

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU102918\  
 Data File : VU027847.D  
 Acq On : 29 Oct 2018 11:22  
 Operator : MD/SY  
 Sample : VU1029MBL01  
 Misc : 5.00g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK53

## 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\SOMULM102218WMA.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      | 1.399    | 64         | 70       | 80        | rBV   | 51280       | 51303      | 13.18%       | 1.647%     |
| 2      | 1.682    | 150        | 158      | 174       | rVB   | 38704       | 49903      | 12.82%       | 1.602%     |
| 3      | 2.276    | 332        | 343      | 354       | rBV   | 79293       | 119633     | 30.74%       | 3.841%     |
| 4      | 2.447    | 394        | 396      | 401       | rVB   | 169         | 102        | 0.03%        | 0.003%     |
| 5      | 2.469    | 401        | 403      | 404       | rBV   | 209         | 105        | 0.03%        | 0.003%     |
| 6      | 2.617    | 444        | 449      | 459       | rVB2  | 316         | 492        | 0.13%        | 0.016%     |
| 7      | 2.836    | 515        | 517      | 520       | rVB   | 180         | 98         | 0.03%        | 0.003%     |
| 8      | 2.858    | 522        | 524      | 528       | rVV   | 114         | 78         | 0.02%        | 0.003%     |
| 9      | 3.469    | 711        | 714      | 717       | rBV   | 114         | 81         | 0.02%        | 0.003%     |
| 10     | 3.524    | 726        | 731      | 733       | rBV   | 92          | 100        | 0.03%        | 0.003%     |
| 11     | 3.659    | 770        | 773      | 777       | rVB   | 206         | 204        | 0.05%        | 0.007%     |
| 12     | 3.685    | 778        | 781      | 786       | rBV   | 150         | 197        | 0.05%        | 0.006%     |
| 13     | 3.772    | 803        | 808      | 813       | rBV   | 143         | 160        | 0.04%        | 0.005%     |
| 14     | 3.900    | 845        | 848      | 854       | rBV   | 200         | 275        | 0.07%        | 0.009%     |
| 15     | 4.003    | 878        | 880      | 883       | rBV   | 146         | 118        | 0.03%        | 0.004%     |
| 16     | 4.177    | 922        | 934      | 960       | rBV   | 37215       | 96958      | 24.92%       | 3.113%     |
| 17     | 4.370    | 989        | 994      | 997       | rVB   | 188         | 173        | 0.04%        | 0.006%     |
| 18     | 4.591    | 1060       | 1063     | 1065      | rBV   | 139         | 122        | 0.03%        | 0.004%     |
| 19     | 4.653    | 1065       | 1082     | 1105      | rVV   | 63536       | 149246     | 38.35%       | 4.792%     |
| 20     | 4.797    | 1121       | 1127     | 1129      | rBV2  | 172         | 201        | 0.05%        | 0.006%     |
| 21     | 4.855    | 1141       | 1145     | 1150      | rBV2  | 155         | 195        | 0.05%        | 0.006%     |
| 22     | 4.932    | 1163       | 1169     | 1171      | rBV   | 159         | 184        | 0.05%        | 0.006%     |
| 23     | 5.241    | 1262       | 1265     | 1267      | rBV   | 158         | 134        | 0.03%        | 0.004%     |
| 24     | 5.344    | 1273       | 1297     | 1317      | rBV2  | 131165      | 389155     | 100.00%      | 12.495%    |
| 25     | 5.495    | 1342       | 1344     | 1347      | rBB   | 242         | 132        | 0.03%        | 0.004%     |
| 26     | 5.517    | 1349       | 1351     | 1353      | rBV   | 128         | 92         | 0.02%        | 0.003%     |
| 27     | 5.598    | 1374       | 1376     | 1379      | rBB   | 141         | 98         | 0.03%        | 0.003%     |
| 28     | 5.620    | 1380       | 1383     | 1385      | rBB   | 128         | 91         | 0.02%        | 0.003%     |
| 29     | 5.633    | 1385       | 1387     | 1388      | rBV   | 122         | 67         | 0.02%        | 0.002%     |
| 30     | 5.697    | 1405       | 1407     | 1412      | rBB   | 162         | 159        | 0.04%        | 0.005%     |
| 31     | 5.723    | 1413       | 1415     | 1418      | rBV   | 164         | 133        | 0.03%        | 0.004%     |
| 32     | 5.842    | 1449       | 1452     | 1453      | rBV   | 126         | 67         | 0.02%        | 0.002%     |
| 33     | 5.887    | 1453       | 1466     | 1493      | rVV   | 139533      | 268673     | 69.04%       | 8.627%     |
| 34     | 6.051    | 1514       | 1517     | 1522      | rBV   | 167         | 90         | 0.02%        | 0.003%     |

