

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU031519\  
 Data File : VU030041.D  
 Acq On : 13 Mar 2019 19:48  
 Operator : JC/SP  
 Sample : K1838-22  
 Misc : 5.31g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BF184

## 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\SOMULM031319WMA.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       | 22            | 27          | 34           | rBV      | 9541           | 10377         | 0.65%           | 0.076%        |
| 2         | 1.396       | 87            | 95          | 111          | rBV      | 151950         | 189379        | 11.79%          | 1.386%        |
| 3         | 1.640       | 166           | 171         | 189          | rBV      | 71978          | 103673        | 6.46%           | 0.759%        |
| 4         | 2.232       | 344           | 355         | 369          | rVB      | 299708         | 463971        | 28.90%          | 3.397%        |
| 5         | 2.335       | 382           | 387         | 389          | rBV3     | 1197           | 1161          | 0.07%           | 0.008%        |
| 6         | 2.518       | 442           | 444         | 448          | rBV3     | 453            | 380           | 0.02%           | 0.003%        |
| 7         | 2.685       | 488           | 496         | 506          | rVB5     | 3349           | 5662          | 0.35%           | 0.041%        |
| 8         | 2.827       | 530           | 540         | 553          | rVV3     | 3795           | 8333          | 0.52%           | 0.061%        |
| 9         | 2.878       | 553           | 556         | 561          | rVB2     | 767            | 458           | 0.03%           | 0.003%        |
| 10        | 2.955       | 576           | 580         | 588          | rVB4     | 926            | 1118          | 0.07%           | 0.008%        |
| 11        | 2.994       | 588           | 592         | 594          | rBV2     | 749            | 638           | 0.04%           | 0.005%        |
| 12        | 3.225       | 659           | 664         | 667          | rVB2     | 584            | 426           | 0.03%           | 0.003%        |
| 13        | 3.261       | 671           | 675         | 677          | rBV4     | 1049           | 752           | 0.05%           | 0.006%        |
| 14        | 3.643       | 791           | 794         | 802          | rVB3     | 554            | 647           | 0.04%           | 0.005%        |
| 15        | 3.724       | 814           | 819         | 822          | rBV2     | 465            | 421           | 0.03%           | 0.003%        |
| 16        | 3.749       | 822           | 827         | 829          | rBV3     | 598            | 426           | 0.03%           | 0.003%        |
| 17        | 3.820       | 843           | 849         | 853          | rBV2     | 680            | 704           | 0.04%           | 0.005%        |
| 18        | 3.843       | 853           | 856         | 862          | rVB2     | 676            | 564           | 0.04%           | 0.004%        |
| 19        | 3.962       | 886           | 893         | 898          | rBV2     | 456            | 639           | 0.04%           | 0.005%        |
| 20        | 4.052       | 917           | 921         | 928          | rVB3     | 459            | 442           | 0.03%           | 0.003%        |
| 21        | 4.113       | 936           | 940         | 945          | rVB2     | 373            | 430           | 0.03%           | 0.003%        |
| 22        | 4.190       | 949           | 964         | 990          | rBV      | 107370         | 351728        | 21.91%          | 2.575%        |
| 23        | 4.640       | 1087          | 1104        | 1127         | rBV2     | 221044         | 550912        | 34.31%          | 4.033%        |
| 24        | 4.791       | 1142          | 1151        | 1160         | rBV5     | 2905           | 6265          | 0.39%           | 0.046%        |
| 25        | 4.862       | 1170          | 1173        | 1175         | rBV      | 997            | 550           | 0.03%           | 0.004%        |
| 26        | 4.962       | 1194          | 1204        | 1223         | rVB3     | 6662           | 17718         | 1.10%           | 0.130%        |
| 27        | 5.084       | 1238          | 1242        | 1249         | rVB      | 766            | 620           | 0.04%           | 0.005%        |
| 28        | 5.174       | 1264          | 1270        | 1272         | rBV4     | 508            | 521           | 0.03%           | 0.004%        |
| 29        | 5.328       | 1295          | 1318        | 1348         | rBV2     | 496249         | 1410479       | 87.85%          | 10.326%       |
| 30        | 5.547       | 1382          | 1386        | 1394         | rBV3     | 551            | 836           | 0.05%           | 0.006%        |
| 31        | 5.611       | 1398          | 1406        | 1407         | rBV3     | 2429           | 2622          | 0.16%           | 0.019%        |
| 32        | 5.707       | 1433          | 1436        | 1442         | rVB2     | 843            | 811           | 0.05%           | 0.006%        |
| 33        | 5.746       | 1442          | 1448        | 1453         | rVB4     | 842            | 1107          | 0.07%           | 0.008%        |
| 34        | 5.878       | 1471          | 1489        | 1521         | rBV      | 552567         | 1155186       | 71.95%          | 8.457%        |

