

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU033019\  
 Data File : VU030560.D  
 Acq On : 29 Mar 2019 22:30  
 Operator : JC/SP  
 Sample : K2101-16ME  
 Misc : 4.47g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFOE7ME

## 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<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          | 36           | rVB      | 13215          | 14897         | 1.16%           | 0.151%        |
| 2         | 1.396       | 87            | 95          | 112          | rBV      | 105499         | 136255        | 10.63%          | 1.381%        |
| 3         | 1.640       | 132           | 171         | 181          | rBV      | 143413         | 441707        | 34.46%          | 4.478%        |
| 4         | 2.222       | 342           | 352         | 369          | rVB      | 206364         | 317920        | 24.80%          | 3.223%        |
| 5         | 2.338       | 386           | 388         | 399          | rVB8     | 2358           | 3557          | 0.28%           | 0.036%        |
| 6         | 2.457       | 423           | 425         | 428          | rBV3     | 651            | 401           | 0.03%           | 0.004%        |
| 7         | 2.489       | 432           | 435         | 439          | rBV2     | 561            | 419           | 0.03%           | 0.004%        |
| 8         | 2.515       | 439           | 443         | 446          | rBV2     | 643            | 467           | 0.04%           | 0.005%        |
| 9         | 2.543       | 448           | 452         | 457          | rVV6     | 471            | 481           | 0.04%           | 0.005%        |
| 10        | 2.675       | 485           | 493         | 494          | rBV4     | 2900           | 3069          | 0.24%           | 0.031%        |
| 11        | 2.730       | 508           | 510         | 514          | rVB      | 979            | 489           | 0.04%           | 0.005%        |
| 12        | 2.765       | 518           | 521         | 525          | rVB2     | 493            | 351           | 0.03%           | 0.004%        |
| 13        | 2.820       | 529           | 538         | 540          | rBV3     | 2548           | 3119          | 0.24%           | 0.032%        |
| 14        | 2.894       | 559           | 561         | 565          | rVB2     | 542            | 337           | 0.03%           | 0.003%        |
| 15        | 2.929       | 570           | 572         | 575          | rVV      | 522            | 321           | 0.03%           | 0.003%        |
| 16        | 2.974       | 583           | 586         | 590          | rVV3     | 367            | 317           | 0.02%           | 0.003%        |
| 17        | 2.994       | 590           | 592         | 599          | rVB2     | 514            | 393           | 0.03%           | 0.004%        |
| 18        | 3.026       | 599           | 602         | 605          | rVB2     | 585            | 314           | 0.02%           | 0.003%        |
| 19        | 3.096       | 619           | 624         | 626          | rVV2     | 389            | 340           | 0.03%           | 0.003%        |
| 20        | 3.116       | 626           | 630         | 632          | rVV      | 519            | 354           | 0.03%           | 0.004%        |
| 21        | 3.145       | 635           | 639         | 644          | rVV3     | 333            | 374           | 0.03%           | 0.004%        |
| 22        | 3.254       | 669           | 673         | 674          | rBV2     | 761            | 451           | 0.04%           | 0.005%        |
| 23        | 3.267       | 674           | 677         | 686          | rVV6     | 1134           | 1528          | 0.12%           | 0.015%        |
| 24        | 3.386       | 708           | 714         | 718          | rVB3     | 399            | 408           | 0.03%           | 0.004%        |
| 25        | 3.408       | 718           | 721         | 726          | rBV3     | 412            | 367           | 0.03%           | 0.004%        |
| 26        | 3.486       | 741           | 745         | 747          | rBV2     | 328            | 319           | 0.02%           | 0.003%        |
| 27        | 3.688       | 805           | 808         | 816          | rVB2     | 458            | 426           | 0.03%           | 0.004%        |
| 28        | 3.752       | 823           | 828         | 831          | rBV3     | 471            | 463           | 0.04%           | 0.005%        |
| 29        | 4.199       | 956           | 967         | 1020         | rBV2     | 84739          | 299696        | 23.38%          | 3.038%        |
| 30        | 4.434       | 1037          | 1040        | 1048         | rVB4     | 1183           | 1418          | 0.11%           | 0.014%        |
| 31        | 4.473       | 1048          | 1052        | 1059         | rVB3     | 678            | 649           | 0.05%           | 0.007%        |
| 32        | 4.640       | 1087          | 1104        | 1126         | rBV      | 158029         | 400390        | 31.23%          | 4.059%        |
| 33        | 4.884       | 1174          | 1180        | 1184         | rBV4     | 1266           | 1532          | 0.12%           | 0.016%        |
| 34        | 4.965       | 1202          | 1205        | 1207         | rBV3     | 709            | 460           | 0.04%           | 0.005%        |

