

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU051519\  
 Data File : VU032031.D  
 Acq On : 15 May 2019 14:58  
 Operator : JC/SP  
 Sample : K2737-12ME  
 Misc : 4.51g/5mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DB860ME

## 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\SOMULM051419WMA.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      | 1.396    | 88         | 95       | 116       | rVB   | 322594      | 536229     | 14.40%       | 1.814%     |
| 2      | 1.640    | 166        | 171      | 186       | rBV   | 181678      | 255595     | 6.87%        | 0.865%     |
| 3      | 2.222    | 342        | 352      | 368       | rVB   | 744507      | 1158863    | 31.13%       | 3.921%     |
| 4      | 2.556    | 452        | 456      | 457       | rBV3  | 1254        | 983        | 0.03%        | 0.003%     |
| 5      | 2.598    | 464        | 469      | 471       | rBV3  | 1274        | 1293       | 0.03%        | 0.004%     |
| 6      | 2.875    | 549        | 555      | 556       | rBV3  | 1287        | 1210       | 0.03%        | 0.004%     |
| 7      | 2.916    | 559        | 568      | 569       | rBV7  | 3466        | 4278       | 0.11%        | 0.014%     |
| 8      | 3.112    | 627        | 629      | 632       | rBV2  | 1208        | 773        | 0.02%        | 0.003%     |
| 9      | 3.167    | 643        | 646      | 652       | rVB4  | 1104        | 913        | 0.02%        | 0.003%     |
| 10     | 3.267    | 671        | 677      | 685       | rVB7  | 2817        | 4487       | 0.12%        | 0.015%     |
| 11     | 3.363    | 702        | 707      | 710       | rVB6  | 1335        | 1326       | 0.04%        | 0.004%     |
| 12     | 3.434    | 724        | 729      | 734       | rVB4  | 1116        | 1387       | 0.04%        | 0.005%     |
| 13     | 3.530    | 756        | 759      | 762       | rBV3  | 946         | 735        | 0.02%        | 0.002%     |
| 14     | 3.566    | 767        | 770      | 773       | rVB3  | 1238        | 706        | 0.02%        | 0.002%     |
| 15     | 3.662    | 796        | 800      | 803       | rBV3  | 745         | 692        | 0.02%        | 0.002%     |
| 16     | 3.711    | 811        | 815      | 819       | rVB3  | 846         | 670        | 0.02%        | 0.002%     |
| 17     | 3.797    | 838        | 842      | 846       | rVB3  | 1177        | 1129       | 0.03%        | 0.004%     |
| 18     | 4.039    | 914        | 917      | 922       | rVB3  | 1329        | 1046       | 0.03%        | 0.004%     |
| 19     | 4.061    | 922        | 924      | 930       | rBV4  | 727         | 713        | 0.02%        | 0.002%     |
| 20     | 4.145    | 945        | 950      | 953       | rBV3  | 738         | 614        | 0.02%        | 0.002%     |
| 21     | 4.196    | 953        | 966      | 1018      | rBV   | 230214      | 906819     | 24.36%       | 3.068%     |
| 22     | 4.640    | 1085       | 1104     | 1136      | rBV   | 544486      | 1414031    | 37.98%       | 4.784%     |
| 23     | 4.820    | 1155       | 1160     | 1164      | rVB6  | 1359        | 1431       | 0.04%        | 0.005%     |
| 24     | 4.852    | 1165       | 1170     | 1171      | rBV3  | 1125        | 761        | 0.02%        | 0.003%     |
| 25     | 4.874    | 1173       | 1177     | 1179      | rBV3  | 1939        | 1487       | 0.04%        | 0.005%     |
| 26     | 4.919    | 1189       | 1191     | 1197      | rVB6  | 1514        | 1182       | 0.03%        | 0.004%     |
| 27     | 4.961    | 1197       | 1204     | 1206      | rBV6  | 1992        | 2112       | 0.06%        | 0.007%     |
| 28     | 5.164    | 1260       | 1267     | 1270      | rBV4  | 704         | 862        | 0.02%        | 0.003%     |
| 29     | 5.202    | 1274       | 1279     | 1284      | rBV4  | 935         | 928        | 0.02%        | 0.003%     |
| 30     | 5.228    | 1284       | 1287     | 1290      | rBV4  | 929         | 852        | 0.02%        | 0.003%     |
| 31     | 5.325    | 1295       | 1317     | 1350      | rBV2  | 1307611     | 3722753    | 100.00%      | 12.596%    |
| 32     | 5.527    | 1377       | 1380     | 1383      | rBV2  | 1150        | 886        | 0.02%        | 0.003%     |
| 33     | 5.608    | 1403       | 1405     | 1409      | rVB4  | 1581        | 808        | 0.02%        | 0.003%     |
| 34     | 5.630    | 1409       | 1412     | 1416      | rVB4  | 1444        | 823        | 0.02%        | 0.003%     |