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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\SOMULM031319WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 6.077 | 1546 | 1551 | 1556 | rBV3 | 480    | 588     | 0.04%  | 0.004%  |
| 36 | 6.125 | 1563 | 1566 | 1571 | rVB2 | 547    | 510     | 0.03%  | 0.004%  |
| 37 | 6.161 | 1571 | 1577 | 1579 | rBV2 | 1170   | 1098    | 0.07%  | 0.008%  |
| 38 | 6.180 | 1580 | 1583 | 1590 | rVB8 | 2266   | 2352    | 0.15%  | 0.017%  |
| 39 | 6.244 | 1593 | 1603 | 1604 | rBV4 | 2591   | 2836    | 0.18%  | 0.021%  |
| 40 | 6.325 | 1614 | 1628 | 1651 | rBV  | 292309 | 619181  | 38.56% | 4.533%  |
| 41 | 6.550 | 1696 | 1698 | 1701 | rVB2 | 742    | 440     | 0.03%  | 0.003%  |
| 42 | 6.572 | 1701 | 1705 | 1709 | rBV2 | 394    | 468     | 0.03%  | 0.003%  |
| 43 | 6.614 | 1715 | 1718 | 1722 | rVB2 | 601    | 486     | 0.03%  | 0.004%  |
| 44 | 6.646 | 1722 | 1728 | 1732 | rBV2 | 438    | 394     | 0.02%  | 0.003%  |
| 45 | 6.688 | 1737 | 1741 | 1747 | rBV2 | 575    | 561     | 0.03%  | 0.004%  |
| 46 | 6.897 | 1792 | 1806 | 1811 | rBV9 | 2909   | 6325    | 0.39%  | 0.046%  |
| 47 | 7.039 | 1846 | 1850 | 1853 | rBV2 | 562    | 435     | 0.03%  | 0.003%  |
| 48 | 7.225 | 1896 | 1908 | 1934 | rBV  | 162282 | 323700  | 20.16% | 2.370%  |
| 49 | 7.367 | 1949 | 1952 | 1960 | rVB3 | 894    | 913     | 0.06%  | 0.007%  |
| 50 | 7.408 | 1960 | 1965 | 1966 | rBV2 | 514    | 436     | 0.03%  | 0.003%  |
| 51 | 7.418 | 1966 | 1968 | 1971 | rVB3 | 741    | 382     | 0.02%  | 0.003%  |
| 52 | 7.495 | 1984 | 1992 | 1997 | rVB4 | 732    | 949     | 0.06%  | 0.007%  |
| 53 | 7.560 | 1998 | 2012 | 2038 | rBV  | 628458 | 1157254 | 72.08% | 8.472%  |
| 54 | 7.752 | 2069 | 2072 | 2078 | rVB3 | 1065   | 925     | 0.06%  | 0.007%  |
| 55 | 7.849 | 2092 | 2102 | 2128 | rBV  | 103630 | 215309  | 13.41% | 1.576%  |
| 56 | 8.177 | 2190 | 2204 | 2210 | rBV  | 108825 | 205611  | 12.81% | 1.505%  |
| 57 | 8.222 | 2211 | 2218 | 2233 | rVB  | 239510 | 415832  | 25.90% | 3.044%  |
| 58 | 8.325 | 2239 | 2250 | 2283 | rVB  | 478569 | 941784  | 58.66% | 6.895%  |
| 59 | 8.682 | 2355 | 2361 | 2364 | rBV3 | 635    | 676     | 0.04%  | 0.005%  |
| 60 | 8.894 | 2422 | 2427 | 2429 | rBV2 | 872    | 811     | 0.05%  | 0.006%  |
| 61 | 9.003 | 2457 | 2461 | 2464 | rBV2 | 463    | 391     | 0.02%  | 0.003%  |
| 62 | 9.090 | 2466 | 2488 | 2516 | rBV  | 813323 | 1508023 | 93.92% | 11.041% |
| 63 | 9.338 | 2561 | 2565 | 2572 | rBV4 | 601    | 743     | 0.05%  | 0.005%  |
| 64 | 9.379 | 2572 | 2578 | 2579 | rBV3 | 1086   | 981     | 0.06%  | 0.007%  |
| 65 | 9.502 | 2613 | 2616 | 2620 | rBV3 | 536    | 443     | 0.03%  | 0.003%  |
| 66 | 9.540 | 2625 | 2628 | 2632 | rBV  | 505    | 383     | 0.02%  | 0.003%  |
| 67 | 9.624 | 2650 | 2654 | 2657 | rVB2 | 621    | 407     | 0.03%  | 0.003%  |
| 68 | 9.688 | 2670 | 2674 | 2676 | rBV2 | 491    | 401     | 0.02%  | 0.003%  |
| 69 | 9.768 | 2693 | 2699 | 2702 | rBV3 | 722    | 786     | 0.05%  | 0.006%  |
| 70 | 9.794 | 2703 | 2707 | 2709 | rBV3 | 743    | 491     | 0.03%  | 0.004%  |
| 71 | 9.958 | 2749 | 2758 | 2767 | rBV5 | 3625   | 6279    | 0.39%  | 0.046%  |

