

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083121\
 Data File : VV022034.D
 Acq On : 31 Aug 2021 12:06
 Operator : SY/MD
 Sample : M3579-06MEDL 100X
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB6A8MEDL

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\SFAMVLM082721WMA.M

Title : VOC Analysis

Signal : TIC: VV022034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	92	rBV	138702	135033	11.43%	1.434%
2	1.565	155	163	176	rVB	122391	142777	12.09%	1.517%
3	2.105	322	331	356	rVB	249807	367961	31.15%	3.909%
4	2.510	449	457	467	rVB4	5053	7814	0.66%	0.083%
5	2.751	528	532	535	rBV2	302	209	0.02%	0.002%
6	2.847	558	562	563	rBV2	245	150	0.01%	0.002%
7	2.944	590	592	595	rVB	312	179	0.02%	0.002%
8	3.008	609	612	617	rBV2	384	266	0.02%	0.003%
9	3.156	656	658	661	rVB2	328	152	0.01%	0.002%
10	3.288	697	699	701	rVB	430	170	0.01%	0.002%
11	3.478	754	758	759	rBV2	203	167	0.01%	0.002%
12	3.545	776	779	783	rBV3	397	273	0.02%	0.003%
13	3.593	789	794	798	rBV2	399	305	0.03%	0.003%
14	3.642	804	809	812	rBV2	407	328	0.03%	0.003%
15	3.690	822	824	828	rVB2	360	166	0.01%	0.002%
16	3.770	845	849	852	rBV2	217	152	0.01%	0.002%
17	3.876	872	882	915	rBV	107387	285659	24.18%	3.034%
18	4.349	1014	1029	1057	rBV	174689	465619	39.42%	4.946%
19	4.609	1106	1110	1113	rBV2	476	384	0.03%	0.004%
20	4.661	1124	1126	1129	rBV	543	355	0.03%	0.004%
21	4.796	1166	1168	1170	rVB2	292	159	0.01%	0.002%
22	4.963	1217	1220	1223	rBV	412	363	0.03%	0.004%
23	5.047	1229	1246	1276	rBV2	460247	1181312	100.00%	12.548%
24	5.288	1319	1321	1324	rBV2	537	363	0.03%	0.004%
25	5.619	1410	1424	1457	rBV	380586	778385	65.89%	8.268%
26	5.908	1502	1514	1532	rBV	28955	61429	5.20%	0.653%
27	6.072	1551	1565	1587	rBV	263430	536566	45.42%	5.700%
28	6.349	1647	1651	1658	rVB4	494	513	0.04%	0.005%
29	6.381	1658	1661	1664	rVB	377	219	0.02%	0.002%
30	6.407	1667	1669	1671	rBV	501	271	0.02%	0.003%
31	6.510	1699	1701	1704	rBV2	328	231	0.02%	0.002%
32	6.558	1715	1716	1719	rBV3	400	236	0.02%	0.003%
33	6.603	1727	1730	1731	rBV	287	150	0.01%	0.002%
34	6.645	1739	1743	1744	rBV2	512	320	0.03%	0.003%
35	6.709	1757	1763	1766	rBV2	383	375	0.03%	0.004%
36	6.757	1776	1778	1782	rVB2	296	173	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
 Title : VOC Analysis

