

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU041719\  
 Data File : VU031225.D  
 Acq On : 16 Apr 2019 21:09  
 Operator : JC/SP  
 Sample : K2409-05  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFC28

## 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\SOMULM041719WMA.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         | 1.180       | 23            | 28          | 38           | rVB      | 32556          | 33063         | 1.67%           | 0.210%        |
| 2         | 1.396       | 88            | 95          | 109          | rBV      | 261596         | 293115        | 14.80%          | 1.860%        |
| 3         | 1.682       | 176           | 184         | 195          | rBV      | 254174         | 311624        | 15.73%          | 1.977%        |
| 4         | 2.270       | 356           | 367         | 381          | rBV3     | 572043         | 948609        | 47.90%          | 6.020%        |
| 5         | 2.453       | 422           | 424         | 426          | rBV3     | 1052           | 685           | 0.03%           | 0.004%        |
| 6         | 2.482       | 428           | 433         | 436          | rVV4     | 1546           | 1730          | 0.09%           | 0.011%        |
| 7         | 2.830       | 529           | 541         | 558          | rBV3     | 7768           | 18032         | 0.91%           | 0.114%        |
| 8         | 2.977       | 583           | 587         | 588          | rBV      | 1354           | 705           | 0.04%           | 0.004%        |
| 9         | 3.003       | 592           | 595         | 602          | rVB5     | 1467           | 1519          | 0.08%           | 0.010%        |
| 10        | 3.251       | 668           | 672         | 674          | rBV2     | 679            | 518           | 0.03%           | 0.003%        |
| 11        | 3.440       | 719           | 731         | 752          | rBV3     | 17789          | 40294         | 2.03%           | 0.256%        |
| 12        | 3.585       | 770           | 776         | 779          | rVB      | 628            | 510           | 0.03%           | 0.003%        |
| 13        | 3.611       | 779           | 784         | 786          | rBV      | 497            | 476           | 0.02%           | 0.003%        |
| 14        | 3.891       | 868           | 871         | 877          | rVB3     | 870            | 746           | 0.04%           | 0.005%        |
| 15        | 3.981       | 892           | 899         | 901          | rBV2     | 602            | 564           | 0.03%           | 0.004%        |
| 16        | 4.077       | 926           | 929         | 933          | rVB3     | 845            | 592           | 0.03%           | 0.004%        |
| 17        | 4.186       | 951           | 963         | 988          | rBV2     | 154415         | 514674        | 25.99%          | 3.266%        |
| 18        | 4.479       | 1051          | 1054        | 1056         | rBV2     | 1979           | 1004          | 0.05%           | 0.006%        |
| 19        | 4.643       | 1089          | 1105        | 1130         | rBV2     | 314993         | 754805        | 38.11%          | 4.790%        |
| 20        | 4.907       | 1173          | 1187        | 1202         | rVV9     | 5502           | 14119         | 0.71%           | 0.090%        |
| 21        | 4.977       | 1206          | 1209        | 1212         | rVV3     | 964            | 736           | 0.04%           | 0.005%        |
| 22        | 5.148       | 1258          | 1262        | 1264         | rBV2     | 763            | 531           | 0.03%           | 0.003%        |
| 23        | 5.334       | 1294          | 1320        | 1355         | rBV2     | 648438         | 1980599       | 100.00%         | 12.568%       |
| 24        | 5.595       | 1399          | 1401        | 1404         | rBV2     | 713            | 483           | 0.02%           | 0.003%        |
| 25        | 5.646       | 1415          | 1417        | 1420         | rVV      | 665            | 479           | 0.02%           | 0.003%        |
| 26        | 5.714       | 1436          | 1438        | 1442         | rVB3     | 896            | 562           | 0.03%           | 0.004%        |
| 27        | 5.746       | 1442          | 1448        | 1451         | rBV4     | 943            | 888           | 0.04%           | 0.006%        |
| 28        | 5.884       | 1475          | 1491        | 1521         | rBV      | 577452         | 1221195       | 61.66%          | 7.749%        |
| 29        | 6.183       | 1571          | 1584        | 1606         | rBV      | 269324         | 539836        | 27.26%          | 3.426%        |
| 30        | 6.328       | 1614          | 1629        | 1664         | rBV      | 421944         | 878386        | 44.35%          | 5.574%        |
| 31        | 6.604       | 1713          | 1715        | 1721         | rVB6     | 987            | 687           | 0.03%           | 0.004%        |
| 32        | 6.717       | 1745          | 1750        | 1753         | rBV3     | 564            | 530           | 0.03%           | 0.003%        |
| 33        | 6.913       | 1808          | 1811        | 1817         | rVB3     | 893            | 775           | 0.04%           | 0.005%        |
| 34        | 6.990       | 1830          | 1835        | 1839         | rBV5     | 627            | 645           | 0.03%           | 0.004%        |