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## Integration Parameters: LSCINT.P

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 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\SOMULM031319WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |         |         |         |         |
|-----|--------|------|------|------|------|---------|---------|---------|---------|
| 72  | 10.045 | 2779 | 2785 | 2786 | rBV2 | 382     | 392     | 0.02%   | 0.003%  |
| 73  | 10.225 | 2836 | 2841 | 2847 | rVB5 | 1145    | 1404    | 0.09%   | 0.010%  |
| 74  | 10.257 | 2848 | 2851 | 2856 | rBV2 | 385     | 406     | 0.03%   | 0.003%  |
| 75  | 10.321 | 2866 | 2871 | 2875 | rVB  | 878     | 798     | 0.05%   | 0.006%  |
| 76  | 10.357 | 2879 | 2882 | 2886 | rBV2 | 443     | 448     | 0.03%   | 0.003%  |
| 77  | 10.434 | 2893 | 2906 | 2931 | rBV  | 584489  | 940682  | 58.59%  | 6.887%  |
| 78  | 10.608 | 2949 | 2960 | 2972 | rBV  | 44601   | 75680   | 4.71%   | 0.554%  |
| 79  | 10.781 | 3010 | 3014 | 3017 | rBV  | 621     | 544     | 0.03%   | 0.004%  |
| 80  | 10.878 | 3038 | 3044 | 3053 | rVB5 | 2091    | 2924    | 0.18%   | 0.021%  |
| 81  | 11.164 | 3129 | 3133 | 3136 | rBV  | 707     | 447     | 0.03%   | 0.003%  |
| 82  | 11.215 | 3147 | 3149 | 3153 | rVB  | 669     | 386     | 0.02%   | 0.003%  |
| 83  | 11.244 | 3153 | 3158 | 3161 | rBV3 | 599     | 669     | 0.04%   | 0.005%  |
| 84  | 11.428 | 3210 | 3215 | 3219 | rBV3 | 1332    | 1282    | 0.08%   | 0.009%  |
| 85  | 11.482 | 3219 | 3232 | 3264 | rVV  | 1020309 | 1605621 | 100.00% | 11.755% |
| 86  | 11.739 | 3309 | 3312 | 3314 | rBV2 | 782     | 527     | 0.03%   | 0.004%  |
| 87  | 11.797 | 3328 | 3330 | 3333 | rVB2 | 726     | 423     | 0.03%   | 0.003%  |
| 88  | 11.858 | 3334 | 3349 | 3372 | rBV  | 767119  | 1275849 | 79.46%  | 9.341%  |
| 89  | 12.479 | 3532 | 3542 | 3555 | rVB2 | 13892   | 24543   | 1.53%   | 0.180%  |
| 90  | 12.762 | 3625 | 3630 | 3633 | rBV2 | 642     | 698     | 0.04%   | 0.005%  |
| 91  | 13.109 | 3735 | 3738 | 3741 | rVV  | 564     | 421     | 0.03%   | 0.003%  |
| 92  | 13.238 | 3773 | 3778 | 3784 | rBV3 | 693     | 1001    | 0.06%   | 0.007%  |
| 93  | 13.321 | 3801 | 3804 | 3808 | rBV2 | 553     | 491     | 0.03%   | 0.004%  |
| 94  | 13.714 | 3918 | 3926 | 3930 | rBV3 | 651     | 1063    | 0.07%   | 0.008%  |
| 95  | 13.797 | 3947 | 3952 | 3954 | rBV3 | 723     | 698     | 0.04%   | 0.005%  |
| 96  | 13.923 | 3988 | 3991 | 3996 | rBV3 | 556     | 516     | 0.03%   | 0.004%  |
| 97  | 14.186 | 4070 | 4073 | 4075 | rBV2 | 596     | 390     | 0.02%   | 0.003%  |
| 98  | 14.273 | 4094 | 4100 | 4114 | rVB  | 6268    | 10134   | 0.63%   | 0.074%  |
| 99  | 14.739 | 4242 | 4245 | 4248 | rBV3 | 729     | 550     | 0.03%   | 0.004%  |
| 100 | 15.009 | 4327 | 4329 | 4333 | rBV3 | 778     | 474     | 0.03%   | 0.003%  |

