

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011822\
 Data File : VV024385.D
 Acq On : 18 Jan 2022 10:44
 Operator : SY/MD
 Sample : VV0118MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK301

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: VV024385.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	51	55	61	rVB	13156	11063	0.91%	0.116%
2	1.307	77	83	99	rVB	151619	157725	12.98%	1.659%
3	1.568	157	164	177	rVB	129168	144953	11.93%	1.525%
4	2.108	321	332	349	rBV	271337	406204	33.44%	4.273%
5	2.298	384	391	399	rVB5	1621	2403	0.20%	0.025%
6	2.384	416	418	420	rBV5	392	236	0.02%	0.002%
7	2.439	427	435	440	rBV3	1109	1462	0.12%	0.015%
8	2.577	476	478	480	rVV	394	159	0.01%	0.002%
9	2.593	480	483	487	rVV3	298	214	0.02%	0.002%
10	2.741	523	529	530	rBV3	265	233	0.02%	0.002%
11	2.754	530	533	534	rBV2	339	168	0.01%	0.002%
12	2.841	556	560	562	rBV	181	146	0.01%	0.002%
13	2.953	586	595	605	rBV5	2590	5572	0.46%	0.059%
14	3.050	618	625	627	rBV2	249	253	0.02%	0.003%
15	3.121	645	647	650	rVB2	262	145	0.01%	0.002%
16	3.278	692	696	698	rBV	369	245	0.02%	0.003%
17	3.339	713	715	718	rBV2	524	279	0.02%	0.003%
18	3.355	718	720	723	rVV	298	174	0.01%	0.002%
19	3.429	742	743	747	rVB	316	148	0.01%	0.002%
20	3.465	751	754	756	rBV	293	185	0.02%	0.002%
21	3.555	780	782	785	rVV	372	246	0.02%	0.003%
22	3.642	806	809	811	rBV	223	140	0.01%	0.001%
23	3.654	811	813	814	rBV	346	175	0.01%	0.002%
24	3.773	847	850	854	rBV2	224	176	0.01%	0.002%
25	3.793	854	856	860	rBV	222	138	0.01%	0.001%
26	3.886	874	885	930	rBV	67612	232293	19.12%	2.444%
27	4.281	1006	1008	1009	rBV	447	226	0.02%	0.002%
28	4.342	1012	1027	1052	rVV2	201710	493595	40.63%	5.192%
29	4.751	1149	1154	1156	rBV3	426	341	0.03%	0.004%
30	4.921	1204	1207	1209	rBV2	246	158	0.01%	0.002%
31	5.043	1227	1245	1274	rBV2	466077	1214865	100.00%	12.780%
32	5.355	1338	1342	1344	rBV2	307	223	0.02%	0.002%
33	5.432	1364	1366	1368	rVB3	549	283	0.02%	0.003%
34	5.452	1368	1372	1376	rBV2	424	409	0.03%	0.004%
35	5.506	1385	1389	1392	rBV2	315	267	0.02%	0.003%
36	5.542	1397	1400	1404	rBV	182	157	0.01%	0.002%

