

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030633.D
 Acq On : 15 Aug 2022 17:45
 Operator : JC/MD
 Sample : N4168-09
 Misc : 10.16g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9B6

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: VX030633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	25	29	30	rBV3	5144	6207	0.54%	0.054%
2	1.367	42	46	54	rVB	94380	143323	12.56%	1.254%
3	1.605	83	85	88	rBV4	3313	5177	0.45%	0.045%
4	1.660	90	94	101	rVV	50213	78636	6.89%	0.688%
5	2.166	176	177	181	rBV4	1042	997	0.09%	0.009%
6	2.270	187	194	207	rBV	240837	388643	34.06%	3.400%
7	2.465	224	226	231	rVB5	1493	2043	0.18%	0.018%
8	2.721	264	268	269	rBV2	1715	1813	0.16%	0.016%
9	2.776	272	277	283	rVV3	3798	8327	0.73%	0.073%
10	2.836	283	287	289	rVB5	1080	1782	0.16%	0.016%
11	2.946	296	305	322	rBV2	24871	75909	6.65%	0.664%
12	3.135	330	336	343	rVB4	1877	4854	0.43%	0.042%
13	3.599	409	412	415	rVV4	1373	2142	0.19%	0.019%
14	4.507	550	561	589	rBV2	52122	247319	21.67%	2.164%
15	4.702	591	593	595	rBV3	1258	1083	0.09%	0.009%
16	5.056	643	651	690	rVB3	193770	964013	84.48%	8.433%
17	5.549	728	732	737	rVB6	2064	4363	0.38%	0.038%
18	5.964	785	800	815	rBV2	408344	1141052	100.00%	9.982%
19	6.379	861	868	872	rBV7	1645	4592	0.40%	0.040%
20	6.757	920	930	944	rBV	292791	689496	60.43%	6.032%
