

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031122\
 Data File : VV024963.D
 Acq On : 11 Mar 2022 14:35
 Operator : SY/MD
 Sample : N1880-01
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0DA9

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\SFAMVLM022822WMA.M
 Title : VOC Analysis

Signal : TIC: VV024963.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	76	83	99	rVB	230835	229223	16.33%	2.314%
2	1.568	156	164	180	rVB	173250	194086	13.83%	1.960%
3	2.108	321	332	354	rBV	352674	511362	36.43%	5.163%
4	2.439	432	435	437	rBV	329	218	0.02%	0.002%
5	2.500	453	454	455	rBV	391	99	0.01%	0.001%
6	2.741	526	529	532	rVB2	249	156	0.01%	0.002%
7	2.786	540	543	545	rBV	193	139	0.01%	0.001%
8	3.327	708	711	714	rBV	275	230	0.02%	0.002%
9	3.629	799	805	807	rBV	213	227	0.02%	0.002%
10	3.802	857	859	860	rBV	136	67	0.00%	0.001%
11	3.892	877	887	938	rBV	73916	256207	18.25%	2.587%
12	4.349	1014	1029	1055	rBV	220740	549486	39.15%	5.548%
13	4.658	1122	1125	1130	rVV	251	202	0.01%	0.002%
14	4.693	1134	1136	1139	rBV3	181	109	0.01%	0.001%
15	4.712	1139	1142	1144	rBV	240	131	0.01%	0.001%
16	4.822	1174	1176	1179	rVB	146	81	0.01%	0.001%
17	4.835	1179	1180	1181	rBV	127	35	0.00%	0.000%
18	4.934	1209	1211	1213	rBV	210	125	0.01%	0.001%
19	5.047	1229	1246	1285	rBV2	551639	1403533	100.00%	14.172%
20	5.397	1351	1355	1356	rBV2	262	215	0.02%	0.002%
21	5.433	1363	1366	1373	rVB3	256	350	0.02%	0.004%
22	5.484	1377	1382	1383	rBV	331	236	0.02%	0.002%
23	5.564	1405	1407	1411	rBV	167	72	0.01%	0.001%
24	5.616	1411	1423	1447	rBV	348019	700848	49.93%	7.077%
25	5.905	1503	1513	1540	rVB3	24946	52321	3.73%	0.528%
26	5.998	1540	1542	1543	rBV	201	83	0.01%	0.001%
27	6.069	1550	1564	1598	rBV	304889	617045	43.96%	6.230%
28	6.269	1623	1626	1631	rVB	372	282	0.02%	0.003%
29	6.291	1631	1633	1638	rVB2	194	113	0.01%	0.001%
30	6.317	1638	1641	1645	rVB	281	181	0.01%	0.002%
31	6.336	1645	1647	1650	rBV2	132	88	0.01%	0.001%
32	6.371	1654	1658	1660	rBV	132	105	0.01%	0.001%
33	6.474	1687	1690	1695	rBV	177	151	0.01%	0.002%
34	6.638	1738	1741	1744	rBV	322	270	0.02%	0.003%
35	6.744	1771	1774	1780	rBV2	176	175	0.01%	0.002%
36	6.986	1837	1849	1874	rBV	161216	291081	20.74%	2.939%

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Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
 Title : VOC Analysis