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 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\SOMULM041719WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |         |
|----|--------|------|------|------|------|--------|---------|--------|---------|
| 35 | 7.225  | 1894 | 1908 | 1937 | rBV  | 226985 | 437765  | 22.10% | 2.778%  |
| 36 | 7.360  | 1947 | 1950 | 1952 | rBV3 | 1172   | 696     | 0.04%  | 0.004%  |
| 37 | 7.562  | 2000 | 2013 | 2059 | rBV  | 747105 | 1463217 | 73.88% | 9.285%  |
| 38 | 7.849  | 2090 | 2102 | 2123 | rBV  | 150992 | 290135  | 14.65% | 1.841%  |
| 39 | 7.993  | 2144 | 2147 | 2152 | rVB4 | 1410   | 1290    | 0.07%  | 0.008%  |
| 40 | 8.177  | 2190 | 2204 | 2215 | rBV2 | 16141  | 30958   | 1.56%  | 0.196%  |
| 41 | 8.234  | 2220 | 2222 | 2227 | rVB5 | 1319   | 955     | 0.05%  | 0.006%  |
| 42 | 8.312  | 2231 | 2246 | 2278 | rBV  | 545090 | 1063745 | 53.71% | 6.750%  |
| 43 | 8.620  | 2339 | 2342 | 2345 | rBV3 | 1025   | 754     | 0.04%  | 0.005%  |
| 44 | 8.736  | 2375 | 2378 | 2382 | rBV4 | 666    | 561     | 0.03%  | 0.004%  |
| 45 | 8.842  | 2409 | 2411 | 2418 | rVB3 | 668    | 625     | 0.03%  | 0.004%  |
| 46 | 8.871  | 2418 | 2420 | 2423 | rVB3 | 791    | 509     | 0.03%  | 0.003%  |
| 47 | 8.951  | 2439 | 2445 | 2447 | rBV3 | 1132   | 1165    | 0.06%  | 0.007%  |
| 48 | 8.971  | 2449 | 2451 | 2455 | rBV2 | 604    | 499     | 0.03%  | 0.003%  |
| 49 | 9.087  | 2474 | 2487 | 2520 | rBV  | 913561 | 1632120 | 82.41% | 10.357% |
| 50 | 9.244  | 2533 | 2536 | 2537 | rBV4 | 1410   | 808     | 0.04%  | 0.005%  |
| 51 | 9.379  | 2576 | 2578 | 2581 | rBV3 | 936    | 506     | 0.03%  | 0.003%  |
| 52 | 9.617  | 2648 | 2652 | 2654 | rBV2 | 885    | 652     | 0.03%  | 0.004%  |
| 53 | 9.659  | 2660 | 2665 | 2667 | rBV3 | 489    | 517     | 0.03%  | 0.003%  |
| 54 | 9.752  | 2690 | 2694 | 2696 | rBV3 | 750    | 494     | 0.02%  | 0.003%  |
| 55 | 9.852  | 2722 | 2725 | 2728 | rBV3 | 953    | 586     | 0.03%  | 0.004%  |
| 56 | 9.877  | 2730 | 2733 | 2736 | rVB2 | 840    | 582     | 0.03%  | 0.004%  |
| 57 | 9.897  | 2736 | 2739 | 2746 | rVB2 | 704    | 670     | 0.03%  | 0.004%  |
| 58 | 9.968  | 2757 | 2761 | 2764 | rBV5 | 883    | 871     | 0.04%  | 0.006%  |
| 59 | 10.177 | 2821 | 2826 | 2830 | rVB4 | 1102   | 1094    | 0.06%  | 0.007%  |
| 60 | 10.244 | 2842 | 2847 | 2850 | rBV3 | 525    | 624     | 0.03%  | 0.004%  |
| 61 | 10.328 | 2870 | 2873 | 2878 | rVB3 | 866    | 854     | 0.04%  | 0.005%  |
| 62 | 10.353 | 2878 | 2881 | 2885 | rBV  | 548    | 526     | 0.03%  | 0.003%  |
| 63 | 10.427 | 2891 | 2904 | 2927 | rBV  | 559079 | 910950  | 45.99% | 5.781%  |
| 64 | 10.530 | 2934 | 2936 | 2940 | rVB  | 778    | 500     | 0.03%  | 0.003%  |
| 65 | 10.566 | 2944 | 2947 | 2950 | rBV2 | 829    | 712     | 0.04%  | 0.005%  |
| 66 | 10.604 | 2950 | 2959 | 2970 | rVV2 | 11160  | 18928   | 0.96%  | 0.120%  |
| 67 | 10.730 | 2995 | 2998 | 3002 | rBV  | 523    | 479     | 0.02%  | 0.003%  |
| 68 | 10.820 | 3019 | 3026 | 3027 | rBV3 | 949    | 931     | 0.05%  | 0.006%  |
| 69 | 10.868 | 3037 | 3041 | 3045 | rBV3 | 622    | 756     | 0.04%  | 0.005%  |
| 70 | 11.061 | 3097 | 3101 | 3104 | rVB2 | 796    | 466     | 0.02%  | 0.003%  |
| 71 | 11.083 | 3104 | 3108 | 3112 | rBV2 | 952    | 941     | 0.05%  | 0.006%  |

