

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042423.D
 Acq On : 19 Jul 2024 23:30
 Operator : JC/MD
 Sample : P3298-12 100X
 Misc : 5.01g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB42

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: VX042423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	36	rBV	32524	44541	6.31%	0.807%
2	1.368	43	46	58	rVB	66174	84986	12.05%	1.540%
3	1.648	88	92	102	rVB	53211	75457	10.70%	1.367%
4	2.294	192	198	210	rBV	118473	187237	26.54%	3.393%
5	2.392	212	214	220	rVB2	552	633	0.09%	0.011%
6	2.465	223	226	228	rVB2	159	166	0.02%	0.003%
7	2.508	228	233	234	rBV3	248	303	0.04%	0.005%
8	2.666	258	259	262	rBV2	108	125	0.02%	0.002%
9	2.782	274	278	284	rBB5	1077	1996	0.28%	0.036%
10	2.940	297	304	315	rVB	5016	11586	1.64%	0.210%
11	3.093	327	329	332	rBV2	106	141	0.02%	0.003%
12	3.184	342	344	346	rBV	155	115	0.02%	0.002%
13	3.331	365	368	369	rBV2	124	109	0.02%	0.002%
14	3.355	369	372	375	rVB2	208	247	0.04%	0.004%
15	3.379	375	376	378	rBV2	166	148	0.02%	0.003%
16	3.690	425	427	429	rBV2	121	104	0.01%	0.002%
17	4.038	482	484	487	rVV	163	141	0.02%	0.003%
18	4.087	491	492	493	rBV	219	133	0.02%	0.002%
19	4.135	498	500	505	rVB	162	217	0.03%	0.004%
20	4.294	522	526	527	rVV2	116	149	0.02%	0.003%
21	4.471	546	555	572	rBV	49534	151943	21.54%	2.753%
22	4.861	618	619	621	rBV	177	104	0.01%	0.002%
23	4.916	624	628	631	rVB	180	250	0.04%	0.005%
24	4.946	631	633	638	rVB2	182	221	0.03%	0.004%
25	5.056	638	651	668	rBV	89754	271419	38.47%	4.919%
26	5.342	696	698	699	rVB	182	104	0.01%	0.002%
27	5.385	702	705	711	rVB3	392	774	0.11%	0.014%
28	5.513	723	726	728	rVB2	167	153	0.02%	0.003%
29	5.544	728	731	732	rBV2	235	246	0.03%	0.004%
30	5.964	789	800	819	rBV2	238270	705522	100.00%	12.785%
31	6.537	892	894	895	rBV	184	133	0.02%	0.002%
32	6.623	906	908	909	rVB	205	102	0.01%	0.002%
33	6.641	909	911	913	rBV2	134	102	0.01%	0.002%
34	6.684	916	918	921	rBV	111	126	0.02%	0.002%
35	6.757	922	930	947	rBV	210431	510797	72.40%	9.256%
36	7.117	984	989	997	rVB6	1217	3089	0.44%	0.056%

