

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU041219\  
 Data File : VU031128.D  
 Acq On : 12 Apr 2019 15:10  
 Operator : JC/SP  
 Sample : VU0412MBL01  
 Misc : 5.00g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK58

## 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\SOMULM040519WMA.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       | 23            | 27          | 39           | rVB      | 23090          | 23038         | 1.13%           | 0.150%        |
| 2         | 1.392       | 87            | 94          | 108          | rBV      | 314589         | 332473        | 16.34%          | 2.160%        |
| 3         | 1.675       | 174           | 182         | 195          | rBV      | 233993         | 300592        | 14.78%          | 1.953%        |
| 4         | 2.267       | 355           | 366         | 378          | rVB      | 473875         | 731368        | 35.95%          | 4.752%        |
| 5         | 2.389       | 402           | 404         | 407          | rVB3     | 1126           | 610           | 0.03%           | 0.004%        |
| 6         | 2.476       | 423           | 431         | 440          | rVB4     | 3662           | 5951          | 0.29%           | 0.039%        |
| 7         | 2.695       | 490           | 499         | 507          | rBV6     | 4089           | 6482          | 0.32%           | 0.042%        |
| 8         | 2.868       | 549           | 553         | 555          | rBV2     | 554            | 475           | 0.02%           | 0.003%        |
| 9         | 2.971       | 582           | 585         | 586          | rVV2     | 934            | 545           | 0.03%           | 0.004%        |
| 10        | 2.984       | 586           | 589         | 593          | rVB4     | 1073           | 879           | 0.04%           | 0.006%        |
| 11        | 3.318       | 688           | 693         | 697          | rBV2     | 818            | 830           | 0.04%           | 0.005%        |
| 12        | 3.441       | 726           | 731         | 734          | rBV3     | 444            | 455           | 0.02%           | 0.003%        |
| 13        | 3.479       | 740           | 743         | 749          | rVB2     | 649            | 442           | 0.02%           | 0.003%        |
| 14        | 3.733       | 819           | 822         | 825          | rVB3     | 742            | 490           | 0.02%           | 0.003%        |
| 15        | 3.752       | 825           | 828         | 831          | rBV2     | 793            | 550           | 0.03%           | 0.004%        |
| 16        | 3.910       | 872           | 877         | 882          | rBV4     | 469            | 504           | 0.02%           | 0.003%        |
| 17        | 3.955       | 889           | 891         | 895          | rBV3     | 607            | 447           | 0.02%           | 0.003%        |
| 18        | 4.055       | 918           | 922         | 927          | rBV3     | 802            | 858           | 0.04%           | 0.006%        |
| 19        | 4.170       | 944           | 958         | 982          | rBV      | 192080         | 512154        | 25.18%          | 3.328%        |
| 20        | 4.550       | 1073          | 1076        | 1080         | rVB3     | 854            | 521           | 0.03%           | 0.003%        |
| 21        | 4.640       | 1084          | 1104        | 1131         | rBV      | 327843         | 799253        | 39.29%          | 5.193%        |
| 22        | 4.862       | 1171          | 1173        | 1176         | rBV3     | 799            | 504           | 0.02%           | 0.003%        |
| 23        | 4.884       | 1176          | 1180        | 1186         | rVB6     | 1388           | 1715          | 0.08%           | 0.011%        |
| 24        | 4.916       | 1186          | 1190        | 1194         | rVB5     | 1019           | 1041          | 0.05%           | 0.007%        |
| 25        | 4.974       | 1204          | 1208        | 1210         | rBV3     | 1200           | 908           | 0.04%           | 0.006%        |
| 26        | 5.103       | 1244          | 1248        | 1251         | rVB2     | 544            | 442           | 0.02%           | 0.003%        |