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 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\SOMULM102218WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |        |        |         |
|----|-------|------|------|------|------|--------|--------|--------|---------|
| 35 | 6.096 | 1526 | 1531 | 1537 | rBV  | 193    | 286    | 0.07%  | 0.009%  |
| 36 | 6.180 | 1555 | 1557 | 1559 | rBV  | 218    | 88     | 0.02%  | 0.003%  |
| 37 | 6.234 | 1572 | 1574 | 1576 | rBV  | 153    | 106    | 0.03%  | 0.003%  |
| 38 | 6.334 | 1590 | 1605 | 1623 | rBV  | 91456  | 181475 | 46.63% | 5.827%  |
| 39 | 6.398 | 1623 | 1625 | 1629 | rVB  | 234    | 125    | 0.03%  | 0.004%  |
| 40 | 6.456 | 1641 | 1643 | 1646 | rBV  | 165    | 134    | 0.03%  | 0.004%  |
| 41 | 6.505 | 1655 | 1658 | 1661 | rBV  | 194    | 185    | 0.05%  | 0.006%  |
| 42 | 6.595 | 1682 | 1686 | 1690 | rBV  | 180    | 230    | 0.06%  | 0.007%  |
| 43 | 6.669 | 1706 | 1709 | 1711 | rBB  | 133    | 93     | 0.02%  | 0.003%  |
| 44 | 6.688 | 1711 | 1715 | 1717 | rBV  | 196    | 176    | 0.05%  | 0.006%  |
| 45 | 6.791 | 1743 | 1747 | 1751 | rVB  | 165    | 200    | 0.05%  | 0.006%  |
| 46 | 6.816 | 1752 | 1755 | 1758 | rBV  | 129    | 134    | 0.03%  | 0.004%  |
| 47 | 6.861 | 1762 | 1769 | 1781 | rVV2 | 1180   | 2189   | 0.56%  | 0.070%  |
| 48 | 6.939 | 1790 | 1793 | 1796 | rBV  | 175    | 166    | 0.04%  | 0.005%  |
| 49 | 7.228 | 1872 | 1883 | 1918 | rVB  | 53697  | 94105  | 24.18% | 3.022%  |
| 50 | 7.360 | 1921 | 1924 | 1926 | rBV  | 235    | 185    | 0.05%  | 0.006%  |
| 51 | 7.373 | 1926 | 1928 | 1930 | rVV  | 178    | 130    | 0.03%  | 0.004%  |
| 52 | 7.386 | 1930 | 1932 | 1936 | rVV2 | 306    | 222    | 0.06%  | 0.007%  |
| 53 | 7.405 | 1936 | 1938 | 1943 | rVB  | 218    | 206    | 0.05%  | 0.007%  |
| 54 | 7.431 | 1943 | 1946 | 1948 | rBV  | 149    | 129    | 0.03%  | 0.004%  |
| 55 | 7.566 | 1974 | 1988 | 2006 | rBV  | 173868 | 301112 | 77.38% | 9.668%  |
| 56 | 7.675 | 2020 | 2022 | 2024 | rVB  | 283    | 153    | 0.04%  | 0.005%  |
| 57 | 7.707 | 2029 | 2032 | 2034 | rVV  | 147    | 99     | 0.03%  | 0.003%  |
| 58 | 7.816 | 2061 | 2066 | 2067 | rBV  | 141    | 124    | 0.03%  | 0.004%  |
| 59 | 7.852 | 2067 | 2077 | 2093 | rVV2 | 35885  | 60961  | 15.66% | 1.957%  |
| 60 | 7.951 | 2104 | 2108 | 2110 | rBV2 | 196    | 168    | 0.04%  | 0.005%  |
| 61 | 7.977 | 2112 | 2116 | 2118 | rBV2 | 289    | 232    | 0.06%  | 0.007%  |
| 62 | 8.025 | 2127 | 2131 | 2133 | rBV  | 155    | 71     | 0.02%  | 0.002%  |
| 63 | 8.041 | 2133 | 2136 | 2141 | rVB2 | 181    | 167    | 0.04%  | 0.005%  |
| 64 | 8.183 | 2167 | 2180 | 2192 | rBV2 | 20033  | 47415  | 12.18% | 1.522%  |
| 65 | 8.312 | 2210 | 2220 | 2245 | rVB  | 129080 | 225083 | 57.84% | 7.227%  |
| 66 | 8.562 | 2295 | 2298 | 2302 | rVB  | 113    | 80     | 0.02%  | 0.003%  |
| 67 | 8.620 | 2308 | 2316 | 2325 | rVV2 | 1055   | 1602   | 0.41%  | 0.051%  |
| 68 | 8.955 | 2415 | 2420 | 2423 | rVB  | 111    | 111    | 0.03%  | 0.004%  |
| 69 | 9.090 | 2450 | 2462 | 2485 | rBV  | 197743 | 322223 | 82.80% | 10.346% |
| 70 | 9.308 | 2527 | 2530 | 2534 | rVV  | 133    | 100    | 0.03%  | 0.003%  |
| 71 | 9.636 | 2629 | 2632 | 2636 | rBV  | 151    | 98     | 0.03%  | 0.003%  |

