

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030621.D
 Acq On : 15 Aug 2022 12:24
 Operator : JC/MD
 Sample : N4168-01
 Misc : 8.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9B0

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	56	rVB	98597	131832	12.87%	1.520%
2	1.673	91	96	103	rBV	59529	102241	9.98%	1.179%
3	2.276	189	195	205	rVB	221281	356940	34.85%	4.115%
4	2.563	239	242	245	rBV3	408	600	0.06%	0.007%
5	2.642	251	255	258	rBV3	487	923	0.09%	0.011%
6	2.721	266	268	273	rVV3	1055	1824	0.18%	0.021%
7	2.782	273	278	281	rVV4	3241	6099	0.60%	0.070%
8	2.831	283	286	296	rVB3	5866	12278	1.20%	0.142%
9	2.941	296	304	317	rBV2	9401	25043	2.45%	0.289%
10	3.166	337	341	342	rBV2	686	914	0.09%	0.011%
11	3.672	422	424	426	rBV	470	436	0.04%	0.005%
12	4.392	539	542	544	rBV2	538	536	0.05%	0.006%
13	4.507	550	561	587	rBV2	38820	203502	19.87%	2.346%
14	5.056	640	651	667	rBV	133183	418137	40.82%	4.821%
15	5.294	689	690	694	rBV2	474	583	0.06%	0.007%
16	5.355	698	700	703	rVV2	438	510	0.05%	0.006%
17	5.379	703	704	706	rVV	746	586	0.06%	0.007%
18	5.404	706	708	709	rVV2	806	550	0.05%	0.006%
19	5.446	712	715	716	rVV3	465	518	0.05%	0.006%
20	5.465	716	718	720	rVV2	879	749	0.07%	0.009%
21	5.964	785	800	815	rBV3	370524	1024250	100.00%	11.809%
22	6.361	862	865	866	rBV3	1218	1256	0.12%	0.014%
23	6.592	900	903	905	rVB2	439	440	0.04%	0.005%
