

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021935.D
 Acq On : 23 Aug 2021 16:59
 Operator : SY/MD
 Sample : M3486-06ME
 Misc : 5.22g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AR5ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	112	rVB	123499	177278	13.13%	1.610%
2	2.072	311	321	334	rBV	257701	368029	27.25%	3.343%
3	2.490	443	451	464	rVB	17178	28717	2.13%	0.261%
4	2.696	513	515	519	rVB3	508	296	0.02%	0.003%
5	2.738	523	528	533	rBV2	629	460	0.03%	0.004%
6	2.799	543	547	549	rVB2	344	243	0.02%	0.002%
7	2.825	553	555	559	rVV	359	181	0.01%	0.002%
8	2.873	564	570	573	rBV5	599	577	0.04%	0.005%
9	2.944	588	592	595	rBV2	587	412	0.03%	0.004%
10	3.015	605	614	616	rBV4	772	828	0.06%	0.008%
11	3.047	623	624	629	rBV2	342	192	0.01%	0.002%
12	3.207	671	674	682	rBV3	338	311	0.02%	0.003%
13	3.519	769	771	776	rVV2	188	185	0.01%	0.002%
14	3.616	793	801	804	rVB3	353	417	0.03%	0.004%
15	3.635	804	807	808	rBV	323	178	0.01%	0.002%
16	3.741	839	840	844	rVB2	398	191	0.01%	0.002%
17	3.793	851	856	858	rBV3	280	265	0.02%	0.002%
18	3.899	878	889	947	rBV3	68439	317139	23.49%	2.881%
19	4.346	1012	1028	1058	rBV2	192385	517898	38.35%	4.705%
20	4.645	1119	1121	1124	rBV4	593	365	0.03%	0.003%
21	4.664	1124	1127	1129	rVB2	395	213	0.02%	0.002%
