

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040419\  
 Data File : VU030669.D  
 Acq On : 04 Apr 2019 08:02  
 Operator : JC/SP  
 Sample : K2246-08  
 Misc : 5.94g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 47 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BF155

## 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\SOMULM032319WMA.M  
 Title : VOC Analysis

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 1.392    | 88         | 94       | 107       | rVB   | 124317      | 151571     | 9.99%        | 1.621%     |
| 2      | 1.640    | 167        | 171      | 180       | rVB   | 71828       | 78550      | 5.18%        | 0.840%     |
| 3      | 2.238    | 347        | 357      | 372       | rVB   | 218899      | 336832     | 22.20%       | 3.602%     |
| 4      | 2.521    | 443        | 445      | 447       | rBV2  | 886         | 471        | 0.03%        | 0.005%     |
| 5      | 2.543    | 450        | 452      | 454       | rVB2  | 992         | 499        | 0.03%        | 0.005%     |
| 6      | 2.685    | 487        | 496      | 509       | rBV4  | 7362        | 15115      | 1.00%        | 0.162%     |
| 7      | 2.836    | 538        | 543      | 550       | rVB7  | 1550        | 1763       | 0.12%        | 0.019%     |
| 8      | 2.968    | 577        | 584      | 586       | rBV3  | 849         | 814        | 0.05%        | 0.009%     |
| 9      | 3.000    | 591        | 594      | 598       | rVB3  | 608         | 424        | 0.03%        | 0.005%     |
| 10     | 3.042    | 603        | 607      | 610       | rBV2  | 902         | 695        | 0.05%        | 0.007%     |
| 11     | 3.096    | 622        | 624      | 629       | rVB3  | 735         | 516        | 0.03%        | 0.006%     |
| 12     | 3.264    | 669        | 676      | 677       | rBV4  | 1029        | 978        | 0.06%        | 0.010%     |
| 13     | 3.331    | 692        | 697      | 701       | rVB3  | 674         | 581        | 0.04%        | 0.006%     |
| 14     | 3.350    | 701        | 703      | 705       | rBV2  | 767         | 489        | 0.03%        | 0.005%     |
| 15     | 3.502    | 747        | 750      | 753       | rBV3  | 639         | 421        | 0.03%        | 0.005%     |
| 16     | 3.582    | 768        | 775      | 778       | rBV2  | 700         | 630        | 0.04%        | 0.007%     |
| 17     | 3.646    | 790        | 795      | 799       | rVB3  | 924         | 940        | 0.06%        | 0.010%     |
| 18     | 3.714    | 814        | 816      | 822       | rVB3  | 875         | 711        | 0.05%        | 0.008%     |
| 19     | 3.765    | 828        | 832      | 833       | rBV2  | 558         | 432        | 0.03%        | 0.005%     |
| 20     | 4.045    | 917        | 919      | 925       | rVB2  | 613         | 476        | 0.03%        | 0.005%     |
| 21     | 4.080    | 925        | 930      | 931       | rBV2  | 612         | 444        | 0.03%        | 0.005%     |
| 22     | 4.138    | 944        | 948      | 951       | rBV4  | 466         | 467        | 0.03%        | 0.005%     |
| 23     | 4.193    | 951        | 965      | 994       | rBV2  | 62079       | 226965     | 14.96%       | 2.427%     |
| 24     | 4.553    | 1075       | 1077     | 1081      | rVB2  | 699         | 459        | 0.03%        | 0.005%     |
| 25     | 4.640    | 1087       | 1104     | 1134      | rBV2  | 138211      | 359925     | 23.72%       | 3.849%     |
| 26     | 4.826    | 1159       | 1162     | 1165      | rVB3  | 816         | 487        | 0.03%        | 0.005%     |
| 27     | 4.855    | 1168       | 1171     | 1173      | rBV3  | 1048        | 644        | 0.04%        | 0.007%     |
| 28     | 4.878    | 1175       | 1178     | 1180      | rVV3  | 1107        | 699        | 0.05%        | 0.007%     |
| 29     | 4.903    | 1184       | 1186     | 1191      | rVB2  | 1243        | 708        | 0.05%        | 0.008%     |
| 30     | 4.948    | 1197       | 1200     | 1202      | rBV2  | 1042        | 607        | 0.04%        | 0.006%     |
| 31     | 4.993    | 1210       | 1214     | 1218      | rBV7  | 812         | 730        | 0.05%        | 0.008%     |
| 32     | 5.093    | 1241       | 1245     | 1249      | rBV2  | 634         | 603        | 0.04%        | 0.006%     |
| 33     | 5.132    | 1254       | 1257     | 1261      | rBV2  | 960         | 562        | 0.04%        | 0.006%     |
| 34     | 5.196    | 1273       | 1277     | 1283      | rVB3  | 659         | 747        | 0.05%        | 0.008%     |