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Integrator: RTE  
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Filtering: 5  
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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\SOMULM051419WMA.M  
 Title : VOC Analysis

|    |       |      |      |      |      |         |         |        |         |
|----|-------|------|------|------|------|---------|---------|--------|---------|
| 35 | 5.749 | 1444 | 1449 | 1452 | rVV5 | 1241    | 1326    | 0.04%  | 0.004%  |
| 36 | 5.878 | 1474 | 1489 | 1522 | rBV  | 1215337 | 2692641 | 72.33% | 9.110%  |
| 37 | 6.135 | 1566 | 1569 | 1570 | rBV2 | 1797    | 973     | 0.03%  | 0.003%  |
| 38 | 6.177 | 1573 | 1582 | 1598 | rVB2 | 7997    | 20177   | 0.54%  | 0.068%  |
| 39 | 6.325 | 1613 | 1628 | 1657 | rBV  | 761207  | 1669184 | 44.84% | 5.648%  |
| 40 | 6.698 | 1737 | 1744 | 1747 | rBV4 | 668     | 835     | 0.02%  | 0.003%  |
| 41 | 6.749 | 1755 | 1760 | 1764 | rBV5 | 751     | 741     | 0.02%  | 0.003%  |
| 42 | 6.897 | 1799 | 1806 | 1812 | rBV7 | 4088    | 6598    | 0.18%  | 0.022%  |
| 43 | 6.984 | 1831 | 1833 | 1840 | rBV5 | 651     | 643     | 0.02%  | 0.002%  |
| 44 | 7.016 | 1840 | 1843 | 1846 | rBV3 | 843     | 624     | 0.02%  | 0.002%  |
| 45 | 7.058 | 1853 | 1856 | 1863 | rVB7 | 1818    | 1598    | 0.04%  | 0.005%  |
| 46 | 7.093 | 1863 | 1867 | 1869 | rBV2 | 836     | 731     | 0.02%  | 0.002%  |
| 47 | 7.225 | 1895 | 1908 | 1933 | rBV  | 388052  | 805309  | 21.63% | 2.725%  |
| 48 | 7.357 | 1947 | 1949 | 1953 | rBV4 | 966     | 620     | 0.02%  | 0.002%  |
| 49 | 7.559 | 1998 | 2012 | 2053 | rBV  | 1484177 | 2913399 | 78.26% | 9.857%  |
| 50 | 7.849 | 2091 | 2102 | 2130 | rBV  | 247038  | 536972  | 14.42% | 1.817%  |
| 51 | 8.035 | 2157 | 2160 | 2165 | rBV5 | 1458    | 1116    | 0.03%  | 0.004%  |
| 52 | 8.141 | 2189 | 2193 | 2197 | rVB4 | 1161    | 1060    | 0.03%  | 0.004%  |
| 53 | 8.167 | 2197 | 2201 | 2202 | rBV2 | 1259    | 834     | 0.02%  | 0.003%  |
| 54 | 8.228 | 2212 | 2220 | 2221 | rBV5 | 4378    | 4948    | 0.13%  | 0.017%  |
| 55 | 8.328 | 2238 | 2251 | 2286 | rBV  | 884857  | 1939898 | 52.11% | 6.564%  |
| 56 | 8.717 | 2369 | 2372 | 2375 | rBV4 | 1112    | 893     | 0.02%  | 0.003%  |
| 57 | 8.791 | 2390 | 2395 | 2401 | rBV6 | 903     | 1164    | 0.03%  | 0.004%  |
| 58 | 8.852 | 2409 | 2414 | 2418 | rBV6 | 1304    | 1458    | 0.04%  | 0.005%  |
| 59 | 8.906 | 2427 | 2431 | 2433 | rBV3 | 1158    | 795     | 0.02%  | 0.003%  |
| 60 | 8.935 | 2436 | 2440 | 2443 | rVB4 | 870     | 656     | 0.02%  | 0.002%  |
| 61 | 8.968 | 2447 | 2450 | 2453 | rBV4 | 896     | 608     | 0.02%  | 0.002%  |
| 62 | 9.042 | 2468 | 2473 | 2474 | rBV2 | 1129    | 864     | 0.02%  | 0.003%  |
| 63 | 9.090 | 2475 | 2488 | 2531 | rVV  | 1785186 | 3432779 | 92.21% | 11.615% |
| 64 | 9.321 | 2556 | 2560 | 2568 | rVB6 | 1081    | 1496    | 0.04%  | 0.005%  |
| 65 | 9.382 | 2572 | 2579 | 2581 | rBV6 | 5644    | 6021    | 0.16%  | 0.020%  |
| 66 | 9.505 | 2612 | 2617 | 2619 | rBV4 | 1333    | 1367    | 0.04%  | 0.005%  |
| 67 | 9.521 | 2619 | 2622 | 2630 | rVV6 | 1830    | 2452    | 0.07%  | 0.008%  |
| 68 | 9.566 | 2633 | 2636 | 2641 | rVV4 | 822     | 807     | 0.02%  | 0.003%  |
| 69 | 9.636 | 2655 | 2658 | 2660 | rBV3 | 1104    | 784     | 0.02%  | 0.003%  |
| 70 | 9.720 | 2681 | 2684 | 2686 | rVV3 | 929     | 636     | 0.02%  | 0.002%  |
| 71 | 9.742 | 2689 | 2691 | 2696 | rVB3 | 919     | 853     | 0.02%  | 0.003%  |

