

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042821\
 Data File : VV021209.D
 Acq On : 28 Apr 2021 18:35
 Operator : SY/MD
 Sample : M2165-21ME 5X
 Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB3G2ME

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\SFAMVLM042121WMA.M

Title : VOC Analysis

Signal : TIC: VV021209.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	100	rVB	336351	361240	8.93%	1.417%
2	1.568	158	164	178	rVB	268481	309249	7.65%	1.213%
3	2.105	322	331	366	rVB	650448	973550	24.07%	3.819%
4	2.294	384	390	400	rVB	7165	10515	0.26%	0.041%
5	2.375	410	415	420	rBV5	1238	1569	0.04%	0.006%
6	2.397	420	422	425	rBV4	1032	602	0.01%	0.002%
7	2.764	530	536	541	rBV7	3858	4691	0.12%	0.018%
8	2.889	569	575	576	rBV2	821	832	0.02%	0.003%
9	2.953	593	595	598	rBV3	1083	792	0.02%	0.003%
10	3.063	623	629	631	rBV2	744	721	0.02%	0.003%
11	3.114	641	645	650	rBV3	727	710	0.02%	0.003%
12	3.249	683	687	688	rBV3	439	275	0.01%	0.001%
13	3.265	689	692	695	rVV4	720	551	0.01%	0.002%
14	3.323	707	710	713	rBV2	572	302	0.01%	0.001%
15	3.375	723	726	730	rBV	629	479	0.01%	0.002%
16	3.429	742	743	744	rBV	396	146	0.00%	0.001%
17	3.616	798	801	804	rBV2	610	451	0.01%	0.002%
18	3.664	814	816	818	rBV2	468	248	0.01%	0.001%
19	3.722	833	834	836	rBV	244	126	0.00%	0.000%
20	3.767	843	848	851	rBV4	1341	1320	0.03%	0.005%
21	3.847	869	873	876	rVB2	866	648	0.02%	0.003%
22	3.902	876	890	929	rBV2	143542	510574	12.63%	2.003%
23	4.291	1009	1011	1012	rBV	975	495	0.01%	0.002%
24	4.352	1013	1030	1056	rVV	447445	1098165	27.15%	4.308%
25	4.815	1172	1174	1175	rBV2	597	221	0.01%	0.001%
26	4.879	1191	1194	1197	rBV2	839	511	0.01%	0.002%
27	4.908	1201	1203	1205	rBV2	489	196	0.00%	0.001%
28	4.989	1225	1228	1229	rBV2	701	441	0.01%	0.002%
29	5.050	1229	1247	1281	rVV2	1023340	2625641	64.92%	10.300%
30	5.339	1335	1337	1340	rBV3	742	425	0.01%	0.002%
31	5.404	1351	1357	1359	rBV3	1003	1077	0.03%	0.004%
32	5.564	1405	1407	1409	rBV	537	228	0.01%	0.001%
33	5.619	1412	1424	1455	rBV	874347	1764800	43.64%	6.923%
34	5.912	1504	1515	1531	rBV3	42062	91079	2.25%	0.357%
35	6.072	1552	1565	1595	rBV2	571800	1176736	29.10%	4.616%
36	6.346	1648	1650	1653	rBV2	611	383	0.01%	0.002%

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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\SFAMVLM042121WMA.M
 Title : VOC Analysis

