

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042452.D
 Acq On : 22 Jul 2024 18:15
 Operator : JC/MD
 Sample : P3264-11
 Misc : 5.18g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL4

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\SFAMXMLM070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042452.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	32	rBV2	17661	22420	3.43%	0.433%
2	1.368	42	46	49	rBV	22914	35225	5.39%	0.681%
3	2.276	189	195	212	rBV	95202	183129	28.04%	3.541%
4	2.636	251	254	256	rBV2	195	257	0.04%	0.005%
5	2.672	258	260	261	rBV	257	173	0.03%	0.003%
6	2.721	262	268	273	rBV	10311	20147	3.09%	0.390%
7	2.941	298	304	317	rVB2	3441	9169	1.40%	0.177%
8	3.075	324	326	328	rVB2	259	164	0.03%	0.003%
9	3.129	334	335	336	rBV	240	112	0.02%	0.002%
10	3.428	380	384	385	rVV	269	251	0.04%	0.005%
11	3.447	385	387	389	rVB2	191	150	0.02%	0.003%
12	3.483	389	393	395	rVB2	101	147	0.02%	0.003%
13	3.507	395	397	399	rBV2	140	157	0.02%	0.003%
14	3.636	415	418	419	rVB2	196	187	0.03%	0.004%
15	3.654	419	421	422	rBV2	133	114	0.02%	0.002%
16	3.727	431	433	435	rVB2	127	113	0.02%	0.002%
17	4.416	544	546	549	rVB2	177	195	0.03%	0.004%
18	4.495	550	559	575	rBV	38147	130637	20.01%	2.526%
19	5.056	640	651	667	rBV	78481	245182	37.55%	4.741%
20	5.556	724	733	739	rVB4	435	1354	0.21%	0.026%
21	5.605	739	741	743	rBV2	120	121	0.02%	0.002%
22	5.684	752	754	757	rBV2	150	124	0.02%	0.002%
23	5.720	757	760	763	rVB2	96	143	0.02%	0.003%
24	5.861	780	783	785	rBV2	155	187	0.03%	0.004%
25	5.964	789	800	829	rVV2	221439	652998	100.00%	12.626%
26	6.318	855	858	859	rVB	201	158	0.02%	0.003%
27	6.373	864	867	868	rBV	159	174	0.03%	0.003%
28	6.391	868	870	872	rBV2	296	300	0.05%	0.006%
29	6.483	883	885	886	rBV2	134	114	0.02%	0.002%
30	6.544	893	895	899	rVB2	142	166	0.03%	0.003%
31	6.757	921	930	952	rBV	208050	510308	78.15%	9.867%
32	7.123	983	990	997	rVB6	1707	4209	0.64%	0.081%
33	7.306	1012	1020	1042	rBV	128014	293381	44.93%	5.673%
34	7.488	1048	1050	1052	rBV2	303	208	0.03%	0.004%
35	7.507	1052	1053	1055	rVB2	267	179	0.03%	0.003%
36	7.574	1062	1064	1067	rBV2	161	180	0.03%	0.003%