37	7.124	1891	1892	1895	rVB2	391	155	0.01%	0.002%
38	7.143	1896	1898	1901	rBV2	413	223	0.02%	0.002%
39	7.188	1910	1912	1914	rBV2	366	180	0.01%	0.002%
40	7.314	1939	1951	1971	rBV	668991	1144855	81.57%	11.560%
41	7.619	2036	2046	2073	rBV	107065	187616	13.37%	1.894%
42	7.773	2091	2094	2097	rBV2	295	230	0.02%	0.002%
43	7.873	2122	2125	2128	rBV	214	136	0.01%	0.001%
44	7.931	2139	2143	2147	rBV2	376	395	0.03%	0.004%
45	7.969	2152	2155	2157	rBV	259	186	0.01%	0.002%
46	8.027	2171	2173	2175	rBV2	173	55	0.00%	0.001%
47	8.088	2182	2192	2227	rBV	285826	553840	39.46%	5.592%
48	8.468	2307	2310	2311	rBV	298	142	0.01%	0.001%
49	8.481	2311	2314	2316	rVV2	176	131	0.01%	0.001%
50	8.593	2346	2349	2352	rBV2	206	157	0.01%	0.002%
51	8.706	2381	2384	2387	rBV	235	215	0.02%	0.002%
52	8.850	2418	2429	2457	rBV	556692	876322	62.44%	8.848%
53	9.111	2507	2510	2512	rVB	248	130	0.01%	0.001%
54	9.149	2516	2522	2526	rBV2	727	813	0.06%	0.008%
55	9.413	2601	2604	2610	rBV2	160	148	0.01%	0.001%
56	9.455	2610	2617	2619	rBV	221	282	0.02%	0.003%
57	9.555	2646	2648	2652	rBV2	152	98	0.01%	0.001%
58	9.905	2754	2757	2764	rBV2	221	336	0.02%	0.003%
59	10.076	2807	2810	2817	rVB2	173	171	0.01%	0.002%
60	10.127	2817	2826	2838	rBV3	3752	5846	0.42%	0.059%
61	10.214	2841	2853	2880	rVV	371406	574097	40.90%	5.797%
62	10.461	2928	2930	2933	rBB	171	72	0.01%	0.001%
63	10.574	2958	2965	2971	rBV4	1069	1578	0.11%	0.016%
64	10.657	2989	2991	2995	rVB2	519	311	0.02%	0.003%
65	10.741	3011	3017	3020	rBV	387	359	0.03%	0.004%
66	10.915	3062	3071	3081	rBV4	2678	4183	0.30%	0.042%
67	11.027	3102	3106	3111	rBV3	480	510	0.04%	0.005%
68	11.143	3135	3142	3149	rBV4	1751	2312	0.16%	0.023%
69	11.246	3163	3174	3193	rBV	532841	818595	58.32%	8.265%
70	11.474	3241	3245	3249	rBV2	221	236	0.02%	0.002%
71	11.522	3258	3260	3262	rBB	213	44	0.00%	0.000%
72	11.622	3279	3291	3313	rBV	596742	918019	65.41%	9.269%
73	12.053	3422	3425	3429	rBV	287	250	0.02%	0.003%
74	12.198	3468	3470	3471	rBV	173	51	0.00%	0.001%
75	12.722	3630	3633	3636	rBV	301	277	0.02%	0.003%
76	12.780	3647	3651	3654	rBV	272	238	0.02%	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\SFAMVLM022822WMA.M
Title : VOC Analysis

77	13.082	3743	3745	3752	rBV	256	230	0.02%	0.002%
78	13.362	3828	3832	3834	rBV	331	268	0.02%	0.003%
79	14.394	4150	4153	4155	rBV	358	219	0.02%	0.002%

