

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021271.D
 Acq On : 04 May 2021 15:15
 Operator : SY/MD
 Sample : M2232-09ME
 Misc : 3.21g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG5B2ME

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\SFAMVLM050321WMA.M

Title : VOC Analysis

Signal : TIC: VV021271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	77	83	89	rBV	139132	151460	6.48%	0.820%
2	1.568	159	164	184	rVB	106845	175417	7.50%	0.950%
3	2.609	480	488	501	rBV3	16249	32162	1.38%	0.174%
4	2.924	584	586	589	rVB4	1758	813	0.03%	0.004%
5	2.992	605	607	609	rBV3	1047	471	0.02%	0.003%
6	3.005	609	611	613	rBV2	1401	837	0.04%	0.005%
7	3.111	641	644	647	rBV3	1294	818	0.03%	0.004%
8	3.130	647	650	655	rVV5	1796	1332	0.06%	0.007%
9	3.182	661	666	668	rVB4	1447	1098	0.05%	0.006%
10	3.207	668	674	676	rBV5	1704	1787	0.08%	0.010%
11	3.281	695	697	701	rVV5	1005	681	0.03%	0.004%
12	3.330	709	712	715	rBV4	1449	1117	0.05%	0.006%
13	3.368	719	724	726	rBV5	1298	1150	0.05%	0.006%
14	3.407	733	736	738	rBV3	1540	1040	0.04%	0.006%
15	3.471	754	756	758	rBV2	962	529	0.02%	0.003%
16	3.519	768	771	773	rBV3	723	418	0.02%	0.002%
17	3.596	793	795	797	rVB3	1094	423	0.02%	0.002%
18	3.670	814	818	822	rBV3	1366	951	0.04%	0.005%
19	3.719	831	833	838	rVB4	1087	721	0.03%	0.004%
20	3.744	838	841	844	rBV5	1099	957	0.04%	0.005%
21	3.783	851	853	855	rVB3	1177	483	0.02%	0.003%
22	3.802	857	859	862	rBV2	905	418	0.02%	0.002%
23	3.822	862	865	868	rVB5	1207	696	0.03%	0.004%
24	3.841	868	871	873	rVB4	848	436	0.02%	0.002%
25	3.860	873	877	882	rVB6	1116	801	0.03%	0.004%
26	3.921	882	896	903	rBV	67732	166545	7.12%	0.902%
27	4.349	1015	1029	1056	rVB2	400649	970346	41.51%	5.257%
28	4.558	1090	1094	1096	rBV5	2118	1496	0.06%	0.008%
29	4.629	1114	1116	1117	rBV2	1290	540	0.02%	0.003%
30	4.651	1120	1123	1125	rBV3	1222	741	0.03%	0.004%
31	4.776	1160	1162	1166	rVB4	1352	814	0.03%	0.004%
32	4.799	1166	1169	1171	rBV4	1297	976	0.04%	0.005%
33	4.834	1178	1180	1181	rBV2	759	395	0.02%	0.002%
34	4.912	1202	1204	1206	rBV2	1266	735	0.03%	0.004%
35	4.973	1221	1223	1226	rVB3	785	464	0.02%	0.003%
36	5.043	1227	1245	1289	rBV3	908040	2337595	100.00%	12.663%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
 Title : VOC Analysis