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Instrument :  
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 BFOE7ME

## Integration Parameters: LSCINT.P

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 Sampling : 1  
 Start Thrs: 0.2  
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 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM032319WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |        |         |        |         |
|----|-------|------|------|------|------|--------|---------|--------|---------|
| 35 | 5.090 | 1239 | 1244 | 1247 | rBV2 | 443    | 357     | 0.03%  | 0.004%  |
| 36 | 5.190 | 1269 | 1275 | 1278 | rBV2 | 584    | 651     | 0.05%  | 0.007%  |
| 37 | 5.325 | 1295 | 1317 | 1357 | rBV2 | 357162 | 1026421 | 80.07% | 10.406% |
| 38 | 5.460 | 1357 | 1359 | 1362 | rVV3 | 528    | 328     | 0.03%  | 0.003%  |
| 39 | 5.521 | 1374 | 1378 | 1382 | rBV2 | 507    | 562     | 0.04%  | 0.006%  |
| 40 | 5.543 | 1382 | 1385 | 1390 | rVV2 | 661    | 602     | 0.05%  | 0.006%  |
| 41 | 5.611 | 1396 | 1406 | 1407 | rBV6 | 2143   | 2234    | 0.17%  | 0.023%  |
| 42 | 5.624 | 1407 | 1410 | 1413 | rVV3 | 1517   | 1193    | 0.09%  | 0.012%  |
| 43 | 5.694 | 1429 | 1432 | 1435 | rBV2 | 514    | 333     | 0.03%  | 0.003%  |
| 44 | 5.762 | 1451 | 1453 | 1457 | rVB2 | 651    | 369     | 0.03%  | 0.004%  |
| 45 | 5.878 | 1472 | 1489 | 1518 | rBV  | 486485 | 1017820 | 79.40% | 10.318% |
| 46 | 6.019 | 1530 | 1533 | 1537 | rVB3 | 776    | 638     | 0.05%  | 0.006%  |
| 47 | 6.125 | 1564 | 1566 | 1569 | rBV2 | 741    | 442     | 0.03%  | 0.004%  |
| 48 | 6.186 | 1575 | 1585 | 1594 | rVB2 | 2681   | 5760    | 0.45%  | 0.058%  |
| 49 | 6.254 | 1594 | 1606 | 1615 | rBV4 | 4784   | 10073   | 0.79%  | 0.102%  |
| 50 | 6.325 | 1615 | 1628 | 1657 | rVB  | 223337 | 477448  | 37.24% | 4.840%  |
| 51 | 6.495 | 1678 | 1681 | 1685 | rVB2 | 593    | 368     | 0.03%  | 0.004%  |
| 52 | 6.601 | 1712 | 1714 | 1720 | rVB3 | 582    | 475     | 0.04%  | 0.005%  |
| 53 | 6.640 | 1724 | 1726 | 1732 | rVB3 | 403    | 322     | 0.03%  | 0.003%  |
| 54 | 6.688 | 1737 | 1741 | 1744 | rBV2 | 479    | 481     | 0.04%  | 0.005%  |
| 55 | 6.823 | 1776 | 1783 | 1785 | rBV3 | 423    | 450     | 0.04%  | 0.005%  |
| 56 | 6.891 | 1794 | 1804 | 1812 | rBV6 | 2480   | 4356    | 0.34%  | 0.044%  |
| 57 | 6.968 | 1824 | 1828 | 1829 | rBV2 | 815    | 531     | 0.04%  | 0.005%  |
| 58 | 7.225 | 1894 | 1908 | 1934 | rBV  | 109086 | 220202  | 17.18% | 2.232%  |
| 59 | 7.350 | 1944 | 1947 | 1950 | rBV3 | 628    | 430     | 0.03%  | 0.004%  |
| 60 | 7.418 | 1965 | 1968 | 1970 | rBV3 | 835    | 575     | 0.04%  | 0.006%  |
| 61 | 7.479 | 1983 | 1987 | 1991 | rVB3 | 426    | 447     | 0.03%  | 0.005%  |
| 62 | 7.563 | 1996 | 2013 | 2036 | rBV  | 393965 | 733639  | 57.23% | 7.437%  |
| 63 | 7.781 | 2078 | 2081 | 2083 | rBV2 | 506    | 322     | 0.03%  | 0.003%  |
| 64 | 7.852 | 2091 | 2103 | 2123 | rBV  | 72777  | 152441  | 11.89% | 1.545%  |
| 65 | 8.042 | 2157 | 2162 | 2166 | rVV3 | 1133   | 1177    | 0.09%  | 0.012%  |
| 66 | 8.083 | 2170 | 2175 | 2181 | rVB4 | 510    | 610     | 0.05%  | 0.006%  |
| 67 | 8.161 | 2196 | 2199 | 2201 | rBV2 | 567    | 397     | 0.03%  | 0.004%  |
| 68 | 8.222 | 2207 | 2218 | 2232 | rBV2 | 88551  | 153783  | 12.00% | 1.559%  |
| 69 | 8.325 | 2236 | 2250 | 2287 | rBV  | 329405 | 710709  | 55.44% | 7.205%  |
| 70 | 8.730 | 2369 | 2376 | 2380 | rBV3 | 874    | 1065    | 0.08%  | 0.011%  |
| 71 | 8.778 | 2387 | 2391 | 2396 | rBV3 | 698    | 624     | 0.05%  | 0.006%  |