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 Title : VOC Analysis

37	5.612	1406	1422	1450	rBV	398303	799308	65.79%	8.408%
38	5.905	1501	1513	1535	rVB4	20025	44960	3.70%	0.473%
39	6.066	1549	1563	1589	rBV	267149	549071	45.20%	5.776%
40	6.301	1632	1636	1637	rBV2	1883	1162	0.10%	0.012%
41	6.407	1667	1669	1672	rBV2	270	195	0.02%	0.002%
42	6.513	1695	1702	1706	rBV3	1025	1153	0.09%	0.012%
43	6.690	1755	1757	1761	rBV3	438	251	0.02%	0.003%
44	6.812	1792	1795	1797	rBV2	355	246	0.02%	0.003%
45	6.899	1817	1822	1824	rBV2	196	181	0.01%	0.002%
46	6.982	1837	1848	1881	rBV	157801	286015	23.54%	3.009%
47	7.194	1912	1914	1915	rBV	471	213	0.02%	0.002%
48	7.313	1939	1951	1968	rBV	582434	1008189	82.99%	10.605%
49	7.619	2036	2046	2070	rBV	106454	190052	15.64%	1.999%
50	7.764	2089	2091	2094	rBV3	361	159	0.01%	0.002%
51	7.870	2121	2124	2127	rBV2	349	275	0.02%	0.003%
52	7.998	2162	2164	2168	rVB2	398	235	0.02%	0.002%
53	8.085	2181	2191	2227	rBV	254225	514509	42.35%	5.412%
54	8.625	2355	2359	2362	rBV2	638	413	0.03%	0.004%
55	8.712	2383	2386	2387	rVB2	359	171	0.01%	0.002%
56	8.722	2387	2389	2392	rBV2	468	248	0.02%	0.003%
57	8.767	2401	2403	2406	rVB2	310	152	0.01%	0.002%
58	8.850	2416	2429	2456	rBV	582842	951764	78.34%	10.012%
59	9.397	2597	2599	2602	rBV2	275	143	0.01%	0.002%
60	9.551	2638	2647	2651	rBV4	1574	2104	0.17%	0.022%
61	9.680	2684	2687	2688	rBV4	242	160	0.01%	0.002%
62	9.767	2711	2714	2716	rBV	251	174	0.01%	0.002%
63	9.818	2723	2730	2733	rBV4	1156	1332	0.11%	0.014%
64	9.889	2749	2752	2755	rBV	411	256	0.02%	0.003%
65	9.908	2755	2758	2761	rVV2	544	432	0.04%	0.005%
66	9.934	2762	2766	2775	rVB5	1642	1925	0.16%	0.020%
67	10.127	2819	2826	2835	rVB6	3201	4867	0.40%	0.051%
68	10.214	2840	2853	2876	rBV	340231	529948	43.62%	5.575%
69	10.538	2949	2954	2960	rBV4	1021	1520	0.13%	0.016%
70	10.564	2960	2962	2963	rBV	545	202	0.02%	0.002%
71	10.651	2987	2989	2994	rVV4	381	272	0.02%	0.003%
72	10.815	3036	3040	3045	rBV5	582	703	0.06%	0.007%
73	10.873	3055	3058	3061	rBV2	545	325	0.03%	0.003%
74	10.918	3064	3072	3082	rVB5	3035	5128	0.42%	0.054%
75	11.033	3103	3108	3110	rBV3	638	630	0.05%	0.007%
76	11.246	3163	3174	3197	rBV	607188	936575	77.09%	9.852%

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 Title : VOC Analysis

77	11.378	3211	3215	3217	rBV2	1491	1067	0.09%	0.011%
78	11.622	3278	3291	3316	rBV	601764	948956	78.11%	9.982%
79	11.763	3333	3335	3336	rBV	484	175	0.01%	0.002%
80	11.834	3354	3357	3360	rBV4	695	515	0.04%	0.005%
81	11.924	3383	3385	3387	rBV2	484	249	0.02%	0.003%
82	12.046	3421	3423	3425	rVB2	412	161	0.01%	0.002%
83	12.091	3434	3437	3440	rBV3	551	411	0.03%	0.004%
84	12.146	3450	3454	3456	rBV2	202	197	0.02%	0.002%
85	12.230	3478	3480	3482	rBV	275	159	0.01%	0.002%
86	12.265	3489	3491	3495	rVB2	537	280	0.02%	0.003%
87	12.355	3512	3519	3527	rBV6	1450	2183	0.18%	0.023%
88	12.522	3569	3571	3573	rBV2	484	225	0.02%	0.002%
89	12.583	3588	3590	3592	rBV	239	144	0.01%	0.002%
90	12.654	3605	3612	3619	rVB5	2279	3123	0.26%	0.033%
91	12.747	3639	3641	3643	rBV2	286	151	0.01%	0.002%
92	12.824	3662	3665	3669	rVB2	346	269	0.02%	0.003%
93	12.847	3669	3672	3675	rBV2	518	393	0.03%	0.004%
94	13.024	3725	3727	3730	rVB2	296	136	0.01%	0.001%
95	13.207	3781	3784	3786	rBV2	379	248	0.02%	0.003%
96	13.265	3792	3802	3811	rBV8	4438	6959	0.57%	0.073%
97	13.506	3868	3877	3891	rBV	11771	19368	1.59%	0.204%
98	13.603	3905	3907	3911	rBV3	365	183	0.02%	0.002%
99	13.747	3942	3952	3963	rBV7	5670	9220	0.76%	0.097%
100	14.503	4184	4187	4188	rBV2	530	296	0.02%	0.003%