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## Integration Parameters: LSCINT.P

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 Sampling : 1  
 Start Thrs: 0.2  
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Filtering: 5  
 Min Area: 0 % of largest Peak  
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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\SOMULM102218WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 72  | 9.861  | 2700 | 2702 | 2705 | rBV  | 119    | 71     | 0.02%  | 0.002% |
| 73  | 9.881  | 2705 | 2708 | 2713 | rVB  | 106    | 94     | 0.02%  | 0.003% |
| 74  | 9.951  | 2728 | 2730 | 2733 | rBV  | 185    | 93     | 0.02%  | 0.003% |
| 75  | 10.270 | 2826 | 2829 | 2831 | rBV  | 111    | 79     | 0.02%  | 0.003% |
| 76  | 10.279 | 2831 | 2832 | 2837 | rVB  | 169    | 75     | 0.02%  | 0.002% |
| 77  | 10.430 | 2868 | 2879 | 2895 | rBV  | 113607 | 180440 | 46.37% | 5.794% |
| 78  | 10.617 | 2925 | 2937 | 2948 | rVB4 | 5810   | 12009  | 3.09%  | 0.386% |
| 79  | 10.877 | 3010 | 3018 | 3031 | rVB2 | 658    | 1078   | 0.28%  | 0.035% |
| 80  | 11.041 | 3066 | 3069 | 3071 | rBV  | 100    | 71     | 0.02%  | 0.002% |
| 81  | 11.334 | 3157 | 3160 | 3162 | rBV  | 107    | 74     | 0.02%  | 0.002% |
| 82  | 11.382 | 3172 | 3175 | 3178 | rBV  | 115    | 88     | 0.02%  | 0.003% |
| 83  | 11.485 | 3195 | 3207 | 3229 | rBV  | 184198 | 287663 | 73.92% | 9.236% |
| 84  | 11.861 | 3312 | 3324 | 3340 | rBV  | 159213 | 252648 | 64.92% | 8.112% |
| 85  | 11.967 | 3354 | 3357 | 3361 | rBV  | 197    | 171    | 0.04%  | 0.005% |
| 86  | 11.990 | 3362 | 3364 | 3365 | rVV  | 164    | 72     | 0.02%  | 0.002% |
| 87  | 12.009 | 3368 | 3370 | 3374 | rVB  | 232    | 106    | 0.03%  | 0.003% |
| 88  | 12.192 | 3425 | 3427 | 3433 | rBV  | 112    | 103    | 0.03%  | 0.003% |
| 89  | 12.479 | 3507 | 3516 | 3528 | rVB2 | 2141   | 3749   | 0.96%  | 0.120% |
| 90  | 12.832 | 3623 | 3626 | 3629 | rBV  | 169    | 127    | 0.03%  | 0.004% |
| 91  | 13.909 | 3958 | 3961 | 3964 | rVB2 | 248    | 155    | 0.04%  | 0.005% |
| 92  | 14.093 | 4015 | 4018 | 4019 | rBV  | 162    | 96     | 0.02%  | 0.003% |
| 93  | 14.231 | 4059 | 4061 | 4062 | rBV  | 168    | 80     | 0.02%  | 0.003% |
| 94  | 14.276 | 4067 | 4075 | 4087 | rBV2 | 3169   | 5104   | 1.31%  | 0.164% |
| 95  | 14.543 | 4156 | 4158 | 4159 | rBV2 | 199    | 88     | 0.02%  | 0.003% |
| 96  | 14.601 | 4173 | 4176 | 4179 | rBV  | 245    | 198    | 0.05%  | 0.006% |
| 97  | 14.659 | 4191 | 4194 | 4196 | rBV2 | 249    | 154    | 0.04%  | 0.005% |
| 98  | 14.736 | 4215 | 4218 | 4224 | rBV2 | 243    | 276    | 0.07%  | 0.009% |
| 99  | 15.032 | 4307 | 4310 | 4313 | rBV  | 271    | 210    | 0.05%  | 0.007% |
| 100 | 16.411 | 4737 | 4739 | 4740 | rBV  | 357    | 153    | 0.04%  | 0.005% |

