

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120923\  
 Data File : VX039124.D  
 Acq On : 08 Dec 2023 22:39  
 Operator : JC/MD  
 Sample : 05646-20 40X  
 Misc : 3.11g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AT9

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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

Signal : TIC: VX039124.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.246       | 23            | 26          | 27           | rBV      | 3833           | 3138          | 0.12%           | 0.027%        |
| 2         | 1.307       | 34            | 36          | 39           | rVB2     | 1892           | 1702          | 0.07%           | 0.015%        |
| 3         | 1.368       | 42            | 46          | 53           | rVV      | 135633         | 140993        | 5.39%           | 1.212%        |
| 4         | 1.502       | 66            | 68          | 73           | rVB      | 5428           | 8887          | 0.34%           | 0.076%        |
| 5         | 1.556       | 73            | 77          | 78           | rBV3     | 3195           | 4149          | 0.16%           | 0.036%        |
| 6         | 1.581       | 80            | 81          | 83           | rBV      | 3417           | 3366          | 0.13%           | 0.029%        |
| 7         | 1.605       | 83            | 85          | 87           | rVV3     | 3047           | 3584          | 0.14%           | 0.031%        |
| 8         | 1.666       | 91            | 95          | 106          | rVV      | 90004          | 133865        | 5.12%           | 1.150%        |
| 9         | 1.880       | 129           | 130         | 133          | rBV      | 1145           | 1450          | 0.06%           | 0.012%        |
| 10        | 2.142       | 171           | 173         | 178          | rVB2     | 1635           | 2661          | 0.10%           | 0.023%        |
| 11        | 2.251       | 185           | 191         | 193          | rBV2     | 5303           | 10945         | 0.42%           | 0.094%        |
| 12        | 2.306       | 194           | 200         | 210          | rVB      | 231381         | 362181        | 13.85%          | 3.113%        |
| 13        | 2.770       | 273           | 276         | 277          | rBV      | 2038           | 1913          | 0.07%           | 0.016%        |
| 14        | 2.794       | 278           | 280         | 283          | rVV3     | 2748           | 3055          | 0.12%           | 0.026%        |
| 15        | 2.940       | 297           | 304         | 311          | rBV      | 11622          | 25084         | 0.96%           | 0.216%        |
| 16        | 3.416       | 379           | 382         | 383          | rBV      | 1129           | 1237          | 0.05%           | 0.011%        |
| 17        | 3.629       | 416           | 417         | 421          | rBV      | 1531           | 2194          | 0.08%           | 0.019%        |
| 18        | 3.666       | 421           | 423         | 427          | rVV      | 1250           | 1620          | 0.06%           | 0.014%        |
| 19        | 3.757       | 434           | 438         | 439          | rVB      | 2056           | 2031          | 0.08%           | 0.017%        |
| 20        | 3.776       | 439           | 441         | 445          | rBV      | 1110           | 1796          | 0.07%           | 0.015%        |
| 21        | 3.855       | 453           | 454         | 455          | rBV      | 2105           | 1178          | 0.05%           | 0.010%        |
| 22        | 3.952       | 469           | 470         | 472          | rBV      | 1352           | 1113          | 0.04%           | 0.010%        |
| 23        | 4.111       | 494           | 496         | 499          | rVB      | 1532           | 1220          | 0.05%           | 0.010%        |
| 24        | 4.355       | 534           | 536         | 538          | rBV      | 1489           | 1345          | 0.05%           | 0.012%        |
| 25        | 4.446       | 543           | 551         | 564          | rBV      | 97127          | 279134        | 10.68%          | 2.399%        |
| 26        | 4.696       | 588           | 592         | 596          | rBV      | 1803           | 3265          | 0.12%           | 0.028%        |
| 27        | 4.971       | 636           | 637         | 639          | rVB      | 1908           | 1256          | 0.05%           | 0.011%        |
| 28        | 5.056       | 639           | 651         | 665          | rBV      | 132273         | 435130        | 16.64%          | 3.739%        |
| 29        | 5.257       | 683           | 684         | 687          | rBV      | 1589           | 1487          | 0.06%           | 0.013%        |
| 30        | 5.288       | 687           | 689         | 690          | rVV      | 1653           | 1238          | 0.05%           | 0.011%        |
| 31        | 5.324       | 693           | 695         | 697          | rVB      | 1890           | 1537          | 0.06%           | 0.013%        |
| 32        | 5.409       | 707           | 709         | 712          | rVB      | 2369           | 2652          | 0.10%           | 0.023%        |
| 33        | 5.617       | 742           | 743         | 746          | rVB      | 1546           | 1458          | 0.06%           | 0.013%        |
| 34        | 5.659       | 746           | 750         | 751          | rBV      | 2050           | 2478          | 0.09%           | 0.021%        |
| 35        | 5.757       | 763           | 766         | 769          | rBV      | 1917           | 2820          | 0.11%           | 0.024%        |
| 36        | 5.842       | 778           | 780         | 784          | rVB      | 2039           | 2559          | 0.10%           | 0.022%        |