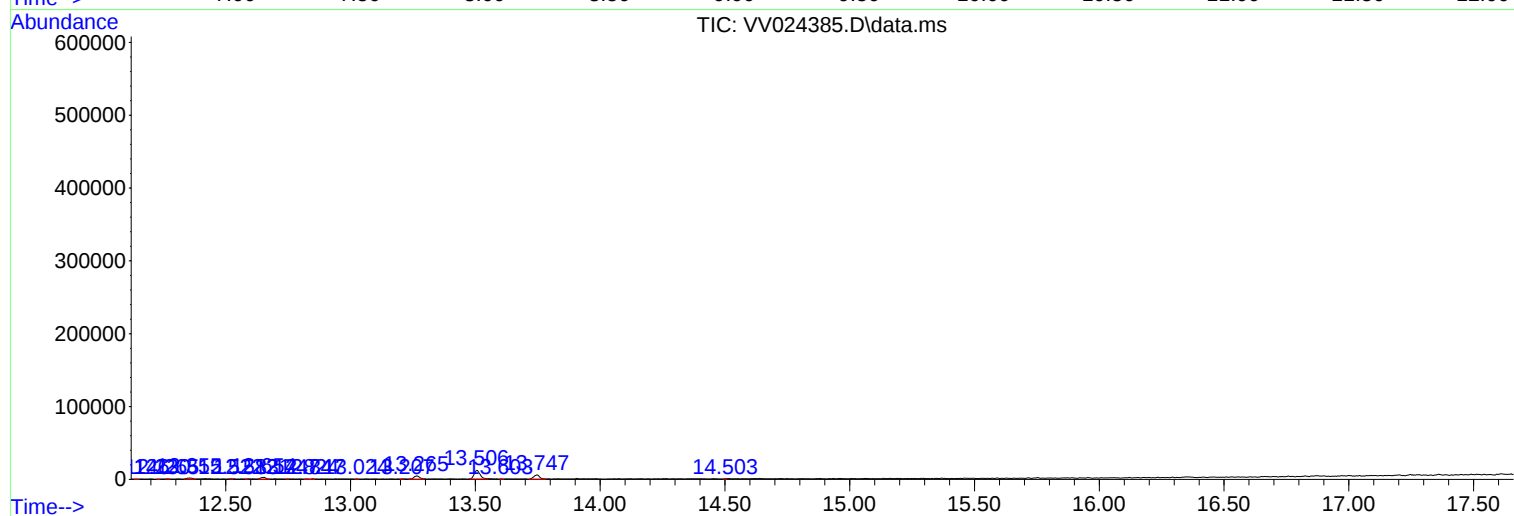
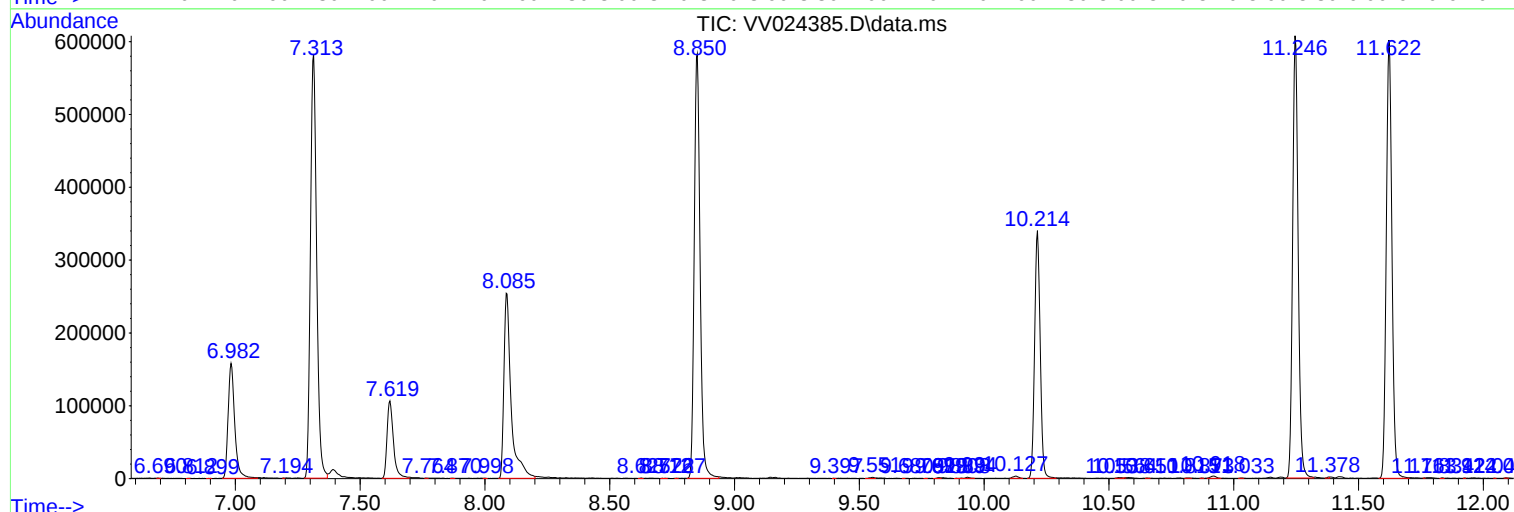