24	6.757	919	930	944	rBV	302118	742118	72.45%	8.556%
25	7.111	980	988	998	rBV5	6485	16472	1.61%	0.190%
26	7.214	1000	1005	1012	rBV3	2060	5483	0.54%	0.063%
27	7.312	1012	1021	1034	rVB2	201273	461474	45.05%	5.321%
28	7.428	1039	1040	1043	rVV2	775	718	0.07%	0.008%
29	7.476	1045	1048	1052	rBV2	980	1761	0.17%	0.020%
30	7.708	1080	1086	1096	rBV3	13405	29263	2.86%	0.337%
31	7.799	1099	1101	1104	rVB2	386	478	0.05%	0.006%
32	7.964	1120	1128	1134	rBV6	2531	6465	0.63%	0.075%
33	8.098	1148	1150	1155	rVB2	804	861	0.08%	0.010%
34	8.159	1156	1160	1163	rVB2	854	1194	0.12%	0.014%
35	8.251	1172	1175	1176	rBV2	531	514	0.05%	0.006%
36	8.324	1181	1187	1200	rBV	137282	235582	23.00%	2.716%

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 Title : VOC Analysis

37	8.501	1213	1216	1217	rVB3	624	422	0.04%	0.005%
38	8.647	1233	1240	1246	rBV	516127	820353	80.09%	9.458%
39	8.720	1246	1252	1262	rVB	388139	616157	60.16%	7.104%
40	8.903	1279	1282	1285	rBV4	2317	3129	0.31%	0.036%
41	8.952	1285	1290	1298	rVB	100619	149499	14.60%	1.724%
42	9.196	1328	1330	1333	rBV2	539	461	0.05%	0.005%
43	9.275	1340	1343	1345	rBV	698	735	0.07%	0.008%
44	9.403	1357	1364	1379	rBV	169066	433097	42.28%	4.993%
45	9.537	1383	1386	1390	rVV5	2754	4002	0.39%	0.046%
46	9.586	1391	1394	1407	rVB3	8331	18511	1.81%	0.213%
47	9.683	1407	1410	1412	rBV2	458	419	0.04%	0.005%
48	9.726	1412	1417	1422	rBV5	1181	2013	0.20%	0.023%
