

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062624\
 Data File : VU059531.D
 Acq On : 26 Jun 2024 18:03
 Operator : MD/SY
 Sample : P2987-04ME
 Misc : 4.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COT88ME

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: VU059531.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	40333	74605	12.35%	1.544%
2	2.531	376	386	403	rVB	109179	182010	30.13%	3.766%
3	2.827	476	478	482	rBV2	400	192	0.03%	0.004%
4	3.027	530	540	549	rBV3	5041	10517	1.74%	0.218%
5	3.165	577	583	597	rBV4	897	2176	0.36%	0.045%
6	3.248	605	609	611	rBV2	274	177	0.03%	0.004%
7	3.435	663	667	673	rBV2	216	262	0.04%	0.005%
8	3.670	730	740	744	rBV3	640	995	0.16%	0.021%
9	3.686	744	745	749	rVV2	315	146	0.02%	0.003%
10	3.718	753	755	758	rBV	151	104	0.02%	0.002%
11	3.898	808	811	815	rVB2	195	157	0.03%	0.003%
12	4.017	847	848	850	rVB	202	74	0.01%	0.002%
13	4.091	868	871	877	rBV2	108	107	0.02%	0.002%
14	4.120	877	880	883	rBV2	182	126	0.02%	0.003%
15	4.219	906	911	913	rBV2	136	159	0.03%	0.003%
16	4.303	935	937	943	rVB	209	173	0.03%	0.004%
17	4.416	968	972	975	rBV2	145	137	0.02%	0.003%
18	4.464	984	987	991	rBV2	123	104	0.02%	0.002%
19	4.625	1028	1037	1077	rBV	46058	144013	23.84%	2.980%
20	4.978	1144	1147	1149	rVB2	257	126	0.02%	0.003%
21	4.994	1150	1152	1154	rVB	515	168	0.03%	0.003%
22	5.052	1154	1170	1194	rBV	97846	222466	36.83%	4.604%
23	5.194	1210	1214	1216	rVB2	343	205	0.03%	0.004%
24	5.242	1225	1229	1231	rBV2	209	146	0.02%	0.003%
25	5.364	1264	1267	1270	rVB	141	79	0.01%	0.002%
26	5.396	1275	1277	1279	rBV	122	78	0.01%	0.002%
27	5.480	1298	1303	1306	rBV2	242	280	0.05%	0.006%
28	5.528	1315	1318	1320	rBV2	280	186	0.03%	0.004%
29	5.644	1350	1354	1356	rBV2	119	82	0.01%	0.002%
30	5.711	1356	1375	1403	rBV2	215292	567984	94.02%	11.754%
31	5.914	1436	1438	1441	rVB	273	180	0.03%	0.004%
32	5.933	1441	1444	1445	rBV	184	106	0.02%	0.002%
33	5.975	1449	1457	1458	rBV4	1511	1523	0.25%	0.032%
34	6.039	1475	1477	1479	rBV	254	114	0.02%	0.002%
35	6.174	1514	1519	1525	rBV2	260	317	0.05%	0.007%
36	6.239	1527	1539	1566	rBV	238150	472614	78.23%	9.780%