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 Title : VOC Analysis

37	7.220	1001	1006	1007	rBV3	321	541	0.08%	0.010%
38	7.306	1012	1020	1037	rVV	138638	310071	43.95%	5.619%
39	7.440	1041	1042	1044	rVV	360	183	0.03%	0.003%
40	7.464	1044	1046	1050	rVB3	235	274	0.04%	0.005%
41	7.684	1080	1082	1085	rVV2	118	115	0.02%	0.002%
42	7.720	1087	1088	1092	rBV	195	162	0.02%	0.003%
43	7.854	1106	1110	1111	rBV2	123	185	0.03%	0.003%
44	7.903	1115	1118	1119	rVV2	122	146	0.02%	0.003%
45	7.952	1122	1126	1138	rVV3	544	1541	0.22%	0.028%
46	8.031	1138	1139	1143	rVV2	207	199	0.03%	0.004%
47	8.086	1146	1148	1150	rBV	210	195	0.03%	0.004%
48	8.171	1160	1162	1165	rVB	233	204	0.03%	0.004%
49	8.202	1165	1167	1168	rBV	170	127	0.02%	0.002%
50	8.257	1171	1176	1177	rBV2	114	138	0.02%	0.003%
51	8.324	1181	1187	1201	rBV	75181	131057	18.58%	2.375%
52	8.525	1212	1220	1224	rBV4	580	1182	0.17%	0.021%
53	8.647	1232	1240	1256	rBV	364074	574468	81.42%	10.410%
54	8.952	1285	1290	1302	rBV	54610	83250	11.80%	1.509%
55	9.104	1313	1315	1316	rBV2	147	129	0.02%	0.002%
56	9.226	1334	1335	1338	rVB	172	122	0.02%	0.002%
57	9.275	1340	1343	1349	rBV2	560	852	0.12%	0.015%
58	9.384	1356	1361	1383	rBV	220249	337478	47.83%	6.116%
59	9.708	1409	1414	1419	rVB4	1102	1881	0.27%	0.034%
60	9.805	1429	1430	1432	rVB	167	103	0.01%	0.002%
61	9.951	1450	1454	1456	rBV	245	271	0.04%	0.005%
62	10.012	1462	1464	1465	rBV	216	155	0.02%	0.003%
63	10.055	1465	1471	1485	rVV	435546	599317	84.95%	10.860%
64	10.305	1508	1512	1518	rVB3	486	850	0.12%	0.015%
65	10.470	1537	1539	1541	rVB2	117	115	0.02%	0.002%
66	10.500	1541	1544	1545	rBV	243	173	0.02%	0.003%
67	10.567	1553	1555	1556	rBV	198	131	0.02%	0.002%
68	10.640	1566	1567	1572	rBV3	209	212	0.03%	0.004%
69	10.707	1576	1578	1581	rVB	161	117	0.02%	0.002%
70	10.829	1596	1598	1601	rVV2	136	115	0.02%	0.002%
71	10.872	1603	1605	1608	rBV2	94	128	0.02%	0.002%
72	11.134	1646	1648	1650	rBV2	195	161	0.02%	0.003%
73	11.189	1652	1657	1668	rVV	276633	364302	51.64%	6.602%
74	11.378	1686	1688	1689	rBV2	143	103	0.01%	0.002%
75	11.421	1694	1695	1700	rVB2	151	133	0.02%	0.002%
76	11.463	1700	1702	1706	rBV2	98	128	0.02%	0.002%

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 Title : VOC Analysis

77	11.500	1706	1708	1711	rVV2	101	119	0.02%	0.002%
78	11.555	1714	1717	1718	rBV2	136	123	0.02%	0.002%
79	11.762	1749	1751	1752	rVB	164	118	0.02%	0.002%
80	11.939	1778	1780	1782	rBV2	160	132	0.02%	0.002%
81	12.024	1788	1794	1806	rBV	407318	543915	77.09%	9.857%
82	12.225	1825	1827	1828	rBV	161	144	0.02%	0.003%
83	12.317	1837	1842	1855	rBV	390409	503355	71.35%	9.122%
84	12.488	1868	1870	1875	rVB4	269	437	0.06%	0.008%
85	12.524	1875	1876	1879	rVV	281	170	0.02%	0.003%
86	12.573	1881	1884	1885	rVB	134	105	0.01%	0.002%
87	12.707	1903	1906	1907	rBV2	147	158	0.02%	0.003%
88	12.737	1910	1911	1913	rBV	128	133	0.02%	0.002%
89	12.762	1913	1915	1918	rVB4	334	380	0.05%	0.007%
90	12.872	1929	1933	1934	rBV	141	127	0.02%	0.002%
91	12.981	1950	1951	1953	rVB2	208	128	0.02%	0.002%
92	13.036	1958	1960	1962	rVB	194	158	0.02%	0.003%
93	13.493	2034	2035	2038	rBV2	91	106	0.02%	0.002%
94	13.737	2072	2075	2077	rBV2	156	162	0.02%	0.003%
95	13.756	2077	2078	2080	rBV	213	116	0.02%	0.002%
96	13.902	2099	2102	2104	rBV2	168	242	0.03%	0.004%
97	14.030	2121	2123	2124	rVB	211	102	0.01%	0.002%
98	14.127	2136	2139	2145	rVB2	960	1287	0.18%	0.023%
99	14.451	2190	2192	2194	rVB2	246	192	0.03%	0.003%
100	15.389	2343	2346	2352	rVB4	1202	1781	0.25%	0.032%