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 ClientSampleId :  
 C0AT9

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMXLM120523WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 5.897  | 787  | 789  | 790  | rBV  | 1557    | 1286    | 0.05%   | 0.011%  |
| 38 | 5.970  | 790  | 801  | 816  | rVV2 | 360848  | 1105841 | 42.30%  | 9.503%  |
| 39 | 6.086  | 819  | 820  | 822  | rBV  | 2215    | 1348    | 0.05%   | 0.012%  |
| 40 | 6.269  | 848  | 850  | 854  | rVB  | 1662    | 1549    | 0.06%   | 0.013%  |
| 41 | 6.519  | 889  | 891  | 893  | rBV  | 1662    | 1448    | 0.06%   | 0.012%  |
| 42 | 6.757  | 921  | 930  | 945  | rBV  | 267815  | 659344  | 25.22%  | 5.666%  |
| 43 | 6.885  | 948  | 951  | 954  | rBV2 | 1770    | 3074    | 0.12%   | 0.026%  |
| 44 | 7.062  | 979  | 980  | 981  | rBV  | 2117    | 1169    | 0.04%   | 0.010%  |
| 45 | 7.104  | 981  | 987  | 990  | rVV2 | 2751    | 6704    | 0.26%   | 0.058%  |
| 46 | 7.305  | 1011 | 1020 | 1036 | rBV  | 226577  | 507629  | 19.42%  | 4.362%  |
| 47 | 7.708  | 1083 | 1086 | 1087 | rBV  | 1172    | 1176    | 0.04%   | 0.010%  |
| 48 | 7.836  | 1103 | 1107 | 1108 | rBV  | 1438    | 1631    | 0.06%   | 0.014%  |
| 49 | 7.885  | 1113 | 1115 | 1117 | rVB  | 1387    | 1255    | 0.05%   | 0.011%  |
| 50 | 8.324  | 1181 | 1187 | 1198 | rBV  | 167072  | 269726  | 10.32%  | 2.318%  |
| 51 | 8.500  | 1214 | 1216 | 1218 | rVB  | 1728    | 1483    | 0.06%   | 0.013%  |
| 52 | 8.531  | 1218 | 1221 | 1222 | rBV  | 1134    | 1195    | 0.05%   | 0.010%  |
| 53 | 8.647  | 1234 | 1240 | 1255 | rVB  | 551320  | 869047  | 33.24%  | 7.468%  |
| 54 | 8.945  | 1284 | 1289 | 1298 | rBV  | 115857  | 181227  | 6.93%   | 1.557%  |
| 55 | 9.336  | 1351 | 1353 | 1355 | rBV  | 1931    | 1457    | 0.06%   | 0.013%  |
| 56 | 9.384  | 1355 | 1361 | 1372 | rVV  | 441948  | 656135  | 25.10%  | 5.639%  |
| 57 | 9.695  | 1409 | 1412 | 1415 | rBV2 | 3649    | 5737    | 0.22%   | 0.049%  |
| 58 | 9.781  | 1425 | 1426 | 1428 | rBV  | 1477    | 1400    | 0.05%   | 0.012%  |
| 59 | 9.945  | 1451 | 1453 | 1456 | rVB2 | 1366    | 1503    | 0.06%   | 0.013%  |
| 60 | 10.055 | 1465 | 1471 | 1482 | rBV  | 548109  | 871980  | 33.35%  | 7.494%  |
| 61 | 10.238 | 1500 | 1501 | 1503 | rBV  | 1903    | 1208    | 0.05%   | 0.010%  |
| 62 | 10.591 | 1557 | 1559 | 1560 | rVB  | 2284    | 1430    | 0.05%   | 0.012%  |
| 63 | 10.604 | 1560 | 1561 | 1562 | rBV  | 2174    | 1334    | 0.05%   | 0.011%  |
| 64 | 10.659 | 1567 | 1570 | 1571 | rBV  | 1372    | 1604    | 0.06%   | 0.014%  |
| 65 | 10.939 | 1614 | 1616 | 1619 | rVB  | 1281    | 1246    | 0.05%   | 0.011%  |
| 66 | 11.012 | 1624 | 1628 | 1630 | rVV  | 1652    | 1438    | 0.06%   | 0.012%  |
| 67 | 11.189 | 1652 | 1657 | 1667 | rVB  | 422790  | 537295  | 20.55%  | 4.617%  |
| 68 | 11.402 | 1689 | 1692 | 1693 | rBV  | 1348    | 1366    | 0.05%   | 0.012%  |
| 69 | 11.421 | 1693 | 1695 | 1698 | rVB  | 1251    | 1277    | 0.05%   | 0.011%  |
| 70 | 11.463 | 1701 | 1702 | 1706 | rVB  | 1580    | 1137    | 0.04%   | 0.010%  |
| 71 | 11.579 | 1719 | 1721 | 1723 | rVB  | 2072    | 1614    | 0.06%   | 0.014%  |
| 72 | 11.597 | 1723 | 1724 | 1726 | rBV  | 1437    | 1410    | 0.05%   | 0.012%  |
| 73 | 11.640 | 1730 | 1731 | 1735 | rBV  | 1667    | 1465    | 0.06%   | 0.013%  |
| 74 | 11.701 | 1739 | 1741 | 1743 | rBV  | 2009    | 2088    | 0.08%   | 0.018%  |
| 75 | 11.969 | 1780 | 1785 | 1789 | rBV  | 47893   | 61322   | 2.35%   | 0.527%  |
| 76 | 12.036 | 1789 | 1796 | 1804 | rVB2 | 1512856 | 2614393 | 100.00% | 22.468% |

