

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021422\
 Data File : VX027015.D
 Acq On : 14 Feb 2022 13:26
 Operator : JC/MD
 Sample : VX0214MBL01
 Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK653

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_X\Method\SFAMXML021422WMA.M
 Title : VOC Analysis

Signal : TIC: VX027015.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	53	rVB	86494	89707	13.85%	1.906%
2	1.673	92	96	106	rVB	62669	75253	11.62%	1.599%
3	2.313	194	201	212	rBV	149592	244176	37.71%	5.187%
4	2.447	218	223	228	rBV5	286	608	0.09%	0.013%
5	2.520	231	235	239	rVB	843	1207	0.19%	0.026%
6	2.709	263	266	268	rVB	225	246	0.04%	0.005%
7	2.794	277	280	285	rVB2	400	598	0.09%	0.013%
8	3.032	317	319	321	rBV	143	104	0.02%	0.002%
9	3.130	334	335	338	rVB	152	101	0.02%	0.002%
10	3.184	341	344	346	rBV	141	185	0.03%	0.004%
11	3.581	407	409	411	rVB	211	132	0.02%	0.003%
12	3.617	411	415	417	rBV2	164	208	0.03%	0.004%
13	3.678	422	425	427	rVB	174	124	0.02%	0.003%
14	3.733	432	434	436	rBV	88	107	0.02%	0.002%
15	3.825	446	449	450	rBV	138	136	0.02%	0.003%
16	4.166	504	505	508	rVB	158	108	0.02%	0.002%
17	4.196	508	510	513	rBV	126	144	0.02%	0.003%
18	4.227	513	515	516	rBV	111	101	0.02%	0.002%
19	4.453	543	552	568	rBV	50342	147061	22.71%	3.124%
20	4.745	598	600	603	rVV2	105	97	0.01%	0.002%
21	5.062	639	652	667	rBV	83696	255861	39.51%	5.435%
22	5.288	685	689	690	rVB	125	159	0.02%	0.003%
23	5.306	690	692	695	rBV	117	180	0.03%	0.004%
24	5.379	700	704	705	rBV2	343	363	0.06%	0.008%
25	5.556	726	733	740	rVB2	667	1797	0.28%	0.038%
26	5.617	740	743	745	rBV2	110	179	0.03%	0.004%
27	5.684	752	754	755	rVB	152	107	0.02%	0.002%
28	5.708	755	758	759	rBV	137	163	0.03%	0.003%
29	5.855	781	782	784	rBV	97	99	0.02%	0.002%
30	5.971	789	801	815	rBV2	216916	647575	100.00%	13.757%
31	6.221	840	842	844	rVB	111	108	0.02%	0.002%
32	6.257	844	848	850	rBV2	152	203	0.03%	0.004%
33	6.403	867	872	873	rBV2	158	260	0.04%	0.006%
34	6.440	877	878	882	rVB	151	127	0.02%	0.003%
35	6.470	882	883	885	rBV	135	91	0.01%	0.002%
36	6.544	891	895	897	rVB3	129	216	0.03%	0.005%