37	5.539	1397	1399	1402	rBV4	1200	696	0.03%	0.004%
38	5.619	1411	1424	1451	rBV2	857150	1794446	76.76%	9.721%
39	5.908	1501	1514	1529	rBV5	42421	91062	3.90%	0.493%
40	6.072	1551	1565	1593	rBV2	459274	1007248	43.09%	5.457%
41	6.288	1629	1632	1635	rBV4	1364	1065	0.05%	0.006%
42	6.307	1635	1638	1641	rBV4	1013	859	0.04%	0.005%
43	6.358	1651	1654	1658	rBV5	1159	808	0.03%	0.004%
44	6.420	1670	1673	1678	rVB5	2059	1538	0.07%	0.008%
45	6.448	1679	1682	1683	rBV	1141	570	0.02%	0.003%
46	6.487	1690	1694	1695	rBV4	1262	923	0.04%	0.005%
47	6.542	1708	1711	1715	rVB4	1177	640	0.03%	0.003%
48	6.600	1726	1729	1732	rVB4	2675	1664	0.07%	0.009%
49	6.632	1735	1739	1741	rBV5	1568	1279	0.05%	0.007%
50	6.741	1771	1773	1777	rBV4	1285	874	0.04%	0.005%
51	6.802	1790	1792	1797	rVB6	1509	1054	0.05%	0.006%
52	6.857	1807	1809	1813	rBV3	1037	619	0.03%	0.003%
53	6.992	1838	1851	1880	rBV2	276771	578888	24.76%	3.136%
54	7.165	1903	1905	1908	rBV3	1485	931	0.04%	0.005%
55	7.227	1921	1924	1925	rBV	1675	1106	0.05%	0.006%
56	7.320	1941	1953	1975	rBV	1047772	1894942	81.06%	10.265%
57	7.590	2035	2037	2039	rBV2	1029	566	0.02%	0.003%
58	7.628	2039	2049	2074	rVV2	191018	398575	17.05%	2.159%
59	7.863	2119	2122	2124	rBV4	1425	834	0.04%	0.005%
60	8.120	2187	2202	2240	rBV5	281472	975941	41.75%	5.287%
61	8.497	2318	2319	2322	rBV3	1163	611	0.03%	0.003%
62	8.567	2338	2341	2345	rVB5	1101	916	0.04%	0.005%
63	8.606	2350	2353	2356	rBV3	1067	808	0.03%	0.004%
64	8.690	2377	2379	2381	rBV2	769	481	0.02%	0.003%
65	8.722	2387	2389	2390	rBV	1249	518	0.02%	0.003%
66	8.744	2393	2396	2399	rVV4	1588	948	0.04%	0.005%
67	8.860	2420	2432	2459	rBV	1238468	2250777	96.29%	12.193%
68	9.056	2488	2493	2496	rBV7	1464	1513	0.06%	0.008%
69	9.300	2566	2569	2572	rBV3	1489	1131	0.05%	0.006%
70	9.316	2572	2574	2578	rVB3	1599	947	0.04%	0.005%
71	9.339	2578	2581	2584	rBV4	1424	1022	0.04%	0.006%
72	9.387	2594	2596	2603	rBV5	1387	1520	0.07%	0.008%
73	9.503	2630	2632	2636	rBV4	799	707	0.03%	0.004%
74	9.561	2647	2650	2654	rBV3	2632	2105	0.09%	0.011%
75	9.603	2661	2663	2666	rVB4	1028	526	0.02%	0.003%
76	9.628	2669	2671	2673	rBV	1484	835	0.04%	0.005%

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Instrument :
 MSVOA_V
 ClientSampleId :
 BG5B2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
 Title : VOC Analysis

77	9.767	2712	2714	2715	rBV	1210	538	0.02%	0.003%
78	9.779	2715	2718	2722	rVV5	1557	1286	0.06%	0.007%
79	9.882	2746	2750	2756	rVB6	1224	1030	0.04%	0.006%
80	9.908	2756	2758	2760	rBV2	1923	1100	0.05%	0.006%
81	10.136	2820	2829	2835	rBV5	8480	12352	0.53%	0.067%
82	10.230	2845	2858	2876	rBV	651599	1146687	49.05%	6.212%
83	10.423	2916	2918	2920	rBV3	1189	720	0.03%	0.004%
84	10.522	2947	2949	2953	rVB3	2917	1794	0.08%	0.010%
85	10.551	2953	2958	2960	rBV5	2479	2132	0.09%	0.012%
86	10.734	3012	3015	3020	rBV5	1915	1649	0.07%	0.009%
87	10.796	3029	3034	3040	rBV6	1813	2160	0.09%	0.012%
88	11.008	3097	3100	3103	rBV3	1211	689	0.03%	0.004%
89	11.098	3126	3128	3132	rBV4	1022	651	0.03%	0.004%
90	11.259	3167	3178	3198	rBV	1488762	2278731	97.48%	12.344%
91	11.480	3244	3247	3249	rBV2	1711	1308	0.06%	0.007%
92	11.558	3269	3271	3273	rBV2	1868	1097	0.05%	0.006%
93	11.635	3283	3295	3316	rBV	1314401	2059013	88.08%	11.154%
94	11.988	3401	3405	3410	rBV6	2461	2566	0.11%	0.014%
95	12.262	3478	3490	3499	rBV4	31816	55006	2.35%	0.298%
96	12.422	3539	3540	3543	rBV3	1252	886	0.04%	0.005%
97	12.529	3571	3573	3575	rBV3	1801	873	0.04%	0.005%
98	13.111	3751	3754	3755	rBV3	1743	1023	0.04%	0.006%
99	13.197	3774	3781	3789	rBV3	3172	5411	0.23%	0.029%
100	13.268	3801	3803	3805	rBV3	1556	724	0.03%	0.004%