22	4.905	1200	1202	1205	rVB	501	251	0.02%	0.002%
23	4.973	1220	1223	1226	rBV	335	233	0.02%	0.002%
24	5.040	1226	1244	1276	rBV2	541489	1350348	100.00%	12.266%
25	5.339	1326	1337	1355	rBV7	5181	16460	1.22%	0.150%
26	5.561	1402	1406	1410	rBV4	511	518	0.04%	0.005%
27	5.613	1410	1422	1461	rBV	438922	924862	68.49%	8.401%
28	5.847	1492	1495	1496	rBV2	339	197	0.01%	0.002%
29	5.902	1500	1512	1529	rBV3	28244	62825	4.65%	0.571%
30	6.069	1552	1564	1587	rBV	277347	591009	43.77%	5.369%
31	6.358	1653	1654	1659	rVB2	490	263	0.02%	0.002%
32	6.445	1674	1681	1682	rBV3	413	458	0.03%	0.004%
33	6.535	1707	1709	1713	rVB2	371	178	0.01%	0.002%
34	6.593	1724	1727	1729	rBV	307	184	0.01%	0.002%
35	6.780	1784	1785	1789	rVB	474	204	0.02%	0.002%
36	6.879	1811	1816	1817	rBV	390	281	0.02%	0.003%

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 Title : VOC Analysis

37	6.924	1824	1830	1835	rBV4	475	519	0.04%	0.005%
38	6.989	1837	1850	1878	rBV	157735	313048	23.18%	2.844%
39	7.265	1934	1936	1939	rVB	491	197	0.01%	0.002%
40	7.317	1939	1952	1970	rBV	637357	1147438	84.97%	10.423%
41	7.625	2037	2048	2076	rBV	103389	204458	15.14%	1.857%
42	7.760	2087	2090	2099	rVB6	1009	1068	0.08%	0.010%
43	7.799	2099	2102	2105	rBV3	546	511	0.04%	0.005%
44	7.931	2141	2143	2148	rVB	330	218	0.02%	0.002%