37	6.590	1724	1726	1729	rBV3	611	368	0.01%	0.001%
38	6.715	1762	1765	1770	rVB5	1004	947	0.02%	0.004%
39	6.770	1779	1782	1785	rVB4	1357	722	0.02%	0.003%
40	6.989	1839	1850	1880	rBV	314069	595215	14.72%	2.335%
41	7.227	1921	1924	1929	rBV5	1173	1128	0.03%	0.004%
42	7.320	1940	1953	1970	rBV	1258186	2179296	53.89%	8.549%
43	7.625	2039	2048	2072	rBV2	221111	391649	9.68%	1.536%
44	7.979	2144	2158	2182	rBV	2441894	4044124	100.00%	15.865%
45	8.095	2185	2194	2231	rVV	569335	1128523	27.91%	4.427%
46	8.522	2322	2327	2332	rBV4	940	1019	0.03%	0.004%
47	8.690	2376	2379	2384	rBV4	920	697	0.02%	0.003%
48	8.857	2419	2431	2457	rBV	1344032	2197302	54.33%	8.620%
49	9.153	2515	2523	2529	rBV5	4955	7448	0.18%	0.029%
50	9.358	2585	2587	2588	rBV	621	305	0.01%	0.001%
51	9.391	2595	2597	2599	rBV	700	364	0.01%	0.001%
52	9.487	2621	2627	2629	rBV2	662	808	0.02%	0.003%
53	9.561	2641	2650	2654	rBV7	3319	4911	0.12%	0.019%
54	9.738	2701	2705	2708	rBV4	1160	997	0.02%	0.004%
55	9.850	2738	2740	2745	rVB4	1176	669	0.02%	0.003%
56	9.944	2764	2769	2776	rVB9	3135	4008	0.10%	0.016%
57	10.056	2801	2804	2805	rBV	453	269	0.01%	0.001%
58	10.136	2821	2829	2841	rVB7	5382	9549	0.24%	0.037%
59	10.223	2841	2856	2880	rBV	869510	1364288	33.74%	5.352%
60	10.458	2925	2929	2931	rBV2	1279	927	0.02%	0.004%
61	10.548	2949	2957	2960	rBV6	3444	4292	0.11%	0.017%
62	10.635	2981	2984	2985	rBV	751	383	0.01%	0.002%
63	10.863	3052	3055	3058	rBV3	686	560	0.01%	0.002%
64	10.924	3067	3074	3086	rBV4	11072	17385	0.43%	0.068%
65	10.985	3091	3093	3097	rVB3	589	266	0.01%	0.001%
66	11.085	3121	3124	3126	rBV	713	433	0.01%	0.002%
67	11.159	3139	3147	3150	rBV7	3351	4922	0.12%	0.019%
68	11.255	3166	3177	3204	rBV	1457101	2254032	55.74%	8.842%
69	11.632	3282	3294	3314	rBV	1388929	2231571	55.18%	8.754%
70	12.172	3460	3462	3465	rVB2	846	404	0.01%	0.002%
71	12.439	3541	3545	3554	rBV5	2199	2491	0.06%	0.010%
72	12.657	3605	3613	3628	rVB3	14943	24072	0.60%	0.094%
73	13.046	3729	3734	3738	rBV3	1159	1511	0.04%	0.006%
74	13.127	3757	3759	3762	rVB2	785	351	0.01%	0.001%
75	13.175	3772	3774	3775	rBV	587	250	0.01%	0.001%
76	13.275	3798	3805	3821	rVB4	16143	24778	0.61%	0.097%

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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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Title : VOC Analysis

77	13.513	3874	3879	3891	rVB2	11909	20200	0.50%	0.079%
78	13.754	3947	3954	3966	rVB4	16569	27909	0.69%	0.109%