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Instrument :  
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 ClientSampleId :  
 BFOE7ME

## Integration Parameters: LSCINT.P

Integrator: RTE  
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Filtering: 5  
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM032319WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |         |         |
|-----|--------|------|------|------|------|--------|---------|---------|---------|
| 72  | 9.013  | 2461 | 2464 | 2469 | rVB2 | 553    | 396     | 0.03%   | 0.004%  |
| 73  | 9.090  | 2474 | 2488 | 2516 | rBV  | 702284 | 1281923 | 100.00% | 12.996% |
| 74  | 9.614  | 2648 | 2651 | 2656 | rVB3 | 493    | 366     | 0.03%   | 0.004%  |
| 75  | 9.640  | 2656 | 2659 | 2663 | rBV2 | 417    | 346     | 0.03%   | 0.004%  |
| 76  | 9.887  | 2734 | 2736 | 2741 | rVB3 | 582    | 441     | 0.03%   | 0.004%  |
| 77  | 9.932  | 2748 | 2750 | 2756 | rVV2 | 515    | 556     | 0.04%   | 0.006%  |
| 78  | 9.968  | 2758 | 2761 | 2767 | rVB2 | 520    | 388     | 0.03%   | 0.004%  |
| 79  | 10.434 | 2893 | 2906 | 2933 | rBV  | 353850 | 586789  | 45.77%  | 5.949%  |
| 80  | 10.730 | 2994 | 2998 | 3001 | rVB2 | 497    | 400     | 0.03%   | 0.004%  |
| 81  | 10.839 | 3029 | 3032 | 3035 | rBV  | 404    | 335     | 0.03%   | 0.003%  |
| 82  | 11.009 | 3082 | 3085 | 3089 | rVB  | 487    | 323     | 0.03%   | 0.003%  |
| 83  | 11.038 | 3089 | 3094 | 3095 | rBV  | 452    | 324     | 0.03%   | 0.003%  |
| 84  | 11.090 | 3108 | 3110 | 3115 | rBV2 | 466    | 373     | 0.03%   | 0.004%  |
| 85  | 11.144 | 3122 | 3127 | 3132 | rVB3 | 530    | 475     | 0.04%   | 0.005%  |
| 86  | 11.199 | 3141 | 3144 | 3149 | rVB  | 614    | 449     | 0.04%   | 0.005%  |
| 87  | 11.234 | 3151 | 3155 | 3157 | rBV  | 669    | 458     | 0.04%   | 0.005%  |
| 88  | 11.395 | 3200 | 3205 | 3206 | rBV2 | 555    | 449     | 0.04%   | 0.005%  |
| 89  | 11.482 | 3220 | 3232 | 3258 | rBV  | 685424 | 1126539 | 87.88%  | 11.421% |
| 90  | 11.861 | 3338 | 3350 | 3378 | rBV  | 404882 | 687790  | 53.65%  | 6.973%  |
| 91  | 12.299 | 3484 | 3486 | 3490 | rVB2 | 770    | 411     | 0.03%   | 0.004%  |
| 92  | 12.450 | 3530 | 3533 | 3534 | rBV2 | 619    | 343     | 0.03%   | 0.003%  |
| 93  | 12.472 | 3535 | 3540 | 3550 | rVB4 | 2202   | 3292    | 0.26%   | 0.033%  |
| 94  | 12.572 | 3568 | 3571 | 3572 | rBV  | 712    | 392     | 0.03%   | 0.004%  |
| 95  | 12.662 | 3596 | 3599 | 3604 | rBV3 | 646    | 535     | 0.04%   | 0.005%  |
| 96  | 12.922 | 3677 | 3680 | 3683 | rVB2 | 545    | 316     | 0.02%   | 0.003%  |
| 97  | 12.955 | 3687 | 3690 | 3693 | rBV2 | 632    | 375     | 0.03%   | 0.004%  |
| 98  | 13.649 | 3903 | 3906 | 3909 | rBV2 | 508    | 334     | 0.03%   | 0.003%  |
| 99  | 13.768 | 3940 | 3943 | 3946 | rBV2 | 486    | 434     | 0.03%   | 0.004%  |
| 100 | 14.273 | 4094 | 4100 | 4113 | rVB3 | 3803   | 5902    | 0.46%   | 0.060%  |