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## Integration Parameters: LSCINT.P

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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\SOMULM041719WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 72  | 11.324 | 3175 | 3183 | 3190 | rVV4 | 2883   | 4539    | 0.23%  | 0.029% |
| 73  | 11.482 | 3218 | 3232 | 3255 | rBV  | 690914 | 1136605 | 57.39% | 7.212% |
| 74  | 11.736 | 3309 | 3311 | 3317 | rVB4 | 1300   | 935     | 0.05%  | 0.006% |
| 75  | 11.775 | 3318 | 3323 | 3325 | rBV4 | 883    | 843     | 0.04%  | 0.005% |
| 76  | 11.855 | 3336 | 3348 | 3374 | rBV  | 678565 | 1159520 | 58.54% | 7.358% |
| 77  | 12.157 | 3439 | 3442 | 3445 | rBV3 | 1114   | 769     | 0.04%  | 0.005% |
| 78  | 12.205 | 3453 | 3457 | 3462 | rBV5 | 1011   | 1044    | 0.05%  | 0.007% |
| 79  | 12.270 | 3474 | 3477 | 3479 | rBV3 | 836    | 530     | 0.03%  | 0.003% |
| 80  | 12.472 | 3532 | 3540 | 3542 | rBV6 | 2462   | 3011    | 0.15%  | 0.019% |
| 81  | 12.646 | 3590 | 3594 | 3597 | rBV2 | 1198   | 929     | 0.05%  | 0.006% |
| 82  | 12.681 | 3599 | 3605 | 3610 | rBV6 | 1394   | 1874    | 0.09%  | 0.012% |
| 83  | 12.746 | 3621 | 3625 | 3626 | rBV2 | 908    | 610     | 0.03%  | 0.004% |
| 84  | 12.884 | 3665 | 3668 | 3670 | rBV2 | 1149   | 736     | 0.04%  | 0.005% |
| 85  | 13.061 | 3720 | 3723 | 3726 | rVB2 | 810    | 503     | 0.03%  | 0.003% |
| 86  | 13.160 | 3748 | 3754 | 3763 | rBV5 | 1153   | 1582    | 0.08%  | 0.010% |
| 87  | 13.199 | 3763 | 3766 | 3768 | rBV2 | 1027   | 604     | 0.03%  | 0.004% |
| 88  | 13.356 | 3811 | 3815 | 3818 | rBV2 | 1114   | 825     | 0.04%  | 0.005% |
| 89  | 13.607 | 3890 | 3893 | 3896 | rVB2 | 941    | 599     | 0.03%  | 0.004% |
| 90  | 13.623 | 3896 | 3898 | 3904 | rBV3 | 693    | 578     | 0.03%  | 0.004% |
| 91  | 13.649 | 3904 | 3906 | 3909 | rBV2 | 793    | 511     | 0.03%  | 0.003% |
| 92  | 13.733 | 3928 | 3932 | 3936 | rBV3 | 914    | 933     | 0.05%  | 0.006% |
| 93  | 14.099 | 4043 | 4046 | 4050 | rBV3 | 946    | 604     | 0.03%  | 0.004% |
| 94  | 14.122 | 4051 | 4053 | 4058 | rVV4 | 741    | 652     | 0.03%  | 0.004% |
| 95  | 14.170 | 4064 | 4068 | 4069 | rBV  | 952    | 639     | 0.03%  | 0.004% |
| 96  | 14.630 | 4208 | 4211 | 4215 | rBV4 | 1424   | 1081    | 0.05%  | 0.007% |
| 97  | 15.048 | 4339 | 4341 | 4344 | rBV  | 1017   | 814     | 0.04%  | 0.005% |
| 98  | 15.192 | 4384 | 4386 | 4389 | rBV3 | 1020   | 571     | 0.03%  | 0.004% |
| 99  | 15.671 | 4532 | 4535 | 4538 | rBV  | 2812   | 2132    | 0.11%  | 0.014% |
| 100 | 16.064 | 4654 | 4657 | 4662 | rVB4 | 2765   | 2180    | 0.11%  | 0.014% |