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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\SOMULM032319WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |         |         |
|----|-------|------|------|------|------|--------|---------|---------|---------|
| 35 | 5.328 | 1297 | 1318 | 1342 | rBV3 | 322578 | 937453  | 61.78%  | 10.024% |
| 36 | 5.595 | 1398 | 1401 | 1402 | rBV2 | 1541   | 822     | 0.05%   | 0.009%  |
| 37 | 5.617 | 1402 | 1408 | 1415 | rVV9 | 3296   | 5132    | 0.34%   | 0.055%  |
| 38 | 5.791 | 1458 | 1462 | 1464 | rBV4 | 574    | 504     | 0.03%   | 0.005%  |
| 39 | 5.881 | 1474 | 1490 | 1520 | rBV  | 557481 | 1209842 | 79.73%  | 12.936% |
| 40 | 6.074 | 1548 | 1550 | 1553 | rBV2 | 846    | 430     | 0.03%   | 0.005%  |
| 41 | 6.251 | 1595 | 1605 | 1612 | rBV8 | 5531   | 10250   | 0.68%   | 0.110%  |
| 42 | 6.325 | 1616 | 1628 | 1651 | rVB  | 182501 | 398917  | 26.29%  | 4.265%  |
| 43 | 6.450 | 1663 | 1667 | 1669 | rBV3 | 916    | 684     | 0.05%   | 0.007%  |
| 44 | 6.534 | 1691 | 1693 | 1697 | rBV4 | 607    | 453     | 0.03%   | 0.005%  |
| 45 | 6.633 | 1717 | 1724 | 1726 | rBV5 | 867    | 825     | 0.05%   | 0.009%  |
| 46 | 6.720 | 1745 | 1751 | 1753 | rBV3 | 470    | 557     | 0.04%   | 0.006%  |
| 47 | 6.768 | 1759 | 1766 | 1768 | rBV3 | 840    | 960     | 0.06%   | 0.010%  |
| 48 | 6.784 | 1768 | 1771 | 1777 | rVB2 | 716    | 712     | 0.05%   | 0.008%  |
| 49 | 6.897 | 1795 | 1806 | 1808 | rBV5 | 2196   | 2909    | 0.19%   | 0.031%  |
| 50 | 6.936 | 1815 | 1818 | 1822 | rVB3 | 1265   | 938     | 0.06%   | 0.010%  |
| 51 | 6.958 | 1822 | 1825 | 1832 | rVB6 | 1239   | 959     | 0.06%   | 0.010%  |
| 52 | 6.997 | 1835 | 1837 | 1841 | rVB4 | 849    | 529     | 0.03%   | 0.006%  |
| 53 | 7.045 | 1848 | 1852 | 1854 | rBV2 | 1064   | 848     | 0.06%   | 0.009%  |
| 54 | 7.167 | 1886 | 1890 | 1892 | rBV2 | 933    | 476     | 0.03%   | 0.005%  |
| 55 | 7.228 | 1897 | 1909 | 1936 | rBV2 | 92144  | 199777  | 13.17%  | 2.136%  |
| 56 | 7.476 | 1984 | 1986 | 1990 | rVB3 | 755    | 446     | 0.03%   | 0.005%  |
| 57 | 7.563 | 2001 | 2013 | 2040 | rBV  | 374942 | 702932  | 46.33%  | 7.516%  |
| 58 | 7.855 | 2093 | 2104 | 2127 | rBV2 | 60170  | 131709  | 8.68%   | 1.408%  |
| 59 | 8.090 | 2174 | 2177 | 2180 | rVB3 | 848    | 617     | 0.04%   | 0.007%  |
| 60 | 8.177 | 2197 | 2204 | 2211 | rVB4 | 1797   | 2130    | 0.14%   | 0.023%  |
| 61 | 8.225 | 2211 | 2219 | 2220 | rBV7 | 6906   | 7658    | 0.50%   | 0.082%  |
| 62 | 8.325 | 2236 | 2250 | 2277 | rBV  | 244192 | 493952  | 32.55%  | 5.282%  |
| 63 | 8.755 | 2382 | 2384 | 2388 | rVB4 | 654    | 534     | 0.04%   | 0.006%  |
| 64 | 8.794 | 2394 | 2396 | 2403 | rVB2 | 1344   | 1095    | 0.07%   | 0.012%  |
| 65 | 9.090 | 2474 | 2488 | 2518 | rBV  | 832840 | 1517368 | 100.00% | 16.225% |
| 66 | 9.302 | 2549 | 2554 | 2556 | rBV5 | 868    | 738     | 0.05%   | 0.008%  |
| 67 | 9.318 | 2556 | 2559 | 2562 | rVV3 | 761    | 545     | 0.04%   | 0.006%  |
| 68 | 9.424 | 2588 | 2592 | 2594 | rBV2 | 589    | 472     | 0.03%   | 0.005%  |
| 69 | 9.472 | 2603 | 2607 | 2610 | rVB4 | 827    | 578     | 0.04%   | 0.006%  |
| 70 | 9.492 | 2610 | 2613 | 2620 | rBV4 | 880    | 918     | 0.06%   | 0.010%  |
| 71 | 9.624 | 2651 | 2654 | 2658 | rVB3 | 566    | 446     | 0.03%   | 0.005%  |

