

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032119\  
 Data File : VU030289.D  
 Acq On : 22 Mar 2019 00:19  
 Operator : JC/SP  
 Sample : K2017-21  
 Misc : 5.04g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 40 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BF0F0

## 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         | 1.174       | 22            | 26          | 34           | rVB2     | 11127          | 10817         | 0.73%           | 0.098%        |
| 2         | 1.396       | 87            | 95          | 110          | rVB      | 149359         | 180326        | 12.22%          | 1.632%        |
| 3         | 1.640       | 165           | 171         | 182          | rBV      | 71752          | 95326         | 6.46%           | 0.863%        |
| 4         | 2.225       | 342           | 353         | 370          | rBV      | 273218         | 422758        | 28.64%          | 3.827%        |
| 5         | 2.473       | 426           | 430         | 434          | rBV      | 1373           | 1538          | 0.10%           | 0.014%        |
| 6         | 2.547       | 450           | 453         | 457          | rBV      | 1139           | 942           | 0.06%           | 0.009%        |
| 7         | 2.608       | 470           | 472         | 477          | rVB      | 1167           | 810           | 0.05%           | 0.007%        |
| 8         | 2.775       | 521           | 524         | 527          | rVB      | 2063           | 1156          | 0.08%           | 0.010%        |
| 9         | 2.794       | 527           | 530         | 533          | rBV      | 882            | 834           | 0.06%           | 0.008%        |
| 10        | 2.836       | 540           | 543         | 549          | rVB2     | 1362           | 1332          | 0.09%           | 0.012%        |
| 11        | 2.945       | 572           | 577         | 578          | rBV      | 1431           | 1183          | 0.08%           | 0.011%        |
| 12        | 3.039       | 600           | 606         | 607          | rBV3     | 1412           | 1299          | 0.09%           | 0.012%        |
| 13        | 3.235       | 664           | 667         | 675          | rBV      | 1069           | 1000          | 0.07%           | 0.009%        |
| 14        | 3.270       | 675           | 678         | 682          | rVB      | 1373           | 1071          | 0.07%           | 0.010%        |
| 15        | 3.293       | 682           | 685         | 690          | rBV      | 1474           | 1398          | 0.09%           | 0.013%        |
| 16        | 3.360       | 697           | 706         | 709          | rBV      | 1807           | 2460          | 0.17%           | 0.022%        |
| 17        | 3.428       | 723           | 727         | 732          | rBV      | 1678           | 1524          | 0.10%           | 0.014%        |
| 18        | 3.640       | 790           | 793         | 799          | rVB2     | 1557           | 1434          | 0.10%           | 0.013%        |
| 19        | 3.778       | 831           | 836         | 841          | rVB      | 1281           | 1594          | 0.11%           | 0.014%        |
| 20        | 3.846       | 854           | 857         | 860          | rBV      | 1439           | 1174          | 0.08%           | 0.011%        |
| 21        | 3.987       | 898           | 901         | 906          | rVB      | 1770           | 1400          | 0.09%           | 0.013%        |
| 22        | 4.051       | 917           | 921         | 923          | rBV2     | 1511           | 1143          | 0.08%           | 0.010%        |
| 23        | 4.199       | 949           | 967         | 999          | rBV      | 84202          | 292390        | 19.81%          | 2.647%        |
| 24        | 4.396       | 1024          | 1028        | 1030         | rBV      | 1350           | 1352          | 0.09%           | 0.012%        |
| 25        | 4.572       | 1079          | 1083        | 1086         | rBV      | 1291           | 1129          | 0.08%           | 0.010%        |
| 26        | 4.640       | 1087          | 1104        | 1127         | rVV      | 180627         | 456145        | 30.91%          | 4.129%        |
| 27        | 4.942       | 1195          | 1198        | 1202         | rBV      | 1403           | 1402          | 0.09%           | 0.013%        |
| 28        | 5.003       | 1215          | 1217        | 1221         | rVB      | 1437           | 1058          | 0.07%           | 0.010%        |
| 29        | 5.029       | 1221          | 1225        | 1228         | rVB2     | 976            | 897           | 0.06%           | 0.008%        |
| 30        | 5.061       | 1228          | 1235        | 1240         | rBV2     | 1303           | 2169          | 0.15%           | 0.020%        |
| 31        | 5.116       | 1249          | 1252        | 1257         | rVB      | 1910           | 1384          | 0.09%           | 0.013%        |
| 32        | 5.190       | 1271          | 1275        | 1277         | rBV      | 1321           | 853           | 0.06%           | 0.008%        |
| 33        | 5.325       | 1296          | 1317        | 1346         | rVV2     | 419466         | 1184751       | 80.27%          | 10.725%       |
| 34        | 5.624       | 1399          | 1410        | 1413         | rBV6     | 3134           | 5010          | 0.34%           | 0.045%        |

