

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091721\
 Data File : VV022217.D
 Acq On : 18 Sep 2021 04:19
 Operator : SY/MD
 Sample : M3787-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0CJ5

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: VV022217.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	75	82	101	rVB	169115	176719	15.19%	2.084%
2	1.564	156	163	177	rBV	135844	156387	13.44%	1.845%
3	2.104	321	331	345	rBV	293497	419258	36.04%	4.945%
4	2.683	508	511	512	rBV	277	156	0.01%	0.002%
5	2.719	518	522	526	rVB2	410	351	0.03%	0.004%
6	2.757	529	534	537	rBV2	540	436	0.04%	0.005%
7	2.857	561	565	567	rBV	243	193	0.02%	0.002%
8	2.902	574	579	583	rBV	383	368	0.03%	0.004%
9	2.928	584	587	591	rVB3	357	282	0.02%	0.003%
10	2.989	604	606	609	rVB2	333	164	0.01%	0.002%
11	3.021	613	616	619	rBV2	232	148	0.01%	0.002%
12	3.204	670	673	675	rBV2	236	167	0.01%	0.002%
13	3.239	680	684	688	rBV3	332	277	0.02%	0.003%
14	3.378	722	727	729	rBV3	416	266	0.02%	0.003%
15	3.394	729	732	735	rVB	335	199	0.02%	0.002%
16	3.706	824	829	831	rBV2	387	276	0.02%	0.003%
17	3.744	836	841	850	rBV3	566	847	0.07%	0.010%
18	3.818	861	864	868	rBV3	257	175	0.02%	0.002%
19	3.905	880	891	926	rBV2	71018	266522	22.91%	3.144%
20	4.352	1014	1030	1052	rBV	182719	453800	39.01%	5.352%
21	4.600	1101	1107	1110	rBV4	545	559	0.05%	0.007%
22	4.815	1171	1174	1176	rBV2	234	147	0.01%	0.002%
23	4.924	1204	1208	1211	rBV2	333	262	0.02%	0.003%
24	5.046	1229	1246	1281	rBV2	461539	1163291	100.00%	13.721%
25	5.558	1403	1405	1411	rVB2	348	216	0.02%	0.003%
26	5.619	1411	1424	1452	rBV	332469	669255	57.53%	7.894%
27	5.908	1503	1514	1536	rBV2	25544	53885	4.63%	0.636%
28	6.072	1551	1565	1588	rBV	256921	524169	45.06%	6.182%
29	6.300	1632	1636	1639	rVB3	816	525	0.05%	0.006%
30	6.349	1648	1651	1655	rVB4	515	297	0.03%	0.004%
31	6.381	1659	1661	1668	rVB3	432	395	0.03%	0.005%
32	6.439	1675	1679	1682	rBV2	489	339	0.03%	0.004%
33	6.519	1701	1704	1712	rBV3	338	312	0.03%	0.004%
34	6.606	1728	1731	1733	rBV2	298	157	0.01%	0.002%
35	6.747	1770	1775	1779	rBV2	372	313	0.03%	0.004%
36	6.825	1797	1799	1806	rVB2	252	227	0.02%	0.003%