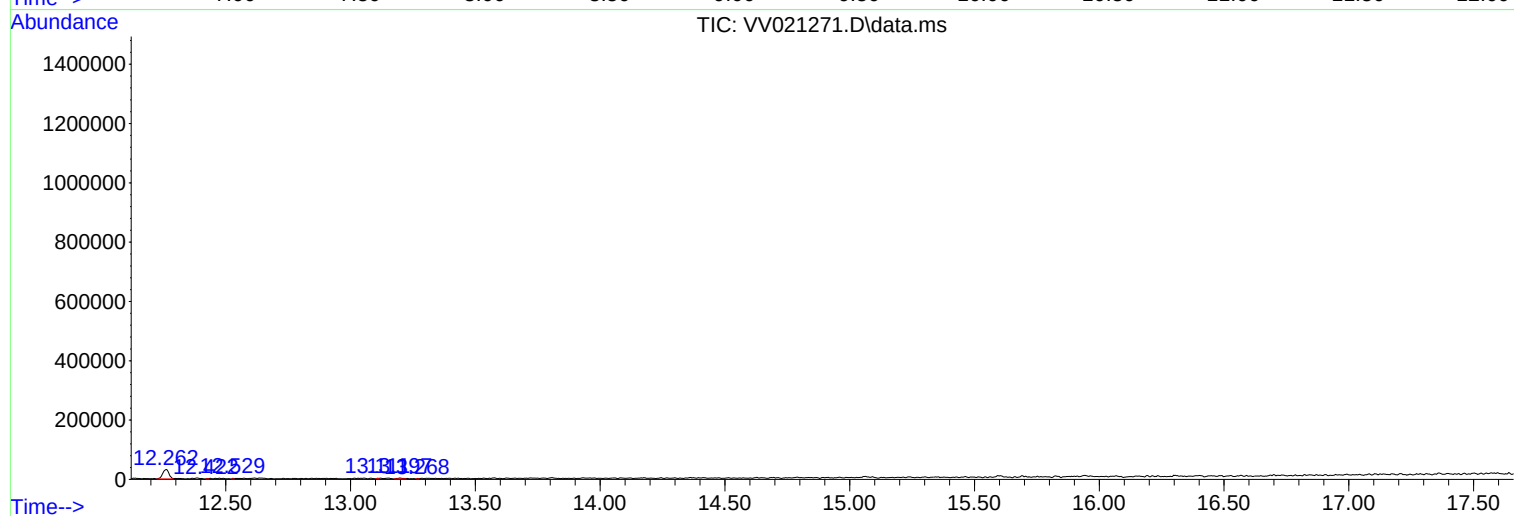
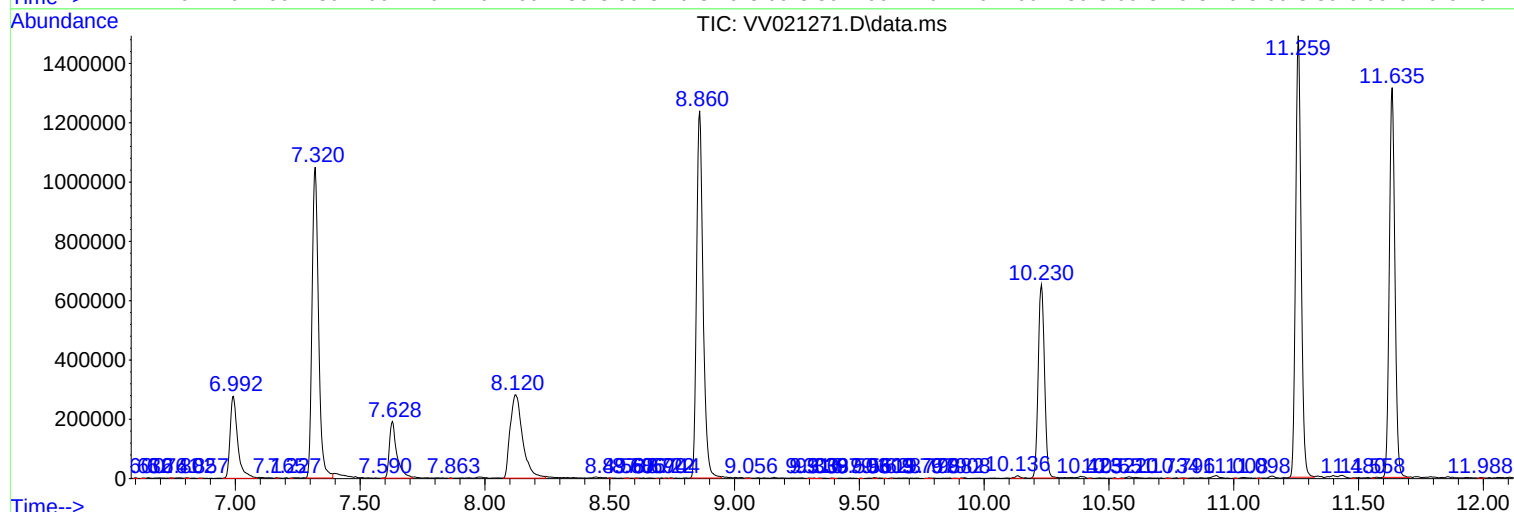