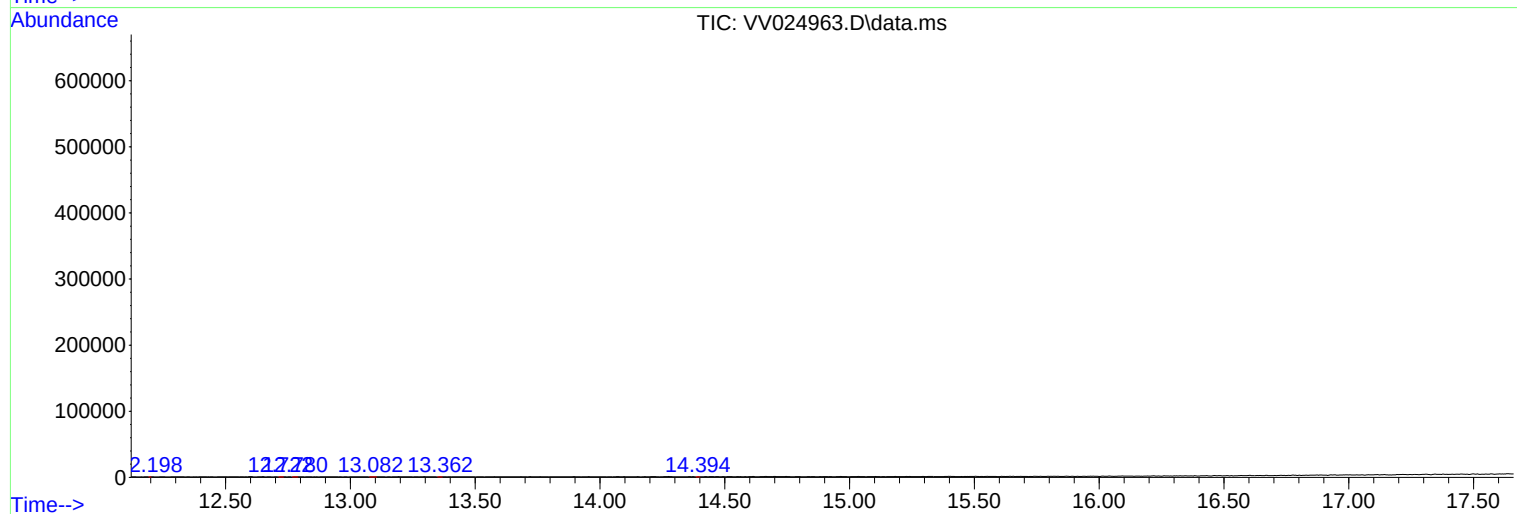
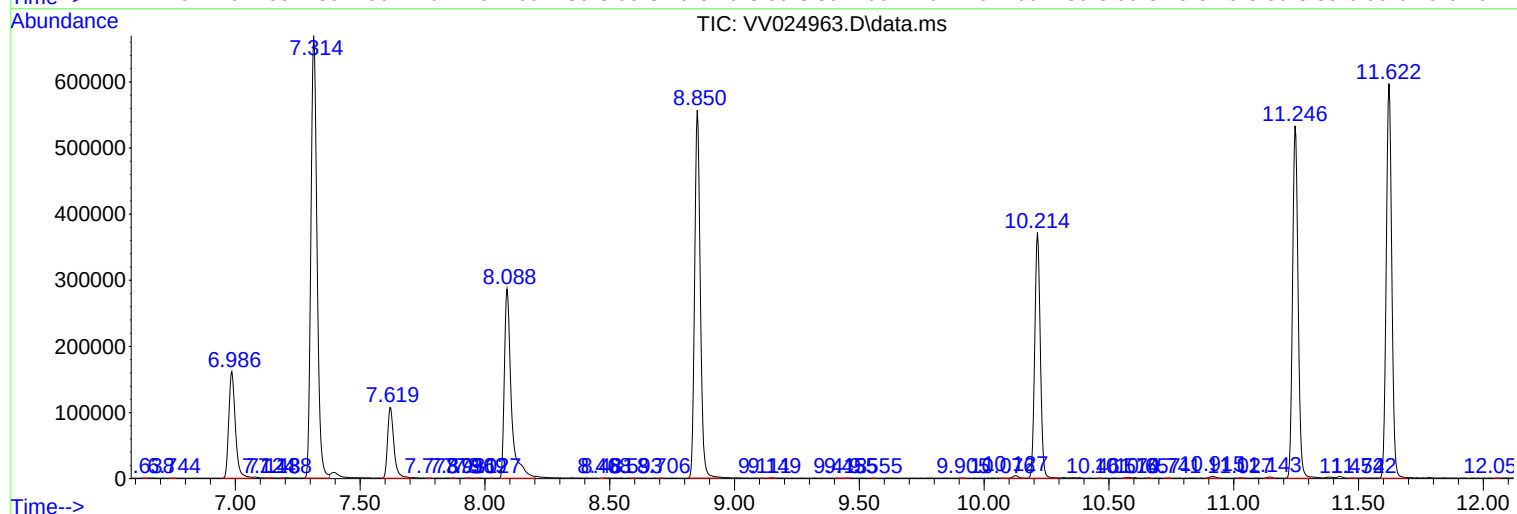
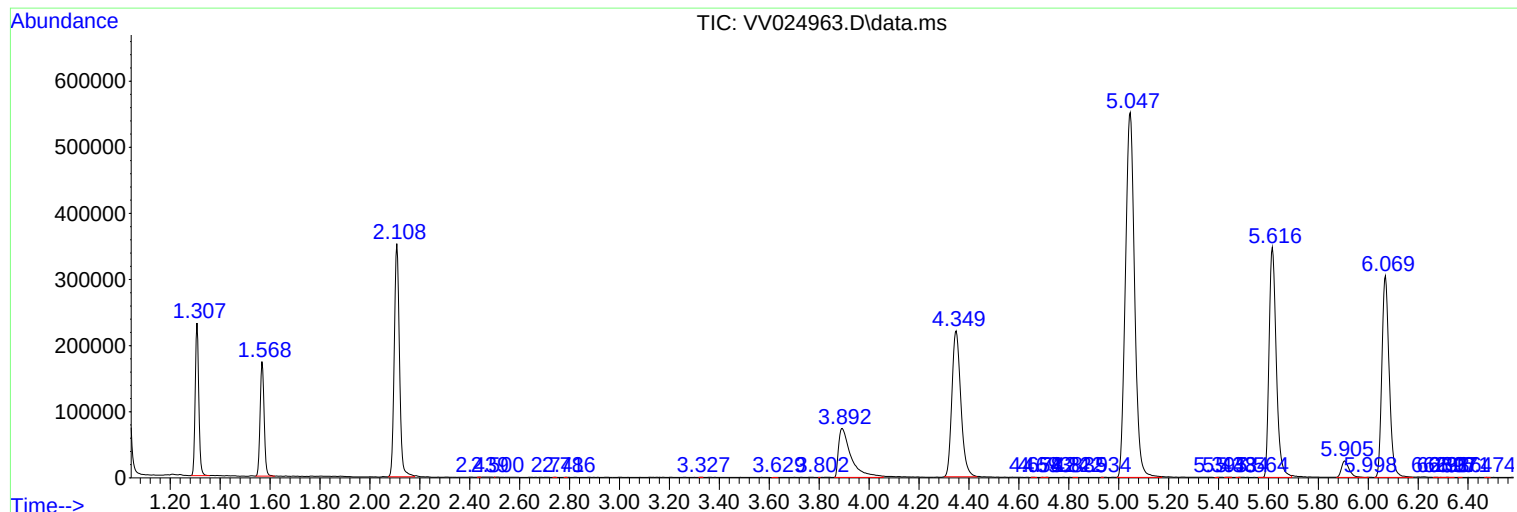
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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



