

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072322\
 Data File : VV026926.D
 Acq On : 23 Jul 2022 16:50
 Operator : SY/MD
 Sample : N3766-06ME
 Misc : 6.15g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0ZD1ME

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_V\Method\SFAMVLM072222WMA.M
 Title : VOC Analysis

Signal : TIC: VV026926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.207	48	52	58	rBV	9195	9062	0.32%	0.039%
2	1.301	74	81	88	rBV	181359	211413	7.50%	0.901%
3	1.558	155	161	169	rBV	102560	123097	4.37%	0.525%
4	2.079	312	323	340	rVB	568850	810564	28.74%	3.455%
5	2.494	444	452	465	rVB3	14667	28089	1.00%	0.120%
6	2.609	480	488	501	rVB4	4317	9262	0.33%	0.039%
7	2.715	518	521	523	rVV2	1179	855	0.03%	0.004%
8	2.735	523	527	538	rVB8	3142	4909	0.17%	0.021%
9	2.809	548	550	554	rVB3	642	471	0.02%	0.002%
10	2.834	554	558	560	rBV2	451	342	0.01%	0.001%
11	2.934	586	589	595	rBV4	585	666	0.02%	0.003%
12	3.011	605	613	615	rBV3	3503	3925	0.14%	0.017%
13	3.101	637	641	644	rBV2	425	340	0.01%	0.001%
14	3.124	644	648	654	rBV2	332	414	0.01%	0.002%
15	3.670	811	818	820	rBV2	428	538	0.02%	0.002%
16	3.725	832	835	836	rBV2	636	371	0.01%	0.002%
17	3.899	877	889	950	rBV	175901	767718	27.22%	3.273%
18	4.339	1009	1026	1056	rBV	447601	1133967	40.21%	4.834%
19	4.567	1092	1097	1100	rBV4	496	463	0.02%	0.002%
20	4.590	1100	1104	1106	rBV4	722	616	0.02%	0.003%
21	4.651	1116	1123	1124	rBV4	1744	1925	0.07%	0.008%
22	4.738	1146	1150	1152	rBV4	749	534	0.02%	0.002%
23	4.792	1162	1167	1174	rVB5	597	756	0.03%	0.003%
24	4.863	1183	1189	1190	rBV3	473	425	0.02%	0.002%
25	4.883	1192	1195	1196	rBV2	853	483	0.02%	0.002%
26	4.899	1197	1200	1209	rVB5	1384	1461	0.05%	0.006%
27	5.034	1223	1242	1277	rBV2	1145914	2820035	100.00%	12.022%
28	5.249	1307	1309	1312	rVB3	964	488	0.02%	0.002%
29	5.333	1325	1335	1357	rBV6	12588	35385	1.25%	0.151%
30	5.477	1375	1380	1395	rVB8	3502	7532	0.27%	0.032%
31	5.548	1399	1402	1404	rBV3	1075	734	0.03%	0.003%
32	5.609	1408	1421	1456	rBV	794567	1640734	58.18%	6.994%
33	5.908	1501	1514	1532	rBV2	189478	399361	14.16%	1.702%
34	6.063	1549	1562	1597	rVB	618774	1326436	47.04%	5.655%
35	6.329	1640	1645	1648	rBV5	1221	1438	0.05%	0.006%
36	6.400	1663	1667	1672	rVB5	710	844	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072222WMA.M
 Title : VOC Analysis