37	6.780	1782	1785	1788	rVB2	385	167	0.01%	0.002%
38	6.857	1807	1809	1812	rVB2	399	182	0.02%	0.002%
39	6.989	1838	1850	1873	rBV	139467	259219	21.94%	2.754%
40	7.275	1936	1939	1940	rBV2	342	196	0.02%	0.002%
41	7.317	1941	1952	1972	rBV	552007	966241	81.79%	10.264%
42	7.625	2038	2048	2068	rBV	95165	167289	14.16%	1.777%
43	7.815	2105	2107	2108	rBV	375	161	0.01%	0.002%
44	7.895	2128	2132	2135	rBV2	315	281	0.02%	0.003%
45	7.979	2148	2158	2173	rVV3	18791	33952	2.87%	0.361%
46	8.092	2183	2193	2226	rBV2	296051	586634	49.66%	6.231%
47	8.365	2276	2278	2281	rBV	354	156	0.01%	0.002%
48	8.436	2297	2300	2303	rBV3	484	257	0.02%	0.003%
49	8.542	2331	2333	2335	rVB	339	151	0.01%	0.002%
50	8.638	2359	2363	2366	rBV3	452	416	0.04%	0.004%
51	8.699	2380	2382	2385	rVB3	419	256	0.02%	0.003%
52	8.757	2398	2400	2405	rVB2	323	209	0.02%	0.002%
53	8.854	2413	2430	2459	rBV	590296	951938	80.58%	10.112%
54	9.104	2506	2508	2513	rBV4	383	212	0.02%	0.002%
55	9.223	2542	2545	2547	rBV3	403	220	0.02%	0.002%
56	9.272	2555	2560	2562	rVV2	259	202	0.02%	0.002%
57	9.420	2604	2606	2611	rBV3	277	182	0.02%	0.002%
58	9.493	2625	2629	2631	rVB	293	164	0.01%	0.002%
59	9.532	2637	2641	2643	rBV	293	242	0.02%	0.003%
60	9.625	2667	2670	2673	rBV3	369	269	0.02%	0.003%
61	9.674	2683	2685	2688	rVV2	303	225	0.02%	0.002%
62	9.789	2718	2721	2726	rBV2	275	196	0.02%	0.002%
63	10.075	2809	2810	2813	rVB	391	168	0.01%	0.002%
64	10.133	2820	2828	2836	rBV8	2125	3547	0.30%	0.038%
65	10.217	2842	2854	2873	rBV	356774	565315	47.85%	6.005%
66	10.352	2894	2896	2897	rBV	347	164	0.01%	0.002%
67	10.452	2925	2927	2930	rBV2	238	150	0.01%	0.002%
68	10.513	2942	2946	2948	rBV	342	222	0.02%	0.002%
69	10.545	2951	2956	2960	rBV4	310	330	0.03%	0.004%
70	10.661	2989	2992	2996	rVB3	346	235	0.02%	0.002%
71	10.702	3002	3005	3007	rBV2	291	171	0.01%	0.002%
72	10.767	3021	3025	3028	rBV2	364	260	0.02%	0.003%
73	10.805	3034	3037	3042	rBV2	410	438	0.04%	0.005%
74	10.873	3054	3058	3059	rBV	370	207	0.02%	0.002%
75	10.921	3067	3073	3083	rVV5	2045	3051	0.26%	0.032%
76	11.001	3096	3098	3101	rBV	226	159	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
 Title : VOC Analysis

77	11.034	3105	3108	3109	rBV	522	235	0.02%	0.002%
78	11.133	3135	3139	3140	rBV	532	348	0.03%	0.004%
79	11.198	3156	3159	3161	rVB2	415	191	0.02%	0.002%
80	11.252	3164	3176	3198	rBV	623955	961829	81.42%	10.217%
81	11.529	3260	3262	3264	rBV	322	187	0.02%	0.002%
82	11.545	3264	3267	3270	rVV4	431	271	0.02%	0.003%
83	11.625	3278	3292	3317	rBV	586463	933478	79.02%	9.916%
84	11.828	3352	3355	3358	rVB3	383	211	0.02%	0.002%
85	11.876	3368	3370	3372	rVB	382	192	0.02%	0.002%
86	11.889	3372	3374	3379	rVB3	461	322	0.03%	0.003%
87	11.976	3399	3401	3403	rBV2	344	156	0.01%	0.002%
88	12.101	3437	3440	3444	rBV3	468	385	0.03%	0.004%
89	12.156	3455	3457	3460	rVB2	630	277	0.02%	0.003%
90	12.243	3482	3484	3488	rBV2	574	438	0.04%	0.005%
91	12.304	3499	3503	3504	rBV	347	195	0.02%	0.002%
92	12.355	3516	3519	3522	rBV	299	165	0.01%	0.002%
93	12.657	3611	3613	3619	rVB3	533	314	0.03%	0.003%
94	12.821	3662	3664	3668	rVB	375	193	0.02%	0.002%
95	13.246	3794	3796	3798	rBV	307	152	0.01%	0.002%
96	13.310	3813	3816	3819	rBV2	554	327	0.03%	0.003%
97	13.554	3889	3892	3895	rBV	424	338	0.03%	0.004%
98	13.853	3981	3985	3986	rBV2	290	201	0.02%	0.002%
99	14.226	4097	4101	4102	rBV	339	193	0.02%	0.002%
100	15.689	4555	4556	4557	rBV	784	257	0.02%	0.003%