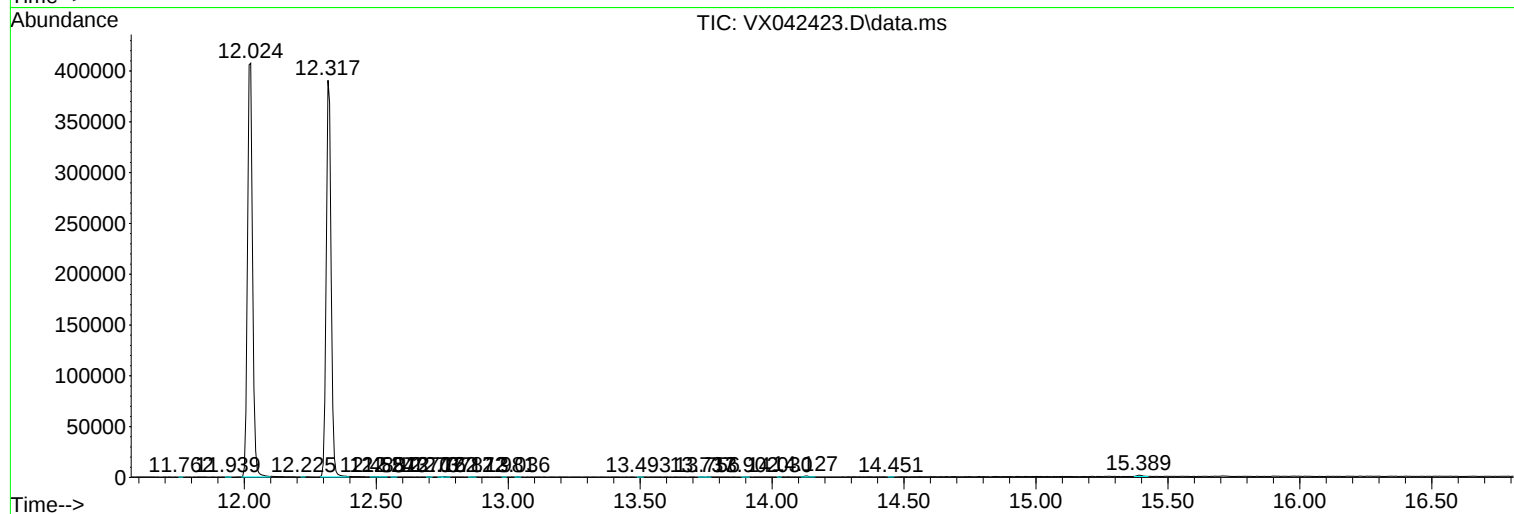
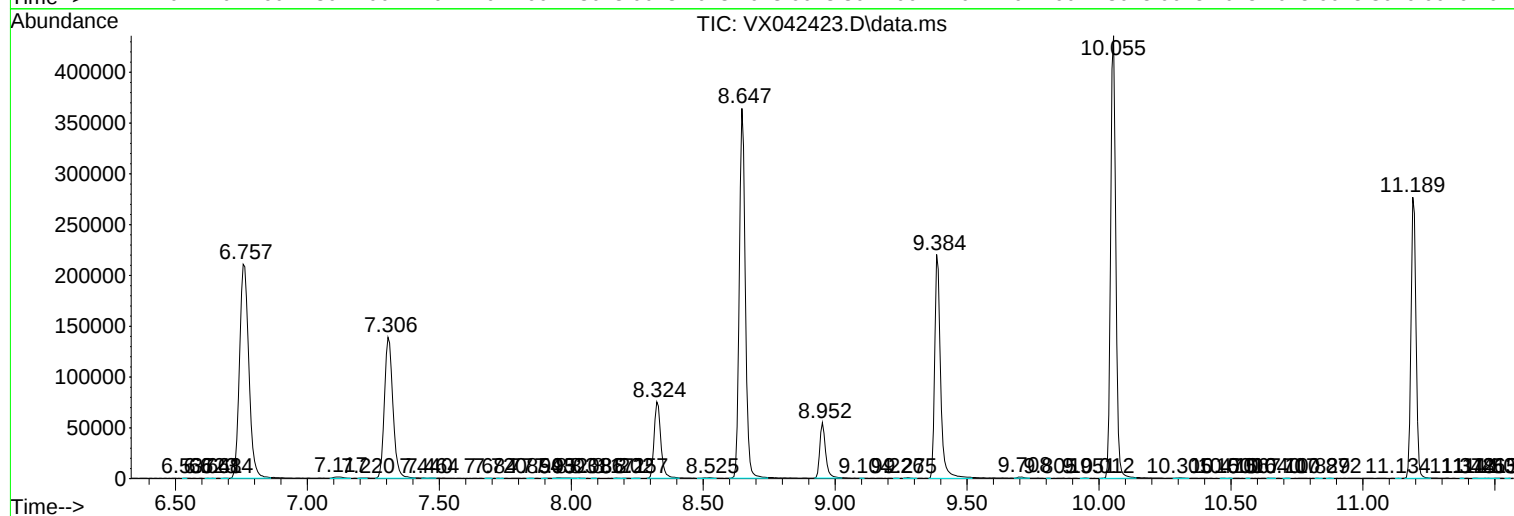
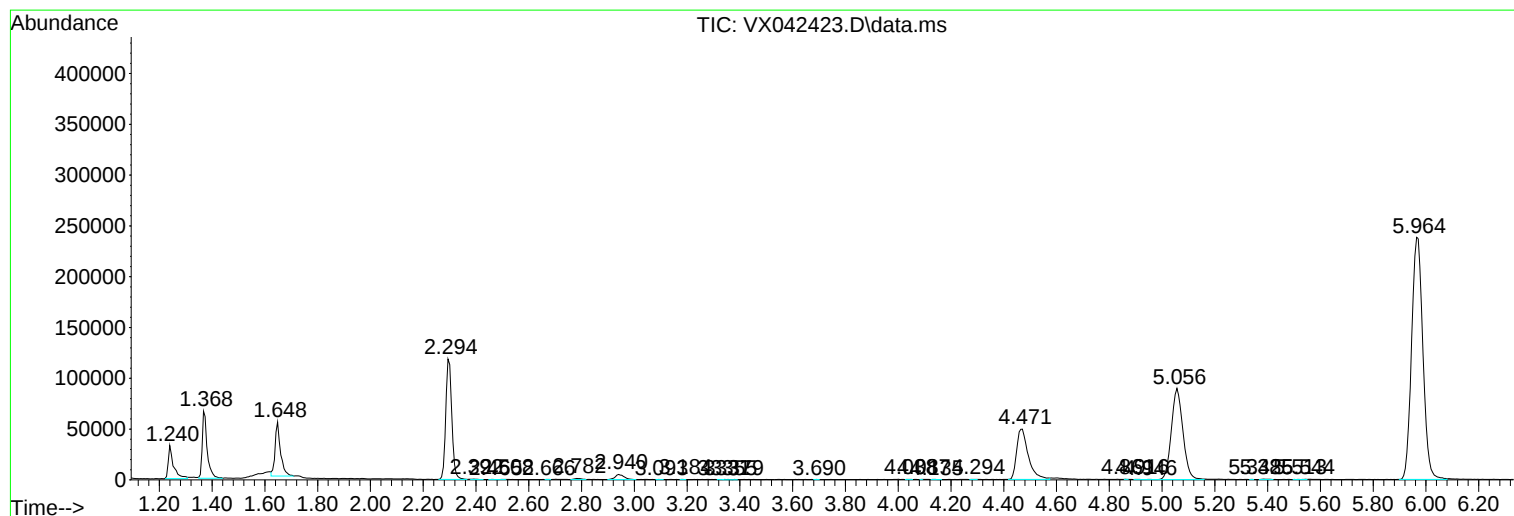
Sum of corrected areas: 5518323

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

TIC Library :
TIC Integration Parameters: LSCINT.P



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No Library Search Compounds Detected

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