37	6.493	1693	1696	1699	rVB3	579	438	0.02%	0.002%
38	6.574	1718	1721	1726	rVB2	534	439	0.02%	0.002%
39	6.599	1726	1729	1730	rBV2	800	428	0.02%	0.002%
40	6.638	1730	1741	1742	rBV5	6495	9063	0.32%	0.039%
41	6.796	1786	1790	1793	rBV5	715	475	0.02%	0.002%
42	6.808	1793	1794	1799	rVB3	547	399	0.01%	0.002%
43	6.828	1799	1800	1806	rBV3	704	670	0.02%	0.003%
44	6.915	1819	1827	1836	rBV8	3226	6322	0.22%	0.027%
45	6.982	1836	1848	1872	rBV	277790	533154	18.91%	2.273%
46	7.136	1894	1896	1900	rVB	795	508	0.02%	0.002%
47	7.239	1920	1928	1938	rBV3	16089	35297	1.25%	0.150%
48	7.310	1939	1950	1965	rVV	1195141	2104474	74.63%	8.971%
49	7.387	1966	1974	2007	rVB	163499	339461	12.04%	1.447%
50	7.567	2023	2030	2037	rVB8	5148	7760	0.28%	0.033%
51	7.619	2037	2046	2069	rBV	192841	365037	12.94%	1.556%
52	7.776	2092	2095	2096	rBV3	1687	963	0.03%	0.004%
53	7.789	2096	2099	2106	rVB6	2690	2973	0.11%	0.013%
54	7.834	2111	2113	2121	rVB8	953	728	0.03%	0.003%
55	7.972	2146	2156	2175	rVB	74456	130267	4.62%	0.555%
56	8.095	2182	2194	2232	rBV	458267	1466491	52.00%	6.252%
57	8.574	2333	2343	2346	rBV9	2783	4732	0.17%	0.020%
58	8.664	2363	2371	2382	rVB6	6807	11948	0.42%	0.051%
59	8.786	2402	2409	2417	rVB4	4340	6626	0.23%	0.028%
60	8.850	2417	2429	2453	rBV	1192335	2042532	72.43%	8.707%
61	9.017	2472	2481	2497	rVB	27589	48856	1.73%	0.208%
62	9.136	2507	2518	2532	rBV	243516	411542	14.59%	1.754%
63	9.320	2574	2575	2579	rVB3	1095	620	0.02%	0.003%
64	9.445	2610	2614	2615	rBV2	836	542	0.02%	0.002%
65	9.468	2615	2621	2634	rVB2	3833	6442	0.23%	0.027%
66	9.545	2634	2645	2668	rBV	183046	314740	11.16%	1.342%
67	9.709	2690	2696	2705	rVB10	6584	10355	0.37%	0.044%
68	9.750	2707	2709	2711	rBV3	1103	613	0.02%	0.003%
69	9.802	2716	2725	2732	rBV8	6528	11212	0.40%	0.048%
70	9.895	2752	2754	2755	rBV	908	463	0.02%	0.002%
71	9.934	2761	2766	2777	rVB5	3533	5840	0.21%	0.025%
72	10.014	2785	2791	2793	rBV3	3895	3628	0.13%	0.015%
73	10.088	2801	2814	2818	rBV8	5076	9881	0.35%	0.042%
74	10.217	2837	2854	2875	rVV	874559	1531495	54.31%	6.529%
75	10.384	2894	2906	2918	rVB3	9624	20357	0.72%	0.087%
76	10.451	2918	2927	2939	rBV2	14042	28200	1.00%	0.120%

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Title : VOC Analysis

77	10.541	2951	2955	2960	rBV3	10015	13080	0.46%	0.056%
78	10.577	2961	2966	2982	rVB	48342	71107	2.52%	0.303%
79	10.699	2995	3004	3012	rBV2	29674	50304	1.78%	0.214%
80	10.879	3053	3060	3065	rBV6	10489	14659	0.52%	0.062%
81	10.918	3065	3072	3093	rVB2	35011	67099	2.38%	0.286%
82	11.030	3100	3107	3113	rBV7	6825	10355	0.37%	0.044%
83	11.152	3134	3145	3154	rBV10	12541	25040	0.89%	0.107%
84	11.191	3155	3157	3164	rVB6	4490	4885	0.17%	0.021%
85	11.249	3164	3175	3194	rBV	1261562	1996816	70.81%	8.512%
86	11.458	3236	3240	3249	rVB9	3630	4715	0.17%	0.020%
87	11.625	3281	3292	3313	rVB	1241443	1980809	70.24%	8.444%
88	11.789	3336	3343	3350	rBV2	30756	38515	1.37%	0.164%
89	11.918	3375	3383	3384	rBV6	6548	8195	0.29%	0.035%
90	12.262	3478	3490	3500	rBV6	8265	16698	0.59%	0.071%
91	12.416	3532	3538	3546	rVB6	7120	10475	0.37%	0.045%
92	12.467	3547	3554	3563	rBV2	11767	17873	0.63%	0.076%
93	12.599	3586	3595	3608	rVB4	24968	47796	1.69%	0.204%
94	12.721	3630	3633	3642	rVB7	6679	9039	0.32%	0.039%
95	12.885	3677	3684	3691	rBV7	15579	22675	0.80%	0.097%
96	13.410	3838	3847	3849	rBV6	6412	8873	0.31%	0.038%
97	13.506	3870	3877	3889	rBV	24000	37501	1.33%	0.160%
98	13.699	3934	3937	3940	rBV4	1719	1175	0.04%	0.005%
99	14.387	4146	4151	4158	rVB5	9904	12634	0.45%	0.054%
100	15.262	4414	4423	4435	rVB2	111544	165573	5.87%	0.706%