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 Title : VOC Analysis

37	7.641	1072	1075	1077	rBV2	118	156	0.02%	0.003%
38	7.659	1077	1078	1081	rVV	176	144	0.02%	0.003%
39	7.720	1086	1088	1093	rVB2	163	205	0.03%	0.004%
40	7.842	1104	1108	1110	rBV2	149	166	0.03%	0.003%
41	7.891	1115	1116	1119	rBV2	135	128	0.02%	0.002%
42	7.958	1122	1127	1135	rBV4	630	1836	0.28%	0.035%
43	8.037	1138	1140	1143	rVB2	176	198	0.03%	0.004%
44	8.324	1181	1187	1199	rBV	65212	117137	17.94%	2.265%
45	8.507	1214	1217	1218	rBV	335	317	0.05%	0.006%
46	8.543	1222	1223	1229	rVB2	381	330	0.05%	0.006%
47	8.592	1229	1231	1233	rBV2	201	202	0.03%	0.004%
48	8.647	1234	1240	1250	rBV	326877	516502	79.10%	9.987%
49	8.952	1285	1290	1304	rBV	47963	76542	11.72%	1.480%
50	9.275	1337	1343	1354	rVB	39489	60824	9.31%	1.176%
51	9.391	1357	1362	1382	rBV	156830	316644	48.49%	6.122%
52	9.708	1412	1414	1418	rBV2	579	698	0.11%	0.013%
53	9.811	1428	1431	1435	rVB2	187	217	0.03%	0.004%
54	10.055	1465	1471	1489	rBV	423136	589888	90.34%	11.406%
55	10.305	1509	1512	1520	rVB4	964	1692	0.26%	0.033%
56	10.372	1522	1523	1525	rBV2	142	118	0.02%	0.002%
57	10.646	1564	1568	1572	rBV4	528	982	0.15%	0.019%
58	10.756	1582	1586	1588	rBV	120	119	0.02%	0.002%
59	10.896	1606	1609	1612	rBV	155	164	0.03%	0.003%
60	10.970	1617	1621	1624	rBV3	1090	1399	0.21%	0.027%
61	11.104	1641	1643	1644	rVB	223	117	0.02%	0.002%
62	11.122	1644	1646	1649	rBV2	149	141	0.02%	0.003%
63	11.195	1652	1658	1664	rBV	255404	336006	51.46%	6.497%
64	11.317	1676	1678	1683	rVB3	460	465	0.07%	0.009%
65	11.451	1694	1700	1702	rBV3	469	655	0.10%	0.013%
66	11.628	1728	1729	1732	rBV2	101	119	0.02%	0.002%
67	11.762	1747	1751	1754	rVB3	590	990	0.15%	0.019%
68	11.927	1775	1778	1779	rBV	183	162	0.02%	0.003%
69	11.982	1783	1787	1789	rBV3	1620	2175	0.33%	0.042%
70	12.024	1789	1794	1809	rVB	416020	529795	81.13%	10.244%
71	12.219	1822	1826	1835	rBV	10561	14912	2.28%	0.288%
72	12.323	1837	1843	1853	rVV	362677	464517	71.14%	8.982%
73	12.494	1870	1871	1875	rVB2	254	244	0.04%	0.005%
74	12.603	1886	1889	1890	rBV	183	158	0.02%	0.003%
75	12.634	1893	1894	1898	rVB2	309	209	0.03%	0.004%
76	12.670	1898	1900	1902	rBV2	146	163	0.02%	0.003%

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 Title : VOC Analysis

77	12.762	1911	1915	1919	rBV2	700	882	0.14%	0.017%
78	12.872	1929	1933	1940	rBV2	4526	6574	1.01%	0.127%
79	13.116	1968	1973	1974	rBV2	356	304	0.05%	0.006%
80	13.176	1981	1983	1985	rBV2	141	112	0.02%	0.002%
81	13.201	1985	1987	1989	rBV	158	147	0.02%	0.003%
82	13.250	1994	1995	1998	rVB	231	163	0.02%	0.003%
83	13.280	1998	2000	2002	rBV2	130	145	0.02%	0.003%
84	13.305	2002	2004	2006	rVB	192	131	0.02%	0.003%
85	13.408	2015	2021	2026	rBV3	2183	3093	0.47%	0.060%
86	13.445	2026	2027	2031	rBV	142	151	0.02%	0.003%
87	13.500	2034	2036	2038	rBV	215	147	0.02%	0.003%
88	13.591	2048	2051	2056	rVB3	593	775	0.12%	0.015%
89	13.682	2063	2066	2072	rVB3	1561	2235	0.34%	0.043%
90	13.780	2079	2082	2087	rBV	1330	1980	0.30%	0.038%
91	13.865	2094	2096	2100	rVB2	197	240	0.04%	0.005%
92	13.920	2104	2105	2109	rBV2	146	153	0.02%	0.003%
93	13.969	2110	2113	2117	rVB3	391	500	0.08%	0.010%
94	14.060	2126	2128	2129	rVB2	214	121	0.02%	0.002%
95	14.073	2129	2130	2132	rBV2	218	191	0.03%	0.004%
96	14.134	2135	2140	2144	rVV2	1857	2464	0.38%	0.048%
97	14.280	2160	2164	2166	rVB2	206	266	0.04%	0.005%
98	14.432	2186	2189	2192	rBV2	758	839	0.13%	0.016%
99	14.786	2245	2247	2249	rVB2	475	430	0.07%	0.008%
100	14.810	2249	2251	2252	rBV	282	156	0.02%	0.003%