21	7.110	978	988	998	rVB8	8401	22800	2.00%	0.199%
22	7.220	998	1006	1012	rBV5	2400	6944	0.61%	0.061%
23	7.305	1012	1020	1031	rBV	226406	507086	44.44%	4.436%
24	7.433	1038	1041	1045	rVV4	1388	1570	0.14%	0.014%
25	7.476	1045	1048	1051	rVB5	1072	1308	0.11%	0.011%
26	7.708	1078	1086	1096	rBV	12115	26588	2.33%	0.233%
27	7.823	1101	1105	1112	rVB5	1452	3096	0.27%	0.027%
28	7.970	1118	1129	1134	rBV7	2943	7717	0.68%	0.068%
29	8.159	1155	1160	1165	rVB3	1426	2601	0.23%	0.023%
30	8.323	1181	1187	1199	rBV	147495	246120	21.57%	2.153%
31	8.488	1211	1214	1216	rBV3	895	1150	0.10%	0.010%
32	8.592	1225	1231	1233	rVV5	2569	4327	0.38%	0.038%
33	8.646	1233	1240	1246	rVV	579715	901910	79.04%	7.890%
34	8.720	1246	1252	1265	rVV	334011	530284	46.47%	4.639%
35	8.866	1269	1276	1278	rBV5	1083	2329	0.20%	0.020%
36	8.909	1278	1283	1285	rVV3	3585	5767	0.51%	0.050%

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37	8.951	1285	1290	1299	rVB	104016	160658	14.08%	1.405%
38	9.159	1320	1324	1329	rVB4	2247	3571	0.31%	0.031%
39	9.274	1339	1343	1349	rVB4	3751	5964	0.52%	0.052%
40	9.402	1354	1364	1378	rBV	221521	518447	45.44%	4.535%
41	9.537	1381	1386	1390	rVV5	2867	5079	0.45%	0.044%
42	9.591	1391	1395	1402	rVV3	7326	14246	1.25%	0.125%
43	9.646	1402	1404	1410	rVB4	1647	2535	0.22%	0.022%
