

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
 Data File : VV024380.D
 Acq On : 17 Jan 2022 17:31
 Operator : SY/MD
 Sample : N1115-13ME
 Misc : 6.31g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLS3ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	49	55	61	rBV2	22846	21474	0.84%	0.119%
2	1.307	75	83	96	rVB	305581	321734	12.54%	1.776%
3	1.510	144	146	148	rBV3	832	538	0.02%	0.003%
4	1.535	148	154	156	rVV3	2080	2130	0.08%	0.012%
5	1.568	156	164	177	rVV	247674	282219	11.00%	1.558%
6	2.104	319	331	369	rVB	575830	861691	33.59%	4.756%
7	2.294	382	390	396	rVB2	2973	3639	0.14%	0.020%
8	2.510	449	457	469	rVB8	2882	5015	0.20%	0.028%
9	2.619	489	491	497	rVB4	627	560	0.02%	0.003%
10	2.760	529	535	547	rBV5	1710	2535	0.10%	0.014%
11	2.957	586	596	609	rBV7	4443	9155	0.36%	0.051%
12	3.883	869	884	939	rBV	167771	520050	20.27%	2.870%
13	4.239	992	995	1001	rVB4	580	605	0.02%	0.003%
14	4.346	1012	1028	1063	rBV	432291	1058654	41.27%	5.843%
15	4.674	1127	1130	1133	rVV4	737	474	0.02%	0.003%
16	4.690	1133	1135	1141	rVB3	447	464	0.02%	0.003%
17	5.043	1227	1245	1287	rVV2	995554	2565096	100.00%	14.157%
18	5.243	1306	1307	1315	rBV4	545	585	0.02%	0.003%
19	5.336	1329	1336	1341	rBV3	1695	2074	0.08%	0.011%
20	5.497	1380	1386	1389	rBV5	631	581	0.02%	0.003%
21	5.616	1410	1423	1453	rBV	469467	946149	36.89%	5.222%