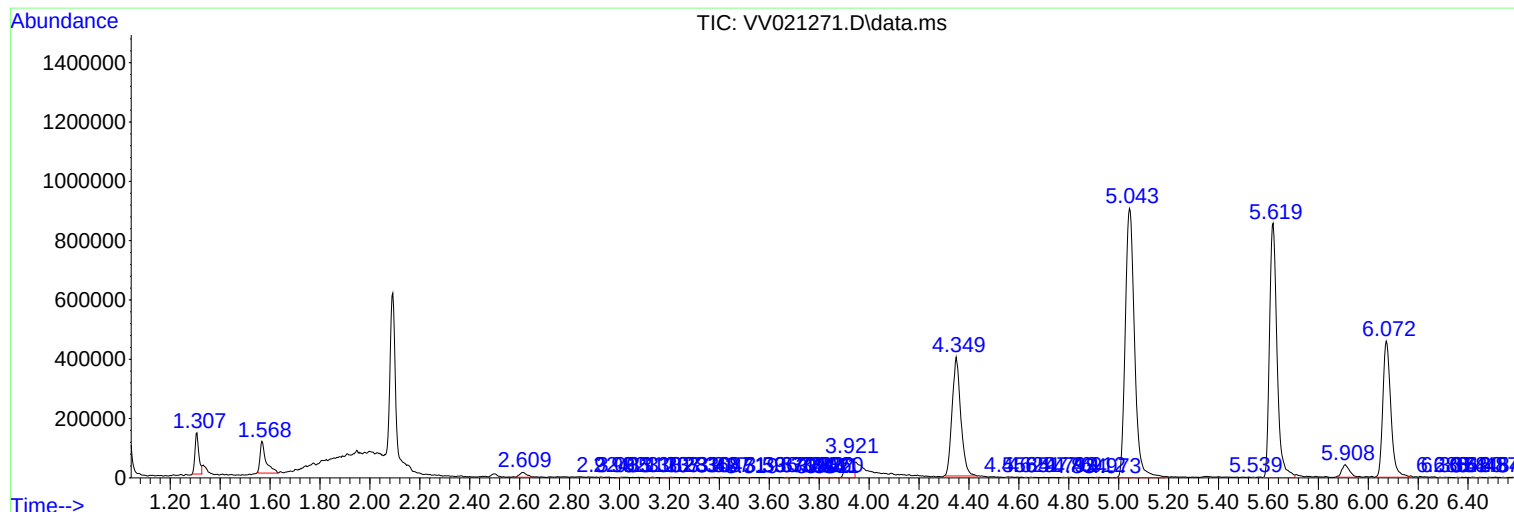
Sum of corrected areas: 18459582