44	9.725	1410	1417	1421	rBV6	2349	5381	0.47%	0.047%
45	9.854	1435	1438	1444	rVB3	2411	3260	0.29%	0.029%
46	10.055	1465	1471	1481	rBV	582456	785695	68.86%	6.873%
47	10.195	1490	1494	1501	rBV2	6092	8633	0.76%	0.076%
48	10.347	1507	1519	1529	rBV	235063	429637	37.65%	3.758%
49	10.652	1564	1569	1580	rBV2	31744	52793	4.63%	0.462%
50	10.805	1590	1594	1598	rVV4	2139	3104	0.27%	0.027%
51	10.847	1599	1601	1604	rVV3	1198	1335	0.12%	0.012%
52	10.902	1607	1610	1614	rBV4	1072	1306	0.11%	0.011%
53	10.963	1614	1620	1625	rVV2	5215	7012	0.61%	0.061%
54	11.195	1653	1658	1665	rBV	333031	463523	40.62%	4.055%
55	11.317	1674	1678	1681	rVB	1014	1379	0.12%	0.012%
56	11.457	1696	1701	1703	rBV3	5243	6704	0.59%	0.059%
57	11.481	1703	1705	1707	rVV	1257	962	0.08%	0.008%
58	11.530	1707	1713	1724	rVV	489035	737832	64.66%	6.455%
59	11.756	1745	1750	1755	rVB2	4926	6789	0.59%	0.059%
60	11.884	1766	1771	1772	rBV3	661	1100	0.10%	0.010%
61	11.926	1772	1778	1784	rBV	446828	625226	54.79%	5.469%
62	12.024	1789	1794	1802	rVB	577873	715674	62.72%	6.261%
63	12.128	1809	1811	1815	rVB5	913	1205	0.11%	0.011%
64	12.213	1822	1825	1826	rBV3	809	1022	0.09%	0.009%
65	12.237	1826	1829	1837	rVV4	3230	6437	0.56%	0.056%
66	12.323	1837	1843	1851	rBV	531432	683887	59.93%	5.983%
67	12.463	1864	1866	1871	rVB6	1744	2426	0.21%	0.021%
68	12.512	1871	1874	1877	rBV4	957	1155	0.10%	0.010%