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 Title : VOC Analysis

37	6.406	1589	1591	1595	rVB3	375	233	0.04%	0.005%
38	6.496	1616	1619	1621	rBV2	195	116	0.02%	0.002%
39	6.525	1621	1628	1640	rVB9	2357	4352	0.72%	0.090%
40	6.596	1640	1650	1663	rBV4	2592	5380	0.89%	0.111%
41	6.682	1664	1677	1704	rVV2	126801	253152	41.91%	5.239%
42	6.776	1704	1706	1710	rVB2	297	170	0.03%	0.004%
43	6.798	1710	1713	1715	rBV	232	148	0.02%	0.003%
44	6.866	1730	1734	1738	rBV2	154	169	0.03%	0.003%
45	6.901	1742	1745	1749	rBV	202	141	0.02%	0.003%
46	6.923	1749	1752	1755	rBV2	139	94	0.02%	0.002%
47	7.187	1831	1834	1835	rBV2	378	223	0.04%	0.005%
48	7.258	1854	1856	1861	rBV2	232	229	0.04%	0.005%
49	7.316	1871	1874	1875	rBV	181	84	0.01%	0.002%
50	7.428	1905	1909	1912	rBV	165	141	0.02%	0.003%
51	7.470	1919	1922	1924	rBV	168	139	0.02%	0.003%
52	7.560	1938	1950	1967	rBV	66359	118896	19.68%	2.460%
53	7.743	2004	2007	2011	rVB3	200	165	0.03%	0.003%
54	7.772	2011	2016	2018	rBV	118	129	0.02%	0.003%
55	7.891	2040	2053	2073	rBV	243101	427730	70.80%	8.851%
56	8.068	2104	2108	2111	rVB2	351	264	0.04%	0.005%
57	8.087	2111	2114	2119	rBV2	245	269	0.04%	0.006%
58	8.113	2119	2122	2126	rVB2	205	151	0.02%	0.003%
59	8.139	2126	2130	2131	rBV	174	98	0.02%	0.002%
60	8.174	2131	2141	2157	rVV	44046	79785	13.21%	1.651%
61	8.232	2157	2159	2163	rVB2	506	294	0.05%	0.006%
62	8.345	2191	2194	2201	rVB3	379	401	0.07%	0.008%
63	8.412	2212	2215	2218	rVB	180	112	0.02%	0.002%
64	8.464	2225	2231	2237	rBV2	342	579	0.10%	0.012%
65	8.518	2243	2248	2251	rBV2	187	160	0.03%	0.003%
66	8.541	2251	2255	2257	rBV2	138	106	0.02%	0.002%
67	8.570	2261	2264	2265	rBV	165	105	0.02%	0.002%
68	8.637	2273	2285	2319	rBV	141462	311958	51.64%	6.456%
69	8.878	2358	2360	2362	rBV2	185	108	0.02%	0.002%
70	8.936	2376	2378	2383	rVB2	195	147	0.02%	0.003%
71	9.412	2513	2526	2553	rBV	348648	604101	100.00%	12.501%
72	10.226	2772	2779	2782	rBV2	396	412	0.07%	0.009%
73	10.290	2793	2799	2801	rBV	295	269	0.04%	0.006%
74	10.332	2808	2812	2816	rBV2	173	167	0.03%	0.003%
75	10.354	2816	2819	2821	rVV	220	117	0.02%	0.002%
76	10.547	2877	2879	2882	rBV2	193	134	0.02%	0.003%

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77	10.595	2891	2894	2895	rBV	158	100	0.02%	0.002%
78	10.621	2897	2902	2908	rVB2	845	1078	0.18%	0.022%
79	10.650	2908	2911	2913	rBV	234	173	0.03%	0.004%
80	10.753	2930	2943	2962	rBV	206692	347279	57.49%	7.186%
81	10.878	2978	2982	2983	rBV	365	251	0.04%	0.005%
82	10.959	3004	3007	3010	rBV2	227	174	0.03%	0.004%
83	11.052	3034	3036	3038	rBV	335	198	0.03%	0.004%
84	11.254	3096	3099	3101	rBV2	279	202	0.03%	0.004%
85	11.312	3113	3117	3125	rVB4	628	786	0.13%	0.016%
86	11.341	3125	3126	3130	rBV	197	134	0.02%	0.003%
87	11.361	3130	3132	3135	rVV2	394	250	0.04%	0.005%
88	11.377	3135	3137	3139	rVV2	576	391	0.06%	0.008%
89	11.409	3141	3147	3157	rVB4	4048	5814	0.96%	0.120%
90	11.470	3164	3166	3168	rBV2	314	171	0.03%	0.004%
91	11.570	3195	3197	3202	rBV3	300	187	0.03%	0.004%
92	11.698	3234	3237	3238	rBV	335	202	0.03%	0.004%
93	11.759	3254	3256	3258	rVB	337	141	0.02%	0.003%
94	11.808	3258	3271	3289	rBV	347229	562672	93.14%	11.644%
95	12.026	3335	3339	3344	rBV2	334	417	0.07%	0.009%
96	12.190	3377	3390	3421	rBV	255244	416688	68.98%	8.623%
97	12.505	3486	3488	3491	rBV2	269	157	0.03%	0.003%
98	12.952	3625	3627	3629	rBV	288	136	0.02%	0.003%
99	13.361	3751	3754	3759	rBV2	363	266	0.04%	0.006%
100	14.100	3982	3984	3986	rBV	384	234	0.04%	0.005%