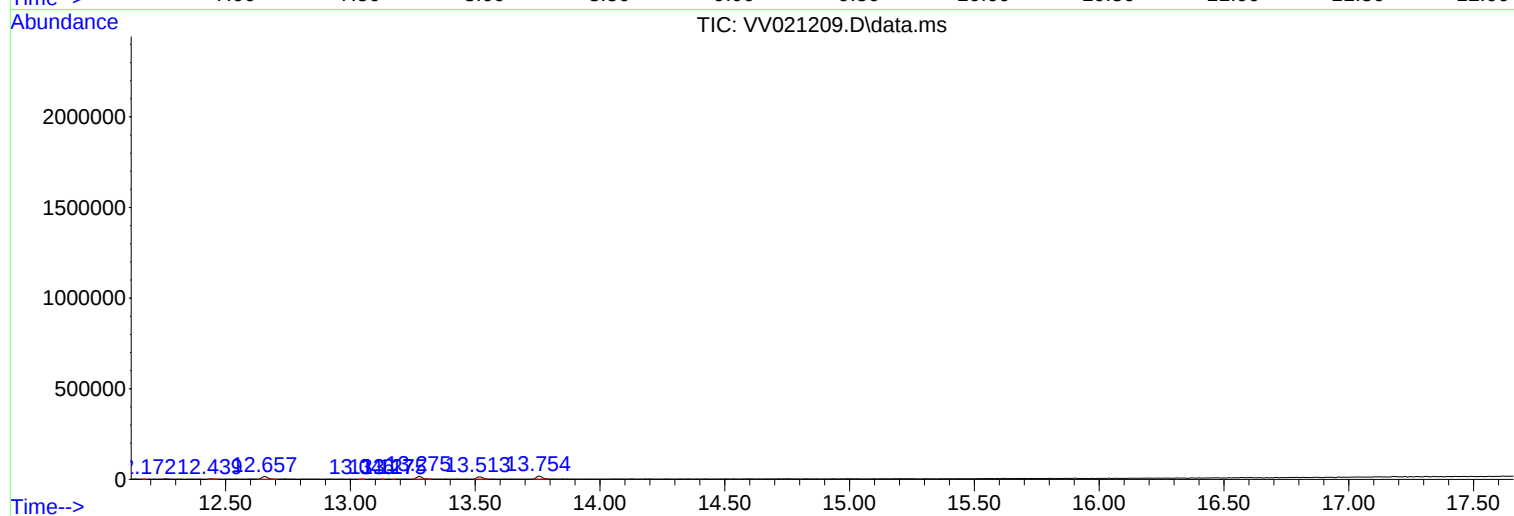
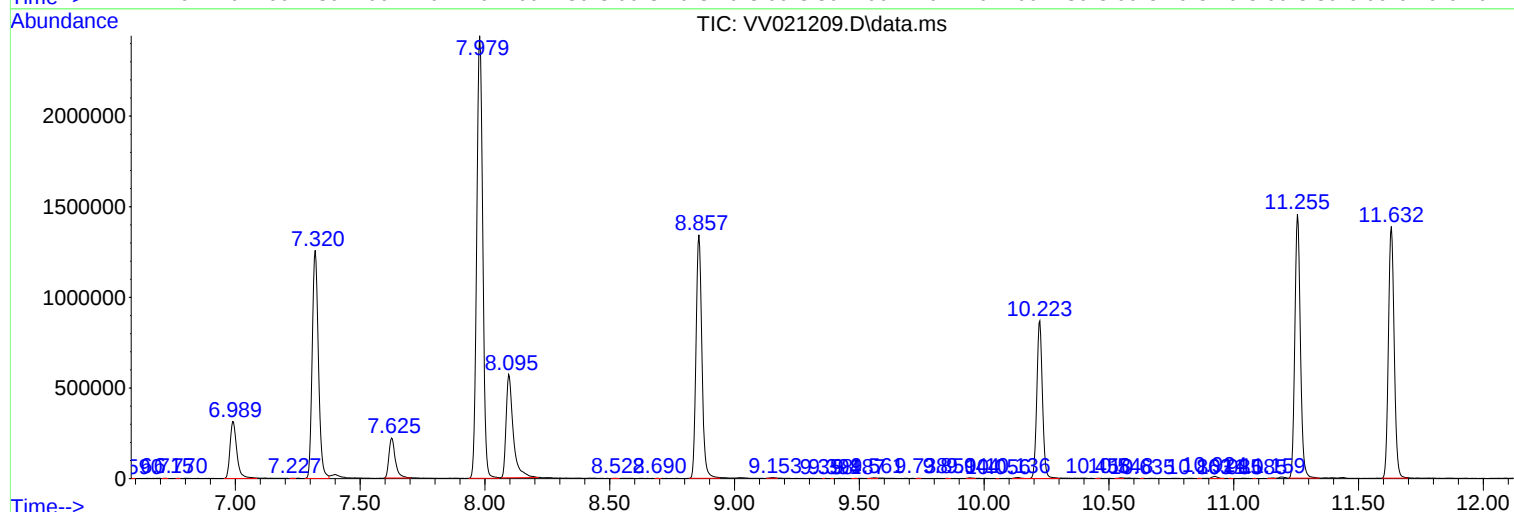
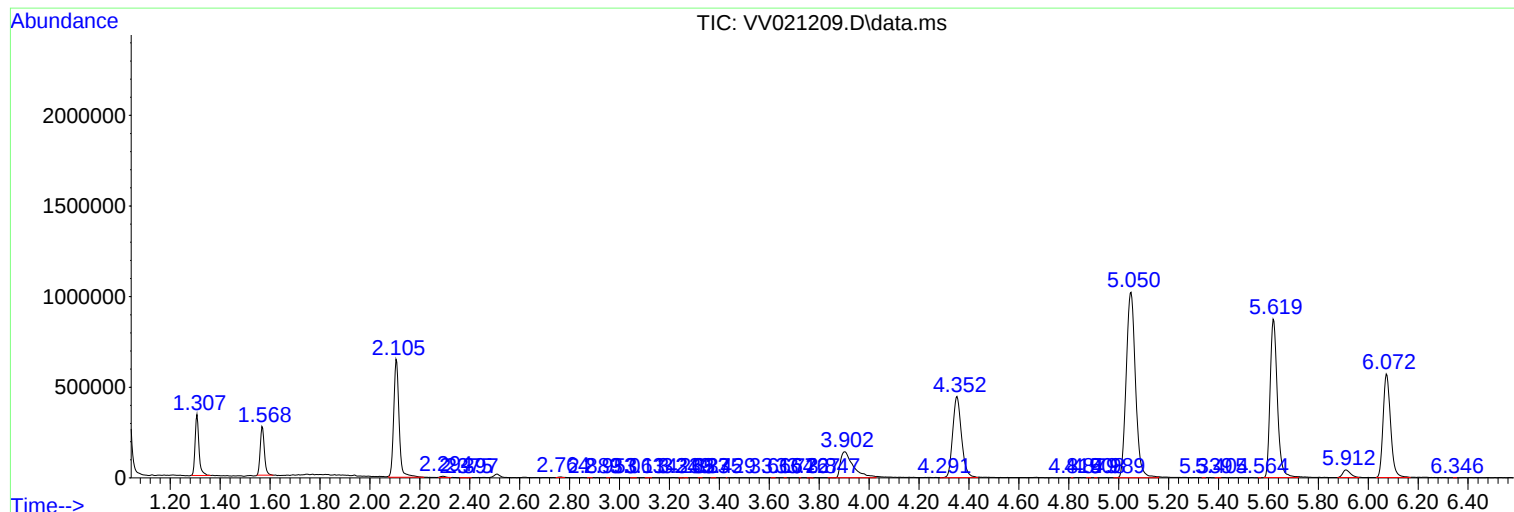
Sum of corrected areas: 25491332