69	12.579	1881	1885	1888	rVV4	817	1280	0.11%	0.011%
70	12.670	1896	1900	1904	rVV2	3463	3625	0.32%	0.032%
71	12.713	1904	1907	1913	rVV4	2462	3185	0.28%	0.028%
72	12.762	1913	1915	1919	rVB2	1991	2611	0.23%	0.023%
73	12.865	1927	1932	1935	rBV5	1912	2892	0.25%	0.025%
74	12.938	1941	1944	1948	rVV5	1160	2228	0.20%	0.019%
75	12.999	1950	1954	1959	rVB2	10645	13827	1.21%	0.121%
76	13.103	1966	1971	1978	rBV4	5983	11652	1.02%	0.102%

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 Title : VOC Analysis

77	13.182	1981	1984	1990	rVB4	1332	1857	0.16%	0.016%
78	13.261	1995	1997	2001	rVB3	1180	1517	0.13%	0.013%
79	13.389	2017	2018	2024	rVB2	1093	1332	0.12%	0.012%
80	13.438	2024	2026	2028	rBV3	866	1116	0.10%	0.010%
81	13.475	2028	2032	2037	rVB7	1708	2818	0.25%	0.025%
82	13.591	2047	2051	2054	rBV4	4043	5325	0.47%	0.047%
83	13.700	2065	2069	2072	rVB6	1764	2827	0.25%	0.025%
84	13.755	2073	2078	2080	rBV3	7173	10230	0.90%	0.089%
85	13.889	2095	2100	2101	rBV4	1391	1854	0.16%	0.016%
86	13.969	2109	2113	2116	rBV5	2932	3615	0.32%	0.032%
87	14.115	2133	2137	2144	rVB	5313	9954	0.87%	0.087%
88	14.206	2149	2152	2155	rBV5	902	1611	0.14%	0.014%
89	14.231	2155	2156	2160	rVV4	1693	1648	0.14%	0.014%
90	14.298	2164	2167	2168	rBV2	1098	1114	0.10%	0.010%
91	14.603	2213	2217	2222	rVV6	1517	3231	0.28%	0.028%