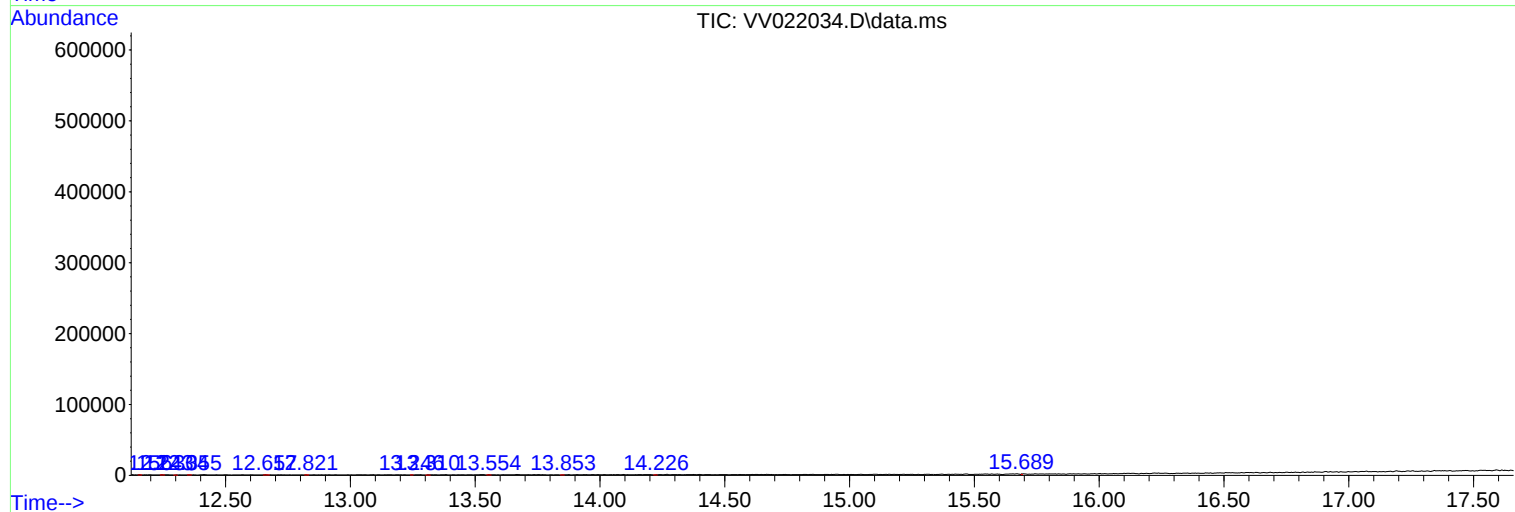
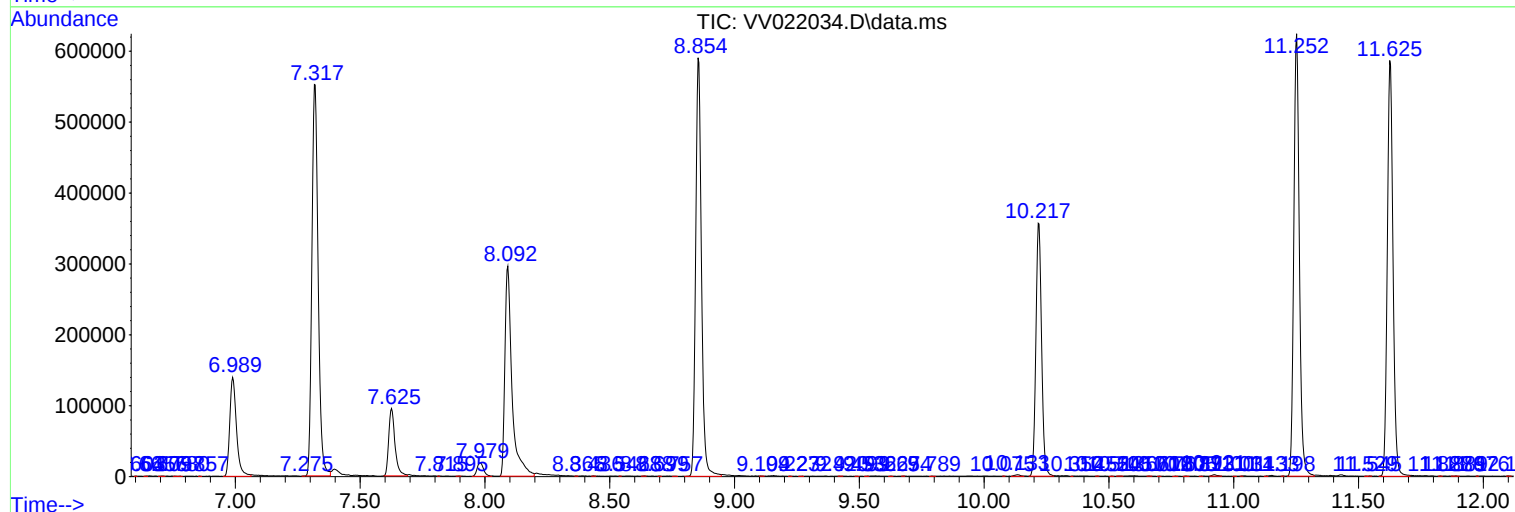
