

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092021\
 Data File : VV022253.D
 Acq On : 20 Sep 2021 23:51
 Operator : SY/MD
 Sample : M3788-15
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0CL8

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: VV022253.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	96	rBV	154942	158606	14.83%	1.941%
2	1.561	155	162	174	rVB	133342	151831	14.20%	1.858%
3	2.105	321	331	346	rBV2	289387	449482	42.03%	5.502%
4	2.503	450	455	458	rBV5	1500	1585	0.15%	0.019%
5	2.793	542	545	548	rBV2	193	145	0.01%	0.002%
6	2.818	551	553	557	rBV2	304	177	0.02%	0.002%
7	3.130	646	650	654	rBV3	257	252	0.02%	0.003%
8	3.240	681	684	687	rVB2	471	311	0.03%	0.004%
9	3.262	687	691	693	rBV	471	304	0.03%	0.004%
10	3.346	715	717	718	rBV	167	63	0.01%	0.001%
11	3.449	746	749	752	rBV2	326	289	0.03%	0.004%
12	3.709	826	830	833	rBV3	277	230	0.02%	0.003%
13	3.876	872	882	923	rBV	94988	310666	29.05%	3.803%
14	4.252	997	999	1002	rBV2	305	216	0.02%	0.003%
15	4.349	1014	1029	1058	rBV	171023	424914	39.73%	5.201%
16	4.850	1183	1185	1191	rVB	407	271	0.03%	0.003%
17	4.947	1213	1215	1218	rVB2	333	150	0.01%	0.002%
18	4.969	1219	1222	1223	rBV	191	87	0.01%	0.001%
19	5.047	1230	1246	1274	rBV2	417375	1069381	100.00%	13.090%
20	5.262	1308	1313	1315	rBV3	435	360	0.03%	0.004%
21	5.336	1334	1336	1338	rBV2	351	174	0.02%	0.002%
22	5.416	1357	1361	1365	rBV3	245	278	0.03%	0.003%
23	5.436	1365	1367	1370	rVB	319	122	0.01%	0.001%
24	5.538	1395	1399	1401	rBV2	332	207	0.02%	0.003%
25	5.561	1404	1406	1408	rBV	178	54	0.01%	0.001%
26	5.619	1411	1424	1453	rBV	327438	667432	62.41%	8.170%
27	5.908	1503	1514	1533	rBV4	28351	61661	5.77%	0.755%
28	6.011	1543	1546	1549	rVB	202	140	0.01%	0.002%
29	6.072	1551	1565	1589	rBV	238662	485881	45.44%	5.947%
30	6.297	1633	1635	1636	rBV	397	123	0.01%	0.002%
31	6.333	1642	1646	1649	rBV2	353	303	0.03%	0.004%
32	6.368	1655	1657	1661	rBV3	332	206	0.02%	0.003%
33	6.500	1694	1698	1702	rVB2	260	205	0.02%	0.003%
34	6.522	1702	1705	1707	rBV2	162	102	0.01%	0.001%
35	6.538	1708	1710	1712	rVB	285	106	0.01%	0.001%
36	6.616	1732	1734	1737	rBV	293	116	0.01%	0.001%