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 Title : VOC Analysis

37	6.853	1806	1808	1811	rBV	334	212	0.02%	0.003%
38	6.911	1823	1826	1836	rBV4	356	462	0.04%	0.005%
39	6.989	1839	1850	1872	rBV	123293	224024	19.26%	2.642%
40	7.275	1936	1939	1940	rBV	326	150	0.01%	0.002%
41	7.320	1940	1953	1971	rBV	518346	916063	78.75%	10.805%
42	7.625	2035	2048	2071	rBV	82538	149108	12.82%	1.759%
43	7.921	2136	2140	2146	rBV3	448	404	0.03%	0.005%
44	7.953	2146	2150	2152	rVV2	384	283	0.02%	0.003%
45	7.979	2155	2158	2166	rVB5	930	1060	0.09%	0.013%
46	8.095	2183	2194	2229	rBV2	278773	567818	48.81%	6.697%
47	8.503	2318	2321	2323	rBV3	267	190	0.02%	0.002%
48	8.632	2356	2361	2365	rBV2	308	397	0.03%	0.005%
49	8.673	2372	2374	2379	rVB2	355	218	0.02%	0.003%
50	8.712	2382	2386	2388	rBV2	437	272	0.02%	0.003%
51	8.776	2404	2406	2409	rVB2	461	168	0.01%	0.002%
52	8.799	2409	2413	2415	rBV2	382	343	0.03%	0.004%
53	8.853	2419	2430	2453	rBV	484505	797051	68.52%	9.401%
54	9.053	2489	2492	2495	rVB3	612	381	0.03%	0.004%
55	9.072	2495	2498	2499	rVV2	311	194	0.02%	0.002%
56	9.091	2502	2504	2506	rVB2	465	158	0.01%	0.002%
57	9.117	2510	2512	2517	rVB3	368	182	0.02%	0.002%
58	9.149	2517	2522	2524	rBV3	589	635	0.05%	0.007%
59	9.175	2528	2530	2533	rVV	294	160	0.01%	0.002%
60	9.246	2549	2552	2555	rVB2	273	176	0.02%	0.002%
61	9.268	2555	2559	2561	rBV	307	271	0.02%	0.003%
62	9.349	2582	2584	2587	rBV	313	212	0.02%	0.003%
63	9.381	2591	2594	2597	rVV2	207	169	0.01%	0.002%
64	9.397	2597	2599	2602	rVV2	423	255	0.02%	0.003%
65	9.432	2605	2610	2613	rVB	299	212	0.02%	0.003%
66	9.770	2708	2715	2717	rBV2	339	295	0.03%	0.003%
67	9.799	2722	2724	2727	rVB	308	166	0.01%	0.002%
68	9.931	2762	2765	2768	rBV2	247	146	0.01%	0.002%
69	9.992	2780	2784	2786	rBV2	460	258	0.02%	0.003%
70	10.043	2794	2800	2803	rBV3	368	366	0.03%	0.004%
71	10.088	2810	2814	2816	rBV2	224	153	0.01%	0.002%
72	10.130	2822	2827	2834	rVB4	1375	1845	0.16%	0.022%
73	10.217	2841	2854	2874	rBV	312218	495780	42.62%	5.848%
74	10.410	2911	2914	2915	rBV	274	147	0.01%	0.002%
75	10.458	2926	2929	2932	rBV	391	342	0.03%	0.004%
76	10.644	2984	2987	2989	rBV	308	218	0.02%	0.003%

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 Title : VOC Analysis

77	10.783	3026	3030	3033	rBV3	270	224	0.02%	0.003%
78	10.918	3066	3072	3081	rVB6	1381	2017	0.17%	0.024%
79	11.078	3119	3122	3125	rBV2	334	247	0.02%	0.003%
80	11.156	3143	3146	3153	rVB4	781	527	0.05%	0.006%
81	11.252	3164	3176	3195	rBV	427672	669738	57.57%	7.899%
82	11.535	3258	3264	3265	rBV4	2902	2349	0.20%	0.028%
83	11.625	3281	3292	3317	rBV	474957	744718	64.02%	8.784%
84	11.789	3339	3343	3344	rBV2	672	425	0.04%	0.005%
85	11.850	3356	3362	3367	rVB4	838	923	0.08%	0.011%
86	11.879	3369	3371	3374	rBV2	302	200	0.02%	0.002%
87	12.004	3404	3410	3418	rVB3	1553	1727	0.15%	0.020%
88	12.101	3437	3440	3442	rVB	515	262	0.02%	0.003%
89	12.149	3452	3455	3457	rBV2	291	216	0.02%	0.003%
90	12.191	3465	3468	3470	rBV2	266	150	0.01%	0.002%
91	12.268	3488	3492	3493	rBV	684	417	0.04%	0.005%
92	12.355	3516	3519	3522	rVB3	482	240	0.02%	0.003%
93	12.500	3562	3564	3567	rBV	283	176	0.02%	0.002%
94	12.898	3685	3688	3690	rBV2	258	185	0.02%	0.002%
95	12.956	3703	3706	3709	rBV3	306	220	0.02%	0.003%
96	12.975	3710	3712	3715	rVB	441	192	0.02%	0.002%
97	13.033	3728	3730	3734	rBV2	358	228	0.02%	0.003%
98	13.332	3821	3823	3825	rVB	389	174	0.01%	0.002%
99	13.583	3897	3901	3903	rBV2	410	328	0.03%	0.004%
100	14.541	4196	4199	4201	rBV2	344	256	0.02%	0.003%

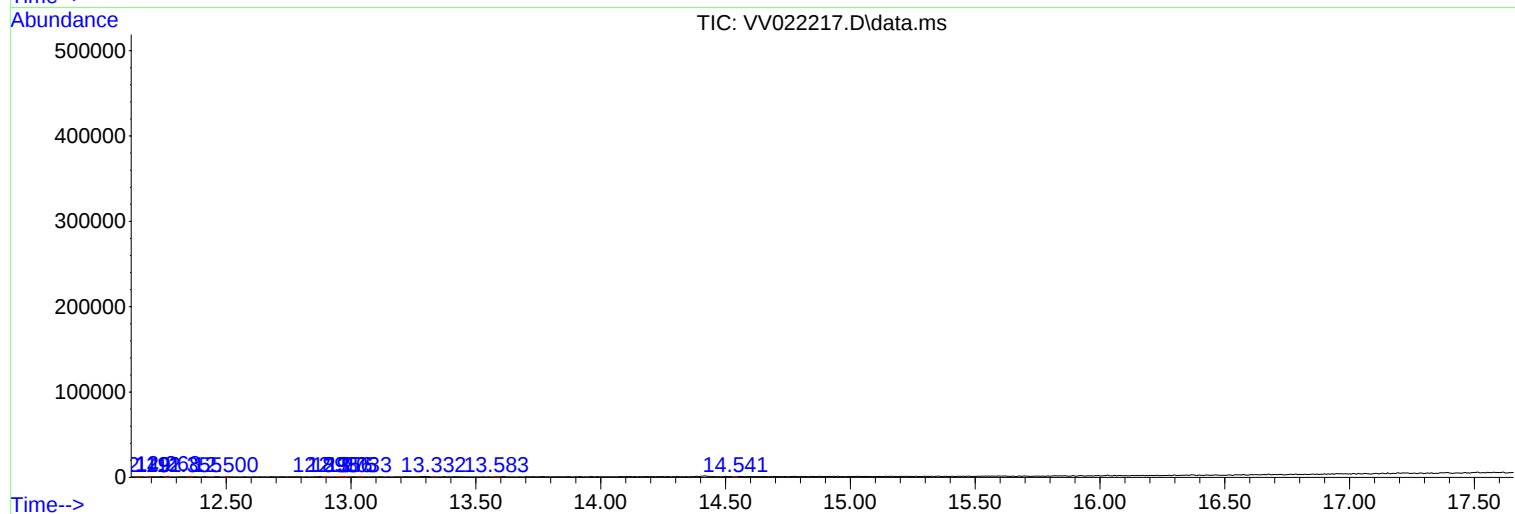
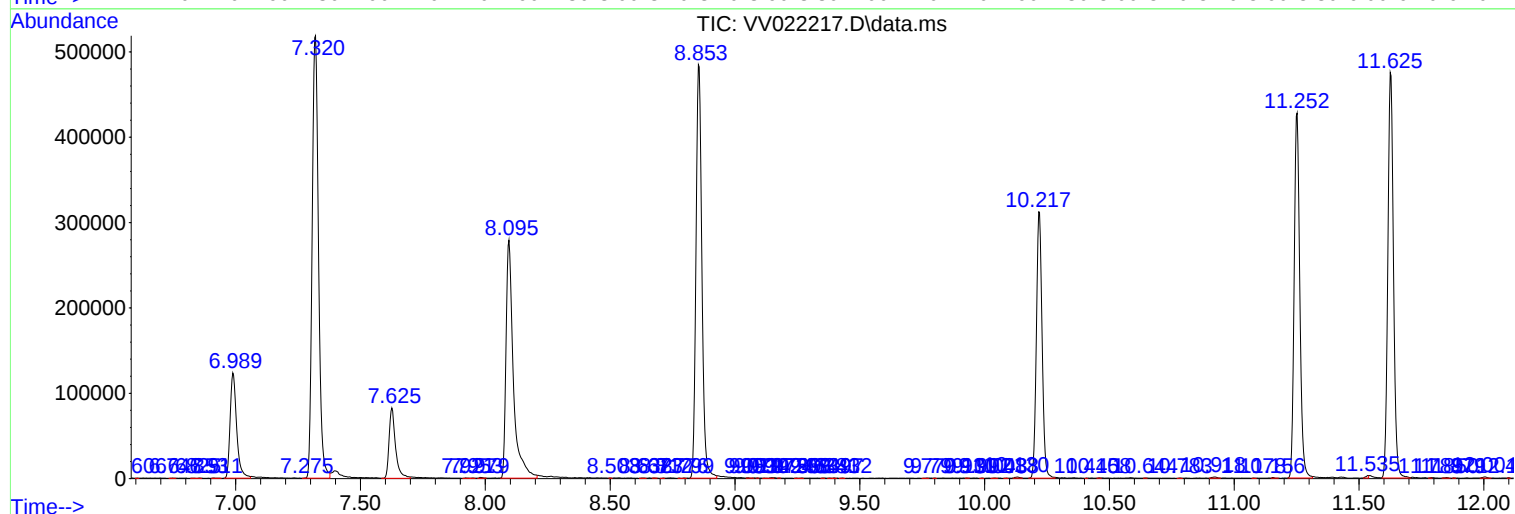
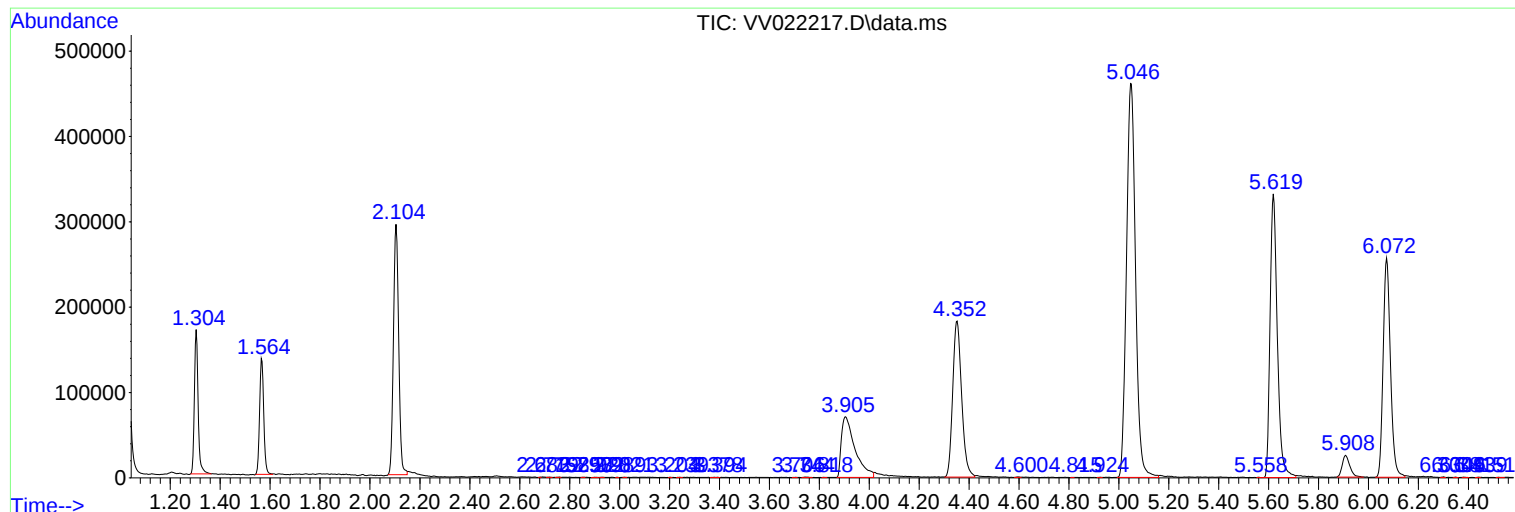
Sum of corrected areas: 8478423