49	9.854	1433	1438	1443	rVB7	1552	2562	0.25%	0.030%
50	9.909	1443	1447	1453	rVB3	816	1358	0.13%	0.016%
51	9.994	1457	1461	1462	rBV2	535	500	0.05%	0.006%
52	10.055	1465	1471	1480	rBV	630319	857422	83.71%	9.886%
53	10.195	1492	1494	1496	rBV3	1110	1264	0.12%	0.015%
54	10.305	1507	1512	1519	rBV4	2256	3497	0.34%	0.040%
55	10.653	1563	1569	1576	rBV	36898	53623	5.24%	0.618%
56	10.787	1589	1591	1593	rVB2	693	449	0.04%	0.005%
57	10.945	1611	1617	1622	rBV3	1447	2899	0.28%	0.033%
58	11.018	1624	1629	1630	rBV	660	836	0.08%	0.010%
59	11.116	1643	1645	1648	rVB	568	459	0.04%	0.005%
60	11.201	1653	1659	1667	rBV	297251	413064	40.33%	4.762%
61	11.311	1674	1677	1681	rVB4	846	1330	0.13%	0.015%
62	11.384	1685	1689	1690	rVV2	621	750	0.07%	0.009%
63	11.445	1694	1699	1701	rBV4	750	1227	0.12%	0.014%
64	11.482	1702	1705	1711	rVB2	3106	4654	0.45%	0.054%
65	11.726	1743	1745	1748	rBV2	436	556	0.05%	0.006%
66	11.750	1748	1749	1753	rVB4	728	795	0.08%	0.009%
67	11.890	1769	1772	1775	rVB2	492	531	0.05%	0.006%
68	11.933	1777	1779	1783	rVV2	569	641	0.06%	0.007%
69	12.024	1789	1794	1801	rBV	626691	771606	75.33%	8.896%
70	12.238	1825	1829	1837	rBV6	2725	5608	0.55%	0.065%
71	12.323	1837	1843	1849	rBV	541980	661753	64.61%	7.630%
72	12.683	1900	1902	1906	rVB3	663	813	0.08%	0.009%
73	12.732	1906	1910	1911	rBV2	746	1031	0.10%	0.012%
74	12.866	1926	1932	1936	rBV5	2184	3835	0.37%	0.044%