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 Title : VOC Analysis

37	6.586	897	902	903	rBV2	100	135	0.02%	0.003%
38	6.623	903	908	909	rBV	122	128	0.02%	0.003%
39	6.690	917	919	921	rBV	144	155	0.02%	0.003%
40	6.763	921	931	948	rVV	129897	311214	48.06%	6.611%
41	7.050	976	978	979	rBV	100	104	0.02%	0.002%
42	7.111	981	988	996	rVV2	7381	16251	2.51%	0.345%
43	7.251	1008	1011	1012	rBV2	129	159	0.02%	0.003%
44	7.306	1012	1020	1035	rVV	130649	286560	44.25%	6.088%
45	7.482	1044	1049	1054	rVB2	323	553	0.09%	0.012%
46	7.769	1094	1096	1097	rBV2	148	137	0.02%	0.003%
47	7.934	1118	1123	1127	rBV2	685	1279	0.20%	0.027%
48	8.080	1145	1147	1149	rBV2	88	106	0.02%	0.002%
49	8.324	1181	1187	1199	rVV	91219	144680	22.34%	3.074%
50	8.476	1207	1212	1219	rBV4	447	932	0.14%	0.020%
51	8.647	1234	1240	1248	rVV	344423	539398	83.30%	11.459%
52	8.720	1248	1252	1258	rVB	4696	7441	1.15%	0.158%
53	8.952	1284	1290	1299	rBV	62430	91613	14.15%	1.946%
54	9.122	1316	1318	1322	rVB2	111	116	0.02%	0.002%
55	9.208	1331	1332	1335	rBV	107	121	0.02%	0.003%
56	9.281	1341	1344	1349	rVB3	413	553	0.09%	0.012%
57	9.324	1349	1351	1352	rBV	144	91	0.01%	0.002%
58	9.385	1355	1361	1377	rBV	238690	342642	52.91%	7.279%
59	9.702	1411	1413	1417	rBV2	121	176	0.03%	0.004%
60	9.927	1448	1450	1452	rBV2	137	166	0.03%	0.004%
61	9.994	1459	1461	1463	rVB2	138	94	0.01%	0.002%
62	10.055	1465	1471	1480	rBV	279263	379265	58.57%	8.057%
63	10.195	1491	1494	1498	rBV2	436	550	0.08%	0.012%
64	10.250	1501	1503	1504	rBV	141	107	0.02%	0.002%
65	10.305	1508	1512	1517	rBV2	919	1253	0.19%	0.027%
66	10.415	1528	1530	1531	rBV	117	99	0.02%	0.002%
67	10.543	1549	1551	1553	rBV	133	133	0.02%	0.003%
68	10.647	1564	1568	1574	rVB5	621	1253	0.19%	0.027%
69	10.750	1583	1585	1588	rBV	145	170	0.03%	0.004%
70	10.964	1617	1620	1625	rVB2	483	643	0.10%	0.014%
71	11.122	1642	1646	1650	rBV	2341	2918	0.45%	0.062%
72	11.195	1652	1658	1664	rBV	210701	276585	42.71%	5.876%
73	11.384	1686	1689	1692	rVB2	177	196	0.03%	0.004%
74	11.451	1697	1700	1702	rBV	522	594	0.09%	0.013%
75	11.677	1734	1737	1739	rBV	228	265	0.04%	0.006%
76	11.750	1745	1749	1755	rVB2	2931	3356	0.52%	0.071%

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 Title : VOC Analysis

77	11.848	1759	1765	1769	rVB2	337	473	0.07%	0.010%
78	11.878	1769	1770	1775	rVB	145	161	0.02%	0.003%
79	11.933	1775	1779	1782	rBV2	1072	1350	0.21%	0.029%
80	11.969	1782	1785	1788	rBV2	892	949	0.15%	0.020%
81	12.024	1789	1794	1800	rBV	298712	369764	57.10%	7.855%
82	12.128	1807	1811	1812	rBV2	855	922	0.14%	0.020%
83	12.146	1812	1814	1819	rVB	1758	2000	0.31%	0.042%
84	12.323	1835	1843	1856	rVB	336794	442639	68.35%	9.403%
85	12.427	1857	1860	1865	rVB2	618	735	0.11%	0.016%
86	12.482	1867	1869	1872	rVB2	376	276	0.04%	0.006%
87	12.579	1883	1885	1888	rBV2	139	155	0.02%	0.003%
88	12.658	1895	1898	1902	rVV3	275	334	0.05%	0.007%
89	12.738	1909	1911	1913	rVB	124	95	0.01%	0.002%
90	12.762	1913	1915	1917	rBV2	122	124	0.02%	0.003%
91	13.049	1960	1962	1967	rBV2	174	201	0.03%	0.004%
92	13.116	1969	1973	1977	rBV3	860	940	0.15%	0.020%
93	13.591	2047	2051	2056	rBB2	1542	1627	0.25%	0.035%
94	13.725	2072	2073	2075	rBV	105	105	0.02%	0.002%
95	13.780	2078	2082	2086	rBV	1827	1976	0.31%	0.042%
96	13.963	2108	2112	2117	rVV	1634	1850	0.29%	0.039%
97	14.024	2120	2122	2123	rBV	153	100	0.02%	0.002%
98	14.451	2191	2192	2195	rBV	172	153	0.02%	0.003%
99	14.609	2216	2218	2223	rBV	165	193	0.03%	0.004%
100	15.902	2428	2430	2431	rVB	205	93	0.01%	0.002%