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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\SOMULM032319WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |         |
|-----|--------|------|------|------|------|--------|---------|--------|---------|
| 72  | 9.681  | 2670 | 2672 | 2679 | rVB2 | 1122   | 733     | 0.05%  | 0.008%  |
| 73  | 9.784  | 2701 | 2704 | 2706 | rBV3 | 782    | 489     | 0.03%  | 0.005%  |
| 74  | 9.861  | 2724 | 2728 | 2730 | rVV2 | 956    | 598     | 0.04%  | 0.006%  |
| 75  | 9.878  | 2730 | 2733 | 2738 | rVV2 | 705    | 504     | 0.03%  | 0.005%  |
| 76  | 9.948  | 2751 | 2755 | 2759 | rBV3 | 830    | 795     | 0.05%  | 0.009%  |
| 77  | 10.083 | 2795 | 2797 | 2803 | rBV3 | 575    | 516     | 0.03%  | 0.006%  |
| 78  | 10.135 | 2809 | 2813 | 2818 | rBV3 | 535    | 562     | 0.04%  | 0.006%  |
| 79  | 10.164 | 2818 | 2822 | 2825 | rBV2 | 586    | 488     | 0.03%  | 0.005%  |
| 80  | 10.189 | 2825 | 2830 | 2837 | rBV4 | 1920   | 2545    | 0.17%  | 0.027%  |
| 81  | 10.434 | 2893 | 2906 | 2930 | rBV  | 279204 | 465984  | 30.71% | 4.983%  |
| 82  | 10.553 | 2941 | 2943 | 2949 | rVB4 | 611    | 634     | 0.04%  | 0.007%  |
| 83  | 10.595 | 2952 | 2956 | 2960 | rBV3 | 813    | 683     | 0.05%  | 0.007%  |
| 84  | 10.691 | 2982 | 2986 | 2991 | rBV3 | 1061   | 970     | 0.06%  | 0.010%  |
| 85  | 10.720 | 2991 | 2995 | 2999 | rBV2 | 569    | 608     | 0.04%  | 0.007%  |
| 86  | 10.890 | 3044 | 3048 | 3051 | rBV2 | 689    | 623     | 0.04%  | 0.007%  |
| 87  | 10.987 | 3075 | 3078 | 3081 | rBV3 | 1086   | 664     | 0.04%  | 0.007%  |
| 88  | 11.035 | 3090 | 3093 | 3097 | rVB2 | 839    | 475     | 0.03%  | 0.005%  |
| 89  | 11.138 | 3122 | 3125 | 3128 | rVB3 | 856    | 532     | 0.04%  | 0.006%  |
| 90  | 11.254 | 3156 | 3161 | 3163 | rBV4 | 623    | 491     | 0.03%  | 0.005%  |
| 91  | 11.424 | 3207 | 3214 | 3219 | rBV6 | 1105   | 1784    | 0.12%  | 0.019%  |
| 92  | 11.482 | 3220 | 3232 | 3258 | rBV  | 880160 | 1439535 | 94.87% | 15.392% |
| 93  | 11.858 | 3338 | 3349 | 3372 | rBV  | 350692 | 603497  | 39.77% | 6.453%  |
| 94  | 12.379 | 3508 | 3511 | 3513 | rBV3 | 1028   | 534     | 0.04%  | 0.006%  |
| 95  | 12.652 | 3593 | 3596 | 3598 | rBV  | 967    | 523     | 0.03%  | 0.006%  |
| 96  | 13.032 | 3711 | 3714 | 3715 | rBV2 | 823    | 463     | 0.03%  | 0.005%  |
| 97  | 13.270 | 3784 | 3788 | 3791 | rBV4 | 781    | 627     | 0.04%  | 0.007%  |
| 98  | 14.488 | 4164 | 4167 | 4171 | rBV4 | 1570   | 1181    | 0.08%  | 0.013%  |
| 99  | 14.533 | 4179 | 4181 | 4184 | rBV2 | 1253   | 703     | 0.05%  | 0.008%  |
| 100 | 15.520 | 4486 | 4488 | 4493 | rBV2 | 1796   | 1513    | 0.10%  | 0.016%  |