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Instrument :  
 MSVOA\_X  
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 C0AT9

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\SFAMXML120523WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 12.177 | 1818 | 1819 | 1821 | rVB  | 2242   | 1463    | 0.06%  | 0.013% |
| 78  | 12.262 | 1831 | 1833 | 1837 | rVB  | 1926   | 1706    | 0.07%  | 0.015% |
| 79  | 12.317 | 1837 | 1842 | 1854 | rBV3 | 639786 | 1054339 | 40.33% | 9.061% |
| 80  | 12.591 | 1886 | 1887 | 1890 | rBV  | 1527   | 1312    | 0.05%  | 0.011% |
| 81  | 12.646 | 1892 | 1896 | 1897 | rVB  | 1556   | 1386    | 0.05%  | 0.012% |
| 82  | 12.725 | 1907 | 1909 | 1911 | rVB  | 1629   | 1382    | 0.05%  | 0.012% |
| 83  | 12.750 | 1911 | 1913 | 1915 | rBV  | 1210   | 1128    | 0.04%  | 0.010% |
| 84  | 13.061 | 1959 | 1964 | 1970 | rBV5 | 9283   | 17920   | 0.69%  | 0.154% |
| 85  | 13.115 | 1970 | 1973 | 1974 | rVB3 | 1988   | 1989    | 0.08%  | 0.017% |
| 86  | 13.152 | 1977 | 1979 | 1982 | rBV  | 1017   | 1210    | 0.05%  | 0.010% |
| 87  | 13.335 | 2007 | 2009 | 2010 | rBV  | 1810   | 1165    | 0.04%  | 0.010% |
| 88  | 13.585 | 2045 | 2050 | 2057 | rVV  | 200792 | 253982  | 9.71%  | 2.183% |
| 89  | 13.634 | 2057 | 2058 | 2060 | rVB  | 2171   | 1173    | 0.04%  | 0.010% |
| 90  | 13.884 | 2096 | 2099 | 2100 | rBV  | 1202   | 1469    | 0.06%  | 0.013% |
| 91  | 13.957 | 2106 | 2111 | 2120 | rVB  | 302055 | 391679  | 14.98% | 3.366% |
| 92  | 14.359 | 2173 | 2177 | 2181 | rBV  | 1961   | 2281    | 0.09%  | 0.020% |
| 93  | 14.451 | 2190 | 2192 | 2194 | rVB  | 1635   | 1194    | 0.05%  | 0.010% |
| 94  | 14.475 | 2194 | 2196 | 2199 | rBV  | 1658   | 2520    | 0.10%  | 0.022% |
| 95  | 14.768 | 2241 | 2244 | 2245 | rBV2 | 2585   | 2609    | 0.10%  | 0.022% |
| 96  | 15.249 | 2318 | 2323 | 2330 | rBV2 | 30879  | 46003   | 1.76%  | 0.395% |
| 97  | 15.383 | 2342 | 2345 | 2347 | rBV  | 1568   | 1850    | 0.07%  | 0.016% |
| 98  | 15.438 | 2353 | 2354 | 2356 | rBV  | 2094   | 1833    | 0.07%  | 0.016% |
| 99  | 15.566 | 2372 | 2375 | 2376 | rBV  | 1427   | 1356    | 0.05%  | 0.012% |
| 100 | 16.578 | 2539 | 2541 | 2544 | rVB  | 1534   | 1569    | 0.06%  | 0.013% |