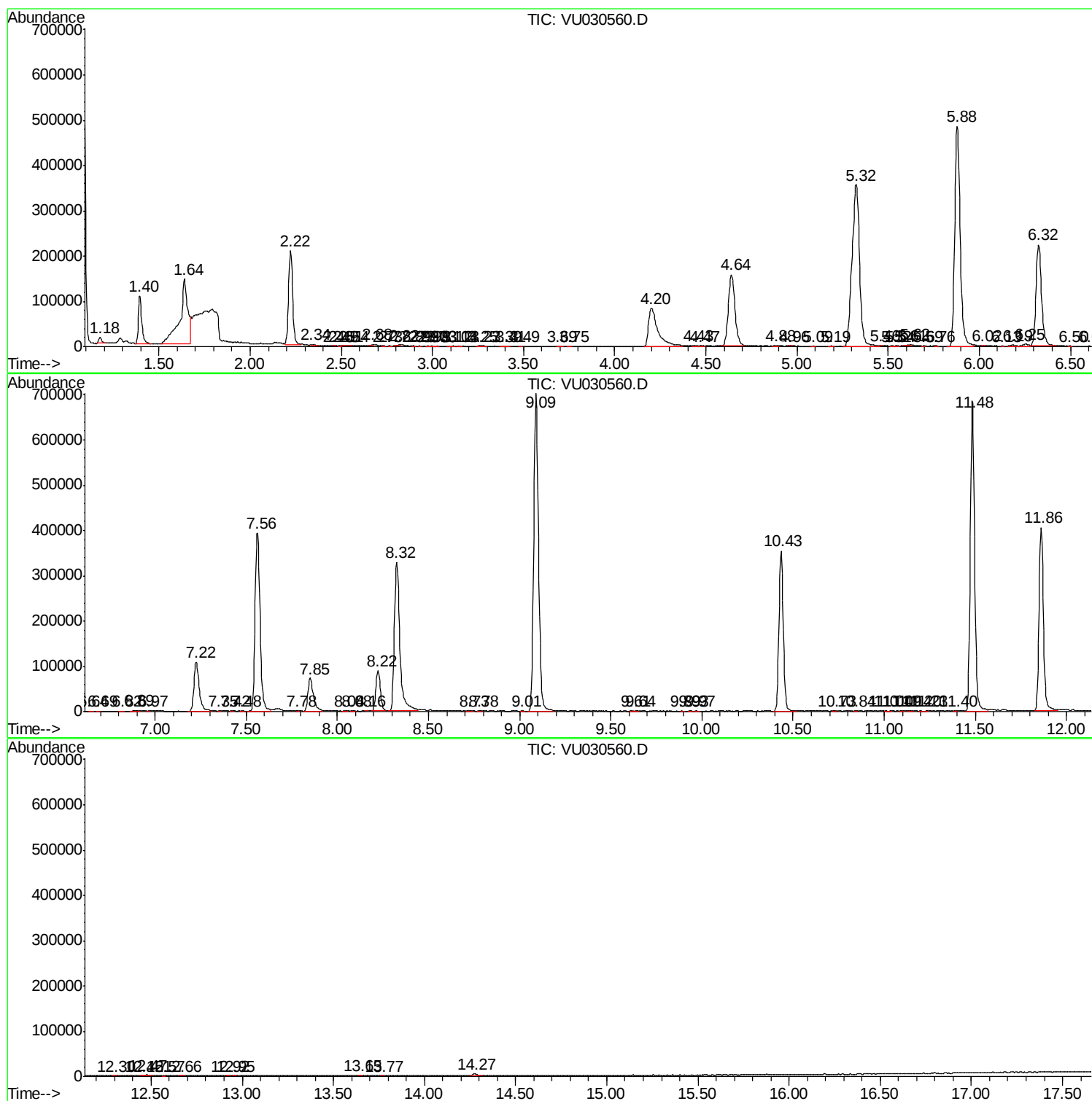
Sum of corrected areas: 9864078

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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\VU033019\  
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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        |