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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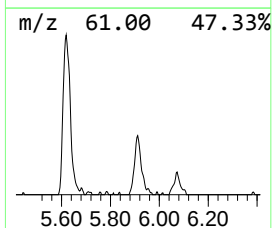
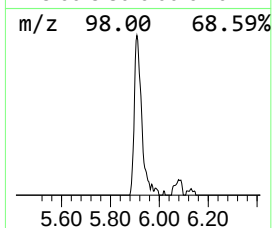
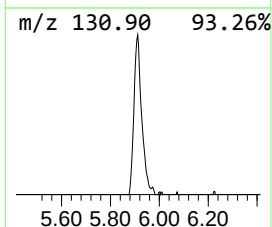
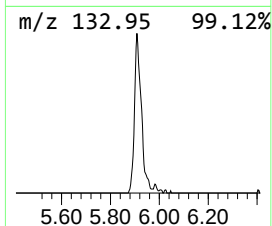
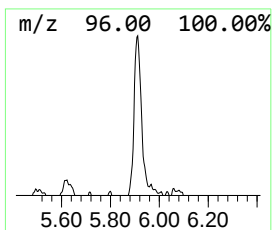
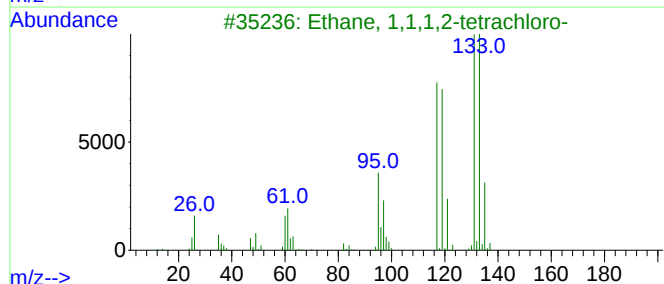
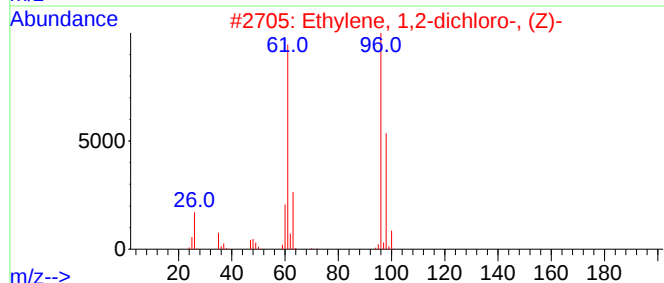
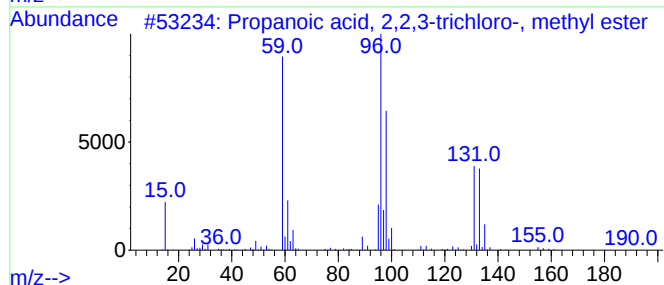
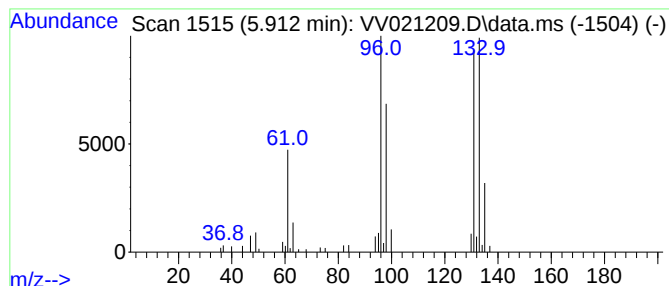
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.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.
5.912	2.58 ug/L	91079	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	37
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			5-Hydroxypyrimidine	96	C4H4N2O	026456-59-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.912	2.6	ug/L	91079	1	5.619	1764800	50.0