75	12.896	1936	1937	1940	rVB2	774	661	0.06%	0.008%
76	12.975	1947	1950	1953	rBV3	497	688	0.07%	0.008%

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 Title : VOC Analysis

77	13.036	1957	1960	1964	rBV2	530	802	0.08%	0.009%
78	13.103	1967	1971	1975	rBV3	3411	4970	0.49%	0.057%
79	13.152	1978	1979	1983	rVB2	704	678	0.07%	0.008%
80	13.189	1983	1985	1987	rBV	412	523	0.05%	0.006%
81	13.439	2024	2026	2028	rBV	436	438	0.04%	0.005%
82	13.542	2041	2043	2045	rBV2	435	455	0.04%	0.005%
83	13.737	2073	2075	2077	rBV2	709	584	0.06%	0.007%
84	13.804	2082	2086	2089	rVB5	1864	2967	0.29%	0.034%
85	14.128	2135	2139	2144	rBV	2520	2894	0.28%	0.033%
86	14.164	2144	2145	2147	rVB2	884	500	0.05%	0.006%
87	14.189	2147	2149	2152	rBV3	708	989	0.10%	0.011%
88	14.262	2159	2161	2164	rVB3	989	664	0.06%	0.008%
89	14.359	2175	2177	2180	rVB2	721	571	0.06%	0.007%
90	14.390	2180	2182	2185	rVB2	460	458	0.04%	0.005%
91	14.432	2185	2189	2192	rBV2	614	977	0.10%	0.011%
92	14.506	2200	2201	2203	rBV2	633	462	0.05%	0.005%
93	14.621	2215	2220	2223	rBV5	1401	2369	0.23%	0.027%
94	14.756	2238	2242	2246	rBV4	5264	7057	0.69%	0.081%
95	15.024	2284	2286	2288	rBV3	642	482	0.05%	0.006%
96	15.219	2314	2318	2323	rBV5	2822	4176	0.41%	0.048%
97	15.390	2344	2346	2352	rBV4	1245	2215	0.22%	0.026%
98	15.542	2370	2371	2373	rBV2	593	431	0.04%	0.005%
99	16.042	2451	2453	2455	rBV2	759	473	0.05%	0.005%