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Integrator: RTE

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Peak separation: 5

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

37	6.648	1742	1744	1747	rBV	181	116	0.01%	0.001%
38	6.754	1776	1777	1778	rBV	238	75	0.01%	0.001%
39	6.764	1778	1780	1784	rVB	356	238	0.02%	0.003%
40	6.953	1838	1839	1840	rBV	241	60	0.01%	0.001%
41	6.989	1840	1850	1875	rBV	117051	213868	20.00%	2.618%
42	7.207	1915	1918	1923	rBV2	401	314	0.03%	0.004%
43	7.320	1940	1953	1970	rBV	487415	844584	78.98%	10.338%
44	7.625	2038	2048	2078	rBV	78830	138850	12.98%	1.700%
45	7.892	2128	2131	2133	rBV2	277	139	0.01%	0.002%
46	7.985	2158	2160	2163	rVB2	993	577	0.05%	0.007%
47	8.005	2163	2166	2167	rBV	266	113	0.01%	0.001%
48	8.091	2183	2193	2235	rBV2	259393	511058	47.79%	6.255%
49	8.458	2305	2307	2311	rBV2	369	181	0.02%	0.002%
50	8.506	2319	2322	2323	rBV	376	207	0.02%	0.003%
51	8.564	2337	2340	2342	rBV2	328	206	0.02%	0.003%
52	8.632	2358	2361	2362	rBV2	218	111	0.01%	0.001%
53	8.699	2381	2382	2385	rBV2	223	118	0.01%	0.001%
54	8.734	2392	2393	2395	rVB2	228	86	0.01%	0.001%
55	8.853	2418	2430	2449	rBV	504087	802459	75.04%	9.822%
56	9.127	2513	2515	2517	rBV2	278	138	0.01%	0.002%
57	9.146	2518	2521	2523	rBV	751	441	0.04%	0.005%
58	9.242	2550	2551	2557	rVB2	272	205	0.02%	0.003%
59	9.336	2578	2580	2581	rBV	161	43	0.00%	0.001%
60	9.381	2592	2594	2597	rBV	160	71	0.01%	0.001%
61	9.693	2688	2691	2693	rBV2	287	174	0.02%	0.002%
62	9.776	2714	2717	2719	rBV	217	113	0.01%	0.001%
63	9.866	2743	2745	2748	rBV	299	132	0.01%	0.002%
64	10.011	2787	2790	2791	rBV	186	99	0.01%	0.001%
65	10.050	2800	2802	2803	rBV	331	100	0.01%	0.001%
66	10.133	2820	2828	2834	rBV6	1546	2518	0.24%	0.031%
67	10.217	2842	2854	2877	rBV	291568	459648	42.98%	5.626%
68	10.345	2892	2894	2897	rBV2	348	236	0.02%	0.003%
69	10.419	2913	2917	2918	rBV2	199	136	0.01%	0.002%
70	10.522	2946	2949	2954	rVB2	316	203	0.02%	0.002%
71	10.815	3037	3040	3041	rBV	255	128	0.01%	0.002%
72	10.914	3066	3071	3073	rBV4	1174	1094	0.10%	0.013%
73	11.050	3109	3113	3118	rBV2	286	305	0.03%	0.004%
74	11.120	3133	3135	3136	rVB2	279	69	0.01%	0.001%
75	11.252	3164	3176	3200	rBV	438401	693410	64.84%	8.488%
76	11.625	3280	3292	3313	rBV	446561	709767	66.37%	8.688%

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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\SFAMVLM082721WMA.M
Title : VOC Analysis

77	12.059	3426	3427	3428	rBV	125	30	0.00%	0.000%
78	12.069	3428	3430	3431	rBV	166	49	0.00%	0.001%
79	12.091	3436	3437	3438	rBV	251	82	0.01%	0.001%
80	12.458	3547	3551	3555	rBV2	419	406	0.04%	0.005%
81	12.541	3575	3577	3578	rBV2	211	80	0.01%	0.001%
82	13.866	3986	3989	3991	rBV2	421	277	0.03%	0.003%