22	5.905	1503	1513	1530	rVV2	32890	67545	2.63%	0.373%
23	6.069	1549	1564	1596	rVV	568474	1155565	45.05%	6.377%
24	6.207	1603	1607	1610	rBV6	1082	992	0.04%	0.005%
25	6.262	1621	1624	1630	rVB5	1117	838	0.03%	0.005%
26	6.310	1632	1639	1642	rBV6	2823	3710	0.14%	0.020%
27	6.429	1673	1676	1682	rVB4	510	548	0.02%	0.003%
28	6.513	1696	1702	1703	rBV3	805	865	0.03%	0.005%
29	6.635	1731	1740	1742	rBV5	1662	2086	0.08%	0.012%
30	6.741	1769	1773	1779	rVB4	633	543	0.02%	0.003%
31	6.982	1837	1848	1875	rBV	349268	629449	24.54%	3.474%
32	7.313	1939	1951	1969	rBV	1276698	2167775	84.51%	11.964%
33	7.619	2035	2046	2070	rBV	249895	424958	16.57%	2.345%
34	7.976	2151	2157	2165	rBV8	1340	2114	0.08%	0.012%
35	8.088	2181	2192	2233	rBV	576409	1200056	46.78%	6.623%
36	8.342	2269	2271	2276	rVB4	845	499	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	8.419	2291	2295	2296	rBV3	1345	838	0.03%	0.005%
38	8.509	2321	2323	2327	rBV2	669	468	0.02%	0.003%
39	8.850	2418	2429	2457	rBV	700358	1131391	44.11%	6.244%
40	9.021	2476	2482	2492	rVB5	1852	2909	0.11%	0.016%
41	9.059	2492	2494	2502	rVB3	746	662	0.03%	0.004%
42	9.149	2514	2522	2535	rVB6	3931	6501	0.25%	0.036%
43	9.423	2602	2607	2614	rBV4	353	463	0.02%	0.003%
44	9.477	2620	2624	2630	rVV4	655	746	0.03%	0.004%
45	9.551	2637	2647	2650	rBV5	1978	2965	0.12%	0.016%