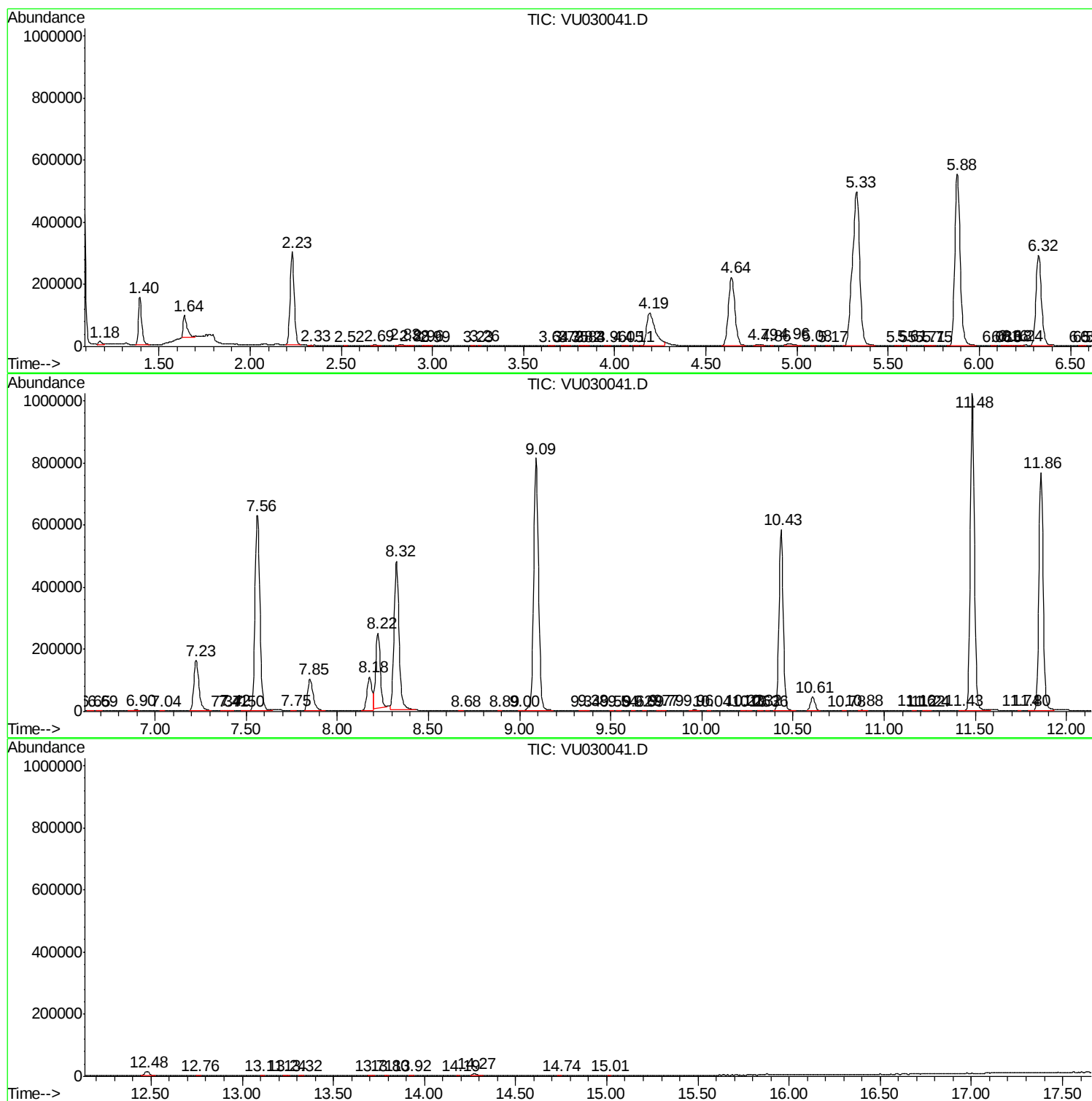
Sum of corrected areas: 13659001

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM031319WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU031519\  
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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        |