	0.02%	0.003%
88	11.811	3260	3272	3291	rBV	303094	494756	57.44%	7.998%
89	12.190	3378	3390	3409	rBV	311588	515501	59.85%	8.333%

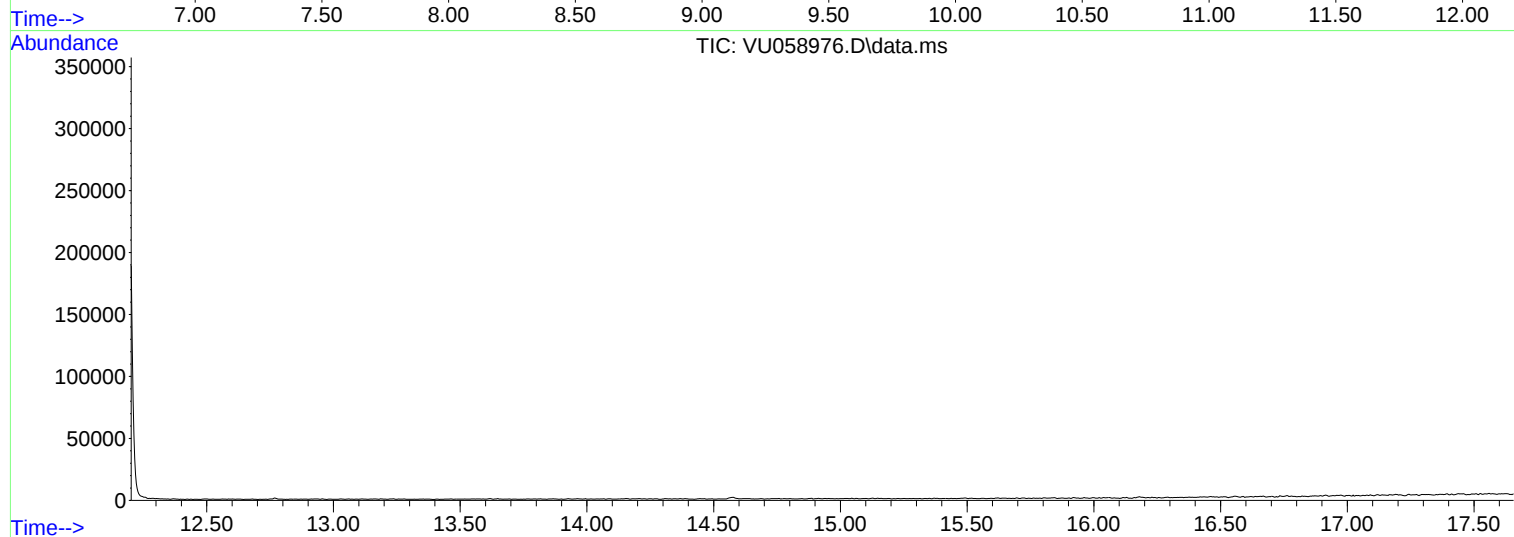
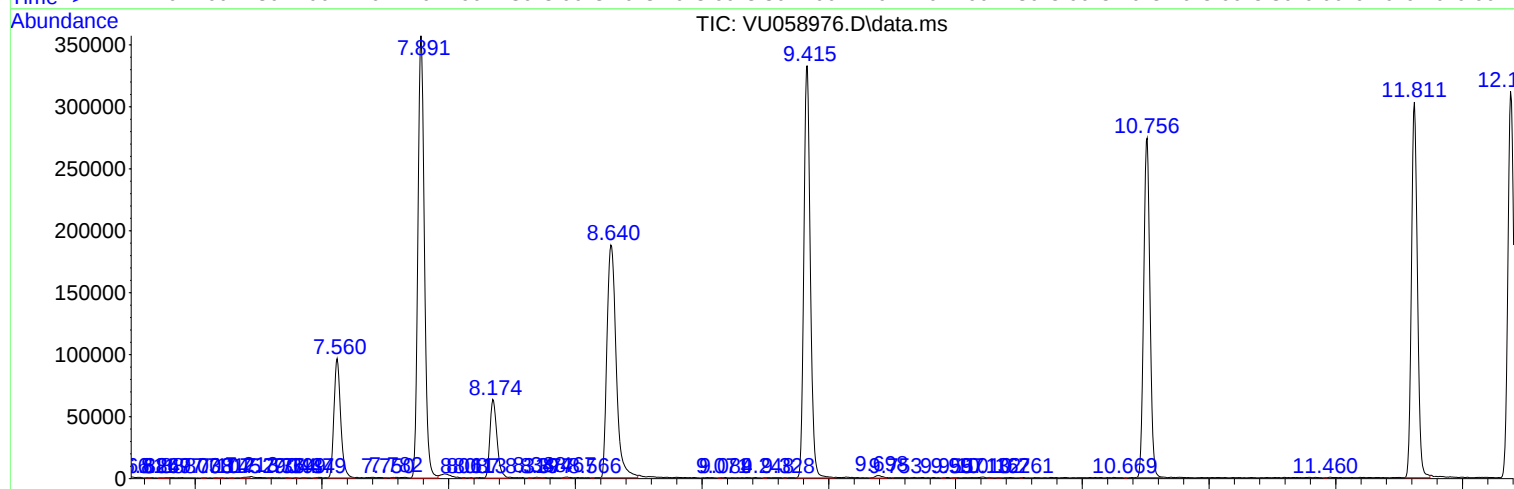
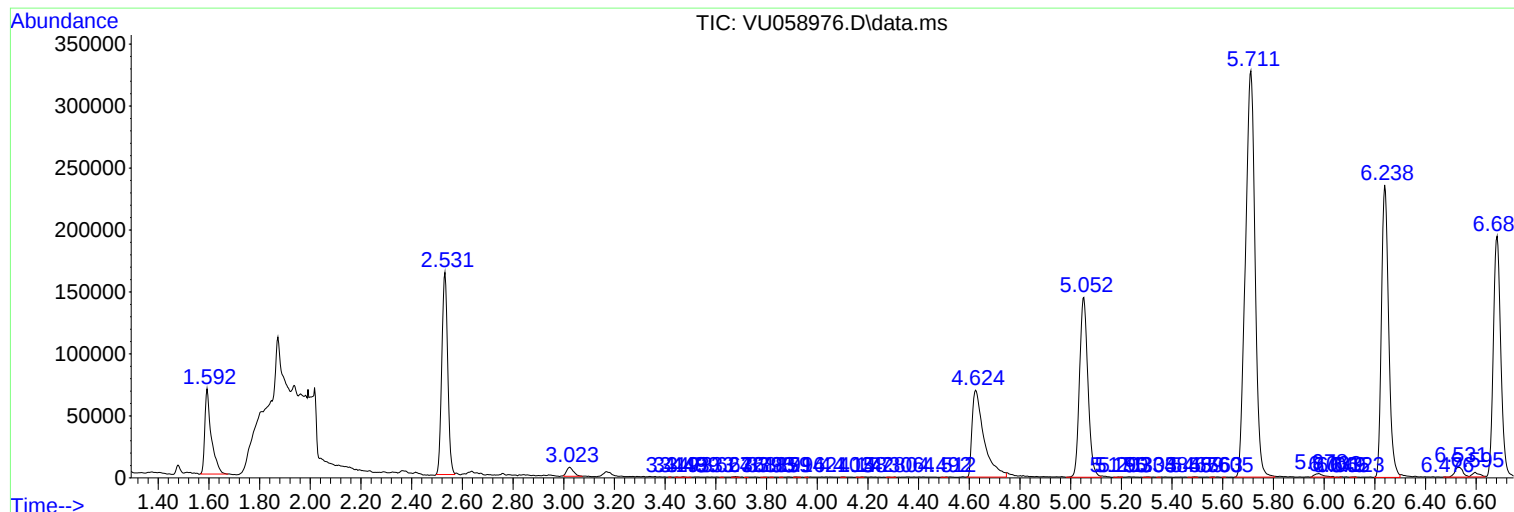
Sum of corrected areas: 6185946

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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\SFAMULM052324WMA.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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