92	14.755	2236	2242	2247	rVV6	3849	7536	0.66%	0.066%
93	14.975	2274	2278	2284	rVB7	2869	5775	0.51%	0.051%
94	15.212	2313	2317	2322	rVB6	1828	2811	0.25%	0.025%
95	15.322	2333	2335	2340	rBV5	878	1496	0.13%	0.013%
96	15.389	2340	2346	2350	rBV5	3230	6243	0.55%	0.055%
97	15.493	2359	2363	2366	rBV4	1902	2522	0.22%	0.022%
98	16.365	2502	2506	2511	rVV7	1678	3752	0.33%	0.033%
99	16.438	2515	2518	2520	rBV4	1203	1411	0.12%	0.012%
100	16.608	2543	2546	2549	rVB3	917	1007	0.09%	0.009%

Sum of corrected areas: 11431247

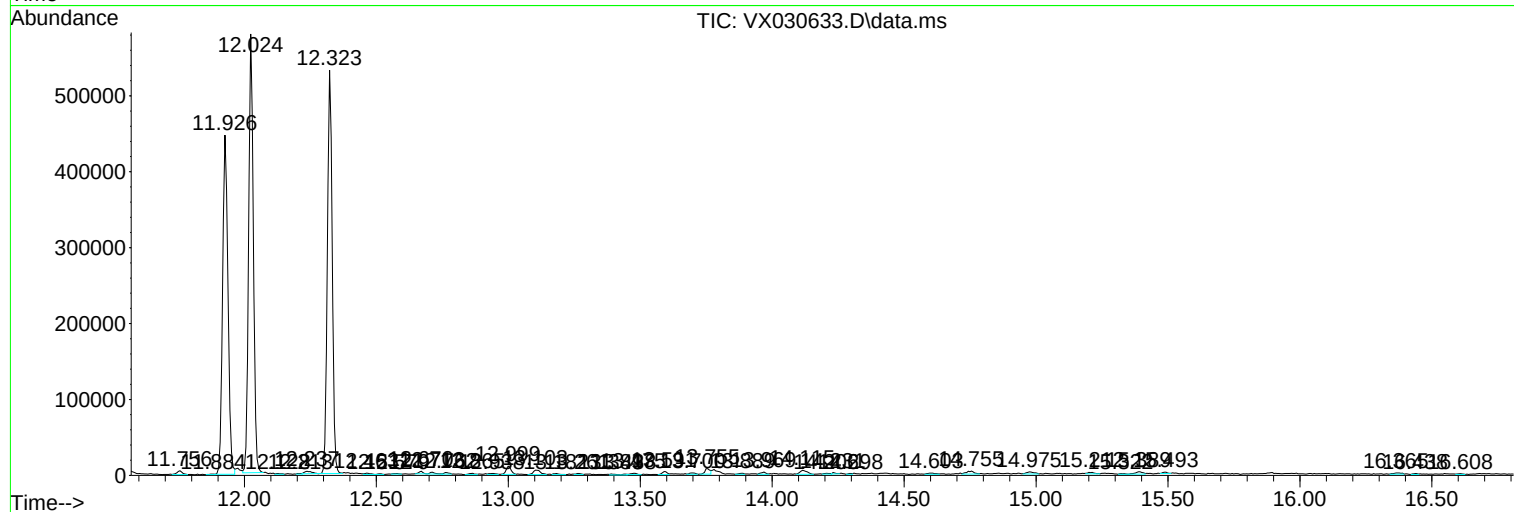
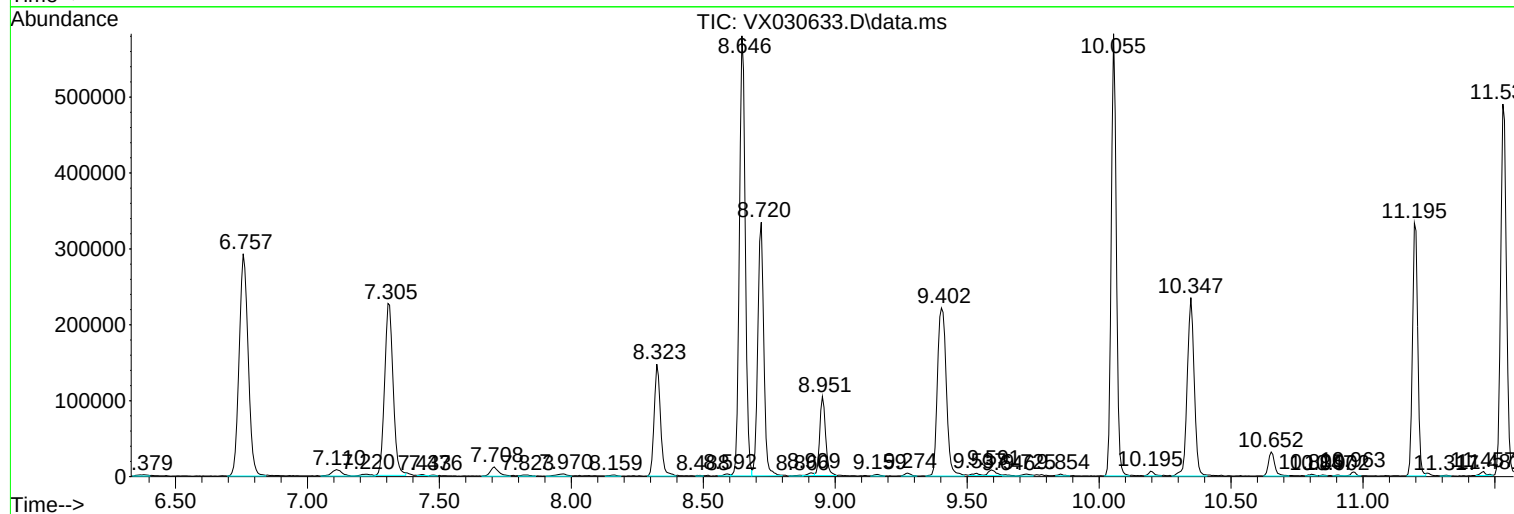
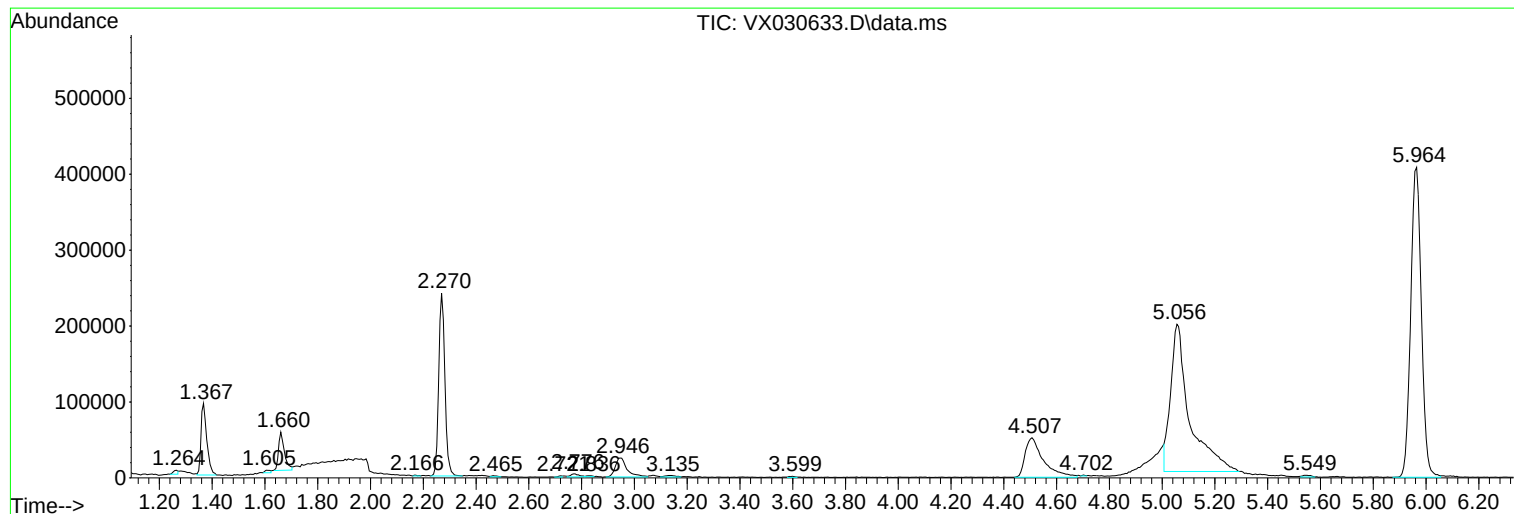
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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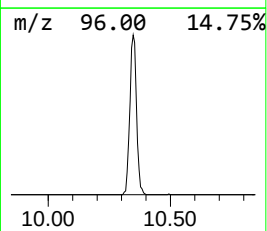
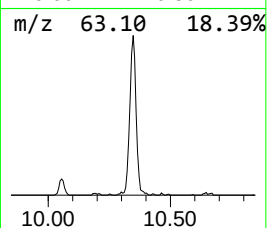
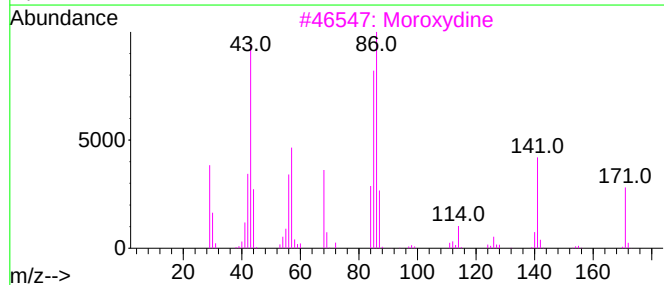
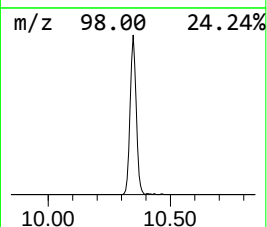
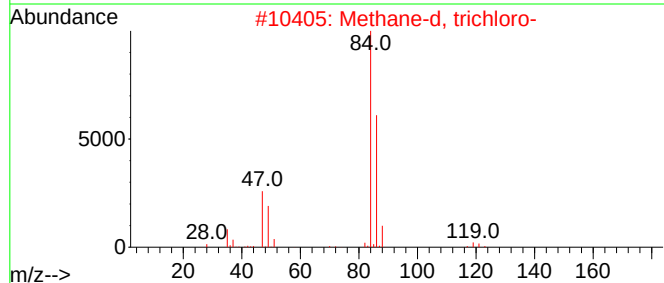
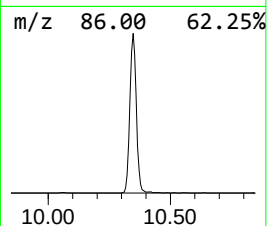
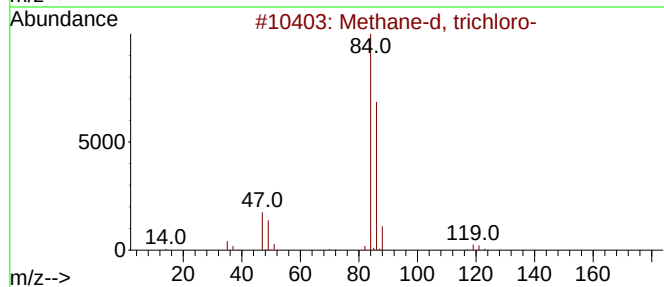
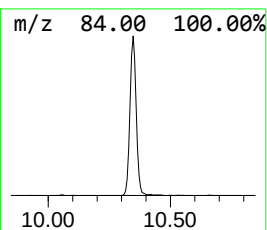
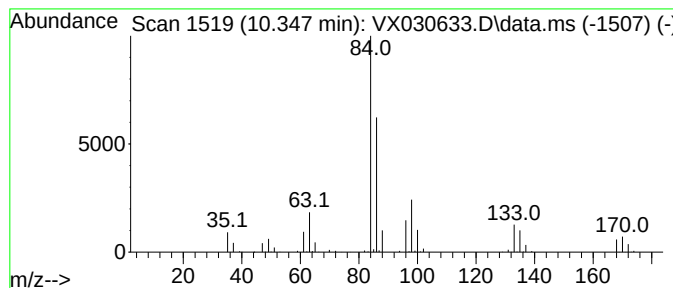
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.347	27.34 ug/L	429637	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane-d, trichloro-	119	CDCl3	000865-49-6	47