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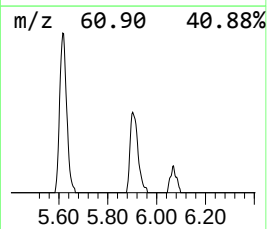
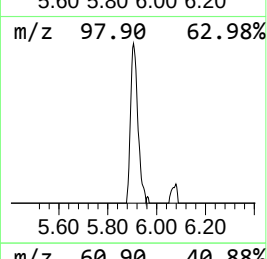
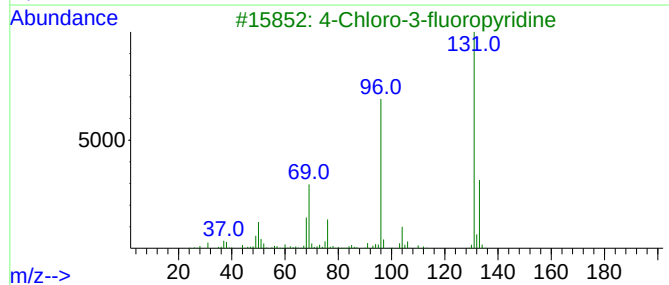
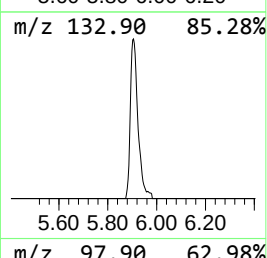
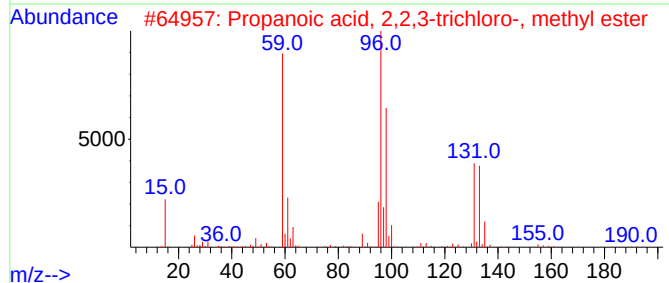
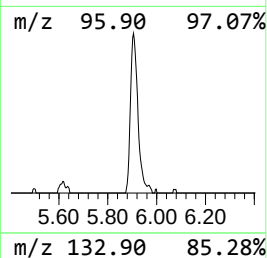
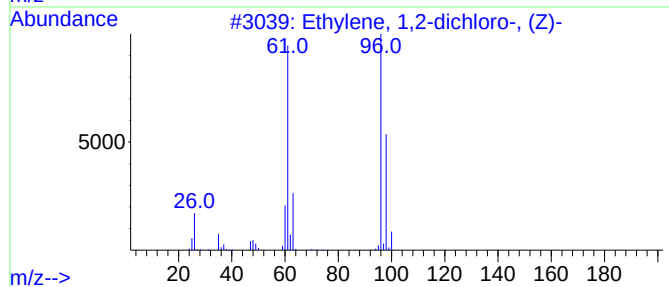
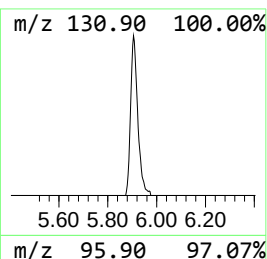
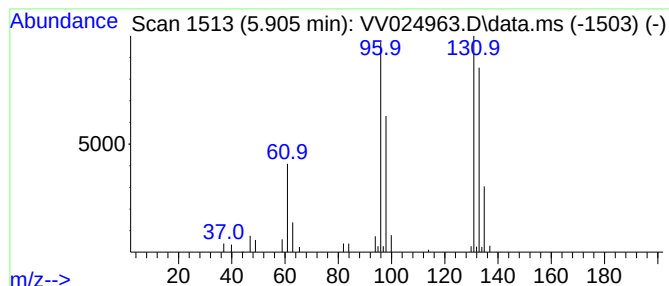
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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.
5.905	3.73 ug/L	52321	1,4-Difluorobenzene	5.616

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	32
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	3.7	ug/L	52321	1	5.616	700848	50.0