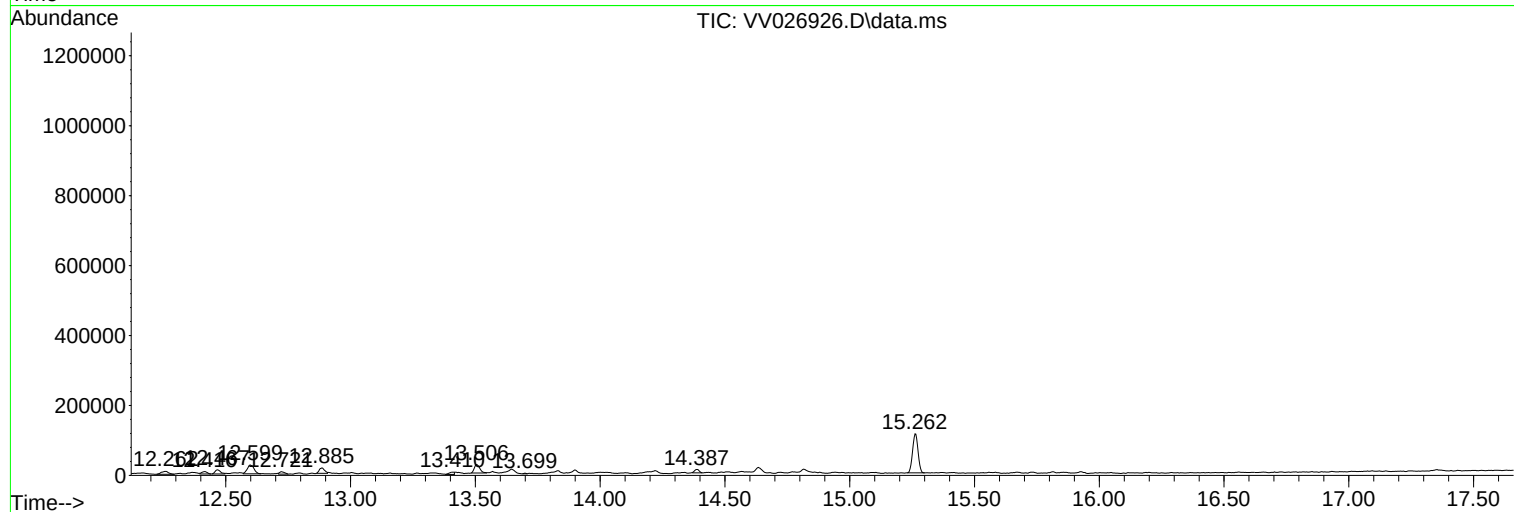
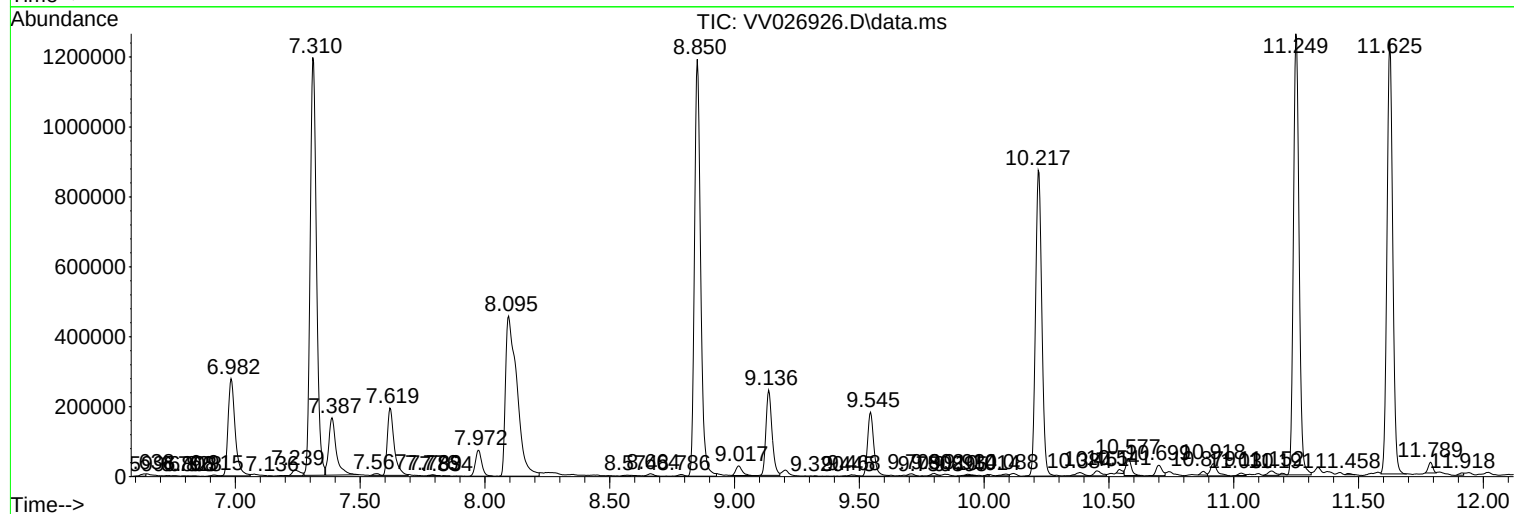