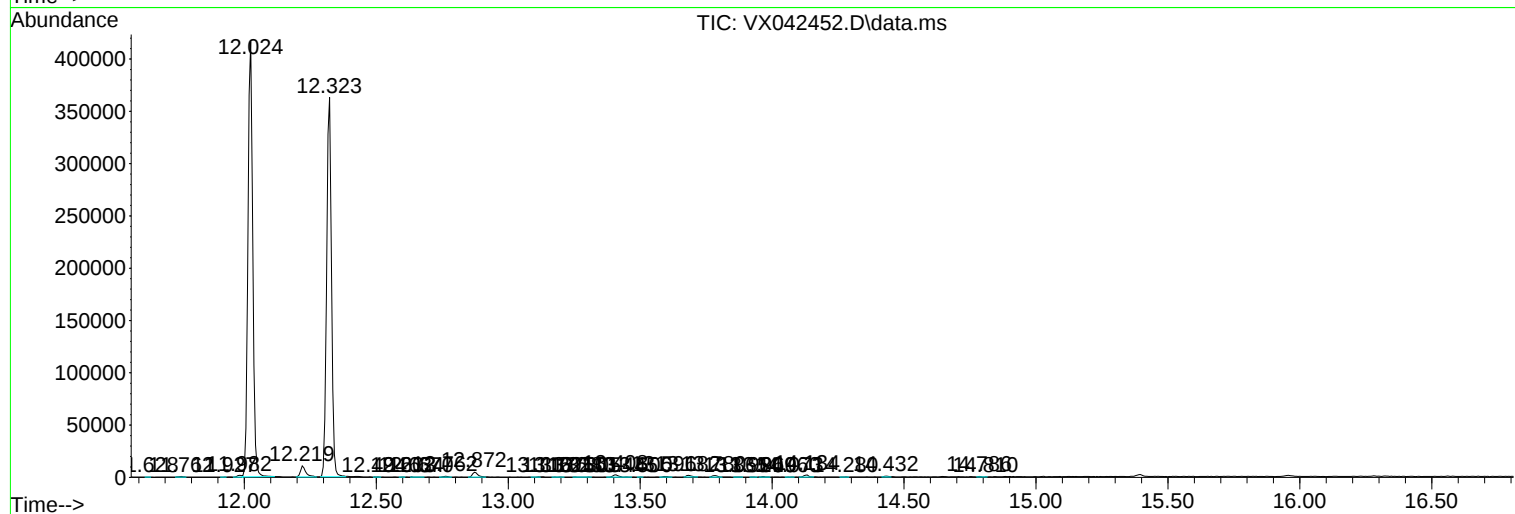
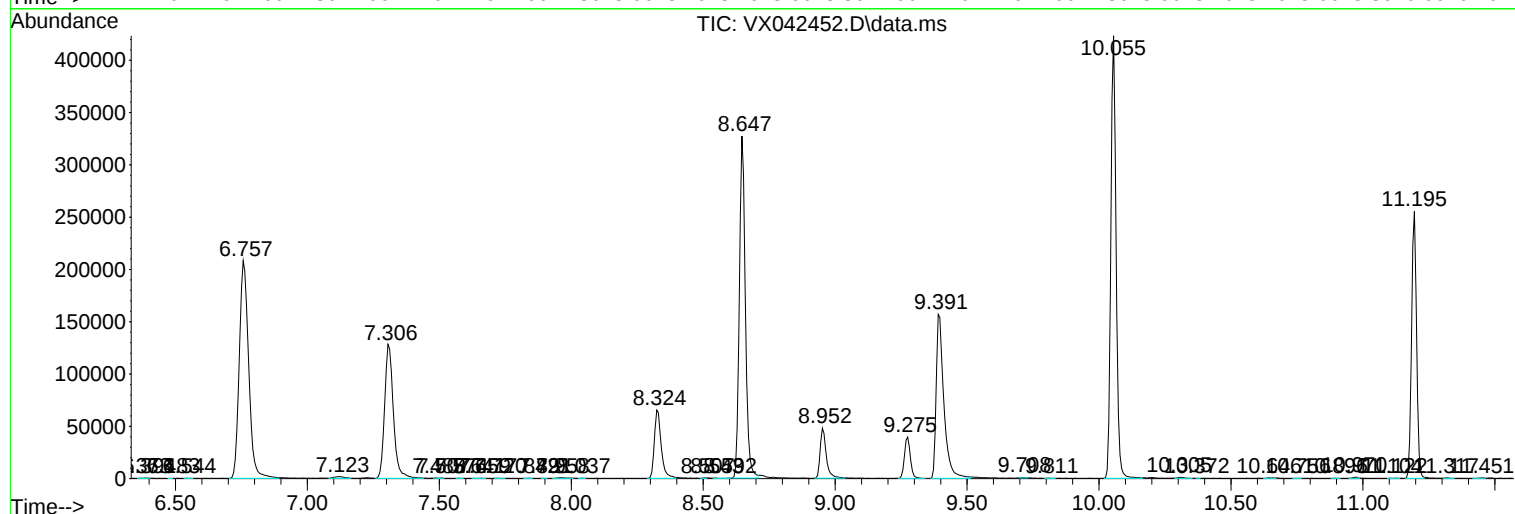
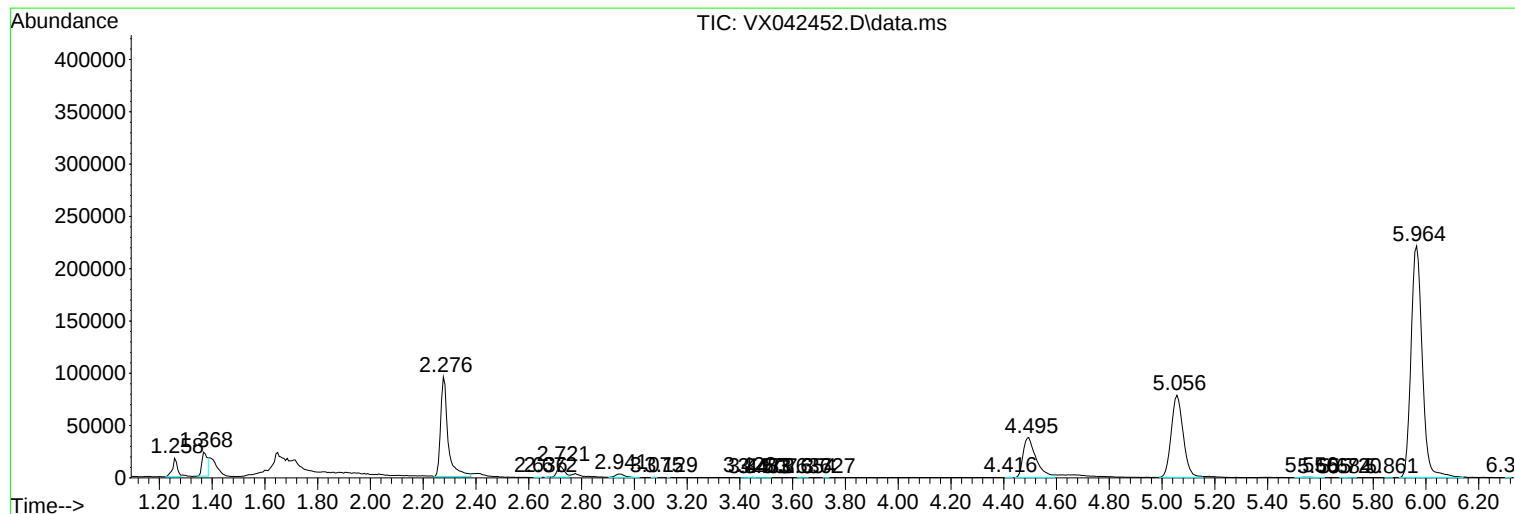
Sum of corrected areas: 5171868

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc