

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040419\  
 Data File : VU030670.D  
 Acq On : 04 Apr 2019 08:25  
 Operator : JC/SP  
 Sample : K2246-09  
 Misc : 5.20g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 48 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BF156

## 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      | 1.174    | 23         | 26       | 33        | rVB2  | 12777       | 11494      | 0.66%        | 0.082%     |
| 2      | 1.392    | 87         | 94       | 107       | rVB   | 204321      | 244769     | 14.10%       | 1.751%     |
| 3      | 1.640    | 166        | 171      | 182       | rVB   | 139046      | 158634     | 9.14%        | 1.135%     |
| 4      | 2.238    | 347        | 357      | 372       | rVB   | 376539      | 583744     | 33.63%       | 4.176%     |
| 5      | 2.511    | 439        | 442      | 449       | rBV5  | 1108        | 1142       | 0.07%        | 0.008%     |
| 6      | 2.566    | 455        | 459      | 460       | rBV4  | 999         | 655        | 0.04%        | 0.005%     |
| 7      | 2.598    | 466        | 469      | 472       | rBV3  | 912         | 689        | 0.04%        | 0.005%     |
| 8      | 2.685    | 486        | 496      | 510       | rVB4  | 7202        | 15542      | 0.90%        | 0.111%     |
| 9      | 2.813    | 532        | 536      | 537       | rBV4  | 821         | 609        | 0.04%        | 0.004%     |
| 10     | 2.852    | 546        | 548      | 551       | rVB2  | 1198        | 675        | 0.04%        | 0.005%     |
| 11     | 2.871    | 551        | 554      | 556       | rVB   | 958         | 504        | 0.03%        | 0.004%     |
| 12     | 3.022    | 599        | 601      | 604       | rVB3  | 978         | 519        | 0.03%        | 0.004%     |
| 13     | 3.061    | 610        | 613      | 617       | rBV2  | 921         | 763        | 0.04%        | 0.005%     |
| 14     | 3.112    | 627        | 629      | 636       | rVB3  | 850         | 847        | 0.05%        | 0.006%     |
| 15     | 3.183    | 648        | 651      | 654       | rBV2  | 601         | 580        | 0.03%        | 0.004%     |
| 16     | 3.280    | 673        | 681      | 689       | rVV7  | 1406        | 2396       | 0.14%        | 0.017%     |
| 17     | 3.534    | 754        | 760      | 763       | rBV2  | 967         | 875        | 0.05%        | 0.006%     |
| 18     | 3.723    | 813        | 819      | 824       | rBV5  | 747         | 705        | 0.04%        | 0.005%     |
| 19     | 3.762    | 829        | 831      | 835       | rVB   | 846         | 548        | 0.03%        | 0.004%     |
| 20     | 3.791    | 835        | 840      | 842       | rBV   | 950         | 814        | 0.05%        | 0.006%     |
| 21     | 3.916    | 876        | 879      | 887       | rBV2  | 750         | 838        | 0.05%        | 0.006%     |
| 22     | 4.186    | 951        | 963      | 996       | rBV   | 125997      | 458437     | 26.41%       | 3.280%     |
| 23     | 4.527    | 1066       | 1069     | 1073      | rVB4  | 1206        | 870        | 0.05%        | 0.006%     |
| 24     | 4.550    | 1073       | 1076     | 1078      | rBV2  | 830         | 525        | 0.03%        | 0.004%     |
| 25     | 4.640    | 1087       | 1104     | 1136      | rBV   | 254044      | 660063     | 38.02%       | 4.722%     |
| 26     | 4.862    | 1170       | 1173     | 1176      | rBV3  | 697         | 659        | 0.04%        | 0.005%     |
| 27     | 5.042    | 1224       | 1229     | 1236      | rBV4  | 1840        | 2188       | 0.13%        | 0.016%     |
| 28     | 5.077    | 1237       | 1240     | 1244      | rVB3  | 794         | 581        | 0.03%        | 0.004%     |
| 29     | 5.112    | 1246       | 1251     | 1253      | rBV3  | 596         | 485        | 0.03%        | 0.003%     |
| 30     | 5.328    | 1296       | 1318     | 1342      | rBV2  | 597540      | 1735910    | 100.00%      | 12.420%    |
| 31     | 5.624    | 1399       | 1410     | 1415      | rBV7  | 4728        | 8402       | 0.48%        | 0.060%     |
| 32     | 5.704    | 1431       | 1435     | 1438      | rVB3  | 1052        | 899        | 0.05%        | 0.006%     |
| 33     | 5.746    | 1444       | 1448     | 1451      | rBV3  | 673         | 501        | 0.03%        | 0.004%     |
| 34     | 5.772    | 1455       | 1456     | 1459      | rVB3  | 1302        | 565        | 0.03%        | 0.004%     |

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

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 35 | 5.881  | 1476 | 1490 | 1518 | rBV  | 561900 | 1218530 | 70.20% | 8.718%  |
| 36 | 6.173  | 1575 | 1581 | 1582 | rBV4 | 2110   | 1940    | 0.11%  | 0.014%  |
| 37 | 6.251  | 1595 | 1605 | 1614 | rBV7 | 5215   | 11183   | 0.64%  | 0.080%  |
| 38 | 6.325  | 1615 | 1628 | 1658 | rVB2 | 355731 | 781043  | 44.99% | 5.588%  |
| 39 | 6.460  | 1668 | 1670 | 1675 | rVB4 | 1339   | 955     | 0.06%  | 0.007%  |
| 40 | 6.588  | 1706 | 1710 | 1714 | rBV4 | 757    | 851     | 0.05%  | 0.006%  |
| 41 | 6.813  | 1778 | 1780 | 1788 | rVB4 | 867    | 752     | 0.04%  | 0.005%  |
| 42 | 6.874  | 1795 | 1799 | 1801 | rBV5 | 1060   | 816     | 0.05%  | 0.006%  |
| 43 | 6.900  | 1803 | 1807 | 1817 | rVV5 | 2123   | 3474    | 0.20%  | 0.025%  |
| 44 | 6.993  | 1832 | 1836 | 1839 | rBV2 | 1319   | 933     | 0.05%  | 0.007%  |
| 45 | 7.087  | 1862 | 1865 | 1868 | rBV2 | 639    | 503     | 0.03%  | 0.004%  |
| 46 | 7.106  | 1868 | 1871 | 1878 | rVB2 | 472    | 490     | 0.03%  | 0.004%  |
| 47 | 7.177  | 1889 | 1893 | 1897 | rBV3 | 995    | 745     | 0.04%  | 0.005%  |
| 48 | 7.225  | 1897 | 1908 | 1936 | rBV2 | 178523 | 376285  | 21.68% | 2.692%  |
| 49 | 7.398  | 1957 | 1962 | 1968 | rVB4 | 867    | 1155    | 0.07%  | 0.008%  |
| 50 | 7.434  | 1968 | 1973 | 1976 | rBV5 | 998    | 1131    | 0.07%  | 0.008%  |
| 51 | 7.472  | 1983 | 1985 | 1992 | rVB4 | 695    | 620     | 0.04%  | 0.004%  |
| 52 | 7.562  | 1998 | 2013 | 2034 | rBV  | 699254 | 1301039 | 74.95% | 9.308%  |
| 53 | 7.852  | 2092 | 2103 | 2134 | rVV  | 122341 | 258145  | 14.87% | 1.847%  |
| 54 | 7.958  | 2134 | 2136 | 2140 | rVB5 | 966    | 623     | 0.04%  | 0.004%  |
| 55 | 8.099  | 2178 | 2180 | 2185 | rVB4 | 1508   | 1021    | 0.06%  | 0.007%  |
| 56 | 8.180  | 2197 | 2205 | 2212 | rBV5 | 1616   | 2978    | 0.17%  | 0.021%  |
| 57 | 8.228  | 2212 | 2220 | 2230 | rVB9 | 5820   | 10033   | 0.58%  | 0.072%  |
| 58 | 8.321  | 2237 | 2249 | 2276 | rBV  | 553905 | 1067939 | 61.52% | 7.641%  |
| 59 | 8.707  | 2365 | 2369 | 2372 | rVB4 | 1014   | 808     | 0.05%  | 0.006%  |
| 60 | 8.836  | 2405 | 2409 | 2414 | rVB4 | 881    | 781     | 0.04%  | 0.006%  |
| 61 | 8.865  | 2414 | 2418 | 2420 | rBV3 | 966    | 554     | 0.03%  | 0.004%  |
| 62 | 8.897  | 2424 | 2428 | 2437 | rVB6 | 1112   | 1627    | 0.09%  | 0.012%  |
| 63 | 9.029  | 2466 | 2469 | 2474 | rBV4 | 1092   | 1095    | 0.06%  | 0.008%  |
| 64 | 9.090  | 2474 | 2488 | 2511 | rBV  | 825356 | 1499106 | 86.36% | 10.725% |
| 65 | 9.389  | 2574 | 2581 | 2587 | rBV6 | 1509   | 2340    | 0.13%  | 0.017%  |
| 66 | 9.469  | 2603 | 2606 | 2612 | rBV4 | 632    | 556     | 0.03%  | 0.004%  |
| 67 | 9.546  | 2627 | 2630 | 2635 | rVB2 | 770    | 625     | 0.04%  | 0.004%  |
| 68 | 9.585  | 2639 | 2642 | 2645 | rVB2 | 920    | 589     | 0.03%  | 0.004%  |
| 69 | 9.881  | 2728 | 2734 | 2736 | rVV2 | 1030   | 816     | 0.05%  | 0.006%  |
| 70 | 9.894  | 2736 | 2738 | 2743 | rVB2 | 1022   | 647     | 0.04%  | 0.005%  |
| 71 | 10.016 | 2770 | 2776 | 2779 | rBV3 | 728    | 637     | 0.04%  | 0.005%  |

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

|     |        |      |      |      |      |        |         |        |         |
|-----|--------|------|------|------|------|--------|---------|--------|---------|
| 72  | 10.164 | 2817 | 2822 | 2825 | rBV3 | 770    | 862     | 0.05%  | 0.006%  |
| 73  | 10.434 | 2893 | 2906 | 2931 | rBV  | 549620 | 912461  | 52.56% | 6.528%  |
| 74  | 10.575 | 2946 | 2950 | 2954 | rBV5 | 649    | 654     | 0.04%  | 0.005%  |
| 75  | 10.662 | 2974 | 2977 | 2982 | rBV4 | 553    | 539     | 0.03%  | 0.004%  |
| 76  | 10.771 | 3005 | 3011 | 3016 | rBV4 | 747    | 955     | 0.06%  | 0.007%  |
| 77  | 10.852 | 3033 | 3036 | 3040 | rVB3 | 922    | 667     | 0.04%  | 0.005%  |
| 78  | 10.874 | 3040 | 3043 | 3050 | rVB3 | 1090   | 895     | 0.05%  | 0.006%  |
| 79  | 10.910 | 3051 | 3054 | 3059 | rBV3 | 595    | 502     | 0.03%  | 0.004%  |
| 80  | 10.977 | 3071 | 3075 | 3078 | rBV4 | 576    | 509     | 0.03%  | 0.004%  |
| 81  | 11.045 | 3092 | 3096 | 3099 | rBV2 | 1140   | 999     | 0.06%  | 0.007%  |
| 82  | 11.122 | 3117 | 3120 | 3125 | rBV3 | 757    | 606     | 0.03%  | 0.004%  |
| 83  | 11.408 | 3207 | 3209 | 3212 | rVB3 | 737    | 486     | 0.03%  | 0.003%  |
| 84  | 11.482 | 3220 | 3232 | 3261 | rBV  | 874853 | 1414356 | 81.48% | 10.119% |
| 85  | 11.858 | 3337 | 3349 | 3376 | rBV  | 701449 | 1179280 | 67.93% | 8.437%  |
| 86  | 12.324 | 3492 | 3494 | 3498 | rVB2 | 1033   | 500     | 0.03%  | 0.004%  |
| 87  | 12.594 | 3576 | 3578 | 3583 | rBV2 | 643    | 485     | 0.03%  | 0.003%  |
| 88  | 12.762 | 3628 | 3630 | 3633 | rBV2 | 877    | 495     | 0.03%  | 0.004%  |
| 89  | 13.279 | 3789 | 3791 | 3794 | rVV2 | 1012   | 576     | 0.03%  | 0.004%  |
| 90  | 13.299 | 3795 | 3797 | 3800 | rVV3 | 1213   | 715     | 0.04%  | 0.005%  |
| 91  | 13.453 | 3842 | 3845 | 3848 | rBV3 | 983    | 697     | 0.04%  | 0.005%  |
| 92  | 13.537 | 3867 | 3871 | 3877 | rBV4 | 1176   | 1275    | 0.07%  | 0.009%  |
| 93  | 13.562 | 3877 | 3879 | 3881 | rBV2 | 829    | 572     | 0.03%  | 0.004%  |
| 94  | 13.668 | 3910 | 3912 | 3916 | rVB2 | 1344   | 818     | 0.05%  | 0.006%  |
| 95  | 13.839 | 3963 | 3965 | 3969 | rVB3 | 1557   | 913     | 0.05%  | 0.007%  |
| 96  | 13.868 | 3969 | 3974 | 3975 | rBV2 | 1283   | 1096    | 0.06%  | 0.008%  |
| 97  | 14.163 | 4063 | 4066 | 4069 | rBV3 | 1072   | 891     | 0.05%  | 0.006%  |
| 98  | 14.266 | 4094 | 4098 | 4099 | rBV3 | 2366   | 1650    | 0.10%  | 0.012%  |
| 99  | 14.639 | 4211 | 4214 | 4215 | rBV3 | 1044   | 566     | 0.03%  | 0.004%  |
| 100 | 15.598 | 4510 | 4512 | 4516 | rBV4 | 1897   | 1330    | 0.08%  | 0.010%  |