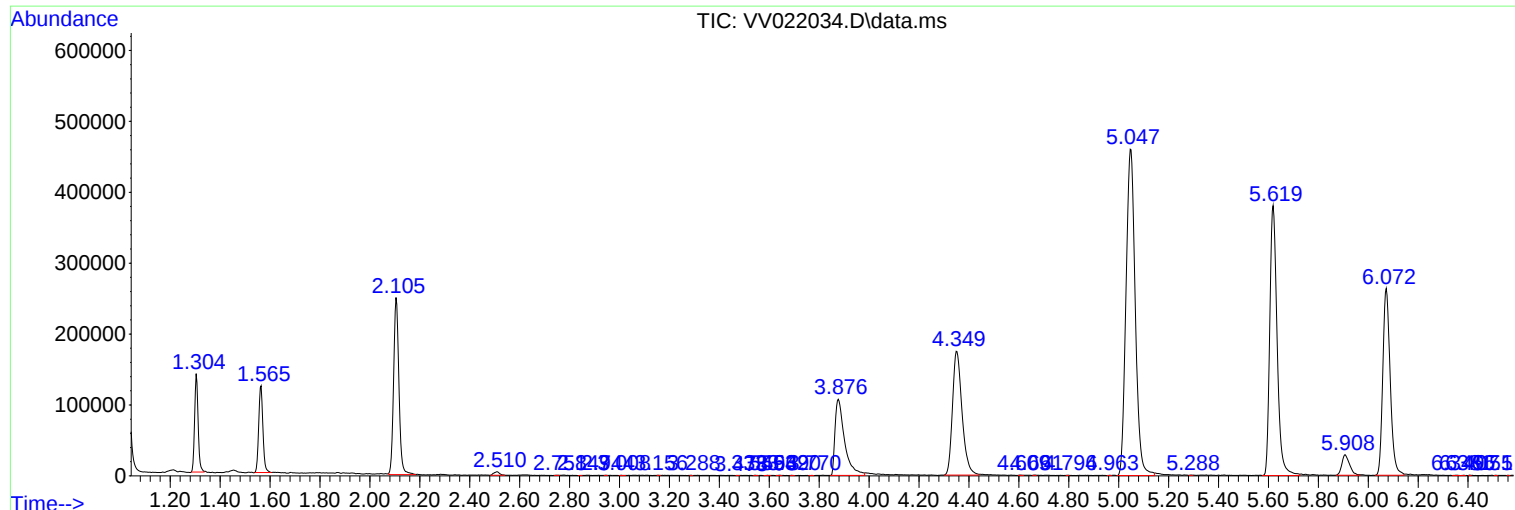
Sum of corrected areas: 9414073