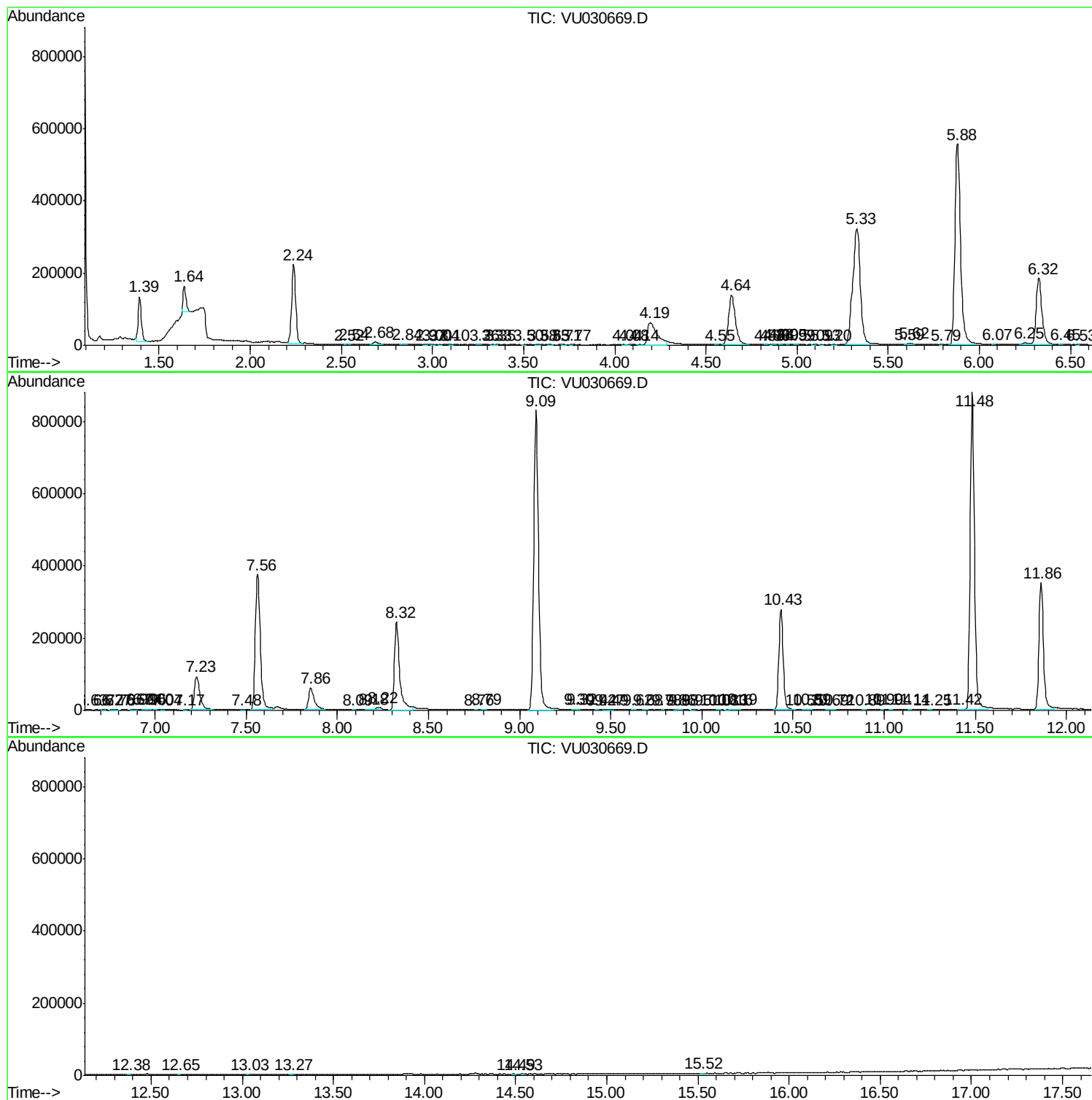
Sum of corrected areas: 9352324

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM032319WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU040419\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM032319WMA.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

\*\*\*\*\*

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TIC Integration Parameters: LSCINT.P

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