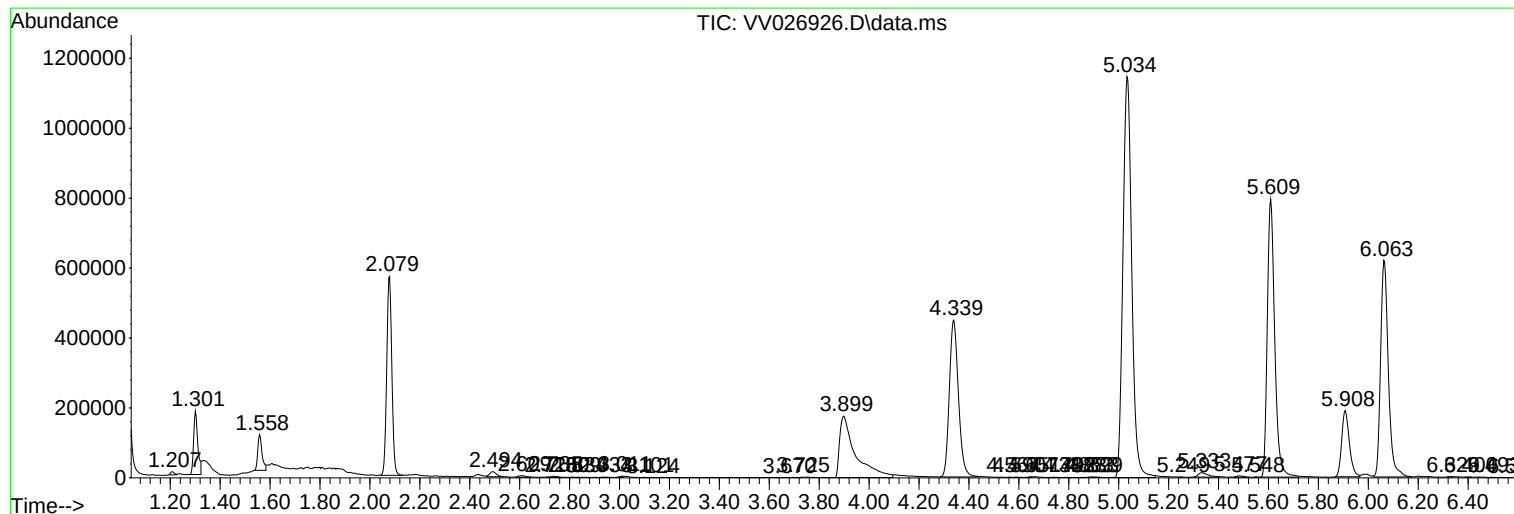
Sum of corrected areas: 23457515