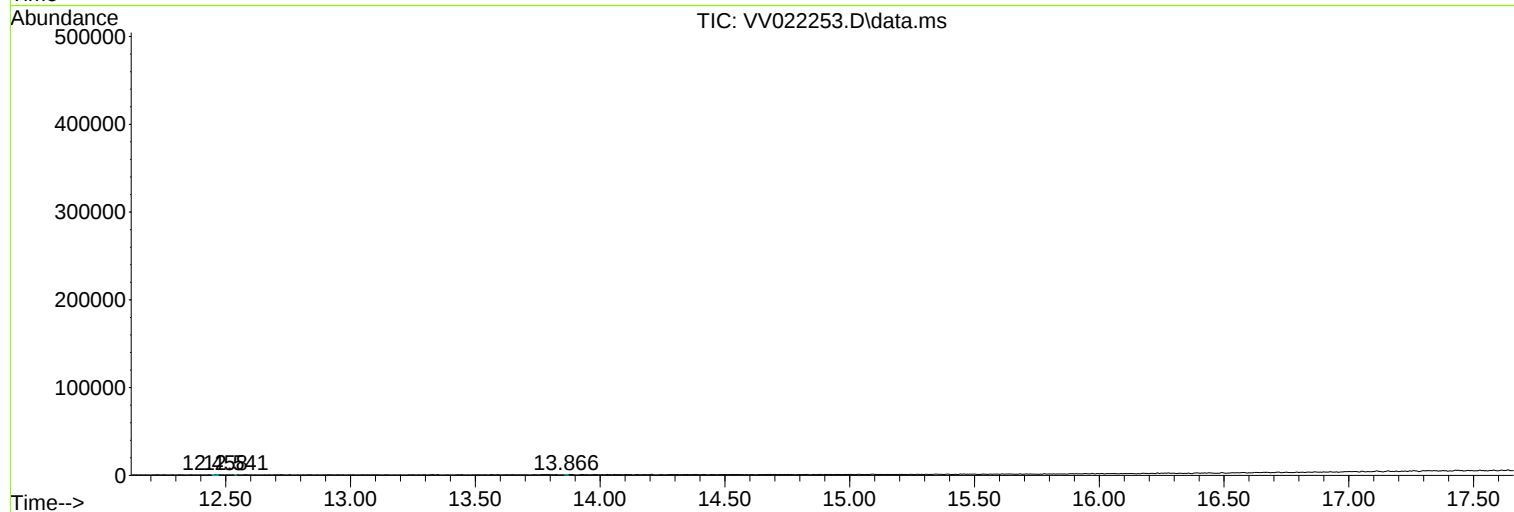
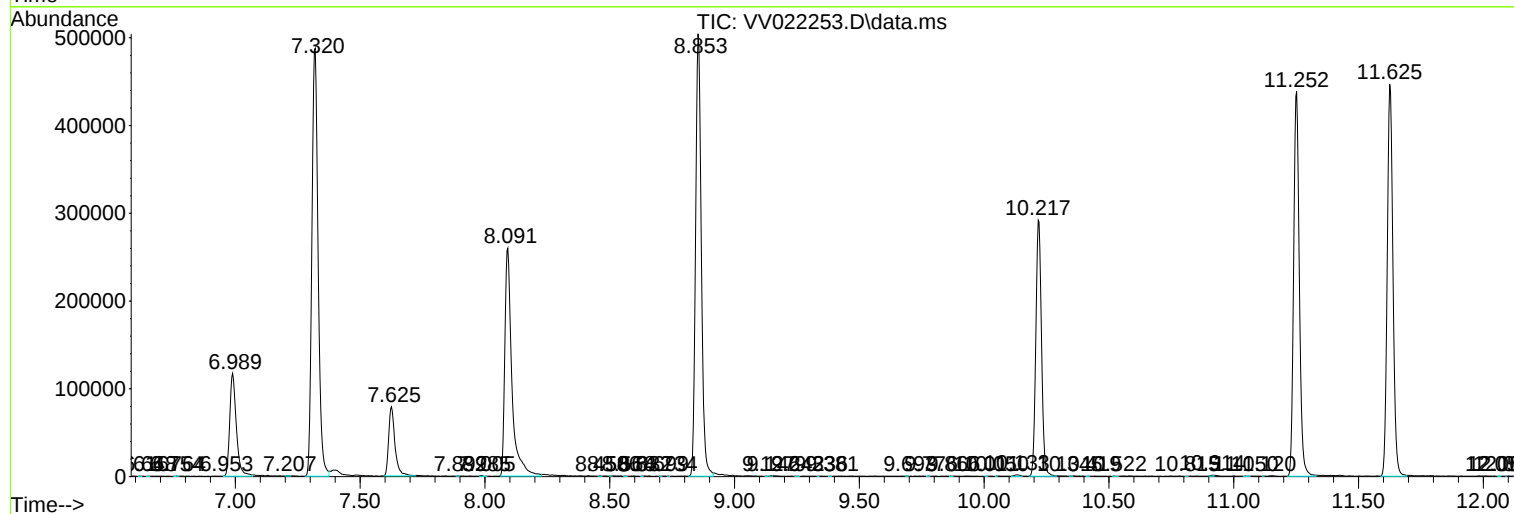
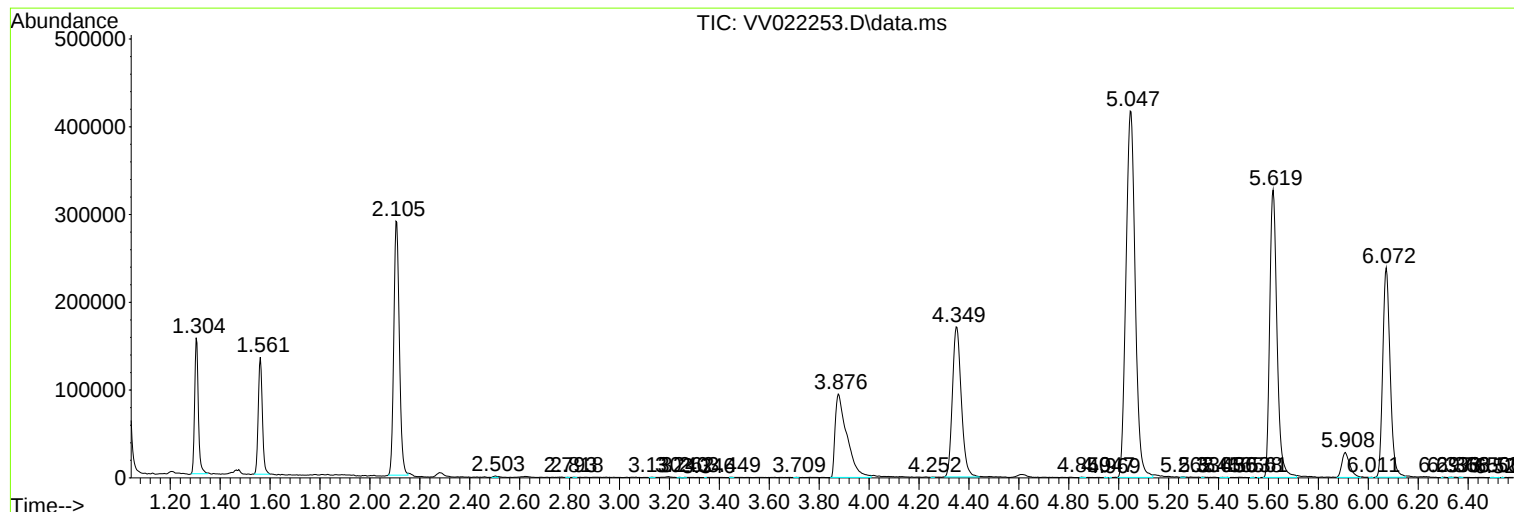
Sum of corrected areas: 8169744