46	9.796	2721	2723	2726	rBV2	652	501	0.02%	0.003%
47	9.934	2756	2766	2775	rBV10	2324	3881	0.15%	0.021%
48	10.017	2788	2792	2794	rBV4	1072	890	0.03%	0.005%
49	10.085	2808	2813	2818	rBV5	1688	1861	0.07%	0.010%
50	10.127	2818	2826	2838	rVB3	7952	14263	0.56%	0.079%
51	10.213	2841	2853	2873	rBV	759133	1207641	47.08%	6.665%
52	10.451	2921	2927	2934	rBV3	1295	1398	0.05%	0.008%
53	10.506	2940	2944	2946	rBV4	1317	926	0.04%	0.005%
54	10.541	2952	2955	2957	rBV2	1447	958	0.04%	0.005%
55	10.657	2987	2991	2992	rBV2	1021	701	0.03%	0.004%
56	10.715	3006	3009	3012	rBV3	873	696	0.03%	0.004%
57	10.834	3040	3046	3048	rBV6	2221	2272	0.09%	0.013%
58	10.876	3054	3059	3066	rBV4	6346	8599	0.34%	0.047%
59	10.914	3066	3071	3081	rVB5	11020	15735	0.61%	0.087%
60	11.037	3100	3109	3114	rBV5	4524	7432	0.29%	0.041%
61	11.094	3122	3127	3133	rVB6	1797	2138	0.08%	0.012%
62	11.149	3136	3144	3151	rBV5	6991	10848	0.42%	0.060%
63	11.249	3164	3175	3196	rBV	749985	1169277	45.58%	6.453%
64	11.384	3211	3217	3225	rVV5	4215	6886	0.27%	0.038%
65	11.426	3225	3230	3238	rVB3	6762	9560	0.37%	0.053%
66	11.461	3238	3241	3246	rVB5	2018	1873	0.07%	0.010%
67	11.538	3262	3265	3268	rBV3	971	768	0.03%	0.004%
68	11.622	3280	3291	3312	rBV	1323247	2092083	81.56%	11.546%
69	11.757	3331	3333	3335	rBV2	1271	809	0.03%	0.004%