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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



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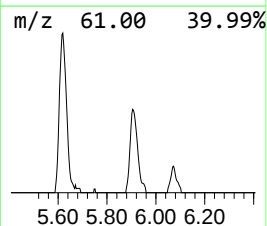
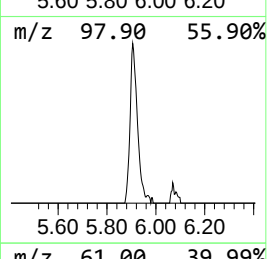
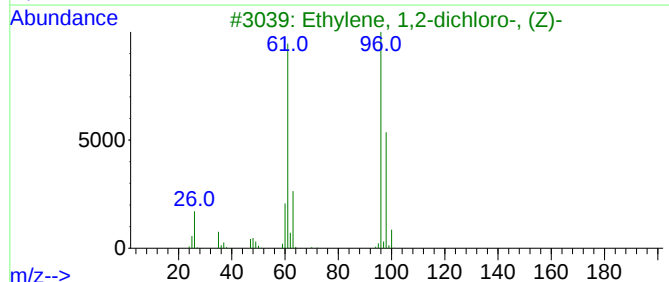
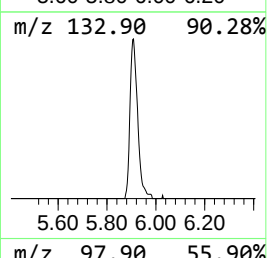
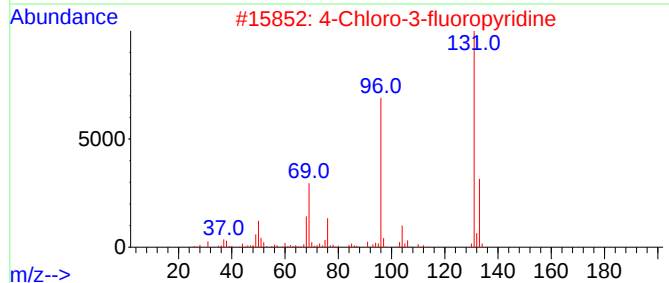
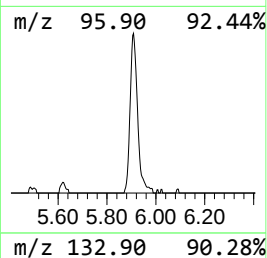
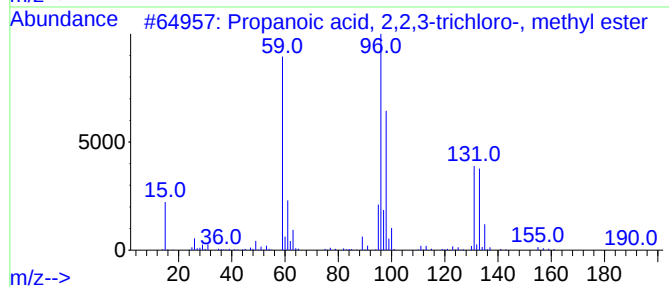
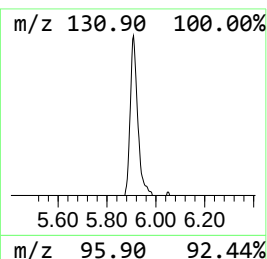
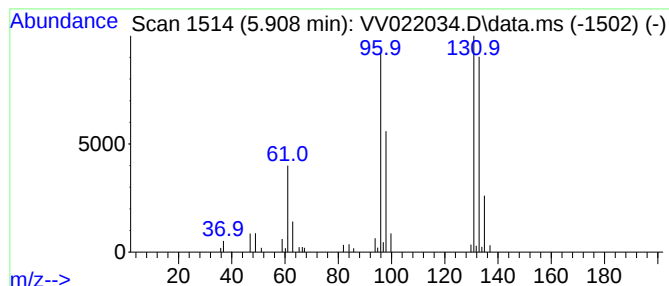
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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.
5.908	3.95 ug/L	61429	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	40
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	4.0	ug/L	61429	1	5.619	778385	50.0