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ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DB860ME

## Integration Parameters: LSCINT.P

Integrator: RTE  
Smoothing : OFF  
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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\SOMULM051419WMA.M  
Title : VOC Analysis

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 72  | 9.787  | 2696 | 2705 | 2718 | rBV6 | 6801    | 12687   | 0.34%  | 0.043% |
| 73  | 9.874  | 2730 | 2732 | 2736 | rBV3 | 915     | 699     | 0.02%  | 0.002% |
| 74  | 10.038 | 2780 | 2783 | 2787 | rVB2 | 1036    | 667     | 0.02%  | 0.002% |
| 75  | 10.135 | 2808 | 2813 | 2817 | rBV4 | 992     | 1021    | 0.03%  | 0.003% |
| 76  | 10.289 | 2856 | 2861 | 2865 | rVB3 | 1815    | 1875    | 0.05%  | 0.006% |
| 77  | 10.321 | 2865 | 2871 | 2875 | rBV5 | 1033    | 1326    | 0.04%  | 0.004% |
| 78  | 10.434 | 2893 | 2906 | 2931 | rBV  | 1209191 | 1990498 | 53.47% | 6.735% |
| 79  | 10.598 | 2953 | 2957 | 2962 | rBV6 | 2583    | 2861    | 0.08%  | 0.010% |
| 80  | 10.672 | 2977 | 2980 | 2984 | rBV4 | 1094    | 895     | 0.02%  | 0.003% |
| 81  | 10.797 | 3016 | 3019 | 3023 | rBV2 | 905     | 738     | 0.02%  | 0.002% |
| 82  | 10.916 | 3051 | 3056 | 3058 | rBV3 | 1110    | 943     | 0.03%  | 0.003% |
| 83  | 10.935 | 3058 | 3062 | 3063 | rBV  | 901     | 652     | 0.02%  | 0.002% |
| 84  | 10.980 | 3073 | 3076 | 3079 | rBV3 | 1422    | 1059    | 0.03%  | 0.004% |
| 85  | 11.086 | 3103 | 3109 | 3113 | rVB6 | 1826    | 1966    | 0.05%  | 0.007% |
| 86  | 11.408 | 3206 | 3209 | 3215 | rBV6 | 1679    | 2007    | 0.05%  | 0.007% |
| 87  | 11.482 | 3220 | 3232 | 3260 | rBV  | 1826916 | 2941754 | 79.02% | 9.953% |
| 88  | 11.858 | 3337 | 3349 | 3374 | rBV  | 1514976 | 2496936 | 67.07% | 8.448% |
| 89  | 12.379 | 3508 | 3511 | 3513 | rBV3 | 1656    | 1169    | 0.03%  | 0.004% |
| 90  | 12.466 | 3535 | 3538 | 3541 | rBV3 | 1533    | 1157    | 0.03%  | 0.004% |
| 91  | 13.003 | 3702 | 3705 | 3708 | rBV3 | 1045    | 847     | 0.02%  | 0.003% |
| 92  | 13.138 | 3743 | 3747 | 3748 | rBV2 | 1067    | 694     | 0.02%  | 0.002% |
| 93  | 13.893 | 3980 | 3982 | 3988 | rBV3 | 1083    | 1221    | 0.03%  | 0.004% |
| 94  | 14.006 | 4014 | 4017 | 4019 | rBV3 | 1045    | 674     | 0.02%  | 0.002% |
| 95  | 14.083 | 4039 | 4041 | 4045 | rBV3 | 1004    | 762     | 0.02%  | 0.003% |
| 96  | 14.270 | 4095 | 4099 | 4102 | rBV5 | 3052    | 2888    | 0.08%  | 0.010% |
| 97  | 14.530 | 4177 | 4180 | 4183 | rBV3 | 1250    | 926     | 0.02%  | 0.003% |
| 98  | 14.572 | 4191 | 4193 | 4195 | rBV3 | 1075    | 650     | 0.02%  | 0.002% |
| 99  | 14.726 | 4238 | 4241 | 4244 | rBV2 | 1765    | 1366    | 0.04%  | 0.005% |
| 100 | 14.835 | 4272 | 4275 | 4279 | rBV3 | 1777    | 1468    | 0.04%  | 0.005% |