70	11.908	3376	3380	3381	rBV3	1149	863	0.03%	0.005%
71	12.365	3513	3522	3531	rBV3	3989	7708	0.30%	0.043%
72	12.590	3589	3592	3594	rBV3	1549	1120	0.04%	0.006%
73	12.651	3602	3611	3623	rVB7	6921	11092	0.43%	0.061%
74	13.033	3727	3730	3731	rBV2	1428	875	0.03%	0.005%
75	13.159	3765	3769	3773	rBV4	1286	970	0.04%	0.005%
76	13.265	3793	3802	3811	rBV5	9080	13672	0.53%	0.075%

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 ClientSampleId :
 BGLS3ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

77	13.429	3848	3853	3857	rBV4	1251	1423	0.06%	0.008%
78	13.474	3864	3867	3869	rBV4	1115	783	0.03%	0.004%
79	13.506	3869	3877	3893	rVB	18777	29787	1.16%	0.164%
80	13.622	3910	3913	3916	rBV3	1192	935	0.04%	0.005%
81	13.696	3932	3936	3939	rVB3	1214	903	0.04%	0.005%
82	13.747	3941	3952	3962	rVB4	9493	15342	0.60%	0.085%
83	13.908	3999	4002	4007	rVB3	1121	883	0.03%	0.005%
84	14.194	4089	4091	4096	rVB4	638	468	0.02%	0.003%
85	14.226	4099	4101	4105	rVV3	923	638	0.02%	0.004%
86	14.393	4150	4153	4161	rBV7	1114	1387	0.05%	0.008%
87	14.499	4183	4186	4194	rVB6	1205	1159	0.05%	0.006%
88	14.590	4211	4214	4216	rBV2	619	480	0.02%	0.003%
89	14.644	4227	4231	4233	rBV4	1606	1319	0.05%	0.007%
90	14.824	4279	4287	4294	rBV8	2623	4231	0.16%	0.023%
91	14.882	4300	4305	4307	rBV6	715	597	0.02%	0.003%
92	15.191	4399	4401	4404	rBV3	773	513	0.02%	0.003%