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 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 | 5.785  | 1457 | 1460 | 1463 | rBV  | 1852   | 1312    | 0.09%  | 0.012%  |
| 36 | 5.878  | 1475 | 1489 | 1519 | rBV  | 520350 | 1101585 | 74.64% | 9.972%  |
| 37 | 6.174  | 1573 | 1581 | 1583 | rBV4 | 2491   | 3010    | 0.20%  | 0.027%  |
| 38 | 6.248  | 1599 | 1604 | 1605 | rBV4 | 2435   | 1906    | 0.13%  | 0.017%  |
| 39 | 6.325  | 1616 | 1628 | 1656 | rVB  | 240118 | 515374  | 34.92% | 4.666%  |
| 40 | 6.463  | 1667 | 1671 | 1677 | rBV  | 2819   | 2796    | 0.19%  | 0.025%  |
| 41 | 6.492  | 1677 | 1680 | 1683 | rVV2 | 1177   | 894     | 0.06%  | 0.008%  |
| 42 | 6.530  | 1687 | 1692 | 1693 | rBV  | 1144   | 821     | 0.06%  | 0.007%  |
| 43 | 6.588  | 1706 | 1710 | 1713 | rBV  | 1431   | 1141    | 0.08%  | 0.010%  |
| 44 | 6.784  | 1766 | 1771 | 1777 | rVB  | 1352   | 1404    | 0.10%  | 0.013%  |
| 45 | 6.817  | 1777 | 1781 | 1784 | rBV2 | 1083   | 1013    | 0.07%  | 0.009%  |
| 46 | 6.887  | 1800 | 1803 | 1805 | rBV2 | 1149   | 769     | 0.05%  | 0.007%  |
| 47 | 6.993  | 1832 | 1836 | 1839 | rBV  | 1165   | 967     | 0.07%  | 0.009%  |
| 48 | 7.225  | 1897 | 1908 | 1931 | rBV  | 124654 | 248150  | 16.81% | 2.246%  |
| 49 | 7.440  | 1971 | 1975 | 1980 | rBV  | 1061   | 1197    | 0.08%  | 0.011%  |
| 50 | 7.563  | 2000 | 2013 | 2036 | rBV  | 513842 | 968096  | 65.59% | 8.764%  |
| 51 | 7.852  | 2093 | 2103 | 2133 | rBV2 | 81648  | 169900  | 11.51% | 1.538%  |
| 52 | 8.167  | 2194 | 2201 | 2202 | rBV  | 2254   | 2246    | 0.15%  | 0.020%  |
| 53 | 8.225  | 2214 | 2219 | 2224 | rVB2 | 2249   | 2554    | 0.17%  | 0.023%  |
| 54 | 8.325  | 2238 | 2250 | 2282 | rBV  | 342459 | 705005  | 47.77% | 6.382%  |
| 55 | 8.585  | 2328 | 2331 | 2335 | rBV  | 1099   | 880     | 0.06%  | 0.008%  |
| 56 | 8.633  | 2343 | 2346 | 2352 | rVB2 | 1084   | 1099    | 0.07%  | 0.010%  |
| 57 | 8.762  | 2382 | 2386 | 2391 | rBV2 | 1076   | 1245    | 0.08%  | 0.011%  |
| 58 | 8.865  | 2413 | 2418 | 2421 | rBV2 | 1100   | 1221    | 0.08%  | 0.011%  |
| 59 | 8.945  | 2440 | 2443 | 2446 | rBV  | 1469   | 876     | 0.06%  | 0.008%  |
| 60 | 9.032  | 2467 | 2470 | 2474 | rVB  | 1962   | 1393    | 0.09%  | 0.013%  |
| 61 | 9.090  | 2474 | 2488 | 2508 | rBV  | 759344 | 1407014 | 95.33% | 12.737% |
| 62 | 9.247  | 2535 | 2537 | 2542 | rVB  | 1083   | 800     | 0.05%  | 0.007%  |
| 63 | 9.328  | 2557 | 2562 | 2564 | rBV3 | 1312   | 1208    | 0.08%  | 0.011%  |
| 64 | 9.357  | 2568 | 2571 | 2573 | rBV  | 1203   | 905     | 0.06%  | 0.008%  |
| 65 | 9.633  | 2654 | 2657 | 2662 | rBV  | 800    | 870     | 0.06%  | 0.008%  |
| 66 | 9.688  | 2671 | 2674 | 2680 | rVV3 | 1126   | 1173    | 0.08%  | 0.011%  |
| 67 | 9.746  | 2689 | 2692 | 2697 | rBV  | 2027   | 2220    | 0.15%  | 0.020%  |
| 68 | 9.852  | 2721 | 2725 | 2729 | rBV  | 1526   | 1678    | 0.11%  | 0.015%  |
| 69 | 10.218 | 2833 | 2839 | 2842 | rBV  | 1911   | 1847    | 0.13%  | 0.017%  |
| 70 | 10.360 | 2879 | 2883 | 2887 | rBV2 | 968    | 834     | 0.06%  | 0.008%  |
| 71 | 10.434 | 2893 | 2906 | 2928 | rVV  | 425786 | 705696  | 47.81% | 6.389%  |