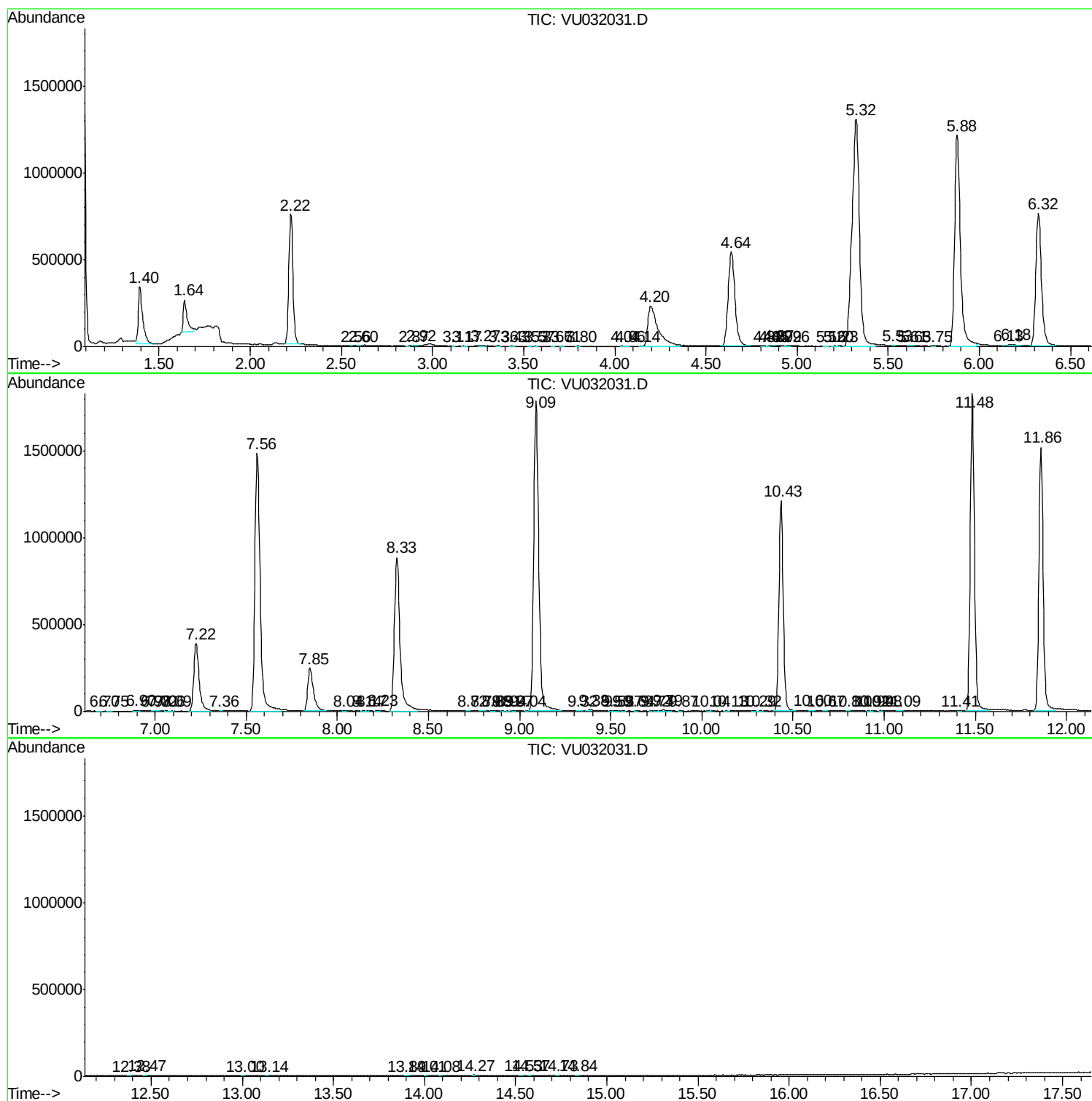
Sum of corrected areas: 29555643

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DB860ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM051419WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_U\DATA\VU051519\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM051419WMA.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

\*\*\*\*\*

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