45	7.960	2148	2152	2153	rBV2	396	241	0.02%	0.002%
46	8.104	2184	2197	2234	rBV2	318019	710640	52.63%	6.455%
47	8.407	2287	2291	2295	rBV4	638	556	0.04%	0.005%
48	8.474	2310	2312	2315	rVB3	424	236	0.02%	0.002%
49	8.497	2315	2319	2322	rVB4	519	383	0.03%	0.003%
50	8.532	2327	2330	2333	rBV2	412	260	0.02%	0.002%
51	8.622	2355	2358	2359	rBV	489	326	0.02%	0.003%
52	8.667	2368	2372	2374	rBV3	506	340	0.03%	0.003%
53	8.728	2389	2391	2398	rVB	276	187	0.01%	0.002%
54	8.854	2418	2430	2460	rBV	665513	1154920	85.53%	10.491%
55	9.088	2500	2503	2505	rBV2	340	246	0.02%	0.002%
56	9.117	2509	2512	2514	rBV	599	368	0.03%	0.003%
57	9.159	2515	2525	2531	rBV8	1483	2313	0.17%	0.021%
58	9.419	2604	2606	2610	rVB2	337	179	0.01%	0.002%
59	9.442	2610	2613	2615	rVB	414	221	0.02%	0.002%
60	9.458	2615	2618	2621	rBV	361	284	0.02%	0.003%
61	9.522	2635	2638	2639	rBV	409	190	0.01%	0.002%
62	9.609	2663	2665	2671	rVB3	546	367	0.03%	0.003%
63	9.661	2678	2681	2684	rBV3	332	240	0.02%	0.002%
64	9.686	2684	2689	2693	rVB4	515	460	0.03%	0.004%
65	9.805	2722	2726	2729	rBV2	337	232	0.02%	0.002%
66	9.944	2764	2769	2770	rBV	439	267	0.02%	0.002%
67	10.017	2790	2792	2795	rVV2	314	206	0.02%	0.002%
68	10.046	2799	2801	2806	rVB2	303	199	0.01%	0.002%
