

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032119\  
 Data File : VU030284.D  
 Acq On : 21 Mar 2019 22:24  
 Operator : JC/SP  
 Sample : K2017-16  
 Misc : 5.59g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BF0E2

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM031919WMA.M  
 Title : VOC Analysis

Signal : TIC

| 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         | 1.177       | 22            | 27          | 33           | rBV      | 10101          | 9922          | 0.65%           | 0.089%        |
| 2         | 1.395       | 87            | 95          | 117          | rBV      | 148460         | 183375        | 11.96%          | 1.648%        |
| 3         | 1.550       | 139           | 143         | 146          | rBV      | 3284           | 3061          | 0.20%           | 0.028%        |
| 4         | 1.640       | 165           | 171         | 185          | rBV      | 76718          | 95558         | 6.23%           | 0.859%        |
| 5         | 2.138       | 321           | 326         | 329          | rBV2     | 5300           | 5518          | 0.36%           | 0.050%        |
| 6         | 2.225       | 343           | 353         | 366          | rVB      | 271164         | 411923        | 26.87%          | 3.701%        |
| 7         | 2.508       | 438           | 441         | 442          | rBV      | 1519           | 948           | 0.06%           | 0.009%        |
| 8         | 2.633       | 475           | 480         | 485          | rVB      | 1571           | 2009          | 0.13%           | 0.018%        |
| 9         | 2.675       | 485           | 493         | 507          | rBV3     | 4371           | 10205         | 0.67%           | 0.092%        |
| 10        | 3.125       | 630           | 633         | 639          | rVB2     | 1310           | 1148          | 0.07%           | 0.010%        |
| 11        | 3.170       | 639           | 647         | 653          | rVB      | 1883           | 3154          | 0.21%           | 0.028%        |
| 12        | 3.212       | 653           | 660         | 663          | rBV2     | 1340           | 2060          | 0.13%           | 0.019%        |
| 13        | 3.344       | 697           | 701         | 705          | rBV      | 1786           | 1524          | 0.10%           | 0.014%        |
| 14        | 3.370       | 707           | 709         | 716          | rVB      | 1645           | 1312          | 0.09%           | 0.012%        |
| 15        | 3.411       | 717           | 722         | 724          | rBV      | 1197           | 1203          | 0.08%           | 0.011%        |
| 16        | 3.627       | 785           | 789         | 794          | rBV      | 1106           | 1245          | 0.08%           | 0.011%        |
| 17        | 3.733       | 816           | 822         | 826          | rVB      | 1398           | 1681          | 0.11%           | 0.015%        |
| 18        | 3.759       | 826           | 830         | 833          | rVB      | 1293           | 918           | 0.06%           | 0.008%        |
| 19        | 3.804       | 840           | 844         | 848          | rVB      | 1912           | 1727          | 0.11%           | 0.016%        |
| 20        | 3.833       | 848           | 853         | 856          | rBV      | 1285           | 1221          | 0.08%           | 0.011%        |
| 21        | 3.977       | 894           | 898         | 904          | rBV      | 1549           | 1746          | 0.11%           | 0.016%        |
| 22        | 4.038       | 911           | 917         | 919          | rBV2     | 1673           | 1823          | 0.12%           | 0.016%        |
| 23        | 4.112       | 937           | 940         | 944          | rVB      | 2171           | 1331          | 0.09%           | 0.012%        |
| 24        | 4.196       | 955           | 966         | 990          | rBV      | 79666          | 255018        | 16.63%          | 2.292%        |
| 25        | 4.424       | 1035          | 1037        | 1041         | rVB2     | 1794           | 1074          | 0.07%           | 0.010%        |
| 26        | 4.479       | 1048          | 1054        | 1055         | rBV      | 1728           | 1613          | 0.11%           | 0.014%        |
| 27        | 4.640       | 1086          | 1104        | 1127         | rBV      | 179430         | 457380        | 29.83%          | 4.110%        |
| 28        | 4.813       | 1152          | 1158        | 1160         | rBV2     | 2150           | 2087          | 0.14%           | 0.019%        |
| 29        | 4.862       | 1169          | 1173        | 1175         | rBV      | 1498           | 1297          | 0.08%           | 0.012%        |
| 30        | 4.961       | 1199          | 1204        | 1210         | rVV4     | 1258           | 1857          | 0.12%           | 0.017%        |
| 31        | 5.054       | 1224          | 1233        | 1237         | rVB      | 1878           | 2886          | 0.19%           | 0.026%        |
| 32        | 5.077       | 1237          | 1240        | 1243         | rBV      | 1501           | 898           | 0.06%           | 0.008%        |
| 33        | 5.325       | 1297          | 1317        | 1340         | rBV2     | 419563         | 1172339       | 76.47%          | 10.534%       |
| 34        | 5.505       | 1369          | 1373        | 1378         | rBV2     | 871            | 950           | 0.06%           | 0.009%        |