2			Methane-d, trichloro-	119	CDCl3	000865-49-6	40
3			Moroxydine	171	C6H13N5O	003731-59-7	9
4			Ethanamine, 2-chloro-N,N-diethyl-	135	C6H14ClN	000100-35-6	9
5			l-Isoleucine, N-(3-methyl-1-oxob...	229	C12H23NO3	118388-30-0	9



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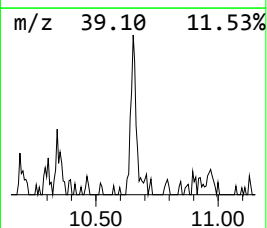
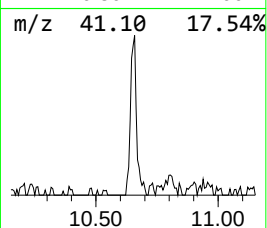
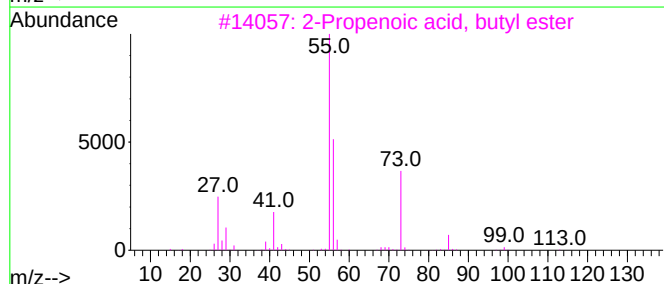
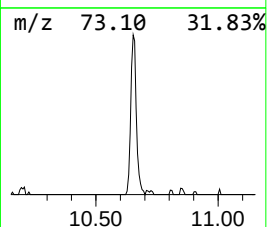
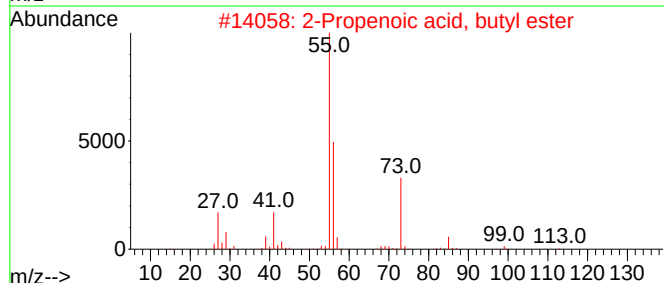
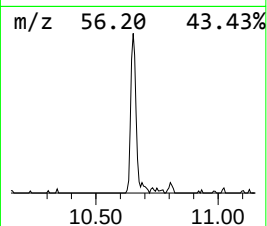
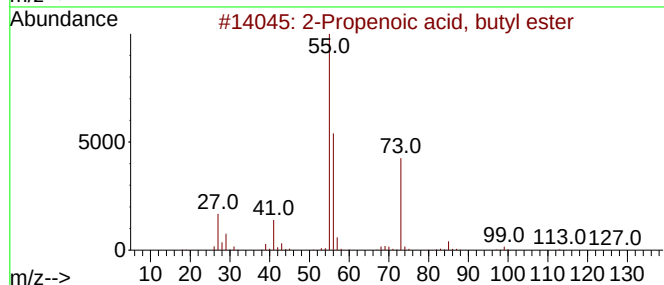
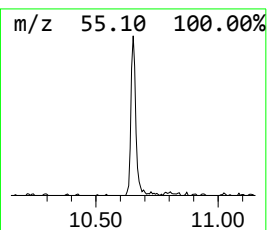
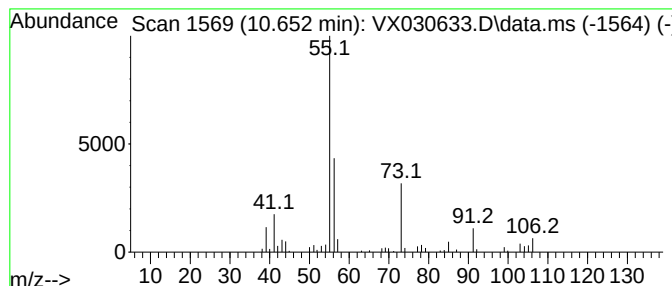
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 2-Propenoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.652	3.36 ug/L	52793	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	59
2			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	59
3			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	45
4			Isobutyl acrylate	128	C7H12O2	000106-63-8	28
5			2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	16



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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.347	27.3	ug/L	429637	2	10.055	785695	50.0
2-Propenoic aci...	10.652	3.4	ug/L	52793	2	10.055	785695	50.0