69	10.130	2817	2827	2840	rBV3	4543	7724	0.57%	0.070%
70	10.223	2844	2856	2877	rVV	420199	675114	50.00%	6.133%
71	10.551	2953	2958	2959	rBV	336	215	0.02%	0.002%
72	10.571	2959	2964	2965	rBV3	1355	964	0.07%	0.009%
73	10.712	3005	3008	3010	rBV3	284	211	0.02%	0.002%
74	10.760	3019	3023	3024	rBV	344	199	0.01%	0.002%
75	10.770	3024	3026	3029	rVV2	558	294	0.02%	0.003%
76	10.828	3040	3044	3045	rBV2	544	364	0.03%	0.003%

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77	10.889	3057	3063	3064	rBV3	601	479	0.04%	0.004%
78	11.085	3120	3124	3126	rVB2	422	281	0.02%	0.003%
79	11.149	3138	3144	3150	rVV4	2132	2698	0.20%	0.025%
80	11.194	3155	3158	3162	rBV4	816	747	0.06%	0.007%
81	11.252	3165	3176	3194	rBV	800220	1245543	92.24%	11.314%
82	11.506	3253	3255	3258	rBV3	561	391	0.03%	0.004%
83	11.538	3263	3265	3269	rBV2	674	567	0.04%	0.005%
84	11.628	3281	3293	3312	rBV	734788	1163670	86.18%	10.571%
85	12.050	3422	3424	3426	rBV3	608	401	0.03%	0.004%
86	12.075	3430	3432	3436	rBV2	920	691	0.05%	0.006%
87	12.169	3458	3461	3464	rVB	392	293	0.02%	0.003%
88	12.249	3481	3486	3488	rBV2	729	591	0.04%	0.005%
89	12.426	3537	3541	3542	rBV	399	193	0.01%	0.002%
90	12.451	3547	3549	3552	rBV	473	248	0.02%	0.002%
91	12.644	3606	3609	3610	rBV	439	248	0.02%	0.002%