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 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM031919WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 35 | 5.620  | 1406 | 1409 | 1412 | rBV2 | 1728   | 1207    | 0.08%  | 0.011%  |
| 36 | 5.762  | 1451 | 1453 | 1462 | rVB2 | 1612   | 1968    | 0.13%  | 0.018%  |
| 37 | 5.878  | 1476 | 1489 | 1515 | rBV  | 541320 | 1139277 | 74.31% | 10.237% |
| 38 | 6.112  | 1558 | 1562 | 1565 | rBV2 | 1339   | 1004    | 0.07%  | 0.009%  |
| 39 | 6.244  | 1597 | 1603 | 1613 | rBV5 | 3790   | 7817    | 0.51%  | 0.070%  |
| 40 | 6.324  | 1614 | 1628 | 1651 | rVV  | 238685 | 505860  | 33.00% | 4.546%  |
| 41 | 6.553  | 1695 | 1699 | 1702 | rBV  | 1007   | 1014    | 0.07%  | 0.009%  |
| 42 | 6.585  | 1706 | 1709 | 1715 | rVB  | 1155   | 934     | 0.06%  | 0.008%  |
| 43 | 6.775  | 1763 | 1768 | 1770 | rBV  | 1248   | 1254    | 0.08%  | 0.011%  |
| 44 | 6.842  | 1784 | 1789 | 1795 | rVB2 | 1139   | 1015    | 0.07%  | 0.009%  |
| 45 | 6.897  | 1802 | 1806 | 1808 | rBV2 | 2202   | 1769    | 0.12%  | 0.016%  |
| 46 | 6.984  | 1830 | 1833 | 1840 | rVB3 | 857    | 980     | 0.06%  | 0.009%  |
| 47 | 7.019  | 1840 | 1844 | 1849 | rBV  | 926    | 1004    | 0.07%  | 0.009%  |
| 48 | 7.045  | 1849 | 1852 | 1855 | rBV  | 1294   | 992     | 0.06%  | 0.009%  |
| 49 | 7.122  | 1873 | 1876 | 1878 | rBV  | 1410   | 995     | 0.06%  | 0.009%  |
| 50 | 7.225  | 1896 | 1908 | 1934 | rBV  | 127466 | 261177  | 17.04% | 2.347%  |
| 51 | 7.395  | 1956 | 1961 | 1966 | rBV2 | 877    | 1076    | 0.07%  | 0.010%  |
| 52 | 7.453  | 1976 | 1979 | 1982 | rBV  | 1762   | 1327    | 0.09%  | 0.012%  |
| 53 | 7.562  | 1997 | 2013 | 2031 | rBV  | 513262 | 962752  | 62.80% | 8.651%  |
| 54 | 7.775  | 2076 | 2079 | 2086 | rVB  | 1159   | 1404    | 0.09%  | 0.013%  |
| 55 | 7.849  | 2091 | 2102 | 2128 | rBV  | 84338  | 176225  | 11.50% | 1.584%  |
| 56 | 7.990  | 2143 | 2146 | 2153 | rVB  | 1809   | 1926    | 0.13%  | 0.017%  |
| 57 | 8.032  | 2154 | 2159 | 2162 | rBV3 | 1234   | 1183    | 0.08%  | 0.011%  |
| 58 | 8.109  | 2180 | 2183 | 2186 | rBV  | 1284   | 909     | 0.06%  | 0.008%  |
| 59 | 8.173  | 2193 | 2203 | 2205 | rBV3 | 2815   | 3633    | 0.24%  | 0.033%  |
| 60 | 8.324  | 2238 | 2250 | 2277 | rBV  | 340652 | 689259  | 44.96% | 6.194%  |
| 61 | 8.549  | 2317 | 2320 | 2325 | rVB  | 1459   | 1340    | 0.09%  | 0.012%  |
| 62 | 8.730  | 2372 | 2376 | 2379 | rBV  | 1766   | 1404    | 0.09%  | 0.013%  |
| 63 | 8.855  | 2412 | 2415 | 2417 | rBV  | 1402   | 966     | 0.06%  | 0.009%  |
| 64 | 8.868  | 2417 | 2419 | 2422 | rVB  | 1658   | 937     | 0.06%  | 0.008%  |
| 65 | 9.090  | 2476 | 2488 | 2511 | rBV  | 793523 | 1461736 | 95.35% | 13.135% |
| 66 | 9.440  | 2590 | 2597 | 2598 | rBV2 | 1129   | 1104    | 0.07%  | 0.010%  |
| 67 | 9.627  | 2652 | 2655 | 2663 | rVB2 | 1723   | 2193    | 0.14%  | 0.020%  |
| 68 | 9.742  | 2686 | 2691 | 2694 | rBV  | 1751   | 1477    | 0.10%  | 0.013%  |
| 69 | 9.791  | 2703 | 2706 | 2709 | rVB  | 1619   | 1025    | 0.07%  | 0.009%  |
| 70 | 9.820  | 2709 | 2715 | 2717 | rBV2 | 1494   | 1315    | 0.09%  | 0.012%  |
| 71 | 10.016 | 2774 | 2776 | 2783 | rVB2 | 1846   | 1910    | 0.12%  | 0.017%  |