| 27        | 5.196       | 1274          | 1277        | 1282         | rBV2     | 896            | 1053          | 0.05%           | 0.007%        |
| 28        | 5.219       | 1282          | 1284        | 1288         | rVB      | 852            | 474           | 0.02%           | 0.003%        |
| 29        | 5.334       | 1293          | 1320        | 1349         | rBV2     | 687348         | 2034235       | 100.00%         | 13.218%       |
| 30        | 5.553       | 1385          | 1388        | 1390         | rBV2     | 825            | 610           | 0.03%           | 0.004%        |
| 31        | 5.598       | 1397          | 1402        | 1404         | rBV4     | 794            | 648           | 0.03%           | 0.004%        |
| 32        | 5.649       | 1414          | 1418        | 1422         | rBV5     | 1329           | 1092          | 0.05%           | 0.007%        |
| 33        | 5.694       | 1430          | 1432        | 1436         | rVB2     | 1111           | 728           | 0.04%           | 0.005%        |
| 34        | 5.733       | 1440          | 1444        | 1447         | rBV4     | 440            | 445           | 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\SOMULM040519WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 5.807 | 1464 | 1467 | 1473 | rVB4 | 699    | 543     | 0.03%  | 0.004%  |
| 36 | 5.881 | 1477 | 1490 | 1519 | rBV  | 577604 | 1160837 | 57.07% | 7.543%  |
| 37 | 6.109 | 1559 | 1561 | 1568 | rVB2 | 1224   | 690     | 0.03%  | 0.004%  |
| 38 | 6.177 | 1571 | 1582 | 1583 | rBV9 | 3320   | 3990    | 0.20%  | 0.026%  |
| 39 | 6.325 | 1613 | 1628 | 1648 | rBV  | 448330 | 911275  | 44.80% | 5.921%  |
| 40 | 6.585 | 1705 | 1709 | 1712 | rVB5 | 741    | 635     | 0.03%  | 0.004%  |
| 41 | 6.733 | 1753 | 1755 | 1758 | rVB2 | 780    | 467     | 0.02%  | 0.003%  |
| 42 | 6.775 | 1762 | 1768 | 1772 | rBV5 | 987    | 1169    | 0.06%  | 0.008%  |
| 43 | 6.887 | 1801 | 1803 | 1807 | rVV3 | 718    | 545     | 0.03%  | 0.004%  |
| 44 | 6.923 | 1809 | 1814 | 1816 | rVB2 | 1013   | 670     | 0.03%  | 0.004%  |
| 45 | 6.939 | 1816 | 1819 | 1825 | rBV2 | 775    | 733     | 0.04%  | 0.005%  |
| 46 | 7.006 | 1834 | 1840 | 1844 | rBV2 | 967    | 1066    | 0.05%  | 0.007%  |
| 47 | 7.170 | 1887 | 1891 | 1896 | rVB2 | 810    | 748     | 0.04%  | 0.005%  |
| 48 | 7.225 | 1896 | 1908 | 1929 | rBV  | 240344 | 447066  | 21.98% | 2.905%  |
| 49 | 7.418 | 1966 | 1968 | 1972 | rVV4 | 1191   | 995     | 0.05%  | 0.006%  |
| 50 | 7.466 | 1976 | 1983 | 1993 | rVV4 | 6350   | 11792   | 0.58%  | 0.077%  |
| 51 | 7.559 | 2000 | 2012 | 2036 | rBV  | 869654 | 1549727 | 76.18% | 10.070% |
| 52 | 7.846 | 2089 | 2101 | 2123 | rBV  | 166047 | 304219  | 14.95% | 1.977%  |
| 53 | 8.077 | 2170 | 2173 | 2179 | rVB5 | 1347   | 1472    | 0.07%  | 0.010%  |
| 54 | 8.103 | 2179 | 2181 | 2186 | rVB3 | 1061   | 799     | 0.04%  | 0.005%  |
| 55 | 8.170 | 2199 | 2202 | 2204 | rBV3 | 1315   | 768     | 0.04%  | 0.005%  |
| 56 | 8.231 | 2212 | 2221 | 2233 | rVB3 | 3381   | 6912    | 0.34%  | 0.045%  |
| 57 | 8.309 | 2233 | 2245 | 2289 | rBV  | 562592 | 1154770 | 56.77% | 7.503%  |
| 58 | 8.746 | 2378 | 2381 | 2386 | rVB5 | 1027   | 759     | 0.04%  | 0.005%  |
| 59 | 8.772 | 2386 | 2389 | 2393 | rBV2 | 435    | 482     | 0.02%  | 0.003%  |
| 60 | 8.839 | 2407 | 2410 | 2413 | rBV3 | 717    | 444     | 0.02%  | 0.003%  |
| 61 | 9.087 | 2474 | 2487 | 2513 | rBV  | 841019 | 1439337 | 70.76% | 9.352%  |
| 62 | 9.254 | 2534 | 2539 | 2542 | rBV4 | 2187   | 2436    | 0.12%  | 0.016%  |
| 63 | 9.296 | 2549 | 2552 | 2556 | rVV2 | 914    | 629     | 0.03%  | 0.004%  |
| 64 | 9.344 | 2565 | 2567 | 2572 | rBV3 | 572    | 517     | 0.03%  | 0.003%  |
| 65 | 9.447 | 2594 | 2599 | 2604 | rVB7 | 933    | 1026    | 0.05%  | 0.007%  |
| 66 | 9.501 | 2613 | 2616 | 2621 | rBV3 | 1004   | 680     | 0.03%  | 0.004%  |
| 67 | 9.530 | 2621 | 2625 | 2631 | rVB3 | 941    | 1042    | 0.05%  | 0.007%  |
| 68 | 9.569 | 2634 | 2637 | 2641 | rVB2 | 781    | 453     | 0.02%  | 0.003%  |
| 69 | 9.646 | 2658 | 2661 | 2665 | rVB3 | 1047   | 708     | 0.03%  | 0.005%  |
| 70 | 9.678 | 2665 | 2671 | 2675 | rBV2 | 839    | 1195    | 0.06%  | 0.008%  |
| 71 | 9.762 | 2693 | 2697 | 2699 | rBV2 | 670    | 477     | 0.02%  | 0.003%  |