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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  | 10.598 | 2953 | 2957 | 2960 | rVV3 | 1786   | 1426    | 0.10%   | 0.013%  |
| 73  | 10.636 | 2966 | 2969 | 2976 | rBV  | 1417   | 1196    | 0.08%   | 0.011%  |
| 74  | 10.681 | 2977 | 2983 | 2992 | rBV  | 2428   | 3965    | 0.27%   | 0.036%  |
| 75  | 10.784 | 3011 | 3015 | 3019 | rBV3 | 1336   | 1109    | 0.08%   | 0.010%  |
| 76  | 10.836 | 3028 | 3031 | 3036 | rBV  | 982    | 1067    | 0.07%   | 0.010%  |
| 77  | 10.884 | 3042 | 3046 | 3051 | rBV  | 1068   | 992     | 0.07%   | 0.009%  |
| 78  | 11.009 | 3080 | 3085 | 3087 | rBV  | 1519   | 1305    | 0.09%   | 0.012%  |
| 79  | 11.058 | 3095 | 3100 | 3103 | rBV  | 1157   | 963     | 0.07%   | 0.009%  |
| 80  | 11.173 | 3133 | 3136 | 3140 | rBV  | 1079   | 807     | 0.05%   | 0.007%  |
| 81  | 11.260 | 3160 | 3163 | 3167 | rVB  | 1319   | 833     | 0.06%   | 0.008%  |
| 82  | 11.398 | 3203 | 3206 | 3208 | rBV  | 1657   | 1139    | 0.08%   | 0.010%  |
| 83  | 11.482 | 3221 | 3232 | 3253 | rBV  | 914072 | 1475909 | 100.00% | 13.361% |
| 84  | 11.707 | 3300 | 3302 | 3305 | rBV  | 1435   | 892     | 0.06%   | 0.008%  |
| 85  | 11.861 | 3337 | 3350 | 3375 | rBV  | 594811 | 995748  | 67.47%  | 9.014%  |
| 86  | 12.064 | 3410 | 3413 | 3416 | rBV2 | 1394   | 996     | 0.07%   | 0.009%  |
| 87  | 12.112 | 3426 | 3428 | 3433 | rVB  | 1380   | 913     | 0.06%   | 0.008%  |
| 88  | 12.556 | 3562 | 3566 | 3572 | rVV2 | 1637   | 1964    | 0.13%   | 0.018%  |
| 89  | 13.119 | 3738 | 3741 | 3744 | rBV  | 1352   | 1019    | 0.07%   | 0.009%  |
| 90  | 13.440 | 3837 | 3841 | 3845 | rBV  | 1806   | 1636    | 0.11%   | 0.015%  |
| 91  | 13.476 | 3849 | 3852 | 3855 | rVB  | 1278   | 784     | 0.05%   | 0.007%  |
| 92  | 13.578 | 3880 | 3884 | 3888 | rBV2 | 1303   | 1363    | 0.09%   | 0.012%  |
| 93  | 13.685 | 3914 | 3917 | 3920 | rBV  | 1536   | 880     | 0.06%   | 0.008%  |
| 94  | 13.971 | 4003 | 4006 | 4013 | rVB2 | 2029   | 2093    | 0.14%   | 0.019%  |
| 95  | 14.019 | 4018 | 4021 | 4023 | rVB  | 1439   | 759     | 0.05%   | 0.007%  |
| 96  | 14.713 | 4235 | 4237 | 4242 | rVB2 | 1559   | 981     | 0.07%   | 0.009%  |
| 97  | 14.739 | 4242 | 4245 | 4247 | rBV2 | 1074   | 849     | 0.06%   | 0.008%  |
| 98  | 14.784 | 4256 | 4259 | 4261 | rBV  | 1254   | 858     | 0.06%   | 0.008%  |
| 99  | 14.861 | 4280 | 4283 | 4285 | rBV2 | 1583   | 901     | 0.06%   | 0.008%  |
| 100 | 15.074 | 4346 | 4349 | 4351 | rBV3 | 1345   | 783     | 0.05%   | 0.007%  |

Sum of corrected areas: 11046288



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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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\V0ASRV\HPCHEM1\MSV0A\_U\DATA\VU032119\  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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