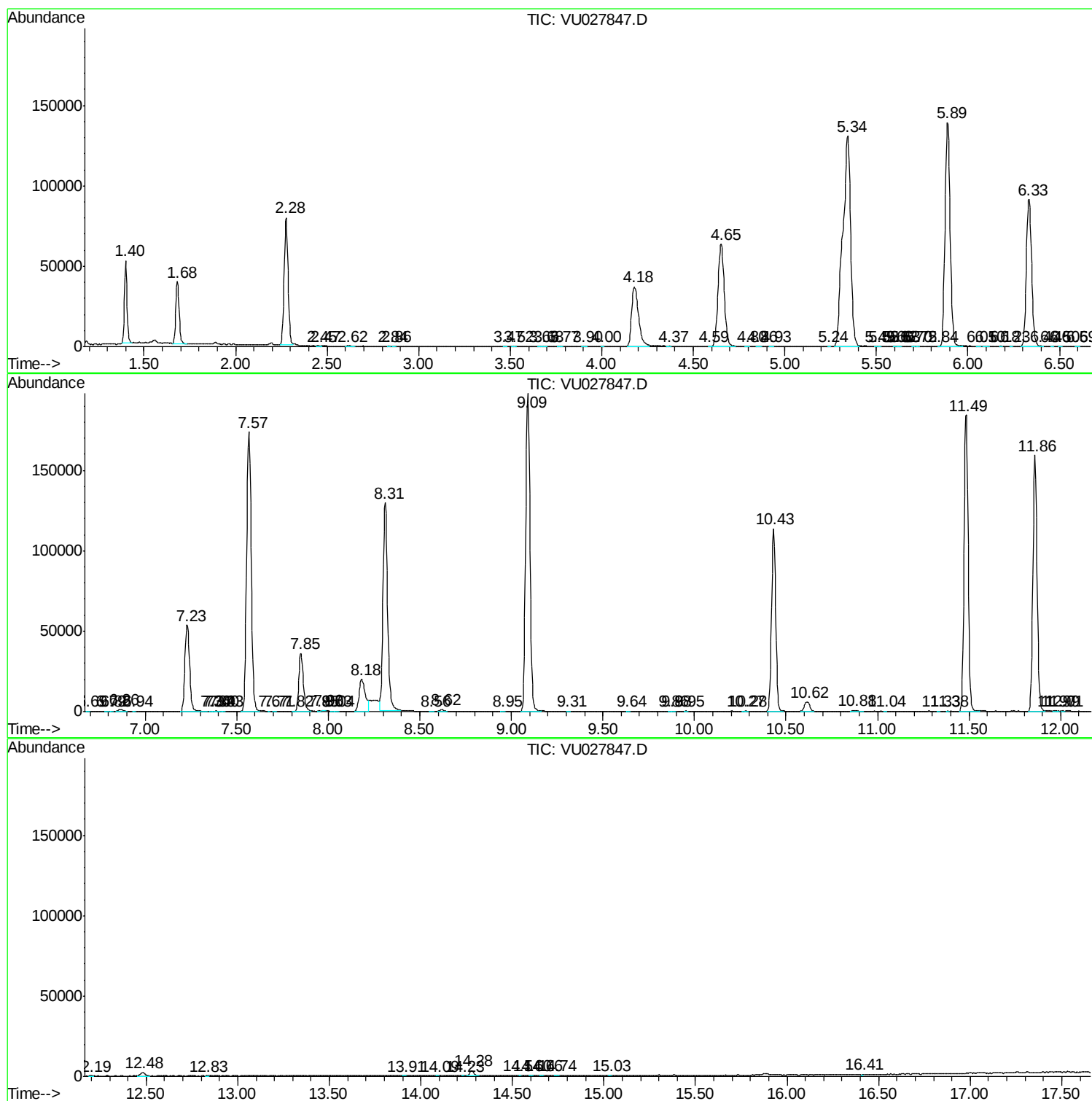
Sum of corrected areas: 3114507

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM102218WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU102918\  
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Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Data Path : Z:\V0ASRV\HPCHEM1\MSV0A\_U\DATA\VU102918\  
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| TIC Top Hit name | RT | EstConc | Units | Response | ---Internal Standard--- |
|------------------|----|---------|-------|----------|-------------------------|
|                  |    |         |       |          | # RT Resp Conc          |