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 Max Peaks: 100  
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM031919WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |         |         |
|-----|--------|------|------|------|------|--------|---------|---------|---------|
| 72  | 10.048 | 2783 | 2786 | 2788 | rBV  | 1494   | 995     | 0.06%   | 0.009%  |
| 73  | 10.218 | 2833 | 2839 | 2841 | rBV2 | 878    | 1108    | 0.07%   | 0.010%  |
| 74  | 10.434 | 2893 | 2906 | 2922 | rBV  | 432393 | 700517  | 45.69%  | 6.295%  |
| 75  | 10.569 | 2944 | 2948 | 2952 | rBV  | 1474   | 1421    | 0.09%   | 0.013%  |
| 76  | 10.607 | 2954 | 2960 | 2964 | rVV  | 1863   | 2165    | 0.14%   | 0.019%  |
| 77  | 10.652 | 2970 | 2974 | 2981 | rBV2 | 1354   | 1608    | 0.10%   | 0.014%  |
| 78  | 10.755 | 3004 | 3006 | 3015 | rVB  | 1289   | 1158    | 0.08%   | 0.010%  |
| 79  | 10.871 | 3040 | 3042 | 3048 | rVB  | 1185   | 1121    | 0.07%   | 0.010%  |
| 80  | 10.913 | 3052 | 3055 | 3061 | rVB  | 1206   | 1267    | 0.08%   | 0.011%  |
| 81  | 10.964 | 3067 | 3071 | 3074 | rVB  | 1585   | 1254    | 0.08%   | 0.011%  |
| 82  | 10.990 | 3074 | 3079 | 3082 | rBV2 | 1147   | 1156    | 0.08%   | 0.010%  |
| 83  | 11.138 | 3120 | 3125 | 3129 | rBV  | 1417   | 1434    | 0.09%   | 0.013%  |
| 84  | 11.282 | 3166 | 3170 | 3175 | rBV2 | 1575   | 1807    | 0.12%   | 0.016%  |
| 85  | 11.434 | 3212 | 3217 | 3220 | rBV3 | 2378   | 2264    | 0.15%   | 0.020%  |
| 86  | 11.482 | 3220 | 3232 | 3252 | rBV  | 951572 | 1533053 | 100.00% | 13.776% |
| 87  | 11.787 | 3324 | 3327 | 3334 | rBV3 | 1568   | 1945    | 0.13%   | 0.017%  |
| 88  | 11.861 | 3338 | 3350 | 3374 | rVV  | 582638 | 971719  | 63.38%  | 8.732%  |
| 89  | 12.205 | 3454 | 3457 | 3461 | rBV  | 1306   | 1116    | 0.07%   | 0.010%  |
| 90  | 12.299 | 3482 | 3486 | 3491 | rBV  | 1355   | 1476    | 0.10%   | 0.013%  |
| 91  | 12.495 | 3544 | 3547 | 3552 | rBV  | 1088   | 948     | 0.06%   | 0.009%  |
| 92  | 12.861 | 3653 | 3661 | 3666 | rBV  | 2366   | 3813    | 0.25%   | 0.034%  |
| 93  | 12.993 | 3700 | 3702 | 3707 | rVB2 | 1571   | 1181    | 0.08%   | 0.011%  |
| 94  | 14.118 | 4049 | 4052 | 4056 | rVB2 | 1661   | 1266    | 0.08%   | 0.011%  |
| 95  | 14.588 | 4195 | 4198 | 4199 | rBV  | 1493   | 927     | 0.06%   | 0.008%  |
| 96  | 14.675 | 4219 | 4225 | 4228 | rBV2 | 1817   | 2084    | 0.14%   | 0.019%  |
| 97  | 15.060 | 4343 | 4345 | 4347 | rBV  | 1467   | 897     | 0.06%   | 0.008%  |
| 98  | 15.105 | 4355 | 4359 | 4360 | rBV2 | 1240   | 937     | 0.06%   | 0.008%  |
| 99  | 15.433 | 4458 | 4461 | 4464 | rBV  | 2086   | 1441    | 0.09%   | 0.013%  |
| 100 | 15.765 | 4561 | 4564 | 4568 | rBV2 | 1470   | 1135    | 0.07%   | 0.010%  |