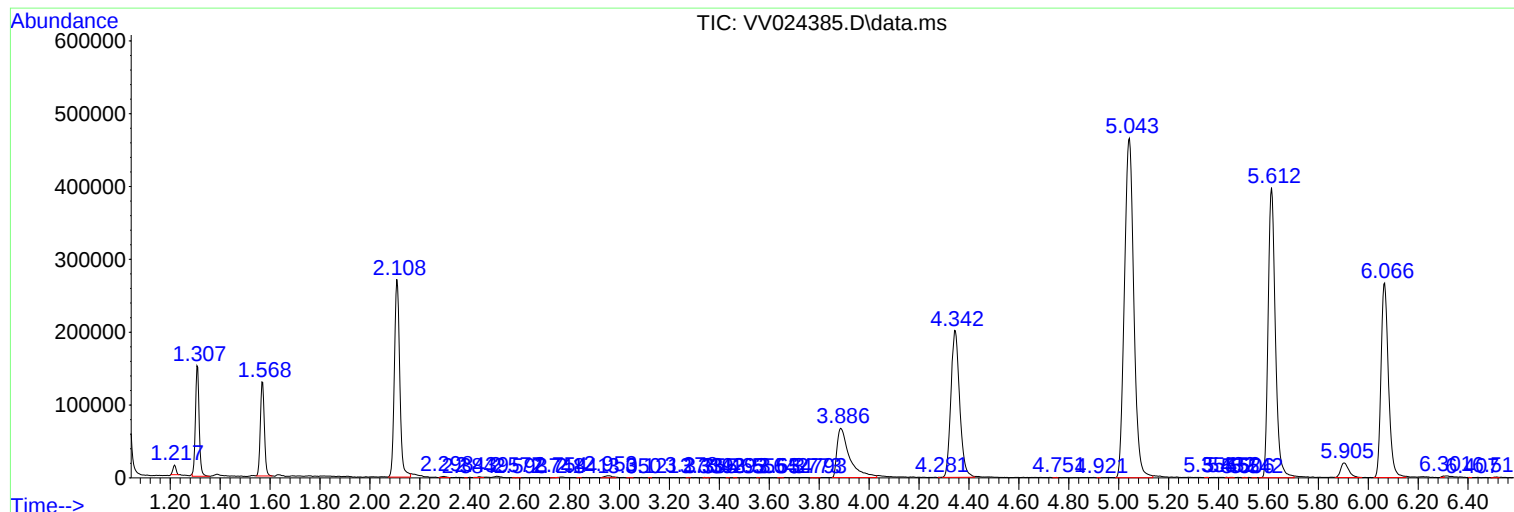
Sum of corrected areas: 9506345