Sum of corrected areas: 4707297

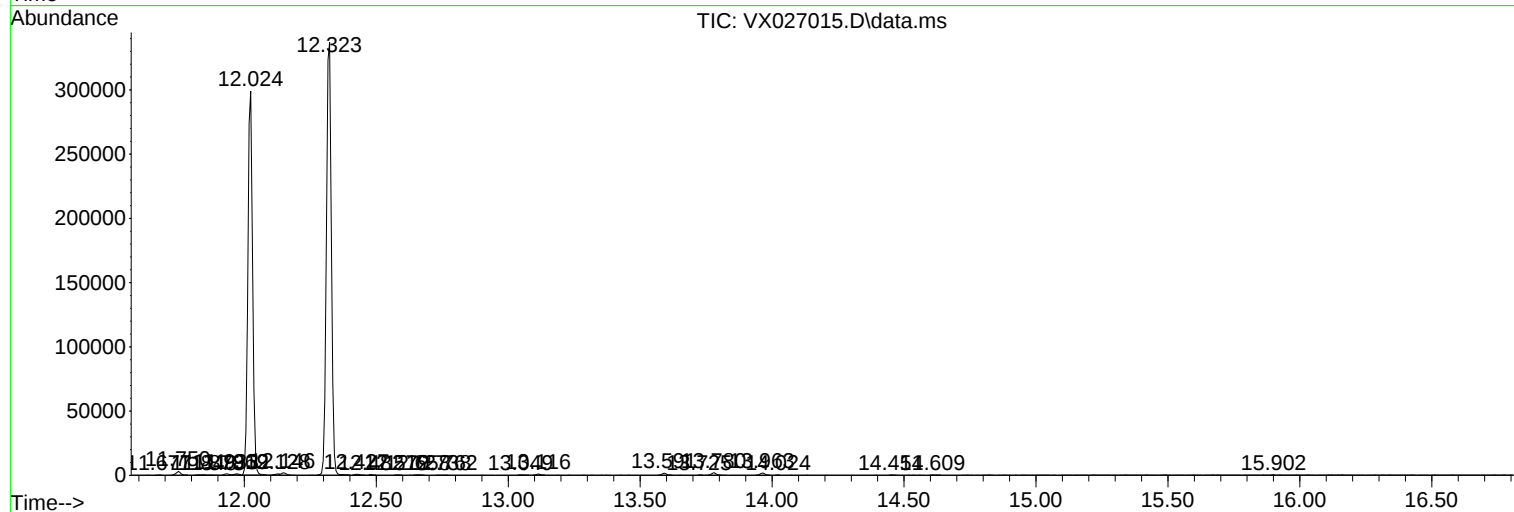
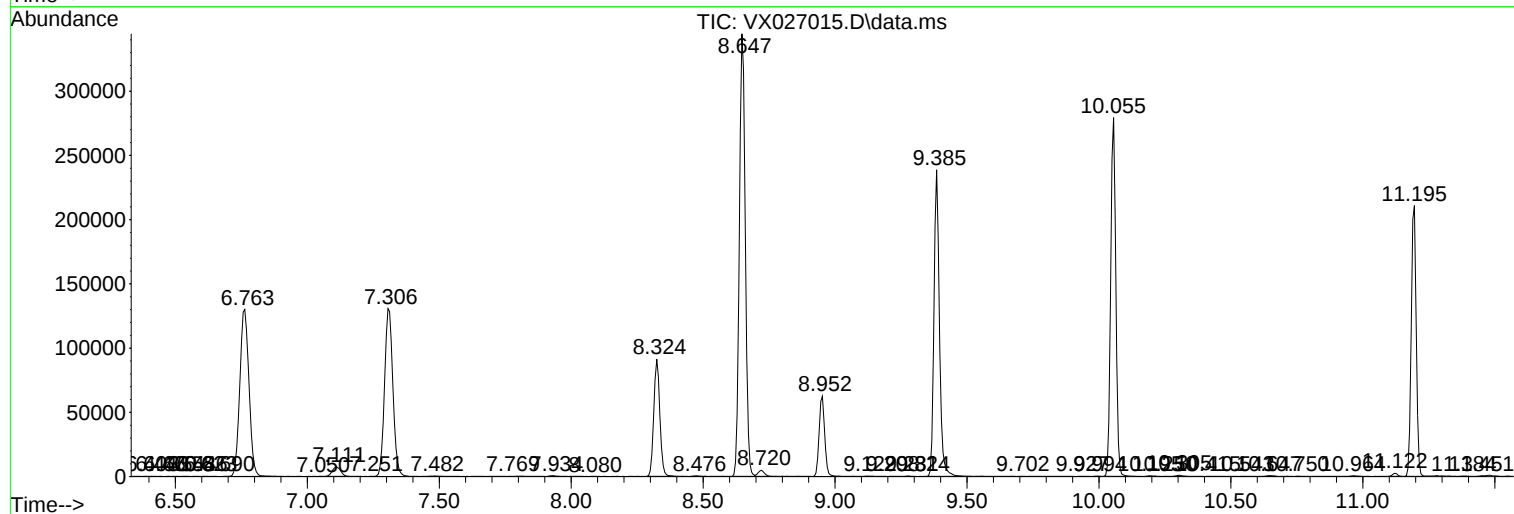
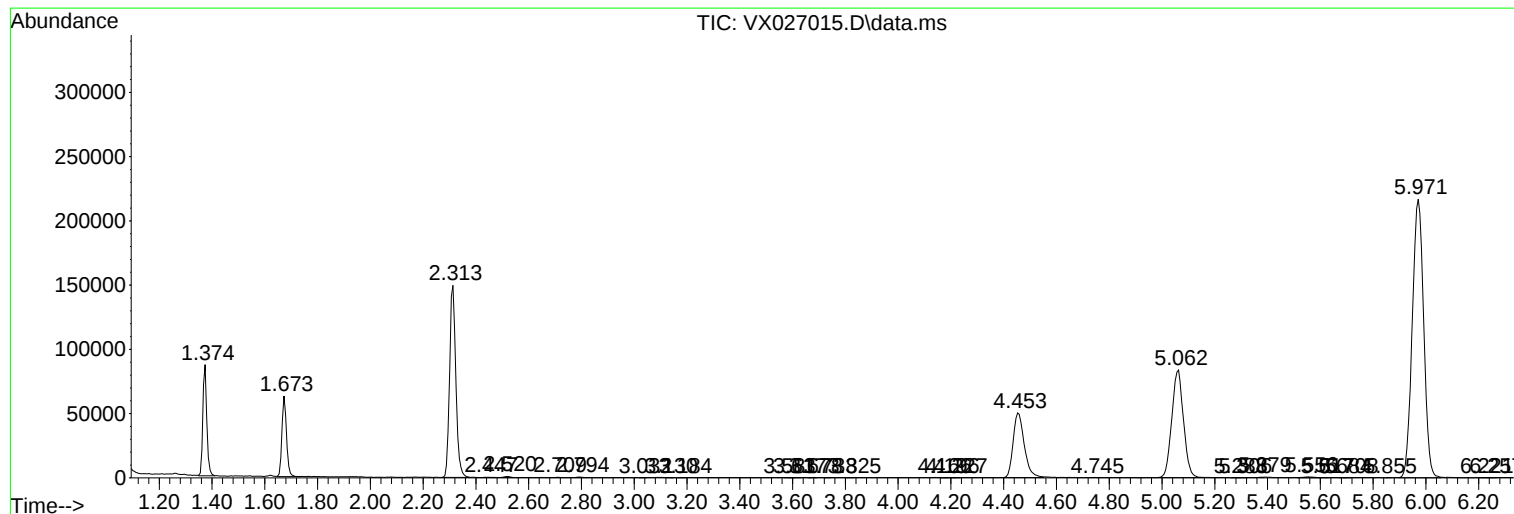
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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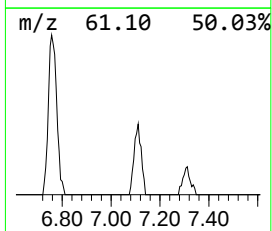