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## Integration Parameters: LSCINT.P

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Filtering: 5  
 Min Area: 0 % of largest Peak  
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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\SOMULM040519WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |       |        |         |        |        |
|-----|--------|------|------|------|-------|--------|---------|--------|--------|
| 72  | 9.781  | 2699 | 2703 | 2705 | rBV4  | 1642   | 1491    | 0.07%  | 0.010% |
| 73  | 10.058 | 2784 | 2789 | 2793 | rVB3  | 953    | 869     | 0.04%  | 0.006% |
| 74  | 10.167 | 2818 | 2823 | 2826 | rBV3  | 3109   | 2911    | 0.14%  | 0.019% |
| 75  | 10.325 | 2869 | 2872 | 2877 | rVB3  | 1047   | 846     | 0.04%  | 0.005% |
| 76  | 10.427 | 2890 | 2904 | 2921 | rBV   | 595724 | 968219  | 47.60% | 6.291% |
| 77  | 10.630 | 2964 | 2967 | 2970 | rBV3  | 918    | 606     | 0.03%  | 0.004% |
| 78  | 10.723 | 2990 | 2996 | 2999 | rBV3  | 701    | 954     | 0.05%  | 0.006% |
| 79  | 10.971 | 3068 | 3073 | 3077 | rVV3  | 734    | 843     | 0.04%  | 0.005% |
| 80  | 11.173 | 3132 | 3136 | 3139 | rBV2  | 884    | 728     | 0.04%  | 0.005% |
| 81  | 11.222 | 3149 | 3151 | 3155 | rBV2  | 692    | 456     | 0.02%  | 0.003% |
| 82  | 11.424 | 3206 | 3214 | 3220 | rBV4  | 5360   | 7387    | 0.36%  | 0.048% |
| 83  | 11.482 | 3220 | 3232 | 3256 | rBV   | 766260 | 1266738 | 62.27% | 8.231% |
| 84  | 11.855 | 3334 | 3348 | 3377 | rBV   | 775040 | 1315274 | 64.66% | 8.546% |
| 85  | 12.308 | 3486 | 3489 | 3491 | rBV2  | 983    | 691     | 0.03%  | 0.004% |
| 86  | 12.379 | 3505 | 3511 | 3512 | rBV2  | 863    | 826     | 0.04%  | 0.005% |
| 87  | 12.437 | 3527 | 3529 | 3532 | rBV2  | 779    | 470     | 0.02%  | 0.003% |
| 88  | 12.540 | 3558 | 3561 | 3564 | rBV3  | 650    | 529     | 0.03%  | 0.003% |
| 89  | 12.659 | 3593 | 3598 | 3602 | rBV5  | 1539   | 1733    | 0.09%  | 0.011% |
| 90  | 12.797 | 3638 | 3641 | 3646 | rBV3  | 757    | 721     | 0.04%  | 0.005% |
| 91  | 12.836 | 3647 | 3653 | 3656 | rVB4  | 842    | 976     | 0.05%  | 0.006% |
| 92  | 12.897 | 3666 | 3672 | 3674 | rBV4  | 4228   | 4515    | 0.22%  | 0.029% |
| 93  | 13.164 | 3752 | 3755 | 3758 | rBV3  | 1032   | 524     | 0.03%  | 0.003% |
| 94  | 13.521 | 3858 | 3866 | 3870 | rBV7  | 4294   | 6752    | 0.33%  | 0.044% |
| 95  | 13.762 | 3933 | 3941 | 3944 | rBV3  | 7290   | 10600   | 0.52%  | 0.069% |
| 96  | 14.000 | 4006 | 4015 | 4022 | rBV10 | 6621   | 14694   | 0.72%  | 0.095% |
| 97  | 14.135 | 4054 | 4057 | 4061 | rBV5  | 1396   | 1210    | 0.06%  | 0.008% |
| 98  | 14.334 | 4115 | 4119 | 4121 | rBV2  | 1138   | 888     | 0.04%  | 0.006% |
| 99  | 15.299 | 4416 | 4419 | 4422 | rBV4  | 1535   | 1246    | 0.06%  | 0.008% |
| 100 | 15.556 | 4496 | 4499 | 4503 | rBV5  | 1404   | 1627    | 0.08%  | 0.011% |