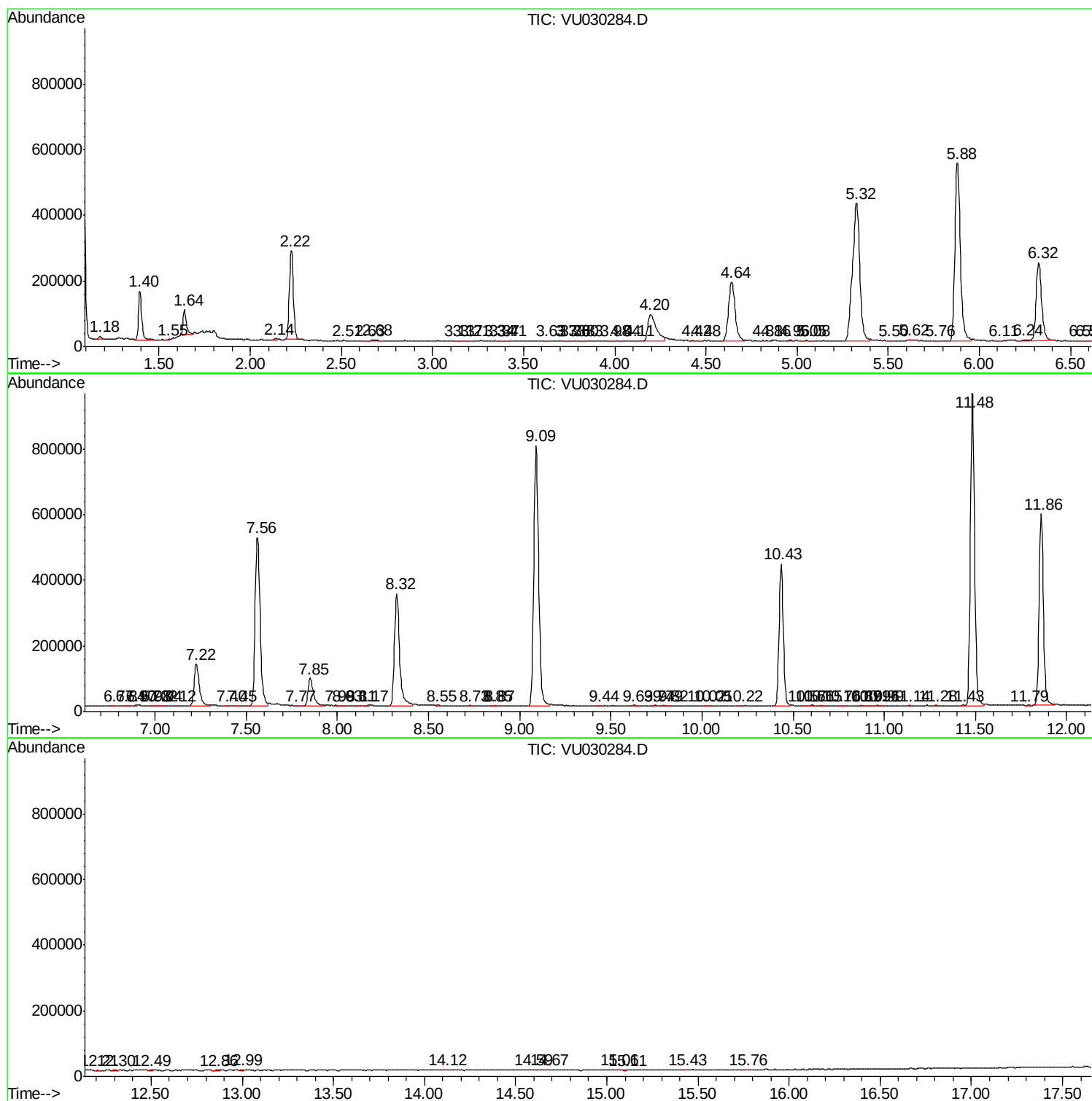
Sum of corrected areas: 11128592

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM031919WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.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        |