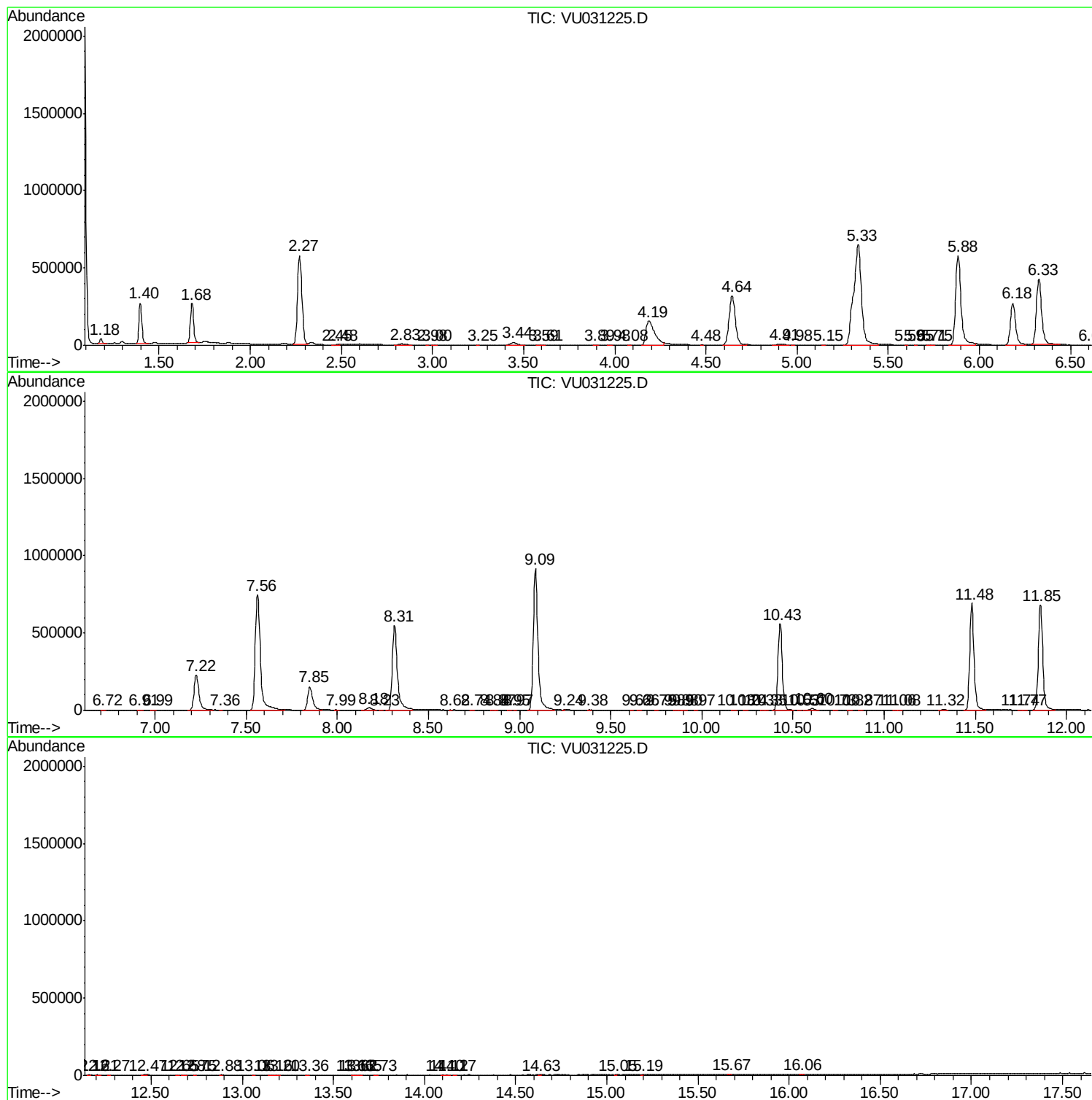
Sum of corrected areas: 15758910

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM041719WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU041719\  
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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          |