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ALS Vial : 49 Sample Multiplier: 1

Instrument :
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C0CJ5

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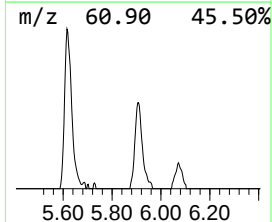
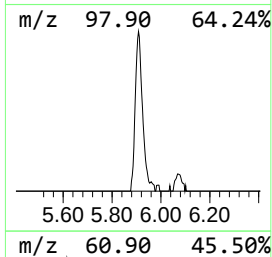
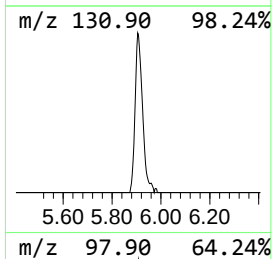
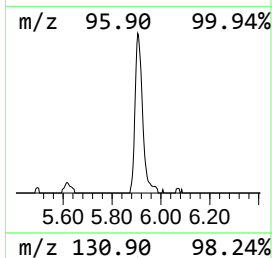
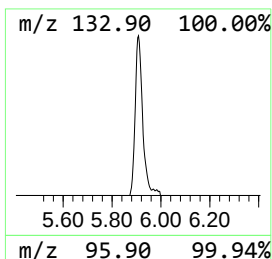
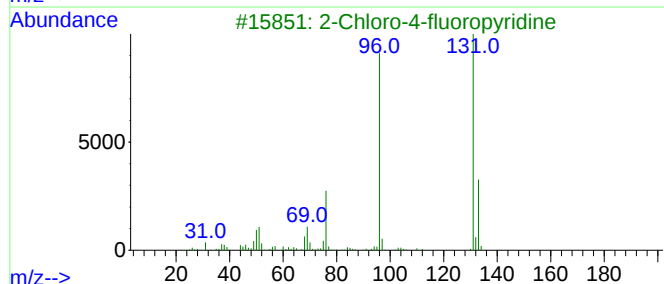
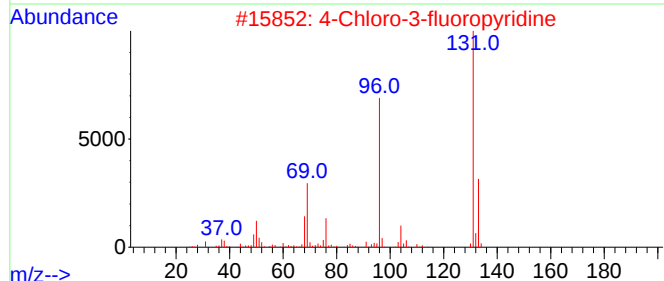
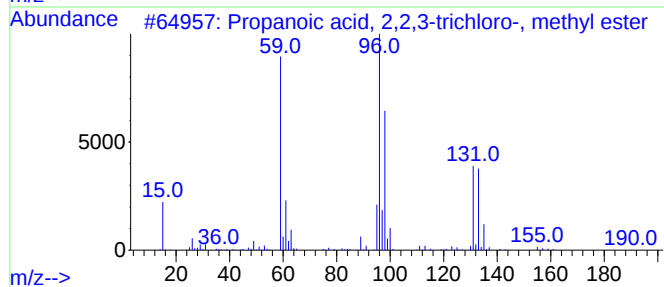
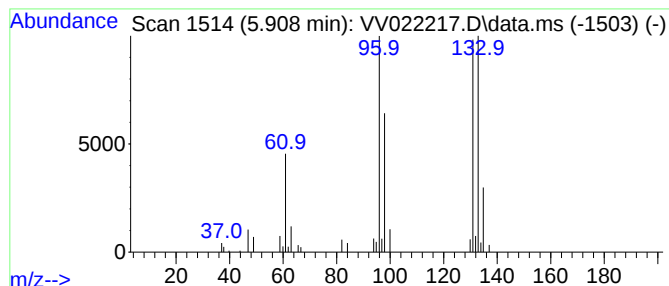
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	4.03 ug/L	53885	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			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	43
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	4.0	ug/L	53885	1	5.619	669255	50.0