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ALS Vial : 3 Sample Multiplier: 1

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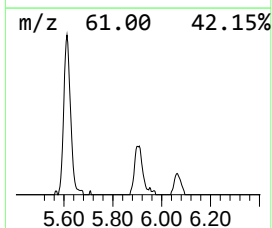
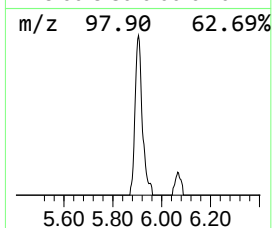
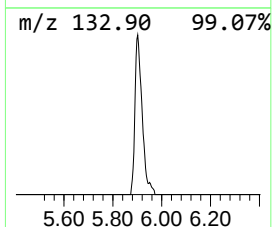
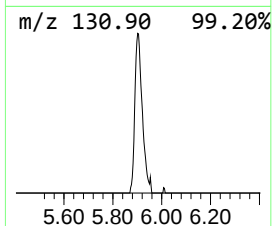
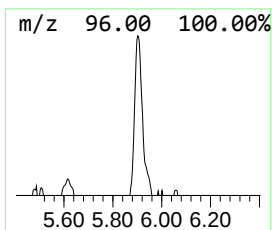
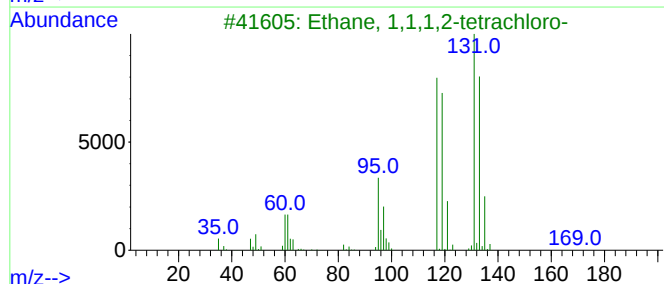
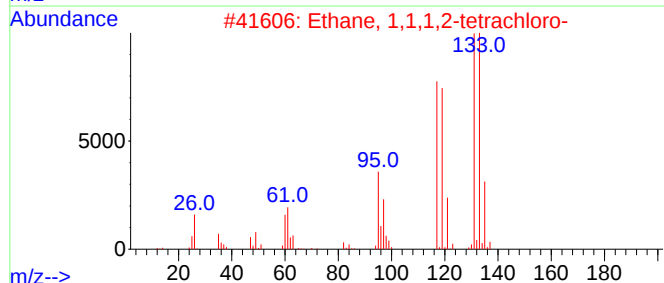
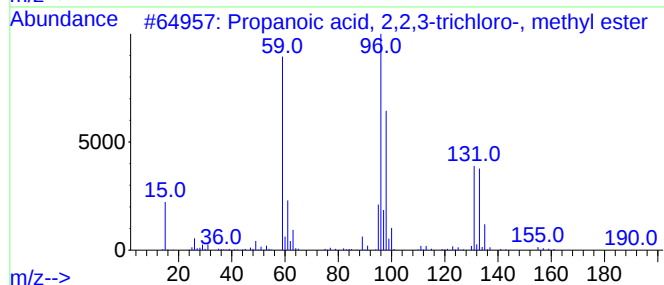
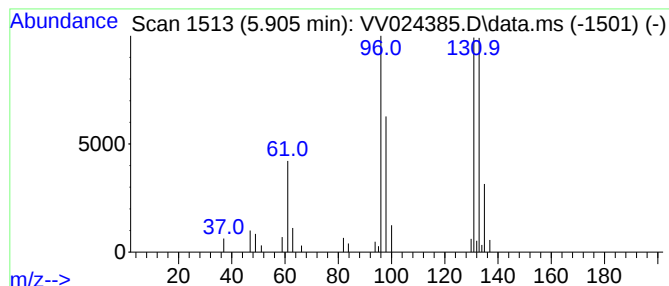
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	2.81 ug/L	44960	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
5			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.905	2.8	ug/L	44960	1	5.612	799308	50.0