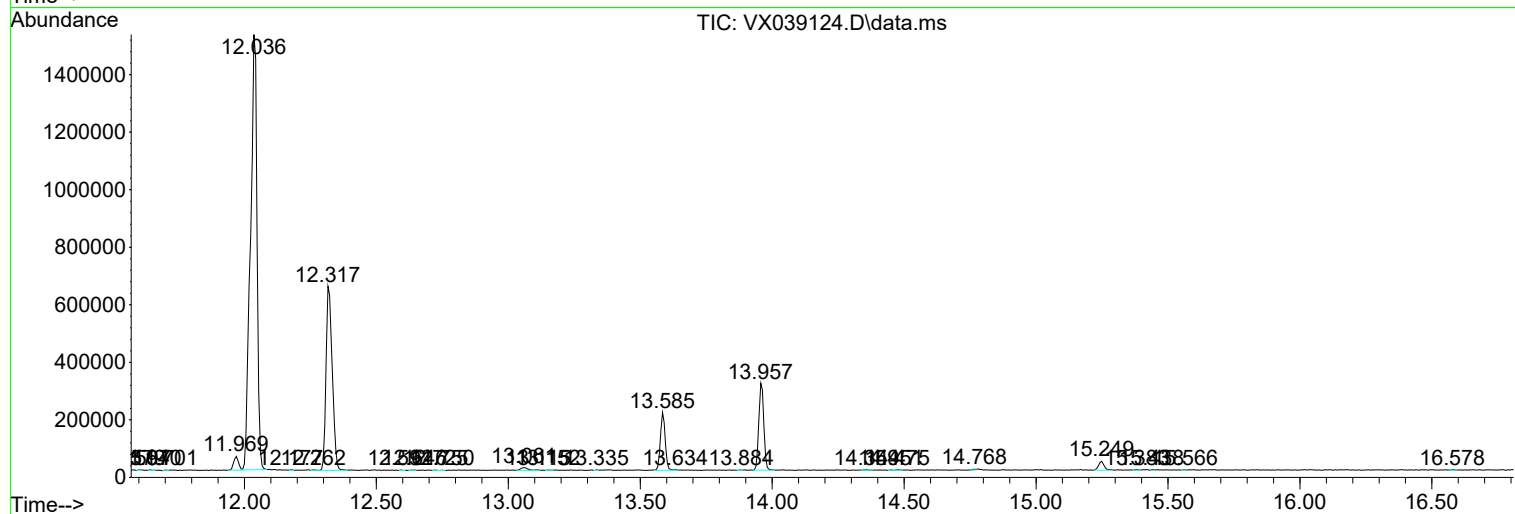
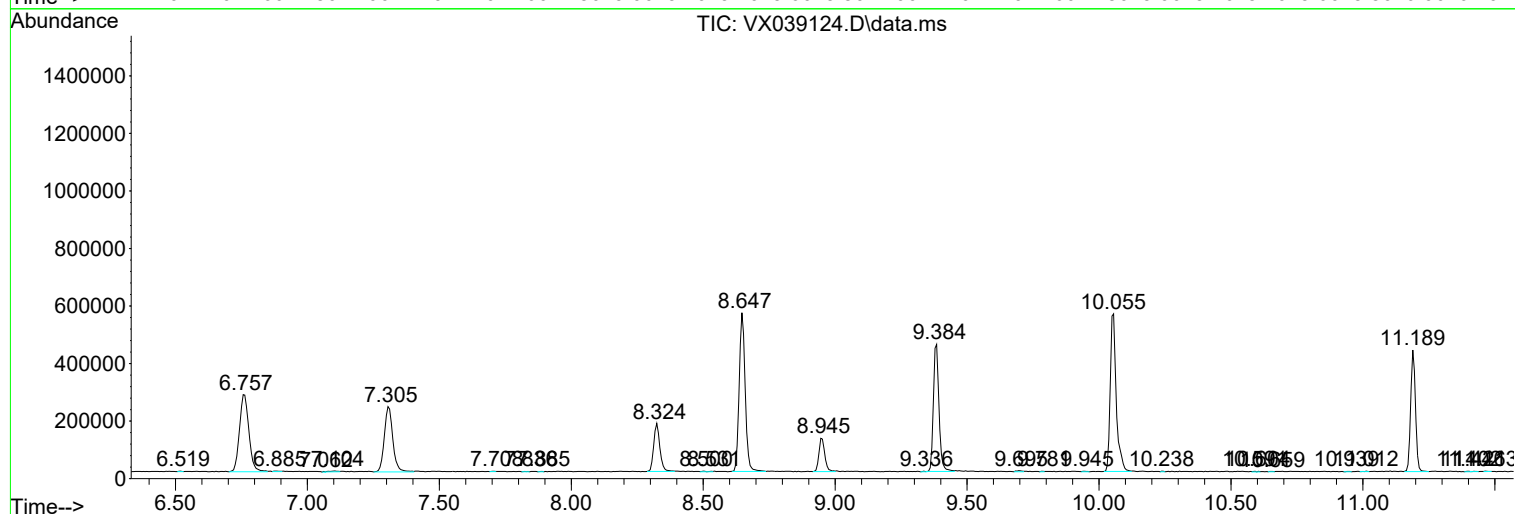
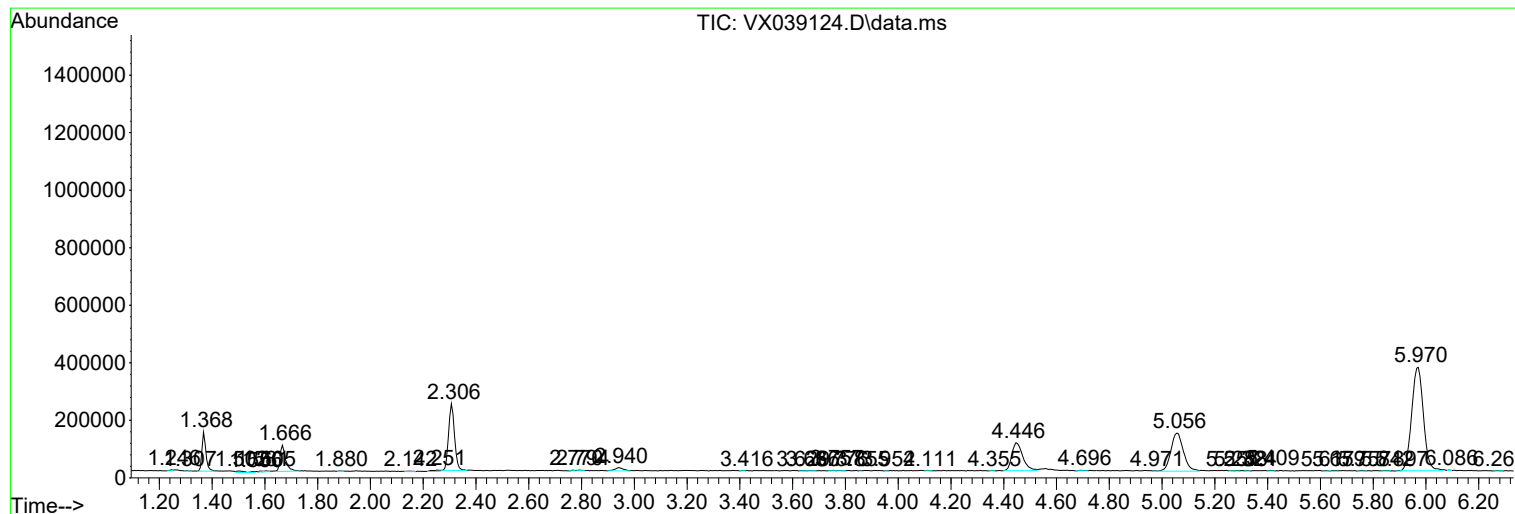
Sum of corrected areas: 11636210

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C0AT9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM120523WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
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 |