100	16.450	2518	2520	2522	rBV	994	1000	0.10%	0.012%

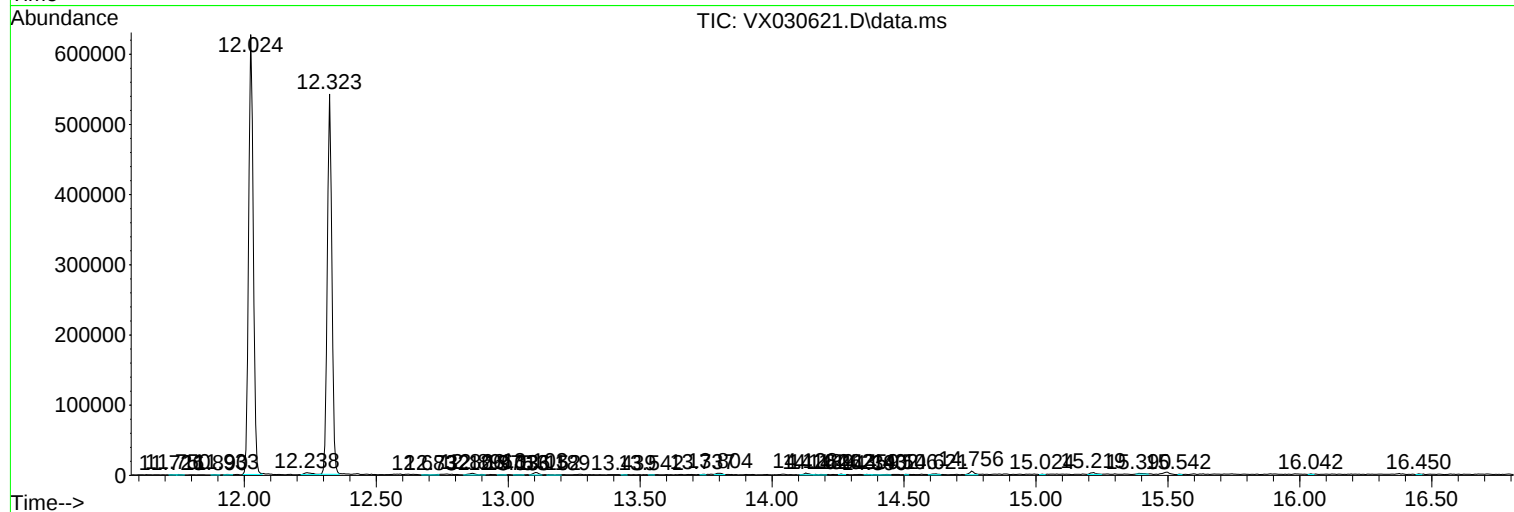
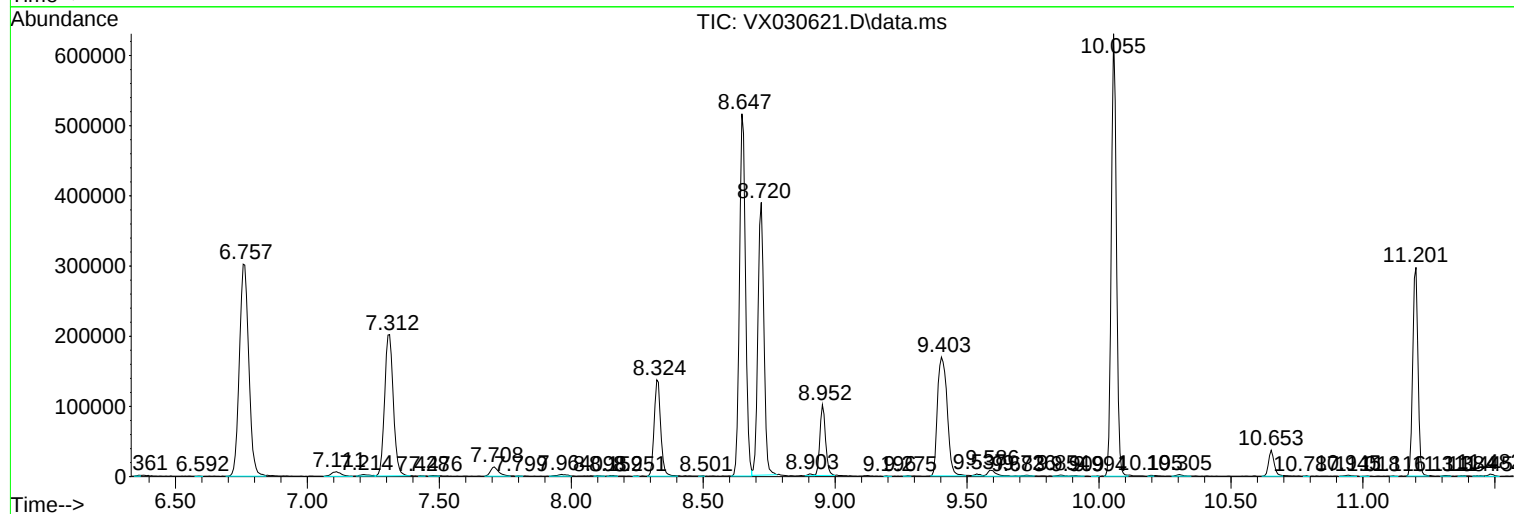
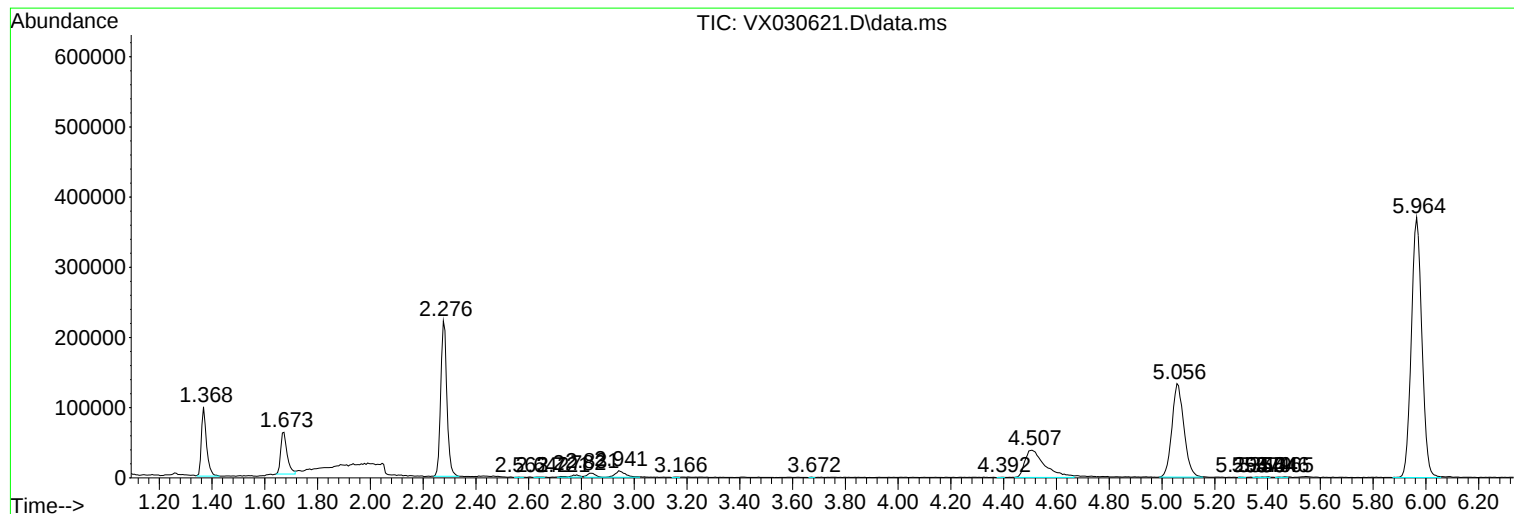
Sum of corrected areas: 8673475

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Instrument :
MSVOA_X
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EX9B0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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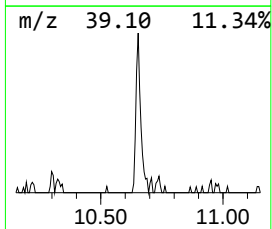
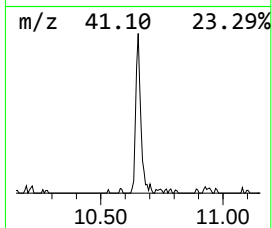
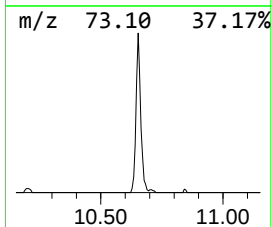
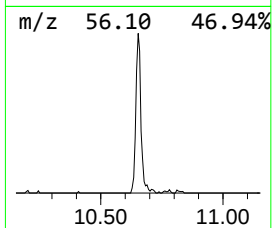
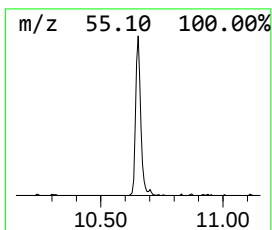
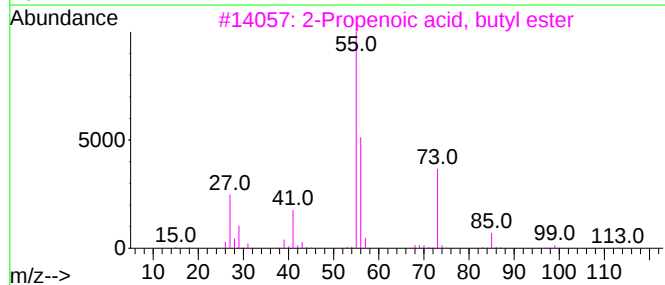
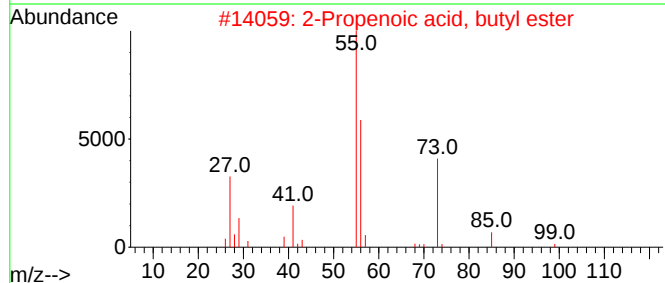
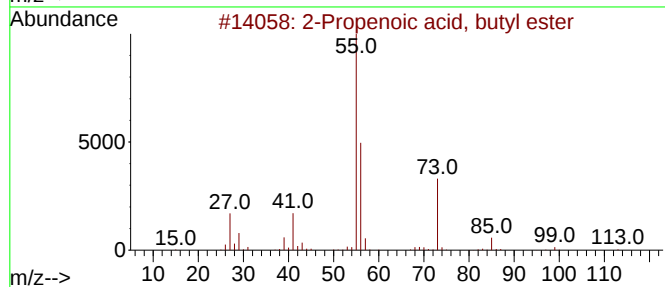
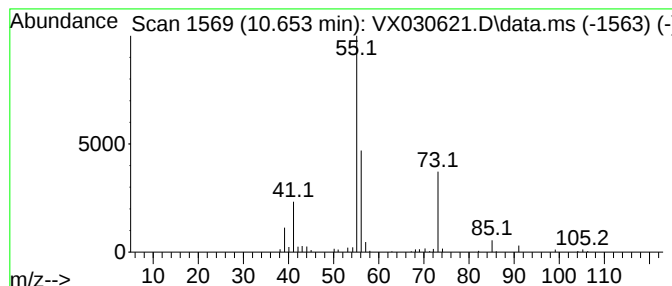
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Propenoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.653	3.13 ug/L	53623	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	78
2			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	78
3			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	72
4			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	56
5			Aminoacetonitrile	56	C2H4N2	000540-61-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propenoic aci...	10.653	3.1	ug/L	53623	2	10.055	857422	50.0