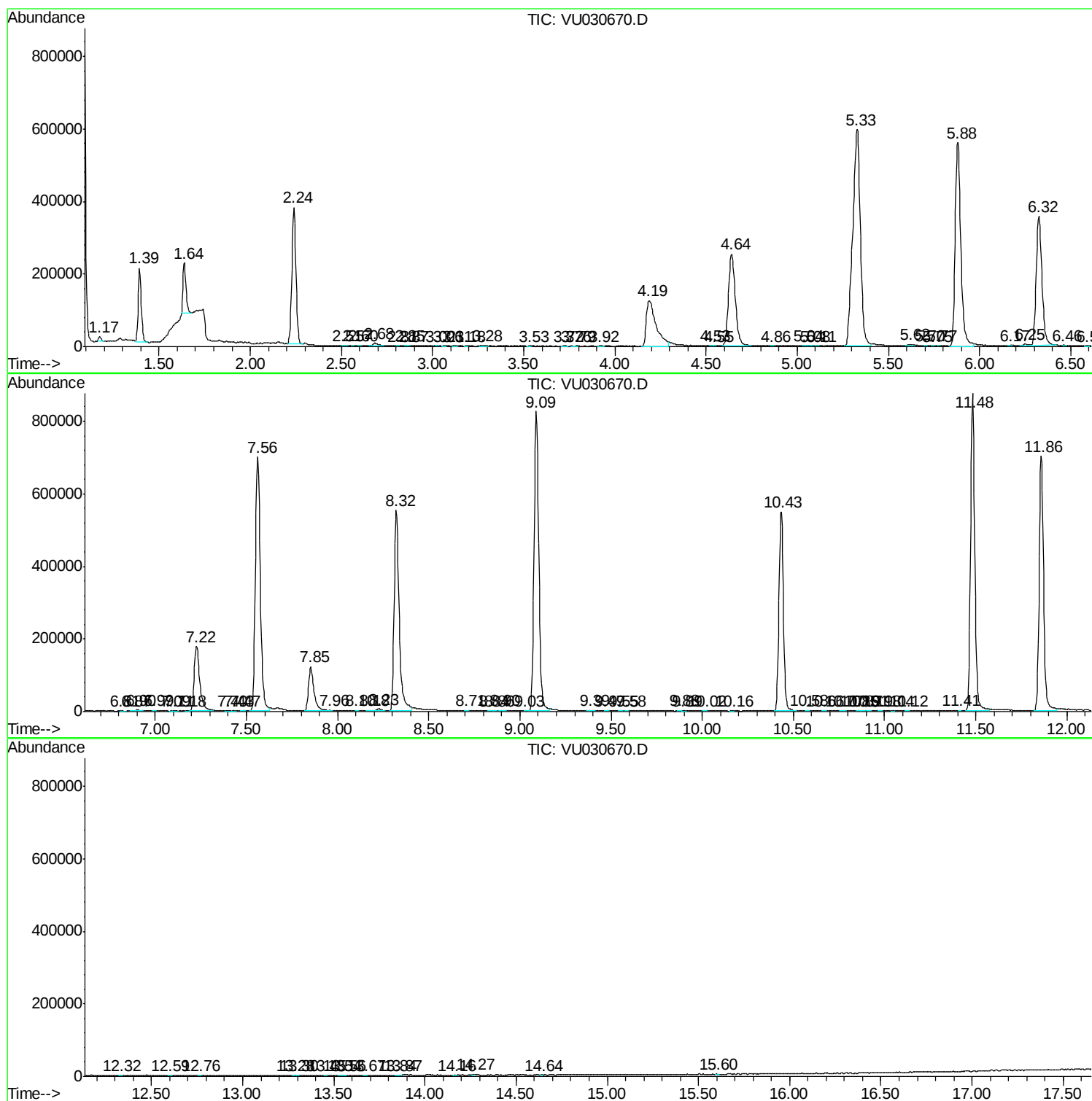
Sum of corrected areas: 13977142

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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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No Library Search Compounds Detected

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