93	15.310	4436	4438	4440	rVB2	1208	499	0.02%	0.003%
94	15.348	4441	4450	4451	rBV8	1881	2457	0.10%	0.014%
95	15.448	4478	4481	4488	rBV8	1351	1812	0.07%	0.010%
96	15.525	4503	4505	4509	rBV5	1143	594	0.02%	0.003%
97	15.670	4542	4550	4562	rVB3	12584	21559	0.84%	0.119%
98	15.760	4576	4578	4582	rBV4	1056	488	0.02%	0.003%
99	15.815	4587	4595	4601	rBV4	12233	17828	0.70%	0.098%
100	16.287	4737	4742	4745	rBV6	4822	5145	0.20%	0.028%

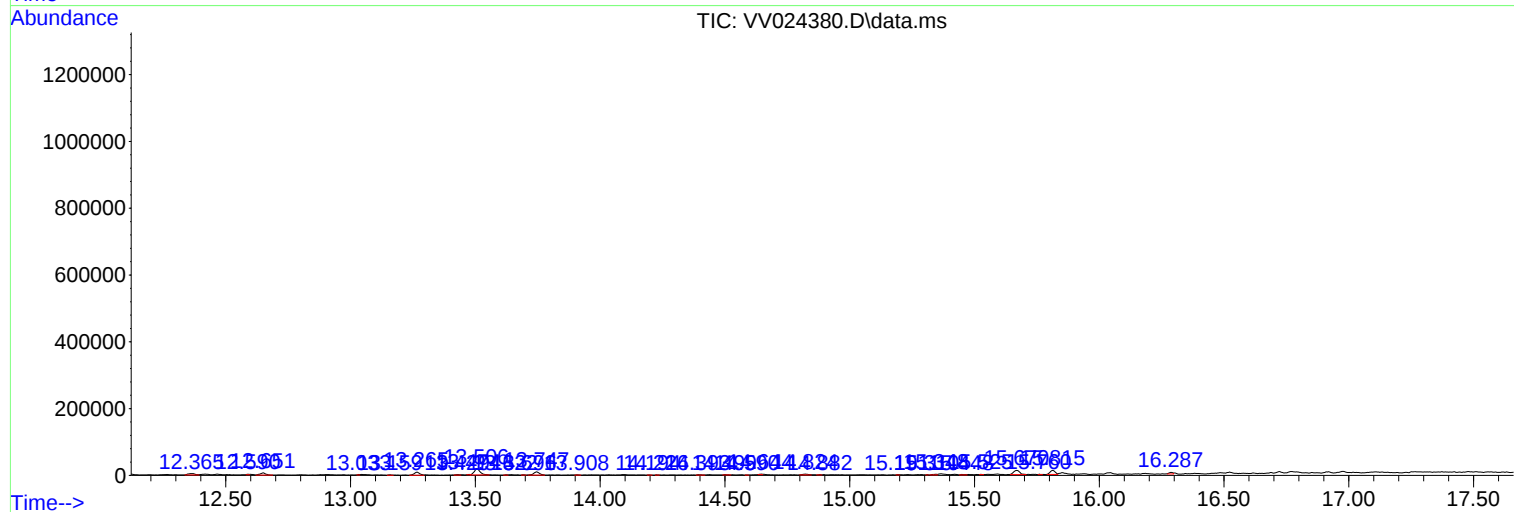
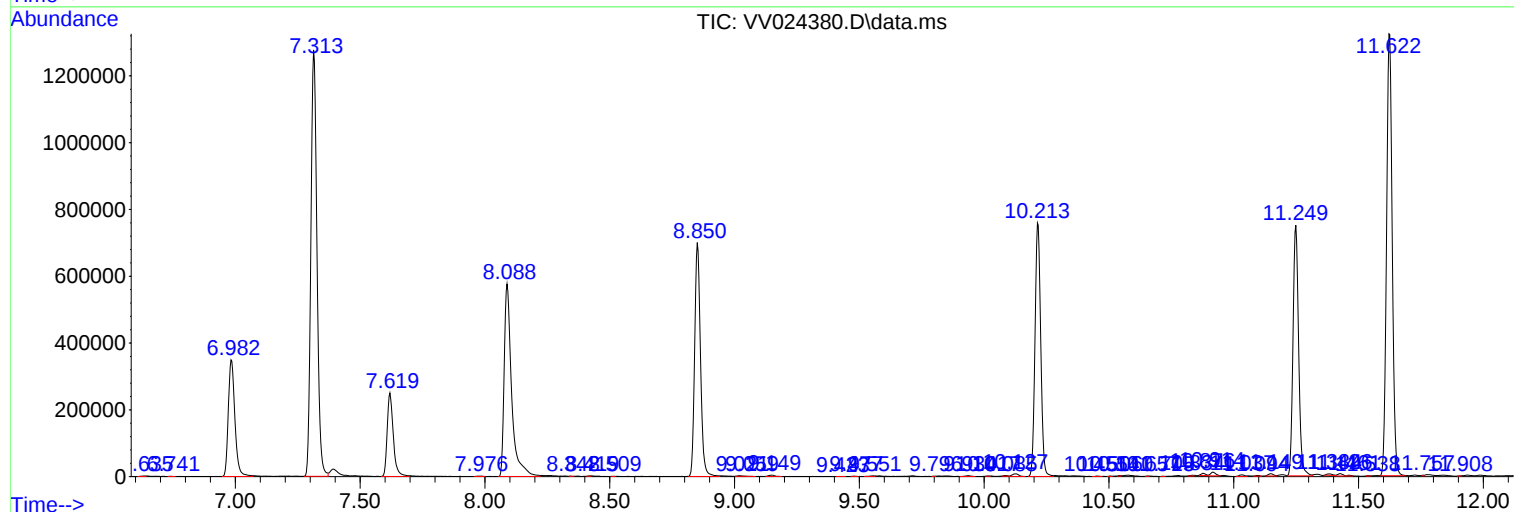
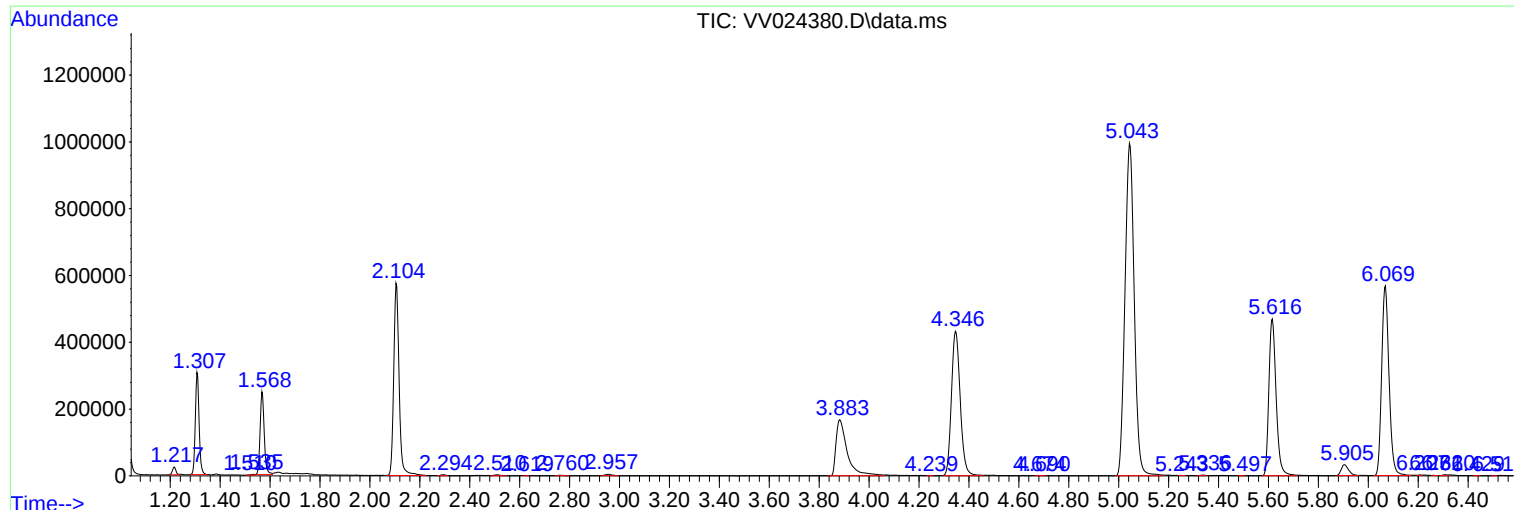
Sum of corrected areas: 18119434

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLS3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
ClientSampleId :
BGLS3ME

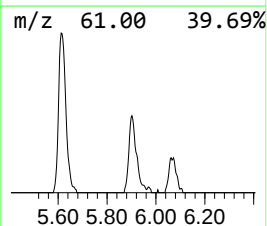
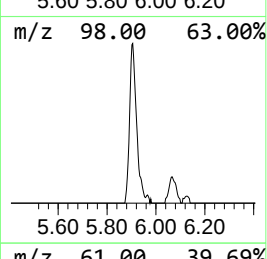
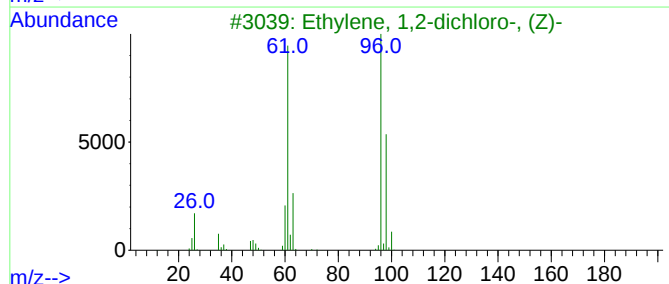
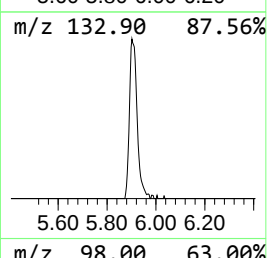
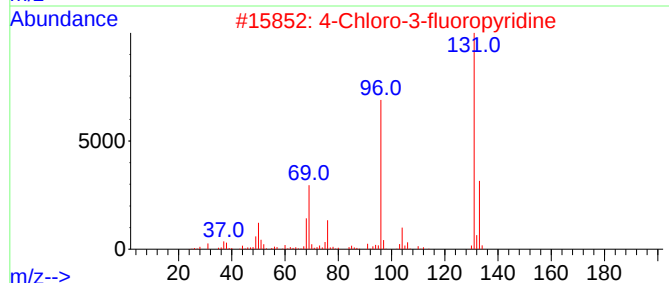
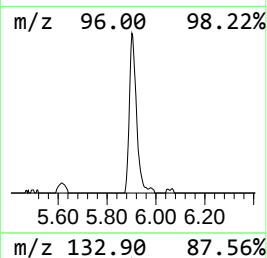
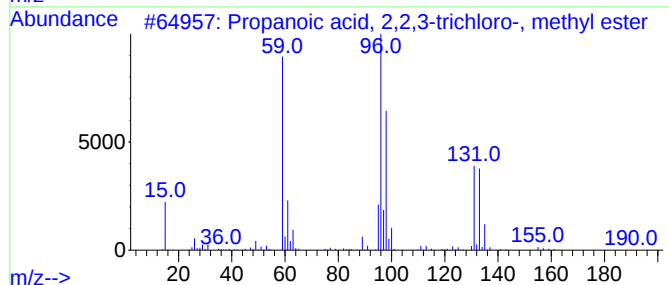
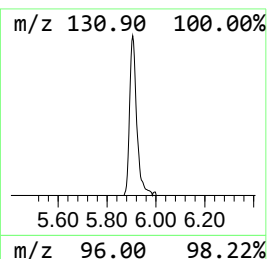
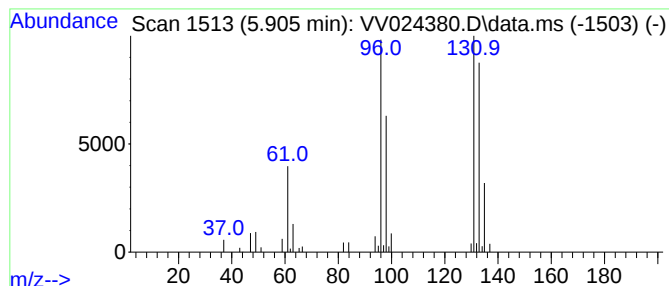
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	3.57 ug/L	67545	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	42
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	3.6	ug/L	67545	1	5.616	946149	50.0