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG5B2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Operator : SY/MD
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Misc : 3.21g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG5B2ME

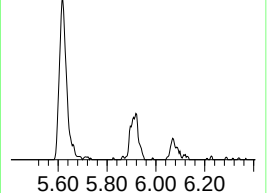
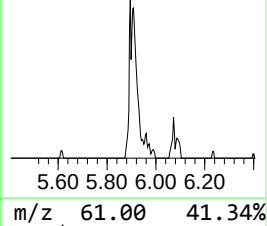
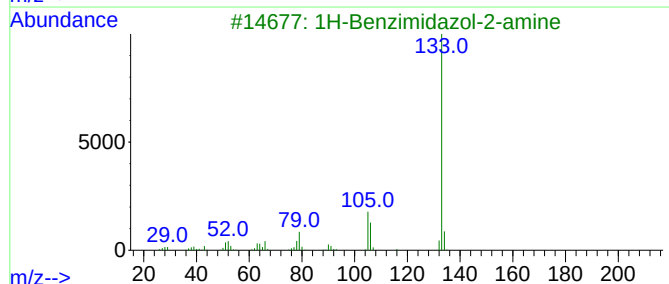
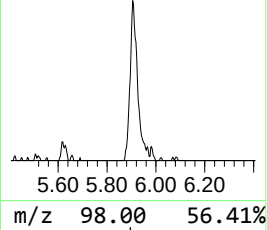
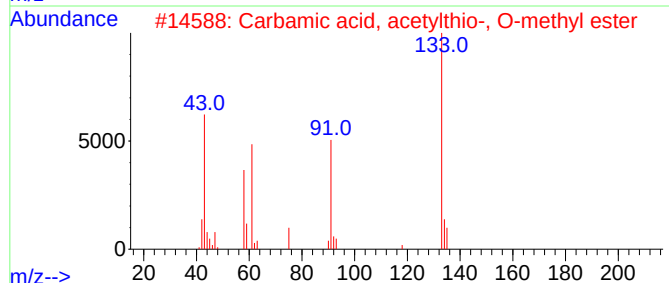
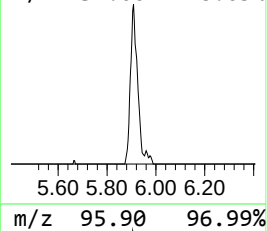
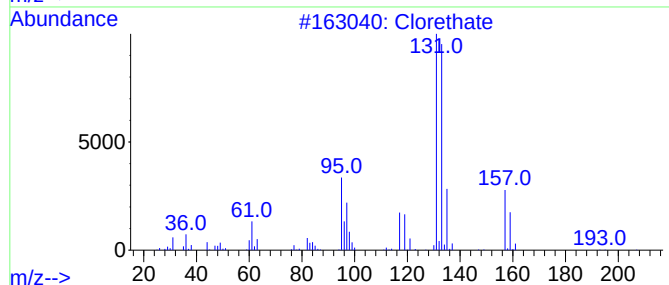
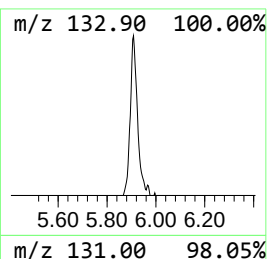
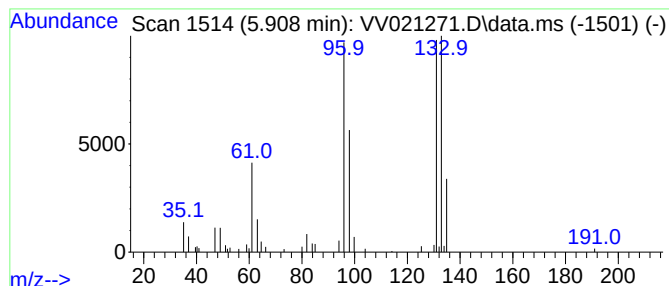
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	2.54 ug/L	91062	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Clorethate	322	C5H4Cl6O3	005634-37-7	25
2			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	9
3			1H-Benzimidazol-2-amine	133	C7H7N3	000934-32-7	9
4			1H-Benzimidazol-2-amine	133	C7H7N3	000934-32-7	9
5			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	2.5	ug/L	91062	1	5.619	1794450	50.0