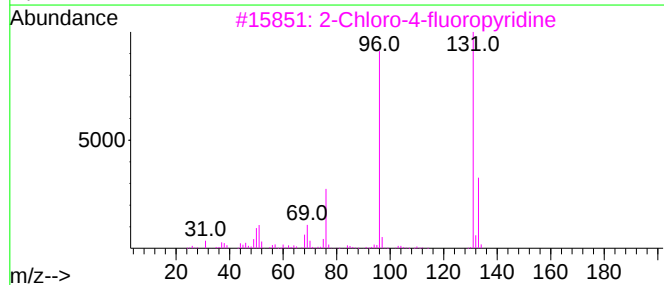
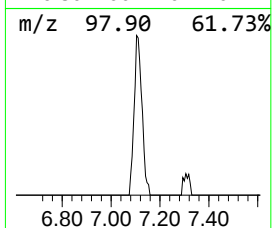
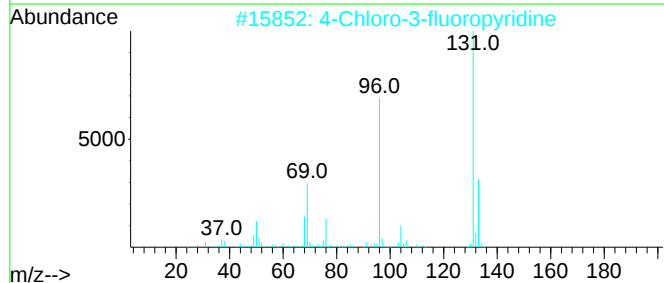
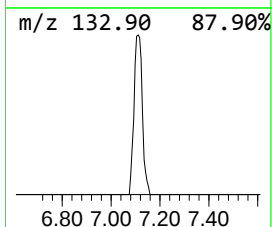
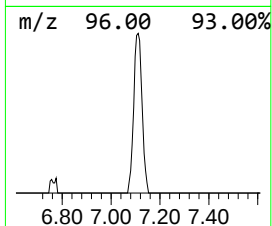
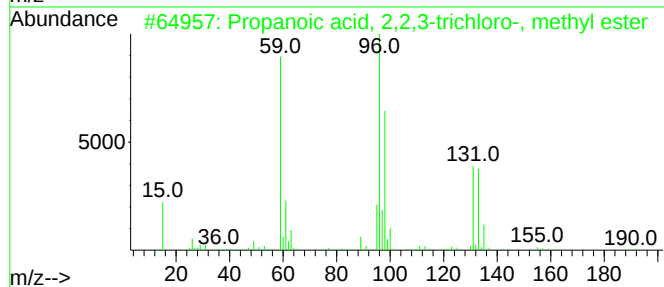
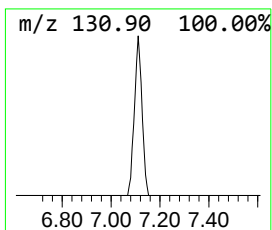
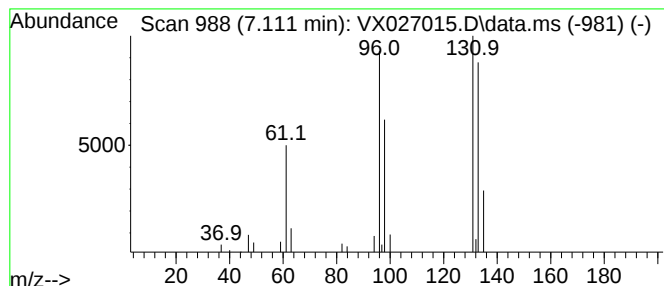
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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.
7.111	2.61 ug/L	16251	1,4-Difluorobenzene	6.763

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			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	7.111	2.6	ug/L	16251	1	6.763	311214	50.0