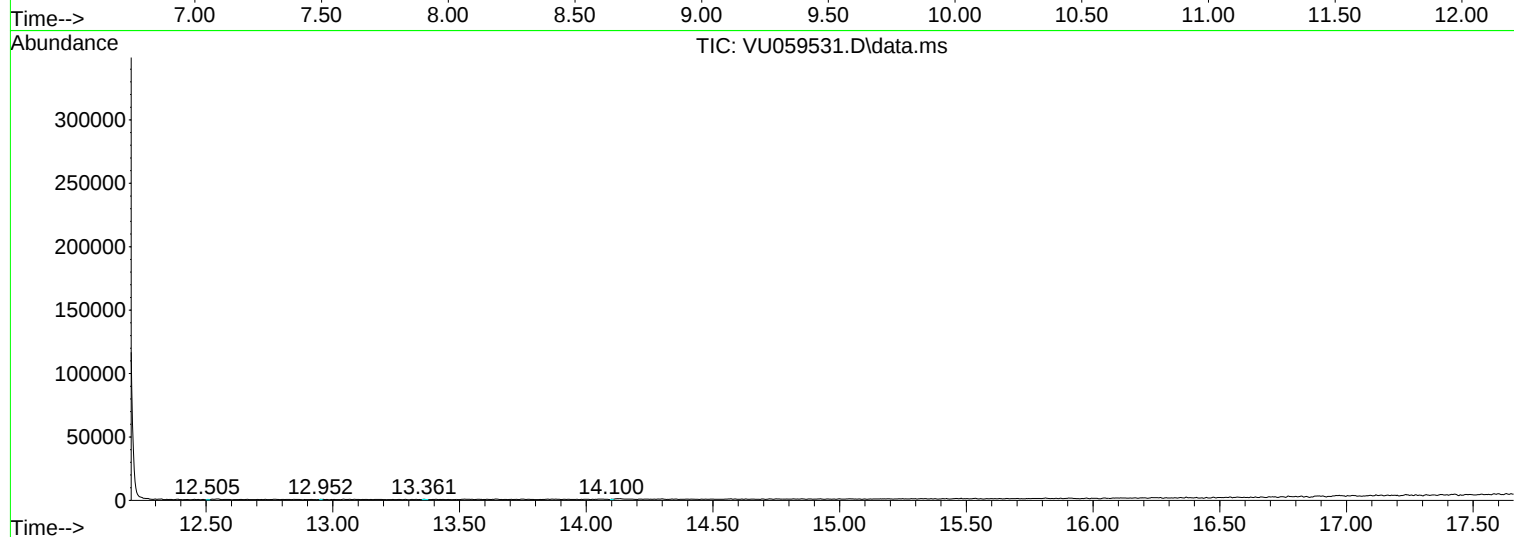
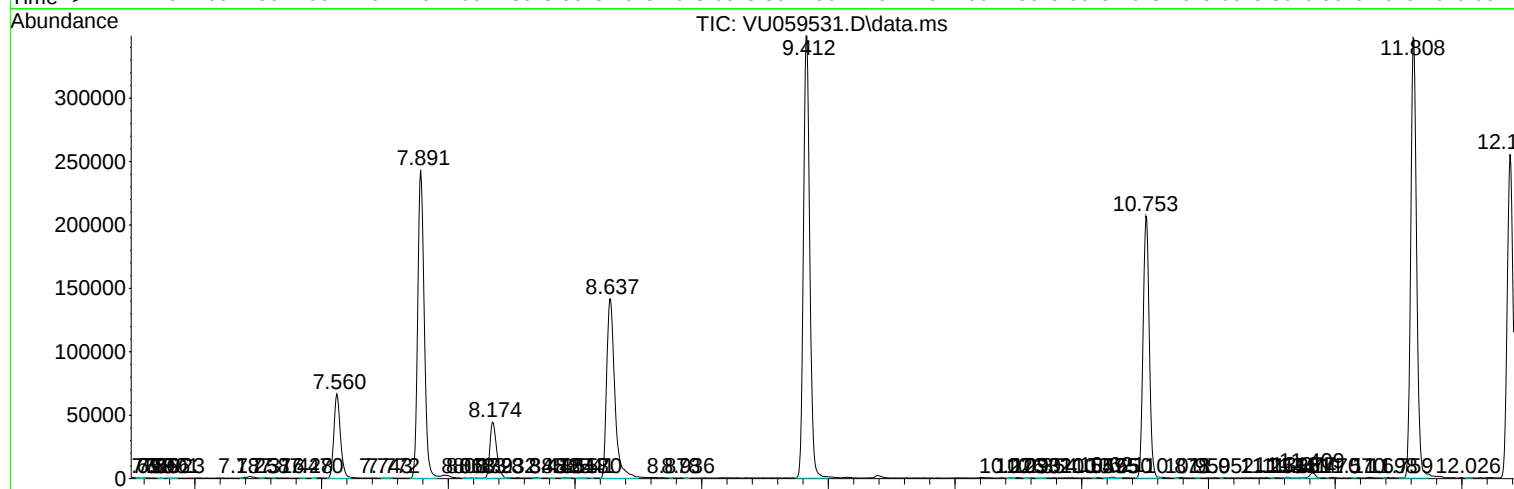
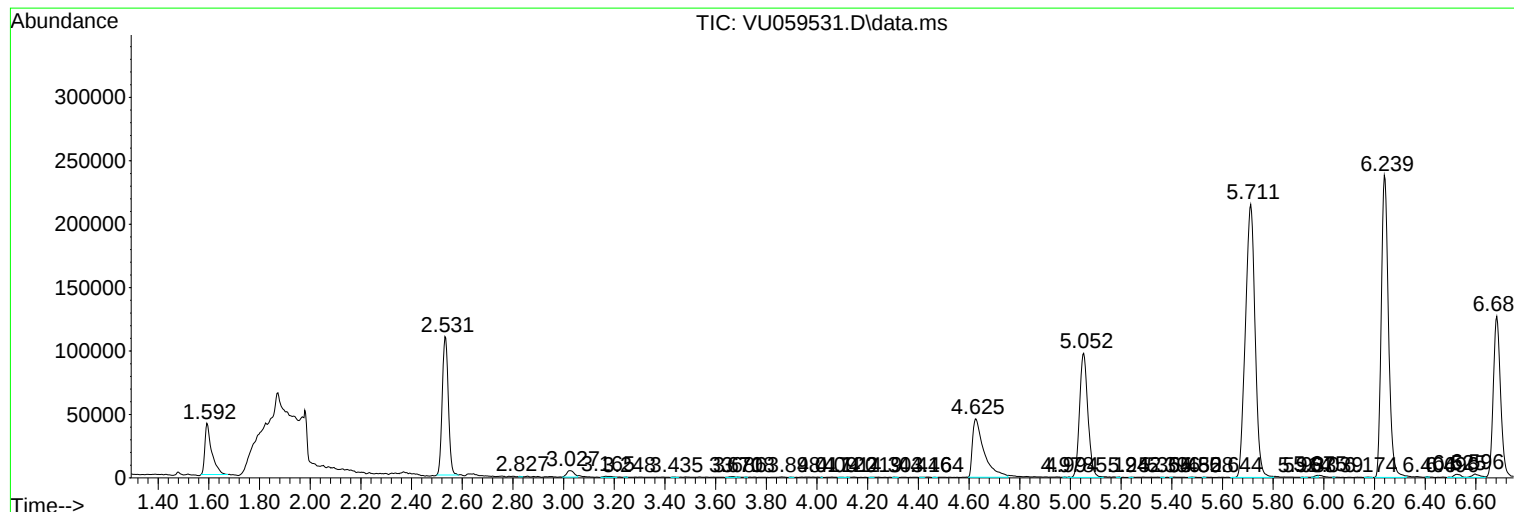
Sum of corrected areas: 4832417

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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 :
MSVOA_U
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C0T88ME

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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