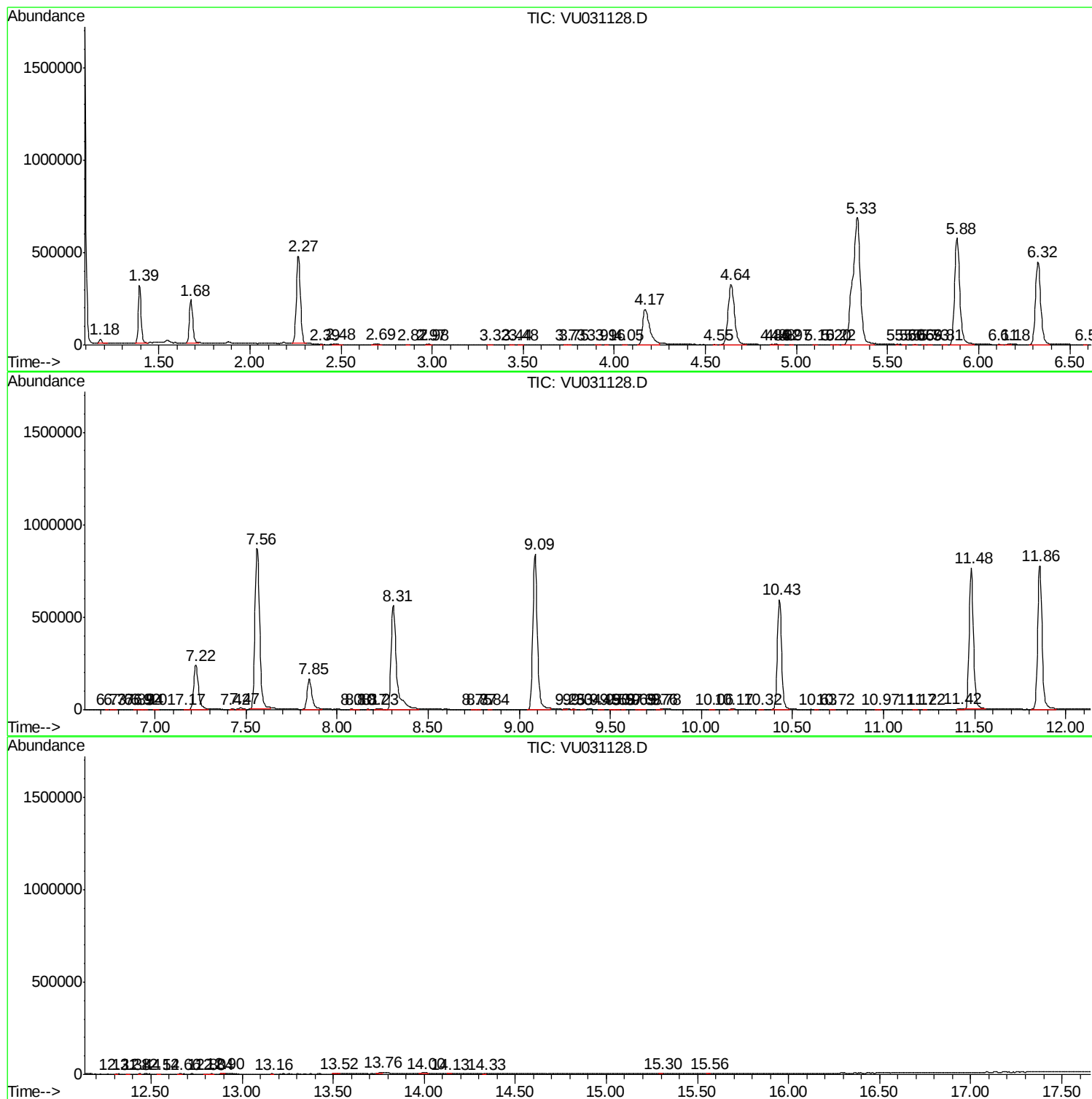
Sum of corrected areas: 15390209

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM040519WMA.M  
Quant Title : VOC Analysis

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



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TIC Library : C:\DATABASE\NIST11.L  
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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        |