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Instrument :
MSVOA_V
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C0ZD1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072222WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_V
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C0ZD1ME

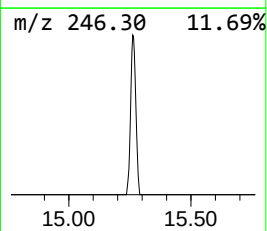
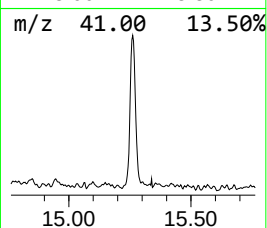
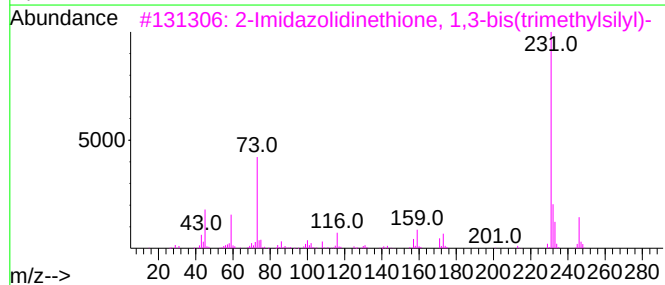
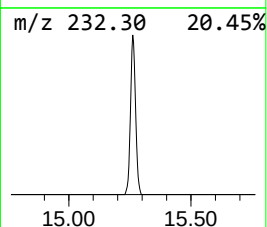
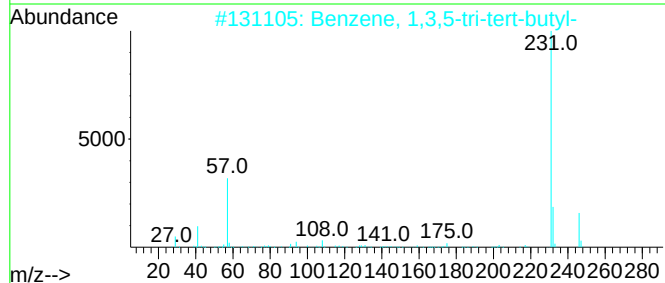
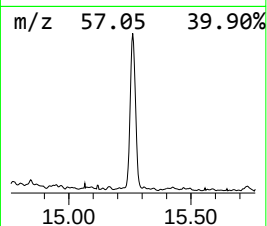
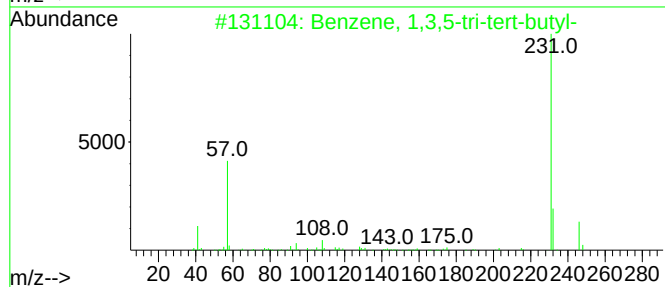
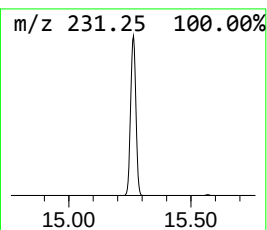
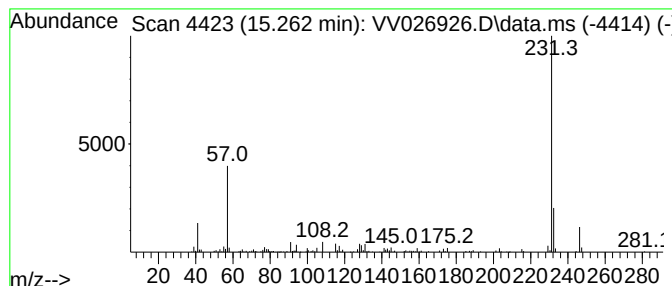
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072222WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,3,5-tri-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.262	4.15 ug/L	165573	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	90
2			Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	72
3			2-Imidazolidinethione, 1,3-bis(t...	246	C9H22N2SSi2	069859-14-9	59
4			2-Cyano-3-phenylquinoxaline	231	C15H9N3	059393-45-2	53
5			Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3,5-...	15.262	4.2	ug/L	165573	3	11.249	1996820	50.0