92	12.824	3663	3665	3669	rVB2	420	203	0.02%	0.002%
93	13.072	3739	3742	3744	rBV2	480	279	0.02%	0.003%
94	13.156	3765	3768	3773	rBV	446	277	0.02%	0.003%
95	13.339	3823	3825	3829	rVB2	391	233	0.02%	0.002%
96	13.397	3839	3843	3844	rBV2	290	192	0.01%	0.002%
97	13.455	3858	3861	3863	rBV	597	342	0.03%	0.003%
98	13.599	3904	3906	3908	rBV	389	221	0.02%	0.002%
99	14.008	4031	4033	4036	rBV2	522	350	0.03%	0.003%
100	14.721	4253	4255	4258	rBV3	628	376	0.03%	0.003%

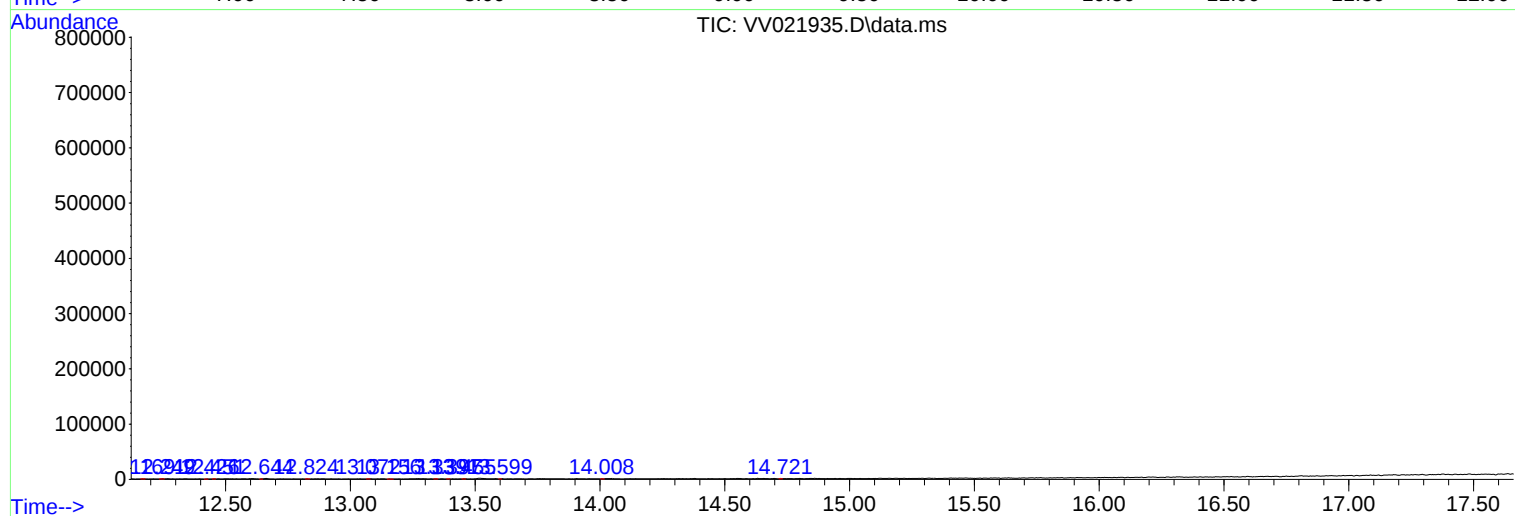
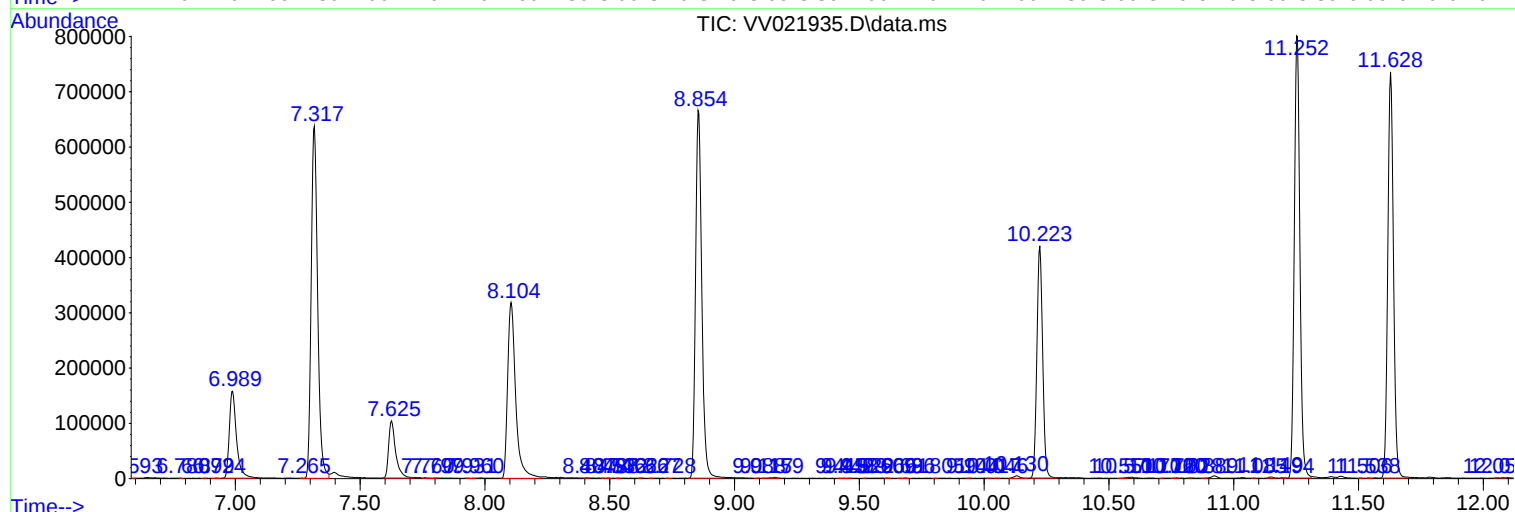
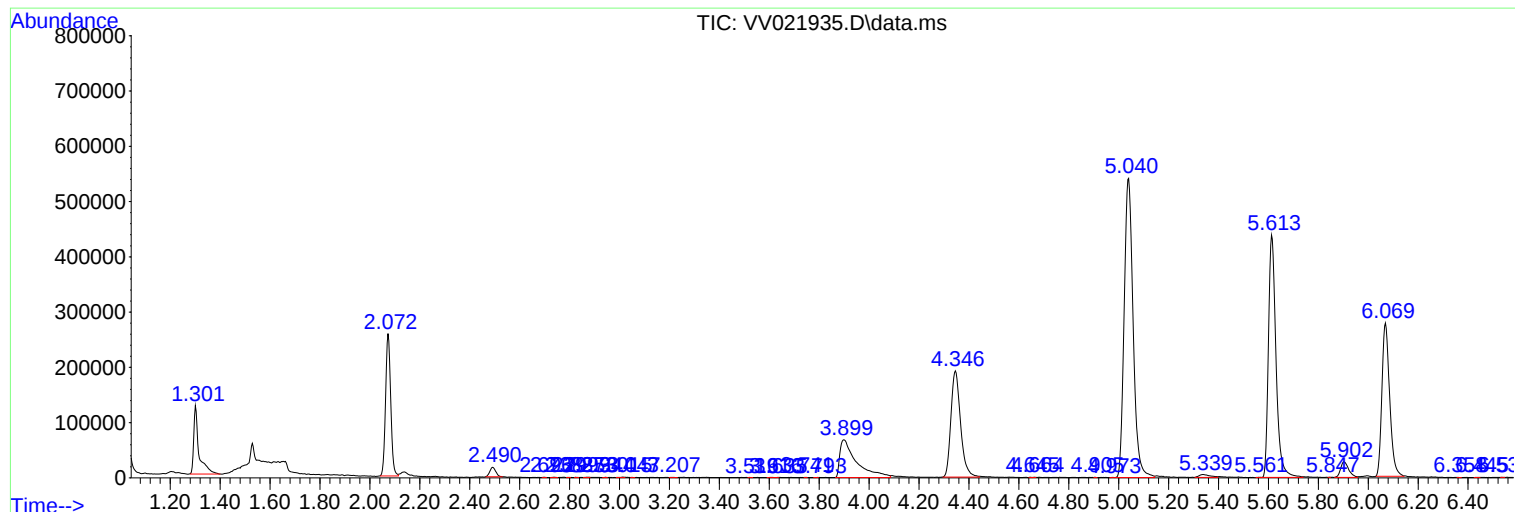
Sum of corrected areas: 11008563

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C0AR5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



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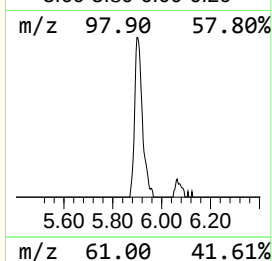
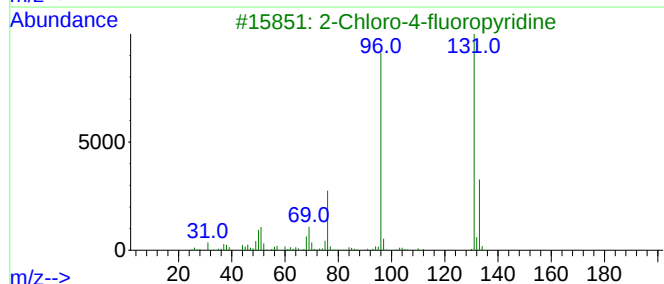
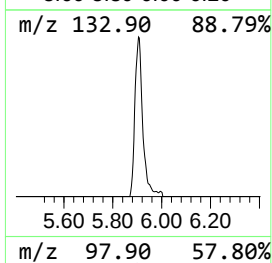
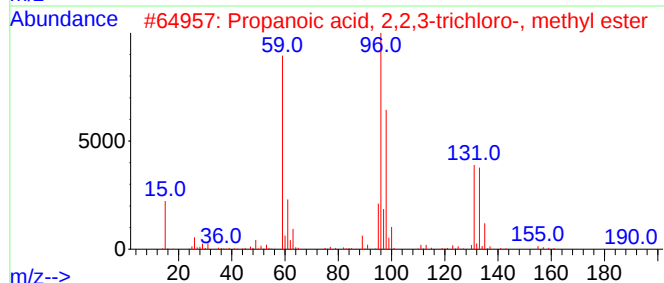
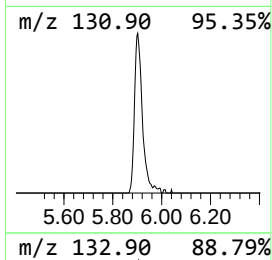
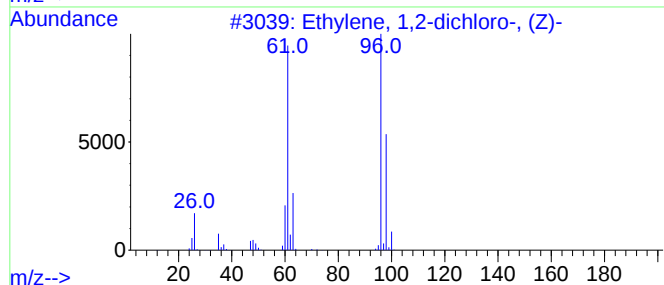
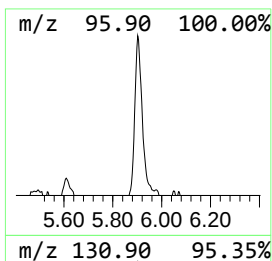
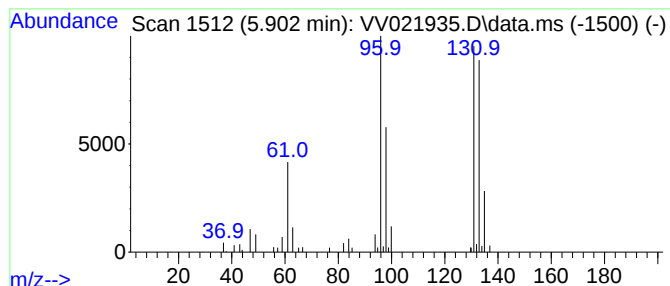
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.40 ug/L	62825	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	3.4	ug/L	62825	1	5.613	924862	50.0