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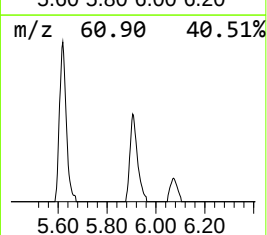
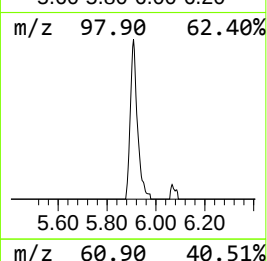
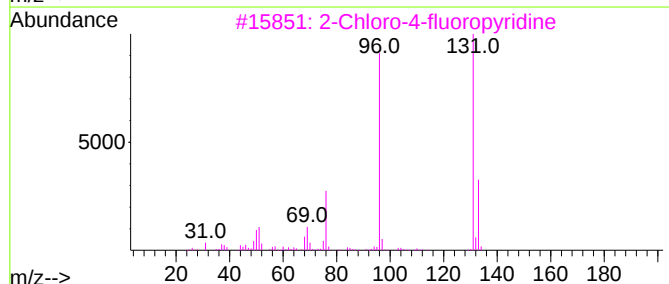
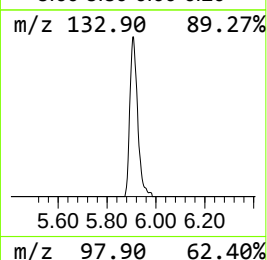
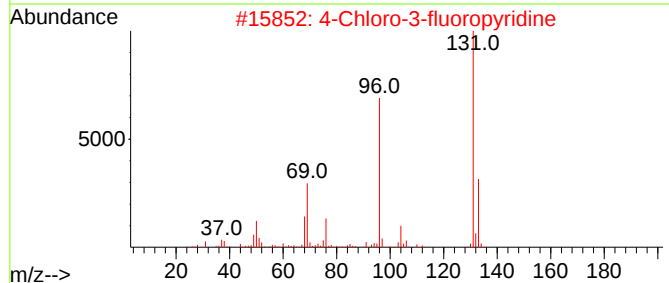
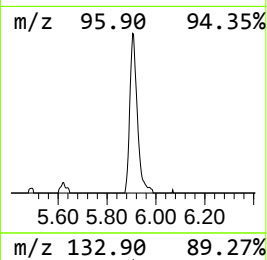
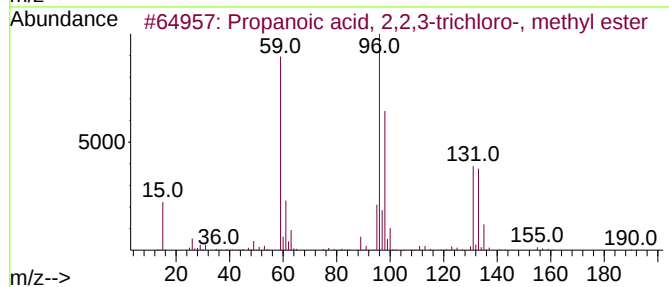
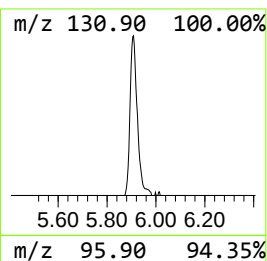
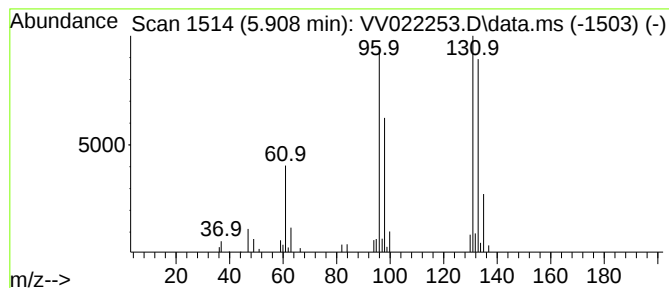
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	4.62 ug/L	61661	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	45
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	43
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	4.6	ug/L	61661	1	5.619	667432	50.0